



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 11:52 PM EDT

PDB ID : 1S5L / pdb_00001s5l
Title : Architecture of the photosynthetic oxygen evolving center
Authors : Ferreira, K.N.; Iverson, T.M.; Maghlaoui, K.; Barber, J.; Iwata, S.
Deposited on : 2004-01-21
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

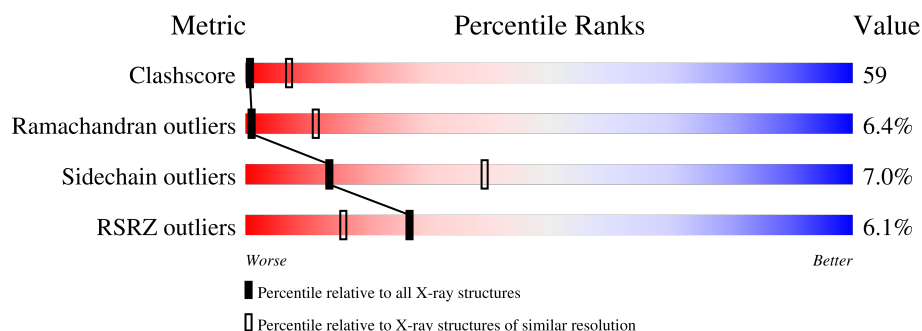
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	5% 23% 55% 17% • •
1	a	344	6% 24% 52% 19% • •
2	B	510	7% 27% 54% 12% • 7%
2	b	510	5% 28% 52% 13% • 7%
3	C	473	5% 18% 56% 14% • 11%
3	c	473	6% 22% 54% 13% • 11%

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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	246	
13	o	246	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	X	50	
17	x	50	
18	N	37	
18	n	37	
19	Z	62	
19	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	524	-	-	X	-
23	CLA	b	2524	-	-	X	-
23	CLA	c	2486	-	-	X	-
28	HEC	E	84	X	-	-	-
28	HEC	V	138	X	-	-	-
28	HEC	e	2084	X	-	-	-
28	HEC	v	2138	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 45945 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2616	1714	430	457	15			

- Molecule 2 is a protein called photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			
2	b	476	Total	C	N	O	S	0	0	0
			3739	2455	625	646	13			

- Molecule 3 is a protein called photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			
3	c	421	Total	C	N	O	S	0	0	0
			3253	2140	544	557	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	insertion	UNP Q8DIF8
C	2	LYS	-	insertion	UNP Q8DIF8
C	3	THR	-	insertion	UNP Q8DIF8
C	4	LEU	-	insertion	UNP Q8DIF8
C	5	SER	-	insertion	UNP Q8DIF8
C	6	SER	-	insertion	UNP Q8DIF8
C	7	GLN	-	insertion	UNP Q8DIF8
C	8	LYS	-	insertion	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ARG	-	insertion	UNP Q8DIF8
C	10	TYR	-	insertion	UNP Q8DIF8
C	11	SER	-	insertion	UNP Q8DIF8
C	12	PRO	-	insertion	UNP Q8DIF8
C	13	VAL	-	insertion	UNP Q8DIF8
c	2001	MET	-	insertion	UNP Q8DIF8
c	2002	LYS	-	insertion	UNP Q8DIF8
c	2003	THR	-	insertion	UNP Q8DIF8
c	2004	LEU	-	insertion	UNP Q8DIF8
c	2005	SER	-	insertion	UNP Q8DIF8
c	2006	SER	-	insertion	UNP Q8DIF8
c	2007	GLN	-	insertion	UNP Q8DIF8
c	2008	LYS	-	insertion	UNP Q8DIF8
c	2009	ARG	-	insertion	UNP Q8DIF8
c	2010	TYR	-	insertion	UNP Q8DIF8
c	2011	SER	-	insertion	UNP Q8DIF8
c	2012	PRO	-	insertion	UNP Q8DIF8
c	2013	VAL	-	insertion	UNP Q8DIF8

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			
4	d	339	Total	C	N	O	S	0	0	0
			2702	1792	439	459	12			

- Molecule 5 is a protein called Cytochrome b559 alpha subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	0
			624	411	99	114			
5	e	76	Total	C	N	O	0	0	0
			624	411	99	114			

- Molecule 6 is a protein called Cytochrome b559 beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

- Molecule 7 is a protein called photosystem II PsbH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			
7	h	53	Total	C	N	O	S	0	0	0
			409	276	60	71	2			

- Molecule 8 is a protein called Photosystem II reaction center I protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

- Molecule 9 is a protein called Photosystem II reaction center J protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center L protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center M protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			
12	m	30	Total	C	N	O	S	0	0	0
			234	159	33	41	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			
13	o	246	Total	C	N	O	S	0	0	0
			1888	1179	320	385	4			

- Molecule 14 is a protein called photosystem II PsbT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			
14	t	31	Total	C	N	O	S	0	0	0
			265	186	38	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	105	Total	C	N	O		0	0	0
			827	521	137	169				
15	u	105	Total	C	N	O		0	0	0
			827	521	137	169				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called photosystem II PsbX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	X	40	Total	C	N	O		0	0	0
			296	197	47	52				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	x	40	Total	C	N	O	0	0	0
			296	197	47	52			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	insertion	UNP Q9F1R6
X	2	ILE	-	insertion	UNP Q9F1R6
X	3	GLN	-	insertion	UNP Q9F1R6
X	4	SER	-	insertion	UNP Q9F1R6
X	5	ALA	-	insertion	UNP Q9F1R6
X	6	SER	-	insertion	UNP Q9F1R6
X	7	SER	-	insertion	UNP Q9F1R6
X	8	LEU	-	insertion	UNP Q9F1R6
X	9	LEU	-	insertion	UNP Q9F1R6
X	10	LEU	-	insertion	UNP Q9F1R6
x	2001	MET	-	insertion	UNP Q9F1R6
x	2002	ILE	-	insertion	UNP Q9F1R6
x	2003	GLN	-	insertion	UNP Q9F1R6
x	2004	SER	-	insertion	UNP Q9F1R6
x	2005	ALA	-	insertion	UNP Q9F1R6
x	2006	SER	-	insertion	UNP Q9F1R6
x	2007	SER	-	insertion	UNP Q9F1R6
x	2008	LEU	-	insertion	UNP Q9F1R6
x	2009	LEU	-	insertion	UNP Q9F1R6
x	2010	LEU	-	insertion	UNP Q9F1R6

- Molecule 18 is a protein called Photosystem II PsbN protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	N	37	Total	C	N	O	0	0	0
			186	111	37	38			
18	n	37	Total	C	N	O	0	0	0
			186	111	37	38			

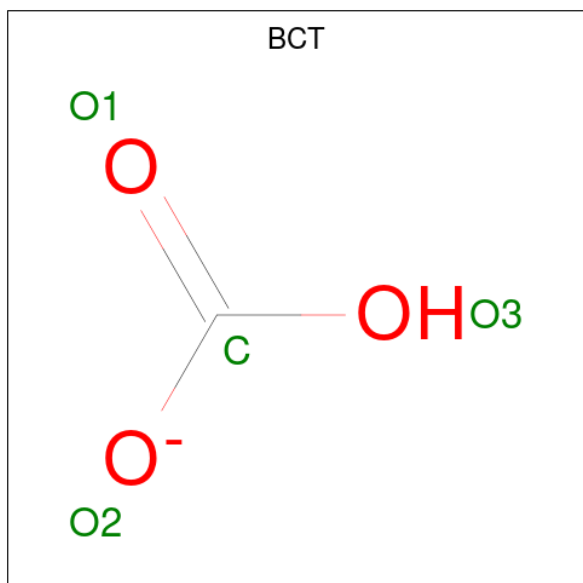
- Molecule 19 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			
19	z	58	Total	C	N	O	S	0	0	0
			442	300	68	72	2			

- Molecule 20 is FE (III) ION (CCD ID: FE) (formula: Fe).

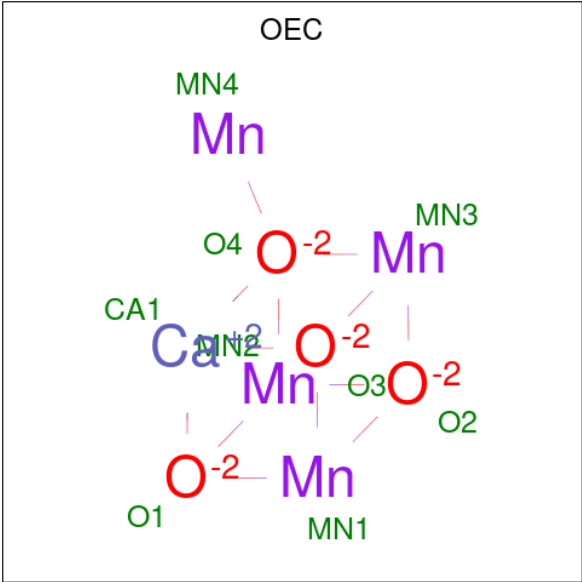
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



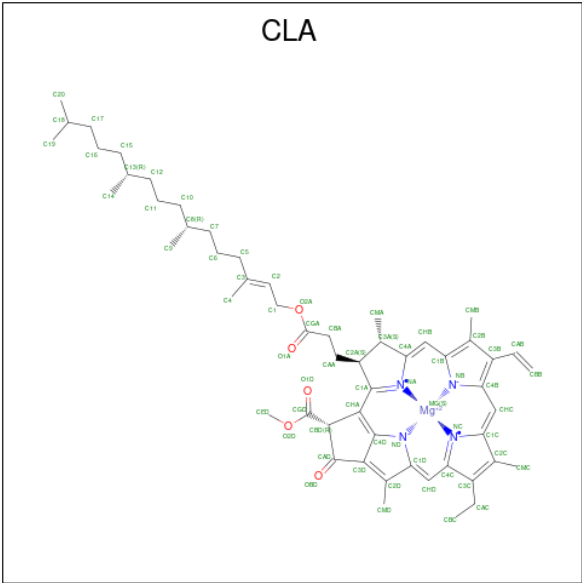
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	1	3		
21	D	1	Total	C	O	0	0
			4	1	3		
21	a	1	Total	C	O	0	0
			4	1	3		
21	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 22 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	Ca	Mn	O	0	0
			9	1	4	4		
22	a	1	Total	Ca	Mn	O	0	0
			9	1	4	4		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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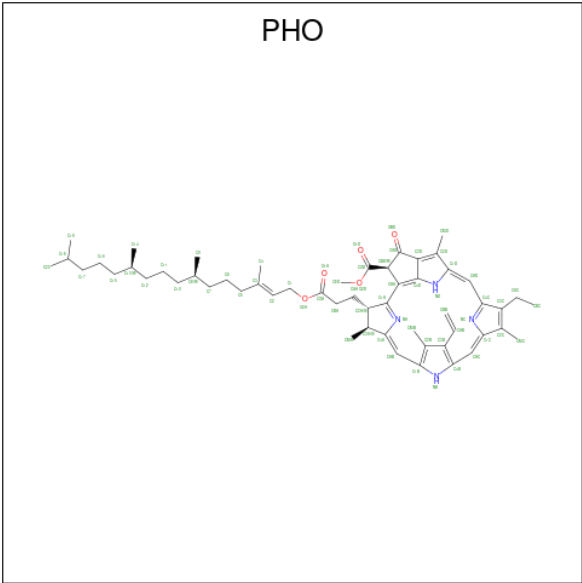
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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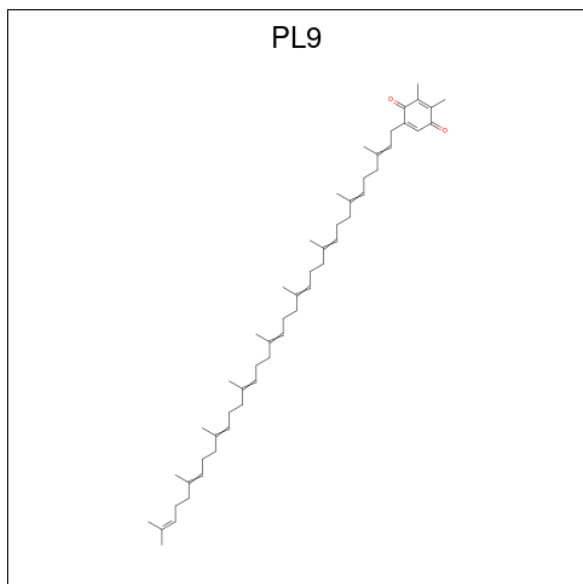
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



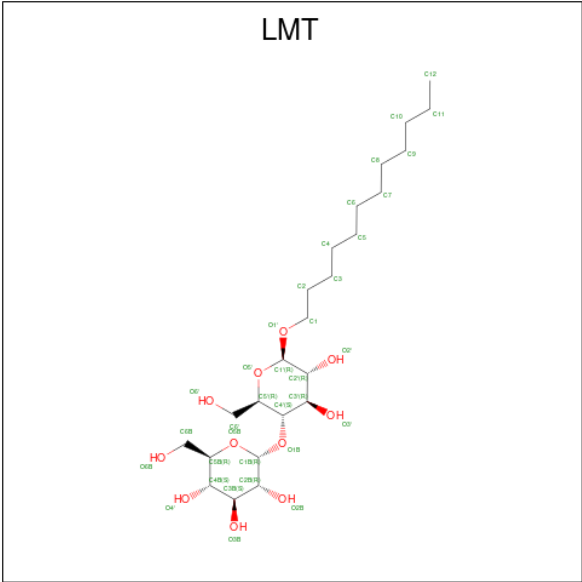
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



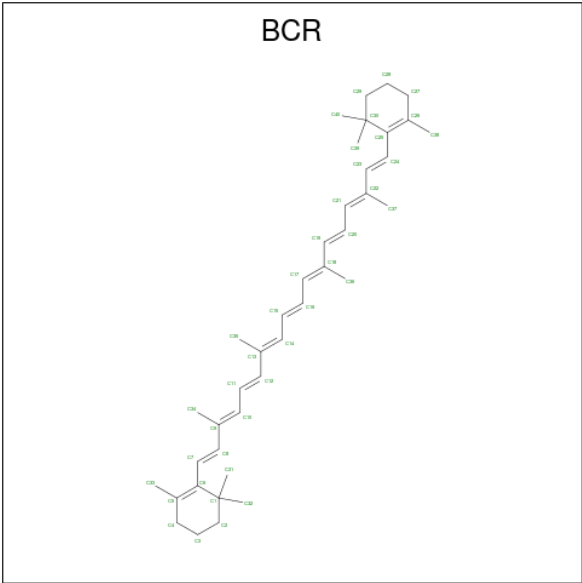
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			45	43	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			45	43	2		

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	B	1	Total	C	O	0
			35	24	11	
26	d	1	Total	C	O	0
			35	24	11	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



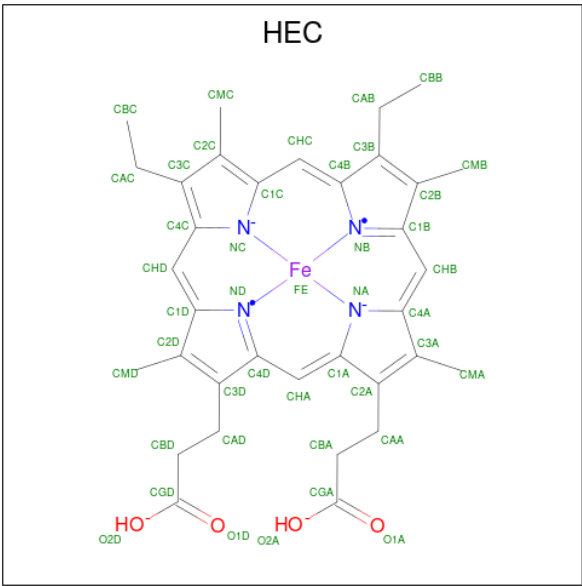
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total	C		0
			40	40		
27	B	1	Total	C		0
			40	40		

Continued on next page...

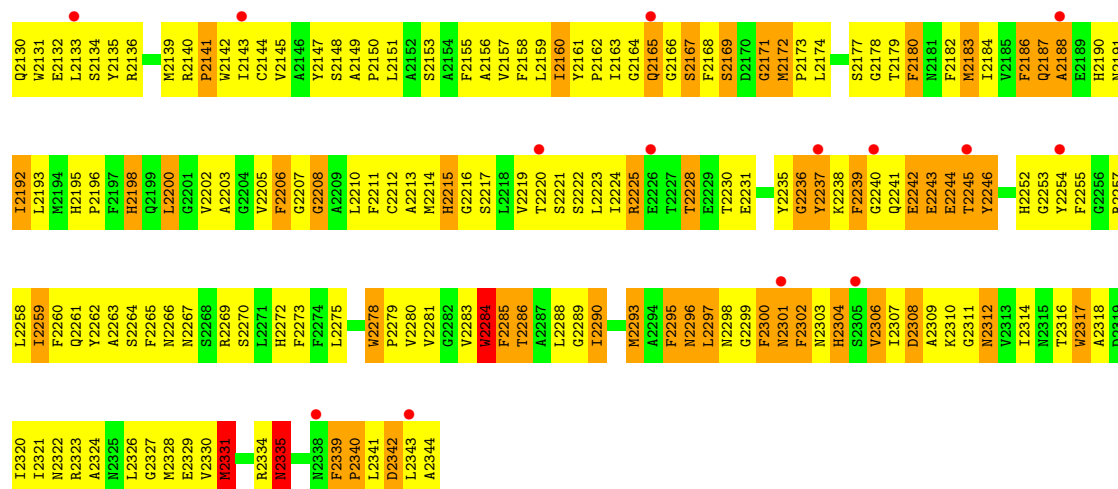
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	F	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

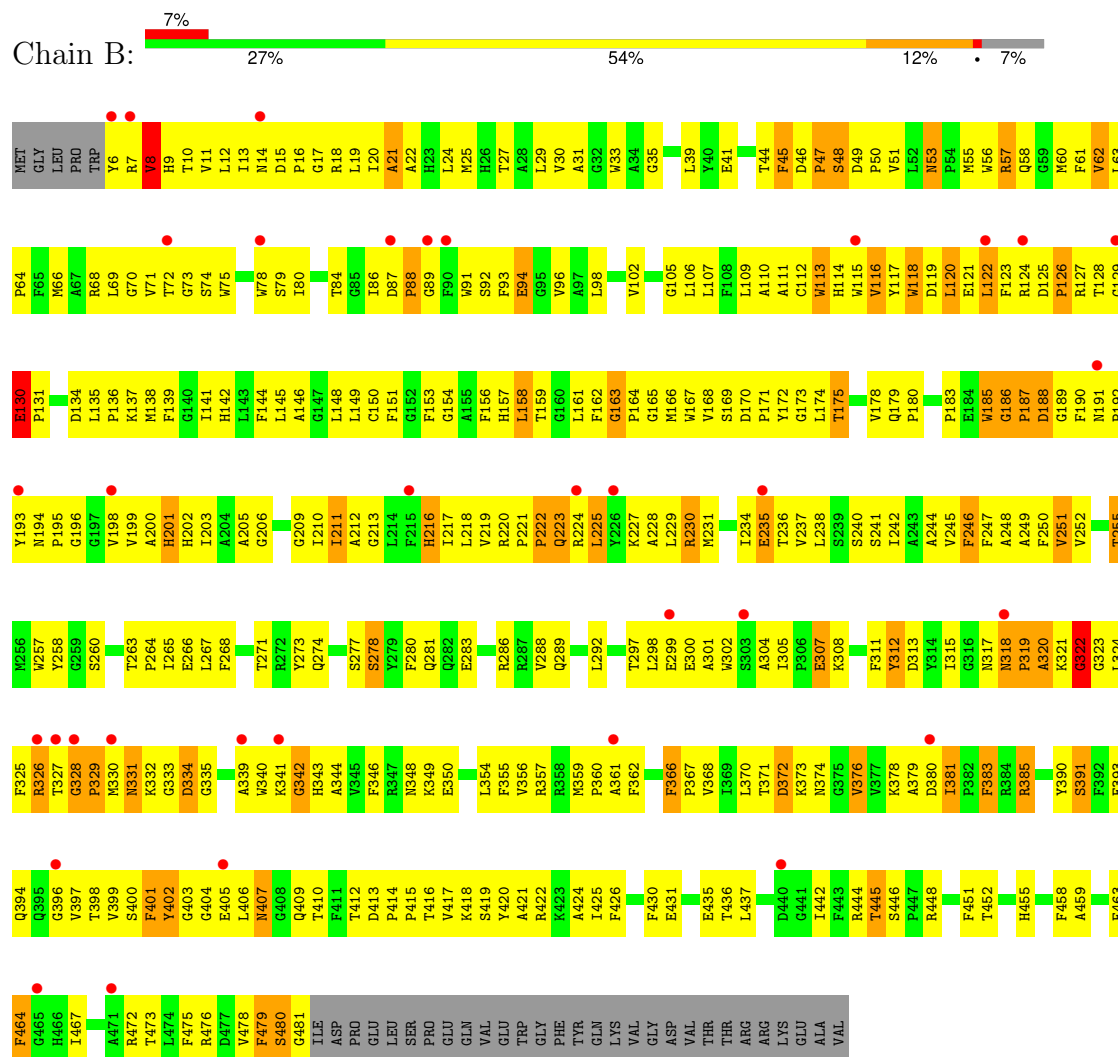
- Molecule 28 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
28	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
28	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
28	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



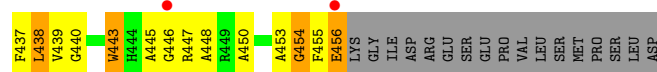
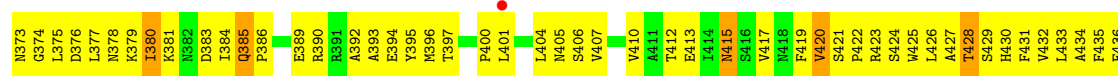
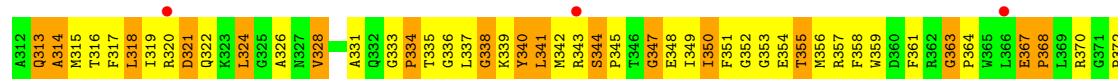
• Molecule 2: photosystem II core light harvesting protein



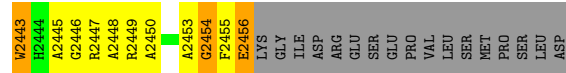
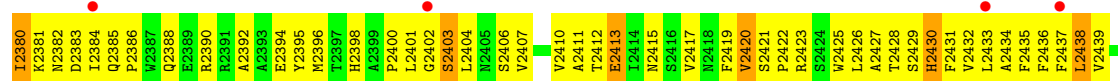
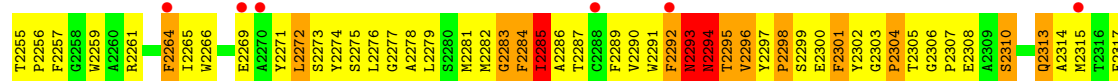
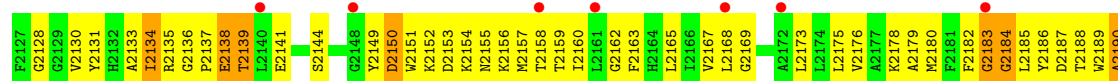
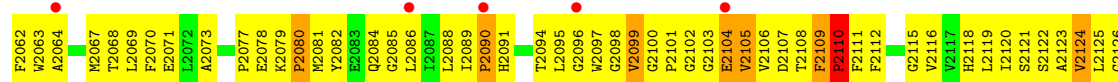
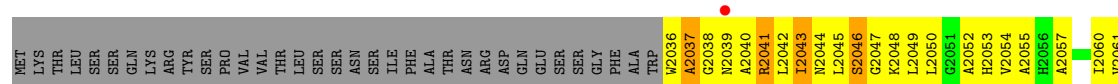
• Molecule 2: photosystem II core light harvesting protein





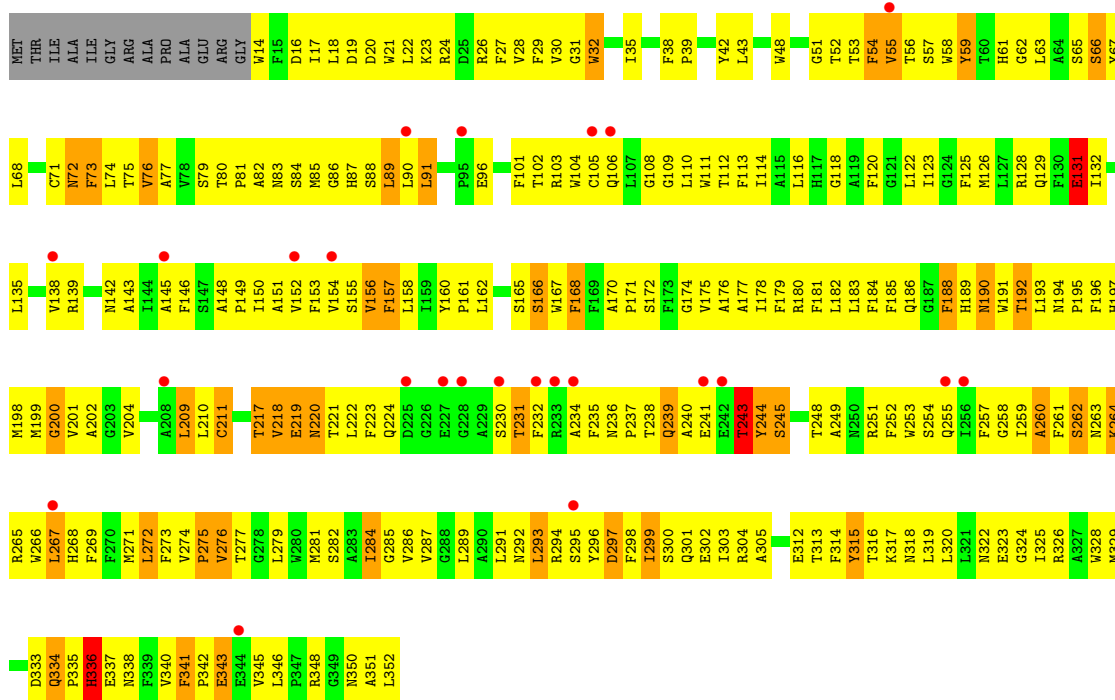


• Molecule 3: photosystem II CP43 protein

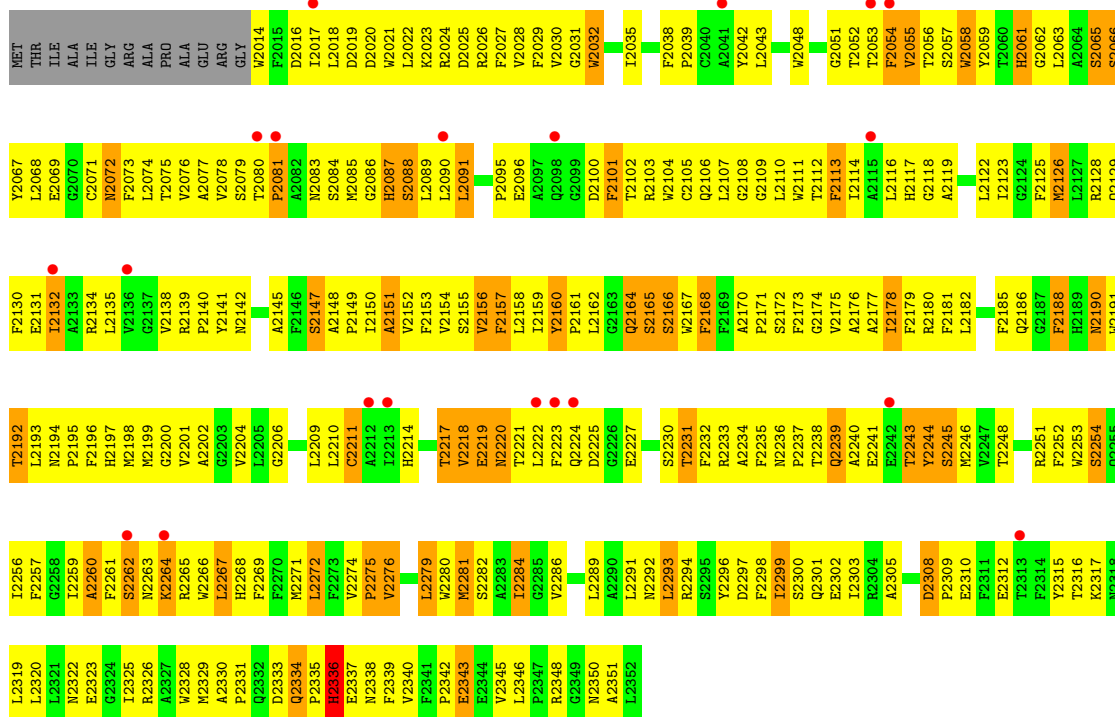


• Molecule 4: photosystem II reaction center D2 protein



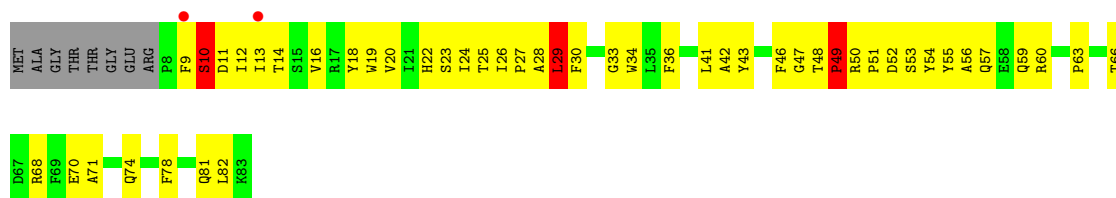


- Molecule 4: photosystem II reaction center D2 protein

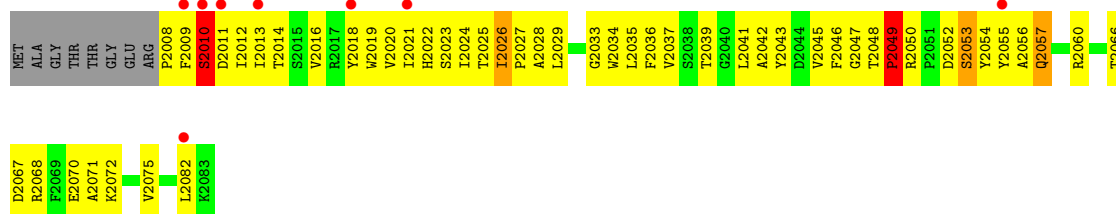


- Molecule 5: Cytochrome b559 alpha subunit

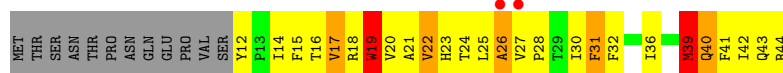




• Molecule 5: Cytochrome b559 alpha subunit



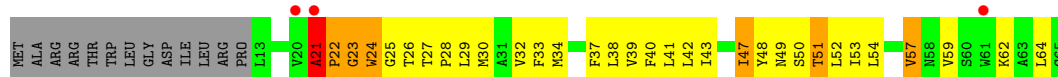
• Molecule 6: Cytochrome b559 beta subunit



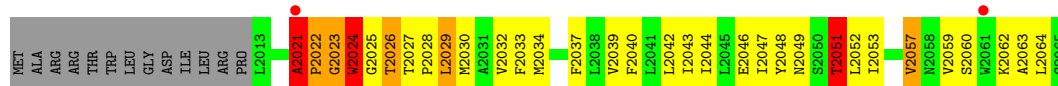
• Molecule 6: Cytochrome b559 beta subunit



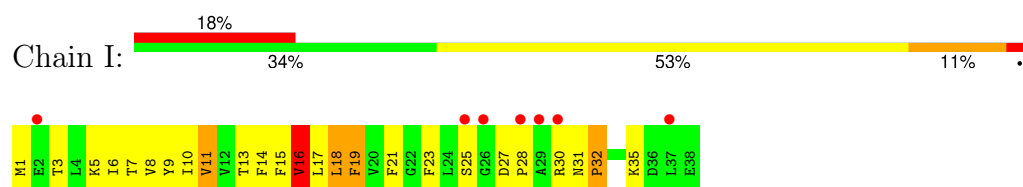
• Molecule 7: photosystem II PsbH protein



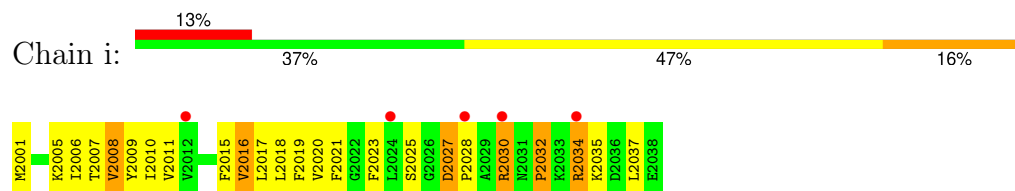
• Molecule 7: photosystem II PsbH protein



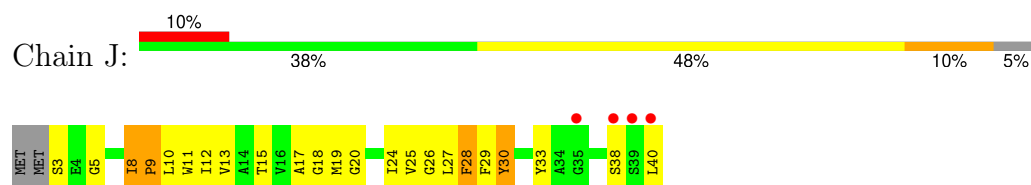
• Molecule 8: Photosystem II reaction center I protein



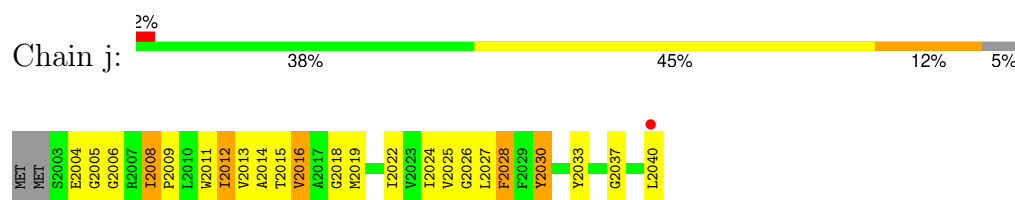
• Molecule 8: Photosystem II reaction center I protein



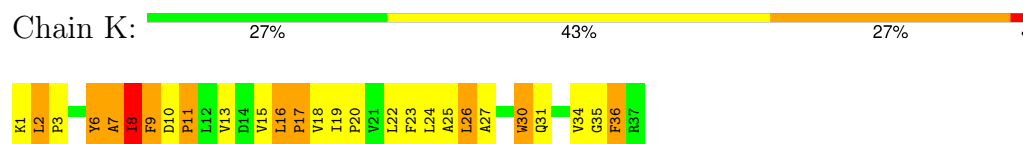
• Molecule 9: Photosystem II reaction center J protein



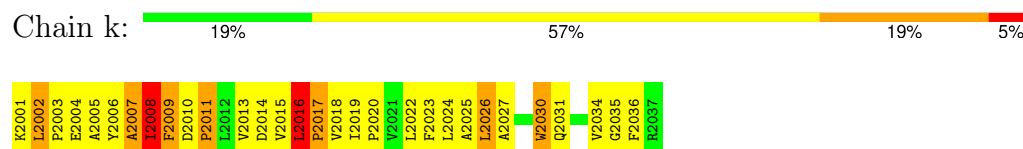
• Molecule 9: Photosystem II reaction center J protein



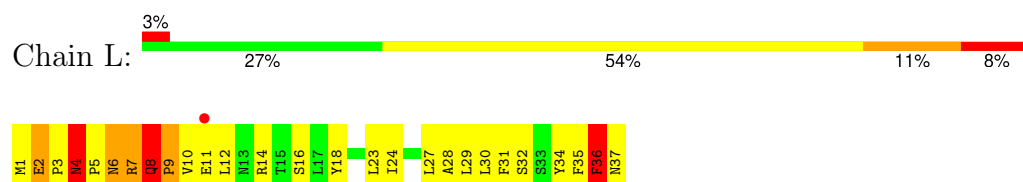
• Molecule 10: Photosystem II reaction center protein K



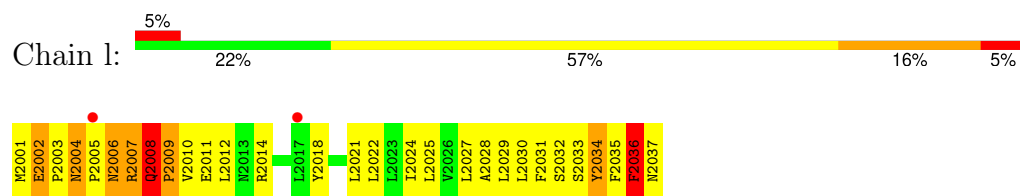
• Molecule 10: Photosystem II reaction center protein K



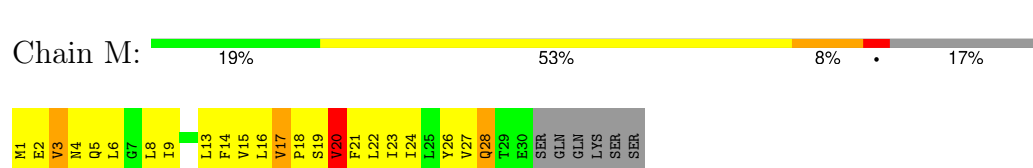
• Molecule 11: Photosystem II reaction center L protein



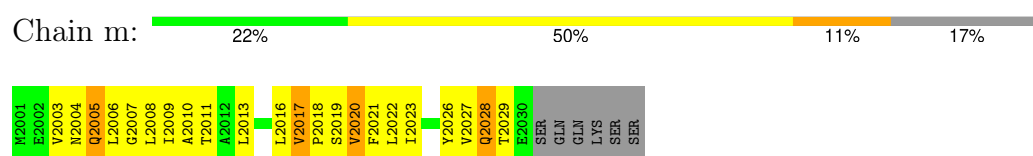
- Molecule 11: Photosystem II reaction center L protein



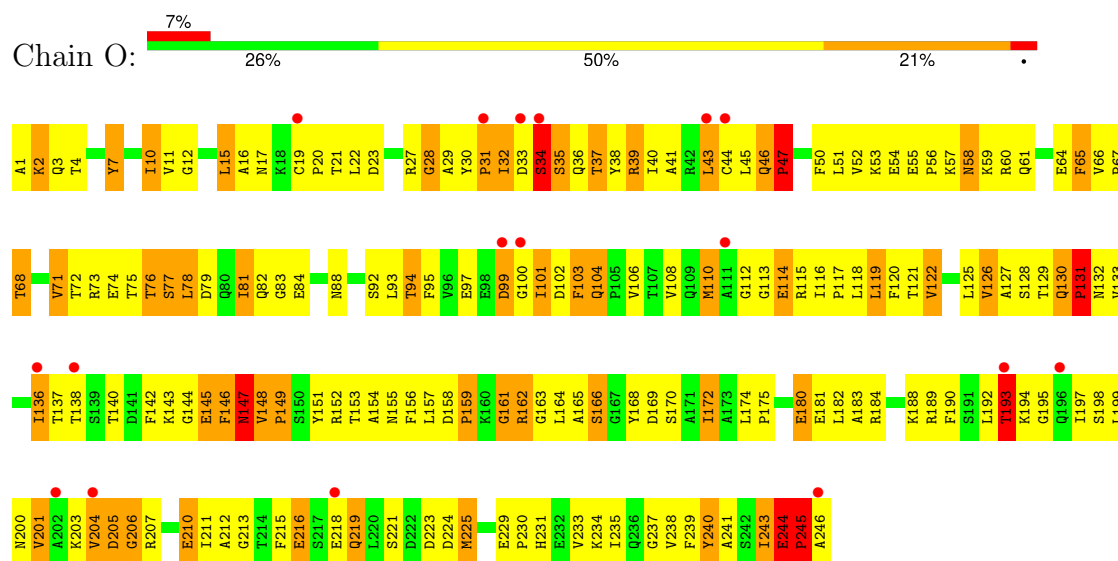
- Molecule 12: Photosystem II reaction center M protein



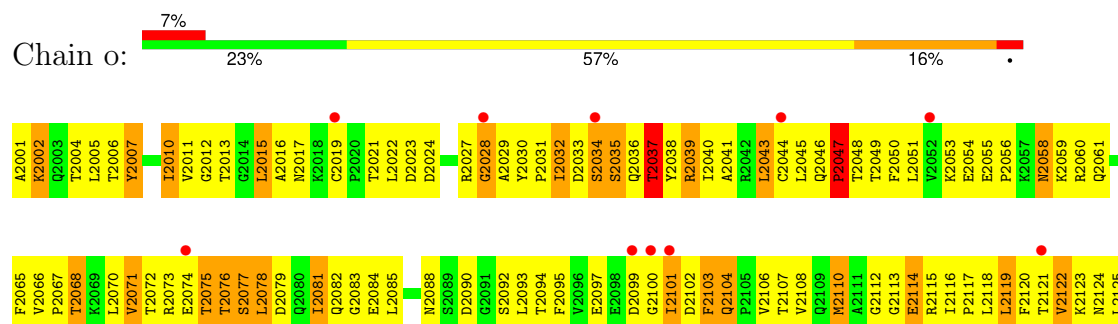
- Molecule 12: Photosystem II reaction center M protein

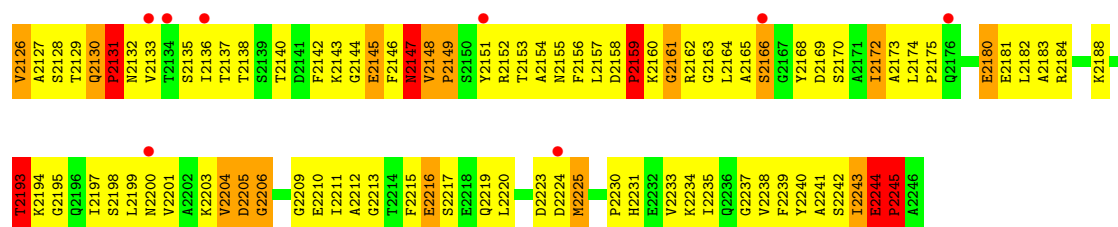


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

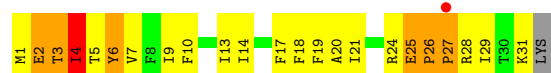


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

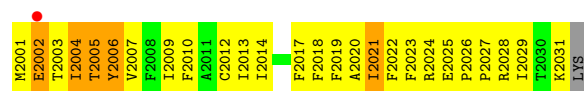




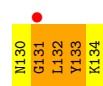
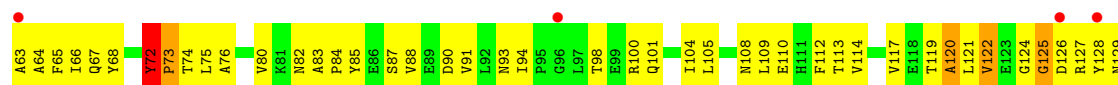
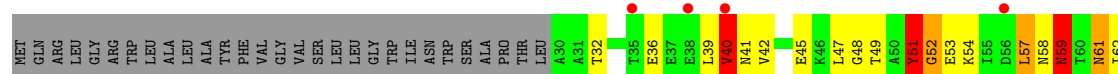
• Molecule 14: photosystem II PsbT protein



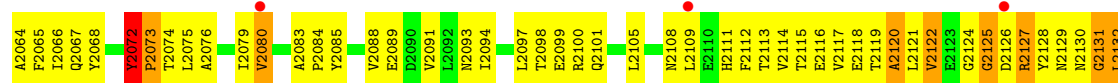
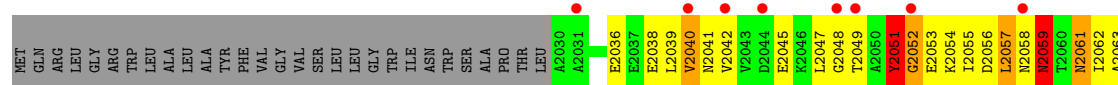
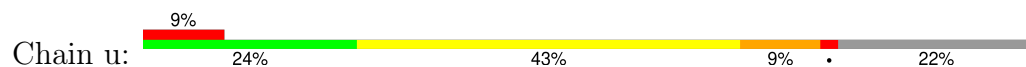
• Molecule 14: photosystem II PsbT protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

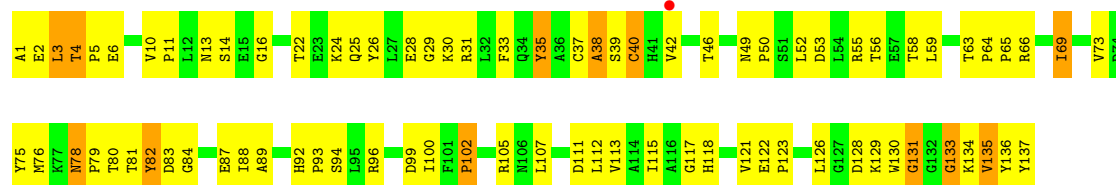


• Molecule 15: Photosystem II 12 kDa extrinsic protein

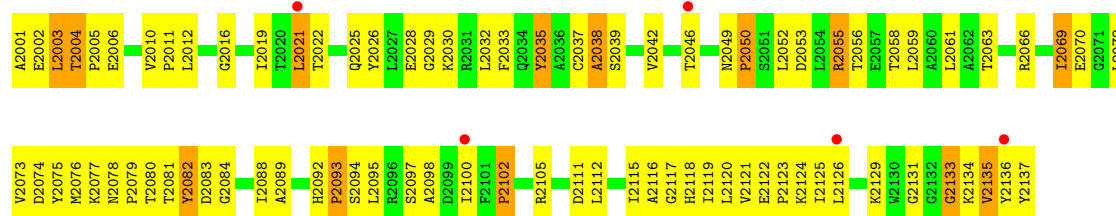


Y2133
K2134

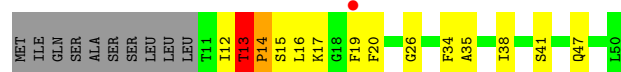
• Molecule 16: Cytochrome c-550



• Molecule 16: Cytochrome c-550



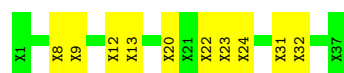
• Molecule 17: photosystem II PsbX protein



• Molecule 17: photosystem II PsbX protein



• Molecule 18: Photosystem II PsbN protein



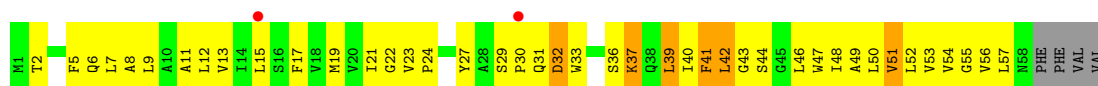
• Molecule 18: Photosystem II PsbN protein

Chain n:  73% 27%



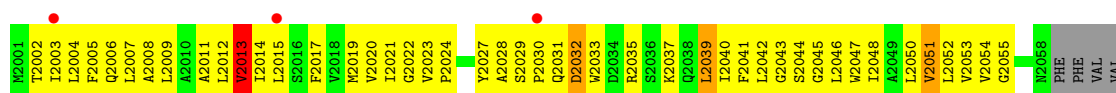
- Molecule 19: Photosystem II reaction center Z protein

Chain Z:  3% 26% 58% 10% 6%



- Molecule 19: Photosystem II reaction center Z protein

Chain z:  5% 21% 66% 5% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 228.85Å 309.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 85.2 (20.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.296 , 0.342 0.309 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	118.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	45945	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, PL9, LMT, BCR, HEC, CLA, PHO, OEC, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	5/2702 (0.2%)	1.28	43/3685 (1.2%)
1	a	0.76	1/2701 (0.0%)	1.27	40/3685 (1.1%)
2	B	0.72	0/3870	1.23	48/5271 (0.9%)
2	b	0.71	0/3870	1.23	53/5271 (1.0%)
3	C	0.74	1/3361 (0.0%)	1.26	45/4579 (1.0%)
3	c	0.69	0/3361	1.24	39/4579 (0.9%)
4	D	0.75	1/2797 (0.0%)	1.26	30/3813 (0.8%)
4	d	0.74	0/2797	1.27	36/3813 (0.9%)
5	E	0.73	0/643	1.26	8/876 (0.9%)
5	e	0.77	1/643 (0.2%)	1.26	9/876 (1.0%)
6	F	0.90	1/278 (0.4%)	1.26	4/379 (1.1%)
6	f	0.88	2/278 (0.7%)	1.30	7/379 (1.8%)
7	H	0.75	0/419	1.29	6/570 (1.1%)
7	h	0.73	0/419	1.23	6/570 (1.1%)
8	I	0.70	0/319	1.08	3/429 (0.7%)
8	i	0.68	0/319	1.07	2/429 (0.5%)
9	J	0.74	0/278	1.34	7/376 (1.9%)
9	j	0.73	0/278	1.38	8/376 (2.1%)
10	K	0.81	0/303	1.27	3/416 (0.7%)
10	k	0.77	0/303	1.25	4/416 (1.0%)
11	L	0.85	0/311	1.20	3/422 (0.7%)
11	l	0.90	0/311	1.18	3/422 (0.7%)
12	M	0.85	0/237	1.21	1/324 (0.3%)
12	m	0.87	0/237	1.18	1/324 (0.3%)
13	O	0.80	0/1919	1.44	38/2601 (1.5%)
13	o	0.80	0/1919	1.44	40/2601 (1.5%)
14	T	0.81	0/274	1.34	8/370 (2.2%)
14	t	0.84	0/274	1.30	4/370 (1.1%)
15	U	0.84	1/838 (0.1%)	1.23	5/1137 (0.4%)
15	u	0.75	0/838	1.21	7/1137 (0.6%)
16	V	0.77	1/1085 (0.1%)	1.09	4/1473 (0.3%)
16	v	0.66	0/1085	1.08	4/1473 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.67	0/299	1.12	3/403 (0.7%)
17	x	0.70	0/299	1.18	2/403 (0.5%)
19	Z	0.68	0/451	1.10	0/617
19	z	0.67	0/451	1.05	1/617 (0.2%)
All	All	0.76	14/40767 (0.0%)	1.26	525/55482 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	b	0	1
11	l	0	1
13	O	0	1
15	U	0	2
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	MET	SD-CE	-10.50	1.53	1.79
1	A	328	MET	SD-CE	-7.79	1.60	1.79
1	A	172	MET	SD-CE	-6.34	1.63	1.79
16	V	113	VAL	CA-CB	-5.88	1.47	1.54
1	A	290	ILE	CA-CB	-5.87	1.47	1.54
15	U	40	VAL	CA-CB	5.74	1.62	1.54
4	D	76	VAL	CA-CB	-5.46	1.48	1.54
5	e	2026	ILE	CA-CB	5.43	1.57	1.54
6	f	2039	MET	SD-CE	-5.41	1.66	1.79
6	f	2042	ILE	CA-CB	5.40	1.59	1.54
1	A	172	MET	CG-SD	5.20	1.93	1.80
6	F	39	MET	SD-CE	-5.16	1.66	1.79
3	C	350	ILE	CA-CB	-5.09	1.47	1.55
1	a	2183	MET	SD-CE	-5.05	1.67	1.79

All (525) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	193	THR	N-CA-C	13.08	125.47	108.34

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	2193	THR	N-CA-C	11.98	125.75	108.86
14	T	2	GLU	N-CA-C	-10.92	99.16	111.71
4	D	334	GLN	CA-C-N	10.88	131.25	119.28
4	D	334	GLN	C-N-CA	10.88	131.25	119.28
1	a	2245	THR	N-CA-C	10.87	123.13	111.28
13	O	23	ASP	N-CA-C	10.66	125.00	111.24
4	D	231	THR	N-CA-C	-10.55	93.98	108.86
4	d	2334	GLN	CA-C-N	10.46	130.79	119.28
4	d	2334	GLN	C-N-CA	10.46	130.79	119.28
4	d	2231	THR	N-CA-C	-10.33	94.30	108.86
2	b	2114	HIS	N-CA-C	-10.29	99.81	114.12
5	e	2053	SER	N-CA-C	10.26	125.10	112.59
14	t	2002	GLU	N-CA-C	-10.16	100.03	111.71
13	O	244	GLU	CA-C-N	10.14	132.52	119.84
13	O	244	GLU	C-N-CA	10.14	132.52	119.84
13	o	2023	ASP	N-CA-C	10.14	124.32	111.24
13	o	2132	ASN	N-CA-C	10.11	124.24	109.69
1	A	22	THR	N-CA-C	10.03	122.30	111.36
13	O	132	ASN	N-CA-C	10.03	124.13	109.69
5	E	53	SER	N-CA-C	9.90	124.66	112.59
2	B	114	HIS	N-CA-C	-9.71	100.63	114.12
1	A	245	THR	N-CA-C	9.48	121.70	111.36
13	o	2113	GLY	N-CA-C	-9.39	103.50	115.42
4	d	2244	TYR	N-CA-C	9.03	122.60	108.79
1	a	2022	THR	N-CA-C	8.92	121.09	111.36
16	V	69	ILE	N-CA-C	8.87	118.94	110.42
4	D	157	PHE	N-CA-C	8.85	123.73	113.19
15	u	2122	VAL	N-CA-C	8.85	120.97	111.58
4	d	2157	PHE	N-CA-C	8.79	123.64	113.19
2	b	2329	PRO	N-CA-C	-8.62	98.46	111.57
2	B	329	PRO	N-CA-C	-8.60	98.49	111.57
1	A	83	VAL	CA-C-N	8.51	130.47	119.84
1	A	83	VAL	C-N-CA	8.51	130.47	119.84
1	a	2083	VAL	CA-C-N	8.49	130.45	119.84
1	a	2083	VAL	C-N-CA	8.49	130.45	119.84
2	b	2435	GLU	N-CA-C	8.47	121.45	111.71
3	C	431	PHE	N-CA-C	-8.39	101.71	111.03
15	U	59	ASN	N-CA-C	8.39	123.46	112.72
14	t	2026	PRO	N-CA-C	8.38	120.93	110.70
4	D	244	TYR	N-CA-C	8.30	121.50	108.79
2	B	51	VAL	N-CA-C	8.28	119.06	110.62
3	c	2431	PHE	N-CA-C	-8.26	101.86	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	U	122	VAL	N-CA-C	8.25	120.32	111.58
13	O	113	GLY	N-CA-C	-8.24	104.96	115.42
3	c	2294	ASN	N-CA-C	-8.22	96.88	109.95
3	C	293	ASN	N-CA-C	8.22	122.45	110.28
4	D	243	THR	N-CA-C	8.22	122.66	113.21
2	B	435	GLU	N-CA-C	8.21	121.15	111.71
2	b	2051	VAL	N-CA-C	8.19	118.98	110.62
3	c	2293	ASN	N-CA-C	8.18	122.39	110.28
13	O	170	SER	N-CA-C	8.12	118.97	108.34
2	b	2158	LEU	N-CA-C	8.05	120.97	111.71
13	o	2244	GLU	CA-C-N	8.04	129.89	119.84
13	o	2244	GLU	C-N-CA	8.04	129.89	119.84
2	B	383	PHE	N-CA-C	-8.04	101.99	112.68
4	D	66	SER	N-CA-C	8.03	123.44	109.80
3	C	294	ASN	N-CA-C	-8.02	97.19	109.95
2	B	53	ASN	CA-C-N	8.00	127.95	120.03
2	B	53	ASN	C-N-CA	8.00	127.95	120.03
13	O	131	PRO	N-CA-C	8.00	128.95	112.47
2	B	332	LYS	N-CA-C	-7.98	103.99	112.93
3	C	136	GLY	CA-C-N	7.95	129.77	119.84
3	C	136	GLY	C-N-CA	7.95	129.77	119.84
4	d	2066	SER	N-CA-C	7.94	123.30	109.80
13	O	30	TYR	CA-C-N	7.83	129.63	119.84
13	O	30	TYR	C-N-CA	7.83	129.63	119.84
4	d	2054	PHE	N-CA-C	7.80	124.96	114.12
3	c	2232	ASP	N-CA-C	-7.80	102.47	110.97
2	b	2383	PHE	N-CA-C	-7.76	101.03	111.96
13	O	32	ILE	N-CA-C	-7.75	103.89	112.80
3	c	2318	LEU	N-CA-C	-7.73	102.80	111.07
1	a	2171	GLY	N-CA-C	-7.71	94.91	113.18
1	A	171	GLY	N-CA-C	-7.70	94.93	113.18
13	o	2032	ILE	N-CA-C	-7.62	104.03	112.80
13	o	2030	TYR	CA-C-N	7.57	129.31	119.84
13	o	2030	TYR	C-N-CA	7.57	129.31	119.84
1	A	60	ILE	N-CA-C	7.56	118.09	110.23
2	b	2332	LYS	N-CA-C	-7.55	104.48	112.93
4	d	2243	THR	N-CA-C	7.55	122.13	113.15
2	b	2335	GLY	N-CA-C	-7.53	99.60	110.60
2	B	464	PHE	N-CA-C	-7.52	103.02	111.07
2	B	129	GLY	N-CA-C	-7.50	98.35	111.62
13	o	2131	PRO	N-CA-C	7.49	127.89	112.47
15	u	2059	ASN	N-CA-C	7.48	123.12	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ILE	CB-CA-C	-7.47	102.13	111.92
7	H	21	ALA	CA-C-N	-7.47	110.50	119.84
7	H	21	ALA	C-N-CA	-7.47	110.50	119.84
1	A	198	HIS	N-CA-C	-7.46	104.20	113.38
13	o	2170	SER	N-CA-C	7.46	119.38	108.86
4	D	245	SER	N-CA-C	7.44	121.82	109.46
2	b	2053	ASN	CA-C-N	7.44	127.40	120.03
2	b	2053	ASN	C-N-CA	7.44	127.40	120.03
4	d	2272	LEU	N-CA-C	-7.44	103.82	113.12
4	d	2284	ILE	N-CA-C	-7.42	103.55	110.53
3	C	232	ASP	N-CA-C	-7.42	103.13	111.07
2	B	158	LEU	N-CA-C	7.39	120.20	111.71
13	o	2010	ILE	N-CA-C	7.37	120.26	111.05
3	c	2209	ILE	N-CA-C	7.37	118.14	110.62
4	d	2245	SER	N-CA-C	7.37	121.69	109.46
1	a	2296	ASN	N-CA-C	7.35	121.20	111.28
13	o	2034	SER	N-CA-C	-7.34	103.21	111.14
2	b	2045	PHE	N-CA-C	7.34	119.78	110.24
6	F	26	ALA	N-CA-C	7.33	120.15	111.71
10	k	2009	PHE	N-CA-C	7.31	121.91	112.92
1	a	2200	LEU	N-CA-C	-7.31	103.34	111.82
13	O	34	SER	N-CA-C	-7.29	103.27	111.14
2	B	185	TRP	N-CA-C	7.25	121.23	112.38
2	b	2129	GLY	N-CA-C	-7.25	98.78	111.62
1	A	296	ASN	N-CA-C	7.23	121.04	111.28
9	j	2008	ILE	CA-C-N	7.19	127.18	119.78
9	j	2008	ILE	C-N-CA	7.19	127.18	119.78
2	B	335	GLY	N-CA-C	-7.17	100.13	110.60
2	b	2366	PHE	CA-C-N	7.16	128.79	119.84
2	b	2366	PHE	C-N-CA	7.16	128.79	119.84
9	j	2011	TRP	N-CA-C	-7.16	104.51	113.18
13	O	15	LEU	N-CA-C	-7.13	105.11	113.88
14	T	26	PRO	N-CA-C	7.11	119.37	110.70
3	C	222	GLY	N-CA-C	-7.11	99.83	110.71
1	a	2198	HIS	N-CA-C	-7.11	104.42	113.23
2	B	225	LEU	N-CA-C	7.10	118.67	111.07
2	B	74	SER	N-CA-C	-7.03	98.33	109.23
13	o	2097	GLU	N-CA-C	6.98	120.71	110.59
9	J	11	TRP	N-CA-C	-6.96	104.78	113.20
10	K	9	PHE	N-CA-C	6.96	121.48	112.92
13	o	2002	LYS	N-CA-C	6.96	125.62	110.80
1	A	297	LEU	N-CA-C	-6.94	100.03	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	29	LEU	N-CA-C	-6.94	104.44	113.12
4	D	59	TYR	N-CA-C	-6.93	103.81	112.90
2	b	2225	LEU	N-CA-C	6.91	118.46	111.07
1	A	61	ASP	N-CA-C	6.90	120.37	112.57
4	D	272	LEU	N-CA-C	-6.89	104.51	113.12
3	C	283	GLY	N-CA-C	-6.87	104.33	112.64
4	d	2059	TYR	N-CA-C	-6.85	103.93	112.90
4	d	2160	TYR	CA-C-N	-6.85	111.75	119.28
4	d	2160	TYR	C-N-CA	-6.85	111.75	119.28
4	d	2276	VAL	N-CA-C	6.84	117.54	110.36
2	b	2407	ASN	N-CA-C	6.84	120.11	107.60
14	T	28	ARG	N-CA-C	6.80	120.76	109.95
3	c	2136	GLY	CA-C-N	6.80	128.34	119.84
3	c	2136	GLY	C-N-CA	6.80	128.34	119.84
2	B	45	PHE	N-CA-C	6.78	119.06	110.24
9	J	30	TYR	N-CA-C	-6.78	103.58	110.97
1	A	321	ILE	N-CA-C	-6.77	104.41	111.58
3	C	318	LEU	N-CA-C	-6.76	103.84	111.07
13	O	10	ILE	N-CA-C	6.74	119.48	111.05
13	o	2035	SER	N-CA-C	-6.74	103.18	111.33
1	A	145	VAL	N-CA-C	6.74	117.52	110.72
16	v	2003	LEU	N-CA-C	-6.74	99.86	109.96
12	m	2020	VAL	N-CA-C	-6.73	103.23	110.23
1	a	2236	GLY	N-CA-C	6.72	129.12	113.18
13	o	2071	VAL	N-CA-C	-6.72	105.20	111.45
3	c	2283	GLY	N-CA-C	-6.72	104.51	112.64
6	f	2026	ALA	N-CA-C	6.71	119.43	111.71
3	C	150	ASP	N-CA-C	6.71	120.12	109.65
3	C	41	ARG	N-CA-C	-6.69	103.80	112.23
2	b	2185	TRP	N-CA-C	6.69	120.54	112.38
2	B	366	PHE	CA-C-N	6.68	128.19	119.84
2	B	366	PHE	C-N-CA	6.68	128.19	119.84
1	A	36	ILE	N-CA-C	-6.67	106.50	111.90
11	L	7	ARG	N-CA-C	-6.66	97.68	108.41
4	d	2190	ASN	N-CA-C	-6.65	102.21	111.52
2	B	407	ASN	N-CA-C	6.63	119.73	107.60
13	O	7	TYR	N-CA-C	-6.62	104.10	111.71
13	o	2015	LEU	N-CA-C	-6.62	105.74	113.88
1	a	2145	VAL	N-CA-C	6.62	117.40	110.72
1	a	2206	PHE	N-CA-C	-6.61	104.31	112.38
1	A	236	GLY	N-CA-C	6.60	128.83	113.18
3	c	2106	VAL	N-CA-C	-6.59	104.59	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	22	VAL	N-CA-C	6.58	117.27	110.36
3	c	2344	SER	N-CA-C	-6.57	100.04	110.10
2	b	2113	TRP	N-CA-C	6.57	120.91	113.02
13	O	2	LYS	N-CA-C	6.57	124.80	110.80
3	C	209	ILE	N-CA-C	6.55	117.24	110.36
4	D	234	ALA	N-CA-C	6.54	119.66	109.52
13	O	243	ILE	CB-CA-C	-6.54	102.72	111.80
3	c	2363	GLY	CA-C-N	6.54	126.47	119.28
3	c	2363	GLY	C-N-CA	6.54	126.47	119.28
2	b	2218	LEU	N-CA-C	6.52	118.27	111.03
2	b	2401	PHE	N-CA-C	6.52	118.91	108.41
4	d	2072	ASN	N-CA-C	-6.51	102.13	110.53
3	c	2324	LEU	N-CA-C	-6.50	105.31	112.72
1	a	2285	PHE	N-CA-C	6.50	118.02	111.07
13	O	97	GLU	N-CA-C	6.49	120.00	110.59
2	B	401	PHE	N-CA-C	6.48	118.84	108.41
4	D	276	VAL	N-CA-C	6.47	117.15	110.36
15	u	2074	THR	N-CA-C	6.47	121.44	112.45
2	b	2257	TRP	N-CA-C	6.46	119.15	111.33
3	c	2379	LYS	N-CA-C	-6.46	104.09	112.23
14	t	2028	ARG	N-CA-C	6.45	120.56	110.17
1	a	2179	THR	N-CA-C	-6.43	104.19	111.07
1	a	2339	PHE	CA-C-N	6.43	125.93	119.24
1	a	2339	PHE	C-N-CA	6.43	125.93	119.24
4	D	72	ASN	N-CA-C	-6.43	102.24	110.53
3	C	109	PHE	N-CA-C	6.42	124.01	109.81
7	h	2034	MET	N-CA-C	-6.42	104.71	112.54
7	H	51	THR	N-CA-C	-6.41	105.50	113.38
7	H	34	MET	N-CA-C	-6.40	104.74	112.54
2	b	2074	SER	N-CA-C	-6.39	99.32	109.23
1	A	179	THR	N-CA-C	-6.39	104.23	111.07
13	O	145	GLU	N-CA-C	6.39	119.42	109.52
3	C	344	SER	N-CA-C	-6.38	100.34	110.10
2	b	2331	ASN	N-CA-C	6.38	120.16	112.38
15	U	72	TYR	N-CA-C	6.35	123.84	109.81
11	l	2007	ARG	N-CA-C	-6.33	98.21	108.41
5	E	11	ASP	CA-C-N	-6.33	110.64	121.09
5	E	11	ASP	C-N-CA	-6.33	110.64	121.09
9	j	2030	TYR	N-CA-C	-6.33	104.07	110.97
5	e	2011	ASP	CA-C-N	-6.32	110.66	121.09
5	e	2011	ASP	C-N-CA	-6.32	110.66	121.09
13	O	4	THR	N-CA-C	6.32	118.92	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	379	LYS	N-CA-C	-6.32	104.27	112.23
1	A	284	TRP	N-CA-C	-6.31	103.32	111.02
1	a	2169	SER	N-CA-C	-6.30	101.35	110.24
15	U	57	LEU	N-CA-C	6.30	120.80	113.18
1	A	89	ILE	N-CA-C	-6.30	103.75	112.50
2	B	307	GLU	N-CA-C	6.30	118.22	111.36
3	c	2109	PHE	N-CA-C	6.30	123.72	109.81
13	O	58	ASN	N-CA-C	6.29	119.16	110.35
3	c	2222	GLY	N-CA-C	-6.29	101.08	110.71
13	o	2043	LEU	N-CA-C	6.26	119.60	109.40
2	B	331	ASN	N-CA-C	6.26	120.01	112.38
6	f	2022	VAL	N-CA-C	6.26	116.93	110.36
3	C	314	ALA	N-CA-C	-6.25	104.09	111.03
12	M	20	VAL	N-CA-C	-6.25	103.72	110.23
2	B	216	HIS	N-CA-C	-6.25	105.43	114.12
1	a	2061	ASP	N-CA-C	6.25	120.75	112.25
1	a	2076	ASN	N-CA-C	-6.25	99.98	109.85
13	o	2099	ASP	N-CA-C	6.25	118.17	111.36
2	b	2464	PHE	N-CA-C	-6.24	104.40	111.07
16	v	2069	ILE	N-CA-C	6.22	116.39	110.42
3	c	2124	VAL	CB-CA-C	-6.21	102.99	112.05
2	B	218	LEU	N-CA-C	6.20	117.91	111.03
2	B	113	TRP	N-CA-C	6.20	120.45	113.02
13	O	43	LEU	N-CA-C	6.20	119.50	109.40
1	A	200	LEU	N-CA-C	-6.19	104.64	111.82
5	e	2020	VAL	N-CA-C	6.19	116.97	110.72
4	D	54	PHE	N-CA-C	6.17	123.33	114.39
3	c	2383	ASP	N-CA-C	6.16	119.24	110.68
5	E	10	SER	CA-C-N	-6.16	109.78	121.54
5	E	10	SER	C-N-CA	-6.16	109.78	121.54
5	e	2010	SER	CA-C-N	-6.15	109.79	121.54
5	e	2010	SER	C-N-CA	-6.15	109.79	121.54
9	J	12	ILE	N-CA-C	-6.15	105.73	111.45
9	j	2012	ILE	N-CA-C	-6.14	105.73	111.45
4	d	2234	ALA	N-CA-C	6.14	119.55	109.85
13	o	2145	GLU	N-CA-C	6.14	118.74	109.41
1	A	331	MET	N-CA-C	6.13	120.79	112.88
9	j	2005	GLY	N-CA-C	-6.13	105.98	115.73
1	a	2192	ILE	CB-CA-C	-6.13	103.89	111.92
13	O	37	THR	N-CA-C	6.12	116.08	108.19
14	t	2006	TYR	N-CA-C	-6.11	105.31	112.89
15	U	74	THR	N-CA-C	6.11	120.94	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	2031	PRO	N-CA-C	6.10	125.03	112.47
11	L	11	GLU	N-CA-C	6.09	119.41	109.06
9	J	8	ILE	CA-C-N	6.09	126.05	119.78
9	J	8	ILE	C-N-CA	6.09	126.05	119.78
8	I	16	VAL	N-CA-C	-6.08	105.80	111.45
11	l	2011	GLU	N-CA-C	6.08	119.40	109.06
11	L	36	PHE	N-CA-C	6.07	117.58	110.97
1	A	340	PRO	N-CA-C	6.06	121.95	113.53
10	k	2030	TRP	N-CA-C	-6.05	104.68	111.28
4	D	190	ASN	N-CA-C	-6.05	103.05	111.39
1	A	169	SER	N-CA-C	-6.02	101.75	110.24
16	V	3	LEU	N-CA-C	-6.01	100.95	109.96
1	A	206	PHE	N-CA-C	-6.01	105.05	112.38
15	u	2127	ARG	N-CA-C	6.00	117.90	111.36
13	O	204	VAL	N-CA-C	-6.00	99.08	108.86
3	c	2057	ALA	N-CA-C	-6.00	105.92	113.18
5	e	2026	ILE	CA-C-N	-6.00	113.46	120.12
5	e	2026	ILE	C-N-CA	-6.00	113.46	120.12
1	A	161	TYR	CA-C-N	-5.98	112.36	119.84
1	A	161	TYR	C-N-CA	-5.98	112.36	119.84
2	b	2216	HIS	N-CA-C	-5.98	105.81	114.12
7	h	2051	THR	N-CA-C	-5.97	106.04	113.38
13	o	2103	PHE	N-CA-C	5.95	118.01	109.14
1	a	2246	TYR	N-CA-C	5.95	119.25	109.85
13	O	205	ASP	N-CA-C	5.95	116.41	108.38
4	D	151	ALA	N-CA-C	-5.94	104.44	111.03
3	c	2150	ASP	N-CA-C	5.94	118.91	109.65
7	h	2024	TRP	N-CA-C	-5.93	105.14	112.38
1	a	2089	ILE	N-CA-C	-5.93	104.26	112.50
13	o	2007	TYR	N-CA-C	-5.92	104.91	111.71
4	d	2151	ALA	N-CA-C	-5.91	104.47	111.03
3	C	341	LEU	N-CA-C	5.91	118.53	108.90
1	A	76	ASN	N-CA-C	-5.90	100.52	109.85
2	b	2412	THR	N-CA-C	5.90	120.28	112.72
3	C	57	ALA	N-CA-C	-5.90	106.04	113.18
2	B	412	THR	N-CA-C	5.89	120.26	112.72
13	O	100	GLY	N-CA-C	5.89	124.77	114.76
4	d	2346	LEU	N-CA-C	5.88	116.80	109.57
3	C	347	GLY	N-CA-C	5.87	125.91	114.16
7	h	2021	ALA	CA-C-N	-5.87	112.50	119.84
7	h	2021	ALA	C-N-CA	-5.87	112.50	119.84
3	C	44	ASN	N-CA-C	5.87	120.16	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	175	THR	N-CA-C	-5.86	104.33	112.30
5	E	20	VAL	CB-CA-C	-5.85	104.48	111.97
3	C	106	VAL	N-CA-C	-5.85	105.38	111.58
4	D	284	ILE	N-CA-C	-5.84	104.64	110.30
8	I	11	VAL	CB-CA-C	-5.84	104.41	111.88
8	i	2034	ARG	N-CA-C	5.84	119.59	112.23
13	o	2100	GLY	N-CA-C	5.84	124.68	114.76
13	o	2147	ASN	N-CA-C	-5.83	98.57	108.26
17	x	2013	THR	CA-C-N	5.82	127.12	119.84
17	x	2013	THR	C-N-CA	5.82	127.12	119.84
13	O	147	ASN	N-CA-C	-5.82	98.60	108.26
3	c	2347	GLY	N-CA-C	5.82	125.80	114.16
8	i	2016	VAL	N-CA-C	-5.82	105.41	111.58
13	o	2037	THR	N-CA-C	5.82	116.10	108.07
13	O	35	SER	N-CA-C	-5.81	104.31	111.75
2	B	257	TRP	N-CA-C	5.80	118.35	111.33
4	D	135	LEU	N-CA-C	-5.80	104.96	112.68
17	X	26	GLY	N-CA-C	-5.79	105.48	112.49
3	C	126	GLY	N-CA-C	-5.79	105.78	112.73
2	B	342	GLY	N-CA-C	5.79	119.14	111.03
4	d	2065	SER	N-CA-C	5.79	118.46	111.40
3	C	322	GLN	N-CA-C	-5.78	105.06	111.71
3	c	2134	ILE	N-CA-C	5.76	121.33	109.34
3	c	2353	GLY	N-CA-C	-5.76	104.10	112.17
1	a	2290	ILE	CB-CA-C	-5.75	104.61	111.97
1	A	188	ALA	N-CA-C	-5.75	106.10	113.23
4	d	2200	GLY	N-CA-C	-5.75	105.68	112.64
16	V	35	TYR	N-CA-C	5.74	117.34	111.14
2	B	118	TRP	N-CA-C	5.74	119.36	112.93
3	c	2341	LEU	N-CA-C	5.74	118.25	108.90
4	D	200	GLY	N-CA-C	-5.73	105.70	112.64
1	A	304	HIS	N-CA-C	5.72	118.82	108.69
13	o	2004	THR	N-CA-C	5.71	117.99	109.25
3	C	142	GLU	N-CA-C	5.71	117.96	111.11
2	b	2342	GLY	N-CA-C	5.71	119.02	111.03
1	A	285	PHE	N-CA-C	5.70	117.17	111.07
3	C	211	GLY	N-CA-C	-5.70	105.89	112.73
2	b	2175	THR	N-CA-C	-5.70	104.55	112.30
3	c	2284	PHE	N-CA-C	-5.69	104.77	110.97
1	A	147	TYR	N-CA-C	-5.69	105.16	111.36
13	o	2058	ASN	N-CA-C	5.69	118.31	110.35
2	b	2307	GLU	N-CA-C	5.68	117.56	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	2031	PHE	N-CA-C	-5.68	105.17	111.36
1	A	288	LEU	N-CA-C	-5.68	104.47	111.40
3	C	428	THR	N-CA-C	5.68	117.33	111.03
3	c	2099	VAL	N-CA-C	5.68	115.81	107.75
3	C	284	PHE	N-CA-C	-5.67	104.79	110.97
16	V	135	VAL	N-CA-C	-5.66	104.85	110.62
3	C	99	VAL	N-CA-C	5.66	115.78	107.75
2	B	128	THR	N-CA-C	5.65	119.45	109.96
13	o	2245	PRO	N-CA-C	-5.65	100.84	112.47
4	D	297	ASP	N-CA-C	5.64	117.68	108.76
2	b	2163	GLY	N-CA-C	5.64	123.85	112.34
1	a	2119	PHE	N-CA-C	5.63	117.41	111.28
4	D	336	HIS	N-CA-C	5.62	117.49	111.36
4	d	2114	ILE	N-CA-C	5.62	116.26	110.36
13	O	99	ASP	N-CA-C	5.62	117.49	111.36
1	a	2331	MET	N-CA-C	5.62	120.12	112.88
3	c	2272	LEU	N-CA-C	-5.61	104.79	111.69
15	u	2072	TYR	N-CA-C	5.61	122.20	109.81
2	b	2118	TRP	N-CA-C	5.60	119.21	112.93
2	b	2320	ALA	N-CA-C	5.60	121.42	110.56
13	o	2210	GLU	N-CA-C	5.60	120.38	112.93
2	B	163	GLY	N-CA-C	5.59	123.75	112.34
14	T	6	TYR	N-CA-C	-5.59	105.95	112.89
3	C	134	ILE	N-CA-C	5.59	120.97	109.34
7	h	2029	LEU	N-CA-C	-5.59	105.11	111.14
2	b	2381	ILE	CA-C-N	5.58	126.82	119.84
2	b	2381	ILE	C-N-CA	5.58	126.82	119.84
2	B	445	THR	N-CA-C	5.58	118.82	109.95
13	o	2205	ASP	N-CA-C	5.58	116.74	108.60
15	u	2057	LEU	N-CA-C	5.57	119.70	113.01
8	I	19	PHE	N-CA-C	-5.56	104.07	111.24
5	e	2029	LEU	N-CA-C	-5.55	106.18	113.12
3	C	56	HIS	N-CA-C	-5.54	106.02	112.89
2	b	2122	LEU	N-CA-C	5.53	118.87	108.65
4	d	2315	TYR	N-CA-C	-5.51	104.30	111.02
2	B	87	ASP	N-CA-C	5.50	118.32	108.47
4	d	2164	GLN	N-CA-C	5.50	118.38	109.86
1	a	2038	ILE	CA-C-N	-5.50	112.97	119.84
1	a	2038	ILE	C-N-CA	-5.50	112.97	119.84
1	a	2186	PHE	N-CA-C	5.50	116.95	111.07
4	D	341	PHE	CA-C-N	5.48	126.34	119.98
4	D	341	PHE	C-N-CA	5.48	126.34	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	VAL	N-CA-C	-5.47	107.10	111.81
2	B	146	ALA	N-CA-C	-5.47	104.16	112.04
2	b	2146	ALA	N-CA-C	-5.47	104.16	112.04
9	J	5	GLY	N-CA-C	-5.47	107.03	115.73
4	d	2055	VAL	N-CA-C	5.47	117.20	108.89
4	D	295	SER	N-CA-C	-5.47	100.83	108.54
2	b	2128	THR	N-CA-C	5.47	119.14	109.96
3	c	2438	LEU	N-CA-C	-5.46	105.41	111.36
2	b	2092	SER	CB-CA-C	-5.46	107.58	114.40
1	A	246	TYR	N-CA-C	5.46	118.48	109.85
3	C	385	GLN	CA-C-N	5.46	124.65	118.97
3	C	385	GLN	C-N-CA	5.46	124.65	118.97
1	a	2188	ALA	N-CA-C	-5.46	106.46	113.23
3	C	383	ASP	N-CA-C	5.46	119.67	111.81
1	A	87	ASN	N-CA-C	-5.45	106.63	113.28
4	d	2336	HIS	N-CA-C	5.45	117.22	111.28
1	A	103	ASP	N-CA-C	-5.44	105.35	111.28
2	B	251	VAL	N-CA-C	-5.44	105.79	110.74
3	c	2126	GLY	N-CA-C	-5.43	106.21	112.73
2	b	2193	TYR	N-CA-C	5.43	120.04	113.41
2	b	2014	ASN	N-CA-C	5.42	119.61	112.89
3	c	2041	ARG	N-CA-C	-5.41	105.41	112.23
2	b	2087	ASP	N-CA-C	5.40	118.14	108.47
1	a	2284	TRP	N-CA-C	-5.40	104.43	111.02
11	l	2036	PHE	N-CA-C	5.40	117.61	111.02
1	a	2165	GLN	N-CA-C	5.40	119.03	112.23
6	F	19	TRP	N-CA-C	5.39	122.29	110.80
1	A	335	ASN	N-CA-C	5.39	122.28	110.80
2	b	2115	TRP	N-CA-C	-5.38	105.84	112.90
13	O	81	ILE	N-CA-C	5.38	120.53	109.34
1	a	2335	ASN	N-CA-C	5.37	122.25	110.80
3	C	324	LEU	N-CA-C	-5.36	106.61	112.72
2	b	2251	VAL	N-CA-C	-5.36	105.87	110.74
2	B	14	ASN	N-CA-C	5.35	119.52	112.89
2	b	2322	GLY	N-CA-C	5.34	125.84	113.18
13	o	2119	LEU	N-CA-C	-5.33	100.04	108.73
13	O	31	PRO	N-CA-C	5.33	123.45	112.47
1	a	2312	ASN	CB-CA-C	-5.33	103.25	109.80
16	v	2135	VAL	N-CA-C	-5.32	105.19	110.62
13	O	119	LEU	N-CA-C	-5.32	100.06	108.73
3	c	2336	GLY	N-CA-C	-5.32	107.88	115.64
4	d	2135	LEU	N-CA-C	-5.32	105.61	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	103	PHE	N-CA-C	5.30	117.03	109.14
3	C	151	TRP	N-CA-C	5.29	116.75	110.19
7	H	24	TRP	N-CA-C	-5.29	105.93	112.38
13	o	2081	ILE	N-CA-C	5.29	120.34	109.34
4	d	2303	ILE	N-CA-C	5.29	115.91	110.36
17	X	13	THR	CA-C-N	5.28	126.44	119.84
17	X	13	THR	C-N-CA	5.28	126.44	119.84
2	B	381	ILE	CA-C-N	5.28	126.44	119.84
2	B	381	ILE	C-N-CA	5.28	126.44	119.84
9	J	9	PRO	N-CA-C	5.28	119.60	111.21
2	B	278	SER	N-CA-C	-5.28	104.36	111.54
3	c	2448	ALA	N-CA-C	-5.28	106.34	112.89
2	B	193	TYR	N-CA-C	5.27	119.83	113.41
4	d	2085	MET	N-CA-C	5.27	119.86	113.38
13	o	2243	ILE	CB-CA-C	-5.26	104.49	111.80
19	z	2045	GLY	N-CA-C	-5.25	106.13	112.49
2	B	122	LEU	N-CA-C	5.25	118.36	108.65
3	C	138	GLU	N-CA-C	5.24	115.97	108.74
5	E	20	VAL	N-CA-C	5.24	115.45	110.42
3	c	2322	GLN	N-CA-C	-5.24	105.69	111.71
3	c	2223	TRP	CA-CB-CG	5.23	123.53	113.60
2	B	322	GLY	N-CA-C	5.22	125.55	113.18
13	O	210	GLU	N-CA-C	5.22	119.87	112.93
14	T	26	PRO	CA-C-N	5.21	126.35	119.84
14	T	26	PRO	C-N-CA	5.21	126.35	119.84
6	f	2019	TRP	N-CA-C	5.21	121.90	110.80
2	B	320	ALA	N-CA-C	5.18	120.62	110.56
13	O	172	ILE	N-CA-C	5.18	115.40	110.42
3	C	353	GLY	N-CA-C	-5.18	104.92	112.17
2	b	2021	ALA	N-CA-C	-5.18	104.56	111.24
3	c	2430	HIS	N-CA-C	5.18	117.66	111.71
1	A	77	ILE	N-CA-C	5.18	120.11	109.34
4	D	114	ILE	N-CA-C	5.18	115.80	110.36
13	o	2204	VAL	N-CA-C	-5.18	100.42	108.86
16	v	2035	TYR	N-CA-C	5.18	116.61	111.07
10	K	8	ILE	N-CA-C	5.17	120.10	109.34
4	D	89	LEU	CA-C-N	-5.17	114.07	122.34
4	D	89	LEU	C-N-CA	-5.17	114.07	122.34
7	H	47	ILE	CB-CA-C	-5.17	105.36	111.97
4	d	2217	THR	N-CA-C	-5.17	104.72	111.02
6	f	2015	PHE	N-CA-C	5.16	117.09	108.99
2	b	2411	PHE	N-CA-C	5.15	117.64	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	363	GLY	CA-C-N	5.14	124.94	119.28
3	C	363	GLY	C-N-CA	5.14	124.94	119.28
4	D	326	ARG	N-CA-C	5.14	116.58	111.07
1	a	2293	MET	N-CA-C	-5.14	106.78	113.16
2	b	2463	PHE	N-CA-C	-5.14	105.75	111.36
3	C	438	LEU	N-CA-C	-5.14	105.75	111.36
2	b	2217	ILE	N-CA-C	-5.14	106.13	111.58
13	O	71	VAL	N-CA-C	-5.14	106.13	111.58
2	B	480	SER	N-CA-C	-5.13	106.72	112.87
1	a	2311	GLY	N-CA-C	-5.13	108.04	115.27
1	A	56	PRO	N-CA-C	-5.12	104.45	110.70
1	A	307	ILE	CB-CA-C	-5.12	102.89	111.29
13	o	2024	ASP	N-CA-C	5.12	119.18	111.96
10	K	30	TRP	N-CA-C	-5.12	105.14	111.33
3	c	2233	VAL	N-CA-C	5.12	116.45	110.62
1	a	2036	ILE	N-CA-C	-5.12	107.75	111.90
3	C	448	ALA	N-CA-C	-5.11	107.05	113.28
13	O	30	TYR	N-CA-C	-5.11	98.53	109.81
4	d	2297	ASP	N-CA-C	5.10	117.00	108.99
2	B	21	ALA	N-CA-C	-5.10	104.67	111.24
3	c	2367	GLU	N-CA-C	5.09	119.68	112.75
15	u	2080	VAL	CB-CA-C	-5.09	105.19	112.22
14	T	25	GLU	CA-C-N	5.09	125.62	120.38
14	T	25	GLU	C-N-CA	5.09	125.62	120.38
10	k	2016	LEU	CA-C-N	5.09	126.20	119.84
10	k	2016	LEU	C-N-CA	5.09	126.20	119.84
1	A	123	ALA	N-CA-C	-5.08	105.82	111.36
1	a	2340	PRO	N-CA-C	5.08	122.02	113.78
2	b	2116	VAL	N-CA-C	-5.08	107.44	111.81
1	a	2304	HIS	N-CA-C	5.07	117.69	109.06
2	b	2445	THR	N-CA-C	5.07	118.02	109.95
1	A	48	PHE	N-CA-C	5.06	117.45	111.33
4	D	55	VAL	N-CA-C	5.06	116.59	108.89
1	a	2297	LEU	N-CA-C	-5.06	100.14	108.49
4	D	315	TYR	N-CA-C	-5.06	105.04	111.11
9	j	2037	GLY	N-CA-C	5.06	120.46	113.99
2	b	2328	GLY	CA-C-N	-5.05	115.36	120.31
2	b	2328	GLY	C-N-CA	-5.05	115.36	120.31
3	C	272	LEU	N-CA-C	-5.05	105.48	111.69
2	B	130	GLU	N-CA-C	5.04	120.96	109.81
6	F	31	PHE	N-CA-C	-5.04	105.49	111.69
2	b	2130	GLU	N-CA-C	5.04	120.95	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	2148	VAL	CA-C-N	5.04	126.14	119.84
13	o	2148	VAL	C-N-CA	5.04	126.14	119.84
1	A	29	TYR	N-CA-C	-5.04	100.08	108.34
1	a	2056	PRO	N-CA-C	-5.04	104.56	110.70
3	C	328	VAL	N-CA-C	5.04	119.14	111.89
4	d	2308	ASP	CA-C-N	5.04	125.86	120.47
4	d	2308	ASP	C-N-CA	5.04	125.86	120.47
1	A	119	PHE	N-CA-C	5.03	116.76	111.28
1	A	311	GLY	N-CA-C	-5.03	108.30	115.64
13	o	2172	ILE	N-CA-C	5.02	115.24	110.42
3	C	296	VAL	CB-CA-C	-5.02	105.46	112.04
3	c	2138	GLU	N-CA-C	5.02	115.66	108.74
13	O	146	PHE	CB-CA-C	-5.02	101.90	111.48
4	d	2117	HIS	N-CA-C	-5.01	105.10	111.11
4	d	2126	MET	N-CA-C	-5.01	106.34	112.90
1	a	2306	VAL	N-CA-C	5.01	119.75	109.34
9	j	2009	PRO	N-CA-C	5.00	119.17	111.21
3	C	367	GLU	N-CA-C	5.00	119.56	112.75
6	f	2012	TYR	CA-C-N	5.00	126.09	119.84
6	f	2012	TYR	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	TYR	Sidechain
2	B	273	TYR	Sidechain
13	O	240	TYR	Sidechain
15	U	133	TYR	Sidechain
15	U	51	TYR	Sidechain
2	b	2273	TYR	Sidechain
11	l	2034	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	468	0
1	a	2616	0	2514	493	0
2	B	3739	0	3613	491	0
2	b	3739	0	3613	494	0
3	C	3253	0	3192	553	0
3	c	3253	0	3192	519	0
4	D	2702	0	2605	428	0
4	d	2702	0	2605	467	0
5	E	624	0	613	98	0
5	e	624	0	613	91	0
6	F	269	0	277	45	0
6	f	269	0	277	46	0
7	H	409	0	424	52	0
7	h	409	0	424	57	0
8	I	312	0	329	29	0
8	i	312	0	326	35	0
9	J	272	0	279	45	0
9	j	272	0	279	42	0
10	K	293	0	308	59	0
10	k	293	0	305	63	0
11	L	304	0	316	50	0
11	l	304	0	313	64	0
12	M	234	0	255	43	0
12	m	234	0	252	45	0
13	O	1888	0	1867	297	6
13	o	1888	0	1864	297	0
14	T	265	0	275	42	0
14	t	265	0	272	36	0
15	U	827	0	819	125	0
15	u	827	0	819	117	0
16	V	1064	0	1075	131	0
16	v	1064	0	1070	117	0
17	X	296	0	328	13	0
17	x	296	0	328	16	0
18	N	186	0	40	10	0
18	n	186	0	40	10	6
19	Z	442	0	480	64	0
19	z	442	0	477	65	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	4	0	0	0	0
21	D	4	0	0	0	0
21	a	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	d	4	0	0	0	0
22	A	9	0	0	1	0
22	a	9	0	0	0	0
23	A	260	0	288	22	0
23	B	1040	0	1152	113	0
23	C	910	0	1008	100	0
23	D	130	0	144	16	0
23	a	195	0	216	20	0
23	b	1040	0	1152	109	0
23	c	910	0	1008	104	0
23	d	195	0	216	30	0
24	A	64	0	74	5	0
24	D	64	0	74	7	0
24	a	64	0	74	5	0
24	d	64	0	74	10	0
25	A	45	0	61	8	0
25	D	45	0	61	6	0
25	a	45	0	61	11	0
25	d	45	0	61	8	0
26	B	35	0	46	0	0
26	d	35	0	46	5	0
27	B	80	0	112	18	0
27	C	80	0	112	23	0
27	F	40	0	56	3	0
27	J	40	0	56	2	0
27	K	40	0	56	13	0
27	b	80	0	112	19	0
27	c	80	0	112	22	0
27	d	40	0	56	2	0
27	j	40	0	56	2	0
27	k	40	0	56	16	0
28	E	43	0	32	17	0
28	V	43	0	32	9	0
28	e	43	0	32	15	0
28	v	43	0	31	1	0
All	All	45945	0	45919	5461	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (5461) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:138:HEC:C2B	28:V:138:HEC:CMB	1.74	1.58
28:V:138:HEC:C2C	28:V:138:HEC:CMC	1.75	1.57
16:V:37:CYS:SG	28:V:138:HEC:HAB	1.57	1.44
5:E:12:ILE:CG2	5:E:18:TYR:HB2	1.44	1.43
5:e:2012:ILE:CG2	5:e:2018:TYR:HB2	1.46	1.42
5:e:2012:ILE:HD12	28:e:2084:HEC:O2D	1.22	1.25
5:E:12:ILE:HD12	28:E:84:HEC:O2D	1.31	1.25
6:F:40:GLN:NE2	9:J:27:LEU:HG	1.52	1.24
5:e:2012:ILE:CD1	28:e:2084:HEC:O2D	1.88	1.22
5:E:12:ILE:HG22	5:E:18:TYR:CB	1.71	1.21
3:c:2326:ALA:HB2	15:u:2127:ARG:HD2	1.22	1.20
5:e:2012:ILE:HG22	5:e:2018:TYR:CB	1.72	1.19
13:O:40:ILE:HG12	13:O:84:GLU:OE1	1.07	1.19
2:B:75:TRP:H	2:B:94:GLU:HG3	1.07	1.18
3:C:158:THR:HG22	3:C:251:HIS:HB3	1.23	1.17
5:E:14:THR:HG22	9:J:8:ILE:HB	1.24	1.16
3:C:158:THR:CG2	3:C:251:HIS:HB3	1.75	1.16
16:v:2079:PRO:HB2	16:v:2088:ILE:HG13	1.29	1.15
4:D:195:PRO:HA	4:D:198:MET:HE2	1.24	1.15
4:d:2298:PHE:HA	11:l:2037:ASN:HD21	1.04	1.15
6:F:39:MET:O	6:F:42:ILE:HG22	1.47	1.14
2:B:326:ARG:CD	2:B:327:THR:H	1.61	1.14
5:E:12:ILE:CD1	28:E:84:HEC:O2D	1.96	1.12
5:e:2026:ILE:HG13	5:e:2027:PRO:HD3	1.22	1.12
13:O:122:VAL:HA	13:O:146:PHE:CE2	1.85	1.12
5:e:2014:THR:HG22	9:j:2008:ILE:HB	1.30	1.11
2:b:2075:TRP:H	2:b:2094:GLU:HG3	1.08	1.10
3:C:308:GLU:HG2	3:C:361:PHE:CE1	1.85	1.10
5:E:60:ARG:HH22	16:V:129:LYS:HE3	1.05	1.10
2:b:2326:ARG:CD	2:b:2327:THR:H	1.63	1.10
3:C:455:PHE:HE1	4:D:224:GLN:HA	1.07	1.10
3:C:138:GLU:HG2	3:C:139:THR:H	1.09	1.09
13:O:146:PHE:HB2	13:O:195:GLY:HA3	1.10	1.09
1:A:214:MET:HA	1:A:214:MET:HE3	1.28	1.09
4:D:298:PHE:HA	11:L:37:ASN:HD21	0.93	1.09
4:D:298:PHE:HA	11:L:37:ASN:ND2	1.67	1.09
5:E:14:THR:CG2	9:J:8:ILE:HB	1.83	1.08
13:o:2130:GLN:HB3	13:o:2131:PRO:HD2	1.08	1.08
1:A:186:PHE:HD2	1:A:192:ILE:HD11	1.05	1.08
3:C:344:SER:HB3	3:C:350:ILE:HD11	1.34	1.08
13:o:2040:ILE:HG12	13:o:2084:GLU:OE1	1.53	1.08
13:O:130:GLN:HB3	13:O:131:PRO:CD	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:TRP:CD1	3:C:224:ILE:HG13	1.90	1.07
5:E:12:ILE:HG22	5:E:18:TYR:HB2	1.10	1.07
15:U:57:LEU:HD21	15:U:112:PHE:HD2	1.02	1.07
16:V:37:CYS:SG	28:V:138:HEC:CAB	2.41	1.07
5:E:10:SER:HA	5:E:13:ILE:HD12	1.37	1.07
1:a:2225:ARG:HB3	2:b:2481:GLY:C	1.79	1.07
1:A:150:PRO:HB2	23:A:348:CLA:H62	1.38	1.06
15:U:59:ASN:HD22	15:U:59:ASN:N	1.33	1.06
5:E:14:THR:CG2	9:J:8:ILE:HD12	1.85	1.06
13:O:121:THR:HG21	13:O:148:VAL:HG22	1.37	1.06
13:O:40:ILE:CG1	13:O:84:GLU:OE1	2.04	1.05
2:b:2192:PRO:HG3	7:h:2048:TYR:CE1	1.91	1.05
2:B:326:ARG:HD2	2:B:327:THR:H	0.88	1.05
2:b:2057:ARG:HD3	2:b:2331:ASN:HD21	1.19	1.05
13:o:2047:PRO:HG3	13:o:2076:THR:HG21	1.33	1.05
5:E:60:ARG:NH2	16:V:129:LYS:HE3	1.71	1.05
1:a:2230:THR:HG22	1:a:2231:GLU:H	1.21	1.05
2:b:2326:ARG:HD2	2:b:2327:THR:H	0.89	1.05
15:u:2059:ASN:HD22	15:u:2059:ASN:N	1.53	1.05
13:O:47:PRO:HG3	13:O:76:THR:HG21	1.36	1.04
3:C:223:TRP:HD1	3:C:224:ILE:HG13	1.19	1.04
2:B:57:ARG:HD3	2:B:331:ASN:HD21	1.17	1.04
15:U:57:LEU:HD21	15:U:112:PHE:CD2	1.93	1.03
3:c:2159:THR:HG23	3:c:2252:ILE:HG23	1.40	1.03
3:c:2141:GLU:HB2	3:c:2144:SER:HB2	1.40	1.03
5:e:2010:SER:HA	5:e:2013:ILE:HD12	1.37	1.03
3:C:343:ARG:HD2	3:C:343:ARG:C	1.84	1.02
1:a:2012:ASN:O	1:a:2015:GLU:HG3	1.59	1.02
5:e:2012:ILE:HG22	5:e:2018:TYR:HB2	1.08	1.02
2:b:2138:MET:HG2	23:b:2522:CLA:HBC2	1.37	1.02
2:B:47:PRO:HB3	2:B:78:TRP:CD1	1.94	1.02
2:B:138:MET:HG2	23:B:522:CLA:HBC2	1.37	1.02
3:C:294:ASN:HD22	3:C:294:ASN:N	1.52	1.02
5:E:14:THR:HG21	9:J:8:ILE:CD1	1.89	1.02
5:e:2014:THR:CG2	9:j:2008:ILE:HB	1.88	1.02
4:d:2274:VAL:HB	4:d:2275:PRO:HD3	1.42	1.01
6:f:2040:GLN:OE1	9:j:2028:PHE:HA	1.57	1.01
2:B:326:ARG:HD2	2:B:327:THR:N	1.74	1.01
2:b:2047:PRO:HB3	2:b:2078:TRP:CD1	1.95	1.01
2:b:2222:PRO:HB3	7:h:2025:GLY:HA2	1.43	1.01
2:b:2326:ARG:HD2	2:b:2327:THR:N	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:THR:HG21	9:J:8:ILE:HD12	1.38	1.01
13:o:2146:PHE:HB2	13:o:2195:GLY:CA	1.90	1.00
3:C:77:PRO:HA	3:C:104:GLU:OE2	1.59	1.00
13:O:81:ILE:HG22	13:O:82:GLN:H	1.24	1.00
1:A:186:PHE:CD2	1:A:192:ILE:HD11	1.95	1.00
3:C:62:PHE:CZ	10:K:19:ILE:HD11	1.95	1.00
4:D:336:HIS:H	4:D:336:HIS:CD2	1.78	1.00
15:U:132:LEU:HD23	15:U:132:LEU:H	1.20	1.00
4:d:2154:VAL:HG13	4:d:2158:LEU:HD12	1.40	1.00
6:f:2039:MET:O	6:f:2042:ILE:HG22	1.60	1.00
13:o:2146:PHE:CB	13:o:2195:GLY:HA3	1.92	1.00
3:C:104:GLU:HG2	3:C:105:VAL:HG23	1.40	0.99
6:F:40:GLN:OE1	9:J:28:PHE:HA	1.61	0.99
13:O:130:GLN:CB	13:O:131:PRO:HD2	1.91	0.99
13:o:2146:PHE:HB2	13:o:2195:GLY:HA3	1.01	0.99
5:E:12:ILE:CG2	5:E:18:TYR:CB	2.35	0.99
3:c:2350:ILE:HG21	3:c:2359:TRP:HB3	1.45	0.99
13:O:106:VAL:HG13	13:O:117:PRO:HG3	1.43	0.99
3:c:2339:LYS:HE2	15:u:2129:ASN:OD1	1.63	0.99
5:e:2026:ILE:HG13	5:e:2027:PRO:CD	1.93	0.99
2:B:222:PRO:HB3	7:H:25:GLY:HA2	1.43	0.98
3:c:2104:GLU:HG2	3:c:2105:VAL:HG23	1.43	0.98
13:o:2130:GLN:HB3	13:o:2131:PRO:CD	1.92	0.98
2:b:2130:GLU:HG2	2:b:2131:PRO:HD3	1.44	0.98
4:d:2298:PHE:HA	11:l:2037:ASN:ND2	1.78	0.98
13:O:193:THR:HG22	13:O:194:LYS:H	1.27	0.98
2:B:136:PRO:HD3	2:B:231:MET:HE1	1.45	0.98
13:O:39:ARG:HB3	13:O:245:PRO:HG3	1.42	0.98
1:A:225:ARG:HB3	2:B:481:GLY:C	1.88	0.97
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.46	0.97
3:c:2305:THR:HG22	3:c:2307:PRO:HD2	1.44	0.97
3:c:2212:TYR:O	3:c:2223:TRP:HB2	1.64	0.97
3:c:2320:ARG:HE	15:u:2128:TYR:HE2	1.06	0.97
3:c:2344:SER:HB3	3:c:2350:ILE:HD11	1.42	0.97
3:C:158:THR:HG22	3:C:251:HIS:CB	1.95	0.97
3:C:455:PHE:CE1	4:D:224:GLN:HA	1.97	0.97
3:c:2158:THR:HG23	3:c:2251:HIS:HB3	1.45	0.96
4:d:2158:LEU:O	4:d:2162:LEU:HG	1.65	0.96
13:o:2047:PRO:HG3	13:o:2076:THR:CG2	1.95	0.96
3:C:320:ARG:NE	15:U:128:TYR:CE2	2.33	0.96
3:c:2158:THR:CG2	3:c:2251:HIS:HB3	1.96	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:2130:GLN:CB	13:o:2131:PRO:HD2	1.94	0.96
13:O:47:PRO:HA	13:O:237:GLY:HA3	1.47	0.95
6:F:40:GLN:HE22	9:J:27:LEU:C	1.74	0.95
2:B:130:GLU:HG2	2:B:131:PRO:HD3	1.48	0.95
19:Z:19:MET:O	19:Z:23:VAL:HG23	1.65	0.95
23:b:2521:CLA:HAB	23:b:2526:CLA:HED1	1.48	0.95
23:C:478:CLA:H62	23:C:485:CLA:H12	1.48	0.95
4:D:158:LEU:O	4:D:162:LEU:HG	1.66	0.95
4:d:2103:ARG:HH11	5:e:2072:LYS:HG2	1.27	0.95
2:B:326:ARG:HH11	2:B:327:THR:CB	1.80	0.95
1:a:2150:PRO:HB2	23:a:2348:CLA:H62	1.46	0.95
2:B:475:PHE:HB3	2:B:478:VAL:HB	1.46	0.95
4:D:88:SER:HB3	5:E:68:ARG:HH21	1.29	0.95
1:a:2334:ARG:HH11	4:d:2320:LEU:HD11	1.32	0.95
2:b:2475:PHE:HB3	2:b:2478:VAL:HB	1.47	0.95
15:U:59:ASN:N	15:U:59:ASN:ND2	2.05	0.95
13:o:2043:LEU:HD12	13:o:2240:TYR:O	1.67	0.95
2:b:2136:PRO:HD3	2:b:2231:MET:HE1	1.47	0.94
2:b:2326:ARG:HH11	2:b:2327:THR:CB	1.80	0.94
13:O:130:GLN:HB3	13:O:131:PRO:HD2	0.96	0.94
15:u:2132:LEU:HD23	15:u:2132:LEU:H	1.31	0.94
3:C:42:LEU:HG	23:C:486:CLA:HED1	1.49	0.94
23:B:521:CLA:HAB	23:B:527:CLA:HED1	1.47	0.94
5:E:14:THR:HG21	9:J:8:ILE:CG1	1.95	0.94
4:d:2236:ASN:OD1	4:d:2239:GLN:HB2	1.67	0.94
4:D:198:MET:HE3	11:L:30:LEU:HD11	1.50	0.94
3:c:2062:PHE:CZ	10:k:2019:ILE:HD11	2.03	0.94
1:a:2326:LEU:HD13	3:c:2412:THR:HG21	1.49	0.94
13:O:81:ILE:HG22	13:O:82:GLN:N	1.80	0.94
1:a:2096:ILE:HG22	8:i:2001:MET:HE1	1.47	0.94
2:B:6:TYR:OH	12:M:21:PHE:HZ	1.48	0.93
3:C:326:ALA:HB2	15:U:127:ARG:HD2	1.50	0.93
3:c:2138:GLU:HG2	3:c:2139:THR:H	1.32	0.93
16:V:133:GLY:O	16:V:137:TYR:HB2	1.69	0.93
16:v:2004:THR:HG22	16:v:2005:PRO:HD2	1.50	0.93
15:U:72:TYR:CD2	15:U:73:PRO:N	2.36	0.93
3:C:71:GLU:OE1	3:C:86:LEU:HB3	1.69	0.93
1:a:2037:MET:HE1	1:a:2129:ARG:HD2	1.50	0.93
3:C:320:ARG:HE	15:U:128:TYR:HE2	1.08	0.93
15:U:59:ASN:HD22	15:U:59:ASN:H	0.99	0.93
13:o:2047:PRO:HA	13:o:2237:GLY:HA3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:271:TYR:HA	3:C:274:TYR:CD1	2.04	0.93
13:O:44:CYS:HB3	13:O:240:TYR:HB3	1.51	0.93
3:c:2294:ASN:N	3:c:2294:ASN:HD22	1.63	0.92
23:c:2478:CLA:H62	23:c:2485:CLA:H12	1.50	0.92
3:c:2282:MET:HA	3:c:2285:ILE:HG13	1.51	0.92
3:C:308:GLU:OE2	3:C:361:PHE:HZ	1.52	0.92
16:v:2079:PRO:HB2	16:v:2088:ILE:CG1	1.99	0.92
15:u:2057:LEU:HD21	15:u:2112:PHE:CD2	2.05	0.92
3:c:2343:ARG:C	3:c:2343:ARG:HD2	1.94	0.92
10:k:2002:LEU:N	10:k:2003:PRO:HD3	1.84	0.92
4:D:319:LEU:HA	4:D:322:ASN:HD22	1.34	0.92
13:o:2121:THR:HG21	13:o:2148:VAL:HG22	1.50	0.92
4:D:52:THR:HG22	4:D:67:TYR:HE1	1.35	0.91
3:C:344:SER:HB3	3:C:350:ILE:CD1	1.99	0.91
3:C:62:PHE:HZ	10:K:19:ILE:HD11	1.32	0.91
1:a:2104:GLU:OE2	13:o:2073:ARG:HD3	1.69	0.91
11:L:7:ARG:C	11:L:9:PRO:HD3	1.96	0.91
13:O:60:ARG:HH22	2:b:2341:LYS:CE	1.82	0.91
1:a:2056:PRO:HA	1:a:2073:TYR:CE1	2.05	0.91
27:C:488:BCR:H312	19:Z:9:LEU:HD11	1.50	0.91
5:e:2026:ILE:CG1	5:e:2027:PRO:HD3	2.00	0.91
19:z:2051:VAL:HG12	19:z:2052:LEU:HD23	1.52	0.90
1:A:237:TYR:CZ	1:A:245:THR:HG23	2.06	0.90
2:B:57:ARG:HD3	2:B:331:ASN:ND2	1.85	0.90
15:u:2059:ASN:N	15:u:2059:ASN:ND2	2.12	0.90
1:A:317:TRP:HA	4:D:63:LEU:HD13	1.54	0.90
1:a:2317:TRP:HA	4:d:2063:LEU:HD13	1.54	0.90
2:b:2326:ARG:HD3	27:b:2528:BCR:H402	1.51	0.90
13:o:2193:THR:HG22	13:o:2194:LYS:H	1.33	0.90
2:b:2056:TRP:CZ3	2:b:2266:GLU:HA	2.07	0.90
4:d:2068:LEU:HA	6:f:2039:MET:HE1	1.54	0.90
5:e:2060:ARG:HH22	16:v:2129:LYS:CE	1.84	0.90
13:O:43:LEU:HD12	13:O:240:TYR:O	1.72	0.90
1:a:2159:LEU:HG	1:a:2163:ILE:HD11	1.54	0.90
15:u:2072:TYR:HB3	15:u:2073:PRO:HD3	1.50	0.90
2:B:56:TRP:CZ3	2:B:266:GLU:HA	2.07	0.90
13:o:2140:THR:CG2	13:o:2201:VAL:HB	2.01	0.90
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.54	0.89
5:e:2056:ALA:HB2	5:e:2082:LEU:HD23	1.54	0.89
16:v:2079:PRO:CB	16:v:2088:ILE:HG13	2.01	0.89
1:A:300:PHE:HB3	1:A:302:PHE:HE1	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:GLU:HG2	3:C:139:THR:N	1.87	0.89
5:E:12:ILE:HG21	5:E:18:TYR:HB2	1.53	0.89
5:E:14:THR:HG22	9:J:8:ILE:CB	2.02	0.89
4:d:2150:ILE:O	4:d:2154:VAL:HG23	1.73	0.89
6:f:2040:GLN:HE22	9:j:2027:LEU:C	1.80	0.89
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.51	0.89
15:u:2059:ASN:HD22	15:u:2059:ASN:H	0.93	0.89
2:B:318:ASN:HD22	2:B:319:PRO:N	1.70	0.89
16:V:4:THR:HG22	16:V:5:PRO:HD2	1.53	0.89
4:d:2186:GLN:HE21	4:d:2186:GLN:HA	1.36	0.89
5:e:2012:ILE:HD12	28:e:2084:HEC:CGD	2.00	0.89
13:o:2043:LEU:HD13	13:o:2241:ALA:HB2	1.52	0.89
13:O:104:GLN:OE1	13:O:104:GLN:N	2.05	0.89
3:c:2320:ARG:HH11	16:v:2049:ASN:HA	1.37	0.89
5:e:2012:ILE:HG22	5:e:2018:TYR:CG	2.07	0.89
3:C:43:ILE:HG13	3:C:44:ASN:H	1.36	0.89
16:V:46:THR:HG22	16:V:49:ASN:H	1.38	0.89
1:a:2156:ALA:HA	1:a:2160:ILE:HD12	1.52	0.89
3:c:2089:ILE:HB	3:c:2090:PRO:HD3	1.53	0.89
4:d:2090:LEU:HD11	4:d:2096:GLU:HB3	1.55	0.89
1:A:307:ILE:CG1	1:A:314:ILE:HD11	2.03	0.88
2:B:318:ASN:HD22	2:B:318:ASN:C	1.79	0.88
2:b:2057:ARG:HD3	2:b:2331:ASN:ND2	1.87	0.88
6:f:2040:GLN:NE2	9:j:2027:LEU:HG	1.88	0.88
1:A:89:ILE:HG12	13:O:73:ARG:NH2	1.88	0.88
1:a:2190:HIS:HB3	1:a:2293:MET:HE2	1.55	0.88
3:c:2055:ALA:HB1	27:c:2488:BCR:H373	1.53	0.88
3:c:2320:ARG:NE	15:u:2128:TYR:CE2	2.41	0.88
1:A:239:PHE:HZ	4:D:223:PHE:HZ	1.22	0.88
2:B:56:TRP:HZ3	2:B:266:GLU:HA	1.38	0.88
3:C:55:ALA:HB1	27:C:488:BCR:H373	1.55	0.88
4:D:198:MET:CE	11:L:30:LEU:HD11	2.03	0.88
19:Z:33:TRP:HE3	19:Z:37:LYS:HD3	1.37	0.88
2:b:2120:LEU:HD23	2:b:2130:GLU:HA	1.55	0.88
19:z:2005:PHE:CE2	19:z:2054:VAL:HG13	2.08	0.88
4:d:2152:VAL:HG21	4:d:2279:LEU:HD13	1.55	0.88
2:B:322:GLY:HA2	2:B:325:PHE:CE1	2.08	0.88
1:A:334:ARG:HH11	4:D:320:LEU:HD11	1.38	0.88
2:b:2056:TRP:HZ3	2:b:2266:GLU:HA	1.39	0.88
13:o:2140:THR:HB	13:o:2201:VAL:H	1.38	0.88
1:A:286:THR:HG22	23:A:348:CLA:O1D	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:2015:THR:HA	27:k:2050:BCR:H372	1.56	0.88
16:v:2133:GLY:O	16:v:2137:TYR:HB2	1.73	0.88
4:D:71:CYS:HB2	4:D:76:VAL:HG23	1.55	0.87
2:b:2318:ASN:C	2:b:2318:ASN:HD22	1.79	0.87
5:e:2060:ARG:HH22	16:v:2129:LYS:HE3	1.34	0.87
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.38	0.87
3:C:116:VAL:HG13	27:C:488:BCR:H332	1.57	0.87
3:C:307:PRO:HB3	3:C:358:PHE:CD2	2.09	0.87
13:O:146:PHE:HB2	13:O:195:GLY:CA	2.01	0.87
13:O:164:LEU:HD23	15:U:42:VAL:HG13	1.56	0.87
3:C:285:ILE:HA	23:C:487:CLA:HMB3	1.56	0.87
3:c:2285:ILE:HA	23:c:2487:CLA:HMB3	1.54	0.87
25:d:2358:PL9:H38	14:t:2018:PHE:HB2	1.56	0.87
17:x:2012:ILE:HA	17:x:2016:LEU:HD12	1.54	0.87
3:C:305:THR:HA	3:C:423:ARG:NH1	1.90	0.87
13:O:163:GLY:HA2	13:O:188:LYS:HG3	1.57	0.87
13:O:155:ASN:HD22	15:U:129:ASN:ND2	1.72	0.87
3:c:2295:THR:O	3:c:2298:PRO:HD3	1.75	0.87
5:e:2012:ILE:CG2	5:e:2018:TYR:CB	2.37	0.87
13:o:2223:ASP:HB3	13:o:2230:PRO:HG3	1.54	0.87
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.56	0.87
13:o:2040:ILE:O	13:o:2243:ILE:HG23	1.74	0.87
1:A:230:THR:HG22	1:A:231:GLU:H	1.39	0.87
13:O:140:THR:HB	13:O:201:VAL:H	1.40	0.87
1:a:2095:PRO:HD2	1:a:2098:GLU:HB3	1.54	0.87
13:O:146:PHE:CB	13:O:195:GLY:HA3	2.01	0.86
19:Z:51:VAL:HG12	19:Z:52:LEU:HD23	1.53	0.86
2:b:2318:ASN:HD22	2:b:2319:PRO:N	1.73	0.86
3:c:2061:VAL:HG11	3:c:2121:SER:HB2	1.57	0.86
4:d:2090:LEU:CD1	4:d:2096:GLU:HB3	2.05	0.86
1:a:2307:ILE:HG13	1:a:2314:ILE:HD11	1.57	0.86
4:d:2068:LEU:HA	6:f:2039:MET:CE	2.04	0.86
11:l:2007:ARG:C	11:l:2009:PRO:HD3	2.00	0.86
2:B:326:ARG:HD3	27:B:529:BCR:H402	1.56	0.86
3:c:2285:ILE:HG21	23:c:2479:CLA:H51	1.54	0.86
4:d:2268:HIS:HA	4:d:2271:MET:HE3	1.54	0.86
2:B:9:HIS:HB2	23:B:523:CLA:HBA2	1.55	0.86
2:B:341:LYS:NZ	13:o:2060:ARG:HH22	1.74	0.86
13:O:155:ASN:ND2	15:U:129:ASN:ND2	2.23	0.86
5:E:60:ARG:HH22	16:V:129:LYS:CE	1.87	0.86
13:O:140:THR:HG21	13:O:201:VAL:O	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2200:LEU:HD13	1:a:2285:PHE:HD1	1.37	0.86
3:c:2116:VAL:HG21	27:c:2489:BCR:H323	1.58	0.86
4:d:2096:GLU:CD	5:e:2068:ARG:O	2.19	0.86
4:d:2148:ALA:HB3	4:d:2149:PRO:HD3	1.58	0.86
13:o:2180:GLU:HG3	13:o:2181:GLU:H	1.41	0.86
1:A:57:PRO:HG2	13:O:115:ARG:NH1	1.91	0.86
5:E:14:THR:CG2	9:J:8:ILE:CB	2.53	0.86
2:b:2322:GLY:HA2	2:b:2325:PHE:CE1	2.11	0.86
3:C:269:GLU:OE2	3:C:447:ARG:HG2	1.75	0.86
1:A:214:MET:HA	1:A:214:MET:CE	2.05	0.86
16:V:75:TYR:HE2	16:V:80:THR:H	1.22	0.86
5:e:2014:THR:HG22	9:j:2008:ILE:CB	2.05	0.86
13:o:2106:VAL:HG22	13:o:2117:PRO:HB3	1.57	0.85
1:a:2239:PHE:HZ	4:d:2223:PHE:HZ	1.21	0.85
16:v:2004:THR:HG22	16:v:2005:PRO:CD	2.05	0.85
2:B:120:LEU:HD23	2:B:130:GLU:HA	1.58	0.85
7:H:39:VAL:O	7:H:43:ILE:HG13	1.76	0.85
13:o:2140:THR:HG21	13:o:2201:VAL:O	1.76	0.85
1:A:142:TRP:NE1	3:C:443:TRP:CH2	2.45	0.85
2:B:341:LYS:HZ3	13:o:2060:ARG:HH22	1.25	0.85
13:O:40:ILE:HG12	13:O:84:GLU:CD	2.02	0.85
4:d:2191:TRP:CE3	4:d:2289:LEU:HD11	2.11	0.85
11:L:31:PHE:HB3	11:L:35:PHE:HE1	1.40	0.85
23:b:2518:CLA:H141	23:b:2524:CLA:HMA1	1.58	0.85
2:B:280:PHE:CE1	2:B:312:TYR:HB3	2.12	0.85
16:V:55:ARG:HH21	16:V:131:GLY:HA3	1.39	0.85
13:o:2104:GLN:HB3	13:o:2151:TYR:HE1	1.42	0.85
1:A:223:LEU:HD22	1:A:245:THR:HG22	1.57	0.85
3:C:305:THR:H	3:C:308:GLU:HG3	1.41	0.85
3:c:2279:LEU:HB3	23:c:2481:CLA:HBC1	1.58	0.85
1:A:29:TYR:HD2	1:A:133:LEU:CD1	1.90	0.85
1:A:307:ILE:HG13	1:A:314:ILE:HD11	1.58	0.85
4:D:197:HIS:O	4:D:201:VAL:HG23	1.76	0.85
13:O:47:PRO:HG3	13:O:76:THR:CG2	2.06	0.85
2:b:2302:TRP:O	2:b:2341:LYS:HE3	1.77	0.85
1:a:2200:LEU:HD13	1:a:2285:PHE:CD1	2.12	0.84
2:b:2144:PHE:HE1	2:b:2210:ILE:HG23	1.42	0.84
19:Z:19:MET:HE1	19:Z:43:GLY:HA3	1.59	0.84
3:c:2223:TRP:CD1	3:c:2224:ILE:HG13	2.11	0.84
10:k:2019:ILE:HD12	27:k:2050:BCR:H342	1.57	0.84
1:A:29:TYR:C	1:A:29:TYR:HD1	1.85	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:19:SER:O	12:M:23:ILE:HG12	1.77	0.84
1:a:2334:ARG:NH1	4:d:2320:LEU:HD11	1.92	0.84
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.12	0.84
1:a:2057:PRO:HG2	13:o:2115:ARG:NH1	1.93	0.84
3:C:257:PHE:O	3:C:261:ARG:HG3	1.77	0.84
3:C:282:MET:HA	3:C:285:ILE:HG13	1.57	0.84
4:D:90:LEU:HD11	4:D:96:GLU:OE1	1.78	0.84
13:O:126:VAL:O	13:O:144:GLY:HA3	1.78	0.84
3:c:2296:VAL:HG11	23:c:2479:CLA:H2A	1.59	0.84
3:c:2048:LYS:HZ2	23:c:2486:CLA:HBA1	1.43	0.84
2:b:2127:ARG:HG3	2:b:2127:ARG:HH11	1.42	0.84
13:O:43:LEU:CD1	13:O:241:ALA:HB2	2.08	0.84
5:e:2060:ARG:NH2	16:v:2129:LYS:HE3	1.92	0.84
2:B:357:ARG:HH22	4:D:337:GLU:HB3	1.41	0.83
3:c:2344:SER:HB3	3:c:2350:ILE:CD1	2.08	0.83
2:B:339:ALA:HB3	2:B:430:PHE:HD1	1.43	0.83
5:e:2014:THR:CG2	9:j:2008:ILE:HD12	2.08	0.83
3:c:2048:LYS:NZ	23:c:2486:CLA:HBA1	1.93	0.83
3:c:2071:GLU:HB3	3:c:2089:ILE:HD11	1.61	0.83
13:o:2143:LYS:HE2	13:o:2198:SER:HB2	1.60	0.83
2:B:322:GLY:HA2	2:B:325:PHE:CD1	2.13	0.83
4:d:2051:GLY:HA2	4:d:2055:VAL:HG23	1.60	0.83
1:A:296:ASN:CG	3:C:401:LEU:HD23	2.04	0.83
1:A:334:ARG:NH1	4:D:320:LEU:HD11	1.93	0.83
1:a:2238:LYS:HD2	14:t:2031:LYS:HD2	1.61	0.83
3:c:2042:LEU:HG	23:c:2486:CLA:HED1	1.61	0.83
1:A:221:SER:HA	4:D:139:ARG:HB2	1.60	0.83
1:A:243:GLU:HA	4:D:240:ALA:HB1	1.58	0.83
3:C:294:ASN:N	3:C:294:ASN:ND2	2.21	0.83
5:E:14:THR:CG2	9:J:8:ILE:CG1	2.56	0.83
11:l:2032:SER:HG	14:t:2006:TYR:HE2	1.22	0.83
2:B:144:PHE:HE1	2:B:210:ILE:HG23	1.43	0.83
23:B:512:CLA:H191	23:B:520:CLA:H151	1.61	0.83
1:a:2307:ILE:CG1	1:a:2314:ILE:HD11	2.09	0.83
2:b:2145:LEU:HD13	23:b:2522:CLA:HMB2	1.59	0.83
23:a:2349:CLA:HED1	4:d:2175:VAL:HG13	1.59	0.83
13:o:2081:ILE:HG22	13:o:2082:GLN:H	1.42	0.83
3:C:279:LEU:HB3	23:C:481:CLA:HBC1	1.59	0.83
4:d:2334:GLN:HB3	4:d:2336:HIS:HE2	1.41	0.83
2:B:339:ALA:HB3	2:B:430:PHE:CD1	2.14	0.82
10:K:25:ALA:HB1	27:K:50:BCR:H19C	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:2080:THR:HG23	16:v:2084:GLY:HA2	1.60	0.82
3:C:55:ALA:HB1	27:C:488:BCR:C37	2.09	0.82
4:D:174:GLY:O	4:D:178:ILE:HG12	1.80	0.82
2:b:2009:HIS:HB2	23:b:2523:CLA:HBA2	1.58	0.82
2:b:2322:GLY:HA2	2:b:2325:PHE:CD1	2.14	0.82
23:A:350:CLA:HED1	4:D:175:VAL:HG13	1.61	0.82
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.14	0.82
3:c:2138:GLU:HG2	3:c:2139:THR:N	1.93	0.82
15:u:2057:LEU:HD21	15:u:2112:PHE:HD2	1.44	0.82
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.14	0.82
2:b:2118:TRP:CZ2	11:l:2003:PRO:HB3	2.15	0.82
2:b:2264:PRO:HG3	2:b:2267:LEU:HD12	1.60	0.82
3:c:2098:GLY:O	3:c:2105:VAL:HG13	1.77	0.82
4:d:2186:GLN:HA	4:d:2186:GLN:NE2	1.94	0.82
4:D:195:PRO:CA	4:D:198:MET:HE2	2.09	0.82
5:E:12:ILE:HD12	28:E:84:HEC:CGD	2.09	0.82
1:A:306:VAL:HG22	1:A:307:ILE:H	1.42	0.82
1:A:330:VAL:CG1	4:D:348:ARG:HG3	2.10	0.82
13:o:2126:VAL:O	13:o:2144:GLY:HA3	1.78	0.82
14:t:2010:PHE:CE2	14:t:2014:ILE:HD11	2.14	0.82
3:C:203:THR:HG22	3:C:208:VAL:HG11	1.62	0.82
4:D:195:PRO:HA	4:D:198:MET:CE	2.09	0.82
15:U:91:VAL:O	15:U:94:ILE:HG13	1.80	0.82
3:c:2101:PRO:N	3:c:2195:ASP:HB3	1.95	0.82
16:V:80:THR:HG23	16:V:84:GLY:HA2	1.62	0.81
4:D:71:CYS:HB2	4:D:76:VAL:CG2	2.09	0.81
1:a:2040:THR:HG22	1:a:2041:LEU:HD23	1.62	0.81
1:a:2334:ARG:HH22	13:o:2159:PRO:HA	1.44	0.81
7:h:2059:VAL:O	7:h:2059:VAL:HG12	1.80	0.81
1:A:156:ALA:HA	1:A:160:ILE:HD12	1.62	0.81
1:A:301:ASN:HD21	3:C:407:VAL:CG2	1.93	0.81
3:C:292:PHE:HD2	3:C:292:PHE:N	1.78	0.81
4:D:102:THR:HG22	4:D:106:GLN:HE21	1.43	0.81
16:V:56:THR:HA	16:V:59:LEU:HD12	1.60	0.81
3:c:2455:PHE:HE1	4:d:2224:GLN:HA	1.46	0.81
4:d:2176:ALA:HA	4:d:2179:PHE:HD1	1.44	0.81
2:B:413:ASP:HB3	2:B:415:PRO:HD2	1.60	0.81
1:a:2161:TYR:HB3	1:a:2162:PRO:HD3	1.61	0.81
3:c:2055:ALA:HB1	27:c:2488:BCR:C37	2.10	0.81
13:O:95:PHE:CB	13:O:127:ALA:HB3	2.10	0.81
1:A:92:HIS:HD2	3:C:219:GLY:HA3	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:HD13	3:C:412:THR:HG21	1.60	0.81
13:O:39:ARG:CB	13:O:245:PRO:HG3	2.10	0.81
13:O:81:ILE:CG2	13:O:82:GLN:H	1.94	0.81
23:b:2512:CLA:H191	23:b:2520:CLA:H151	1.61	0.81
25:d:2358:PL9:H261	14:t:2021:ILE:HD11	1.60	0.81
13:O:40:ILE:HG22	13:O:41:ALA:H	1.46	0.81
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.62	0.81
2:b:2324:LEU:CD1	11:l:2034:TYR:HB3	2.11	0.81
2:B:145:LEU:HD13	23:B:522:CLA:HMB2	1.63	0.80
2:B:222:PRO:HB3	7:H:25:GLY:CA	2.11	0.80
2:B:248:ALA:HA	23:B:517:CLA:H42	1.62	0.80
3:C:295:THR:O	3:C:298:PRO:HD3	1.79	0.80
2:b:2305:ILE:O	2:b:2305:ILE:HG13	1.80	0.80
2:B:170:ASP:OD1	2:B:175:THR:HG22	1.81	0.80
3:C:199:ILE:HD12	3:C:234:VAL:HG21	1.62	0.80
9:J:40:LEU:HD23	16:V:30:LYS:HE2	1.61	0.80
2:b:2326:ARG:NH1	2:b:2327:THR:OG1	2.15	0.80
3:c:2307:PRO:HB3	3:c:2358:PHE:CD2	2.16	0.80
3:C:120:ILE:O	3:C:124:VAL:HG23	1.82	0.80
1:a:2056:PRO:HA	1:a:2073:TYR:HE1	1.44	0.80
2:b:2248:ALA:HA	23:b:2517:CLA:H42	1.64	0.80
3:C:212:TYR:O	3:C:223:TRP:HB2	1.81	0.80
4:d:2145:ALA:HB2	4:d:2272:LEU:HD11	1.63	0.80
2:B:63:LEU:HB3	2:B:64:PRO:HD3	1.62	0.80
3:c:2141:GLU:HB2	3:c:2144:SER:CB	2.12	0.80
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.17	0.80
2:B:302:TRP:O	2:B:341:LYS:HE3	1.81	0.80
3:C:126:GLY:O	3:C:130:VAL:HG23	1.80	0.80
2:b:2222:PRO:HB3	7:h:2025:GLY:CA	2.11	0.80
4:d:2298:PHE:CA	11:l:2037:ASN:HD21	1.93	0.80
13:o:2081:ILE:HG22	13:o:2082:GLN:N	1.95	0.80
2:B:75:TRP:N	2:B:94:GLU:HG3	1.93	0.80
4:d:2155:SER:HA	4:d:2159:ILE:HD12	1.62	0.80
2:B:478:VAL:HG11	4:D:139:ARG:HA	1.64	0.80
3:C:308:GLU:HG2	3:C:361:PHE:HE1	1.42	0.80
4:D:138:VAL:HG12	4:D:139:ARG:N	1.97	0.80
4:D:190:ASN:HB2	4:D:296:TYR:HD1	1.44	0.80
19:Z:8:ALA:O	19:Z:11:ALA:HB3	1.82	0.80
1:a:2221:SER:HA	4:d:2139:ARG:HB2	1.62	0.80
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.64	0.80
2:b:2478:VAL:HG11	4:d:2139:ARG:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:2132:LEU:HD23	15:u:2132:LEU:N	1.96	0.80
1:A:246:TYR:CE1	1:A:248:ILE:HG12	2.17	0.79
3:C:405:ASN:HB2	3:C:407:VAL:HG23	1.62	0.79
1:a:2131:TRP:HZ2	3:c:2449:ARG:HG3	1.46	0.79
2:b:2280:PHE:CE1	2:b:2312:TYR:HB3	2.17	0.79
11:L:12:LEU:HD11	11:L:16:SER:HB3	1.64	0.79
13:O:122:VAL:HA	13:O:146:PHE:HE2	1.47	0.79
16:V:4:THR:HG22	16:V:5:PRO:CD	2.12	0.79
1:a:2202:VAL:HG21	23:a:2349:CLA:OBD	1.81	0.79
1:a:2243:GLU:HA	4:d:2240:ALA:HB1	1.64	0.79
2:b:2113:TRP:HB3	23:b:2525:CLA:HED1	1.63	0.79
3:c:2199:ILE:HD12	3:c:2234:VAL:HG21	1.62	0.79
8:i:2025:SER:HB2	8:i:2028:PRO:HD2	1.62	0.79
4:D:336:HIS:H	4:D:336:HIS:HD2	1.28	0.79
1:a:2159:LEU:O	1:a:2162:PRO:HD2	1.81	0.79
3:c:2285:ILE:HA	23:c:2487:CLA:CMB	2.11	0.79
4:d:2161:PRO:CG	4:d:2170:ALA:HB2	2.12	0.79
8:i:2027:ASP:HB2	8:i:2028:PRO:CD	2.13	0.79
1:A:210:LEU:HD12	1:A:210:LEU:O	1.82	0.79
3:C:334:PRO:HA	13:O:153:THR:HB	1.65	0.79
5:E:56:ALA:HB2	5:E:82:LEU:HD23	1.62	0.79
23:B:512:CLA:H193	23:B:523:CLA:H102	1.62	0.79
3:C:292:PHE:N	3:C:292:PHE:CD2	2.50	0.79
15:U:132:LEU:HD23	15:U:132:LEU:N	1.96	0.79
3:c:2326:ALA:CB	15:u:2127:ARG:HD2	2.09	0.79
5:E:14:THR:CG2	9:J:8:ILE:CD1	2.54	0.79
1:a:2306:VAL:HG22	1:a:2307:ILE:N	1.97	0.79
3:c:2347:GLY:HA3	13:o:2017:ASN:OD1	1.81	0.79
3:c:2363:GLY:O	3:c:2367:GLU:HG2	1.81	0.79
4:d:2103:ARG:NH1	5:e:2072:LYS:HG2	1.96	0.79
2:B:341:LYS:CE	13:o:2060:ARG:HH22	1.96	0.79
3:C:285:ILE:HA	23:C:487:CLA:CMB	2.11	0.79
3:C:293:ASN:C	3:C:294:ASN:HD22	1.89	0.79
4:d:2197:HIS:O	4:d:2201:VAL:HG23	1.83	0.79
5:e:2014:THR:CG2	9:j:2008:ILE:CB	2.59	0.79
3:C:225:VAL:HB	23:C:487:CLA:HMC3	1.65	0.79
3:C:264:PHE:N	3:C:264:PHE:HD2	1.81	0.79
16:V:79:PRO:HB2	16:V:88:ILE:CG1	2.13	0.79
4:d:2088:SER:HB3	5:e:2068:ARG:NH2	1.97	0.79
1:A:14:TRP:CZ3	1:A:18:CYS:SG	2.76	0.79
16:v:2055:ARG:HG3	16:v:2056:THR:N	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:HZ	4:D:223:PHE:CZ	2.01	0.79
13:O:95:PHE:HB3	13:O:127:ALA:HB3	1.65	0.79
1:a:2339:PHE:HB3	1:a:2340:PRO:HD2	1.66	0.78
4:D:68:LEU:HA	6:F:39:MET:HE1	1.65	0.78
3:C:223:TRP:CD1	3:C:224:ILE:H	2.01	0.78
3:C:273:SER:HB3	3:C:445:ALA:HB2	1.66	0.78
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.18	0.78
2:B:264:PRO:HG3	2:B:267:LEU:HD12	1.64	0.78
13:O:140:THR:HB	13:O:201:VAL:HG23	1.64	0.78
1:a:2300:PHE:HB3	1:a:2302:PHE:HE1	1.47	0.78
10:K:16:LEU:HB3	10:K:17:PRO:CD	2.13	0.78
13:O:75:THR:HG22	13:O:103:PHE:HD2	1.47	0.78
8:I:27:ASP:HB2	8:I:28:PRO:CD	2.13	0.78
2:b:2063:LEU:HB3	2:b:2064:PRO:HD3	1.66	0.78
2:b:2170:ASP:OD1	2:b:2175:THR:HG22	1.82	0.78
4:d:2280:TRP:O	4:d:2284:ILE:HG13	1.83	0.78
13:o:2040:ILE:HG12	13:o:2084:GLU:CD	2.08	0.78
1:A:239:PHE:CE1	4:D:245:SER:HA	2.19	0.78
1:A:253:GLY:O	1:A:257:ARG:HG2	1.83	0.78
23:A:350:CLA:H121	25:A:353:PL9:H162	1.66	0.78
2:B:221:PRO:HG3	2:B:225:LEU:HD12	1.64	0.78
4:D:236:ASN:OD1	4:D:239:GLN:HB2	1.83	0.78
2:b:2221:PRO:HG3	2:b:2225:LEU:HD12	1.66	0.78
5:e:2014:THR:HG21	9:j:2008:ILE:CG1	2.14	0.78
1:A:301:ASN:ND2	3:C:407:VAL:HG21	1.99	0.78
3:C:86:LEU:HD13	3:C:89:ILE:HD12	1.64	0.78
5:E:22:HIS:HA	5:E:25:THR:HB	1.64	0.77
13:O:20:PRO:HB2	13:O:240:TYR:CD1	2.18	0.77
4:d:2068:LEU:CA	6:f:2039:MET:HE1	2.14	0.77
3:C:347:GLY:HA3	13:O:17:ASN:OD1	1.85	0.77
4:D:298:PHE:CA	11:L:37:ASN:HD21	1.87	0.77
1:a:2083:VAL:CG1	1:a:2084:PRO:HD2	2.14	0.77
1:a:2239:PHE:HZ	4:d:2223:PHE:CZ	2.02	0.77
13:o:2140:THR:HG21	13:o:2201:VAL:HB	1.64	0.77
19:z:2019:MET:O	19:z:2023:VAL:HG23	1.83	0.77
4:D:176:ALA:HA	4:D:179:PHE:HD1	1.48	0.77
1:a:2162:PRO:HB3	1:a:2168:PHE:HA	1.66	0.77
6:F:36:ILE:HA	6:F:39:MET:HG3	1.67	0.77
10:K:2:LEU:N	10:K:3:PRO:HD3	1.98	0.77
2:b:2413:ASP:HB3	2:b:2415:PRO:HD2	1.66	0.77
1:A:29:TYR:C	1:A:29:TYR:CD1	2.59	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:522:CLA:H171	23:B:525:CLA:CMD	2.14	0.77
5:e:2060:ARG:HH22	16:v:2129:LYS:NZ	1.82	0.77
5:E:12:ILE:HG22	5:E:18:TYR:CG	2.20	0.77
1:a:2095:PRO:HD2	1:a:2098:GLU:CB	2.14	0.77
4:d:2238:THR:O	4:d:2240:ALA:N	2.16	0.77
3:C:320:ARG:HH12	16:V:50:PRO:HD2	1.46	0.77
2:B:327:THR:HG22	2:B:329:PRO:HD3	1.67	0.77
2:B:478:VAL:CG1	4:D:139:ARG:HA	2.15	0.77
2:b:2075:TRP:N	2:b:2094:GLU:HG3	1.93	0.77
1:A:53:ILE:HG12	1:A:71:LEU:HD12	1.67	0.77
1:A:63:ILE:HD11	1:A:336:ALA:HB2	1.67	0.77
16:V:79:PRO:HB2	16:V:88:ILE:HG12	1.67	0.77
1:a:2186:PHE:CD2	1:a:2192:ILE:HD11	2.20	0.77
3:C:320:ARG:NH1	16:V:50:PRO:HD2	1.99	0.77
1:A:206:PHE:HE1	23:A:348:CLA:HMB1	1.49	0.76
1:A:306:VAL:HG22	1:A:307:ILE:N	1.99	0.76
2:B:326:ARG:CD	2:B:327:THR:N	2.41	0.76
25:D:357:PL9:H38	14:T:18:PHE:HB2	1.66	0.76
1:a:2116:ILE:HG22	1:a:2117:PHE:N	2.00	0.76
2:b:2068:ARG:HH12	23:b:2516:CLA:HED1	1.50	0.76
8:i:2007:THR:O	8:i:2011:VAL:HG23	1.86	0.76
13:o:2075:THR:HG23	13:o:2103:PHE:CD2	2.20	0.76
2:B:326:ARG:NH1	2:B:327:THR:OG1	2.17	0.76
1:a:2219:VAL:HG11	4:d:2268:HIS:CG	2.20	0.76
2:b:2025:MET:HB3	27:b:2528:BCR:H332	1.68	0.76
2:B:113:TRP:HB3	23:B:525:CLA:HED1	1.67	0.76
3:C:437:PHE:HA	23:C:483:CLA:HMC1	1.68	0.76
1:a:2341:LEU:HD11	15:u:2134:LYS:HZ2	1.51	0.76
3:c:2293:ASN:N	3:c:2293:ASN:HD22	1.84	0.76
8:I:7:THR:O	8:I:11:VAL:HG23	1.85	0.76
13:O:60:ARG:HH12	2:b:2341:LYS:HZ2	1.32	0.76
4:d:2071:CYS:HB3	4:d:2075:THR:HB	1.68	0.76
4:d:2072:ASN:OD1	4:d:2074:LEU:HB2	1.84	0.76
1:A:295:PHE:HB3	3:C:291:TRP:CZ3	2.20	0.76
1:A:301:ASN:HD21	3:C:407:VAL:HG21	1.48	0.76
2:B:142:HIS:CE1	23:B:524:CLA:H142	2.21	0.76
4:D:323:GLU:HG2	13:O:168:TYR:OH	1.86	0.76
5:e:2071:ALA:O	5:e:2075:VAL:HG23	1.85	0.76
1:A:142:TRP:HE1	3:C:443:TRP:HH2	1.33	0.76
1:A:29:TYR:HD1	1:A:30:VAL:N	1.83	0.76
3:C:175:LEU:HD11	23:C:479:CLA:HED3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2285:ILE:HD12	23:c:2479:CLA:H71	1.66	0.76
13:o:2122:VAL:HA	13:o:2146:PHE:CE2	2.21	0.76
1:a:2300:PHE:HB3	1:a:2302:PHE:CE1	2.20	0.76
3:c:2345:PRO:O	13:o:2074:GLU:HB2	1.86	0.76
13:o:2022:LEU:O	13:o:2203:LYS:HD2	1.86	0.76
1:A:87:ASN:HD21	3:C:357:ARG:HH11	1.32	0.76
5:E:12:ILE:CD1	28:E:84:HEC:O1A	2.34	0.76
9:J:15:THR:HA	27:K:50:BCR:H372	1.67	0.76
4:d:2052:THR:HG22	4:d:2067:TYR:HE1	1.50	0.76
2:b:2327:THR:HG22	2:b:2329:PRO:HD3	1.68	0.76
2:b:2348:ASN:OD1	2:b:2349:LYS:N	2.15	0.76
3:c:2176:VAL:O	3:c:2180:MET:HG2	1.86	0.76
6:f:2025:LEU:O	6:f:2028:PRO:HD2	1.85	0.76
2:B:326:ARG:HH11	2:B:327:THR:HB	1.48	0.75
4:d:2172:SER:HB2	4:d:2177:ALA:HB1	1.67	0.75
23:c:2477:CLA:CMD	23:c:2485:CLA:HAB	2.16	0.75
3:c:2293:ASN:C	3:c:2294:ASN:HD22	1.94	0.75
13:o:2104:GLN:N	13:o:2104:GLN:CD	2.43	0.75
15:u:2036:GLU:O	15:u:2040:VAL:HG23	1.86	0.75
1:A:141:PRO:HG2	3:C:443:TRP:HZ3	1.52	0.75
1:A:148:SER:HB2	1:A:284:TRP:HH2	1.50	0.75
2:B:118:TRP:CZ2	11:L:3:PRO:HB3	2.21	0.75
23:C:479:CLA:H92	23:C:479:CLA:HAB	1.69	0.75
4:D:31:GLY:HA3	4:D:131:GLU:OE1	1.86	0.75
1:a:2041:LEU:HD21	1:a:2122:GLY:HA3	1.68	0.75
2:b:2172:TYR:CE2	2:b:2283:GLU:HB2	2.21	0.75
3:c:2062:PHE:HZ	10:k:2019:ILE:HD11	1.52	0.75
3:c:2292:PHE:HD2	3:c:2292:PHE:N	1.85	0.75
2:B:305:ILE:O	2:B:305:ILE:HG13	1.86	0.75
2:b:2478:VAL:CG1	4:d:2139:ARG:HA	2.16	0.75
3:c:2308:GLU:OE2	3:c:2361:PHE:HZ	1.70	0.75
3:C:264:PHE:N	3:C:264:PHE:CD2	2.54	0.75
4:d:2161:PRO:HG2	4:d:2170:ALA:HB2	1.68	0.75
13:o:2140:THR:CB	13:o:2201:VAL:H	1.99	0.75
1:A:56:PRO:HA	1:A:73:TYR:CE1	2.22	0.75
1:A:57:PRO:HB3	1:A:68:SER:HB3	1.68	0.75
2:B:25:MET:HB3	27:B:529:BCR:H332	1.69	0.75
4:D:304:ARG:HD3	12:M:1:MET:HE3	1.68	0.75
13:O:7:TYR:O	13:O:11:VAL:HG23	1.86	0.75
1:a:2158:PHE:HE2	1:a:2172:MET:HE3	1.51	0.75
2:b:2326:ARG:HH11	2:b:2327:THR:HB	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2061:VAL:HG12	3:c:2118:HIS:O	1.87	0.75
1:A:159:LEU:HD21	23:C:487:CLA:HBD	1.69	0.75
4:D:336:HIS:CD2	4:D:336:HIS:N	2.52	0.75
23:b:2522:CLA:H171	23:b:2525:CLA:CMD	2.16	0.75
1:a:2157:VAL:HG22	1:a:2290:ILE:HD13	1.69	0.74
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.68	0.74
3:C:98:GLY:O	3:C:99:VAL:HG23	1.86	0.74
1:a:2159:LEU:HG	1:a:2163:ILE:CD1	2.17	0.74
4:d:2032:TRP:HB2	4:d:2131:GLU:OE2	1.87	0.74
16:v:2072:LEU:O	16:v:2076:MET:HG3	1.87	0.74
2:B:187:PRO:O	2:B:190:PHE:N	2.20	0.74
3:C:89:ILE:HB	3:C:90:PRO:HD3	1.69	0.74
4:D:88:SER:CB	5:E:68:ARG:HH21	1.98	0.74
5:e:2009:PHE:O	5:e:2010:SER:HB3	1.85	0.74
3:C:285:ILE:HG21	23:C:479:CLA:H51	1.69	0.74
3:C:374:GLY:HA2	13:O:7:TYR:CE1	2.22	0.74
4:D:19:ASP:OD1	4:D:23:LYS:HD2	1.87	0.74
11:L:4:ASN:N	11:L:5:PRO:HD3	2.03	0.74
2:b:2339:ALA:HB3	2:b:2430:PHE:CD1	2.22	0.74
3:c:2123:ALA:HB1	19:z:2047:TRP:HH2	1.52	0.74
4:d:2129:GLN:HE21	4:d:2142:ASN:HB3	1.52	0.74
2:B:172:TYR:CE2	2:B:283:GLU:HB2	2.23	0.74
2:b:2066:MET:O	2:b:2071:VAL:HG23	1.88	0.74
23:b:2520:CLA:HBC3	23:b:2523:CLA:H41	1.70	0.74
3:c:2264:PHE:HD1	23:c:2485:CLA:HMC1	1.53	0.74
2:B:112:CYS:O	2:B:116:VAL:HG23	1.87	0.74
3:C:308:GLU:HG2	3:C:361:PHE:CZ	2.22	0.74
3:C:363:GLY:O	3:C:367:GLU:HG2	1.87	0.74
3:C:229:ASN:HB3	3:C:232:ASP:OD1	1.88	0.74
4:D:235:PHE:HA	4:D:239:GLN:OE1	1.86	0.74
5:E:9:PHE:O	5:E:10:SER:HB3	1.85	0.74
5:E:43:TYR:CD2	5:E:50:ARG:HG2	2.22	0.74
13:O:60:ARG:HH22	2:b:2341:LYS:HE2	1.51	0.74
23:b:2512:CLA:H193	23:b:2523:CLA:H102	1.69	0.74
3:c:2043:ILE:HG13	3:c:2044:ASN:H	1.52	0.74
7:h:2022:PRO:HG2	7:h:2023:GLY:H	1.53	0.74
14:t:2024:ARG:HG2	14:t:2025:GLU:N	2.02	0.74
2:B:63:LEU:HD11	2:B:93:PHE:CE1	2.22	0.74
3:C:350:ILE:HG12	3:C:359:TRP:HB2	1.70	0.74
4:d:2186:GLN:HB2	23:d:2354:CLA:HBC1	1.68	0.74
4:D:51:GLY:HA2	4:D:55:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:CYS:HB3	4:D:75:THR:HB	1.68	0.74
4:D:90:LEU:HD11	4:D:96:GLU:CD	2.13	0.74
5:E:19:TRP:HZ2	9:J:13:VAL:HG22	1.50	0.74
1:A:78:ILE:HD11	11:L:34:TYR:CE1	2.23	0.74
3:C:41:ARG:HB2	23:C:486:CLA:HED3	1.69	0.74
3:C:61:VAL:HG22	23:C:480:CLA:HAC2	1.70	0.74
3:C:227:VAL:HG23	3:C:294:ASN:HB3	1.68	0.74
3:C:320:ARG:NE	15:U:128:TYR:HE2	1.79	0.74
4:D:152:VAL:O	4:D:156:VAL:HG23	1.88	0.74
10:K:19:ILE:HA	10:K:22:LEU:HD12	1.70	0.74
1:a:2306:VAL:HG22	1:a:2307:ILE:H	1.51	0.74
3:C:101:PRO:N	3:C:195:ASP:HB3	2.03	0.73
4:d:2262:SER:O	4:d:2263:ASN:ND2	2.21	0.73
9:j:2040:LEU:HD23	16:v:2030:LYS:HE3	1.68	0.73
13:o:2163:GLY:CA	13:o:2188:LYS:HE2	2.18	0.73
12:M:20:VAL:HG22	12:m:2020:VAL:HG11	1.70	0.73
13:O:43:LEU:HD13	13:O:241:ALA:HB2	1.69	0.73
5:e:2012:ILE:HG23	5:e:2018:TYR:HB2	1.62	0.73
10:K:2:LEU:H	10:K:3:PRO:HD3	1.51	0.73
2:b:2414:PRO:HG2	2:b:2415:PRO:HD3	1.71	0.73
2:B:27:THR:O	23:B:518:CLA:HBC1	1.88	0.73
3:C:138:GLU:CG	3:C:139:THR:H	1.96	0.73
4:D:267:LEU:O	4:D:271:MET:HG3	1.87	0.73
1:a:2078:ILE:O	1:a:2177:SER:HB2	1.88	0.73
3:c:2203:THR:HG22	3:c:2208:VAL:HG11	1.70	0.73
1:A:317:TRP:HA	4:D:63:LEU:CD1	2.19	0.73
2:B:357:ARG:NH2	4:D:337:GLU:HB3	2.04	0.73
2:B:368:VAL:HA	2:B:425:ILE:HD11	1.69	0.73
4:D:56:THR:HB	5:E:48:THR:HG23	1.71	0.73
4:d:2302:GLU:OE1	4:d:2302:GLU:HA	1.89	0.73
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.69	0.73
2:b:2339:ALA:HB3	2:b:2430:PHE:HD1	1.53	0.73
4:d:2267:LEU:O	4:d:2271:MET:HG3	1.89	0.73
9:j:2015:THR:HA	27:k:2050:BCR:C37	2.19	0.73
3:C:248:GLY:O	3:C:252:ILE:HG13	1.89	0.73
14:T:18:PHE:HD2	14:T:19:PHE:CD1	2.07	0.73
3:c:2350:ILE:HG21	3:c:2359:TRP:CB	2.19	0.73
23:c:2479:CLA:H92	23:c:2479:CLA:HAB	1.69	0.73
3:C:343:ARG:C	3:C:343:ARG:CD	2.59	0.73
4:d:2195:PRO:HA	4:d:2198:MET:CE	2.19	0.73
11:l:2004:ASN:H	11:l:2004:ASN:HD22	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:2004:ASN:N	11:l:2005:PRO:HD3	2.02	0.73
3:C:123:ALA:HB1	19:Z:47:TRP:HH2	1.53	0.73
2:b:2047:PRO:HB3	2:b:2078:TRP:HD1	1.54	0.73
3:c:2178:LYS:HA	3:c:2182:PHE:HB2	1.70	0.73
4:d:2322:ASN:HA	4:d:2325:ILE:HD12	1.70	0.73
13:O:50:PHE:HZ	13:O:76:THR:HG23	1.54	0.72
13:O:68:THR:HA	13:O:110:MET:HE1	1.71	0.72
4:d:2160:TYR:HB3	4:d:2161:PRO:HD3	1.70	0.72
1:A:334:ARG:HH12	13:O:159:PRO:HA	1.53	0.72
2:b:2017:GLY:O	2:b:2020:ILE:HG22	1.89	0.72
13:o:2164:LEU:O	13:o:2165:ALA:HB3	1.87	0.72
1:A:76:ASN:HB3	14:T:2:GLU:OE2	1.90	0.72
2:B:246:PHE:HE1	2:B:463:PHE:HB2	1.53	0.72
4:D:238:THR:O	4:D:240:ALA:N	2.20	0.72
2:b:2326:ARG:CD	2:b:2327:THR:N	2.43	0.72
3:c:2299:SER:HB2	3:c:2303:GLY:O	1.89	0.72
4:d:2195:PRO:HA	4:d:2198:MET:HE2	1.70	0.72
1:A:69:GLY:HA2	1:A:75:ASN:OD1	1.90	0.72
2:B:66:MET:O	2:B:71:VAL:HG23	1.89	0.72
4:d:2091:LEU:HD23	4:d:2091:LEU:N	2.04	0.72
13:o:2163:GLY:HA3	13:o:2188:LYS:HE2	1.72	0.72
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.71	0.72
19:Z:41:PHE:HD1	19:Z:41:PHE:H	1.35	0.72
1:a:2083:VAL:HG13	1:a:2084:PRO:HD2	1.72	0.72
2:b:2086:ILE:O	2:b:2088:PRO:HD3	1.89	0.72
1:A:182:PHE:O	1:A:186:PHE:HB2	1.88	0.72
2:B:172:TYR:CZ	2:B:283:GLU:HB2	2.25	0.72
2:B:400:SER:OG	2:B:410:THR:HG23	1.88	0.72
3:C:271:TYR:HA	3:C:274:TYR:HD1	1.50	0.72
2:b:2142:HIS:CE1	23:b:2524:CLA:H142	2.23	0.72
15:u:2055:ILE:HD11	15:u:2068:TYR:HE1	1.53	0.72
2:B:340:TRP:CZ3	2:B:342:GLY:HA3	2.24	0.72
4:D:194:ASN:O	4:D:198:MET:HG3	1.88	0.72
4:D:235:PHE:CD1	4:D:236:ASN:N	2.57	0.72
13:O:162:ARG:O	13:O:162:ARG:HG2	1.90	0.72
23:a:2349:CLA:H121	25:a:2352:PL9:H162	1.71	0.72
2:b:2340:TRP:CZ3	2:b:2342:GLY:HA3	2.25	0.72
3:c:2322:GLN:NE2	3:c:2322:GLN:HA	2.03	0.72
4:d:2019:ASP:OD1	4:d:2023:LYS:HD2	1.90	0.72
4:d:2118:GLY:HA3	24:d:2356:PHO:H71	1.72	0.72
5:e:2014:THR:CG2	9:j:2008:ILE:CG1	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:CG	23:C:486:CLA:HED1	2.18	0.72
4:D:86:GLY:C	4:D:87:HIS:HD2	1.98	0.72
4:D:319:LEU:HA	4:D:322:ASN:ND2	2.04	0.72
15:U:132:LEU:H	15:U:132:LEU:CD2	1.96	0.72
2:b:2339:ALA:HB2	2:b:2431:GLU:H	1.55	0.72
8:I:15:PHE:HA	8:I:18:LEU:HG	1.72	0.72
15:U:83:ALA:HA	15:U:85:TYR:CE2	2.25	0.72
2:b:2172:TYR:CZ	2:b:2283:GLU:HB2	2.24	0.72
13:o:2095:PHE:HB3	13:o:2127:ALA:HB3	1.70	0.72
15:u:2039:LEU:C	15:u:2041:ASN:H	1.97	0.72
23:C:477:CLA:CMD	23:C:485:CLA:HAB	2.19	0.72
5:E:14:THR:HG21	9:J:8:ILE:HG13	1.71	0.72
13:O:201:VAL:HG13	13:O:211:ILE:HG23	1.71	0.72
13:O:223:ASP:HB3	13:O:230:PRO:HG3	1.71	0.72
1:a:2069:GLY:HA2	1:a:2075:ASN:OD1	1.90	0.72
2:b:2113:TRP:O	2:b:2117:TYR:HB2	1.89	0.72
2:b:2478:VAL:HG12	4:d:2139:ARG:HG2	1.71	0.72
3:c:2450:ALA:HA	3:c:2454:GLY:HA3	1.72	0.72
13:o:2153:THR:HG22	13:o:2154:ALA:N	2.05	0.72
13:o:2201:VAL:HG13	13:o:2211:ILE:HG23	1.71	0.72
2:B:68:ARG:HH12	23:B:516:CLA:HED1	1.54	0.71
12:M:18:PRO:O	12:M:22:LEU:HG	1.89	0.71
3:c:2039:ASN:HA	3:c:2042:LEU:HD12	1.70	0.71
4:d:2052:THR:O	4:d:2076:VAL:HG11	1.91	0.71
5:e:2033:GLY:HA2	6:f:2031:PHE:CE2	2.24	0.71
17:x:2042:GLN:O	17:x:2045:LYS:HG3	1.90	0.71
1:A:29:TYR:CD2	1:A:133:LEU:CD1	2.72	0.71
1:A:326:LEU:CD1	3:C:412:THR:HG21	2.20	0.71
23:B:520:CLA:HBC3	23:B:523:CLA:H41	1.72	0.71
3:C:99:VAL:HG22	3:C:104:GLU:O	1.90	0.71
3:C:343:ARG:HA	3:C:348:GLU:O	1.90	0.71
2:B:248:ALA:O	2:B:252:VAL:HG23	1.89	0.71
3:c:2266:TRP:HA	3:c:2271:TYR:HE2	1.54	0.71
4:d:2054:PHE:HB3	5:e:2046:PHE:CD1	2.25	0.71
8:i:2027:ASP:HB2	8:i:2028:PRO:HD3	1.72	0.71
1:A:239:PHE:CZ	4:D:223:PHE:HZ	2.08	0.71
4:D:68:LEU:HA	6:F:39:MET:CE	2.19	0.71
2:b:2271:THR:OG1	2:b:2274:GLN:HG3	1.90	0.71
2:b:2315:ILE:HD13	2:b:2359:MET:HE2	1.72	0.71
4:d:2319:LEU:HA	4:d:2322:ASN:HD22	1.53	0.71
8:i:2019:PHE:CE1	8:i:2023:PHE:HE1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD11	1:A:336:ALA:CB	2.20	0.71
2:B:17:GLY:O	2:B:20:ILE:HG22	1.89	0.71
3:C:385:GLN:OE1	3:C:386:PRO:HD2	1.91	0.71
3:C:437:PHE:HA	23:C:483:CLA:CMC	2.19	0.71
3:c:2417:VAL:HG22	16:v:2038:ALA:HB1	1.71	0.71
10:k:2025:ALA:HB1	27:k:2050:BCR:H19C	1.71	0.71
1:A:330:VAL:HG11	4:D:348:ARG:HG3	1.72	0.71
2:B:47:PRO:HB3	2:B:78:TRP:HD1	1.51	0.71
2:B:397:VAL:HG12	2:B:398:THR:N	2.05	0.71
3:C:43:ILE:HG13	3:C:44:ASN:N	2.06	0.71
13:O:104:GLN:N	13:O:104:GLN:CD	2.46	0.71
1:a:2040:THR:HG22	1:a:2041:LEU:N	2.04	0.71
1:a:2142:TRP:NE1	3:c:2443:TRP:CH2	2.59	0.71
2:b:2397:VAL:HG12	2:b:2398:THR:N	2.06	0.71
4:d:2056:THR:HB	5:e:2048:THR:HG23	1.72	0.71
1:A:309:ALA:O	16:V:3:LEU:N	2.24	0.71
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.72	0.71
4:D:244:TYR:OH	4:D:264:LYS:NZ	2.21	0.71
4:D:274:VAL:HB	4:D:275:PRO:HD3	1.71	0.71
2:b:2063:LEU:HD11	2:b:2093:PHE:CE1	2.25	0.71
4:d:2056:THR:HA	4:d:2065:SER:HB3	1.71	0.71
16:v:2063:THR:HB	16:v:2083:ASP:O	1.89	0.71
1:A:29:TYR:HE1	1:A:31:GLY:CA	2.03	0.71
1:A:243:GLU:CA	4:D:240:ALA:HB1	2.21	0.71
2:B:418:LYS:HZ1	15:U:45:GLU:CD	1.99	0.71
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.54	0.71
4:D:190:ASN:CB	4:D:296:TYR:HD1	2.04	0.71
4:D:262:SER:O	4:D:263:ASN:ND2	2.24	0.71
1:a:2296:ASN:CG	3:c:2401:LEU:HD23	2.16	0.71
2:b:2112:CYS:O	2:b:2116:VAL:HG23	1.91	0.71
2:b:2400:SER:OG	2:b:2410:THR:HG23	1.90	0.71
3:c:2042:LEU:CG	23:c:2486:CLA:HED1	2.21	0.71
3:c:2248:GLY:O	3:c:2252:ILE:HG13	1.91	0.71
4:d:2148:ALA:HB2	4:d:2276:VAL:HG13	1.72	0.71
16:v:2075:TYR:CD2	16:v:2079:PRO:HA	2.26	0.71
1:A:159:LEU:HG	1:A:163:ILE:HD11	1.73	0.71
2:B:339:ALA:HB2	2:B:431:GLU:H	1.56	0.71
3:C:345:PRO:O	13:O:74:GLU:HB2	1.90	0.71
13:O:40:ILE:HG22	13:O:41:ALA:N	2.04	0.71
1:a:2334:ARG:HH11	4:d:2320:LEU:CD1	2.03	0.71
2:b:2266:GLU:O	2:b:2266:GLU:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2318:ASN:C	2:b:2318:ASN:ND2	2.46	0.71
4:d:2068:LEU:N	6:f:2039:MET:HE1	2.05	0.71
4:d:2235:PHE:CD1	4:d:2236:ASN:N	2.59	0.71
4:d:2261:PHE:HD2	14:t:2024:ARG:HH22	1.38	0.71
23:d:2357:CLA:H12	7:h:2042:LEU:HD21	1.71	0.71
1:A:341:LEU:HD21	15:U:134:LYS:HZ2	1.56	0.71
2:B:57:ARG:NH1	2:B:317:ASN:OD1	2.23	0.71
2:B:321:LYS:CE	2:B:325:PHE:HZ	2.04	0.71
2:B:348:ASN:OD1	2:B:349:LYS:N	2.17	0.71
15:U:73:PRO:HB2	16:V:83:ASP:OD2	1.91	0.71
1:a:2184:ILE:HG22	1:a:2328:MET:HE3	1.73	0.71
1:a:2214:MET:HE2	4:d:2142:ASN:HD21	1.55	0.71
4:d:2138:VAL:HG12	4:d:2139:ARG:N	2.05	0.71
1:A:89:ILE:HG21	1:A:94:TYR:HB2	1.73	0.70
13:O:71:VAL:HG21	13:O:108:VAL:HG23	1.71	0.70
5:e:2014:THR:HG21	9:j:2008:ILE:HD12	1.72	0.70
1:A:307:ILE:O	1:A:309:ALA:N	2.23	0.70
3:C:269:GLU:CD	3:C:447:ARG:HG2	2.16	0.70
4:D:221:THR:O	4:D:221:THR:HG22	1.90	0.70
13:O:17:ASN:O	13:O:46:GLN:HG3	1.91	0.70
2:b:2368:VAL:HA	2:b:2425:ILE:HD11	1.71	0.70
3:C:350:ILE:HG21	3:C:359:TRP:HB3	1.73	0.70
13:O:164:LEU:O	13:O:165:ALA:HB3	1.89	0.70
2:b:2248:ALA:O	2:b:2252:VAL:HG23	1.90	0.70
3:c:2108:THR:HG23	10:k:2002:LEU:HD23	1.74	0.70
4:D:16:ASP:O	4:D:19:ASP:HB3	1.90	0.70
3:c:2042:LEU:CD2	23:c:2486:CLA:HED1	2.20	0.70
4:d:2090:LEU:HD11	4:d:2096:GLU:CB	2.20	0.70
13:o:2043:LEU:CD1	13:o:2241:ALA:HB2	2.20	0.70
1:A:159:LEU:HD11	23:C:487:CLA:OBD	1.92	0.70
5:E:52:ASP:O	16:V:1:ALA:HB3	1.90	0.70
10:K:15:VAL:HG11	18:N:13:UNK:CB	2.21	0.70
13:O:155:ASN:ND2	15:U:129:ASN:HD22	1.88	0.70
13:O:211:ILE:HB	13:O:241:ALA:HB3	1.73	0.70
1:a:2228:THR:HG22	1:a:2228:THR:O	1.90	0.70
1:a:2330:VAL:HG13	4:d:2348:ARG:HG3	1.73	0.70
7:h:2057:VAL:HG12	7:h:2057:VAL:O	1.90	0.70
1:A:142:TRP:NE1	3:C:443:TRP:HH2	1.89	0.70
3:C:316:THR:HG21	3:C:396:MET:HE1	1.73	0.70
3:C:450:ALA:HA	3:C:454:GLY:HA3	1.73	0.70
6:F:31:PHE:HD2	6:F:31:PHE:O	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2364:GLU:HG3	4:d:2296:TYR:CE2	2.26	0.70
3:c:2294:ASN:N	3:c:2294:ASN:ND2	2.28	0.70
3:c:2350:ILE:HG12	3:c:2359:TRP:HB2	1.72	0.70
1:a:2210:LEU:O	1:a:2210:LEU:HD12	1.91	0.70
1:a:2303:ASN:O	1:a:2304:HIS:ND1	2.25	0.70
2:b:2264:PRO:CG	2:b:2267:LEU:HD12	2.20	0.70
2:b:2380:ASP:OD1	2:b:2390:TYR:HB2	1.90	0.70
1:A:75:ASN:ND2	1:A:79:THR:HG21	2.05	0.70
7:H:59:VAL:O	7:H:59:VAL:HG12	1.91	0.70
12:M:15:VAL:HG12	12:M:16:LEU:HD23	1.73	0.70
1:a:2335:ASN:C	1:a:2335:ASN:HD22	1.99	0.70
5:e:2012:ILE:CD1	28:e:2084:HEC:O1A	2.38	0.70
28:e:2084:HEC:HAC	6:f:2026:ALA:HB1	1.72	0.70
13:o:2124:ASN:HD22	13:o:2147:ASN:CB	2.05	0.70
2:B:414:PRO:HG2	2:B:415:PRO:HD3	1.72	0.70
19:Z:19:MET:HE1	19:Z:43:GLY:CA	2.21	0.70
2:b:2027:THR:O	23:b:2518:CLA:HBC1	1.92	0.70
2:b:2057:ARG:HH11	2:b:2057:ARG:HG3	1.56	0.70
2:b:2092:SER:O	2:b:2096:VAL:HG23	1.92	0.70
8:i:2025:SER:OG	8:i:2028:PRO:HG2	1.90	0.70
1:A:317:TRP:CA	4:D:63:LEU:HD13	2.22	0.70
4:D:90:LEU:CD1	4:D:96:GLU:HB3	2.21	0.70
13:O:224:ASP:C	13:O:225:MET:HG2	2.16	0.70
4:d:2176:ALA:HA	4:d:2179:PHE:CD1	2.27	0.70
3:C:121:SER:O	3:C:125:LEU:HG	1.91	0.69
4:D:18:LEU:O	4:D:22:LEU:HB3	1.92	0.69
4:D:118:GLY:HA3	24:D:355:PHO:H71	1.72	0.69
1:a:2042:LEU:O	1:a:2046:ILE:HG12	1.93	0.69
2:b:2041:GLU:OE1	2:b:2063:LEU:HB2	1.91	0.69
4:d:2310:GLU:HG2	13:o:2224:ASP:OD2	1.93	0.69
7:h:2042:LEU:O	7:h:2046:GLU:HG3	1.92	0.69
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.22	0.69
1:a:2303:ASN:C	1:a:2304:HIS:HD1	1.99	0.69
2:b:2145:LEU:HD13	23:b:2522:CLA:CMB	2.21	0.69
3:c:2229:ASN:HB3	3:c:2232:ASP:OD1	1.91	0.69
3:c:2308:GLU:HG2	3:c:2361:PHE:CE1	2.27	0.69
4:d:2071:CYS:HB2	4:d:2076:VAL:HG23	1.73	0.69
4:d:2087:HIS:CD2	26:d:2359:LMT:O4'	2.45	0.69
4:d:2180:ARG:C	4:d:2180:ARG:HD3	2.17	0.69
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.26	0.69
2:B:397:VAL:HG12	2:B:398:THR:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:ALA:CB	19:Z:47:TRP:HH2	2.04	0.69
3:C:150:ASP:O	3:C:157:MET:HE3	1.92	0.69
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.74	0.69
16:V:37:CYS:O	16:V:39:SER:N	2.26	0.69
2:b:2124:ARG:HG2	2:b:2125:ASP:N	2.07	0.69
2:b:2397:VAL:HG12	2:b:2398:THR:H	1.57	0.69
13:o:2104:GLN:HB3	13:o:2151:TYR:CE1	2.27	0.69
2:B:41:GLU:OE1	2:B:63:LEU:HB2	1.91	0.69
3:C:305:THR:HA	3:C:423:ARG:HH11	1.56	0.69
4:D:29:PHE:C	4:D:29:PHE:CD2	2.67	0.69
13:O:118:LEU:CD1	13:O:233:VAL:HG11	2.23	0.69
16:V:75:TYR:CD2	16:V:79:PRO:HA	2.26	0.69
2:b:2187:PRO:O	2:b:2190:PHE:N	2.19	0.69
3:c:2292:PHE:N	3:c:2292:PHE:CD2	2.58	0.69
1:A:235:TYR:HA	4:D:265:ARG:NH2	2.06	0.69
2:B:324:LEU:CD1	11:L:34:TYR:HB3	2.22	0.69
10:K:30:TRP:CE3	10:K:31:GLN:NE2	2.60	0.69
5:e:2012:ILE:CG1	28:e:2084:HEC:O2D	2.40	0.69
1:A:219:VAL:HG11	4:D:268:HIS:CG	2.28	0.69
1:A:320:ILE:HG22	1:A:320:ILE:O	1.93	0.69
4:D:87:HIS:NE2	4:D:166:SER:HA	2.08	0.69
4:D:186:GLN:HB2	23:D:354:CLA:HBC1	1.73	0.69
16:V:133:GLY:O	16:V:137:TYR:CB	2.41	0.69
1:a:2317:TRP:HA	4:d:2063:LEU:CD1	2.23	0.69
23:b:2522:CLA:H171	23:b:2525:CLA:HMD1	1.75	0.69
13:o:2040:ILE:HG22	13:o:2041:ALA:H	1.57	0.69
1:A:161:TYR:HB3	1:A:162:PRO:CD	2.21	0.69
3:C:342:MET:HE3	3:C:352:GLY:CA	2.22	0.69
13:O:28:GLY:HA3	13:O:137:THR:HG22	1.73	0.69
1:a:2092:HIS:CD2	3:c:2219:GLY:HA3	2.28	0.69
1:a:2096:ILE:CG2	8:i:2001:MET:HE1	2.20	0.69
3:c:2162:GLY:O	3:c:2165:LEU:HB2	1.92	0.69
4:d:2077:ALA:HB2	4:d:2174:GLY:HA3	1.73	0.69
1:A:281:VAL:O	1:A:281:VAL:HG12	1.91	0.69
2:B:30:VAL:HG12	23:B:518:CLA:HHD	1.73	0.69
2:B:341:LYS:HZ3	13:o:2060:ARG:NH2	1.90	0.69
3:C:176:VAL:O	3:C:180:MET:HG2	1.93	0.69
3:C:343:ARG:HD2	3:C:343:ARG:O	1.92	0.69
1:a:2222:SER:O	1:a:2246:TYR:HB2	1.91	0.69
2:b:2030:VAL:HG12	23:b:2518:CLA:HHD	1.75	0.69
2:b:2057:ARG:HH11	2:b:2057:ARG:CG	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2130:GLU:HG2	2:b:2131:PRO:CD	2.22	0.69
3:c:2291:TRP:O	3:c:2305:THR:HG23	1.92	0.69
3:c:2320:ARG:NH1	16:v:2049:ASN:HA	2.06	0.69
4:d:2108:GLY:C	4:d:2110:LEU:H	1.99	0.69
4:d:2206:GLY:O	4:d:2210:LEU:HG	1.93	0.69
5:e:2012:ILE:HG21	5:e:2018:TYR:HB2	1.68	0.69
13:o:2039:ARG:HA	13:o:2245:PRO:HG3	1.75	0.69
13:o:2112:GLY:C	13:o:2114:GLU:H	1.98	0.69
3:C:319:ILE:HD13	3:C:389:GLU:HG2	1.74	0.69
3:C:342:MET:HE3	3:C:352:GLY:HA3	1.74	0.69
13:O:47:PRO:CG	13:O:76:THR:HG21	2.20	0.69
13:O:75:THR:HG22	13:O:103:PHE:CD2	2.28	0.69
3:c:2086:LEU:HD13	3:c:2089:ILE:HD12	1.75	0.69
3:c:2437:PHE:HA	23:c:2483:CLA:HMC1	1.74	0.69
4:d:2336:HIS:H	4:d:2336:HIS:CD2	2.11	0.69
11:l:2032:SER:OG	14:t:2006:TYR:HE2	1.76	0.69
2:B:57:ARG:HH11	2:B:57:ARG:CG	2.06	0.69
2:B:268:PHE:HB2	2:B:448:ARG:HE	1.56	0.69
13:O:211:ILE:HG22	13:O:212:ALA:N	2.08	0.69
1:A:29:TYR:HD2	1:A:133:LEU:HD13	1.59	0.68
2:B:57:ARG:HH11	2:B:57:ARG:HG3	1.56	0.68
3:C:158:THR:HG23	3:C:251:HIS:HB3	1.74	0.68
4:D:138:VAL:HG12	4:D:139:ARG:H	1.55	0.68
13:O:140:THR:CB	13:O:201:VAL:H	2.06	0.68
15:U:39:LEU:C	15:U:41:ASN:H	2.01	0.68
15:U:62:ILE:HG23	15:U:76:ALA:HB1	1.74	0.68
1:a:2237:TYR:N	1:a:2237:TYR:CD1	2.61	0.68
1:a:2239:PHE:CZ	4:d:2223:PHE:HZ	2.10	0.68
2:b:2246:PHE:HE1	2:b:2463:PHE:HB2	1.55	0.68
5:e:2014:THR:HG21	9:j:2008:ILE:CD1	2.23	0.68
1:A:76:ASN:HD21	4:D:298:PHE:HE2	1.39	0.68
1:A:301:ASN:OD1	3:C:407:VAL:HG21	1.94	0.68
3:C:203:THR:CG2	3:C:208:VAL:HG11	2.23	0.68
13:O:22:LEU:O	13:O:203:LYS:HD3	1.94	0.68
2:b:2414:PRO:CD	2:b:2415:PRO:HD3	2.23	0.68
3:c:2305:THR:H	3:c:2308:GLU:HG3	1.58	0.68
3:c:2343:ARG:HB3	13:o:2078:LEU:CD1	2.24	0.68
27:c:2488:BCR:H312	19:z:2009:LEU:HD11	1.74	0.68
3:C:116:VAL:HG21	27:C:489:BCR:H323	1.75	0.68
13:o:2078:LEU:O	13:o:2079:ASP:OD1	2.10	0.68
13:o:2211:ILE:HG22	13:o:2212:ALA:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:THR:HA	4:D:67:TYR:CD1	2.29	0.68
1:A:81:ALA:HB3	1:A:174:LEU:O	1.93	0.68
2:B:145:LEU:HD13	23:B:522:CLA:CMB	2.23	0.68
2:B:185:TRP:CD1	2:B:185:TRP:H	2.10	0.68
3:C:443:TRP:CE3	3:C:443:TRP:HA	2.28	0.68
4:D:261:PHE:HA	14:T:24:ARG:HH22	1.59	0.68
15:u:2057:LEU:HD11	15:u:2088:VAL:HG13	1.76	0.68
13:O:163:GLY:HA3	13:O:188:LYS:HE2	1.76	0.68
1:a:2182:PHE:O	1:a:2186:PHE:HB2	1.94	0.68
1:a:2309:ALA:O	16:v:2003:LEU:N	2.25	0.68
3:c:2094:THR:C	3:c:2096:GLY:H	2.00	0.68
4:d:2195:PRO:O	4:d:2198:MET:HB2	1.94	0.68
8:i:2005:LYS:HG3	8:i:2009:TYR:HE1	1.59	0.68
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.29	0.68
2:B:105:GLY:HA2	27:B:528:BCR:H383	1.75	0.68
3:C:78:GLU:H	3:C:104:GLU:CD	2.01	0.68
3:C:156:LYS:O	3:C:160:ILE:HG13	1.93	0.68
23:C:475:CLA:HBD	27:J:53:BCR:HC21	1.76	0.68
25:D:357:PL9:H261	14:T:21:ILE:HD11	1.74	0.68
1:a:2237:TYR:CZ	1:a:2245:THR:HG23	2.28	0.68
3:c:2042:LEU:HD13	23:c:2486:CLA:HMA2	1.75	0.68
2:B:86:ILE:O	2:B:88:PRO:HD3	1.93	0.68
1:a:2174:LEU:HD13	24:a:2350:PHO:H143	1.76	0.68
2:b:2225:LEU:HD13	2:b:2231:MET:SD	2.34	0.68
4:d:2029:PHE:HD2	4:d:2029:PHE:C	2.01	0.68
8:i:2005:LYS:O	8:i:2009:TYR:HD1	1.76	0.68
15:u:2072:TYR:CB	15:u:2073:PRO:HD3	2.24	0.68
1:A:61:ASP:HA	1:A:87:ASN:HB2	1.75	0.68
2:B:6:TYR:HH	12:M:21:PHE:HZ	0.74	0.68
2:B:124:ARG:HG2	2:B:125:ASP:N	2.07	0.68
3:C:275:SER:HB3	23:C:485:CLA:HAA1	1.76	0.68
4:D:80:THR:HG21	4:D:167:TRP:O	1.94	0.68
4:d:2261:PHE:CD2	14:t:2024:ARG:NH2	2.61	0.68
5:e:2022:HIS:HA	5:e:2025:THR:HB	1.76	0.68
2:B:383:PHE:O	13:O:166:SER:HA	1.93	0.68
9:J:9:PRO:O	9:J:10:LEU:HD23	1.94	0.68
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.74	0.68
4:d:2261:PHE:HD2	14:t:2024:ARG:NH2	1.92	0.68
13:o:2045:LEU:HD21	13:o:2215:PHE:CE1	2.29	0.68
27:C:488:BCR:H341	27:K:50:BCR:HC31	1.76	0.67
7:H:57:VAL:O	7:H:57:VAL:CG1	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:2133:GLY:O	16:v:2137:TYR:CB	2.43	0.67
2:B:406:LEU:HD12	13:o:2059:LYS:HD2	1.76	0.67
23:B:522:CLA:H171	23:B:525:CLA:HMD1	1.74	0.67
5:E:33:GLY:HA2	6:F:31:PHE:CE2	2.29	0.67
7:H:53:ILE:HG23	17:X:13:THR:OG1	1.94	0.67
3:c:2156:LYS:O	3:c:2160:ILE:HG13	1.94	0.67
19:z:2048:ILE:O	19:z:2052:LEU:HG	1.94	0.67
2:B:113:TRP:O	2:B:117:TYR:HB2	1.94	0.67
2:B:318:ASN:C	2:B:318:ASN:ND2	2.44	0.67
3:C:149:TYR:CD2	3:C:156:LYS:HG3	2.29	0.67
3:C:308:GLU:OE2	3:C:361:PHE:CZ	2.43	0.67
13:O:60:ARG:HH22	2:b:2341:LYS:NZ	1.91	0.67
2:b:2105:GLY:HA2	27:b:2527:BCR:H383	1.76	0.67
3:c:2348:GLU:HG2	13:o:2007:TYR:HE1	1.59	0.67
4:d:2350:ASN:HD22	4:d:2351:ALA:N	1.92	0.67
5:e:2035:LEU:O	5:e:2039:THR:OG1	2.07	0.67
13:o:2081:ILE:CG2	13:o:2082:GLN:H	2.07	0.67
15:u:2072:TYR:CD2	15:u:2073:PRO:N	2.63	0.67
3:C:108:THR:HG21	10:K:2:LEU:HG	1.76	0.67
4:D:279:LEU:HD11	24:D:355:PHO:HMC3	1.75	0.67
1:a:2190:HIS:CB	1:a:2293:MET:HE2	2.24	0.67
3:c:2041:ARG:HB2	23:c:2486:CLA:HED3	1.75	0.67
3:c:2123:ALA:CB	19:z:2047:TRP:HH2	2.07	0.67
3:c:2443:TRP:CE3	3:c:2443:TRP:HA	2.30	0.67
27:c:2488:BCR:HC22	19:z:2009:LEU:HD11	1.75	0.67
24:A:351:PHO:NC	4:D:209:LEU:HD12	2.09	0.67
2:B:326:ARG:NH1	2:B:327:THR:CB	2.56	0.67
3:C:141:GLU:HB3	3:C:144:SER:OG	1.93	0.67
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.76	0.67
3:C:305:THR:CA	3:C:423:ARG:NH1	2.57	0.67
19:Z:48:ILE:O	19:Z:52:LEU:HG	1.95	0.67
2:b:2414:PRO:CG	2:b:2415:PRO:HD3	2.25	0.67
3:c:2050:LEU:O	3:c:2054:VAL:HG23	1.95	0.67
15:u:2059:ASN:ND2	15:u:2059:ASN:H	1.73	0.67
2:B:266:GLU:O	2:B:266:GLU:HG2	1.93	0.67
3:C:141:GLU:HB2	3:C:144:SER:HB2	1.75	0.67
3:C:282:MET:HA	3:C:285:ILE:CG1	2.24	0.67
4:D:108:GLY:O	4:D:110:LEU:N	2.27	0.67
10:K:34:VAL:O	10:K:34:VAL:HG12	1.93	0.67
1:a:2225:ARG:CB	2:b:2481:GLY:C	2.64	0.67
2:b:2364:GLU:HB2	4:d:2326:ARG:HH12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2216:SER:O	3:c:2221:GLU:O	2.12	0.67
3:c:2257:PHE:O	3:c:2261:ARG:HG3	1.94	0.67
4:d:2108:GLY:O	4:d:2110:LEU:N	2.28	0.67
16:v:2037:CYS:O	16:v:2039:SER:N	2.27	0.67
1:A:75:ASN:ND2	1:A:79:THR:CG2	2.57	0.67
2:B:86:ILE:O	2:B:86:ILE:HG22	1.94	0.67
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.09	0.67
4:D:108:GLY:C	4:D:110:LEU:H	2.02	0.67
13:O:168:TYR:CE1	13:O:172:ILE:HD11	2.29	0.67
3:c:2208:VAL:HG13	3:c:2209:ILE:N	2.09	0.67
5:e:2056:ALA:O	5:e:2057:GLN:C	2.37	0.67
15:u:2061:ASN:HB3	15:u:2126:ASP:O	1.93	0.67
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.24	0.67
5:E:26:ILE:CG1	5:E:27:PRO:HD3	2.25	0.67
13:O:125:LEU:HD12	13:O:145:GLU:O	1.93	0.67
2:b:2229:LEU:O	2:b:2230:ARG:C	2.38	0.67
4:d:2236:ASN:HB2	4:d:2237:PRO:HD2	1.76	0.67
4:d:2342:PRO:HG2	4:d:2345:VAL:HG21	1.77	0.67
13:o:2110:MET:H	13:o:2110:MET:HE2	1.60	0.67
2:B:324:LEU:HD12	11:L:34:TYR:HB3	1.77	0.67
2:B:414:PRO:CD	2:B:415:PRO:HD3	2.24	0.67
3:C:291:TRP:HB3	3:C:292:PHE:CD2	2.29	0.67
3:C:419:PHE:O	3:C:420:VAL:HG23	1.95	0.67
13:O:243:ILE:O	13:O:244:GLU:HB2	1.95	0.67
1:a:2255:PHE:HD2	1:a:2264:SER:HA	1.60	0.67
2:b:2268:PHE:HB2	2:b:2448:ARG:HE	1.59	0.67
3:c:2070:PHE:O	3:c:2073:ALA:HB3	1.95	0.67
3:c:2343:ARG:C	3:c:2343:ARG:CD	2.68	0.67
4:d:2274:VAL:CB	4:d:2275:PRO:HD3	2.22	0.67
13:o:2092:SER:HB2	13:o:2129:THR:O	1.95	0.67
1:A:141:PRO:HG3	3:C:446:GLY:O	1.94	0.67
28:E:84:HEC:HAC	6:F:26:ALA:HB1	1.75	0.67
6:F:40:GLN:HE21	9:J:27:LEU:HG	1.55	0.67
1:a:2069:GLY:O	1:a:2081:ALA:HA	1.95	0.67
1:a:2284:TRP:CE3	3:c:2435:PHE:HZ	2.13	0.67
2:b:2326:ARG:NH1	2:b:2327:THR:CB	2.57	0.67
3:c:2455:PHE:CE1	4:d:2224:GLN:HA	2.28	0.67
13:o:2075:THR:HG23	13:o:2103:PHE:CE2	2.30	0.67
3:C:131:TYR:HE1	3:C:135:ARG:HD3	1.60	0.66
13:O:164:LEU:H	13:O:188:LYS:HE2	1.60	0.66
4:d:2071:CYS:HB2	4:d:2076:VAL:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:2016:LEU:HB3	10:k:2017:PRO:CD	2.25	0.66
1:A:180:PHE:CE2	4:D:192:THR:HG22	2.31	0.66
1:A:290:ILE:HD11	23:A:348:CLA:CGD	2.25	0.66
5:E:56:ALA:O	5:E:57:GLN:C	2.37	0.66
14:T:3:THR:O	14:T:5:THR:N	2.28	0.66
1:a:2184:ILE:CG2	1:a:2328:MET:HE3	2.25	0.66
4:d:2029:PHE:C	4:d:2029:PHE:CD2	2.73	0.66
23:A:348:CLA:H192	25:D:357:PL9:H252	1.77	0.66
2:B:380:ASP:OD1	2:B:390:TYR:HB2	1.95	0.66
13:o:2050:PHE:HZ	13:o:2076:THR:HG23	1.59	0.66
13:o:2071:VAL:HG21	13:o:2108:VAL:HG23	1.76	0.66
1:A:222:SER:O	1:A:246:TYR:HB2	1.96	0.66
1:A:255:PHE:HD2	1:A:264:SER:HA	1.60	0.66
3:C:37:ALA:HA	23:C:483:CLA:O1A	1.95	0.66
3:C:103:GLY:O	3:C:104:GLU:C	2.39	0.66
13:O:140:THR:CG2	13:O:201:VAL:HB	2.24	0.66
13:O:164:LEU:CD2	15:U:42:VAL:HG13	2.25	0.66
1:a:2263:ALA:HB1	25:a:2352:PL9:H151	1.77	0.66
2:b:2357:ARG:HH22	4:d:2337:GLU:HB3	1.60	0.66
11:l:2036:PHE:HE2	12:m:2008:LEU:N	1.93	0.66
2:b:2006:TYR:OH	12:m:2021:PHE:HZ	1.79	0.66
2:b:2058:GLN:O	2:b:2329:PRO:HB2	1.95	0.66
2:b:2192:PRO:HG3	7:h:2048:TYR:CD1	2.31	0.66
23:b:2513:CLA:H91	23:b:2516:CLA:HAA1	1.78	0.66
3:c:2343:ARG:HB3	13:o:2078:LEU:HD12	1.77	0.66
5:e:2014:THR:HG21	9:j:2008:ILE:HG13	1.77	0.66
2:B:58:GLN:O	2:B:329:PRO:CB	2.43	0.66
3:C:450:ALA:HB1	3:C:455:PHE:O	1.96	0.66
13:O:102:ASP:OD2	13:O:119:LEU:HD11	1.96	0.66
16:V:78:ASN:HB2	16:V:96:ARG:HH11	1.60	0.66
1:a:2307:ILE:O	1:a:2309:ALA:N	2.28	0.66
3:c:2343:ARG:HA	3:c:2348:GLU:O	1.95	0.66
4:d:2067:TYR:C	6:f:2039:MET:HE1	2.21	0.66
15:u:2055:ILE:HD11	15:u:2068:TYR:CE1	2.29	0.66
15:U:39:LEU:O	15:U:41:ASN:N	2.28	0.66
3:c:2293:ASN:OD1	3:c:2423:ARG:NH2	2.28	0.66
11:l:2032:SER:OG	14:t:2006:TYR:CE2	2.47	0.66
13:o:2027:ARG:C	13:o:2029:ALA:H	2.03	0.66
19:z:2005:PHE:CZ	19:z:2054:VAL:HG13	2.30	0.66
1:A:214:MET:HE1	4:D:142:ASN:OD1	1.95	0.66
2:B:58:GLN:O	2:B:329:PRO:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:LEU:CA	6:F:39:MET:HE1	2.25	0.66
5:E:12:ILE:HD13	28:E:84:HEC:O1A	1.95	0.66
1:a:2029:TYR:HE1	1:a:2031:GLY:HA3	1.61	0.66
2:b:2171:PRO:HD3	7:h:2064:LEU:HD11	1.76	0.66
2:b:2321:LYS:CE	2:b:2325:PHE:HZ	2.09	0.66
19:z:2008:ALA:O	19:z:2011:ALA:HB3	1.96	0.66
3:C:443:TRP:HA	3:C:443:TRP:HE3	1.61	0.66
5:E:19:TRP:CZ2	9:J:13:VAL:HG22	2.30	0.66
15:U:88:VAL:HG22	15:U:114:VAL:HG23	1.78	0.66
19:Z:7:LEU:O	19:Z:11:ALA:HB2	1.95	0.66
4:d:2350:ASN:HD22	4:d:2351:ALA:H	1.44	0.66
19:z:2013:VAL:HG12	19:z:2014:ILE:N	2.11	0.66
1:A:301:ASN:CG	3:C:407:VAL:HG21	2.19	0.66
4:D:189:HIS:ND1	4:D:294:ARG:NE	2.43	0.66
13:O:118:LEU:HD13	13:O:233:VAL:HG11	1.78	0.66
13:o:2044:CYS:HB3	13:o:2240:TYR:HB3	1.77	0.66
13:o:2180:GLU:HG3	13:o:2181:GLU:N	2.11	0.66
2:B:92:SER:O	2:B:96:VAL:HG23	1.96	0.65
3:C:208:VAL:HG13	3:C:209:ILE:N	2.10	0.65
3:C:380:ILE:HG22	3:C:381:LYS:N	2.10	0.65
1:a:2330:VAL:HG21	4:d:2328:TRP:CZ2	2.31	0.65
3:c:2162:GLY:HA2	3:c:2248:GLY:HA2	1.79	0.65
1:A:119:PHE:O	1:A:123:ALA:HB2	1.96	0.65
3:C:42:LEU:HD13	23:C:486:CLA:HMA2	1.78	0.65
4:D:14:TRP:HA	4:D:17:ILE:HD12	1.78	0.65
8:I:18:LEU:N	8:I:18:LEU:HD23	2.10	0.65
16:V:76:MET:HE3	28:V:138:HEC:HMB2	1.78	0.65
2:b:2144:PHE:CE1	2:b:2210:ILE:HG23	2.29	0.65
2:b:2154:GLY:HA2	2:b:2158:LEU:HD12	1.78	0.65
3:c:2437:PHE:HA	23:c:2483:CLA:CMC	2.26	0.65
4:d:2274:VAL:HB	4:d:2275:PRO:CD	2.21	0.65
1:A:29:TYR:CE1	1:A:31:GLY:N	2.63	0.65
1:A:219:VAL:HG11	4:D:268:HIS:CD2	2.30	0.65
4:D:180:ARG:C	4:D:180:ARG:HD3	2.21	0.65
1:a:2341:LEU:HD21	15:u:2134:LYS:NZ	2.12	0.65
2:b:2138:MET:CG	23:b:2522:CLA:HBC2	2.20	0.65
3:c:2199:ILE:HG23	3:c:2231:GLU:HG2	1.78	0.65
10:k:2019:ILE:HG22	10:k:2022:LEU:HD12	1.77	0.65
13:o:2143:LYS:CE	13:o:2198:SER:HB2	2.26	0.65
15:u:2039:LEU:O	15:u:2041:ASN:N	2.26	0.65
19:z:2002:THR:O	19:z:2006:GLN:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD13	1:A:285:PHE:CD1	2.31	0.65
2:B:84:THR:O	2:B:84:THR:HG22	1.95	0.65
3:C:108:THR:HG23	10:K:2:LEU:HD23	1.79	0.65
3:C:320:ARG:HH12	16:V:50:PRO:CD	2.10	0.65
13:O:112:GLY:C	13:O:114:GLU:H	2.03	0.65
13:O:158:ASP:HB2	13:O:159:PRO:HD2	1.78	0.65
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.27	0.65
1:a:2097:TRP:HZ3	8:i:2008:VAL:HG21	1.61	0.65
1:a:2143:ILE:HD12	4:d:2252:PHE:CE2	2.31	0.65
1:a:2184:ILE:HG22	1:a:2328:MET:CE	2.27	0.65
2:b:2185:TRP:CD1	2:b:2185:TRP:H	2.12	0.65
4:d:2302:GLU:OE2	13:o:2173:ALA:HB2	1.96	0.65
4:D:210:LEU:HD13	4:D:271:MET:HG2	1.79	0.65
7:H:27:THR:N	7:H:28:PRO:HD2	2.10	0.65
13:O:27:ARG:HG3	13:O:29:ALA:HB3	1.77	0.65
1:a:2214:MET:HE1	4:d:2142:ASN:OD1	1.97	0.65
1:a:2295:PHE:HB3	3:c:2291:TRP:CZ3	2.32	0.65
4:d:2016:ASP:O	4:d:2019:ASP:HB3	1.96	0.65
1:A:29:TYR:HE1	1:A:31:GLY:N	1.95	0.65
3:C:249:ILE:HA	3:C:252:ILE:HD12	1.78	0.65
15:U:72:TYR:HD2	15:U:73:PRO:N	1.93	0.65
1:a:2045:THR:HG22	1:a:2046:ILE:N	2.11	0.65
26:d:2359:LMT:H21	7:h:2060:SER:HB3	1.78	0.65
10:k:2006:TYR:O	10:k:2007:ALA:C	2.40	0.65
2:B:229:LEU:O	2:B:230:ARG:C	2.40	0.65
13:O:128:SER:O	13:O:142:PHE:HA	1.96	0.65
1:a:2258:LEU:O	4:d:2128:ARG:NH2	2.30	0.65
3:c:2322:GLN:HA	3:c:2322:GLN:HE21	1.62	0.65
4:d:2052:THR:CG2	4:d:2067:TYR:HE1	2.08	0.65
4:d:2103:ARG:HH11	5:e:2072:LYS:CG	2.05	0.65
13:o:2140:THR:HB	13:o:2201:VAL:HG23	1.79	0.65
2:B:414:PRO:CG	2:B:415:PRO:HD3	2.26	0.65
3:C:243:ILE:O	23:C:474:CLA:HMC1	1.97	0.65
8:I:17:LEU:O	8:I:21:PHE:HB2	1.96	0.65
1:a:2159:LEU:HD21	23:c:2487:CLA:HBD	1.79	0.65
3:c:2297:TYR:CD2	3:c:2302:TYR:HE1	2.15	0.65
11:l:2018:TYR:CE2	14:t:2020:ALA:HA	2.31	0.65
15:u:2058:ASN:HD21	15:u:2114:VAL:HG13	1.61	0.65
2:B:280:PHE:CZ	2:B:312:TYR:HB3	2.32	0.65
4:D:28:VAL:HB	6:F:17:VAL:HG13	1.79	0.65
1:a:2317:TRP:CA	4:d:2063:LEU:HD13	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2334:ARG:HH12	13:o:2159:PRO:HA	1.62	0.65
2:b:2012:LEU:HD11	2:b:2018:ARG:C	2.22	0.65
4:d:2122:LEU:HD21	23:d:2354:CLA:C9	2.26	0.65
1:A:97:TRP:HZ3	8:I:8:VAL:HG21	1.62	0.65
1:A:221:SER:HB3	4:D:138:VAL:HG12	1.78	0.65
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.11	0.65
3:C:61:VAL:HG22	23:C:480:CLA:CAC	2.25	0.65
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.79	0.65
10:K:25:ALA:HB1	27:K:50:BCR:C19	2.27	0.65
13:O:152:ARG:NH1	13:O:156:PHE:CZ	2.65	0.65
4:d:2053:THR:HA	4:d:2067:TYR:CD1	2.32	0.65
4:d:2168:PHE:C	4:d:2168:PHE:CD2	2.75	0.65
13:o:2040:ILE:HG22	13:o:2041:ALA:N	2.12	0.65
13:o:2110:MET:H	13:o:2110:MET:CE	2.10	0.65
2:B:238:LEU:O	2:B:242:ILE:HG13	1.97	0.64
23:B:520:CLA:H161	12:M:17:VAL:HG11	1.79	0.64
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.78	0.64
7:H:49:ASN:OD1	7:H:49:ASN:O	2.15	0.64
1:a:2334:ARG:HH22	13:o:2159:PRO:CA	2.10	0.64
2:b:2006:TYR:HH	12:m:2021:PHE:HZ	1.42	0.64
3:c:2284:PHE:HD1	3:c:2434:ALA:HB1	1.61	0.64
23:c:2475:CLA:HBD	27:j:2053:BCR:HC21	1.79	0.64
4:d:2168:PHE:C	4:d:2168:PHE:HD2	2.04	0.64
10:k:2034:VAL:HG12	10:k:2034:VAL:O	1.97	0.64
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.78	0.64
3:C:293:ASN:OD1	3:C:297:TYR:O	2.15	0.64
11:L:1:MET:C	11:L:3:PRO:HD2	2.23	0.64
1:a:2198:HIS:HA	1:a:2286:THR:HG23	1.79	0.64
2:b:2058:GLN:O	2:b:2329:PRO:CB	2.46	0.64
3:c:2320:ARG:NH2	15:u:2128:TYR:CE2	2.64	0.64
4:d:2194:ASN:OD1	4:d:2195:PRO:HD2	1.98	0.64
2:B:154:GLY:HA2	2:B:158:LEU:HD12	1.79	0.64
1:a:2180:PHE:CD2	4:d:2192:THR:HB	2.33	0.64
2:b:2135:LEU:HD23	2:b:2138:MET:SD	2.37	0.64
3:c:2285:ILE:CA	23:c:2487:CLA:HMB3	2.27	0.64
3:c:2292:PHE:HE1	23:c:2487:CLA:HBC3	1.63	0.64
4:d:2325:ILE:HG22	4:d:2329:MET:HE2	1.80	0.64
13:o:2075:THR:CG2	13:o:2103:PHE:HD2	2.10	0.64
4:D:52:THR:HG22	4:D:67:TYR:CE1	2.26	0.64
9:J:15:THR:HA	27:K:50:BCR:C37	2.27	0.64
10:K:6:TYR:O	10:K:7:ALA:C	2.41	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:27:ARG:C	13:O:29:ALA:H	2.04	0.64
15:U:132:LEU:N	15:U:132:LEU:CD2	2.57	0.64
1:a:2142:TRP:N	4:d:2220:ASN:OD1	2.30	0.64
1:a:2220:THR:O	1:a:2223:LEU:HG	1.97	0.64
2:b:2122:LEU:HD12	23:b:2525:CLA:HMA2	1.79	0.64
3:c:2067:MET:O	3:c:2071:GLU:HG3	1.97	0.64
13:o:2047:PRO:CG	13:o:2076:THR:HG21	2.19	0.64
13:o:2071:VAL:CG2	13:o:2108:VAL:HG23	2.27	0.64
13:o:2121:THR:HG22	13:o:2219:GLN:CD	2.23	0.64
13:o:2158:ASP:HB2	13:o:2159:PRO:HD2	1.78	0.64
1:A:285:PHE:O	1:A:288:LEU:HB2	1.97	0.64
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.29	0.64
23:B:513:CLA:H91	23:B:516:CLA:HAA1	1.77	0.64
23:B:520:CLA:H161	12:M:17:VAL:CG1	2.27	0.64
6:F:40:GLN:NE2	9:J:27:LEU:CG	2.46	0.64
4:d:2066:SER:HA	4:d:2076:VAL:HG13	1.79	0.64
4:d:2190:ASN:HB2	4:d:2296:TYR:CD1	2.32	0.64
7:h:2059:VAL:O	7:h:2059:VAL:CG1	2.46	0.64
14:t:2010:PHE:CD2	14:t:2014:ILE:HD11	2.32	0.64
1:A:221:SER:HB3	4:D:138:VAL:CG1	2.27	0.64
3:C:349:ILE:C	3:C:350:ILE:HG13	2.22	0.64
6:F:25:LEU:O	6:F:28:PRO:HD2	1.98	0.64
10:K:9:PHE:O	10:K:13:VAL:HG23	1.96	0.64
11:L:2:GLU:N	11:L:3:PRO:CD	2.61	0.64
12:M:28:GLN:HB2	12:m:2027:VAL:CG1	2.28	0.64
13:O:20:PRO:HB2	13:O:240:TYR:CE1	2.33	0.64
13:O:66:VAL:HG13	13:O:67:PRO:HD2	1.80	0.64
13:o:2007:TYR:O	13:o:2011:VAL:HG23	1.96	0.64
2:B:478:VAL:HG12	4:D:139:ARG:HG2	1.80	0.64
3:C:42:LEU:HG	23:C:486:CLA:CED	2.24	0.64
3:C:319:ILE:CD1	3:C:389:GLU:HG2	2.28	0.64
4:D:57:SER:OG	4:D:65:SER:HB2	1.98	0.64
5:E:59:GLN:HE21	5:E:81:GLN:NE2	1.96	0.64
1:a:2206:PHE:HD2	24:d:2356:PHO:CBB	2.11	0.64
2:b:2234:ILE:O	2:b:2236:THR:N	2.31	0.64
2:b:2327:THR:OG1	27:b:2528:BCR:H401	1.97	0.64
3:c:2443:TRP:HA	3:c:2443:TRP:HE3	1.62	0.64
4:d:2088:SER:HB3	5:e:2068:ARG:HH21	1.63	0.64
2:B:12:LEU:HD11	2:B:18:ARG:C	2.23	0.64
2:B:130:GLU:HG2	2:B:131:PRO:CD	2.26	0.64
2:B:138:MET:CG	23:B:522:CLA:HBC2	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:THR:OG1	2:B:274:GLN:HG3	1.97	0.64
4:D:281:MET:HE2	4:D:281:MET:HA	1.80	0.64
1:a:2224:ILE:HG13	1:a:2245:THR:O	1.97	0.64
1:a:2235:TYR:HA	4:d:2265:ARG:NH2	2.13	0.64
2:b:2263:THR:HG22	2:b:2448:ARG:NH2	2.12	0.64
3:c:2243:ILE:O	23:c:2474:CLA:HMC1	1.96	0.64
3:c:2376:ASP:O	3:c:2380:ILE:HG13	1.97	0.64
4:d:2171:PRO:HG3	4:d:2181:PHE:CE1	2.32	0.64
5:e:2014:THR:CG2	9:j:2008:ILE:CD1	2.75	0.64
16:v:2100:ILE:C	16:v:2102:PRO:HD3	2.23	0.64
1:A:310:LYS:HB3	1:A:312:ASN:ND2	2.13	0.64
10:K:2:LEU:N	10:K:3:PRO:CD	2.60	0.64
3:c:2342:MET:HE3	3:c:2352:GLY:HA3	1.78	0.64
3:c:2350:ILE:HG22	3:c:2351:PHE:N	2.12	0.64
3:c:2426:LEU:O	3:c:2430:HIS:HB2	1.97	0.64
4:d:2190:ASN:ND2	4:d:2193:LEU:HD12	2.13	0.64
7:h:2027:THR:N	7:h:2028:PRO:HD2	2.13	0.64
2:B:73:GLY:O	2:B:92:SER:HB2	1.98	0.64
3:C:162:GLY:O	3:C:165:LEU:HB2	1.95	0.64
1:a:2057:PRO:HB3	1:a:2068:SER:HB3	1.79	0.64
2:b:2380:ASP:OD1	2:b:2390:TYR:CB	2.45	0.64
3:c:2067:MET:HE2	3:c:2067:MET:HA	1.80	0.64
3:c:2189:TRP:NE1	3:c:2295:THR:OG1	2.30	0.64
7:h:2039:VAL:O	7:h:2043:ILE:HG13	1.98	0.64
19:z:2019:MET:HE1	19:z:2043:GLY:HA3	1.78	0.64
1:A:159:LEU:HG	1:A:163:ILE:CD1	2.28	0.63
2:B:405:GLU:HB3	13:o:2059:LYS:HB3	1.80	0.63
8:I:27:ASP:HB2	8:I:28:PRO:HD3	1.80	0.63
19:Z:47:TRP:CD1	19:Z:47:TRP:C	2.76	0.63
1:a:2173:PRO:HG3	1:a:2178:GLY:C	2.23	0.63
2:b:2324:LEU:HD12	11:l:2034:TYR:HB3	1.79	0.63
4:d:2052:THR:HG22	4:d:2067:TYR:CE1	2.33	0.63
1:A:281:VAL:HA	1:A:284:TRP:CD1	2.33	0.63
3:C:305:THR:CA	3:C:423:ARG:HH12	2.11	0.63
3:C:348:GLU:OE1	3:C:348:GLU:N	2.31	0.63
4:D:263:ASN:O	4:D:265:ARG:N	2.31	0.63
1:a:2063:ILE:HG22	3:c:2335:THR:CG2	2.29	0.63
1:a:2290:ILE:HD11	23:a:2348:CLA:OBD	1.98	0.63
2:b:2257:TRP:CZ3	4:d:2291:LEU:HD22	2.33	0.63
2:B:221:PRO:HB3	2:B:225:LEU:HB2	1.78	0.63
3:C:426:LEU:O	3:C:430:HIS:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:39:ARG:CA	13:O:245:PRO:HG3	2.28	0.63
13:O:59:LYS:HB3	2:b:2405:GLU:HB3	1.80	0.63
13:O:155:ASN:HD22	15:U:129:ASN:HD21	1.42	0.63
13:O:238:VAL:HG12	13:O:239:PHE:N	2.12	0.63
1:a:2243:GLU:CA	4:d:2240:ALA:HB1	2.27	0.63
1:a:2283:VAL:HG21	24:a:2350:PHO:HBC3	1.79	0.63
1:a:2322:ASN:OD1	3:c:2412:THR:HG23	1.99	0.63
1:a:2342:ASP:O	1:a:2343:LEU:HD23	1.98	0.63
23:a:2348:CLA:H192	25:d:2358:PL9:H252	1.80	0.63
2:B:221:PRO:CG	2:B:225:LEU:HD12	2.29	0.63
2:B:326:ARG:NH1	2:B:327:THR:HB	2.13	0.63
12:M:27:VAL:CG1	12:m:2028:GLN:HB2	2.28	0.63
1:a:2037:MET:SD	1:a:2126:TYR:HA	2.37	0.63
1:a:2119:PHE:O	1:a:2123:ALA:HB2	1.99	0.63
4:d:2110:LEU:O	4:d:2113:PHE:HB3	1.98	0.63
4:d:2138:VAL:CG1	4:d:2139:ARG:N	2.60	0.63
1:A:29:TYR:HD2	1:A:133:LEU:HD12	1.63	0.63
4:D:39:PRO:O	4:D:43:LEU:HG	1.99	0.63
1:a:2061:ASP:HA	1:a:2087:ASN:HB2	1.81	0.63
2:b:2127:ARG:HG3	2:b:2127:ARG:NH1	2.11	0.63
3:c:2282:MET:HG2	23:c:2479:CLA:H62	1.79	0.63
13:o:2201:VAL:CG1	13:o:2211:ILE:HG23	2.29	0.63
1:A:63:ILE:HG23	3:C:335:THR:CG2	2.28	0.63
1:A:206:PHE:HE1	23:A:348:CLA:CMB	2.11	0.63
3:C:160:ILE:O	3:C:163:PHE:HB2	1.98	0.63
8:I:19:PHE:CZ	8:I:23:PHE:HE1	2.16	0.63
1:a:2029:TYR:CD1	1:a:2029:TYR:C	2.77	0.63
3:c:2450:ALA:HB1	3:c:2455:PHE:O	1.99	0.63
7:h:2057:VAL:O	7:h:2057:VAL:CG1	2.46	0.63
19:Z:46:LEU:O	19:Z:50:LEU:HG	1.99	0.63
2:b:2221:PRO:HB3	2:b:2225:LEU:HB2	1.79	0.63
3:c:2213:LEU:HD11	23:c:2474:CLA:H171	1.81	0.63
4:D:52:THR:HG23	4:D:76:VAL:HG12	1.81	0.63
4:D:222:LEU:HA	4:D:243:THR:O	1.98	0.63
4:D:253:TRP:HA	4:D:253:TRP:CE3	2.33	0.63
8:I:25:SER:HB2	8:I:28:PRO:HD2	1.80	0.63
16:V:75:TYR:HE2	16:V:80:THR:N	1.95	0.63
1:a:2180:PHE:N	1:a:2180:PHE:HD1	1.97	0.63
5:e:2012:ILE:HD13	28:e:2084:HEC:O1A	1.99	0.63
10:k:2002:LEU:N	10:k:2003:PRO:CD	2.60	0.63
13:o:2137:THR:O	13:o:2140:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD2	1:A:63:ILE:O	2.17	0.63
2:B:327:THR:OG1	27:B:529:BCR:H401	1.99	0.63
2:B:341:LYS:HZ2	13:o:2060:ARG:HH12	1.47	0.63
4:D:42:TYR:CZ	6:F:24:THR:HG23	2.33	0.63
15:U:113:THR:HG22	15:U:114:VAL:N	2.13	0.63
1:a:2306:VAL:CG2	1:a:2307:ILE:H	2.11	0.63
2:b:2190:PHE:HZ	7:h:2040:PHE:HE1	1.47	0.63
3:C:119:LEU:O	3:C:122:SER:OG	2.17	0.62
4:D:298:PHE:CA	11:L:37:ASN:ND2	2.54	0.62
12:M:8:LEU:HD22	14:T:1:MET:CE	2.29	0.62
1:a:2195:HIS:ND1	1:a:2196:PRO:HD2	2.13	0.62
2:b:2479:PHE:HD2	2:b:2479:PHE:C	2.07	0.62
3:c:2078:GLU:HB3	16:v:2102:PRO:HB3	1.79	0.62
13:o:2083:GLY:HA3	13:o:2095:PHE:CZ	2.33	0.62
1:A:322:ASN:OD1	3:C:412:THR:HG23	1.99	0.62
3:C:120:ILE:HG21	27:C:489:BCR:H353	1.81	0.62
3:C:370:ARG:HD3	3:C:375:LEU:CD2	2.29	0.62
27:C:489:BCR:H312	19:Z:55:GLY:HA2	1.81	0.62
5:E:12:ILE:HD11	28:E:84:HEC:O1A	1.99	0.62
16:V:102:PRO:HA	16:V:105:ARG:HG3	1.81	0.62
1:a:2095:PRO:HG2	1:a:2098:GLU:HB2	1.80	0.62
1:a:2259:ILE:HG22	1:a:2260:PHE:CD2	2.34	0.62
2:b:2327:THR:C	2:b:2329:PRO:HD3	2.23	0.62
3:c:2349:ILE:C	3:c:2350:ILE:HG13	2.24	0.62
27:c:2488:BCR:H341	27:k:2050:BCR:HC31	1.80	0.62
15:u:2126:ASP:OD1	15:u:2127:ARG:N	2.31	0.62
1:A:161:TYR:CE1	1:A:186:PHE:HE1	2.17	0.62
23:A:350:CLA:HED1	4:D:175:VAL:CG1	2.29	0.62
2:B:106:LEU:HD22	23:B:522:CLA:H143	1.80	0.62
2:B:234:ILE:O	2:B:236:THR:N	2.32	0.62
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.67	0.62
3:c:2157:MET:HE2	3:c:2160:ILE:HD12	1.81	0.62
15:u:2061:ASN:HD22	15:u:2061:ASN:N	1.95	0.62
2:B:225:LEU:HD13	2:B:231:MET:SD	2.38	0.62
23:B:520:CLA:HAA2	23:B:520:CLA:HBD	1.81	0.62
3:C:70:PHE:O	3:C:73:ALA:HB3	1.99	0.62
4:D:56:THR:HG23	4:D:56:THR:O	1.98	0.62
1:a:2237:TYR:HA	1:a:2241:GLN:NE2	2.14	0.62
4:d:2058:TRP:HA	4:d:2062:GLY:H	1.63	0.62
9:j:2040:LEU:HD21	16:v:2118:HIS:CE1	2.34	0.62
1:A:180:PHE:HE2	4:D:192:THR:O	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:HE1	4:D:245:SER:HA	1.61	0.62
3:c:2291:TRP:HB3	3:c:2292:PHE:CD2	2.34	0.62
3:c:2292:PHE:CE1	23:c:2487:CLA:HBC3	2.34	0.62
23:c:2486:CLA:H172	19:z:2023:VAL:HG21	1.81	0.62
4:d:2244:TYR:OH	4:d:2264:LYS:NZ	2.24	0.62
1:A:141:PRO:HG3	3:C:446:GLY:C	2.24	0.62
1:A:309:ALA:HB1	16:V:1:ALA:O	2.00	0.62
10:K:15:VAL:HG21	18:N:9:UNK:O	1.99	0.62
12:M:5:GLN:HG2	12:m:2005:GLN:HG2	1.80	0.62
13:O:162:ARG:O	13:O:162:ARG:CG	2.48	0.62
19:Z:37:LYS:O	19:Z:41:PHE:CD1	2.52	0.62
1:a:2142:TRP:HE1	3:c:2443:TRP:HH2	1.47	0.62
2:b:2069:LEU:HD12	23:b:2518:CLA:HBA2	1.81	0.62
3:c:2053:HIS:ND1	23:c:2478:CLA:H141	2.15	0.62
3:c:2308:GLU:OE2	3:c:2361:PHE:CZ	2.50	0.62
5:e:2009:PHE:O	5:e:2010:SER:CB	2.47	0.62
2:B:323:GLY:HA2	4:D:293:LEU:HG	1.81	0.62
3:C:94:THR:C	3:C:96:GLY:H	2.07	0.62
1:a:2041:LEU:HD21	1:a:2122:GLY:CA	2.30	0.62
2:b:2348:ASN:CG	2:b:2349:LYS:H	2.05	0.62
23:c:2477:CLA:HMD2	23:c:2485:CLA:HAB	1.80	0.62
4:d:2087:HIS:CD2	4:d:2087:HIS:N	2.68	0.62
11:l:2002:GLU:N	11:l:2003:PRO:CD	2.63	0.62
16:v:2052:LEU:HD23	28:v:2138:HEC:HAD2	1.81	0.62
3:C:216:SER:O	3:C:221:GLU:O	2.18	0.62
3:C:320:ARG:NH1	16:V:49:ASN:HA	2.15	0.62
4:D:186:GLN:HA	4:D:186:GLN:NE2	2.14	0.62
10:K:10:ASP:HB3	10:K:11:PRO:HD3	1.81	0.62
13:O:168:TYR:CD1	13:O:172:ILE:HD11	2.35	0.62
1:a:2093:PHE:CE1	1:a:2095:PRO:HG3	2.35	0.62
1:a:2142:TRP:NE1	3:c:2443:TRP:HH2	1.97	0.62
2:b:2383:PHE:O	13:o:2166:SER:HA	2.00	0.62
23:b:2521:CLA:CAB	23:b:2526:CLA:HED1	2.27	0.62
3:c:2095:LEU:HA	3:c:2185:LEU:HD12	1.80	0.62
3:c:2176:VAL:HG13	3:c:2234:VAL:HG13	1.82	0.62
3:c:2282:MET:HA	3:c:2285:ILE:CG1	2.28	0.62
4:d:2096:GLU:OE1	5:e:2068:ARG:HG2	1.99	0.62
11:l:2006:ASN:H	11:l:2006:ASN:HD22	1.48	0.62
16:v:2012:LEU:O	16:v:2070:GLU:HG3	1.99	0.62
19:z:2051:VAL:HG12	19:z:2052:LEU:CD2	2.29	0.62
1:A:180:PHE:HD1	1:A:180:PHE:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLN:HG3	1:A:262:TYR:N	2.13	0.62
2:B:479:PHE:HD2	2:B:479:PHE:C	2.07	0.62
4:D:268:HIS:HA	4:D:271:MET:HE3	1.82	0.62
5:E:12:ILE:HD13	28:E:84:HEC:CGA	2.30	0.62
13:O:11:VAL:HG12	13:O:11:VAL:O	2.00	0.62
15:U:57:LEU:CD2	15:U:112:PHE:HD2	1.95	0.62
1:a:2180:PHE:N	1:a:2180:PHE:CD1	2.68	0.62
1:a:2252:HIS:CE1	1:a:2264:SER:HG	2.14	0.62
3:c:2225:VAL:HG13	3:c:2294:ASN:HD21	1.62	0.62
23:c:2474:CLA:H8	23:c:2477:CLA:H143	1.82	0.62
9:j:2019:MET:SD	27:k:2050:BCR:H361	2.40	0.62
13:o:2108:VAL:HG22	13:o:2115:ARG:HG2	1.81	0.62
13:o:2224:ASP:C	13:o:2225:MET:HG2	2.21	0.62
2:B:29:LEU:HB3	27:B:528:BCR:H351	1.82	0.62
2:B:69:LEU:HD12	23:B:518:CLA:HBA2	1.82	0.62
27:B:528:BCR:HC8	27:B:528:BCR:H331	1.82	0.62
3:C:120:ILE:CG2	27:C:489:BCR:H353	2.30	0.62
3:C:169:GLY:HA2	3:C:241:GLY:HA2	1.81	0.62
3:C:284:PHE:O	3:C:285:ILE:C	2.42	0.62
4:D:168:PHE:HD2	4:D:168:PHE:C	2.08	0.62
16:V:129:LYS:CE	16:V:135:VAL:HG23	2.30	0.62
4:d:2048:TRP:CE3	24:d:2356:PHO:H161	2.35	0.62
4:d:2329:MET:HG2	4:d:2329:MET:O	2.00	0.62
13:o:2128:SER:O	13:o:2142:PHE:HA	2.00	0.62
1:A:237:TYR:CE2	1:A:245:THR:HA	2.35	0.61
1:A:335:ASN:C	1:A:335:ASN:HD22	2.08	0.61
23:B:524:CLA:H13	23:B:524:CLA:OBD	2.00	0.61
5:E:9:PHE:O	5:E:10:SER:CB	2.47	0.61
19:Z:44:SER:O	19:Z:48:ILE:HG22	2.00	0.61
1:a:2081:ALA:HB3	1:a:2174:LEU:O	2.01	0.61
2:b:2414:PRO:O	2:b:2418:LYS:HG3	1.99	0.61
23:b:2521:CLA:H201	4:d:2123:ILE:HD11	1.82	0.61
3:c:2223:TRP:HD1	3:c:2224:ILE:HG13	1.64	0.61
27:c:2489:BCR:H341	19:z:2051:VAL:HG13	1.81	0.61
4:d:2296:TYR:CG	4:d:2296:TYR:O	2.53	0.61
16:v:2080:THR:CG2	16:v:2084:GLY:HA2	2.29	0.61
3:C:38:GLY:HA2	3:C:41:ARG:HE	1.64	0.61
3:C:321:ASP:OD1	3:C:321:ASP:N	2.31	0.61
3:C:405:ASN:HB2	3:C:407:VAL:CG2	2.30	0.61
4:D:91:LEU:N	4:D:91:LEU:HD23	2.14	0.61
13:O:53:LYS:HE2	13:O:234:LYS:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2326:LEU:CD1	3:c:2412:THR:HG21	2.28	0.61
2:b:2235:GLU:HB3	2:b:2473:THR:OG1	2.00	0.61
2:b:2280:PHE:CZ	2:b:2312:TYR:HB3	2.35	0.61
27:b:2527:BCR:HC8	27:b:2527:BCR:H331	1.81	0.61
3:c:2169:GLY:HA2	3:c:2241:GLY:HA2	1.81	0.61
13:o:2233:VAL:HG12	13:o:2234:LYS:N	2.14	0.61
27:C:489:BCR:H341	19:Z:51:VAL:HG13	1.82	0.61
4:D:86:GLY:C	4:D:87:HIS:CD2	2.78	0.61
4:d:2014:TRP:HA	4:d:2017:ILE:HD12	1.81	0.61
4:d:2032:TRP:HA	4:d:2032:TRP:CE3	2.36	0.61
4:d:2342:PRO:HG2	4:d:2345:VAL:CG2	2.29	0.61
28:e:2084:HEC:C4A	6:f:2019:TRP:HH2	2.13	0.61
19:z:2044:SER:O	19:z:2048:ILE:HG22	2.00	0.61
1:A:89:ILE:HD12	1:A:108:ASN:HB3	1.83	0.61
2:B:479:PHE:C	2:B:479:PHE:CD2	2.78	0.61
4:D:29:PHE:C	4:D:29:PHE:HD2	2.08	0.61
5:E:12:ILE:CG1	28:E:84:HEC:O2D	2.47	0.61
13:O:50:PHE:HZ	13:O:76:THR:CG2	2.13	0.61
15:U:59:ASN:ND2	15:U:59:ASN:H	1.80	0.61
3:c:2151:TRP:C	3:c:2153:ASP:H	2.08	0.61
3:c:2227:VAL:HG23	3:c:2294:ASN:HB3	1.82	0.61
2:B:348:ASN:CG	2:B:349:LYS:H	2.07	0.61
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.31	0.61
13:O:102:ASP:O	13:O:103:PHE:CD1	2.53	0.61
13:O:163:GLY:CA	13:O:188:LYS:HE2	2.30	0.61
14:T:4:ILE:HG13	14:T:5:THR:N	2.15	0.61
1:a:2269:ARG:HD3	1:a:2270:SER:N	2.15	0.61
2:b:2057:ARG:CG	2:b:2057:ARG:NH1	2.64	0.61
1:A:114:LEU:CD1	1:A:118:HIS:CE1	2.84	0.61
2:B:135:LEU:HD23	2:B:138:MET:SD	2.40	0.61
27:C:489:BCR:C34	19:Z:51:VAL:HG13	2.31	0.61
13:O:94:THR:HA	13:O:127:ALA:O	2.01	0.61
2:b:2394:GLN:NE2	15:u:2052:GLY:HA3	2.16	0.61
3:c:2320:ARG:CZ	15:u:2128:TYR:CZ	2.83	0.61
27:c:2489:BCR:H312	19:z:2055:GLY:HA2	1.81	0.61
4:d:2106:GLN:HE21	5:e:2047:GLY:HA3	1.65	0.61
13:o:2238:VAL:HG12	13:o:2239:PHE:N	2.16	0.61
3:C:265:ILE:HG22	3:C:266:TRP:H	1.66	0.61
3:C:282:MET:HA	3:C:285:ILE:HB	1.83	0.61
3:C:283:GLY:HA3	3:C:434:ALA:HB2	1.81	0.61
13:O:40:ILE:CG2	13:O:41:ALA:H	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2034:GLY:HA2	1:a:2037:MET:HB3	1.83	0.61
1:a:2188:ALA:HB2	1:a:2328:MET:HE2	1.82	0.61
2:b:2057:ARG:NH1	2:b:2317:ASN:OD1	2.29	0.61
11:l:2024:ILE:CD1	12:m:2018:PRO:HB2	2.30	0.61
13:o:2039:ARG:CA	13:o:2245:PRO:HG3	2.30	0.61
13:o:2102:ASP:O	13:o:2103:PHE:CD1	2.53	0.61
2:B:271:THR:HG22	2:B:448:ARG:NH1	2.15	0.61
25:D:357:PL9:H401	27:b:2527:BCR:H382	1.82	0.61
15:U:82:ASN:O	15:U:85:TYR:HE2	1.84	0.61
1:a:2063:ILE:HG22	3:c:2335:THR:HG23	1.83	0.61
1:a:2224:ILE:HD11	1:a:2243:GLU:HG3	1.82	0.61
1:a:2306:VAL:CG2	1:a:2307:ILE:N	2.64	0.61
2:b:2014:ASN:OD1	11:l:2007:ARG:NH2	2.34	0.61
2:b:2302:TRP:O	2:b:2305:ILE:HG12	2.00	0.61
3:c:2265:ILE:HD11	3:c:2449:ARG:HH11	1.66	0.61
13:o:2124:ASN:HD22	13:o:2147:ASN:HB3	1.66	0.61
1:A:110:GLY:O	1:A:111:PRO:C	2.43	0.61
1:A:149:ALA:HA	1:A:284:TRP:CZ3	2.36	0.61
3:C:36:TRP:O	3:C:38:GLY:N	2.31	0.61
3:C:227:VAL:HG23	3:C:227:VAL:O	2.00	0.61
4:D:22:LEU:HD21	4:D:32:TRP:CE3	2.35	0.61
4:D:157:PHE:O	4:D:158:LEU:HD23	2.00	0.61
4:D:171:PRO:HG3	4:D:181:PHE:CE1	2.36	0.61
13:O:92:SER:HB2	13:O:129:THR:O	2.01	0.61
15:U:127:ARG:O	15:U:128:TYR:HD1	1.82	0.61
4:d:2186:GLN:NE2	4:d:2186:GLN:CA	2.62	0.61
4:d:2222:LEU:HA	4:d:2243:THR:O	2.00	0.61
4:d:2330:ALA:N	4:d:2331:PRO:HD3	2.15	0.61
13:o:2211:ILE:HG22	13:o:2212:ALA:H	1.65	0.61
16:v:2076:MET:O	16:v:2094:SER:HA	2.01	0.61
1:A:224:ILE:HG21	1:A:227:THR:OG1	2.01	0.61
1:A:306:VAL:CG2	1:A:307:ILE:H	2.13	0.61
3:C:39:ASN:HA	3:C:42:LEU:HD12	1.82	0.61
3:C:285:ILE:HG23	23:C:487:CLA:HMB3	1.81	0.61
3:C:333:GLY:O	3:C:335:THR:N	2.34	0.61
4:D:18:LEU:HA	17:X:41:SER:OG	2.01	0.61
13:O:137:THR:O	13:O:140:THR:HG23	2.01	0.61
1:a:2334:ARG:NH2	13:o:2159:PRO:HA	2.14	0.61
2:b:2174:LEU:O	2:b:2174:LEU:HG	2.01	0.61
3:c:2265:ILE:HG22	3:c:2266:TRP:N	2.16	0.61
4:d:2084:SER:HB2	5:e:2066:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2263:ASN:O	4:d:2265:ARG:N	2.34	0.61
1:A:180:PHE:CD2	4:D:192:THR:HB	2.37	0.60
1:A:322:ASN:O	1:A:326:LEU:HB2	2.00	0.60
2:B:136:PRO:CD	2:B:231:MET:HE1	2.27	0.60
3:C:272:LEU:O	3:C:276:LEU:HB2	2.00	0.60
4:D:83:ASN:ND2	4:D:83:ASN:O	2.34	0.60
13:O:95:PHE:HB2	13:O:127:ALA:HB3	1.81	0.60
23:b:2520:CLA:HAA2	23:b:2520:CLA:HBD	1.81	0.60
3:c:2289:PHE:CD1	23:c:2487:CLA:HBB2	2.35	0.60
4:d:2165:SER:O	4:d:2166:SER:HB3	2.01	0.60
13:o:2164:LEU:HG	13:o:2188:LYS:HB2	1.83	0.60
14:t:2021:ILE:C	14:t:2022:PHE:HD2	2.09	0.60
1:A:187:GLN:HG3	1:A:193:LEU:HG	1.83	0.60
2:B:57:ARG:NH1	2:B:57:ARG:CG	2.64	0.60
2:B:98:LEU:O	2:B:102:VAL:HG23	2.01	0.60
3:C:81:MET:HE2	3:C:90:PRO:HG3	1.83	0.60
4:D:68:LEU:N	6:F:39:MET:HE1	2.16	0.60
13:O:28:GLY:HA3	13:O:137:THR:CG2	2.30	0.60
1:a:2133:LEU:HD22	4:d:2256:ILE:HG13	1.83	0.60
1:a:2135:TYR:OH	8:i:2032:PRO:HG3	2.01	0.60
2:b:2046:ASP:HB3	2:b:2058:GLN:OE1	2.00	0.60
4:d:2323:GLU:HG2	13:o:2168:TYR:OH	2.01	0.60
2:B:321:LYS:HE3	2:B:325:PHE:HZ	1.66	0.60
3:C:433:LEU:O	3:C:437:PHE:HB2	2.02	0.60
23:C:486:CLA:H61	27:C:488:BCR:H393	1.83	0.60
2:b:2190:PHE:HZ	7:h:2040:PHE:CE1	2.20	0.60
2:b:2479:PHE:C	2:b:2479:PHE:CD2	2.79	0.60
3:c:2158:THR:HG22	3:c:2251:HIS:HB3	1.81	0.60
3:c:2333:GLY:O	3:c:2335:THR:N	2.34	0.60
4:d:2334:GLN:HB3	4:d:2336:HIS:NE2	2.13	0.60
13:o:2140:THR:HG22	13:o:2201:VAL:HB	1.82	0.60
1:A:214:MET:HE2	4:D:142:ASN:HD21	1.64	0.60
1:A:279:PRO:HG2	4:D:211:CYS:HB3	1.81	0.60
2:B:7:ARG:HA	23:B:523:CLA:O1A	2.01	0.60
4:D:253:TRP:HA	4:D:253:TRP:HE3	1.67	0.60
10:K:6:TYR:O	10:K:8:ILE:N	2.34	0.60
1:a:2162:PRO:HG3	1:a:2171:GLY:HA2	1.84	0.60
3:c:2071:GLU:OE1	3:c:2086:LEU:HB3	2.01	0.60
3:c:2101:PRO:CA	3:c:2195:ASP:HB3	2.32	0.60
3:c:2320:ARG:NE	15:u:2128:TYR:OH	2.35	0.60
1:A:96:ILE:HG22	8:I:1:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD22	1:A:245:THR:CG2	2.30	0.60
1:A:316:THR:O	1:A:317:TRP:C	2.43	0.60
2:B:399:VAL:HG23	2:B:417:VAL:HG13	1.83	0.60
3:C:95:LEU:HD21	23:C:479:CLA:OBD	2.01	0.60
3:C:275:SER:CB	23:C:485:CLA:HAA1	2.30	0.60
4:D:77:ALA:CB	4:D:174:GLY:HA3	2.31	0.60
4:D:138:VAL:CG1	4:D:139:ARG:N	2.65	0.60
4:D:168:PHE:C	4:D:168:PHE:CD2	2.79	0.60
4:D:188:PHE:N	4:D:188:PHE:CD1	2.69	0.60
4:D:196:PHE:HD1	4:D:285:GLY:HA2	1.66	0.60
11:L:23:LEU:O	11:L:27:LEU:HB2	2.01	0.60
1:a:2141:PRO:HG3	3:c:2446:GLY:O	2.01	0.60
2:b:2006:TYR:CE1	2:b:2008:VAL:HG21	2.37	0.60
3:c:2308:GLU:HG2	3:c:2361:PHE:CZ	2.35	0.60
1:A:261:GLN:HG3	1:A:262:TYR:H	1.66	0.60
2:B:123:PHE:CG	2:B:123:PHE:O	2.54	0.60
2:B:142:HIS:ND1	23:B:524:CLA:H142	2.16	0.60
3:C:78:GLU:OE1	3:C:78:GLU:HA	2.01	0.60
3:C:95:LEU:HA	3:C:185:LEU:HD12	1.84	0.60
23:C:486:CLA:H42	10:K:30:TRP:NE1	2.17	0.60
7:H:30:MET:O	7:H:33:PHE:N	2.35	0.60
13:O:95:PHE:HB3	13:O:127:ALA:CB	2.31	0.60
13:o:2233:VAL:CG1	13:o:2234:LYS:N	2.63	0.60
15:u:2075:LEU:O	15:u:2079:ILE:HG13	2.02	0.60
1:A:321:ILE:O	1:A:325:ASN:ND2	2.34	0.60
2:B:191:ASN:HB2	2:B:192:PRO:HD2	1.83	0.60
23:C:474:CLA:H8	23:C:477:CLA:H143	1.84	0.60
4:D:145:ALA:HB2	4:D:272:LEU:HD11	1.83	0.60
13:O:88:ASN:ND2	13:O:92:SER:OG	2.34	0.60
1:a:2041:LEU:CD2	1:a:2122:GLY:HA3	2.31	0.60
3:c:2320:ARG:NE	15:u:2128:TYR:CZ	2.70	0.60
3:c:2343:ARG:HD2	3:c:2343:ARG:O	2.00	0.60
8:i:2017:LEU:O	8:i:2021:PHE:HB2	2.01	0.60
16:v:2136:TYR:CD2	16:v:2136:TYR:O	2.54	0.60
1:A:104:GLU:OE2	13:O:73:ARG:HD3	2.02	0.60
1:A:206:PHE:CE1	23:A:348:CLA:HMB1	2.35	0.60
2:B:372:ASP:OD2	2:B:376:VAL:HG23	2.02	0.60
1:a:2312:ASN:HB3	5:e:2055:TYR:CE1	2.37	0.60
3:c:2103:GLY:O	3:c:2104:GLU:C	2.44	0.60
3:c:2189:TRP:CD1	3:c:2295:THR:HG1	2.19	0.60
4:d:2023:LYS:HZ1	4:d:2032:TRP:CD1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:2006:TYR:O	10:k:2008:ILE:N	2.35	0.60
13:o:2040:ILE:CG1	13:o:2084:GLU:OE1	2.41	0.60
2:B:321:LYS:CE	2:B:325:PHE:CZ	2.84	0.60
3:C:297:TYR:CD2	3:C:302:TYR:HE1	2.19	0.60
4:D:261:PHE:HD1	4:D:266:TRP:CD1	2.19	0.60
11:L:8:GLN:N	11:L:9:PRO:HD3	2.17	0.60
16:V:38:ALA:O	16:V:42:VAL:HG23	2.01	0.60
17:X:12:ILE:HG22	17:X:16:LEU:HD13	1.82	0.60
1:a:2159:LEU:HD11	23:c:2487:CLA:OBD	2.02	0.60
1:a:2278:TRP:HB3	1:a:2279:PRO:HD3	1.84	0.60
2:b:2123:PHE:CG	2:b:2123:PHE:O	2.55	0.60
3:c:2158:THR:HG21	3:c:2254:THR:O	2.02	0.60
7:h:2021:ALA:HB3	7:h:2022:PRO:CD	2.31	0.60
10:k:2030:TRP:CE3	10:k:2031:GLN:NE2	2.70	0.60
2:B:355:PHE:CE1	2:B:373:LYS:HB3	2.36	0.60
3:C:285:ILE:CA	23:C:487:CLA:HMB3	2.29	0.60
23:C:477:CLA:HMD2	23:C:485:CLA:HAB	1.83	0.60
4:D:58:TRP:HA	4:D:62:GLY:H	1.67	0.60
5:E:12:ILE:HG23	5:E:18:TYR:HB2	1.70	0.60
5:E:59:GLN:HE21	5:E:81:GLN:HE22	1.50	0.60
7:H:28:PRO:O	7:H:32:VAL:HG23	2.02	0.60
11:L:36:PHE:O	12:M:3:VAL:HG23	2.01	0.60
24:a:2350:PHO:HED2	4:d:2257:PHE:CD1	2.37	0.60
2:b:2422:ARG:NH2	13:o:2169:ASP:HB3	2.17	0.60
3:c:2099:VAL:HG12	3:c:2100:GLY:O	2.02	0.60
3:c:2121:SER:O	3:c:2125:LEU:HG	2.02	0.60
13:o:2077:SER:OG	13:o:2078:LEU:N	2.34	0.60
2:B:122:LEU:HD12	23:B:525:CLA:HMA2	1.84	0.59
3:C:62:PHE:CZ	10:K:19:ILE:CD1	2.81	0.59
3:C:240:ILE:HG22	3:C:244:CYS:SG	2.42	0.59
5:E:26:ILE:HG12	5:E:27:PRO:HD3	1.84	0.59
16:V:118:HIS:CD2	16:V:122:GLU:OE1	2.55	0.59
1:a:2089:ILE:HG12	13:o:2073:ARG:NH2	2.17	0.59
1:a:2265:PHE:CE2	1:a:2270:SER:HB3	2.37	0.59
2:b:2371:THR:HG22	2:b:2372:ASP:O	2.02	0.59
2:b:2394:GLN:CD	15:u:2052:GLY:HA3	2.27	0.59
3:c:2096:GLY:HA3	3:c:2196:VAL:HG22	1.84	0.59
4:d:2268:HIS:CA	4:d:2271:MET:HE3	2.30	0.59
13:o:2027:ARG:HG3	13:o:2029:ALA:HB3	1.84	0.59
1:A:57:PRO:HG2	13:O:115:ARG:HH11	1.67	0.59
1:A:281:VAL:O	1:A:281:VAL:CG1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:PHE:CE1	23:B:527:CLA:HED3	2.38	0.59
2:B:235:GLU:HB3	2:B:473:THR:OG1	2.02	0.59
1:a:2230:THR:HG22	1:a:2231:GLU:N	2.02	0.59
2:b:2084:THR:O	2:b:2084:THR:HG22	2.01	0.59
3:c:2037:ALA:HA	23:c:2483:CLA:O1A	2.02	0.59
3:c:2201:ASN:CG	3:c:2201:ASN:O	2.43	0.59
3:c:2285:ILE:HG23	23:c:2487:CLA:HMB3	1.84	0.59
13:o:2164:LEU:O	13:o:2165:ALA:CB	2.49	0.59
3:C:169:GLY:O	3:C:173:LEU:HG	2.02	0.59
4:D:101:PHE:CE2	4:D:105:CYS:SG	2.95	0.59
13:O:194:LYS:HG3	13:O:194:LYS:O	2.01	0.59
24:a:2350:PHO:HED2	4:d:2257:PHE:CE1	2.37	0.59
2:b:2171:PRO:HG3	7:h:2062:LYS:HA	1.84	0.59
2:b:2414:PRO:N	2:b:2415:PRO:HD3	2.17	0.59
23:b:2519:CLA:H142	23:d:2357:CLA:H42	1.84	0.59
3:c:2109:PHE:CZ	27:c:2489:BCR:HC32	2.38	0.59
3:c:2265:ILE:HD11	3:c:2449:ARG:NH1	2.17	0.59
27:c:2489:BCR:C34	19:z:2051:VAL:HG13	2.33	0.59
1:A:281:VAL:HG22	1:A:284:TRP:HD1	1.67	0.59
1:A:296:ASN:OD1	3:C:401:LEU:HD23	2.00	0.59
2:B:171:PRO:CG	7:H:62:LYS:HA	2.33	0.59
3:C:299:SER:HB2	3:C:303:GLY:O	2.02	0.59
23:C:486:CLA:H172	19:Z:23:VAL:HG21	1.84	0.59
6:F:40:GLN:HE22	9:J:27:LEU:HG	1.58	0.59
15:U:124:GLY:O	15:U:125:GLY:C	2.46	0.59
16:V:69:ILE:O	16:V:73:VAL:HG23	2.01	0.59
1:a:2036:ILE:O	1:a:2040:THR:HB	2.02	0.59
1:a:2261:GLN:HG2	4:d:2027:PHE:HE1	1.67	0.59
2:b:2142:HIS:ND1	23:b:2524:CLA:H142	2.16	0.59
2:b:2221:PRO:CG	2:b:2225:LEU:HD12	2.31	0.59
3:c:2213:LEU:HD11	23:c:2474:CLA:H203	1.84	0.59
10:k:2024:LEU:O	10:k:2027:ALA:HB3	2.02	0.59
15:u:2132:LEU:N	15:u:2132:LEU:CD2	2.65	0.59
3:C:141:GLU:HB2	3:C:144:SER:CB	2.32	0.59
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.84	0.59
13:O:233:VAL:HG12	13:O:234:LYS:N	2.17	0.59
2:b:2086:ILE:O	2:b:2086:ILE:HG22	2.03	0.59
2:b:2234:ILE:HG21	23:b:2513:CLA:HAC1	1.85	0.59
2:b:2368:VAL:HG21	2:b:2422:ARG:HG2	1.85	0.59
3:c:2305:THR:HA	3:c:2423:ARG:HH11	1.66	0.59
13:o:2137:THR:CG2	13:o:2138:THR:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ASP:OD1	2:B:390:TYR:CB	2.50	0.59
15:U:58:ASN:C	15:U:59:ASN:HD22	2.08	0.59
16:V:117:GLY:O	16:V:121:VAL:HG23	2.03	0.59
23:a:2349:CLA:HED1	4:d:2175:VAL:CG1	2.31	0.59
3:c:2036:TRP:O	3:c:2038:GLY:N	2.31	0.59
3:c:2042:LEU:HG	23:c:2486:CLA:CED	2.30	0.59
3:c:2272:LEU:O	3:c:2276:LEU:HB2	2.01	0.59
3:c:2285:ILE:O	23:c:2487:CLA:HBB1	2.03	0.59
3:c:2291:TRP:HB3	3:c:2292:PHE:HD2	1.68	0.59
4:d:2261:PHE:HA	14:t:2024:ARG:HH22	1.67	0.59
13:o:2039:ARG:CB	13:o:2245:PRO:HG3	2.32	0.59
1:A:303:ASN:C	1:A:304:HIS:HD1	2.10	0.59
3:C:223:TRP:CD1	3:C:224:ILE:N	2.71	0.59
4:D:66:SER:HA	4:D:76:VAL:HG13	1.85	0.59
4:D:67:TYR:C	6:F:39:MET:HE1	2.27	0.59
10:K:9:PHE:O	10:K:10:ASP:C	2.44	0.59
16:V:55:ARG:HG3	16:V:56:THR:N	2.16	0.59
2:b:2326:ARG:NH1	2:b:2327:THR:HB	2.17	0.59
2:B:15:ASP:C	2:B:15:ASP:OD1	2.45	0.59
2:B:174:LEU:HG	2:B:174:LEU:O	2.01	0.59
2:B:302:TRP:O	2:B:305:ILE:HG12	2.02	0.59
2:B:327:THR:C	2:B:329:PRO:HD3	2.27	0.59
2:B:372:ASP:CG	2:B:373:LYS:N	2.60	0.59
3:C:36:TRP:C	3:C:38:GLY:H	2.10	0.59
3:C:200:THR:C	3:C:201:ASN:HD22	2.10	0.59
2:b:2106:LEU:HD22	23:b:2522:CLA:H143	1.84	0.59
2:b:2110:ALA:O	2:b:2113:TRP:N	2.36	0.59
2:b:2110:ALA:O	2:b:2111:ALA:C	2.46	0.59
2:b:2263:THR:HG22	2:b:2263:THR:O	2.03	0.59
3:c:2266:TRP:HA	3:c:2271:TYR:CE2	2.38	0.59
23:c:2486:CLA:H42	10:k:2030:TRP:NE1	2.18	0.59
4:d:2080:THR:CG2	4:d:2168:PHE:HA	2.32	0.59
4:d:2281:MET:HE2	4:d:2284:ILE:HD12	1.83	0.59
7:h:2026:THR:C	7:h:2028:PRO:HD2	2.28	0.59
15:u:2124:GLY:O	15:u:2125:GLY:C	2.45	0.59
1:A:265:PHE:HB2	1:A:271:LEU:HD21	1.85	0.59
2:B:321:LYS:HE2	2:B:325:PHE:CZ	2.37	0.59
3:C:374:GLY:HA2	13:O:7:TYR:HE1	1.65	0.59
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.37	0.59
4:D:235:PHE:CG	4:D:236:ASN:N	2.70	0.59
7:H:53:ILE:HG22	17:X:15:SER:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:164:LEU:O	13:O:165:ALA:CB	2.51	0.59
15:U:32:THR:O	15:U:36:GLU:HG3	2.03	0.59
1:a:2217:SER:OG	4:d:2142:ASN:ND2	2.35	0.59
3:c:2299:SER:HB3	3:c:2423:ARG:HH22	1.67	0.59
3:c:2320:ARG:NH2	15:u:2128:TYR:CZ	2.71	0.59
3:c:2376:ASP:OD1	3:c:2378:ASN:HB2	2.02	0.59
9:j:2040:LEU:HD23	16:v:2030:LYS:CE	2.32	0.59
10:k:2009:PHE:O	10:k:2010:ASP:C	2.45	0.59
2:B:225:LEU:O	2:B:231:MET:HG2	2.03	0.59
2:B:301:ALA:O	2:B:304:ALA:HB3	2.02	0.59
3:C:284:PHE:HD1	3:C:434:ALA:HB1	1.66	0.59
3:C:429:SER:O	3:C:432:VAL:HB	2.03	0.59
1:a:2105:TRP:NE1	1:a:2110:GLY:HA3	2.18	0.59
1:a:2307:ILE:HG13	1:a:2314:ILE:CD1	2.30	0.59
1:a:2321:ILE:HD11	4:d:2176:ALA:HB1	1.84	0.59
2:b:2340:TRP:CD1	2:b:2340:TRP:H	2.21	0.59
3:c:2043:ILE:HG13	3:c:2044:ASN:N	2.17	0.59
3:c:2089:ILE:HB	3:c:2090:PRO:CD	2.30	0.59
3:c:2189:TRP:NE1	3:c:2295:THR:HG1	2.00	0.59
3:c:2334:PRO:HA	13:o:2153:THR:HB	1.85	0.59
4:d:2191:TRP:NE1	4:d:2197:HIS:CD2	2.71	0.59
4:d:2312:GLU:HB2	13:o:2159:PRO:HG3	1.84	0.59
3:C:239:TRP:O	3:C:243:ILE:HG13	2.03	0.58
5:E:30:PHE:O	5:E:30:PHE:HD2	1.84	0.58
10:K:15:VAL:O	10:K:15:VAL:HG12	2.02	0.58
1:a:2041:LEU:HD21	1:a:2122:GLY:C	2.28	0.58
1:a:2093:PHE:HB2	3:c:2218:PHE:CD1	2.38	0.58
1:a:2110:GLY:O	1:a:2111:PRO:C	2.44	0.58
2:b:2313:ASP:O	2:b:2313:ASP:OD1	2.21	0.58
2:b:2414:PRO:N	2:b:2415:PRO:CD	2.66	0.58
3:c:2318:LEU:HD22	3:c:2328:VAL:HG11	1.85	0.58
16:v:2061:LEU:HB2	16:v:2082:TYR:OH	2.03	0.58
2:B:46:ASP:HB3	2:B:58:GLN:OE1	2.03	0.58
2:B:171:PRO:HG3	7:H:62:LYS:HA	1.86	0.58
2:B:223:GLN:HG3	2:B:227:LYS:HE3	1.85	0.58
2:B:340:TRP:N	2:B:340:TRP:CD1	2.71	0.58
4:D:88:SER:OG	5:E:68:ARG:NE	2.36	0.58
1:a:2235:TYR:HA	4:d:2265:ARG:HH22	1.67	0.58
2:b:2136:PRO:CD	2:b:2231:MET:HE1	2.27	0.58
2:b:2340:TRP:CD1	2:b:2340:TRP:N	2.70	0.58
23:b:2522:CLA:HMD2	23:b:2524:CLA:H202	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2257:PHE:CZ	25:d:2358:PL9:H253	2.38	0.58
1:A:29:TYR:CD2	1:A:133:LEU:HD12	2.37	0.58
1:A:307:ILE:HG13	1:A:314:ILE:CD1	2.30	0.58
2:B:234:ILE:HG21	23:B:513:CLA:HAC1	1.85	0.58
3:C:62:PHE:CE1	3:C:119:LEU:HD11	2.39	0.58
4:D:27:PHE:HB3	6:F:17:VAL:HG11	1.84	0.58
8:I:19:PHE:CE1	8:I:23:PHE:HE1	2.21	0.58
13:O:156:PHE:O	13:O:188:LYS:NZ	2.36	0.58
13:O:221:SER:OG	13:O:231:HIS:N	2.36	0.58
1:a:2142:TRP:HB2	4:d:2220:ASN:OD1	2.03	0.58
3:c:2036:TRP:C	3:c:2038:GLY:H	2.09	0.58
3:c:2279:LEU:HB3	23:c:2481:CLA:CBC	2.32	0.58
3:c:2305:THR:HA	3:c:2423:ARG:NH1	2.18	0.58
3:c:2354:GLU:C	3:c:2356:MET:H	2.11	0.58
3:c:2433:LEU:O	3:c:2437:PHE:HB2	2.03	0.58
7:h:2047:ILE:HG12	7:h:2052:LEU:HD23	1.84	0.58
7:h:2053:ILE:HG22	17:x:2015:SER:OG	2.03	0.58
13:o:2094:THR:HA	13:o:2127:ALA:O	2.03	0.58
1:A:210:LEU:HD13	24:D:355:PHO:ND	2.18	0.58
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.31	0.58
3:C:77:PRO:O	3:C:78:GLU:HB2	2.03	0.58
3:C:151:TRP:C	3:C:153:ASP:H	2.10	0.58
3:C:266:TRP:HA	3:C:271:TYR:HE2	1.68	0.58
4:D:32:TRP:N	4:D:131:GLU:OE2	2.35	0.58
13:O:32:ILE:C	13:O:34:SER:H	2.10	0.58
2:b:2098:LEU:O	2:b:2102:VAL:HG23	2.03	0.58
2:b:2271:THR:HG22	2:b:2448:ARG:NH1	2.18	0.58
23:b:2524:CLA:H13	23:b:2524:CLA:OBD	2.02	0.58
4:d:2086:GLY:C	4:d:2087:HIS:HD2	2.11	0.58
6:f:2022:VAL:O	6:f:2026:ALA:HB3	2.04	0.58
13:o:2039:ARG:HB3	13:o:2245:PRO:HG3	1.84	0.58
13:o:2075:THR:HG23	13:o:2103:PHE:HD2	1.67	0.58
1:A:98:GLU:O	1:A:98:GLU:HG3	2.02	0.58
3:C:71:GLU:HB3	3:C:89:ILE:HD11	1.85	0.58
3:C:293:ASN:OD1	3:C:423:ARG:NH2	2.37	0.58
3:C:373:ASN:OD1	13:O:16:ALA:HA	2.03	0.58
4:D:29:PHE:HE2	4:D:31:GLY:CA	2.16	0.58
16:V:63:THR:HB	16:V:83:ASP:O	2.03	0.58
1:a:2021:VAL:HG13	1:a:2030:VAL:O	2.04	0.58
1:a:2097:TRP:CD1	8:i:2005:LYS:HD3	2.39	0.58
3:c:2318:LEU:CD2	3:c:2328:VAL:HG11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2152:VAL:HG13	23:d:2354:CLA:CED	2.34	0.58
4:d:2231:THR:HG22	4:d:2232:PHE:N	2.19	0.58
5:e:2048:THR:O	5:e:2048:THR:HG22	2.02	0.58
11:l:2007:ARG:O	11:l:2009:PRO:HD3	2.03	0.58
12:m:2018:PRO:O	12:m:2021:PHE:HB3	2.03	0.58
13:o:2114:GLU:OE2	13:o:2231:HIS:NE2	2.36	0.58
16:v:2073:VAL:O	16:v:2077:LYS:HG3	2.03	0.58
27:B:529:BCR:H311	27:B:529:BCR:H342	1.86	0.58
3:C:113:VAL:O	3:C:117:VAL:HG23	2.03	0.58
3:C:271:TYR:HA	3:C:274:TYR:CE1	2.39	0.58
13:O:215:PHE:O	13:O:216:GLU:HB2	2.02	0.58
15:U:73:PRO:HG2	16:V:83:ASP:CG	2.28	0.58
1:a:2057:PRO:HG2	13:o:2115:ARG:HH12	1.67	0.58
1:a:2161:TYR:HB3	1:a:2162:PRO:CD	2.34	0.58
3:c:2281:MET:O	3:c:2284:PHE:HB2	2.04	0.58
3:c:2320:ARG:CZ	15:u:2128:TYR:CE2	2.87	0.58
13:o:2217:SER:OG	13:o:2235:ILE:HB	2.03	0.58
4:D:35:ILE:O	4:D:39:PRO:HD2	2.03	0.58
4:D:96:GLU:CD	5:E:68:ARG:O	2.46	0.58
13:O:40:ILE:HG23	13:O:84:GLU:OE2	2.04	0.58
13:O:60:ARG:NH2	2:b:2341:LYS:HZ3	2.02	0.58
13:O:215:PHE:HB3	13:O:237:GLY:H	1.69	0.58
3:c:2271:TYR:HA	3:c:2274:TYR:CD1	2.38	0.58
4:d:2195:PRO:HG2	4:d:2196:PHE:N	2.19	0.58
13:o:2118:LEU:HD13	13:o:2233:VAL:HG11	1.85	0.58
15:u:2065:PHE:HD1	15:u:2076:ALA:HB1	1.69	0.58
1:A:334:ARG:HH11	4:D:320:LEU:CD1	2.13	0.58
3:C:63:TRP:CE2	3:C:67:MET:HG3	2.39	0.58
23:C:477:CLA:H142	23:C:477:CLA:H101	1.84	0.58
13:O:60:ARG:NH2	2:b:2341:LYS:NZ	2.52	0.58
17:X:34:PHE:O	17:X:38:ILE:HG13	2.04	0.58
1:a:2307:ILE:HG22	1:a:2309:ALA:HB3	1.85	0.58
2:b:2045:PHE:CE2	2:b:2078:TRP:CZ2	2.91	0.58
3:c:2293:ASN:CG	3:c:2423:ARG:NH2	2.62	0.58
13:o:2075:THR:CG2	13:o:2103:PHE:CD2	2.87	0.58
13:o:2125:LEU:HD12	13:o:2126:VAL:H	1.69	0.58
17:x:2034:PHE:O	17:x:2038:ILE:HG13	2.04	0.58
2:B:225:LEU:C	2:B:231:MET:HG2	2.28	0.58
13:O:39:ARG:HA	13:O:245:PRO:HG3	1.85	0.58
14:T:3:THR:O	14:T:6:TYR:N	2.33	0.58
16:V:75:TYR:CE2	16:V:79:PRO:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2225:LEU:C	2:b:2231:MET:HG2	2.29	0.58
2:b:2355:PHE:CE1	2:b:2373:LYS:HB3	2.39	0.58
3:c:2320:ARG:NH1	16:v:2050:PRO:HD2	2.19	0.58
23:c:2477:CLA:H142	23:c:2477:CLA:H101	1.86	0.58
4:d:2112:THR:O	4:d:2116:LEU:HG	2.03	0.58
5:e:2012:ILE:HD11	28:e:2084:HEC:O1A	2.04	0.58
10:k:2009:PHE:CE1	19:z:2009:LEU:HD23	2.39	0.58
13:o:2142:PHE:HB2	13:o:2199:LEU:HB2	1.86	0.58
16:v:2079:PRO:HG3	16:v:2088:ILE:C	2.28	0.58
1:A:14:TRP:HH2	8:I:25:SER:HB3	1.68	0.58
23:B:521:CLA:CAB	23:B:527:CLA:HED1	2.27	0.58
3:C:63:TRP:CZ2	3:C:67:MET:HG3	2.39	0.58
3:C:123:ALA:HB1	19:Z:47:TRP:CH2	2.37	0.58
4:D:108:GLY:C	4:D:110:LEU:N	2.60	0.58
13:O:60:ARG:NH1	2:b:2341:LYS:HZ2	2.00	0.58
1:a:2320:ILE:HG22	1:a:2320:ILE:O	2.04	0.58
3:c:2134:ILE:HD11	23:c:2486:CLA:H2	1.84	0.58
3:c:2188:THR:OG1	3:c:2298:PRO:HB3	2.03	0.58
3:c:2273:SER:OG	3:c:2445:ALA:CA	2.52	0.58
4:d:2145:ALA:CB	4:d:2272:LEU:HD11	2.32	0.58
5:e:2021:ILE:O	5:e:2025:THR:OG1	2.19	0.58
13:o:2125:LEU:HG	13:o:2126:VAL:N	2.18	0.58
19:z:2023:VAL:HB	19:z:2024:PRO:HD3	1.86	0.58
1:A:78:ILE:O	1:A:177:SER:HB2	2.03	0.57
1:A:228:THR:HG22	1:A:228:THR:O	2.04	0.57
23:B:520:CLA:HAA2	23:B:520:CLA:CBD	2.33	0.57
3:C:188:THR:HG22	3:C:188:THR:O	2.03	0.57
4:D:28:VAL:H	6:F:17:VAL:HG11	1.69	0.57
11:L:27:LEU:HD23	12:M:14:PHE:CE2	2.39	0.57
13:O:53:LYS:HG2	13:O:65:PHE:CD2	2.39	0.57
16:V:76:MET:O	16:V:94:SER:HA	2.04	0.57
16:V:100:ILE:C	16:V:102:PRO:HD3	2.29	0.57
5:e:2012:ILE:HD13	28:e:2084:HEC:CGA	2.33	0.57
13:o:2200:ASN:O	13:o:2213:GLY:HA3	2.04	0.57
15:u:2065:PHE:HD1	15:u:2076:ALA:CB	2.17	0.57
2:B:135:LEU:HB2	2:B:231:MET:HE1	1.86	0.57
23:B:518:CLA:H142	23:B:524:CLA:HBA1	1.86	0.57
27:B:528:BCR:H382	25:d:2358:PL9:H401	1.85	0.57
3:C:286:ALA:O	3:C:289:PHE:HB3	2.03	0.57
3:C:305:THR:O	3:C:308:GLU:HB2	2.04	0.57
3:C:344:SER:O	3:C:347:GLY:N	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:436:PHE:O	3:C:439:VAL:HB	2.04	0.57
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.39	0.57
6:F:14:ILE:O	6:F:14:ILE:HG13	2.03	0.57
8:I:5:LYS:O	8:I:9:TYR:HD1	1.86	0.57
10:K:11:PRO:HB3	18:N:9:UNK:CB	2.34	0.57
13:O:200:ASN:O	13:O:213:GLY:HA3	2.04	0.57
13:O:215:PHE:HB3	13:O:237:GLY:N	2.19	0.57
16:V:38:ALA:O	16:V:42:VAL:CG2	2.52	0.57
2:b:2012:LEU:HD21	2:b:2019:LEU:HA	1.86	0.57
3:c:2314:ALA:HB3	3:c:2351:PHE:CD1	2.39	0.57
4:d:2227:GLU:HG3	4:d:2230:SER:H	1.69	0.57
4:d:2298:PHE:O	4:d:2299:ILE:C	2.47	0.57
13:o:2032:ILE:C	13:o:2034:SER:N	2.61	0.57
16:v:2122:GLU:HB3	16:v:2123:PRO:CD	2.33	0.57
1:A:89:ILE:HD13	1:A:94:TYR:CG	2.39	0.57
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.19	0.57
1:A:218:LEU:CD2	4:D:142:ASN:HD22	2.16	0.57
1:A:286:THR:CG2	23:A:348:CLA:O1D	2.50	0.57
1:A:307:ILE:C	1:A:309:ALA:N	2.62	0.57
2:B:315:ILE:HD13	2:B:359:MET:HE2	1.86	0.57
2:B:368:VAL:HG21	2:B:422:ARG:HG2	1.86	0.57
3:C:318:LEU:HD22	3:C:328:VAL:HG21	1.87	0.57
10:K:24:LEU:O	10:K:27:ALA:HB3	2.04	0.57
19:Z:12:LEU:HD12	19:Z:12:LEU:O	2.04	0.57
1:a:2258:LEU:C	1:a:2259:ILE:HG13	2.30	0.57
1:a:2310:LYS:O	16:v:2125:ILE:HD13	2.05	0.57
1:a:2330:VAL:CG1	4:d:2348:ARG:HG3	2.34	0.57
2:b:2328:GLY:HA3	23:b:2514:CLA:O1A	2.04	0.57
3:c:2406:SER:OG	23:c:2475:CLA:O1A	2.23	0.57
3:c:2419:PHE:O	3:c:2420:VAL:HG23	2.05	0.57
11:l:2006:ASN:H	11:l:2006:ASN:ND2	2.02	0.57
13:o:2011:VAL:O	13:o:2011:VAL:HG12	2.04	0.57
17:x:2012:ILE:HA	17:x:2016:LEU:CD1	2.33	0.57
1:A:15:GLU:O	1:A:19:ASN:ND2	2.38	0.57
1:A:69:GLY:O	1:A:81:ALA:HA	2.04	0.57
1:A:142:TRP:CD1	3:C:443:TRP:CH2	2.92	0.57
1:A:161:TYR:CE2	1:A:165:GLN:HG3	2.40	0.57
1:A:263:ALA:HB1	25:A:353:PL9:H151	1.86	0.57
1:A:341:LEU:HD21	15:U:134:LYS:NZ	2.19	0.57
2:B:192:PRO:HG3	7:H:48:TYR:CE1	2.40	0.57
3:C:222:GLY:O	3:C:223:TRP:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:TRP:HB3	3:C:292:PHE:CE2	2.39	0.57
4:D:72:ASN:OD1	4:D:74:LEU:HB2	2.03	0.57
14:T:9:ILE:O	14:T:9:ILE:HG22	2.05	0.57
15:U:75:LEU:HD21	15:U:101:GLN:HE21	1.69	0.57
1:a:2143:ILE:HD13	4:d:2253:TRP:CH2	2.39	0.57
1:a:2210:LEU:HD13	24:d:2356:PHO:ND	2.20	0.57
2:b:2012:LEU:HG	2:b:2019:LEU:HB2	1.86	0.57
2:b:2135:LEU:HB2	2:b:2231:MET:HE1	1.85	0.57
2:b:2236:THR:O	2:b:2240:SER:HB3	2.04	0.57
2:b:2250:PHE:CD1	2:b:2459:ALA:HB1	2.39	0.57
27:b:2528:BCR:H311	27:b:2528:BCR:H342	1.86	0.57
3:c:2282:MET:HE3	23:c:2479:CLA:H61	1.86	0.57
6:f:2040:GLN:NE2	9:j:2027:LEU:O	2.32	0.57
16:v:2037:CYS:O	16:v:2038:ALA:C	2.47	0.57
1:A:142:TRP:HB2	4:D:220:ASN:HB2	1.86	0.57
3:C:155:ASN:HB3	3:C:255:THR:OG1	2.05	0.57
4:D:261:PHE:CD1	4:D:266:TRP:CD1	2.93	0.57
14:T:24:ARG:HG2	14:T:25:GLU:N	2.19	0.57
16:V:79:PRO:HG3	16:V:88:ILE:C	2.30	0.57
1:a:2058:VAL:HG13	1:a:2107:TYR:O	2.04	0.57
1:a:2131:TRP:CE3	1:a:2132:GLU:N	2.72	0.57
2:b:2010:THR:O	2:b:2013:ILE:HG22	2.04	0.57
2:b:2372:ASP:OD2	2:b:2376:VAL:HG23	2.03	0.57
2:b:2399:VAL:HG23	2:b:2417:VAL:HG13	1.87	0.57
2:b:2458:PHE:CE1	23:b:2516:CLA:HBB1	2.40	0.57
1:A:143:ILE:HD13	4:D:253:TRP:CH2	2.40	0.57
2:B:45:PHE:CE2	2:B:78:TRP:CZ2	2.92	0.57
23:B:524:CLA:O1A	23:B:524:CLA:H2	2.04	0.57
4:D:122:LEU:HD21	23:D:354:CLA:C9	2.35	0.57
4:D:302:GLU:OE1	4:D:302:GLU:HA	2.03	0.57
1:a:2092:HIS:HD2	3:c:2219:GLY:HA3	1.67	0.57
2:b:2029:LEU:HB3	27:b:2527:BCR:H351	1.85	0.57
2:b:2357:ARG:NH2	4:d:2337:GLU:HB3	2.18	0.57
23:c:2477:CLA:H8	8:i:2020:VAL:HG22	1.87	0.57
4:d:2188:PHE:N	4:d:2188:PHE:CD1	2.73	0.57
8:i:2015:PHE:HD2	8:i:2018:LEU:HD12	1.69	0.57
13:o:2137:THR:HG23	13:o:2138:THR:N	2.18	0.57
13:o:2153:THR:CG2	13:o:2154:ALA:N	2.67	0.57
1:A:225:ARG:CB	2:B:481:GLY:C	2.72	0.57
1:A:316:THR:O	1:A:318:ALA:N	2.37	0.57
2:B:247:PHE:CE1	23:B:521:CLA:H72	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:PHE:CD1	2:B:459:ALA:HB1	2.40	0.57
2:B:414:PRO:N	2:B:415:PRO:CD	2.67	0.57
4:D:110:LEU:O	4:D:113:PHE:HB3	2.05	0.57
1:a:2023:SER:OG	1:a:2024:THR:N	2.37	0.57
1:a:2085:SER:HA	1:a:2109:GLY:HA3	1.87	0.57
2:b:2015:ASP:C	2:b:2015:ASP:OD1	2.47	0.57
3:c:2283:GLY:HA3	3:c:2434:ALA:HB2	1.86	0.57
4:d:2071:CYS:HB3	4:d:2075:THR:CB	2.34	0.57
4:d:2077:ALA:CB	4:d:2174:GLY:HA3	2.35	0.57
4:d:2138:VAL:CG1	4:d:2139:ARG:H	2.18	0.57
13:o:2032:ILE:C	13:o:2034:SER:H	2.10	0.57
3:C:42:LEU:CD2	23:C:486:CLA:HED1	2.35	0.57
3:C:81:MET:HE1	3:C:89:ILE:HG22	1.87	0.57
3:C:157:MET:HE2	3:C:157:MET:HA	1.86	0.57
3:C:292:PHE:HE1	23:C:487:CLA:HBC3	1.69	0.57
16:V:22:THR:H	16:V:25:GLN:NE2	2.03	0.57
1:a:2131:TRP:CZ2	3:c:2449:ARG:HG3	2.35	0.57
1:a:2221:SER:CA	4:d:2139:ARG:HB2	2.33	0.57
1:a:2254:TYR:HD1	4:d:2132:ILE:HG22	1.70	0.57
2:b:2321:LYS:CE	2:b:2325:PHE:CZ	2.88	0.57
3:c:2433:LEU:HB3	23:c:2481:CLA:HMC2	1.85	0.57
13:o:2093:LEU:O	13:o:2128:SER:HA	2.04	0.57
16:v:2118:HIS:NE2	16:v:2122:GLU:OE1	2.37	0.57
2:B:414:PRO:N	2:B:415:PRO:HD3	2.20	0.57
3:C:282:MET:CA	3:C:285:ILE:HG13	2.32	0.57
13:O:78:LEU:O	13:O:79:ASP:OD1	2.23	0.57
2:b:2007:ARG:HA	23:b:2523:CLA:O1A	2.05	0.57
4:d:2335:PRO:O	4:d:2338:ASN:ND2	2.37	0.57
13:o:2095:PHE:CB	13:o:2127:ALA:HB3	2.34	0.57
13:o:2162:ARG:HG3	13:o:2162:ARG:O	2.03	0.57
2:B:10:THR:O	2:B:13:ILE:HG22	2.04	0.57
2:B:110:ALA:O	2:B:111:ALA:C	2.46	0.57
3:C:155:ASN:OD1	3:C:156:LYS:HG2	2.04	0.57
4:D:52:THR:O	4:D:67:TYR:HD1	1.88	0.57
13:O:39:ARG:HA	13:O:245:PRO:CB	2.35	0.57
13:O:102:ASP:O	13:O:103:PHE:HD1	1.85	0.57
15:U:40:VAL:O	15:U:40:VAL:HG12	2.05	0.57
1:a:2133:LEU:CD2	4:d:2256:ILE:HG13	2.35	0.57
2:b:2372:ASP:OD2	2:b:2374:ASN:HB2	2.05	0.57
3:c:2199:ILE:HD12	3:c:2234:VAL:CG2	2.32	0.57
7:h:2022:PRO:CG	7:h:2023:GLY:H	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:CD1	1:A:30:VAL:N	2.69	0.56
2:B:414:PRO:O	2:B:418:LYS:HG3	2.04	0.56
3:C:141:GLU:CB	3:C:144:SER:OG	2.53	0.56
3:C:314:ALA:HB3	3:C:351:PHE:CD1	2.40	0.56
3:C:326:ALA:CB	15:U:127:ARG:HD2	2.31	0.56
3:C:412:THR:HG22	16:V:136:TYR:HE2	1.69	0.56
3:C:417:VAL:HG21	16:V:42:VAL:HG22	1.86	0.56
8:I:31:ASN:CG	8:I:31:ASN:O	2.48	0.56
13:O:53:LYS:CE	13:O:234:LYS:HB2	2.35	0.56
13:O:66:VAL:CG1	13:O:67:PRO:HD2	2.35	0.56
17:X:12:ILE:HA	17:X:16:LEU:HD12	1.87	0.56
1:a:2307:ILE:HD13	5:e:2054:TYR:HB2	1.86	0.56
2:b:2190:PHE:CE2	7:h:2044:ILE:HD11	2.40	0.56
4:d:2222:LEU:HD23	4:d:2244:TYR:HB3	1.86	0.56
13:o:2168:TYR:CD2	13:o:2172:ILE:HD11	2.40	0.56
13:o:2215:PHE:HB3	13:o:2237:GLY:H	1.69	0.56
1:A:52:PHE:CE1	1:A:81:ALA:HB2	2.40	0.56
1:A:114:LEU:HD11	1:A:118:HIS:CE1	2.39	0.56
1:A:237:TYR:CD1	1:A:237:TYR:N	2.73	0.56
23:B:512:CLA:H203	23:B:523:CLA:H192	1.87	0.56
4:D:138:VAL:CG1	4:D:139:ARG:H	2.17	0.56
4:D:186:GLN:HA	4:D:186:GLN:HE21	1.69	0.56
4:D:329:MET:HG2	4:D:329:MET:O	2.05	0.56
1:a:2278:TRP:HE1	23:a:2349:CLA:C4	2.19	0.56
2:b:2061:PHE:O	2:b:2064:PRO:HD2	2.04	0.56
2:b:2246:PHE:C	2:b:2246:PHE:CD2	2.82	0.56
2:b:2372:ASP:CG	2:b:2373:LYS:N	2.63	0.56
23:b:2524:CLA:O1A	23:b:2524:CLA:H2	2.05	0.56
13:o:2013:THR:O	13:o:2013:THR:HG22	2.05	0.56
13:o:2039:ARG:HD2	13:o:2245:PRO:HG3	1.86	0.56
13:o:2053:LYS:HE2	13:o:2234:LYS:HB2	1.86	0.56
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.87	0.56
2:B:458:PHE:CE1	23:B:516:CLA:HBB1	2.41	0.56
3:C:88:LEU:O	3:C:91:HIS:HB2	2.05	0.56
3:C:229:ASN:OD1	3:C:231:GLU:HG3	2.05	0.56
3:C:324:LEU:HD21	15:U:72:TYR:OH	2.05	0.56
23:C:476:CLA:H12	23:C:483:CLA:H2	1.86	0.56
4:D:261:PHE:HA	14:T:24:ARG:NH2	2.20	0.56
7:H:53:ILE:HG23	7:H:53:ILE:O	2.04	0.56
11:L:7:ARG:O	11:L:9:PRO:HD3	2.05	0.56
13:O:149:PRO:HA	13:O:192:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2172:MET:HE2	23:d:2355:CLA:HMC2	1.87	0.56
2:b:2326:ARG:HD3	27:b:2528:BCR:C40	2.29	0.56
3:c:2108:THR:HG21	10:k:2002:LEU:HG	1.88	0.56
3:c:2155:ASN:OD1	3:c:2156:LYS:HG2	2.05	0.56
3:c:2160:ILE:O	3:c:2163:PHE:HB2	2.05	0.56
4:d:2026:ARG:HD3	6:f:2017:VAL:CG2	2.36	0.56
4:d:2253:TRP:HA	4:d:2253:TRP:CE3	2.39	0.56
4:d:2329:MET:O	4:d:2333:ASP:HB2	2.05	0.56
7:h:2053:ILE:HG23	17:x:2013:THR:OG1	2.05	0.56
10:k:2001:LYS:HG2	10:k:2003:PRO:CD	2.35	0.56
11:l:2010:VAL:O	12:m:2028:GLN:NE2	2.37	0.56
2:B:231:MET:HE3	2:B:231:MET:O	2.05	0.56
2:B:451:PHE:CD1	2:B:451:PHE:C	2.84	0.56
3:C:281:MET:O	3:C:284:PHE:HB2	2.05	0.56
4:D:231:THR:HG22	4:D:232:PHE:N	2.20	0.56
13:O:43:LEU:HD12	13:O:241:ALA:HB2	1.87	0.56
1:a:2242:GLU:O	4:d:2241:GLU:HA	2.06	0.56
3:c:2037:ALA:HA	23:c:2483:CLA:HBA1	1.86	0.56
11:l:2025:LEU:HD11	14:t:2012:CYS:HB3	1.87	0.56
16:v:2075:TYR:CE2	16:v:2079:PRO:HA	2.40	0.56
16:v:2079:PRO:CG	16:v:2088:ILE:HG13	2.35	0.56
1:A:133:LEU:HD23	4:D:252:PHE:CD1	2.41	0.56
1:A:195:HIS:O	1:A:199:GLN:HG3	2.06	0.56
2:B:372:ASP:OD2	2:B:374:ASN:HB2	2.03	0.56
3:C:284:PHE:CD1	3:C:434:ALA:HB1	2.41	0.56
14:T:24:ARG:HG2	14:T:25:GLU:H	1.70	0.56
16:V:129:LYS:NZ	16:V:135:VAL:CG2	2.69	0.56
1:a:2074:GLY:C	1:a:2075:ASN:HD22	2.13	0.56
1:a:2114:LEU:HD12	23:a:2351:CLA:O1D	2.06	0.56
1:a:2286:THR:HG22	23:a:2348:CLA:O1D	2.05	0.56
1:a:2340:PRO:HD3	15:u:2132:LEU:CD1	2.36	0.56
2:b:2318:ASN:O	2:b:2320:ALA:N	2.38	0.56
2:b:2356:VAL:HG23	2:b:2370:LEU:HD23	1.88	0.56
3:c:2063:TRP:CH2	3:c:2088:LEU:HD21	2.39	0.56
4:d:2026:ARG:HD3	6:f:2017:VAL:HG21	1.86	0.56
4:d:2102:THR:OG1	5:e:2045:VAL:O	2.20	0.56
7:h:2022:PRO:HG2	7:h:2023:GLY:N	2.18	0.56
7:h:2022:PRO:O	7:h:2023:GLY:O	2.23	0.56
1:A:114:LEU:CD1	1:A:118:HIS:HE1	2.19	0.56
1:A:330:VAL:HG13	4:D:348:ARG:HG3	1.87	0.56
2:B:246:PHE:CD2	2:B:246:PHE:C	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:GLN:NE2	15:U:52:GLY:HA3	2.21	0.56
3:C:350:ILE:CG2	3:C:359:TRP:HB3	2.35	0.56
4:D:87:HIS:CD2	4:D:166:SER:HA	2.41	0.56
11:L:12:LEU:HD11	11:L:16:SER:CB	2.34	0.56
13:O:192:LEU:HD22	15:U:119:THR:HG23	1.88	0.56
2:b:2041:GLU:HG2	2:b:2060:MET:SD	2.46	0.56
2:b:2045:PHE:HE1	2:b:2055:MET:HA	1.70	0.56
2:b:2321:LYS:HE3	2:b:2325:PHE:HZ	1.69	0.56
11:l:2001:MET:C	11:l:2003:PRO:HD2	2.30	0.56
1:A:93:PHE:CZ	23:A:352:CLA:HBA1	2.41	0.56
2:B:371:THR:HG22	2:B:372:ASP:O	2.05	0.56
23:B:518:CLA:C14	23:B:524:CLA:HMA2	2.35	0.56
3:C:279:LEU:HB3	23:C:481:CLA:CBC	2.35	0.56
7:H:47:ILE:HG12	7:H:52:LEU:HD23	1.87	0.56
13:O:32:ILE:C	13:O:34:SER:N	2.59	0.56
16:V:22:THR:H	16:V:25:GLN:HE21	1.52	0.56
1:a:2063:ILE:CG2	3:c:2335:THR:HG21	2.34	0.56
1:a:2190:HIS:O	1:a:2298:ASN:HB3	2.05	0.56
3:c:2079:LYS:O	3:c:2080:PRO:C	2.49	0.56
4:d:2058:TRP:HB3	4:d:2063:LEU:O	2.05	0.56
10:k:2025:ALA:HB1	27:k:2050:BCR:C19	2.35	0.56
2:B:41:GLU:HG2	2:B:60:MET:SD	2.45	0.56
4:D:32:TRP:CE3	4:D:32:TRP:HA	2.41	0.56
2:b:2012:LEU:CD2	2:b:2019:LEU:HD12	2.35	0.56
3:c:2062:PHE:CD2	10:k:2020:PRO:HG3	2.41	0.56
3:c:2071:GLU:CB	3:c:2089:ILE:HD11	2.35	0.56
7:h:2043:ILE:HG12	17:x:2019:PHE:CZ	2.41	0.56
13:o:2053:LYS:CE	13:o:2234:LYS:HB2	2.35	0.56
13:o:2168:TYR:CG	13:o:2172:ILE:HD11	2.41	0.56
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.36	0.56
1:A:281:VAL:HG22	1:A:284:TRP:CD1	2.41	0.56
3:C:61:VAL:HG11	3:C:121:SER:HB2	1.88	0.56
28:E:84:HEC:C4A	6:F:19:TRP:HH2	2.18	0.56
10:K:16:LEU:HB3	10:K:17:PRO:HD3	1.88	0.56
1:a:2029:TYR:C	1:a:2029:TYR:HD1	2.12	0.56
1:a:2183:MET:HG2	23:d:2355:CLA:HBC1	1.87	0.56
2:b:2174:LEU:HD22	2:b:2308:LYS:HZ2	1.70	0.56
4:d:2329:MET:O	4:d:2333:ASP:CB	2.54	0.56
13:o:2038:TYR:O	13:o:2245:PRO:CG	2.53	0.56
15:u:2040:VAL:O	15:u:2040:VAL:HG12	2.04	0.56
16:v:2010:VAL:HG13	16:v:2011:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:2012:LEU:O	19:z:2012:LEU:HD12	2.06	0.56
1:A:95:PRO:HD2	1:A:98:GLU:HB3	1.87	0.56
1:A:205:VAL:HG12	4:D:204:VAL:HG12	1.87	0.56
23:B:519:CLA:H142	23:D:356:CLA:H42	1.88	0.56
4:D:87:HIS:CD2	4:D:87:HIS:N	2.73	0.56
5:E:59:GLN:NE2	5:E:81:GLN:NE2	2.54	0.56
13:O:118:LEU:CD1	13:O:233:VAL:HG21	2.35	0.56
16:V:75:TYR:HE1	28:V:138:HEC:C2A	2.19	0.56
4:d:2231:THR:HG22	4:d:2232:PHE:H	1.70	0.56
5:e:2008:PRO:HB3	6:f:2018:ARG:HH22	1.71	0.56
13:o:2238:VAL:CG1	13:o:2239:PHE:N	2.69	0.56
14:t:2003:THR:O	14:t:2005:THR:N	2.38	0.56
2:B:340:TRP:CD1	2:B:340:TRP:H	2.23	0.55
3:C:354:GLU:C	3:C:356:MET:H	2.13	0.55
10:K:30:TRP:CZ3	10:K:31:GLN:NE2	2.74	0.55
14:T:3:THR:O	14:T:4:ILE:C	2.48	0.55
1:a:2295:PHE:CD1	1:a:2295:PHE:N	2.74	0.55
2:b:2191:ASN:HB2	2:b:2192:PRO:HD2	1.88	0.55
2:b:2205:ALA:O	23:b:2518:CLA:H191	2.07	0.55
23:b:2512:CLA:H203	23:b:2523:CLA:H192	1.88	0.55
3:c:2120:ILE:O	3:c:2124:VAL:HG23	2.06	0.55
4:d:2068:LEU:HA	6:f:2039:MET:HE3	1.86	0.55
4:d:2108:GLY:C	4:d:2110:LEU:N	2.59	0.55
4:d:2316:THR:HG23	13:o:2160:LYS:NZ	2.20	0.55
5:e:2060:ARG:NH2	16:v:2129:LYS:CE	2.59	0.55
1:A:159:LEU:CG	1:A:163:ILE:HD11	2.36	0.55
3:C:101:PRO:CA	3:C:195:ASP:HB3	2.36	0.55
3:C:331:ALA:O	3:C:338:GLY:HA2	2.05	0.55
4:D:257:PHE:CZ	25:D:357:PL9:H253	2.41	0.55
4:D:298:PHE:O	4:D:299:ILE:C	2.49	0.55
4:D:302:GLU:O	4:D:305:ALA:HB3	2.06	0.55
11:L:2:GLU:N	11:L:3:PRO:HD2	2.21	0.55
1:a:2183:MET:HB3	23:a:2348:CLA:HBC2	1.88	0.55
2:b:2110:ALA:HA	23:b:2522:CLA:H203	1.86	0.55
3:c:2284:PHE:O	3:c:2285:ILE:C	2.47	0.55
4:d:2072:ASN:OD1	4:d:2074:LEU:CB	2.54	0.55
4:d:2238:THR:C	4:d:2240:ALA:N	2.64	0.55
4:d:2281:MET:O	4:d:2284:ILE:N	2.38	0.55
13:o:2215:PHE:HB3	13:o:2237:GLY:N	2.21	0.55
16:v:2046:THR:HG22	16:v:2049:ASN:H	1.71	0.55
1:A:221:SER:CA	4:D:139:ARG:HB2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:LEU:HA	3:C:176:VAL:HG23	1.88	0.55
4:D:118:GLY:CA	24:D:355:PHO:H71	2.37	0.55
1:a:2269:ARG:HD3	1:a:2269:ARG:C	2.31	0.55
2:b:2047:PRO:HA	2:b:2078:TRP:HE1	1.71	0.55
2:b:2073:GLY:O	2:b:2092:SER:HB2	2.06	0.55
2:b:2223:GLN:HG3	2:b:2227:LYS:HE3	1.88	0.55
3:c:2094:THR:C	3:c:2096:GLY:N	2.65	0.55
23:c:2478:CLA:H162	23:c:2482:CLA:HMD2	1.87	0.55
4:d:2118:GLY:CA	24:d:2356:PHO:H71	2.36	0.55
13:o:2046:GLN:HG2	13:o:2047:PRO:N	2.20	0.55
14:t:2024:ARG:HG2	14:t:2025:GLU:H	1.68	0.55
1:A:142:TRP:HH2	1:A:273:PHE:HE1	1.54	0.55
1:A:189:GLU:CD	22:A:347:OEC:O1	2.37	0.55
1:a:2192:ILE:O	1:a:2193:LEU:C	2.50	0.55
1:a:2334:ARG:NH2	4:d:2312:GLU:OE2	2.40	0.55
2:b:2159:THR:O	2:b:2159:THR:HG22	2.06	0.55
3:c:2149:TYR:CG	3:c:2156:LYS:HG3	2.42	0.55
4:d:2052:THR:O	4:d:2066:SER:HB2	2.07	0.55
4:d:2153:PHE:CE1	24:d:2356:PHO:H92	2.41	0.55
4:d:2336:HIS:CD2	4:d:2336:HIS:N	2.69	0.55
13:o:2051:LEU:HD23	13:o:2066:VAL:O	2.06	0.55
19:z:2013:VAL:HG13	19:z:2017:PHE:CE1	2.41	0.55
1:A:12:ASN:O	1:A:15:GLU:HG3	2.06	0.55
2:B:326:ARG:HD3	27:B:529:BCR:C40	2.31	0.55
23:B:511:CLA:HBC3	7:H:33:PHE:CD2	2.42	0.55
3:C:285:ILE:HG12	23:C:487:CLA:CMB	2.37	0.55
3:C:285:ILE:HG12	23:C:487:CLA:HMB1	1.88	0.55
3:C:294:ASN:O	3:C:296:VAL:N	2.40	0.55
4:D:59:TYR:HE1	5:E:49:PRO:HG2	1.72	0.55
16:V:55:ARG:O	16:V:59:LEU:HG	2.07	0.55
1:a:2253:GLY:O	1:a:2257:ARG:HG2	2.06	0.55
1:a:2260:PHE:HB2	4:d:2027:PHE:CZ	2.41	0.55
1:a:2341:LEU:HD21	15:u:2134:LYS:HZ2	1.70	0.55
2:b:2153:PHE:O	2:b:2158:LEU:HG	2.06	0.55
2:b:2225:LEU:O	2:b:2231:MET:HG2	2.06	0.55
16:v:2022:THR:OG1	16:v:2025:GLN:HG3	2.07	0.55
16:v:2066:ARG:HE	16:v:2075:TYR:HB2	1.71	0.55
19:z:2019:MET:HE1	19:z:2043:GLY:CA	2.36	0.55
1:A:297:LEU:HD22	3:C:428:THR:HG21	1.87	0.55
1:A:325:ASN:HD22	1:A:325:ASN:N	2.05	0.55
2:B:12:LEU:HG	2:B:19:LEU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:522:CLA:HMD2	23:B:524:CLA:H202	1.89	0.55
13:O:153:THR:HG22	13:O:154:ALA:N	2.22	0.55
15:U:88:VAL:CG2	15:U:114:VAL:HG23	2.36	0.55
1:a:2097:TRP:CZ3	8:i:2008:VAL:HG21	2.40	0.55
1:a:2142:TRP:HH2	1:a:2273:PHE:HE1	1.55	0.55
1:a:2161:TYR:OH	1:a:2190:HIS:NE2	2.35	0.55
1:a:2193:LEU:HD13	4:d:2179:PHE:HB3	1.87	0.55
1:a:2272:HIS:ND1	4:d:2218:VAL:HG11	2.21	0.55
2:b:2044:THR:HB	2:b:2060:MET:HE1	1.87	0.55
2:b:2137:LYS:O	2:b:2141:ILE:HG12	2.06	0.55
2:b:2247:PHE:CE1	23:b:2521:CLA:H72	2.41	0.55
2:b:2297:THR:O	2:b:2298:LEU:C	2.48	0.55
3:c:2318:LEU:HD11	3:c:2351:PHE:HE2	1.71	0.55
27:c:2489:BCR:C31	19:z:2055:GLY:HA2	2.37	0.55
4:d:2235:PHE:CG	4:d:2236:ASN:N	2.75	0.55
16:v:2069:ILE:O	16:v:2073:VAL:HG23	2.07	0.55
16:v:2072:LEU:HD11	16:v:2120:LEU:HD21	1.89	0.55
1:A:224:ILE:O	1:A:224:ILE:HG22	2.06	0.55
2:B:6:TYR:N	2:B:6:TYR:CD2	2.75	0.55
2:B:12:LEU:HD21	2:B:19:LEU:HA	1.88	0.55
3:C:187:ASP:O	3:C:194:GLY:O	2.25	0.55
3:C:377:LEU:HD21	13:O:99:ASP:CG	2.32	0.55
7:H:21:ALA:HB3	7:H:22:PRO:CD	2.37	0.55
13:O:19:CYS:HB3	13:O:240:TYR:HB2	1.89	0.55
16:V:63:THR:HB	16:V:83:ASP:C	2.32	0.55
1:a:2184:ILE:CG2	1:a:2328:MET:CE	2.85	0.55
2:b:2321:LYS:HE2	2:b:2325:PHE:CZ	2.42	0.55
2:b:2451:PHE:CD1	2:b:2451:PHE:C	2.85	0.55
23:c:2476:CLA:H12	23:c:2483:CLA:H2	1.88	0.55
6:f:2040:GLN:OE1	9:j:2028:PHE:CD2	2.59	0.55
10:k:2016:LEU:HB3	10:k:2017:PRO:HD3	1.89	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.88	0.55
1:A:301:ASN:HD21	3:C:407:VAL:HG23	1.71	0.55
2:B:47:PRO:HA	2:B:78:TRP:HE1	1.72	0.55
3:C:98:GLY:O	3:C:105:VAL:HG13	2.07	0.55
3:C:116:VAL:HG13	27:C:488:BCR:C33	2.33	0.55
3:C:158:THR:O	3:C:161:LEU:HB3	2.07	0.55
3:C:447:ARG:HG3	3:C:447:ARG:O	2.06	0.55
23:C:478:CLA:C9	23:C:482:CLA:HAA1	2.36	0.55
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.41	0.55
6:F:31:PHE:HD2	6:F:31:PHE:C	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:54:GLU:CD	13:O:231:HIS:CE1	2.85	0.55
1:a:2029:TYR:CD2	1:a:2133:LEU:HD13	2.42	0.55
1:a:2083:VAL:HG12	1:a:2084:PRO:HD2	1.88	0.55
1:a:2302:PHE:N	1:a:2302:PHE:CD1	2.74	0.55
3:c:2264:PHE:N	3:c:2264:PHE:HD2	2.05	0.55
3:c:2320:ARG:CZ	15:u:2128:TYR:OH	2.55	0.55
4:d:2174:GLY:O	4:d:2178:ILE:HG12	2.07	0.55
9:j:2012:ILE:O	9:j:2016:VAL:HG23	2.05	0.55
1:A:180:PHE:CD2	4:D:192:THR:CG2	2.90	0.55
1:A:224:ILE:HD11	1:A:243:GLU:HG3	1.89	0.55
2:B:356:VAL:HG23	2:B:370:LEU:HD23	1.89	0.55
4:D:29:PHE:HE2	4:D:31:GLY:HA3	1.72	0.55
15:U:57:LEU:HD11	15:U:112:PHE:HB3	1.89	0.55
15:U:108:ASN:O	15:U:109:LEU:C	2.50	0.55
16:V:129:LYS:HZ3	16:V:135:VAL:CG2	2.20	0.55
1:a:2052:PHE:CE1	1:a:2081:ALA:HB2	2.42	0.55
1:a:2214:MET:CE	4:d:2142:ASN:OD1	2.55	0.55
2:b:2171:PRO:CG	7:h:2062:LYS:HA	2.37	0.55
2:b:2192:PRO:HG3	7:h:2048:TYR:HE1	1.64	0.55
3:c:2077:PRO:HA	3:c:2104:GLU:OE2	2.07	0.55
13:o:2112:GLY:C	13:o:2114:GLU:N	2.65	0.55
12:M:17:VAL:HG12	12:M:18:PRO:N	2.22	0.55
16:V:66:ARG:HH11	16:V:66:ARG:HG3	1.72	0.55
2:b:2302:TRP:CZ3	2:b:2343:HIS:HB2	2.42	0.55
3:c:2063:TRP:CZ3	3:c:2088:LEU:HD21	2.42	0.55
4:d:2057:SER:OG	4:d:2065:SER:HB2	2.07	0.55
10:k:2011:PRO:HB3	18:n:2009:UNK:CB	2.37	0.55
11:l:2028:ALA:O	11:l:2029:LEU:C	2.50	0.55
12:m:2016:LEU:O	12:m:2020:VAL:HG23	2.06	0.55
1:A:14:TRP:CH2	8:I:25:SER:HB3	2.42	0.54
1:A:291:SER:O	1:A:295:PHE:CE1	2.59	0.54
2:B:342:GLY:HA2	2:B:403:GLY:HA3	1.89	0.54
3:C:90:PRO:HB2	3:C:302:TYR:HE2	1.72	0.54
2:b:2046:ASP:OD1	2:b:2048:SER:OG	2.24	0.54
2:b:2231:MET:O	2:b:2231:MET:HE3	2.08	0.54
23:b:2518:CLA:H142	23:b:2524:CLA:HBA1	1.88	0.54
3:c:2071:GLU:C	3:c:2073:ALA:H	2.15	0.54
3:c:2131:TYR:HE1	3:c:2135:ARG:HD3	1.72	0.54
3:c:2138:GLU:CG	3:c:2139:THR:H	2.14	0.54
3:c:2264:PHE:N	3:c:2264:PHE:CD2	2.75	0.54
23:c:2478:CLA:C9	23:c:2482:CLA:HAA1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2195:PRO:HG2	4:d:2196:PHE:H	1.72	0.54
5:e:2043:TYR:O	5:e:2047:GLY:N	2.37	0.54
11:l:2006:ASN:HD22	11:l:2006:ASN:N	2.04	0.54
13:o:2106:VAL:HG22	13:o:2117:PRO:CB	2.34	0.54
1:A:139:MET:HE2	4:D:248:THR:CG2	2.37	0.54
2:B:302:TRP:CZ3	2:B:343:HIS:HB2	2.43	0.54
3:C:182:PHE:O	3:C:184:GLY:N	2.41	0.54
4:D:71:CYS:HB3	4:D:75:THR:CB	2.38	0.54
10:K:19:ILE:HG13	10:K:20:PRO:HD3	1.89	0.54
13:O:211:ILE:CG2	13:O:212:ALA:N	2.70	0.54
15:U:51:TYR:O	15:U:53:GLU:N	2.40	0.54
15:U:84:PRO:C	15:U:85:TYR:CD2	2.85	0.54
1:a:2135:TYR:CZ	8:i:2032:PRO:HG3	2.42	0.54
13:o:2120:PHE:HE1	13:o:2235:ILE:HG21	1.71	0.54
13:o:2136:ILE:HG22	13:o:2137:THR:N	2.22	0.54
1:A:97:TRP:CE3	8:I:5:LYS:HA	2.43	0.54
1:A:142:TRP:N	4:D:220:ASN:OD1	2.40	0.54
1:A:334:ARG:O	1:A:335:ASN:ND2	2.40	0.54
2:B:6:TYR:OH	12:M:21:PHE:CZ	2.35	0.54
2:B:159:THR:O	2:B:159:THR:HG22	2.07	0.54
3:C:50:LEU:O	3:C:54:VAL:HG23	2.07	0.54
4:D:30:VAL:HG22	4:D:38:PHE:HE1	1.71	0.54
13:O:22:LEU:O	13:O:203:LYS:CD	2.55	0.54
16:V:92:HIS:ND1	16:V:93:PRO:HD2	2.22	0.54
19:Z:17:PHE:O	19:Z:21:ILE:HG13	2.06	0.54
1:a:2261:GLN:HG3	1:a:2262:TYR:H	1.72	0.54
2:b:2021:ALA:O	2:b:2024:LEU:HB2	2.08	0.54
2:b:2324:LEU:HD13	11:l:2034:TYR:HB3	1.88	0.54
3:c:2120:ILE:HG21	27:c:2489:BCR:H353	1.89	0.54
23:c:2486:CLA:H61	27:c:2488:BCR:H393	1.89	0.54
4:d:2071:CYS:HB3	4:d:2075:THR:CG2	2.37	0.54
10:k:2002:LEU:H	10:k:2003:PRO:HD3	1.71	0.54
13:o:2050:PHE:HZ	13:o:2076:THR:CG2	2.19	0.54
19:z:2003:ILE:O	19:z:2007:LEU:HG	2.06	0.54
1:A:278:TRP:HE1	23:A:350:CLA:H42	1.73	0.54
2:B:45:PHE:HE1	2:B:55:MET:HA	1.72	0.54
3:C:199:ILE:CD1	3:C:234:VAL:HG21	2.33	0.54
4:D:90:LEU:HD13	4:D:96:GLU:HB3	1.87	0.54
13:O:140:THR:HG21	13:O:201:VAL:HB	1.88	0.54
13:O:243:ILE:HG22	13:O:244:GLU:N	2.22	0.54
1:a:2202:VAL:O	1:a:2206:PHE:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2062:VAL:O	2:b:2063:LEU:C	2.51	0.54
23:b:2513:CLA:H18	23:b:2524:CLA:CGA	2.37	0.54
4:d:2122:LEU:HD21	23:d:2354:CLA:H92	1.89	0.54
4:d:2199:MET:O	4:d:2202:ALA:HB3	2.07	0.54
11:l:2008:GLN:N	11:l:2009:PRO:HD3	2.22	0.54
13:o:2045:LEU:HD12	13:o:2239:PHE:HB2	1.90	0.54
1:A:308:ASP:O	1:A:309:ALA:C	2.50	0.54
2:B:321:LYS:HE2	2:B:325:PHE:HZ	1.71	0.54
3:C:88:LEU:O	3:C:89:ILE:C	2.50	0.54
1:a:2334:ARG:O	1:a:2335:ASN:ND2	2.39	0.54
4:d:2161:PRO:HG2	4:d:2170:ALA:CB	2.37	0.54
4:d:2188:PHE:O	4:d:2294:ARG:NH1	2.41	0.54
10:k:2001:LYS:HG2	10:k:2003:PRO:HD2	1.89	0.54
15:u:2108:ASN:O	15:u:2109:LEU:C	2.51	0.54
1:A:63:ILE:HG23	3:C:335:THR:HG21	1.89	0.54
1:A:133:LEU:HD21	4:D:252:PHE:HA	1.90	0.54
1:A:180:PHE:HD2	4:D:192:THR:HB	1.72	0.54
1:A:302:PHE:N	1:A:302:PHE:CD1	2.75	0.54
2:B:297:THR:O	2:B:298:LEU:C	2.48	0.54
2:B:371:THR:HG22	2:B:372:ASP:N	2.23	0.54
2:B:402:TYR:N	2:B:402:TYR:HD1	2.06	0.54
3:C:88:LEU:O	3:C:91:HIS:N	2.40	0.54
4:D:29:PHE:HD2	4:D:29:PHE:O	1.91	0.54
6:F:31:PHE:C	6:F:31:PHE:CD2	2.83	0.54
1:a:2254:TYR:OH	4:d:2129:GLN:HG2	2.08	0.54
1:a:2281:VAL:O	1:a:2281:VAL:HG12	2.07	0.54
2:b:2324:LEU:HD12	11:l:2034:TYR:HD2	1.73	0.54
2:b:2326:ARG:C	27:b:2528:BCR:H292	2.33	0.54
3:c:2040:ALA:O	3:c:2043:ILE:HG23	2.07	0.54
3:c:2062:PHE:HE2	10:k:2020:PRO:HD3	1.72	0.54
7:h:2024:TRP:HA	7:h:2024:TRP:CE3	2.42	0.54
10:k:2016:LEU:N	10:k:2017:PRO:HD2	2.23	0.54
1:A:258:LEU:O	4:D:128:ARG:NH2	2.40	0.54
2:B:110:ALA:O	2:B:113:TRP:N	2.37	0.54
4:D:52:THR:O	4:D:76:VAL:HG11	2.08	0.54
4:D:87:HIS:CE1	4:D:162:LEU:HA	2.43	0.54
4:D:336:HIS:HD2	4:D:336:HIS:N	1.99	0.54
6:F:19:TRP:CH2	6:F:23:HIS:NE2	2.76	0.54
16:V:76:MET:HE3	28:V:138:HEC:CMB	2.38	0.54
19:Z:37:LYS:O	19:Z:41:PHE:HD1	1.90	0.54
3:c:2278:ALA:HB1	23:c:2479:CLA:H142	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:2007:LEU:O	19:z:2011:ALA:HB2	2.07	0.54
1:A:89:ILE:CG2	1:A:94:TYR:HB2	2.38	0.54
1:A:243:GLU:HA	4:D:240:ALA:CB	2.34	0.54
2:B:66:MET:HE3	2:B:96:VAL:HG11	1.89	0.54
2:B:134:ASP:OD2	2:B:220:ARG:NH2	2.40	0.54
2:B:183:PRO:HD3	2:B:199:VAL:HG11	1.90	0.54
27:C:489:BCR:C31	19:Z:55:GLY:HA2	2.37	0.54
4:D:221:THR:O	4:D:221:THR:CG2	2.56	0.54
4:D:281:MET:O	4:D:284:ILE:N	2.40	0.54
13:O:193:THR:HG22	13:O:194:LYS:N	2.11	0.54
1:a:2307:ILE:O	1:a:2307:ILE:HG22	2.07	0.54
2:b:2183:PRO:HD3	2:b:2199:VAL:HG11	1.90	0.54
2:b:2247:PHE:O	2:b:2251:VAL:HG23	2.07	0.54
3:c:2169:GLY:O	3:c:2173:LEU:HG	2.08	0.54
5:e:2014:THR:HG22	9:j:2008:ILE:HD12	1.89	0.54
13:o:2101:ILE:HG22	13:o:2102:ASP:N	2.22	0.54
15:u:2056:ASP:CG	15:u:2059:ASN:HD21	2.16	0.54
16:v:2063:THR:HB	16:v:2083:ASP:C	2.33	0.54
1:A:131:TRP:CE3	1:A:132:GLU:N	2.76	0.54
1:A:320:ILE:O	1:A:320:ILE:CG2	2.55	0.54
2:B:153:PHE:O	2:B:158:LEU:HG	2.07	0.54
3:C:285:ILE:O	23:C:487:CLA:HBB1	2.07	0.54
3:C:297:TYR:O	3:C:298:PRO:C	2.51	0.54
4:D:83:ASN:HB3	4:D:336:HIS:ND1	2.23	0.54
6:F:17:VAL:O	6:F:18:ARG:C	2.50	0.54
7:H:57:VAL:O	7:H:57:VAL:HG12	2.07	0.54
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.07	0.54
16:V:37:CYS:O	16:V:38:ALA:C	2.50	0.54
1:a:2308:ASP:O	1:a:2309:ALA:C	2.49	0.54
23:b:2520:CLA:HAA2	23:b:2520:CLA:CBD	2.33	0.54
3:c:2040:ALA:O	3:c:2043:ILE:HG12	2.08	0.54
1:A:114:LEU:HD12	1:A:118:HIS:CE1	2.43	0.54
4:D:156:VAL:CG1	4:D:171:PRO:HG2	2.38	0.54
15:U:72:TYR:HD2	15:U:73:PRO:CD	2.20	0.54
2:b:2209:GLY:HA3	23:b:2518:CLA:H201	1.89	0.54
2:b:2360:PRO:C	2:b:2362:PHE:H	2.16	0.54
23:b:2521:CLA:HAB	23:b:2526:CLA:CED	2.31	0.54
13:o:2197:ILE:HD11	13:o:2215:PHE:CE1	2.43	0.54
15:u:2083:ALA:HB1	15:u:2084:PRO:HA	1.89	0.54
2:B:21:ALA:O	2:B:24:LEU:HB2	2.08	0.53
2:B:209:GLY:HA3	23:B:518:CLA:H201	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:152:VAL:HG13	23:D:354:CLA:CED	2.38	0.53
1:a:2029:TYR:HE1	1:a:2031:GLY:CA	2.21	0.53
1:a:2187:GLN:NE2	1:a:2187:GLN:C	2.66	0.53
1:a:2316:THR:O	1:a:2317:TRP:C	2.48	0.53
2:b:2402:TYR:N	2:b:2402:TYR:HD1	2.06	0.53
4:d:2083:ASN:O	4:d:2083:ASN:ND2	2.40	0.53
13:o:2010:ILE:HG23	13:o:2015:LEU:HB2	1.90	0.53
1:A:301:ASN:CG	1:A:301:ASN:O	2.51	0.53
2:B:360:PRO:C	2:B:362:PHE:H	2.16	0.53
3:C:60:ILE:HG22	23:C:480:CLA:HMD3	1.91	0.53
3:C:324:LEU:HD12	15:U:128:TYR:CZ	2.43	0.53
3:C:417:VAL:HG22	16:V:38:ALA:HB1	1.90	0.53
4:D:20:ASP:O	4:D:21:TRP:C	2.50	0.53
4:D:319:LEU:CA	4:D:322:ASN:HD22	2.14	0.53
5:E:68:ARG:HH12	7:H:50:SER:HB3	1.72	0.53
13:O:152:ARG:HD2	13:O:156:PHE:CD2	2.43	0.53
16:V:22:THR:N	16:V:25:GLN:HE21	2.06	0.53
19:Z:36:SER:HA	19:Z:39:LEU:HD12	1.89	0.53
1:a:2214:MET:CE	4:d:2142:ASN:HD21	2.22	0.53
1:a:2285:PHE:O	1:a:2288:LEU:HB2	2.09	0.53
2:b:2190:PHE:CE1	23:b:2526:CLA:HED3	2.43	0.53
3:c:2305:THR:CA	3:c:2423:ARG:NH1	2.70	0.53
4:d:2078:VAL:HB	4:d:2173:PHE:HB2	1.90	0.53
4:d:2080:THR:HG21	4:d:2167:TRP:O	2.08	0.53
4:d:2257:PHE:CD2	4:d:2259:ILE:HG22	2.43	0.53
6:f:2017:VAL:O	6:f:2018:ARG:C	2.51	0.53
12:m:2019:SER:O	12:m:2023:ILE:HG12	2.09	0.53
14:t:2022:PHE:C	14:t:2023:PHE:HD1	2.15	0.53
2:B:6:TYR:CE1	2:B:8:VAL:HG21	2.42	0.53
2:B:44:THR:HB	2:B:60:MET:HE1	1.89	0.53
2:B:62:VAL:O	2:B:63:LEU:C	2.51	0.53
2:B:137:LYS:O	2:B:141:ILE:HG12	2.09	0.53
23:B:513:CLA:H18	23:B:524:CLA:CGA	2.38	0.53
23:B:518:CLA:C14	23:B:524:CLA:HBA1	2.38	0.53
3:C:55:ALA:HB1	27:C:488:BCR:H371	1.90	0.53
3:C:88:LEU:HD22	23:C:480:CLA:CGD	2.39	0.53
4:D:179:PHE:HA	4:D:182:LEU:CD1	2.38	0.53
4:D:195:PRO:O	4:D:198:MET:HB2	2.09	0.53
13:O:133:VAL:O	13:O:133:VAL:HG12	2.07	0.53
15:U:47:LEU:C	15:U:49:THR:H	2.16	0.53
1:a:2031:GLY:O	1:a:2034:GLY:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2258:LEU:C	4:d:2128:ARG:NH2	2.67	0.53
2:b:2148:LEU:O	2:b:2151:PHE:HB3	2.09	0.53
3:c:2054:VAL:O	3:c:2054:VAL:HG12	2.08	0.53
3:c:2071:GLU:C	3:c:2073:ALA:N	2.66	0.53
4:d:2028:VAL:HB	6:f:2017:VAL:HG13	1.91	0.53
27:k:2050:BCR:H333	19:z:2017:PHE:HA	1.90	0.53
13:o:2065:PHE:N	13:o:2065:PHE:CD1	2.76	0.53
14:t:2022:PHE:N	14:t:2022:PHE:CD2	2.74	0.53
1:A:213:ALA:O	1:A:217:SER:HB2	2.08	0.53
1:A:292:THR:HG23	3:C:428:THR:HG23	1.91	0.53
2:B:194:ASN:C	2:B:196:GLY:N	2.66	0.53
2:B:234:ILE:CG2	23:B:524:CLA:H193	2.38	0.53
2:B:475:PHE:O	2:B:476:ARG:C	2.51	0.53
23:B:518:CLA:H141	23:B:524:CLA:HMA2	1.90	0.53
3:C:165:LEU:HD21	23:C:474:CLA:CBB	2.38	0.53
4:D:83:ASN:CB	4:D:336:HIS:HD1	2.22	0.53
4:D:201:VAL:O	4:D:201:VAL:HG12	2.09	0.53
13:O:79:ASP:HA	13:O:101:ILE:HG21	1.91	0.53
2:b:2393:GLU:OE1	2:b:2393:GLU:N	2.41	0.53
3:c:2340:TYR:CD1	3:c:2340:TYR:N	2.77	0.53
4:d:2154:VAL:CG1	4:d:2158:LEU:HD12	2.27	0.53
13:o:2054:GLU:CD	13:o:2231:HIS:CE1	2.86	0.53
13:o:2143:LYS:CD	13:o:2198:SER:HB2	2.39	0.53
14:t:2009:ILE:HG22	14:t:2009:ILE:O	2.06	0.53
16:v:2055:ARG:HG3	16:v:2056:THR:H	1.72	0.53
2:B:321:LYS:HE3	2:B:325:PHE:CZ	2.43	0.53
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.91	0.53
3:C:186:TYR:C	3:C:186:TYR:CD2	2.86	0.53
3:C:255:THR:HG23	3:C:256:PRO:HD2	1.89	0.53
3:C:293:ASN:CG	3:C:423:ARG:NH2	2.67	0.53
3:C:318:LEU:HD22	3:C:328:VAL:CG2	2.38	0.53
15:U:75:LEU:HD21	15:U:101:GLN:NE2	2.24	0.53
1:a:2205:VAL:HG21	23:a:2348:CLA:HMA2	1.91	0.53
1:a:2223:LEU:O	1:a:2225:ARG:HG3	2.07	0.53
3:c:2317:PHE:O	3:c:2321:ASP:OD1	2.27	0.53
23:c:2487:CLA:HBC2	23:c:2487:CLA:HHD	1.89	0.53
5:e:2012:ILE:HD12	28:e:2084:HEC:CBD	2.38	0.53
7:h:2024:TRP:HA	7:h:2024:TRP:HE3	1.73	0.53
1:A:307:ILE:C	1:A:309:ALA:H	2.16	0.53
2:B:313:ASP:O	2:B:313:ASP:OD1	2.26	0.53
3:C:176:VAL:HG13	3:C:234:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:ILE:HG13	5:E:27:PRO:HD3	1.89	0.53
12:M:5:GLN:HG2	12:m:2005:GLN:CG	2.38	0.53
12:M:8:LEU:HD22	14:T:1:MET:HE3	1.89	0.53
16:V:40:CYS:SG	28:V:138:HEC:CAC	2.97	0.53
2:b:2342:GLY:HA2	2:b:2403:GLY:HA3	1.90	0.53
23:b:2519:CLA:C14	23:d:2357:CLA:H11	2.39	0.53
3:c:2188:THR:HG22	3:c:2364:PRO:HG2	1.90	0.53
4:d:2055:VAL:HG12	4:d:2056:THR:N	2.22	0.53
4:d:2253:TRP:HA	4:d:2253:TRP:HE3	1.74	0.53
5:e:2019:TRP:HZ2	9:j:2013:VAL:HG22	1.73	0.53
7:h:2030:MET:O	7:h:2033:PHE:N	2.39	0.53
13:o:2152:ARG:HD2	13:o:2156:PHE:CD1	2.43	0.53
13:o:2193:THR:HG21	13:o:2220:LEU:HD12	1.89	0.53
13:o:2211:ILE:HB	13:o:2241:ALA:HB3	1.90	0.53
15:u:2115:THR:HG22	15:u:2116:GLU:N	2.24	0.53
18:n:2031:UNK:HA	19:z:2030:PRO:CG	2.39	0.53
2:B:308:LYS:HE2	2:B:312:TYR:CE2	2.43	0.53
3:C:291:TRP:O	3:C:305:THR:HG23	2.08	0.53
3:C:384:ILE:HG23	3:C:384:ILE:O	2.06	0.53
15:U:72:TYR:CG	15:U:73:PRO:N	2.74	0.53
16:V:122:GLU:HB3	16:V:123:PRO:CD	2.39	0.53
1:a:2335:ASN:C	1:a:2335:ASN:ND2	2.66	0.53
2:b:2371:THR:HG22	2:b:2372:ASP:N	2.23	0.53
23:b:2518:CLA:C14	23:b:2524:CLA:HBA1	2.39	0.53
3:c:2123:ALA:HB1	19:z:2047:TRP:CH2	2.38	0.53
3:c:2305:THR:HG22	3:c:2307:PRO:CD	2.30	0.53
4:d:2191:TRP:HE1	4:d:2197:HIS:CD2	2.26	0.53
5:e:2048:THR:O	5:e:2049:PRO:O	2.26	0.53
13:o:2046:GLN:O	13:o:2238:VAL:O	2.27	0.53
1:A:29:TYR:HE1	1:A:31:GLY:HA3	1.73	0.53
1:A:31:GLY:O	1:A:34:GLY:N	2.38	0.53
1:A:306:VAL:CG2	1:A:307:ILE:N	2.69	0.53
2:B:62:VAL:HG11	23:B:518:CLA:HED3	1.91	0.53
2:B:263:THR:HG22	2:B:263:THR:O	2.09	0.53
2:B:302:TRP:C	2:B:304:ALA:H	2.17	0.53
2:B:340:TRP:CE3	2:B:342:GLY:HA3	2.44	0.53
2:B:381:ILE:HG22	2:B:381:ILE:O	2.09	0.53
2:B:479:PHE:O	4:D:139:ARG:NH2	2.29	0.53
14:T:10:PHE:CE2	14:T:14:ILE:HD11	2.43	0.53
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.33	0.53
16:V:13:ASN:C	16:V:13:ASN:OD1	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:52:LEU:HD23	28:V:138:HEC:HAD2	1.90	0.53
1:a:2150:PRO:O	1:a:2153:SER:HB3	2.09	0.53
1:a:2214:MET:HE2	4:d:2142:ASN:ND2	2.24	0.53
2:b:2324:LEU:HD12	11:l:2034:TYR:CD2	2.43	0.53
3:c:2249:ILE:HA	3:c:2252:ILE:HD12	1.91	0.53
3:c:2344:SER:O	3:c:2347:GLY:N	2.34	0.53
1:A:180:PHE:HE2	4:D:192:THR:C	2.17	0.53
4:D:83:ASN:CG	4:D:336:HIS:HD1	2.16	0.53
6:F:20:VAL:O	6:F:21:ALA:C	2.52	0.53
16:V:78:ASN:ND2	16:V:87:GLU:OE2	2.42	0.53
1:a:2063:ILE:CG2	3:c:2335:THR:CG2	2.86	0.53
1:a:2149:ALA:HB3	1:a:2150:PRO:CD	2.39	0.53
1:a:2180:PHE:O	1:a:2184:ILE:HG13	2.09	0.53
1:a:2200:LEU:O	1:a:2203:ALA:HB3	2.08	0.53
2:b:2045:PHE:CE2	2:b:2046:ASP:O	2.61	0.53
2:b:2234:ILE:CG2	23:b:2524:CLA:H193	2.39	0.53
23:b:2517:CLA:HMA2	23:b:2521:CLA:HED3	1.90	0.53
3:c:2120:ILE:CG2	27:c:2489:BCR:H353	2.39	0.53
3:c:2187:ASP:O	3:c:2194:GLY:O	2.27	0.53
4:d:2325:ILE:HG22	4:d:2329:MET:CE	2.39	0.53
7:h:2027:THR:N	7:h:2028:PRO:CD	2.72	0.53
7:h:2049:ASN:OD1	7:h:2049:ASN:O	2.27	0.53
8:i:2019:PHE:CE1	8:i:2023:PHE:CE1	2.94	0.53
1:A:23:SER:OG	1:A:24:THR:N	2.41	0.53
2:B:236:THR:O	2:B:240:SER:HB3	2.09	0.53
3:C:112:PHE:O	3:C:116:VAL:HG23	2.09	0.53
3:C:294:ASN:O	3:C:295:THR:C	2.50	0.53
6:F:30:ILE:O	6:F:30:ILE:HG22	2.09	0.53
1:a:2040:THR:HG21	1:a:2122:GLY:HA3	1.91	0.53
1:a:2168:PHE:O	1:a:2169:SER:C	2.52	0.53
1:a:2278:TRP:HE1	23:a:2349:CLA:H42	1.73	0.53
2:b:2199:VAL:O	2:b:2203:ILE:HG13	2.08	0.53
3:c:2080:PRO:O	3:c:2081:MET:C	2.52	0.53
3:c:2284:PHE:CD1	3:c:2434:ALA:HB1	2.44	0.53
4:d:2020:ASP:O	4:d:2021:TRP:C	2.51	0.53
4:d:2052:THR:HG23	4:d:2076:VAL:CG1	2.39	0.53
4:d:2086:GLY:C	4:d:2087:HIS:CD2	2.87	0.53
4:d:2087:HIS:HA	4:d:2167:TRP:NE1	2.24	0.53
4:d:2130:PHE:HE2	4:d:2140:PRO:HB2	1.74	0.53
9:j:2015:THR:CA	27:k:2050:BCR:H372	2.36	0.53
15:u:2094:ILE:HB	15:u:2097:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:2098:ALA:HB1	16:v:2105:ARG:HG2	1.90	0.53
1:A:63:ILE:CD1	1:A:336:ALA:HB2	2.38	0.52
2:B:344:ALA:HB2	2:B:401:PHE:HE1	1.74	0.52
2:B:421:ALA:O	2:B:424:ALA:HB3	2.08	0.52
3:C:71:GLU:C	3:C:73:ALA:H	2.15	0.52
10:K:16:LEU:HB3	10:K:17:PRO:HD2	1.90	0.52
19:Z:37:LYS:HA	19:Z:40:ILE:HD12	1.91	0.52
1:a:2283:VAL:O	1:a:2284:TRP:C	2.53	0.52
2:b:2057:ARG:HH12	2:b:2317:ASN:CG	2.17	0.52
2:b:2183:PRO:HB2	2:b:2200:ALA:HB2	1.91	0.52
2:b:2272:ARG:HH12	4:d:2164:GLN:HG2	1.73	0.52
3:c:2088:LEU:O	3:c:2091:HIS:N	2.41	0.52
3:c:2134:ILE:HD11	23:c:2486:CLA:H52	1.92	0.52
4:d:2302:GLU:OE2	13:o:2173:ALA:CB	2.57	0.52
15:u:2062:ILE:O	15:u:2064:ALA:N	2.42	0.52
15:u:2109:LEU:HA	15:u:2112:PHE:CD1	2.44	0.52
19:z:2040:ILE:HG22	19:z:2041:PHE:N	2.23	0.52
19:z:2041:PHE:H	19:z:2041:PHE:HD1	1.57	0.52
1:A:217:SER:OG	4:D:142:ASN:HA	2.09	0.52
3:C:71:GLU:C	3:C:73:ALA:N	2.67	0.52
3:C:292:PHE:CE1	23:C:487:CLA:HBC3	2.43	0.52
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.44	0.52
5:E:48:THR:O	5:E:49:PRO:O	2.27	0.52
7:H:22:PRO:O	7:H:23:GLY:O	2.26	0.52
16:V:25:GLN:O	16:V:26:TYR:C	2.52	0.52
1:a:2054:ALA:O	1:a:2055:ALA:C	2.52	0.52
3:c:2287:THR:O	3:c:2290:VAL:HB	2.09	0.52
4:d:2244:TYR:CZ	4:d:2264:LYS:NZ	2.75	0.52
4:d:2337:GLU:HB2	4:d:2339:PHE:CE1	2.44	0.52
6:f:2036:ILE:HA	6:f:2039:MET:HG3	1.91	0.52
13:o:2201:VAL:HG11	13:o:2204:VAL:HG23	1.91	0.52
15:u:2099:GLU:OE1	15:u:2099:GLU:HA	2.09	0.52
1:A:218:LEU:HD23	4:D:142:ASN:HD22	1.74	0.52
1:A:223:LEU:O	1:A:225:ARG:HG3	2.09	0.52
2:B:46:ASP:OD1	2:B:48:SER:OG	2.19	0.52
2:B:328:GLY:HA3	23:B:514:CLA:O1A	2.10	0.52
13:O:27:ARG:C	13:O:29:ALA:N	2.68	0.52
14:T:18:PHE:HD2	14:T:19:PHE:HD1	1.56	0.52
2:b:2134:ASP:OD2	2:b:2220:ARG:NH2	2.42	0.52
2:b:2149:LEU:O	2:b:2150:CYS:C	2.51	0.52
3:c:2150:ASP:O	3:c:2157:MET:HE3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2273:SER:HB3	3:c:2445:ALA:HB2	1.91	0.52
13:o:2122:VAL:O	13:o:2122:VAL:HG12	2.07	0.52
13:o:2157:LEU:HD21	13:o:2166:SER:HB3	1.90	0.52
1:A:246:TYR:HE1	1:A:248:ILE:HG12	1.74	0.52
2:B:213:GLY:O	2:B:217:ILE:HG13	2.10	0.52
2:B:326:ARG:C	27:B:529:BCR:H292	2.34	0.52
2:B:394:GLN:CD	15:U:52:GLY:HA3	2.34	0.52
3:C:201:ASN:O	3:C:201:ASN:ND2	2.41	0.52
4:D:83:ASN:OD1	4:D:336:HIS:ND1	2.39	0.52
23:D:356:CLA:H12	7:H:42:LEU:HD21	1.91	0.52
5:E:43:TYR:O	5:E:47:GLY:N	2.42	0.52
10:K:19:ILE:CG1	10:K:20:PRO:HD3	2.39	0.52
2:b:2321:LYS:HE3	2:b:2325:PHE:CZ	2.44	0.52
7:h:2053:ILE:HG22	17:x:2015:SER:CB	2.38	0.52
13:o:2001:ALA:O	13:o:2002:LYS:HB2	2.09	0.52
13:o:2017:ASN:CG	13:o:2077:SER:OG	2.52	0.52
1:A:52:PHE:CD2	1:A:52:PHE:O	2.63	0.52
1:A:283:VAL:O	1:A:284:TRP:C	2.52	0.52
2:B:62:VAL:CG1	23:B:518:CLA:HED3	2.40	0.52
4:D:268:HIS:O	4:D:271:MET:HB2	2.10	0.52
7:H:51:THR:HG22	7:H:51:THR:O	2.10	0.52
13:O:201:VAL:CG1	13:O:211:ILE:HG23	2.37	0.52
1:a:2165:GLN:HE22	1:a:2344:ALA:C	2.16	0.52
1:a:2205:VAL:HG12	4:d:2204:VAL:HG12	1.92	0.52
1:a:2261:GLN:HG3	1:a:2262:TYR:N	2.25	0.52
1:a:2307:ILE:C	1:a:2309:ALA:N	2.66	0.52
2:b:2213:GLY:O	2:b:2217:ILE:HG13	2.10	0.52
2:b:2307:GLU:O	2:b:2308:LYS:C	2.52	0.52
23:b:2521:CLA:H112	23:d:2357:CLA:H92	1.92	0.52
3:c:2297:TYR:CG	3:c:2302:TYR:HE1	2.26	0.52
3:c:2297:TYR:O	3:c:2298:PRO:C	2.52	0.52
6:f:2019:TRP:CZ3	6:f:2023:HIS:CE1	2.98	0.52
13:o:2039:ARG:HA	13:o:2245:PRO:CG	2.40	0.52
13:o:2239:PHE:CD1	13:o:2239:PHE:C	2.88	0.52
16:v:2095:LEU:HD11	16:v:2112:LEU:HD11	1.92	0.52
1:A:53:ILE:O	1:A:53:ILE:HG22	2.10	0.52
1:A:295:PHE:CD1	1:A:295:PHE:N	2.76	0.52
4:D:87:HIS:HA	4:D:167:TRP:NE1	2.25	0.52
2:b:2091:TRP:CB	23:b:2515:CLA:H43	2.40	0.52
2:b:2301:ALA:O	2:b:2304:ALA:HB3	2.10	0.52
5:e:2060:ARG:HH22	16:v:2129:LYS:HZ2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:2058:ASN:ND2	15:u:2114:VAL:HG13	2.24	0.52
1:A:303:ASN:O	1:A:304:HIS:ND1	2.40	0.52
2:B:110:ALA:HA	23:B:522:CLA:H203	1.90	0.52
2:B:247:PHE:O	2:B:251:VAL:HG23	2.09	0.52
23:B:520:CLA:H201	12:M:18:PRO:HB3	1.92	0.52
3:C:122:SER:O	27:C:488:BCR:H363	2.09	0.52
3:C:278:ALA:O	3:C:282:MET:HG3	2.09	0.52
4:D:286:VAL:HG21	23:D:354:CLA:HED2	1.92	0.52
19:Z:5:PHE:CZ	19:Z:54:VAL:HG13	2.45	0.52
1:a:2330:VAL:CG1	4:d:2348:ARG:HA	2.39	0.52
2:b:2402:TYR:N	2:b:2402:TYR:CD1	2.77	0.52
15:u:2117:VAL:HG13	15:u:2122:VAL:HG21	1.92	0.52
16:v:2129:LYS:HE2	16:v:2135:VAL:HG23	1.91	0.52
1:A:153:SER:OG	23:A:348:CLA:HED1	2.09	0.52
1:A:192:ILE:HG12	1:A:293:MET:HE1	1.92	0.52
3:C:264:PHE:CZ	23:C:474:CLA:CGA	2.92	0.52
3:C:289:PHE:O	3:C:289:PHE:HD2	1.92	0.52
4:D:83:ASN:HB3	4:D:336:HIS:HD1	1.75	0.52
4:D:122:LEU:HD21	23:D:354:CLA:H92	1.92	0.52
13:O:38:TYR:O	13:O:245:PRO:HB2	2.09	0.52
13:O:52:VAL:HG11	13:O:116:ILE:HD13	1.91	0.52
13:O:122:VAL:HA	13:O:146:PHE:CD2	2.43	0.52
14:T:18:PHE:CD2	14:T:19:PHE:CD1	2.95	0.52
15:U:62:ILE:O	15:U:64:ALA:N	2.42	0.52
1:a:2307:ILE:HG12	1:a:2314:ILE:HD11	1.90	0.52
2:b:2029:LEU:HD11	27:b:2528:BCR:H331	1.92	0.52
2:b:2238:LEU:O	2:b:2242:ILE:HG13	2.10	0.52
2:b:2421:ALA:O	2:b:2424:ALA:HB3	2.10	0.52
23:b:2520:CLA:H161	12:m:2017:VAL:CG1	2.40	0.52
3:c:2063:TRP:CZ3	3:c:2088:LEU:HD11	2.45	0.52
3:c:2182:PHE:O	3:c:2184:GLY:N	2.43	0.52
3:c:2413:GLU:OE1	16:v:2042:VAL:HG11	2.10	0.52
6:f:2031:PHE:O	6:f:2031:PHE:HD2	1.92	0.52
7:h:2028:PRO:O	7:h:2032:VAL:HG23	2.09	0.52
10:k:2019:ILE:HG13	10:k:2020:PRO:HD3	1.92	0.52
13:o:2153:THR:HG22	13:o:2154:ALA:H	1.74	0.52
3:C:131:TYR:HE1	3:C:135:ARG:CD	2.23	0.52
3:C:316:THR:HG21	3:C:396:MET:CE	2.39	0.52
8:I:32:PRO:HG2	8:I:35:LYS:O	2.09	0.52
1:a:2112:TYR:CZ	1:a:2116:ILE:HD11	2.45	0.52
1:a:2252:HIS:CE1	1:a:2264:SER:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2250:PHE:CE1	2:b:2459:ALA:HB1	2.45	0.52
23:b:2518:CLA:C14	23:b:2524:CLA:HMA1	2.37	0.52
3:c:2269:GLU:OE1	3:c:2447:ARG:HG2	2.10	0.52
3:c:2342:MET:HE3	3:c:2352:GLY:CA	2.40	0.52
4:d:2147:SER:HG	4:d:2280:TRP:HZ2	1.56	0.52
6:f:2040:GLN:OE1	9:j:2028:PHE:HD2	1.93	0.52
11:l:2003:PRO:C	11:l:2005:PRO:HD3	2.35	0.52
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.45	0.52
1:A:260:PHE:O	1:A:263:ALA:HB3	2.09	0.52
1:A:340:PRO:O	4:D:352:LEU:HD23	2.10	0.52
23:B:522:CLA:H171	23:B:525:CLA:HMD3	1.92	0.52
3:C:79:LYS:O	3:C:80:PRO:C	2.53	0.52
3:C:350:ILE:HG22	3:C:351:PHE:O	2.10	0.52
23:C:478:CLA:H162	23:C:482:CLA:HMD2	1.92	0.52
13:O:17:ASN:ND2	13:O:77:SER:OG	2.43	0.52
13:O:233:VAL:CG1	13:O:234:LYS:N	2.72	0.52
1:a:2236:GLY:N	4:d:2265:ARG:NH2	2.58	0.52
2:b:2340:TRP:CH2	2:b:2342:GLY:HA3	2.45	0.52
2:b:2359:MET:HB2	2:b:2425:ILE:CG2	2.40	0.52
2:b:2475:PHE:O	2:b:2476:ARG:C	2.52	0.52
3:c:2199:ILE:CG2	3:c:2231:GLU:HG2	2.39	0.52
13:o:2121:THR:HG22	13:o:2219:GLN:OE1	2.10	0.52
1:A:210:LEU:HD12	1:A:210:LEU:C	2.36	0.51
1:A:337:HIS:CE1	4:D:352:LEU:HD12	2.44	0.51
23:B:521:CLA:H112	23:D:356:CLA:H92	1.92	0.51
3:C:390:ARG:NH1	16:V:100:ILE:CG2	2.73	0.51
23:C:486:CLA:H42	10:K:30:TRP:HE1	1.74	0.51
4:D:343:GLU:OE2	16:V:134:LYS:NZ	2.40	0.51
1:a:2075:ASN:ND2	1:a:2079:THR:HG21	2.25	0.51
1:a:2076:ASN:C	1:a:2076:ASN:OD1	2.51	0.51
1:a:2225:ARG:HA	2:b:2481:GLY:HA3	1.91	0.51
3:c:2273:SER:OG	3:c:2445:ALA:N	2.42	0.51
3:c:2274:TYR:CE2	23:c:2477:CLA:HED3	2.45	0.51
4:d:2218:VAL:HG12	4:d:2219:GLU:N	2.25	0.51
7:h:2023:GLY:C	7:h:2025:GLY:N	2.65	0.51
7:h:2049:ASN:O	7:h:2049:ASN:CG	2.53	0.51
9:j:2030:TYR:O	9:j:2033:TYR:HB2	2.10	0.51
13:o:2156:PHE:O	13:o:2188:LYS:NZ	2.44	0.51
2:B:393:GLU:OE1	2:B:393:GLU:N	2.43	0.51
3:C:305:THR:O	3:C:306:GLY:C	2.52	0.51
3:C:340:TYR:CD1	3:C:340:TYR:N	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:21:ALA:CB	7:H:22:PRO:CD	2.87	0.51
1:a:2254:TYR:CD1	4:d:2132:ILE:HG22	2.45	0.51
2:b:2308:LYS:HE2	2:b:2312:TYR:CE2	2.45	0.51
3:c:2158:THR:HG22	3:c:2251:HIS:O	2.10	0.51
4:d:2291:LEU:C	4:d:2293:LEU:N	2.68	0.51
9:j:2040:LEU:O	16:v:2126:LEU:HD11	2.09	0.51
10:k:2010:ASP:HB3	10:k:2011:PRO:HD3	1.91	0.51
16:v:2063:THR:O	16:v:2080:THR:HG21	2.10	0.51
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.68	0.51
3:C:138:GLU:O	3:C:139:THR:HB	2.09	0.51
4:D:318:ASN:O	4:D:322:ASN:ND2	2.44	0.51
5:E:70:GLU:O	5:E:71:ALA:C	2.52	0.51
7:H:37:PHE:O	7:H:40:PHE:HB3	2.11	0.51
12:M:5:GLN:HG3	12:M:5:GLN:O	2.10	0.51
13:O:93:LEU:O	13:O:128:SER:HA	2.11	0.51
1:a:2021:VAL:HG12	1:a:2031:GLY:HA2	1.92	0.51
1:a:2048:PHE:HA	1:a:2115:ILE:HD11	1.91	0.51
1:a:2150:PRO:O	1:a:2151:LEU:C	2.53	0.51
2:b:2006:TYR:CD2	2:b:2006:TYR:N	2.79	0.51
2:b:2289:GLN:HA	2:b:2289:GLN:OE1	2.11	0.51
2:b:2344:ALA:HB2	2:b:2401:PHE:HE1	1.76	0.51
2:b:2420:TYR:O	2:b:2424:ALA:N	2.43	0.51
8:i:2030:ARG:O	8:i:2032:PRO:HD3	2.11	0.51
10:k:2010:ASP:O	10:k:2014:ASP:OD1	2.29	0.51
19:z:2033:TRP:O	19:z:2037:LYS:HB2	2.10	0.51
1:A:307:ILE:HG22	1:A:309:ALA:CB	2.40	0.51
2:B:168:VAL:HG12	2:B:169:SER:N	2.24	0.51
2:B:250:PHE:CE1	2:B:459:ALA:HB1	2.45	0.51
3:C:67:MET:HA	3:C:67:MET:HE2	1.92	0.51
4:D:220:ASN:O	4:D:220:ASN:ND2	2.44	0.51
11:L:27:LEU:HD23	12:M:14:PHE:HE2	1.75	0.51
1:a:2221:SER:HB3	4:d:2138:VAL:CG1	2.40	0.51
1:a:2243:GLU:HA	4:d:2240:ALA:CB	2.38	0.51
1:a:2318:ALA:HA	1:a:2321:ILE:HD12	1.92	0.51
3:c:2154:LYS:NZ	3:c:2261:ARG:HD3	2.26	0.51
3:c:2331:ALA:O	3:c:2338:GLY:HA2	2.10	0.51
4:d:2035:ILE:O	4:d:2039:PRO:HD2	2.10	0.51
4:d:2119:ALA:O	4:d:2123:ILE:HG13	2.08	0.51
11:l:2036:PHE:CE2	12:m:2008:LEU:N	2.76	0.51
13:o:2055:GLU:HB3	13:o:2061:GLN:NE2	2.26	0.51
15:u:2073:PRO:CG	16:v:2081:THR:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:SER:O	1:A:75:ASN:HB2	2.10	0.51
1:A:131:TRP:O	1:A:134:SER:HB2	2.10	0.51
1:A:288:LEU:O	1:A:289:GLY:C	2.54	0.51
2:B:164:PRO:HB3	23:B:515:CLA:HED2	1.93	0.51
2:B:234:ILE:O	2:B:235:GLU:C	2.53	0.51
3:C:68:THR:HB	3:C:115:GLY:HA2	1.93	0.51
4:D:80:THR:HG22	4:D:81:PRO:HD2	1.92	0.51
4:D:90:LEU:HD11	4:D:96:GLU:HB3	1.90	0.51
4:D:198:MET:HE1	11:L:30:LEU:HD11	1.86	0.51
13:O:1:ALA:O	13:O:2:LYS:HB2	2.10	0.51
13:O:164:LEU:HG	13:O:188:LYS:HB2	1.93	0.51
16:V:63:THR:CG2	16:V:83:ASP:O	2.59	0.51
1:a:2148:SER:HB2	1:a:2284:TRP:HH2	1.74	0.51
1:a:2317:TRP:CZ3	1:a:2320:ILE:HD12	2.45	0.51
2:b:2315:ILE:HG22	2:b:2426:PHE:HB3	1.91	0.51
3:c:2112:PHE:O	3:c:2116:VAL:HG23	2.10	0.51
4:d:2080:THR:HG21	4:d:2168:PHE:HA	1.91	0.51
10:k:2015:VAL:O	10:k:2015:VAL:HG12	2.10	0.51
1:A:162:PRO:HG3	1:A:171:GLY:HA2	1.93	0.51
2:B:318:ASN:O	2:B:320:ALA:N	2.43	0.51
3:C:105:VAL:HG12	3:C:107:ASP:O	2.10	0.51
3:C:264:PHE:HD1	23:C:485:CLA:HMC1	1.76	0.51
3:C:343:ARG:HB3	13:O:78:LEU:CD1	2.40	0.51
4:D:258:GLY:O	14:T:21:ILE:HG23	2.10	0.51
5:E:26:ILE:HA	5:E:29:LEU:HD12	1.93	0.51
5:E:68:ARG:HH12	7:H:50:SER:CB	2.24	0.51
13:O:152:ARG:HD2	13:O:156:PHE:CE2	2.46	0.51
1:a:2031:GLY:HA3	1:a:2132:GLU:OE2	2.10	0.51
1:a:2047:CYS:SG	1:a:2114:LEU:HD23	2.50	0.51
1:a:2180:PHE:HE2	4:d:2192:THR:O	1.94	0.51
1:a:2301:ASN:HD21	3:c:2407:VAL:HB	1.75	0.51
2:b:2194:ASN:C	2:b:2196:GLY:N	2.65	0.51
3:c:2256:PRO:HA	23:c:2474:CLA:HED3	1.93	0.51
3:c:2286:ALA:O	3:c:2289:PHE:HB3	2.11	0.51
3:c:2385:GLN:HB2	3:c:2388:GLN:OE1	2.11	0.51
26:d:2359:LMT:H21	7:h:2060:SER:CB	2.40	0.51
7:h:2021:ALA:CB	7:h:2022:PRO:CD	2.88	0.51
13:o:2194:LYS:HG3	13:o:2194:LYS:O	2.09	0.51
19:z:2005:PHE:HE2	19:z:2054:VAL:HG13	1.69	0.51
19:z:2020:VAL:O	19:z:2020:VAL:HG12	2.09	0.51
1:A:333:GLU:OE1	3:C:354:GLU:OE2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:LYS:HE2	2:B:312:TYR:CZ	2.46	0.51
2:B:340:TRP:CZ3	2:B:342:GLY:CA	2.92	0.51
23:B:521:CLA:H172	23:D:356:CLA:H72	1.92	0.51
3:C:166:ILE:O	3:C:170:ILE:HG13	2.10	0.51
4:D:58:TRP:HB3	4:D:63:LEU:O	2.10	0.51
6:F:36:ILE:CA	6:F:39:MET:HG3	2.40	0.51
13:O:188:LYS:HD2	13:O:225:MET:HG3	1.93	0.51
16:V:64:PRO:HD2	16:V:66:ARG:HH22	1.76	0.51
19:Z:41:PHE:CD1	19:Z:41:PHE:N	2.73	0.51
1:a:2265:PHE:CD2	1:a:2270:SER:HB3	2.46	0.51
1:a:2316:THR:O	1:a:2318:ALA:N	2.43	0.51
2:b:2025:MET:HB3	27:b:2528:BCR:C33	2.40	0.51
2:b:2340:TRP:CZ3	2:b:2342:GLY:CA	2.93	0.51
3:c:2151:TRP:C	3:c:2153:ASP:N	2.68	0.51
3:c:2291:TRP:HD1	3:c:2292:PHE:CE2	2.29	0.51
3:c:2301:PHE:CD2	3:c:2301:PHE:N	2.78	0.51
23:c:2479:CLA:HAB	23:c:2479:CLA:C9	2.39	0.51
13:o:2223:ASP:HB3	13:o:2230:PRO:CG	2.35	0.51
1:A:33:PHE:CD1	1:A:128:GLY:C	2.89	0.51
1:A:176:ILE:O	1:A:179:THR:HB	2.11	0.51
2:B:174:LEU:HD22	2:B:308:LYS:HZ2	1.74	0.51
2:B:452:THR:HG22	4:D:291:LEU:HD11	1.92	0.51
4:D:175:VAL:HG12	4:D:179:PHE:HE1	1.76	0.51
1:a:2089:ILE:HG21	1:a:2094:TYR:HB2	1.93	0.51
2:b:2472:ARG:NE	2:b:2479:PHE:HE1	2.09	0.51
3:c:2097:TRP:CD1	3:c:2110:PRO:HB3	2.46	0.51
3:c:2271:TYR:N	3:c:2271:TYR:CD2	2.79	0.51
4:d:2048:TRP:CH2	24:d:2356:PHO:H18	2.46	0.51
1:A:34:GLY:HA2	1:A:37:MET:HE2	1.93	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
1:A:116:ILE:HG22	1:A:117:PHE:N	2.25	0.51
3:C:318:LEU:HD21	3:C:340:TYR:CB	2.40	0.51
3:C:343:ARG:NH1	3:C:345:PRO:HD3	2.25	0.51
4:D:52:THR:O	4:D:67:TYR:CD1	2.64	0.51
4:D:238:THR:C	4:D:240:ALA:N	2.68	0.51
4:D:261:PHE:CD2	14:T:24:ARG:NH2	2.79	0.51
13:O:27:ARG:O	13:O:29:ALA:N	2.44	0.51
16:V:30:LYS:HG2	16:V:118:HIS:CD2	2.46	0.51
19:Z:23:VAL:O	19:Z:27:TYR:CD1	2.64	0.51
1:a:2048:PHE:HB2	1:a:2115:ILE:HD13	1.91	0.51
1:a:2104:GLU:O	1:a:2105:TRP:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2168:VAL:HG12	2:b:2169:SER:N	2.25	0.51
2:b:2283:GLU:OE1	2:b:2283:GLU:HA	2.11	0.51
2:b:2418:LYS:O	2:b:2419:SER:C	2.53	0.51
4:d:2198:MET:CE	11:l:2030:LEU:HD11	2.40	0.51
13:o:2118:LEU:HD22	13:o:2233:VAL:HG21	1.91	0.51
14:t:2003:THR:O	14:t:2004:ILE:C	2.53	0.51
16:v:2134:LYS:C	16:v:2137:TYR:H	2.19	0.51
2:B:62:VAL:HG13	23:B:518:CLA:O1D	2.11	0.51
2:B:307:GLU:O	2:B:308:LYS:C	2.48	0.51
2:B:402:TYR:N	2:B:402:TYR:CD1	2.78	0.51
4:D:71:CYS:HB2	4:D:76:VAL:HG22	1.89	0.51
4:D:82:ALA:H	4:D:85:MET:CE	2.24	0.51
4:D:199:MET:O	4:D:202:ALA:HB3	2.11	0.51
11:L:4:ASN:N	11:L:5:PRO:CD	2.72	0.51
14:T:20:ALA:O	14:T:24:ARG:HB2	2.11	0.51
1:a:2160:ILE:O	1:a:2164:GLY:N	2.43	0.51
1:a:2334:ARG:NH1	4:d:2320:LEU:CD1	2.69	0.51
2:b:2206:GLY:O	2:b:2210:ILE:HG13	2.11	0.51
3:c:2205:ASP:O	3:c:2208:VAL:HG12	2.11	0.51
3:c:2275:SER:CB	23:c:2485:CLA:HAA1	2.41	0.51
3:c:2282:MET:HE3	23:c:2479:CLA:C6	2.41	0.51
4:d:2024:ARG:O	4:d:2026:ARG:HG3	2.11	0.51
5:e:2070:GLU:O	5:e:2071:ALA:C	2.52	0.51
15:u:2047:LEU:O	15:u:2051:TYR:HB2	2.11	0.51
16:v:2005:PRO:O	16:v:2006:GLU:C	2.53	0.51
1:A:109:GLY:O	1:A:110:GLY:C	2.53	0.50
1:A:126:TYR:O	1:A:130:GLN:HG3	2.11	0.50
1:A:210:LEU:HD13	24:D:355:PHO:C1D	2.40	0.50
2:B:420:TYR:O	2:B:424:ALA:N	2.44	0.50
3:C:37:ALA:HA	23:C:483:CLA:HBA1	1.92	0.50
3:C:157:MET:HE2	3:C:160:ILE:HD12	1.92	0.50
4:D:54:PHE:HB3	5:E:46:PHE:CD1	2.46	0.50
16:V:33:PHE:CD2	16:V:37:CYS:SG	3.04	0.50
16:V:133:GLY:O	16:V:137:TYR:CA	2.59	0.50
1:a:2341:LEU:CD1	15:u:2134:LYS:HZ2	2.23	0.50
3:c:2250:TRP:CD1	3:c:2250:TRP:C	2.88	0.50
4:d:2195:PRO:HG2	4:d:2196:PHE:CD2	2.46	0.50
4:d:2286:VAL:HG21	23:d:2354:CLA:HED2	1.92	0.50
11:l:2031:PHE:O	11:l:2032:SER:C	2.52	0.50
13:o:2075:THR:O	13:o:2076:THR:C	2.54	0.50
15:u:2056:ASP:CG	15:u:2059:ASN:ND2	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:2064:ALA:O	15:u:2067:GLN:HG2	2.11	0.50
15:u:2091:VAL:CG1	15:u:2105:LEU:HD13	2.40	0.50
1:A:57:PRO:CB	1:A:68:SER:HB3	2.37	0.50
1:A:316:THR:HB	4:D:75:THR:CG2	2.40	0.50
1:A:317:TRP:N	4:D:63:LEU:HD13	2.26	0.50
2:B:340:TRP:CH2	2:B:342:GLY:HA3	2.45	0.50
2:B:400:SER:HG	2:B:410:THR:HG23	1.76	0.50
3:C:123:ALA:CB	19:Z:47:TRP:CH2	2.91	0.50
3:C:301:PHE:CD2	3:C:301:PHE:N	2.79	0.50
11:L:28:ALA:O	11:L:29:LEU:C	2.53	0.50
1:a:2040:THR:HG21	1:a:2122:GLY:CA	2.41	0.50
1:a:2159:LEU:O	1:a:2162:PRO:CD	2.56	0.50
3:c:2062:PHE:CZ	10:k:2019:ILE:CD1	2.88	0.50
3:c:2157:MET:HE2	3:c:2157:MET:HA	1.94	0.50
3:c:2275:SER:HB3	23:c:2485:CLA:HAA1	1.93	0.50
3:c:2435:PHE:O	3:c:2436:PHE:C	2.52	0.50
5:e:2033:GLY:HA2	6:f:2031:PHE:HE2	1.73	0.50
8:i:2005:LYS:CG	8:i:2009:TYR:HE1	2.22	0.50
13:o:2032:ILE:O	13:o:2035:SER:N	2.44	0.50
13:o:2041:ALA:N	13:o:2083:GLY:O	2.44	0.50
13:o:2085:LEU:HD11	13:o:2093:LEU:HB3	1.92	0.50
13:o:2102:ASP:O	13:o:2103:PHE:HD1	1.93	0.50
16:v:2025:GLN:O	16:v:2026:TYR:C	2.54	0.50
16:v:2136:TYR:O	16:v:2137:TYR:CG	2.65	0.50
1:A:316:THR:HB	4:D:75:THR:HG21	1.93	0.50
3:C:305:THR:H	3:C:308:GLU:CG	2.19	0.50
3:C:420:VAL:HG12	3:C:425:TRP:CD1	2.46	0.50
4:D:315:TYR:CZ	4:D:319:LEU:HD11	2.46	0.50
13:O:54:GLU:OE1	13:O:231:HIS:CD2	2.64	0.50
16:V:64:PRO:O	16:V:66:ARG:NH1	2.44	0.50
1:a:2225:ARG:HG2	2:b:2481:GLY:O	2.11	0.50
2:b:2006:TYR:CE1	2:b:2008:VAL:CG2	2.94	0.50
2:b:2194:ASN:C	2:b:2196:GLY:H	2.20	0.50
27:b:2528:BCR:H371	27:b:2528:BCR:H393	1.93	0.50
3:c:2109:PHE:O	3:c:2111:PHE:N	2.45	0.50
3:c:2123:ALA:CB	19:z:2047:TRP:CH2	2.93	0.50
4:d:2029:PHE:HD2	4:d:2030:VAL:N	2.10	0.50
13:o:2146:PHE:HZ	13:o:2197:ILE:HD12	1.76	0.50
13:o:2211:ILE:CG2	13:o:2212:ALA:N	2.74	0.50
13:o:2215:PHE:O	13:o:2216:GLU:HB2	2.10	0.50
16:v:2079:PRO:HG3	16:v:2089:ALA:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:O	1:A:180:PHE:HB2	2.12	0.50
1:A:237:TYR:CE2	1:A:245:THR:HG23	2.46	0.50
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.94	0.50
2:B:246:PHE:CE1	2:B:463:PHE:HB2	2.42	0.50
2:B:280:PHE:O	2:B:281:GLN:C	2.55	0.50
3:C:157:MET:CE	3:C:160:ILE:HD12	2.41	0.50
13:O:41:ALA:N	13:O:83:GLY:O	2.43	0.50
13:O:60:ARG:HH12	2:b:2341:LYS:NZ	2.08	0.50
13:O:121:THR:HG21	13:O:148:VAL:CG2	2.26	0.50
15:U:42:VAL:HG12	15:U:45:GLU:H	1.76	0.50
15:U:85:TYR:CD2	15:U:85:TYR:N	2.75	0.50
2:b:2297:THR:O	2:b:2300:GLU:N	2.45	0.50
3:c:2062:PHE:HD2	10:k:2020:PRO:HG3	1.75	0.50
3:c:2208:VAL:CG1	3:c:2209:ILE:N	2.75	0.50
13:o:2243:ILE:HG22	13:o:2244:GLU:N	2.26	0.50
1:A:148:SER:HB2	1:A:284:TRP:CH2	2.37	0.50
1:A:200:LEU:O	1:A:203:ALA:HB3	2.11	0.50
1:A:278:TRP:CB	1:A:279:PRO:HD3	2.35	0.50
1:A:334:ARG:NH1	13:O:159:PRO:HA	2.25	0.50
3:C:183:GLY:O	3:C:184:GLY:O	2.30	0.50
3:C:350:ILE:HG22	3:C:351:PHE:N	2.27	0.50
8:I:6:ILE:O	8:I:10:ILE:HG13	2.11	0.50
3:c:2290:VAL:O	3:c:2293:ASN:ND2	2.45	0.50
4:d:2257:PHE:HD2	4:d:2259:ILE:HG22	1.76	0.50
4:d:2350:ASN:ND2	4:d:2351:ALA:N	2.58	0.50
19:z:2023:VAL:O	19:z:2027:TYR:CD1	2.64	0.50
1:A:78:ILE:HD13	11:L:34:TYR:OH	2.10	0.50
1:A:180:PHE:N	1:A:180:PHE:CD1	2.77	0.50
1:A:237:TYR:CD2	1:A:241:GLN:OE1	2.65	0.50
3:C:151:TRP:C	3:C:153:ASP:N	2.70	0.50
3:C:456:GLU:C	4:D:230:SER:CB	2.85	0.50
6:F:40:GLN:OE1	9:J:28:PHE:CD2	2.65	0.50
13:O:120:PHE:HE1	13:O:235:ILE:HG21	1.77	0.50
14:T:17:PHE:O	14:T:18:PHE:C	2.55	0.50
15:U:54:LYS:HD2	15:U:113:THR:OG1	2.11	0.50
15:U:105:LEU:O	15:U:109:LEU:N	2.41	0.50
2:b:2136:PRO:HD3	2:b:2231:MET:CE	2.33	0.50
13:o:2077:SER:HG	13:o:2078:LEU:H	1.57	0.50
13:o:2119:LEU:O	13:o:2219:GLN:NE2	2.42	0.50
15:u:2062:ILE:HG12	15:u:2080:VAL:HG21	1.93	0.50
1:A:24:THR:CB	4:D:251:ARG:NH2	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HG2	1:A:98:GLU:CB	2.41	0.50
2:B:29:LEU:HD11	27:B:529:BCR:H331	1.94	0.50
2:B:240:SER:OG	2:B:241:SER:N	2.44	0.50
3:C:287:THR:O	3:C:290:VAL:HB	2.11	0.50
3:C:302:TYR:O	3:C:422:PRO:HD2	2.12	0.50
23:C:487:CLA:HBC2	23:C:487:CLA:HHD	1.94	0.50
4:D:200:GLY:O	4:D:204:VAL:HG23	2.11	0.50
4:D:222:LEU:HD22	4:D:243:THR:HB	1.93	0.50
4:D:261:PHE:HD2	14:T:24:ARG:NH2	2.10	0.50
11:L:6:ASN:HD22	11:L:6:ASN:H	1.59	0.50
13:O:168:TYR:CZ	13:O:172:ILE:HD11	2.46	0.50
16:V:75:TYR:CE2	16:V:80:THR:N	2.70	0.50
19:Z:5:PHE:CE2	19:Z:54:VAL:HG13	2.47	0.50
2:b:2078:TRP:HZ3	2:b:2093:PHE:CE1	2.29	0.50
2:b:2235:GLU:OE1	2:b:2235:GLU:HA	2.12	0.50
2:b:2340:TRP:CE3	2:b:2342:GLY:HA3	2.46	0.50
3:c:2122:SER:O	27:c:2488:BCR:H363	2.12	0.50
3:c:2305:THR:N	3:c:2423:ARG:NH1	2.60	0.50
13:o:2211:ILE:CG2	13:o:2212:ALA:H	2.24	0.50
1:A:320:ILE:HG21	4:D:333:ASP:OD2	2.12	0.50
2:B:206:GLY:O	2:B:210:ILE:HG13	2.11	0.50
2:B:479:PHE:C	2:B:481:GLY:N	2.69	0.50
3:C:435:PHE:O	3:C:436:PHE:C	2.55	0.50
6:F:40:GLN:OE1	9:J:28:PHE:HD2	1.95	0.50
15:U:100:ARG:O	15:U:101:GLN:C	2.55	0.50
1:a:2015:GLU:O	1:a:2019:ASN:ND2	2.44	0.50
1:a:2288:LEU:O	1:a:2289:GLY:C	2.55	0.50
1:a:2330:VAL:HG12	4:d:2348:ARG:HA	1.94	0.50
2:b:2250:PHE:HB3	23:b:2521:CLA:H142	1.94	0.50
2:b:2264:PRO:O	2:b:2448:ARG:NH2	2.45	0.50
3:c:2337:LEU:HB3	3:c:2342:MET:HE2	1.94	0.50
5:e:2034:TRP:CD1	5:e:2034:TRP:C	2.90	0.50
13:o:2140:THR:HG21	13:o:2201:VAL:C	2.36	0.50
15:u:2072:TYR:HD2	15:u:2073:PRO:CD	2.24	0.50
19:z:2002:THR:HG22	19:z:2006:GLN:CD	2.37	0.50
1:A:89:ILE:HD13	1:A:94:TYR:CD2	2.46	0.50
1:A:150:PRO:O	1:A:153:SER:HB3	2.12	0.50
1:A:300:PHE:CB	1:A:302:PHE:HE1	2.16	0.50
3:C:41:ARG:HH21	23:C:486:CLA:HMD2	1.77	0.50
3:C:225:VAL:CB	23:C:487:CLA:HMC3	2.39	0.50
4:D:24:ARG:HB3	4:D:26:ARG:HE	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:23:GLY:C	7:H:25:GLY:N	2.66	0.50
13:O:39:ARG:HA	13:O:245:PRO:HB3	1.92	0.50
13:O:238:VAL:CG1	13:O:239:PHE:N	2.75	0.50
15:U:72:TYR:HD2	15:U:73:PRO:HG3	1.77	0.50
1:a:2140:ARG:CZ	4:d:2232:PHE:CZ	2.95	0.50
1:a:2180:PHE:HD1	1:a:2180:PHE:H	1.59	0.50
1:a:2340:PRO:HD3	15:u:2132:LEU:HD12	1.93	0.50
2:b:2308:LYS:HE2	2:b:2312:TYR:CZ	2.47	0.50
3:c:2079:LYS:HG2	3:c:2084:GLN:HE21	1.76	0.50
3:c:2339:LYS:HB2	3:c:2340:TYR:CE1	2.47	0.50
4:d:2057:SER:CB	4:d:2079:SER:HB2	2.41	0.50
6:f:2020:VAL:O	6:f:2021:ALA:C	2.54	0.50
15:u:2098:THR:N	15:u:2101:GLN:OE1	2.44	0.50
2:B:205:ALA:O	23:B:518:CLA:H191	2.12	0.49
3:C:98:GLY:O	3:C:99:VAL:CG2	2.58	0.49
23:C:487:CLA:H102	23:C:487:CLA:H51	1.94	0.49
13:O:189:ARG:NE	15:U:39:LEU:HD23	2.27	0.49
1:a:2242:GLU:O	1:a:2244:GLU:N	2.45	0.49
1:a:2284:TRP:CE3	1:a:2284:TRP:HA	2.47	0.49
1:a:2295:PHE:HB3	3:c:2291:TRP:CH2	2.47	0.49
2:b:2360:PRO:O	2:b:2362:PHE:N	2.45	0.49
3:c:2294:ASN:O	3:c:2296:VAL:N	2.45	0.49
3:c:2328:VAL:O	3:c:2328:VAL:HG12	2.12	0.49
4:d:2188:PHE:N	4:d:2188:PHE:HD1	2.10	0.49
1:A:183:MET:HB3	23:A:348:CLA:HBC2	1.94	0.49
23:A:348:CLA:HBB1	23:D:354:CLA:NC	2.27	0.49
2:B:244:ALA:O	2:B:247:PHE:HB3	2.11	0.49
3:C:91:HIS:O	3:C:94:THR:HB	2.11	0.49
3:C:128:GLY:HA3	23:C:484:CLA:HMC2	1.94	0.49
23:C:486:CLA:H192	19:Z:19:MET:HG2	1.94	0.49
7:H:24:TRP:CE3	7:H:24:TRP:HA	2.46	0.49
16:V:122:GLU:HG3	16:V:126:LEU:HD12	1.94	0.49
1:a:2029:TYR:CE1	1:a:2031:GLY:N	2.80	0.49
1:a:2036:ILE:HD13	23:c:2487:CLA:H141	1.94	0.49
2:b:2156:PHE:HA	2:b:2161:LEU:HB2	1.92	0.49
2:b:2478:VAL:CG1	4:d:2139:ARG:HG2	2.41	0.49
3:c:2042:LEU:HD21	23:c:2486:CLA:HED1	1.93	0.49
4:d:2029:PHE:HE2	4:d:2031:GLY:CA	2.25	0.49
8:i:2032:PRO:HD2	8:i:2035:LYS:O	2.12	0.49
13:o:2164:LEU:HD21	13:o:2188:LYS:O	2.12	0.49
15:u:2108:ASN:C	15:u:2112:PHE:HE1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:2133:GLY:O	16:v:2137:TYR:CA	2.59	0.49
2:B:25:MET:HE2	27:B:529:BCR:H332	1.93	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.49
2:B:341:LYS:HE2	13:o:2060:ARG:HH22	1.75	0.49
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.42	0.49
3:C:85:GLY:C	3:C:86:LEU:HD23	2.37	0.49
3:C:278:ALA:HB1	23:C:479:CLA:H142	1.94	0.49
3:C:294:ASN:C	3:C:296:VAL:N	2.70	0.49
3:C:345:PRO:HB3	13:O:73:ARG:CZ	2.41	0.49
3:C:349:ILE:O	3:C:350:ILE:HG13	2.13	0.49
3:C:395:TYR:O	3:C:396:MET:C	2.55	0.49
12:M:8:LEU:HD22	14:T:1:MET:HE1	1.93	0.49
16:V:5:PRO:O	16:V:6:GLU:C	2.55	0.49
16:V:33:PHE:HD2	16:V:37:CYS:SG	2.34	0.49
1:a:2272:HIS:HD1	4:d:2218:VAL:HG11	1.75	0.49
1:a:2307:ILE:C	1:a:2309:ALA:H	2.21	0.49
1:a:2317:TRP:CE3	4:d:2063:LEU:CD1	2.95	0.49
23:a:2348:CLA:HBB1	23:d:2354:CLA:NC	2.26	0.49
2:b:2025:MET:HE2	27:b:2528:BCR:H332	1.92	0.49
2:b:2234:ILE:O	2:b:2237:VAL:N	2.43	0.49
2:b:2327:THR:O	2:b:2329:PRO:N	2.46	0.49
2:b:2385:ARG:HG3	13:o:2165:ALA:C	2.37	0.49
3:c:2428:THR:HG22	3:c:2429:SER:N	2.25	0.49
4:d:2302:GLU:O	4:d:2305:ALA:HB3	2.12	0.49
4:d:2319:LEU:HA	4:d:2322:ASN:ND2	2.22	0.49
11:l:2033:SER:HA	14:t:2006:TYR:OH	2.12	0.49
13:o:2110:MET:HE2	13:o:2110:MET:N	2.27	0.49
13:o:2135:SER:C	13:o:2136:ILE:HD12	2.37	0.49
1:A:215:HIS:HA	25:A:353:PL9:O1	2.12	0.49
2:B:472:ARG:NE	2:B:479:PHE:HE1	2.11	0.49
3:C:149:TYR:CG	3:C:156:LYS:HG3	2.47	0.49
3:C:291:TRP:HB3	3:C:292:PHE:HD2	1.74	0.49
3:C:337:LEU:HA	13:O:104:GLN:HE21	1.75	0.49
5:E:26:ILE:HG13	5:E:27:PRO:CD	2.42	0.49
13:O:118:LEU:CD2	13:O:233:VAL:HG21	2.43	0.49
1:a:2242:GLU:HG3	1:a:2243:GLU:H	1.78	0.49
1:a:2284:TRP:CZ3	3:c:2435:PHE:HZ	2.30	0.49
2:b:2066:MET:HE3	2:b:2096:VAL:HG11	1.94	0.49
2:b:2070:GLY:HA2	2:b:2178:VAL:HG21	1.94	0.49
3:c:2305:THR:N	3:c:2423:ARG:HH12	2.09	0.49
4:d:2298:PHE:CA	11:l:2037:ASN:ND2	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2334:GLN:CB	4:d:2336:HIS:HE2	2.18	0.49
5:e:2055:TYR:O	16:v:2001:ALA:HB2	2.13	0.49
11:l:2024:ILE:HD13	12:m:2018:PRO:HB2	1.94	0.49
1:A:192:ILE:O	1:A:193:LEU:C	2.55	0.49
1:A:234:ASN:C	4:D:265:ARG:HH22	2.19	0.49
2:B:12:LEU:CD2	2:B:19:LEU:HD12	2.43	0.49
2:B:260:SER:H	2:B:263:THR:HB	1.77	0.49
2:B:289:GLN:HA	2:B:289:GLN:OE1	2.12	0.49
3:C:80:PRO:O	3:C:81:MET:C	2.53	0.49
3:C:450:ALA:HA	3:C:454:GLY:CA	2.42	0.49
5:E:48:THR:O	5:E:48:THR:HG22	2.13	0.49
27:K:50:BCR:H333	19:Z:17:PHE:HA	1.94	0.49
1:a:2131:TRP:HB2	1:a:2144:CYS:SG	2.53	0.49
1:a:2156:ALA:CA	1:a:2160:ILE:HD12	2.35	0.49
1:a:2215:HIS:CD2	4:d:2268:HIS:HD2	2.31	0.49
23:c:2486:CLA:CHB	27:c:2488:BCR:H402	2.42	0.49
14:t:2017:PHE:O	14:t:2018:PHE:C	2.55	0.49
16:v:2033:PHE:O	16:v:2037:CYS:HB2	2.12	0.49
16:v:2079:PRO:HG3	16:v:2089:ALA:HA	1.95	0.49
16:v:2134:LYS:HA	16:v:2137:TYR:OXT	2.11	0.49
1:A:75:ASN:HD22	1:A:79:THR:HG21	1.77	0.49
2:B:61:PHE:O	2:B:64:PRO:HD2	2.12	0.49
3:C:138:GLU:CG	3:C:139:THR:N	2.61	0.49
3:C:286:ALA:HA	3:C:289:PHE:HB3	1.95	0.49
1:a:2214:MET:HG2	25:a:2352:PL9:HC8	1.94	0.49
2:b:2234:ILE:O	2:b:2235:GLU:C	2.54	0.49
3:c:2251:HIS:HD1	3:c:2251:HIS:H	1.60	0.49
12:m:2026:TYR:O	12:m:2026:TYR:CG	2.65	0.49
13:o:2047:PRO:HG3	13:o:2076:THR:HG22	1.88	0.49
13:o:2152:ARG:HD2	13:o:2156:PHE:CG	2.47	0.49
13:o:2161:GLY:O	13:o:2168:TYR:N	2.40	0.49
14:t:2022:PHE:HD2	14:t:2022:PHE:N	2.08	0.49
1:A:166:GLY:O	1:A:167:SER:HB3	2.13	0.49
2:B:311:PHE:O	2:B:313:ASP:N	2.45	0.49
2:B:326:ARG:HG2	12:M:4:ASN:HD22	1.78	0.49
2:B:341:LYS:NZ	13:o:2060:ARG:NH2	2.51	0.49
2:B:451:PHE:CZ	2:B:455:HIS:ND1	2.80	0.49
3:C:66:ALA:HB1	10:K:17:PRO:HB3	1.95	0.49
11:L:12:LEU:CD1	11:L:16:SER:HB3	2.39	0.49
13:O:50:PHE:O	13:O:68:THR:OG1	2.31	0.49
13:O:65:PHE:N	13:O:65:PHE:CD1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:112:GLY:C	13:O:114:GLU:N	2.71	0.49
15:U:75:LEU:CD2	15:U:101:GLN:HE21	2.25	0.49
1:a:2076:ASN:O	1:a:2079:THR:HB	2.12	0.49
1:a:2109:GLY:O	1:a:2110:GLY:C	2.53	0.49
1:a:2334:ARG:NH1	13:o:2159:PRO:HA	2.26	0.49
2:b:2061:PHE:CZ	23:b:2514:CLA:HBB1	2.48	0.49
3:c:2165:LEU:HD21	23:c:2474:CLA:CBB	2.43	0.49
15:u:2051:TYR:O	15:u:2053:GLU:N	2.45	0.49
1:A:124:SER:O	1:A:127:MET:HB3	2.12	0.49
1:A:238:LYS:O	1:A:239:PHE:C	2.55	0.49
2:B:45:PHE:CE2	2:B:46:ASP:O	2.66	0.49
2:B:156:PHE:HA	2:B:161:LEU:HB2	1.93	0.49
2:B:397:VAL:CG1	2:B:398:THR:N	2.76	0.49
2:B:422:ARG:NH2	13:O:169:ASP:HB3	2.28	0.49
3:C:99:VAL:CG1	3:C:100:GLY:N	2.74	0.49
3:C:109:PHE:CZ	27:C:489:BCR:HC32	2.47	0.49
4:D:188:PHE:N	4:D:188:PHE:HD1	2.10	0.49
5:E:12:ILE:HD12	28:E:84:HEC:CBD	2.42	0.49
5:E:63:PRO:HB3	5:E:78:PHE:CD2	2.47	0.49
1:a:2140:ARG:NH2	4:d:2232:PHE:CE1	2.81	0.49
1:a:2142:TRP:HH2	1:a:2273:PHE:CE1	2.31	0.49
1:a:2147:TYR:CE1	1:a:2151:LEU:HD13	2.47	0.49
2:b:2012:LEU:HG	2:b:2019:LEU:CD1	2.43	0.49
2:b:2185:TRP:O	2:b:2186:GLY:O	2.30	0.49
2:b:2249:ALA:CB	2:b:2459:ALA:HB2	2.43	0.49
3:c:2271:TYR:N	3:c:2271:TYR:HD2	2.11	0.49
3:c:2282:MET:HA	3:c:2285:ILE:HB	1.93	0.49
3:c:2294:ASN:HB2	3:c:2296:VAL:HG23	1.95	0.49
4:d:2027:PHE:HB3	6:f:2017:VAL:HG11	1.95	0.49
8:i:2008:VAL:O	8:i:2009:TYR:C	2.56	0.49
14:t:2003:THR:O	14:t:2006:TYR:N	2.36	0.49
15:u:2054:LYS:HB3	15:u:2111:HIS:O	2.11	0.49
15:u:2057:LEU:CD1	15:u:2088:VAL:HG13	2.41	0.49
2:B:6:TYR:CE1	2:B:8:VAL:CG2	2.96	0.49
2:B:24:LEU:HD12	2:B:111:ALA:HA	1.93	0.49
2:B:78:TRP:HZ3	2:B:93:PHE:CE1	2.30	0.49
2:B:305:ILE:O	2:B:341:LYS:HD2	2.12	0.49
2:B:326:ARG:HG2	12:M:4:ASN:ND2	2.27	0.49
4:D:18:LEU:HD12	17:X:41:SER:OG	2.12	0.49
8:I:27:ASP:OD1	8:I:27:ASP:N	2.46	0.49
16:V:128:ASP:HB3	16:V:134:LYS:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:53:VAL:O	19:Z:57:LEU:HG	2.13	0.49
1:a:2107:TYR:CD1	13:o:2115:ARG:NH1	2.81	0.49
1:a:2140:ARG:C	4:d:2220:ASN:HD21	2.20	0.49
2:b:2170:ASP:HB2	2:b:2171:PRO:CD	2.42	0.49
3:c:2088:LEU:O	3:c:2089:ILE:C	2.54	0.49
23:c:2476:CLA:HBD	23:c:2486:CLA:CBB	2.43	0.49
12:m:2009:ILE:O	12:m:2013:LEU:HG	2.12	0.49
13:o:2039:ARG:HA	13:o:2245:PRO:CB	2.43	0.49
1:A:104:GLU:O	1:A:105:TRP:C	2.56	0.49
1:A:243:GLU:N	4:D:240:ALA:HB1	2.28	0.49
1:A:255:PHE:CE2	25:A:353:PL9:H152	2.48	0.49
2:B:194:ASN:C	2:B:196:GLY:H	2.20	0.49
2:B:479:PHE:C	2:B:481:GLY:H	2.21	0.49
3:C:97:TRP:HA	3:C:97:TRP:CE3	2.48	0.49
3:C:296:VAL:O	3:C:298:PRO:HD2	2.13	0.49
3:C:304:PRO:HB3	3:C:395:TYR:CG	2.48	0.49
4:D:102:THR:HG23	5:E:46:PHE:C	2.38	0.49
6:F:43:GLN:HG2	6:F:44:ARG:HG2	1.94	0.49
11:L:10:VAL:O	12:M:28:GLN:NE2	2.46	0.49
12:M:9:ILE:O	12:M:13:LEU:HG	2.13	0.49
1:a:2107:TYR:HD1	13:o:2115:ARG:NH1	2.10	0.49
1:a:2155:PHE:O	1:a:2159:LEU:N	2.42	0.49
1:a:2219:VAL:HG21	4:d:2268:HIS:CD2	2.48	0.49
2:b:2062:VAL:HG13	23:b:2518:CLA:O1D	2.13	0.49
2:b:2327:THR:O	2:b:2329:PRO:HD3	2.12	0.49
4:d:2052:THR:O	4:d:2067:TYR:HD1	1.96	0.49
4:d:2110:LEU:O	4:d:2111:TRP:C	2.55	0.49
4:d:2261:PHE:HD1	4:d:2266:TRP:CD1	2.31	0.49
4:d:2291:LEU:O	4:d:2293:LEU:N	2.46	0.49
4:d:2316:THR:O	4:d:2317:LYS:C	2.55	0.49
11:l:2036:PHE:O	12:m:2003:VAL:HG23	2.13	0.49
13:o:2039:ARG:HD2	13:o:2245:PRO:CG	2.42	0.49
13:o:2193:THR:HG22	13:o:2194:LYS:N	2.14	0.49
16:v:2117:GLY:O	16:v:2121:VAL:HG23	2.13	0.49
18:n:2022:UNK:C	18:n:2024:UNK:N	2.75	0.49
2:B:31:ALA:N	23:B:518:CLA:HBC3	2.28	0.48
4:D:158:LEU:O	4:D:161:PRO:HD2	2.13	0.48
4:D:158:LEU:C	4:D:161:PRO:HD2	2.37	0.48
4:D:196:PHE:HD1	4:D:285:GLY:CA	2.25	0.48
4:D:315:TYR:CE2	4:D:319:LEU:HD11	2.48	0.48
13:O:38:TYR:O	13:O:245:PRO:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2161:TYR:O	1:a:2162:PRO:C	2.54	0.48
2:b:2321:LYS:HE2	2:b:2325:PHE:HZ	1.78	0.48
2:b:2397:VAL:CG1	2:b:2398:THR:N	2.75	0.48
3:c:2217:PRO:HA	3:c:2222:GLY:HA2	1.95	0.48
4:d:2091:LEU:HD22	23:d:2357:CLA:HED1	1.95	0.48
4:d:2243:THR:O	4:d:2243:THR:HG22	2.12	0.48
4:d:2291:LEU:C	4:d:2293:LEU:H	2.20	0.48
4:d:2330:ALA:N	4:d:2331:PRO:CD	2.76	0.48
10:k:2015:VAL:HG21	18:n:2009:UNK:O	2.12	0.48
13:o:2053:LYS:HG2	13:o:2065:PHE:CD2	2.48	0.48
15:u:2039:LEU:C	15:u:2041:ASN:N	2.65	0.48
2:B:200:ALA:C	23:B:521:CLA:HBB1	2.38	0.48
23:B:512:CLA:H2A	23:B:512:CLA:O2A	2.13	0.48
23:B:517:CLA:HMA3	23:B:521:CLA:HED3	1.95	0.48
3:C:201:ASN:O	3:C:201:ASN:CG	2.57	0.48
3:C:282:MET:O	3:C:285:ILE:HB	2.13	0.48
23:C:486:CLA:CHB	27:C:488:BCR:H402	2.43	0.48
4:D:333:ASP:O	4:D:333:ASP:OD1	2.31	0.48
9:J:24:ILE:O	9:J:27:LEU:HB3	2.12	0.48
1:a:2037:MET:O	1:a:2041:LEU:HG	2.13	0.48
1:a:2187:GLN:C	1:a:2187:GLN:HE21	2.21	0.48
1:a:2236:GLY:N	4:d:2265:ARG:CZ	2.76	0.48
2:b:2340:TRP:HH2	2:b:2401:PHE:CD1	2.32	0.48
3:c:2249:ILE:HG13	3:c:2250:TRP:N	2.28	0.48
3:c:2321:ASP:OD1	3:c:2321:ASP:N	2.46	0.48
4:d:2282:SER:OG	23:d:2354:CLA:O1D	2.31	0.48
6:f:2035:ALA:O	6:f:2039:MET:HG3	2.13	0.48
16:v:2133:GLY:O	16:v:2137:TYR:OXT	2.31	0.48
1:A:89:ILE:CG1	13:O:73:ARG:NH2	2.71	0.48
1:A:107:TYR:HD1	13:O:115:ARG:CZ	2.26	0.48
1:A:200:LEU:HD13	1:A:285:PHE:HD1	1.75	0.48
1:A:242:GLU:O	4:D:241:GLU:HA	2.12	0.48
2:B:84:THR:O	2:B:84:THR:CG2	2.61	0.48
3:C:153:ASP:OD1	3:C:155:ASN:OD1	2.30	0.48
3:C:208:VAL:CG1	3:C:209:ILE:N	2.77	0.48
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.48	0.48
4:D:110:LEU:O	4:D:111:TRP:C	2.55	0.48
4:D:112:THR:HG22	4:D:116:LEU:CD1	2.43	0.48
4:D:236:ASN:HB2	4:D:237:PRO:HD2	1.96	0.48
6:F:22:VAL:O	6:F:26:ALA:HB3	2.13	0.48
6:F:39:MET:O	6:F:41:PHE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:72:TYR:HD2	15:U:73:PRO:CG	2.26	0.48
1:a:2075:ASN:CG	1:a:2079:THR:HG21	2.38	0.48
7:h:2042:LEU:HD23	7:h:2042:LEU:HA	1.62	0.48
11:l:2012:LEU:O	12:m:2029:THR:OG1	2.22	0.48
15:u:2072:TYR:CD2	15:u:2073:PRO:CD	2.96	0.48
15:u:2091:VAL:O	15:u:2094:ILE:HG13	2.13	0.48
1:A:161:TYR:O	1:A:162:PRO:C	2.54	0.48
1:A:211:PHE:CE2	1:A:278:TRP:CD1	3.02	0.48
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.43	0.48
2:B:225:LEU:CD2	23:B:524:CLA:HMC1	2.43	0.48
2:B:302:TRP:C	2:B:304:ALA:N	2.71	0.48
3:C:162:GLY:CA	3:C:248:GLY:HA2	2.43	0.48
3:C:316:THR:OG1	3:C:392:ALA:HB1	2.14	0.48
3:C:320:ARG:HH11	16:V:49:ASN:HA	1.78	0.48
3:C:347:GLY:O	13:O:16:ALA:HB3	2.13	0.48
4:D:84:SER:HB2	5:E:66:THR:O	2.13	0.48
4:D:154:VAL:HG13	4:D:158:LEU:HD12	1.94	0.48
10:K:19:ILE:HD12	27:K:50:BCR:H342	1.95	0.48
15:U:72:TYR:CD2	15:U:73:PRO:CA	2.96	0.48
15:U:76:ALA:O	15:U:80:VAL:HG23	2.14	0.48
16:V:133:GLY:O	16:V:137:TYR:N	2.47	0.48
1:a:2033:PHE:CD1	1:a:2128:GLY:C	2.92	0.48
1:a:2063:ILE:HG23	3:c:2335:THR:HG21	1.95	0.48
1:a:2183:MET:HG2	23:d:2355:CLA:CBC	2.43	0.48
1:a:2295:PHE:O	3:c:2291:TRP:CH2	2.67	0.48
2:b:2012:LEU:HD23	2:b:2019:LEU:HD12	1.94	0.48
2:b:2024:LEU:HD12	2:b:2111:ALA:HA	1.95	0.48
2:b:2164:PRO:HB3	23:b:2515:CLA:HED2	1.95	0.48
2:b:2224:ARG:O	2:b:2228:ALA:HB3	2.13	0.48
3:c:2302:TYR:O	3:c:2422:PRO:HD2	2.13	0.48
23:c:2487:CLA:H102	23:c:2487:CLA:H51	1.95	0.48
4:d:2194:ASN:O	4:d:2198:MET:HG3	2.14	0.48
13:o:2125:LEU:CG	13:o:2126:VAL:N	2.76	0.48
2:B:57:ARG:HA	2:B:330:MET:HG3	1.96	0.48
23:B:519:CLA:C14	23:D:356:CLA:H11	2.43	0.48
3:C:40:ALA:O	3:C:43:ILE:HG23	2.12	0.48
3:C:109:PHE:O	3:C:111:PHE:N	2.47	0.48
13:O:45:LEU:HD11	13:O:215:PHE:CE1	2.48	0.48
13:O:59:LYS:O	2:b:2405:GLU:HG2	2.13	0.48
13:O:182:LEU:O	13:O:183:ALA:C	2.55	0.48
1:a:2131:TRP:O	1:a:2134:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2187:PRO:HA	2:b:2190:PHE:HB2	1.95	0.48
2:b:2280:PHE:O	2:b:2281:GLN:C	2.56	0.48
2:b:2311:PHE:HA	2:b:2430:PHE:CZ	2.49	0.48
2:b:2372:ASP:HB3	2:b:2376:VAL:HB	1.95	0.48
3:c:2222:GLY:O	3:c:2223:TRP:C	2.51	0.48
3:c:2266:TRP:HB3	3:c:2271:TYR:OH	2.13	0.48
4:d:2161:PRO:HG3	4:d:2170:ALA:HB2	1.91	0.48
7:h:2022:PRO:CG	7:h:2023:GLY:N	2.76	0.48
13:o:2116:ILE:HG22	13:o:2118:LEU:HD21	1.95	0.48
16:v:2075:TYR:HD2	16:v:2079:PRO:HA	1.76	0.48
19:z:2013:VAL:HG13	19:z:2017:PHE:HE1	1.77	0.48
1:A:129:ARG:NH2	4:D:255:GLN:O	2.46	0.48
1:A:224:ILE:CG2	1:A:227:THR:OG1	2.61	0.48
1:A:259:ILE:HD13	25:A:353:PL9:H172	1.95	0.48
2:B:136:PRO:HD3	2:B:231:MET:CE	2.32	0.48
2:B:405:GLU:HG2	13:o:2059:LYS:O	2.12	0.48
2:B:418:LYS:O	2:B:419:SER:C	2.55	0.48
3:C:367:GLU:O	3:C:370:ARG:N	2.37	0.48
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.96	0.48
23:C:479:CLA:HAB	23:C:479:CLA:C9	2.41	0.48
5:E:30:PHE:C	5:E:30:PHE:CD2	2.91	0.48
15:U:61:ASN:CB	15:U:126:ASP:O	2.62	0.48
16:V:33:PHE:CD2	16:V:37:CYS:HB2	2.48	0.48
16:V:134:LYS:C	16:V:137:TYR:H	2.22	0.48
2:b:2113:TRP:HB3	23:b:2525:CLA:CED	2.39	0.48
2:b:2364:GLU:HG2	4:d:2294:ARG:HH12	1.78	0.48
3:c:2159:THR:HA	3:c:2252:ILE:HA	1.95	0.48
3:c:2183:GLY:O	3:c:2184:GLY:O	2.31	0.48
3:c:2367:GLU:O	3:c:2370:ARG:HB2	2.12	0.48
3:c:2419:PHE:O	3:c:2420:VAL:CG2	2.61	0.48
23:c:2486:CLA:H121	19:z:2020:VAL:HG13	1.96	0.48
6:f:2027:VAL:N	6:f:2028:PRO:CD	2.76	0.48
10:k:2009:PHE:O	10:k:2013:VAL:HG23	2.14	0.48
15:u:2038:GLU:O	15:u:2041:ASN:HB3	2.13	0.48
15:u:2056:ASP:OD1	15:u:2059:ASN:ND2	2.45	0.48
17:x:2034:PHE:O	17:x:2035:ALA:C	2.54	0.48
1:A:172:MET:HE2	23:A:349:CLA:HMC3	1.96	0.48
1:A:284:TRP:HA	1:A:284:TRP:CE3	2.49	0.48
2:B:71:VAL:O	2:B:93:PHE:HE2	1.96	0.48
2:B:360:PRO:O	2:B:362:PHE:N	2.46	0.48
2:B:372:ASP:HB3	2:B:376:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:129:GLN:HE21	4:D:142:ASN:HB3	1.78	0.48
5:E:22:HIS:C	5:E:24:ILE:N	2.70	0.48
7:H:29:LEU:O	7:H:33:PHE:HD1	1.96	0.48
12:M:20:VAL:O	12:M:21:PHE:C	2.55	0.48
15:U:65:PHE:HD1	15:U:76:ALA:HB1	1.78	0.48
16:V:46:THR:HG22	16:V:49:ASN:N	2.19	0.48
16:V:63:THR:O	16:V:80:THR:HG21	2.14	0.48
1:a:2089:ILE:HD13	1:a:2094:TYR:CG	2.49	0.48
1:a:2119:PHE:O	1:a:2123:ALA:CB	2.61	0.48
1:a:2279:PRO:HG2	4:d:2211:CYS:HB3	1.95	0.48
25:a:2352:PL9:H271	25:a:2352:PL9:H23	1.42	0.48
2:b:2246:PHE:CE1	2:b:2463:PHE:HB2	2.44	0.48
2:b:2302:TRP:C	2:b:2304:ALA:H	2.20	0.48
2:b:2328:GLY:HA2	2:b:2444:ARG:HD3	1.96	0.48
2:b:2346:PHE:O	2:b:2354:LEU:HB2	2.13	0.48
2:b:2360:PRO:C	2:b:2362:PHE:N	2.70	0.48
3:c:2037:ALA:O	3:c:2038:GLY:C	2.56	0.48
3:c:2088:LEU:O	3:c:2091:HIS:HB2	2.12	0.48
3:c:2191:PRO:O	3:c:2193:GLY:N	2.45	0.48
3:c:2398:HIS:HB3	3:c:2419:PHE:CZ	2.48	0.48
4:d:2101:PHE:O	4:d:2104:TRP:N	2.47	0.48
4:d:2110:LEU:O	4:d:2113:PHE:CB	2.61	0.48
13:o:2103:PHE:O	13:o:2119:LEU:HD12	2.13	0.48
15:u:2130:ASN:O	15:u:2131:GLY:C	2.57	0.48
16:v:2056:THR:HA	16:v:2059:LEU:HD12	1.93	0.48
1:A:96:ILE:CG2	8:I:1:MET:HE1	2.44	0.48
1:A:119:PHE:O	1:A:123:ALA:CB	2.62	0.48
1:A:150:PRO:O	1:A:153:SER:N	2.47	0.48
1:A:278:TRP:CE3	1:A:278:TRP:HA	2.48	0.48
2:B:63:LEU:HB3	2:B:64:PRO:CD	2.38	0.48
2:B:91:TRP:CB	23:B:515:CLA:H43	2.44	0.48
2:B:199:VAL:O	2:B:203:ILE:HG13	2.13	0.48
3:C:289:PHE:CE2	3:C:294:ASN:OD1	2.67	0.48
3:C:372:PRO:O	3:C:373:ASN:HB2	2.14	0.48
4:D:181:PHE:O	4:D:182:LEU:C	2.57	0.48
10:K:26:LEU:HD21	18:N:20:UNK:CB	2.43	0.48
13:O:32:ILE:O	13:O:35:SER:N	2.45	0.48
13:O:34:SER:O	13:O:35:SER:C	2.57	0.48
13:O:71:VAL:CG2	13:O:108:VAL:HG23	2.39	0.48
13:O:161:GLY:O	13:O:168:TYR:N	2.43	0.48
15:U:61:ASN:HB3	15:U:126:ASP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:72:TYR:CD2	15:U:73:PRO:CD	2.96	0.48
1:a:2089:ILE:HD12	1:a:2108:ASN:HB3	1.96	0.48
1:a:2166:GLY:O	1:a:2167:SER:HB3	2.13	0.48
1:a:2255:PHE:CD2	1:a:2264:SER:HA	2.46	0.48
3:c:2042:LEU:HD22	3:c:2048:LYS:HB3	1.95	0.48
3:c:2436:PHE:O	3:c:2439:VAL:HB	2.14	0.48
23:c:2486:CLA:H42	10:k:2030:TRP:HE1	1.79	0.48
10:k:2010:ASP:N	10:k:2011:PRO:CD	2.77	0.48
12:m:2017:VAL:HB	12:m:2018:PRO:CD	2.44	0.48
13:o:2072:THR:HG22	13:o:2075:THR:HB	1.95	0.48
2:B:311:PHE:C	2:B:313:ASP:N	2.71	0.48
3:C:282:MET:HA	3:C:285:ILE:CB	2.44	0.48
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.48	0.48
8:I:27:ASP:HB2	8:I:28:PRO:HD2	1.94	0.48
8:I:31:ASN:O	8:I:31:ASN:OD1	2.31	0.48
13:O:45:LEU:HB3	13:O:79:ASP:HB2	1.96	0.48
13:O:137:THR:HG23	13:O:138:THR:N	2.29	0.48
15:U:47:LEU:O	15:U:49:THR:N	2.46	0.48
1:a:2205:VAL:CG1	4:d:2204:VAL:HG12	2.43	0.48
1:a:2312:ASN:CG	5:e:2055:TYR:CD1	2.92	0.48
1:a:2323:ARG:HG2	4:d:2329:MET:HA	1.96	0.48
2:b:2062:VAL:CG1	23:b:2518:CLA:HED3	2.43	0.48
2:b:2062:VAL:HG11	23:b:2518:CLA:HED3	1.96	0.48
2:b:2479:PHE:C	2:b:2481:GLY:N	2.69	0.48
27:b:2528:BCR:H361	27:b:2528:BCR:H20C	1.61	0.48
27:c:2488:BCR:C20	10:k:2023:PHE:HE2	2.27	0.48
5:e:2008:PRO:HB3	6:f:2018:ARG:NH2	2.28	0.48
19:z:2015:LEU:CD2	19:z:2047:TRP:HB2	2.44	0.48
1:A:234:ASN:C	4:D:265:ARG:HH12	2.22	0.48
1:A:238:LYS:O	1:A:240:GLY:N	2.47	0.48
1:A:242:GLU:O	1:A:244:GLU:N	2.47	0.48
1:A:307:ILE:HD13	5:E:54:TYR:HB2	1.95	0.48
2:B:57:ARG:NH2	2:B:334:ASP:OD2	2.45	0.48
2:B:235:GLU:OE1	2:B:235:GLU:HA	2.14	0.48
2:B:237:VAL:HG22	23:B:524:CLA:HBC2	1.96	0.48
2:B:385:ARG:HG3	13:O:165:ALA:HA	1.95	0.48
3:C:64:ALA:HB3	3:C:118:HIS:HB3	1.95	0.48
3:C:305:THR:N	3:C:308:GLU:HG3	2.21	0.48
4:D:56:THR:O	4:D:56:THR:CG2	2.60	0.48
4:D:152:VAL:CG1	23:D:354:CLA:H43	2.44	0.48
6:F:27:VAL:N	6:F:28:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:66:ILE:O	15:U:66:ILE:HG22	2.13	0.48
1:a:2142:TRP:HB2	4:d:2220:ASN:HB2	1.95	0.48
1:a:2192:ILE:HG12	1:a:2293:MET:SD	2.54	0.48
1:a:2215:HIS:HA	25:a:2352:PL9:O1	2.13	0.48
2:b:2045:PHE:CE2	2:b:2078:TRP:HZ2	2.30	0.48
2:b:2234:ILE:HG13	23:b:2524:CLA:H191	1.96	0.48
3:c:2060:ILE:HG22	23:c:2480:CLA:HMD3	1.96	0.48
3:c:2067:MET:HE3	10:k:2017:PRO:HB2	1.96	0.48
3:c:2395:TYR:O	3:c:2396:MET:C	2.57	0.48
4:d:2043:LEU:HD22	27:d:2360:BCR:H323	1.96	0.48
4:d:2178:ILE:O	4:d:2181:PHE:HB3	2.14	0.48
25:d:2358:PL9:H271	25:d:2358:PL9:H251	1.79	0.48
5:e:2041:LEU:O	5:e:2042:ALA:C	2.57	0.48
11:l:2004:ASN:N	11:l:2005:PRO:CD	2.74	0.48
13:o:2153:THR:CG2	13:o:2154:ALA:H	2.26	0.48
14:t:2007:VAL:O	14:t:2010:PHE:HB3	2.14	0.48
1:A:104:GLU:HG2	1:A:105:TRP:N	2.29	0.47
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.47
1:A:284:TRP:HA	1:A:284:TRP:HE3	1.79	0.47
2:B:12:LEU:HG	2:B:19:LEU:CD1	2.43	0.47
2:B:148:LEU:O	2:B:151:PHE:HB3	2.13	0.47
2:B:265:ILE:C	2:B:267:LEU:H	2.22	0.47
2:B:328:GLY:HA2	2:B:444:ARG:HD3	1.95	0.47
3:C:208:VAL:HG13	3:C:209:ILE:H	1.79	0.47
3:C:370:ARG:HD3	3:C:375:LEU:HD23	1.94	0.47
4:D:90:LEU:HD11	4:D:96:GLU:CB	2.44	0.47
4:D:191:TRP:HE1	4:D:197:HIS:CD2	2.31	0.47
10:K:35:GLY:O	10:K:36:PHE:HB2	2.13	0.47
12:M:27:VAL:HG12	12:m:2028:GLN:HB2	1.96	0.47
13:O:34:SER:C	13:O:36:GLN:N	2.69	0.47
13:O:46:GLN:O	13:O:238:VAL:O	2.31	0.47
16:V:79:PRO:HG3	16:V:89:ALA:N	2.29	0.47
1:a:2037:MET:HE1	1:a:2129:ARG:CD	2.35	0.47
1:a:2334:ARG:HH12	13:o:2159:PRO:CA	2.26	0.47
2:b:2006:TYR:OH	12:m:2021:PHE:CZ	2.54	0.47
2:b:2400:SER:HG	2:b:2410:THR:HG23	1.75	0.47
3:c:2098:GLY:C	3:c:2099:VAL:HG23	2.38	0.47
3:c:2305:THR:O	3:c:2306:GLY:C	2.56	0.47
4:d:2052:THR:O	4:d:2076:VAL:CG1	2.62	0.47
13:o:2017:ASN:ND2	13:o:2077:SER:OG	2.47	0.47
19:z:2048:ILE:O	19:z:2048:ILE:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:HD21	4:D:313:THR:HG21	1.79	0.47
1:A:168:PHE:O	1:A:169:SER:C	2.57	0.47
1:A:205:VAL:CG1	4:D:204:VAL:HG12	2.44	0.47
2:B:88:PRO:O	2:B:89:GLY:C	2.57	0.47
2:B:149:LEU:O	2:B:150:CYS:C	2.56	0.47
2:B:247:PHE:HE1	23:B:521:CLA:H72	1.77	0.47
3:C:339:LYS:HB2	3:C:340:TYR:CE1	2.49	0.47
3:C:376:ASP:OD1	3:C:378:ASN:HB2	2.14	0.47
4:D:83:ASN:CB	4:D:336:HIS:ND1	2.77	0.47
4:D:178:ILE:O	4:D:182:LEU:HG	2.14	0.47
4:D:243:THR:O	4:D:243:THR:HG22	2.13	0.47
7:H:49:ASN:O	7:H:49:ASN:CG	2.57	0.47
9:J:25:VAL:O	9:J:26:GLY:C	2.54	0.47
12:M:16:LEU:O	12:M:17:VAL:C	2.53	0.47
13:O:164:LEU:N	13:O:188:LYS:HE2	2.29	0.47
2:b:2056:TRP:CD1	2:b:2056:TRP:C	2.92	0.47
2:b:2124:ARG:CG	2:b:2125:ASP:N	2.75	0.47
2:b:2327:THR:C	2:b:2329:PRO:CD	2.86	0.47
23:b:2516:CLA:H111	23:b:2522:CLA:H42	1.95	0.47
23:b:2520:CLA:H201	12:m:2018:PRO:HB3	1.96	0.47
3:c:2162:GLY:CA	3:c:2248:GLY:HA2	2.43	0.47
3:c:2349:ILE:O	3:c:2350:ILE:HG13	2.14	0.47
4:d:2269:PHE:C	4:d:2269:PHE:CD2	2.90	0.47
23:d:2357:CLA:H203	7:h:2048:TYR:CD2	2.49	0.47
5:e:2052:ASP:O	16:v:2001:ALA:HB3	2.14	0.47
13:o:2053:LYS:HE3	13:o:2233:VAL:C	2.39	0.47
13:o:2058:ASN:O	13:o:2059:LYS:HB2	2.14	0.47
14:t:2004:ILE:HG13	14:t:2005:THR:N	2.29	0.47
16:v:2081:THR:O	16:v:2083:ASP:N	2.47	0.47
19:z:2046:LEU:O	19:z:2050:LEU:HG	2.15	0.47
1:A:42:LEU:O	1:A:46:ILE:HG12	2.14	0.47
1:A:54:ALA:O	1:A:55:ALA:C	2.55	0.47
23:A:348:CLA:H191	14:T:17:PHE:CZ	2.49	0.47
3:C:42:LEU:CD1	23:C:486:CLA:HMA2	2.44	0.47
4:D:80:THR:CG2	4:D:168:PHE:HA	2.43	0.47
4:D:348:ARG:NH1	15:U:133:TYR:CE1	2.82	0.47
5:E:48:THR:O	5:E:49:PRO:C	2.57	0.47
13:O:193:THR:CG2	13:O:194:LYS:H	2.05	0.47
15:U:61:ASN:HB3	15:U:130:ASN:ND2	2.28	0.47
16:V:35:TYR:C	16:V:35:TYR:CD2	2.92	0.47
16:V:53:ASP:OD1	16:V:55:ARG:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2084:PRO:HA	1:a:2112:TYR:CG	2.49	0.47
2:b:2071:VAL:O	2:b:2093:PHE:HE2	1.97	0.47
2:b:2264:PRO:HG2	2:b:2267:LEU:HB2	1.96	0.47
3:c:2264:PHE:CD1	23:c:2485:CLA:HMC1	2.42	0.47
23:c:2477:CLA:HAA2	23:c:2477:CLA:HBD	1.95	0.47
4:d:2087:HIS:NE2	26:d:2359:LMT:O4'	2.47	0.47
4:d:2246:MET:HE3	4:d:2246:MET:HB3	1.77	0.47
17:x:2013:THR:O	17:x:2015:SER:N	2.47	0.47
1:A:159:LEU:O	1:A:160:ILE:C	2.56	0.47
1:A:301:ASN:HB2	1:A:303:ASN:HD21	1.79	0.47
2:B:198:VAL:O	2:B:201:HIS:HB3	2.14	0.47
3:C:199:ILE:HD12	3:C:234:VAL:CG2	2.39	0.47
6:F:19:TRP:CZ3	6:F:23:HIS:CE1	3.03	0.47
10:K:10:ASP:O	10:K:11:PRO:C	2.58	0.47
15:U:58:ASN:C	15:U:59:ASN:ND2	2.70	0.47
17:X:12:ILE:O	17:X:12:ILE:HG13	2.15	0.47
1:a:2219:VAL:HG11	4:d:2268:HIS:CD2	2.48	0.47
2:b:2237:VAL:HG22	23:b:2524:CLA:HBC2	1.96	0.47
2:b:2323:GLY:N	4:d:2294:ARG:O	2.47	0.47
3:c:2350:ILE:HD13	3:c:2359:TRP:CG	2.49	0.47
4:d:2018:LEU:O	4:d:2022:LEU:CB	2.62	0.47
4:d:2048:TRP:CZ3	24:d:2356:PHO:H161	2.50	0.47
5:e:2025:THR:O	5:e:2028:ALA:HB3	2.13	0.47
7:h:2053:ILE:HG22	17:x:2015:SER:HB2	1.94	0.47
13:o:2027:ARG:O	13:o:2029:ALA:N	2.46	0.47
15:u:2072:TYR:HB3	15:u:2073:PRO:CD	2.33	0.47
1:A:150:PRO:O	1:A:151:LEU:C	2.55	0.47
1:A:161:TYR:CE1	1:A:186:PHE:CE1	3.00	0.47
1:A:180:PHE:CE2	4:D:192:THR:CG2	2.97	0.47
1:A:202:VAL:HG21	23:A:350:CLA:OBD	2.15	0.47
2:B:264:PRO:HG2	2:B:267:LEU:HB2	1.96	0.47
23:B:514:CLA:H202	11:L:27:LEU:HD11	1.96	0.47
3:C:94:THR:C	3:C:96:GLY:N	2.71	0.47
3:C:213:LEU:HD21	23:C:474:CLA:H171	1.97	0.47
3:C:249:ILE:O	3:C:252:ILE:HB	2.15	0.47
3:C:392:ALA:O	3:C:396:MET:HB3	2.15	0.47
23:C:478:CLA:H91	23:C:482:CLA:HAA1	1.96	0.47
4:D:101:PHE:O	4:D:102:THR:C	2.56	0.47
5:E:74:GLN:O	5:E:78:PHE:CD1	2.67	0.47
13:O:81:ILE:CG2	13:O:82:GLN:N	2.52	0.47
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2130:GLN:OE1	1:a:2143:ILE:HG22	2.14	0.47
1:a:2334:ARG:HH12	13:o:2159:PRO:C	2.21	0.47
2:b:2027:THR:HG22	2:b:2107:LEU:CD1	2.44	0.47
2:b:2472:ARG:NE	2:b:2479:PHE:CE1	2.82	0.47
3:c:2184:GLY:HA3	3:c:2196:VAL:CG1	2.44	0.47
3:c:2297:TYR:OH	23:c:2481:CLA:O1D	2.31	0.47
3:c:2318:LEU:CD2	3:c:2328:VAL:CG1	2.92	0.47
4:d:2301:GLN:O	4:d:2302:GLU:C	2.57	0.47
26:d:2359:LMT:H121	7:h:2053:ILE:HD11	1.96	0.47
10:k:2019:ILE:CG1	10:k:2020:PRO:HD3	2.44	0.47
13:o:2076:THR:HB	13:o:2077:SER:H	1.42	0.47
14:t:2022:PHE:C	14:t:2023:PHE:CD1	2.93	0.47
1:A:44:ALA:CB	24:A:351:PHO:H91	2.44	0.47
1:A:315:ASN:HB2	4:D:63:LEU:HD23	1.95	0.47
2:B:464:PHE:HD2	23:B:523:CLA:HAC2	1.79	0.47
4:D:170:ALA:O	4:D:171:PRO:C	2.56	0.47
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.97	0.47
4:D:316:THR:O	4:D:317:LYS:C	2.58	0.47
5:E:30:PHE:HD2	5:E:30:PHE:C	2.23	0.47
7:H:24:TRP:HA	7:H:24:TRP:HE3	1.78	0.47
13:O:211:ILE:HG22	13:O:212:ALA:H	1.79	0.47
15:U:73:PRO:HG2	16:V:83:ASP:OD1	2.13	0.47
15:U:112:PHE:N	15:U:112:PHE:CD1	2.82	0.47
15:U:130:ASN:O	15:U:131:GLY:C	2.57	0.47
1:a:2157:VAL:CG2	1:a:2290:ILE:HD13	2.42	0.47
1:a:2260:PHE:O	1:a:2263:ALA:HB3	2.15	0.47
2:b:2397:VAL:CG1	2:b:2398:THR:H	2.27	0.47
2:b:2479:PHE:C	2:b:2481:GLY:H	2.21	0.47
23:b:2521:CLA:H172	23:d:2357:CLA:H72	1.95	0.47
23:b:2522:CLA:H171	23:b:2525:CLA:HMD3	1.95	0.47
3:c:2294:ASN:O	3:c:2295:THR:C	2.57	0.47
3:c:2297:TYR:HB3	3:c:2302:TYR:HD1	1.79	0.47
3:c:2299:SER:O	3:c:2303:GLY:O	2.33	0.47
4:d:2038:PHE:HB2	4:d:2039:PRO:HD3	1.97	0.47
4:d:2066:SER:C	4:d:2076:VAL:HG22	2.40	0.47
4:d:2160:TYR:CZ	4:d:2164:GLN:NE2	2.83	0.47
5:e:2055:TYR:O	16:v:2001:ALA:CB	2.63	0.47
13:o:2040:ILE:CG2	13:o:2041:ALA:H	2.23	0.47
13:o:2045:LEU:HD12	13:o:2239:PHE:CB	2.45	0.47
15:u:2091:VAL:HG12	15:u:2105:LEU:HD13	1.96	0.47
15:u:2125:GLY:O	15:u:2129:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CD1	1:A:81:ALA:HB2	2.50	0.47
1:A:143:ILE:HG21	4:D:253:TRP:HH2	1.80	0.47
2:B:124:ARG:CG	2:B:125:ASP:N	2.76	0.47
2:B:252:VAL:O	2:B:255:THR:HB	2.15	0.47
2:B:331:ASN:C	2:B:333:GLY:H	2.21	0.47
23:B:519:CLA:CBB	4:D:123:ILE:HG12	2.44	0.47
3:C:100:GLY:O	3:C:101:PRO:C	2.53	0.47
23:C:476:CLA:HED3	23:C:483:CLA:H71	1.96	0.47
4:D:71:CYS:HB3	4:D:75:THR:CG2	2.45	0.47
4:D:291:LEU:O	4:D:293:LEU:N	2.48	0.47
7:H:54:LEU:HB2	7:H:57:VAL:HB	1.97	0.47
10:K:31:GLN:HB3	10:K:36:PHE:HD2	1.80	0.47
12:M:21:PHE:CD2	12:M:22:LEU:HD23	2.50	0.47
13:O:39:ARG:HA	13:O:245:PRO:CG	2.44	0.47
13:O:118:LEU:HD13	13:O:233:VAL:HG21	1.96	0.47
13:O:147:ASN:HD22	13:O:147:ASN:HA	1.43	0.47
15:U:66:ILE:HG23	16:V:82:TYR:CE2	2.49	0.47
17:X:13:THR:O	17:X:15:SER:N	2.47	0.47
1:a:2077:ILE:HD13	11:l:2029:LEU:HG	1.97	0.47
1:a:2173:PRO:CG	1:a:2178:GLY:C	2.88	0.47
1:a:2202:VAL:HG11	23:a:2349:CLA:CAD	2.45	0.47
1:a:2214:MET:HA	1:a:2214:MET:HE3	1.97	0.47
1:a:2275:LEU:HD22	4:d:2211:CYS:SG	2.54	0.47
1:a:2309:ALA:HB1	16:v:2001:ALA:O	2.15	0.47
2:b:2057:ARG:HA	2:b:2330:MET:HG3	1.96	0.47
2:b:2198:VAL:O	2:b:2201:HIS:HB3	2.14	0.47
2:b:2401:PHE:HZ	2:b:2420:TYR:CD2	2.33	0.47
2:b:2418:LYS:HZ1	15:u:2045:GLU:CG	2.27	0.47
3:c:2188:THR:HG22	3:c:2188:THR:O	2.15	0.47
3:c:2299:SER:CB	3:c:2303:GLY:O	2.62	0.47
3:c:2385:GLN:HB3	3:c:2386:PRO:HD2	1.97	0.47
3:c:2450:ALA:HA	3:c:2454:GLY:CA	2.42	0.47
4:d:2042:TYR:CZ	6:f:2024:THR:HG23	2.50	0.47
4:d:2156:VAL:CG1	4:d:2171:PRO:HG2	2.45	0.47
4:d:2316:THR:HG23	13:o:2160:LYS:HZ1	1.80	0.47
5:e:2048:THR:O	5:e:2049:PRO:C	2.58	0.47
8:i:2005:LYS:O	8:i:2009:TYR:CD1	2.64	0.47
10:k:2030:TRP:HE3	10:k:2031:GLN:NE2	2.13	0.47
11:l:2037:ASN:ND2	11:l:2037:ASN:OXT	2.48	0.47
13:o:2133:VAL:O	13:o:2133:VAL:HG12	2.15	0.47
15:u:2057:LEU:CD2	15:u:2112:PHE:HD2	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:2098:THR:OG1	15:u:2101:GLN:HG3	2.15	0.47
16:v:2133:GLY:O	16:v:2137:TYR:N	2.47	0.47
1:A:261:GLN:CG	1:A:262:TYR:H	2.28	0.47
2:B:11:VAL:HG13	11:L:6:ASN:CB	2.45	0.47
2:B:187:PRO:HA	2:B:190:PHE:HB2	1.95	0.47
2:B:277:SER:O	2:B:278:SER:C	2.57	0.47
3:C:37:ALA:O	3:C:38:GLY:C	2.57	0.47
3:C:39:ASN:HB2	23:C:483:CLA:HBA2	1.96	0.47
3:C:97:TRP:CZ3	3:C:178:LYS:HE3	2.50	0.47
3:C:227:VAL:HG23	3:C:294:ASN:CB	2.42	0.47
4:D:153:PHE:CZ	24:D:355:PHO:H92	2.50	0.47
5:E:23:SER:O	5:E:27:PRO:HG2	2.15	0.47
1:a:2174:LEU:N	1:a:2174:LEU:HD23	2.30	0.47
1:a:2180:PHE:CD2	4:d:2192:THR:CG2	2.98	0.47
2:b:2315:ILE:HD13	2:b:2359:MET:CE	2.41	0.47
23:c:2476:CLA:H61	23:c:2483:CLA:H72	1.97	0.47
4:d:2090:LEU:HD13	4:d:2096:GLU:HB3	1.89	0.47
4:d:2091:LEU:HD22	23:d:2357:CLA:O2D	2.14	0.47
25:d:2358:PL9:H38	14:t:2018:PHE:CB	2.39	0.47
13:o:2015:LEU:O	13:o:2016:ALA:C	2.58	0.47
13:o:2033:ASP:O	13:o:2037:THR:N	2.46	0.47
15:u:2066:ILE:O	15:u:2066:ILE:HG22	2.15	0.47
1:A:139:MET:HE2	4:D:248:THR:HG21	1.97	0.47
1:A:186:PHE:CD2	1:A:192:ILE:CD1	2.85	0.47
1:A:271:LEU:O	1:A:275:LEU:HG	2.15	0.47
2:B:153:PHE:O	2:B:157:HIS:HB3	2.14	0.47
2:B:250:PHE:HB3	23:B:521:CLA:H142	1.96	0.47
23:B:522:CLA:H152	23:B:525:CLA:HMD3	1.95	0.47
3:C:320:ARG:HG2	15:U:128:TYR:HE2	1.80	0.47
3:C:343:ARG:HB3	13:O:78:LEU:HD12	1.97	0.47
23:C:476:CLA:HBD	23:C:486:CLA:CBB	2.45	0.47
5:E:14:THR:CB	9:J:8:ILE:HD12	2.43	0.47
9:J:27:LEU:O	9:J:30:TYR:N	2.48	0.47
13:O:158:ASP:CB	13:O:159:PRO:CD	2.92	0.47
15:U:72:TYR:CB	15:U:73:PRO:CD	2.91	0.47
18:N:31:UNK:HA	19:Z:30:PRO:CG	2.45	0.47
19:Z:37:LYS:O	19:Z:41:PHE:CE1	2.68	0.47
1:a:2215:HIS:CD2	4:d:2268:HIS:CD2	3.03	0.47
1:a:2300:PHE:CB	1:a:2302:PHE:HE1	2.22	0.47
2:b:2012:LEU:HG	2:b:2019:LEU:HD13	1.96	0.47
2:b:2244:ALA:O	2:b:2247:PHE:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2048:LYS:HZ3	23:c:2486:CLA:HBA1	1.77	0.47
3:c:2068:THR:HB	3:c:2115:GLY:HA2	1.97	0.47
3:c:2100:GLY:O	3:c:2101:PRO:C	2.57	0.47
4:d:2221:THR:O	4:d:2221:THR:HG22	2.15	0.47
13:o:2027:ARG:C	13:o:2029:ALA:N	2.67	0.47
13:o:2040:ILE:HG12	13:o:2084:GLU:OE2	2.14	0.47
15:u:2047:LEU:C	15:u:2049:THR:H	2.22	0.47
16:v:2080:THR:HG22	16:v:2081:THR:O	2.14	0.47
19:z:2017:PHE:O	19:z:2021:ILE:HG13	2.15	0.47
1:A:291:SER:O	1:A:295:PHE:HE1	1.98	0.47
2:B:224:ARG:O	2:B:228:ALA:HB3	2.15	0.47
2:B:340:TRP:HH2	2:B:401:PHE:CD1	2.33	0.47
2:B:390:TYR:O	2:B:391:SER:O	2.33	0.47
4:D:52:THR:HG23	4:D:76:VAL:CG1	2.44	0.47
7:H:27:THR:N	7:H:28:PRO:CD	2.78	0.47
11:L:36:PHE:C	12:M:3:VAL:HG23	2.40	0.47
13:O:54:GLU:OE1	13:O:231:HIS:NE2	2.48	0.47
13:O:152:ARG:HD2	13:O:156:PHE:CG	2.50	0.47
13:O:210:GLU:OE1	13:O:210:GLU:HA	2.15	0.47
1:a:2255:PHE:HZ	25:a:2352:PL9:H112	1.79	0.47
1:a:2341:LEU:HD21	15:u:2134:LYS:CD	2.45	0.47
2:b:2478:VAL:O	2:b:2481:GLY:N	2.46	0.47
3:c:2050:LEU:O	3:c:2054:VAL:CG2	2.61	0.47
3:c:2343:ARG:NE	13:o:2075:THR:OG1	2.33	0.47
4:d:2091:LEU:HD22	23:d:2357:CLA:CED	2.45	0.47
4:d:2181:PHE:CZ	4:d:2185:PHE:CE1	3.03	0.47
5:e:2067:ASP:HB3	5:e:2070:GLU:HG3	1.97	0.47
9:j:2014:ALA:O	27:k:2050:BCR:H24C	2.15	0.47
10:k:2011:PRO:O	10:k:2014:ASP:HB2	2.15	0.47
12:m:2016:LEU:O	12:m:2017:VAL:C	2.58	0.47
13:o:2116:ILE:HG22	13:o:2118:LEU:CD2	2.44	0.47
13:o:2182:LEU:O	13:o:2183:ALA:C	2.57	0.47
1:A:36:ILE:HD13	23:C:487:CLA:H141	1.97	0.46
2:B:45:PHE:CE2	2:B:78:TRP:HZ2	2.32	0.46
2:B:183:PRO:HB2	2:B:200:ALA:HB2	1.96	0.46
2:B:401:PHE:HZ	2:B:420:TYR:CD2	2.34	0.46
2:B:467:ILE:HD13	4:D:126:MET:CE	2.45	0.46
23:B:519:CLA:HBB2	4:D:123:ILE:HG12	1.97	0.46
3:C:307:PRO:O	3:C:308:GLU:C	2.57	0.46
3:C:337:LEU:HA	13:O:104:GLN:NE2	2.29	0.46
4:D:188:PHE:HD1	4:D:188:PHE:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:21:ALA:HB3	7:H:22:PRO:HD2	1.97	0.46
13:O:110:MET:CE	13:O:110:MET:H	2.28	0.46
13:O:122:VAL:O	13:O:122:VAL:HG12	2.15	0.46
16:V:126:LEU:O	16:V:129:LYS:HG3	2.15	0.46
2:b:2091:TRP:HB3	23:b:2515:CLA:H43	1.96	0.46
2:b:2212:ALA:HB2	23:b:2511:CLA:HMC3	1.96	0.46
2:b:2265:ILE:C	2:b:2267:LEU:H	2.23	0.46
2:b:2305:ILE:O	2:b:2341:LYS:HD2	2.15	0.46
3:c:2285:ILE:CB	23:c:2487:CLA:HMB3	2.44	0.46
3:c:2417:VAL:HG21	16:v:2042:VAL:HG22	1.96	0.46
4:d:2322:ASN:O	4:d:2325:ILE:N	2.48	0.46
15:u:2061:ASN:N	15:u:2061:ASN:ND2	2.60	0.46
19:z:2031:GLN:O	19:z:2032:ASP:C	2.58	0.46
1:A:230:THR:HG22	1:A:231:GLU:N	2.18	0.46
2:B:25:MET:HB3	27:B:529:BCR:C33	2.42	0.46
2:B:119:ASP:HB3	2:B:121:GLU:HG3	1.97	0.46
3:C:292:PHE:HD2	3:C:292:PHE:H	1.56	0.46
3:C:412:THR:HG22	3:C:412:THR:O	2.14	0.46
23:C:480:CLA:H42	23:C:481:CLA:HBD	1.98	0.46
11:L:12:LEU:CD1	11:L:16:SER:CB	2.93	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.97	0.46
13:O:180:GLU:HG3	13:O:181:GLU:H	1.80	0.46
1:a:2083:VAL:CG1	1:a:2084:PRO:CD	2.90	0.46
2:b:2381:ILE:HG22	2:b:2381:ILE:O	2.13	0.46
3:c:2135:ARG:O	3:c:2135:ARG:HG2	2.15	0.46
3:c:2305:THR:CB	3:c:2308:GLU:HG3	2.45	0.46
3:c:2306:GLY:HA2	3:c:2400:PRO:HG2	1.97	0.46
3:c:2350:ILE:HD13	3:c:2359:TRP:CB	2.45	0.46
4:d:2080:THR:CG2	4:d:2081:PRO:HD2	2.46	0.46
4:d:2210:LEU:HD11	4:d:2274:VAL:HG21	1.98	0.46
13:o:2034:SER:O	13:o:2035:SER:C	2.58	0.46
13:o:2040:ILE:CG2	13:o:2041:ALA:N	2.79	0.46
13:o:2205:ASP:OD1	13:o:2209:GLY:O	2.32	0.46
15:u:2061:ASN:CB	15:u:2126:ASP:O	2.60	0.46
15:u:2072:TYR:HD2	15:u:2073:PRO:HG3	1.80	0.46
15:u:2113:THR:CG2	15:u:2114:VAL:N	2.77	0.46
16:v:2129:LYS:CE	16:v:2135:VAL:HG23	2.45	0.46
1:A:31:GLY:O	1:A:33:PHE:N	2.48	0.46
27:B:529:BCR:H371	27:B:529:BCR:H393	1.97	0.46
4:D:301:GLN:O	4:D:302:GLU:C	2.58	0.46
13:O:32:ILE:O	13:O:34:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:75:THR:O	13:O:76:THR:C	2.57	0.46
13:O:114:GLU:OE2	13:O:231:HIS:NE2	2.47	0.46
1:a:2242:GLU:C	1:a:2244:GLU:H	2.23	0.46
1:a:2329:GLU:OE2	3:c:2410:VAL:HG11	2.16	0.46
2:b:2463:PHE:CZ	2:b:2467:ILE:HD11	2.50	0.46
3:c:2378:ASN:O	3:c:2382:ASN:HB2	2.15	0.46
3:c:2456:GLU:C	4:d:2230:SER:CB	2.89	0.46
4:d:2156:VAL:HG23	23:d:2354:CLA:HED1	1.95	0.46
23:d:2357:CLA:H12	7:h:2042:LEU:CD2	2.43	0.46
13:o:2130:GLN:CB	13:o:2131:PRO:CD	2.73	0.46
19:z:2012:LEU:CD1	19:z:2047:TRP:CD1	2.99	0.46
1:A:37:MET:HB3	1:A:37:MET:HE2	1.75	0.46
1:A:211:PHE:HE2	1:A:278:TRP:CD1	2.33	0.46
2:B:297:THR:O	2:B:300:GLU:N	2.49	0.46
23:B:518:CLA:H61	23:B:518:CLA:H41	1.79	0.46
3:C:93:ALA:HB3	3:C:301:PHE:CE1	2.51	0.46
3:C:108:THR:CG2	10:K:2:LEU:HD23	2.44	0.46
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.50	0.46
4:D:72:ASN:OD1	4:D:74:LEU:CB	2.63	0.46
4:D:325:ILE:O	4:D:329:MET:HB3	2.14	0.46
5:E:41:LEU:O	5:E:42:ALA:C	2.59	0.46
9:J:19:MET:SD	27:K:50:BCR:H361	2.55	0.46
15:U:100:ARG:HG3	15:U:104:ILE:HD11	1.98	0.46
1:a:2102:LEU:O	1:a:2106:LEU:HG	2.14	0.46
1:a:2295:PHE:O	3:c:2291:TRP:HH2	1.98	0.46
2:b:2057:ARG:NH2	2:b:2334:ASP:OD2	2.46	0.46
2:b:2166:MET:CE	2:b:2195:PRO:HB3	2.44	0.46
3:c:2108:THR:CG2	10:k:2002:LEU:HD23	2.44	0.46
3:c:2265:ILE:HD11	3:c:2449:ARG:HD3	1.97	0.46
3:c:2279:LEU:HD22	23:c:2480:CLA:C14	2.46	0.46
3:c:2372:PRO:O	3:c:2373:ASN:HB2	2.15	0.46
5:e:2010:SER:HA	5:e:2013:ILE:CD1	2.27	0.46
11:l:2004:ASN:HD22	11:l:2004:ASN:N	2.04	0.46
13:o:2028:GLY:O	13:o:2136:ILE:HB	2.14	0.46
13:o:2104:GLN:N	13:o:2104:GLN:OE1	2.42	0.46
1:A:315:ASN:C	4:D:63:LEU:HD22	2.39	0.46
2:B:163:GLY:O	2:B:165:GLY:N	2.46	0.46
2:B:185:TRP:O	2:B:186:GLY:O	2.33	0.46
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.15	0.46
2:B:321:LYS:NZ	4:D:297:ASP:OD2	2.42	0.46
3:C:77:PRO:HA	3:C:104:GLU:CD	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:THR:O	3:C:201:ASN:ND2	2.32	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD1	2.38	0.46
4:D:337:GLU:O	4:D:338:ASN:HB2	2.14	0.46
27:K:50:BCR:HC42	19:Z:17:PHE:CD1	2.49	0.46
11:L:31:PHE:O	11:L:32:SER:C	2.57	0.46
16:V:33:PHE:CD2	16:V:37:CYS:CB	2.99	0.46
17:X:34:PHE:O	17:X:35:ALA:C	2.58	0.46
1:a:2173:PRO:HG3	1:a:2178:GLY:O	2.15	0.46
1:a:2180:PHE:HD2	4:d:2192:THR:HB	1.78	0.46
2:b:2119:ASP:HB3	2:b:2121:GLU:HG3	1.98	0.46
3:c:2101:PRO:HA	3:c:2195:ASP:HB3	1.97	0.46
3:c:2273:SER:CB	3:c:2445:ALA:HB2	2.45	0.46
10:k:2001:LYS:HE3	10:k:2010:ASP:HB2	1.97	0.46
12:m:2020:VAL:O	12:m:2021:PHE:C	2.58	0.46
12:m:2028:GLN:HE21	12:m:2028:GLN:HB3	1.45	0.46
13:o:2081:ILE:CG2	13:o:2082:GLN:N	2.63	0.46
16:v:2012:LEU:HD13	16:v:2019:ILE:HG21	1.98	0.46
1:A:75:ASN:ND2	1:A:79:THR:HG22	2.31	0.46
1:A:140:ARG:HB2	4:D:220:ASN:CG	2.41	0.46
1:A:261:GLN:CG	1:A:262:TYR:N	2.78	0.46
3:C:71:GLU:O	3:C:75:PHE:HB2	2.15	0.46
3:C:73:ALA:O	10:K:1:LYS:HA	2.14	0.46
3:C:218:PHE:O	3:C:219:GLY:C	2.58	0.46
3:C:281:MET:O	3:C:285:ILE:HG13	2.16	0.46
3:C:343:ARG:HD3	3:C:344:SER:C	2.40	0.46
3:C:347:GLY:O	13:O:16:ALA:CB	2.64	0.46
13:O:46:GLN:HE21	13:O:46:GLN:HB3	1.50	0.46
14:T:1:MET:C	14:T:3:THR:N	2.68	0.46
1:a:2133:LEU:HD23	4:d:2252:PHE:CD1	2.50	0.46
1:a:2150:PRO:O	1:a:2153:SER:N	2.48	0.46
1:a:2230:THR:CG2	1:a:2231:GLU:H	2.04	0.46
1:a:2284:TRP:HA	1:a:2284:TRP:HE3	1.79	0.46
2:b:2019:LEU:HD21	23:b:2524:CLA:H192	1.98	0.46
23:b:2512:CLA:H2A	23:b:2512:CLA:O2A	2.16	0.46
3:c:2042:LEU:CD1	23:c:2486:CLA:HMA2	2.45	0.46
3:c:2158:THR:HG22	3:c:2251:HIS:CB	2.45	0.46
3:c:2225:VAL:HG13	3:c:2294:ASN:ND2	2.28	0.46
3:c:2294:ASN:C	3:c:2296:VAL:N	2.73	0.46
3:c:2321:ASP:CG	15:u:2128:TYR:CD2	2.94	0.46
23:c:2476:CLA:HED3	23:c:2483:CLA:H71	1.97	0.46
4:d:2152:VAL:CG2	4:d:2279:LEU:HD13	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:2019:TRP:HA	6:f:2019:TRP:CE3	2.50	0.46
7:h:2063:ALA:O	7:h:2064:LEU:HD23	2.16	0.46
9:j:2027:LEU:O	9:j:2030:TYR:N	2.49	0.46
1:A:307:ILE:O	1:A:308:ASP:C	2.58	0.46
1:A:312:ASN:HB3	5:E:55:TYR:CE1	2.51	0.46
2:B:53:ASN:ND2	2:B:58:GLN:OE1	2.49	0.46
3:C:98:GLY:C	3:C:99:VAL:HG23	2.41	0.46
3:C:293:ASN:N	3:C:293:ASN:HD22	2.12	0.46
3:C:335:THR:HG22	3:C:335:THR:O	2.16	0.46
4:D:110:LEU:O	4:D:113:PHE:N	2.49	0.46
10:K:10:ASP:N	10:K:11:PRO:CD	2.79	0.46
1:a:2033:PHE:CD1	1:a:2128:GLY:HA3	2.51	0.46
1:a:2063:ILE:HG22	3:c:2335:THR:HG21	1.97	0.46
1:a:2187:GLN:NE2	1:a:2187:GLN:O	2.48	0.46
1:a:2266:ASN:OD1	1:a:2267:ASN:N	2.45	0.46
1:a:2330:VAL:HG12	1:a:2331:MET:HG2	1.98	0.46
2:b:2006:TYR:OH	23:b:2520:CLA:HMD2	2.15	0.46
2:b:2127:ARG:NH1	2:b:2127:ARG:CG	2.79	0.46
2:b:2471:ALA:HB2	4:d:2130:PHE:CZ	2.50	0.46
23:b:2516:CLA:HAA2	23:b:2516:CLA:HBD	1.98	0.46
4:d:2089:LEU:HB2	4:d:2091:LEU:HD21	1.96	0.46
4:d:2170:ALA:O	4:d:2171:PRO:C	2.59	0.46
4:d:2340:VAL:HG23	4:d:2340:VAL:O	2.16	0.46
2:B:222:PRO:CB	7:H:25:GLY:HA2	2.30	0.46
2:B:234:ILE:HG13	23:B:524:CLA:H191	1.97	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.97	0.46
3:C:99:VAL:HG12	3:C:100:GLY:O	2.15	0.46
3:C:286:ALA:HA	3:C:289:PHE:CB	2.46	0.46
3:C:321:ASP:CG	15:U:128:TYR:CD2	2.94	0.46
4:D:87:HIS:HE1	4:D:162:LEU:HA	1.80	0.46
4:D:165:SER:O	4:D:166:SER:HB3	2.16	0.46
4:D:329:MET:O	4:D:333:ASP:HB2	2.15	0.46
13:O:40:ILE:CG2	13:O:41:ALA:N	2.72	0.46
13:O:238:VAL:HG12	13:O:239:PHE:H	1.78	0.46
15:U:84:PRO:C	15:U:85:TYR:HD2	2.22	0.46
16:V:81:THR:O	16:V:83:ASP:N	2.49	0.46
1:a:2238:LYS:O	1:a:2239:PHE:C	2.59	0.46
1:a:2307:ILE:HG22	1:a:2309:ALA:CB	2.45	0.46
3:c:2305:THR:HB	3:c:2308:GLU:HG3	1.96	0.46
3:c:2307:PRO:O	3:c:2308:GLU:C	2.59	0.46
4:d:2089:LEU:CB	4:d:2091:LEU:HD21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:2019:MET:CG	27:k:2050:BCR:H361	2.46	0.46
1:A:141:PRO:HG2	3:C:443:TRP:CZ3	2.41	0.46
1:A:218:LEU:CD2	4:D:142:ASN:ND2	2.79	0.46
2:B:19:LEU:HD21	23:B:524:CLA:H192	1.97	0.46
23:B:519:CLA:HMD3	23:B:524:CLA:HAB	1.98	0.46
3:C:82:TYR:CD1	3:C:82:TYR:C	2.94	0.46
3:C:95:LEU:HD11	23:C:480:CLA:HBA2	1.97	0.46
3:C:281:MET:C	3:C:285:ILE:HG13	2.41	0.46
3:C:406:SER:OG	23:C:475:CLA:O1A	2.34	0.46
4:D:218:VAL:O	4:D:219:GLU:C	2.59	0.46
13:O:40:ILE:O	13:O:243:ILE:HG23	2.16	0.46
13:O:137:THR:CG2	13:O:138:THR:N	2.77	0.46
13:O:152:ARG:NH1	13:O:156:PHE:CE2	2.84	0.46
14:T:7:VAL:O	14:T:10:PHE:HB3	2.16	0.46
16:V:78:ASN:HB2	16:V:96:ARG:NH1	2.28	0.46
19:Z:31:GLN:O	19:Z:32:ASP:C	2.59	0.46
19:Z:48:ILE:O	19:Z:48:ILE:HG12	2.15	0.46
1:a:2135:TYR:HH	8:i:2032:PRO:HG3	1.81	0.46
4:d:2190:ASN:CB	4:d:2296:TYR:CD1	2.99	0.46
10:k:2015:VAL:HG11	18:n:2013:UNK:CB	2.46	0.46
13:o:2028:GLY:HA3	13:o:2137:THR:HG22	1.97	0.46
2:B:346:PHE:O	2:B:354:LEU:HB2	2.16	0.46
2:B:385:ARG:HG3	13:O:165:ALA:C	2.41	0.46
3:C:48:LYS:NZ	23:C:486:CLA:HBA1	2.31	0.46
4:D:148:ALA:HB1	4:D:279:LEU:HB2	1.98	0.46
5:E:43:TYR:CE2	5:E:50:ARG:HG2	2.51	0.46
6:F:39:MET:HE2	6:F:39:MET:HB3	1.79	0.46
11:L:24:ILE:HD13	12:M:18:PRO:HB2	1.97	0.46
13:O:15:LEU:O	13:O:16:ALA:C	2.59	0.46
13:O:28:GLY:HA2	13:O:204:VAL:HB	1.96	0.46
2:b:2225:LEU:CD2	23:b:2524:CLA:HMC1	2.46	0.46
3:c:2063:TRP:CH2	3:c:2088:LEU:HD11	2.50	0.46
3:c:2134:ILE:HG12	23:c:2486:CLA:O1A	2.16	0.46
3:c:2297:TYR:CG	3:c:2302:TYR:CE1	3.04	0.46
4:d:2103:ARG:C	4:d:2105:CYS:N	2.73	0.46
4:d:2181:PHE:O	4:d:2182:LEU:C	2.59	0.46
4:d:2190:ASN:CB	4:d:2296:TYR:HD1	2.29	0.46
12:m:2018:PRO:O	12:m:2022:LEU:HG	2.16	0.46
13:o:2045:LEU:HD12	13:o:2045:LEU:HA	1.78	0.46
13:o:2201:VAL:HG11	13:o:2204:VAL:CG2	2.46	0.46
13:o:2224:ASP:O	13:o:2225:MET:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD21	1:A:122:GLY:C	2.40	0.45
1:A:159:LEU:CD2	1:A:163:ILE:HD11	2.46	0.45
2:B:360:PRO:C	2:B:362:PHE:N	2.71	0.45
3:C:210:PHE:O	3:C:213:LEU:HB2	2.16	0.45
3:C:390:ARG:NH1	16:V:100:ILE:HG23	2.31	0.45
7:H:53:ILE:HG22	17:X:15:SER:CB	2.45	0.45
13:O:53:LYS:HB3	13:O:64:GLU:O	2.16	0.45
13:O:136:ILE:HG22	13:O:204:VAL:HG21	1.98	0.45
18:N:22:UNK:C	18:N:24:UNK:N	2.75	0.45
1:a:2065:GLU:O	1:a:2065:GLU:HG2	2.15	0.45
2:b:2135:LEU:HB2	2:b:2231:MET:CE	2.45	0.45
2:b:2166:MET:HE1	2:b:2195:PRO:HB3	1.98	0.45
2:b:2445:THR:HG22	2:b:2446:SER:N	2.31	0.45
23:b:2511:CLA:H102	7:h:2037:PHE:CD1	2.51	0.45
3:c:2390:ARG:HD3	16:v:2100:ILE:CG2	2.47	0.45
9:j:2025:VAL:O	9:j:2026:GLY:C	2.57	0.45
13:o:2088:ASN:ND2	13:o:2090:ASP:OD2	2.49	0.45
15:u:2105:LEU:O	15:u:2109:LEU:N	2.47	0.45
1:A:112:TYR:CZ	1:A:116:ILE:HD11	2.51	0.45
1:A:169:SER:O	1:A:170:ASP:HB2	2.16	0.45
1:A:225:ARG:HA	2:B:481:GLY:HA3	1.99	0.45
1:A:320:ILE:HD13	4:D:333:ASP:HA	1.98	0.45
2:B:19:LEU:HD21	23:B:524:CLA:C19	2.46	0.45
2:B:249:ALA:CB	2:B:459:ALA:HB2	2.47	0.45
23:B:521:CLA:HAB	23:B:527:CLA:CED	2.31	0.45
3:C:285:ILE:HD12	23:C:479:CLA:H71	1.98	0.45
3:C:341:LEU:HD22	3:C:349:ILE:HG22	1.97	0.45
3:C:390:ARG:NH1	16:V:100:ILE:HG21	2.32	0.45
28:E:84:HEC:C4A	6:F:19:TRP:CH2	2.99	0.45
16:V:66:ARG:HG3	16:V:66:ARG:NH1	2.31	0.45
1:a:2014:TRP:HH2	8:i:2025:SER:HB3	1.82	0.45
1:a:2052:PHE:O	1:a:2052:PHE:CD2	2.69	0.45
1:a:2243:GLU:HG3	1:a:2243:GLU:O	2.15	0.45
2:b:2135:LEU:O	2:b:2138:MET:N	2.49	0.45
3:c:2247:GLY:O	3:c:2248:GLY:C	2.57	0.45
3:c:2404:LEU:C	3:c:2406:SER:H	2.25	0.45
4:d:2232:PHE:N	4:d:2232:PHE:CD1	2.84	0.45
28:e:2084:HEC:HMC2	6:f:2030:ILE:HD12	1.97	0.45
13:o:2068:THR:HA	13:o:2110:MET:HE1	1.96	0.45
13:o:2076:THR:O	13:o:2077:SER:C	2.60	0.45
13:o:2143:LYS:HG2	13:o:2198:SER:HB2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:2152:ARG:HD2	13:o:2156:PHE:CE1	2.51	0.45
1:A:155:PHE:O	1:A:159:LEU:N	2.41	0.45
2:B:118:TRP:CD1	2:B:118:TRP:H	2.33	0.45
2:B:171:PRO:HD3	7:H:64:LEU:HD11	1.98	0.45
27:B:529:BCR:H361	27:B:529:BCR:H20C	1.66	0.45
3:C:285:ILE:CB	23:C:487:CLA:HMB3	2.47	0.45
4:D:65:SER:OG	4:D:77:ALA:O	2.31	0.45
11:L:37:ASN:ND2	11:L:37:ASN:OXT	2.50	0.45
14:T:3:THR:C	14:T:5:THR:N	2.74	0.45
15:U:72:TYR:O	15:U:76:ALA:HB3	2.16	0.45
19:Z:51:VAL:HG12	19:Z:52:LEU:CD2	2.36	0.45
1:a:2159:LEU:O	1:a:2160:ILE:C	2.59	0.45
1:a:2213:ALA:O	1:a:2217:SER:CB	2.64	0.45
3:c:2286:ALA:HA	3:c:2289:PHE:HB3	1.99	0.45
3:c:2304:PRO:C	3:c:2423:ARG:NH1	2.74	0.45
27:c:2488:BCR:C21	10:k:2023:PHE:HE2	2.29	0.45
4:d:2322:ASN:O	4:d:2323:GLU:C	2.58	0.45
15:u:2100:ARG:O	15:u:2101:GLN:C	2.58	0.45
1:A:14:TRP:CH2	1:A:18:CYS:SG	3.09	0.45
1:A:117:PHE:O	1:A:121:LEU:HG	2.16	0.45
23:A:350:CLA:H121	25:A:353:PL9:C16	2.43	0.45
2:B:135:LEU:HB2	2:B:231:MET:CE	2.47	0.45
2:B:194:ASN:O	2:B:196:GLY:N	2.50	0.45
3:C:169:GLY:O	3:C:173:LEU:CD1	2.65	0.45
27:C:488:BCR:C21	10:K:23:PHE:HE2	2.29	0.45
12:M:28:GLN:HB2	12:m:2027:VAL:HG11	1.97	0.45
16:V:30:LYS:HG2	16:V:118:HIS:NE2	2.32	0.45
19:Z:2:THR:O	19:Z:6:GLN:HG3	2.17	0.45
1:a:2101:SER:O	1:a:2104:GLU:HB3	2.17	0.45
1:a:2237:TYR:HA	1:a:2241:GLN:CD	2.40	0.45
2:b:2018:ARG:NH1	2:b:2115:TRP:O	2.50	0.45
23:b:2522:CLA:H152	23:b:2525:CLA:HMD3	1.99	0.45
3:c:2211:GLY:O	3:c:2215:LYS:HG2	2.16	0.45
9:j:2019:MET:SD	27:k:2050:BCR:C36	3.05	0.45
16:v:2038:ALA:O	16:v:2042:VAL:HG23	2.16	0.45
19:z:2015:LEU:HD13	19:z:2046:LEU:HD23	1.98	0.45
1:A:52:PHE:O	1:A:52:PHE:HD2	1.98	0.45
1:A:63:ILE:HD11	1:A:336:ALA:HB1	1.99	0.45
1:A:303:ASN:HB2	3:C:415:ASN:OD1	2.16	0.45
2:B:212:ALA:HB2	23:B:511:CLA:HMC3	1.98	0.45
3:C:178:LYS:CG	3:C:178:LYS:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:313:GLN:O	3:C:317:PHE:HD1	2.00	0.45
4:D:279:LEU:N	4:D:279:LEU:HD23	2.32	0.45
16:V:76:MET:HE2	16:V:112:LEU:HD22	1.97	0.45
1:a:2052:PHE:O	1:a:2052:PHE:HD2	2.00	0.45
2:b:2118:TRP:CD1	2:b:2118:TRP:H	2.34	0.45
2:b:2418:LYS:HZ1	15:u:2045:GLU:HG2	1.81	0.45
3:c:2055:ALA:HB1	27:c:2488:BCR:H371	1.95	0.45
3:c:2080:PRO:HB3	3:c:2082:TYR:CZ	2.52	0.45
3:c:2179:ALA:HB2	3:c:2185:LEU:HD22	1.98	0.45
4:d:2175:VAL:HG12	4:d:2179:PHE:CE1	2.51	0.45
4:d:2201:VAL:O	4:d:2201:VAL:HG12	2.16	0.45
9:j:2018:GLY:O	9:j:2022:ILE:HG13	2.17	0.45
1:A:303:ASN:OD1	1:A:322:ASN:ND2	2.49	0.45
2:B:12:LEU:HG	2:B:19:LEU:HD13	1.97	0.45
2:B:113:TRP:HB3	23:B:525:CLA:CED	2.41	0.45
2:B:422:ARG:H	2:B:422:ARG:HG3	1.57	0.45
3:C:229:ASN:HD21	3:C:231:GLU:HB2	1.82	0.45
3:C:336:GLY:O	13:O:104:GLN:HG2	2.17	0.45
23:C:477:CLA:HAA2	23:C:477:CLA:HBD	1.97	0.45
4:D:231:THR:HG22	4:D:232:PHE:H	1.81	0.45
4:D:267:LEU:C	4:D:271:MET:HE3	2.42	0.45
5:E:25:THR:HG23	28:E:84:HEC:HAB	1.98	0.45
8:I:5:LYS:HG3	8:I:9:TYR:HE1	1.82	0.45
10:K:9:PHE:HE2	19:Z:13:VAL:HG21	1.81	0.45
13:O:38:TYR:O	13:O:245:PRO:CB	2.65	0.45
14:T:18:PHE:HD2	14:T:19:PHE:CE1	2.35	0.45
14:T:29:ILE:O	14:T:29:ILE:HG22	2.16	0.45
15:U:108:ASN:C	15:U:112:PHE:HE1	2.25	0.45
16:V:111:ASP:O	16:V:115:ILE:HG13	2.16	0.45
1:a:2070:SER:O	1:a:2075:ASN:HB2	2.16	0.45
23:a:2349:CLA:HMD2	4:d:2182:LEU:HD11	1.97	0.45
2:b:2187:PRO:O	2:b:2188:ASP:C	2.59	0.45
2:b:2187:PRO:O	2:b:2189:GLY:N	2.50	0.45
2:b:2302:TRP:CH2	2:b:2343:HIS:CG	3.05	0.45
2:b:2311:PHE:O	2:b:2313:ASP:N	2.50	0.45
2:b:2422:ARG:H	2:b:2422:ARG:HG3	1.56	0.45
3:c:2158:THR:HG22	3:c:2251:HIS:C	2.41	0.45
3:c:2273:SER:OG	3:c:2445:ALA:HA	2.17	0.45
3:c:2421:SER:O	3:c:2422:PRO:C	2.60	0.45
4:d:2090:LEU:HD11	4:d:2096:GLU:CG	2.46	0.45
4:d:2148:ALA:O	4:d:2152:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:n:2031:UNK:HA	19:z:2030:PRO:HG3	1.99	0.45
19:z:2015:LEU:HG	19:z:2019:MET:CE	2.46	0.45
19:z:2023:VAL:O	19:z:2027:TYR:HD1	1.98	0.45
1:A:224:ILE:HD11	1:A:243:GLU:CG	2.47	0.45
1:A:289:GLY:O	1:A:293:MET:HG3	2.16	0.45
1:A:300:PHE:CD2	3:C:404:LEU:HB2	2.52	0.45
2:B:341:LYS:NZ	13:o:2060:ARG:HH12	2.14	0.45
3:C:189:TRP:O	3:C:190:ALA:C	2.59	0.45
3:C:297:TYR:CG	3:C:302:TYR:HE1	2.35	0.45
4:D:312:GLU:HB2	13:O:159:PRO:HG3	1.97	0.45
13:O:59:LYS:HB3	2:b:2405:GLU:CB	2.45	0.45
13:O:60:ARG:NE	2:b:2405:GLU:OE1	2.47	0.45
15:U:58:ASN:HB2	15:U:59:ASN:ND2	2.32	0.45
1:a:2093:PHE:HD1	23:a:2351:CLA:H92	1.80	0.45
1:a:2139:MET:HE2	4:d:2248:THR:CG2	2.47	0.45
1:a:2187:GLN:HG2	1:a:2192:ILE:H	1.82	0.45
1:a:2257:ARG:NH1	4:d:2025:ASP:HB3	2.31	0.45
2:b:2194:ASN:O	2:b:2196:GLY:N	2.49	0.45
2:b:2249:ALA:HB3	2:b:2459:ALA:HB2	1.99	0.45
2:b:2302:TRP:CE3	2:b:2343:HIS:HB2	2.51	0.45
23:b:2519:CLA:H142	23:d:2357:CLA:H11	1.97	0.45
3:c:2128:GLY:HA3	23:c:2484:CLA:HMC2	1.98	0.45
3:c:2350:ILE:CG2	3:c:2351:PHE:N	2.78	0.45
4:d:2175:VAL:O	4:d:2178:ILE:HB	2.16	0.45
10:k:2026:LEU:HD11	18:n:2020:UNK:CB	2.47	0.45
11:l:2036:PHE:CD2	12:m:2007:GLY:HA3	2.51	0.45
13:o:2066:VAL:HG13	13:o:2067:PRO:HD2	1.98	0.45
1:A:46:ILE:O	1:A:47:CYS:C	2.59	0.45
1:A:193:LEU:HB3	4:D:179:PHE:CD2	2.52	0.45
2:B:135:LEU:O	2:B:138:MET:N	2.50	0.45
3:C:42:LEU:HD22	3:C:48:LYS:HB3	1.99	0.45
3:C:42:LEU:O	3:C:43:ILE:C	2.59	0.45
3:C:63:TRP:CZ3	3:C:88:LEU:HD11	2.52	0.45
3:C:276:LEU:HD23	3:C:440:GLY:O	2.17	0.45
4:D:129:GLN:NE2	4:D:142:ASN:HB3	2.32	0.45
13:O:205:ASP:O	13:O:206:GLY:C	2.58	0.45
15:U:113:THR:CG2	15:U:114:VAL:N	2.78	0.45
1:a:2159:LEU:CG	1:a:2163:ILE:HD11	2.38	0.45
2:b:2072:THR:HG22	2:b:2079:SER:HB2	1.98	0.45
2:b:2350:GLU:OE1	2:b:2350:GLU:N	2.50	0.45
23:c:2474:CLA:H122	23:c:2485:CLA:H13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2019:ASP:O	4:d:2023:LYS:HG3	2.16	0.45
4:d:2052:THR:HG23	4:d:2076:VAL:HG11	1.96	0.45
4:d:2080:THR:HG23	4:d:2081:PRO:HD2	1.98	0.45
4:d:2227:GLU:HG2	4:d:2231:THR:H	1.81	0.45
4:d:2305:ALA:HB1	13:o:2160:LYS:HE2	1.98	0.45
5:e:2037:VAL:HG21	6:f:2035:ALA:O	2.16	0.45
15:u:2073:PRO:HG2	16:v:2081:THR:HG22	1.99	0.45
2:B:56:TRP:CD1	2:B:56:TRP:C	2.94	0.45
2:B:219:VAL:HG12	2:B:220:ARG:N	2.32	0.45
2:B:271:THR:HG22	2:B:448:ARG:HH11	1.82	0.45
2:B:302:TRP:CH2	2:B:343:HIS:CG	3.05	0.45
2:B:302:TRP:CE3	2:B:343:HIS:HB2	2.52	0.45
2:B:451:PHE:CD1	2:B:451:PHE:O	2.69	0.45
27:B:529:BCR:H403	12:M:6:LEU:HD12	1.99	0.45
3:C:393:ALA:O	3:C:397:THR:OG1	2.33	0.45
4:D:19:ASP:O	4:D:23:LYS:HG3	2.16	0.45
13:O:60:ARG:NH1	2:b:2341:LYS:NZ	2.65	0.45
13:O:163:GLY:HA3	13:O:188:LYS:CE	2.45	0.45
14:T:26:PRO:HA	14:T:27:PRO:HD3	1.83	0.45
14:T:29:ILE:C	14:T:31:LYS:N	2.75	0.45
1:a:2063:ILE:H	1:a:2063:ILE:HG13	1.51	0.45
3:c:2167:VAL:HG13	23:c:2482:CLA:H42	1.99	0.45
3:c:2208:VAL:HG13	3:c:2209:ILE:H	1.79	0.45
4:d:2148:ALA:HB1	4:d:2279:LEU:HB2	1.99	0.45
6:f:2015:PHE:O	6:f:2016:THR:C	2.60	0.45
9:j:2019:MET:HG2	27:k:2050:BCR:H361	1.99	0.45
13:o:2123:LYS:O	13:o:2124:ASN:HB2	2.17	0.45
15:u:2088:VAL:O	15:u:2091:VAL:HG23	2.17	0.45
16:v:2032:LEU:HB3	16:v:2115:ILE:HD11	1.99	0.45
16:v:2063:THR:CB	16:v:2083:ASP:O	2.64	0.45
16:v:2119:ILE:HG22	16:v:2119:ILE:O	2.17	0.45
1:A:38:ILE:O	1:A:42:LEU:HG	2.17	0.45
1:A:52:PHE:CD2	1:A:52:PHE:C	2.95	0.45
1:A:87:ASN:HD21	3:C:357:ARG:NH1	2.08	0.45
1:A:235:TYR:HA	4:D:265:ARG:HH22	1.77	0.45
1:A:307:ILE:HG12	1:A:314:ILE:HD11	1.92	0.45
2:B:156:PHE:HB2	23:B:515:CLA:HAC1	1.99	0.45
3:C:205:ASP:O	3:C:208:VAL:HG12	2.17	0.45
16:V:64:PRO:HB2	16:V:65:PRO:HD2	1.98	0.45
19:Z:9:LEU:C	19:Z:11:ALA:N	2.73	0.45
19:Z:33:TRP:CE3	19:Z:37:LYS:HD3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2017:GLY:C	2:b:2020:ILE:HG22	2.42	0.45
2:b:2302:TRP:C	2:b:2304:ALA:N	2.75	0.45
2:b:2339:ALA:HB1	2:b:2340:TRP:HD1	1.82	0.45
2:b:2451:PHE:CZ	2:b:2455:HIS:ND1	2.85	0.45
3:c:2151:TRP:O	3:c:2153:ASP:N	2.50	0.45
3:c:2285:ILE:HG12	23:c:2487:CLA:CMB	2.47	0.45
4:d:2195:PRO:HA	4:d:2198:MET:HE3	1.95	0.45
6:f:2029:THR:O	6:f:2033:LEU:HG	2.16	0.45
13:o:2032:ILE:O	13:o:2034:SER:N	2.50	0.45
1:A:295:PHE:HB3	3:C:291:TRP:CH2	2.53	0.44
2:B:234:ILE:O	2:B:237:VAL:N	2.43	0.44
2:B:258:TYR:N	2:B:258:TYR:CD2	2.85	0.44
2:B:265:ILE:C	2:B:267:LEU:N	2.75	0.44
3:C:105:VAL:CG1	3:C:107:ASP:O	2.65	0.44
3:C:339:LYS:NZ	15:U:125:GLY:HA3	2.32	0.44
5:E:25:THR:O	5:E:28:ALA:HB3	2.16	0.44
5:E:56:ALA:CB	5:E:82:LEU:HD23	2.38	0.44
9:J:8:ILE:HA	9:J:9:PRO:HD3	1.82	0.44
13:O:140:THR:HG22	13:O:201:VAL:HB	1.98	0.44
16:V:25:GLN:O	16:V:28:GLU:N	2.51	0.44
1:a:2131:TRP:CE3	1:a:2132:GLU:HA	2.53	0.44
1:a:2140:ARG:HB2	4:d:2220:ASN:CG	2.42	0.44
2:b:2031:ALA:N	23:b:2518:CLA:HBC3	2.31	0.44
2:b:2297:THR:HB	2:b:2299:GLU:OE1	2.17	0.44
2:b:2311:PHE:C	2:b:2313:ASP:N	2.72	0.44
3:c:2048:LYS:HD3	3:c:2133:ALA:O	2.18	0.44
3:c:2069:LEU:CD2	3:c:2115:GLY:HA3	2.48	0.44
23:c:2484:CLA:C4B	27:c:2489:BCR:H393	2.47	0.44
4:d:2101:PHE:O	4:d:2102:THR:C	2.60	0.44
4:d:2237:PRO:HG2	4:d:2238:THR:H	1.81	0.44
13:o:2022:LEU:O	13:o:2203:LYS:CD	2.60	0.44
15:u:2072:TYR:CB	15:u:2073:PRO:CD	2.86	0.44
1:A:95:PRO:CG	1:A:98:GLU:HB2	2.48	0.44
1:A:224:ILE:HG13	1:A:245:THR:O	2.18	0.44
2:B:315:ILE:HD13	2:B:359:MET:CE	2.47	0.44
2:B:322:GLY:C	4:D:293:LEU:HG	2.42	0.44
3:C:435:PHE:O	3:C:438:LEU:N	2.48	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
4:D:89:LEU:CB	4:D:91:LEU:HD21	2.47	0.44
5:E:10:SER:HA	5:E:13:ILE:CD1	2.27	0.44
8:I:7:THR:HA	8:I:10:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.83	0.44
15:U:62:ILE:C	15:U:64:ALA:H	2.26	0.44
1:a:2238:LYS:O	1:a:2240:GLY:N	2.50	0.44
1:a:2255:PHE:CE2	25:a:2352:PL9:H152	2.52	0.44
1:a:2307:ILE:HD12	1:a:2312:ASN:HB2	1.98	0.44
1:a:2317:TRP:CD2	4:d:2063:LEU:HD12	2.52	0.44
23:b:2519:CLA:HMB2	4:d:2126:MET:HE3	1.99	0.44
3:c:2104:GLU:O	3:c:2105:VAL:HG22	2.17	0.44
3:c:2386:PRO:C	3:c:2388:GLN:H	2.25	0.44
4:d:2056:THR:HG21	5:e:2049:PRO:HD2	2.00	0.44
4:d:2182:LEU:O	4:d:2185:PHE:HB2	2.17	0.44
5:e:2025:THR:HG21	28:e:2084:HEC:C3B	2.47	0.44
12:m:2007:GLY:O	12:m:2008:LEU:C	2.60	0.44
16:v:2053:ASP:OD1	16:v:2055:ARG:HB3	2.17	0.44
16:v:2075:TYR:HE2	16:v:2079:PRO:CB	2.30	0.44
1:A:29:TYR:CE1	1:A:31:GLY:CA	2.93	0.44
2:B:190:PHE:CE1	23:B:527:CLA:CED	3.01	0.44
3:C:376:ASP:OD1	3:C:378:ASN:N	2.50	0.44
4:D:68:LEU:HD23	5:E:48:THR:HB	1.99	0.44
4:D:156:VAL:O	4:D:161:PRO:HD3	2.17	0.44
4:D:300:SER:N	11:L:37:ASN:OD1	2.51	0.44
10:K:27:ALA:O	10:K:31:GLN:HG2	2.18	0.44
13:O:153:THR:CG2	13:O:154:ALA:N	2.81	0.44
13:O:211:ILE:CG2	13:O:212:ALA:H	2.29	0.44
1:a:2029:TYR:HE2	1:a:2136:ARG:HG3	1.82	0.44
1:a:2076:ASN:ND2	11:l:2033:SER:HB2	2.32	0.44
1:a:2141:PRO:CG	3:c:2446:GLY:O	2.64	0.44
2:b:2153:PHE:O	2:b:2157:HIS:HB3	2.17	0.44
3:c:2343:ARG:CB	13:o:2078:LEU:CD1	2.95	0.44
3:c:2395:TYR:N	3:c:2395:TYR:CD2	2.83	0.44
4:d:2156:VAL:HG11	4:d:2171:PRO:HG2	1.99	0.44
10:k:2010:ASP:O	10:k:2011:PRO:C	2.60	0.44
11:l:2036:PHE:HD2	12:m:2007:GLY:HA3	1.80	0.44
13:o:2140:THR:HG21	13:o:2201:VAL:CB	2.42	0.44
2:B:31:ALA:HB2	23:B:518:CLA:CBC	2.47	0.44
2:B:436:THR:O	2:B:437:LEU:HD23	2.17	0.44
3:C:136:GLY:HA2	3:C:137:PRO:HD3	1.77	0.44
3:C:220:GLY:H	23:C:487:CLA:HBC1	1.82	0.44
3:C:311:GLN:NE2	3:C:355:THR:O	2.50	0.44
4:D:91:LEU:N	4:D:91:LEU:CD2	2.73	0.44
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:15:PHE:O	6:F:16:THR:C	2.60	0.44
13:O:55:GLU:HG2	13:O:64:GLU:HG3	2.00	0.44
13:O:218:GLU:HG3	13:O:233:VAL:O	2.17	0.44
15:U:83:ALA:HB1	15:U:84:PRO:HA	1.98	0.44
1:a:2078:ILE:HD11	11:l:2034:TYR:CE1	2.52	0.44
1:a:2243:GLU:OE1	4:d:2240:ALA:HA	2.18	0.44
2:b:2200:ALA:C	23:b:2521:CLA:HBB1	2.42	0.44
2:b:2247:PHE:HE1	23:b:2521:CLA:H72	1.79	0.44
3:c:2038:GLY:HA3	23:c:2486:CLA:C1D	2.47	0.44
3:c:2195:ASP:N	3:c:2195:ASP:OD1	2.49	0.44
3:c:2218:PHE:O	3:c:2219:GLY:C	2.60	0.44
3:c:2346:THR:C	3:c:2348:GLU:OE1	2.60	0.44
3:c:2384:ILE:HG23	3:c:2384:ILE:O	2.17	0.44
12:m:2011:THR:O	12:m:2011:THR:HG22	2.18	0.44
16:v:2116:ALA:O	16:v:2120:LEU:HG	2.17	0.44
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.52	0.44
2:B:370:LEU:HD12	2:B:379:ALA:HB3	1.99	0.44
2:B:397:VAL:CG1	2:B:398:THR:H	2.28	0.44
2:B:478:VAL:O	2:B:481:GLY:N	2.47	0.44
3:C:286:ALA:O	3:C:290:VAL:N	2.49	0.44
4:D:88:SER:CB	5:E:68:ARG:NH2	2.74	0.44
4:D:154:VAL:O	4:D:155:SER:C	2.60	0.44
4:D:291:LEU:C	4:D:293:LEU:N	2.73	0.44
4:D:296:TYR:CG	4:D:296:TYR:O	2.70	0.44
4:D:322:ASN:O	4:D:323:GLU:C	2.60	0.44
11:L:37:ASN:OXT	11:L:37:ASN:CG	2.59	0.44
13:O:55:GLU:HB3	13:O:61:GLN:NE2	2.32	0.44
14:T:13:ILE:HG22	14:T:13:ILE:O	2.17	0.44
16:V:79:PRO:HG3	16:V:89:ALA:HA	1.99	0.44
16:V:92:HIS:CE1	16:V:93:PRO:HD2	2.52	0.44
1:a:2142:TRP:CD1	3:c:2443:TRP:CH2	3.05	0.44
2:b:2442:ILE:HD12	4:d:2299:ILE:HG12	1.99	0.44
23:b:2519:CLA:HBB1	4:d:2123:ILE:HG23	1.98	0.44
3:c:2061:VAL:HG22	23:c:2480:CLA:CAC	2.48	0.44
3:c:2100:GLY:C	3:c:2195:ASP:HB3	2.42	0.44
3:c:2318:LEU:O	3:c:2322:GLN:HB2	2.18	0.44
4:d:2091:LEU:HD13	23:d:2357:CLA:HBA1	1.99	0.44
4:d:2110:LEU:O	4:d:2113:PHE:N	2.51	0.44
4:d:2134:ARG:HA	4:d:2134:ARG:HD2	1.80	0.44
1:A:97:TRP:CZ3	8:I:8:VAL:HG21	2.49	0.44
1:A:230:THR:CG2	1:A:231:GLU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HD3	1:A:270:SER:N	2.32	0.44
1:A:330:VAL:HG12	4:D:348:ARG:HA	2.00	0.44
2:B:12:LEU:HD21	2:B:22:ALA:CB	2.48	0.44
2:B:405:GLU:CB	13:o:2059:LYS:HB3	2.46	0.44
3:C:270:ALA:O	3:C:274:TYR:CE1	2.71	0.44
3:C:282:MET:O	3:C:283:GLY:C	2.60	0.44
3:C:287:THR:HG23	3:C:427:ALA:HA	1.99	0.44
4:D:42:TYR:CZ	6:F:24:THR:CG2	3.00	0.44
11:L:24:ILE:HD11	12:M:18:PRO:HB2	2.00	0.44
15:U:133:TYR:O	15:U:134:LYS:OXT	2.36	0.44
19:Z:39:LEU:H	19:Z:39:LEU:HG	1.39	0.44
2:b:2031:ALA:HB2	23:b:2518:CLA:CBC	2.47	0.44
2:b:2068:ARG:NH1	23:b:2516:CLA:HED1	2.26	0.44
23:b:2513:CLA:H18	23:b:2524:CLA:O1A	2.18	0.44
3:c:2343:ARG:CB	13:o:2078:LEU:HD12	2.47	0.44
13:o:2068:THR:CG2	13:o:2107:THR:HB	2.47	0.44
16:v:2021:LEU:HD23	16:v:2021:LEU:HA	1.78	0.44
1:A:78:ILE:CD1	11:L:34:TYR:CE1	2.99	0.44
1:A:107:TYR:HD1	13:O:115:ARG:NH1	2.16	0.44
1:A:149:ALA:CA	1:A:284:TRP:CZ3	3.00	0.44
1:A:213:ALA:O	1:A:217:SER:CB	2.65	0.44
2:B:57:ARG:HH12	2:B:317:ASN:CG	2.17	0.44
2:B:350:GLU:OE1	2:B:350:GLU:N	2.50	0.44
3:C:93:ALA:CB	3:C:301:PHE:CE1	3.01	0.44
3:C:131:TYR:CE1	3:C:135:ARG:HB3	2.52	0.44
3:C:217:PRO:HA	3:C:222:GLY:HA2	2.00	0.44
23:C:476:CLA:H61	23:C:483:CLA:H72	1.99	0.44
4:D:57:SER:CB	4:D:79:SER:HB2	2.48	0.44
10:K:6:TYR:N	10:K:6:TYR:CD1	2.86	0.44
15:U:62:ILE:CG2	15:U:76:ALA:HB1	2.47	0.44
19:Z:5:PHE:HD2	19:Z:5:PHE:O	2.01	0.44
19:Z:15:LEU:HG	19:Z:19:MET:HE2	2.00	0.44
1:a:2224:ILE:HD11	1:a:2243:GLU:CG	2.46	0.44
2:b:2016:PRO:HG3	2:b:2133:LEU:HD11	1.99	0.44
2:b:2058:GLN:HB2	2:b:2060:MET:HG2	2.00	0.44
2:b:2088:PRO:O	2:b:2089:GLY:C	2.59	0.44
2:b:2219:VAL:HG12	2:b:2220:ARG:N	2.33	0.44
23:b:2513:CLA:HMD2	23:b:2524:CLA:H172	2.00	0.44
23:b:2514:CLA:H161	11:l:2027:LEU:HD21	2.00	0.44
3:c:2178:LYS:HG2	3:c:2178:LYS:O	2.17	0.44
3:c:2318:LEU:HD11	3:c:2351:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2178:ILE:HD13	4:d:2178:ILE:HA	1.79	0.44
4:d:2195:PRO:CG	4:d:2196:PHE:N	2.79	0.44
4:d:2299:ILE:O	4:d:2300:SER:C	2.60	0.44
5:e:2022:HIS:C	5:e:2024:ILE:N	2.72	0.44
6:f:2018:ARG:HD2	6:f:2018:ARG:HA	1.74	0.44
10:k:2019:ILE:HA	10:k:2022:LEU:HD12	1.98	0.44
13:o:2048:THR:O	13:o:2049:THR:HG23	2.18	0.44
13:o:2193:THR:CG2	13:o:2194:LYS:H	2.12	0.44
15:u:2062:ILE:C	15:u:2064:ALA:H	2.25	0.44
1:A:315:ASN:O	4:D:63:LEU:HD22	2.16	0.44
2:B:325:PHE:O	2:B:326:ARG:C	2.60	0.44
4:D:350:ASN:HD22	4:D:351:ALA:N	2.16	0.44
4:D:350:ASN:ND2	4:D:351:ALA:N	2.65	0.44
12:M:9:ILE:HG12	12:m:2009:ILE:HG12	1.99	0.44
13:O:33:ASP:O	13:O:36:GLN:HB2	2.17	0.44
1:a:2180:PHE:CE2	4:d:2192:THR:HG22	2.52	0.44
1:a:2324:ALA:C	1:a:2326:LEU:N	2.75	0.44
2:b:2187:PRO:C	2:b:2189:GLY:N	2.75	0.44
2:b:2327:THR:O	2:b:2328:GLY:C	2.59	0.44
3:c:2049:LEU:O	3:c:2052:ALA:N	2.51	0.44
3:c:2297:TYR:HB3	3:c:2302:TYR:CD1	2.53	0.44
3:c:2315:MET:CE	3:c:2392:ALA:HB2	2.47	0.44
3:c:2321:ASP:O	3:c:2324:LEU:N	2.45	0.44
3:c:2343:ARG:HE	13:o:2075:THR:HG1	1.63	0.44
4:d:2233:ARG:HG3	4:d:2233:ARG:O	2.18	0.44
10:k:2019:ILE:O	10:k:2020:PRO:C	2.61	0.44
19:z:2013:VAL:CG1	19:z:2014:ILE:N	2.80	0.44
1:A:229:GLU:CD	2:B:480:SER:O	2.60	0.44
25:A:353:PL9:H23	25:A:353:PL9:H271	1.42	0.44
23:B:519:CLA:H142	23:D:356:CLA:H11	1.99	0.44
3:C:36:TRP:C	3:C:38:GLY:N	2.76	0.44
3:C:89:ILE:HB	3:C:90:PRO:CD	2.44	0.44
3:C:274:TYR:HB3	23:C:485:CLA:C3B	2.48	0.44
3:C:299:SER:O	3:C:303:GLY:O	2.36	0.44
3:C:317:PHE:O	3:C:321:ASP:OD1	2.36	0.44
4:D:146:PHE:O	4:D:149:PRO:HD2	2.18	0.44
4:D:161:PRO:HG3	4:D:170:ALA:CB	2.46	0.44
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.44
5:E:68:ARG:NH1	7:H:50:SER:O	2.50	0.44
13:O:31:PRO:HB2	13:O:33:ASP:H	1.83	0.44
13:O:190:PHE:CE1	15:U:120:ALA:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:75:LEU:CD2	15:U:101:GLN:NE2	2.81	0.44
1:a:2161:TYR:CE2	1:a:2165:GLN:HG3	2.52	0.44
1:a:2316:THR:HB	4:d:2075:THR:HG21	1.99	0.44
1:a:2322:ASN:O	1:a:2326:LEU:HB2	2.18	0.44
2:b:2163:GLY:O	2:b:2165:GLY:N	2.47	0.44
2:b:2164:PRO:C	2:b:2165:GLY:O	2.59	0.44
2:b:2327:THR:N	27:b:2528:BCR:H292	2.32	0.44
2:b:2331:ASN:C	2:b:2333:GLY:H	2.25	0.44
2:b:2333:GLY:HA2	2:b:2442:ILE:O	2.17	0.44
3:c:2251:HIS:O	3:c:2252:ILE:C	2.61	0.44
3:c:2265:ILE:CG2	3:c:2266:TRP:N	2.81	0.44
3:c:2315:MET:HE2	3:c:2392:ALA:HB2	2.00	0.44
4:d:2231:THR:C	4:d:2232:PHE:CD1	2.96	0.44
14:t:2001:MET:HG3	14:t:2002:GLU:N	2.32	0.44
16:v:2083:ASP:OD1	16:v:2084:GLY:N	2.51	0.44
1:A:41:LEU:HD13	24:A:351:PHO:C2	2.48	0.43
1:A:187:GLN:HE21	1:A:187:GLN:HB3	1.50	0.43
1:A:326:LEU:HD13	3:C:412:THR:CG2	2.39	0.43
2:B:264:PRO:HD2	2:B:268:PHE:HE1	1.83	0.43
5:E:33:GLY:O	5:E:36:PHE:N	2.48	0.43
6:F:40:GLN:NE2	9:J:27:LEU:O	2.48	0.43
11:L:29:LEU:O	11:L:30:LEU:C	2.61	0.43
15:U:47:LEU:HB3	15:U:51:TYR:HD1	1.83	0.43
19:Z:49:ALA:O	19:Z:53:VAL:HG23	2.18	0.43
1:a:2069:GLY:CA	1:a:2075:ASN:OD1	2.64	0.43
1:a:2147:TYR:O	1:a:2150:PRO:HG2	2.18	0.43
1:a:2205:VAL:C	1:a:2207:GLY:N	2.75	0.43
2:b:2006:TYR:HE1	2:b:2008:VAL:HG21	1.78	0.43
2:b:2340:TRP:H	2:b:2340:TRP:HD1	1.66	0.43
4:d:2080:THR:HG21	4:d:2168:PHE:CA	2.47	0.43
4:d:2161:PRO:CG	4:d:2170:ALA:CB	2.90	0.43
13:o:2140:THR:HB	13:o:2201:VAL:N	2.19	0.43
19:z:2035:ARG:O	19:z:2039:LEU:HG	2.18	0.43
2:B:93:PHE:O	2:B:94:GLU:C	2.61	0.43
2:B:234:ILE:HG21	23:B:524:CLA:H193	2.00	0.43
3:C:189:TRP:O	3:C:190:ALA:O	2.36	0.43
4:D:101:PHE:O	4:D:104:TRP:N	2.52	0.43
13:O:32:ILE:HA	13:O:133:VAL:HG11	2.00	0.43
15:U:88:VAL:HG12	15:U:109:LEU:CD1	2.48	0.43
1:a:2033:PHE:CE1	1:a:2128:GLY:HA3	2.52	0.43
1:a:2135:TYR:HH	8:i:2030:ARG:C	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2207:GLY:O	1:a:2208:GLY:C	2.61	0.43
1:a:2236:GLY:H	4:d:2265:ARG:NH2	2.16	0.43
1:a:2237:TYR:CD2	1:a:2241:GLN:OE1	2.71	0.43
1:a:2297:LEU:HD22	3:c:2428:THR:HG21	2.00	0.43
2:b:2258:TYR:N	2:b:2258:TYR:CD2	2.86	0.43
2:b:2385:ARG:HG3	13:o:2165:ALA:HA	2.00	0.43
3:c:2245:ILE:C	3:c:2247:GLY:N	2.74	0.43
3:c:2293:ASN:OD1	3:c:2297:TYR:HB3	2.18	0.43
10:k:2027:ALA:O	10:k:2031:GLN:HG2	2.17	0.43
15:u:2057:LEU:HB2	15:u:2114:VAL:HG22	2.00	0.43
18:n:2031:UNK:HA	19:z:2030:PRO:HG2	1.98	0.43
19:z:2012:LEU:HD13	19:z:2047:TRP:CD1	2.53	0.43
1:A:160:ILE:H	1:A:160:ILE:HG13	1.66	0.43
2:B:18:ARG:NH1	2:B:115:TRP:O	2.50	0.43
2:B:91:TRP:HB3	23:B:515:CLA:H43	2.00	0.43
2:B:156:PHE:CD1	2:B:156:PHE:N	2.86	0.43
2:B:166:MET:HE1	2:B:195:PRO:HB3	2.00	0.43
2:B:405:GLU:OE1	13:o:2060:ARG:NH2	2.51	0.43
3:C:48:LYS:HD3	3:C:133:ALA:O	2.18	0.43
3:C:187:ASP:OD1	3:C:189:TRP:N	2.51	0.43
3:C:421:SER:O	3:C:422:PRO:C	2.60	0.43
4:D:178:ILE:O	4:D:181:PHE:HB3	2.19	0.43
5:E:55:TYR:O	16:V:1:ALA:HB2	2.17	0.43
7:H:59:VAL:O	7:H:59:VAL:CG1	2.64	0.43
13:O:243:ILE:CG2	13:O:244:GLU:N	2.81	0.43
16:V:35:TYR:CD2	16:V:35:TYR:O	2.71	0.43
1:a:2131:TRP:CE3	1:a:2132:GLU:CA	3.02	0.43
1:a:2281:VAL:O	1:a:2281:VAL:CG1	2.66	0.43
1:a:2320:ILE:O	1:a:2320:ILE:CG2	2.65	0.43
2:b:2161:LEU:HD23	2:b:2161:LEU:HA	1.87	0.43
2:b:2193:TYR:O	2:b:2195:PRO:HD3	2.18	0.43
3:c:2394:GLU:OE1	3:c:2394:GLU:HA	2.18	0.43
3:c:2426:LEU:HD13	23:c:2481:CLA:CED	2.48	0.43
23:c:2480:CLA:H42	23:c:2481:CLA:HBD	2.01	0.43
4:d:2220:ASN:O	4:d:2220:ASN:ND2	2.52	0.43
4:d:2261:PHE:HA	14:t:2024:ARG:NH2	2.32	0.43
5:e:2014:THR:HG22	9:j:2008:ILE:CD1	2.47	0.43
11:l:2029:LEU:O	11:l:2032:SER:HB3	2.17	0.43
12:m:2008:LEU:HD12	12:m:2008:LEU:HA	1.85	0.43
16:v:2004:THR:CG2	16:v:2005:PRO:CD	2.89	0.43
1:A:242:GLU:C	1:A:244:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:PRO:O	3:C:193:GLY:N	2.48	0.43
3:C:286:ALA:O	3:C:287:THR:C	2.61	0.43
3:C:394:GLU:O	3:C:397:THR:HB	2.18	0.43
5:E:24:ILE:O	5:E:24:ILE:HG22	2.18	0.43
7:H:57:VAL:O	7:H:57:VAL:HG13	2.17	0.43
10:K:9:PHE:N	10:K:9:PHE:CD1	2.86	0.43
13:O:57:LYS:HG3	13:O:57:LYS:O	2.18	0.43
16:V:92:HIS:O	16:V:93:PRO:C	2.60	0.43
2:b:2190:PHE:CZ	7:h:2040:PHE:HE1	2.30	0.43
3:c:2102:GLY:CA	3:c:2186:TYR:OH	2.66	0.43
4:d:2196:PHE:HE2	11:l:2031:PHE:HZ	1.66	0.43
4:d:2218:VAL:O	4:d:2219:GLU:C	2.62	0.43
11:l:2022:LEU:O	11:l:2022:LEU:HG	2.18	0.43
13:o:2205:ASP:O	13:o:2206:GLY:C	2.60	0.43
16:v:2038:ALA:O	16:v:2042:VAL:CG2	2.66	0.43
16:v:2058:THR:O	16:v:2082:TYR:OH	2.31	0.43
17:x:2012:ILE:HG22	17:x:2016:LEU:HD13	2.00	0.43
19:z:2033:TRP:CE3	19:z:2037:LYS:HD3	2.54	0.43
1:A:162:PRO:CG	1:A:171:GLY:HA2	2.48	0.43
1:A:339:PHE:CE1	3:C:314:ALA:HA	2.53	0.43
3:C:155:ASN:O	3:C:159:THR:OG1	2.27	0.43
3:C:167:VAL:CG1	23:C:482:CLA:H11	2.48	0.43
3:C:223:TRP:HD1	3:C:224:ILE:N	2.14	0.43
4:D:189:HIS:CE1	4:D:294:ARG:HH21	2.36	0.43
4:D:218:VAL:O	4:D:220:ASN:N	2.52	0.43
4:D:273:PHE:O	4:D:277:THR:HB	2.17	0.43
4:D:297:ASP:C	4:D:298:PHE:HD1	2.26	0.43
23:D:356:CLA:H12	7:H:42:LEU:CD2	2.48	0.43
7:H:23:GLY:C	7:H:25:GLY:H	2.27	0.43
10:K:19:ILE:O	10:K:20:PRO:C	2.59	0.43
12:M:20:VAL:HG13	12:m:2020:VAL:HG13	2.01	0.43
19:Z:13:VAL:HG13	19:Z:17:PHE:CE1	2.54	0.43
19:Z:42:LEU:O	19:Z:46:LEU:HB2	2.18	0.43
1:a:2147:TYR:O	1:a:2150:PRO:HD2	2.17	0.43
2:b:2019:LEU:HD21	23:b:2524:CLA:C19	2.48	0.43
2:b:2139:PHE:C	2:b:2139:PHE:CD2	2.95	0.43
2:b:2364:GLU:HG2	4:d:2294:ARG:NH1	2.33	0.43
4:d:2039:PRO:O	4:d:2043:LEU:HG	2.18	0.43
4:d:2168:PHE:HD2	4:d:2168:PHE:O	2.01	0.43
13:o:2095:PHE:HB3	13:o:2127:ALA:CB	2.44	0.43
16:v:2066:ARG:NH2	16:v:2080:THR:HB	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:2079:PRO:HG3	16:v:2089:ALA:CA	2.48	0.43
16:v:2094:SER:OG	16:v:2097:SER:HB2	2.18	0.43
2:B:63:LEU:HD12	2:B:63:LEU:HA	1.87	0.43
2:B:161:LEU:HD23	2:B:161:LEU:HA	1.84	0.43
2:B:234:ILE:HG23	23:B:524:CLA:H193	2.01	0.43
2:B:354:LEU:CD2	2:B:378:LYS:HG3	2.48	0.43
2:B:416:THR:O	2:B:417:VAL:C	2.62	0.43
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.18	0.43
4:D:195:PRO:O	4:D:199:MET:HG3	2.19	0.43
6:F:32:PHE:CE1	27:F:48:BCR:H14C	2.54	0.43
13:O:240:TYR:C	13:O:240:TYR:CD2	2.97	0.43
1:a:2105:TRP:CE2	1:a:2110:GLY:HA3	2.53	0.43
1:a:2149:ALA:HB2	1:a:2280:VAL:HG13	2.00	0.43
2:b:2045:PHE:CE1	2:b:2055:MET:HA	2.52	0.43
2:b:2179:GLN:O	2:b:2180:PRO:C	2.58	0.43
2:b:2464:PHE:HD2	23:b:2523:CLA:HAC2	1.83	0.43
3:c:2078:GLU:HA	3:c:2078:GLU:OE1	2.18	0.43
3:c:2105:VAL:HG12	3:c:2107:ASP:O	2.17	0.43
3:c:2157:MET:CE	3:c:2160:ILE:HD12	2.48	0.43
3:c:2265:ILE:O	3:c:2266:TRP:CG	2.72	0.43
3:c:2276:LEU:HD12	3:c:2276:LEU:HA	1.86	0.43
7:h:2023:GLY:C	7:h:2025:GLY:H	2.26	0.43
13:o:2019:CYS:HB3	13:o:2240:TYR:HB2	2.00	0.43
13:o:2126:VAL:O	13:o:2126:VAL:HG12	2.19	0.43
19:z:2033:TRP:HB2	19:z:2037:LYS:HD2	2.00	0.43
1:A:239:PHE:C	1:A:241:GLN:N	2.73	0.43
1:A:295:PHE:O	3:C:291:TRP:CH2	2.72	0.43
2:B:17:GLY:C	2:B:20:ILE:HG22	2.42	0.43
2:B:252:VAL:HG22	23:B:517:CLA:O1A	2.19	0.43
2:B:297:THR:HB	2:B:299:GLU:OE1	2.18	0.43
2:B:327:THR:O	2:B:329:PRO:HD3	2.18	0.43
3:C:229:ASN:ND2	3:C:231:GLU:HB2	2.33	0.43
4:D:22:LEU:CD2	4:D:32:TRP:CE3	3.01	0.43
10:K:31:GLN:HB3	10:K:36:PHE:CD2	2.54	0.43
13:O:76:THR:O	13:O:77:SER:C	2.61	0.43
13:O:183:ALA:O	13:O:184:ARG:C	2.60	0.43
16:V:22:THR:N	16:V:25:GLN:NE2	2.65	0.43
1:a:2243:GLU:N	4:d:2240:ALA:HB1	2.34	0.43
1:a:2307:ILE:O	1:a:2308:ASP:C	2.61	0.43
2:b:2122:LEU:HB3	2:b:2123:PHE:H	1.62	0.43
2:b:2235:GLU:O	2:b:2238:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:2418:LYS:HZ1	15:u:2045:GLU:CD	2.26	0.43
2:b:2478:VAL:C	2:b:2481:GLY:H	2.26	0.43
3:c:2265:ILE:HG22	3:c:2266:TRP:H	1.82	0.43
3:c:2346:THR:O	3:c:2348:GLU:OE1	2.36	0.43
3:c:2354:GLU:O	3:c:2356:MET:N	2.52	0.43
4:d:2043:LEU:CD2	27:d:2360:BCR:H323	2.48	0.43
4:d:2077:ALA:HB1	4:d:2173:PHE:O	2.18	0.43
4:d:2101:PHE:O	4:d:2104:TRP:HB3	2.18	0.43
10:k:2022:LEU:HB3	27:k:2050:BCR:C15	2.49	0.43
13:o:2125:LEU:CD1	13:o:2126:VAL:H	2.32	0.43
14:t:2013:ILE:O	14:t:2013:ILE:HG22	2.18	0.43
16:v:2010:VAL:HG22	16:v:2124:LYS:NZ	2.34	0.43
16:v:2032:LEU:O	16:v:2035:TYR:HB3	2.18	0.43
19:z:2009:LEU:C	19:z:2011:ALA:N	2.75	0.43
19:z:2015:LEU:HG	19:z:2019:MET:HE2	2.01	0.43
1:A:290:ILE:HD11	23:A:348:CLA:OBD	2.19	0.43
1:A:301:ASN:HD22	1:A:301:ASN:N	2.16	0.43
3:C:256:PRO:HA	23:C:474:CLA:HED3	2.01	0.43
3:C:285:ILE:CG2	23:C:487:CLA:HMB3	2.48	0.43
3:C:377:LEU:HD21	13:O:99:ASP:OD2	2.18	0.43
4:D:103:ARG:C	4:D:105:CYS:N	2.72	0.43
10:K:34:VAL:O	10:K:34:VAL:CG1	2.64	0.43
11:L:6:ASN:HD22	11:L:6:ASN:N	2.15	0.43
13:O:10:ILE:C	13:O:12:GLY:H	2.27	0.43
13:O:58:ASN:O	13:O:59:LYS:HB2	2.19	0.43
13:O:126:VAL:O	13:O:126:VAL:HG12	2.18	0.43
14:T:10:PHE:HE2	14:T:14:ILE:HD11	1.83	0.43
15:U:82:ASN:C	15:U:85:TYR:HE2	2.27	0.43
19:Z:7:LEU:O	19:Z:11:ALA:CB	2.63	0.43
19:Z:40:ILE:C	19:Z:42:LEU:N	2.77	0.43
1:a:2059:ASP:O	1:a:2059:ASP:CG	2.62	0.43
1:a:2097:TRP:CB	8:i:2005:LYS:HB2	2.48	0.43
1:a:2299:GLY:O	3:c:2403:SER:HB3	2.19	0.43
1:a:2301:ASN:CG	1:a:2301:ASN:O	2.61	0.43
2:b:2277:SER:O	2:b:2278:SER:C	2.60	0.43
2:b:2327:THR:O	2:b:2329:PRO:CD	2.67	0.43
2:b:2348:ASN:CG	2:b:2349:LYS:N	2.71	0.43
2:b:2368:VAL:HG22	2:b:2425:ILE:HD12	2.00	0.43
23:b:2512:CLA:OBD	23:b:2520:CLA:HHC	2.19	0.43
23:b:2520:CLA:H51	27:b:2528:BCR:H313	2.00	0.43
3:c:2104:GLU:C	3:c:2105:VAL:CG2	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2286:ALA:O	3:c:2290:VAL:N	2.49	0.43
3:c:2310:SER:HB3	3:c:2355:THR:OG1	2.19	0.43
4:d:2088:SER:OG	5:e:2068:ARG:NE	2.52	0.43
4:d:2125:PHE:CD2	4:d:2125:PHE:O	2.71	0.43
4:d:2129:GLN:HE21	4:d:2142:ASN:CB	2.28	0.43
4:d:2225:ASP:C	4:d:2227:GLU:N	2.77	0.43
4:d:2308:ASP:HA	4:d:2309:PRO:HD2	1.89	0.43
13:o:2058:ASN:O	13:o:2059:LYS:CB	2.66	0.43
13:o:2122:VAL:O	13:o:2122:VAL:CG1	2.66	0.43
15:u:2065:PHE:CD1	15:u:2076:ALA:CB	3.01	0.43
1:A:12:ASN:HA	1:A:15:GLU:CD	2.44	0.43
1:A:29:TYR:CE1	1:A:31:GLY:HA3	2.53	0.43
1:A:196:PRO:HA	1:A:199:GLN:HB2	2.01	0.43
2:B:135:LEU:N	2:B:136:PRO:HD2	2.33	0.43
2:B:237:VAL:CG2	23:B:524:CLA:HBC2	2.49	0.43
4:D:21:TRP:O	4:D:26:ARG:NH2	2.40	0.43
4:D:217:THR:O	4:D:218:VAL:C	2.60	0.43
15:U:73:PRO:CG	16:V:83:ASP:CG	2.92	0.43
16:V:112:LEU:HD23	16:V:112:LEU:HA	1.80	0.43
1:a:2131:TRP:O	1:a:2134:SER:CB	2.67	0.43
1:a:2157:VAL:HG12	1:a:2172:MET:HB2	2.00	0.43
1:a:2278:TRP:HA	1:a:2278:TRP:CE3	2.52	0.43
2:b:2381:ILE:HA	2:b:2382:PRO:HD2	1.80	0.43
3:c:2347:GLY:O	13:o:2016:ALA:HB3	2.17	0.43
3:c:2354:GLU:C	3:c:2356:MET:N	2.77	0.43
6:f:2040:GLN:NE2	9:j:2027:LEU:C	2.63	0.43
10:k:2016:LEU:O	10:k:2018:VAL:N	2.52	0.43
19:z:2022:GLY:O	19:z:2023:VAL:C	2.62	0.43
19:z:2028:ALA:C	19:z:2030:PRO:HD2	2.44	0.43
1:A:89:ILE:HD13	1:A:94:TYR:CD1	2.54	0.43
1:A:104:GLU:O	1:A:107:TYR:N	2.41	0.43
2:B:6:TYR:HE1	2:B:8:VAL:HG21	1.83	0.43
2:B:478:VAL:C	2:B:481:GLY:H	2.27	0.43
23:C:484:CLA:C4B	27:C:489:BCR:H393	2.48	0.43
4:D:55:VAL:O	4:D:65:SER:HB3	2.18	0.43
4:D:103:ARG:O	4:D:104:TRP:C	2.61	0.43
4:D:328:TRP:CE2	4:D:346:LEU:HD13	2.54	0.43
5:E:33:GLY:O	5:E:36:PHE:HB3	2.18	0.43
10:K:8:ILE:H	10:K:8:ILE:HG13	1.68	0.43
13:O:152:ARG:HD2	13:O:156:PHE:CZ	2.54	0.43
15:U:87:SER:HB3	15:U:90:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:100:ILE:O	16:V:102:PRO:HD3	2.19	0.43
1:a:2205:VAL:HG12	4:d:2204:VAL:CG1	2.48	0.43
1:a:2239:PHE:CE1	4:d:2245:SER:HA	2.53	0.43
2:b:2025:MET:O	2:b:2028:ALA:N	2.52	0.43
2:b:2240:SER:OG	2:b:2241:SER:N	2.51	0.43
2:b:2371:THR:HG23	2:b:2376:VAL:O	2.18	0.43
3:c:2101:PRO:O	3:c:2102:GLY:C	2.60	0.43
3:c:2109:PHE:HZ	27:c:2489:BCR:HC32	1.83	0.43
3:c:2291:TRP:CD1	3:c:2292:PHE:CE2	3.07	0.43
4:d:2018:LEU:O	4:d:2019:ASP:C	2.62	0.43
4:d:2032:TRP:HA	4:d:2032:TRP:HE3	1.81	0.43
4:d:2058:TRP:HA	4:d:2062:GLY:N	2.30	0.43
4:d:2069:GLU:OE1	5:e:2054:TYR:OH	2.32	0.43
4:d:2090:LEU:HD11	4:d:2096:GLU:CD	2.44	0.43
8:i:2034:ARG:HD3	8:i:2034:ARG:HA	1.75	0.43
9:j:2004:GLU:C	9:j:2006:GLY:H	2.26	0.43
15:u:2062:ILE:HG23	15:u:2076:ALA:HB1	1.99	0.43
15:u:2108:ASN:C	15:u:2112:PHE:CE1	2.97	0.43
15:u:2127:ARG:O	15:u:2128:TYR:HD1	2.02	0.43
2:B:315:ILE:C	2:B:317:ASN:H	2.27	0.42
2:B:327:THR:O	2:B:328:GLY:C	2.61	0.42
2:B:368:VAL:HG22	2:B:425:ILE:HD12	2.01	0.42
3:C:274:TYR:CE2	23:C:477:CLA:HED3	2.53	0.42
11:L:6:ASN:OD1	11:L:8:GLN:HG2	2.19	0.42
13:O:33:ASP:O	13:O:37:THR:N	2.50	0.42
16:V:79:PRO:CB	16:V:88:ILE:HG12	2.44	0.42
18:N:31:UNK:HA	19:Z:30:PRO:HG2	2.01	0.42
1:a:2281:VAL:HA	1:a:2284:TRP:CD1	2.54	0.42
2:b:2315:ILE:C	2:b:2317:ASN:H	2.27	0.42
3:c:2036:TRP:C	3:c:2038:GLY:N	2.76	0.42
3:c:2109:PHE:O	3:c:2112:PHE:N	2.52	0.42
3:c:2223:TRP:CD1	3:c:2224:ILE:H	2.37	0.42
3:c:2278:ALA:HB1	23:c:2479:CLA:C14	2.49	0.42
3:c:2435:PHE:O	3:c:2438:LEU:N	2.50	0.42
3:c:2443:TRP:CE3	3:c:2443:TRP:CA	3.00	0.42
23:c:2481:CLA:HBD	23:c:2481:CLA:HAA2	2.01	0.42
4:d:2031:GLY:HA3	4:d:2131:GLU:OE1	2.18	0.42
4:d:2087:HIS:HA	4:d:2167:TRP:CD1	2.54	0.42
4:d:2209:LEU:HD22	23:d:2355:CLA:H42	2.00	0.42
4:d:2217:THR:O	4:d:2218:VAL:C	2.62	0.42
8:i:2005:LYS:CG	8:i:2009:TYR:CE1	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:2007:ARG:H	11:l:2007:ARG:HD2	1.84	0.42
13:o:2201:VAL:CG1	13:o:2204:VAL:HG23	2.49	0.42
15:u:2083:ALA:HA	15:u:2085:TYR:CE2	2.53	0.42
2:B:323:GLY:N	4:D:294:ARG:O	2.49	0.42
3:C:116:VAL:HG11	27:C:489:BCR:H321	2.00	0.42
3:C:276:LEU:HD13	23:C:483:CLA:HBB1	2.01	0.42
4:D:221:THR:HG22	4:D:245:SER:H	1.84	0.42
28:E:84:HEC:O1D	6:F:18:ARG:NE	2.48	0.42
9:J:3:SER:N	18:N:32:UNK:CB	2.82	0.42
10:K:30:TRP:HE3	10:K:31:GLN:HE21	1.65	0.42
13:O:43:LEU:HD11	13:O:239:PHE:CD1	2.53	0.42
13:O:54:GLU:OE1	13:O:114:GLU:OE1	2.37	0.42
13:O:122:VAL:O	13:O:125:LEU:HB2	2.19	0.42
16:V:76:MET:HE1	16:V:115:ILE:HG21	2.00	0.42
1:a:2239:PHE:C	1:a:2241:GLN:N	2.74	0.42
1:a:2317:TRP:N	4:d:2063:LEU:HD13	2.33	0.42
2:b:2053:ASN:ND2	2:b:2058:GLN:OE1	2.51	0.42
2:b:2234:ILE:HG23	23:b:2524:CLA:H193	2.01	0.42
3:c:2285:ILE:CG2	23:c:2487:CLA:HMB3	2.49	0.42
4:d:2021:TRP:CZ2	17:x:2040:ILE:HG21	2.54	0.42
4:d:2289:LEU:C	4:d:2291:LEU:N	2.75	0.42
4:d:2329:MET:O	4:d:2333:ASP:HB3	2.17	0.42
6:f:2039:MET:O	6:f:2041:PHE:N	2.52	0.42
17:x:2017:LYS:O	17:x:2020:PHE:N	2.53	0.42
19:z:2004:LEU:O	19:z:2008:ALA:N	2.45	0.42
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.02	0.42
1:A:142:TRP:HH2	1:A:273:PHE:CE1	2.34	0.42
1:A:307:ILE:HG22	1:A:309:ALA:HB3	2.00	0.42
2:B:327:THR:O	2:B:329:PRO:N	2.53	0.42
3:C:108:THR:HG21	10:K:2:LEU:CG	2.47	0.42
3:C:204:LEU:HD12	3:C:239:TRP:HE1	1.84	0.42
3:C:251:HIS:O	3:C:252:ILE:C	2.61	0.42
3:C:315:MET:O	3:C:319:ILE:HG13	2.18	0.42
5:E:14:THR:HG22	9:J:8:ILE:CD1	2.44	0.42
5:E:14:THR:HG22	9:J:8:ILE:HD12	1.88	0.42
7:H:41:LEU:O	7:H:42:LEU:C	2.60	0.42
13:O:104:GLN:HB3	13:O:151:TYR:HE1	1.85	0.42
15:U:51:TYR:HB3	15:U:52:GLY:H	1.34	0.42
1:a:2288:LEU:HD13	3:c:2432:VAL:HG13	2.00	0.42
2:b:2049:ASP:HA	2:b:2050:PRO:HD3	1.85	0.42
2:b:2234:ILE:HG21	23:b:2524:CLA:H193	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:2098:GLY:O	3:c:2099:VAL:HG23	2.19	0.42
3:c:2261:ARG:O	8:i:2030:ARG:NH2	2.52	0.42
3:c:2377:LEU:O	3:c:2381:LYS:HG2	2.19	0.42
3:c:2386:PRO:C	3:c:2388:GLN:N	2.75	0.42
4:d:2057:SER:O	4:d:2061:HIS:HB2	2.19	0.42
4:d:2222:LEU:HD22	4:d:2243:THR:HB	2.01	0.42
8:i:2008:VAL:O	8:i:2011:VAL:N	2.52	0.42
9:j:2024:ILE:O	9:j:2027:LEU:HB3	2.19	0.42
11:l:2007:ARG:HD2	11:l:2007:ARG:N	2.35	0.42
11:l:2036:PHE:HD2	11:l:2036:PHE:HA	1.68	0.42
13:o:2037:THR:HB	13:o:2038:TYR:H	1.74	0.42
15:u:2118:GLU:O	15:u:2119:THR:C	2.62	0.42
16:v:2092:HIS:O	16:v:2093:PRO:C	2.61	0.42
1:A:57:PRO:CA	1:A:68:SER:HB3	2.49	0.42
1:A:64:ARG:O	13:O:152:ARG:NH2	2.50	0.42
1:A:77:ILE:HD11	14:T:6:TYR:CD2	2.54	0.42
1:A:139:MET:CE	4:D:248:THR:CG2	2.97	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.01	0.42
2:B:327:THR:C	2:B:329:PRO:CD	2.90	0.42
23:B:524:CLA:O1D	23:B:524:CLA:H93	2.20	0.42
3:C:139:THR:O	3:C:139:THR:HG23	2.19	0.42
3:C:159:THR:HA	3:C:252:ILE:HA	2.01	0.42
3:C:168:LEU:HD21	23:C:478:CLA:H72	2.02	0.42
3:C:213:LEU:HD11	23:C:474:CLA:H171	2.01	0.42
3:C:324:LEU:HD23	3:C:324:LEU:HA	1.77	0.42
3:C:443:TRP:CE3	3:C:443:TRP:CA	3.00	0.42
4:D:28:VAL:O	4:D:28:VAL:HG12	2.17	0.42
4:D:126:MET:SD	4:D:143:ALA:O	2.77	0.42
4:D:273:PHE:O	4:D:277:THR:CB	2.67	0.42
8:I:13:THR:O	8:I:16:VAL:HB	2.19	0.42
13:O:229:GLU:HA	13:O:230:PRO:HD3	1.91	0.42
15:U:47:LEU:C	15:U:49:THR:N	2.77	0.42
16:V:37:CYS:HB2	16:V:38:ALA:H	1.71	0.42
17:X:17:LYS:O	17:X:20:PHE:N	2.52	0.42
1:a:2133:LEU:HD21	4:d:2252:PHE:HA	2.01	0.42
2:b:2008:VAL:C	2:b:2010:THR:H	2.27	0.42
2:b:2118:TRP:HZ2	11:l:2003:PRO:HB3	1.76	0.42
2:b:2475:PHE:CD2	4:d:2140:PRO:HD3	2.54	0.42
3:c:2190:ALA:HA	3:c:2191:PRO:HA	1.44	0.42
6:f:2022:VAL:O	6:f:2026:ALA:CB	2.67	0.42
8:i:2035:LYS:HE2	8:i:2037:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:2117:PRO:HB2	13:o:2151:TYR:CE2	2.54	0.42
16:v:2081:THR:O	16:v:2084:GLY:N	2.52	0.42
19:z:2015:LEU:HD21	19:z:2047:TRP:HB2	2.01	0.42
1:A:55:ALA:HA	1:A:56:PRO:HD3	1.92	0.42
1:A:297:LEU:CD2	3:C:428:THR:HG21	2.50	0.42
1:A:316:THR:C	1:A:318:ALA:N	2.78	0.42
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.49	0.42
2:B:49:ASP:HA	2:B:50:PRO:HD3	1.87	0.42
2:B:139:PHE:C	2:B:139:PHE:CD2	2.96	0.42
2:B:168:VAL:CG1	2:B:169:SER:N	2.83	0.42
2:B:245:VAL:HG22	23:B:513:CLA:H172	2.02	0.42
3:C:97:TRP:CE3	3:C:178:LYS:CE	3.02	0.42
3:C:404:LEU:C	3:C:406:SER:H	2.26	0.42
4:D:20:ASP:O	4:D:24:ARG:N	2.52	0.42
4:D:249:ALA:O	4:D:252:PHE:HB3	2.20	0.42
6:F:32:PHE:CD1	27:F:48:BCR:H14C	2.54	0.42
9:J:15:THR:CA	27:K:50:BCR:H372	2.45	0.42
10:K:18:VAL:C	10:K:20:PRO:HD2	2.45	0.42
15:U:108:ASN:O	15:U:110:GLU:N	2.53	0.42
16:V:94:SER:C	16:V:96:ARG:N	2.75	0.42
1:a:2263:ALA:HB1	25:a:2352:PL9:C15	2.46	0.42
1:a:2326:LEU:O	1:a:2327:GLY:C	2.61	0.42
24:a:2350:PHO:NC	4:d:2209:LEU:HD12	2.35	0.42
2:b:2084:THR:O	2:b:2084:THR:CG2	2.67	0.42
2:b:2091:TRP:HB2	23:b:2515:CLA:H43	2.01	0.42
2:b:2191:ASN:OD1	2:b:2191:ASN:C	2.62	0.42
2:b:2234:ILE:HD13	2:b:2234:ILE:HA	1.89	0.42
2:b:2252:VAL:HG22	23:b:2517:CLA:O1A	2.20	0.42
3:c:2259:TRP:HZ3	23:c:2474:CLA:O2A	2.03	0.42
3:c:2350:ILE:CG2	3:c:2359:TRP:CB	2.92	0.42
9:j:2040:LEU:HD21	16:v:2118:HIS:HE1	1.84	0.42
11:l:2036:PHE:HZ	12:m:2008:LEU:HD13	1.85	0.42
13:o:2183:ALA:O	13:o:2184:ARG:C	2.63	0.42
16:v:2029:GLY:HA3	16:v:2118:HIS:HB2	2.02	0.42
1:A:31:GLY:HA3	1:A:132:GLU:OE2	2.19	0.42
1:A:76:ASN:CB	14:T:2:GLU:OE2	2.64	0.42
1:A:142:TRP:CH2	1:A:273:PHE:HE1	2.35	0.42
1:A:180:PHE:CE2	4:D:192:THR:O	2.68	0.42
1:A:258:LEU:C	1:A:259:ILE:HG13	2.43	0.42
2:B:35:GLY:O	2:B:39:LEU:HG	2.19	0.42
3:C:393:ALA:HA	3:C:396:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:350:ASN:O	4:D:351:ALA:HB3	2.19	0.42
9:J:15:THR:HG23	27:K:50:BCR:H372	2.01	0.42
10:K:16:LEU:O	10:K:18:VAL:N	2.52	0.42
19:Z:47:TRP:HE1	19:Z:51:VAL:HG23	1.85	0.42
1:a:2237:TYR:O	1:a:2238:LYS:HG3	2.19	0.42
1:a:2297:LEU:HD12	1:a:2297:LEU:HA	1.73	0.42
2:b:2063:LEU:HB3	2:b:2064:PRO:CD	2.42	0.42
2:b:2225:LEU:HD23	2:b:2225:LEU:HA	1.79	0.42
2:b:2288:VAL:O	2:b:2292:LEU:CB	2.68	0.42
2:b:2474:LEU:C	2:b:2475:PHE:HD1	2.28	0.42
23:c:2478:CLA:H91	23:c:2482:CLA:HAA1	2.00	0.42
4:d:2139:ARG:NH1	4:d:2141:TYR:CZ	2.88	0.42
4:d:2198:MET:HE3	11:l:2030:LEU:HD11	2.00	0.42
6:f:2031:PHE:C	6:f:2031:PHE:CD2	2.97	0.42
13:o:2068:THR:HG22	13:o:2107:THR:HB	2.02	0.42
1:A:160:ILE:O	1:A:164:GLY:N	2.46	0.42
1:A:184:ILE:O	1:A:185:VAL:C	2.63	0.42
2:B:106:LEU:HB3	23:B:522:CLA:H121	2.02	0.42
2:B:340:TRP:CE3	2:B:342:GLY:CA	3.02	0.42
23:B:511:CLA:H102	7:H:37:PHE:CD1	2.55	0.42
23:B:523:CLA:HAA2	23:B:523:CLA:HBD	2.01	0.42
3:C:38:GLY:HA3	23:C:486:CLA:C1D	2.50	0.42
3:C:101:PRO:O	3:C:102:GLY:C	2.61	0.42
4:D:116:LEU:O	4:D:120:PHE:HD1	2.03	0.42
4:D:146:PHE:O	4:D:150:ILE:HG13	2.20	0.42
4:D:289:LEU:C	4:D:291:LEU:N	2.76	0.42
4:D:291:LEU:C	4:D:293:LEU:H	2.27	0.42
7:H:51:THR:O	7:H:51:THR:CG2	2.68	0.42
13:O:51:LEU:HD23	13:O:67:PRO:HA	2.02	0.42
15:U:72:TYR:O	15:U:73:PRO:C	2.63	0.42
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.42
16:V:29:GLY:HA3	16:V:118:HIS:HB2	2.02	0.42
1:a:2265:PHE:HE2	1:a:2270:SER:HB3	1.80	0.42
1:a:2309:ALA:HB1	16:v:2002:GLU:HA	2.02	0.42
2:b:2020:ILE:O	2:b:2024:LEU:HG	2.20	0.42
23:b:2519:CLA:H141	23:d:2357:CLA:H11	2.02	0.42
3:c:2119:LEU:O	3:c:2119:LEU:HD12	2.20	0.42
23:c:2475:CLA:H51	27:j:2053:BCR:H342	2.00	0.42
4:d:2087:HIS:N	4:d:2087:HIS:HD2	2.14	0.42
13:o:2034:SER:C	13:o:2036:GLN:N	2.72	0.42
1:A:63:ILE:HG23	3:C:335:THR:HG23	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:N	1:A:73:TYR:CD2	2.88	0.42
1:A:140:ARG:C	4:D:220:ASN:OD1	2.63	0.42
1:A:142:TRP:O	1:A:145:VAL:N	2.49	0.42
1:A:339:PHE:HB3	3:C:313:GLN:OE1	2.19	0.42
2:B:122:LEU:HD12	23:B:525:CLA:CMA	2.49	0.42
2:B:164:PRO:C	2:B:165:GLY:O	2.60	0.42
2:B:366:PHE:HA	2:B:367:PRO:HD3	1.71	0.42
2:B:399:VAL:CG2	2:B:417:VAL:HG13	2.49	0.42
2:B:451:PHE:CZ	2:B:455:HIS:CE1	3.08	0.42
2:B:463:PHE:CZ	2:B:467:ILE:HD11	2.54	0.42
3:C:210:PHE:O	3:C:214:LEU:HG	2.20	0.42
23:C:475:CLA:H51	27:J:53:BCR:H342	2.01	0.42
4:D:30:VAL:HG22	4:D:38:PHE:CE1	2.53	0.42
4:D:80:THR:CG2	4:D:81:PRO:HD2	2.49	0.42
4:D:186:GLN:NE2	4:D:192:THR:OG1	2.53	0.42
4:D:281:MET:O	4:D:284:ILE:HB	2.19	0.42
9:J:17:ALA:O	9:J:20:GLY:N	2.53	0.42
9:J:19:MET:HG2	27:K:50:BCR:H361	2.01	0.42
9:J:30:TYR:O	9:J:33:TYR:HB2	2.20	0.42
15:U:67:GLN:O	15:U:68:TYR:CD2	2.73	0.42
16:V:81:THR:HB	16:V:83:ASP:OD1	2.19	0.42
1:a:2038:ILE:HD13	1:a:2038:ILE:HA	1.85	0.42
1:a:2210:LEU:HD12	1:a:2210:LEU:C	2.43	0.42
1:a:2211:PHE:CE2	1:a:2278:TRP:CD1	3.07	0.42
2:b:2056:TRP:HH2	2:b:2312:TYR:HE2	1.67	0.42
2:b:2212:ALA:HB2	23:b:2511:CLA:CMC	2.49	0.42
2:b:2308:LYS:HE2	2:b:2312:TYR:OH	2.20	0.42
2:b:2315:ILE:C	2:b:2317:ASN:N	2.78	0.42
3:c:2073:ALA:O	10:k:2001:LYS:HA	2.19	0.42
3:c:2199:ILE:HG22	3:c:2200:THR:N	2.35	0.42
3:c:2265:ILE:C	3:c:2266:TRP:CG	2.96	0.42
3:c:2420:VAL:HB	3:c:2425:TRP:HE1	1.84	0.42
4:d:2201:VAL:HG13	23:d:2354:CLA:CMB	2.49	0.42
4:d:2214:HIS:O	4:d:2218:VAL:HG23	2.19	0.42
4:d:2253:TRP:O	4:d:2254:SER:C	2.63	0.42
10:k:2035:GLY:O	10:k:2036:PHE:HB2	2.20	0.42
13:o:2033:ASP:O	13:o:2036:GLN:HB2	2.19	0.42
15:u:2088:VAL:CG1	15:u:2112:PHE:HB2	2.50	0.42
1:A:21:VAL:HG13	1:A:30:VAL:O	2.19	0.42
1:A:183:MET:HE2	23:A:349:CLA:HMD2	2.02	0.42
1:A:327:GLY:HA3	4:D:324:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:TRP:HH2	2:B:312:TYR:HE2	1.67	0.42
2:B:179:GLN:O	2:B:180:PRO:C	2.62	0.42
2:B:187:PRO:O	2:B:188:ASP:C	2.62	0.42
2:B:223:GLN:HG2	2:B:227:LYS:HG3	2.01	0.42
2:B:325:PHE:O	2:B:328:GLY:N	2.52	0.42
23:B:512:CLA:OBD	23:B:520:CLA:HHC	2.20	0.42
23:B:516:CLA:H111	23:B:522:CLA:H42	2.00	0.42
3:C:173:LEU:HA	3:C:176:VAL:CG2	2.49	0.42
3:C:259:TRP:HZ3	23:C:474:CLA:O2A	2.03	0.42
3:C:289:PHE:CD1	23:C:487:CLA:HBB2	2.55	0.42
3:C:425:TRP:CE2	23:C:475:CLA:HBA2	2.54	0.42
4:D:43:LEU:HD22	27:F:48:BCR:H323	2.02	0.42
5:E:25:THR:HG21	28:E:84:HEC:C4B	2.50	0.42
5:E:68:ARG:NH1	7:H:50:SER:HB3	2.34	0.42
13:O:198:SER:O	13:O:199:LEU:HD23	2.20	0.42
14:T:18:PHE:CD2	14:T:19:PHE:CE1	3.08	0.42
16:V:30:LYS:O	16:V:31:ARG:C	2.62	0.42
19:Z:9:LEU:HD12	19:Z:9:LEU:HA	1.83	0.42
1:a:2024:THR:HB	4:d:2251:ARG:NH2	2.35	0.42
1:a:2037:MET:CE	1:a:2129:ARG:HD2	2.36	0.42
1:a:2049:VAL:O	1:a:2053:ILE:HG13	2.20	0.42
1:a:2140:ARG:CZ	4:d:2232:PHE:CE1	3.02	0.42
2:b:2288:VAL:O	2:b:2292:LEU:HB2	2.20	0.42
2:b:2390:TYR:O	2:b:2391:SER:O	2.37	0.42
3:c:2102:GLY:HA2	3:c:2186:TYR:OH	2.19	0.42
3:c:2208:VAL:HG13	3:c:2209:ILE:HG12	2.01	0.42
4:d:2201:VAL:HG13	23:d:2354:CLA:HMB1	2.01	0.42
4:d:2343:GLU:OE1	15:u:2133:TYR:CE1	2.73	0.42
10:k:2016:LEU:HD11	27:k:2050:BCR:H322	2.01	0.42
11:l:2014:ARG:HA	12:m:2026:TYR:CE1	2.54	0.42
13:o:2155:ASN:HD22	15:u:2129:ASN:ND2	2.17	0.42
16:v:2012:LEU:HD13	16:v:2019:ILE:CG2	2.49	0.42
1:A:214:MET:HG2	25:A:353:PL9:HC8	2.02	0.42
2:B:19:LEU:HD23	23:B:524:CLA:H201	2.02	0.42
2:B:72:THR:HG22	2:B:79:SER:HB2	2.02	0.42
2:B:264:PRO:O	2:B:448:ARG:NH2	2.52	0.42
3:C:172:ALA:N	23:C:479:CLA:HAC1	2.35	0.42
3:C:245:ILE:C	3:C:247:GLY:N	2.77	0.42
4:D:90:LEU:HD11	4:D:96:GLU:CG	2.49	0.42
25:D:357:PL9:H38	14:T:18:PHE:CB	2.44	0.42
5:E:34:TRP:CD1	5:E:34:TRP:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:47:ILE:CG1	7:H:52:LEU:HD23	2.50	0.42
13:O:142:PHE:O	13:O:143:LYS:HG2	2.19	0.42
16:V:2:GLU:H	16:V:2:GLU:CD	2.27	0.42
1:a:2215:HIS:HD2	4:d:2268:HIS:HD2	1.67	0.42
2:b:2091:TRP:HB2	23:b:2515:CLA:C4	2.50	0.42
2:b:2093:PHE:O	2:b:2094:GLU:C	2.63	0.42
2:b:2458:PHE:HB3	23:b:2516:CLA:HMC1	2.02	0.42
3:c:2067:MET:HE1	3:c:2070:PHE:CD2	2.54	0.42
3:c:2168:LEU:HD21	23:c:2478:CLA:H72	2.02	0.42
3:c:2298:PRO:C	3:c:2300:GLU:H	2.28	0.42
3:c:2348:GLU:HG2	13:o:2007:TYR:CE1	2.46	0.42
10:k:2030:TRP:O	10:k:2034:VAL:HG23	2.19	0.42
11:l:2021:LEU:O	11:l:2022:LEU:C	2.63	0.42
19:z:2040:ILE:C	19:z:2042:LEU:N	2.74	0.42
1:A:89:ILE:HG21	1:A:94:TYR:CB	2.46	0.41
1:A:141:PRO:O	3:C:443:TRP:CZ3	2.73	0.41
1:A:220:THR:O	1:A:223:LEU:HG	2.20	0.41
1:A:291:SER:O	1:A:295:PHE:CD1	2.73	0.41
3:C:170:ILE:O	3:C:171:GLY:C	2.62	0.41
3:C:273:SER:CB	3:C:445:ALA:HB2	2.44	0.41
3:C:339:LYS:HE2	15:U:129:ASN:OD1	2.19	0.41
4:D:48:TRP:CE3	24:D:355:PHO:H161	2.55	0.41
4:D:189:HIS:CE1	4:D:294:ARG:HE	2.38	0.41
4:D:334:GLN:N	4:D:335:PRO:HD3	2.35	0.41
10:K:16:LEU:CB	10:K:17:PRO:CD	2.85	0.41
13:O:101:ILE:HG22	13:O:102:ASP:N	2.35	0.41
13:O:118:LEU:HD22	13:O:233:VAL:HG21	2.01	0.41
1:a:2298:ASN:ND2	3:c:2402:GLY:O	2.53	0.41
2:b:2135:LEU:N	2:b:2136:PRO:HD2	2.35	0.41
2:b:2211:ILE:HG22	2:b:2212:ALA:N	2.35	0.41
2:b:2370:LEU:HD12	2:b:2379:ALA:HB3	2.02	0.41
3:c:2225:VAL:O	3:c:2225:VAL:HG12	2.20	0.41
11:l:2029:LEU:O	11:l:2030:LEU:C	2.62	0.41
2:B:145:LEU:CD1	23:B:522:CLA:HAB	2.49	0.41
23:B:516:CLA:HAA2	23:B:516:CLA:HBD	2.02	0.41
3:C:49:LEU:O	3:C:52:ALA:N	2.53	0.41
3:C:199:ILE:HG22	3:C:200:THR:N	2.35	0.41
3:C:339:LYS:HB2	3:C:340:TYR:CD1	2.54	0.41
3:C:350:ILE:CG2	3:C:351:PHE:N	2.81	0.41
23:C:474:CLA:HBB2	23:C:485:CLA:HED1	2.01	0.41
9:J:19:MET:CG	27:K:50:BCR:H361	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:197:ILE:HG12	13:O:198:SER:N	2.35	0.41
13:O:207:ARG:O	13:O:210:GLU:OE2	2.38	0.41
14:T:9:ILE:O	14:T:9:ILE:CG2	2.68	0.41
16:V:129:LYS:NZ	16:V:135:VAL:HG23	2.35	0.41
19:Z:52:LEU:O	19:Z:56:VAL:HG23	2.21	0.41
1:a:2053:ILE:HG22	1:a:2053:ILE:O	2.20	0.41
1:a:2183:MET:CE	23:d:2355:CLA:HMD2	2.50	0.41
1:a:2317:TRP:HA	1:a:2317:TRP:CE3	2.55	0.41
2:b:2190:PHE:CE2	7:h:2044:ILE:CD1	3.02	0.41
2:b:2265:ILE:C	2:b:2267:LEU:N	2.77	0.41
3:c:2067:MET:HE3	10:k:2017:PRO:CB	2.49	0.41
3:c:2175:LEU:HD13	23:c:2479:CLA:HMD1	2.02	0.41
4:d:2281:MET:O	4:d:2284:ILE:HB	2.21	0.41
6:f:2039:MET:HE2	6:f:2039:MET:HB3	1.87	0.41
1:A:143:ILE:HD12	4:D:252:PHE:CE2	2.56	0.41
1:A:337:HIS:ND1	4:D:352:LEU:HD12	2.35	0.41
2:B:46:ASP:HA	2:B:47:PRO:HD3	1.68	0.41
2:B:175:THR:O	2:B:175:THR:HG23	2.21	0.41
2:B:212:ALA:HB2	23:B:511:CLA:CMC	2.50	0.41
2:B:235:GLU:O	2:B:238:LEU:HB3	2.21	0.41
2:B:372:ASP:OD1	2:B:373:LYS:N	2.53	0.41
3:C:78:GLU:HG3	16:V:105:ARG:NH1	2.35	0.41
3:C:89:ILE:O	3:C:92:ILE:N	2.53	0.41
3:C:195:ASP:N	3:C:195:ASP:OD1	2.53	0.41
3:C:247:GLY:O	3:C:248:GLY:C	2.61	0.41
3:C:412:THR:HG22	16:V:136:TYR:CE2	2.52	0.41
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.37	0.41
8:I:27:ASP:CB	8:I:28:PRO:CD	2.88	0.41
11:L:14:ARG:HA	12:M:26:TYR:CE1	2.55	0.41
13:O:137:THR:O	13:O:138:THR:C	2.63	0.41
13:O:224:ASP:O	13:O:225:MET:C	2.63	0.41
15:U:62:ILE:HG12	15:U:80:VAL:HG21	2.02	0.41
16:V:22:THR:OG1	16:V:25:GLN:HG3	2.20	0.41
16:V:63:THR:HG21	16:V:83:ASP:O	2.19	0.41
1:a:2141:PRO:O	3:c:2443:TRP:CZ3	2.73	0.41
3:c:2305:THR:H	3:c:2308:GLU:CG	2.28	0.41
3:c:2335:THR:HG22	3:c:2335:THR:O	2.19	0.41
4:d:2020:ASP:O	4:d:2024:ARG:N	2.53	0.41
4:d:2154:VAL:O	4:d:2155:SER:C	2.63	0.41
4:d:2180:ARG:HD3	4:d:2181:PHE:N	2.34	0.41
4:d:2218:VAL:O	4:d:2220:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2269:PHE:O	4:d:2272:LEU:N	2.35	0.41
11:l:2002:GLU:N	11:l:2003:PRO:HD2	2.34	0.41
13:o:2010:ILE:C	13:o:2012:GLY:H	2.27	0.41
13:o:2125:LEU:HD12	13:o:2145:GLU:O	2.20	0.41
13:o:2163:GLY:HA2	13:o:2188:LYS:HG3	2.02	0.41
15:u:2073:PRO:HD2	16:v:2083:ASP:HB3	2.02	0.41
1:A:160:ILE:HG21	1:A:291:SER:OG	2.20	0.41
1:A:331:MET:HE2	1:A:331:MET:HB3	1.84	0.41
1:A:339:PHE:CB	3:C:313:GLN:OE1	2.68	0.41
2:B:8:VAL:C	2:B:10:THR:H	2.29	0.41
3:C:320:ARG:NE	15:U:128:TYR:CZ	2.77	0.41
23:C:474:CLA:H122	23:C:485:CLA:H13	2.03	0.41
4:D:199:MET:O	4:D:202:ALA:N	2.51	0.41
9:J:29:PHE:O	9:J:30:TYR:C	2.63	0.41
13:O:77:SER:O	13:O:78:LEU:C	2.63	0.41
1:a:2055:ALA:HA	1:a:2056:PRO:HD3	1.87	0.41
1:a:2095:PRO:CD	1:a:2098:GLU:CB	2.94	0.41
2:b:2019:LEU:HD23	23:b:2524:CLA:H201	2.03	0.41
2:b:2026:HIS:HB2	23:b:2513:CLA:HMB3	2.02	0.41
2:b:2364:GLU:HG3	4:d:2296:TYR:CD2	2.54	0.41
23:b:2523:CLA:HAA2	23:b:2523:CLA:HBD	2.02	0.41
3:c:2306:GLY:N	3:c:2307:PRO:HD2	2.35	0.41
6:f:2014:ILE:O	6:f:2014:ILE:HG13	2.19	0.41
10:k:2001:LYS:C	10:k:2003:PRO:HD3	2.40	0.41
12:m:2011:THR:O	12:m:2011:THR:CG2	2.68	0.41
15:u:2072:TYR:O	15:u:2076:ALA:HB3	2.20	0.41
15:u:2120:ALA:O	15:u:2122:VAL:N	2.54	0.41
1:A:210:LEU:O	1:A:214:MET:HB2	2.20	0.41
2:B:66:MET:HE1	2:B:93:PHE:HA	2.03	0.41
2:B:265:ILE:O	2:B:267:LEU:N	2.54	0.41
2:B:288:VAL:O	2:B:292:LEU:HB2	2.21	0.41
3:C:222:GLY:O	3:C:223:TRP:O	2.38	0.41
3:C:333:GLY:C	3:C:335:THR:N	2.79	0.41
4:D:29:PHE:CD2	4:D:29:PHE:O	2.72	0.41
4:D:342:PRO:HG2	4:D:345:VAL:CG2	2.51	0.41
10:K:6:TYR:HD1	10:K:6:TYR:H	1.67	0.41
14:T:27:PRO:HG2	14:T:27:PRO:O	2.21	0.41
16:V:79:PRO:CB	16:V:88:ILE:CG1	2.93	0.41
18:N:22:UNK:O	18:N:23:UNK:C	2.68	0.41
19:Z:47:TRP:CD1	19:Z:51:VAL:HG23	2.55	0.41
1:a:2093:PHE:HB2	3:c:2218:PHE:HD1	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2193:LEU:HD22	4:d:2179:PHE:CD2	2.55	0.41
1:a:2301:ASN:OD1	3:c:2407:VAL:HG21	2.20	0.41
2:b:2311:PHE:O	2:b:2312:TYR:C	2.64	0.41
2:b:2366:PHE:HA	2:b:2367:PRO:HD3	1.70	0.41
2:b:2462:PHE:HA	23:b:2523:CLA:HMC2	2.01	0.41
3:c:2277:GLY:C	23:c:2477:CLA:HBC2	2.44	0.41
3:c:2282:MET:O	3:c:2283:GLY:C	2.62	0.41
3:c:2365:TRP:CZ3	3:c:2366:LEU:HB2	2.55	0.41
3:c:2412:THR:O	3:c:2412:THR:HG22	2.19	0.41
4:d:2073:PHE:CD1	4:d:2073:PHE:C	2.99	0.41
4:d:2153:PHE:CE1	24:d:2356:PHO:C9	3.04	0.41
4:d:2155:SER:O	4:d:2159:ILE:HB	2.20	0.41
4:d:2252:PHE:CE2	4:d:2256:ILE:HD12	2.55	0.41
10:k:2004:GLU:HB3	10:k:2005:ALA:H	1.47	0.41
11:l:2035:PHE:CD2	12:m:2010:ALA:HB1	2.55	0.41
12:m:2003:VAL:HG22	12:m:2004:ASN:N	2.34	0.41
13:o:2106:VAL:HA	13:o:2117:PRO:HA	2.02	0.41
15:u:2113:THR:HG22	15:u:2114:VAL:N	2.35	0.41
16:v:2003:LEU:HD12	16:v:2003:LEU:HA	1.89	0.41
16:v:2134:LYS:O	16:v:2137:TYR:C	2.63	0.41
1:A:58:VAL:HG13	1:A:107:TYR:O	2.21	0.41
1:A:207:GLY:HA3	1:A:278:TRP:CD1	2.56	0.41
2:B:308:LYS:HE2	2:B:312:TYR:OH	2.20	0.41
2:B:315:ILE:C	2:B:317:ASN:N	2.78	0.41
3:C:90:PRO:CB	3:C:302:TYR:HE2	2.33	0.41
3:C:190:ALA:HA	3:C:191:PRO:HA	1.49	0.41
3:C:320:ARG:HG2	15:U:128:TYR:CE2	2.56	0.41
3:C:333:GLY:O	3:C:334:PRO:C	2.62	0.41
4:D:259:ILE:O	4:D:260:ALA:HB2	2.20	0.41
7:H:22:PRO:HG2	7:H:23:GLY:H	1.85	0.41
7:H:43:ILE:HG12	17:X:19:PHE:CZ	2.56	0.41
13:O:76:THR:HB	13:O:77:SER:H	1.29	0.41
13:O:157:LEU:HD23	13:O:157:LEU:HA	1.79	0.41
14:T:14:ILE:O	14:T:17:PHE:HB2	2.21	0.41
1:a:2040:THR:CG2	1:a:2122:GLY:HA3	2.50	0.41
1:a:2045:THR:O	1:a:2046:ILE:C	2.62	0.41
1:a:2192:ILE:HG22	1:a:2198:HIS:HB2	2.03	0.41
1:a:2206:PHE:HD2	24:d:2356:PHO:HBB2	1.85	0.41
2:b:2162:PHE:HB3	23:b:2515:CLA:HMD2	2.02	0.41
2:b:2354:LEU:CD2	2:b:2378:LYS:HG3	2.49	0.41
23:b:2511:CLA:H111	23:b:2511:CLA:H152	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:2518:CLA:H61	23:b:2518:CLA:H41	1.80	0.41
3:c:2282:MET:HA	3:c:2285:ILE:CB	2.50	0.41
3:c:2365:TRP:CE3	3:c:2366:LEU:HB2	2.56	0.41
23:d:2357:CLA:H151	23:d:2357:CLA:H112	1.90	0.41
28:e:2084:HEC:C4A	6:f:2019:TRP:CH2	2.99	0.41
9:j:2028:PHE:CD2	9:j:2028:PHE:N	2.88	0.41
14:t:2018:PHE:HD2	14:t:2019:PHE:CD1	2.38	0.41
16:v:2111:ASP:O	16:v:2115:ILE:HG13	2.20	0.41
1:A:95:PRO:HG2	1:A:98:GLU:HB2	2.02	0.41
1:A:140:ARG:C	4:D:220:ASN:HD21	2.29	0.41
1:A:149:ALA:HA	1:A:284:TRP:CE3	2.56	0.41
1:A:159:LEU:HD21	1:A:163:ILE:HD11	2.03	0.41
2:B:311:PHE:O	2:B:312:TYR:C	2.61	0.41
2:B:339:ALA:HB1	2:B:340:TRP:HD1	1.86	0.41
23:B:513:CLA:H18	23:B:524:CLA:O1A	2.20	0.41
3:C:45:LEU:O	3:C:47:GLY:N	2.54	0.41
3:C:54:VAL:O	3:C:54:VAL:HG12	2.21	0.41
3:C:395:TYR:N	3:C:395:TYR:CD2	2.87	0.41
4:D:217:THR:OG1	4:D:253:TRP:HZ2	2.03	0.41
4:D:322:ASN:O	4:D:325:ILE:N	2.53	0.41
13:O:71:VAL:HG21	13:O:108:VAL:CG2	2.46	0.41
1:a:2131:TRP:CD2	1:a:2131:TRP:C	2.98	0.41
1:a:2183:MET:HE1	23:d:2355:CLA:HMD2	2.02	0.41
1:a:2223:LEU:HD22	1:a:2245:THR:HG22	2.03	0.41
2:b:2122:LEU:HD12	23:b:2525:CLA:CMA	2.47	0.41
2:b:2470:GLY:O	2:b:2473:THR:HB	2.20	0.41
3:c:2064:ALA:HB3	3:c:2118:HIS:HB3	2.02	0.41
3:c:2313:GLN:HE21	3:c:2313:GLN:HB2	1.71	0.41
27:c:2488:BCR:C21	10:k:2023:PHE:CE2	3.04	0.41
5:e:2022:HIS:O	5:e:2023:SER:C	2.63	0.41
7:h:2051:THR:O	7:h:2051:THR:HG22	2.21	0.41
10:k:2022:LEU:HB2	27:k:2050:BCR:H352	2.03	0.41
12:m:2017:VAL:HG12	12:m:2018:PRO:N	2.34	0.41
13:o:2077:SER:O	13:o:2078:LEU:C	2.63	0.41
13:o:2137:THR:O	13:o:2138:THR:C	2.64	0.41
15:u:2042:VAL:HG12	15:u:2045:GLU:H	1.85	0.41
15:u:2089:GLU:H	15:u:2089:GLU:HG3	1.50	0.41
16:v:2025:GLN:O	16:v:2028:GLU:N	2.52	0.41
1:A:40:THR:CG2	1:A:118:HIS:O	2.69	0.41
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.21	0.41
1:A:208:GLY:O	1:A:212:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ALA:C	1:A:326:LEU:N	2.77	0.41
2:B:12:LEU:HD11	2:B:19:LEU:N	2.36	0.41
2:B:288:VAL:O	2:B:292:LEU:CB	2.68	0.41
3:C:53:HIS:ND1	23:C:478:CLA:H141	2.35	0.41
3:C:175:LEU:HD23	3:C:237:HIS:CD2	2.55	0.41
3:C:273:SER:HB2	23:C:477:CLA:HED1	2.02	0.41
3:C:275:SER:OG	23:C:485:CLA:HAA1	2.21	0.41
3:C:355:THR:O	3:C:355:THR:OG1	2.37	0.41
4:D:58:TRP:HA	4:D:62:GLY:N	2.32	0.41
5:E:19:TRP:HZ2	9:J:13:VAL:CG2	2.27	0.41
13:O:118:LEU:HD22	13:O:221:SER:HA	2.01	0.41
13:O:224:ASP:C	13:O:225:MET:CG	2.91	0.41
15:U:57:LEU:HA	15:U:57:LEU:HD23	1.78	0.41
15:U:113:THR:HG22	15:U:114:VAL:H	1.82	0.41
19:Z:22:GLY:O	19:Z:23:VAL:C	2.64	0.41
1:a:2221:SER:HB3	4:d:2138:VAL:HG12	2.01	0.41
1:a:2342:ASP:OD1	1:a:2342:ASP:C	2.61	0.41
2:b:2062:VAL:HG12	2:b:2063:LEU:N	2.35	0.41
2:b:2109:LEU:O	2:b:2113:TRP:HE3	2.04	0.41
2:b:2237:VAL:CG2	23:b:2524:CLA:HBC2	2.51	0.41
2:b:2340:TRP:CE3	2:b:2342:GLY:CA	3.03	0.41
27:b:2528:BCR:H15C	27:b:2528:BCR:H351	1.93	0.41
3:c:2045:LEU:O	3:c:2047:GLY:N	2.54	0.41
3:c:2078:GLU:H	3:c:2104:GLU:CD	2.29	0.41
3:c:2433:LEU:HD13	23:c:2481:CLA:HMC2	2.02	0.41
4:d:2151:ALA:O	4:d:2152:VAL:C	2.62	0.41
4:d:2246:MET:SD	4:d:2264:LYS:HG2	2.61	0.41
5:e:2060:ARG:HG3	5:e:2060:ARG:O	2.21	0.41
11:l:2004:ASN:H	11:l:2004:ASN:ND2	2.12	0.41
13:o:2188:LYS:HD2	13:o:2225:MET:HG3	2.03	0.41
15:u:2093:ASN:O	15:u:2094:ILE:C	2.64	0.41
1:A:24:THR:OG1	4:D:251:ARG:NH2	2.53	0.41
1:A:29:TYR:OH	1:A:132:GLU:OE2	2.35	0.41
1:A:180:PHE:HD1	1:A:180:PHE:N	2.12	0.41
1:A:309:ALA:HB1	16:V:2:GLU:HA	2.03	0.41
2:B:6:TYR:OH	23:B:520:CLA:HMD2	2.21	0.41
2:B:9:HIS:HE1	23:B:512:CLA:HED1	1.86	0.41
2:B:12:LEU:HG	2:B:19:LEU:CB	2.51	0.41
2:B:33:TRP:HE1	23:B:514:CLA:HBC2	1.86	0.41
2:B:126:PRO:C	2:B:127:ARG:HG3	2.46	0.41
2:B:187:PRO:O	2:B:189:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ASN:OD1	2:B:191:ASN:C	2.64	0.41
2:B:340:TRP:CZ3	2:B:407:ASN:HB3	2.55	0.41
2:B:403:GLY:O	2:B:404:GLY:C	2.64	0.41
2:B:404:GLY:O	2:B:405:GLU:C	2.64	0.41
2:B:472:ARG:O	2:B:472:ARG:HG2	2.19	0.41
23:B:514:CLA:H61	23:B:514:CLA:H41	1.93	0.41
23:B:520:CLA:H51	27:B:529:BCR:H313	2.02	0.41
3:C:62:PHE:CD2	10:K:20:PRO:HG3	2.56	0.41
3:C:101:PRO:HA	3:C:195:ASP:HB3	2.02	0.41
3:C:172:ALA:N	23:C:479:CLA:CAC	2.84	0.41
3:C:249:ILE:HG13	3:C:250:TRP:N	2.36	0.41
3:C:263:ALA:HB3	3:C:264:PHE:CD2	2.55	0.41
3:C:290:VAL:HG12	3:C:291:TRP:N	2.35	0.41
27:C:488:BCR:C20	10:K:23:PHE:HE2	2.33	0.41
4:D:18:LEU:O	4:D:19:ASP:C	2.64	0.41
4:D:51:GLY:HA2	4:D:55:VAL:CG2	2.46	0.41
4:D:73:PHE:CD1	4:D:73:PHE:C	2.99	0.41
4:D:125:PHE:CD2	4:D:125:PHE:O	2.74	0.41
4:D:156:VAL:HG23	23:D:354:CLA:HED1	2.03	0.41
4:D:199:MET:O	4:D:200:GLY:C	2.61	0.41
4:D:269:PHE:C	4:D:269:PHE:CD2	2.98	0.41
4:D:299:ILE:O	4:D:300:SER:C	2.64	0.41
7:H:29:LEU:HA	7:H:29:LEU:HD12	1.79	0.41
9:J:25:VAL:O	9:J:28:PHE:N	2.54	0.41
13:O:224:ASP:O	13:O:224:ASP:OD1	2.38	0.41
15:U:65:PHE:CD1	15:U:76:ALA:CB	3.04	0.41
15:U:100:ARG:O	15:U:104:ILE:HG13	2.21	0.41
19:Z:47:TRP:NE1	19:Z:51:VAL:HG23	2.36	0.41
1:a:2029:TYR:CD2	1:a:2133:LEU:CD1	3.03	0.41
1:a:2040:THR:HG21	1:a:2122:GLY:N	2.35	0.41
1:a:2186:PHE:HD2	1:a:2192:ILE:HD11	1.79	0.41
1:a:2212:CYS:SG	4:d:2210:LEU:HB2	2.60	0.41
23:a:2348:CLA:H191	14:t:2017:PHE:CE1	2.56	0.41
2:b:2190:PHE:CE1	23:b:2526:CLA:CED	3.04	0.41
2:b:2346:PHE:N	2:b:2346:PHE:CD1	2.89	0.41
2:b:2472:ARG:O	2:b:2472:ARG:HG2	2.19	0.41
3:c:2071:GLU:O	3:c:2073:ALA:N	2.54	0.41
4:d:2100:ASP:O	4:d:2101:PHE:C	2.64	0.41
4:d:2107:LEU:HD11	5:e:2071:ALA:HB1	2.01	0.41
4:d:2148:ALA:HB3	4:d:2149:PRO:CD	2.40	0.41
12:m:2006:LEU:HD23	12:m:2006:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:t:2029:ILE:C	14:t:2031:LYS:N	2.78	0.41
15:u:2047:LEU:O	15:u:2049:THR:N	2.54	0.41
16:v:2021:LEU:HD22	16:v:2025:GLN:CD	2.46	0.41
19:z:2053:VAL:O	19:z:2054:VAL:C	2.64	0.41
1:A:26:ASN:O	1:A:26:ASN:CG	2.64	0.41
1:A:225:ARG:HG3	1:A:225:ARG:H	1.19	0.41
1:A:325:ASN:HD22	1:A:325:ASN:H	1.69	0.41
2:B:9:HIS:CE1	23:B:512:CLA:HED1	2.55	0.41
2:B:135:LEU:O	2:B:137:LYS:N	2.54	0.41
2:B:166:MET:CE	2:B:195:PRO:HB3	2.51	0.41
2:B:201:HIS:CD2	2:B:202:HIS:N	2.89	0.41
2:B:265:ILE:HG21	2:B:312:TYR:CE1	2.55	0.41
23:B:516:CLA:H61	23:B:516:CLA:H41	1.94	0.41
4:D:32:TRP:HA	4:D:32:TRP:HE3	1.82	0.41
4:D:341:PHE:HA	4:D:342:PRO:HD2	1.73	0.41
5:E:22:HIS:O	5:E:23:SER:C	2.62	0.41
13:O:38:TYR:C	13:O:39:ARG:HD2	2.46	0.41
15:U:93:ASN:O	15:U:94:ILE:C	2.64	0.41
1:a:2096:ILE:HG22	8:i:2001:MET:CE	2.34	0.41
1:a:2203:ALA:O	1:a:2207:GLY:N	2.54	0.41
2:b:2011:VAL:HG13	11:l:2006:ASN:HB3	2.02	0.41
2:b:2106:LEU:O	2:b:2107:LEU:C	2.61	0.41
2:b:2298:LEU:O	2:b:2299:GLU:C	2.64	0.41
23:b:2522:CLA:H102	23:b:2525:CLA:HBC1	2.03	0.41
3:c:2287:THR:HG23	3:c:2427:ALA:HA	2.03	0.41
4:d:2176:ALA:C	4:d:2178:ILE:N	2.79	0.41
4:d:2188:PHE:HD1	4:d:2188:PHE:H	1.69	0.41
5:e:2025:THR:HG21	28:e:2084:HEC:C4B	2.51	0.41
13:o:2162:ARG:O	13:o:2162:ARG:CG	2.69	0.41
13:o:2242:SER:C	13:o:2243:ILE:HG13	2.46	0.41
15:u:2075:LEU:HD21	15:u:2101:GLN:HG2	2.03	0.41
16:v:2010:VAL:HG12	16:v:2011:PRO:N	2.36	0.41
1:A:32:TRP:HA	1:A:35:VAL:CG2	2.51	0.40
1:A:53:ILE:O	1:A:53:ILE:CG2	2.69	0.40
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.65	0.40
2:B:12:LEU:HD23	2:B:19:LEU:HD12	2.02	0.40
2:B:47:PRO:HA	2:B:78:TRP:NE1	2.36	0.40
2:B:91:TRP:CD1	23:B:515:CLA:H51	2.55	0.40
2:B:211:ILE:HG22	2:B:212:ALA:N	2.36	0.40
2:B:249:ALA:HB3	2:B:459:ALA:HB2	2.02	0.40
2:B:271:THR:CG2	2:B:448:ARG:NH1	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:LYS:CG	2:B:322:GLY:N	2.84	0.40
2:B:325:PHE:CZ	4:D:297:ASP:OD2	2.74	0.40
2:B:445:THR:HG22	2:B:446:SER:N	2.35	0.40
23:B:518:CLA:H141	23:B:524:CLA:CMA	2.51	0.40
3:C:154:LYS:O	3:C:158:THR:OG1	2.15	0.40
3:C:291:TRP:HZ3	3:C:424:SER:HA	1.86	0.40
3:C:438:LEU:C	3:C:440:GLY:N	2.75	0.40
4:D:303:ILE:HD13	12:M:2:GLU:OE1	2.21	0.40
5:E:50:ARG:HB3	5:E:51:PRO:HD2	2.03	0.40
7:H:38:LEU:HA	7:H:38:LEU:HD23	1.87	0.40
7:H:42:LEU:HD23	7:H:42:LEU:HA	1.72	0.40
13:O:152:ARG:HD2	13:O:156:PHE:CD1	2.56	0.40
13:O:238:VAL:CG1	13:O:239:PHE:H	2.33	0.40
15:U:61:ASN:HB3	15:U:130:ASN:HD22	1.85	0.40
18:N:8:UNK:O	18:N:12:UNK:N	2.54	0.40
19:Z:13:VAL:HG13	19:Z:17:PHE:HE1	1.86	0.40
1:a:2215:HIS:O	1:a:2216:GLY:C	2.64	0.40
1:a:2278:TRP:CB	1:a:2279:PRO:HD3	2.48	0.40
1:a:2331:MET:HE2	1:a:2331:MET:HB3	1.88	0.40
2:b:2225:LEU:HD23	2:b:2229:LEU:HD12	2.02	0.40
2:b:2327:THR:CG2	2:b:2329:PRO:HD3	2.46	0.40
3:c:2155:ASN:OD1	3:c:2156:LYS:N	2.54	0.40
3:c:2341:LEU:HD22	3:c:2349:ILE:HG22	2.02	0.40
4:d:2021:TRP:HB3	17:x:2041:SER:OG	2.20	0.40
4:d:2260:ALA:HB1	25:d:2358:PL9:O1	2.20	0.40
7:h:2021:ALA:HB3	7:h:2022:PRO:HD3	2.02	0.40
7:h:2021:ALA:CB	7:h:2022:PRO:HD3	2.51	0.40
7:h:2028:PRO:HG2	7:h:2029:LEU:N	2.36	0.40
11:l:2036:PHE:HE2	12:m:2008:LEU:H	1.65	0.40
16:v:2074:ASP:C	16:v:2074:ASP:OD1	2.64	0.40
1:A:40:THR:HG22	1:A:41:LEU:N	2.36	0.40
1:A:41:LEU:HD21	1:A:122:GLY:HA3	2.04	0.40
1:A:131:TRP:O	1:A:134:SER:N	2.54	0.40
1:A:174:LEU:HD13	24:A:351:PHO:H143	2.02	0.40
1:A:239:PHE:O	1:A:240:GLY:C	2.64	0.40
2:B:109:LEU:O	2:B:113:TRP:HE3	2.03	0.40
2:B:124:ARG:HG3	23:B:525:CLA:H43	2.03	0.40
2:B:267:LEU:HD23	2:B:267:LEU:HA	1.95	0.40
2:B:327:THR:N	27:B:529:BCR:H292	2.36	0.40
3:C:89:ILE:O	3:C:90:PRO:C	2.63	0.40
3:C:297:TYR:HB3	3:C:302:TYR:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:THR:CB	3:C:308:GLU:HG3	2.51	0.40
23:C:479:CLA:CMD	23:C:481:CLA:H111	2.52	0.40
4:D:183:LEU:O	4:D:184:PHE:C	2.64	0.40
4:D:287:VAL:HG12	4:D:287:VAL:O	2.20	0.40
4:D:314:PHE:O	4:D:315:TYR:C	2.63	0.40
8:I:8:VAL:O	8:I:9:TYR:C	2.64	0.40
8:I:13:THR:O	8:I:14:PHE:C	2.62	0.40
13:O:140:THR:HG21	13:O:201:VAL:C	2.43	0.40
15:U:65:PHE:HD1	15:U:76:ALA:CB	2.34	0.40
1:a:2029:TYR:CE1	1:a:2031:GLY:CA	3.04	0.40
1:a:2090:GLY:C	1:a:2167:SER:HA	2.46	0.40
1:a:2187:GLN:HG3	1:a:2193:LEU:HG	2.03	0.40
1:a:2192:ILE:HG22	1:a:2198:HIS:CB	2.51	0.40
1:a:2215:HIS:CD2	1:a:2219:VAL:HG21	2.56	0.40
1:a:2259:ILE:HD13	25:a:2352:PL9:H172	2.03	0.40
1:a:2303:ASN:OD1	1:a:2322:ASN:ND2	2.54	0.40
1:a:2310:LYS:O	16:v:2125:ILE:CG2	2.69	0.40
2:b:2340:TRP:CZ3	2:b:2407:ASN:HB3	2.56	0.40
27:b:2528:BCR:H11C	27:b:2528:BCR:H341	1.84	0.40
3:c:2062:PHE:HB2	3:c:2122:SER:HB2	2.03	0.40
3:c:2099:VAL:HG12	3:c:2100:GLY:N	2.36	0.40
3:c:2130:VAL:HG21	23:c:2486:CLA:H13	2.02	0.40
3:c:2205:ASP:HA	3:c:2206:PRO:HD3	1.89	0.40
3:c:2254:THR:HG22	3:c:2255:THR:O	2.21	0.40
4:d:2029:PHE:HE2	4:d:2031:GLY:HA2	1.87	0.40
5:e:2033:GLY:O	5:e:2036:PHE:N	2.47	0.40
7:h:2029:LEU:O	7:h:2033:PHE:HD1	2.04	0.40
13:o:2116:ILE:HA	13:o:2117:PRO:HD3	1.77	0.40
18:n:2008:UNK:O	18:n:2012:UNK:N	2.54	0.40
1:A:52:PHE:CD1	1:A:81:ALA:CB	3.04	0.40
1:A:110:GLY:O	1:A:112:TYR:N	2.54	0.40
2:B:55:MET:HE1	2:B:80:ILE:HD13	2.02	0.40
2:B:122:LEU:HB3	2:B:123:PHE:H	1.63	0.40
2:B:162:PHE:HB3	23:B:515:CLA:HMD2	2.02	0.40
2:B:406:LEU:HD12	13:o:2059:LYS:CD	2.49	0.40
3:C:61:VAL:HG13	3:C:118:HIS:HD2	1.86	0.40
3:C:116:VAL:O	3:C:117:VAL:C	2.64	0.40
3:C:176:VAL:HG11	3:C:238:ILE:HG12	2.04	0.40
3:C:271:TYR:N	3:C:271:TYR:CD2	2.90	0.40
3:C:308:GLU:CG	3:C:361:PHE:CZ	2.98	0.40
3:C:425:TRP:NE1	23:C:475:CLA:HBA2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:438:LEU:O	3:C:439:VAL:C	2.63	0.40
27:C:489:BCR:H342	19:Z:51:VAL:HG13	2.03	0.40
4:D:68:LEU:HA	4:D:68:LEU:HD12	1.84	0.40
4:D:281:MET:O	4:D:282:SER:C	2.64	0.40
9:J:17:ALA:O	9:J:18:GLY:C	2.64	0.40
10:K:19:ILE:O	10:K:23:PHE:HD1	2.05	0.40
12:M:24:ILE:CG2	12:m:2027:VAL:HG21	2.51	0.40
13:O:10:ILE:C	13:O:12:GLY:N	2.78	0.40
13:O:137:THR:O	13:O:140:THR:CG2	2.67	0.40
13:O:168:TYR:CE1	13:O:172:ILE:CD1	3.01	0.40
1:a:2237:TYR:N	1:a:2237:TYR:HD1	2.12	0.40
2:b:2047:PRO:HA	2:b:2078:TRP:NE1	2.35	0.40
2:b:2063:LEU:HD12	2:b:2063:LEU:HA	1.92	0.40
2:b:2231:MET:O	2:b:2231:MET:CE	2.69	0.40
3:c:2155:ASN:OD1	3:c:2155:ASN:C	2.64	0.40
3:c:2240:ILE:HG13	23:c:2479:CLA:HBB1	2.04	0.40
3:c:2289:PHE:HD1	23:c:2487:CLA:HBB2	1.81	0.40
3:c:2345:PRO:HB3	13:o:2073:ARG:CZ	2.50	0.40
23:c:2476:CLA:H93	23:c:2483:CLA:H8	2.04	0.40
4:d:2018:LEU:O	4:d:2022:LEU:HB3	2.21	0.40
4:d:2157:PHE:CD1	4:d:2157:PHE:N	2.89	0.40
13:o:2050:PHE:CE1	13:o:2070:LEU:HD21	2.56	0.40
13:o:2201:VAL:HG13	13:o:2211:ILE:CG2	2.45	0.40
15:u:2051:TYR:HB3	15:u:2052:GLY:H	1.31	0.40
16:v:2055:ARG:O	16:v:2059:LEU:HG	2.21	0.40
1:A:44:ALA:HB1	24:A:351:PHO:H91	2.02	0.40
1:A:48:PHE:HB2	1:A:115:ILE:HD13	2.03	0.40
1:A:255:PHE:CD2	1:A:264:SER:HA	2.47	0.40
1:A:301:ASN:OD1	3:C:407:VAL:HG11	2.20	0.40
2:B:92:SER:O	2:B:93:PHE:C	2.61	0.40
2:B:187:PRO:C	2:B:189:GLY:N	2.77	0.40
2:B:258:TYR:N	2:B:258:TYR:HD2	2.19	0.40
2:B:333:GLY:HA2	2:B:442:ILE:O	2.22	0.40
3:C:112:PHE:HE2	10:K:6:TYR:CZ	2.39	0.40
3:C:240:ILE:HG13	23:C:479:CLA:HBB1	2.03	0.40
4:D:66:SER:O	4:D:71:CYS:SG	2.74	0.40
5:E:12:ILE:HB	28:E:84:HEC:HAD2	2.02	0.40
11:L:36:PHE:CE2	12:M:8:LEU:N	2.90	0.40
13:O:27:ARG:HG3	13:O:29:ALA:CB	2.48	0.40
13:O:201:VAL:HG11	13:O:204:VAL:CG2	2.51	0.40
16:V:10:VAL:HA	16:V:11:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:24:LYS:HE2	16:V:28:GLU:OE2	2.21	0.40
16:V:63:THR:CB	16:V:83:ASP:O	2.67	0.40
16:V:75:TYR:HD2	16:V:79:PRO:HA	1.82	0.40
16:V:81:THR:O	16:V:84:GLY:N	2.54	0.40
1:a:2036:ILE:CD1	23:c:2487:CLA:H141	2.51	0.40
1:a:2180:PHE:CD2	4:d:2192:THR:CB	3.04	0.40
1:a:2225:ARG:HB3	2:b:2481:GLY:O	2.17	0.40
1:a:2296:ASN:HB3	3:c:2401:LEU:HA	2.03	0.40
1:a:2296:ASN:ND2	3:c:2401:LEU:HD23	2.36	0.40
25:a:2352:PL9:H122	25:a:2352:PL9:H101	1.95	0.40
2:b:2236:THR:OG1	2:b:2473:THR:HG21	2.21	0.40
2:b:2265:ILE:HG21	2:b:2312:TYR:CE1	2.57	0.40
23:b:2519:CLA:HMD3	23:b:2524:CLA:HAB	2.04	0.40
3:c:2081:MET:HE1	3:c:2089:ILE:HG22	2.03	0.40
3:c:2189:TRP:O	3:c:2190:ALA:O	2.40	0.40
3:c:2289:PHE:HB2	23:c:2487:CLA:CBB	2.52	0.40
4:d:2156:VAL:O	4:d:2161:PRO:HD3	2.21	0.40
4:d:2185:PHE:CE2	4:d:2289:LEU:HD12	2.57	0.40
10:k:2034:VAL:O	10:k:2034:VAL:CG1	2.68	0.40
1:A:181:ASN:O	1:A:182:PHE:C	2.65	0.40
2:B:225:LEU:HD23	2:B:229:LEU:HD12	2.03	0.40
2:B:346:PHE:CE2	2:B:399:VAL:HG22	2.57	0.40
23:B:513:CLA:HMD2	23:B:524:CLA:H172	2.04	0.40
3:C:162:GLY:HA3	3:C:248:GLY:O	2.21	0.40
3:C:343:ARG:CB	13:O:78:LEU:CD1	2.99	0.40
4:D:190:ASN:ND2	4:D:193:LEU:CD1	2.85	0.40
23:D:356:CLA:H112	23:D:356:CLA:H151	1.92	0.40
5:E:25:THR:HG21	28:E:84:HEC:C3B	2.51	0.40
13:O:72:THR:HG22	13:O:75:THR:OG1	2.21	0.40
13:O:120:PHE:HA	13:O:219:GLN:HE22	1.86	0.40
15:U:108:ASN:C	15:U:110:GLU:N	2.79	0.40
16:V:81:THR:C	16:V:83:ASP:N	2.78	0.40
1:a:2089:ILE:CG2	1:a:2094:TYR:HB2	2.51	0.40
1:a:2111:PRO:O	1:a:2112:TYR:C	2.65	0.40
1:a:2153:SER:OG	23:a:2348:CLA:HED1	2.21	0.40
1:a:2310:LYS:HG2	16:v:2125:ILE:HG12	2.03	0.40
1:a:2320:ILE:HD12	4:d:2063:LEU:HD11	2.02	0.40
23:a:2349:CLA:H121	25:a:2352:PL9:C16	2.47	0.40
2:b:2474:LEU:C	2:b:2475:PHE:CD1	2.99	0.40
3:c:2158:THR:CG2	3:c:2251:HIS:CB	2.83	0.40
3:c:2410:VAL:C	3:c:2412:THR:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:2268:HIS:O	4:d:2271:MET:HB2	2.21	0.40
8:i:2006:ILE:O	8:i:2010:ILE:HG13	2.22	0.40
13:o:2118:LEU:CD2	13:o:2233:VAL:HG21	2.51	0.40
13:o:2148:VAL:HA	13:o:2149:PRO:HD3	1.82	0.40
17:x:2024:LEU:HD12	17:x:2024:LEU:HA	1.94	0.40
18:n:2022:UNK:O	18:n:2023:UNK:C	2.68	0.40
19:z:2041:PHE:N	19:z:2041:PHE:CD1	2.90	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:246:ALA:C	18:n:2035:UNK:O[2_555]	1.76	0.44
13:O:246:ALA:N	18:n:2035:UNK:O[2_555]	1.97	0.23
13:O:246:ALA:O	18:n:2035:UNK:O[2_555]	2.07	0.13
13:O:246:ALA:O	18:n:2035:UNK:CB[2_555]	2.15	0.05
13:O:246:ALA:N	18:n:2035:UNK:C[2_555]	2.17	0.03
13:O:246:ALA:CA	18:n:2035:UNK:O[2_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	251 (76%)	58 (18%)	22 (7%)	1	11
1	a	331/344 (96%)	253 (76%)	56 (17%)	22 (7%)	1	11
2	B	474/510 (93%)	367 (77%)	84 (18%)	23 (5%)	1	16
2	b	474/510 (93%)	367 (77%)	83 (18%)	24 (5%)	1	15
3	C	419/473 (89%)	326 (78%)	60 (14%)	33 (8%)	1	8
3	c	419/473 (89%)	326 (78%)	62 (15%)	31 (7%)	1	9
4	D	337/352 (96%)	274 (81%)	49 (14%)	14 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	337/352 (96%)	270 (80%)	51 (15%)	16 (5%)	2	17
5	E	74/84 (88%)	62 (84%)	10 (14%)	2 (3%)	4	27
5	e	74/84 (88%)	57 (77%)	14 (19%)	3 (4%)	2	19
6	F	31/45 (69%)	23 (74%)	5 (16%)	3 (10%)	0	6
6	f	31/45 (69%)	22 (71%)	6 (19%)	3 (10%)	0	6
7	H	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	1	12
7	h	51/66 (77%)	35 (69%)	13 (26%)	3 (6%)	1	12
8	I	36/38 (95%)	25 (69%)	10 (28%)	1 (3%)	4	26
8	i	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	1	13
9	J	36/40 (90%)	32 (89%)	3 (8%)	1 (3%)	4	26
9	j	36/40 (90%)	30 (83%)	4 (11%)	2 (6%)	1	13
10	K	35/37 (95%)	27 (77%)	2 (6%)	6 (17%)	0	2
10	k	35/37 (95%)	26 (74%)	3 (9%)	6 (17%)	0	2
11	L	35/37 (95%)	28 (80%)	3 (9%)	4 (11%)	0	5
11	l	35/37 (95%)	27 (77%)	5 (14%)	3 (9%)	0	7
12	M	28/36 (78%)	22 (79%)	5 (18%)	1 (4%)	2	22
12	m	28/36 (78%)	22 (79%)	4 (14%)	2 (7%)	1	10
13	O	244/246 (99%)	180 (74%)	44 (18%)	20 (8%)	0	8
13	o	244/246 (99%)	179 (73%)	45 (18%)	20 (8%)	0	8
14	T	29/32 (91%)	23 (79%)	3 (10%)	3 (10%)	0	5
14	t	29/32 (91%)	22 (76%)	5 (17%)	2 (7%)	1	10
15	U	103/134 (77%)	78 (76%)	14 (14%)	11 (11%)	0	5
15	u	103/134 (77%)	81 (79%)	11 (11%)	11 (11%)	0	5
16	V	135/137 (98%)	111 (82%)	16 (12%)	8 (6%)	1	12
16	v	135/137 (98%)	106 (78%)	22 (16%)	7 (5%)	1	14
17	X	38/50 (76%)	36 (95%)	1 (3%)	1 (3%)	4	27
17	x	38/50 (76%)	35 (92%)	2 (5%)	1 (3%)	4	27
19	Z	56/62 (90%)	39 (70%)	15 (27%)	2 (4%)	2	22
19	z	56/62 (90%)	40 (71%)	13 (23%)	3 (5%)	1	14
All	All	4984/5446 (92%)	3864 (78%)	801 (16%)	319 (6%)	1	11

All (319) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	GLY
1	A	228	THR
1	A	242	GLU
1	A	308	ASP
2	B	88	PRO
2	B	126	PRO
2	B	173	GLY
2	B	235	GLU
2	B	326	ARG
2	B	391	SER
3	C	37	ALA
3	C	104	GLU
3	C	137	PRO
3	C	184	GLY
3	C	190	ALA
3	C	192	GLY
3	C	227	VAL
3	C	285	ILE
4	D	218	VAL
4	D	264	LYS
5	E	49	PRO
6	F	17	VAL
7	H	21	ALA
10	K	7	ALA
10	K	8	ILE
11	L	8	GLN
11	L	9	PRO
13	O	76	THR
13	O	77	SER
13	O	101	ILE
13	O	130	GLN
13	O	245	PRO
15	U	40	VAL
15	U	52	GLY
15	U	72	TYR
16	V	38	ALA
17	X	14	PRO
1	a	2090	GLY
1	a	2141	PRO
1	a	2228	THR
2	b	2088	PRO
2	b	2126	PRO
2	b	2173	GLY

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Mol	Chain	Res	Type
2	b	2235	GLU
2	b	2326	ARG
2	b	2391	SER
3	c	2037	ALA
3	c	2104	GLU
3	c	2184	GLY
3	c	2190	ALA
3	c	2191	PRO
3	c	2192	GLY
3	c	2285	ILE
4	d	2218	VAL
4	d	2264	LYS
5	e	2049	PRO
6	f	2017	VAL
7	h	2021	ALA
10	k	2007	ALA
10	k	2008	ILE
11	l	2009	PRO
13	o	2076	THR
13	o	2077	SER
13	o	2130	GLN
13	o	2245	PRO
15	u	2040	VAL
15	u	2051	TYR
15	u	2052	GLY
15	u	2072	TYR
16	v	2038	ALA
17	x	2014	PRO
1	A	32	TRP
1	A	141	PRO
1	A	160	ILE
1	A	225	ARG
1	A	239	PHE
1	A	243	GLU
1	A	317	TRP
1	A	335	ASN
2	B	186	GLY
2	B	201	HIS
2	B	230	ARG
2	B	328	GLY
2	B	396	GLY
3	C	43	ILE

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Mol	Chain	Res	Type
3	C	183	GLY
3	C	219	GLY
3	C	295	THR
3	C	453	ALA
4	D	109	GLY
4	D	156	VAL
4	D	219	GLU
4	D	292	ASN
5	E	10	SER
6	F	40	GLN
7	H	23	GLY
10	K	11	PRO
10	K	17	PRO
13	O	56	PRO
13	O	131	PRO
13	O	206	GLY
13	O	216	GLU
14	T	4	ILE
15	U	48	GLY
15	U	51	TYR
15	U	63	ALA
15	U	73	PRO
15	U	120	ALA
15	U	121	LEU
15	U	125	GLY
15	U	131	GLY
16	V	82	TYR
19	Z	32	ASP
1	a	2032	TRP
1	a	2160	ILE
1	a	2225	ARG
1	a	2239	PHE
1	a	2242	GLU
1	a	2243	GLU
1	a	2308	ASP
2	b	2186	GLY
2	b	2201	HIS
2	b	2230	ARG
2	b	2328	GLY
2	b	2396	GLY
3	c	2137	PRO
3	c	2183	GLY

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Mol	Chain	Res	Type
3	c	2219	GLY
3	c	2227	VAL
3	c	2295	THR
3	c	2453	ALA
4	d	2109	GLY
4	d	2219	GLU
4	d	2292	ASN
4	d	2299	ILE
5	e	2010	SER
6	f	2040	GLN
7	h	2023	GLY
10	k	2011	PRO
11	l	2008	GLN
13	o	2056	PRO
13	o	2078	LEU
13	o	2101	ILE
13	o	2161	GLY
13	o	2206	GLY
14	t	2004	ILE
15	u	2048	GLY
15	u	2063	ALA
15	u	2073	PRO
15	u	2120	ALA
15	u	2121	LEU
15	u	2131	GLY
16	v	2082	TYR
1	A	215	HIS
2	B	187	PRO
2	B	222	PRO
2	B	223	GLN
2	B	312	TYR
2	B	319	PRO
2	B	361	ALA
3	C	80	PRO
3	C	110	PRO
3	C	191	PRO
3	C	223	TRP
3	C	334	PRO
3	C	355	THR
3	C	415	ASN
3	C	454	GLY
4	D	260	ALA

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Mol	Chain	Res	Type
4	D	299	ILE
7	H	22	PRO
9	J	28	PHE
13	O	28	GLY
13	O	78	LEU
13	O	149	PRO
13	O	161	GLY
16	V	16	GLY
16	V	99	ASP
1	a	2191	ASN
1	a	2259	ILE
1	a	2317	TRP
2	b	2187	PRO
2	b	2222	PRO
2	b	2223	GLN
2	b	2319	PRO
2	b	2361	ALA
3	c	2110	PRO
3	c	2152	LYS
3	c	2223	TRP
3	c	2355	THR
3	c	2413	GLU
3	c	2415	ASN
4	d	2239	GLN
4	d	2260	ALA
4	d	2343	GLU
6	f	2019	TRP
7	h	2022	PRO
9	j	2028	PHE
10	k	2017	PRO
13	o	2131	PRO
13	o	2149	PRO
13	o	2180	GLU
13	o	2216	GLU
15	u	2125	GLY
16	v	2016	GLY
19	z	2032	ASP
1	A	167	SER
1	A	191	ASN
1	A	208	GLY
1	A	259	ILE
1	A	300	PHE

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Mol	Chain	Res	Type
1	A	301	ASN
1	A	334	ARG
3	C	46	SER
3	C	85	GLY
3	C	152	LYS
3	C	195	ASP
3	C	298	PRO
3	C	420	VAL
4	D	132	ILE
4	D	166	SER
4	D	239	GLN
4	D	343	GLU
13	O	114	GLU
14	T	27	PRO
16	V	133	GLY
19	Z	29	SER
1	a	2167	SER
1	a	2208	GLY
1	a	2215	HIS
1	a	2300	PHE
1	a	2301	ASN
2	b	2188	ASP
2	b	2312	TYR
3	c	2043	ILE
3	c	2334	PRO
3	c	2411	ALA
3	c	2420	VAL
4	d	2166	SER
13	o	2047	PRO
13	o	2114	GLU
14	t	2027	PRO
16	v	2021	LEU
16	v	2102	PRO
16	v	2131	GLY
2	B	188	ASP
3	C	413	GLU
4	D	131	GLU
6	F	19	TRP
8	I	32	PRO
10	K	16	LEU
13	O	47	PRO
13	O	180	GLU

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Mol	Chain	Res	Type
16	V	102	PRO
16	V	107	LEU
16	V	131	GLY
1	a	2116	ILE
1	a	2244	GLU
2	b	2047	PRO
3	c	2046	SER
3	c	2080	PRO
3	c	2454	GLY
4	d	2101	PHE
5	e	2057	GLN
10	k	2016	LEU
12	m	2005	GLN
13	o	2028	GLY
16	v	2133	GLY
19	z	2029	SER
1	A	116	ILE
2	B	47	PRO
3	C	380	ILE
11	L	2	GLU
14	T	3	THR
3	c	2085	GLY
3	c	2195	ASP
3	c	2298	PRO
3	c	2338	GLY
4	d	2113	PHE
4	d	2132	ILE
11	l	2002	GLU
12	m	2017	VAL
13	o	2175	PRO
1	A	63	ILE
2	B	16	PRO
3	C	101	PRO
3	C	117	VAL
13	O	159	PRO
13	O	244	GLU
1	a	2046	ILE
1	a	2063	ILE
2	b	2264	PRO
13	o	2159	PRO
2	B	211	ILE
2	B	322	GLY

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Mol	Chain	Res	Type
3	C	338	GLY
13	O	122	VAL
2	b	2016	PRO
2	b	2211	ILE
2	b	2322	GLY
13	o	2122	VAL
10	K	2	LEU
11	L	4	ASN
2	b	2008	VAL
9	j	2016	VAL
2	B	8	VAL
3	C	410	VAL
4	D	275	PRO
12	M	17	VAL
3	c	2380	ILE
4	d	2156	VAL
8	i	2008	VAL
8	i	2032	PRO
10	k	2002	LEU
13	o	2244	GLU
13	O	175	PRO
4	d	2095	PRO
4	d	2275	PRO
19	z	2013	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	247 (92%)	23 (8%)	10	34
1	a	270/280 (96%)	246 (91%)	24 (9%)	9	32
2	B	377/407 (93%)	357 (95%)	20 (5%)	20	47
2	b	377/407 (93%)	356 (94%)	21 (6%)	19	46
3	C	326/374 (87%)	306 (94%)	20 (6%)	17	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	326/374 (87%)	304 (93%)	22 (7%)	15	41
4	D	275/283 (97%)	256 (93%)	19 (7%)	14	39
4	d	275/283 (97%)	253 (92%)	22 (8%)	11	35
5	E	68/73 (93%)	65 (96%)	3 (4%)	25	51
5	e	68/73 (93%)	64 (94%)	4 (6%)	18	44
6	F	27/39 (69%)	25 (93%)	2 (7%)	13	37
6	f	27/39 (69%)	26 (96%)	1 (4%)	30	56
7	H	44/55 (80%)	42 (96%)	2 (4%)	24	50
7	h	44/55 (80%)	40 (91%)	4 (9%)	9	32
8	I	35/35 (100%)	31 (89%)	4 (11%)	5	24
8	i	35/35 (100%)	32 (91%)	3 (9%)	10	33
9	J	26/28 (93%)	25 (96%)	1 (4%)	29	55
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	28
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	41
11	L	35/35 (100%)	31 (89%)	4 (11%)	5	24
11	l	35/35 (100%)	31 (89%)	4 (11%)	5	24
12	M	27/33 (82%)	24 (89%)	3 (11%)	6	25
12	m	27/33 (82%)	26 (96%)	1 (4%)	30	56
13	O	208/208 (100%)	185 (89%)	23 (11%)	6	25
13	o	208/208 (100%)	190 (91%)	18 (9%)	9	33
14	T	28/29 (97%)	27 (96%)	1 (4%)	31	57
14	t	28/29 (97%)	26 (93%)	2 (7%)	13	38
15	U	89/112 (80%)	85 (96%)	4 (4%)	24	50
15	u	89/112 (80%)	85 (96%)	4 (4%)	24	50
16	V	117/117 (100%)	111 (95%)	6 (5%)	21	48
16	v	117/117 (100%)	112 (96%)	5 (4%)	26	51
17	X	33/42 (79%)	30 (91%)	3 (9%)	9	32
17	x	33/42 (79%)	29 (88%)	4 (12%)	5	22
19	Z	48/52 (92%)	43 (90%)	5 (10%)	7	27
19	z	48/52 (92%)	45 (94%)	3 (6%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4126/4464 (92%)	3836 (93%)	290 (7%)	14	39

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	25	ASP
1	A	27	ARG
1	A	29	TYR
1	A	70	SER
1	A	84	PRO
1	A	162	PRO
1	A	172	MET
1	A	177	SER
1	A	180	PHE
1	A	183	MET
1	A	187	GLN
1	A	212	CYS
1	A	214	MET
1	A	226	GLU
1	A	237	TYR
1	A	284	TRP
1	A	295	PHE
1	A	298	ASN
1	A	301	ASN
1	A	325	ASN
1	A	335	ASN
1	A	342	ASP
2	B	8	VAL
2	B	48	SER
2	B	57	ARG
2	B	62	VAL
2	B	94	GLU
2	B	120	LEU
2	B	130	GLU
2	B	167	TRP
2	B	216	HIS
2	B	246	PHE
2	B	255	THR
2	B	286	ARG
2	B	318	ASN
2	B	334	ASP

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Mol	Chain	Res	Type
2	B	372	ASP
2	B	376	VAL
2	B	385	ARG
2	B	402	TYR
2	B	409	GLN
2	B	479	PHE
3	C	61	VAL
3	C	110	PRO
3	C	139	THR
3	C	198	VAL
3	C	201	ASN
3	C	264	PHE
3	C	285	ILE
3	C	290	VAL
3	C	292	PHE
3	C	293	ASN
3	C	294	ASN
3	C	295	THR
3	C	308	GLU
3	C	313	GLN
3	C	321	ASP
3	C	340	TYR
3	C	368	PRO
3	C	400	PRO
3	C	443	TRP
3	C	456	GLU
4	D	32	TRP
4	D	61	HIS
4	D	73	PHE
4	D	91	LEU
4	D	131	GLU
4	D	168	PHE
4	D	188	PHE
4	D	192	THR
4	D	209	LEU
4	D	211	CYS
4	D	217	THR
4	D	220	ASN
4	D	243	THR
4	D	254	SER
4	D	262	SER
4	D	267	LEU

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Mol	Chain	Res	Type
4	D	293	LEU
4	D	336	HIS
4	D	340	VAL
5	E	16	VAL
5	E	29	LEU
5	E	49	PRO
6	F	12	TYR
6	F	39	MET
7	H	26	THR
7	H	57	VAL
8	I	3	THR
8	I	16	VAL
8	I	18	LEU
8	I	30	ARG
9	J	38	SER
10	K	6	TYR
10	K	26	LEU
10	K	36	PHE
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
11	L	36	PHE
12	M	3	VAL
12	M	20	VAL
12	M	28	GLN
13	O	3	GLN
13	O	21	THR
13	O	34	SER
13	O	39	ARG
13	O	46	GLN
13	O	47	PRO
13	O	65	PHE
13	O	68	THR
13	O	94	THR
13	O	104	GLN
13	O	110	MET
13	O	126	VAL
13	O	136	ILE
13	O	147	ASN
13	O	148	VAL
13	O	162	ARG
13	O	166	SER

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Mol	Chain	Res	Type
13	O	174	LEU
13	O	193	THR
13	O	201	VAL
13	O	219	GLN
13	O	225	MET
13	O	245	PRO
14	T	4	ILE
15	U	51	TYR
15	U	59	ASN
15	U	61	ASN
15	U	132	LEU
16	V	4	THR
16	V	14	SER
16	V	40	CYS
16	V	58	THR
16	V	78	ASN
16	V	130	TRP
17	X	13	THR
17	X	14	PRO
17	X	47	GLN
19	Z	37	LYS
19	Z	39	LEU
19	Z	41	PHE
19	Z	42	LEU
19	Z	51	VAL
1	a	2015	GLU
1	a	2024	THR
1	a	2025	ASP
1	a	2027	ARG
1	a	2028	LEU
1	a	2029	TYR
1	a	2040	THR
1	a	2045	THR
1	a	2063	ILE
1	a	2070	SER
1	a	2084	PRO
1	a	2111	PRO
1	a	2172	MET
1	a	2180	PHE
1	a	2187	GLN
1	a	2237	TYR
1	a	2278	TRP

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Mol	Chain	Res	Type
1	a	2284	TRP
1	a	2286	THR
1	a	2295	PHE
1	a	2302	PHE
1	a	2331	MET
1	a	2335	ASN
1	a	2342	ASP
2	b	2008	VAL
2	b	2048	SER
2	b	2057	ARG
2	b	2062	VAL
2	b	2094	GLU
2	b	2112	CYS
2	b	2120	LEU
2	b	2130	GLU
2	b	2167	TRP
2	b	2216	HIS
2	b	2246	PHE
2	b	2255	THR
2	b	2286	ARG
2	b	2318	ASN
2	b	2334	ASP
2	b	2372	ASP
2	b	2376	VAL
2	b	2385	ARG
2	b	2402	TYR
2	b	2409	GLN
2	b	2479	PHE
3	c	2046	SER
3	c	2090	PRO
3	c	2105	VAL
3	c	2110	PRO
3	c	2139	THR
3	c	2198	VAL
3	c	2201	ASN
3	c	2264	PHE
3	c	2285	ILE
3	c	2292	PHE
3	c	2293	ASN
3	c	2294	ASN
3	c	2296	VAL
3	c	2301	PHE

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Mol	Chain	Res	Type
3	c	2304	PRO
3	c	2310	SER
3	c	2313	GLN
3	c	2321	ASP
3	c	2340	TYR
3	c	2403	SER
3	c	2443	TRP
3	c	2456	GLU
4	d	2032	TRP
4	d	2058	TRP
4	d	2061	HIS
4	d	2081	PRO
4	d	2087	HIS
4	d	2088	SER
4	d	2091	LEU
4	d	2147	SER
4	d	2165	SER
4	d	2168	PHE
4	d	2178	ILE
4	d	2188	PHE
4	d	2192	THR
4	d	2211	CYS
4	d	2220	ASN
4	d	2254	SER
4	d	2262	SER
4	d	2267	LEU
4	d	2279	LEU
4	d	2281	MET
4	d	2293	LEU
4	d	2336	HIS
5	e	2016	VAL
5	e	2049	PRO
5	e	2050	ARG
5	e	2053	SER
6	f	2043	GLN
7	h	2024	TRP
7	h	2026	THR
7	h	2051	THR
7	h	2057	VAL
8	i	2016	VAL
8	i	2027	ASP
8	i	2030	ARG

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Mol	Chain	Res	Type
10	k	2008	ILE
10	k	2026	LEU
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
11	l	2036	PHE
12	m	2028	GLN
13	o	2005	LEU
13	o	2006	THR
13	o	2021	THR
13	o	2037	THR
13	o	2039	ARG
13	o	2047	PRO
13	o	2068	THR
13	o	2075	THR
13	o	2104	GLN
13	o	2110	MET
13	o	2126	VAL
13	o	2147	ASN
13	o	2159	PRO
13	o	2166	SER
13	o	2174	LEU
13	o	2193	THR
13	o	2225	MET
13	o	2245	PRO
14	t	2005	THR
14	t	2021	ILE
15	u	2051	TYR
15	u	2059	ASN
15	u	2061	ASN
15	u	2132	LEU
16	v	2004	THR
16	v	2050	PRO
16	v	2055	ARG
16	v	2078	ASN
16	v	2093	PRO
17	x	2011	THR
17	x	2013	THR
17	x	2014	PRO
17	x	2047	GLN
19	z	2013	VAL
19	z	2039	LEU

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Mol	Chain	Res	Type
19	z	2051	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	92	HIS
1	A	165	GLN
1	A	187	GLN
1	A	191	ASN
1	A	199	GLN
1	A	234	ASN
1	A	247	ASN
1	A	301	ASN
1	A	303	ASN
1	A	312	ASN
1	A	322	ASN
1	A	325	ASN
2	B	157	HIS
2	B	233	ASN
2	B	285	ASN
2	B	318	ASN
2	B	331	ASN
2	B	374	ASN
2	B	409	GLN
2	B	438	ASN
3	C	39	ASN
3	C	201	ASN
3	C	294	ASN
3	C	311	GLN
3	C	327	ASN
4	D	83	ASN
4	D	87	HIS
4	D	106	GLN
4	D	117	HIS
4	D	129	GLN
4	D	142	ASN
4	D	164	GLN
4	D	186	GLN
4	D	255	GLN
4	D	263	ASN
4	D	322	ASN

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Mol	Chain	Res	Type
4	D	338	ASN
4	D	350	ASN
5	E	81	GLN
6	F	43	GLN
7	H	58	ASN
10	K	31	GLN
11	L	4	ASN
11	L	6	ASN
11	L	8	GLN
12	M	4	ASN
12	M	28	GLN
13	O	36	GLN
13	O	46	GLN
13	O	61	GLN
13	O	124	ASN
13	O	132	ASN
13	O	147	ASN
13	O	155	ASN
13	O	200	ASN
13	O	219	GLN
13	O	236	GLN
15	U	59	ASN
15	U	61	ASN
15	U	130	ASN
16	V	25	GLN
19	Z	6	GLN
19	Z	31	GLN
1	a	2019	ASN
1	a	2092	HIS
1	a	2165	GLN
1	a	2199	GLN
1	a	2296	ASN
1	a	2298	ASN
1	a	2303	ASN
1	a	2322	ASN
1	a	2325	ASN
1	a	2335	ASN
2	b	2157	HIS
2	b	2285	ASN
2	b	2318	ASN
2	b	2331	ASN
2	b	2343	HIS

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Mol	Chain	Res	Type
2	b	2374	ASN
2	b	2409	GLN
2	b	2438	ASN
3	c	2039	ASN
3	c	2074	HIS
3	c	2201	ASN
3	c	2294	ASN
3	c	2322	GLN
3	c	2405	ASN
4	d	2087	HIS
4	d	2129	GLN
4	d	2142	ASN
4	d	2186	GLN
4	d	2190	ASN
4	d	2250	ASN
4	d	2263	ASN
4	d	2322	ASN
4	d	2338	ASN
4	d	2350	ASN
6	f	2040	GLN
6	f	2043	GLN
11	l	2004	ASN
11	l	2006	ASN
11	l	2008	GLN
12	m	2004	ASN
12	m	2028	GLN
13	o	2017	ASN
13	o	2046	GLN
13	o	2124	ASN
13	o	2147	ASN
13	o	2155	ASN
13	o	2236	GLN
15	u	2059	ASN
15	u	2061	ASN
15	u	2130	ASN
16	v	2078	ASN
19	z	2031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 2 are monoatomic - leaving 106 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	CLA	A	350	-	69,73,73	1.33	5 (7%)	82,113,113	1.78	12 (14%)
21	BCT	a	2346	22	3,3,3	1.80	1 (33%)	2,3,3	1.34	0
26	LMT	B	526	-	36,36,36	1.35	4 (11%)	47,47,47	1.93	8 (17%)
23	CLA	b	2521	2	69,73,73	1.38	9 (13%)	82,113,113	1.67	8 (9%)
27	BCR	C	489	-	41,41,41	1.78	7 (17%)	56,56,56	2.00	16 (28%)
23	CLA	B	527	-	69,73,73	1.54	12 (17%)	82,113,113	1.96	12 (14%)
23	CLA	D	356	4	69,73,73	1.35	13 (18%)	82,113,113	1.93	10 (12%)
23	CLA	c	2479	3	69,73,73	1.34	8 (11%)	82,113,113	2.17	17 (20%)
24	PHO	d	2356	-	58,69,69	1.65	9 (15%)	55,99,99	2.29	17 (30%)
24	PHO	a	2350	-	58,69,69	1.80	10 (17%)	55,99,99	2.07	16 (29%)
27	BCR	K	50	-	41,41,41	1.97	14 (34%)	56,56,56	1.95	17 (30%)
23	CLA	C	483	3	69,73,73	1.39	11 (15%)	82,113,113	2.11	13 (15%)
23	CLA	B	523	2	69,73,73	1.31	7 (10%)	82,113,113	2.05	11 (13%)
27	BCR	c	2488	-	41,41,41	2.00	9 (21%)	56,56,56	2.01	19 (33%)
23	CLA	d	2355	-	69,73,73	1.27	7 (10%)	82,113,113	2.11	13 (15%)
23	CLA	b	2522	2	69,73,73	1.31	9 (13%)	82,113,113	1.90	12 (14%)
27	BCR	b	2527	-	41,41,41	1.92	7 (17%)	56,56,56	2.24	20 (35%)
23	CLA	c	2477	3	69,73,73	1.46	8 (11%)	82,113,113	2.15	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	486	3	69,73,73	1.39	8 (11%)	82,113,113	1.90	13 (15%)
23	CLA	C	477	3	69,73,73	1.47	10 (14%)	82,113,113	2.16	14 (17%)
23	CLA	B	518	2	69,73,73	1.31	5 (7%)	82,113,113	2.02	12 (14%)
23	CLA	C	480	3	69,73,73	1.26	6 (8%)	82,113,113	1.85	10 (12%)
23	CLA	D	354	4	69,73,73	1.38	9 (13%)	82,113,113	1.94	11 (13%)
23	CLA	A	348	1	69,73,73	1.34	9 (13%)	82,113,113	1.84	14 (17%)
23	CLA	b	2516	2	69,73,73	1.63	13 (18%)	82,113,113	1.94	13 (15%)
23	CLA	b	2517	2	69,73,73	1.28	9 (13%)	82,113,113	1.92	11 (13%)
27	BCR	d	2360	-	41,41,41	2.00	7 (17%)	56,56,56	2.50	21 (37%)
23	CLA	c	2482	3	69,73,73	1.45	10 (14%)	82,113,113	1.90	11 (13%)
23	CLA	B	524	-	69,73,73	1.28	8 (11%)	82,113,113	2.11	11 (13%)
28	HEC	v	2138	16	50,50,50	2.85	26 (52%)	68,82,82	2.38	26 (38%)
23	CLA	C	481	3	69,73,73	1.26	7 (10%)	82,113,113	2.11	10 (12%)
27	BCR	b	2528	-	41,41,41	2.09	10 (24%)	56,56,56	2.25	22 (39%)
23	CLA	B	514	-	69,73,73	1.45	10 (14%)	82,113,113	1.96	13 (15%)
23	CLA	B	519	2	69,73,73	1.55	13 (18%)	82,113,113	2.36	13 (15%)
23	CLA	b	2520	2	69,73,73	1.46	11 (15%)	82,113,113	2.41	13 (15%)
26	LMT	d	2359	-	36,36,36	1.36	4 (11%)	47,47,47	1.93	7 (14%)
23	CLA	b	2519	2	69,73,73	1.49	12 (17%)	82,113,113	2.27	11 (13%)
27	BCR	j	2053	-	41,41,41	2.19	8 (19%)	56,56,56	2.15	21 (37%)
23	CLA	C	487	-	69,73,73	1.58	12 (17%)	82,113,113	1.90	14 (17%)
23	CLA	B	513	2	69,73,73	1.41	10 (14%)	82,113,113	2.23	15 (18%)
23	CLA	A	349	-	69,73,73	1.30	7 (10%)	82,113,113	2.19	13 (15%)
23	CLA	c	2474	3	69,73,73	1.27	8 (11%)	82,113,113	1.97	10 (12%)
23	CLA	a	2349	-	69,73,73	1.31	5 (7%)	82,113,113	1.74	12 (14%)
27	BCR	B	528	-	41,41,41	2.03	7 (17%)	56,56,56	2.23	21 (37%)
23	CLA	C	485	-	69,73,73	1.29	8 (11%)	82,113,113	1.87	13 (15%)
23	CLA	b	2512	2	69,73,73	1.30	9 (13%)	82,113,113	2.04	11 (13%)
23	CLA	B	516	2	69,73,73	1.59	11 (15%)	82,113,113	1.94	13 (15%)
23	CLA	C	482	3	69,73,73	1.43	9 (13%)	82,113,113	1.98	10 (12%)
27	BCR	C	488	-	41,41,41	1.82	9 (21%)	56,56,56	2.02	18 (32%)
23	CLA	c	2475	-	69,73,73	1.60	12 (17%)	82,113,113	1.89	9 (10%)
25	PL9	A	353	-	45,45,55	2.32	19 (42%)	56,57,69	2.18	17 (30%)
23	CLA	B	520	2	69,73,73	1.44	10 (14%)	82,113,113	2.38	12 (14%)
23	CLA	c	2485	-	69,73,73	1.36	8 (11%)	82,113,113	1.91	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	BCR	J	53	-	41,41,41	1.94	6 (14%)	56,56,56	2.14	21 (37%)
23	CLA	B	521	2	69,73,73	1.35	10 (14%)	82,113,113	1.68	10 (12%)
21	BCT	A	346	22	3,3,3	1.14	0	2,3,3	0.80	0
23	CLA	c	2483	3	69,73,73	1.38	9 (13%)	82,113,113	2.08	12 (14%)
23	CLA	B	525	2	69,73,73	1.35	9 (13%)	82,113,113	1.93	10 (12%)
23	CLA	c	2484	3	69,73,73	1.39	10 (14%)	82,113,113	1.89	11 (13%)
23	CLA	C	474	3	69,73,73	1.26	7 (10%)	82,113,113	2.01	13 (15%)
23	CLA	b	2515	2	69,73,73	1.36	10 (14%)	82,113,113	1.95	14 (17%)
23	CLA	b	2525	2	69,73,73	1.38	9 (13%)	82,113,113	1.97	10 (12%)
23	CLA	B	511	2	69,73,73	1.44	14 (20%)	82,113,113	2.15	14 (17%)
23	CLA	c	2480	3	69,73,73	1.27	6 (8%)	82,113,113	1.87	9 (10%)
21	BCT	D	353	20	3,3,3	2.10	1 (33%)	2,3,3	0.22	0
25	PL9	d	2358	-	45,45,55	2.37	19 (42%)	56,57,69	1.75	12 (21%)
23	CLA	a	2348	1	69,73,73	1.36	9 (13%)	82,113,113	1.81	13 (15%)
22	OEC	a	2347	1,3,21	0,13,13	-	-	-	-	-
23	CLA	c	2486	3	69,73,73	1.40	7 (10%)	82,113,113	1.94	15 (18%)
24	PHO	A	351	-	58,69,69	1.62	9 (15%)	55,99,99	2.03	15 (27%)
23	CLA	B	517	2	69,73,73	1.29	7 (10%)	82,113,113	1.96	11 (13%)
27	BCR	F	48	-	41,41,41	2.03	7 (17%)	56,56,56	2.55	22 (39%)
23	CLA	C	478	3	69,73,73	1.35	7 (10%)	82,113,113	2.01	13 (15%)
27	BCR	c	2489	-	41,41,41	1.97	8 (19%)	56,56,56	2.02	18 (32%)
23	CLA	b	2526	-	69,73,73	1.49	11 (15%)	82,113,113	1.98	13 (15%)
23	CLA	B	515	2	69,73,73	1.37	6 (8%)	82,113,113	1.94	15 (18%)
23	CLA	c	2476	3	69,73,73	1.38	11 (15%)	82,113,113	1.87	11 (13%)
22	OEC	A	347	1,3,21	0,13,13	-	-	-	-	-
23	CLA	B	522	2	69,73,73	1.31	8 (11%)	82,113,113	1.91	12 (14%)
23	CLA	C	484	3	69,73,73	1.48	13 (18%)	82,113,113	1.87	12 (14%)
23	CLA	b	2524	-	69,73,73	1.26	9 (13%)	82,113,113	2.11	12 (14%)
23	CLA	d	2354	4	69,73,73	1.37	8 (11%)	82,113,113	1.96	11 (13%)
23	CLA	b	2513	2	69,73,73	1.39	10 (14%)	82,113,113	2.23	16 (19%)
23	CLA	C	479	3	69,73,73	1.31	8 (11%)	82,113,113	2.12	17 (20%)
23	CLA	c	2481	3	69,73,73	1.28	9 (13%)	82,113,113	2.11	13 (15%)
23	CLA	c	2478	3	69,73,73	1.33	6 (8%)	82,113,113	2.03	14 (17%)
23	CLA	b	2518	2	69,73,73	1.37	10 (14%)	82,113,113	1.99	10 (12%)
28	HEC	e	2084	6,5	50,50,50	2.34	21 (42%)	68,82,82	1.32	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	2514	-	69,73,73	1.47	11 (15%)	82,113,113	1.97	13 (15%)
23	CLA	b	2511	2	69,73,73	1.44	12 (17%)	82,113,113	2.14	13 (15%)
27	BCR	k	2050	-	41,41,41	2.02	15 (36%)	56,56,56	1.92	17 (30%)
23	CLA	C	475	-	69,73,73	1.61	12 (17%)	82,113,113	1.96	11 (13%)
23	CLA	b	2523	2	69,73,73	1.34	10 (14%)	82,113,113	2.04	11 (13%)
28	HEC	E	84	6,5	50,50,50	2.27	15 (30%)	68,82,82	1.43	13 (19%)
23	CLA	a	2351	1	69,73,73	1.39	10 (14%)	82,113,113	1.93	12 (14%)
23	CLA	d	2357	4	69,73,73	1.39	9 (13%)	82,113,113	1.93	10 (12%)
25	PL9	a	2352	-	45,45,55	2.32	18 (40%)	56,57,69	2.21	17 (30%)
24	PHO	D	355	-	58,69,69	1.67	8 (13%)	55,99,99	2.30	18 (32%)
23	CLA	C	476	3	69,73,73	1.31	7 (10%)	82,113,113	1.92	12 (14%)
28	HEC	V	138	16	50,50,50	5.90	37 (74%)	68,82,82	2.46	27 (39%)
23	CLA	B	512	2	69,73,73	1.33	9 (13%)	82,113,113	1.98	8 (9%)
25	PL9	D	357	-	45,45,55	2.32	18 (40%)	56,57,69	1.75	12 (21%)
27	BCR	B	529	-	41,41,41	2.12	8 (19%)	56,56,56	2.32	21 (37%)
23	CLA	c	2487	-	69,73,73	1.59	11 (15%)	82,113,113	1.86	15 (18%)
23	CLA	A	352	1	69,73,73	1.36	10 (14%)	82,113,113	1.93	13 (15%)
21	BCT	d	2353	20	3,3,3	1.94	1 (33%)	2,3,3	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	350	-	-	7/39/115/115	-
26	LMT	B	526	-	-	8/21/61/61	0/2/2/2
23	CLA	b	2521	2	-	6/39/115/115	-
27	BCR	C	489	-	-	2/29/63/63	0/2/2/2
23	CLA	B	527	-	-	15/39/115/115	-
23	CLA	D	356	4	-	6/39/115/115	-
23	CLA	c	2479	3	-	11/39/115/115	-
24	PHO	d	2356	-	-	11/37/103/103	0/5/6/6
24	PHO	a	2350	-	-	9/37/103/103	0/5/6/6
27	BCR	K	50	-	-	3/29/63/63	0/2/2/2
23	CLA	C	483	3	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	523	2	-	10/39/115/115	-
27	BCR	c	2488	-	-	5/29/63/63	0/2/2/2
23	CLA	d	2355	-	-	14/39/115/115	-
23	CLA	b	2522	2	-	17/39/115/115	-
27	BCR	b	2527	-	-	5/29/63/63	0/2/2/2
23	CLA	c	2477	3	-	17/39/115/115	-
23	CLA	C	486	3	-	7/39/115/115	-
23	CLA	C	477	3	-	17/39/115/115	-
23	CLA	B	518	2	-	12/39/115/115	-
23	CLA	C	480	3	-	16/39/115/115	-
23	CLA	D	354	4	-	8/39/115/115	-
23	CLA	A	348	1	-	12/39/115/115	-
23	CLA	b	2516	2	-	6/39/115/115	-
23	CLA	b	2517	2	-	15/39/115/115	-
27	BCR	d	2360	-	-	4/29/63/63	0/2/2/2
23	CLA	c	2482	3	-	12/39/115/115	-
28	HEC	v	2138	16	1/1/3/7	6/14/54/54	-
23	CLA	B	524	-	-	15/39/115/115	-
23	CLA	C	481	3	-	9/39/115/115	-
27	BCR	b	2528	-	-	6/29/63/63	0/2/2/2
23	CLA	B	514	-	-	16/39/115/115	-
23	CLA	B	519	2	-	8/39/115/115	-
23	CLA	b	2520	2	-	7/39/115/115	-
26	LMT	d	2359	-	-	8/21/61/61	0/2/2/2
23	CLA	b	2519	2	-	8/39/115/115	-
27	BCR	j	2053	-	-	4/29/63/63	0/2/2/2
23	CLA	C	487	-	-	15/39/115/115	-
23	CLA	B	513	2	-	14/39/115/115	-
23	CLA	A	349	-	-	14/39/115/115	-
23	CLA	c	2474	3	-	13/39/115/115	-
23	CLA	a	2349	-	-	6/39/115/115	-
27	BCR	B	528	-	-	5/29/63/63	0/2/2/2
23	CLA	C	485	-	-	14/39/115/115	-
23	CLA	b	2512	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	516	2	-	6/39/115/115	-
23	CLA	C	482	3	-	11/39/115/115	-
27	BCR	C	488	-	-	6/29/63/63	0/2/2/2
23	CLA	c	2475	-	-	12/39/115/115	-
25	PL9	A	353	-	-	10/41/61/73	0/1/1/1
23	CLA	B	520	2	-	5/39/115/115	-
23	CLA	c	2485	-	-	14/39/115/115	-
27	BCR	J	53	-	-	4/29/63/63	0/2/2/2
23	CLA	B	521	2	-	6/39/115/115	-
23	CLA	c	2483	3	-	12/39/115/115	-
23	CLA	B	525	2	-	14/39/115/115	-
23	CLA	c	2484	3	-	17/39/115/115	-
23	CLA	C	474	3	-	13/39/115/115	-
23	CLA	b	2515	2	-	17/39/115/115	-
23	CLA	b	2525	2	-	13/39/115/115	-
23	CLA	B	511	2	-	16/39/115/115	-
23	CLA	c	2480	3	-	16/39/115/115	-
25	PL9	d	2358	-	-	12/41/61/73	0/1/1/1
23	CLA	a	2348	1	-	12/39/115/115	-
22	OEC	a	2347	1,3,21	-	-	0/6/5/5
23	CLA	c	2486	3	-	7/39/115/115	-
24	PHO	A	351	-	-	9/37/103/103	0/5/6/6
23	CLA	B	517	2	-	15/39/115/115	-
27	BCR	F	48	-	-	3/29/63/63	0/2/2/2
23	CLA	C	478	3	-	14/39/115/115	-
27	BCR	c	2489	-	-	2/29/63/63	0/2/2/2
23	CLA	b	2526	-	-	15/39/115/115	-
23	CLA	B	515	2	-	17/39/115/115	-
23	CLA	c	2476	3	-	12/39/115/115	-
22	OEC	A	347	1,3,21	-	-	0/6/5/5
23	CLA	B	522	2	-	16/39/115/115	-
23	CLA	C	484	3	-	16/39/115/115	-
23	CLA	b	2524	-	-	15/39/115/115	-
23	CLA	d	2354	4	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	2513	2	-	13/39/115/115	-
23	CLA	C	479	3	-	11/39/115/115	-
23	CLA	c	2481	3	-	8/39/115/115	-
23	CLA	c	2478	3	-	14/39/115/115	-
23	CLA	b	2518	2	-	12/39/115/115	-
28	HEC	e	2084	6,5	1/1/3/7	2/14/54/54	-
23	CLA	b	2514	-	-	16/39/115/115	-
23	CLA	b	2511	2	-	16/39/115/115	-
27	BCR	k	2050	-	-	3/29/63/63	0/2/2/2
23	CLA	C	475	-	-	11/39/115/115	-
23	CLA	b	2523	2	-	10/39/115/115	-
28	HEC	E	84	6,5	1/1/3/7	2/14/54/54	-
23	CLA	a	2351	1	-	9/39/115/115	-
23	CLA	d	2357	4	-	6/39/115/115	-
25	PL9	a	2352	-	-	10/41/61/73	0/1/1/1
24	PHO	D	355	-	-	13/37/103/103	0/5/6/6
23	CLA	C	476	3	-	12/39/115/115	-
28	HEC	V	138	16	1/1/3/7	4/14/54/54	-
23	CLA	B	512	2	-	10/39/115/115	-
25	PL9	D	357	-	-	12/41/61/73	0/1/1/1
27	BCR	B	529	-	-	6/29/63/63	0/2/2/2
23	CLA	c	2487	-	-	14/39/115/115	-
23	CLA	A	352	1	-	9/39/115/115	-

All (1004) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	V	138	HEC	CMC-C2C	12.23	1.75	1.50
28	V	138	HEC	CMB-C2B	11.74	1.74	1.50
28	V	138	HEC	C1D-ND	10.84	1.58	1.40
28	V	138	HEC	CHA-C1A	10.42	1.58	1.38
28	V	138	HEC	C4B-NB	10.23	1.57	1.40
28	V	138	HEC	C4A-NA	9.59	1.57	1.39
28	V	138	HEC	C4B-C3B	9.42	1.61	1.45
28	V	138	HEC	C1B-NB	9.20	1.56	1.38
28	V	138	HEC	CMD-C2D	8.75	1.68	1.50
28	V	138	HEC	C1A-NA	8.63	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	V	138	HEC	C2A-C3A	8.29	1.54	1.36
28	V	138	HEC	C3B-C2B	8.27	1.54	1.36
27	j	2053	BCR	C30-C25	8.18	1.64	1.53
28	V	138	HEC	C1C-NC	7.92	1.54	1.39
24	a	2350	PHO	C3B-C4B	7.84	1.49	1.41
28	V	138	HEC	CMA-C3A	7.58	1.66	1.50
27	F	48	BCR	C30-C25	7.53	1.63	1.53
28	v	2138	HEC	CMC-C2C	7.37	1.65	1.50
27	J	53	BCR	C30-C25	6.96	1.62	1.53
28	v	2138	HEC	CMB-C2B	6.91	1.64	1.50
24	D	355	PHO	C3B-C4B	6.77	1.48	1.41
27	B	529	BCR	C30-C25	6.59	1.62	1.53
23	c	2487	CLA	MG-NA	6.54	2.21	2.06
27	B	528	BCR	C30-C25	6.53	1.62	1.53
24	A	351	PHO	C3B-C4B	6.52	1.48	1.41
28	v	2138	HEC	CMD-C2D	6.44	1.64	1.50
27	b	2528	BCR	C30-C25	6.41	1.62	1.53
27	d	2360	BCR	C30-C25	6.36	1.61	1.53
28	V	138	HEC	C4D-ND	6.33	1.51	1.38
28	V	138	HEC	C3D-C2D	6.23	1.50	1.36
23	C	487	CLA	MG-NA	6.16	2.20	2.06
27	C	489	BCR	C30-C25	6.07	1.61	1.53
27	c	2489	BCR	C30-C25	6.04	1.61	1.53
28	e	2084	HEC	CMB-C2B	6.00	1.63	1.50
24	a	2350	PHO	C1B-C2B	5.98	1.46	1.39
23	C	486	CLA	MG-NA	5.76	2.19	2.06
25	D	357	PL9	C31-C29	5.75	1.63	1.51
28	E	84	HEC	CMB-C2B	5.74	1.62	1.50
28	V	138	HEC	CHA-C4D	-5.63	1.26	1.39
23	D	354	CLA	MG-NA	5.63	2.19	2.06
24	D	355	PHO	C1B-C2B	5.61	1.45	1.39
28	V	138	HEC	CHD-C4C	5.60	1.52	1.39
23	b	2526	CLA	MG-NA	5.54	2.19	2.06
23	B	527	CLA	MG-NA	5.52	2.19	2.06
28	v	2138	HEC	CHA-C1A	5.48	1.49	1.38
23	d	2354	CLA	MG-NA	5.47	2.19	2.06
27	c	2488	BCR	C1-C6	5.43	1.60	1.53
24	d	2356	PHO	C1B-C2B	5.36	1.45	1.39
28	E	84	HEC	CMA-C3A	5.34	1.61	1.50
25	d	2358	PL9	C53-C6	-5.33	1.39	1.50
24	d	2356	PHO	C3B-C4B	5.30	1.46	1.41
27	b	2527	BCR	C30-C25	5.28	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2348	CLA	MG-NA	5.25	2.18	2.06
27	B	529	BCR	C26-C25	5.23	1.43	1.34
23	c	2486	CLA	MG-NA	5.22	2.18	2.06
25	D	357	PL9	C53-C6	-5.20	1.40	1.50
25	d	2358	PL9	C52-C5	-5.20	1.40	1.50
28	V	138	HEC	C4C-NC	5.18	1.49	1.39
28	V	138	HEC	C3C-C2C	5.16	1.52	1.38
28	V	138	HEC	C4D-C3D	5.13	1.53	1.45
28	V	138	HEC	FE-NA	5.08	2.11	1.95
27	c	2489	BCR	C1-C6	5.07	1.60	1.53
23	c	2476	CLA	MG-NA	5.03	2.18	2.06
27	j	2053	BCR	C26-C25	5.00	1.42	1.34
23	B	513	CLA	CAA-C2A	5.00	1.63	1.54
23	C	482	CLA	MG-NA	4.99	2.18	2.06
23	c	2482	CLA	MG-NA	4.99	2.18	2.06
25	a	2352	PL9	C53-C6	-4.98	1.40	1.50
27	b	2527	BCR	C5-C6	4.97	1.42	1.34
28	e	2084	HEC	CMD-C2D	4.96	1.60	1.50
25	d	2358	PL9	C31-C29	4.93	1.61	1.51
23	B	516	CLA	MG-NA	4.93	2.18	2.06
23	c	2477	CLA	MG-NA	4.93	2.18	2.06
24	A	351	PHO	C1B-C2B	4.92	1.45	1.39
27	j	2053	BCR	C5-C6	4.91	1.42	1.34
23	C	477	CLA	MG-NA	4.86	2.17	2.06
25	A	353	PL9	C52-C5	-4.84	1.40	1.50
28	V	138	HEC	O2D-CGD	-4.81	1.14	1.30
27	B	528	BCR	C26-C25	4.81	1.42	1.34
23	b	2521	CLA	MG-NA	4.77	2.17	2.06
25	a	2352	PL9	C7-C3	4.76	1.57	1.51
27	c	2488	BCR	C30-C25	4.76	1.59	1.53
28	V	138	HEC	O1A-CGA	4.75	1.37	1.22
25	A	353	PL9	C53-C6	-4.72	1.41	1.50
28	v	2138	HEC	C1A-NA	4.71	1.48	1.39
28	E	84	HEC	CMC-C2C	4.70	1.60	1.50
23	C	484	CLA	MG-NA	4.70	2.17	2.06
27	F	48	BCR	C1-C6	4.68	1.59	1.53
27	b	2528	BCR	C2-C1	4.66	1.64	1.54
23	a	2349	CLA	MG-NA	4.66	2.17	2.06
23	C	481	CLA	MG-NA	4.65	2.17	2.06
28	E	84	HEC	CMD-C2D	4.63	1.60	1.50
25	a	2352	PL9	C22-C23	-4.61	1.36	1.50
23	A	348	CLA	MG-NA	4.60	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	2528	BCR	C26-C25	4.59	1.42	1.34
23	A	350	CLA	MG-NA	4.58	2.17	2.06
27	B	528	BCR	C5-C6	4.56	1.42	1.34
23	C	480	CLA	MG-NA	4.56	2.17	2.06
24	d	2356	PHO	C3A-C2A	-4.54	1.50	1.54
23	c	2487	CLA	MG-NC	4.53	2.17	2.06
23	c	2481	CLA	MG-NA	4.53	2.17	2.06
23	b	2522	CLA	MG-NA	4.51	2.17	2.06
25	a	2352	PL9	C52-C5	-4.51	1.41	1.50
23	c	2484	CLA	MG-NA	4.50	2.17	2.06
23	b	2513	CLA	CAA-C2A	4.50	1.62	1.54
25	A	353	PL9	C22-C23	-4.49	1.36	1.50
23	B	520	CLA	CAA-CBA	-4.48	1.39	1.52
23	b	2516	CLA	MG-NA	4.48	2.16	2.06
25	D	357	PL9	C52-C5	-4.47	1.41	1.50
23	B	515	CLA	MG-NA	4.47	2.16	2.06
23	B	522	CLA	MG-NA	4.46	2.16	2.06
23	c	2480	CLA	MG-NA	4.46	2.16	2.06
28	e	2084	HEC	CHB-C4A	4.44	1.47	1.38
27	C	488	BCR	C30-C25	4.44	1.59	1.53
27	d	2360	BCR	C1-C6	4.44	1.59	1.53
28	e	2084	HEC	C1B-NB	4.44	1.47	1.38
25	A	353	PL9	C7-C3	4.41	1.57	1.51
27	B	529	BCR	C2-C1	4.41	1.64	1.54
27	b	2527	BCR	C26-C25	4.38	1.41	1.34
23	C	478	CLA	MG-NA	4.36	2.16	2.06
27	J	53	BCR	C5-C6	4.36	1.41	1.34
23	B	521	CLA	MG-NA	4.35	2.16	2.06
23	b	2514	CLA	CHB-C1B	-4.35	1.29	1.39
23	b	2520	CLA	CAA-CBA	-4.33	1.39	1.52
23	C	479	CLA	MG-NA	4.32	2.16	2.06
27	c	2488	BCR	C29-C30	4.31	1.64	1.54
23	B	527	CLA	MG-NC	4.31	2.16	2.06
23	b	2526	CLA	MG-NC	4.30	2.16	2.06
27	d	2360	BCR	C5-C6	4.29	1.41	1.34
27	d	2360	BCR	C29-C30	4.29	1.63	1.54
27	k	2050	BCR	C1-C6	4.29	1.59	1.53
23	B	523	CLA	CAA-CBA	-4.28	1.40	1.52
23	b	2515	CLA	MG-NA	4.28	2.16	2.06
23	b	2523	CLA	CAA-CBA	-4.27	1.40	1.52
27	c	2489	BCR	C29-C30	4.25	1.63	1.54
23	c	2478	CLA	MG-NA	4.25	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	525	CLA	MG-NA	4.23	2.16	2.06
25	d	2358	PL9	C23-C24	4.22	1.42	1.33
23	C	475	CLA	MG-NA	4.22	2.16	2.06
23	C	487	CLA	MG-NC	4.22	2.16	2.06
23	c	2475	CLA	MG-NA	4.22	2.16	2.06
28	V	138	HEC	CHC-C4B	4.19	1.46	1.38
23	b	2517	CLA	MG-NA	4.17	2.16	2.06
23	C	487	CLA	C4C-C3C	4.17	1.52	1.45
27	C	488	BCR	C29-C30	4.14	1.63	1.54
25	A	353	PL9	C33-C34	4.14	1.42	1.33
25	d	2358	PL9	C18-C19	4.14	1.42	1.33
23	c	2485	CLA	MG-NA	4.13	2.16	2.06
23	B	514	CLA	CHB-C1B	-4.13	1.30	1.39
23	b	2525	CLA	MG-NA	4.13	2.16	2.06
23	C	483	CLA	MG-NA	4.12	2.16	2.06
27	d	2360	BCR	C26-C25	4.11	1.41	1.34
28	V	138	HEC	CHB-C1B	4.11	1.48	1.39
28	v	2138	HEC	C1C-NC	4.11	1.47	1.39
23	C	475	CLA	CAA-C2A	4.09	1.61	1.54
23	d	2357	CLA	MG-NC	4.09	2.16	2.06
27	b	2527	BCR	C2-C1	4.06	1.63	1.54
23	c	2483	CLA	MG-NA	4.06	2.15	2.06
23	c	2474	CLA	MG-NA	4.03	2.15	2.06
27	C	488	BCR	C1-C6	4.02	1.58	1.53
25	a	2352	PL9	C28-C29	4.02	1.42	1.33
23	c	2477	CLA	CAA-CBA	-4.01	1.40	1.52
23	A	352	CLA	MG-NA	4.01	2.15	2.06
27	b	2527	BCR	C29-C30	4.01	1.63	1.54
23	b	2516	CLA	CAA-C2A	4.01	1.61	1.54
23	B	514	CLA	CAA-CBA	-4.00	1.40	1.52
27	d	2360	BCR	C2-C1	3.99	1.63	1.54
23	b	2514	CLA	CAA-CBA	-3.99	1.40	1.52
27	F	48	BCR	C26-C25	3.98	1.41	1.34
23	A	352	CLA	MG-NC	3.98	2.15	2.06
23	c	2479	CLA	CAA-CBA	-3.98	1.41	1.52
27	j	2053	BCR	C2-C1	3.98	1.63	1.54
27	b	2528	BCR	C1-C6	3.94	1.58	1.53
23	C	484	CLA	MG-NC	3.94	2.15	2.06
27	C	489	BCR	C29-C30	3.94	1.63	1.54
27	B	528	BCR	C29-C30	3.93	1.63	1.54
23	c	2487	CLA	C4C-C3C	3.93	1.51	1.45
28	e	2084	HEC	FE-NB	3.92	2.07	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	J	53	BCR	C29-C30	3.91	1.63	1.54
27	j	2053	BCR	C29-C30	3.90	1.63	1.54
28	v	2138	HEC	C3D-C2D	3.90	1.45	1.36
27	c	2488	BCR	C2-C1	3.89	1.63	1.54
28	V	138	HEC	FE-ND	3.89	2.06	1.94
25	D	357	PL9	C18-C19	3.86	1.42	1.33
23	D	356	CLA	MG-NC	3.86	2.15	2.06
25	d	2358	PL9	C7-C3	3.85	1.56	1.51
23	b	2524	CLA	MG-NA	3.85	2.15	2.06
23	C	476	CLA	MG-NC	3.85	2.15	2.06
27	b	2528	BCR	C29-C30	3.84	1.62	1.54
23	C	477	CLA	C1D-ND	-3.83	1.32	1.37
23	c	2486	CLA	MG-NC	3.83	2.15	2.06
23	A	349	CLA	MG-NA	3.83	2.15	2.06
23	C	487	CLA	CAA-C2A	3.82	1.61	1.54
27	J	53	BCR	C26-C25	3.82	1.40	1.34
23	B	519	CLA	O2A-CGA	3.81	1.44	1.33
25	D	357	PL9	C7-C3	3.81	1.56	1.51
27	B	528	BCR	C2-C1	3.80	1.62	1.54
23	b	2518	CLA	MG-NA	3.80	2.15	2.06
27	C	488	BCR	C2-C1	3.79	1.62	1.54
23	B	512	CLA	MG-NA	3.79	2.15	2.06
28	E	84	HEC	C2A-C3A	3.79	1.44	1.36
23	b	2516	CLA	C2-C3	3.78	1.41	1.33
23	b	2519	CLA	O2A-CGA	3.78	1.44	1.33
23	C	485	CLA	CHB-C1B	-3.78	1.30	1.39
23	B	513	CLA	MG-NC	3.77	2.15	2.06
27	K	50	BCR	C23-C22	-3.77	1.37	1.46
23	B	524	CLA	CHB-C1B	-3.77	1.31	1.39
27	B	529	BCR	C1-C6	3.76	1.58	1.53
23	C	476	CLA	MG-NA	3.76	2.15	2.06
23	a	2351	CLA	MG-NA	3.75	2.15	2.06
23	C	485	CLA	MG-NA	3.74	2.15	2.06
25	A	353	PL9	C28-C29	3.74	1.41	1.33
23	c	2475	CLA	CAA-C2A	3.73	1.60	1.54
23	B	519	CLA	C1D-ND	-3.73	1.33	1.37
27	K	50	BCR	C30-C25	3.72	1.58	1.53
23	B	519	CLA	CHB-C1B	-3.72	1.31	1.39
23	d	2357	CLA	MG-NA	3.72	2.15	2.06
23	C	482	CLA	CAA-C2A	3.72	1.60	1.54
28	v	2138	HEC	CMA-C3A	3.71	1.58	1.50
27	k	2050	BCR	C19-C18	-3.71	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	v	2138	HEC	O1A-CGA	3.71	1.34	1.22
27	k	2050	BCR	C23-C22	-3.70	1.38	1.46
23	d	2355	CLA	C1D-ND	-3.69	1.33	1.37
27	F	48	BCR	C2-C1	3.69	1.62	1.54
23	C	475	CLA	MG-NC	3.68	2.15	2.06
23	C	477	CLA	CAA-CBA	-3.68	1.41	1.52
23	a	2351	CLA	MG-NC	3.67	2.15	2.06
23	c	2475	CLA	C2-C3	3.67	1.41	1.33
23	B	517	CLA	MG-NA	3.67	2.15	2.06
23	B	524	CLA	MG-NA	3.67	2.15	2.06
27	k	2050	BCR	C29-C30	3.66	1.62	1.54
28	E	84	HEC	C1A-C2A	3.66	1.51	1.45
23	B	523	CLA	MG-NA	3.66	2.15	2.06
25	A	353	PL9	C38-C39	3.65	1.43	1.32
24	a	2350	PHO	CBD-CGD	3.65	1.57	1.52
23	c	2487	CLA	CAA-C2A	3.65	1.60	1.54
23	b	2513	CLA	MG-NA	3.65	2.14	2.06
27	c	2489	BCR	C2-C1	3.65	1.62	1.54
23	B	511	CLA	MG-NC	3.64	2.14	2.06
24	A	351	PHO	C3A-C2A	-3.64	1.51	1.54
28	v	2138	HEC	C1B-NB	3.64	1.46	1.38
27	F	48	BCR	C29-C30	3.63	1.62	1.54
23	B	514	CLA	MG-NA	3.63	2.14	2.06
21	D	353	BCT	O1-C	3.62	1.38	1.25
23	c	2485	CLA	MG-NC	3.62	2.14	2.06
27	B	529	BCR	C29-C30	3.61	1.62	1.54
23	B	515	CLA	CHB-C1B	-3.60	1.31	1.39
23	C	475	CLA	C2-C3	3.60	1.41	1.33
27	K	50	BCR	C19-C18	-3.59	1.38	1.46
23	b	2511	CLA	MG-NA	3.58	2.14	2.06
28	E	84	HEC	CHD-C4C	3.58	1.47	1.39
27	C	489	BCR	C2-C1	3.57	1.62	1.54
26	B	526	LMT	C3B-C2B	-3.57	1.43	1.52
28	e	2084	HEC	C3B-C2B	3.57	1.44	1.36
28	V	138	HEC	FE-NB	3.57	2.05	1.94
23	b	2514	CLA	MG-NA	3.56	2.14	2.06
23	c	2479	CLA	MG-NA	3.56	2.14	2.06
23	B	523	CLA	MG-NC	3.56	2.14	2.06
24	d	2356	PHO	C3D-CAD	-3.56	1.41	1.47
23	b	2512	CLA	MG-NA	3.55	2.14	2.06
23	c	2482	CLA	CAA-C2A	3.55	1.60	1.54
28	v	2138	HEC	C3C-C2C	3.55	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2350	PHO	C3A-C2A	-3.54	1.51	1.54
25	D	357	PL9	C23-C24	3.54	1.41	1.33
27	J	53	BCR	C2-C1	3.54	1.62	1.54
23	C	475	CLA	C5-C3	3.54	1.58	1.51
23	B	513	CLA	MG-NA	3.54	2.14	2.06
23	b	2515	CLA	CHB-C1B	-3.52	1.31	1.39
27	K	50	BCR	C29-C30	3.51	1.62	1.54
28	v	2138	HEC	O2D-CGD	-3.50	1.19	1.30
25	a	2352	PL9	C31-C29	3.50	1.58	1.51
23	B	511	CLA	MG-NA	3.50	2.14	2.06
27	c	2489	BCR	C26-C25	3.50	1.40	1.34
23	b	2524	CLA	CHB-C1B	-3.49	1.31	1.39
23	b	2523	CLA	MG-NA	3.49	2.14	2.06
23	C	474	CLA	MG-NA	3.48	2.14	2.06
27	F	48	BCR	C5-C6	3.48	1.40	1.34
23	b	2519	CLA	MG-NA	3.48	2.14	2.06
23	b	2519	CLA	CHB-C1B	-3.47	1.31	1.39
23	D	356	CLA	MG-NA	3.47	2.14	2.06
28	e	2084	HEC	CMA-C3A	3.47	1.57	1.50
23	c	2485	CLA	CHB-C1B	-3.47	1.31	1.39
23	b	2520	CLA	MG-NC	3.47	2.14	2.06
23	b	2513	CLA	MG-NC	3.47	2.14	2.06
23	B	518	CLA	MG-NC	3.46	2.14	2.06
25	a	2352	PL9	C13-C14	3.45	1.41	1.33
23	b	2511	CLA	CHB-C1B	-3.44	1.31	1.39
23	C	474	CLA	MG-NC	3.43	2.14	2.06
25	d	2358	PL9	C33-C34	3.43	1.41	1.33
23	c	2475	CLA	C5-C3	3.43	1.58	1.51
23	b	2516	CLA	C5-C3	3.42	1.58	1.51
23	B	517	CLA	CHB-C1B	-3.42	1.31	1.39
23	b	2516	CLA	C1-C2	3.42	1.58	1.49
23	B	511	CLA	CAA-CBA	-3.41	1.42	1.52
23	b	2511	CLA	MG-NC	3.41	2.14	2.06
28	V	138	HEC	CHB-C4A	3.41	1.45	1.38
23	C	482	CLA	MG-NC	3.41	2.14	2.06
28	E	84	HEC	C3B-C2B	3.41	1.44	1.36
23	B	516	CLA	C5-C3	3.40	1.58	1.51
23	B	512	CLA	MG-NC	3.40	2.14	2.06
23	C	483	CLA	MG-NC	3.40	2.14	2.06
23	B	516	CLA	C1-C2	3.39	1.58	1.49
25	A	353	PL9	C13-C14	3.39	1.40	1.33
23	C	483	CLA	C5-C3	3.39	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	349	CLA	C1D-ND	-3.39	1.33	1.37
23	c	2477	CLA	O2A-CGA	3.39	1.43	1.33
23	C	481	CLA	MG-NC	3.38	2.14	2.06
27	c	2488	BCR	C26-C25	3.38	1.40	1.34
23	c	2484	CLA	MG-NC	3.38	2.14	2.06
23	b	2518	CLA	CAA-CBA	-3.38	1.42	1.52
28	V	138	HEC	C1C-C2C	3.38	1.51	1.43
23	B	520	CLA	MG-NA	3.38	2.14	2.06
27	k	2050	BCR	C2-C1	3.38	1.61	1.54
23	a	2348	CLA	CHB-C1B	-3.37	1.31	1.39
23	C	486	CLA	CAA-C2A	3.37	1.60	1.54
23	c	2475	CLA	O2A-CGA	3.37	1.43	1.33
23	B	520	CLA	MG-NC	3.37	2.14	2.06
25	A	353	PL9	C31-C29	3.37	1.58	1.51
23	B	518	CLA	MG-NA	3.36	2.14	2.06
26	d	2359	LMT	O1'-C1'	3.35	1.45	1.40
24	D	355	PHO	C3D-CAD	-3.35	1.41	1.47
23	b	2520	CLA	MG-NA	3.35	2.14	2.06
28	E	84	HEC	FE-NA	3.35	2.06	1.95
25	a	2352	PL9	C38-C39	3.35	1.42	1.32
21	d	2353	BCT	O1-C	3.34	1.37	1.25
23	c	2482	CLA	MG-NC	3.33	2.14	2.06
28	v	2138	HEC	CHB-C1B	3.33	1.46	1.39
23	c	2477	CLA	MG-NC	3.31	2.14	2.06
23	C	479	CLA	CAA-CBA	-3.30	1.43	1.52
23	d	2355	CLA	MG-NA	3.29	2.14	2.06
23	B	518	CLA	CAA-CBA	-3.29	1.43	1.52
23	c	2478	CLA	MG-NC	3.29	2.14	2.06
23	c	2476	CLA	MG-NC	3.29	2.14	2.06
23	B	516	CLA	C2-C3	3.29	1.40	1.33
23	c	2475	CLA	MG-NC	3.29	2.14	2.06
23	b	2519	CLA	C1D-ND	-3.28	1.33	1.37
23	b	2515	CLA	CAA-CBA	-3.28	1.43	1.52
28	V	138	HEC	CAC-C3C	-3.28	1.42	1.51
27	B	529	BCR	C24-C23	3.28	1.42	1.33
23	b	2525	CLA	MG-NC	3.28	2.14	2.06
27	C	489	BCR	C1-C6	3.28	1.58	1.53
25	D	357	PL9	C28-C29	3.28	1.40	1.33
23	b	2519	CLA	CAA-CBA	-3.27	1.43	1.52
23	b	2521	CLA	C4-C3	3.26	1.58	1.50
23	A	348	CLA	CHB-C1B	-3.26	1.32	1.39
27	c	2489	BCR	C5-C6	3.26	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	357	PL9	C30-C29	3.24	1.58	1.50
23	C	486	CLA	MG-NC	3.23	2.13	2.06
27	k	2050	BCR	C30-C25	3.23	1.57	1.53
23	B	519	CLA	CAA-CBA	-3.23	1.43	1.52
23	B	519	CLA	MG-ND	-3.22	1.99	2.05
28	V	138	HEC	O2A-CGA	-3.22	1.20	1.30
24	D	355	PHO	C3A-C2A	-3.21	1.51	1.54
28	e	2084	HEC	CHB-C1B	3.21	1.46	1.39
23	A	350	CLA	MG-NC	3.21	2.13	2.06
23	B	521	CLA	MG-NC	3.21	2.13	2.06
28	e	2084	HEC	C2A-C3A	3.21	1.43	1.36
23	C	477	CLA	O2A-CGA	3.21	1.42	1.33
23	d	2354	CLA	CAA-C2A	3.21	1.59	1.54
23	A	349	CLA	C1D-C2D	-3.21	1.39	1.45
25	A	353	PL9	C23-C24	3.20	1.40	1.33
23	b	2523	CLA	MG-NC	3.19	2.13	2.06
23	B	515	CLA	CAA-CBA	-3.18	1.43	1.52
25	d	2358	PL9	C13-C14	3.18	1.40	1.33
23	c	2486	CLA	CAA-C2A	3.17	1.59	1.54
23	B	516	CLA	CAA-C2A	3.16	1.59	1.54
23	a	2349	CLA	CAA-CBA	-3.15	1.43	1.52
23	b	2525	CLA	C1D-ND	-3.15	1.33	1.37
23	C	485	CLA	MG-NC	3.15	2.13	2.06
23	A	350	CLA	C1D-C2D	-3.14	1.39	1.45
23	d	2355	CLA	CHB-C1B	-3.14	1.32	1.39
28	E	84	HEC	C1A-NA	3.14	1.45	1.39
23	B	518	CLA	CHB-C1B	-3.14	1.32	1.39
27	C	489	BCR	C26-C25	3.14	1.39	1.34
27	k	2050	BCR	C26-C25	3.14	1.39	1.34
23	c	2483	CLA	C5-C3	3.14	1.57	1.51
23	C	476	CLA	CAA-C2A	3.14	1.59	1.54
23	C	478	CLA	MG-NC	3.13	2.13	2.06
28	V	138	HEC	CBD-CGD	-3.13	1.43	1.50
26	d	2359	LMT	C3B-C2B	-3.13	1.44	1.52
23	C	480	CLA	CAA-CBA	-3.13	1.43	1.52
23	b	2519	CLA	C1-C2	3.13	1.58	1.49
23	B	511	CLA	CHB-C1B	-3.13	1.32	1.39
23	b	2516	CLA	MG-NC	3.13	2.13	2.06
23	b	2511	CLA	CAA-CBA	-3.12	1.43	1.52
27	b	2527	BCR	C1-C6	3.12	1.57	1.53
23	C	475	CLA	O2A-CGA	3.11	1.42	1.33
23	C	477	CLA	MG-NC	3.11	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	50	BCR	C1-C6	3.11	1.57	1.53
25	d	2358	PL9	C28-C29	3.11	1.40	1.33
21	a	2346	BCT	O1-C	3.10	1.36	1.25
28	e	2084	HEC	C4B-C3B	3.10	1.50	1.45
23	C	478	CLA	CHB-C1B	-3.10	1.32	1.39
23	B	522	CLA	C1D-ND	-3.09	1.33	1.37
23	b	2525	CLA	CAA-C2A	3.09	1.59	1.54
23	B	525	CLA	C1D-ND	-3.08	1.33	1.37
25	a	2352	PL9	C33-C34	3.08	1.40	1.33
25	D	357	PL9	C33-C34	3.07	1.40	1.33
23	C	482	CLA	C5-C3	3.07	1.57	1.51
23	c	2481	CLA	CAA-CBA	-3.07	1.43	1.52
23	B	520	CLA	C1-C2	3.06	1.57	1.49
23	B	520	CLA	O2A-CGA	3.06	1.42	1.33
25	a	2352	PL9	C23-C24	3.06	1.40	1.33
23	c	2475	CLA	C4-C3	3.06	1.58	1.50
23	A	350	CLA	C1D-ND	-3.06	1.33	1.37
23	D	354	CLA	CAA-C2A	3.06	1.59	1.54
23	c	2486	CLA	CHB-C1B	-3.06	1.32	1.39
23	c	2484	CLA	CAA-C2A	3.06	1.59	1.54
23	d	2354	CLA	MG-NC	3.05	2.13	2.06
23	b	2520	CLA	C1-C2	3.05	1.57	1.49
23	A	352	CLA	CAA-C2A	3.04	1.59	1.54
24	a	2350	PHO	C4A-C3A	-3.04	1.46	1.51
23	c	2478	CLA	CHB-C1B	-3.03	1.32	1.39
23	A	348	CLA	MG-NC	3.03	2.13	2.06
27	K	50	BCR	C2-C1	3.03	1.61	1.54
23	c	2479	CLA	MG-NC	3.03	2.13	2.06
23	b	2514	CLA	C5-C3	3.03	1.57	1.51
28	e	2084	HEC	O1A-CGA	3.02	1.32	1.22
23	b	2517	CLA	CHB-C1B	-3.02	1.32	1.39
23	B	519	CLA	C1-C2	3.02	1.57	1.49
27	c	2488	BCR	C5-C6	3.01	1.39	1.34
23	C	475	CLA	CHB-C1B	-3.01	1.32	1.39
23	a	2349	CLA	MG-NC	3.00	2.13	2.06
27	K	50	BCR	C26-C25	2.99	1.39	1.34
23	c	2485	CLA	CAA-CBA	-2.99	1.43	1.52
23	B	522	CLA	MG-NC	2.99	2.13	2.06
23	C	484	CLA	CAA-C2A	2.98	1.59	1.54
23	c	2475	CLA	C1-C2	2.98	1.57	1.49
23	c	2480	CLA	MG-NC	2.98	2.13	2.06
23	c	2483	CLA	CAA-CBA	-2.98	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	488	BCR	C5-C6	2.97	1.39	1.34
27	C	489	BCR	C5-C6	2.97	1.39	1.34
23	C	475	CLA	C1-C2	2.97	1.57	1.49
26	d	2359	LMT	C2-C1	2.97	1.63	1.51
23	c	2482	CLA	C5-C3	2.96	1.57	1.51
23	B	521	CLA	C4-C3	2.96	1.57	1.50
23	b	2512	CLA	MG-NC	2.96	2.13	2.06
23	C	474	CLA	CAA-CBA	-2.96	1.44	1.52
28	E	84	HEC	FE-ND	2.96	2.04	1.94
23	B	516	CLA	MG-NC	2.95	2.13	2.06
23	c	2481	CLA	MG-NC	2.95	2.13	2.06
23	c	2474	CLA	MG-NC	2.95	2.13	2.06
23	B	522	CLA	C1D-C2D	-2.95	1.39	1.45
28	e	2084	HEC	FE-NA	2.94	2.04	1.95
23	B	512	CLA	C4-C3	2.94	1.57	1.50
23	B	517	CLA	MG-NC	2.94	2.13	2.06
26	B	526	LMT	C2-C1	2.94	1.63	1.51
27	C	488	BCR	C26-C25	2.94	1.39	1.34
23	C	483	CLA	CAA-CBA	-2.93	1.44	1.52
28	v	2138	HEC	CAD-C3D	-2.92	1.43	1.51
23	C	487	CLA	CHB-C1B	-2.92	1.32	1.39
28	V	138	HEC	FE-NC	2.92	2.04	1.95
23	c	2484	CLA	C4-C3	2.92	1.57	1.50
24	A	351	PHO	C4A-C3A	-2.91	1.46	1.51
23	c	2480	CLA	CAA-CBA	-2.91	1.44	1.52
23	b	2521	CLA	CAA-CBA	-2.90	1.44	1.52
23	c	2474	CLA	C4-C3	2.90	1.57	1.50
27	K	50	BCR	C12-C13	-2.90	1.39	1.46
28	V	138	HEC	CHD-C1D	2.89	1.44	1.38
23	a	2348	CLA	CHC-C1C	2.89	1.44	1.38
23	C	486	CLA	CHB-C1B	-2.88	1.32	1.39
23	B	516	CLA	CAA-CBA	-2.88	1.44	1.52
23	b	2518	CLA	MG-NC	2.88	2.13	2.06
23	C	484	CLA	C4-C3	2.88	1.57	1.50
23	B	524	CLA	O2A-CGA	2.88	1.41	1.33
23	b	2515	CLA	MG-NC	2.88	2.13	2.06
28	E	84	HEC	O1A-CGA	2.87	1.31	1.22
23	d	2357	CLA	C4-C3	2.87	1.57	1.50
23	D	354	CLA	MG-NC	2.87	2.13	2.06
23	b	2520	CLA	C2-C3	2.86	1.39	1.33
23	c	2483	CLA	MG-NC	2.86	2.13	2.06
23	c	2477	CLA	C1D-C2D	-2.86	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	475	CLA	C4-C3	2.85	1.57	1.50
23	A	349	CLA	CHB-C1B	-2.85	1.33	1.39
23	b	2517	CLA	MG-NC	2.85	2.13	2.06
23	b	2511	CLA	C1-C2	2.85	1.57	1.49
23	d	2355	CLA	O2A-CGA	2.85	1.41	1.33
25	d	2358	PL9	C30-C29	2.85	1.57	1.50
23	B	519	CLA	C5-C3	2.85	1.57	1.51
23	b	2521	CLA	MG-NC	2.84	2.13	2.06
23	b	2517	CLA	CAA-CBA	-2.83	1.44	1.52
24	d	2356	PHO	CHA-CBD	2.83	1.55	1.51
23	B	525	CLA	MG-NC	2.83	2.13	2.06
23	b	2512	CLA	CAA-C2A	2.82	1.59	1.54
23	b	2518	CLA	CHB-C1B	-2.82	1.33	1.39
23	c	2479	CLA	CHB-C1B	-2.82	1.33	1.39
23	d	2357	CLA	C5-C3	2.82	1.57	1.51
24	a	2350	PHO	CHA-CBD	2.81	1.54	1.51
25	a	2352	PL9	C17-C18	-2.80	1.42	1.50
23	c	2487	CLA	CHD-C1D	2.80	1.43	1.38
28	e	2084	HEC	C1A-NA	2.80	1.44	1.39
23	c	2474	CLA	CAA-CBA	-2.80	1.44	1.52
23	b	2516	CLA	CAA-CBA	-2.79	1.44	1.52
27	K	50	BCR	C33-C5	2.79	1.55	1.50
23	b	2526	CLA	CMB-C2B	2.79	1.56	1.50
23	b	2520	CLA	C4-C3	2.78	1.57	1.50
23	B	521	CLA	CAA-CBA	-2.78	1.44	1.52
27	B	528	BCR	C33-C5	2.78	1.55	1.50
23	b	2520	CLA	O2A-CGA	2.77	1.41	1.33
23	B	524	CLA	CAA-C2A	2.77	1.59	1.54
23	A	350	CLA	CAA-CBA	-2.77	1.44	1.52
23	c	2483	CLA	C4-C3	2.76	1.57	1.50
23	C	479	CLA	CHB-C1B	-2.76	1.33	1.39
23	c	2475	CLA	CHB-C1B	-2.76	1.33	1.39
23	c	2477	CLA	C1D-ND	-2.75	1.34	1.37
23	C	474	CLA	CHB-C1B	-2.75	1.33	1.39
23	B	525	CLA	CAA-C2A	2.74	1.59	1.54
23	B	516	CLA	C6-C5	2.74	1.62	1.52
23	a	2349	CLA	C1D-ND	-2.74	1.34	1.37
23	C	480	CLA	C1D-ND	-2.74	1.34	1.37
23	B	527	CLA	CMB-C2B	2.74	1.56	1.50
23	C	476	CLA	C1D-C2D	-2.74	1.39	1.45
26	d	2359	LMT	C4'-C5'	2.74	1.60	1.52
23	c	2487	CLA	C4-C3	2.73	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	352	CLA	C4-C3	2.73	1.57	1.50
25	D	357	PL9	C13-C14	2.73	1.39	1.33
23	a	2351	CLA	CHB-C1B	-2.72	1.33	1.39
25	d	2358	PL9	C8-C9	2.72	1.39	1.33
23	b	2519	CLA	C1D-C2D	-2.72	1.40	1.45
23	b	2524	CLA	O2A-CGA	2.72	1.41	1.33
23	a	2351	CLA	C4C-C3C	2.71	1.49	1.45
23	A	348	CLA	CAA-CBA	-2.71	1.44	1.52
25	a	2352	PL9	C35-C34	2.71	1.57	1.50
27	b	2528	BCR	C38-C26	2.71	1.55	1.50
23	A	348	CLA	CHC-C1C	2.71	1.43	1.38
23	b	2511	CLA	O2A-CGA	2.70	1.41	1.33
23	b	2521	CLA	CMB-C2B	2.70	1.56	1.50
23	B	524	CLA	C1D-ND	-2.70	1.34	1.37
23	C	479	CLA	C1D-ND	-2.70	1.34	1.37
23	B	514	CLA	C5-C3	2.70	1.56	1.51
23	B	517	CLA	CAA-CBA	-2.70	1.44	1.52
27	k	2050	BCR	C12-C13	-2.69	1.40	1.46
23	B	527	CLA	C4-C3	2.69	1.57	1.50
23	C	477	CLA	C1D-C2D	-2.69	1.40	1.45
25	d	2358	PL9	C2-C3	2.69	1.41	1.34
25	d	2358	PL9	C35-C34	2.68	1.57	1.50
23	B	511	CLA	C1-C2	2.68	1.56	1.49
23	a	2348	CLA	MG-NC	2.68	2.12	2.06
27	k	2050	BCR	C17-C18	-2.68	1.29	1.35
23	c	2478	CLA	CAA-C2A	2.68	1.59	1.54
23	B	522	CLA	CHB-C1B	-2.68	1.33	1.39
27	K	50	BCR	C17-C18	-2.67	1.29	1.35
23	A	352	CLA	CHB-C1B	-2.67	1.33	1.39
23	B	515	CLA	MG-NC	2.67	2.12	2.06
27	b	2528	BCR	C24-C23	2.67	1.41	1.33
25	A	353	PL9	C30-C29	2.67	1.57	1.50
25	D	357	PL9	C8-C9	2.67	1.39	1.33
23	C	484	CLA	C1D-ND	-2.66	1.34	1.37
23	b	2520	CLA	C5-C3	2.66	1.56	1.51
27	j	2053	BCR	C38-C26	2.66	1.55	1.50
23	B	520	CLA	C2-C3	2.65	1.39	1.33
23	a	2351	CLA	CAA-C2A	2.65	1.58	1.54
23	b	2514	CLA	MG-NC	2.64	2.12	2.06
25	D	357	PL9	C38-C39	2.64	1.40	1.32
25	D	357	PL9	C2-C3	2.64	1.41	1.34
23	B	516	CLA	C4-C3	2.63	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	2476	CLA	CMB-C2B	2.63	1.56	1.50
23	a	2351	CLA	C4-C3	2.63	1.57	1.50
23	A	349	CLA	O2A-CGA	2.63	1.41	1.33
23	b	2522	CLA	MG-NC	2.63	2.12	2.06
23	d	2355	CLA	C1D-C2D	-2.63	1.40	1.45
23	b	2522	CLA	C4-C3	2.63	1.57	1.50
24	A	351	PHO	C3D-CAD	-2.62	1.42	1.47
23	c	2474	CLA	CHB-C1B	-2.62	1.33	1.39
28	v	2138	HEC	FE-ND	2.62	2.03	1.94
25	A	353	PL9	C27-C28	-2.62	1.42	1.50
23	C	485	CLA	CAA-CBA	-2.62	1.45	1.52
27	k	2050	BCR	C33-C5	2.61	1.55	1.50
25	a	2352	PL9	C30-C29	2.61	1.57	1.50
28	e	2084	HEC	C4A-C3A	2.61	1.50	1.45
23	D	356	CLA	C4-C3	2.60	1.57	1.50
23	C	481	CLA	C4-C3	2.60	1.57	1.50
23	C	475	CLA	CAA-CBA	-2.60	1.45	1.52
23	b	2513	CLA	C1D-C2D	-2.60	1.40	1.45
23	c	2477	CLA	CMB-C2B	2.60	1.56	1.50
23	a	2349	CLA	C1D-C2D	-2.60	1.40	1.45
25	d	2358	PL9	C38-C39	2.60	1.40	1.32
23	c	2475	CLA	CAA-CBA	-2.59	1.45	1.52
23	b	2512	CLA	C4-C3	2.59	1.57	1.50
23	b	2521	CLA	C5-C3	2.59	1.56	1.51
28	E	84	HEC	C1B-NB	2.59	1.43	1.38
23	B	514	CLA	MG-NC	2.59	2.12	2.06
25	a	2352	PL9	C27-C28	-2.58	1.42	1.50
23	C	478	CLA	CAA-C2A	2.58	1.58	1.54
26	B	526	LMT	O1'-C1'	2.58	1.44	1.40
23	b	2515	CLA	C4-C3	2.58	1.57	1.50
23	B	512	CLA	CAA-C2A	2.57	1.58	1.54
23	b	2511	CLA	CHC-C1C	2.57	1.43	1.38
25	A	353	PL9	C35-C34	2.57	1.57	1.50
23	B	517	CLA	C1D-ND	-2.57	1.34	1.37
23	b	2523	CLA	C5-C3	2.57	1.56	1.51
23	b	2518	CLA	C4-C3	2.57	1.57	1.50
23	B	521	CLA	CHB-C1B	-2.56	1.33	1.39
25	a	2352	PL9	C8-C9	2.56	1.39	1.33
26	B	526	LMT	C4'-C5'	2.56	1.59	1.52
24	d	2356	PHO	C4A-C3A	-2.56	1.47	1.51
23	c	2480	CLA	CHB-C1B	-2.56	1.33	1.39
23	b	2524	CLA	C1D-ND	-2.55	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	2356	PHO	C1D-C2D	2.55	1.42	1.39
23	c	2476	CLA	CAA-C2A	2.55	1.58	1.54
23	C	481	CLA	CAA-CBA	-2.55	1.45	1.52
23	b	2512	CLA	C1D-C2D	-2.55	1.40	1.45
23	b	2518	CLA	MG-NB	2.55	2.10	2.05
28	E	84	HEC	FE-NB	2.55	2.02	1.94
23	B	511	CLA	O2A-CGA	2.54	1.40	1.33
27	c	2489	BCR	C33-C5	2.54	1.55	1.50
23	C	487	CLA	CHD-C1D	2.54	1.43	1.38
24	a	2350	PHO	CAA-CBA	-2.54	1.45	1.52
25	A	353	PL9	C17-C18	-2.54	1.42	1.50
23	b	2525	CLA	C1D-C2D	-2.53	1.40	1.45
23	B	511	CLA	C1D-C2D	-2.53	1.40	1.45
23	c	2485	CLA	CBA-CGA	-2.53	1.43	1.50
25	D	357	PL9	C35-C34	2.53	1.56	1.50
23	C	478	CLA	O2A-CGA	2.53	1.40	1.33
23	B	519	CLA	C2-C3	2.52	1.38	1.33
27	c	2488	BCR	C19-C18	-2.52	1.40	1.46
23	c	2483	CLA	C1D-ND	-2.52	1.34	1.37
23	A	352	CLA	C1D-C2D	-2.52	1.40	1.45
23	B	527	CLA	C4C-C3C	2.52	1.49	1.45
23	b	2512	CLA	C1D-ND	-2.52	1.34	1.37
23	C	485	CLA	C4-C3	2.52	1.56	1.50
23	b	2522	CLA	CHB-C1B	-2.52	1.33	1.39
25	D	357	PL9	C32-C33	-2.52	1.42	1.50
23	c	2481	CLA	C4-C3	2.52	1.56	1.50
23	B	513	CLA	C1D-C2D	-2.51	1.40	1.45
23	B	523	CLA	CHB-C1B	-2.51	1.33	1.39
23	A	349	CLA	CAA-CBA	-2.51	1.45	1.52
28	e	2084	HEC	C1C-NC	2.51	1.44	1.39
23	c	2485	CLA	C1D-ND	-2.51	1.34	1.37
23	B	519	CLA	MG-NC	2.51	2.12	2.06
23	c	2485	CLA	C4-C3	2.51	1.56	1.50
23	d	2354	CLA	C5-C3	2.50	1.56	1.51
23	c	2483	CLA	C2-C3	2.50	1.38	1.33
23	C	487	CLA	C4-C3	2.50	1.56	1.50
23	b	2513	CLA	C1D-ND	-2.50	1.34	1.37
23	b	2525	CLA	CHB-C1B	-2.50	1.33	1.39
23	c	2481	CLA	C1D-C2D	-2.50	1.40	1.45
23	b	2525	CLA	C4-C3	2.49	1.56	1.50
23	b	2516	CLA	C1D-ND	-2.49	1.34	1.37
27	j	2053	BCR	C33-C5	2.49	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2519	CLA	C4-C3	2.49	1.56	1.50
23	b	2522	CLA	C1D-C2D	-2.49	1.40	1.45
23	B	527	CLA	C1-C2	2.48	1.56	1.49
27	B	529	BCR	C38-C26	2.48	1.54	1.50
23	b	2517	CLA	C1D-C2D	-2.48	1.40	1.45
23	b	2511	CLA	C3B-C4B	2.48	1.50	1.42
23	a	2348	CLA	CAA-CBA	-2.48	1.45	1.52
23	B	520	CLA	CHB-C1B	-2.48	1.33	1.39
25	A	353	PL9	C8-C9	2.47	1.38	1.33
23	b	2519	CLA	C2-C3	2.47	1.38	1.33
23	b	2522	CLA	C5-C3	2.47	1.56	1.51
23	c	2479	CLA	C1D-ND	-2.47	1.34	1.37
23	B	511	CLA	CHC-C1C	2.47	1.43	1.38
23	C	484	CLA	CHB-C4A	2.47	1.43	1.37
23	b	2511	CLA	C1D-C2D	-2.47	1.40	1.45
23	a	2348	CLA	C1D-ND	-2.47	1.34	1.37
23	b	2514	CLA	C4-C3	2.47	1.56	1.50
27	K	50	BCR	C16-C15	-2.47	1.29	1.36
23	D	354	CLA	C1D-C2D	-2.46	1.40	1.45
23	b	2513	CLA	C4-C3	2.46	1.56	1.50
23	A	349	CLA	CAA-C2A	2.46	1.58	1.54
23	A	348	CLA	C1D-C2D	-2.46	1.40	1.45
23	D	356	CLA	C1C-C2C	2.46	1.49	1.44
28	v	2138	HEC	CHA-C4D	-2.46	1.33	1.39
23	b	2526	CLA	C4C-C3C	2.46	1.49	1.45
23	C	475	CLA	C1D-ND	-2.46	1.34	1.37
23	B	519	CLA	MG-NA	2.45	2.12	2.06
23	b	2526	CLA	C4-C3	2.45	1.56	1.50
23	d	2354	CLA	C1D-ND	-2.45	1.34	1.37
27	c	2488	BCR	C33-C5	2.44	1.54	1.50
24	a	2350	PHO	C4-C3	2.44	1.56	1.50
27	k	2050	BCR	C16-C15	-2.44	1.29	1.36
28	e	2084	HEC	C1C-C2C	2.44	1.48	1.43
23	A	352	CLA	CMB-C2B	2.43	1.55	1.50
23	b	2515	CLA	C1D-ND	-2.43	1.34	1.37
23	c	2487	CLA	CHB-C1B	-2.43	1.34	1.39
23	C	486	CLA	C5-C3	2.42	1.56	1.51
23	b	2523	CLA	CHC-C1C	2.42	1.43	1.38
23	b	2522	CLA	CAA-C2A	2.42	1.58	1.54
23	b	2516	CLA	C6-C5	2.42	1.61	1.52
23	B	524	CLA	MG-NC	2.42	2.12	2.06
23	B	512	CLA	CHB-C4A	2.41	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2520	CLA	CHC-C1C	2.41	1.43	1.38
23	B	527	CLA	C2-C3	2.41	1.38	1.33
23	B	527	CLA	MG-NB	2.41	2.10	2.05
23	B	516	CLA	CHB-C4A	2.41	1.43	1.37
23	b	2524	CLA	C1D-C2D	-2.41	1.40	1.45
28	e	2084	HEC	C4A-NA	2.40	1.44	1.39
23	c	2476	CLA	CHC-C1C	2.40	1.43	1.38
23	B	513	CLA	CHB-C4A	2.40	1.43	1.37
23	a	2351	CLA	C1D-C2D	-2.40	1.40	1.45
23	c	2476	CLA	C1D-C2D	-2.40	1.40	1.45
23	D	356	CLA	CAA-CBA	-2.40	1.45	1.52
23	d	2354	CLA	C1D-C2D	-2.40	1.40	1.45
23	B	520	CLA	C4-C3	2.40	1.56	1.50
23	b	2511	CLA	C1C-C2C	2.40	1.49	1.44
23	B	514	CLA	C4-C3	2.40	1.56	1.50
23	b	2522	CLA	C1D-ND	-2.40	1.34	1.37
23	C	480	CLA	MG-NC	2.39	2.12	2.06
23	B	515	CLA	C4-C3	2.38	1.56	1.50
23	B	521	CLA	C1D-ND	-2.38	1.34	1.37
23	C	485	CLA	C1D-ND	-2.38	1.34	1.37
23	c	2487	CLA	C5-C3	2.37	1.56	1.51
23	c	2478	CLA	C2-C3	2.37	1.38	1.33
23	C	477	CLA	C1-C2	2.37	1.55	1.49
23	c	2486	CLA	C4-C3	2.37	1.56	1.50
23	C	482	CLA	C1-C2	2.37	1.55	1.49
23	B	511	CLA	C1D-ND	-2.36	1.34	1.37
23	b	2511	CLA	C1D-ND	-2.36	1.34	1.37
28	V	138	HEC	O1D-CGD	2.36	1.29	1.22
25	d	2358	PL9	C32-C33	-2.35	1.43	1.50
23	B	525	CLA	C4-C3	2.35	1.56	1.50
23	C	477	CLA	CHB-C1B	-2.35	1.34	1.39
23	b	2516	CLA	O2A-CGA	2.34	1.40	1.33
23	C	483	CLA	C4-C3	2.34	1.56	1.50
23	b	2523	CLA	C1C-C2C	2.34	1.49	1.44
28	v	2138	HEC	CBC-CAC	-2.34	1.41	1.51
23	A	348	CLA	CBA-CGA	-2.34	1.43	1.50
23	b	2524	CLA	CAA-C2A	2.34	1.58	1.54
23	b	2523	CLA	C4-C3	2.34	1.56	1.50
23	B	519	CLA	C4-C3	2.33	1.56	1.50
23	D	354	CLA	C1-C2	2.33	1.55	1.49
23	b	2516	CLA	C4-C3	2.33	1.56	1.50
27	J	53	BCR	C38-C26	2.33	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	351	PHO	CBD-CGD	2.33	1.55	1.52
24	D	355	PHO	C4A-C3A	-2.32	1.47	1.51
23	C	482	CLA	C4-C3	2.32	1.56	1.50
23	c	2482	CLA	C4C-C3C	2.32	1.49	1.45
23	b	2514	CLA	C1D-ND	-2.32	1.34	1.37
24	D	355	PHO	CHA-CBD	2.32	1.54	1.51
23	c	2475	CLA	C1D-ND	-2.32	1.34	1.37
23	C	476	CLA	CMB-C2B	2.32	1.55	1.50
23	b	2524	CLA	MG-ND	-2.32	2.01	2.05
23	B	527	CLA	CHB-C1B	-2.31	1.34	1.39
23	b	2521	CLA	C1D-ND	-2.31	1.34	1.37
23	D	356	CLA	C1D-C2D	-2.31	1.40	1.45
23	c	2480	CLA	C4-C3	2.31	1.56	1.50
23	d	2357	CLA	CAA-CBA	-2.31	1.46	1.52
23	d	2357	CLA	CAA-C2A	2.31	1.58	1.54
24	A	351	PHO	C4-C3	2.30	1.56	1.50
28	v	2138	HEC	CAB-C3B	2.30	1.57	1.51
28	e	2084	HEC	C4C-NC	2.30	1.43	1.39
23	B	525	CLA	CHB-C1B	-2.30	1.34	1.39
23	A	352	CLA	C1D-ND	-2.30	1.34	1.37
23	c	2476	CLA	C1D-ND	-2.30	1.34	1.37
23	C	484	CLA	CHC-C1C	2.30	1.43	1.38
23	D	356	CLA	CMD-C2D	2.30	1.55	1.50
23	d	2355	CLA	CHC-C1C	2.30	1.43	1.38
23	C	483	CLA	CAA-C2A	2.29	1.58	1.54
23	B	513	CLA	C2-C3	2.29	1.38	1.33
23	b	2513	CLA	CHB-C1B	-2.29	1.34	1.39
23	C	481	CLA	C1D-ND	-2.29	1.34	1.37
23	B	523	CLA	C5-C3	2.29	1.56	1.51
23	b	2523	CLA	CHB-C1B	-2.28	1.34	1.39
23	C	482	CLA	CHB-C4A	2.28	1.43	1.37
25	A	353	PL9	C2-C3	2.28	1.40	1.34
27	j	2053	BCR	C1-C6	2.28	1.56	1.53
27	C	488	BCR	C23-C22	-2.28	1.41	1.46
23	c	2481	CLA	CHB-C1B	-2.28	1.34	1.39
28	V	138	HEC	CBA-CGA	-2.28	1.45	1.50
23	C	487	CLA	OBD-CAD	2.28	1.26	1.22
28	e	2084	HEC	CMC-C2C	2.27	1.55	1.50
23	B	519	CLA	C1D-C2D	-2.27	1.40	1.45
28	v	2138	HEC	CHD-C4C	2.27	1.44	1.39
23	b	2517	CLA	C4-C3	2.27	1.56	1.50
23	c	2482	CLA	C4-C3	2.27	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	527	CLA	C1B-C2B	2.27	1.48	1.43
25	a	2352	PL9	C40-C39	2.27	1.56	1.50
28	v	2138	HEC	CBA-CGA	-2.27	1.45	1.50
27	b	2527	BCR	C38-C26	2.27	1.54	1.50
23	b	2525	CLA	OBD-CAD	2.26	1.26	1.22
27	K	50	BCR	C20-C21	-2.26	1.36	1.43
23	C	484	CLA	C3B-C4B	2.26	1.49	1.42
23	C	474	CLA	C4-C3	2.26	1.56	1.50
23	b	2515	CLA	C3A-C4A	-2.26	1.44	1.51
23	a	2351	CLA	CMB-C2B	2.26	1.55	1.50
23	c	2476	CLA	CHB-C4A	2.26	1.43	1.37
23	C	486	CLA	C4-C3	2.25	1.56	1.50
24	d	2356	PHO	C4-C3	2.25	1.56	1.50
23	B	520	CLA	CHC-C1C	2.25	1.43	1.38
23	B	523	CLA	C4-C3	2.25	1.56	1.50
25	d	2358	PL9	C37-C38	-2.25	1.43	1.50
23	B	513	CLA	C4-C3	2.25	1.56	1.50
23	C	480	CLA	C4-C3	2.25	1.56	1.50
28	v	2138	HEC	O2A-CGA	-2.25	1.23	1.30
25	A	353	PL9	C21-C19	-2.25	1.46	1.51
27	B	529	BCR	C7-C6	2.25	1.52	1.45
23	c	2487	CLA	CMA-C3A	2.24	1.57	1.53
23	b	2516	CLA	CHB-C4A	2.24	1.43	1.37
23	d	2354	CLA	CHB-C1B	-2.24	1.34	1.39
24	D	355	PHO	CBD-CGD	2.24	1.55	1.52
23	B	525	CLA	OBD-CAD	2.24	1.26	1.22
23	C	484	CLA	C1B-C2B	2.24	1.48	1.43
27	k	2050	BCR	C20-C21	-2.24	1.36	1.43
23	B	524	CLA	C1D-C2D	-2.24	1.40	1.45
23	c	2484	CLA	C1D-ND	-2.24	1.34	1.37
23	B	524	CLA	O2A-C1	2.24	1.52	1.46
28	v	2138	HEC	CBA-CAA	-2.23	1.44	1.51
23	C	481	CLA	CMB-C2B	2.23	1.55	1.50
23	b	2513	CLA	CHB-C4A	2.23	1.43	1.37
23	c	2476	CLA	C4-C3	2.23	1.56	1.50
23	b	2520	CLA	CHB-C1B	-2.23	1.34	1.39
23	C	479	CLA	C1D-C2D	-2.23	1.40	1.45
23	c	2482	CLA	C1-C2	2.23	1.55	1.49
23	c	2478	CLA	O2A-CGA	2.22	1.39	1.33
23	C	474	CLA	C1-C2	2.22	1.55	1.49
23	B	512	CLA	C1D-ND	-2.22	1.34	1.37
23	d	2357	CLA	C1B-C2B	2.22	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	511	CLA	CMB-C2B	2.22	1.55	1.50
27	C	489	BCR	C33-C5	2.22	1.54	1.50
23	b	2512	CLA	CHB-C4A	2.22	1.43	1.37
23	c	2482	CLA	CHB-C4A	2.22	1.43	1.37
23	d	2357	CLA	CHB-C4A	2.22	1.43	1.37
23	B	521	CLA	C1-C2	2.21	1.55	1.49
23	b	2513	CLA	C1B-NB	-2.21	1.35	1.37
23	b	2512	CLA	CMB-C2B	2.21	1.55	1.50
23	C	480	CLA	CHB-C1B	-2.21	1.34	1.39
23	b	2526	CLA	CHB-C1B	-2.21	1.34	1.39
23	b	2519	CLA	C1C-NC	-2.21	1.34	1.37
23	c	2486	CLA	CMB-C2B	2.21	1.55	1.50
27	k	2050	BCR	C5-C6	2.21	1.38	1.34
23	d	2357	CLA	CMD-C2D	2.21	1.55	1.50
23	D	354	CLA	C5-C3	2.20	1.55	1.51
23	c	2483	CLA	CHB-C4A	2.20	1.43	1.37
27	b	2528	BCR	C7-C6	2.20	1.52	1.45
23	c	2476	CLA	C1C-C2C	2.20	1.49	1.44
27	k	2050	BCR	C16-C17	-2.20	1.36	1.43
23	B	515	CLA	C3A-C4A	-2.20	1.44	1.51
23	c	2485	CLA	CHD-C1D	2.20	1.42	1.38
23	b	2511	CLA	CMB-C2B	2.19	1.55	1.50
23	b	2518	CLA	C1D-ND	-2.19	1.35	1.37
27	c	2488	BCR	C23-C22	-2.19	1.41	1.46
23	C	486	CLA	C1D-C2D	-2.19	1.41	1.45
23	B	513	CLA	C1D-ND	-2.19	1.35	1.37
23	b	2523	CLA	CBA-CGA	-2.19	1.44	1.50
23	b	2526	CLA	C1B-C2B	2.19	1.48	1.43
23	d	2355	CLA	CAA-CBA	-2.19	1.46	1.52
27	K	50	BCR	C16-C17	-2.19	1.36	1.43
23	B	521	CLA	MG-NB	2.19	2.10	2.05
27	b	2528	BCR	C5-C6	2.19	1.38	1.34
23	b	2526	CLA	C1D-C2D	-2.19	1.41	1.45
23	C	484	CLA	C1-C2	2.19	1.55	1.49
23	B	512	CLA	C1D-C2D	-2.19	1.41	1.45
23	C	478	CLA	C1D-C2D	-2.19	1.41	1.45
23	B	517	CLA	C3A-C4A	-2.18	1.44	1.51
28	E	84	HEC	C4C-NC	2.18	1.43	1.39
24	a	2350	PHO	C3D-CAD	-2.18	1.43	1.47
23	b	2514	CLA	CMB-C2B	2.18	1.55	1.50
23	B	522	CLA	C4-C3	2.18	1.56	1.50
23	C	487	CLA	C5-C3	2.18	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	2518	CLA	O2A-CGA	2.18	1.39	1.33
23	b	2524	CLA	MG-NC	2.18	2.11	2.06
25	A	353	PL9	C18-C19	2.17	1.38	1.33
23	B	523	CLA	CHC-C1C	2.17	1.42	1.38
23	c	2482	CLA	C1D-ND	-2.17	1.35	1.37
25	a	2352	PL9	C2-C3	2.17	1.40	1.34
23	C	485	CLA	CHD-C1D	2.17	1.42	1.38
23	C	482	CLA	CMB-C2B	2.17	1.55	1.50
23	C	483	CLA	CHB-C1B	-2.17	1.34	1.39
23	B	513	CLA	CHB-C1B	-2.17	1.34	1.39
25	D	357	PL9	C37-C38	-2.17	1.43	1.50
23	c	2479	CLA	C4-C3	2.17	1.56	1.50
24	A	351	PHO	CHA-CBD	2.17	1.54	1.51
23	B	514	CLA	C1-C2	2.16	1.55	1.49
23	b	2514	CLA	C1-C2	2.16	1.55	1.49
27	d	2360	BCR	C24-C23	2.16	1.39	1.33
23	B	511	CLA	C3A-C4A	-2.15	1.44	1.51
23	B	514	CLA	C3A-C4A	-2.15	1.44	1.51
23	C	483	CLA	C2-C3	2.15	1.38	1.33
23	b	2519	CLA	C5-C3	2.15	1.55	1.51
23	C	479	CLA	MG-NC	2.15	2.11	2.06
25	D	357	PL9	C7-C8	-2.14	1.47	1.50
23	B	517	CLA	C4-C3	2.14	1.55	1.50
23	c	2484	CLA	CMB-C2B	2.14	1.55	1.50
23	a	2351	CLA	C1B-C2B	2.14	1.48	1.43
23	D	354	CLA	C1D-ND	-2.13	1.35	1.37
23	D	356	CLA	C5-C3	2.13	1.55	1.51
23	b	2518	CLA	CHC-C1C	2.13	1.42	1.38
28	v	2138	HEC	O1D-CGD	2.13	1.29	1.22
23	b	2526	CLA	MG-NB	2.13	2.10	2.05
28	v	2138	HEC	C3B-C2B	2.13	1.41	1.36
23	B	514	CLA	O2A-CGA	2.13	1.39	1.33
23	b	2515	CLA	C1D-C2D	-2.13	1.41	1.45
23	c	2487	CLA	CMD-C2D	2.13	1.55	1.50
25	a	2352	PL9	C21-C19	-2.13	1.46	1.51
27	C	488	BCR	C19-C18	-2.12	1.41	1.46
23	c	2484	CLA	C5-C3	2.12	1.55	1.51
23	A	352	CLA	C4C-C3C	2.12	1.48	1.45
23	b	2524	CLA	O2A-C1	2.12	1.51	1.46
28	v	2138	HEC	C4D-C3D	-2.12	1.41	1.45
23	B	514	CLA	C1D-ND	-2.12	1.35	1.37
25	A	353	PL9	C40-C39	2.12	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	2354	CLA	C1-C2	2.12	1.55	1.49
23	C	474	CLA	C1C-NC	-2.12	1.34	1.37
23	b	2526	CLA	C3B-C4B	2.12	1.48	1.42
23	B	521	CLA	CHC-C1C	2.12	1.42	1.38
23	C	483	CLA	C1D-ND	-2.12	1.35	1.37
23	b	2521	CLA	C1-C2	2.12	1.55	1.49
23	c	2484	CLA	C1-C2	2.12	1.55	1.49
23	B	511	CLA	C5-C3	2.12	1.55	1.51
23	C	483	CLA	C1-C2	2.11	1.55	1.49
23	C	475	CLA	C1D-C2D	-2.11	1.41	1.45
23	B	511	CLA	C4-C3	2.11	1.55	1.50
23	B	522	CLA	CAA-C2A	2.11	1.57	1.54
23	C	483	CLA	CHB-C4A	2.11	1.43	1.37
23	b	2523	CLA	CHB-C4A	2.10	1.43	1.37
23	B	516	CLA	O2A-CGA	2.10	1.39	1.33
25	d	2358	PL9	C36-C34	-2.10	1.47	1.51
27	K	50	BCR	C15-C14	-2.10	1.36	1.43
23	b	2525	CLA	CHB-C4A	2.10	1.42	1.37
23	c	2480	CLA	CMB-C2B	2.10	1.55	1.50
23	C	481	CLA	C1D-C2D	-2.10	1.41	1.45
23	b	2515	CLA	CBA-CGA	-2.10	1.44	1.50
23	B	521	CLA	C5-C3	2.10	1.55	1.51
23	b	2520	CLA	C1D-C2D	-2.10	1.41	1.45
23	C	479	CLA	C1-C2	2.10	1.55	1.49
23	A	352	CLA	C1B-C2B	2.09	1.48	1.43
23	b	2526	CLA	CHD-C1D	2.09	1.42	1.38
27	B	528	BCR	C38-C26	2.09	1.54	1.50
23	c	2481	CLA	CHB-C4A	2.09	1.42	1.37
23	c	2481	CLA	C1D-ND	-2.09	1.35	1.37
24	d	2356	PHO	CAA-CBA	-2.09	1.46	1.52
23	C	487	CLA	CMA-C3A	2.08	1.57	1.53
23	B	519	CLA	CMB-C2B	2.08	1.55	1.50
23	B	527	CLA	C3B-C4B	2.08	1.48	1.42
24	A	351	PHO	C1D-ND	-2.08	1.34	1.38
23	D	356	CLA	CAA-C2A	2.08	1.57	1.54
23	C	476	CLA	CHB-C4A	2.08	1.42	1.37
23	C	478	CLA	C2-C3	2.08	1.37	1.33
23	C	477	CLA	CMB-C2B	2.07	1.55	1.50
23	b	2512	CLA	C5-C3	2.07	1.55	1.51
23	c	2479	CLA	C3A-C4A	-2.07	1.45	1.51
23	c	2486	CLA	C5-C3	2.07	1.55	1.51
23	c	2474	CLA	C4C-C3C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	2351	CLA	C1D-ND	-2.07	1.35	1.37
23	B	520	CLA	C5-C3	2.07	1.55	1.51
23	b	2516	CLA	CHD-C1D	2.07	1.42	1.38
23	c	2481	CLA	C1C-C2C	2.07	1.48	1.44
23	c	2482	CLA	CMD-C2D	2.07	1.55	1.50
23	C	476	CLA	C4-C3	2.06	1.55	1.50
25	D	357	PL9	C36-C34	-2.06	1.47	1.51
23	C	484	CLA	CMB-C2B	2.06	1.55	1.50
23	a	2348	CLA	C3B-C4B	2.06	1.48	1.42
27	F	48	BCR	C24-C23	2.06	1.39	1.33
23	B	512	CLA	C1B-C2B	2.06	1.48	1.43
23	D	354	CLA	CHB-C1B	-2.06	1.34	1.39
23	b	2515	CLA	CHD-C1D	2.06	1.42	1.38
23	B	513	CLA	MG-ND	-2.06	2.01	2.05
23	c	2484	CLA	CHB-C4A	2.06	1.42	1.37
28	e	2084	HEC	CHC-C1C	2.06	1.44	1.39
28	v	2138	HEC	C2A-C3A	2.06	1.41	1.36
23	C	487	CLA	CMD-C2D	2.05	1.55	1.50
23	b	2522	CLA	C1C-NC	-2.05	1.34	1.37
23	B	518	CLA	C1D-ND	-2.05	1.35	1.37
23	c	2479	CLA	C1-C2	2.05	1.55	1.49
23	C	486	CLA	CMB-C2B	2.05	1.55	1.50
23	c	2484	CLA	C1C-C2C	2.05	1.48	1.44
23	b	2514	CLA	C3A-C4A	-2.05	1.45	1.51
23	D	356	CLA	C1B-C2B	2.04	1.47	1.43
23	b	2514	CLA	O2A-CGA	2.04	1.39	1.33
23	B	522	CLA	C5-C3	2.04	1.55	1.51
23	c	2476	CLA	C1B-C2B	2.04	1.47	1.43
23	C	485	CLA	CBA-CGA	-2.04	1.44	1.50
24	D	355	PHO	C4-C3	2.04	1.55	1.50
28	e	2084	HEC	CBA-CGA	-2.04	1.45	1.50
23	b	2517	CLA	C3A-C4A	-2.04	1.45	1.51
23	C	487	CLA	C4D-CHA	2.03	1.45	1.38
23	D	356	CLA	CMB-C2B	2.03	1.54	1.50
27	C	488	BCR	C40-C30	-2.03	1.49	1.53
23	b	2517	CLA	O2A-CGA	2.03	1.39	1.33
23	A	348	CLA	C4-C3	2.03	1.55	1.50
23	a	2348	CLA	C4-C3	2.03	1.55	1.50
27	k	2050	BCR	C38-C26	2.03	1.54	1.50
23	D	354	CLA	CHB-C4A	2.03	1.42	1.37
23	c	2474	CLA	C1-C2	2.03	1.54	1.49
23	c	2477	CLA	C1-C2	2.03	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	2350	PHO	C1D-ND	-2.02	1.35	1.38
23	B	525	CLA	CMB-C2B	2.02	1.54	1.50
27	c	2489	BCR	C38-C26	2.02	1.54	1.50
23	C	482	CLA	C4C-C3C	2.02	1.48	1.45
25	d	2358	PL9	C22-C23	-2.02	1.44	1.50
23	b	2521	CLA	O2A-CGA	2.02	1.39	1.33
23	b	2513	CLA	C2-C3	2.02	1.37	1.33
23	B	525	CLA	C1D-C2D	-2.02	1.41	1.45
23	a	2348	CLA	CBA-CGA	-2.02	1.44	1.50
25	d	2358	PL9	C7-C8	-2.02	1.47	1.50
23	D	356	CLA	C1D-ND	-2.01	1.35	1.37
23	b	2518	CLA	MG-ND	-2.01	2.01	2.05
23	c	2475	CLA	C6-C5	2.01	1.59	1.52
23	B	511	CLA	C1C-C2C	2.01	1.48	1.44
23	b	2517	CLA	C1D-ND	-2.01	1.35	1.37
23	c	2487	CLA	C4D-CHA	2.01	1.45	1.38
23	b	2519	CLA	MG-NC	2.01	2.11	2.06
23	C	484	CLA	C5-C3	2.01	1.55	1.51
23	C	484	CLA	OBD-CAD	2.01	1.25	1.22
23	c	2483	CLA	CHC-C1C	2.00	1.42	1.38
23	c	2474	CLA	C1D-C2D	-2.00	1.41	1.45
27	b	2528	BCR	C37-C22	2.00	1.54	1.50
23	A	348	CLA	C1B-NB	-2.00	1.35	1.37
23	B	512	CLA	CHC-C1C	2.00	1.42	1.38
23	D	356	CLA	CHB-C4A	2.00	1.42	1.37
23	B	527	CLA	CMD-C2D	2.00	1.54	1.50
23	C	477	CLA	C1C-NC	-2.00	1.34	1.37
23	C	479	CLA	CMB-C2B	2.00	1.54	1.50

All (1364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2513	CLA	C4A-NA-C1A	14.75	113.41	106.68
23	B	513	CLA	C4A-NA-C1A	14.60	113.34	106.68
23	c	2479	CLA	C4A-NA-C1A	14.27	113.19	106.68
23	B	511	CLA	C4A-NA-C1A	14.15	113.13	106.68
23	B	519	CLA	C4A-NA-C1A	13.99	113.06	106.68
23	b	2511	CLA	C4A-NA-C1A	13.96	113.05	106.68
23	d	2357	CLA	C4A-NA-C1A	13.85	113.00	106.68
23	D	356	CLA	C4A-NA-C1A	13.83	112.99	106.68
23	C	479	CLA	C4A-NA-C1A	13.81	112.98	106.68
23	b	2512	CLA	C4A-NA-C1A	13.75	112.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2523	CLA	C4A-NA-C1A	13.68	112.92	106.68
23	B	523	CLA	C4A-NA-C1A	13.52	112.85	106.68
23	B	512	CLA	C4A-NA-C1A	13.41	112.80	106.68
23	B	517	CLA	C4A-NA-C1A	13.35	112.77	106.68
23	C	483	CLA	C4A-NA-C1A	13.32	112.76	106.68
23	A	352	CLA	C4A-NA-C1A	13.32	112.75	106.68
23	A	349	CLA	C4A-NA-C1A	13.25	112.72	106.68
23	b	2525	CLA	C4A-NA-C1A	13.24	112.72	106.68
23	b	2522	CLA	C4A-NA-C1A	13.20	112.70	106.68
23	B	524	CLA	C4A-NA-C1A	13.19	112.70	106.68
23	C	476	CLA	C4A-NA-C1A	13.18	112.69	106.68
23	c	2483	CLA	C4A-NA-C1A	13.16	112.69	106.68
23	c	2478	CLA	C4A-NA-C1A	13.14	112.67	106.68
23	B	522	CLA	C4A-NA-C1A	13.14	112.67	106.68
23	a	2351	CLA	C4A-NA-C1A	13.07	112.64	106.68
23	b	2520	CLA	C4A-NA-C1A	13.07	112.64	106.68
23	C	474	CLA	C4A-NA-C1A	13.05	112.63	106.68
23	C	478	CLA	C4A-NA-C1A	13.01	112.61	106.68
23	C	482	CLA	C4A-NA-C1A	13.00	112.61	106.68
23	b	2518	CLA	C4A-NA-C1A	12.96	112.59	106.68
23	B	518	CLA	C4A-NA-C1A	12.96	112.59	106.68
23	b	2524	CLA	C4A-NA-C1A	12.92	112.57	106.68
23	B	525	CLA	C4A-NA-C1A	12.91	112.57	106.68
23	c	2484	CLA	C4A-NA-C1A	12.90	112.56	106.68
23	C	481	CLA	C4A-NA-C1A	12.84	112.54	106.68
23	b	2519	CLA	C4A-NA-C1A	12.83	112.53	106.68
23	c	2481	CLA	C4A-NA-C1A	12.80	112.52	106.68
23	c	2480	CLA	C4A-NA-C1A	12.78	112.51	106.68
23	b	2517	CLA	C4A-NA-C1A	12.72	112.48	106.68
23	B	520	CLA	C4A-NA-C1A	12.68	112.46	106.68
23	c	2486	CLA	C4A-NA-C1A	12.65	112.45	106.68
23	C	480	CLA	C4A-NA-C1A	12.61	112.43	106.68
23	d	2355	CLA	C4A-NA-C1A	12.61	112.43	106.68
23	C	484	CLA	C4A-NA-C1A	12.60	112.43	106.68
23	B	516	CLA	C4A-NA-C1A	12.60	112.43	106.68
23	b	2516	CLA	C4A-NA-C1A	12.58	112.42	106.68
23	c	2474	CLA	C4A-NA-C1A	12.54	112.40	106.68
23	c	2476	CLA	C4A-NA-C1A	12.50	112.38	106.68
23	C	475	CLA	C4A-NA-C1A	12.43	112.35	106.68
23	c	2482	CLA	C4A-NA-C1A	12.38	112.33	106.68
23	B	514	CLA	C4A-NA-C1A	12.37	112.32	106.68
23	b	2514	CLA	C4A-NA-C1A	12.34	112.31	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	486	CLA	C4A-NA-C1A	12.30	112.29	106.68
23	b	2515	CLA	C4A-NA-C1A	12.10	112.20	106.68
23	b	2526	CLA	C4A-NA-C1A	12.02	112.16	106.68
23	c	2485	CLA	C4A-NA-C1A	11.99	112.15	106.68
23	A	348	CLA	C4A-NA-C1A	11.83	112.08	106.68
23	B	527	CLA	C4A-NA-C1A	11.80	112.06	106.68
23	B	515	CLA	C4A-NA-C1A	11.72	112.03	106.68
23	c	2475	CLA	C4A-NA-C1A	11.69	112.01	106.68
23	C	485	CLA	C4A-NA-C1A	11.56	111.95	106.68
23	d	2354	CLA	C4A-NA-C1A	11.53	111.94	106.68
23	D	354	CLA	C4A-NA-C1A	11.50	111.92	106.68
23	a	2348	CLA	C4A-NA-C1A	11.49	111.92	106.68
23	b	2521	CLA	C4A-NA-C1A	11.33	111.85	106.68
23	A	350	CLA	C4A-NA-C1A	11.28	111.83	106.68
23	c	2477	CLA	C4A-NA-C1A	11.28	111.83	106.68
23	B	521	CLA	C4A-NA-C1A	11.24	111.81	106.68
23	C	477	CLA	C4A-NA-C1A	11.14	111.76	106.68
23	C	487	CLA	C4A-NA-C1A	11.06	111.72	106.68
24	d	2356	PHO	C4D-CHA-CBD	-11.02	103.17	108.45
23	a	2349	CLA	C4A-NA-C1A	10.96	111.68	106.68
24	D	355	PHO	C4D-CHA-CBD	-10.61	103.36	108.45
23	c	2487	CLA	C4A-NA-C1A	10.36	111.41	106.68
23	B	520	CLA	CBA-CAA-C2A	9.79	142.93	113.79
23	b	2520	CLA	CBA-CAA-C2A	9.77	142.88	113.79
26	d	2359	LMT	O1'-C1-C2	9.19	140.53	109.37
26	B	526	LMT	O1'-C1-C2	9.17	140.49	109.37
24	A	351	PHO	C4D-CHA-CBD	-8.89	104.19	108.45
24	a	2350	PHO	C4D-CHA-CBD	-8.86	104.20	108.45
23	A	349	CLA	C1-C2-C3	8.19	139.61	126.20
23	C	477	CLA	CBA-CAA-C2A	7.90	137.30	113.79
23	d	2355	CLA	C1-C2-C3	7.80	138.98	126.20
23	c	2477	CLA	CBA-CAA-C2A	7.80	137.00	113.79
23	B	519	CLA	C1-C2-C3	7.66	138.74	126.20
23	d	2354	CLA	C1-C2-C3	7.61	138.66	126.20
23	D	354	CLA	C1-C2-C3	7.57	138.59	126.20
23	b	2519	CLA	C1-C2-C3	7.52	138.52	126.20
23	B	520	CLA	CAA-C2A-C1A	-7.51	87.37	111.97
23	b	2520	CLA	CAA-C2A-C1A	-7.49	87.43	111.97
23	C	481	CLA	CBA-CAA-C2A	6.96	134.49	113.79
23	b	2524	CLA	C1-C2-C3	6.92	137.53	126.20
27	b	2527	BCR	C33-C5-C6	6.90	132.01	124.48
27	B	528	BCR	C33-C5-C6	6.90	132.01	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2481	CLA	CBA-CAA-C2A	6.74	133.84	113.79
23	B	524	CLA	C1-C2-C3	6.64	137.08	126.20
25	a	2352	PL9	C22-C23-C24	6.49	142.47	127.62
23	b	2520	CLA	CAA-CBA-CGA	-6.48	94.80	113.21
23	B	520	CLA	CAA-CBA-CGA	-6.43	94.95	113.21
23	b	2519	CLA	CBA-CAA-C2A	6.43	132.92	113.79
28	v	2138	HEC	C1C-C2C-C3C	-6.39	99.50	106.82
28	v	2138	HEC	CAC-C3C-C4C	-6.38	116.13	124.91
28	V	138	HEC	CHB-C1B-NB	6.35	131.25	124.42
27	B	529	BCR	C38-C26-C25	6.33	131.40	124.48
25	D	357	PL9	C37-C36-C34	6.27	133.97	113.19
25	d	2358	PL9	C37-C36-C34	6.25	133.88	113.19
23	B	519	CLA	CBA-CAA-C2A	6.23	132.33	113.79
27	d	2360	BCR	C33-C5-C6	6.21	131.26	124.48
23	c	2477	CLA	CAA-C2A-C1A	-6.20	91.66	111.97
23	C	483	CLA	CBA-CAA-C2A	6.19	132.20	113.79
28	V	138	HEC	CBC-CAC-C3C	6.15	129.10	112.42
23	C	477	CLA	CAA-C2A-C1A	-6.11	91.96	111.97
27	F	48	BCR	C33-C5-C6	5.95	130.97	124.48
27	B	529	BCR	C20-C21-C22	-5.94	118.94	127.28
23	c	2483	CLA	CBA-CAA-C2A	5.94	131.48	113.79
27	j	2053	BCR	C33-C5-C6	5.90	130.92	124.48
27	b	2527	BCR	C38-C26-C25	5.90	130.92	124.48
27	F	48	BCR	C16-C17-C18	5.88	135.53	127.28
25	A	353	PL9	C22-C23-C24	5.88	141.08	127.62
28	V	138	HEC	CBD-CAD-C3D	-5.86	96.33	112.53
25	A	353	PL9	C37-C36-C34	5.85	132.56	113.19
23	B	519	CLA	CAA-C2A-C1A	-5.76	93.09	111.97
23	b	2519	CLA	CAA-C2A-C1A	-5.74	93.15	111.97
25	a	2352	PL9	C37-C36-C34	5.74	132.20	113.19
27	B	528	BCR	C38-C26-C25	5.74	130.75	124.48
27	J	53	BCR	C33-C5-C6	5.72	130.72	124.48
27	J	53	BCR	C38-C26-C25	5.71	130.72	124.48
27	d	2360	BCR	C16-C17-C18	5.71	135.29	127.28
27	b	2528	BCR	C38-C26-C25	5.69	130.70	124.48
28	V	138	HEC	CHA-C1A-NA	-5.68	118.27	124.45
27	c	2489	BCR	C33-C5-C6	5.63	130.63	124.48
27	j	2053	BCR	C38-C26-C25	5.54	130.53	124.48
27	b	2528	BCR	C20-C21-C22	-5.52	119.53	127.28
27	C	489	BCR	C33-C5-C6	5.50	130.49	124.48
27	F	48	BCR	C38-C26-C25	5.49	130.47	124.48
23	C	475	CLA	O2A-CGA-CBA	5.43	128.40	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2475	CLA	O2A-CGA-CBA	5.39	128.27	111.83
27	K	50	BCR	C38-C26-C25	5.34	130.31	124.48
23	C	481	CLA	CAA-CBA-CGA	-5.29	98.19	113.21
23	B	516	CLA	O2A-CGA-CBA	5.27	127.90	111.83
23	b	2516	CLA	O2A-CGA-CBA	5.22	127.76	111.83
23	B	512	CLA	C1-C2-C3	5.22	134.75	126.20
23	c	2481	CLA	CAA-CBA-CGA	-5.22	98.38	113.21
27	d	2360	BCR	C38-C26-C25	5.15	130.10	124.48
27	k	2050	BCR	C38-C26-C25	5.06	130.00	124.48
23	b	2512	CLA	C1-C2-C3	5.04	134.46	126.20
27	C	488	BCR	C38-C26-C25	4.99	129.93	124.48
23	c	2478	CLA	C1-C2-C3	4.96	134.32	126.20
25	A	353	PL9	C35-C34-C36	-4.95	106.63	115.23
27	C	488	BCR	C33-C5-C6	4.92	129.85	124.48
27	F	48	BCR	C11-C10-C9	4.89	134.14	127.28
28	v	2138	HEC	CMD-C2D-C1D	-4.84	117.47	125.03
27	K	50	BCR	C33-C5-C6	4.82	129.75	124.48
27	c	2488	BCR	C38-C26-C25	4.82	129.75	124.48
27	c	2488	BCR	C33-C5-C6	4.80	129.72	124.48
24	D	355	PHO	O2D-CGD-CBD	4.78	116.20	110.95
27	d	2360	BCR	C11-C10-C9	4.73	133.92	127.28
28	v	2138	HEC	CMD-C2D-C3D	4.72	138.92	126.15
25	a	2352	PL9	C35-C34-C36	-4.71	107.05	115.23
27	B	529	BCR	C2-C1-C6	4.70	117.27	110.44
23	c	2477	CLA	C7-C6-C5	-4.69	100.77	113.26
23	C	478	CLA	C1-C2-C3	4.68	133.87	126.20
26	d	2359	LMT	C1B-O1B-C4'	-4.68	106.88	117.98
27	k	2050	BCR	C33-C5-C6	4.68	129.59	124.48
23	B	518	CLA	CBA-CAA-C2A	4.67	127.70	113.79
23	c	2483	CLA	CAA-C2A-C1A	-4.66	96.70	111.97
23	C	477	CLA	CAA-CBA-CGA	-4.65	100.00	113.21
28	v	2138	HEC	CHA-C4D-ND	4.63	129.41	124.42
23	C	477	CLA	C7-C6-C5	-4.63	100.93	113.26
27	F	48	BCR	C8-C9-C10	-4.61	111.76	119.01
23	c	2479	CLA	CAA-CBA-CGA	-4.60	100.16	113.21
23	b	2523	CLA	CBA-CAA-C2A	4.58	127.41	113.79
23	B	523	CLA	CBA-CAA-C2A	4.57	127.39	113.79
23	b	2518	CLA	CBA-CAA-C2A	4.56	127.38	113.79
28	v	2138	HEC	CMC-C2C-C3C	4.56	135.30	125.62
23	c	2477	CLA	CAA-CBA-CGA	-4.54	100.31	113.21
27	c	2489	BCR	C38-C26-C25	4.54	129.44	124.48
23	C	483	CLA	CAA-C2A-C1A	-4.54	97.11	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	489	BCR	C38-C26-C25	4.52	129.42	124.48
25	A	353	PL9	C36-C34-C33	4.52	131.30	121.17
27	b	2528	BCR	C2-C1-C6	4.48	116.94	110.44
28	V	138	HEC	C3B-C4B-NB	-4.48	105.26	110.17
24	a	2350	PHO	O2D-CGD-CBD	4.48	115.86	110.95
25	a	2352	PL9	C26-C24-C23	-4.46	111.17	121.17
24	A	351	PHO	O2D-CGD-CBD	4.44	115.82	110.95
26	B	526	LMT	C1B-O1B-C4'	-4.44	107.46	117.98
27	B	529	BCR	C21-C20-C19	4.43	136.04	123.20
23	B	511	CLA	CBA-CAA-C2A	4.43	126.98	113.79
27	F	48	BCR	C7-C8-C9	4.43	132.79	126.23
23	B	527	CLA	C1-O2A-CGA	4.42	127.36	116.65
23	b	2511	CLA	CBA-CAA-C2A	4.42	126.95	113.79
25	a	2352	PL9	C36-C34-C33	4.42	131.08	121.17
27	d	2360	BCR	C8-C9-C10	-4.41	112.07	119.01
23	b	2524	CLA	C1-O2A-CGA	4.39	127.29	116.65
23	b	2513	CLA	CAA-CBA-CGA	4.39	125.68	113.21
25	D	357	PL9	C35-C34-C36	-4.39	107.61	115.23
23	b	2526	CLA	C1-O2A-CGA	4.38	127.26	116.65
27	b	2528	BCR	C21-C20-C19	4.37	135.88	123.20
27	K	50	BCR	C2-C1-C6	4.36	116.77	110.44
27	B	528	BCR	C2-C1-C6	4.33	116.73	110.44
27	k	2050	BCR	C2-C1-C6	4.31	116.70	110.44
23	B	513	CLA	CAA-CBA-CGA	4.31	125.44	113.21
23	B	524	CLA	C1-O2A-CGA	4.30	127.06	116.65
23	D	356	CLA	C1-C2-C3	4.30	133.24	126.20
23	C	479	CLA	CAA-CBA-CGA	-4.28	101.07	113.21
23	a	2351	CLA	C1-C2-C3	4.25	133.16	126.20
23	c	2476	CLA	C1-C2-C3	4.25	133.16	126.20
23	d	2357	CLA	C1-C2-C3	4.25	133.16	126.20
25	d	2358	PL9	C35-C34-C36	-4.24	107.87	115.23
23	C	487	CLA	CAC-C3C-C4C	4.19	130.24	124.79
28	v	2138	HEC	CBD-CAD-C3D	-4.17	101.00	112.53
27	d	2360	BCR	C7-C8-C9	4.16	132.39	126.23
23	B	513	CLA	CBA-CAA-C2A	4.14	126.10	113.79
27	C	488	BCR	C16-C17-C18	4.10	133.03	127.28
23	c	2481	CLA	CAA-C2A-C1A	-4.08	98.59	111.97
28	V	138	HEC	C1B-C2B-C3B	4.07	111.26	106.98
23	B	519	CLA	CAA-CBA-CGA	-4.06	101.67	113.21
27	b	2527	BCR	C33-C5-C4	-4.06	104.94	113.60
23	b	2518	CLA	O2A-CGA-CBA	4.06	124.22	111.83
23	c	2482	CLA	C1-C2-C3	4.06	132.85	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	2527	BCR	C2-C1-C6	4.05	116.33	110.44
27	b	2527	BCR	C29-C30-C25	4.02	116.28	110.44
27	d	2360	BCR	C23-C24-C25	4.02	137.74	127.00
25	A	353	PL9	C26-C24-C23	-4.02	112.15	121.17
27	C	489	BCR	C2-C1-C6	4.02	116.27	110.44
23	B	518	CLA	O2A-CGA-CBA	4.01	124.08	111.83
27	c	2488	BCR	C29-C30-C25	4.01	116.27	110.44
23	C	482	CLA	C1-C2-C3	4.01	132.77	126.20
27	J	53	BCR	C29-C30-C25	4.01	116.27	110.44
23	C	479	CLA	CBA-CAA-C2A	4.00	125.69	113.79
23	C	476	CLA	C1-C2-C3	4.00	132.75	126.20
23	C	482	CLA	C1-O2A-CGA	3.99	126.31	116.65
23	b	2526	CLA	C7-C6-C5	-3.98	102.64	113.26
25	a	2352	PL9	C7-C8-C9	3.98	133.68	126.83
28	V	138	HEC	C4A-NA-C1A	-3.97	99.35	105.82
23	B	511	CLA	CAA-C2A-C1A	-3.96	99.00	111.97
27	C	489	BCR	C29-C30-C25	3.96	116.19	110.44
27	B	528	BCR	C29-C30-C25	3.95	116.18	110.44
27	B	529	BCR	C30-C25-C26	-3.95	117.24	122.64
23	c	2479	CLA	CBA-CAA-C2A	3.94	125.53	113.79
28	e	2084	HEC	C2A-C1A-NA	3.94	114.13	110.32
23	b	2526	CLA	CAA-CBA-CGA	-3.94	102.03	113.21
23	B	527	CLA	C7-C6-C5	-3.93	102.78	113.26
23	a	2348	CLA	C1-O2A-CGA	3.93	126.17	116.65
23	b	2511	CLA	CAA-C2A-C1A	-3.92	99.12	111.97
25	D	357	PL9	C30-C29-C31	3.92	122.03	115.23
23	c	2487	CLA	CAC-C3C-C4C	3.91	129.88	124.79
27	c	2488	BCR	C16-C17-C18	3.90	132.75	127.28
24	a	2350	PHO	C1-C2-C3	3.90	132.59	126.20
25	A	353	PL9	C7-C8-C9	3.90	133.55	126.83
28	v	2138	HEC	C4C-C3C-C2C	3.89	112.89	106.87
23	B	514	CLA	O2A-CGA-CBA	3.88	123.67	111.83
28	V	138	HEC	CHB-C1B-C2B	-3.87	118.92	125.03
23	B	514	CLA	CBA-CAA-C2A	3.86	125.28	113.79
23	C	481	CLA	CAA-C2A-C1A	-3.86	99.33	111.97
27	F	48	BCR	C2-C1-C6	3.86	116.04	110.44
23	b	2516	CLA	O2A-C1-C2	3.85	122.93	108.11
23	b	2513	CLA	CBA-CAA-C2A	3.85	125.25	113.79
23	B	518	CLA	CAA-C2A-C1A	-3.85	99.37	111.97
23	A	348	CLA	C1-O2A-CGA	3.84	125.96	116.65
23	c	2482	CLA	C1-O2A-CGA	3.84	125.96	116.65
23	B	516	CLA	O2A-C1-C2	3.84	122.88	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	511	CLA	CAA-CBA-CGA	-3.84	102.31	113.21
27	b	2528	BCR	C30-C25-C26	-3.82	117.41	122.64
27	c	2489	BCR	C2-C1-C6	3.82	115.99	110.44
27	C	489	BCR	C23-C24-C25	3.81	137.19	127.00
23	b	2514	CLA	CAA-C2A-C3A	-3.81	102.69	113.00
23	b	2512	CLA	C1-O2A-CGA	3.81	125.87	116.65
23	b	2519	CLA	CAA-CBA-CGA	-3.81	102.39	113.21
23	B	513	CLA	C7-C6-C5	-3.81	103.12	113.26
27	F	48	BCR	C23-C24-C25	3.81	137.17	127.00
27	b	2528	BCR	C29-C30-C25	3.81	115.97	110.44
23	B	527	CLA	CAA-CBA-CGA	-3.81	102.40	113.21
27	K	50	BCR	C29-C30-C25	3.80	115.97	110.44
23	c	2476	CLA	C7-C6-C5	-3.80	103.12	113.26
23	A	349	CLA	CBA-CAA-C2A	3.80	125.09	113.79
27	d	2360	BCR	C29-C30-C25	3.79	115.95	110.44
28	V	138	HEC	C3D-C4D-ND	-3.78	106.69	110.35
23	d	2355	CLA	CBA-CAA-C2A	3.78	125.04	113.79
27	B	528	BCR	C33-C5-C4	-3.78	105.53	113.60
27	d	2360	BCR	C2-C1-C6	3.77	115.92	110.44
23	b	2525	CLA	CED-O2D-CGD	3.76	124.45	115.92
25	d	2358	PL9	C30-C29-C31	3.76	121.75	115.23
23	A	349	CLA	O2A-CGA-CBA	3.76	123.29	111.83
23	C	474	CLA	CBA-CAA-C2A	3.75	124.94	113.79
28	V	138	HEC	O1D-CGD-CBD	-3.74	111.22	123.09
23	A	350	CLA	CBA-CAA-C2A	3.74	124.93	113.79
23	B	514	CLA	CAA-C2A-C1A	-3.74	99.71	111.97
24	d	2356	PHO	C2D-C1D-ND	3.74	112.13	109.43
24	a	2350	PHO	OBD-CAD-CBD	-3.74	120.34	125.82
23	b	2518	CLA	CAA-C2A-C1A	-3.73	99.76	111.97
23	B	523	CLA	CAA-CBA-CGA	-3.73	102.63	113.21
23	C	478	CLA	C2A-C1A-CHA	3.72	130.32	123.87
23	c	2474	CLA	CBA-CAA-C2A	3.71	124.84	113.79
25	A	353	PL9	C21-C22-C23	-3.71	93.65	112.02
25	A	353	PL9	C27-C26-C24	-3.71	100.89	113.19
23	b	2514	CLA	CBA-CAA-C2A	3.71	124.83	113.79
24	D	355	PHO	C7-C6-C5	-3.71	103.37	113.26
23	C	479	CLA	CAA-C2A-C1A	-3.71	99.82	111.97
23	B	514	CLA	CAA-C2A-C3A	-3.71	102.98	113.00
23	b	2523	CLA	CAA-CBA-CGA	-3.71	102.68	113.21
23	b	2514	CLA	O2A-CGA-CBA	3.71	123.14	111.83
23	b	2526	CLA	C6-C5-C3	3.71	122.50	113.47
27	c	2489	BCR	C29-C30-C25	3.71	115.82	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	k	2050	BCR	C29-C30-C25	3.70	115.82	110.44
23	B	520	CLA	C1-C2-C3	3.70	132.27	126.20
23	B	523	CLA	CAA-C2A-C1A	-3.70	99.85	111.97
23	B	525	CLA	CED-O2D-CGD	3.69	124.30	115.92
27	b	2527	BCR	C24-C23-C22	3.69	131.70	126.23
23	c	2480	CLA	CBA-CAA-C2A	3.69	124.79	113.79
24	d	2356	PHO	O2D-CGD-CBD	3.68	114.99	110.95
23	B	512	CLA	C1-O2A-CGA	3.68	125.56	116.65
23	B	527	CLA	C6-C5-C3	3.68	122.42	113.47
27	B	529	BCR	C1-C6-C5	-3.67	117.62	122.64
27	c	2489	BCR	C23-C24-C25	3.67	136.80	127.00
23	c	2479	CLA	CAA-C2A-C1A	-3.66	99.97	111.97
23	b	2511	CLA	CAA-CBA-CGA	-3.66	102.81	113.21
23	b	2514	CLA	CAA-C2A-C1A	-3.66	99.98	111.97
27	F	48	BCR	C29-C30-C25	3.65	115.75	110.44
23	c	2478	CLA	C2A-C1A-CHA	3.65	130.21	123.87
27	J	53	BCR	C24-C23-C22	3.65	131.64	126.23
27	b	2528	BCR	C1-C6-C5	-3.65	117.65	122.64
27	B	528	BCR	C24-C23-C22	3.64	131.62	126.23
23	A	352	CLA	C1-C2-C3	3.63	132.15	126.20
23	b	2523	CLA	CAA-C2A-C1A	-3.63	100.09	111.97
23	B	515	CLA	CBA-CAA-C2A	3.62	124.58	113.79
23	b	2520	CLA	C1-C2-C3	3.62	132.13	126.20
24	D	355	PHO	C2D-C1D-ND	3.62	112.05	109.43
23	C	480	CLA	CBA-CAA-C2A	3.62	124.56	113.79
25	a	2352	PL9	C27-C26-C24	-3.62	101.19	113.19
23	b	2513	CLA	C7-C6-C5	-3.62	103.62	113.26
23	a	2349	CLA	CBA-CAA-C2A	3.62	124.55	113.79
27	j	2053	BCR	C24-C23-C22	3.61	131.57	126.23
23	b	2523	CLA	CED-O2D-CGD	3.60	124.08	115.92
27	B	529	BCR	C29-C30-C25	3.60	115.67	110.44
23	d	2355	CLA	O2A-CGA-CBA	3.60	122.81	111.83
23	c	2483	CLA	O2A-CGA-CBA	3.60	122.80	111.83
27	C	488	BCR	C29-C30-C25	3.59	115.66	110.44
23	C	484	CLA	C1-C2-C3	3.59	132.07	126.20
27	F	48	BCR	C16-C15-C14	3.59	130.86	123.52
27	C	488	BCR	C23-C24-C25	3.58	136.57	127.00
25	a	2352	PL9	C21-C22-C23	-3.57	94.33	112.02
23	B	515	CLA	CED-O2D-CGD	3.57	124.02	115.92
23	B	513	CLA	C1-C2-C3	3.57	132.05	126.20
25	D	357	PL9	C36-C34-C33	3.57	129.17	121.17
23	C	479	CLA	C7-C6-C5	-3.56	103.77	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2475	CLA	CED-O2D-CGD	3.56	123.99	115.92
25	a	2352	PL9	C32-C31-C29	3.55	124.94	113.19
23	a	2349	CLA	C7-C6-C5	-3.55	103.81	113.26
23	c	2478	CLA	O2A-CGA-CBA	3.54	122.62	111.83
23	b	2525	CLA	C7-C6-C5	-3.53	103.86	113.26
23	C	478	CLA	O2A-CGA-CBA	3.53	122.59	111.83
23	c	2486	CLA	C1-C2-C3	3.53	131.98	126.20
23	C	474	CLA	C1-O2A-CGA	3.53	125.19	116.65
25	A	353	PL9	C32-C31-C29	3.53	124.87	113.19
23	b	2515	CLA	CBA-CAA-C2A	3.52	124.27	113.79
25	d	2358	PL9	C36-C34-C33	3.52	129.07	121.17
27	d	2360	BCR	C33-C5-C4	-3.52	106.09	113.60
23	b	2515	CLA	C1-C2-C3	3.52	131.96	126.20
23	B	523	CLA	CED-O2D-CGD	3.51	123.88	115.92
23	B	527	CLA	O2A-C1-C2	-3.51	94.60	108.11
23	c	2477	CLA	O2A-CGA-CBA	3.51	122.54	111.83
27	J	53	BCR	C2-C1-C6	3.50	115.53	110.44
23	B	521	CLA	CED-O2D-CGD	3.50	123.86	115.92
23	b	2513	CLA	C1-C2-C3	3.50	131.93	126.20
23	A	350	CLA	C7-C6-C5	-3.50	103.94	113.26
23	C	477	CLA	O2A-CGA-CBA	3.49	122.49	111.83
27	d	2360	BCR	C16-C15-C14	3.49	130.66	123.52
24	A	351	PHO	C1-C2-C3	3.48	131.90	126.20
23	C	483	CLA	O2A-CGA-CBA	3.48	122.45	111.83
27	b	2527	BCR	C38-C26-C27	-3.48	106.17	113.60
23	b	2526	CLA	O2A-C1-C2	-3.48	94.73	108.11
28	v	2138	HEC	CHC-C1C-C2C	-3.48	117.34	127.43
24	a	2350	PHO	C7-C6-C5	-3.47	104.00	113.26
27	c	2488	BCR	C23-C24-C25	3.47	136.27	127.00
23	c	2479	CLA	C7-C6-C5	-3.47	104.01	113.26
24	d	2356	PHO	C7-C6-C5	-3.47	104.02	113.26
27	J	53	BCR	C33-C5-C4	-3.47	106.20	113.60
23	b	2526	CLA	CBA-CAA-C2A	3.46	124.08	113.79
23	C	477	CLA	CED-O2D-CGD	3.45	123.75	115.92
27	j	2053	BCR	C7-C8-C9	3.45	131.34	126.23
23	c	2477	CLA	CED-O2D-CGD	3.45	123.73	115.92
23	c	2484	CLA	C1-C2-C3	3.44	131.84	126.20
23	d	2354	CLA	O2A-CGA-CBA	3.44	122.34	111.83
23	B	524	CLA	C7-C6-C5	-3.44	104.09	113.26
23	B	515	CLA	CAA-C2A-C3A	-3.44	103.70	113.00
23	B	527	CLA	CBA-CAA-C2A	3.43	124.00	113.79
23	C	486	CLA	C7-C6-C5	-3.43	104.13	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2520	CLA	O2D-CGD-CBD	3.42	117.22	111.23
23	D	354	CLA	O2A-CGA-CBA	3.42	122.27	111.83
27	c	2488	BCR	C8-C9-C10	-3.42	113.63	119.01
23	C	485	CLA	CED-O2D-CGD	3.42	123.67	115.92
28	V	138	HEC	CHA-C4D-ND	3.41	128.09	124.42
23	C	476	CLA	C7-C6-C5	-3.41	104.18	113.26
23	c	2481	CLA	C7-C6-C5	-3.41	104.19	113.26
23	b	2515	CLA	CED-O2D-CGD	3.41	123.64	115.92
27	F	48	BCR	C33-C5-C4	-3.40	106.35	113.60
23	C	483	CLA	C1-C2-C3	3.40	131.76	126.20
27	C	488	BCR	C2-C1-C6	3.39	115.37	110.44
28	v	2138	HEC	CHA-C4D-C3D	-3.39	119.83	124.77
23	C	486	CLA	C1-C2-C3	3.37	131.72	126.20
27	j	2053	BCR	C2-C1-C6	3.37	115.33	110.44
27	j	2053	BCR	C33-C5-C4	-3.37	106.41	113.60
23	b	2524	CLA	C5-C3-C2	-3.37	113.61	121.17
23	c	2485	CLA	CED-O2D-CGD	3.37	123.56	115.92
23	b	2515	CLA	C1-O2A-CGA	3.36	124.79	116.65
27	B	528	BCR	C38-C26-C27	-3.36	106.44	113.60
27	j	2053	BCR	C8-C9-C10	-3.35	113.74	119.01
23	B	515	CLA	CAA-CBA-CGA	-3.35	103.70	113.21
24	A	351	PHO	C7-C6-C5	-3.35	104.34	113.26
27	F	48	BCR	C38-C26-C27	-3.35	106.46	113.60
23	B	515	CLA	C1-C2-C3	3.34	131.68	126.20
23	b	2521	CLA	CED-O2D-CGD	3.34	123.49	115.92
23	B	517	CLA	O2A-CGA-CBA	3.34	122.02	111.83
27	b	2527	BCR	C23-C24-C25	3.34	135.92	127.00
27	c	2488	BCR	C2-C1-C6	3.34	115.29	110.44
23	c	2479	CLA	CED-O2D-CGD	3.34	123.48	115.92
27	B	529	BCR	C33-C5-C6	3.34	128.12	124.48
23	c	2487	CLA	CED-O2D-CGD	3.33	123.48	115.92
27	b	2528	BCR	C33-C5-C6	3.33	128.12	124.48
23	b	2515	CLA	CAA-C2A-C3A	-3.33	104.00	113.00
23	B	525	CLA	C1-C2-C3	3.33	131.65	126.20
23	c	2486	CLA	C7-C6-C5	-3.33	104.40	113.26
27	j	2053	BCR	C29-C30-C25	3.32	115.27	110.44
25	D	357	PL9	C32-C31-C29	3.32	124.19	113.19
24	A	351	PHO	OBD-CAD-CBD	-3.32	120.95	125.82
26	B	526	LMT	C1-O1'-C1'	-3.31	108.02	113.68
23	c	2486	CLA	O2A-CGA-CBA	3.31	121.92	111.83
23	B	512	CLA	C7-C6-C5	-3.31	104.45	113.26
23	C	481	CLA	C7-C6-C5	-3.30	104.46	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2513	CLA	O2A-CGA-CBA	3.30	121.90	111.83
27	c	2489	BCR	C7-C8-C9	3.30	131.12	126.23
27	j	2053	BCR	C23-C22-C21	-3.30	113.83	119.01
23	C	475	CLA	CED-O2D-CGD	3.29	123.38	115.92
27	C	488	BCR	C8-C9-C10	-3.29	113.84	119.01
27	B	529	BCR	C38-C26-C27	-3.29	106.59	113.60
25	d	2358	PL9	C32-C31-C29	3.28	124.06	113.19
23	b	2519	CLA	CED-O2D-CGD	3.28	123.35	115.92
28	V	138	HEC	C4A-CHB-C1B	-3.28	119.06	126.02
27	K	50	BCR	C7-C8-C9	3.28	131.08	126.23
23	c	2474	CLA	C7-C6-C5	-3.27	104.54	113.26
23	c	2484	CLA	CED-O2D-CGD	3.27	123.33	115.92
23	B	511	CLA	CED-O2D-CGD	3.27	123.33	115.92
27	B	528	BCR	C23-C24-C25	3.27	135.72	127.00
27	k	2050	BCR	C7-C8-C9	3.26	131.06	126.23
23	c	2478	CLA	CED-O2D-CGD	3.26	123.31	115.92
23	C	474	CLA	C1-C2-C3	3.26	131.54	126.20
23	b	2511	CLA	CED-O2D-CGD	3.26	123.30	115.92
27	C	488	BCR	C38-C26-C27	-3.25	106.66	113.60
23	c	2474	CLA	C1-O2A-CGA	3.25	124.53	116.65
23	B	519	CLA	O2A-CGA-CBA	3.25	121.75	111.83
23	C	485	CLA	C7-C6-C5	-3.25	104.60	113.26
23	B	515	CLA	C1-O2A-CGA	3.25	124.51	116.65
23	c	2474	CLA	O2D-CGD-CBD	3.24	116.89	111.23
23	C	480	CLA	O2A-CGA-CBA	3.23	121.69	111.83
23	b	2512	CLA	C7-C6-C5	-3.22	104.67	113.26
27	C	489	BCR	C33-C5-C4	-3.22	106.72	113.60
23	c	2483	CLA	C1-C2-C3	3.22	131.47	126.20
23	b	2517	CLA	O2A-CGA-CBA	3.22	121.66	111.83
23	C	486	CLA	O2A-CGA-CBA	3.22	121.64	111.83
23	B	525	CLA	C7-C6-C5	-3.21	104.70	113.26
23	b	2513	CLA	CED-O2D-CGD	3.21	123.20	115.92
23	B	524	CLA	C5-C3-C2	-3.21	113.97	121.17
28	v	2138	HEC	C4A-NA-C1A	-3.20	100.60	105.82
27	F	48	BCR	C34-C9-C8	3.20	122.98	118.09
28	v	2138	HEC	C1D-C2D-C3D	-3.20	103.61	106.98
27	d	2360	BCR	C30-C25-C26	-3.20	118.26	122.64
23	b	2524	CLA	C7-C6-C5	-3.19	104.75	113.26
23	b	2515	CLA	CAA-CBA-CGA	-3.19	104.14	113.21
24	D	355	PHO	O2A-CGA-CBA	3.19	121.57	111.83
23	b	2525	CLA	C1-C2-C3	3.19	131.42	126.20
23	B	513	CLA	CED-O2D-CGD	3.19	123.15	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V	138	HEC	CHC-C1C-NC	3.18	129.63	123.86
27	B	528	BCR	C8-C7-C6	3.18	135.50	127.00
23	B	513	CLA	C2A-C1A-CHA	3.18	129.39	123.87
23	b	2522	CLA	CED-O2D-CGD	3.18	123.13	115.92
23	c	2474	CLA	O2A-CGA-CBA	3.18	121.52	111.83
27	F	48	BCR	C30-C25-C26	-3.18	118.29	122.64
26	B	526	LMT	O1B-C1B-C2B	3.18	115.91	108.09
23	a	2351	CLA	CAA-C2A-C3A	-3.18	104.42	113.00
24	D	355	PHO	CED-O2D-CGD	3.17	123.11	115.92
23	c	2480	CLA	O2A-CGA-CBA	3.17	121.51	111.83
26	d	2359	LMT	O1B-C1B-C2B	3.17	115.89	108.09
23	C	479	CLA	CED-O2D-CGD	3.17	123.11	115.92
24	d	2356	PHO	O2A-CGA-CBA	3.17	121.50	111.83
27	d	2360	BCR	C38-C26-C27	-3.17	106.84	113.60
23	b	2519	CLA	O2A-CGA-CBA	3.16	121.48	111.83
23	C	474	CLA	O2A-CGA-CBA	3.16	121.47	111.83
27	J	53	BCR	C8-C7-C6	3.16	135.44	127.00
23	b	2517	CLA	CED-O2D-CGD	3.16	123.08	115.92
24	d	2356	PHO	C12-C11-C10	-3.16	99.13	113.28
23	C	487	CLA	CED-O2D-CGD	3.16	123.08	115.92
23	B	513	CLA	O2A-CGA-CBA	3.15	121.45	111.83
26	d	2359	LMT	C1-O1'-C1'	-3.14	108.31	113.68
23	B	518	CLA	CAA-C2A-C3A	-3.14	104.52	113.00
23	B	516	CLA	CBA-CAA-C2A	3.13	123.11	113.79
23	c	2477	CLA	C6-C5-C3	3.13	121.09	113.47
27	J	53	BCR	C23-C22-C21	-3.12	114.11	119.01
23	B	515	CLA	C7-C6-C5	-3.12	104.95	113.26
23	b	2517	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
23	a	2348	CLA	O2D-CGD-CBD	3.11	116.67	111.23
23	C	484	CLA	CED-O2D-CGD	3.11	122.96	115.92
23	b	2525	CLA	O2A-CGA-CBA	3.11	121.31	111.83
24	a	2350	PHO	CED-O2D-CGD	3.11	122.96	115.92
23	B	525	CLA	O2A-CGA-CBA	3.11	121.31	111.83
24	D	355	PHO	C12-C11-C10	-3.10	99.37	113.28
25	a	2352	PL9	C25-C24-C23	3.10	131.59	123.63
27	d	2360	BCR	C34-C9-C8	3.09	122.81	118.09
23	c	2485	CLA	O2D-CGD-CBD	3.09	116.63	111.23
23	C	481	CLA	O2A-CGA-CBA	3.09	121.25	111.83
23	B	522	CLA	CED-O2D-CGD	3.09	122.92	115.92
23	c	2485	CLA	C7-C6-C5	-3.09	105.04	113.26
23	b	2524	CLA	O2A-CGA-CBA	3.09	121.24	111.83
27	c	2488	BCR	C38-C26-C27	-3.08	107.02	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	348	CLA	C7-C6-C5	-3.08	105.05	113.26
23	C	485	CLA	CBA-CAA-C2A	3.08	122.95	113.79
24	d	2356	PHO	CAA-C2A-C3A	-3.08	104.69	113.00
23	b	2518	CLA	CED-O2D-CGD	3.07	122.89	115.92
24	D	355	PHO	CAA-C2A-C3A	-3.07	104.71	113.00
23	d	2357	CLA	O2D-CGD-CBD	3.07	116.59	111.23
23	b	2526	CLA	C2A-C1A-CHA	3.07	129.19	123.87
23	c	2481	CLA	CED-O2D-CGD	3.07	122.87	115.92
27	C	489	BCR	C7-C8-C9	3.06	130.77	126.23
23	c	2480	CLA	CED-O2D-CGD	3.06	122.86	115.92
27	c	2489	BCR	C33-C5-C4	-3.06	107.08	113.60
23	c	2486	CLA	O2D-CGD-CBD	3.06	116.58	111.23
24	A	351	PHO	CED-O2D-CGD	3.06	122.85	115.92
23	b	2514	CLA	CED-O2D-CGD	3.06	122.85	115.92
27	b	2528	BCR	C38-C26-C27	-3.06	107.08	113.60
23	c	2475	CLA	O2A-C1-C2	3.06	119.87	108.11
24	d	2356	PHO	C4A-C3A-C2A	3.05	105.75	102.84
23	B	511	CLA	C1-C2-C3	3.05	131.20	126.20
23	C	478	CLA	CED-O2D-CGD	3.05	122.84	115.92
23	C	475	CLA	O2A-C1-C2	3.05	119.85	108.11
27	b	2527	BCR	C8-C7-C6	3.05	135.14	127.00
28	e	2084	HEC	CHB-C4A-NA	-3.05	121.14	124.45
28	e	2084	HEC	CBA-CAA-C2A	-3.05	104.11	112.53
23	b	2511	CLA	C3B-C4B-NB	-3.04	107.81	110.53
23	A	352	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
23	a	2348	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
27	J	53	BCR	C7-C8-C9	3.04	130.74	126.23
27	J	53	BCR	C8-C9-C10	-3.04	114.22	119.01
27	B	528	BCR	C30-C25-C26	-3.04	118.48	122.64
27	j	2053	BCR	C8-C7-C6	3.04	135.12	127.00
23	c	2474	CLA	C1-C2-C3	3.04	131.17	126.20
23	b	2516	CLA	CBA-CAA-C2A	3.04	122.83	113.79
23	B	517	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
23	B	524	CLA	CED-O2D-CGD	3.03	122.79	115.92
23	a	2349	CLA	O2A-CGA-CBA	3.03	121.08	111.83
28	V	138	HEC	C4D-C3D-C2D	3.03	111.30	106.89
23	b	2511	CLA	C1-C2-C3	3.03	131.16	126.20
23	b	2513	CLA	C2A-C1A-CHA	3.02	129.11	123.87
27	b	2527	BCR	C30-C25-C26	-3.02	118.50	122.64
23	c	2481	CLA	O2A-CGA-CBA	3.02	121.05	111.83
23	A	349	CLA	CAA-C2A-C1A	-3.02	102.09	111.97
27	B	528	BCR	C1-C6-C5	-3.02	118.51	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	352	CLA	C7-C6-C5	-3.02	105.22	113.26
27	C	488	BCR	C33-C5-C4	-3.02	107.17	113.60
23	B	523	CLA	O2A-CGA-CBA	3.02	121.03	111.83
28	V	138	HEC	C2A-C1A-NA	3.01	113.23	110.32
27	b	2527	BCR	C1-C6-C5	-3.01	118.52	122.64
23	b	2526	CLA	CED-O2D-CGD	3.01	122.75	115.92
23	b	2511	CLA	C1-O2A-CGA	3.01	123.94	116.65
23	C	482	CLA	CBA-CAA-C2A	3.01	122.75	113.79
27	F	48	BCR	C30-C25-C24	3.01	123.81	115.65
23	C	485	CLA	O2D-CGD-CBD	3.01	116.49	111.23
23	B	519	CLA	CED-O2D-CGD	3.01	122.73	115.92
23	C	474	CLA	O2D-CGD-CBD	3.00	116.48	111.23
23	C	482	CLA	O2D-CGD-CBD	3.00	116.48	111.23
24	d	2356	PHO	CED-O2D-CGD	3.00	122.72	115.92
23	c	2487	CLA	C3B-C4B-NB	-3.00	107.85	110.53
27	J	53	BCR	C38-C26-C27	-3.00	107.20	113.60
23	B	524	CLA	O2A-CGA-CBA	3.00	120.97	111.83
23	B	511	CLA	C3B-C4B-NB	-2.99	107.86	110.53
23	B	520	CLA	CED-O2D-CGD	2.99	122.70	115.92
23	A	350	CLA	O2A-CGA-CBA	2.98	120.93	111.83
27	F	48	BCR	C1-C6-C5	-2.98	118.56	122.64
28	E	84	HEC	CBA-CAA-C2A	-2.98	104.30	112.53
23	C	475	CLA	O1A-CGA-CBA	-2.97	112.16	123.78
27	j	2053	BCR	C38-C26-C27	-2.97	107.27	113.60
23	B	520	CLA	O2D-CGD-CBD	2.97	116.42	111.23
23	B	527	CLA	C2A-C1A-CHA	2.97	129.01	123.87
27	c	2489	BCR	C8-C9-C10	-2.96	114.35	119.01
23	c	2475	CLA	O1A-CGA-CBA	-2.96	112.19	123.78
23	b	2524	CLA	CED-O2D-CGD	2.96	122.63	115.92
25	A	353	PL9	C7-C3-C4	2.96	119.35	116.91
23	B	513	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
25	d	2358	PL9	C8-C7-C3	2.96	119.67	112.03
23	B	527	CLA	CED-O2D-CGD	2.96	122.62	115.92
23	A	348	CLA	CED-O2D-CGD	2.96	122.62	115.92
23	B	518	CLA	CED-O2D-CGD	2.95	122.62	115.92
27	C	489	BCR	C30-C25-C24	2.95	123.66	115.65
23	c	2482	CLA	CBA-CAA-C2A	2.95	122.58	113.79
24	D	355	PHO	C4A-C3A-C2A	2.95	105.65	102.84
24	d	2356	PHO	C1-C2-C3	2.95	131.03	126.20
23	B	517	CLA	O2D-CGD-CBD	2.95	116.38	111.23
23	c	2482	CLA	CED-O2D-CGD	2.94	122.59	115.92
23	b	2523	CLA	O2A-CGA-CBA	2.94	120.81	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2517	CLA	O2D-CGD-CBD	2.94	116.37	111.23
23	C	483	CLA	CED-O2D-CGD	2.94	122.58	115.92
23	C	487	CLA	CHB-C1B-NB	2.94	128.45	124.05
23	C	487	CLA	C1-O2A-CGA	2.93	123.74	116.65
23	c	2474	CLA	CAA-C2A-C1A	-2.93	102.37	111.97
23	a	2351	CLA	C1-O2A-CGA	2.93	123.74	116.65
23	d	2355	CLA	CAA-C2A-C1A	-2.93	102.38	111.97
23	a	2351	CLA	CED-O2D-CGD	2.93	122.55	115.92
23	C	487	CLA	C3B-C4B-NB	-2.92	107.92	110.53
23	c	2487	CLA	CHB-C1B-NB	2.92	128.44	124.05
28	e	2084	HEC	O1D-CGD-CBD	-2.92	113.82	123.09
23	c	2483	CLA	CED-O2D-CGD	2.92	122.54	115.92
23	C	477	CLA	C6-C5-C3	2.92	120.58	113.47
23	A	348	CLA	C3B-C4B-NB	-2.92	107.93	110.53
23	d	2354	CLA	CBA-CAA-C2A	2.91	122.46	113.79
23	B	523	CLA	C3B-C4B-NB	-2.91	107.93	110.53
23	c	2486	CLA	C6-C5-C3	2.91	120.55	113.47
23	b	2519	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
23	a	2351	CLA	C7-C6-C5	-2.90	105.53	113.26
23	B	522	CLA	C1-C2-C3	2.90	130.95	126.20
27	c	2489	BCR	C30-C25-C24	2.90	123.52	115.65
27	K	50	BCR	C23-C22-C21	-2.90	114.45	119.01
23	A	348	CLA	O2D-CGD-CBD	2.89	116.29	111.23
23	B	520	CLA	O2A-CGA-CBA	2.89	120.65	111.83
28	v	2138	HEC	C3A-C4A-NA	2.89	114.98	109.64
23	c	2485	CLA	CBA-CAA-C2A	2.89	122.39	113.79
23	C	480	CLA	CED-O2D-CGD	2.88	122.46	115.92
23	b	2518	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
23	B	513	CLA	O2D-CGD-CBD	2.88	116.27	111.23
23	c	2487	CLA	C1-O2A-CGA	2.88	123.62	116.65
23	C	482	CLA	CED-O2D-CGD	2.88	122.44	115.92
28	E	84	HEC	O1D-CGD-CBD	-2.88	113.97	123.09
23	b	2513	CLA	O2D-CGD-CBD	2.87	116.25	111.23
23	D	354	CLA	O2A-C1-C2	2.87	119.14	108.11
23	b	2512	CLA	CED-O2D-CGD	2.86	122.41	115.92
23	C	474	CLA	CED-O2D-CGD	2.86	122.41	115.92
23	B	527	CLA	C1-C2-C3	2.86	130.89	126.20
23	C	486	CLA	C2A-C1A-CHA	2.86	128.83	123.87
23	A	348	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
23	c	2484	CLA	O2A-CGA-CBA	2.86	120.55	111.83
27	c	2489	BCR	C38-C26-C27	-2.86	107.50	113.60
27	k	2050	BCR	C34-C9-C8	2.86	122.45	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	2513	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
23	C	486	CLA	C6-C5-C3	2.86	120.42	113.47
27	C	489	BCR	C38-C26-C27	-2.85	107.51	113.60
23	b	2515	CLA	C7-C6-C5	-2.85	105.67	113.26
28	V	138	HEC	C1C-C2C-C3C	-2.85	103.56	106.82
23	C	475	CLA	C3B-C4B-NB	-2.84	107.99	110.53
23	c	2486	CLA	CED-O2D-CGD	2.84	122.36	115.92
23	B	519	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
23	C	474	CLA	C7-C6-C5	-2.83	105.71	113.26
27	k	2050	BCR	C23-C22-C21	-2.83	114.55	119.01
27	d	2360	BCR	C30-C25-C24	2.83	123.31	115.65
23	C	484	CLA	O2A-CGA-CBA	2.82	120.45	111.83
27	K	50	BCR	C36-C18-C19	2.82	122.40	118.09
28	V	138	HEC	C1C-CHC-C4B	-2.82	119.62	126.25
23	a	2349	CLA	CAA-C2A-C1A	-2.81	102.75	111.97
23	c	2478	CLA	C3B-C4B-NB	-2.81	108.02	110.53
27	K	50	BCR	C23-C24-C25	2.81	134.51	127.00
23	b	2522	CLA	C1-C2-C3	2.81	130.80	126.20
27	B	529	BCR	C1-C6-C7	2.81	123.27	115.65
23	b	2511	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
23	C	474	CLA	CAA-C2A-C1A	-2.81	102.78	111.97
28	E	84	HEC	C3A-C4A-NA	2.80	114.83	109.64
23	b	2513	CLA	C6-C5-C3	2.80	120.30	113.47
27	k	2050	BCR	C8-C9-C10	-2.80	114.60	119.01
23	A	350	CLA	O2D-CGD-CBD	2.80	116.13	111.23
23	B	514	CLA	CED-O2D-CGD	2.80	122.26	115.92
23	c	2485	CLA	O2A-CGA-CBA	2.80	120.36	111.83
23	C	476	CLA	O2A-CGA-CBA	2.80	120.36	111.83
28	v	2138	HEC	C2C-C1C-NC	2.80	114.62	110.14
25	a	2352	PL9	C7-C3-C4	2.79	119.21	116.91
23	b	2520	CLA	O2A-CGA-CBA	2.79	120.36	111.83
28	e	2084	HEC	CHA-C4D-ND	2.79	127.43	124.42
23	b	2520	CLA	CED-O2D-CGD	2.79	122.25	115.92
23	C	486	CLA	CED-O2D-CGD	2.79	122.24	115.92
23	c	2485	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
27	c	2488	BCR	C33-C5-C4	-2.78	107.66	113.60
27	B	528	BCR	C8-C9-C10	-2.78	114.63	119.01
23	B	517	CLA	CED-O2D-CGD	2.78	122.23	115.92
23	b	2515	CLA	C2A-C1A-CHA	2.78	128.70	123.87
27	k	2050	BCR	C36-C18-C19	2.78	122.34	118.09
23	A	352	CLA	C1-O2A-CGA	2.78	123.39	116.65
28	v	2138	HEC	CAB-C3B-C4B	-2.78	121.17	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	2354	CLA	O2D-CGD-CBD	2.78	116.08	111.23
23	B	513	CLA	C6-C5-C3	2.78	120.23	113.47
23	B	519	CLA	O2D-CGD-CBD	2.77	116.08	111.23
28	v	2138	HEC	CAA-C2A-C1A	-2.77	119.21	124.85
25	D	357	PL9	C8-C7-C3	2.77	119.20	112.03
23	A	349	CLA	CED-O2D-CGD	2.77	122.20	115.92
27	k	2050	BCR	C38-C26-C27	-2.77	107.69	113.60
23	C	478	CLA	C3B-C4B-NB	-2.77	108.06	110.53
23	c	2485	CLA	C12-C11-C10	-2.77	100.86	113.28
24	A	351	PHO	C4A-C3A-C2A	2.77	105.47	102.84
23	B	511	CLA	C1-O2A-CGA	2.77	123.35	116.65
23	a	2348	CLA	C7-C6-C5	-2.77	105.89	113.26
23	C	476	CLA	O2D-CGD-CBD	2.76	116.06	111.23
23	c	2485	CLA	C1-C2-C3	2.76	130.72	126.20
23	C	480	CLA	C7-C6-C5	-2.76	105.90	113.26
23	D	356	CLA	O2D-CGD-CBD	2.76	116.06	111.23
23	d	2355	CLA	C5-C3-C2	-2.76	114.97	121.17
23	c	2484	CLA	C1-O2A-CGA	2.76	123.33	116.65
27	F	48	BCR	C24-C23-C22	2.76	130.32	126.23
23	B	522	CLA	C3B-C4B-NB	-2.76	108.07	110.53
23	B	515	CLA	C2A-C1A-CHA	2.76	128.65	123.87
23	c	2483	CLA	C6-C5-C3	2.75	120.18	113.47
23	C	485	CLA	C1-C2-C3	2.75	130.71	126.20
27	K	50	BCR	C8-C9-C10	-2.75	114.68	119.01
25	A	353	PL9	C27-C28-C29	-2.75	121.32	127.62
23	c	2480	CLA	C7-C6-C5	-2.75	105.93	113.26
23	c	2476	CLA	O2D-CGD-CBD	2.75	116.04	111.23
25	d	2358	PL9	C22-C21-C19	-2.75	104.07	113.19
23	C	475	CLA	CAA-C2A-C3A	-2.75	105.57	113.00
27	B	529	BCR	C35-C13-C12	2.75	122.28	118.09
23	b	2514	CLA	CAA-CBA-CGA	-2.75	105.41	113.21
27	k	2050	BCR	C23-C24-C25	2.75	134.33	127.00
23	B	513	CLA	C2A-C3A-C4A	2.74	106.30	101.87
25	a	2352	PL9	C32-C33-C34	-2.74	121.35	127.62
28	V	138	HEC	CHC-C1C-C2C	-2.74	119.47	127.43
27	K	50	BCR	C38-C26-C27	-2.73	107.77	113.60
23	C	486	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
27	b	2528	BCR	C33-C5-C4	-2.73	107.77	113.60
23	b	2513	CLA	C2A-C3A-C4A	2.73	106.28	101.87
23	C	487	CLA	C1-C2-C3	2.73	130.67	126.20
23	b	2520	CLA	C3B-C4B-NB	-2.73	108.10	110.53
26	d	2359	LMT	C3'-C4'-C5'	-2.73	104.89	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	485	CLA	C12-C11-C10	-2.72	101.07	113.28
27	C	488	BCR	C19-C18-C17	-2.72	114.73	119.01
23	C	485	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
26	B	526	LMT	C3'-C4'-C5'	-2.72	104.90	110.93
23	c	2479	CLA	O2A-CGA-CBA	2.72	120.12	111.83
23	C	483	CLA	CAA-CBA-CGA	-2.71	105.50	113.21
23	C	481	CLA	CED-O2D-CGD	2.71	122.07	115.92
27	b	2528	BCR	C1-C6-C7	2.71	123.00	115.65
23	c	2476	CLA	O2A-CGA-CBA	2.71	120.10	111.83
27	d	2360	BCR	C1-C6-C5	-2.71	118.94	122.64
24	d	2356	PHO	C6-C5-C3	2.70	120.05	113.47
27	k	2050	BCR	C37-C22-C23	2.70	122.22	118.09
23	b	2522	CLA	O2A-CGA-CBA	2.70	120.07	111.83
23	d	2354	CLA	CED-O2D-CGD	2.70	122.03	115.92
23	c	2483	CLA	C7-C6-C5	-2.70	106.08	113.26
23	b	2517	CLA	C2A-C1A-CHA	2.70	128.54	123.87
23	B	522	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	d	2354	CLA	O2A-C1-C2	2.69	118.48	108.11
23	B	518	CLA	CMD-C2D-C1D	2.69	129.46	124.73
27	C	489	BCR	C8-C9-C10	-2.69	114.78	119.01
23	C	477	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	C	487	CLA	O2A-CGA-CBA	2.69	120.02	111.83
23	C	482	CLA	C2A-C3A-C4A	2.69	106.21	101.87
23	d	2355	CLA	CED-O2D-CGD	2.68	122.00	115.92
28	V	138	HEC	CHD-C1D-ND	-2.68	121.05	124.37
27	B	529	BCR	C37-C22-C21	-2.68	118.47	122.82
23	D	356	CLA	CED-O2D-CGD	2.68	122.00	115.92
23	A	349	CLA	C5-C3-C2	-2.68	115.15	121.17
23	c	2478	CLA	O2D-CGD-CBD	2.68	115.91	111.23
24	D	355	PHO	C1-C2-C3	2.68	130.58	126.20
23	B	515	CLA	O2D-CGD-CBD	2.67	115.90	111.23
23	C	478	CLA	C1-O2A-CGA	2.67	123.12	116.65
23	c	2486	CLA	C2A-C1A-CHA	2.67	128.50	123.87
23	c	2482	CLA	C2A-C3A-C4A	2.67	106.18	101.87
27	K	50	BCR	C37-C22-C23	2.66	122.16	118.09
27	d	2360	BCR	C24-C23-C22	2.66	130.18	126.23
27	b	2527	BCR	C23-C22-C21	-2.66	114.82	119.01
23	A	350	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
23	c	2474	CLA	CED-O2D-CGD	2.66	121.95	115.92
27	j	2053	BCR	C37-C22-C23	2.66	122.16	118.09
23	B	517	CLA	C2A-C1A-CHA	2.66	128.49	123.87
23	c	2476	CLA	CED-O2D-CGD	2.66	121.95	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	483	CLA	C2A-C3A-C4A	2.66	106.16	101.87
27	K	50	BCR	C33-C5-C4	-2.66	107.93	113.60
23	B	520	CLA	C3B-C4B-NB	-2.65	108.16	110.53
27	F	48	BCR	C8-C7-C6	2.65	134.08	127.00
23	b	2525	CLA	C3B-C4B-NB	-2.65	108.16	110.53
27	c	2489	BCR	C1-C6-C5	-2.65	119.02	122.64
27	J	53	BCR	C30-C25-C26	-2.65	119.02	122.64
27	b	2528	BCR	C35-C13-C12	2.65	122.13	118.09
23	A	352	CLA	CED-O2D-CGD	2.64	121.91	115.92
23	b	2511	CLA	C2A-C1A-CHA	2.64	128.45	123.87
27	c	2488	BCR	C15-C16-C17	-2.64	118.11	123.52
23	B	525	CLA	CBA-CAA-C2A	2.64	121.65	113.79
27	C	489	BCR	C30-C25-C26	-2.64	119.03	122.64
27	C	488	BCR	C36-C18-C19	2.64	122.12	118.09
23	c	2475	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
27	C	489	BCR	C1-C6-C5	-2.64	119.03	122.64
27	c	2489	BCR	C21-C20-C19	2.64	130.84	123.20
23	b	2525	CLA	O2D-CGD-CBD	2.63	115.84	111.23
27	d	2360	BCR	C20-C21-C22	2.63	130.97	127.28
23	c	2483	CLA	CAA-CBA-CGA	-2.63	105.73	113.21
23	c	2487	CLA	C1-C2-C3	2.63	130.50	126.20
23	b	2524	CLA	O2D-CGD-CBD	2.62	115.82	111.23
25	A	353	PL9	C25-C24-C23	2.62	130.37	123.63
23	C	483	CLA	C6-C5-C3	2.62	119.86	113.47
28	v	2138	HEC	CAA-C2A-C3A	2.62	132.78	127.87
28	V	138	HEC	C4C-C3C-C2C	2.62	110.92	106.87
23	C	479	CLA	O2A-CGA-CBA	2.62	119.82	111.83
23	B	524	CLA	O2D-CGD-CBD	2.62	115.81	111.23
23	b	2525	CLA	CBA-CAA-C2A	2.62	121.58	113.79
23	b	2518	CLA	CMD-C2D-C1D	2.61	129.33	124.73
23	B	511	CLA	O2A-CGA-CBA	2.61	119.81	111.83
27	C	488	BCR	C34-C9-C8	2.61	122.08	118.09
23	B	522	CLA	C2A-C1A-CHA	2.61	128.40	123.87
24	a	2350	PHO	C4A-C3A-C2A	2.61	105.33	102.84
28	E	84	HEC	CHC-C1C-C2C	-2.61	119.85	127.43
24	d	2356	PHO	CBA-CAA-C2A	2.61	121.47	113.78
23	b	2513	CLA	CAA-C2A-C1A	-2.61	103.42	111.97
23	B	520	CLA	CMD-C2D-C1D	2.61	129.32	124.73
27	B	529	BCR	C33-C5-C4	-2.61	108.04	113.60
25	a	2352	PL9	C27-C28-C29	-2.60	121.66	127.62
23	d	2355	CLA	CMD-C2D-C1D	2.60	129.31	124.73
23	C	477	CLA	O2D-CGD-CBD	2.60	115.78	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2487	CLA	O2A-CGA-CBA	2.60	119.76	111.83
23	B	514	CLA	CAA-CBA-CGA	-2.60	105.83	113.21
23	A	349	CLA	CAA-C2A-C3A	-2.60	105.99	113.00
23	C	480	CLA	CAA-C2A-C1A	-2.59	103.47	111.97
27	b	2528	BCR	C30-C25-C24	2.59	122.68	115.65
23	b	2519	CLA	O2D-CGD-CBD	2.59	115.76	111.23
28	v	2138	HEC	CAC-C3C-C2C	2.59	130.98	126.89
27	b	2528	BCR	C23-C24-C25	2.59	133.91	127.00
23	a	2348	CLA	C3B-C4B-NB	-2.58	108.23	110.53
23	b	2519	CLA	O2A-C1-C2	2.58	118.03	108.11
23	b	2512	CLA	C6-C5-C3	2.58	119.75	113.47
23	B	511	CLA	C2A-C1A-CHA	2.57	128.34	123.87
27	B	528	BCR	C23-C22-C21	-2.57	114.96	119.01
23	C	478	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
23	C	484	CLA	C1-O2A-CGA	2.57	122.88	116.65
23	b	2525	CLA	C2A-C3A-C4A	2.57	106.02	101.87
25	D	357	PL9	C22-C21-C19	-2.57	104.66	113.19
28	v	2138	HEC	CAB-C3B-C2B	2.57	132.28	127.56
23	C	483	CLA	O2D-CGD-CBD	2.57	115.72	111.23
23	b	2521	CLA	O2A-CGA-CBA	2.57	119.66	111.83
27	d	2360	BCR	C8-C7-C6	2.57	133.86	127.00
24	A	351	PHO	O2A-CGA-CBA	2.57	119.66	111.83
27	C	488	BCR	C15-C16-C17	-2.57	118.27	123.52
27	k	2050	BCR	C33-C5-C4	-2.56	108.13	113.60
24	D	355	PHO	CBA-CAA-C2A	2.56	121.33	113.78
27	b	2528	BCR	C37-C22-C21	-2.56	118.66	122.82
23	c	2477	CLA	O2A-C1-C2	2.56	117.97	108.11
27	c	2488	BCR	C19-C18-C17	-2.56	114.98	119.01
23	B	523	CLA	C7-C6-C5	-2.56	106.43	113.26
27	b	2527	BCR	C7-C8-C9	2.56	130.02	126.23
27	b	2528	BCR	C34-C9-C8	2.56	122.00	118.09
24	a	2350	PHO	O2A-CGA-CBA	2.56	119.63	111.83
27	d	2360	BCR	C15-C16-C17	-2.55	118.29	123.52
24	a	2350	PHO	OBD-CAD-C3D	2.55	131.88	127.89
24	A	351	PHO	C2D-C1D-ND	2.55	111.27	109.43
23	C	479	CLA	C6-C5-C3	2.55	119.68	113.47
23	C	485	CLA	O2A-CGA-CBA	2.55	119.61	111.83
23	a	2348	CLA	C2A-C3A-C4A	2.55	105.98	101.87
27	C	489	BCR	C8-C7-C6	2.55	133.80	127.00
23	B	511	CLA	CAA-C2A-C3A	-2.55	106.12	113.00
23	C	484	CLA	CBA-CAA-C2A	2.55	121.37	113.79
28	V	138	HEC	CMD-C2D-C3D	2.54	133.03	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2487	CLA	C7-C6-C5	-2.54	106.49	113.26
23	b	2523	CLA	C7-C6-C5	-2.54	106.49	113.26
23	b	2522	CLA	C2A-C1A-CHA	2.54	128.27	123.87
23	C	476	CLA	CED-O2D-CGD	2.54	121.67	115.92
23	C	477	CLA	O2A-C1-C2	2.54	117.86	108.11
23	B	513	CLA	CAA-C2A-C1A	-2.54	103.67	111.97
27	C	489	BCR	C21-C20-C19	2.53	130.54	123.20
23	C	485	CLA	C2A-C3A-C4A	2.53	105.96	101.87
23	c	2484	CLA	CBA-CAA-C2A	2.53	121.33	113.79
23	c	2477	CLA	O2D-CGD-CBD	2.53	115.66	111.23
25	d	2358	PL9	C31-C29-C28	-2.53	115.48	121.17
23	B	512	CLA	C6-C5-C3	2.53	119.63	113.47
25	D	357	PL9	C31-C29-C28	-2.53	115.49	121.17
23	c	2478	CLA	C1-O2A-CGA	2.53	122.77	116.65
23	c	2480	CLA	O2D-CGD-CBD	2.53	115.65	111.23
27	b	2527	BCR	C37-C22-C23	2.53	121.95	118.09
23	C	481	CLA	C2A-C3A-C4A	2.52	105.95	101.87
23	B	514	CLA	O2A-C1-C2	2.52	117.82	108.11
27	B	529	BCR	C23-C24-C25	2.52	133.73	127.00
24	a	2350	PHO	CMA-C3A-C4A	-2.52	109.19	114.61
23	b	2517	CLA	CBA-CAA-C2A	2.52	121.28	113.79
23	c	2485	CLA	C2A-C3A-C4A	2.52	105.93	101.87
23	D	354	CLA	CBA-CAA-C2A	2.51	121.28	113.79
24	D	355	PHO	OBD-CAD-CBD	-2.51	122.13	125.82
25	A	353	PL9	C30-C29-C31	2.51	119.58	115.23
23	b	2523	CLA	C3B-C4B-NB	-2.51	108.29	110.53
23	b	2526	CLA	C1-C2-C3	2.50	130.30	126.20
27	c	2488	BCR	C11-C10-C9	2.50	130.79	127.28
27	c	2488	BCR	C34-C9-C8	2.50	121.91	118.09
27	j	2053	BCR	C35-C13-C12	2.50	121.91	118.09
23	c	2483	CLA	O2D-CGD-CBD	2.50	115.60	111.23
27	b	2527	BCR	C8-C9-C10	-2.50	115.08	119.01
23	C	483	CLA	C7-C6-C5	-2.49	106.62	113.26
23	B	519	CLA	O2A-C1-C2	2.49	117.69	108.11
28	V	138	HEC	CMD-C2D-C1D	-2.49	121.14	125.03
25	d	2358	PL9	C7-C3-C4	2.49	118.96	116.91
23	C	486	CLA	C2A-C3A-C4A	2.49	105.89	101.87
23	c	2480	CLA	CAA-C2A-C1A	-2.48	103.83	111.97
23	b	2522	CLA	C3B-C4B-NB	-2.48	108.31	110.53
23	c	2478	CLA	C2A-C3A-C4A	2.48	105.88	101.87
23	c	2479	CLA	C6-C7-C8	2.48	124.21	115.97
23	B	516	CLA	O2D-CGD-CBD	2.48	115.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	2348	CLA	CED-O2D-CGD	2.48	121.54	115.92
23	b	2514	CLA	O2A-C1-C2	2.48	117.64	108.11
23	B	521	CLA	O2A-CGA-CBA	2.48	119.39	111.83
23	A	350	CLA	C1-O2A-CGA	2.48	122.64	116.65
28	E	84	HEC	O1A-CGA-CBA	-2.47	115.24	123.09
24	A	351	PHO	CAA-C2A-C3A	-2.47	106.31	113.00
27	F	48	BCR	C15-C16-C17	-2.47	118.46	123.52
23	c	2486	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
24	a	2350	PHO	C2D-C1D-ND	2.47	111.21	109.43
23	c	2478	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
23	A	352	CLA	O2D-CGD-CBD	2.46	115.54	111.23
23	D	354	CLA	CED-O2D-CGD	2.46	121.50	115.92
27	B	529	BCR	C34-C9-C8	2.46	121.85	118.09
23	c	2477	CLA	C3B-C4B-NB	-2.46	108.33	110.53
27	j	2053	BCR	C30-C25-C26	-2.46	119.27	122.64
23	B	516	CLA	C2A-C3A-C4A	2.46	105.85	101.87
23	c	2486	CLA	C2A-C3A-C4A	2.46	105.84	101.87
23	b	2516	CLA	C5-C3-C2	2.46	126.69	121.17
23	B	522	CLA	C1-O2A-CGA	2.46	122.61	116.65
23	b	2513	CLA	C1-O2A-CGA	2.46	122.61	116.65
23	C	479	CLA	C2A-C1A-CHA	2.46	128.13	123.87
24	d	2356	PHO	OBD-CAD-CBD	-2.46	122.22	125.82
23	c	2475	CLA	CMD-C2D-C1D	2.46	129.06	124.73
24	D	355	PHO	C6-C5-C3	2.46	119.45	113.47
23	C	482	CLA	C6-C5-C3	2.46	119.45	113.47
27	j	2053	BCR	C16-C17-C18	2.45	130.72	127.28
23	a	2351	CLA	O2D-CGD-CBD	2.45	115.52	111.23
23	c	2475	CLA	C3B-C4B-NB	-2.45	108.34	110.53
27	F	48	BCR	C20-C21-C22	2.45	130.72	127.28
25	A	353	PL9	C32-C33-C34	-2.45	122.02	127.62
28	v	2138	HEC	C1C-CHC-C4B	-2.44	120.50	126.25
23	A	348	CLA	O2A-C1-C2	2.44	117.50	108.11
27	B	529	BCR	C24-C23-C22	2.44	129.84	126.23
23	d	2354	CLA	C3B-C4B-NB	-2.44	108.35	110.53
23	A	349	CLA	O2D-CGD-CBD	2.44	115.50	111.23
24	d	2356	PHO	CMB-C2B-C3B	2.44	129.55	124.68
23	c	2476	CLA	C1-O2A-CGA	2.44	122.55	116.65
27	c	2489	BCR	C30-C25-C26	-2.44	119.31	122.64
23	C	480	CLA	O2D-CGD-CBD	2.43	115.49	111.23
27	c	2488	BCR	C32-C1-C6	2.43	114.06	110.24
23	d	2357	CLA	C1-O2A-CGA	2.43	122.53	116.65
23	c	2486	CLA	C3B-C4B-NB	-2.43	108.36	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	486	CLA	CBA-CAA-C2A	2.43	121.02	113.79
24	d	2356	PHO	C4D-ND-C1D	-2.43	105.97	108.87
23	B	525	CLA	O2D-CGD-CBD	2.43	115.47	111.23
23	c	2486	CLA	CBA-CAA-C2A	2.42	121.00	113.79
28	e	2084	HEC	C4A-NA-C1A	-2.42	101.88	105.82
23	c	2479	CLA	C2A-C1A-CHA	2.42	128.06	123.87
23	b	2511	CLA	O2D-CGD-CBD	2.41	115.45	111.23
27	j	2053	BCR	C1-C6-C5	-2.41	119.34	122.64
28	v	2138	HEC	O1D-CGD-CBD	-2.41	115.44	123.09
23	c	2479	CLA	C1-C2-C3	2.41	130.15	126.20
23	A	350	CLA	CMA-C3A-C2A	-2.41	104.66	113.98
23	d	2357	CLA	C7-C6-C5	-2.41	106.84	113.26
23	b	2512	CLA	O2A-CGA-CBA	2.41	119.18	111.83
23	b	2516	CLA	O1A-CGA-CBA	-2.41	114.36	123.78
23	a	2349	CLA	O2D-CGD-CBD	2.41	115.44	111.23
23	a	2349	CLA	C1-O2A-CGA	2.41	122.47	116.65
23	B	520	CLA	C2A-C3A-C4A	2.40	105.75	101.87
23	D	356	CLA	C1-O2A-CGA	2.40	122.47	116.65
25	d	2358	PL9	C20-C19-C21	-2.40	111.06	115.23
23	D	354	CLA	C3B-C4B-NB	-2.40	108.39	110.53
23	C	484	CLA	C7-C6-C5	-2.40	106.87	113.26
23	B	516	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
23	b	2514	CLA	O2D-CGD-CBD	2.40	115.42	111.23
23	D	354	CLA	C2A-C3A-C4A	2.40	105.74	101.87
23	B	517	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
23	b	2511	CLA	O2A-CGA-CBA	2.40	119.15	111.83
23	c	2482	CLA	O2D-CGD-CBD	2.40	115.42	111.23
23	b	2521	CLA	C1-O2A-CGA	2.40	122.45	116.65
28	E	84	HEC	C4C-C3C-C2C	2.40	110.58	106.87
28	v	2138	HEC	C1A-CHA-C4D	-2.40	120.93	126.02
23	B	517	CLA	C7-C6-C5	-2.39	106.88	113.26
27	F	48	BCR	C36-C18-C19	2.39	121.74	118.09
27	B	529	BCR	C30-C25-C24	2.39	122.14	115.65
23	b	2515	CLA	O2D-CGD-CBD	2.39	115.41	111.23
23	B	512	CLA	CED-O2D-CGD	2.39	121.33	115.92
23	C	478	CLA	O2D-CGD-CBD	2.39	115.40	111.23
23	D	356	CLA	C7-C6-C5	-2.39	106.90	113.26
23	A	350	CLA	C2A-C3A-C4A	2.38	105.72	101.87
23	C	486	CLA	O2D-CGD-CBD	2.38	115.39	111.23
23	C	479	CLA	C6-C7-C8	2.38	123.88	115.97
23	B	521	CLA	CMD-C2D-C1D	2.38	128.92	124.73
23	B	516	CLA	O1A-CGA-CBA	-2.38	114.47	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	2352	PL9	C15-C14-C16	-2.38	111.10	115.23
23	d	2355	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
23	B	511	CLA	O2D-CGD-CBD	2.38	115.39	111.23
27	c	2488	BCR	C36-C18-C19	2.38	121.72	118.09
23	B	523	CLA	CMD-C2D-C1D	2.38	128.91	124.73
27	K	50	BCR	C34-C9-C8	2.38	121.72	118.09
23	c	2479	CLA	C6-C5-C3	2.38	119.26	113.47
27	J	53	BCR	C1-C6-C5	-2.38	119.39	122.64
27	b	2528	BCR	C20-C19-C18	-2.38	119.85	126.36
23	c	2477	CLA	C6-C7-C8	2.37	123.85	115.97
27	C	489	BCR	C34-C9-C8	2.37	121.71	118.09
23	d	2354	CLA	C2A-C3A-C4A	2.37	105.70	101.87
23	B	518	CLA	O2D-CGD-CBD	2.37	115.36	111.23
23	b	2516	CLA	CAA-C2A-C1A	-2.36	104.23	111.97
23	c	2487	CLA	CHD-C4C-C3C	2.36	128.22	124.77
23	A	352	CLA	CAA-CBA-CGA	2.36	119.91	113.21
27	B	528	BCR	C16-C17-C18	2.36	130.59	127.28
23	B	516	CLA	C5-C3-C2	2.36	126.46	121.17
23	C	475	CLA	CMD-C2D-C1D	2.35	128.88	124.73
27	J	53	BCR	C37-C22-C23	2.35	121.69	118.09
23	c	2484	CLA	C7-C6-C5	-2.35	106.99	113.26
23	C	487	CLA	C2A-C1A-CHA	2.35	127.94	123.87
23	C	477	CLA	C6-C7-C8	2.35	123.77	115.97
23	b	2515	CLA	CAA-C2A-C1A	-2.35	104.29	111.97
23	C	479	CLA	CAA-C2A-C3A	-2.34	106.66	113.00
28	V	138	HEC	O2D-CGD-O1D	2.34	129.36	123.33
27	j	2053	BCR	C30-C25-C24	2.34	122.00	115.65
23	b	2524	CLA	C2A-C3A-C4A	2.34	105.65	101.87
26	d	2359	LMT	C3-C2-C1	-2.34	103.29	113.47
23	d	2357	CLA	CED-O2D-CGD	2.34	121.22	115.92
28	E	84	HEC	C1C-C2C-C3C	-2.34	104.14	106.82
23	c	2478	CLA	C7-C6-C5	-2.34	107.03	113.26
23	B	525	CLA	C2A-C3A-C4A	2.34	105.65	101.87
23	B	512	CLA	O2A-CGA-CBA	2.34	118.97	111.83
23	C	487	CLA	CHD-C4C-C3C	2.34	128.18	124.77
27	d	2360	BCR	C36-C18-C19	2.34	121.66	118.09
25	D	357	PL9	C7-C8-C9	2.34	130.86	126.83
23	a	2349	CLA	CMA-C3A-C2A	-2.34	104.95	113.98
23	B	523	CLA	C16-C15-C13	2.34	123.73	115.97
23	D	356	CLA	C2A-C3A-C4A	2.34	105.64	101.87
23	A	349	CLA	CMD-C2D-C1D	2.33	128.84	124.73
23	b	2522	CLA	C7-C6-C5	-2.33	107.05	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	528	BCR	C12-C13-C14	-2.33	115.34	119.01
23	c	2487	CLA	C2A-C1A-CHA	2.33	127.91	123.87
23	b	2517	CLA	C3B-C4B-NB	-2.33	108.45	110.53
23	a	2351	CLA	C2A-C3A-C4A	2.32	105.62	101.87
23	B	522	CLA	C7-C6-C5	-2.32	107.07	113.26
27	J	53	BCR	C30-C25-C24	2.32	121.95	115.65
27	c	2488	BCR	C30-C25-C26	-2.32	119.46	122.64
23	C	482	CLA	CAA-CBA-CGA	2.32	119.80	113.21
23	b	2516	CLA	CED-O2D-CGD	2.32	121.17	115.92
23	A	352	CLA	C2A-C3A-C4A	2.32	105.61	101.87
23	B	517	CLA	CBA-CAA-C2A	2.32	120.69	113.79
25	d	2358	PL9	C7-C8-C9	2.32	130.82	126.83
28	V	138	HEC	CAC-C3C-C4C	-2.32	121.72	124.91
25	a	2352	PL9	C30-C29-C31	2.31	119.24	115.23
27	b	2527	BCR	C34-C9-C8	2.31	121.62	118.09
23	b	2523	CLA	C16-C15-C13	2.31	123.65	115.97
23	D	356	CLA	O2A-CGA-CBA	2.31	118.88	111.83
23	c	2483	CLA	C2A-C3A-C4A	2.31	105.60	101.87
23	B	517	CLA	C3B-C4B-NB	-2.31	108.47	110.53
27	b	2527	BCR	C35-C13-C12	2.31	121.61	118.09
23	a	2348	CLA	C12-C11-C10	-2.31	102.95	113.28
28	v	2138	HEC	CHC-C1C-NC	2.30	128.04	123.86
27	c	2489	BCR	C34-C9-C8	2.30	121.61	118.09
28	V	138	HEC	CHA-C1A-C2A	2.30	128.50	124.86
23	A	348	CLA	C12-C11-C10	-2.30	102.96	113.28
23	d	2357	CLA	O2A-CGA-CBA	2.30	118.85	111.83
23	D	354	CLA	C1-O2A-CGA	2.30	122.22	116.65
23	b	2516	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
27	b	2528	BCR	C7-C8-C9	2.30	129.63	126.23
23	c	2482	CLA	CAA-CBA-CGA	2.30	119.73	113.21
23	B	524	CLA	C4-C3-C5	2.30	119.21	115.23
23	b	2521	CLA	CMD-C2D-C1D	2.29	128.77	124.73
25	D	357	PL9	C20-C19-C21	-2.29	111.25	115.23
23	b	2526	CLA	O2D-CGD-CBD	2.29	115.24	111.23
23	b	2511	CLA	C7-C6-C5	-2.29	107.15	113.26
23	C	476	CLA	CBA-CAA-C2A	2.29	120.62	113.79
27	b	2527	BCR	C16-C17-C18	2.29	130.49	127.28
23	b	2523	CLA	CMD-C2D-C1D	2.29	128.76	124.73
23	d	2357	CLA	C2A-C3A-C4A	2.28	105.56	101.87
23	B	521	CLA	C1-O2A-CGA	2.28	122.18	116.65
23	A	348	CLA	O2A-CGA-CBA	2.28	118.80	111.83
23	B	525	CLA	C6-C5-C3	2.28	119.02	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	355	PHO	CBC-CAC-C3C	-2.28	109.61	112.87
24	D	355	PHO	C4D-ND-C1D	-2.28	106.14	108.87
23	C	484	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
23	b	2521	CLA	CAA-CBA-CGA	-2.28	106.75	113.21
23	C	486	CLA	C3B-C4B-NB	-2.27	108.50	110.53
23	c	2479	CLA	O2D-CGD-CBD	2.27	115.20	111.23
23	c	2484	CLA	CMD-C2D-C1D	2.27	128.73	124.73
23	b	2516	CLA	C6-C7-C8	2.27	123.52	115.97
23	C	479	CLA	O2D-CGD-CBD	2.27	115.20	111.23
27	B	528	BCR	C7-C8-C9	2.27	129.60	126.23
23	b	2522	CLA	CBA-CAA-C2A	2.27	120.55	113.79
23	C	480	CLA	CMD-C2D-C1D	2.27	128.73	124.73
27	B	528	BCR	C37-C22-C23	2.27	121.56	118.09
23	C	476	CLA	C2A-C3A-C4A	2.27	105.53	101.87
27	B	529	BCR	C20-C19-C18	-2.27	120.14	126.36
23	b	2514	CLA	C3B-C4B-NB	-2.27	108.50	110.53
23	B	523	CLA	C2A-C3A-C4A	2.27	105.53	101.87
28	V	138	HEC	C3A-C4A-NA	2.26	113.83	109.64
23	d	2354	CLA	C7-C6-C5	-2.26	107.23	113.26
26	B	526	LMT	C3-C2-C1	-2.26	103.63	113.47
23	B	516	CLA	C6-C7-C8	2.26	123.48	115.97
27	c	2489	BCR	C11-C10-C9	2.26	130.45	127.28
23	A	352	CLA	C12-C11-C10	-2.26	103.15	113.28
23	c	2481	CLA	O2D-CGD-CBD	2.26	115.18	111.23
23	C	484	CLA	C2A-C3A-C4A	2.26	105.52	101.87
23	a	2348	CLA	O2A-CGA-CBA	2.26	118.72	111.83
24	A	351	PHO	C12-C11-C10	-2.26	103.16	113.28
24	A	351	PHO	CMA-C3A-C4A	-2.26	109.75	114.61
23	c	2480	CLA	CMD-C2D-C1D	2.26	128.70	124.73
23	A	352	CLA	C2A-C1A-CHA	2.26	127.78	123.87
23	B	516	CLA	CAA-C2A-C1A	-2.26	104.58	111.97
23	C	487	CLA	C7-C6-C5	-2.26	107.25	113.26
23	c	2485	CLA	C3B-C4B-NB	-2.25	108.52	110.53
23	a	2348	CLA	O2A-C1-C2	2.25	116.78	108.11
23	B	514	CLA	C3B-C4B-NB	-2.25	108.52	110.53
23	b	2514	CLA	C3A-C2A-C1A	2.25	104.71	101.34
23	b	2515	CLA	C2A-C3A-C4A	2.25	105.50	101.87
23	b	2526	CLA	C2A-C3A-C4A	2.25	105.50	101.87
27	J	53	BCR	C16-C17-C18	2.25	130.43	127.28
27	j	2053	BCR	C15-C14-C13	2.25	130.43	127.28
23	A	350	CLA	C3B-C4B-NB	-2.24	108.53	110.53
23	B	519	CLA	C3B-C4B-NB	-2.24	108.53	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	521	CLA	CAA-CBA-CGA	-2.24	106.85	113.21
24	A	351	PHO	OBD-CAD-C3D	2.24	131.38	127.89
28	e	2084	HEC	O1A-CGA-CBA	-2.24	115.99	123.09
23	C	475	CLA	C2A-C1A-CHA	2.24	127.75	123.87
23	b	2520	CLA	CMD-C2D-C1D	2.24	128.67	124.73
23	a	2349	CLA	C2A-C3A-C4A	2.24	105.48	101.87
23	A	349	CLA	C1-O2A-CGA	2.24	122.06	116.65
23	b	2517	CLA	CAA-C2A-C1A	-2.24	104.65	111.97
27	c	2489	BCR	C8-C7-C6	2.23	132.97	127.00
23	D	354	CLA	C7-C6-C5	-2.23	107.31	113.26
23	c	2487	CLA	O2D-CGD-CBD	2.23	115.13	111.23
23	A	349	CLA	C2A-C3A-C4A	2.23	105.47	101.87
23	B	515	CLA	C2A-C3A-C4A	2.23	105.47	101.87
27	C	488	BCR	C30-C25-C26	-2.23	119.59	122.64
23	b	2519	CLA	C3B-C4B-NB	-2.23	108.54	110.53
23	D	354	CLA	O2D-CGD-CBD	2.23	115.13	111.23
23	B	511	CLA	C7-C6-C5	-2.23	107.32	113.26
23	B	520	CLA	C1-O2A-CGA	2.23	122.04	116.65
23	C	479	CLA	C1-C2-C3	2.23	129.84	126.20
23	B	522	CLA	CBA-CAA-C2A	2.22	120.41	113.79
23	a	2351	CLA	C12-C11-C10	-2.22	103.31	113.28
23	d	2355	CLA	O2D-CGD-CBD	2.22	115.11	111.23
23	b	2515	CLA	C3B-C4B-NB	-2.22	108.55	110.53
23	c	2479	CLA	C2A-C3A-C4A	2.22	105.45	101.87
27	J	53	BCR	C35-C13-C12	2.21	121.47	118.09
23	C	484	CLA	C3B-C4B-NB	-2.21	108.56	110.53
23	b	2516	CLA	O2D-CGD-CBD	2.21	115.10	111.23
23	b	2516	CLA	C2A-C3A-C4A	2.21	105.44	101.87
23	C	482	CLA	CMD-C2D-C1D	2.21	128.62	124.73
28	E	84	HEC	O2A-CGA-CBA	2.21	120.98	114.00
24	D	355	PHO	CMB-C2B-C3B	2.21	129.10	124.68
23	c	2476	CLA	C12-C11-C10	-2.21	103.38	113.28
24	A	351	PHO	CBC-CAC-C3C	-2.21	109.71	112.87
25	a	2352	PL9	C8-C7-C3	2.21	117.73	112.03
27	F	48	BCR	C40-C30-C25	2.21	113.70	110.24
23	C	478	CLA	C7-C6-C5	-2.20	107.39	113.26
23	b	2517	CLA	C7-C6-C5	-2.20	107.39	113.26
27	B	529	BCR	C7-C8-C9	2.20	129.49	126.23
23	B	521	CLA	C3B-C4B-NB	-2.20	108.56	110.53
23	B	524	CLA	C2A-C3A-C4A	2.20	105.42	101.87
23	B	525	CLA	C3B-C4B-NB	-2.20	108.57	110.53
25	a	2352	PL9	O1-C4-C3	-2.20	118.41	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	513	CLA	C1-O2A-CGA	2.20	121.97	116.65
23	B	514	CLA	O2D-CGD-CBD	2.20	115.07	111.23
23	C	477	CLA	C16-C15-C13	2.20	123.27	115.97
23	B	518	CLA	C3B-C4B-NB	-2.20	108.57	110.53
27	C	488	BCR	C37-C22-C23	2.20	121.44	118.09
23	b	2520	CLA	C2A-C3A-C4A	2.19	105.41	101.87
23	C	485	CLA	C3B-C4B-NB	-2.19	108.57	110.53
23	B	515	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
23	c	2481	CLA	C2A-C3A-C4A	2.19	105.41	101.87
23	B	515	CLA	O2A-CGA-CBA	2.19	118.52	111.83
27	j	2053	BCR	C36-C18-C19	2.19	121.43	118.09
23	b	2516	CLA	CMD-C2D-C1D	2.19	128.58	124.73
24	a	2350	PHO	CAA-C2A-C3A	-2.19	107.09	113.00
27	K	50	BCR	C1-C6-C5	-2.19	119.65	122.64
23	B	514	CLA	C2A-C1A-CHA	2.19	127.66	123.87
28	E	84	HEC	CBB-CAB-C3B	-2.19	106.50	112.42
28	E	84	HEC	CHC-C1C-NC	2.18	127.82	123.86
23	a	2351	CLA	O2A-CGA-CBA	2.18	118.49	111.83
28	e	2084	HEC	CHA-C1A-C2A	-2.18	121.42	124.86
23	b	2525	CLA	C6-C5-C3	2.18	118.78	113.47
23	b	2524	CLA	C4-C3-C5	2.18	119.01	115.23
27	J	53	BCR	C36-C18-C19	2.17	121.41	118.09
23	c	2487	CLA	C2A-C3A-C4A	2.17	105.38	101.87
23	c	2475	CLA	C2A-C1A-CHA	2.17	127.64	123.87
23	d	2355	CLA	C2A-C3A-C4A	2.17	105.38	101.87
23	C	474	CLA	C3B-C4B-NB	-2.17	108.59	110.53
27	c	2488	BCR	C23-C22-C21	-2.17	115.60	119.01
23	a	2351	CLA	CAA-CBA-CGA	2.17	119.37	113.21
23	C	483	CLA	CMD-C2D-C1D	2.17	128.55	124.73
23	C	478	CLA	C2A-C3A-C4A	2.17	105.37	101.87
23	C	481	CLA	C3B-C4B-NB	-2.17	108.60	110.53
27	J	53	BCR	C20-C21-C22	2.17	130.32	127.28
23	a	2351	CLA	C2A-C1A-CHA	2.17	127.62	123.87
23	C	484	CLA	O2D-CGD-CBD	2.16	115.01	111.23
23	C	484	CLA	CMD-C2D-C1D	2.16	128.53	124.73
23	b	2512	CLA	O2D-CGD-CBD	2.16	115.01	111.23
27	C	488	BCR	C11-C10-C9	2.16	130.31	127.28
24	D	355	PHO	C3B-C4B-NB	2.16	108.87	107.46
23	B	522	CLA	C6-C5-C3	2.16	118.73	113.47
27	c	2489	BCR	C32-C1-C6	2.16	113.63	110.24
23	c	2479	CLA	C1-O2A-CGA	2.16	121.87	116.65
27	j	2053	BCR	C34-C9-C8	2.16	121.38	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	2356	PHO	CMA-C3A-C4A	-2.16	109.96	114.61
23	B	518	CLA	C12-C11-C10	-2.16	103.62	113.28
23	b	2514	CLA	C2A-C1A-CHA	2.16	127.61	123.87
23	C	479	CLA	CMD-C2D-C1D	2.15	128.52	124.73
23	c	2486	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
23	c	2481	CLA	C2D-C1D-ND	2.15	112.26	110.13
27	c	2488	BCR	C37-C22-C23	2.15	121.38	118.09
23	C	487	CLA	C2A-C3A-C4A	2.15	105.35	101.87
23	B	514	CLA	CMD-C2D-C1D	2.15	128.52	124.73
23	b	2526	CLA	C6-C7-C8	2.15	123.12	115.97
23	B	521	CLA	C7-C6-C5	-2.15	107.53	113.26
24	A	351	PHO	O1D-CGD-CBD	-2.15	121.46	124.72
25	D	357	PL9	C7-C3-C4	2.15	118.68	116.91
23	b	2522	CLA	C1-O2A-CGA	2.15	121.85	116.65
23	c	2476	CLA	CBA-CAA-C2A	2.15	120.18	113.79
23	C	485	CLA	C1-O2A-CGA	2.14	121.84	116.65
23	A	349	CLA	C2D-C1D-ND	2.14	112.25	110.13
23	B	517	CLA	CMD-C2D-C1D	2.14	128.50	124.73
23	C	477	CLA	C2A-C3A-C4A	2.14	105.33	101.87
23	a	2349	CLA	CED-O2D-CGD	2.14	120.77	115.92
28	e	2084	HEC	CBB-CAB-C3B	-2.14	106.62	112.42
23	C	475	CLA	CAA-CBA-CGA	2.14	119.28	113.21
27	B	529	BCR	C16-C17-C18	2.14	130.28	127.28
23	b	2513	CLA	CMA-C3A-C2A	-2.14	105.72	113.98
23	b	2518	CLA	O2A-C1-C2	2.14	116.33	108.11
28	v	2138	HEC	CBB-CAB-C3B	-2.14	106.63	112.42
24	d	2356	PHO	C3D-C4D-ND	2.13	110.44	107.71
23	C	476	CLA	C12-C11-C10	-2.13	103.72	113.28
28	v	2138	HEC	CHB-C4A-C3A	-2.13	121.05	125.49
23	c	2478	CLA	CAA-CBA-CGA	2.13	119.26	113.21
23	d	2354	CLA	C1-O2A-CGA	2.13	121.81	116.65
27	B	528	BCR	C34-C9-C8	2.13	121.34	118.09
23	c	2476	CLA	C2A-C3A-C4A	2.13	105.31	101.87
27	C	488	BCR	C1-C6-C7	2.13	121.42	115.65
23	a	2349	CLA	C3B-C4B-NB	-2.13	108.63	110.53
23	C	479	CLA	C2A-C3A-C4A	2.13	105.30	101.87
23	B	527	CLA	C2A-C3A-C4A	2.12	105.30	101.87
25	A	353	PL9	C8-C7-C3	2.12	117.52	112.03
27	c	2488	BCR	C1-C6-C7	2.12	121.41	115.65
23	c	2482	CLA	CMD-C2D-C1D	2.12	128.47	124.73
23	B	515	CLA	C3B-C4B-NB	-2.12	108.64	110.53
24	a	2350	PHO	C12-C11-C10	-2.12	103.78	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	519	CLA	CHB-C4A-NA	2.12	127.46	124.40
23	b	2512	CLA	C2A-C3A-C4A	2.12	105.29	101.87
23	c	2476	CLA	CMA-C3A-C2A	-2.12	105.79	113.98
23	C	476	CLA	C1-O2A-CGA	2.12	121.78	116.65
23	b	2514	CLA	CMD-C2D-C1D	2.12	128.45	124.73
23	a	2349	CLA	CAA-C2A-C3A	-2.11	107.28	113.00
24	D	355	PHO	CMA-C3A-C4A	-2.11	110.06	114.61
27	c	2489	BCR	C1-C6-C7	2.11	121.38	115.65
27	b	2528	BCR	C37-C22-C23	2.11	121.32	118.09
23	b	2515	CLA	CMD-C2D-C1D	2.11	128.45	124.73
26	B	526	LMT	O1'-C1'-C2'	2.11	111.48	108.27
28	E	84	HEC	C4A-NA-C1A	-2.11	102.38	105.82
23	c	2479	CLA	CHB-C4A-NA	2.11	127.45	124.40
23	b	2522	CLA	C16-C15-C13	2.11	122.97	115.97
23	C	476	CLA	CMA-C3A-C2A	-2.11	105.83	113.98
23	b	2517	CLA	C3A-C2A-C1A	2.11	104.50	101.34
23	c	2480	CLA	C2A-C3A-C4A	2.11	105.27	101.87
23	A	350	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
23	C	478	CLA	C12-C11-C10	-2.11	103.84	113.28
27	C	488	BCR	C1-C6-C5	-2.10	119.76	122.64
23	b	2518	CLA	C12-C11-C10	-2.10	103.85	113.28
23	C	474	CLA	CAA-C2A-C3A	-2.10	107.31	113.00
23	C	483	CLA	C3B-C4B-NB	-2.10	108.65	110.53
28	E	84	HEC	C1C-CHC-C4B	-2.10	121.31	126.25
23	B	521	CLA	CBA-CAA-C2A	2.10	120.05	113.79
23	c	2484	CLA	C3B-C4B-NB	-2.10	108.66	110.53
27	B	528	BCR	C36-C18-C19	2.10	121.30	118.09
23	c	2474	CLA	C2A-C3A-C4A	2.10	105.26	101.87
27	J	53	BCR	C11-C10-C9	2.10	130.22	127.28
23	B	522	CLA	C2A-C3A-C4A	2.10	105.26	101.87
23	b	2521	CLA	C7-C6-C5	-2.10	107.67	113.26
23	c	2482	CLA	O2A-CGA-CBA	2.10	118.23	111.83
23	C	479	CLA	C1-O2A-CGA	2.10	121.72	116.65
23	B	511	CLA	CHB-C4A-NA	2.09	127.42	124.40
23	B	515	CLA	CMD-C2D-C1D	2.09	128.41	124.73
23	B	514	CLA	C3A-C2A-C1A	2.09	104.47	101.34
23	b	2524	CLA	C12-C11-C10	-2.09	103.90	113.28
27	k	2050	BCR	C1-C6-C7	2.09	121.33	115.65
24	a	2350	PHO	CMB-C2B-C3B	2.09	128.86	124.68
23	B	518	CLA	O2A-C1-C2	2.09	116.15	108.11
27	B	529	BCR	C10-C11-C12	2.09	129.25	123.20
23	d	2357	CLA	C6-C5-C3	2.09	118.56	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	489	BCR	C11-C10-C9	2.09	130.21	127.28
23	c	2478	CLA	C12-C11-C10	-2.09	103.93	113.28
23	A	352	CLA	C3B-C4B-NB	-2.09	108.67	110.53
27	K	50	BCR	C1-C6-C7	2.09	121.31	115.65
23	D	356	CLA	C3B-C4B-NB	-2.09	108.67	110.53
23	a	2348	CLA	CMA-C3A-C2A	-2.08	105.92	113.98
27	k	2050	BCR	C16-C17-C18	2.08	130.20	127.28
23	c	2479	CLA	CMD-C2D-C1D	2.08	128.40	124.73
23	B	521	CLA	C2A-C3A-C4A	2.08	105.23	101.87
23	C	474	CLA	C2A-C3A-C4A	2.08	105.23	101.87
23	b	2518	CLA	C3B-C4B-NB	-2.08	108.67	110.53
23	c	2477	CLA	C16-C15-C13	2.08	122.88	115.97
25	A	353	PL9	O1-C4-C3	-2.08	118.54	120.73
27	J	53	BCR	C23-C24-C25	2.08	132.55	127.00
23	A	348	CLA	CMA-C3A-C2A	-2.08	105.95	113.98
23	B	527	CLA	C6-C7-C8	2.08	122.87	115.97
23	A	348	CLA	C2A-C1A-CHA	2.08	127.47	123.87
23	c	2481	CLA	C4D-CHA-C1A	2.08	123.72	121.24
23	c	2482	CLA	C6-C5-C3	2.07	118.52	113.47
23	A	352	CLA	O2A-CGA-CBA	2.07	118.16	111.83
27	b	2528	BCR	C16-C17-C18	2.07	130.19	127.28
23	B	516	CLA	C3B-C4B-NB	-2.07	108.68	110.53
23	C	487	CLA	CMD-C2D-C1D	2.07	128.38	124.73
27	b	2527	BCR	C12-C13-C14	-2.07	115.75	119.01
26	d	2359	LMT	O6B-C6B-C5B	2.07	118.37	111.33
23	C	486	CLA	CMD-C2D-C1D	2.06	128.36	124.73
23	a	2348	CLA	C16-C15-C13	2.06	122.83	115.97
23	d	2355	CLA	C1-O2A-CGA	2.06	121.64	116.65
28	V	138	HEC	C4C-CHD-C1D	2.06	131.10	126.25
23	A	348	CLA	C2A-C3A-C4A	2.06	105.20	101.87
23	c	2487	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
23	b	2521	CLA	CBA-CAA-C2A	2.06	119.92	113.79
23	b	2512	CLA	C12-C11-C10	-2.06	104.05	113.28
23	b	2520	CLA	C1-O2A-CGA	2.06	121.64	116.65
23	B	522	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
23	B	518	CLA	C2A-C1A-CHA	2.06	127.44	123.87
23	b	2522	CLA	C6-C5-C3	2.06	118.48	113.47
23	B	513	CLA	CMA-C3A-C2A	-2.06	106.03	113.98
27	B	528	BCR	C15-C14-C13	2.06	130.16	127.28
23	c	2478	CLA	CMD-C2D-C1D	2.06	128.35	124.73
23	c	2479	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
27	K	50	BCR	C19-C18-C17	-2.05	115.78	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	2484	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
23	C	487	CLA	O2D-CGD-CBD	2.05	114.82	111.23
27	j	2053	BCR	C23-C24-C25	2.05	132.47	127.00
23	C	480	CLA	C12-C11-C10	-2.05	104.11	113.28
23	C	478	CLA	CAA-CBA-CGA	2.05	119.02	113.21
23	B	512	CLA	C2A-C3A-C4A	2.05	105.17	101.87
23	c	2477	CLA	C2A-C3A-C4A	2.05	105.17	101.87
23	c	2484	CLA	C2A-C3A-C4A	2.04	105.17	101.87
23	C	476	CLA	C6-C5-C3	2.04	118.44	113.47
27	K	50	BCR	C16-C17-C18	2.04	130.14	127.28
23	b	2513	CLA	C12-C11-C10	-2.04	104.13	113.28
23	c	2481	CLA	C3B-C4B-NB	-2.04	108.71	110.53
23	d	2357	CLA	C3B-C4B-NB	-2.04	108.71	110.53
23	D	356	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
23	B	519	CLA	C2A-C1A-CHA	2.04	127.40	123.87
23	C	474	CLA	C6-C7-C8	2.04	122.73	115.97
23	C	480	CLA	C2A-C3A-C4A	2.04	105.16	101.87
28	v	2138	HEC	O2D-CGD-O1D	2.04	128.57	123.33
24	a	2350	PHO	C3D-C4D-ND	2.03	110.31	107.71
23	c	2483	CLA	CMD-C2D-C1D	2.03	128.31	124.73
23	c	2487	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
23	A	348	CLA	C16-C15-C13	2.03	122.70	115.97
23	d	2355	CLA	C4-C3-C5	2.03	118.75	115.23
23	b	2524	CLA	C2A-C1A-CHA	2.03	127.38	123.87
23	c	2486	CLA	C1-O2A-CGA	2.02	121.55	116.65
27	k	2050	BCR	C19-C18-C17	-2.02	115.83	119.01
27	b	2528	BCR	C10-C11-C12	2.02	129.05	123.20
23	C	481	CLA	O2D-CGD-CBD	2.02	114.76	111.23
23	b	2522	CLA	C2A-C3A-C4A	2.02	105.13	101.87
23	C	475	CLA	C12-C11-C10	-2.02	104.23	113.28
25	D	357	PL9	C25-C24-C26	-2.02	111.73	115.23
24	a	2350	PHO	CBC-CAC-C3C	-2.02	109.99	112.87
23	C	485	CLA	CMD-C2D-C1D	2.02	128.28	124.73
23	A	350	CLA	CED-O2D-CGD	2.02	120.49	115.92
27	B	528	BCR	C30-C25-C24	2.02	121.12	115.65
23	B	524	CLA	C3B-C4B-NB	-2.01	108.73	110.53
27	b	2528	BCR	C35-C13-C14	-2.01	119.55	122.82
23	c	2485	CLA	C1-O2A-CGA	2.01	121.52	116.65
28	e	2084	HEC	O2A-CGA-CBA	2.01	120.36	114.00
25	d	2358	PL9	C25-C24-C26	-2.01	111.74	115.23
28	E	84	HEC	CMA-C3A-C2A	2.01	131.59	126.15
25	A	353	PL9	C15-C14-C16	-2.01	111.74	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	526	LMT	C1'-O5'-C5'	2.01	117.64	113.72
23	C	479	CLA	C3A-C2A-C1A	2.01	104.35	101.34
27	k	2050	BCR	C35-C13-C12	2.01	121.15	118.09
23	b	2512	CLA	CMD-C2D-C1D	2.01	128.26	124.73
27	b	2527	BCR	C15-C14-C13	2.01	130.09	127.28
23	b	2523	CLA	C2D-C1D-ND	2.00	112.11	110.13
23	c	2481	CLA	C1-C2-C3	2.00	129.48	126.20
23	B	516	CLA	CMD-C2D-C1D	2.00	128.25	124.73
23	b	2520	CLA	C7-C6-C5	-2.00	107.93	113.26
23	c	2486	CLA	CMD-C2D-C1D	2.00	128.25	124.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	E	84	HEC	NA
28	V	138	HEC	NA
28	e	2084	HEC	NA
28	v	2138	HEC	NA

All (1033) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	348	CLA	C2-C1-O2A-CGA
23	A	349	CLA	C2B-C3B-CAB-CBB
23	A	349	CLA	C4B-C3B-CAB-CBB
23	A	352	CLA	C2B-C3B-CAB-CBB
23	A	352	CLA	C4B-C3B-CAB-CBB
23	B	511	CLA	C2B-C3B-CAB-CBB
23	B	511	CLA	C4B-C3B-CAB-CBB
23	B	512	CLA	CBD-CGD-O2D-CED
23	B	513	CLA	C2B-C3B-CAB-CBB
23	B	513	CLA	C4B-C3B-CAB-CBB
23	B	513	CLA	CAD-CBD-CGD-O1D
23	B	513	CLA	CAD-CBD-CGD-O2D
23	B	513	CLA	O2A-C1-C2-C3
23	B	514	CLA	CBD-CGD-O2D-CED
23	B	514	CLA	C6-C7-C8-C9
23	B	515	CLA	C2B-C3B-CAB-CBB
23	B	515	CLA	C4B-C3B-CAB-CBB
23	B	515	CLA	CAD-CBD-CGD-O1D
23	B	515	CLA	CAD-CBD-CGD-O2D
23	B	515	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	B	517	CLA	C2B-C3B-CAB-CBB
23	B	517	CLA	C4B-C3B-CAB-CBB
23	B	517	CLA	CAD-CBD-CGD-O1D
23	B	517	CLA	CAD-CBD-CGD-O2D
23	B	518	CLA	C2B-C3B-CAB-CBB
23	B	518	CLA	C4B-C3B-CAB-CBB
23	B	518	CLA	C6-C7-C8-C9
23	B	519	CLA	O2A-C1-C2-C3
23	B	520	CLA	CHA-CBD-CGD-O1D
23	B	520	CLA	CHA-CBD-CGD-O2D
23	B	521	CLA	C2B-C3B-CAB-CBB
23	B	521	CLA	C4B-C3B-CAB-CBB
23	B	522	CLA	CBD-CGD-O2D-CED
23	B	524	CLA	C2-C1-O2A-CGA
23	B	524	CLA	C2B-C3B-CAB-CBB
23	B	524	CLA	C4B-C3B-CAB-CBB
23	B	524	CLA	C14-C13-C15-C16
23	B	525	CLA	C2B-C3B-CAB-CBB
23	B	525	CLA	C4B-C3B-CAB-CBB
23	B	525	CLA	CBD-CGD-O2D-CED
23	B	527	CLA	CBD-CGD-O2D-CED
23	B	527	CLA	C6-C7-C8-C9
23	C	474	CLA	C2B-C3B-CAB-CBB
23	C	474	CLA	C4B-C3B-CAB-CBB
23	C	475	CLA	C2B-C3B-CAB-CBB
23	C	475	CLA	C4B-C3B-CAB-CBB
23	C	476	CLA	C2B-C3B-CAB-CBB
23	C	476	CLA	C4B-C3B-CAB-CBB
23	C	476	CLA	CBD-CGD-O2D-CED
23	C	477	CLA	C2B-C3B-CAB-CBB
23	C	477	CLA	C4B-C3B-CAB-CBB
23	C	477	CLA	CBD-CGD-O2D-CED
23	C	478	CLA	CAD-CBD-CGD-O1D
23	C	478	CLA	CAD-CBD-CGD-O2D
23	C	479	CLA	CHA-CBD-CGD-O1D
23	C	479	CLA	CHA-CBD-CGD-O2D
23	C	480	CLA	C2B-C3B-CAB-CBB
23	C	480	CLA	C4B-C3B-CAB-CBB
23	C	481	CLA	C4B-C3B-CAB-CBB
23	C	481	CLA	CBD-CGD-O2D-CED
23	C	482	CLA	C2B-C3B-CAB-CBB
23	C	482	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	482	CLA	CBD-CGD-O2D-CED
23	C	483	CLA	C2B-C3B-CAB-CBB
23	C	483	CLA	C4B-C3B-CAB-CBB
23	C	483	CLA	CHA-CBD-CGD-O1D
23	C	483	CLA	CHA-CBD-CGD-O2D
23	C	483	CLA	C6-C7-C8-C9
23	C	484	CLA	C2B-C3B-CAB-CBB
23	C	484	CLA	C4B-C3B-CAB-CBB
23	C	484	CLA	C6-C7-C8-C9
23	C	485	CLA	C2B-C3B-CAB-CBB
23	C	485	CLA	C4B-C3B-CAB-CBB
23	C	485	CLA	CHA-CBD-CGD-O1D
23	C	485	CLA	CHA-CBD-CGD-O2D
23	C	486	CLA	C2B-C3B-CAB-CBB
23	C	486	CLA	C4B-C3B-CAB-CBB
23	C	486	CLA	CHA-CBD-CGD-O2D
23	C	487	CLA	C2B-C3B-CAB-CBB
23	C	487	CLA	C4B-C3B-CAB-CBB
23	C	487	CLA	CBD-CGD-O2D-CED
23	a	2348	CLA	C2-C1-O2A-CGA
23	a	2351	CLA	C2B-C3B-CAB-CBB
23	a	2351	CLA	C4B-C3B-CAB-CBB
23	b	2511	CLA	C2B-C3B-CAB-CBB
23	b	2511	CLA	C4B-C3B-CAB-CBB
23	b	2512	CLA	CBD-CGD-O2D-CED
23	b	2513	CLA	C2B-C3B-CAB-CBB
23	b	2513	CLA	C4B-C3B-CAB-CBB
23	b	2513	CLA	CAD-CBD-CGD-O1D
23	b	2513	CLA	CAD-CBD-CGD-O2D
23	b	2513	CLA	O2A-C1-C2-C3
23	b	2514	CLA	CBD-CGD-O2D-CED
23	b	2514	CLA	C6-C7-C8-C9
23	b	2515	CLA	C2B-C3B-CAB-CBB
23	b	2515	CLA	C4B-C3B-CAB-CBB
23	b	2515	CLA	CAD-CBD-CGD-O1D
23	b	2515	CLA	CAD-CBD-CGD-O2D
23	b	2515	CLA	O2A-C1-C2-C3
23	b	2517	CLA	C2B-C3B-CAB-CBB
23	b	2517	CLA	C4B-C3B-CAB-CBB
23	b	2517	CLA	CAD-CBD-CGD-O1D
23	b	2517	CLA	CAD-CBD-CGD-O2D
23	b	2518	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	b	2518	CLA	C4B-C3B-CAB-CBB
23	b	2518	CLA	C6-C7-C8-C9
23	b	2519	CLA	O2A-C1-C2-C3
23	b	2520	CLA	CHA-CBD-CGD-O1D
23	b	2520	CLA	CHA-CBD-CGD-O2D
23	b	2521	CLA	C2B-C3B-CAB-CBB
23	b	2521	CLA	C4B-C3B-CAB-CBB
23	b	2522	CLA	CBD-CGD-O2D-CED
23	b	2524	CLA	C2-C1-O2A-CGA
23	b	2524	CLA	C2B-C3B-CAB-CBB
23	b	2524	CLA	C4B-C3B-CAB-CBB
23	b	2524	CLA	C14-C13-C15-C16
23	b	2525	CLA	C2B-C3B-CAB-CBB
23	b	2525	CLA	C4B-C3B-CAB-CBB
23	b	2526	CLA	CBD-CGD-O2D-CED
23	b	2526	CLA	C6-C7-C8-C9
23	c	2474	CLA	C2B-C3B-CAB-CBB
23	c	2474	CLA	C4B-C3B-CAB-CBB
23	c	2475	CLA	C2B-C3B-CAB-CBB
23	c	2475	CLA	C4B-C3B-CAB-CBB
23	c	2476	CLA	C2B-C3B-CAB-CBB
23	c	2476	CLA	C4B-C3B-CAB-CBB
23	c	2476	CLA	CBD-CGD-O2D-CED
23	c	2477	CLA	C2B-C3B-CAB-CBB
23	c	2477	CLA	C4B-C3B-CAB-CBB
23	c	2477	CLA	CBD-CGD-O2D-CED
23	c	2478	CLA	CAD-CBD-CGD-O1D
23	c	2478	CLA	CAD-CBD-CGD-O2D
23	c	2479	CLA	CHA-CBD-CGD-O1D
23	c	2479	CLA	CHA-CBD-CGD-O2D
23	c	2480	CLA	C2B-C3B-CAB-CBB
23	c	2480	CLA	C4B-C3B-CAB-CBB
23	c	2481	CLA	C4B-C3B-CAB-CBB
23	c	2481	CLA	CBD-CGD-O2D-CED
23	c	2482	CLA	C4B-C3B-CAB-CBB
23	c	2482	CLA	CBD-CGD-O2D-CED
23	c	2483	CLA	C2B-C3B-CAB-CBB
23	c	2483	CLA	C4B-C3B-CAB-CBB
23	c	2483	CLA	CHA-CBD-CGD-O1D
23	c	2483	CLA	CHA-CBD-CGD-O2D
23	c	2483	CLA	C6-C7-C8-C9
23	c	2484	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	c	2484	CLA	C4B-C3B-CAB-CBB
23	c	2485	CLA	C2B-C3B-CAB-CBB
23	c	2485	CLA	C4B-C3B-CAB-CBB
23	c	2485	CLA	CHA-CBD-CGD-O1D
23	c	2485	CLA	CHA-CBD-CGD-O2D
23	c	2486	CLA	C2B-C3B-CAB-CBB
23	c	2486	CLA	C4B-C3B-CAB-CBB
23	c	2486	CLA	CHA-CBD-CGD-O2D
23	c	2487	CLA	C2B-C3B-CAB-CBB
23	c	2487	CLA	C4B-C3B-CAB-CBB
23	c	2487	CLA	CBD-CGD-O2D-CED
23	d	2355	CLA	C2B-C3B-CAB-CBB
23	d	2355	CLA	C4B-C3B-CAB-CBB
24	D	355	PHO	CBD-CGD-O2D-CED
24	d	2356	PHO	CBD-CGD-O2D-CED
25	A	353	PL9	C18-C19-C21-C22
25	A	353	PL9	C20-C19-C21-C22
25	d	2358	PL9	C29-C31-C32-C33
26	B	526	LMT	C2'-C1'-O1'-C1
26	B	526	LMT	O5'-C1'-O1'-C1
26	d	2359	LMT	C2'-C1'-O1'-C1
26	d	2359	LMT	O5'-C1'-O1'-C1
27	B	529	BCR	C6-C7-C8-C9
27	B	529	BCR	C7-C8-C9-C10
27	B	529	BCR	C7-C8-C9-C34
27	B	529	BCR	C22-C23-C24-C25
27	C	488	BCR	C6-C7-C8-C9
27	C	488	BCR	C7-C8-C9-C10
27	C	488	BCR	C7-C8-C9-C34
27	C	489	BCR	C6-C7-C8-C9
27	C	489	BCR	C22-C23-C24-C25
27	F	48	BCR	C6-C7-C8-C9
27	F	48	BCR	C22-C23-C24-C25
27	J	53	BCR	C6-C7-C8-C9
27	J	53	BCR	C22-C23-C24-C25
27	K	50	BCR	C22-C23-C24-C25
27	b	2527	BCR	C7-C8-C9-C10
27	b	2528	BCR	C6-C7-C8-C9
27	b	2528	BCR	C7-C8-C9-C10
27	b	2528	BCR	C7-C8-C9-C34
27	b	2528	BCR	C22-C23-C24-C25
27	c	2488	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	c	2488	BCR	C7-C8-C9-C10
27	c	2488	BCR	C7-C8-C9-C34
27	c	2489	BCR	C6-C7-C8-C9
27	c	2489	BCR	C22-C23-C24-C25
27	d	2360	BCR	C6-C7-C8-C9
27	j	2053	BCR	C6-C7-C8-C9
27	j	2053	BCR	C22-C23-C24-C25
27	k	2050	BCR	C22-C23-C24-C25
23	C	480	CLA	O1D-CGD-O2D-CED
23	C	484	CLA	O1D-CGD-O2D-CED
23	c	2480	CLA	O1D-CGD-O2D-CED
23	c	2484	CLA	O1D-CGD-O2D-CED
23	A	349	CLA	O1D-CGD-O2D-CED
23	B	512	CLA	O1D-CGD-O2D-CED
23	B	513	CLA	O1D-CGD-O2D-CED
23	B	527	CLA	O1D-CGD-O2D-CED
23	b	2512	CLA	O1D-CGD-O2D-CED
23	b	2526	CLA	O1D-CGD-O2D-CED
23	c	2478	CLA	O1D-CGD-O2D-CED
23	A	349	CLA	CBD-CGD-O2D-CED
23	B	511	CLA	CBD-CGD-O2D-CED
23	B	513	CLA	CBD-CGD-O2D-CED
23	B	515	CLA	CBD-CGD-O2D-CED
23	B	516	CLA	CBD-CGD-O2D-CED
23	B	524	CLA	CBD-CGD-O2D-CED
23	C	478	CLA	CBD-CGD-O2D-CED
23	C	479	CLA	CBD-CGD-O2D-CED
23	C	480	CLA	CBD-CGD-O2D-CED
23	C	484	CLA	CBD-CGD-O2D-CED
23	b	2511	CLA	CBD-CGD-O2D-CED
23	b	2513	CLA	CBD-CGD-O2D-CED
23	b	2515	CLA	CBD-CGD-O2D-CED
23	b	2516	CLA	CBD-CGD-O2D-CED
23	b	2524	CLA	CBD-CGD-O2D-CED
23	b	2525	CLA	CBD-CGD-O2D-CED
23	c	2478	CLA	CBD-CGD-O2D-CED
23	c	2479	CLA	CBD-CGD-O2D-CED
23	c	2480	CLA	CBD-CGD-O2D-CED
23	c	2484	CLA	CBD-CGD-O2D-CED
23	d	2355	CLA	CBD-CGD-O2D-CED
23	c	2487	CLA	C2C-C3C-CAC-CBC
23	C	487	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	C	478	CLA	O1D-CGD-O2D-CED
23	b	2513	CLA	O1D-CGD-O2D-CED
23	d	2355	CLA	O1D-CGD-O2D-CED
28	v	2138	HEC	C4C-C3C-CAC-CBC
23	C	482	CLA	O1D-CGD-O2D-CED
23	C	487	CLA	O1D-CGD-O2D-CED
23	b	2522	CLA	O1D-CGD-O2D-CED
23	c	2482	CLA	O1D-CGD-O2D-CED
23	c	2487	CLA	O1D-CGD-O2D-CED
24	D	355	PHO	O1D-CGD-O2D-CED
23	B	522	CLA	O1D-CGD-O2D-CED
23	C	476	CLA	O1D-CGD-O2D-CED
23	C	477	CLA	O1D-CGD-O2D-CED
23	C	481	CLA	O1D-CGD-O2D-CED
23	c	2476	CLA	O1D-CGD-O2D-CED
23	c	2477	CLA	O1D-CGD-O2D-CED
23	c	2481	CLA	O1D-CGD-O2D-CED
24	d	2356	PHO	O1D-CGD-O2D-CED
23	A	349	CLA	C13-C15-C16-C17
23	d	2355	CLA	C13-C15-C16-C17
28	V	138	HEC	C4C-C3C-CAC-CBC
23	B	514	CLA	O1D-CGD-O2D-CED
28	V	138	HEC	C2C-C3C-CAC-CBC
28	v	2138	HEC	C2C-C3C-CAC-CBC
23	C	487	CLA	C4C-C3C-CAC-CBC
23	c	2487	CLA	C4C-C3C-CAC-CBC
23	C	474	CLA	CBD-CGD-O2D-CED
23	C	475	CLA	CBD-CGD-O2D-CED
23	C	483	CLA	CBD-CGD-O2D-CED
23	c	2474	CLA	CBD-CGD-O2D-CED
23	c	2475	CLA	CBD-CGD-O2D-CED
23	c	2483	CLA	CBD-CGD-O2D-CED
23	B	515	CLA	O1D-CGD-O2D-CED
23	B	516	CLA	O1D-CGD-O2D-CED
23	B	525	CLA	O1D-CGD-O2D-CED
23	b	2514	CLA	O1D-CGD-O2D-CED
23	b	2525	CLA	O1D-CGD-O2D-CED
23	b	2516	CLA	O1D-CGD-O2D-CED
23	B	517	CLA	C4-C3-C5-C6
23	B	518	CLA	C4-C3-C5-C6
23	B	522	CLA	C4-C3-C5-C6
23	C	479	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	480	CLA	C4-C3-C5-C6
23	b	2517	CLA	C4-C3-C5-C6
23	b	2518	CLA	C4-C3-C5-C6
23	b	2522	CLA	C4-C3-C5-C6
23	c	2479	CLA	C4-C3-C5-C6
23	c	2480	CLA	C4-C3-C5-C6
25	D	357	PL9	C25-C24-C26-C27
25	a	2352	PL9	C20-C19-C21-C22
25	d	2358	PL9	C25-C24-C26-C27
23	B	517	CLA	C2-C3-C5-C6
23	B	518	CLA	C2-C3-C5-C6
23	C	479	CLA	C2-C3-C5-C6
23	C	480	CLA	C2-C3-C5-C6
23	b	2517	CLA	C2-C3-C5-C6
23	b	2518	CLA	C2-C3-C5-C6
23	c	2479	CLA	C2-C3-C5-C6
23	c	2480	CLA	C2-C3-C5-C6
25	a	2352	PL9	C18-C19-C21-C22
23	b	2511	CLA	O1D-CGD-O2D-CED
23	B	511	CLA	O1D-CGD-O2D-CED
23	B	524	CLA	O1D-CGD-O2D-CED
23	b	2515	CLA	O1D-CGD-O2D-CED
23	b	2524	CLA	O1D-CGD-O2D-CED
26	B	526	LMT	O5B-C5B-C6B-O6B
26	d	2359	LMT	O5B-C5B-C6B-O6B
23	c	2479	CLA	O1D-CGD-O2D-CED
23	B	514	CLA	C4-C3-C5-C6
23	B	521	CLA	C4-C3-C5-C6
23	C	484	CLA	C4-C3-C5-C6
23	b	2514	CLA	C4-C3-C5-C6
23	b	2521	CLA	C4-C3-C5-C6
23	c	2484	CLA	C4-C3-C5-C6
25	A	353	PL9	C35-C34-C36-C37
25	D	357	PL9	C35-C34-C36-C37
25	a	2352	PL9	C35-C34-C36-C37
25	d	2358	PL9	C35-C34-C36-C37
23	B	516	CLA	C2-C3-C5-C6
23	B	521	CLA	C2-C3-C5-C6
23	B	522	CLA	C2-C3-C5-C6
23	C	484	CLA	C2-C3-C5-C6
23	b	2516	CLA	C2-C3-C5-C6
23	b	2521	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	2522	CLA	C2-C3-C5-C6
23	c	2484	CLA	C2-C3-C5-C6
25	D	357	PL9	C33-C34-C36-C37
25	d	2358	PL9	C33-C34-C36-C37
25	D	357	PL9	C14-C16-C17-C18
25	D	357	PL9	C29-C31-C32-C33
25	d	2358	PL9	C14-C16-C17-C18
23	A	348	CLA	C2A-CAA-CBA-CGA
23	a	2348	CLA	C2A-CAA-CBA-CGA
23	C	479	CLA	O1D-CGD-O2D-CED
23	B	518	CLA	CBD-CGD-O2D-CED
23	a	2349	CLA	CBD-CGD-O2D-CED
23	b	2518	CLA	CBD-CGD-O2D-CED
23	A	350	CLA	CBD-CGD-O2D-CED
23	B	516	CLA	C4-C3-C5-C6
23	b	2516	CLA	C4-C3-C5-C6
23	B	514	CLA	C2-C3-C5-C6
23	b	2514	CLA	C2-C3-C5-C6
25	A	353	PL9	C33-C34-C36-C37
25	D	357	PL9	C23-C24-C26-C27
25	a	2352	PL9	C33-C34-C36-C37
25	d	2358	PL9	C23-C24-C26-C27
23	A	349	CLA	C6-C7-C8-C9
23	B	511	CLA	C11-C10-C8-C9
23	B	514	CLA	C11-C12-C13-C14
23	B	522	CLA	C14-C13-C15-C16
23	B	523	CLA	C6-C7-C8-C9
23	B	524	CLA	C6-C7-C8-C9
23	C	474	CLA	C11-C12-C13-C14
23	C	475	CLA	C6-C7-C8-C9
23	C	477	CLA	C6-C7-C8-C9
23	C	477	CLA	C14-C13-C15-C16
23	C	481	CLA	C6-C7-C8-C9
23	b	2511	CLA	C11-C10-C8-C9
23	b	2514	CLA	C11-C12-C13-C14
23	b	2522	CLA	C14-C13-C15-C16
23	b	2523	CLA	C6-C7-C8-C9
23	b	2524	CLA	C6-C7-C8-C9
23	c	2474	CLA	C11-C12-C13-C14
23	c	2475	CLA	C6-C7-C8-C9
23	c	2477	CLA	C6-C7-C8-C9
23	c	2477	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	2481	CLA	C6-C7-C8-C9
23	c	2484	CLA	C6-C7-C8-C9
23	d	2355	CLA	C6-C7-C8-C9
23	C	475	CLA	O1D-CGD-O2D-CED
23	C	483	CLA	O1D-CGD-O2D-CED
23	c	2483	CLA	O1D-CGD-O2D-CED
27	B	528	BCR	C7-C8-C9-C34
27	J	53	BCR	C7-C8-C9-C34
27	b	2527	BCR	C7-C8-C9-C34
27	j	2053	BCR	C7-C8-C9-C34
27	J	53	BCR	C7-C8-C9-C10
27	j	2053	BCR	C7-C8-C9-C10
23	A	349	CLA	C2A-CAA-CBA-CGA
23	B	524	CLA	C2A-CAA-CBA-CGA
23	b	2524	CLA	C2A-CAA-CBA-CGA
23	d	2355	CLA	C2A-CAA-CBA-CGA
26	B	526	LMT	C4B-C5B-C6B-O6B
26	d	2359	LMT	C4B-C5B-C6B-O6B
23	C	478	CLA	C2-C1-O2A-CGA
23	c	2478	CLA	C2-C1-O2A-CGA
23	B	516	CLA	C15-C16-C17-C18
23	a	2351	CLA	C13-C15-C16-C17
23	b	2516	CLA	C15-C16-C17-C18
23	A	348	CLA	C12-C13-C15-C16
23	B	512	CLA	C11-C10-C8-C7
23	B	517	CLA	C11-C12-C13-C15
23	B	523	CLA	C12-C13-C15-C16
23	C	478	CLA	C6-C7-C8-C10
23	a	2348	CLA	C12-C13-C15-C16
23	b	2511	CLA	C11-C12-C13-C15
23	b	2512	CLA	C11-C10-C8-C7
23	b	2517	CLA	C11-C12-C13-C15
23	b	2523	CLA	C12-C13-C15-C16
23	c	2478	CLA	C6-C7-C8-C10
23	A	352	CLA	C13-C15-C16-C17
23	a	2348	CLA	C10-C11-C12-C13
23	c	2474	CLA	O1D-CGD-O2D-CED
25	A	353	PL9	C29-C31-C32-C33
25	a	2352	PL9	C29-C31-C32-C33
26	B	526	LMT	O1'-C1-C2-C3
23	A	348	CLA	C10-C11-C12-C13
23	b	2513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	B	513	CLA	C15-C16-C17-C18
23	C	484	CLA	C10-C11-C12-C13
23	a	2348	CLA	C5-C6-C7-C8
23	c	2481	CLA	C5-C6-C7-C8
23	c	2484	CLA	C10-C11-C12-C13
23	B	511	CLA	C2A-CAA-CBA-CGA
23	B	519	CLA	C2A-CAA-CBA-CGA
23	C	479	CLA	C2A-CAA-CBA-CGA
23	b	2511	CLA	C2A-CAA-CBA-CGA
23	b	2519	CLA	C2A-CAA-CBA-CGA
23	c	2479	CLA	C2A-CAA-CBA-CGA
23	c	2474	CLA	C13-C15-C16-C17
26	d	2359	LMT	O1'-C1-C2-C3
23	c	2475	CLA	O1D-CGD-O2D-CED
27	d	2360	BCR	C22-C23-C24-C25
23	A	348	CLA	C5-C6-C7-C8
23	B	514	CLA	C10-C11-C12-C13
23	C	480	CLA	C5-C6-C7-C8
23	C	481	CLA	C5-C6-C7-C8
23	C	482	CLA	C13-C15-C16-C17
23	D	354	CLA	C5-C6-C7-C8
23	b	2514	CLA	C10-C11-C12-C13
23	c	2480	CLA	C5-C6-C7-C8
23	c	2482	CLA	C13-C15-C16-C17
23	d	2354	CLA	C5-C6-C7-C8
23	B	527	CLA	C15-C16-C17-C18
23	b	2525	CLA	C10-C11-C12-C13
23	C	474	CLA	O1D-CGD-O2D-CED
23	B	525	CLA	C10-C11-C12-C13
23	C	474	CLA	C13-C15-C16-C17
23	b	2526	CLA	C15-C16-C17-C18
23	b	2525	CLA	C15-C16-C17-C18
23	d	2357	CLA	C5-C6-C7-C8
23	B	521	CLA	C2A-CAA-CBA-CGA
23	C	478	CLA	C2A-CAA-CBA-CGA
23	b	2517	CLA	C2A-CAA-CBA-CGA
23	b	2521	CLA	C2A-CAA-CBA-CGA
23	c	2478	CLA	C2A-CAA-CBA-CGA
23	B	515	CLA	C5-C6-C7-C8
23	C	485	CLA	C5-C6-C7-C8
23	b	2522	CLA	C5-C6-C7-C8
23	c	2482	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	B	512	CLA	C10-C11-C12-C13
23	B	513	CLA	C5-C6-C7-C8
23	B	525	CLA	C15-C16-C17-C18
23	b	2512	CLA	C10-C11-C12-C13
23	b	2515	CLA	C15-C16-C17-C18
23	d	2357	CLA	C13-C15-C16-C17
23	B	515	CLA	C15-C16-C17-C18
23	B	522	CLA	C5-C6-C7-C8
23	D	356	CLA	C5-C6-C7-C8
23	D	356	CLA	C13-C15-C16-C17
23	c	2485	CLA	C5-C6-C7-C8
23	b	2514	CLA	C5-C6-C7-C8
23	C	482	CLA	C5-C6-C7-C8
23	C	484	CLA	C5-C6-C7-C8
25	D	357	PL9	C9-C11-C12-C13
25	d	2358	PL9	C9-C11-C12-C13
23	B	518	CLA	C10-C11-C12-C13
23	b	2513	CLA	C5-C6-C7-C8
27	B	528	BCR	C7-C8-C9-C10
23	B	517	CLA	C2A-CAA-CBA-CGA
23	c	2474	CLA	C2A-CAA-CBA-CGA
23	D	354	CLA	O2A-C1-C2-C3
23	d	2354	CLA	O2A-C1-C2-C3
23	B	522	CLA	C13-C15-C16-C17
23	b	2518	CLA	C10-C11-C12-C13
23	B	518	CLA	O1D-CGD-O2D-CED
23	B	514	CLA	C5-C6-C7-C8
23	C	474	CLA	C2-C1-O2A-CGA
23	c	2474	CLA	C2-C1-O2A-CGA
23	d	2355	CLA	C2-C1-O2A-CGA
26	B	526	LMT	C2-C1-O1'-C1'
26	d	2359	LMT	C2-C1-O1'-C1'
23	b	2518	CLA	O1D-CGD-O2D-CED
23	B	515	CLA	C10-C11-C12-C13
23	b	2515	CLA	C5-C6-C7-C8
23	B	514	CLA	C4B-C3B-CAB-CBB
23	B	523	CLA	C4B-C3B-CAB-CBB
23	B	527	CLA	C4B-C3B-CAB-CBB
23	D	356	CLA	C4B-C3B-CAB-CBB
23	b	2523	CLA	C4B-C3B-CAB-CBB
23	b	2526	CLA	C4B-C3B-CAB-CBB
23	d	2357	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	B	525	CLA	C2A-CAA-CBA-CGA
23	b	2525	CLA	C2A-CAA-CBA-CGA
23	B	513	CLA	C13-C15-C16-C17
23	b	2522	CLA	C13-C15-C16-C17
23	B	511	CLA	C11-C12-C13-C15
23	c	2483	CLA	C15-C16-C17-C18
23	c	2484	CLA	C5-C6-C7-C8
23	b	2515	CLA	C10-C11-C12-C13
23	A	350	CLA	C10-C11-C12-C13
23	C	479	CLA	C10-C11-C12-C13
23	a	2349	CLA	C10-C11-C12-C13
23	B	523	CLA	C2B-C3B-CAB-CBB
23	C	481	CLA	C2B-C3B-CAB-CBB
23	D	356	CLA	C2B-C3B-CAB-CBB
23	b	2523	CLA	C2B-C3B-CAB-CBB
23	c	2481	CLA	C2B-C3B-CAB-CBB
23	c	2482	CLA	C2B-C3B-CAB-CBB
23	d	2357	CLA	C2B-C3B-CAB-CBB
27	B	528	BCR	C1-C6-C7-C8
27	B	528	BCR	C5-C6-C7-C8
27	B	529	BCR	C1-C6-C7-C8
27	B	529	BCR	C5-C6-C7-C8
27	b	2527	BCR	C1-C6-C7-C8
27	b	2527	BCR	C5-C6-C7-C8
27	b	2528	BCR	C1-C6-C7-C8
27	b	2528	BCR	C5-C6-C7-C8
23	C	483	CLA	C15-C16-C17-C18
23	b	2513	CLA	C13-C15-C16-C17
23	C	474	CLA	C2A-CAA-CBA-CGA
23	B	515	CLA	C4-C3-C5-C6
23	a	2349	CLA	O1D-CGD-O2D-CED
23	B	520	CLA	C10-C11-C12-C13
27	B	528	BCR	C6-C7-C8-C9
23	B	523	CLA	C5-C6-C7-C8
23	c	2478	CLA	C5-C6-C7-C8
23	A	350	CLA	C4-C3-C5-C6
23	a	2349	CLA	C2-C3-C5-C6
23	c	2476	CLA	C10-C11-C12-C13
23	c	2477	CLA	C5-C6-C7-C8
23	c	2479	CLA	C10-C11-C12-C13
23	d	2355	CLA	C10-C11-C12-C13
23	B	523	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	C	478	CLA	C5-C6-C7-C8
23	C	483	CLA	C10-C11-C12-C13
23	b	2523	CLA	C15-C16-C17-C18
23	B	522	CLA	C15-C16-C17-C18
23	C	477	CLA	C5-C6-C7-C8
23	b	2520	CLA	C10-C11-C12-C13
24	d	2356	PHO	C10-C11-C12-C13
23	C	476	CLA	C10-C11-C12-C13
23	b	2522	CLA	C15-C16-C17-C18
23	c	2477	CLA	C15-C16-C17-C18
24	D	355	PHO	C10-C11-C12-C13
23	b	2522	CLA	C2C-C3C-CAC-CBC
23	a	2349	CLA	C4-C3-C5-C6
23	A	350	CLA	C2-C3-C5-C6
23	A	349	CLA	C10-C11-C12-C13
23	B	527	CLA	C13-C15-C16-C17
23	b	2523	CLA	C5-C6-C7-C8
24	a	2350	PHO	C10-C11-C12-C13
23	c	2480	CLA	C15-C16-C17-C18
23	c	2483	CLA	C10-C11-C12-C13
23	B	511	CLA	C6-C7-C8-C10
23	B	512	CLA	C11-C12-C13-C15
23	B	514	CLA	C6-C7-C8-C10
23	B	514	CLA	C11-C12-C13-C15
23	B	519	CLA	C11-C12-C13-C15
23	C	477	CLA	C11-C10-C8-C7
23	C	477	CLA	C12-C13-C15-C16
23	C	480	CLA	C11-C10-C8-C7
23	C	482	CLA	C11-C12-C13-C15
23	b	2511	CLA	C6-C7-C8-C10
23	b	2512	CLA	C11-C12-C13-C15
23	b	2513	CLA	C11-C12-C13-C15
23	b	2514	CLA	C11-C12-C13-C15
23	b	2519	CLA	C11-C12-C13-C15
23	c	2477	CLA	C11-C10-C8-C7
23	c	2477	CLA	C12-C13-C15-C16
23	c	2482	CLA	C11-C12-C13-C15
24	D	355	PHO	C11-C10-C8-C7
24	d	2356	PHO	C6-C7-C8-C10
23	B	517	CLA	C5-C6-C7-C8
23	c	2487	CLA	C5-C6-C7-C8
23	B	522	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	C	477	CLA	C15-C16-C17-C18
23	A	349	CLA	C11-C10-C8-C9
23	B	512	CLA	C11-C10-C8-C9
23	B	513	CLA	C11-C12-C13-C14
23	B	522	CLA	C11-C10-C8-C9
23	B	525	CLA	C11-C12-C13-C14
23	C	477	CLA	C11-C10-C8-C9
23	C	480	CLA	C11-C10-C8-C9
23	C	485	CLA	C6-C7-C8-C9
23	b	2512	CLA	C11-C10-C8-C9
23	c	2477	CLA	C11-C10-C8-C9
23	c	2480	CLA	C11-C10-C8-C9
23	d	2355	CLA	C11-C10-C8-C9
24	A	351	PHO	C6-C7-C8-C9
24	D	355	PHO	C11-C10-C8-C9
24	D	355	PHO	C14-C13-C15-C16
24	a	2350	PHO	C6-C7-C8-C9
24	a	2350	PHO	C11-C12-C13-C14
24	d	2356	PHO	C11-C10-C8-C9
23	b	2526	CLA	C13-C15-C16-C17
23	A	350	CLA	O1D-CGD-O2D-CED
23	A	348	CLA	C13-C15-C16-C17
23	a	2348	CLA	C13-C15-C16-C17
23	b	2517	CLA	C5-C6-C7-C8
23	B	525	CLA	C5-C6-C7-C8
24	A	351	PHO	C10-C11-C12-C13
23	C	477	CLA	C13-C15-C16-C17
23	C	487	CLA	C5-C6-C7-C8
23	c	2477	CLA	C13-C15-C16-C17
23	A	350	CLA	C5-C6-C7-C8
23	a	2349	CLA	C5-C6-C7-C8
24	A	351	PHO	O2A-C1-C2-C3
24	D	355	PHO	O2A-C1-C2-C3
24	a	2350	PHO	O2A-C1-C2-C3
24	d	2356	PHO	O2A-C1-C2-C3
27	b	2527	BCR	C6-C7-C8-C9
26	B	526	LMT	C11-C10-C9-C8
23	C	475	CLA	CAA-CBA-CGA-O2A
23	b	2525	CLA	C5-C6-C7-C8
23	A	349	CLA	C2-C1-O2A-CGA
23	b	2511	CLA	C4-C3-C5-C6
25	A	353	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
23	c	2486	CLA	C10-C11-C12-C13
28	v	2138	HEC	C1A-C2A-CAA-CBA
23	B	511	CLA	C6-C7-C8-C9
23	B	515	CLA	C6-C7-C8-C9
23	B	517	CLA	C11-C10-C8-C9
23	B	523	CLA	C14-C13-C15-C16
23	C	482	CLA	C11-C12-C13-C14
23	b	2511	CLA	C6-C7-C8-C9
23	b	2513	CLA	C11-C12-C13-C14
23	b	2514	CLA	C14-C13-C15-C16
23	b	2517	CLA	C11-C10-C8-C9
23	b	2522	CLA	C11-C10-C8-C9
23	b	2523	CLA	C14-C13-C15-C16
23	b	2525	CLA	C11-C12-C13-C14
23	c	2482	CLA	C11-C12-C13-C14
23	c	2485	CLA	C6-C7-C8-C9
24	A	351	PHO	C11-C12-C13-C14
24	D	355	PHO	C6-C7-C8-C9
24	d	2356	PHO	C6-C7-C8-C9
24	d	2356	PHO	C14-C13-C15-C16
26	d	2359	LMT	C11-C10-C9-C8
23	b	2514	CLA	C15-C16-C17-C18
23	b	2514	CLA	C4B-C3B-CAB-CBB
28	v	2138	HEC	C3A-C2A-CAA-CBA
23	C	486	CLA	C10-C11-C12-C13
23	c	2475	CLA	CAA-CBA-CGA-O2A
23	A	352	CLA	C6-C7-C8-C10
23	B	513	CLA	C11-C12-C13-C15
23	B	514	CLA	C12-C13-C15-C16
23	B	517	CLA	C11-C10-C8-C7
23	B	518	CLA	C6-C7-C8-C10
23	B	522	CLA	C11-C10-C8-C7
23	B	524	CLA	C6-C7-C8-C10
23	B	524	CLA	C12-C13-C15-C16
23	B	525	CLA	C11-C12-C13-C15
23	B	527	CLA	C6-C7-C8-C10
23	C	474	CLA	C11-C12-C13-C15
23	C	474	CLA	C12-C13-C15-C16
23	C	475	CLA	C11-C10-C8-C7
23	C	483	CLA	C6-C7-C8-C10
23	C	485	CLA	C6-C7-C8-C10
23	a	2351	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	2514	CLA	C6-C7-C8-C10
23	b	2514	CLA	C12-C13-C15-C16
23	b	2517	CLA	C11-C10-C8-C7
23	b	2518	CLA	C6-C7-C8-C10
23	b	2522	CLA	C11-C10-C8-C7
23	b	2523	CLA	C6-C7-C8-C10
23	b	2524	CLA	C12-C13-C15-C16
23	b	2526	CLA	C6-C7-C8-C10
23	c	2474	CLA	C11-C12-C13-C15
23	c	2475	CLA	C11-C10-C8-C7
23	c	2480	CLA	C11-C10-C8-C7
23	c	2483	CLA	C6-C7-C8-C10
23	c	2485	CLA	C6-C7-C8-C10
24	A	351	PHO	C6-C7-C8-C10
24	A	351	PHO	C11-C12-C13-C15
24	D	355	PHO	C6-C7-C8-C10
24	D	355	PHO	C12-C13-C15-C16
24	a	2350	PHO	C6-C7-C8-C10
24	a	2350	PHO	C11-C12-C13-C15
24	d	2356	PHO	C11-C10-C8-C7
24	d	2356	PHO	C12-C13-C15-C16
23	C	480	CLA	C15-C16-C17-C18
25	a	2352	PL9	C25-C24-C26-C27
25	A	353	PL9	C23-C24-C26-C27
23	B	511	CLA	C4-C3-C5-C6
25	a	2352	PL9	C23-C24-C26-C27
27	K	50	BCR	C1-C6-C7-C8
27	d	2360	BCR	C5-C6-C7-C8
27	k	2050	BCR	C1-C6-C7-C8
23	B	511	CLA	C5-C6-C7-C8
23	B	514	CLA	C15-C16-C17-C18
25	D	357	PL9	C4-C3-C7-C8
25	d	2358	PL9	C4-C3-C7-C8
23	A	348	CLA	C14-C13-C15-C16
23	B	514	CLA	C14-C13-C15-C16
23	B	522	CLA	C6-C7-C8-C9
23	C	479	CLA	C14-C13-C15-C16
23	a	2348	CLA	C14-C13-C15-C16
23	b	2515	CLA	C6-C7-C8-C9
23	b	2522	CLA	C6-C7-C8-C9
23	b	2511	CLA	C5-C6-C7-C8
23	B	523	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	B	525	CLA	C11-C10-C8-C7
23	b	2524	CLA	C6-C7-C8-C10
23	b	2525	CLA	C11-C10-C8-C7
23	b	2525	CLA	C11-C12-C13-C15
23	b	2526	CLA	C12-C13-C15-C16
23	c	2474	CLA	C12-C13-C15-C16
23	c	2483	CLA	C11-C12-C13-C15
23	b	2515	CLA	C4-C3-C5-C6
23	b	2517	CLA	O1D-CGD-O2D-CED
23	A	352	CLA	C4-C3-C5-C6
24	d	2356	PHO	C5-C6-C7-C8
23	b	2518	CLA	C11-C12-C13-C14
23	c	2479	CLA	C14-C13-C15-C16
23	b	2522	CLA	C4C-C3C-CAC-CBC
23	C	486	CLA	CAA-CBA-CGA-O2A
23	c	2486	CLA	CAA-CBA-CGA-O2A
24	D	355	PHO	C5-C6-C7-C8
23	B	519	CLA	C4-C3-C5-C6
23	c	2487	CLA	C4-C3-C5-C6
23	b	2524	CLA	C10-C11-C12-C13
23	c	2475	CLA	C10-C11-C12-C13
23	B	519	CLA	C4B-C3B-CAB-CBB
23	B	520	CLA	C4B-C3B-CAB-CBB
23	b	2520	CLA	C4B-C3B-CAB-CBB
23	a	2351	CLA	C4-C3-C5-C6
23	b	2519	CLA	C4-C3-C5-C6
23	B	522	CLA	C4C-C3C-CAC-CBC
23	C	477	CLA	C2A-CAA-CBA-CGA
23	c	2477	CLA	C2A-CAA-CBA-CGA
23	b	2517	CLA	CBD-CGD-O2D-CED
23	B	511	CLA	C12-C13-C15-C16
23	B	512	CLA	C12-C13-C15-C16
23	B	523	CLA	C11-C10-C8-C7
23	B	527	CLA	C12-C13-C15-C16
23	C	477	CLA	C11-C12-C13-C15
23	C	478	CLA	C12-C13-C15-C16
23	C	481	CLA	C6-C7-C8-C10
23	C	483	CLA	C11-C12-C13-C15
23	b	2511	CLA	C12-C13-C15-C16
23	b	2512	CLA	C12-C13-C15-C16
23	b	2523	CLA	C11-C10-C8-C7
23	c	2477	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	c	2478	CLA	C12-C13-C15-C16
23	c	2481	CLA	C6-C7-C8-C10
23	B	524	CLA	C10-C11-C12-C13
23	A	352	CLA	C6-C7-C8-C9
23	B	512	CLA	C14-C13-C15-C16
23	B	518	CLA	C11-C12-C13-C14
23	C	478	CLA	C14-C13-C15-C16
23	b	2511	CLA	C14-C13-C15-C16
23	b	2525	CLA	C11-C10-C8-C9
23	c	2474	CLA	C14-C13-C15-C16
23	c	2478	CLA	C14-C13-C15-C16
24	A	351	PHO	C5-C6-C7-C8
24	a	2350	PHO	C5-C6-C7-C8
23	C	476	CLA	C4-C3-C5-C6
23	c	2476	CLA	C4-C3-C5-C6
23	A	352	CLA	C2-C3-C5-C6
23	C	476	CLA	CAD-CBD-CGD-O2D
23	C	480	CLA	CAD-CBD-CGD-O2D
23	c	2476	CLA	CAD-CBD-CGD-O2D
23	c	2480	CLA	CAD-CBD-CGD-O2D
23	C	476	CLA	CAD-CBD-CGD-O1D
23	C	480	CLA	CAD-CBD-CGD-O1D
23	C	486	CLA	CHA-CBD-CGD-O1D
23	c	2476	CLA	CAD-CBD-CGD-O1D
23	c	2480	CLA	CAD-CBD-CGD-O1D
23	c	2486	CLA	CHA-CBD-CGD-O1D
23	B	514	CLA	C2B-C3B-CAB-CBB
23	B	527	CLA	C2B-C3B-CAB-CBB
23	b	2514	CLA	C2B-C3B-CAB-CBB
23	b	2526	CLA	C2B-C3B-CAB-CBB
27	C	488	BCR	C23-C24-C25-C30
27	F	48	BCR	C5-C6-C7-C8
23	B	515	CLA	C2-C3-C5-C6
23	B	519	CLA	C2-C3-C5-C6
23	C	475	CLA	C10-C11-C12-C13
23	a	2348	CLA	CBD-CGD-O2D-CED
25	A	353	PL9	C4-C3-C7-C8
25	a	2352	PL9	C4-C3-C7-C8
25	D	357	PL9	C2-C3-C7-C8
23	B	511	CLA	C14-C13-C15-C16
23	B	525	CLA	C11-C10-C8-C9
23	C	474	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	C	475	CLA	C11-C10-C8-C9
23	a	2351	CLA	C6-C7-C8-C9
23	b	2512	CLA	C14-C13-C15-C16
23	d	2354	CLA	C11-C12-C13-C15
23	B	517	CLA	O1D-CGD-O2D-CED
23	C	478	CLA	C4-C3-C5-C6
23	d	2354	CLA	C4-C3-C5-C6
25	D	357	PL9	C16-C17-C18-C19
25	d	2358	PL9	C16-C17-C18-C19
23	a	2348	CLA	O1D-CGD-O2D-CED
23	d	2355	CLA	CAA-CBA-CGA-O2A
25	A	353	PL9	C12-C11-C9-C10
23	B	511	CLA	CAA-CBA-CGA-O2A
23	A	349	CLA	CAA-CBA-CGA-O2A
23	C	484	CLA	CAA-CBA-CGA-O2A
23	A	348	CLA	O1D-CGD-O2D-CED
23	b	2511	CLA	CAA-CBA-CGA-O2A
23	C	487	CLA	C4-C3-C5-C6
23	d	2355	CLA	C4-C3-C5-C6
23	C	480	CLA	CAA-CBA-CGA-O2A
23	c	2484	CLA	CAA-CBA-CGA-O2A
23	a	2351	CLA	C2-C3-C5-C6
23	B	527	CLA	C5-C6-C7-C8
25	d	2358	PL9	C2-C3-C7-C8
23	B	515	CLA	C14-C13-C15-C16
23	B	517	CLA	C11-C12-C13-C14
23	C	478	CLA	C6-C7-C8-C9
23	C	485	CLA	C11-C10-C8-C9
23	c	2475	CLA	C11-C10-C8-C9
23	c	2478	CLA	C6-C7-C8-C9
23	c	2482	CLA	C6-C7-C8-C9
23	c	2485	CLA	C11-C10-C8-C9
23	b	2519	CLA	C4B-C3B-CAB-CBB
23	C	476	CLA	C13-C15-C16-C17
23	C	479	CLA	C15-C16-C17-C18
23	A	349	CLA	C4-C3-C5-C6
23	c	2478	CLA	C4-C3-C5-C6
23	A	349	CLA	C2-C3-C5-C6
23	C	476	CLA	C2-C3-C5-C6
23	b	2519	CLA	C2-C3-C5-C6
23	c	2476	CLA	C2-C3-C5-C6
23	b	2516	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	c	2482	CLA	C6-C7-C8-C10
23	B	514	CLA	C13-C15-C16-C17
23	B	516	CLA	CAA-CBA-CGA-O2A
23	b	2526	CLA	C5-C6-C7-C8
23	c	2480	CLA	CAA-CBA-CGA-O2A
23	d	2355	CLA	C2-C3-C5-C6
23	B	518	CLA	C5-C6-C7-C8
23	b	2514	CLA	C13-C15-C16-C17
23	c	2479	CLA	C15-C16-C17-C18
23	A	348	CLA	CBD-CGD-O2D-CED
23	C	485	CLA	C2-C1-O2A-CGA
23	c	2476	CLA	C13-C15-C16-C17
25	a	2352	PL9	C12-C11-C9-C10
23	C	475	CLA	CAA-CBA-CGA-O1A
28	v	2138	HEC	CAD-CBD-CGD-O1D
23	A	352	CLA	C11-C12-C13-C14
23	B	512	CLA	C6-C7-C8-C9
23	B	527	CLA	C14-C13-C15-C16
23	C	474	CLA	C6-C7-C8-C9
23	C	482	CLA	C6-C7-C8-C9
23	C	482	CLA	C14-C13-C15-C16
23	D	354	CLA	C6-C7-C8-C9
23	D	354	CLA	C11-C12-C13-C14
23	a	2351	CLA	C11-C12-C13-C14
23	b	2512	CLA	C6-C7-C8-C9
23	b	2526	CLA	C14-C13-C15-C16
23	c	2474	CLA	C6-C7-C8-C9
23	c	2482	CLA	C14-C13-C15-C16
23	c	2483	CLA	C11-C12-C13-C14
23	d	2354	CLA	C11-C12-C13-C14
28	E	84	HEC	CAD-CBD-CGD-O1D
23	B	519	CLA	C2B-C3B-CAB-CBB
23	B	520	CLA	C2B-C3B-CAB-CBB
23	B	522	CLA	C2B-C3B-CAB-CBB
23	b	2519	CLA	C2B-C3B-CAB-CBB
23	b	2520	CLA	C2B-C3B-CAB-CBB
23	b	2522	CLA	C2B-C3B-CAB-CBB
27	c	2488	BCR	C23-C24-C25-C30
27	k	2050	BCR	C5-C6-C7-C8
28	V	138	HEC	CAD-CBD-CGD-O1D
28	e	2084	HEC	CAD-CBD-CGD-O1D
23	c	2478	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B	512	CLA	C5-C6-C7-C8
23	B	511	CLA	C11-C10-C8-C7
23	B	515	CLA	C12-C13-C15-C16
23	B	522	CLA	C12-C13-C15-C16
23	B	527	CLA	C11-C10-C8-C7
23	C	482	CLA	C6-C7-C8-C10
23	C	485	CLA	C11-C10-C8-C7
23	C	487	CLA	C12-C13-C15-C16
23	D	354	CLA	C11-C12-C13-C15
23	a	2348	CLA	C11-C10-C8-C7
23	b	2511	CLA	C11-C10-C8-C7
23	b	2515	CLA	C12-C13-C15-C16
23	b	2522	CLA	C12-C13-C15-C16
23	b	2526	CLA	C11-C10-C8-C7
23	c	2485	CLA	C11-C10-C8-C7
23	c	2487	CLA	C12-C13-C15-C16
23	c	2475	CLA	CAA-CBA-CGA-O1A
23	B	517	CLA	CBD-CGD-O2D-CED
23	B	527	CLA	C2A-CAA-CBA-CGA
23	b	2526	CLA	C2A-CAA-CBA-CGA
23	b	2518	CLA	C5-C6-C7-C8
23	c	2484	CLA	C15-C16-C17-C18
23	B	517	CLA	CAA-CBA-CGA-O2A
23	C	478	CLA	C2-C3-C5-C6
23	c	2476	CLA	C2-C1-O2A-CGA
28	v	2138	HEC	CAD-CBD-CGD-O2D
23	B	524	CLA	C11-C12-C13-C14
23	C	487	CLA	C14-C13-C15-C16
23	b	2517	CLA	C11-C12-C13-C14
23	b	2524	CLA	C11-C12-C13-C14
27	C	488	BCR	C22-C23-C24-C25
27	c	2488	BCR	C22-C23-C24-C25
24	a	2350	PHO	C4-C3-C5-C6
25	d	2358	PL9	C20-C19-C21-C22
28	E	84	HEC	CAD-CBD-CGD-O2D
23	b	2517	CLA	CAA-CBA-CGA-O2A
23	B	511	CLA	C2-C3-C5-C6
23	b	2511	CLA	C2-C3-C5-C6
23	b	2515	CLA	C2-C3-C5-C6
23	C	485	CLA	C10-C11-C12-C13
23	a	2351	CLA	C5-C6-C7-C8
28	e	2084	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	C	484	CLA	C15-C16-C17-C18
23	B	518	CLA	CAA-CBA-CGA-O2A
23	c	2485	CLA	C2A-CAA-CBA-CGA
23	C	476	CLA	CAA-CBA-CGA-O2A
23	b	2524	CLA	C4-C3-C5-C6
24	A	351	PHO	C4-C3-C5-C6
25	D	357	PL9	C20-C19-C21-C22
23	B	519	CLA	CAA-CBA-CGA-O2A
23	b	2519	CLA	CAA-CBA-CGA-O2A
23	d	2354	CLA	C2-C3-C5-C6
23	B	522	CLA	C4B-C3B-CAB-CBB
23	b	2522	CLA	C4B-C3B-CAB-CBB
23	b	2518	CLA	CAA-CBA-CGA-O2A
23	c	2476	CLA	CAA-CBA-CGA-O2A
28	V	138	HEC	CAD-CBD-CGD-O2D
24	D	355	PHO	CHA-CBD-CGD-O1D
25	A	353	PL9	C12-C11-C9-C8
23	b	2512	CLA	C5-C6-C7-C8
23	B	524	CLA	C11-C12-C13-C15
23	B	521	CLA	C11-C10-C8-C9
23	C	483	CLA	C11-C12-C13-C14
23	C	484	CLA	C11-C12-C13-C14
23	b	2515	CLA	C14-C13-C15-C16
23	b	2521	CLA	C11-C10-C8-C9
23	c	2477	CLA	C11-C12-C13-C14
23	c	2484	CLA	C11-C12-C13-C14
23	c	2487	CLA	C14-C13-C15-C16
23	d	2354	CLA	C6-C7-C8-C9
23	C	484	CLA	C2A-CAA-CBA-CGA
23	B	513	CLA	C2-C1-O2A-CGA
23	C	476	CLA	C2-C1-O2A-CGA
23	c	2484	CLA	C2-C1-O2A-CGA
23	c	2485	CLA	C2-C1-O2A-CGA
23	c	2487	CLA	C2-C3-C5-C6
23	c	2487	CLA	O2A-C1-C2-C3
26	d	2359	LMT	C4-C5-C6-C7
23	c	2485	CLA	C10-C11-C12-C13
26	B	526	LMT	C4-C5-C6-C7
23	c	2484	CLA	C2A-CAA-CBA-CGA
23	b	2520	CLA	CBD-CGD-O2D-CED
23	C	477	CLA	C11-C12-C13-C14
23	D	356	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	2523	CLA	C11-C10-C8-C9
23	d	2357	CLA	C14-C13-C15-C16
23	c	2485	CLA	CAA-CBA-CGA-O2A
23	A	348	CLA	CAA-CBA-CGA-O2A
23	C	485	CLA	CAA-CBA-CGA-O2A
23	a	2348	CLA	CAA-CBA-CGA-O2A
23	A	348	CLA	C11-C10-C8-C7
23	C	475	CLA	C6-C7-C8-C10
23	C	477	CLA	C6-C7-C8-C10
23	C	484	CLA	C11-C12-C13-C15
23	D	354	CLA	C6-C7-C8-C10
23	b	2524	CLA	C11-C12-C13-C15
23	b	2526	CLA	C11-C12-C13-C15
23	c	2477	CLA	C6-C7-C8-C10
23	c	2480	CLA	C11-C12-C13-C15
23	c	2484	CLA	C11-C12-C13-C15
23	d	2354	CLA	C6-C7-C8-C10
23	d	2355	CLA	C6-C7-C8-C10
27	C	488	BCR	C23-C24-C25-C26
27	K	50	BCR	C5-C6-C7-C8
27	d	2360	BCR	C1-C6-C7-C8
23	C	480	CLA	C2-C1-O2A-CGA
23	C	484	CLA	C2-C1-O2A-CGA
24	A	351	PHO	C2-C1-O2A-CGA
24	a	2350	PHO	C2-C1-O2A-CGA
23	A	352	CLA	C5-C6-C7-C8
23	c	2487	CLA	CAA-CBA-CGA-O2A
23	B	524	CLA	C4-C3-C5-C6
23	D	354	CLA	C4-C3-C5-C6
23	b	2515	CLA	CAA-CBA-CGA-O2A
25	a	2352	PL9	C12-C11-C9-C8
23	B	525	CLA	C14-C13-C15-C16
23	b	2525	CLA	C14-C13-C15-C16
23	b	2526	CLA	C11-C12-C13-C14
23	c	2480	CLA	C11-C12-C13-C14
23	C	479	CLA	C4B-C3B-CAB-CBB
23	c	2479	CLA	C4B-C3B-CAB-CBB
23	c	2475	CLA	C4-C3-C5-C6
23	D	354	CLA	C2-C3-C5-C6
23	B	515	CLA	CAA-CBA-CGA-O2A
23	C	485	CLA	C2A-CAA-CBA-CGA
23	C	487	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	C	477	CLA	C2-C1-O2A-CGA
23	b	2513	CLA	C2-C1-O2A-CGA
23	c	2477	CLA	C2-C1-O2A-CGA
23	c	2480	CLA	C2-C1-O2A-CGA
24	D	355	PHO	C2-C1-O2A-CGA
23	A	349	CLA	C6-C7-C8-C10
23	B	527	CLA	C11-C12-C13-C15
23	C	478	CLA	C11-C12-C13-C15
23	C	480	CLA	C11-C12-C13-C15
23	C	484	CLA	C6-C7-C8-C10
23	c	2475	CLA	C6-C7-C8-C10
23	c	2478	CLA	C11-C12-C13-C15
23	c	2484	CLA	C6-C7-C8-C10
23	C	487	CLA	O2A-C1-C2-C3
23	b	2524	CLA	C5-C6-C7-C8
23	D	356	CLA	C2A-CAA-CBA-CGA
23	b	2520	CLA	O1D-CGD-O2D-CED
23	c	2482	CLA	C4-C3-C5-C6
25	D	357	PL9	C15-C14-C16-C17
25	d	2358	PL9	C15-C14-C16-C17
23	C	481	CLA	C15-C16-C17-C18
23	B	523	CLA	C11-C10-C8-C9
23	B	527	CLA	C11-C12-C13-C14
23	C	480	CLA	C11-C12-C13-C14
23	C	486	CLA	CAA-CBA-CGA-O1A
23	C	487	CLA	C10-C11-C12-C13
23	a	2348	CLA	CAA-CBA-CGA-O1A
23	C	485	CLA	CAA-CBA-CGA-O1A
23	B	524	CLA	C5-C6-C7-C8
23	B	515	CLA	CAA-CBA-CGA-O1A
23	c	2485	CLA	CAA-CBA-CGA-O1A
23	c	2481	CLA	C15-C16-C17-C18
23	A	348	CLA	CAA-CBA-CGA-O1A
23	b	2515	CLA	CAA-CBA-CGA-O1A
23	d	2357	CLA	C2A-CAA-CBA-CGA
23	c	2486	CLA	CAA-CBA-CGA-O1A
23	C	487	CLA	C2-C3-C5-C6
23	A	350	CLA	CAD-CBD-CGD-O2D
23	C	481	CLA	CAD-CBD-CGD-O2D
23	c	2484	CLA	CAD-CBD-CGD-O2D
23	B	525	CLA	C2-C1-O2A-CGA
23	C	487	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	c	2487	CLA	CAA-CBA-CGA-O1A
23	b	2522	CLA	CAA-CBA-CGA-O2A
23	B	513	CLA	C2A-CAA-CBA-CGA
23	c	2474	CLA	CAA-CBA-CGA-O2A
23	C	474	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

100 monomers are involved in 707 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	350	CLA	6	0
23	b	2521	CLA	11	0
27	C	489	BCR	11	0
23	B	527	CLA	5	0
23	D	356	CLA	8	0
23	c	2479	CLA	12	0
24	d	2356	PHO	10	0
24	a	2350	PHO	5	0
27	K	50	BCR	13	0
23	C	483	CLA	9	0
23	B	523	CLA	7	0
27	c	2488	BCR	12	0
23	d	2355	CLA	6	0
23	b	2522	CLA	13	0
27	b	2527	BCR	4	0
23	c	2477	CLA	8	0
23	C	486	CLA	17	0
23	C	477	CLA	7	0
23	B	518	CLA	16	0
23	C	480	CLA	6	0
23	D	354	CLA	8	0
23	A	348	CLA	13	0
23	b	2516	CLA	7	0
23	b	2517	CLA	3	0
27	d	2360	BCR	2	0
23	c	2482	CLA	4	0
23	B	524	CLA	25	0
28	v	2138	HEC	1	0
23	C	481	CLA	4	0
27	b	2528	BCR	15	0
23	B	514	CLA	4	0
23	B	519	CLA	6	0

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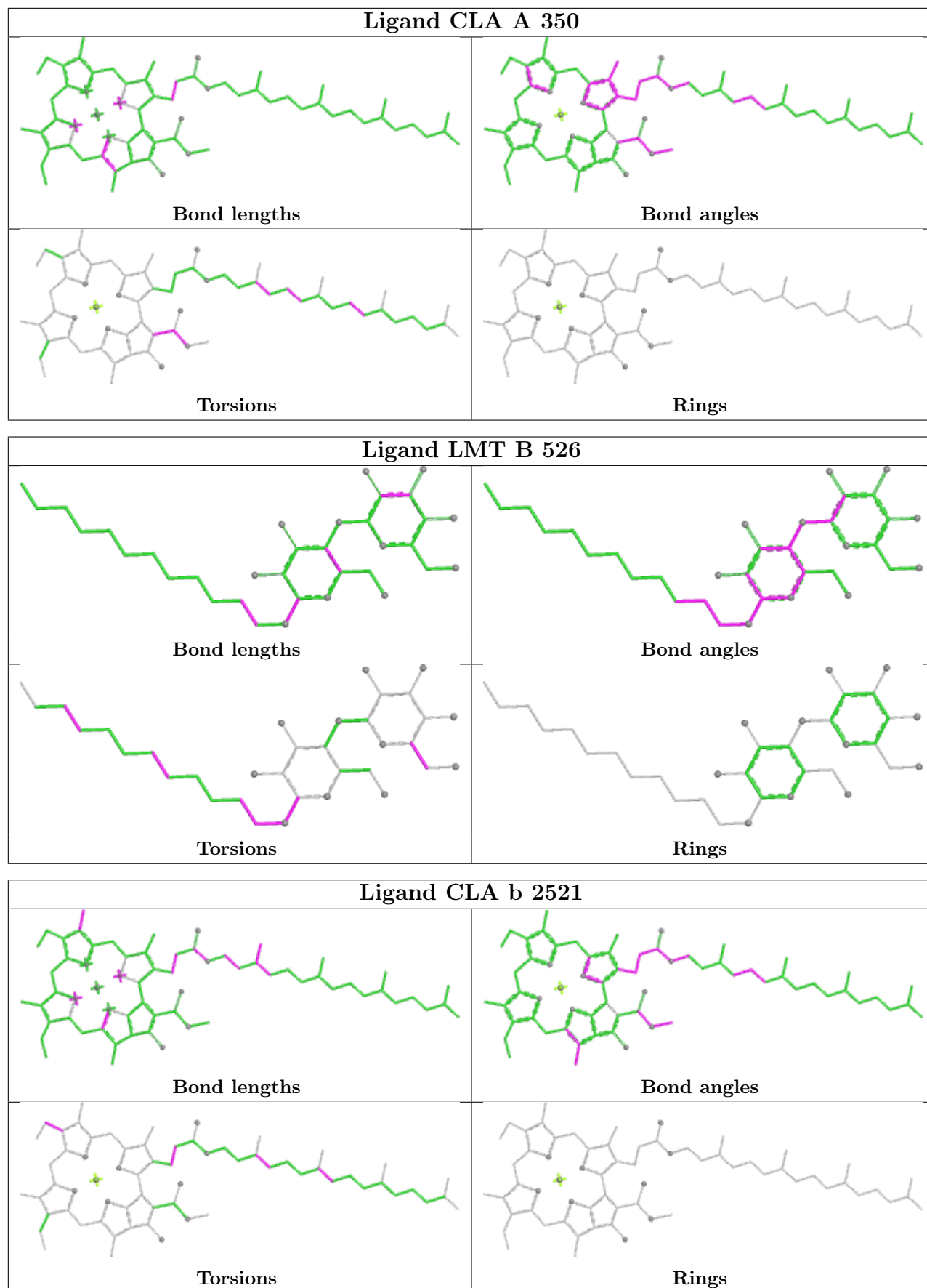
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	2520	CLA	9	0
26	d	2359	LMT	5	0
23	b	2519	CLA	7	0
27	j	2053	BCR	2	0
23	C	487	CLA	20	0
23	B	513	CLA	6	0
23	A	349	CLA	2	0
23	c	2474	CLA	8	0
23	a	2349	CLA	9	0
27	B	528	BCR	4	0
23	C	485	CLA	10	0
23	b	2512	CLA	5	0
23	B	516	CLA	6	0
23	C	482	CLA	4	0
27	C	488	BCR	12	0
23	c	2475	CLA	3	0
25	A	353	PL9	8	0
23	B	520	CLA	10	0
23	c	2485	CLA	8	0
27	J	53	BCR	2	0
23	B	521	CLA	10	0
23	c	2483	CLA	8	0
23	B	525	CLA	9	0
23	c	2484	CLA	2	0
23	C	474	CLA	10	0
23	b	2515	CLA	6	0
23	b	2525	CLA	9	0
23	B	511	CLA	4	0
23	c	2480	CLA	4	0
25	d	2358	PL9	8	0
23	a	2348	CLA	9	0
23	c	2486	CLA	23	0
24	A	351	PHO	5	0
23	B	517	CLA	3	0
27	F	48	BCR	3	0
23	C	478	CLA	6	0
27	c	2489	BCR	10	0
23	b	2526	CLA	5	0
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23	c	2476	CLA	5	0
22	A	347	OEC	1	0
23	B	522	CLA	14	0

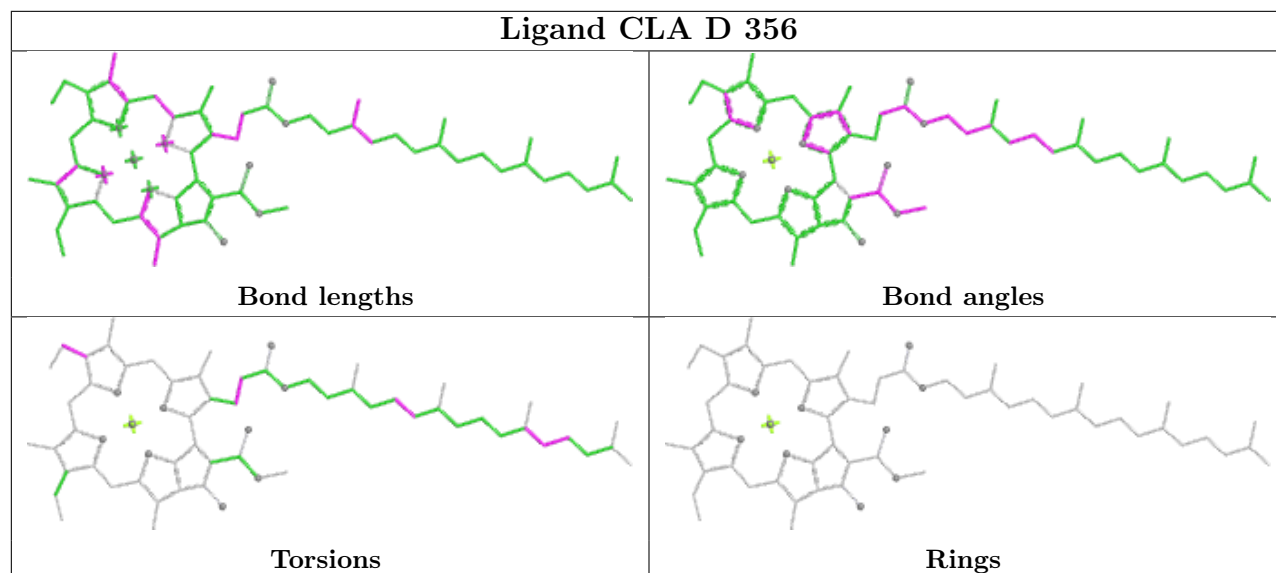
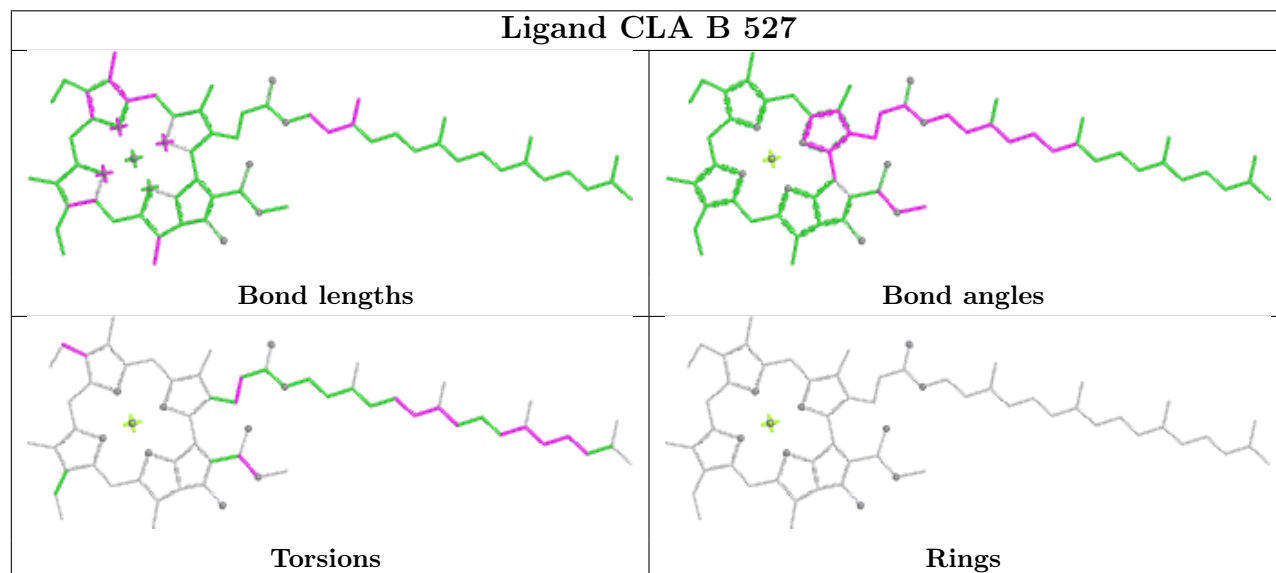
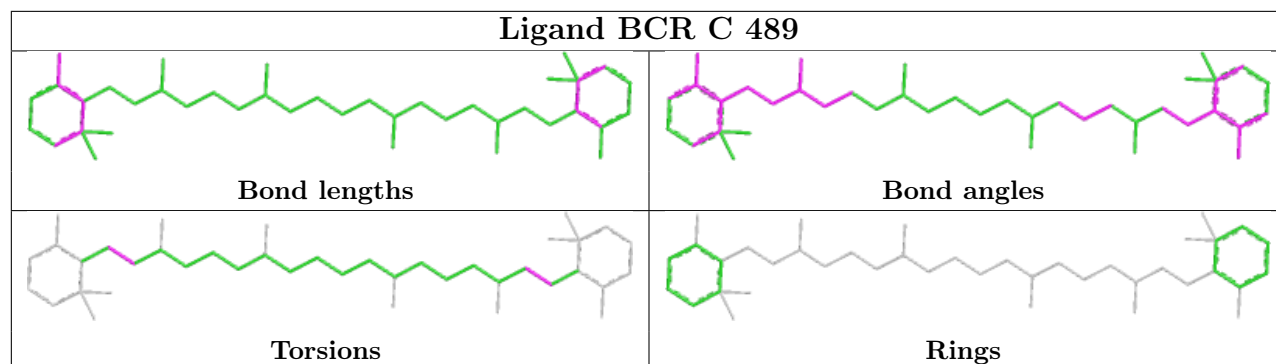
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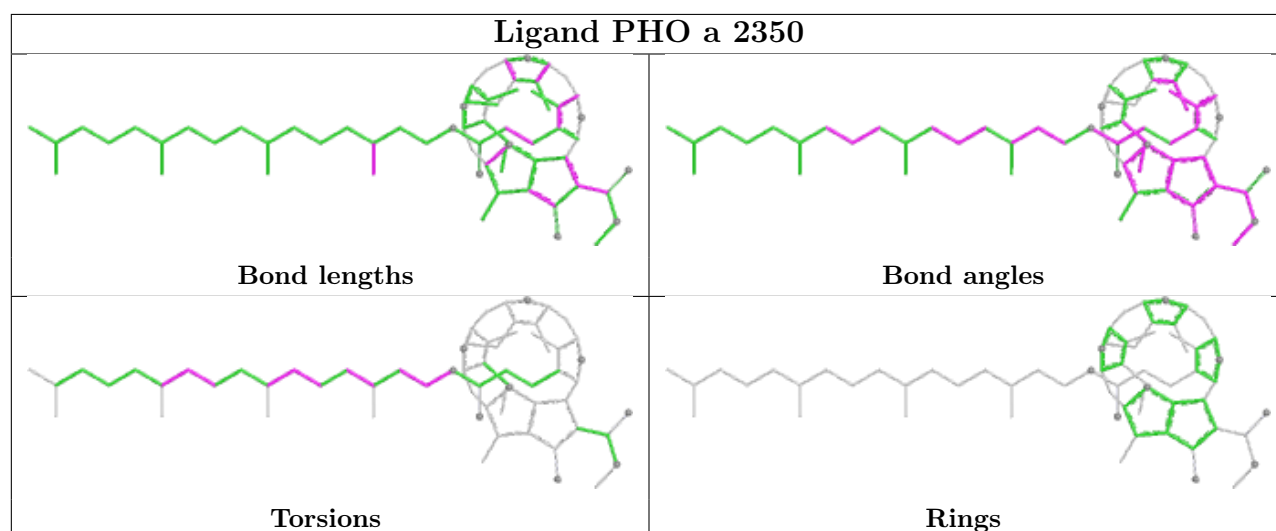
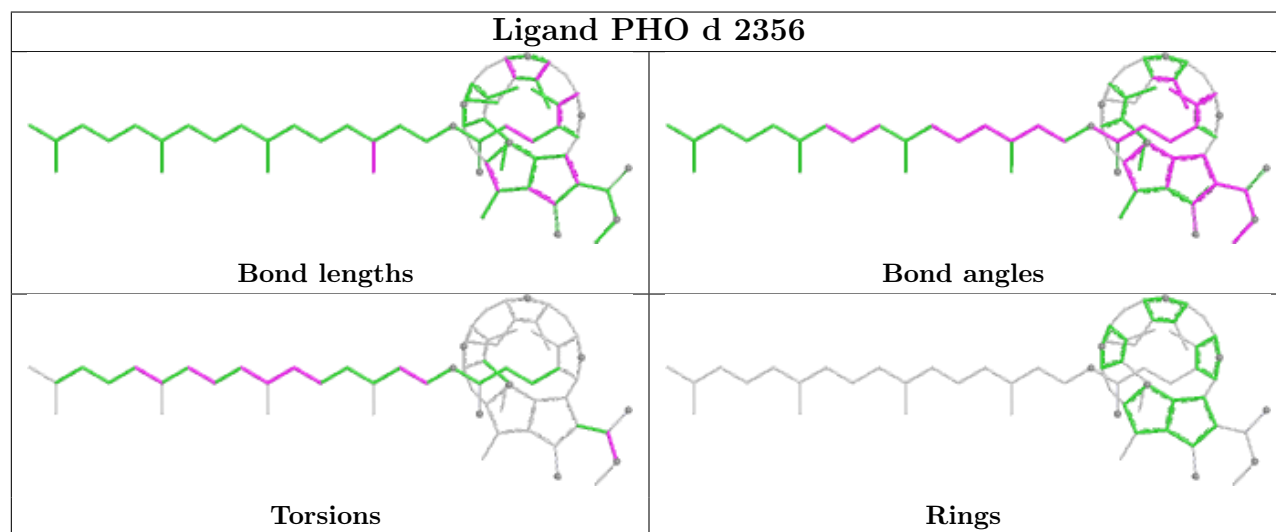
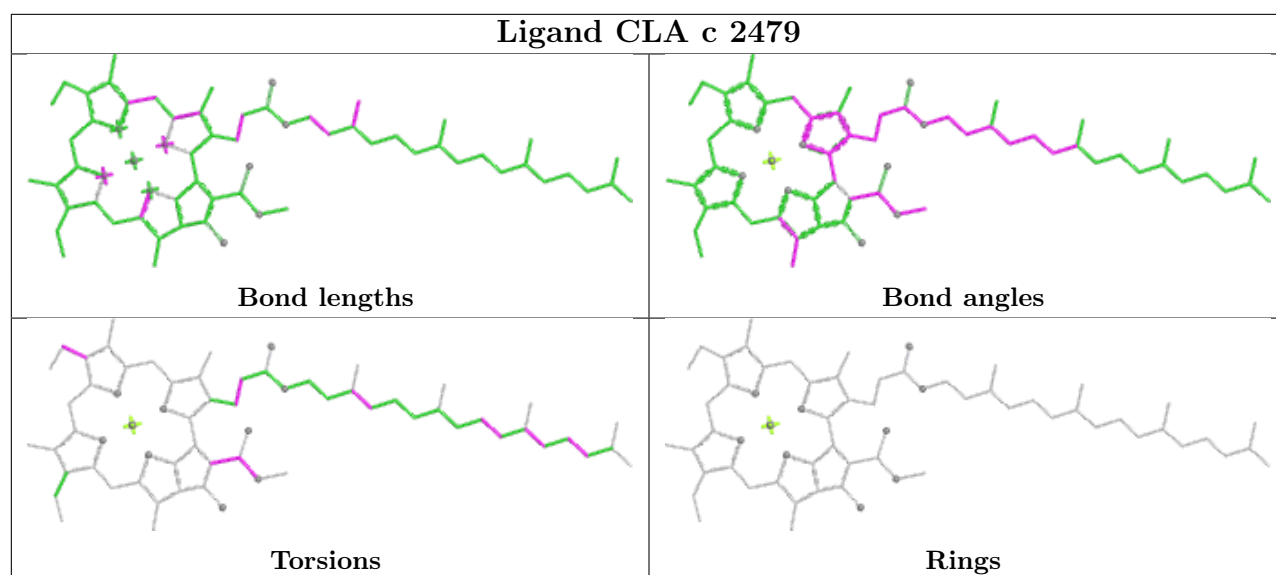
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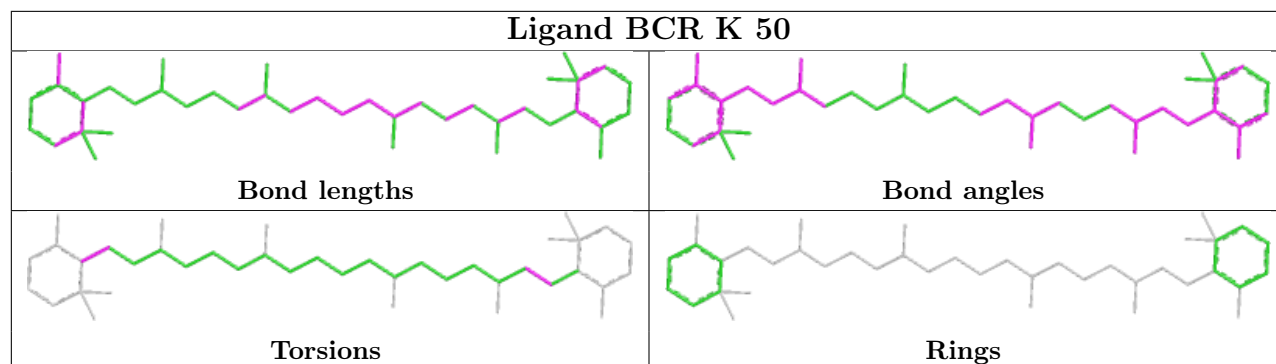
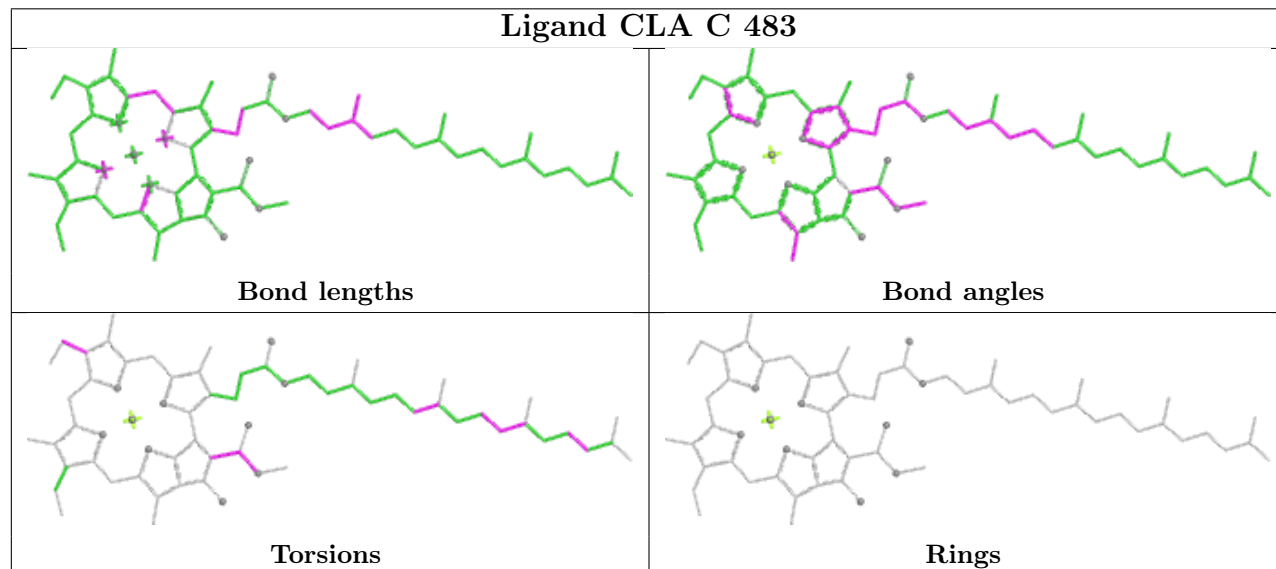
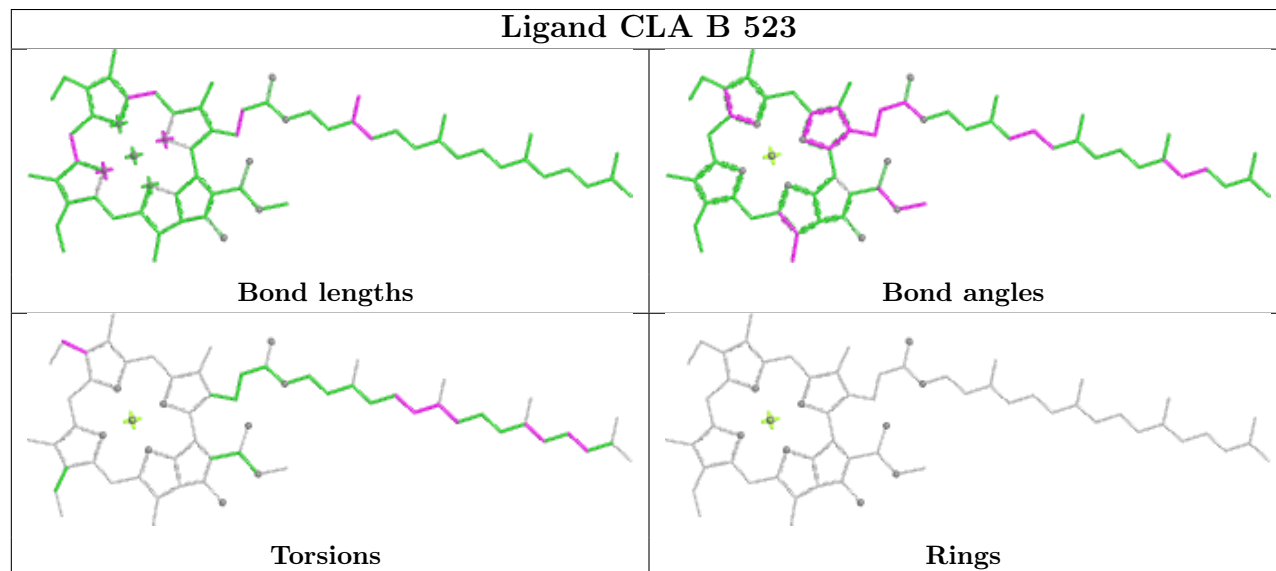
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	484	CLA	2	0
23	b	2524	CLA	23	0
23	d	2354	CLA	10	0
23	b	2513	CLA	6	0
23	C	479	CLA	11	0
23	c	2481	CLA	8	0
23	c	2478	CLA	6	0
23	b	2518	CLA	15	0
28	e	2084	HEC	15	0
23	b	2514	CLA	3	0
23	b	2511	CLA	4	0
27	k	2050	BCR	16	0
23	C	475	CLA	5	0
23	b	2523	CLA	8	0
28	E	84	HEC	17	0
23	a	2351	CLA	2	0
23	d	2357	CLA	14	0
25	a	2352	PL9	11	0
24	D	355	PHO	7	0
23	C	476	CLA	4	0
28	V	138	HEC	9	0
23	B	512	CLA	7	0
25	D	357	PL9	6	0
27	B	529	BCR	14	0
23	c	2487	CLA	19	0
23	A	352	CLA	1	0

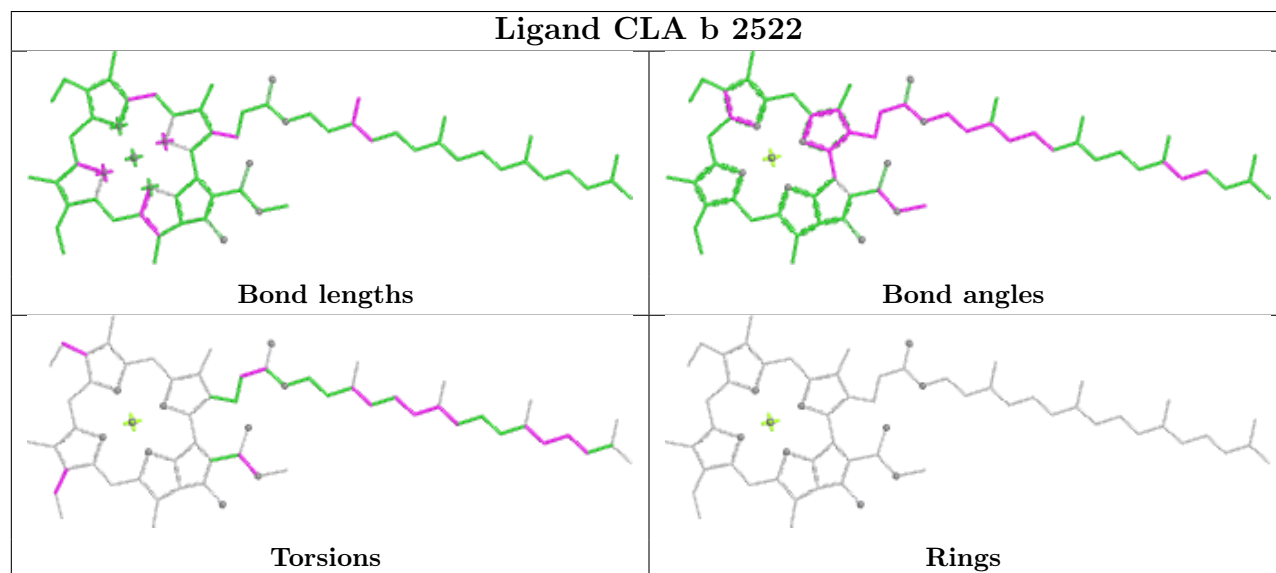
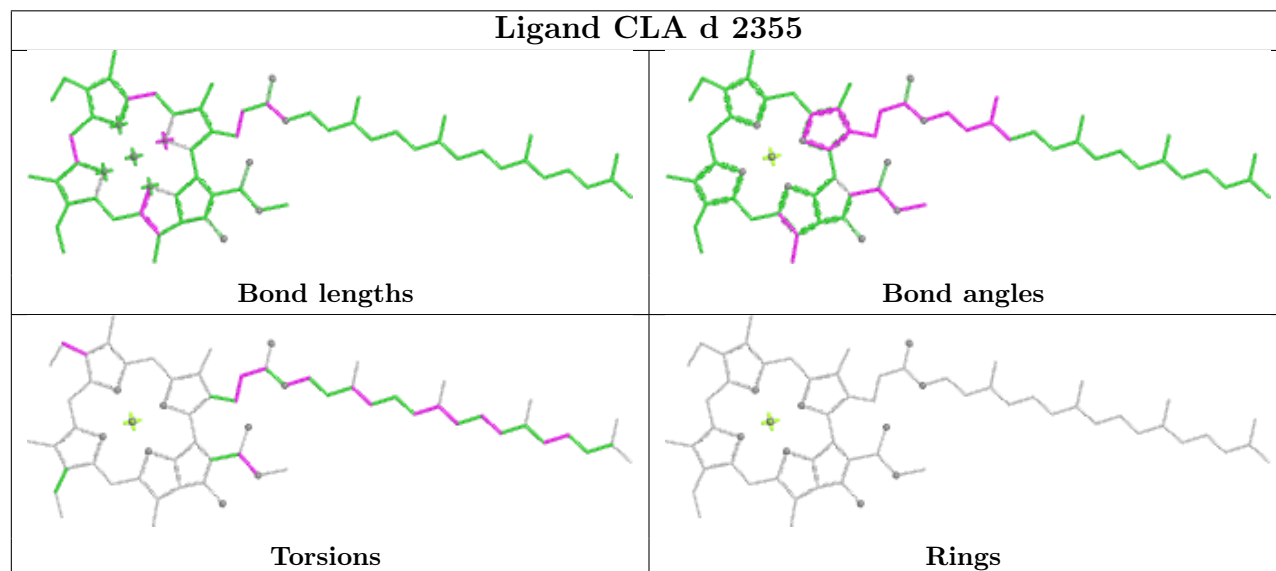
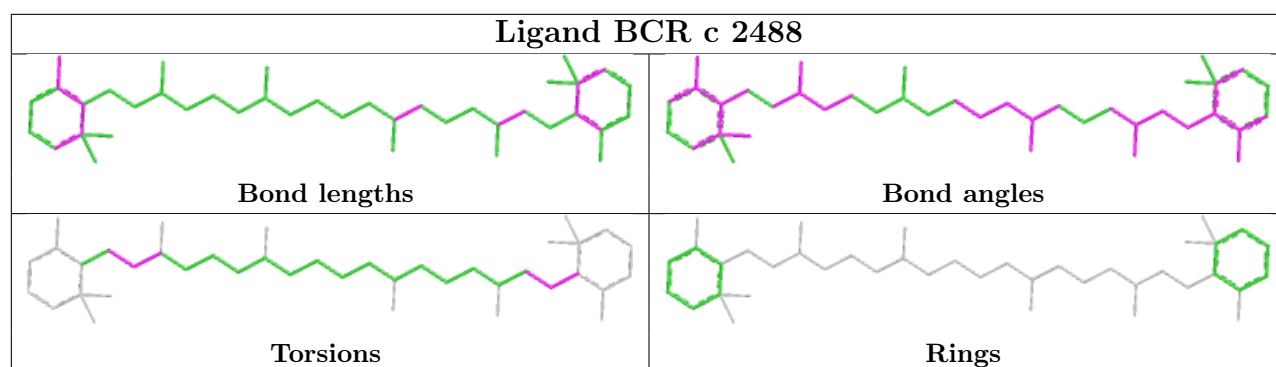
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

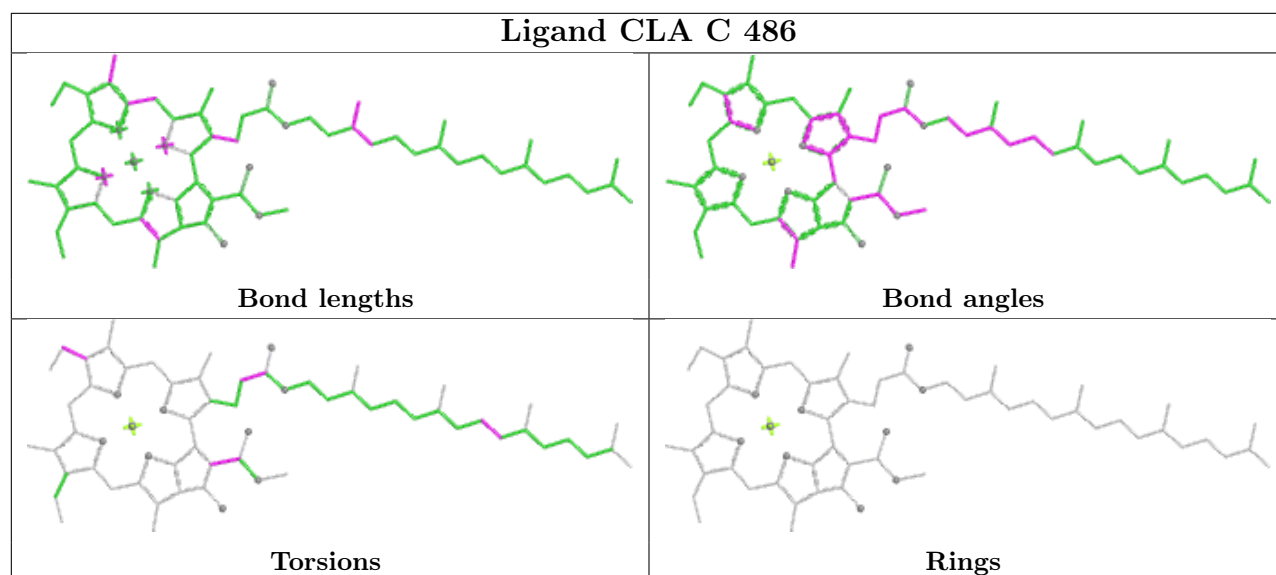
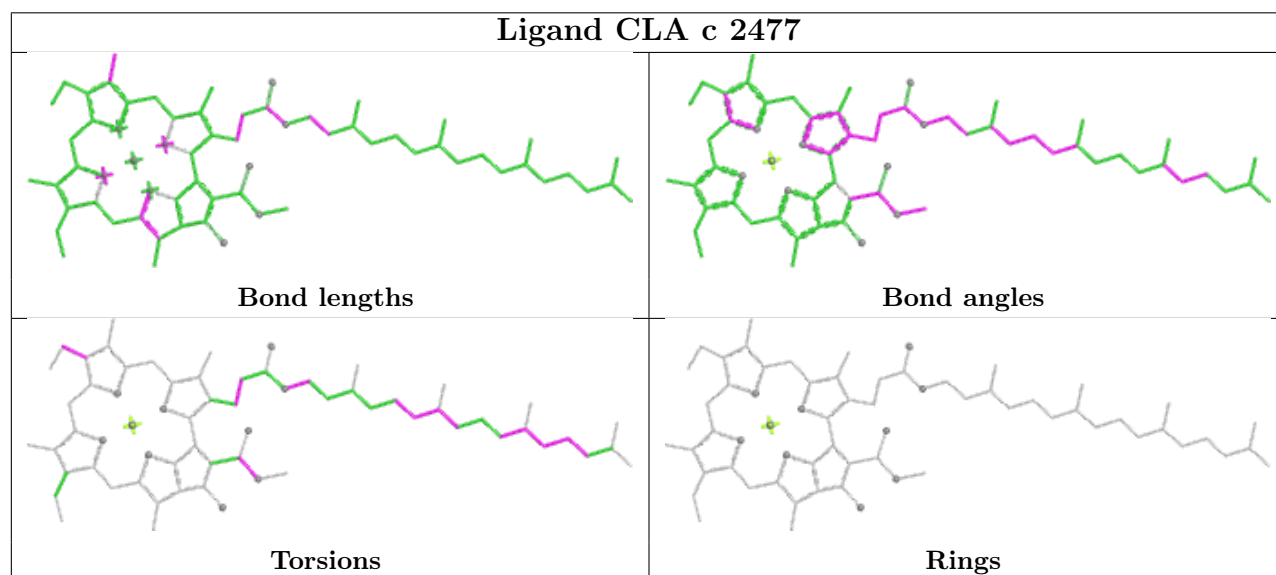
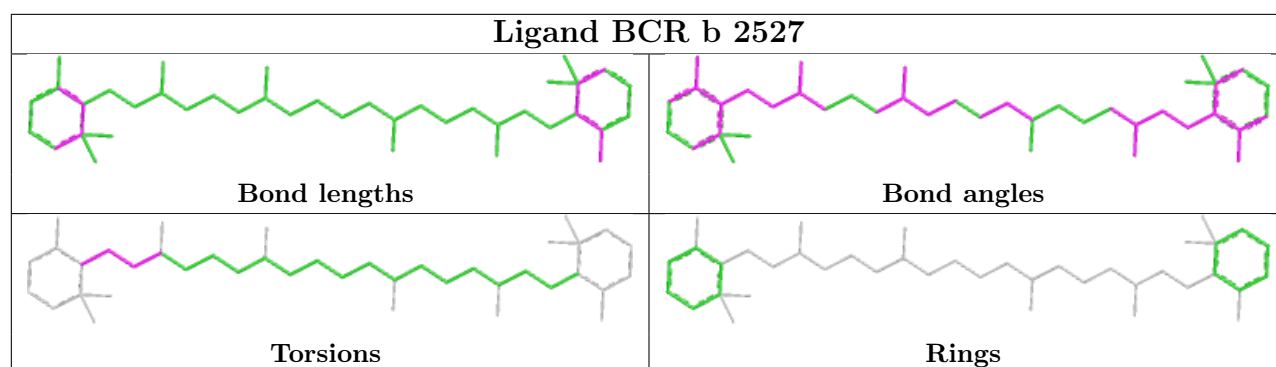




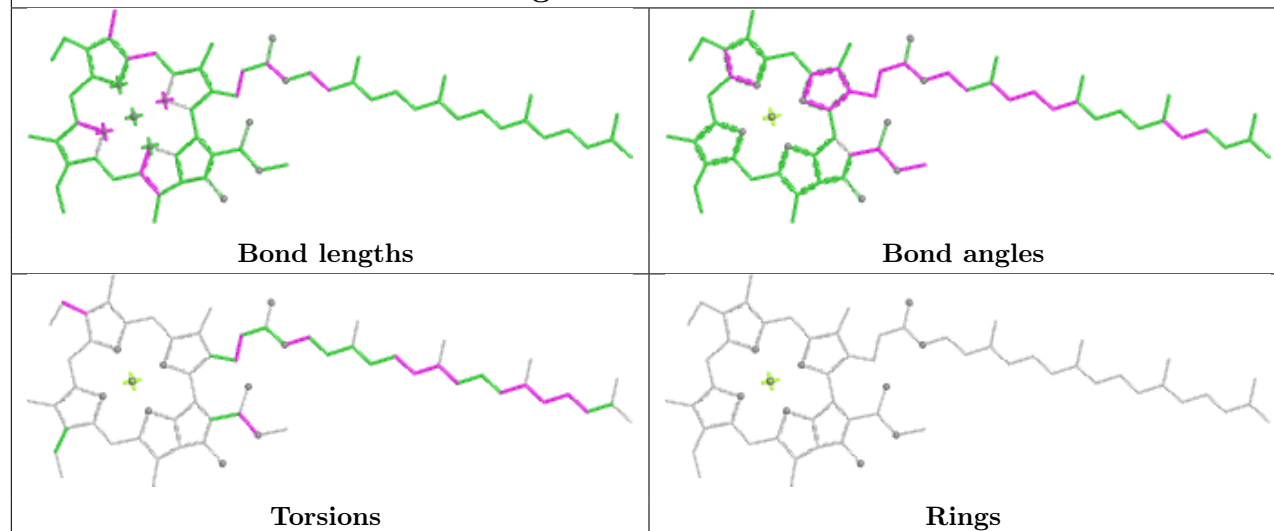


Ligand BCR K 50**Ligand CLA C 483****Ligand CLA B 523**

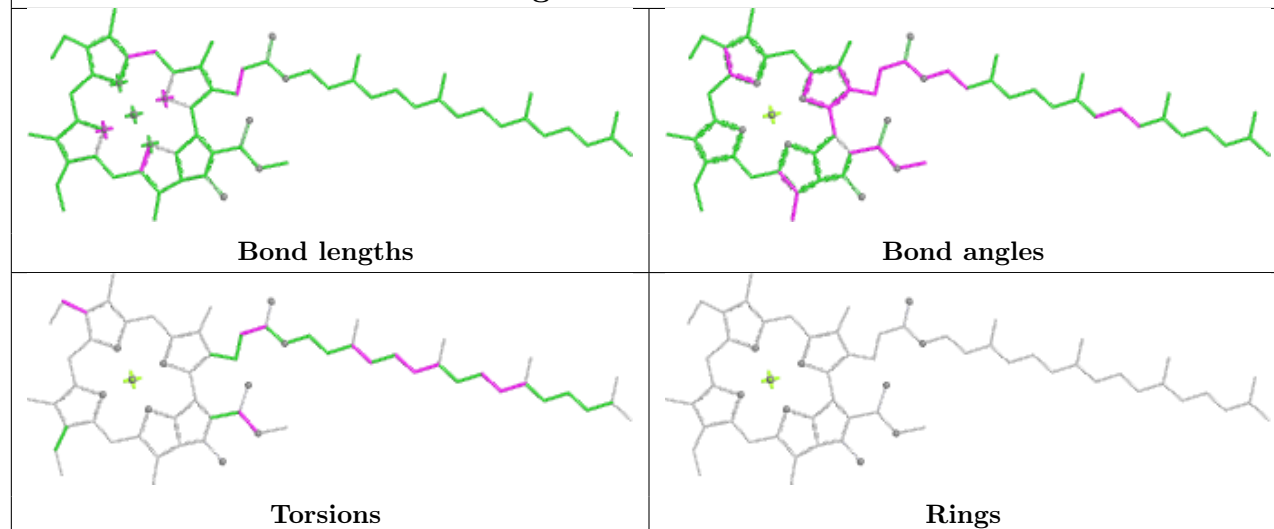




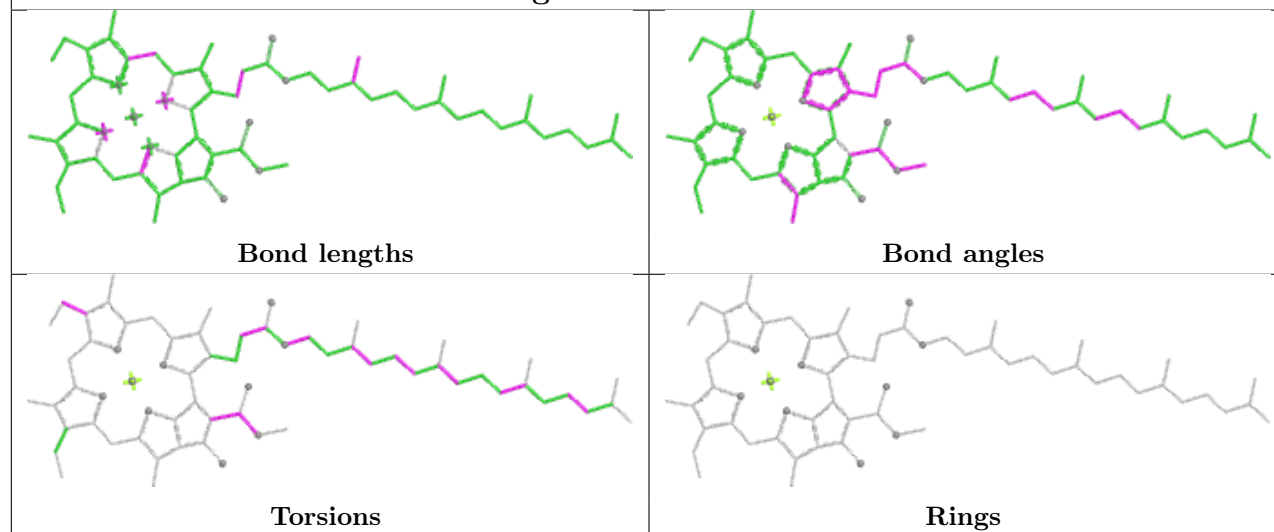
Ligand CLA C 477

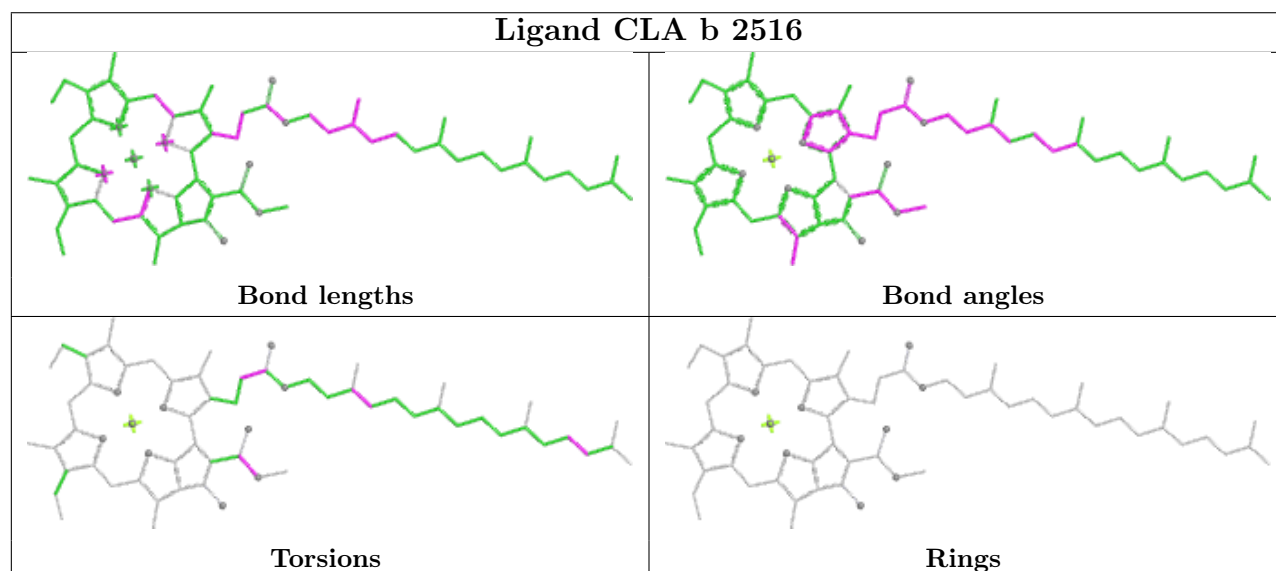
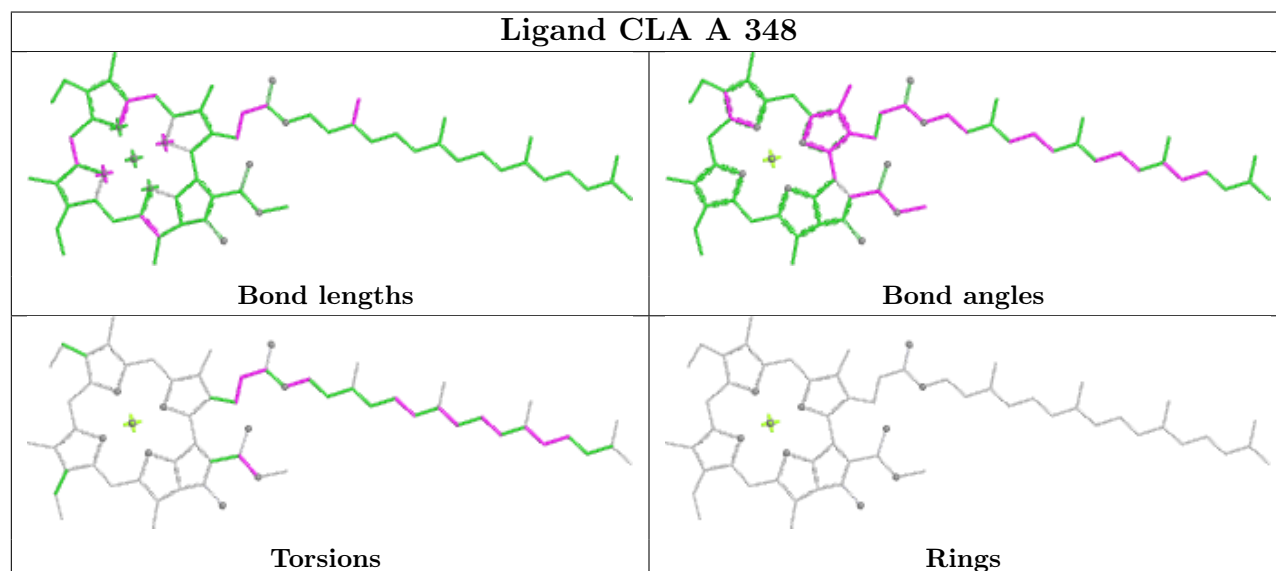
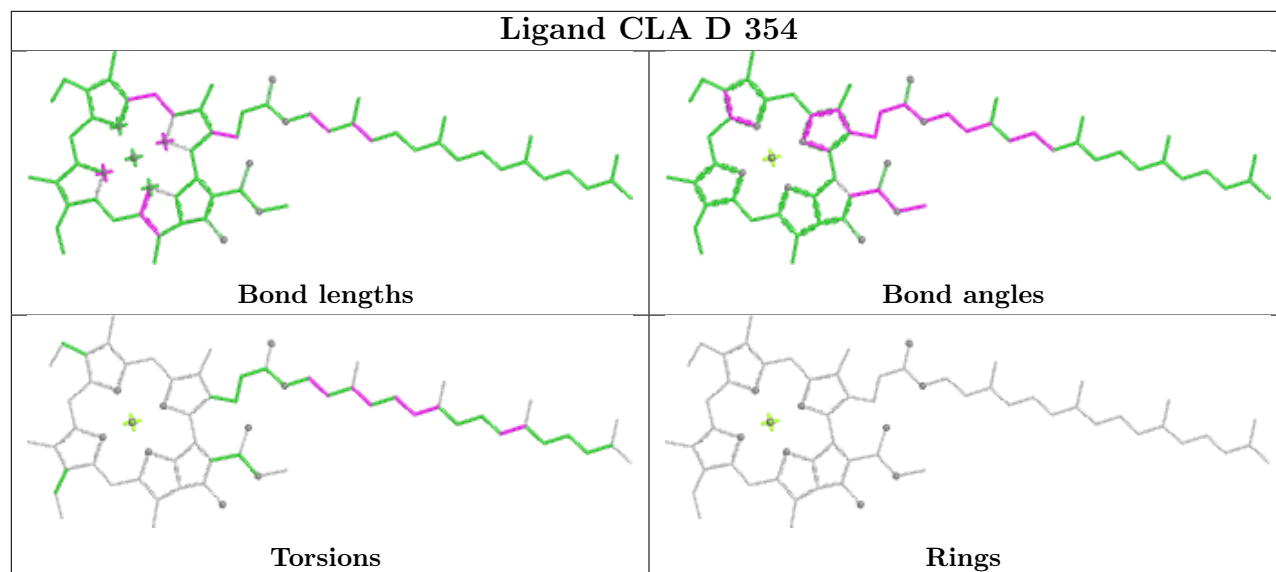


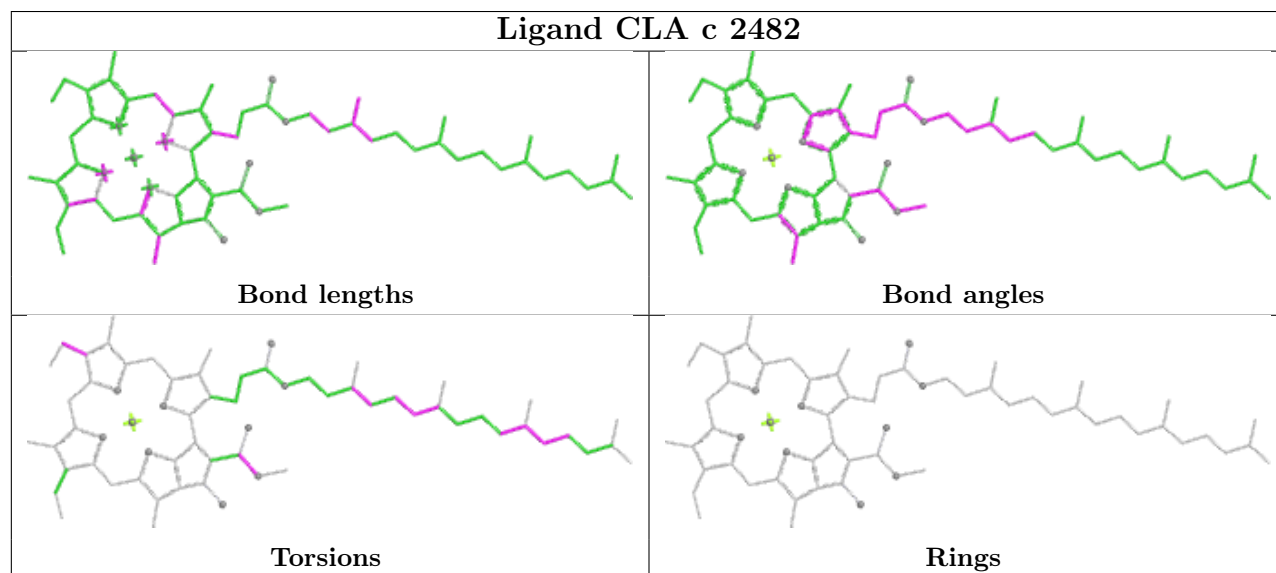
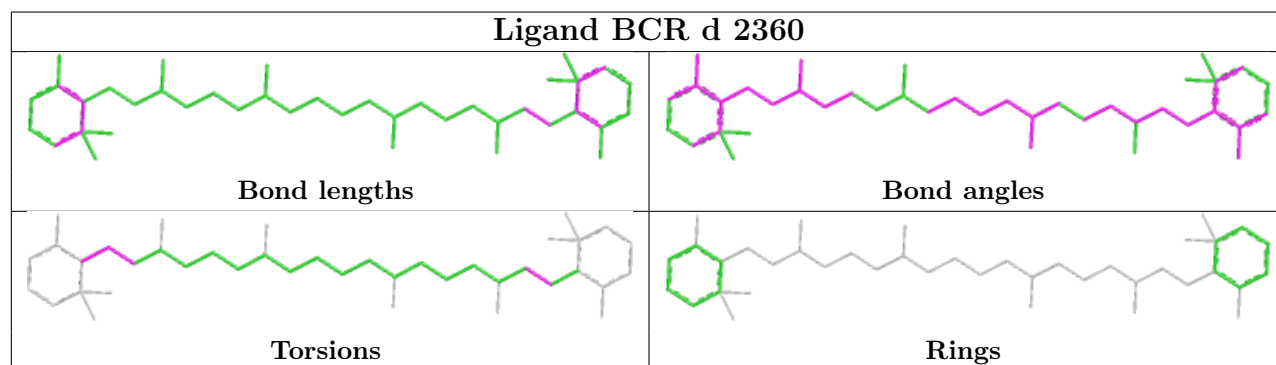
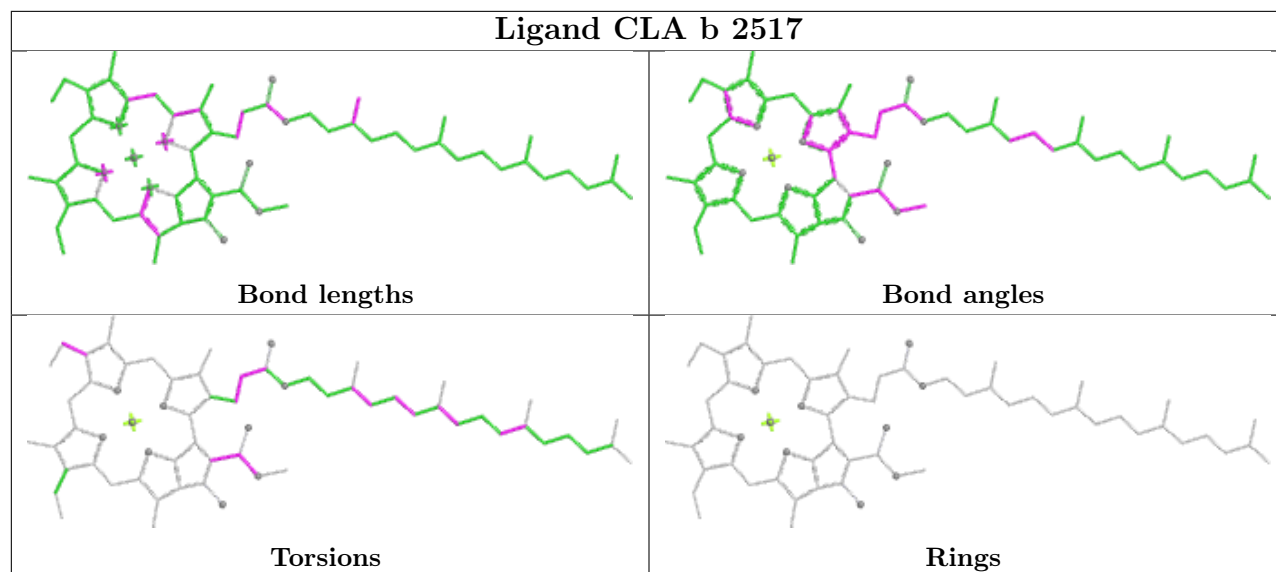
Ligand CLA B 518



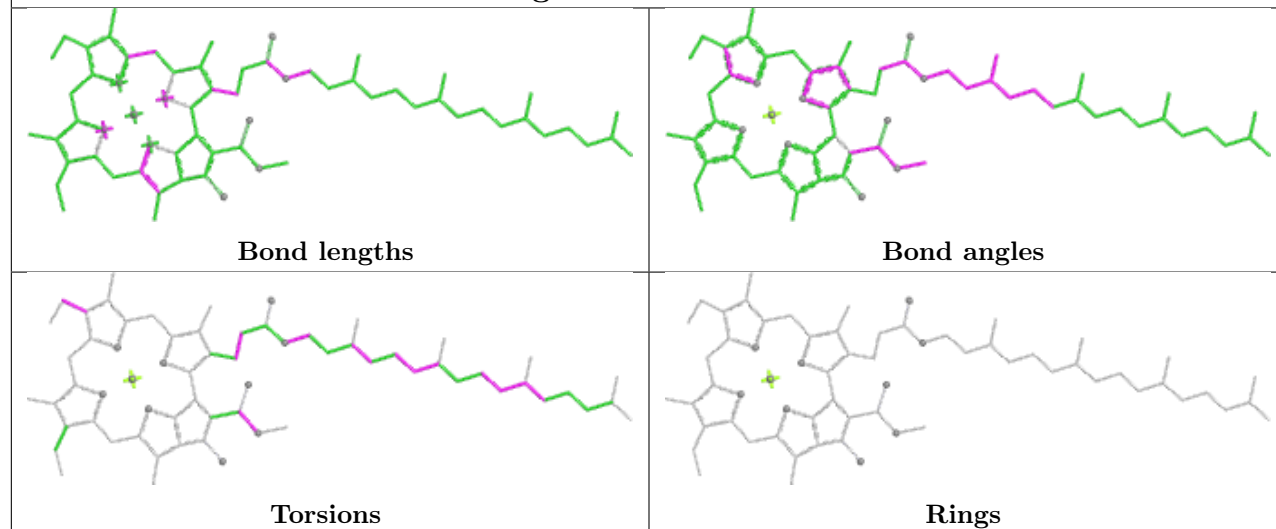
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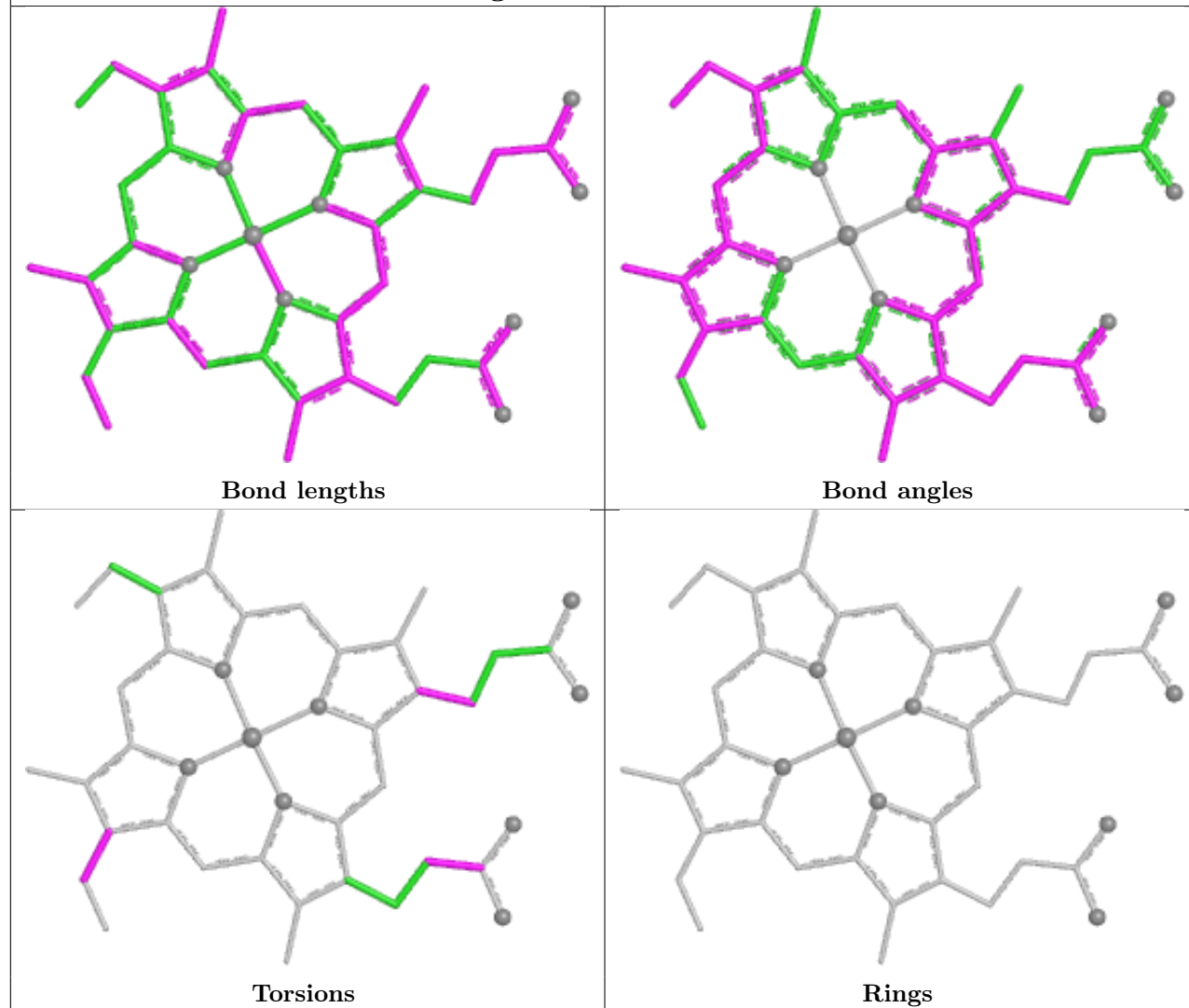


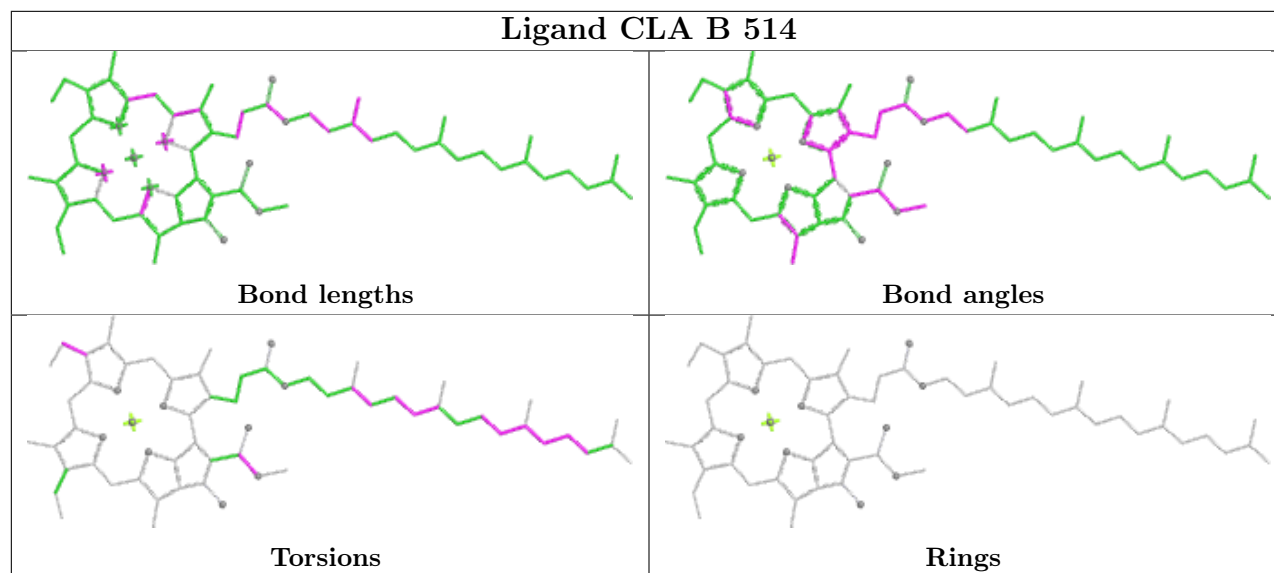
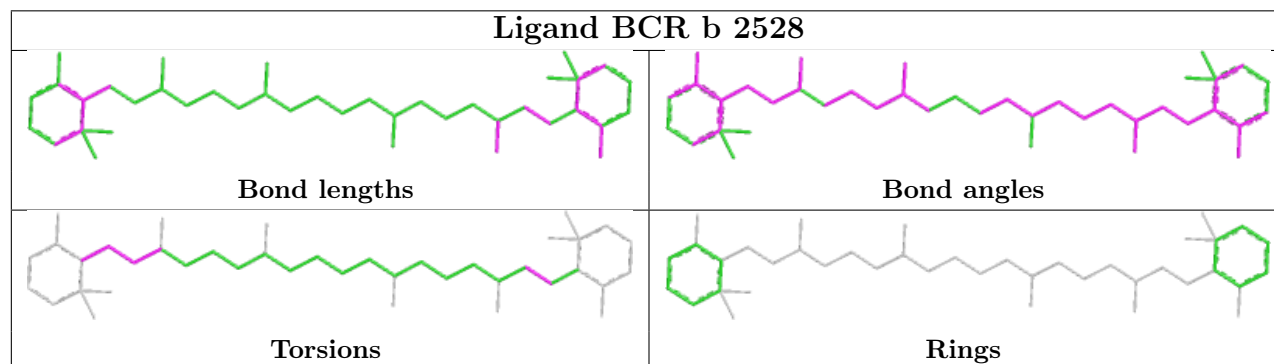
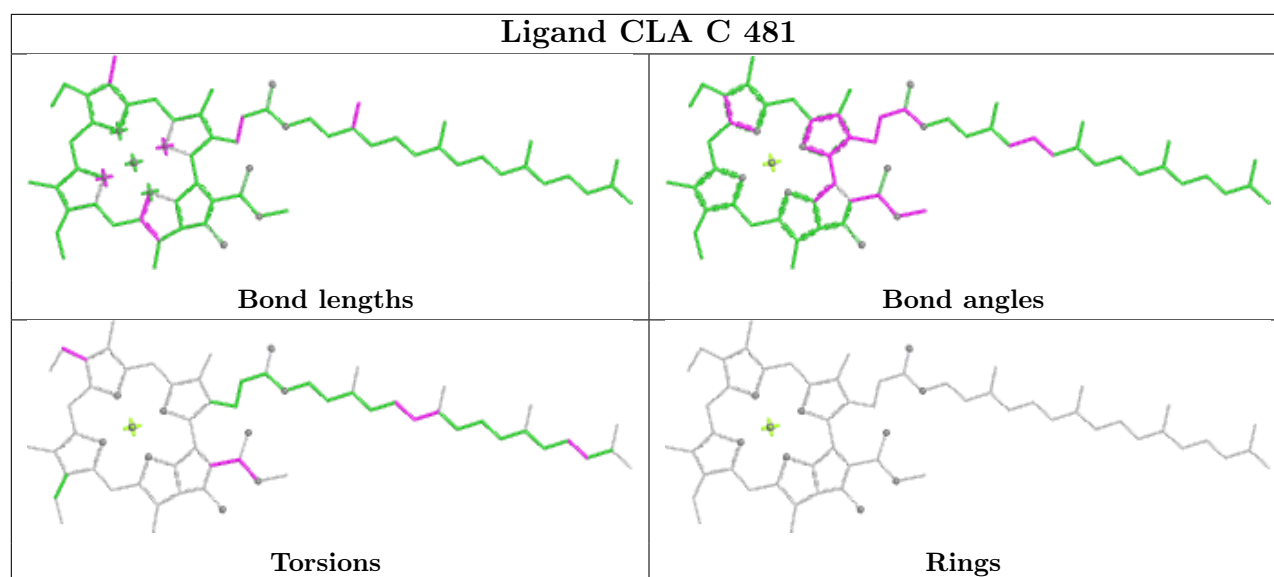


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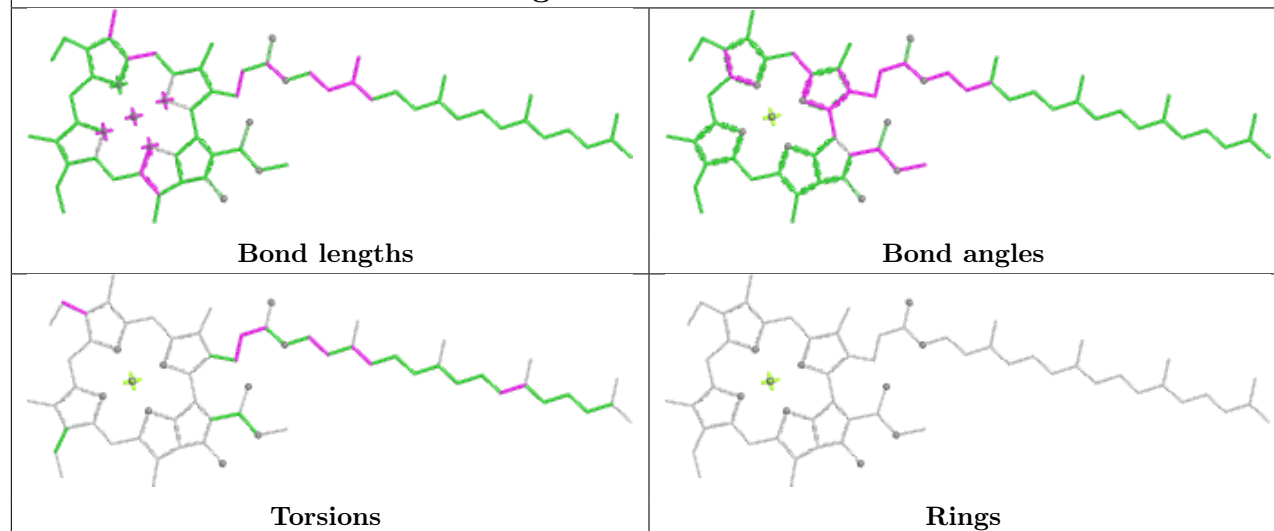


Ligand HEC v 2138

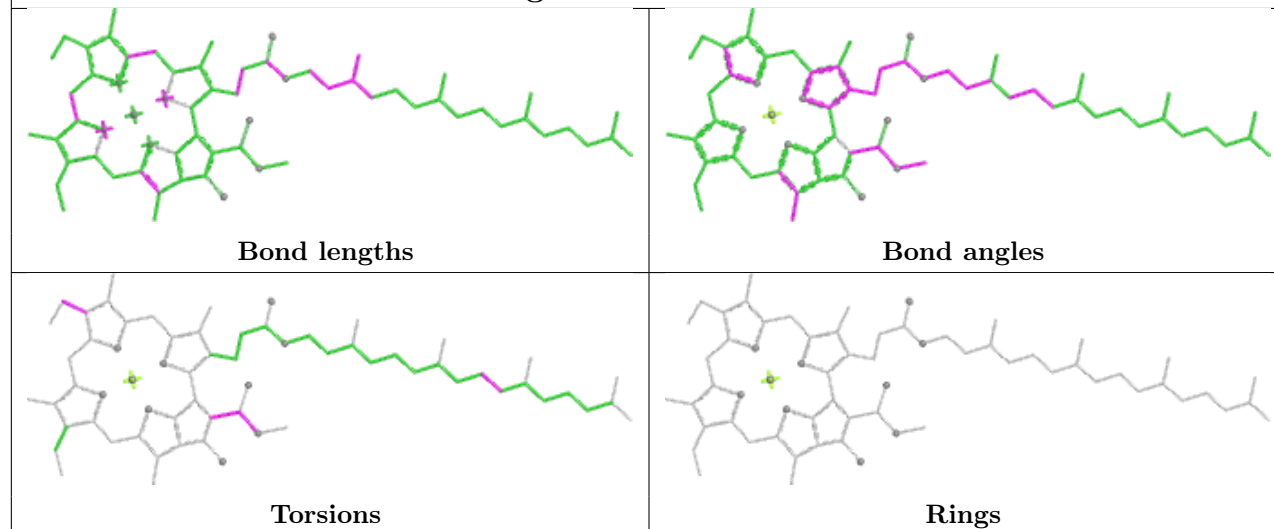




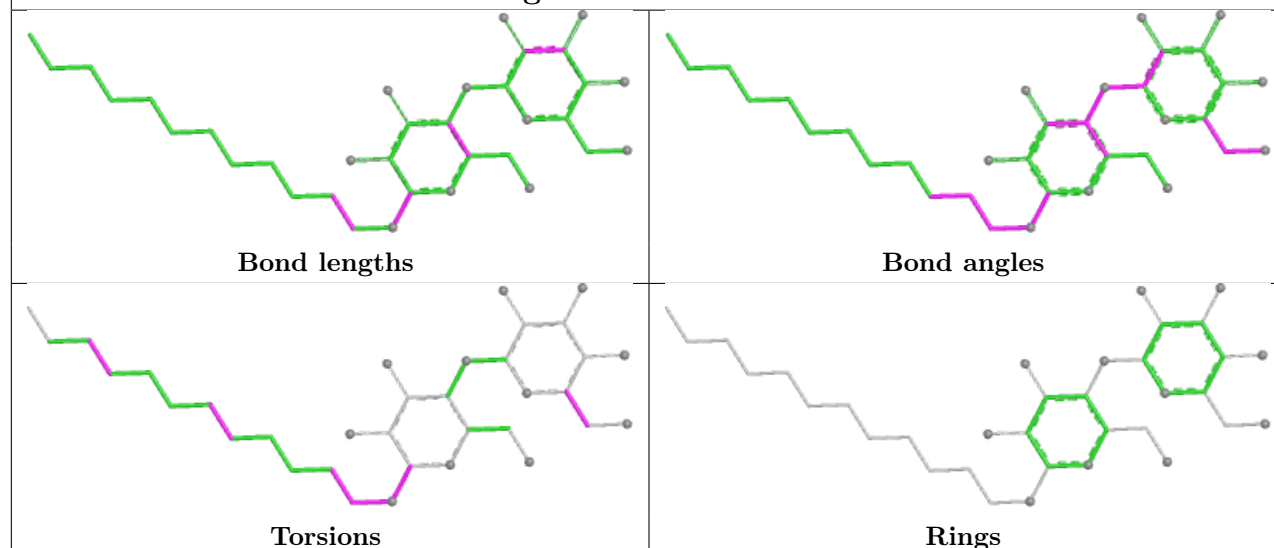
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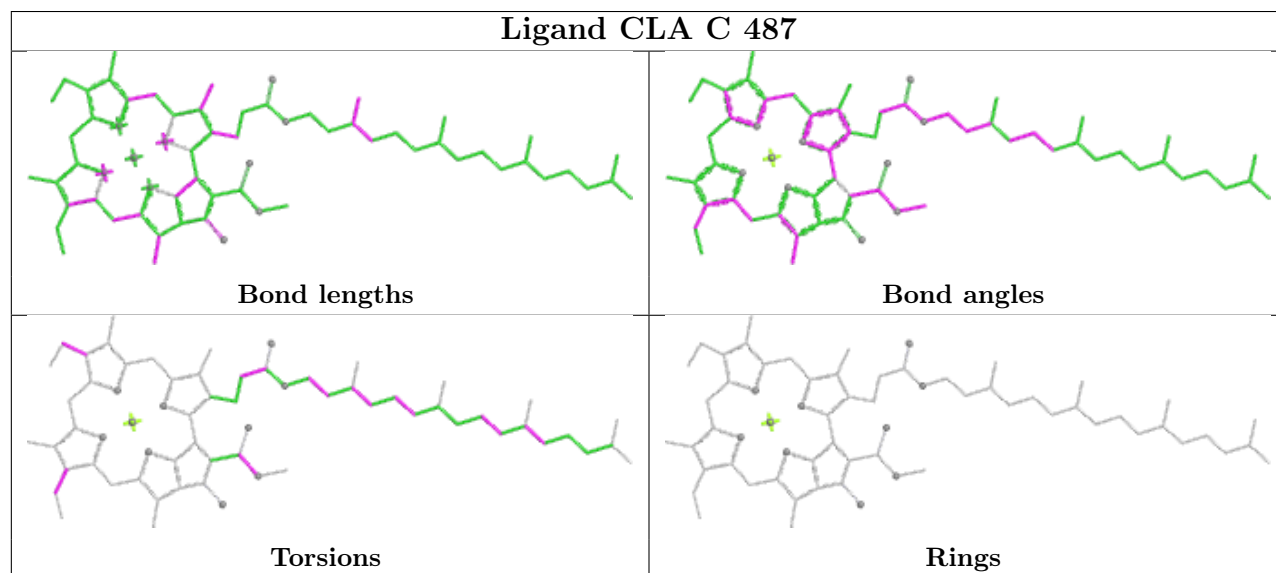
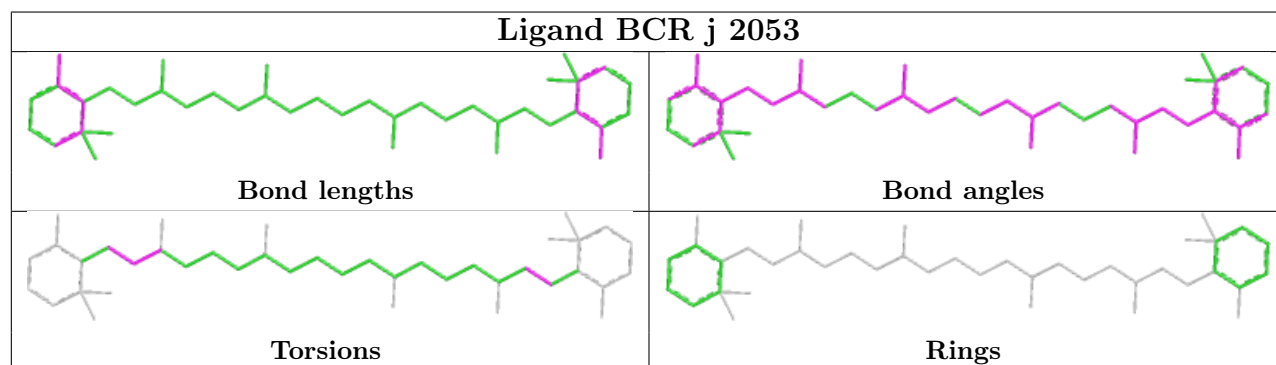
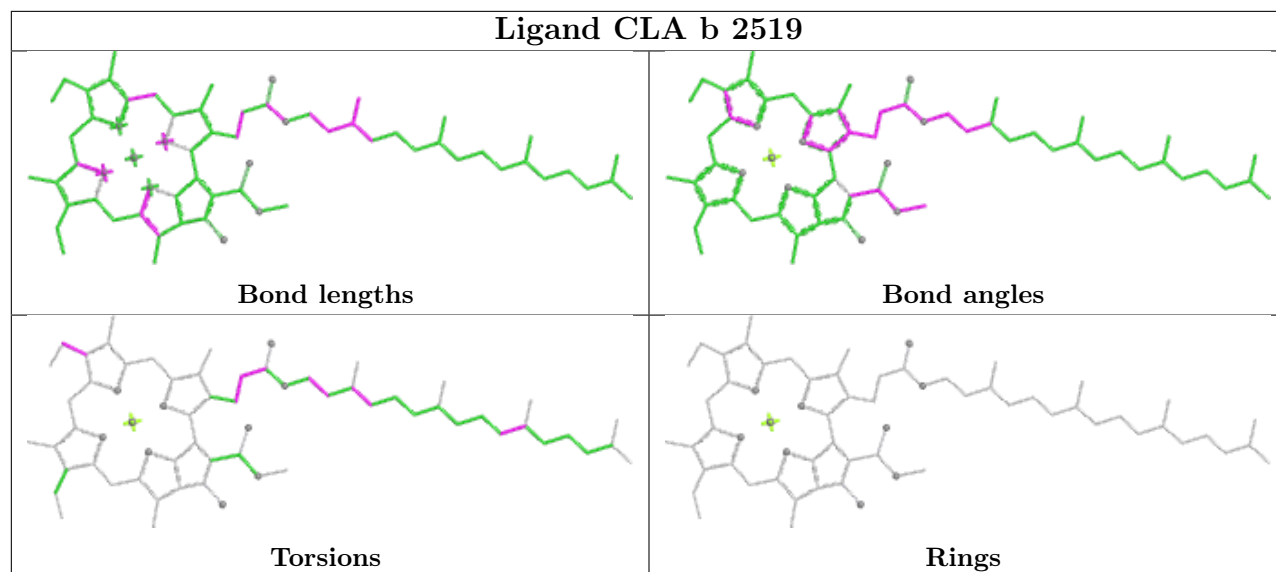


Ligand CLA b 2520

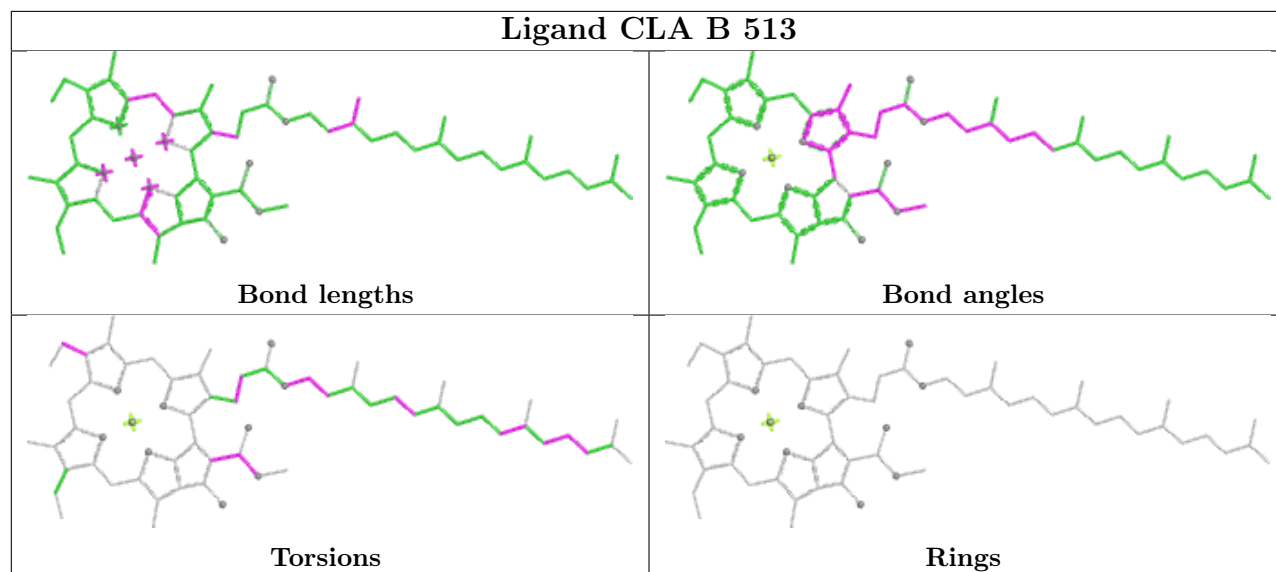


Ligand LMT d 2359

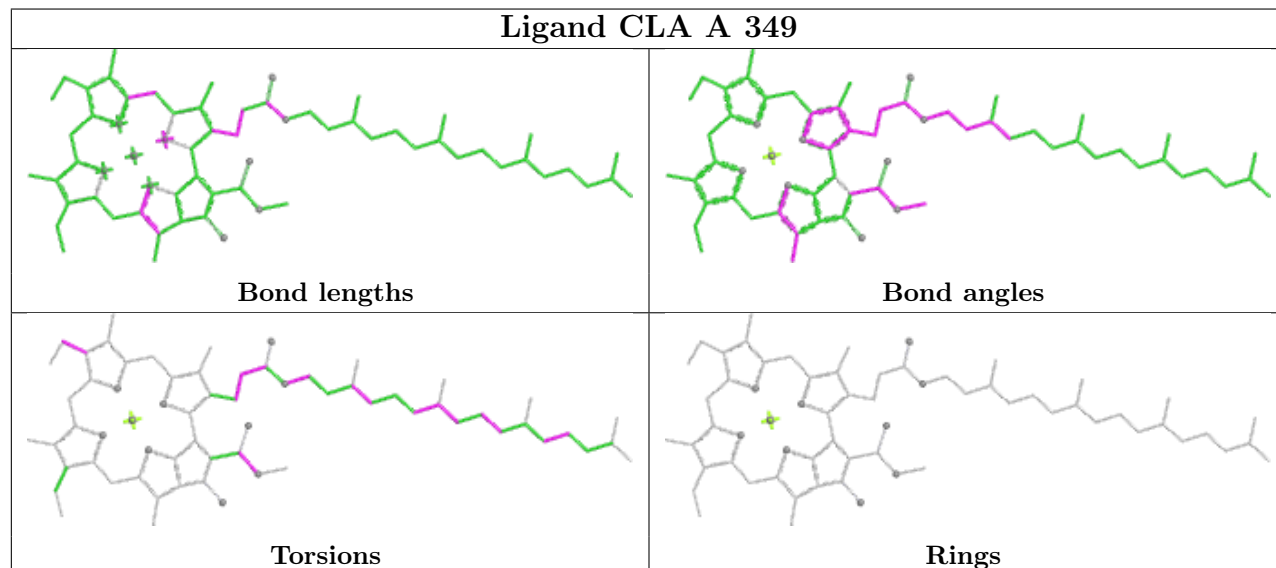




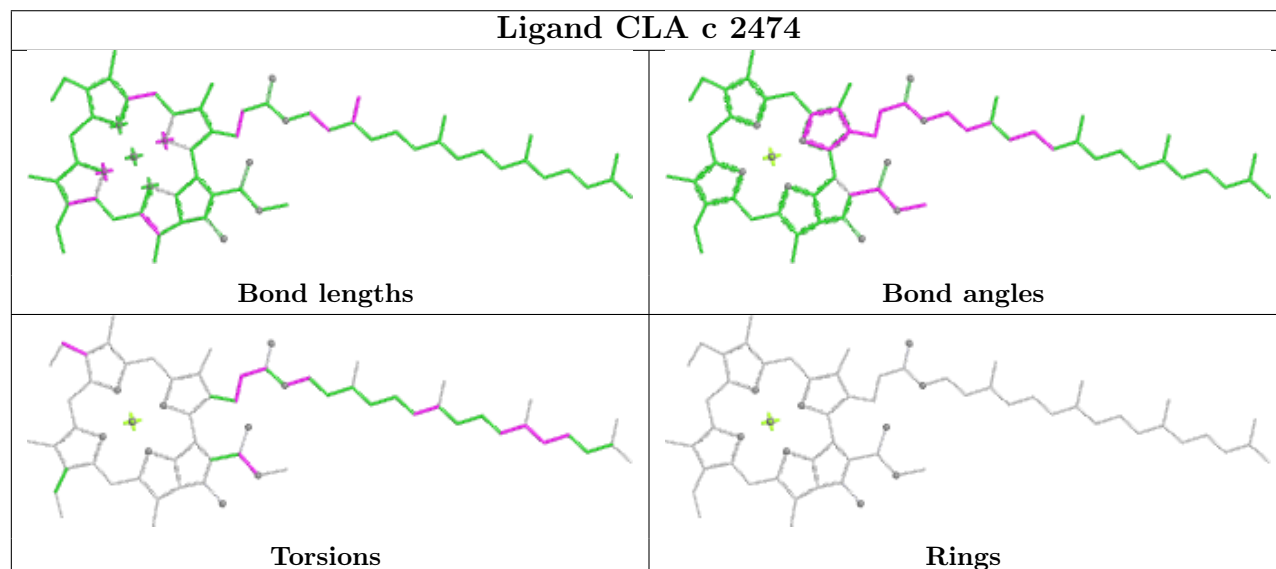
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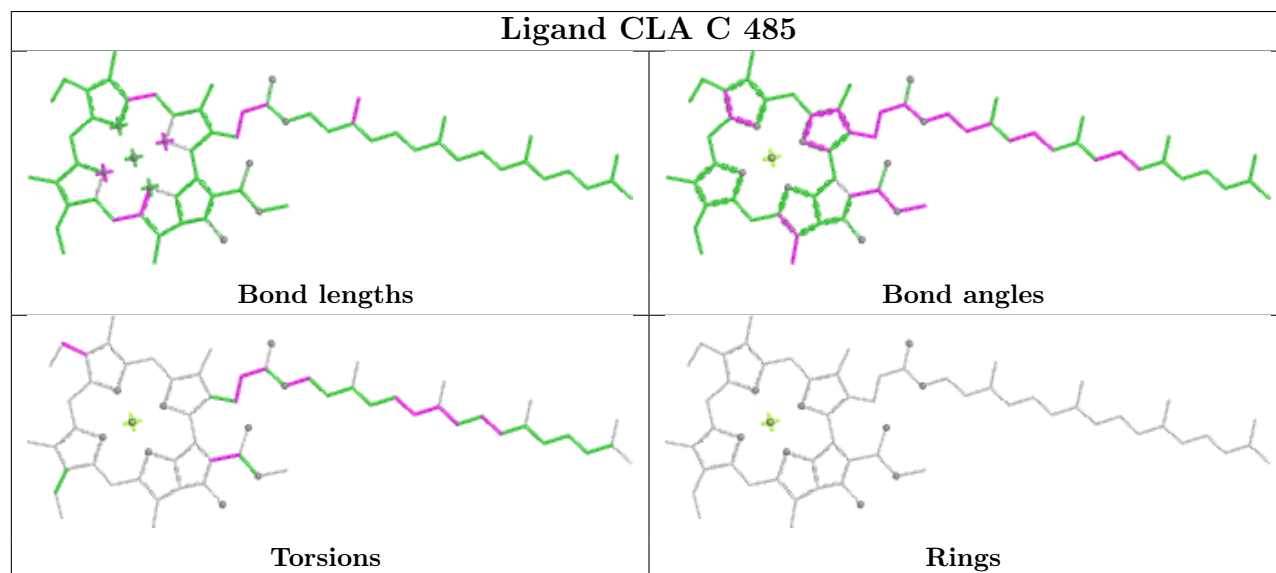
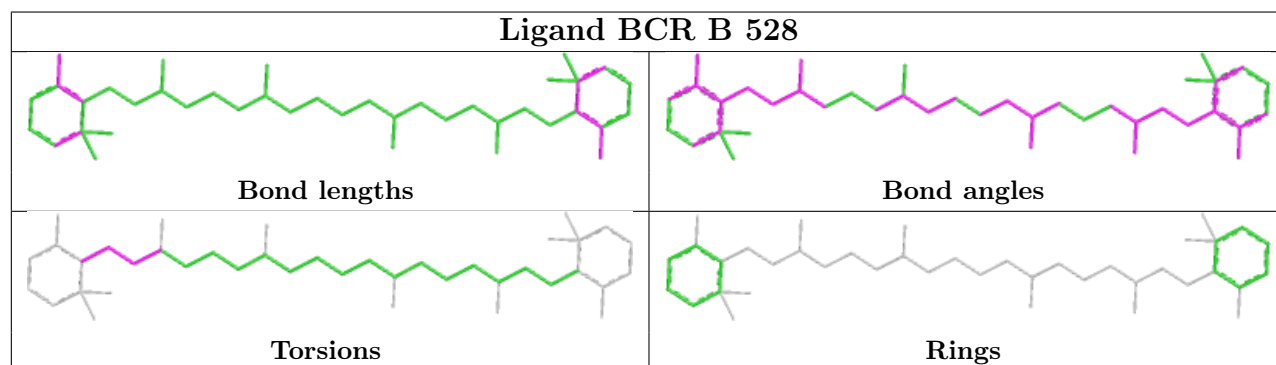
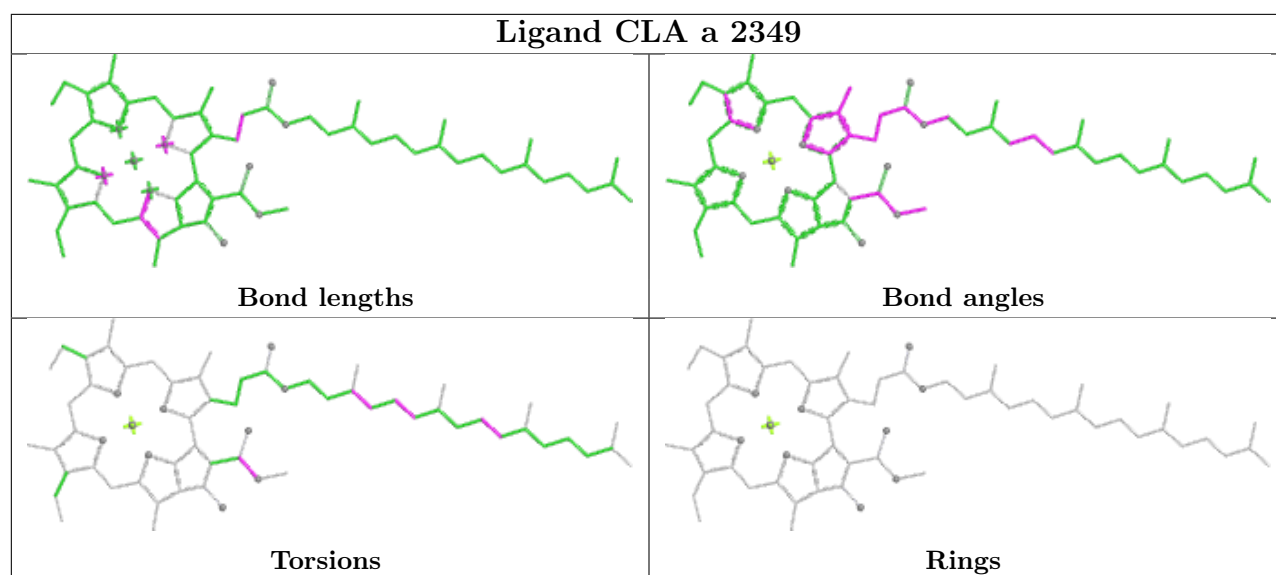


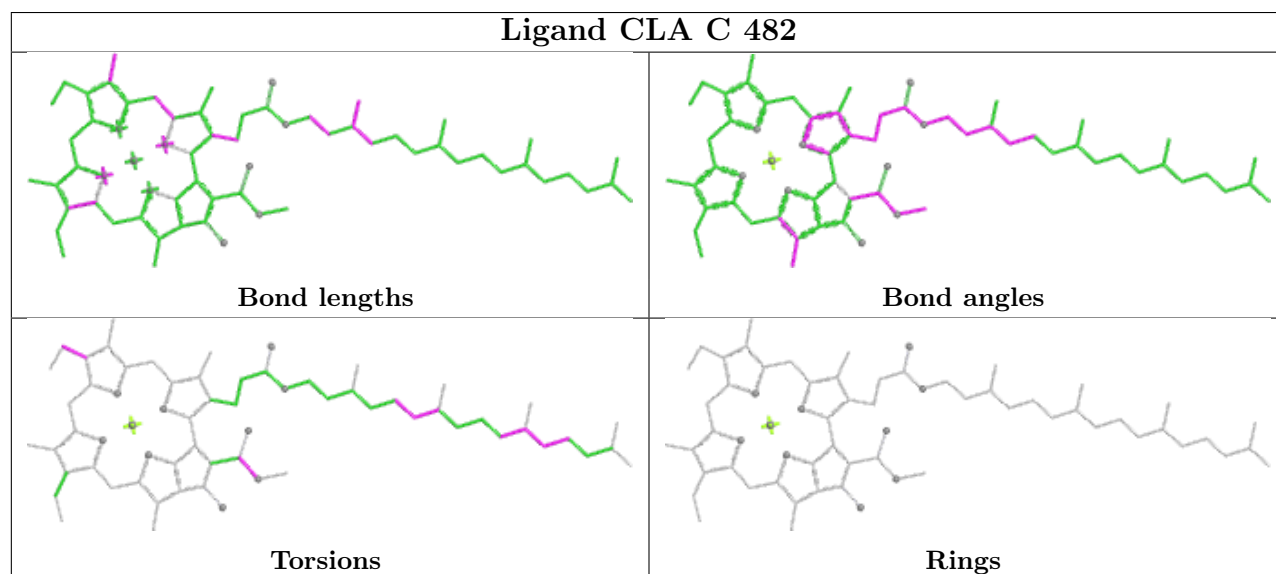
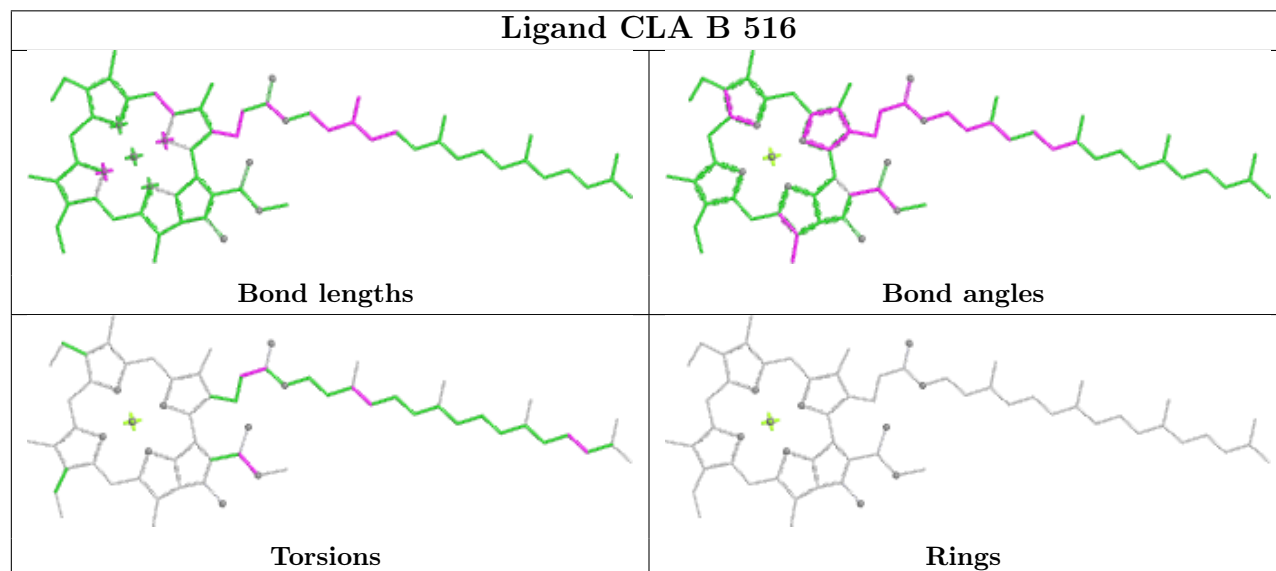
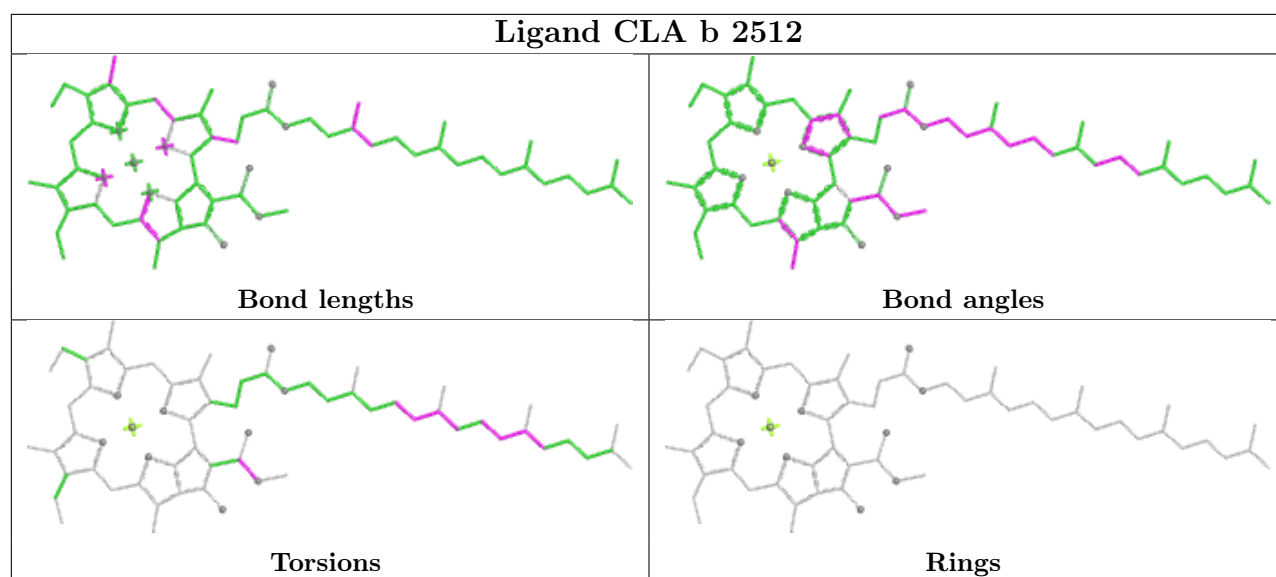
Ligand CLA A 349

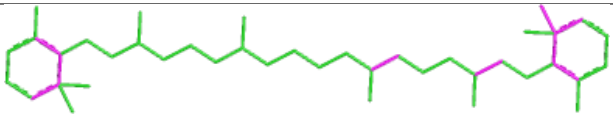
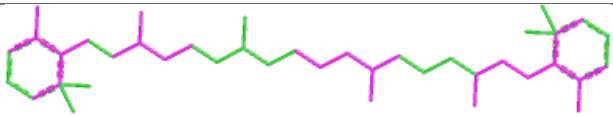
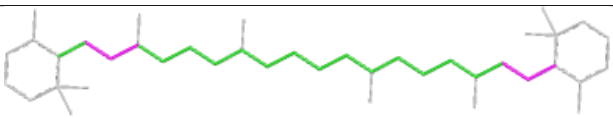
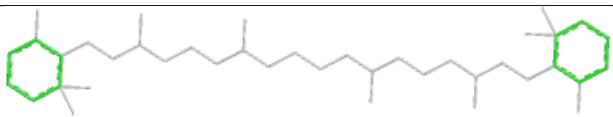


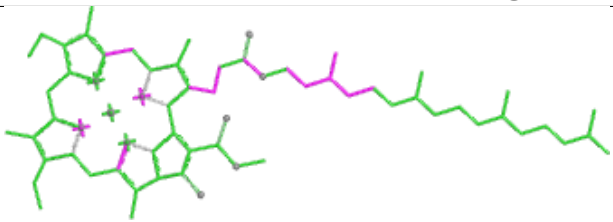
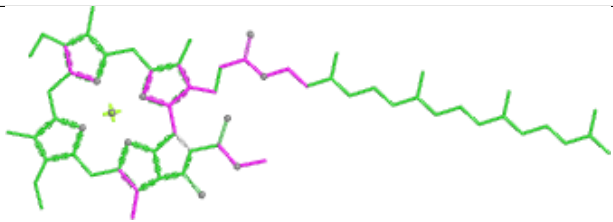
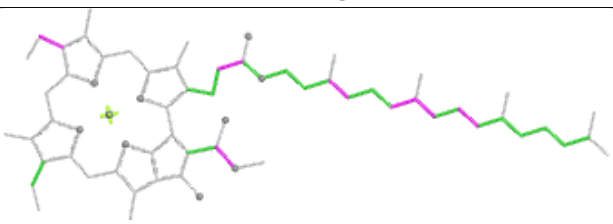
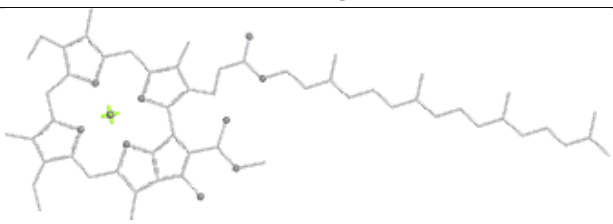
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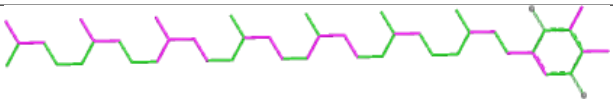
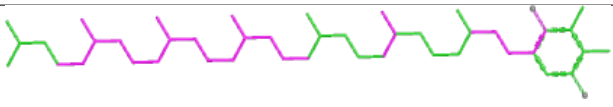
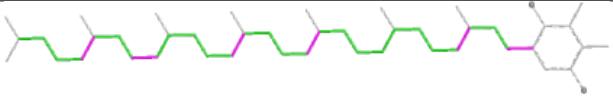
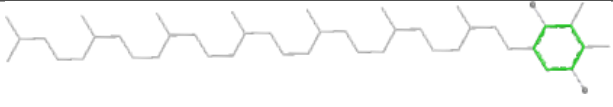


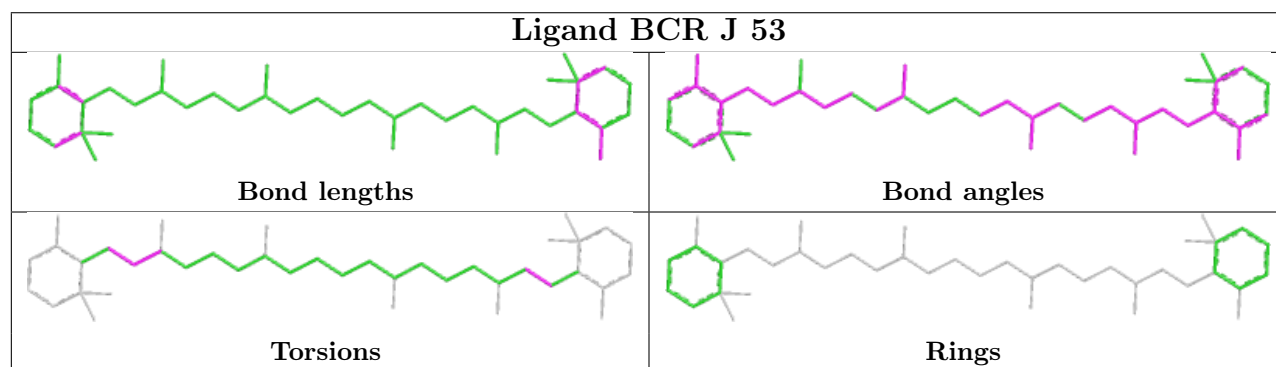
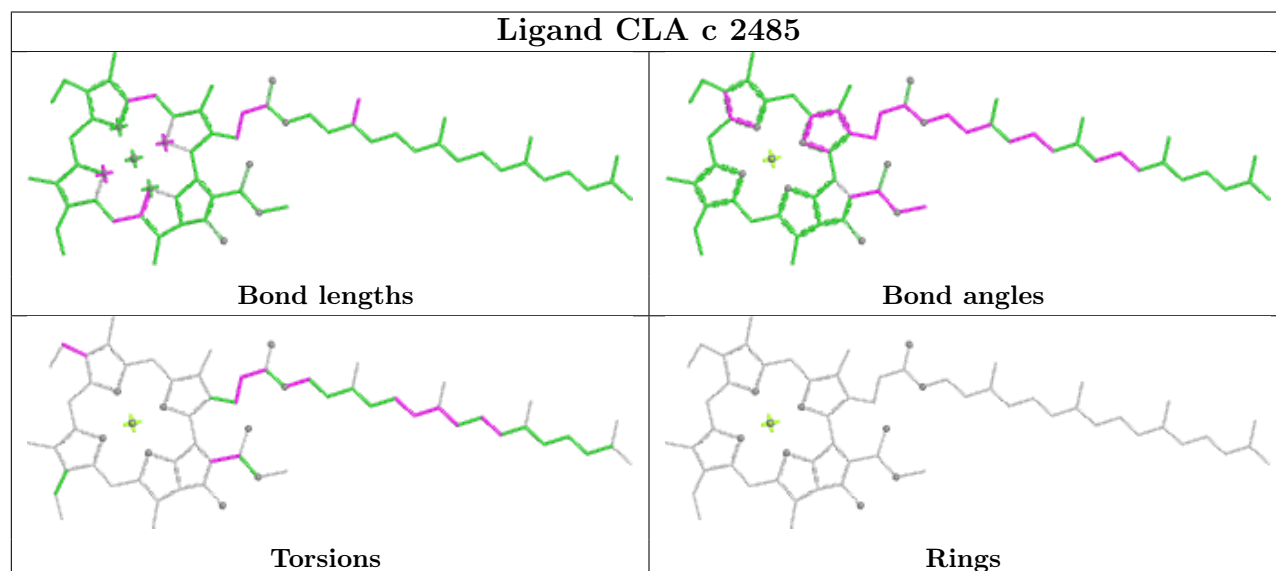
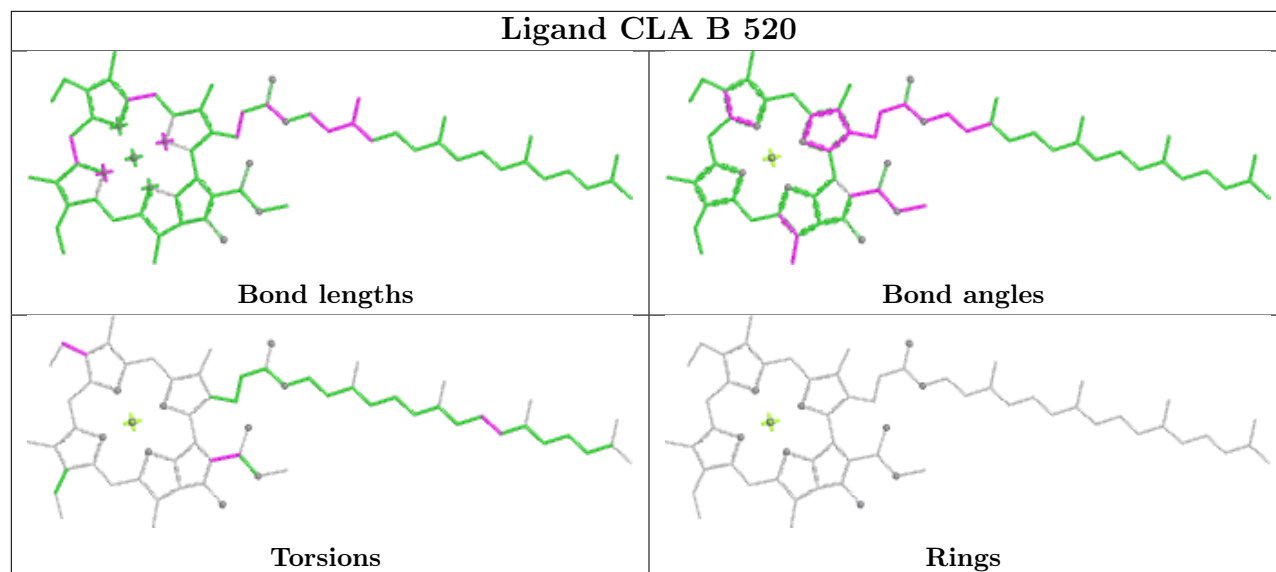




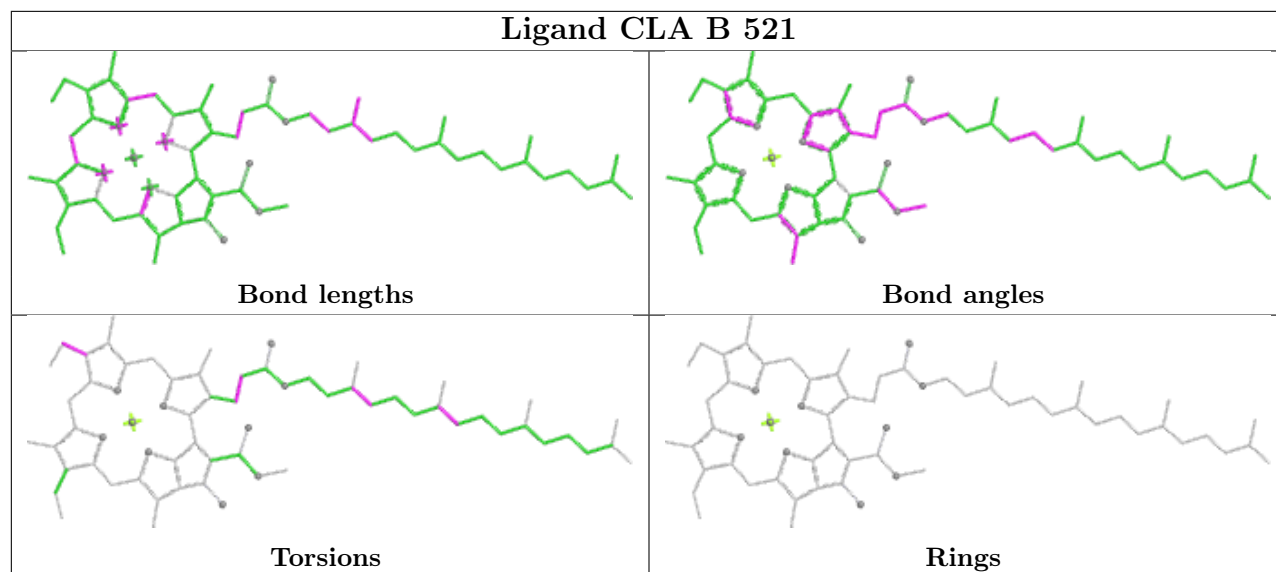
Ligand BCR C 488	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 2475	
	
Bond lengths	Bond angles
	
Torsions	Rings

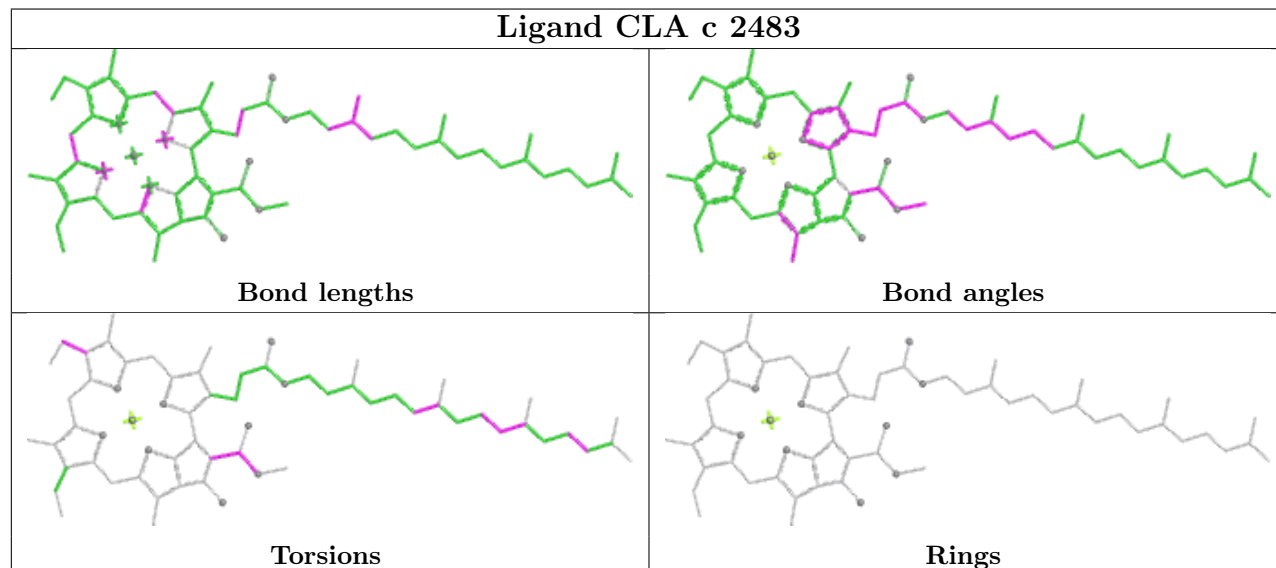
Ligand PL9 A 353	
	
Bond lengths	Bond angles
	
Torsions	Rings



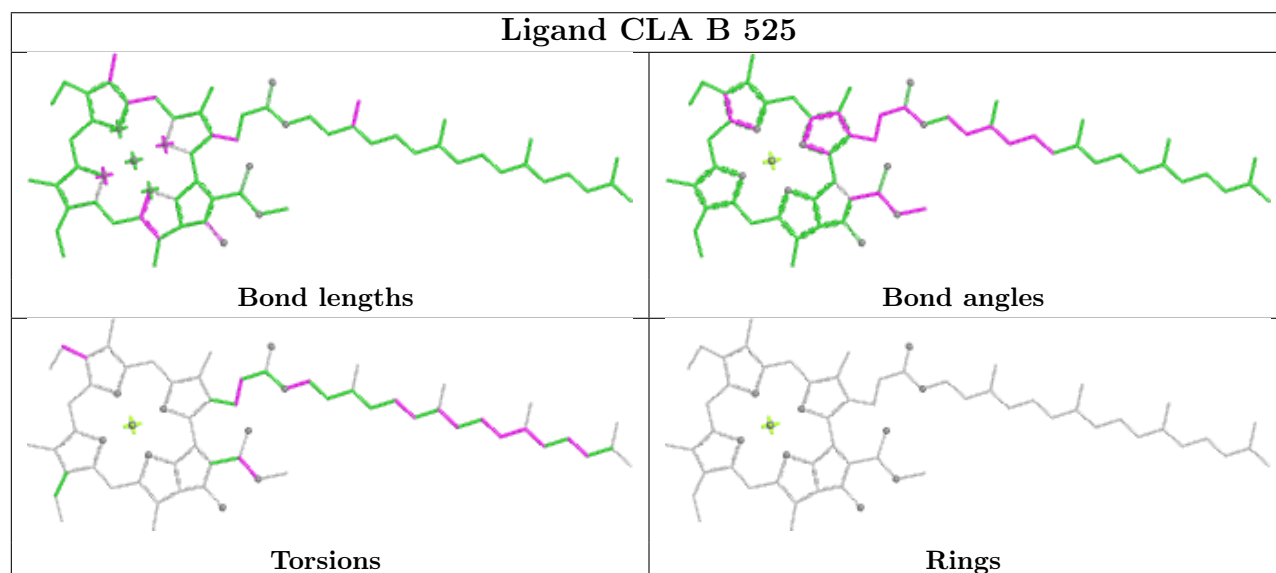
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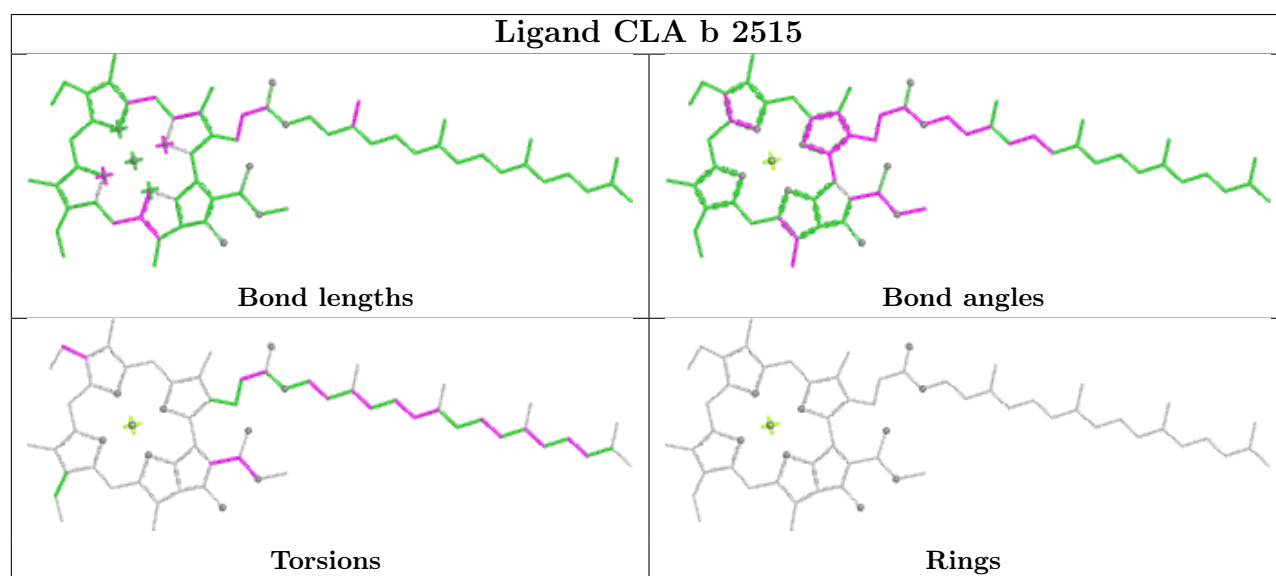
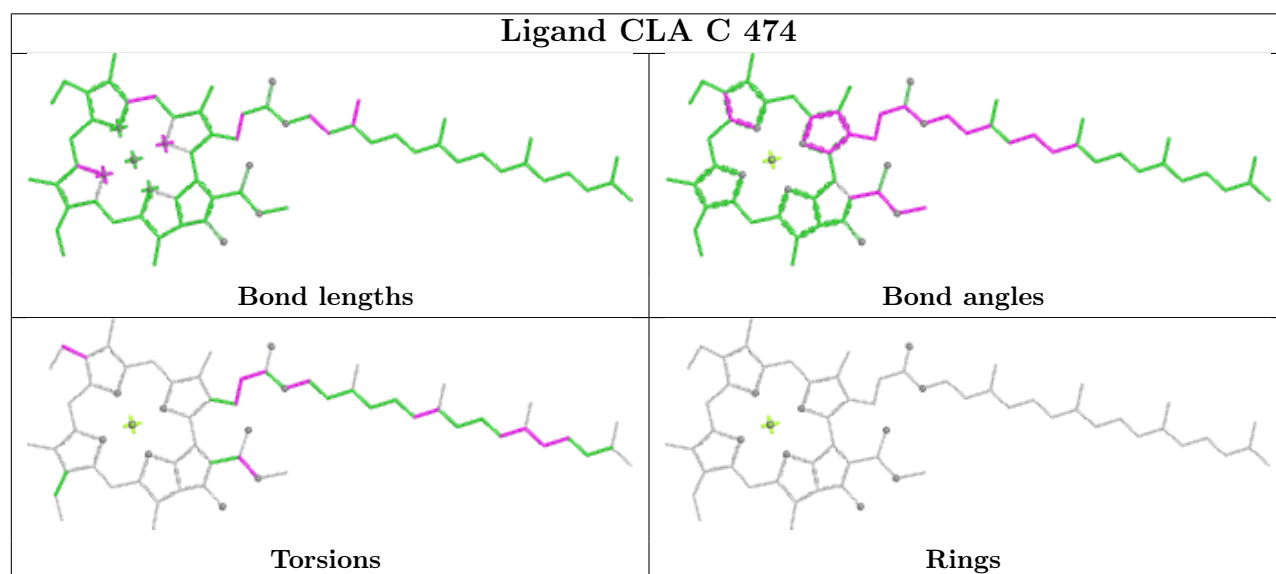
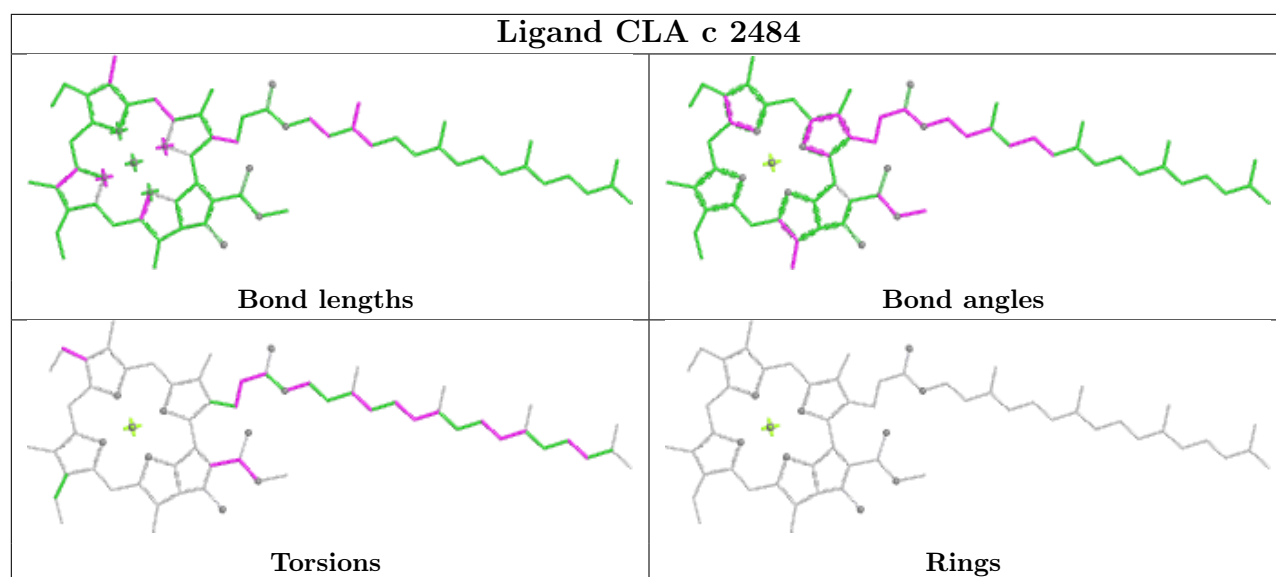


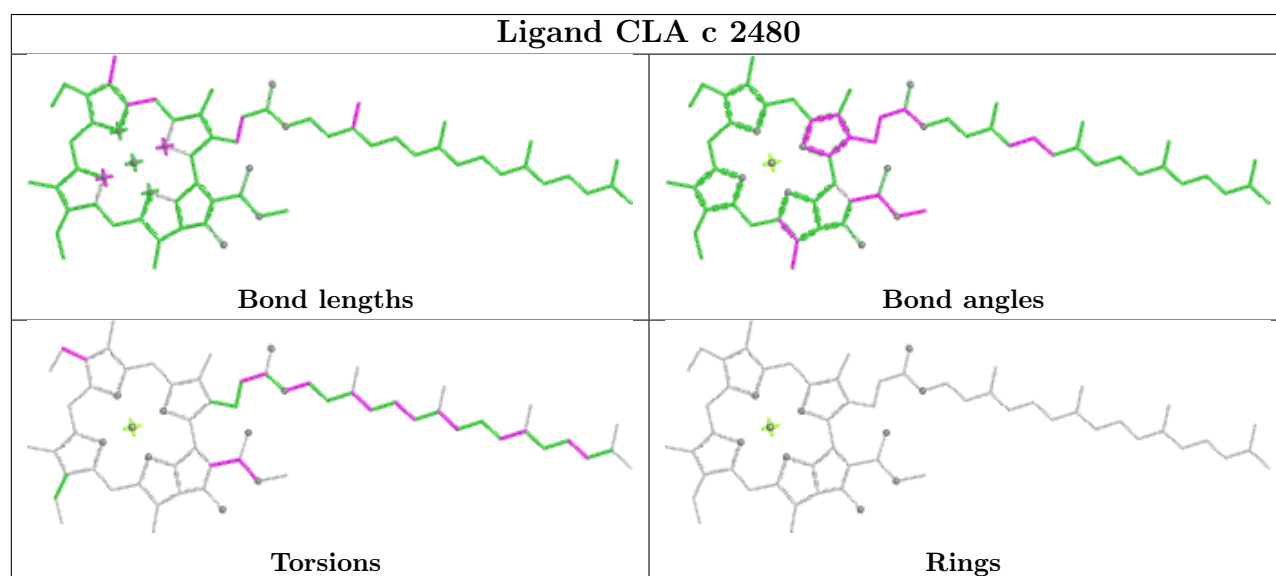
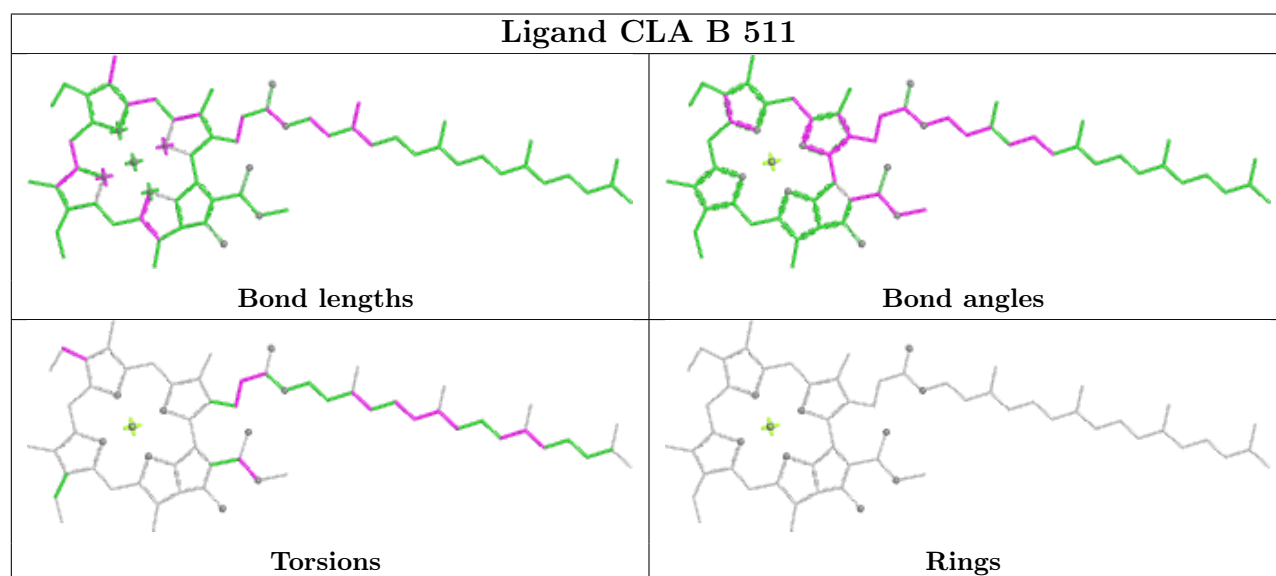
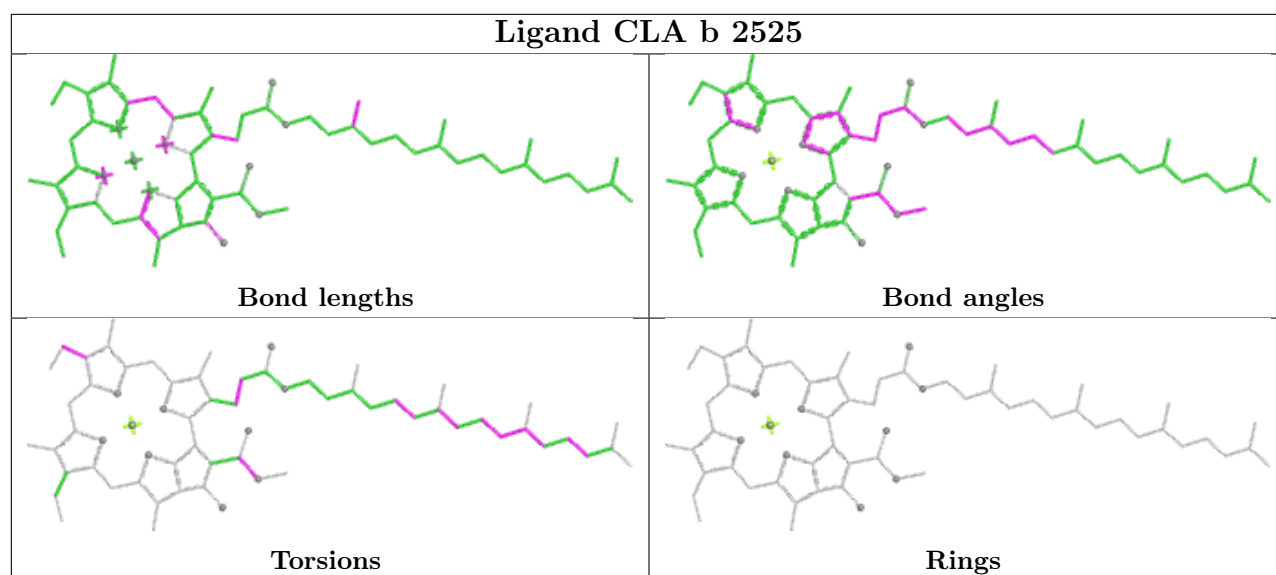
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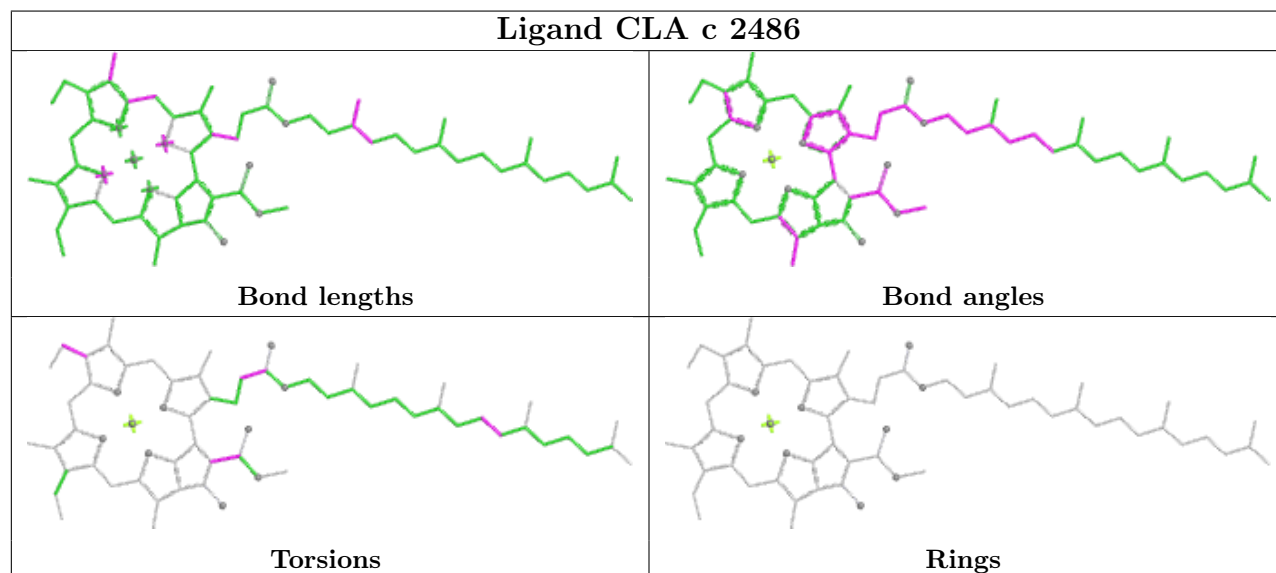
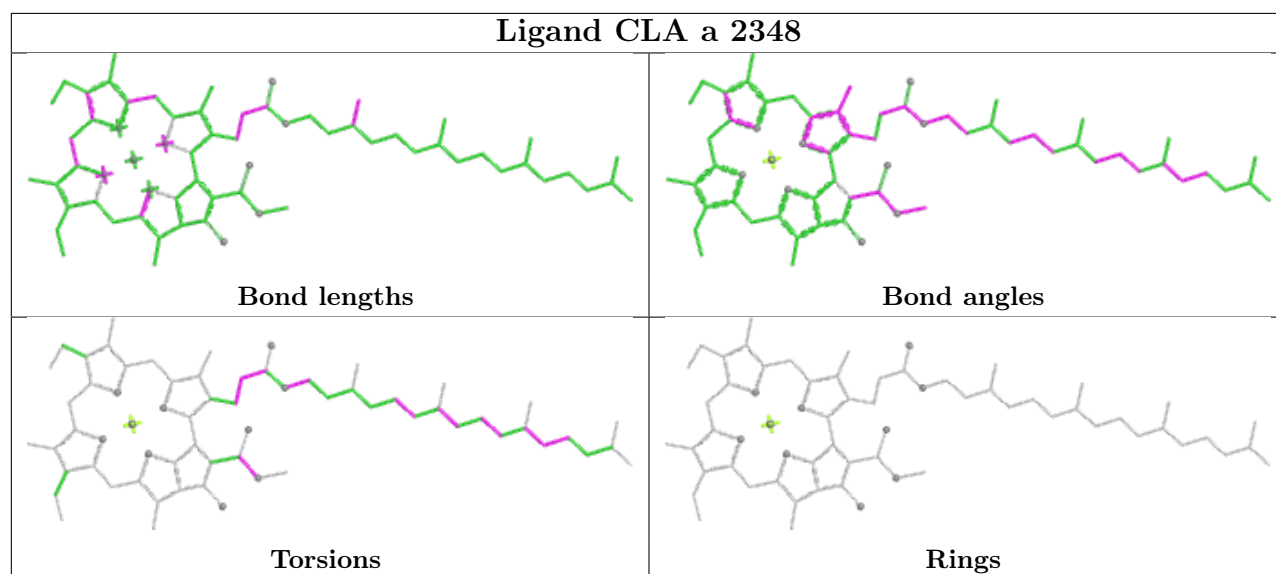
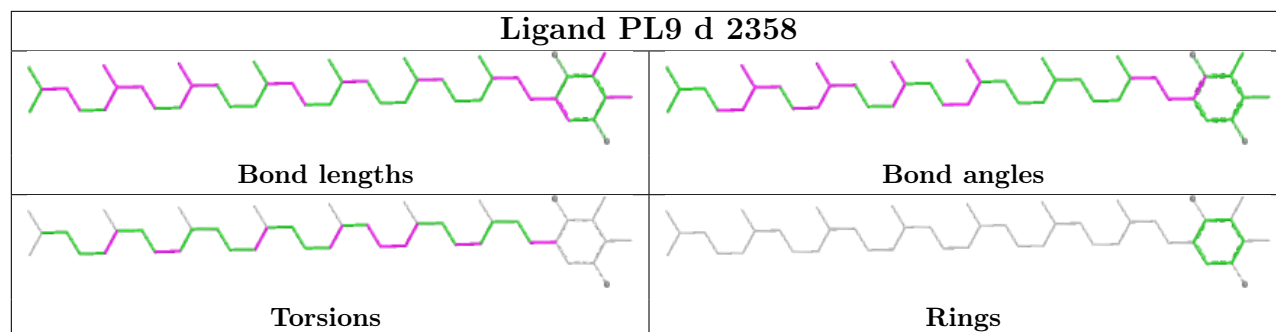


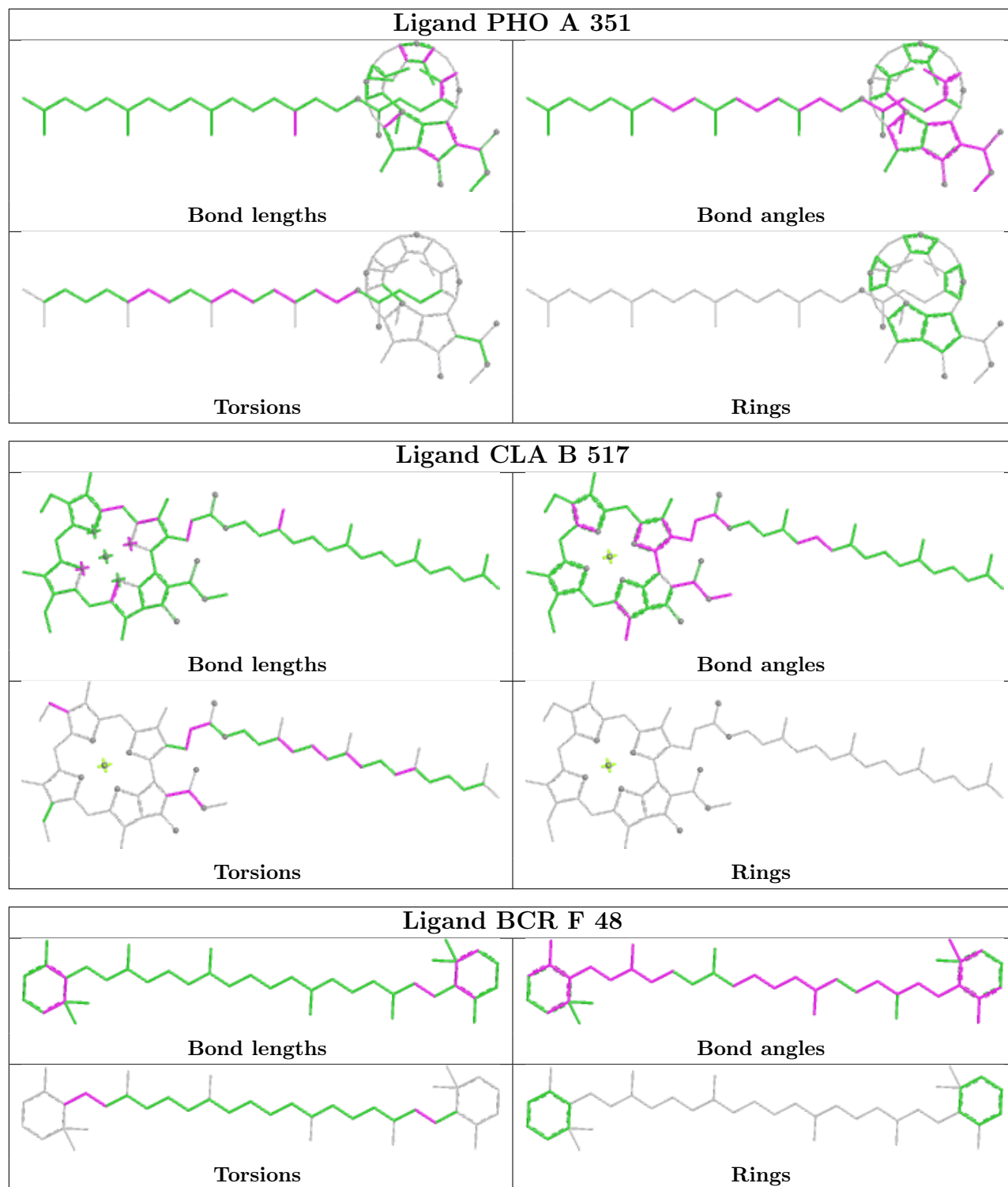
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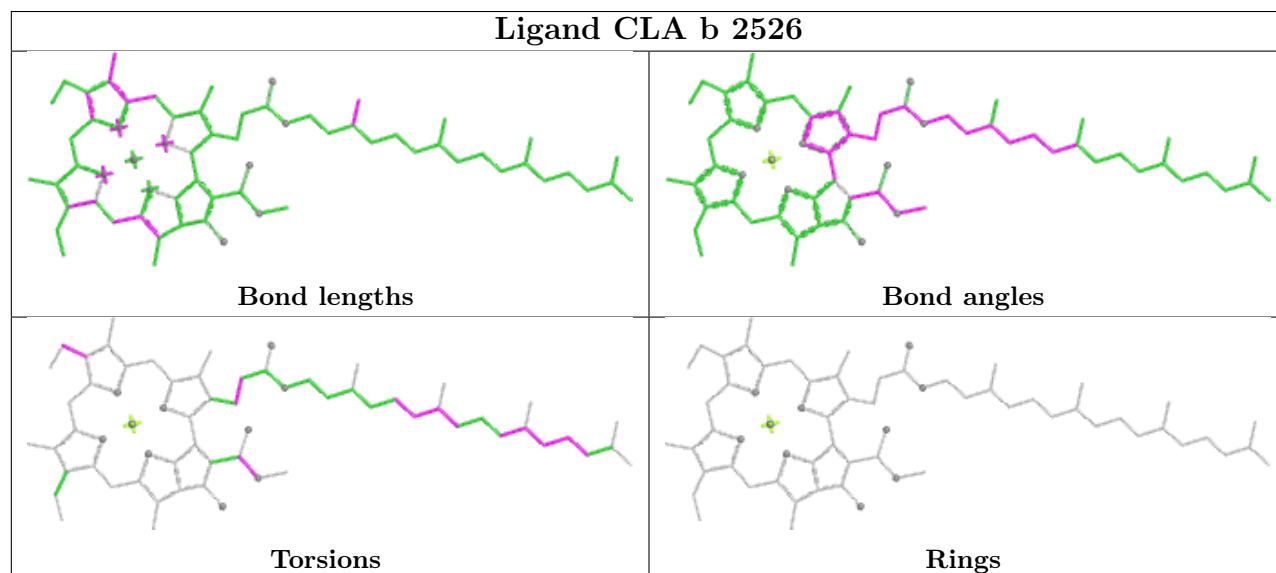
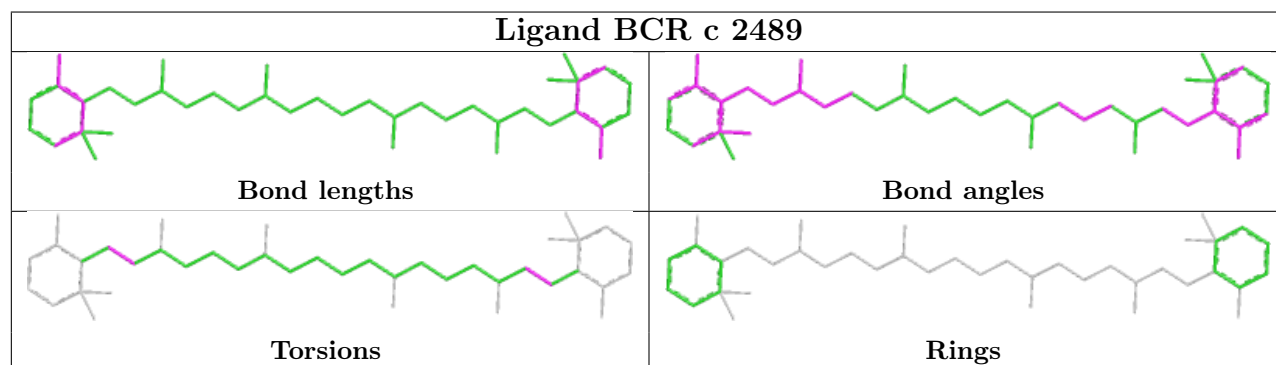
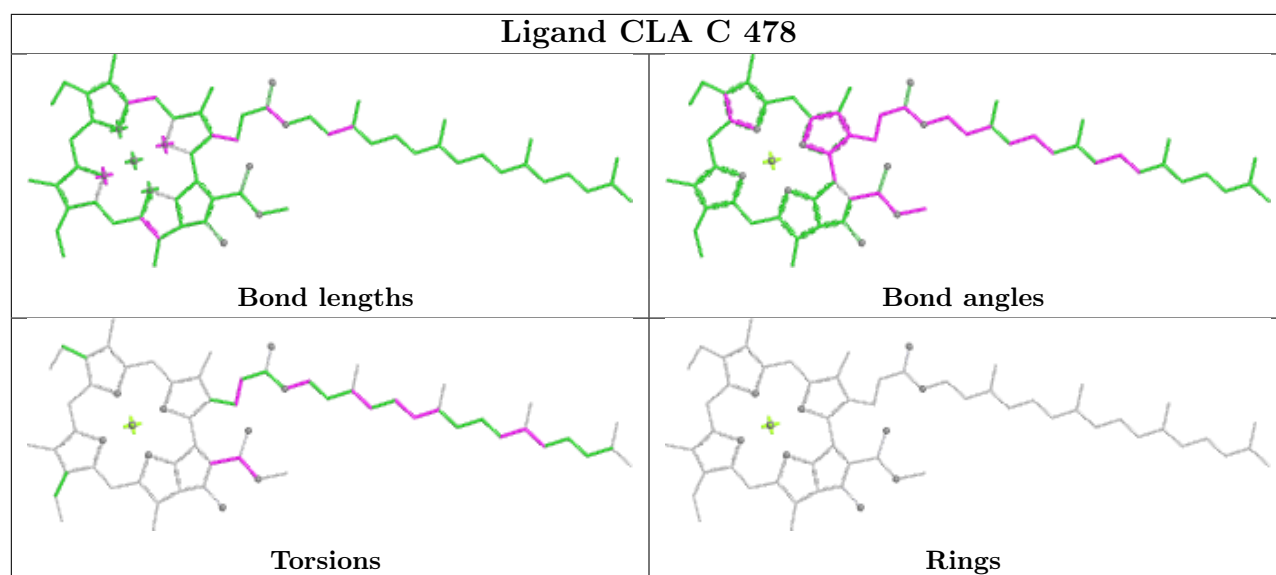




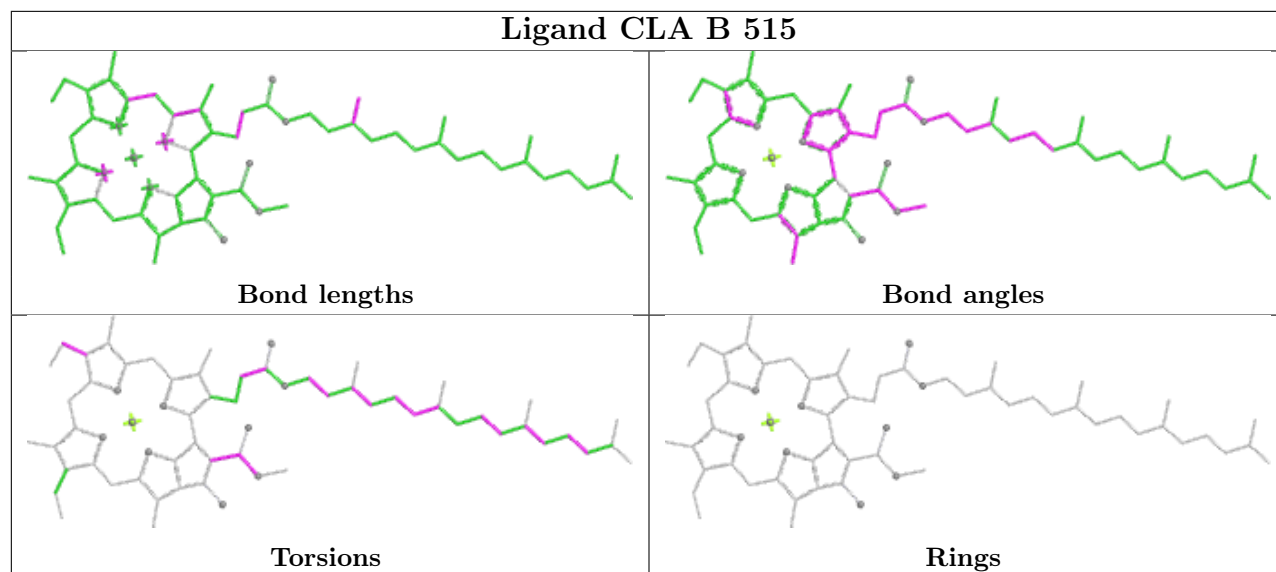




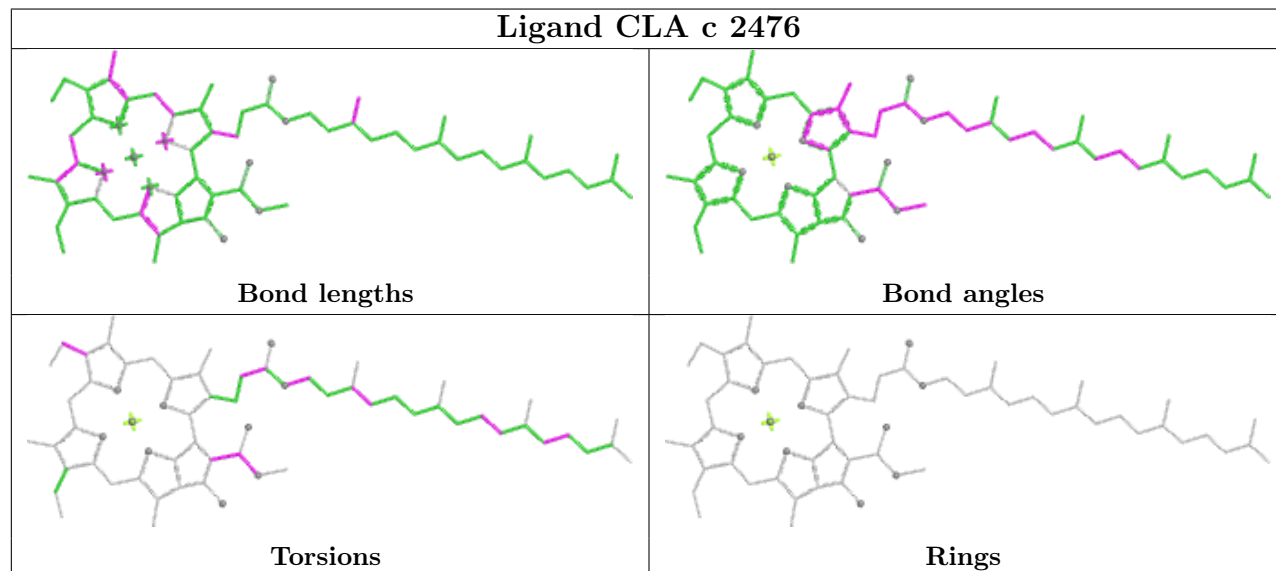




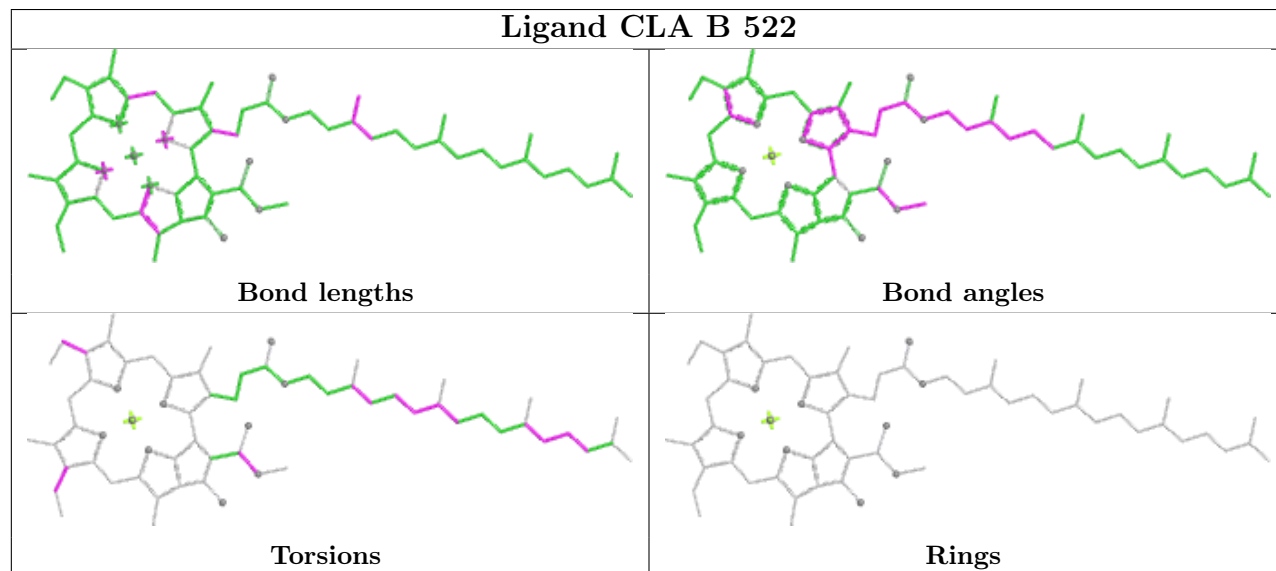
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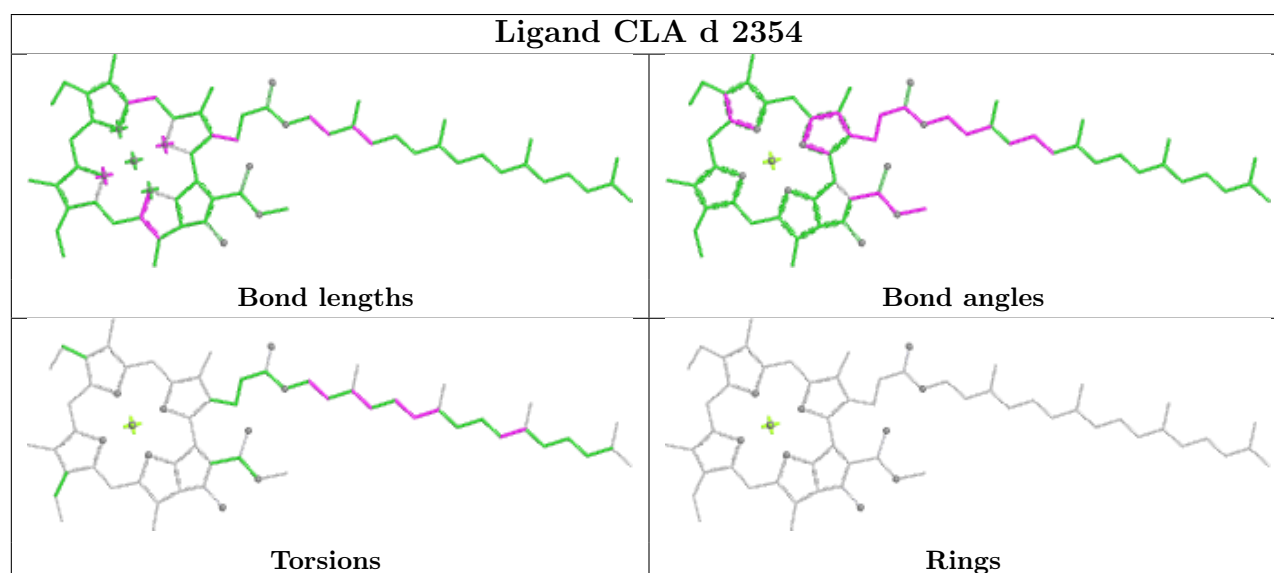
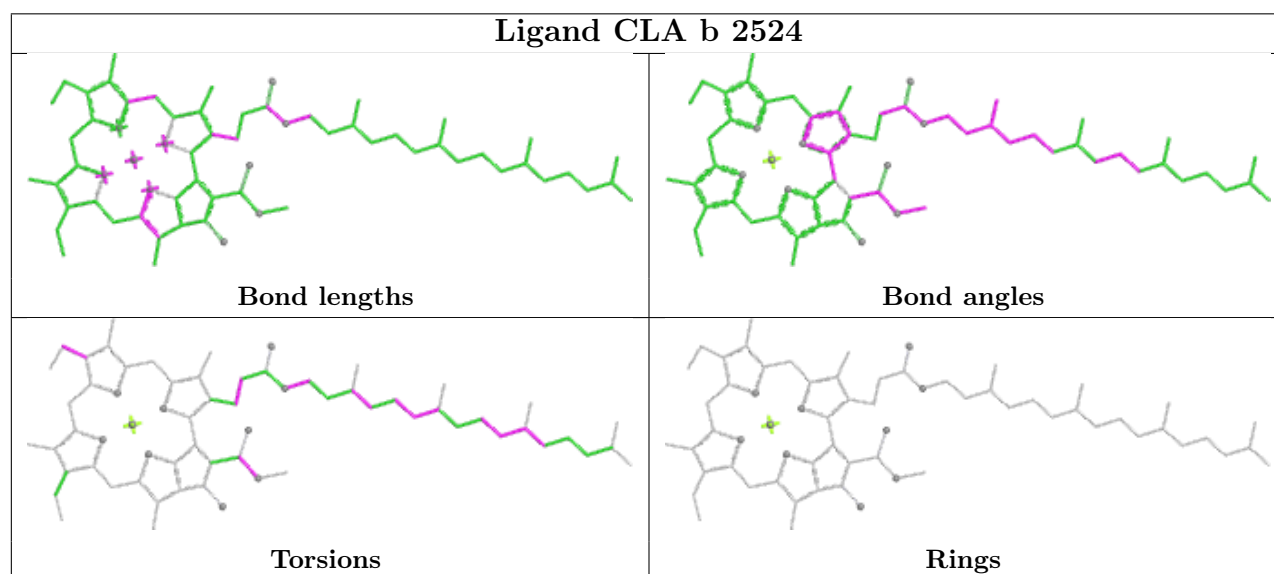
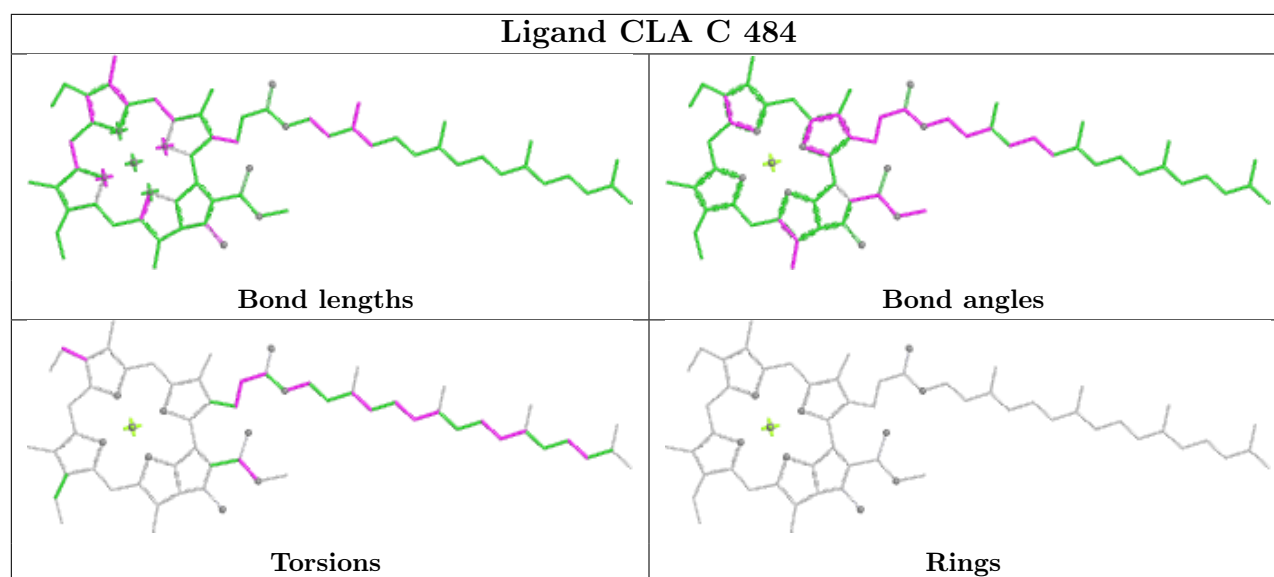


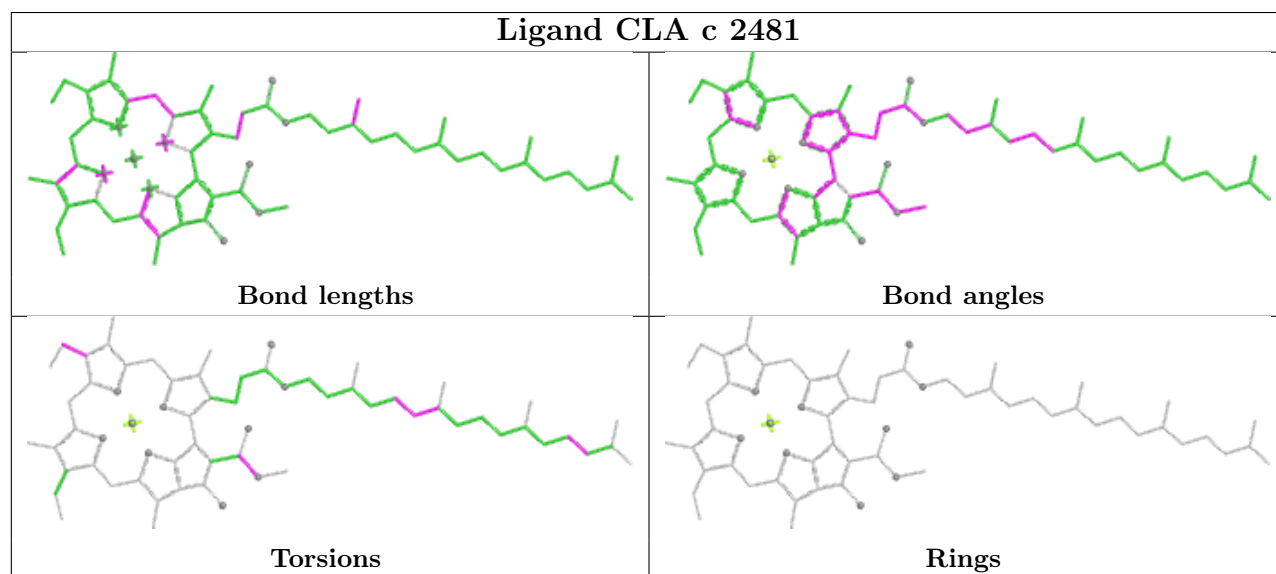
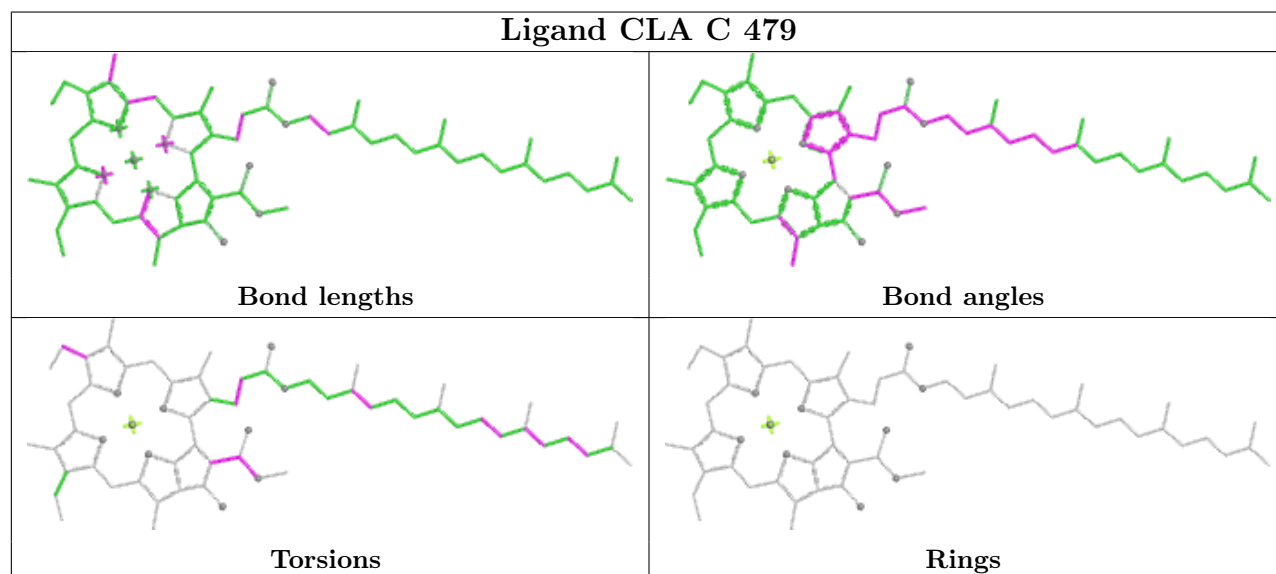
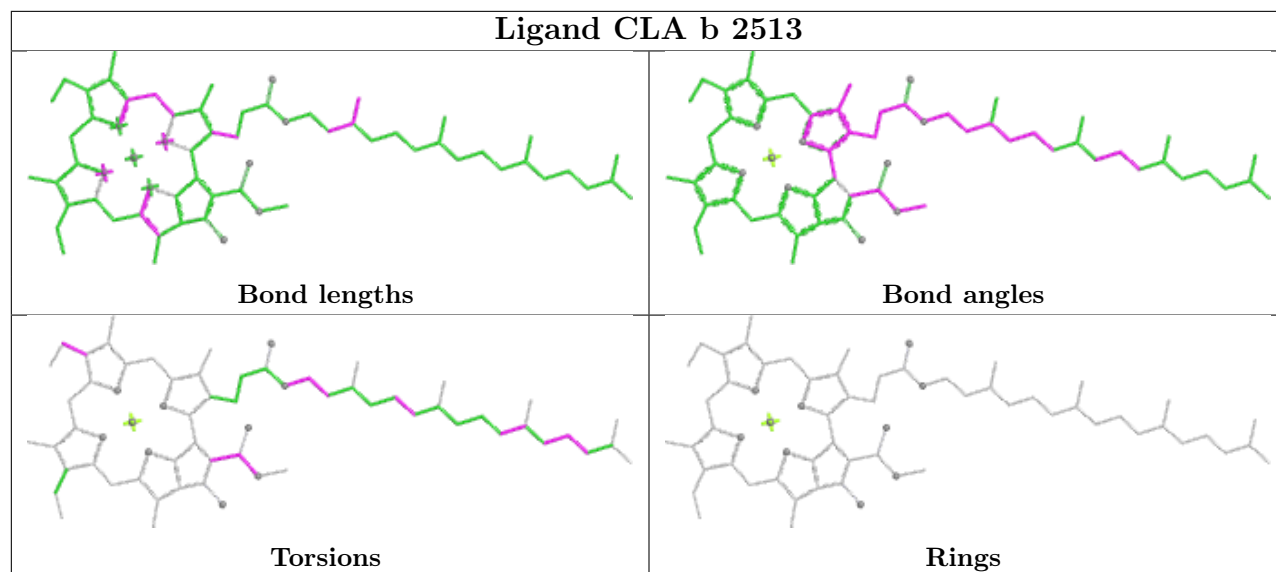
Ligand CLA c 2476

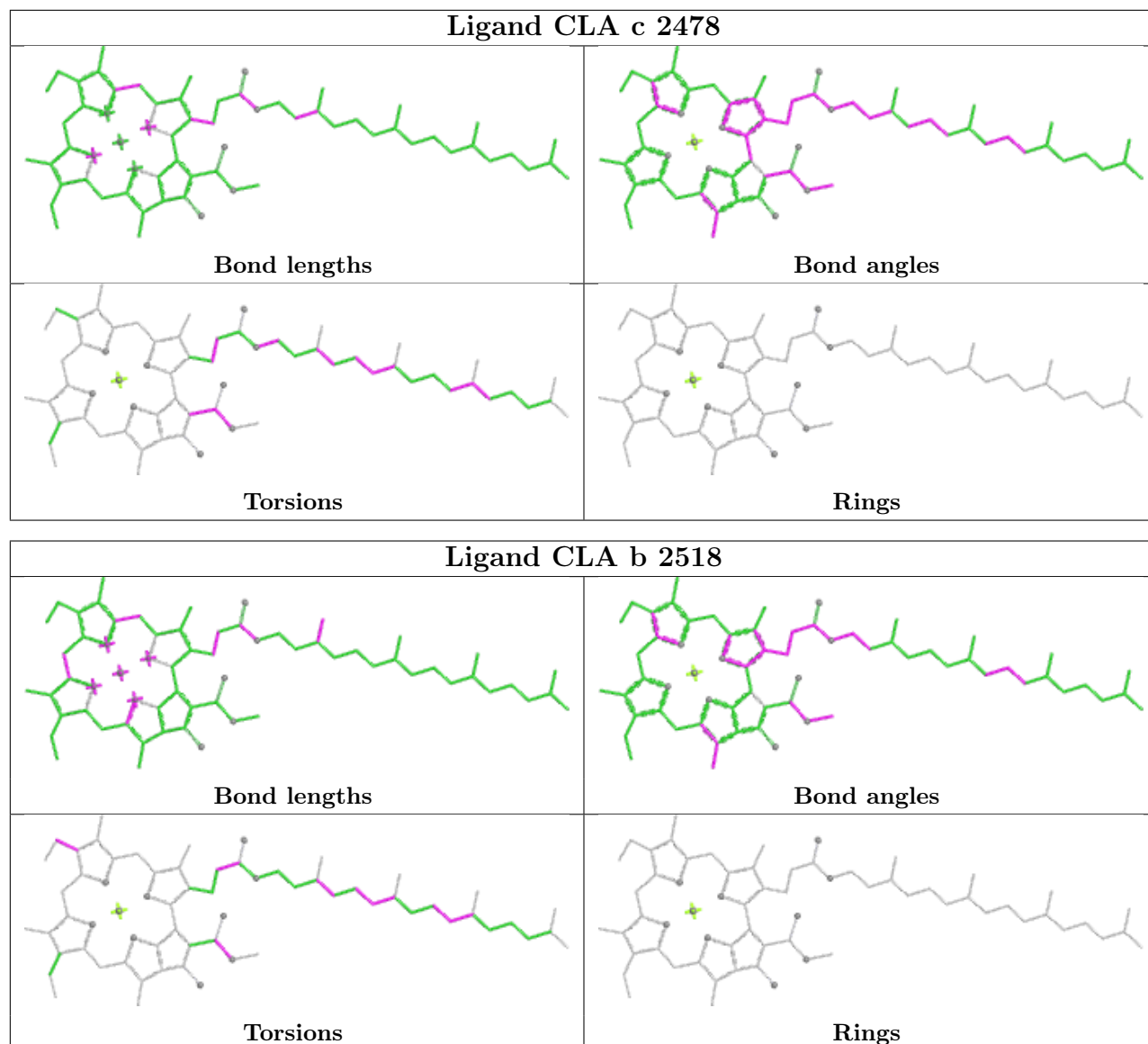


Ligand CLA B 522

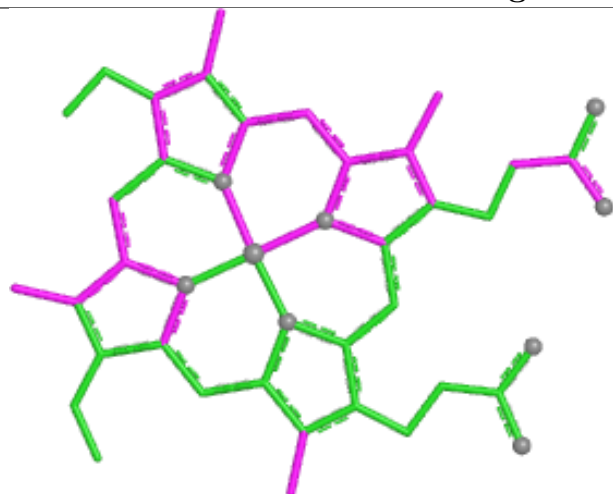




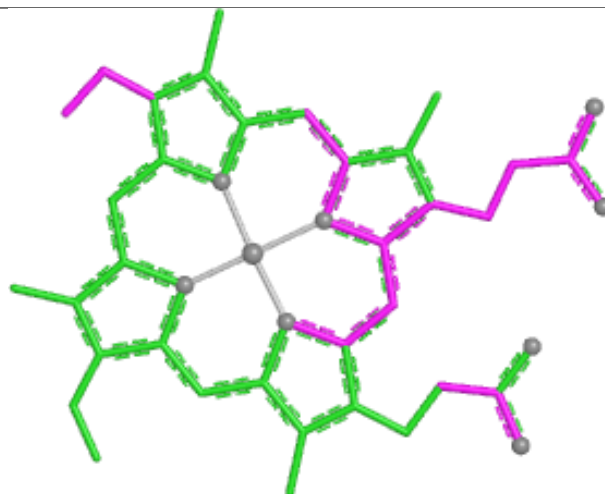




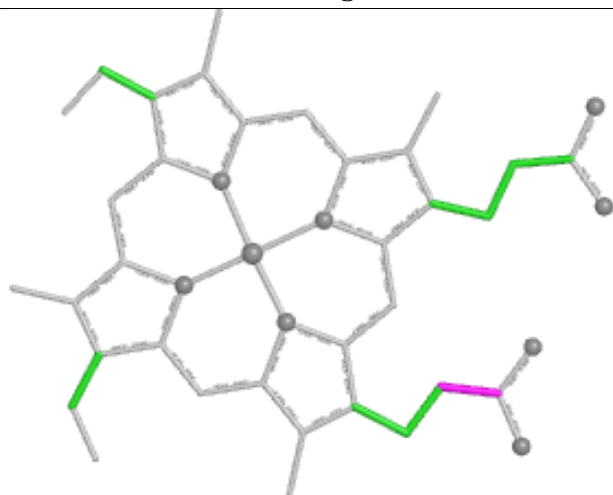
Ligand HEC e 2084



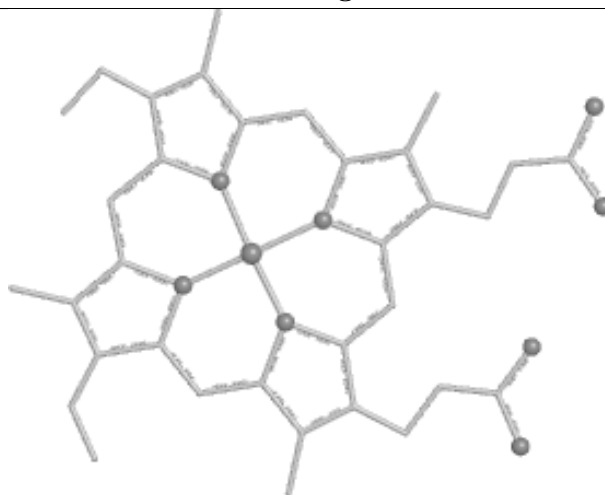
Bond lengths



Bond angles

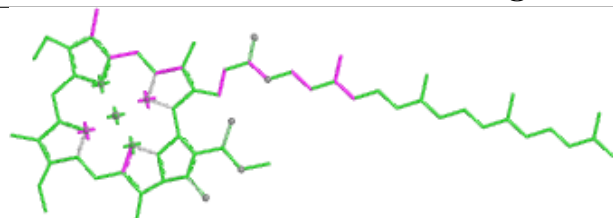


Torsions

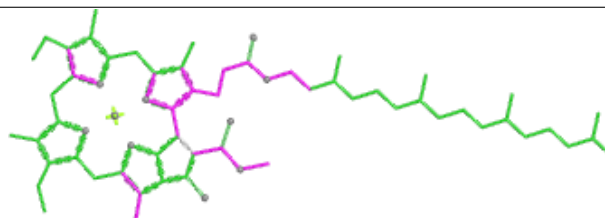


Rings

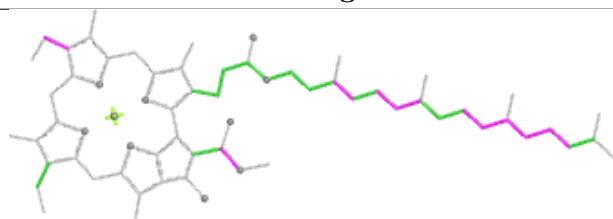
Ligand CLA b 2514



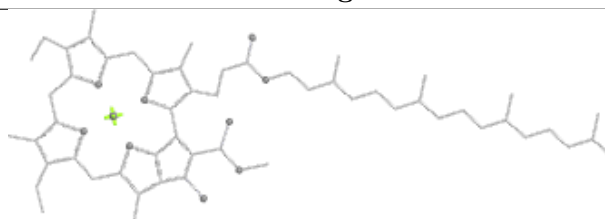
Bond lengths



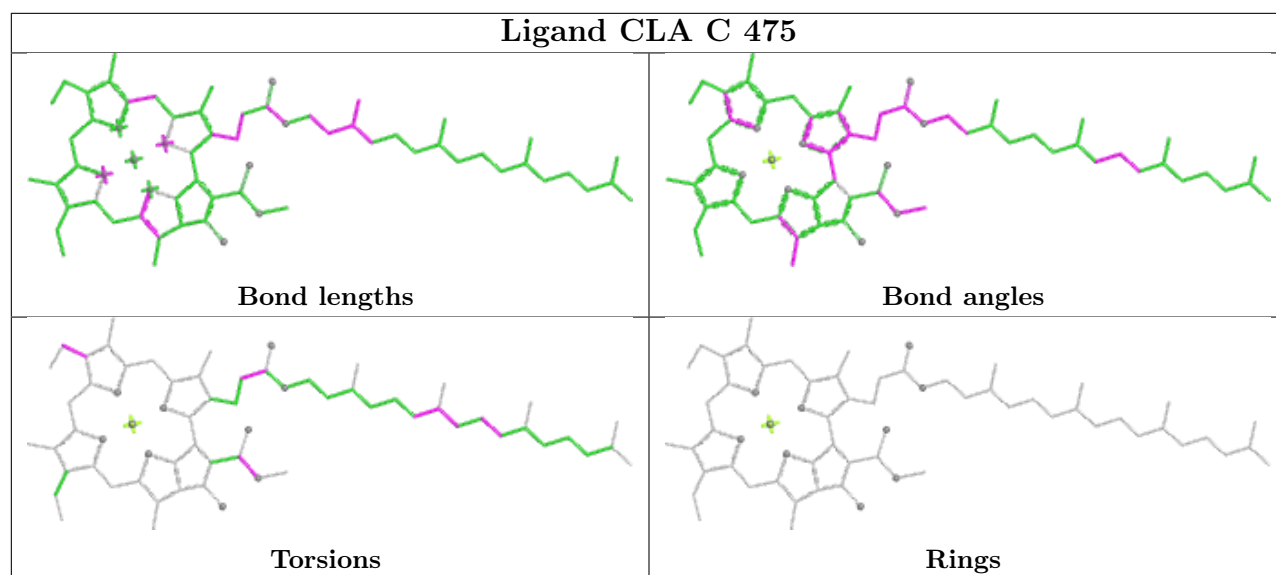
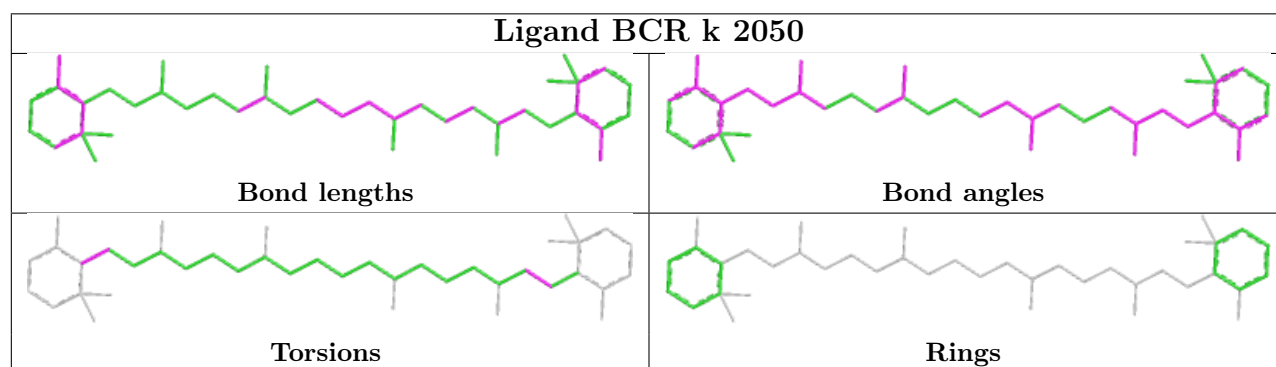
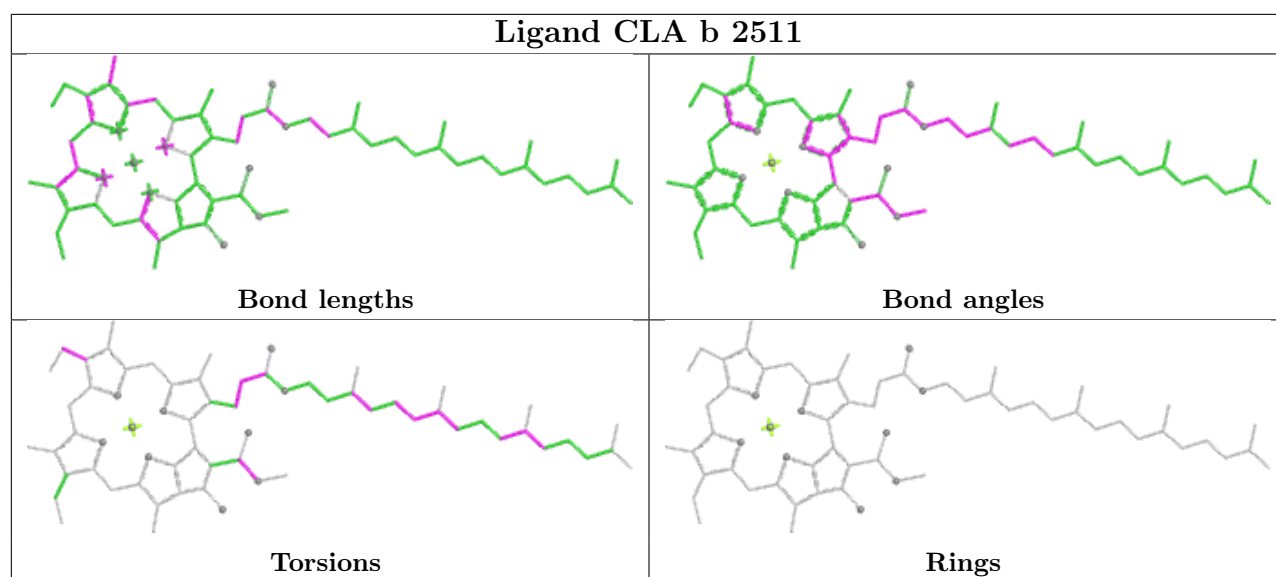
Bond angles

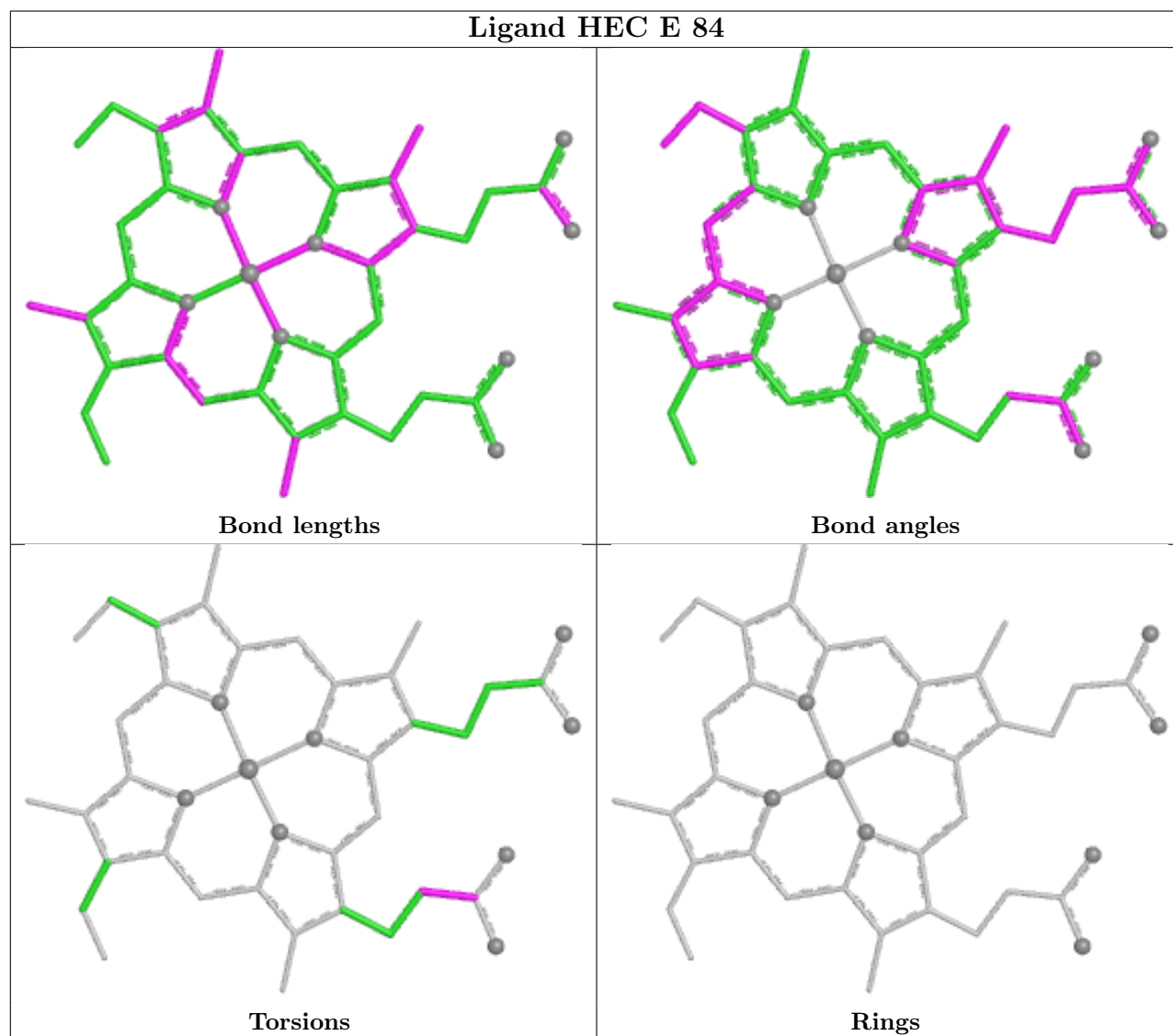
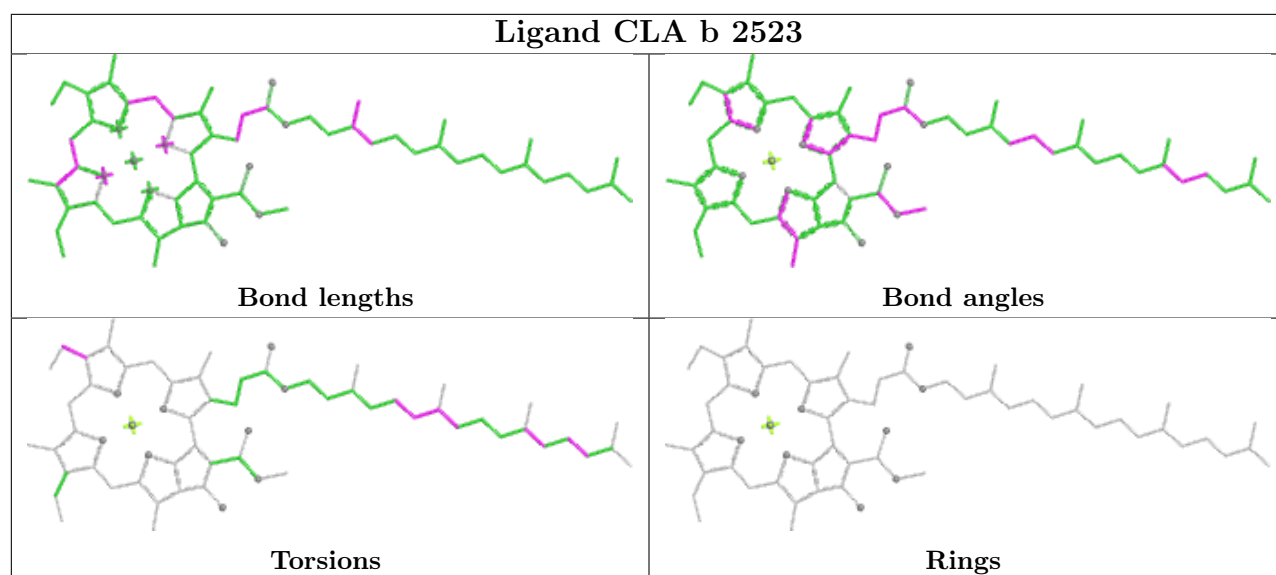


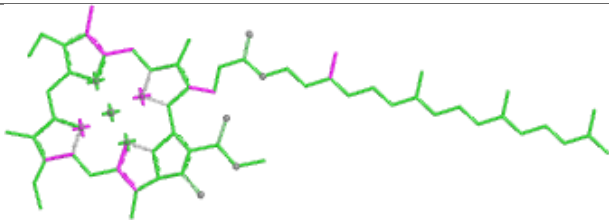
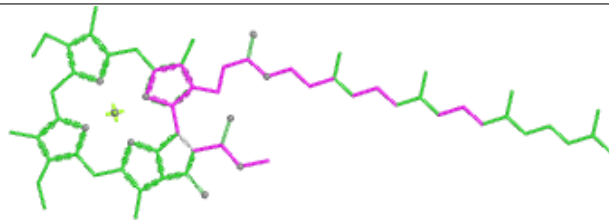
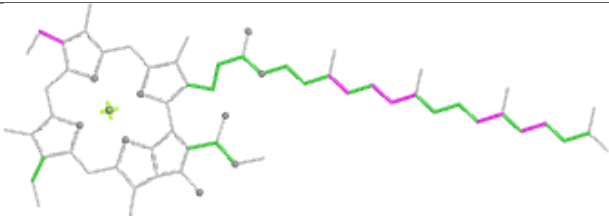
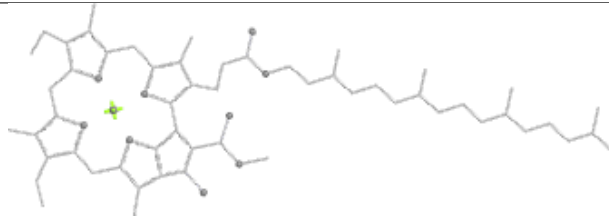
Torsions

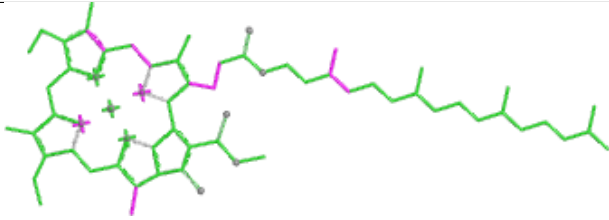
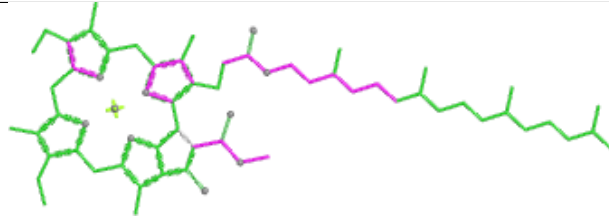
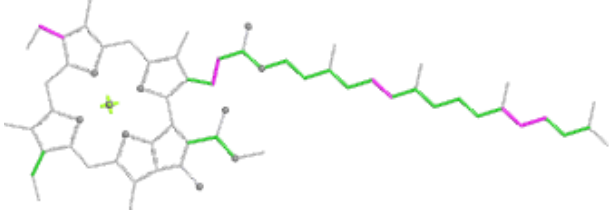
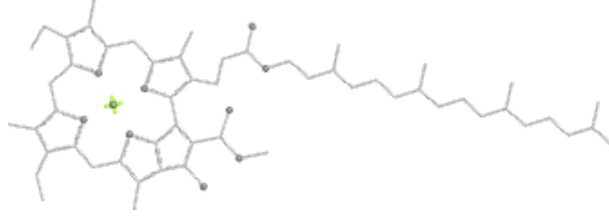


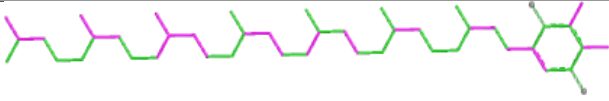
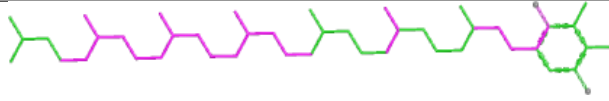
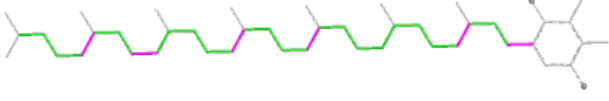
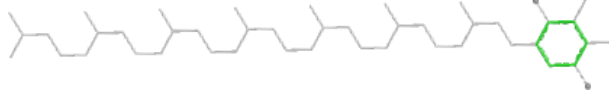
Rings

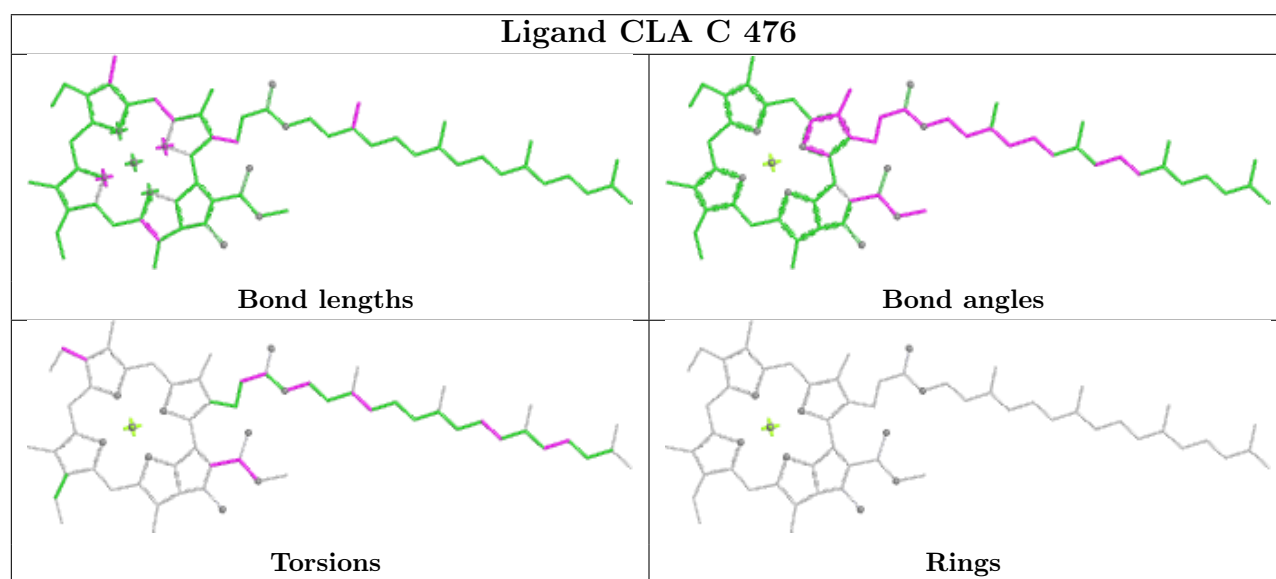
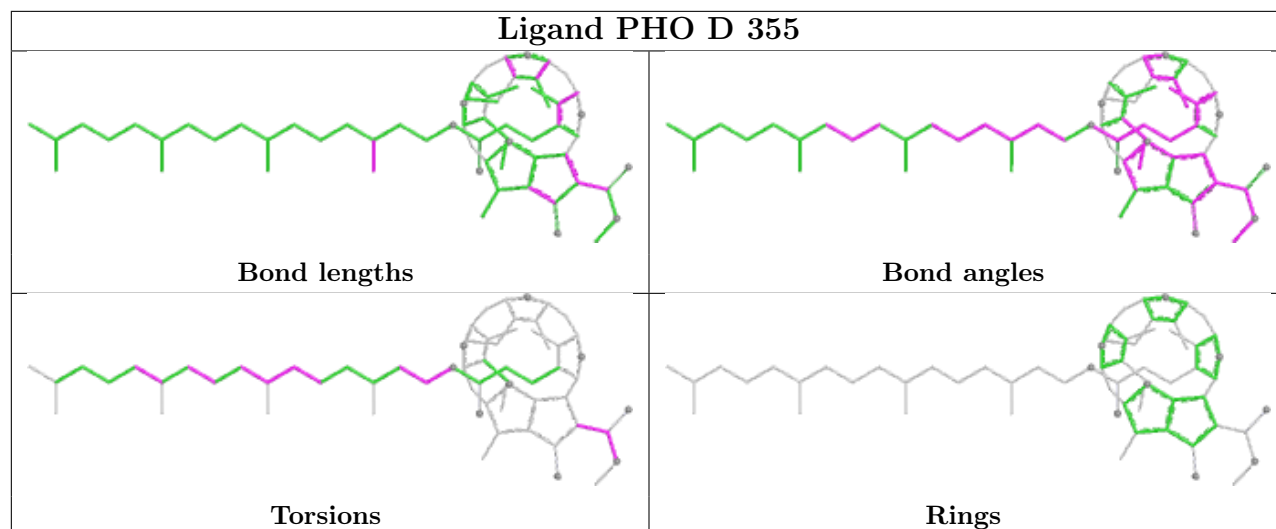




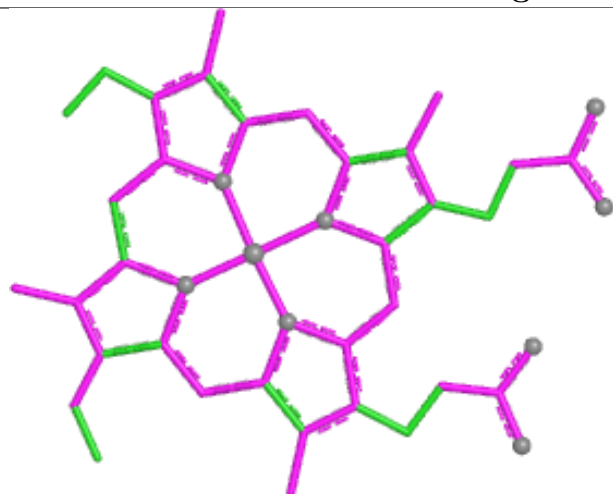
Ligand CLA a 2351	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 2357	
	
Bond lengths	Bond angles
	
Torsions	Rings

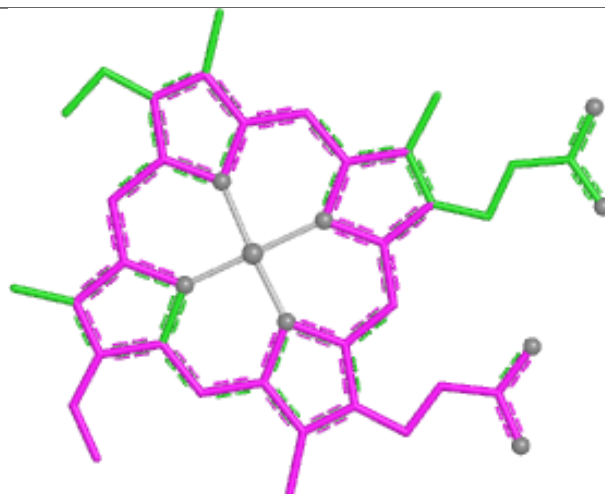
Ligand PL9 a 2352	
	
Bond lengths	Bond angles
	
Torsions	Rings



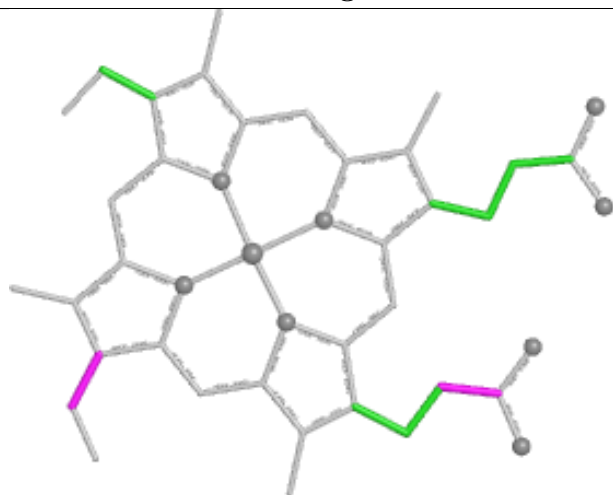
Ligand HEC V 138



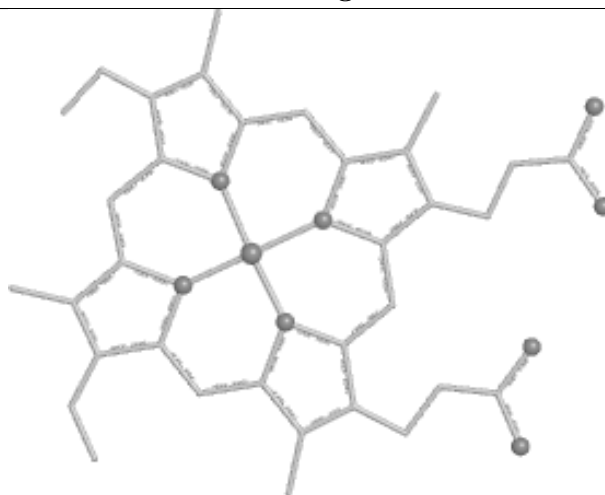
Bond lengths



Bond angles

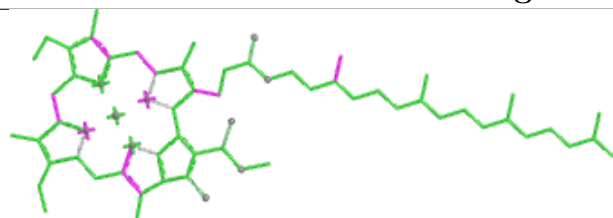


Torsions

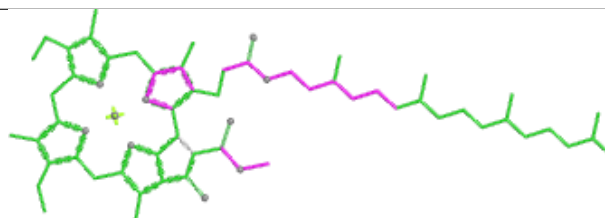


Rings

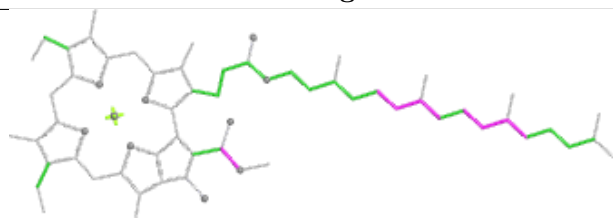
Ligand CLA B 512



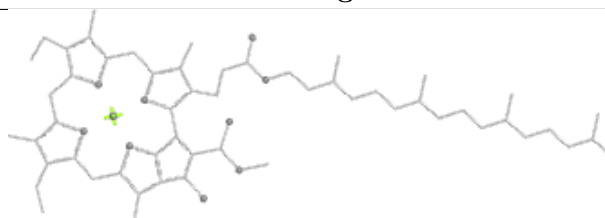
Bond lengths



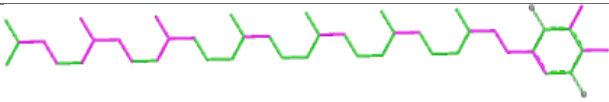
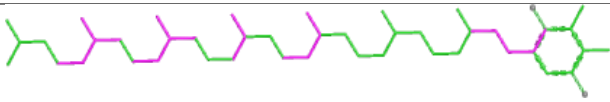
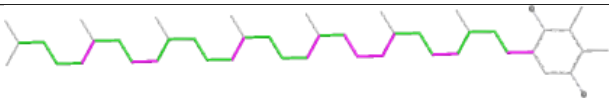
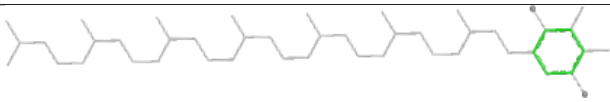
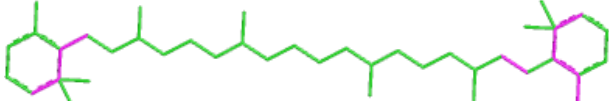
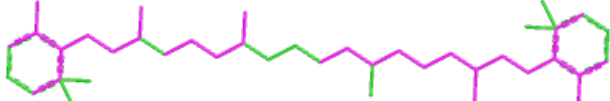
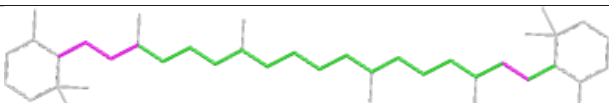
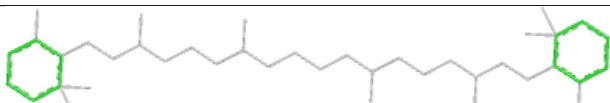
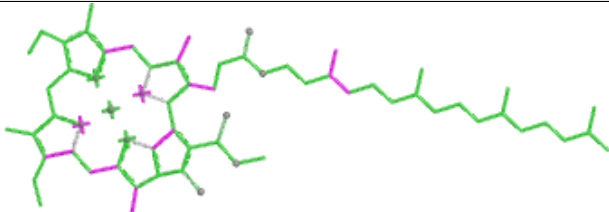
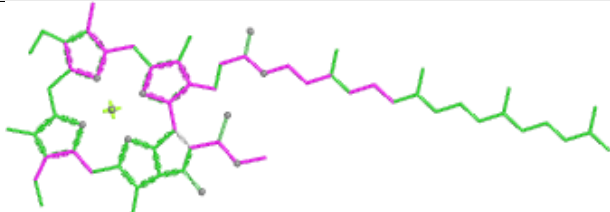
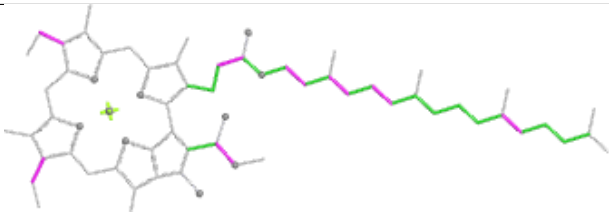
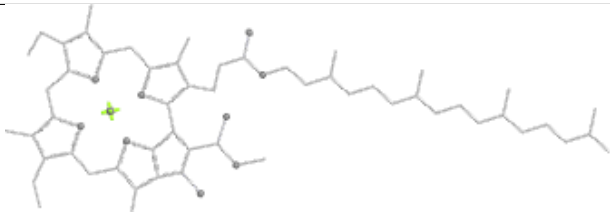
Bond angles

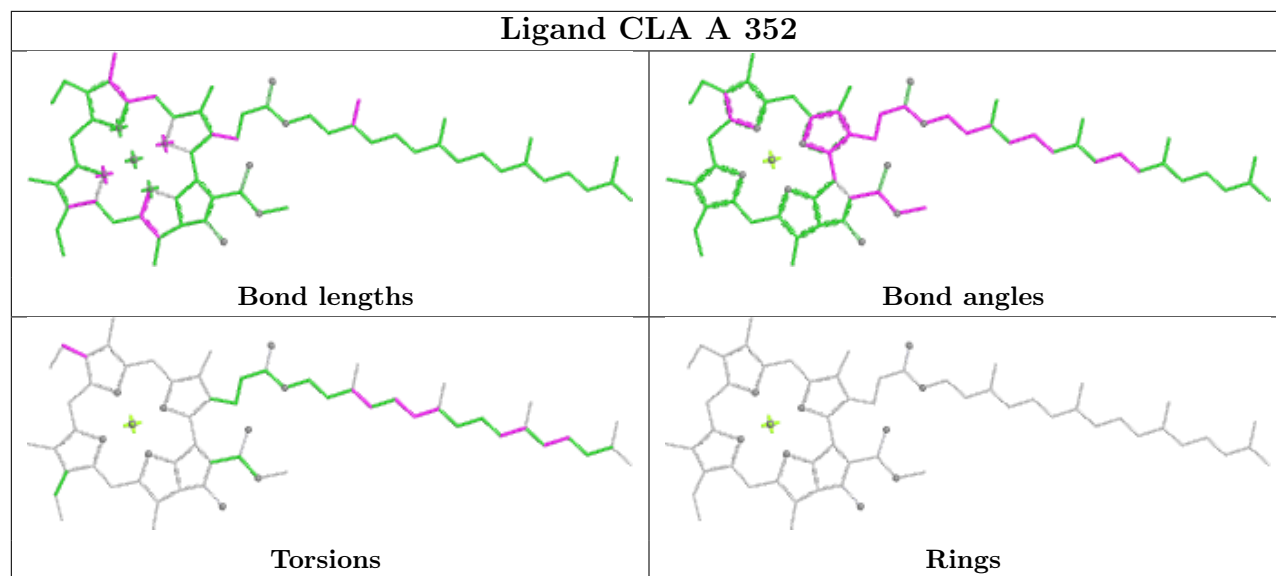


Torsions



Rings

Ligand PL9 D 357	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 529	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 2487	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	333/344 (96%)	0.59	18 (5%)	31	18	33, 60, 91, 104	0
1	a	333/344 (96%)	0.56	20 (6%)	27	16	39, 63, 92, 105	0
2	B	476/510 (93%)	0.65	35 (7%)	20	13	39, 65, 89, 105	0
2	b	476/510 (93%)	0.59	23 (4%)	35	19	39, 65, 89, 106	0
3	C	421/473 (89%)	0.63	25 (5%)	28	16	34, 69, 89, 103	0
3	c	421/473 (89%)	0.70	30 (7%)	22	14	36, 71, 90, 107	0
4	D	339/352 (96%)	0.53	24 (7%)	22	14	22, 60, 92, 106	0
4	d	339/352 (96%)	0.52	20 (5%)	28	16	31, 62, 92, 106	0
5	E	76/84 (90%)	0.61	2 (2%)	57	33	55, 76, 94, 107	0
5	e	76/84 (90%)	0.88	8 (10%)	11	8	60, 79, 96, 107	0
6	F	33/45 (73%)	0.49	2 (6%)	27	16	49, 68, 92, 107	0
6	f	33/45 (73%)	0.59	2 (6%)	27	16	49, 70, 92, 101	0
7	H	53/66 (80%)	0.41	3 (5%)	29	17	46, 73, 104, 106	0
7	h	53/66 (80%)	0.45	2 (3%)	44	24	56, 74, 106, 109	0
8	I	38/38 (100%)	1.04	7 (18%)	3	4	60, 76, 100, 102	0
8	i	38/38 (100%)	0.66	5 (13%)	7	6	59, 76, 100, 104	0
9	J	38/40 (95%)	0.47	4 (10%)	11	8	60, 79, 99, 103	0
9	j	38/40 (95%)	0.85	1 (2%)	57	33	61, 82, 98, 107	0
10	K	37/37 (100%)	0.30	0	100	100	61, 71, 95, 95	0
10	k	37/37 (100%)	0.45	0	100	100	65, 73, 96, 97	0
11	L	37/37 (100%)	0.47	1 (2%)	56	33	39, 58, 101, 104	0
11	l	37/37 (100%)	0.52	2 (5%)	31	18	34, 61, 99, 101	0
12	M	30/36 (83%)	0.11	0	100	100	45, 56, 78, 88	0
12	m	30/36 (83%)	0.26	0	100	100	44, 56, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	246/246 (100%)	0.76	17 (6%) 23 14	41, 75, 100, 110	0
13	o	246/246 (100%)	0.80	18 (7%) 21 13	46, 75, 99, 107	0
14	T	31/32 (96%)	0.23	1 (3%) 50 29	27, 54, 86, 89	0
14	t	31/32 (96%)	0.18	1 (3%) 50 29	32, 53, 90, 93	0
15	U	105/134 (78%)	0.68	9 (8%) 16 11	41, 67, 91, 104	0
15	u	105/134 (78%)	0.68	12 (11%) 10 7	46, 68, 92, 103	0
16	V	137/137 (100%)	0.36	1 (0%) 84 63	42, 66, 80, 88	0
16	v	137/137 (100%)	0.47	5 (3%) 46 25	46, 70, 85, 90	0
17	X	40/50 (80%)	0.28	1 (2%) 58 35	67, 74, 102, 109	0
17	x	40/50 (80%)	0.26	2 (5%) 34 19	67, 77, 104, 108	0
18	N	0/37	-	-	-	-
18	n	0/37	-	-	-	-
19	Z	58/62 (93%)	0.43	2 (3%) 48 27	62, 80, 93, 102	0
19	z	58/62 (93%)	0.56	3 (5%) 33 19	70, 81, 94, 106	0
All	All	5056/5520 (91%)	0.59	306 (6%) 27 16	22, 68, 95, 110	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	2006	TYR	6.9
8	I	28	PRO	6.3
4	D	242	GLU	6.2
2	B	328	GLY	6.0
3	C	47	GLY	5.8
13	O	246	ALA	5.7
1	a	2026	ASN	5.6
9	j	2040	LEU	5.3
3	C	293	ASN	5.2
8	I	25	SER	5.1
8	I	2	GLU	5.0
2	B	224	ARG	4.9
15	U	35	THR	4.9
1	A	245	THR	4.8
15	u	2052	GLY	4.7
1	A	264	SER	4.5
2	B	6	TYR	4.4
14	t	2002	GLU	4.4
5	e	2009	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
15	U	38	GLU	4.4
1	a	2226	GLU	4.3
3	c	2172	ALA	4.3
2	b	2091	TRP	4.3
9	J	39	SER	4.2
2	B	72	THR	4.1
5	e	2010	SER	4.1
13	o	2134	THR	4.0
16	v	2100	ILE	4.0
2	b	2471	ALA	4.0
4	d	2041	ALA	4.0
2	B	87	ASP	4.0
11	L	11	GLU	3.9
1	A	342	ASP	3.8
13	o	2100	GLY	3.8
9	J	40	LEU	3.8
2	B	235	GLU	3.8
13	O	34	SER	3.7
2	b	2078	TRP	3.7
7	H	21	ALA	3.7
4	D	55	VAL	3.6
3	C	366	LEU	3.6
2	b	2271	THR	3.5
13	O	218	GLU	3.5
2	b	2441	GLY	3.5
2	b	2188	ASP	3.4
2	b	2122	LEU	3.4
13	o	2034	SER	3.4
8	I	29	ALA	3.4
4	d	2053	THR	3.3
2	b	2326	ARG	3.3
1	A	263	ALA	3.3
13	O	99	ASP	3.3
15	u	2134	LYS	3.3
19	Z	30	PRO	3.3
4	d	2054	PHE	3.3
5	E	13	ILE	3.3
8	I	26	GLY	3.3
5	E	9	PHE	3.3
2	B	198	VAL	3.3
1	A	344	ALA	3.2
4	d	2262	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	74	GLY	3.2
1	A	112	TYR	3.2
3	C	294	ASN	3.2
3	c	2148	GLY	3.1
2	B	327	THR	3.1
2	b	2163	GLY	3.1
2	B	361	ALA	3.1
3	c	2288	CYS	3.1
15	U	128	TYR	3.1
17	X	19	PHE	3.1
13	o	2099	ASP	3.1
1	A	166	GLY	3.0
3	c	2064	ALA	3.0
11	l	2017	LEU	3.0
2	B	226	TYR	3.0
2	B	115	TRP	3.0
2	B	405	GLU	2.9
3	C	104	GLU	2.9
16	v	2126	LEU	2.9
4	D	105	CYS	2.9
1	a	2133	LEU	2.9
2	b	2388	SER	2.9
13	O	196	GLN	2.9
7	h	2021	ALA	2.9
13	o	2019	CYS	2.9
3	C	72	LEU	2.9
3	C	195	ASP	2.9
4	D	230	SER	2.8
15	u	2044	ASP	2.8
4	D	255	GLN	2.8
3	c	2270	ALA	2.8
1	a	2305	SER	2.8
3	C	277	GLY	2.8
2	B	89	GLY	2.8
15	U	56	ASP	2.8
2	B	326	ARG	2.8
16	v	2136	TYR	2.8
2	B	440	ASP	2.8
15	u	2126	ASP	2.8
4	d	2090	LEU	2.8
8	i	2024	LEU	2.8
3	c	2086	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	d	2213	ILE	2.7
6	F	27	VAL	2.7
15	u	2042	VAL	2.7
1	A	26	ASN	2.7
2	B	78	TRP	2.7
3	C	257	PHE	2.7
13	O	31	PRO	2.7
2	B	193	TYR	2.7
13	o	2166	SER	2.7
15	U	126	ASP	2.7
4	D	95	PRO	2.7
1	A	142	TRP	2.7
3	c	2090	PRO	2.7
3	C	270	ALA	2.7
3	C	142	GLU	2.7
1	A	167	SER	2.7
6	f	2013	PRO	2.7
8	i	2028	PRO	2.7
13	o	2101	ILE	2.7
1	a	2338	ASN	2.7
3	c	2437	PHE	2.7
3	C	446	GLY	2.6
6	F	26	ALA	2.6
4	d	2223	PHE	2.6
5	e	2018	TYR	2.6
9	J	38	SER	2.6
13	o	2052	VAL	2.6
2	B	122	LEU	2.6
3	c	2366	LEU	2.6
2	B	330	MET	2.6
19	Z	15	LEU	2.6
13	O	204	VAL	2.5
1	a	2165	GLN	2.5
4	d	2224	GLN	2.5
15	U	131	GLY	2.5
2	b	2181	VAL	2.5
13	O	19	CYS	2.5
2	B	7	ARG	2.5
7	H	61	TRP	2.5
1	a	2188	ALA	2.5
15	U	96	GLY	2.5
3	c	2158	THR	2.5

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Mol	Chain	Res	Type	RSRZ
15	U	40	VAL	2.5
2	b	2344	ALA	2.5
13	O	33	ASP	2.5
2	B	124	ARG	2.5
13	O	111	ALA	2.5
3	c	2161	LEU	2.5
4	D	225	ASP	2.5
3	C	138	GLU	2.4
4	D	234	ALA	2.4
13	O	202	ALA	2.4
15	u	2031	ALA	2.4
8	I	30	ARG	2.4
1	A	139	MET	2.4
4	D	241	GLU	2.4
3	C	320	ARG	2.4
4	d	2017	ILE	2.4
4	d	2132	ILE	2.4
3	c	2269	GLU	2.4
8	i	2030	ARG	2.4
11	l	2005	PRO	2.4
17	x	2038	ILE	2.4
4	d	2242	GLU	2.4
13	O	100	GLY	2.4
1	A	222	SER	2.4
1	a	2143	ILE	2.4
4	D	256	ILE	2.4
4	d	2222	LEU	2.4
2	B	465	GLY	2.4
3	c	2384	ILE	2.4
13	O	138	THR	2.4
4	d	2115	ALA	2.4
1	a	2301	ASN	2.3
3	C	288	CYS	2.3
13	o	2200	ASN	2.3
1	a	2082	VAL	2.3
3	c	2104	GLU	2.3
4	D	344	GLU	2.3
4	D	90	LEU	2.3
15	u	2048	GLY	2.3
5	e	2082	LEU	2.3
16	v	2046	THR	2.3
2	B	299	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	c	2183	GLY	2.3
7	H	20	VAL	2.3
1	a	2245	THR	2.3
15	u	2058	ASN	2.3
7	h	2061	TRP	2.3
1	A	261	GLN	2.3
4	D	228	GLY	2.3
19	z	2003	ILE	2.3
5	e	2055	TYR	2.3
4	d	2264	LYS	2.3
4	D	233	ARG	2.3
13	o	2176	GLN	2.2
2	B	341	LYS	2.2
5	e	2011	ASP	2.2
13	o	2121	THR	2.2
3	c	2373	ASN	2.2
5	e	2013	ILE	2.2
15	U	63	ALA	2.2
15	u	2080	VAL	2.2
15	u	2109	LEU	2.2
3	c	2292	PHE	2.2
2	b	2097	ALA	2.2
1	a	2037	MET	2.2
3	c	2315	MET	2.2
1	a	2343	LEU	2.2
19	z	2015	LEU	2.2
3	c	2096	GLY	2.2
3	c	2346	THR	2.2
13	O	136	ILE	2.2
4	D	145	ALA	2.2
4	D	106	GLN	2.2
1	A	135	TYR	2.2
4	D	138	VAL	2.2
13	o	2133	VAL	2.2
16	V	42	VAL	2.2
2	b	2129	GLY	2.2
3	C	98	GLY	2.2
4	D	232	PHE	2.2
1	A	19	ASN	2.2
3	C	260	ALA	2.2
8	i	2034	ARG	2.2
1	a	2237	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
13	o	2151	TYR	2.2
1	a	2090	GLY	2.2
2	B	90	PHE	2.2
4	D	227	GLU	2.2
4	d	2080	THR	2.2
4	d	2313	THR	2.2
2	B	14	ASN	2.2
2	B	318	ASN	2.2
1	a	2240	GLY	2.1
3	C	298	PRO	2.1
2	b	2084	THR	2.1
13	O	43	LEU	2.1
2	B	339	ALA	2.1
2	B	471	ALA	2.1
3	c	2039	ASN	2.1
4	D	208	ALA	2.1
2	b	2343	HIS	2.1
13	o	2044	CYS	2.1
3	c	2264	PHE	2.1
4	d	2081	PRO	2.1
2	b	2225	LEU	2.1
2	B	191	ASN	2.1
3	C	190	ALA	2.1
3	C	343	ARG	2.1
15	u	2040	VAL	2.1
2	B	129	GLY	2.1
2	b	2154	GLY	2.1
3	c	2402	GLY	2.1
3	c	2364	PRO	2.1
3	C	401	LEU	2.1
4	D	267	LEU	2.1
13	o	2074	GLU	2.1
2	b	2072	THR	2.1
2	B	303	SER	2.1
3	c	2229	ASN	2.1
4	D	295	SER	2.1
4	D	154	VAL	2.1
4	d	2136	VAL	2.1
8	i	2012	VAL	2.1
3	C	251	HIS	2.1
1	a	2254	TYR	2.1
1	A	244	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	2220	THR	2.1
2	b	2153	PHE	2.1
2	B	396	GLY	2.1
19	z	2030	PRO	2.1
13	o	2136	ILE	2.1
3	c	2168	LEU	2.1
1	A	138	GLY	2.0
13	o	2028	GLY	2.0
2	B	380	ASP	2.0
2	b	2128	THR	2.0
13	O	193	THR	2.0
13	o	2224	ASP	2.0
3	C	456	GLU	2.0
17	x	2048	ARG	2.0
3	c	2224	ILE	2.0
3	C	179	ALA	2.0
4	d	2098	GLN	2.0
9	J	35	GLY	2.0
14	T	27	PRO	2.0
1	a	2089	ILE	2.0
3	C	265	ILE	2.0
2	b	2046	ASP	2.0
1	a	2023	SER	2.0
2	B	215	PHE	2.0
3	c	2140	LEU	2.0
3	c	2375	LEU	2.0
3	c	2433	LEU	2.0
4	d	2212	ALA	2.0
4	D	152	VAL	2.0
6	f	2039	MET	2.0
13	O	44	CYS	2.0
5	e	2021	ILE	2.0
15	u	2049	THR	2.0
8	I	37	LEU	2.0
16	v	2021	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	487	65/65	0.49	0.24	87,101,114,118	0
23	CLA	c	2487	65/65	0.53	0.22	88,101,114,118	0
27	BCR	c	2489	40/40	0.53	0.20	85,90,100,100	0
26	LMT	d	2359	35/35	0.55	0.26	73,82,91,92	0
27	BCR	j	2053	40/40	0.56	0.14	71,87,100,101	0
27	BCR	k	2050	40/40	0.57	0.25	80,85,97,101	0
27	BCR	B	529	40/40	0.59	0.23	76,93,105,106	0
27	BCR	J	53	40/40	0.63	0.15	70,88,100,100	0
27	BCR	K	50	40/40	0.65	0.22	79,85,96,101	0
27	BCR	C	489	40/40	0.66	0.24	85,90,100,100	0
25	PL9	D	357	45/55	0.66	0.24	71,80,86,88	0
25	PL9	d	2358	45/55	0.67	0.22	70,80,87,89	0
23	CLA	c	2475	65/65	0.67	0.19	66,80,97,102	0
27	BCR	b	2528	40/40	0.67	0.23	77,92,105,106	0
23	CLA	B	527	65/65	0.68	0.16	84,89,106,109	0
23	CLA	b	2526	65/65	0.70	0.16	82,89,106,110	0
23	CLA	C	482	65/65	0.71	0.17	71,80,97,98	0
23	CLA	c	2486	65/65	0.71	0.22	79,84,92,94	0
27	BCR	d	2360	40/40	0.72	0.21	67,79,91,93	0
23	CLA	d	2357	65/65	0.72	0.21	68,77,91,95	0
23	CLA	c	2484	65/65	0.72	0.17	77,87,101,102	0
27	BCR	c	2488	40/40	0.73	0.23	76,84,93,96	0
23	CLA	b	2511	65/65	0.75	0.20	58,81,92,97	0
23	CLA	B	511	65/65	0.75	0.21	58,81,92,97	0
25	PL9	a	2352	45/55	0.75	0.15	77,85,90,91	0
25	PL9	A	353	45/55	0.76	0.16	77,86,91,92	0
23	CLA	B	523	65/65	0.76	0.18	60,64,94,109	0
23	CLA	C	484	65/65	0.76	0.16	76,87,101,102	0
26	LMT	B	526	35/35	0.77	0.21	72,82,90,91	0
23	CLA	c	2482	65/65	0.77	0.15	72,81,97,98	0
23	CLA	C	477	65/65	0.77	0.17	71,79,97,100	0
23	CLA	b	2525	65/65	0.77	0.17	73,80,89,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	BCT	d	2353	4/4	0.78	0.13	66,68,69,69	0
21	BCT	A	346	4/4	0.78	0.14	70,70,71,74	0
23	CLA	c	2480	65/65	0.78	0.17	65,80,82,87	0
23	CLA	c	2474	65/65	0.79	0.17	70,76,88,89	0
23	CLA	b	2517	65/65	0.79	0.17	64,71,80,89	0
23	CLA	B	520	65/65	0.79	0.15	63,68,79,79	0
23	CLA	A	352	65/65	0.79	0.18	48,65,101,102	0
23	CLA	b	2523	65/65	0.80	0.16	59,64,94,108	0
23	CLA	c	2477	65/65	0.80	0.16	73,79,98,101	0
23	CLA	B	514	65/65	0.80	0.17	60,67,79,82	0
27	BCR	B	528	40/40	0.80	0.19	63,79,85,87	0
23	CLA	C	483	65/65	0.80	0.14	67,73,101,106	0
23	CLA	c	2483	65/65	0.80	0.16	68,74,100,106	0
23	CLA	B	525	65/65	0.80	0.16	72,80,89,92	0
23	CLA	C	474	65/65	0.81	0.17	69,76,87,89	0
23	CLA	b	2513	65/65	0.81	0.18	45,57,102,106	0
23	CLA	C	485	65/65	0.81	0.18	64,75,91,95	0
27	BCR	b	2527	40/40	0.81	0.15	64,78,84,86	0
23	CLA	B	519	65/65	0.81	0.15	58,67,90,91	0
23	CLA	a	2349	65/65	0.82	0.14	36,54,93,95	0
23	CLA	c	2479	65/65	0.82	0.16	57,76,80,84	0
23	CLA	a	2351	65/65	0.82	0.16	50,66,101,102	0
23	CLA	c	2481	65/65	0.82	0.15	55,60,85,89	0
23	CLA	b	2520	65/65	0.82	0.14	61,68,78,79	0
23	CLA	B	516	65/65	0.82	0.16	44,55,92,93	0
23	CLA	c	2476	65/65	0.82	0.16	50,64,75,78	0
23	CLA	B	515	65/65	0.83	0.16	45,66,84,87	0
23	CLA	c	2485	65/65	0.83	0.17	61,75,90,94	0
23	CLA	b	2514	65/65	0.83	0.17	59,67,79,82	0
23	CLA	b	2516	65/65	0.83	0.14	42,54,93,94	0
21	BCT	a	2346	4/4	0.83	0.14	71,72,73,76	0
24	PHO	a	2350	64/64	0.83	0.18	56,66,81,82	0
23	CLA	D	356	65/65	0.83	0.15	69,77,90,95	0
23	CLA	b	2521	65/65	0.83	0.18	67,71,80,82	0
27	BCR	C	488	40/40	0.84	0.23	75,83,92,95	0
23	CLA	C	486	65/65	0.84	0.18	78,84,91,95	0
27	BCR	F	48	40/40	0.84	0.15	66,80,91,92	0
23	CLA	C	475	65/65	0.84	0.17	66,80,97,103	0
24	PHO	D	355	64/64	0.84	0.16	62,69,103,111	0
23	CLA	B	524	65/65	0.84	0.17	56,68,75,88	0
23	CLA	B	521	65/65	0.85	0.16	67,72,80,81	0
23	CLA	b	2522	65/65	0.85	0.15	69,75,87,88	0

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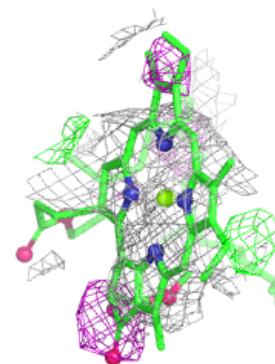
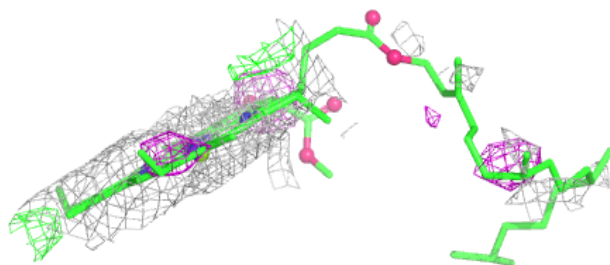
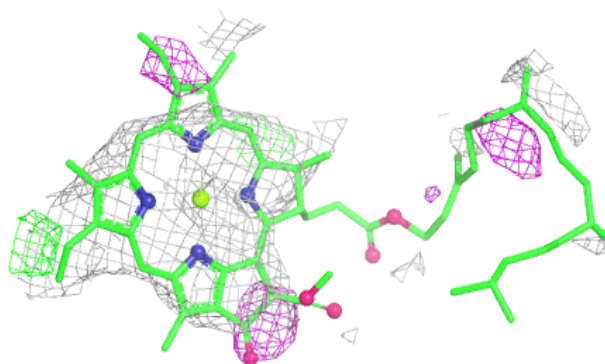
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	C	476	65/65	0.85	0.15	49,62,75,78	0
24	PHO	d	2356	64/64	0.85	0.16	62,70,103,111	0
28	HEC	e	2084	43/43	0.85	0.23	75,79,100,108	0
23	CLA	b	2519	65/65	0.86	0.13	60,66,90,91	0
23	CLA	B	512	65/65	0.86	0.13	37,50,63,67	0
23	CLA	C	481	65/65	0.86	0.16	54,60,84,88	0
23	CLA	B	522	65/65	0.86	0.16	71,75,87,88	0
23	CLA	B	518	65/65	0.86	0.15	51,61,86,89	0
23	CLA	c	2478	65/65	0.87	0.19	55,66,87,92	0
23	CLA	C	480	65/65	0.87	0.16	64,79,82,87	0
23	CLA	B	517	65/65	0.87	0.16	65,71,79,89	0
23	CLA	b	2515	65/65	0.87	0.15	43,66,84,87	0
23	CLA	A	350	65/65	0.87	0.15	36,52,92,95	0
23	CLA	C	478	65/65	0.87	0.18	55,65,87,91	0
23	CLA	b	2524	65/65	0.87	0.17	56,68,76,89	0
23	CLA	b	2518	65/65	0.88	0.18	53,60,86,88	0
23	CLA	b	2512	65/65	0.88	0.13	34,50,63,66	0
23	CLA	A	348	65/65	0.88	0.14	44,50,65,70	0
23	CLA	d	2354	65/65	0.88	0.12	40,47,75,80	0
23	CLA	B	513	65/65	0.88	0.16	46,57,102,106	0
24	PHO	A	351	64/64	0.88	0.15	55,65,80,82	0
23	CLA	d	2355	65/65	0.89	0.14	19,32,75,86	0
23	CLA	a	2348	65/65	0.89	0.14	44,50,65,69	0
23	CLA	D	354	65/65	0.89	0.14	42,46,76,81	0
23	CLA	C	479	65/65	0.90	0.14	57,76,80,83	0
21	BCT	D	353	4/4	0.90	0.12	66,66,69,69	0
23	CLA	A	349	65/65	0.91	0.12	19,31,76,86	0
28	HEC	E	84	43/43	0.93	0.18	64,79,100,108	0
28	HEC	V	138	43/43	0.94	0.17	44,49,56,57	0
22	OEC	A	347	9/9	0.94	0.06	66,69,73,74	0
28	HEC	v	2138	43/43	0.94	0.12	40,50,55,57	0
22	OEC	a	2347	9/9	0.95	0.06	68,70,74,75	0
20	FE	a	2345	1/1	0.98	0.03	67,67,67,67	0
20	FE	A	345	1/1	0.99	0.04	58,58,58,58	0

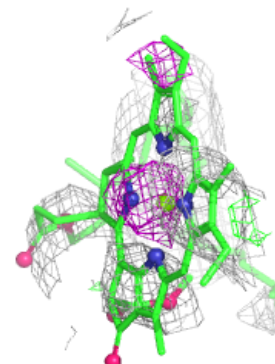
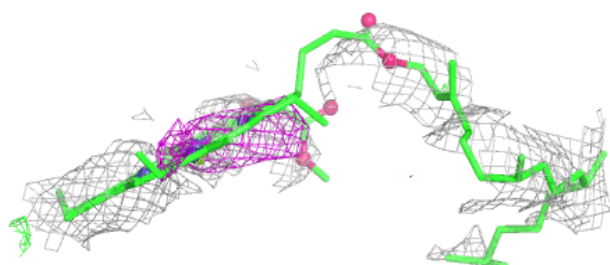
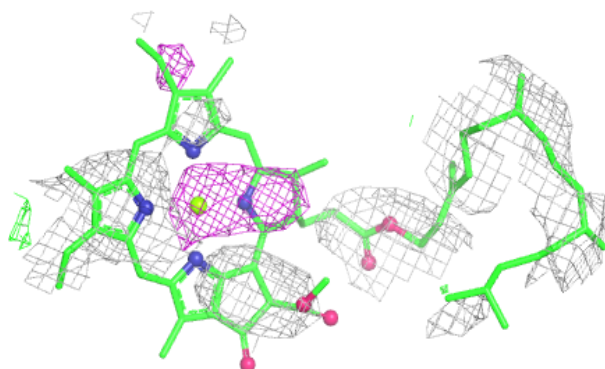
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLA C 487:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

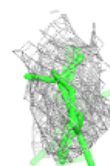
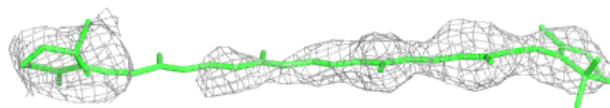
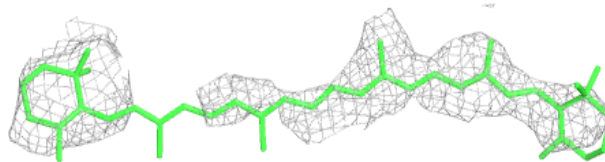
**Electron density around CLA c 2487:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

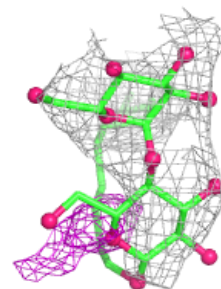
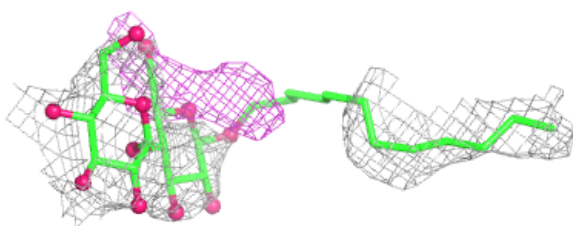
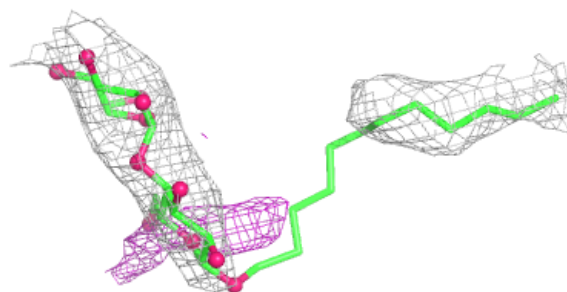


Electron density around BCR c 2489:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

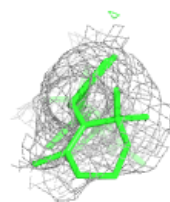
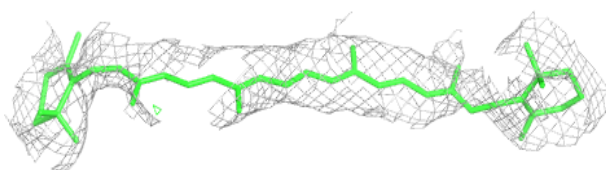
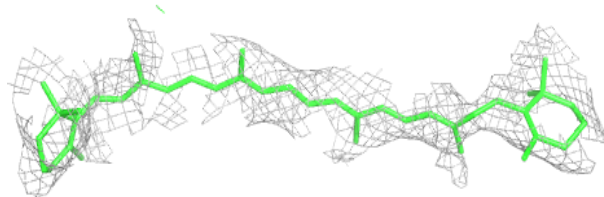
**Electron density around LMT d 2359:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

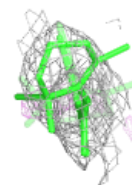
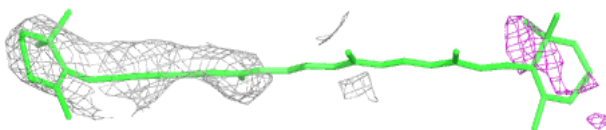
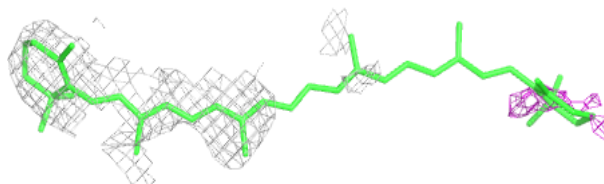


Electron density around BCR j 2053:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

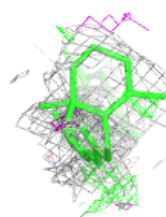
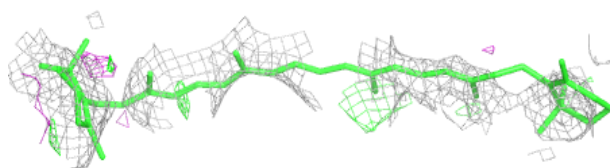
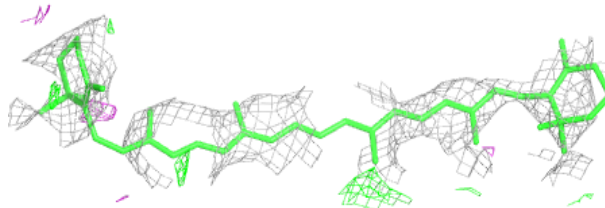
**Electron density around BCR k 2050:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

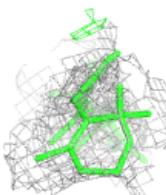
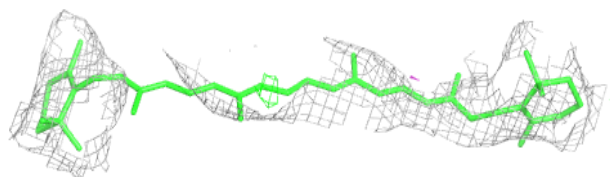
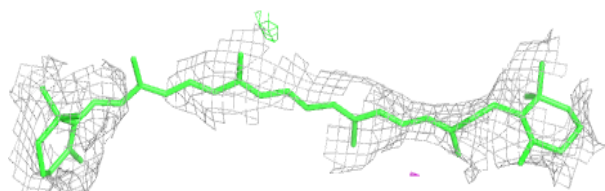


Electron density around BCR B 529:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

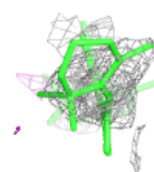
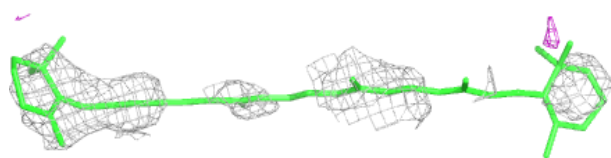
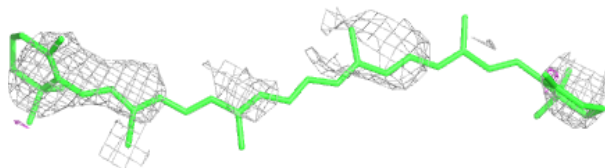
**Electron density around BCR J 53:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

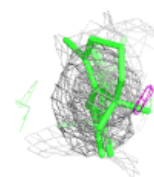
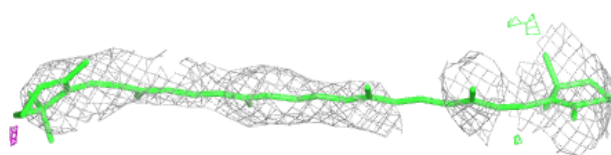
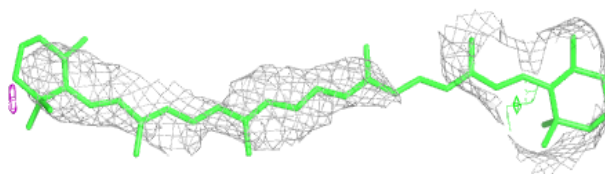


Electron density around BCR K 50:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

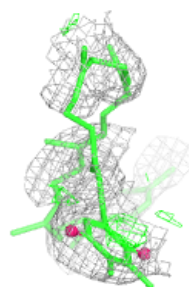
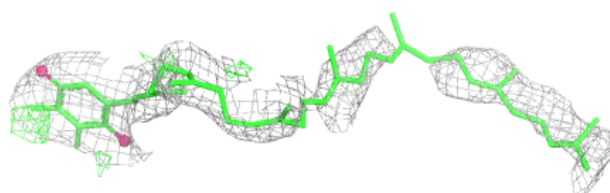
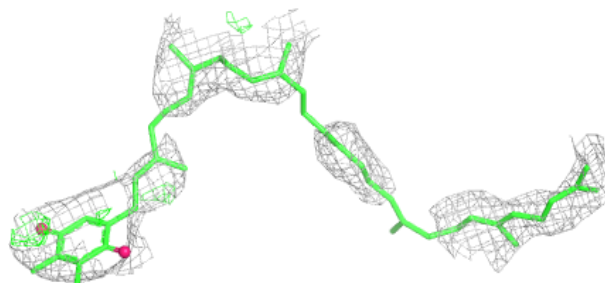
**Electron density around BCR C 489:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

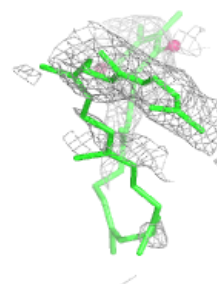
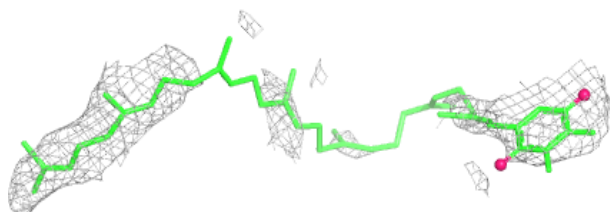


Electron density around PL9 D 357:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

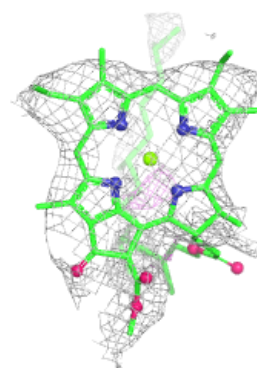
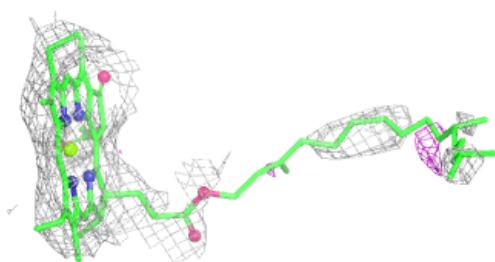
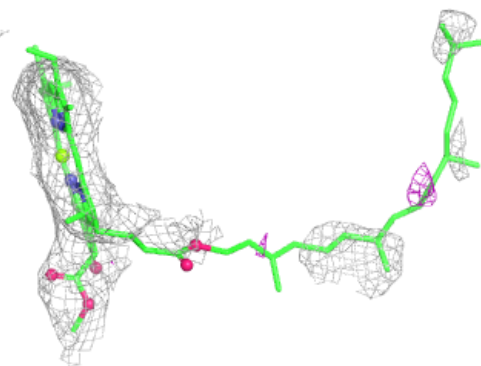
**Electron density around PL9 d 2358:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

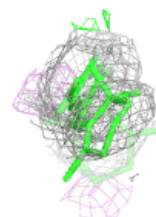
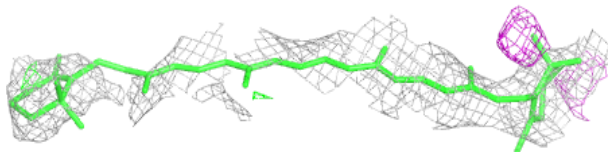
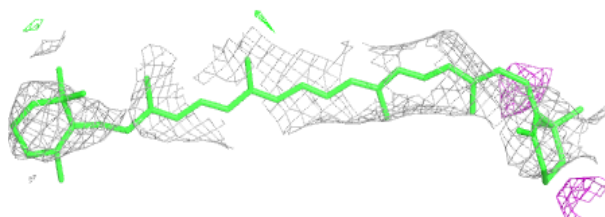


Electron density around CLA c 2475:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

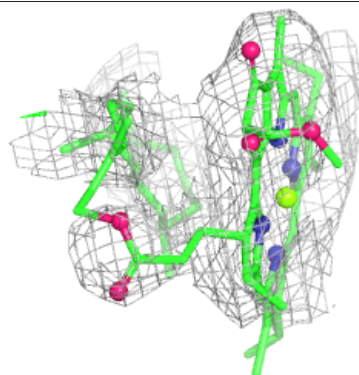
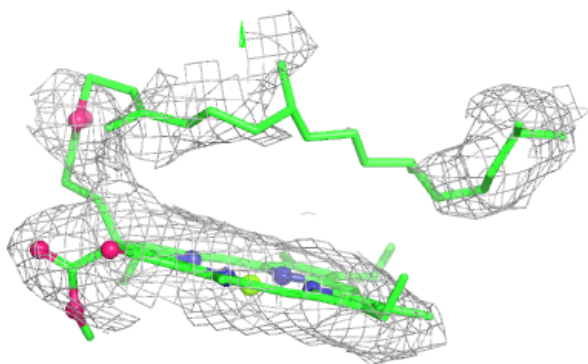
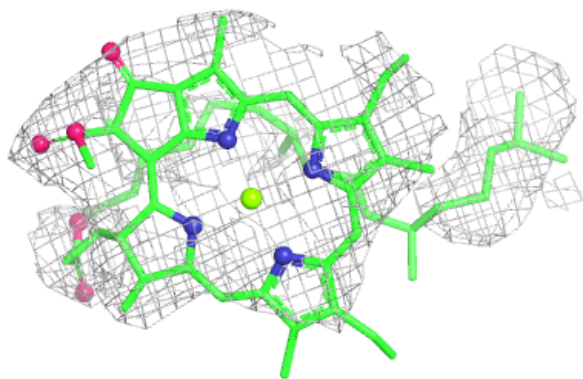
**Electron density around BCR b 2528:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

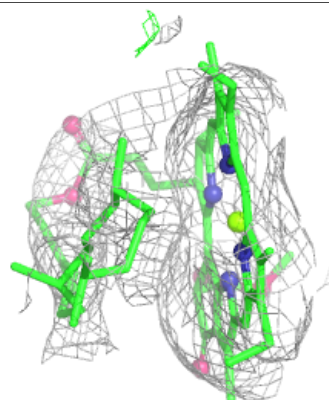
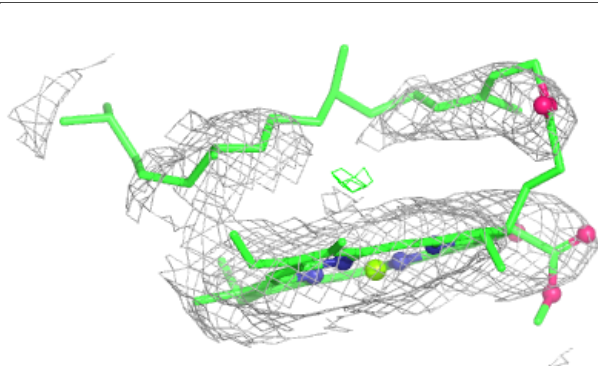
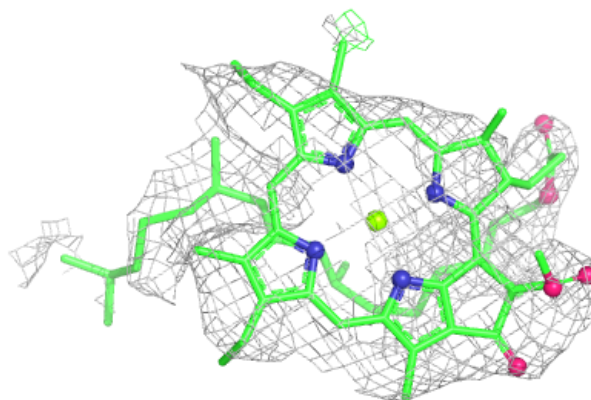


Electron density around CLA B 527:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

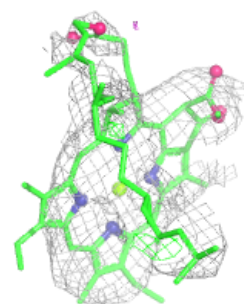
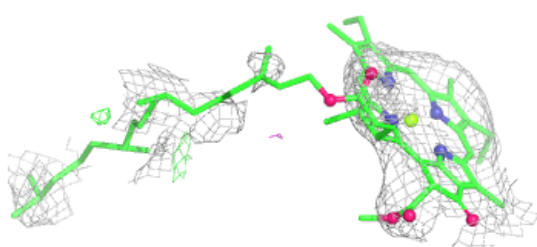
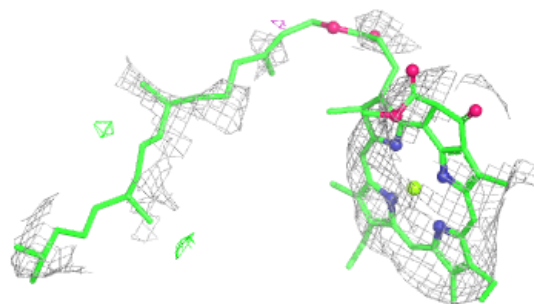
**Electron density around CLA b 2526:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

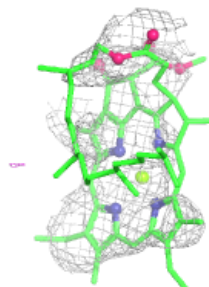
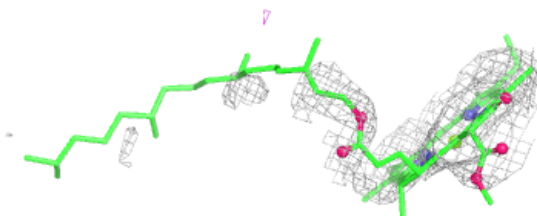


Electron density around CLA C 482:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

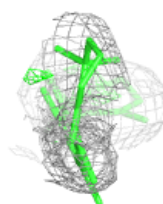
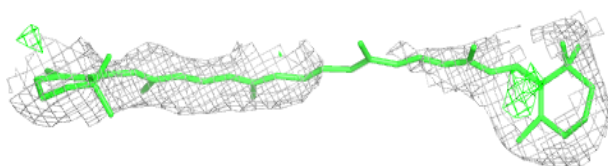
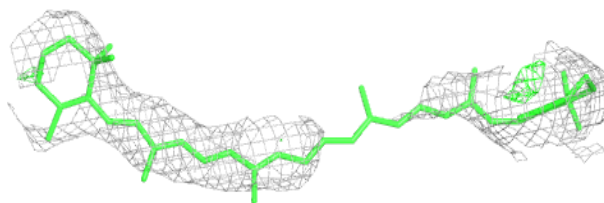
**Electron density around CLA c 2486:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

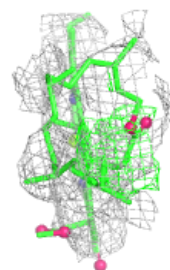
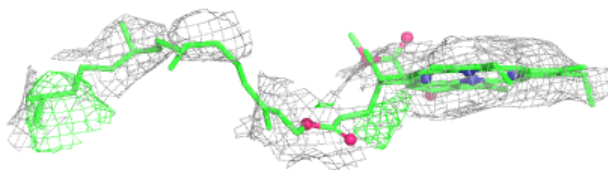
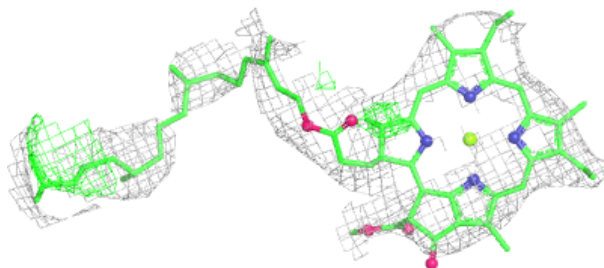


Electron density around BCR d 2360:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

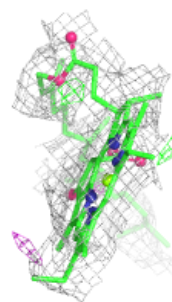
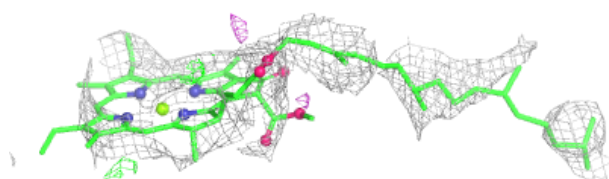
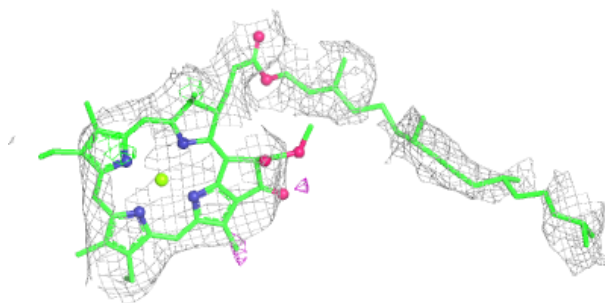
**Electron density around CLA d 2357:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

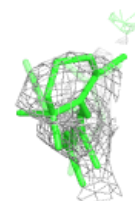
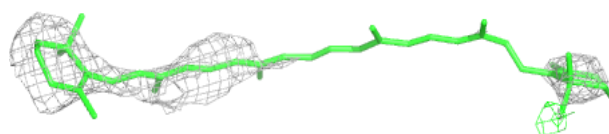
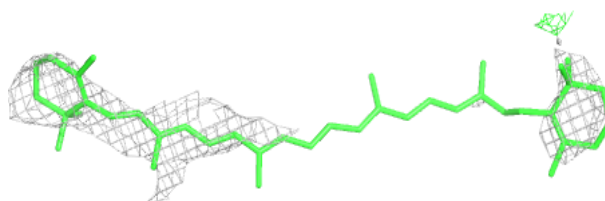


Electron density around CLA c 2484:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

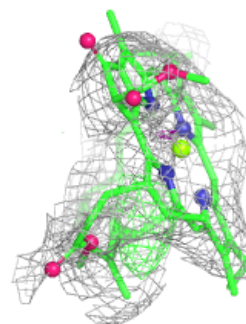
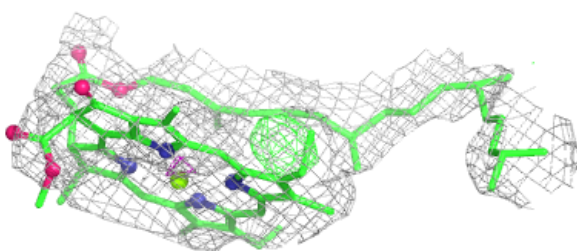
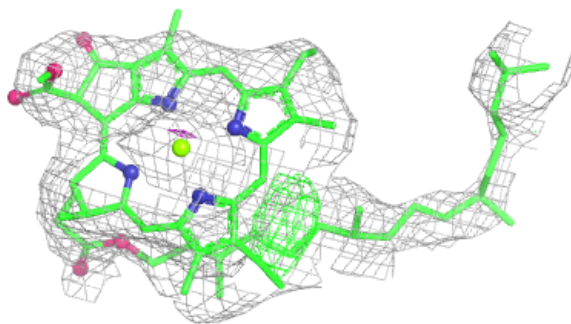
**Electron density around BCR c 2488:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

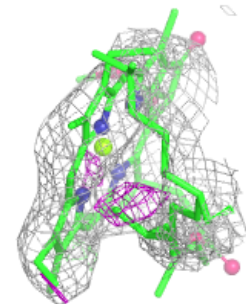
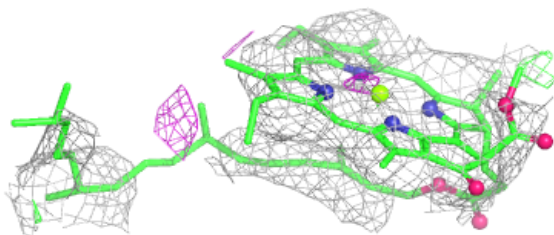
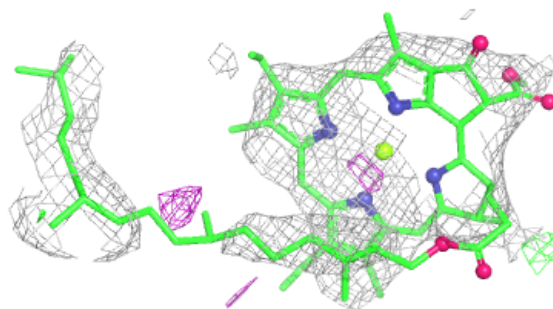


Electron density around CLA b 2511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

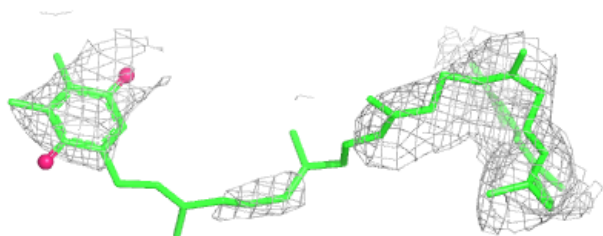
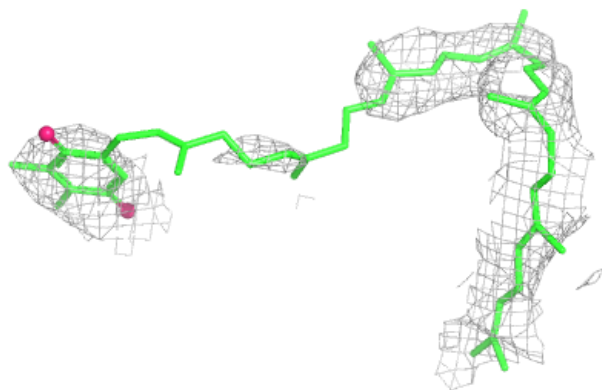
**Electron density around CLA B 511:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

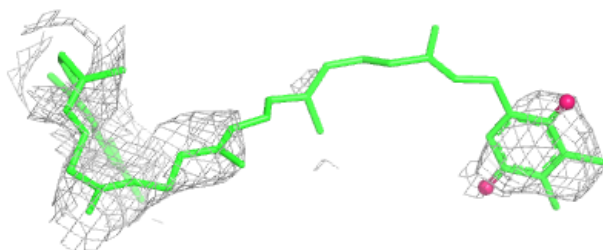
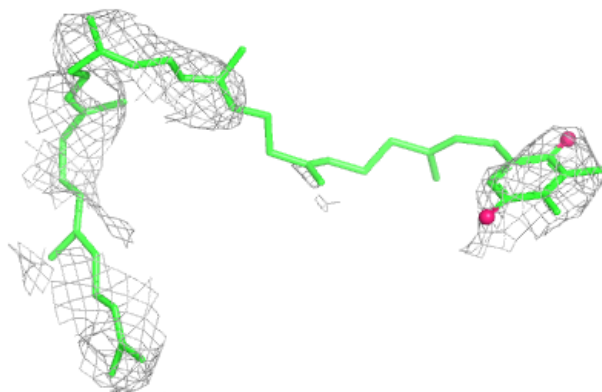


Electron density around PL9 a 2352:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

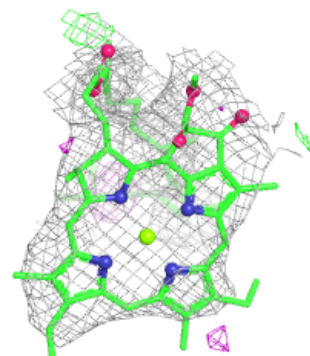
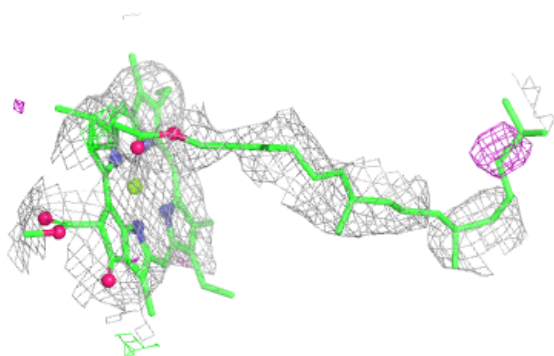
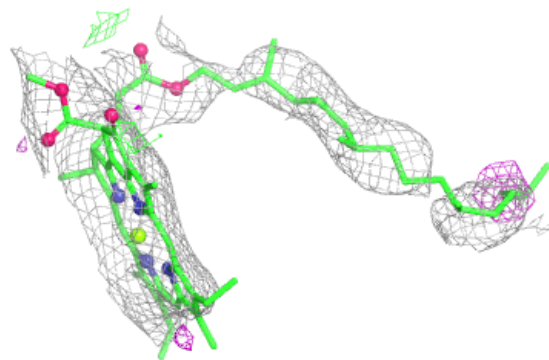
**Electron density around PL9 A 353:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

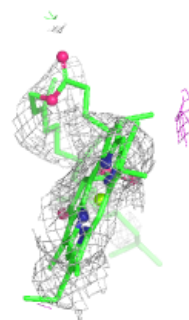
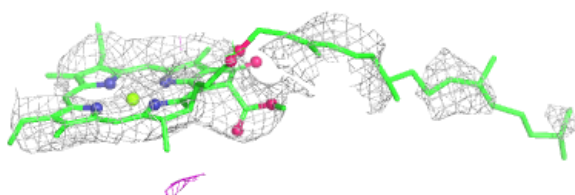
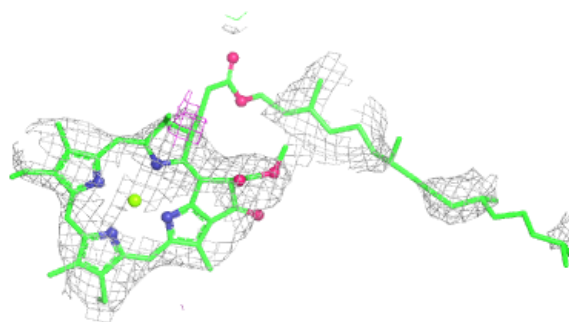


Electron density around CLA B 523:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

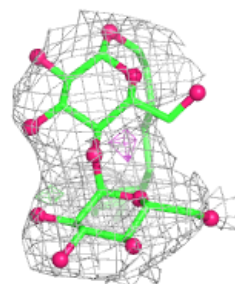
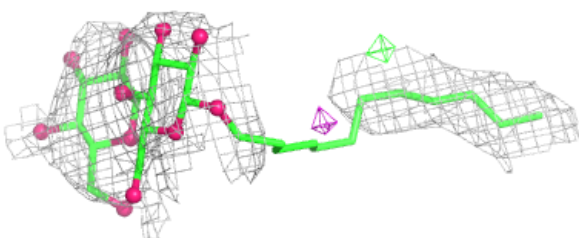
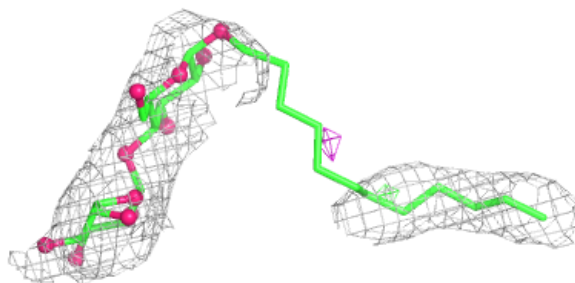
**Electron density around CLA C 484:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

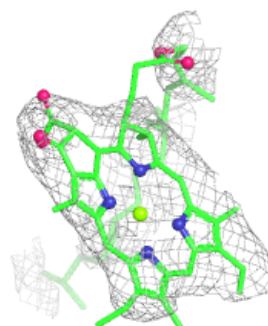
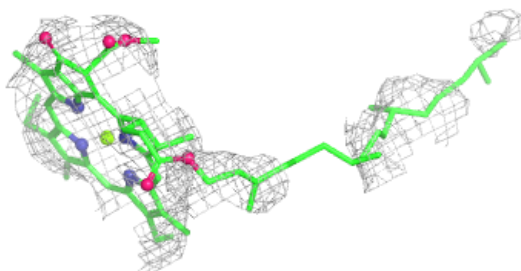
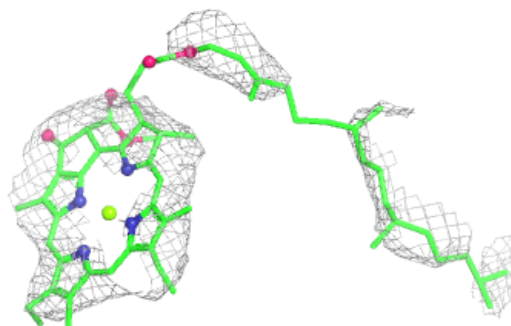


Electron density around LMT B 526:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

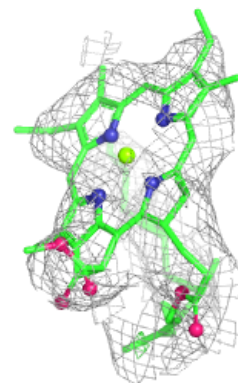
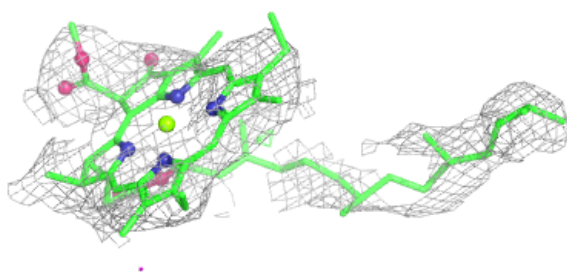
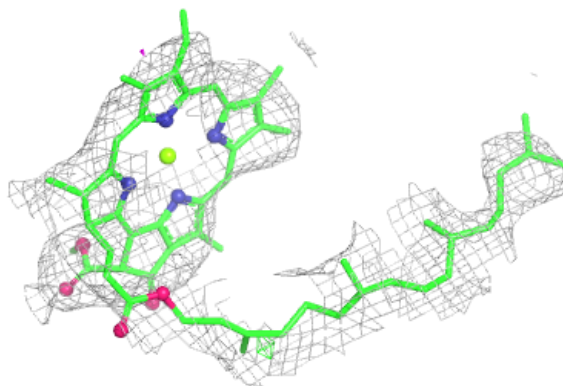
**Electron density around CLA c 2482:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



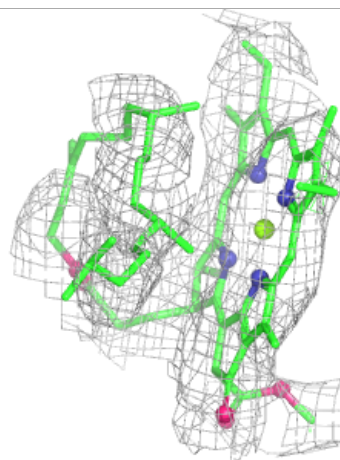
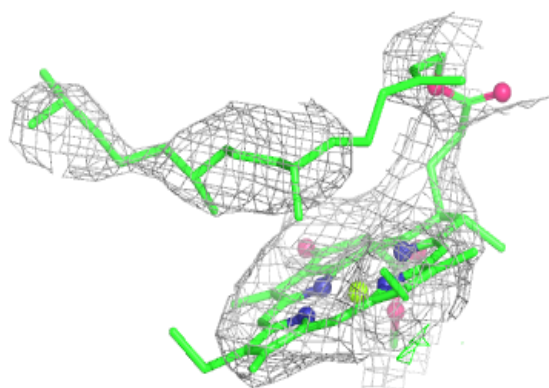
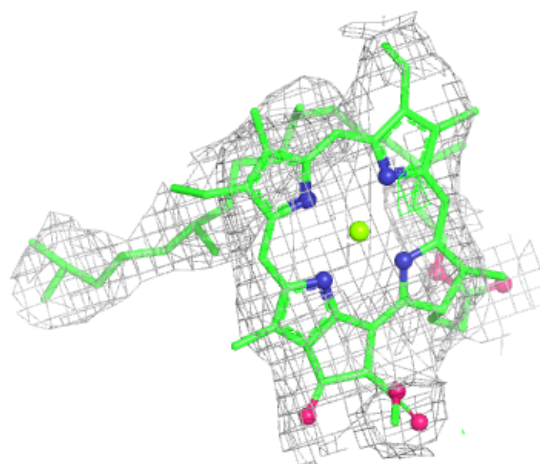
Electron density around CLA C 477:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



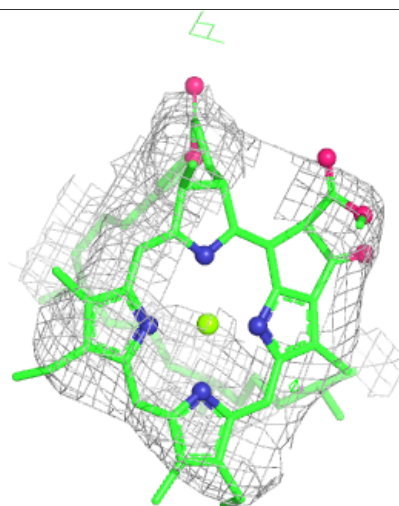
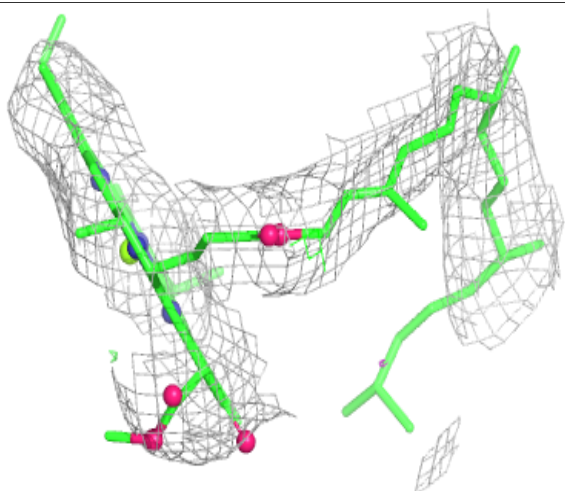
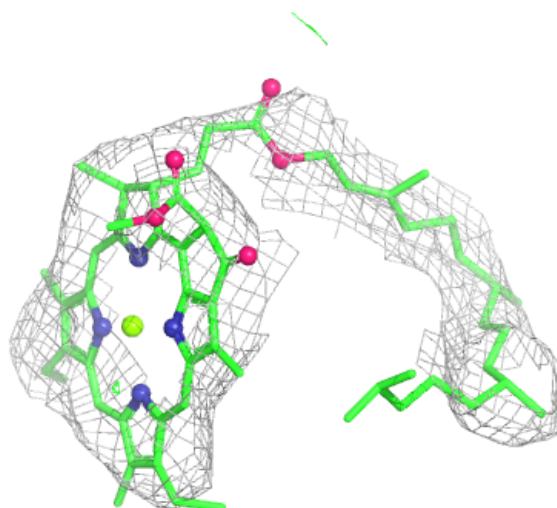
Electron density around CLA b 2525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



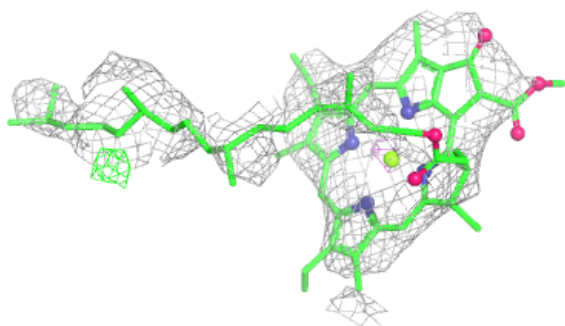
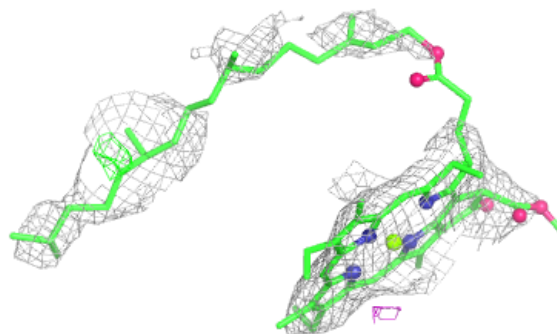
Electron density around CLA c 2480:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

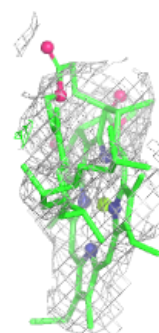
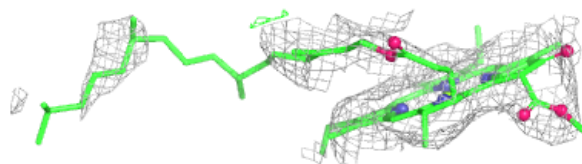
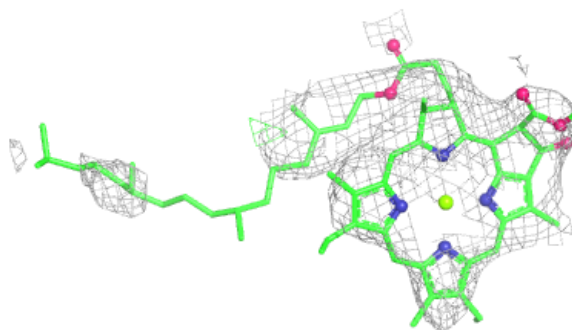


Electron density around CLA c 2474:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

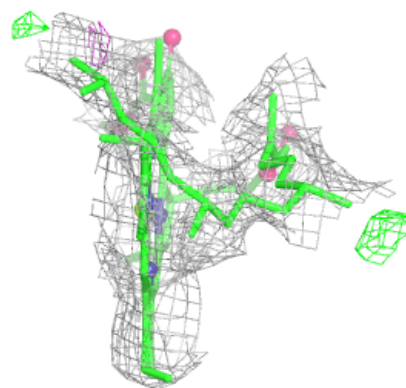
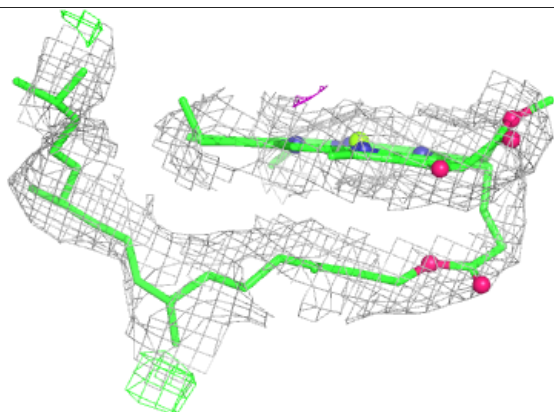
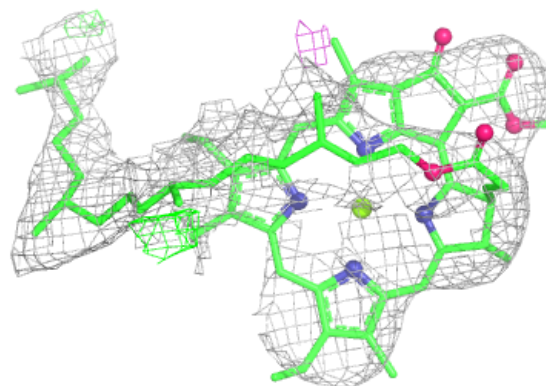
**Electron density around CLA b 2517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

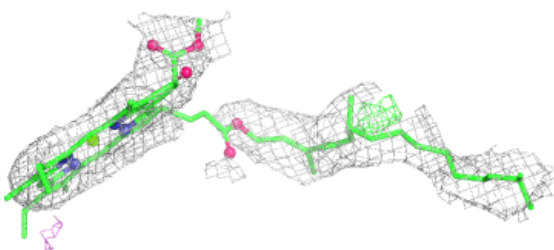
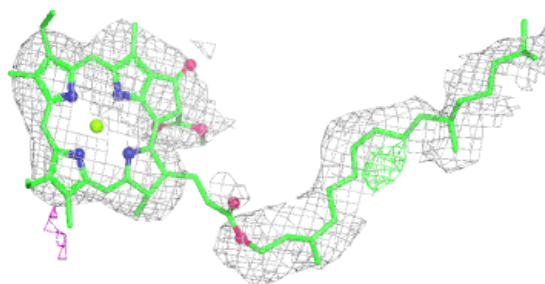


Electron density around CLA B 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

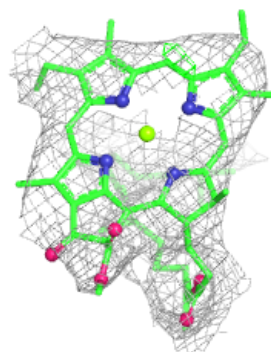
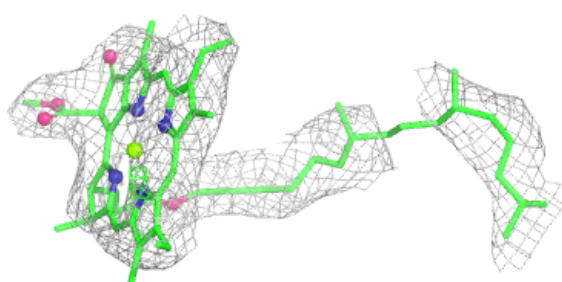
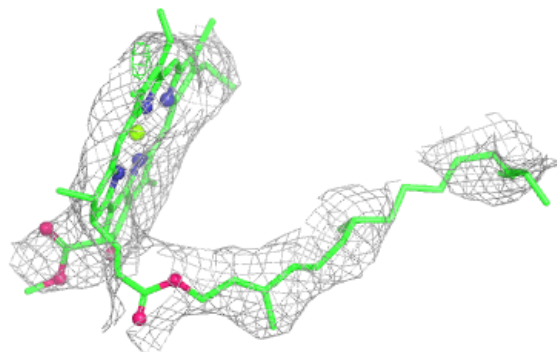
**Electron density around CLA A 352:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

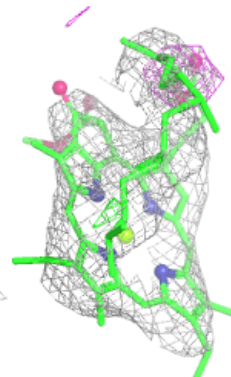
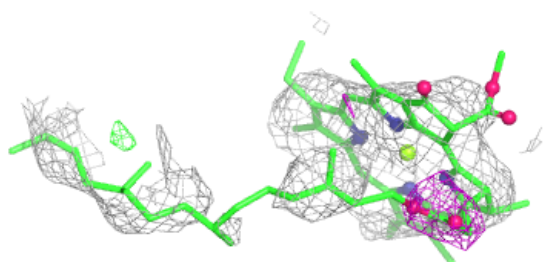
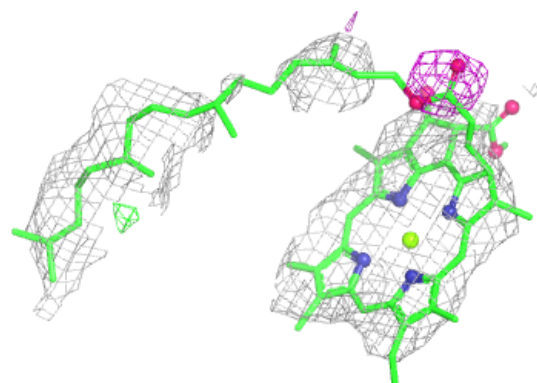


Electron density around CLA b 2523:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

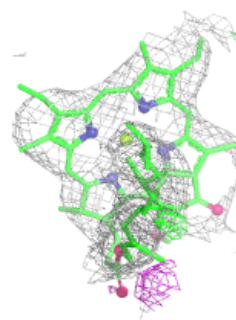
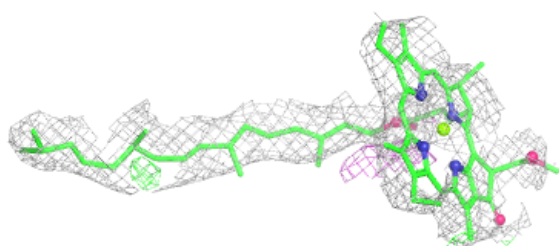
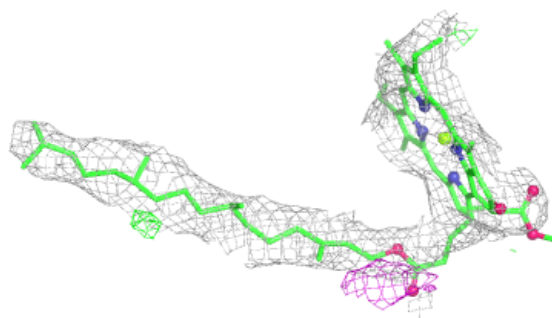
**Electron density around CLA c 2477:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

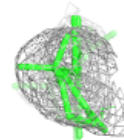
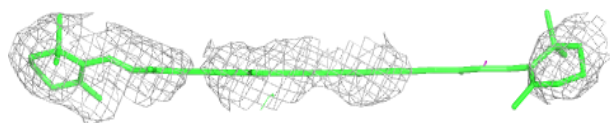
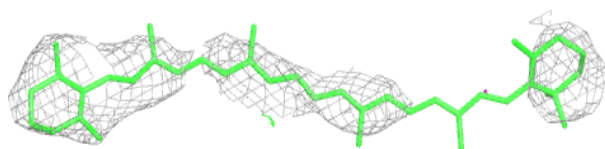


Electron density around CLA B 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

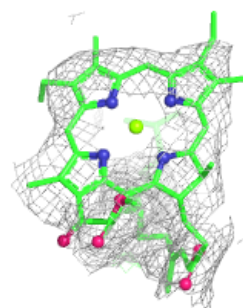
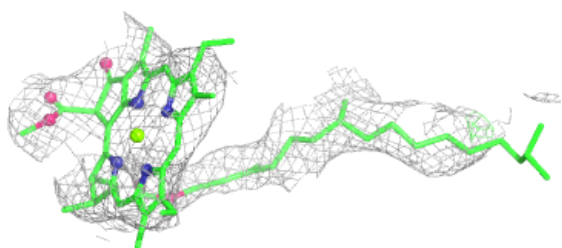
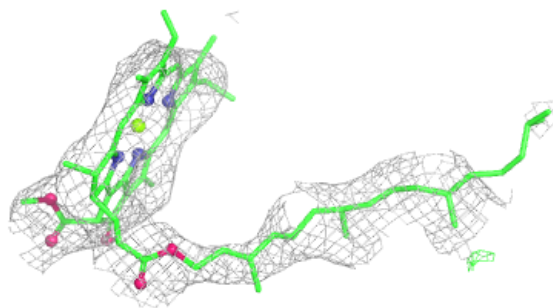
**Electron density around BCR B 528:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

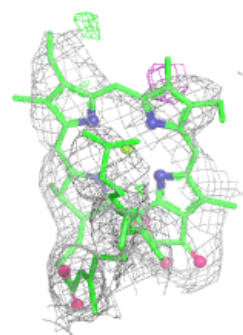
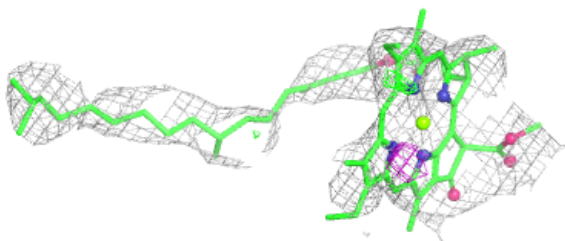
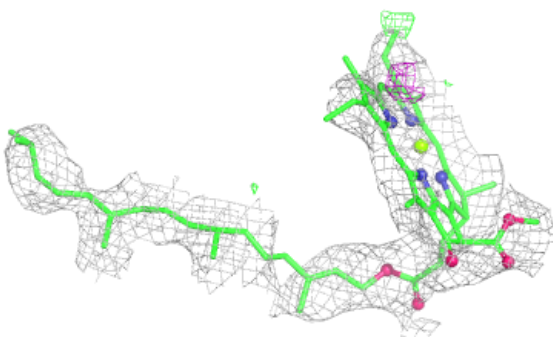


Electron density around CLA C 483:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

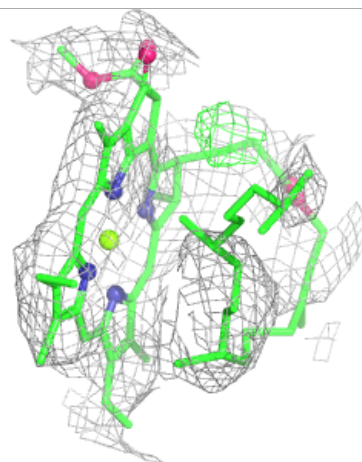
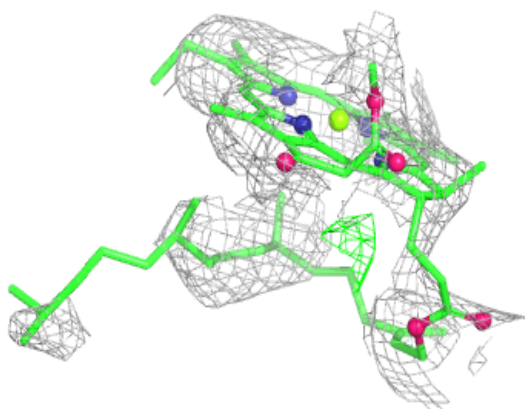
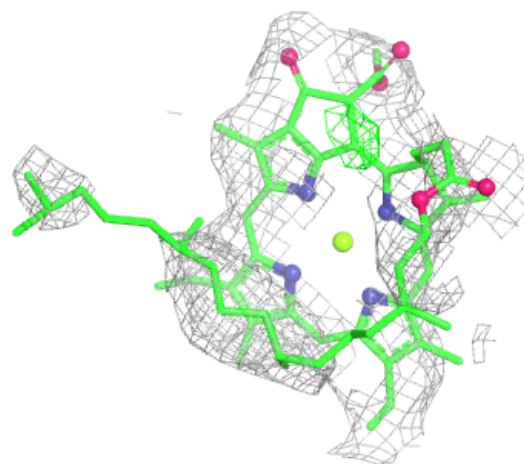
**Electron density around CLA c 2483:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



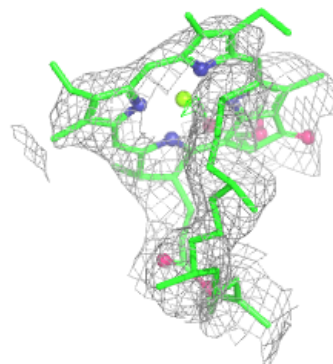
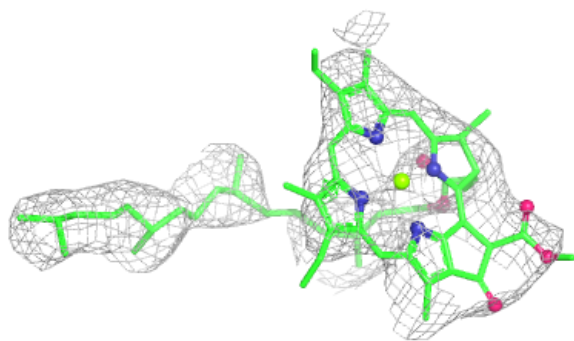
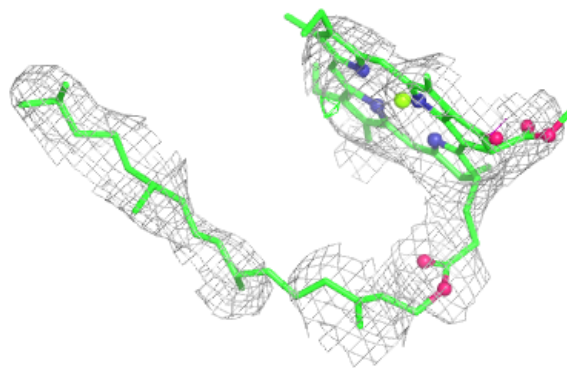
Electron density around CLA B 525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



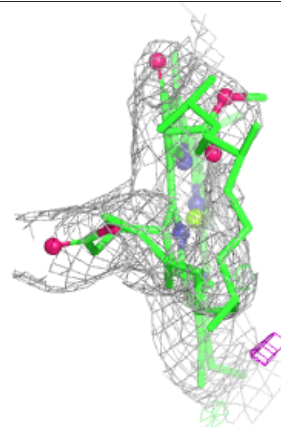
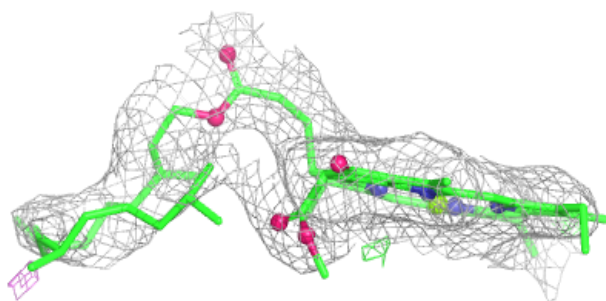
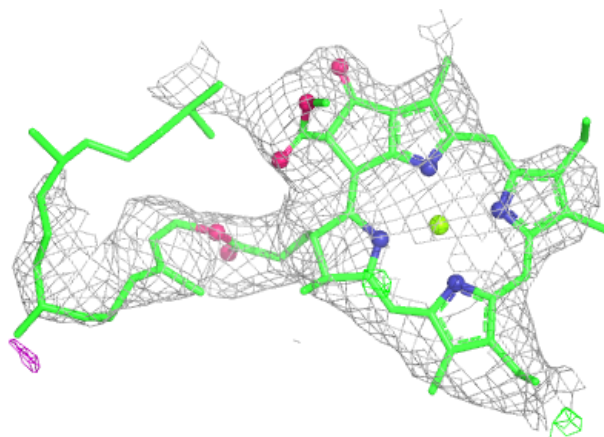
Electron density around CLA C 474:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



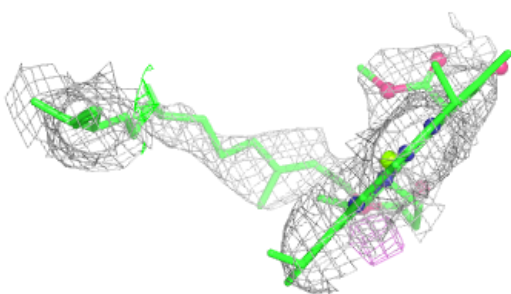
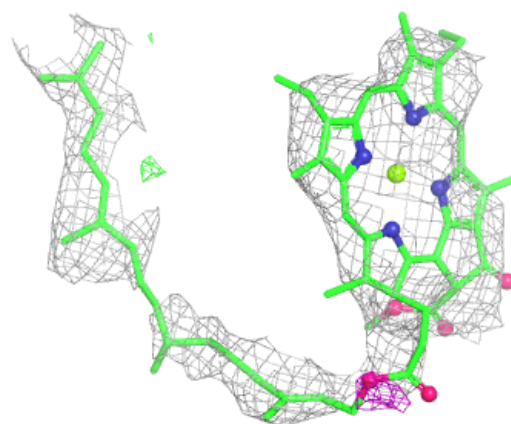
Electron density around CLA b 2513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

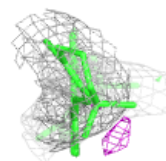
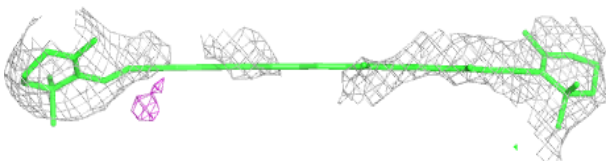
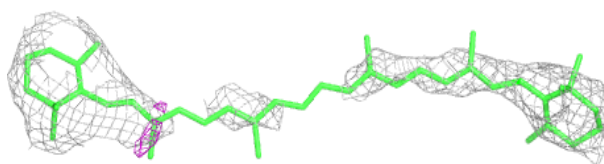


Electron density around CLA C 485:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

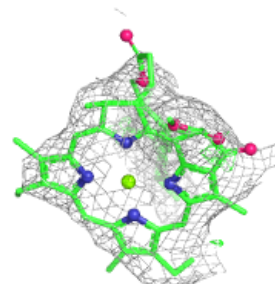
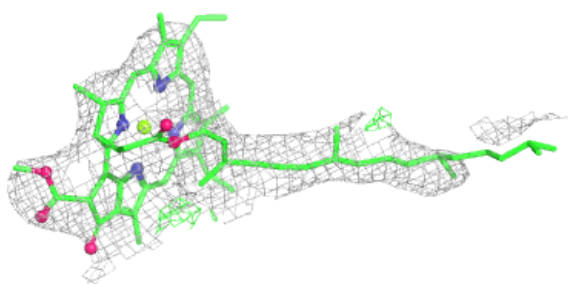
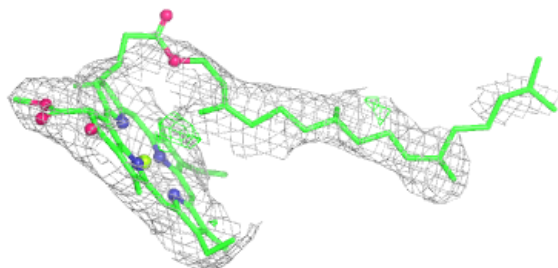
**Electron density around BCR b 2527:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

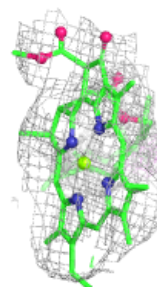
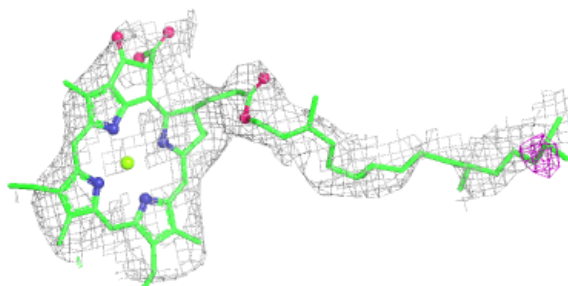


Electron density around CLA B 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

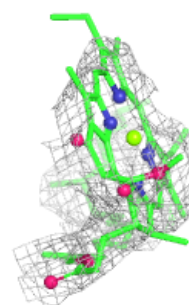
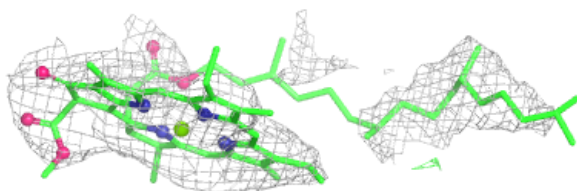
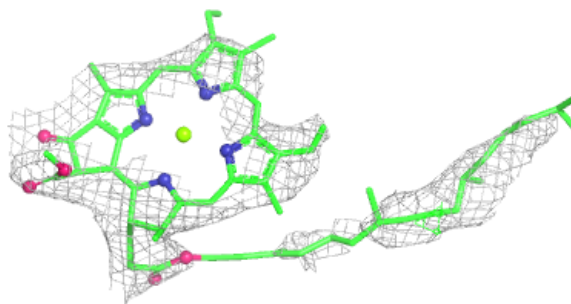
**Electron density around CLA a 2349:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

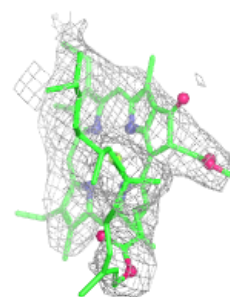
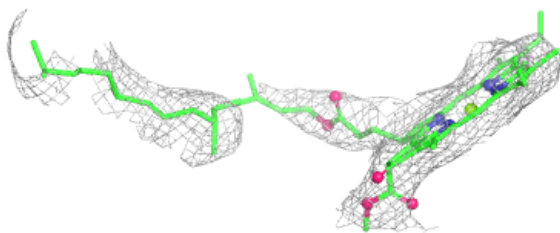
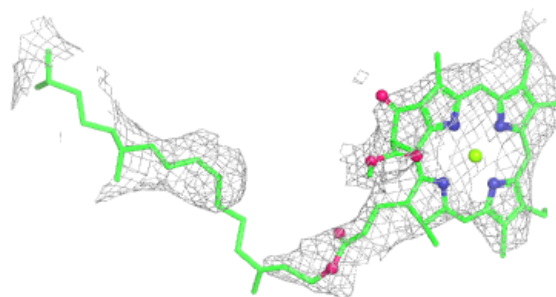


Electron density around CLA c 2479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

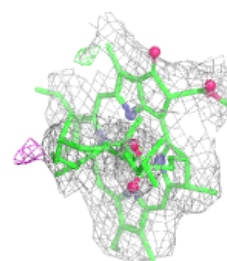
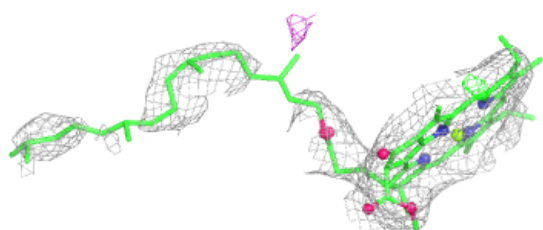
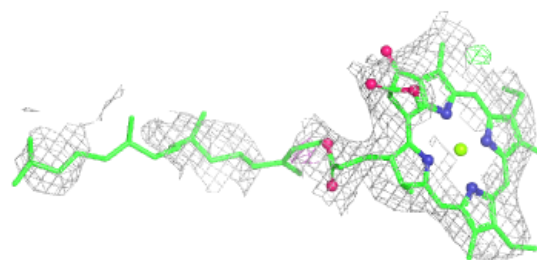
**Electron density around CLA a 2351:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

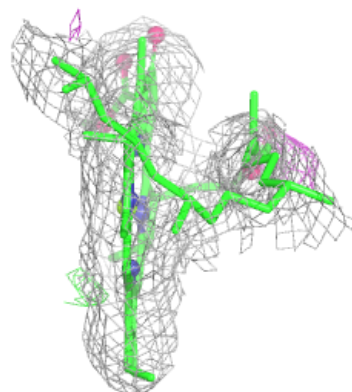
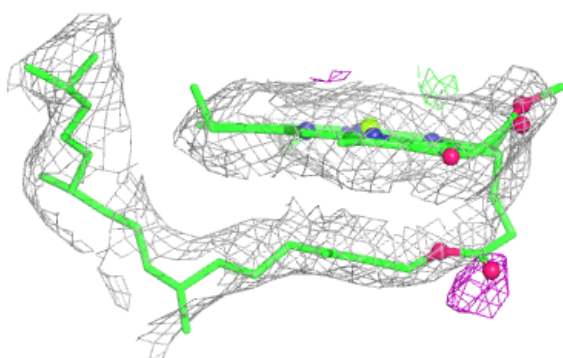
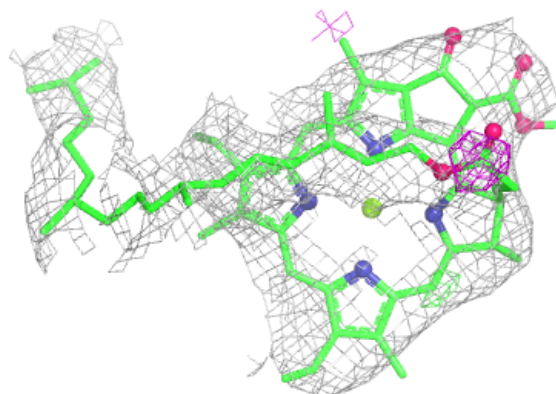


Electron density around CLA c 2481:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

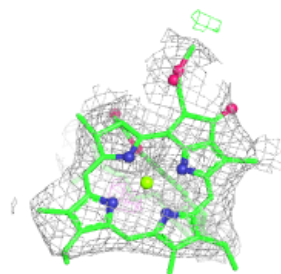
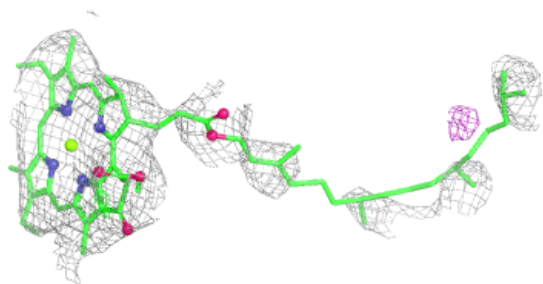
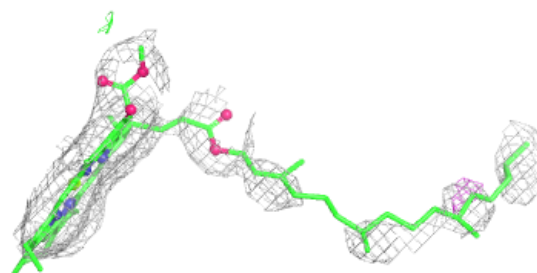
**Electron density around CLA b 2520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



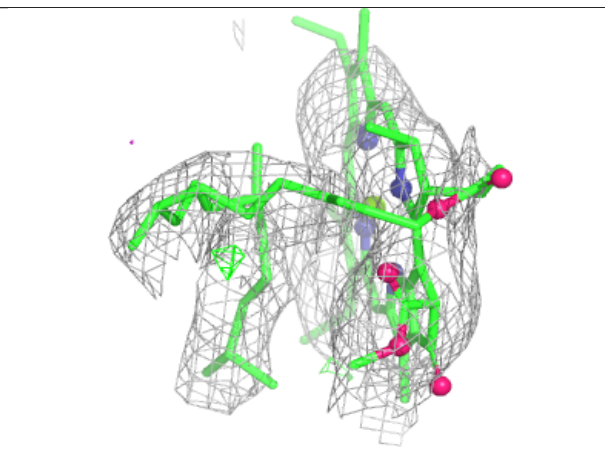
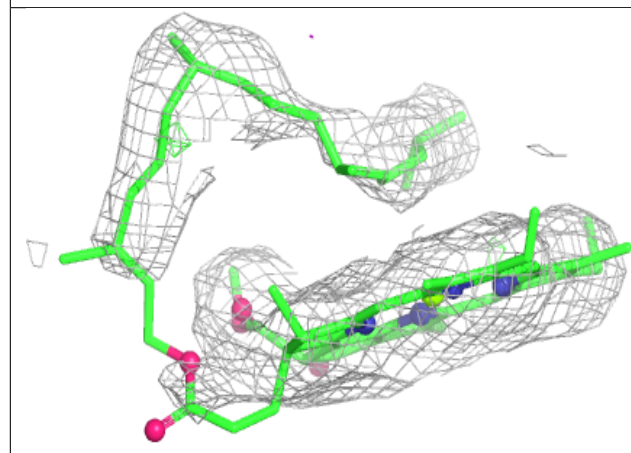
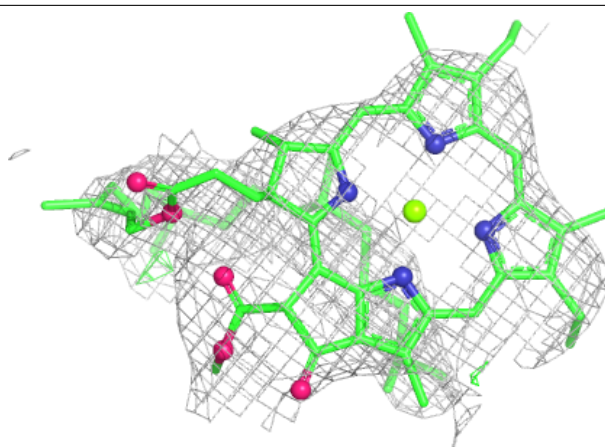
Electron density around CLA B 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



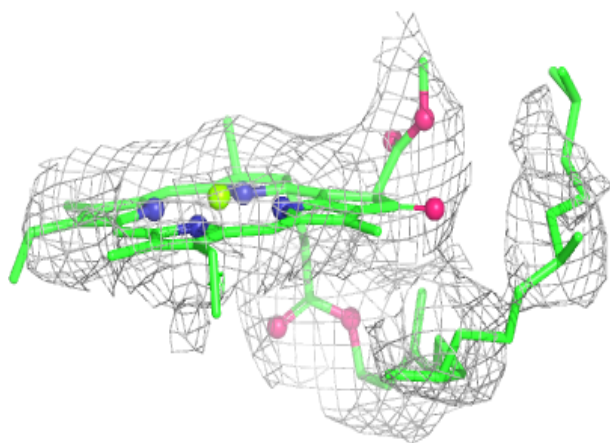
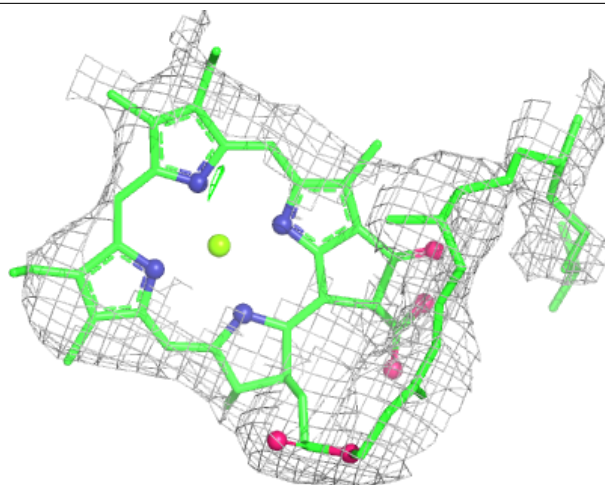
Electron density around CLA c 2476:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



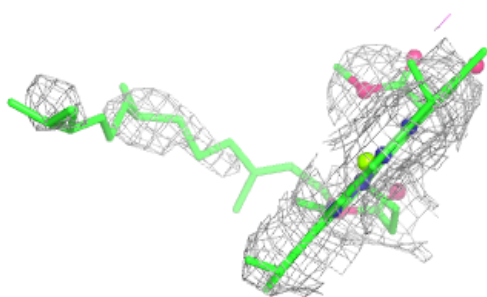
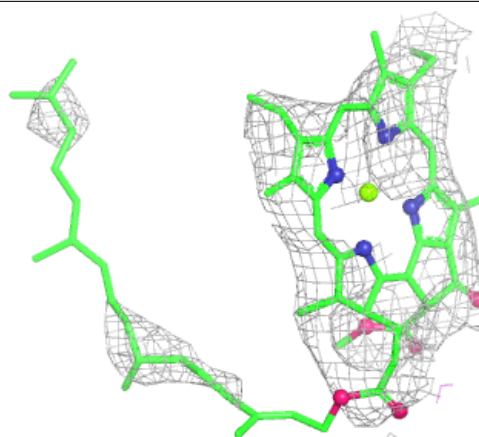
Electron density around CLA B 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



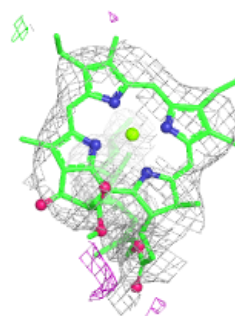
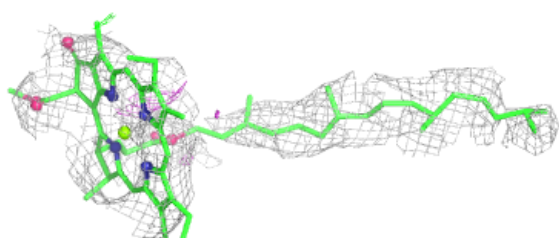
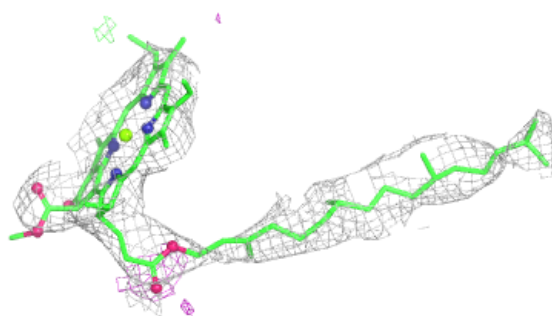
Electron density around CLA c 2485:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

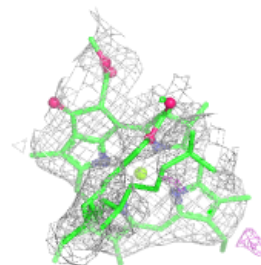
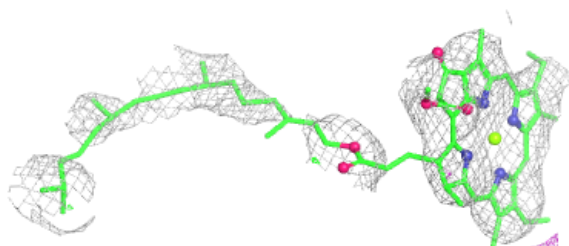
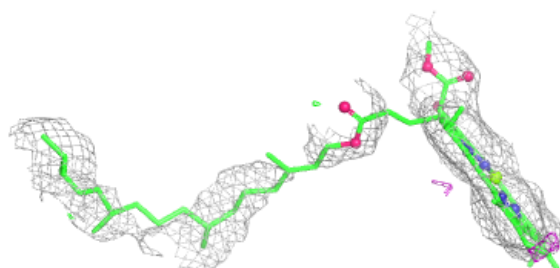


Electron density around CLA b 2514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

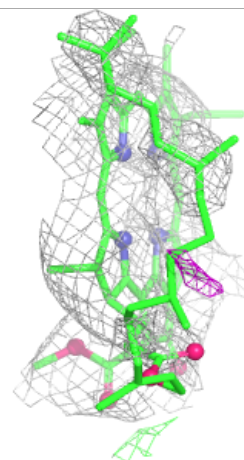
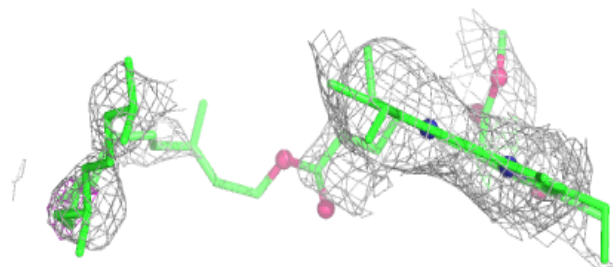
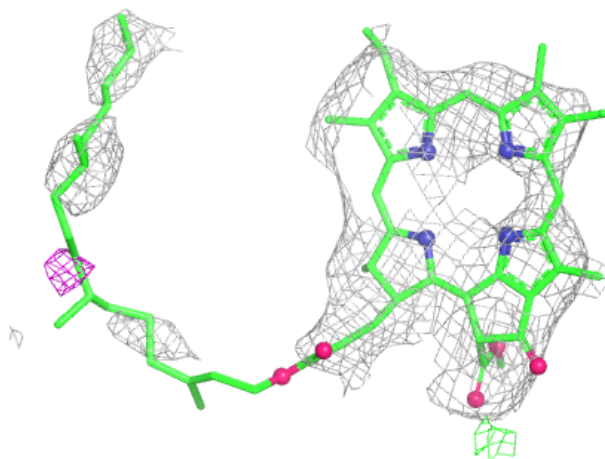
**Electron density around CLA b 2516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



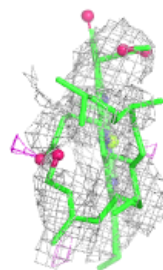
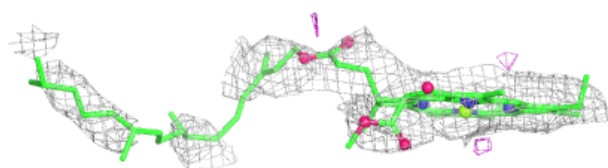
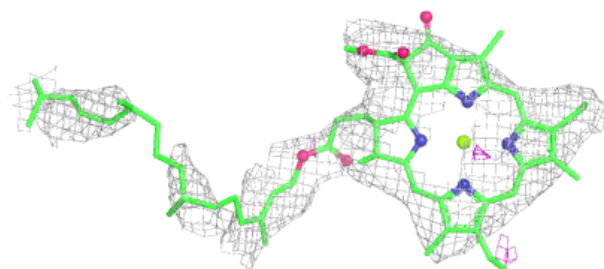
Electron density around PHO a 2350:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

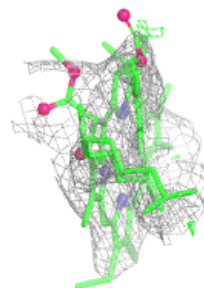
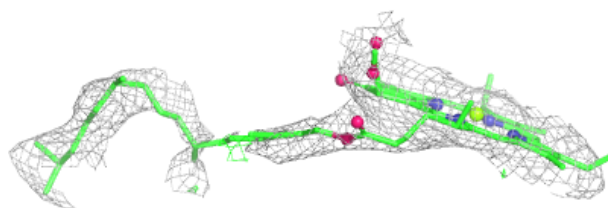
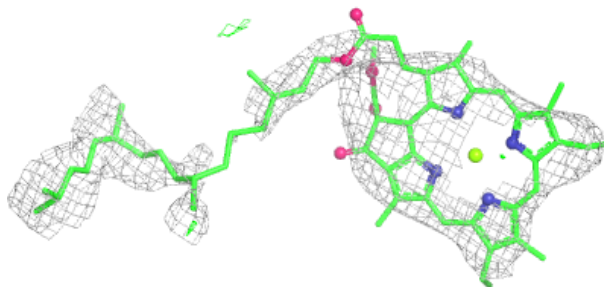


Electron density around CLA D 356:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

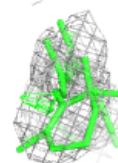
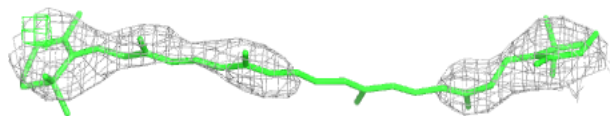
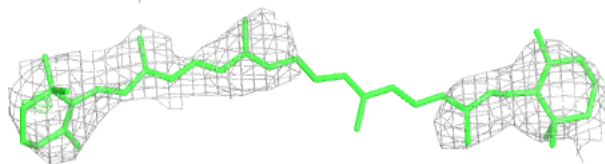
**Electron density around CLA b 2521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

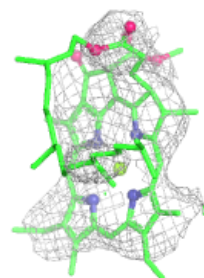
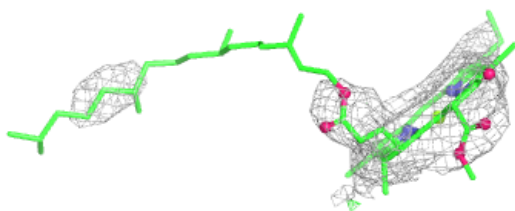
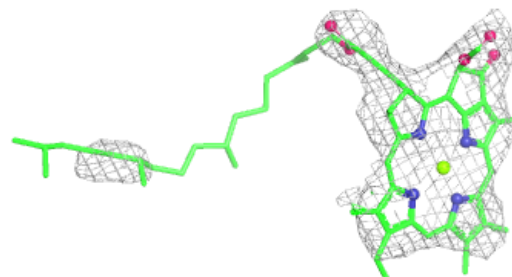


Electron density around BCR C 488:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

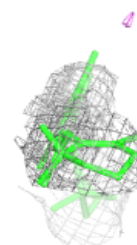
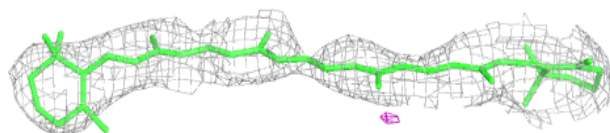
**Electron density around CLA C 486:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

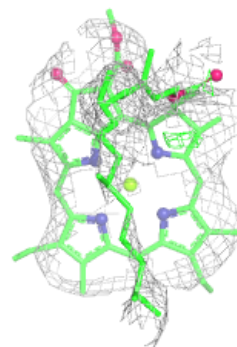
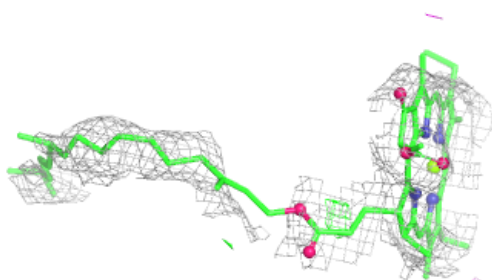


Electron density around BCR F 48:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

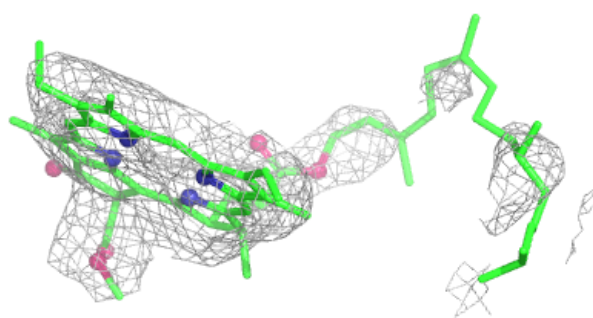
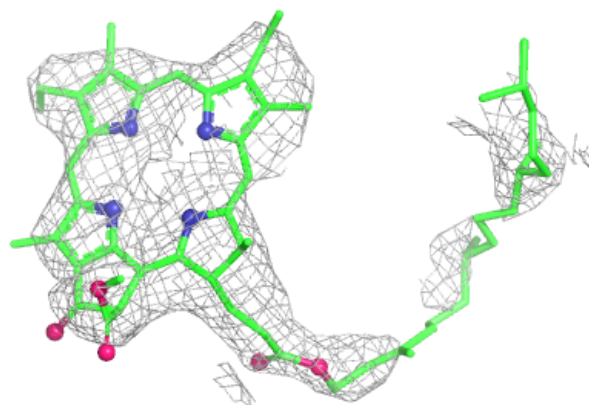
**Electron density around CLA C 475:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



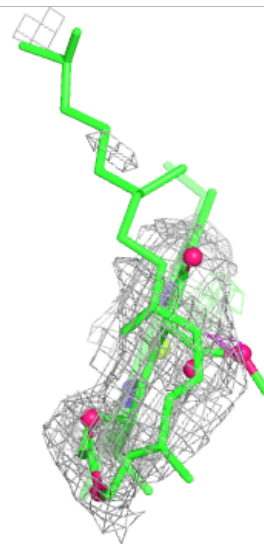
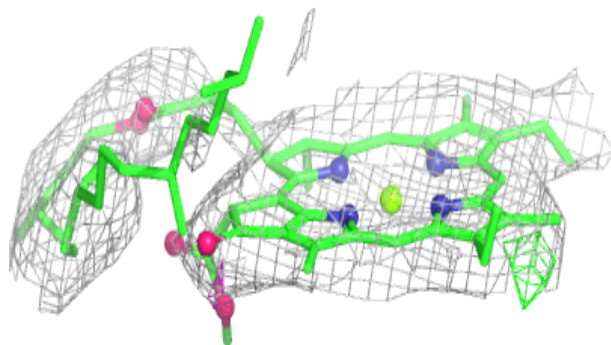
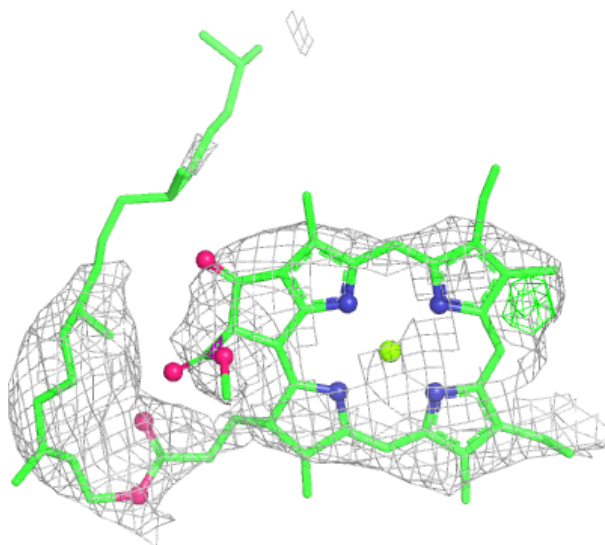
Electron density around PHO D 355:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



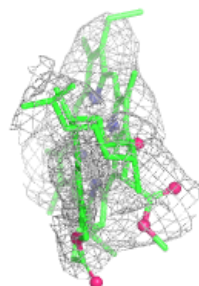
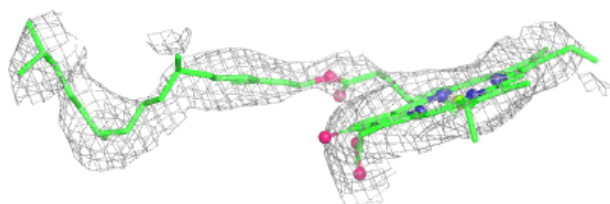
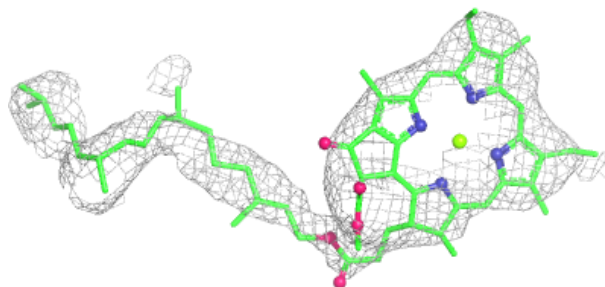
Electron density around CLA B 524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

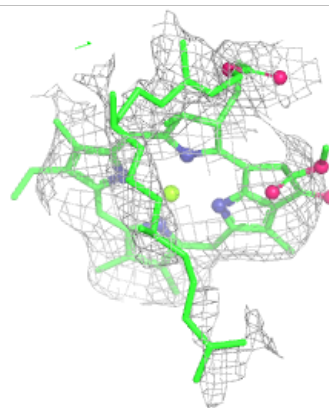
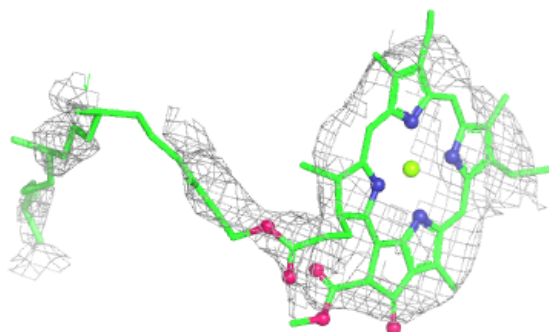
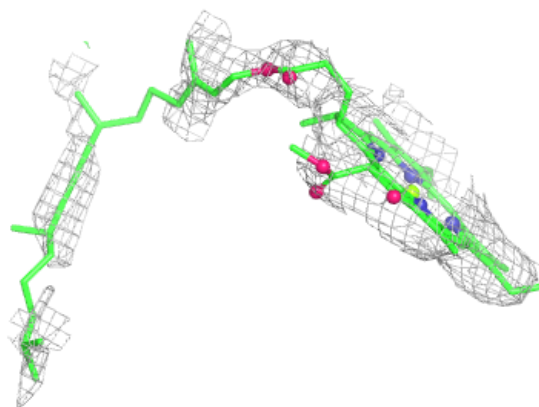


Electron density around CLA B 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

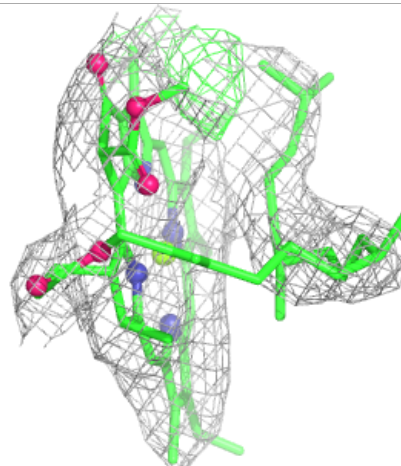
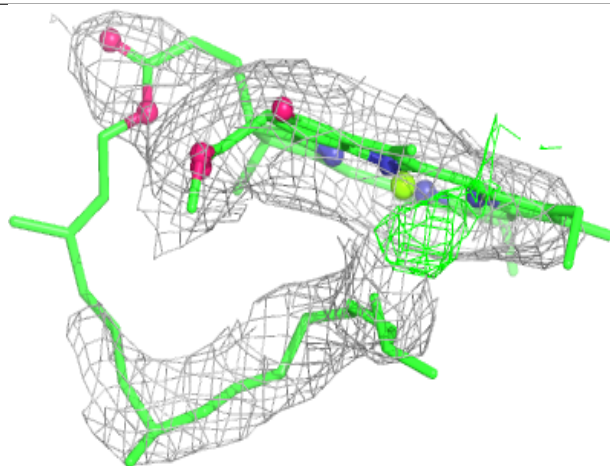
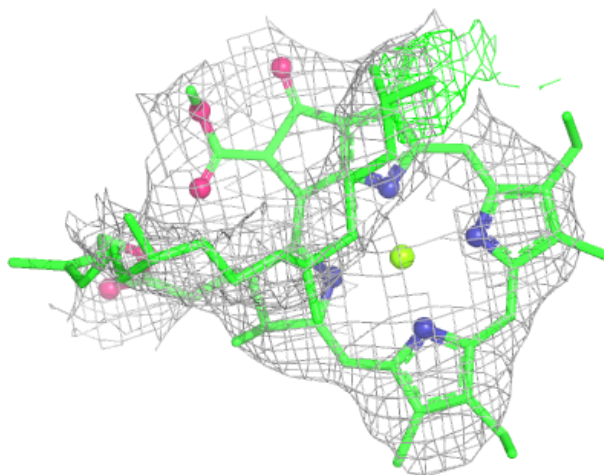
**Electron density around CLA b 2522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



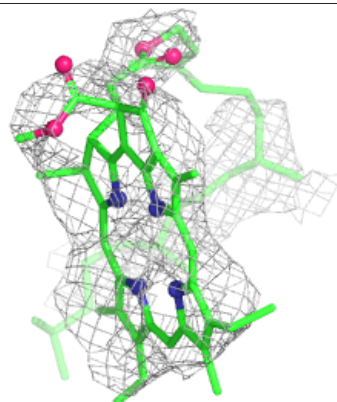
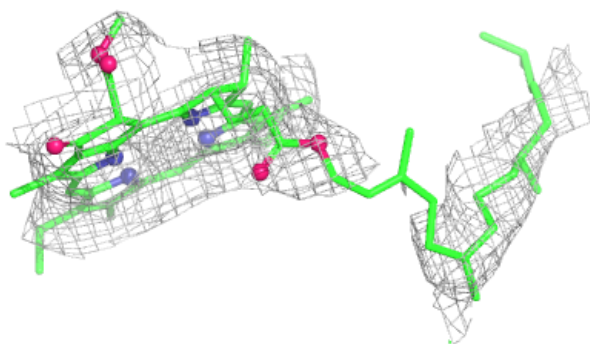
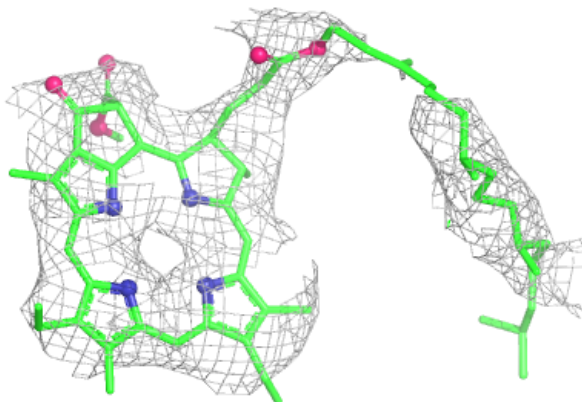
Electron density around CLA C 476:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



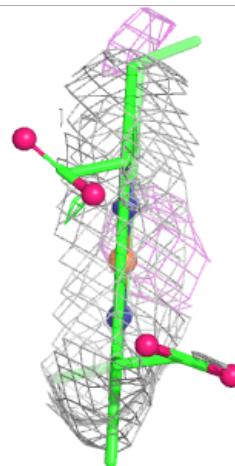
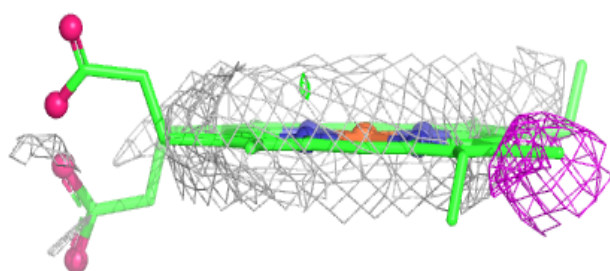
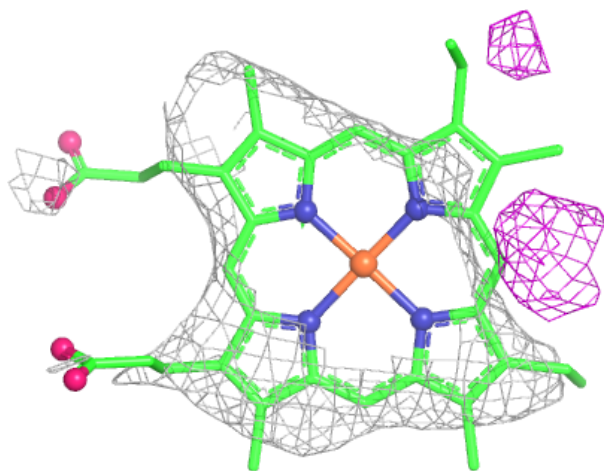
Electron density around PHO d 2356:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



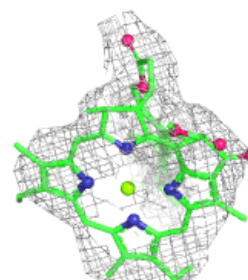
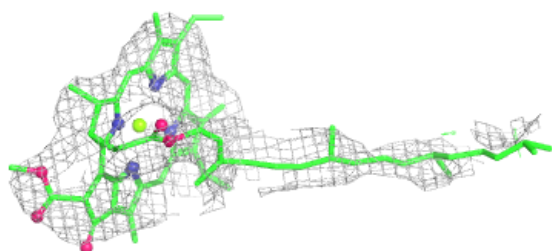
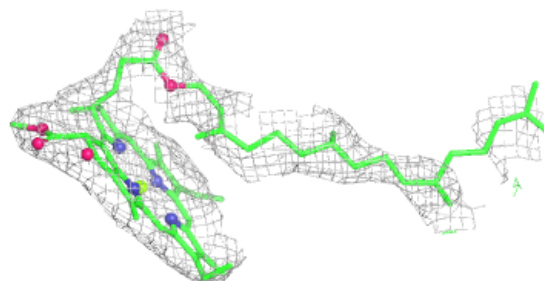
Electron density around HEC e 2084:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



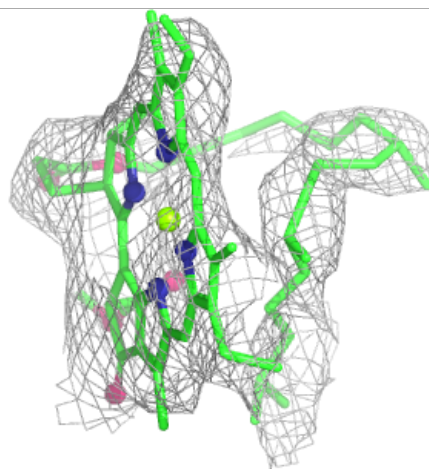
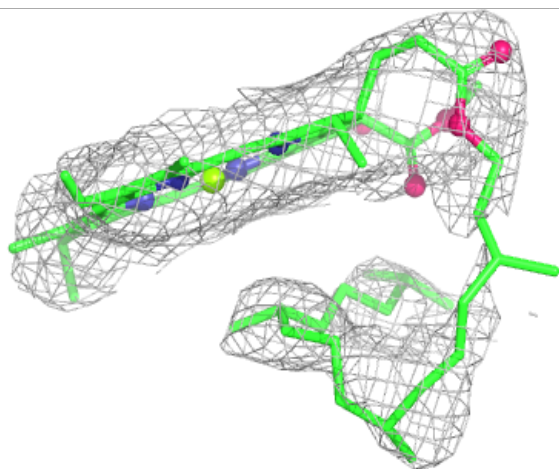
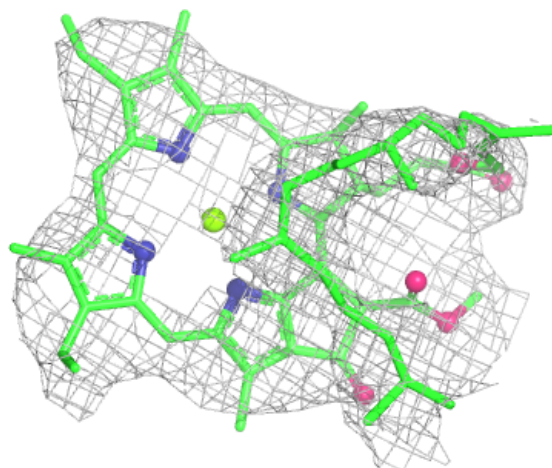
Electron density around CLA b 2519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



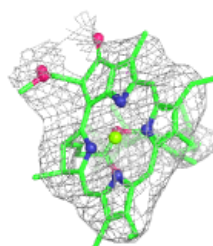
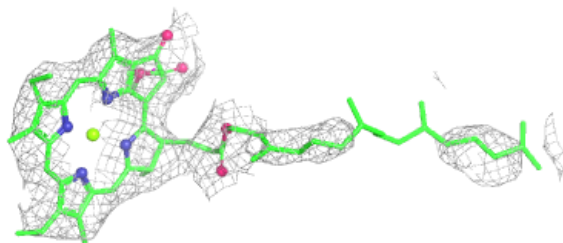
Electron density around CLA B 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

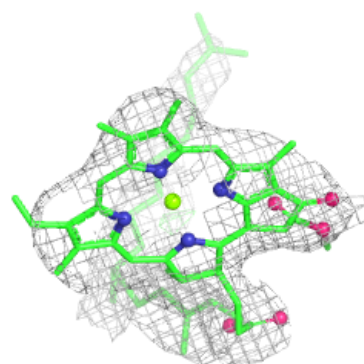
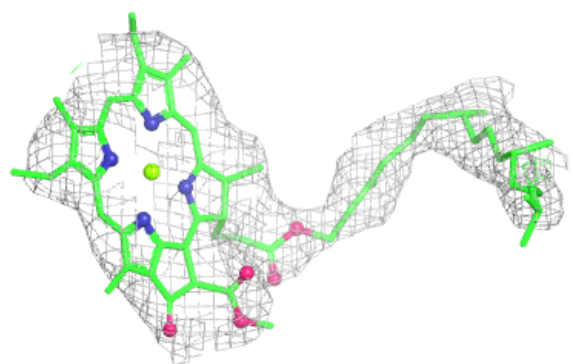
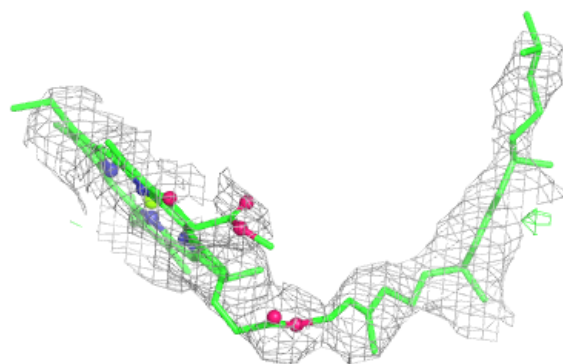


Electron density around CLA C 481:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

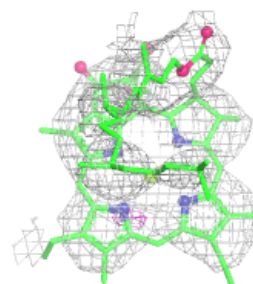
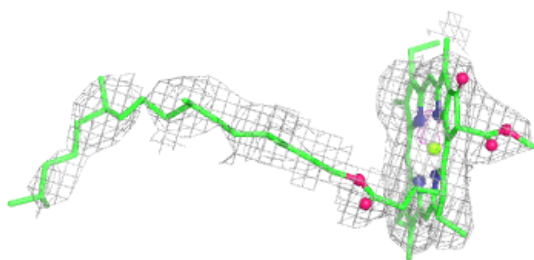
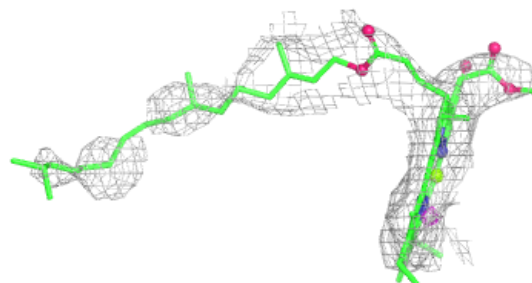
**Electron density around CLA B 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

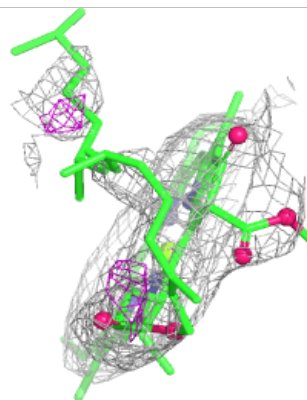
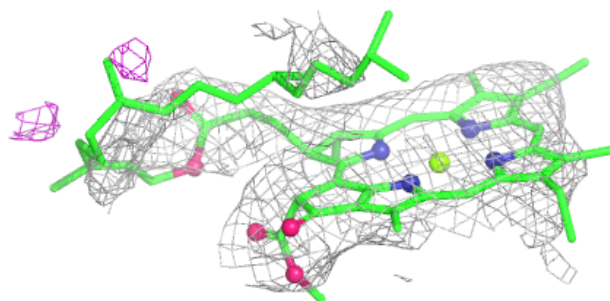
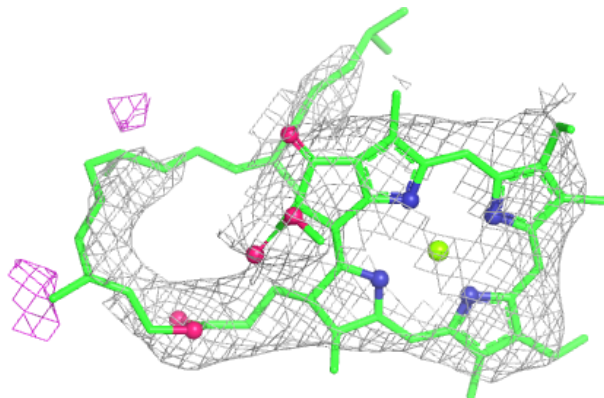


Electron density around CLA B 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

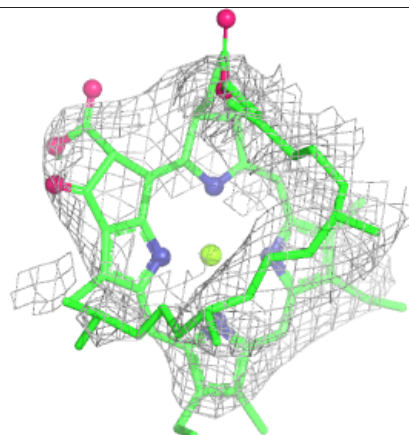
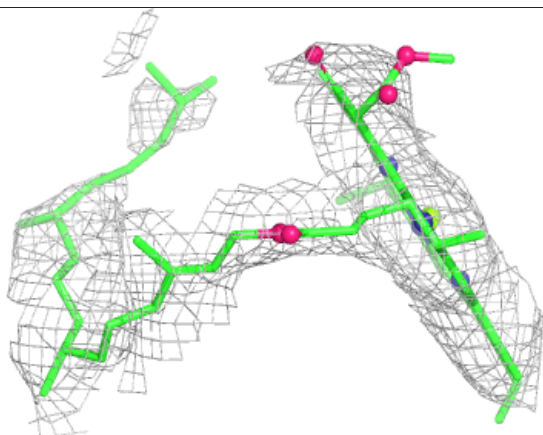
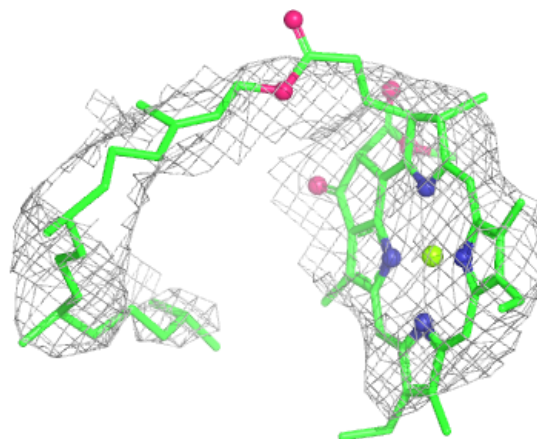
**Electron density around CLA c 2478:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



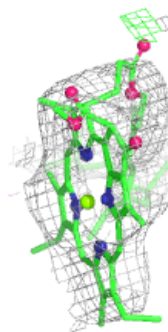
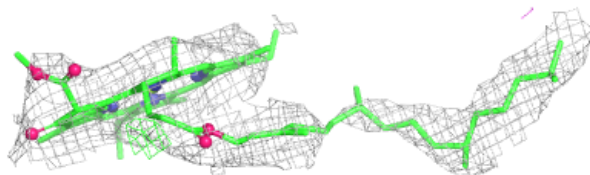
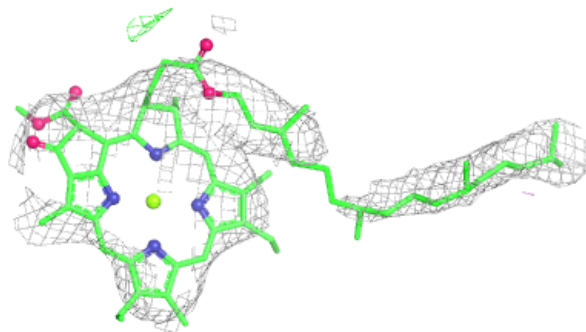
Electron density around CLA C 480:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

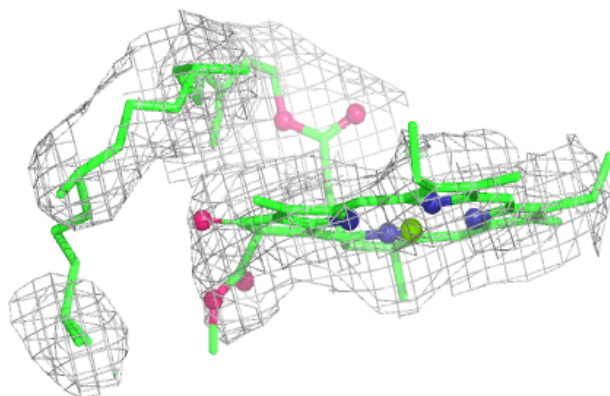
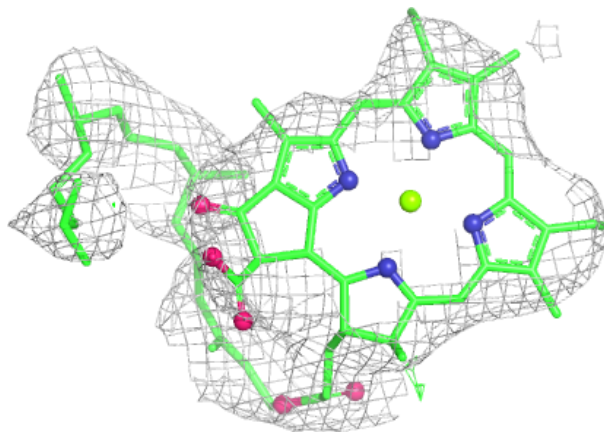


Electron density around CLA B 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

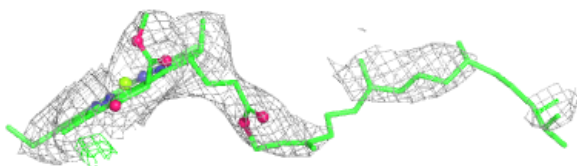
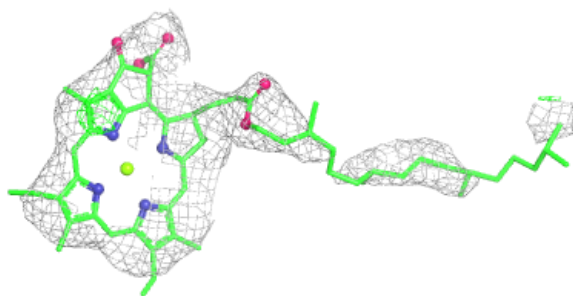
**Electron density around CLA b 2515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



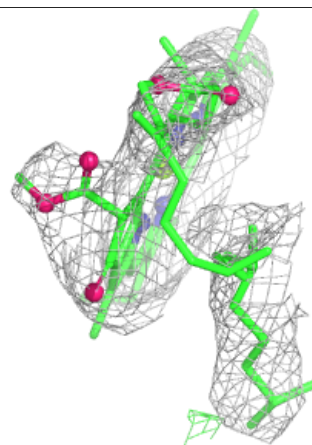
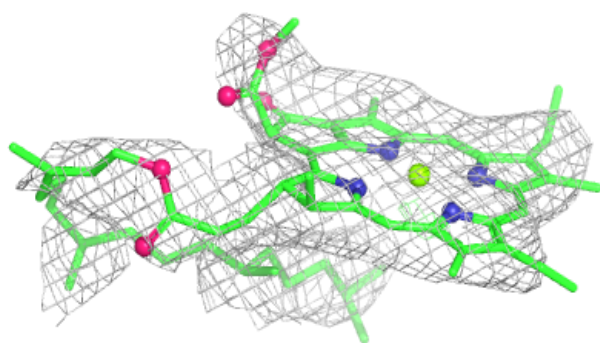
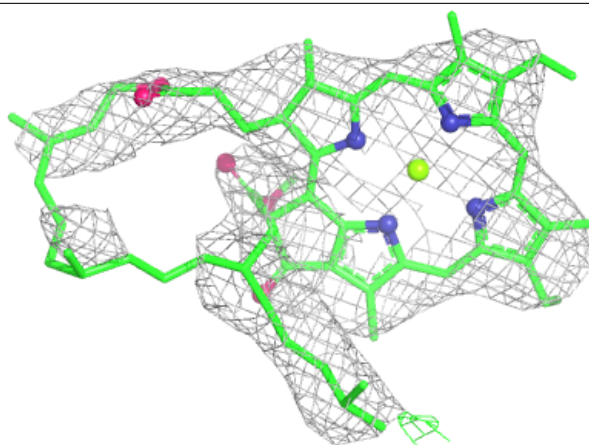
Electron density around CLA A 350:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



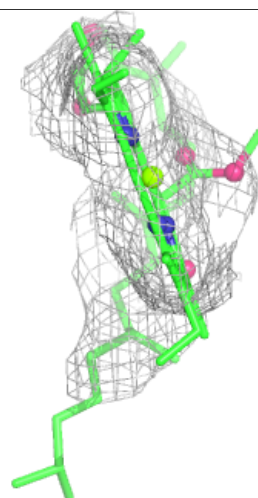
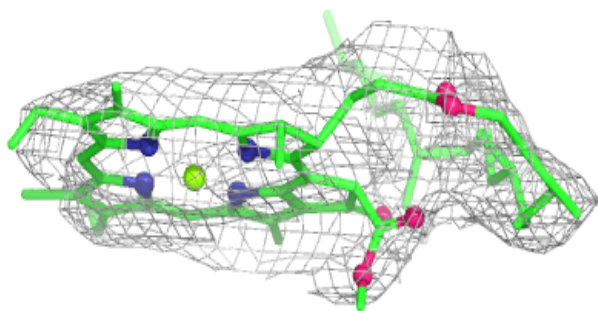
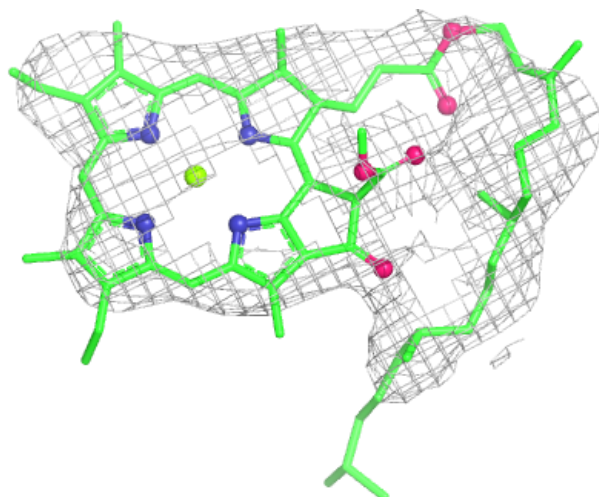
Electron density around CLA C 478:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



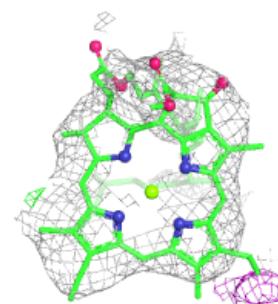
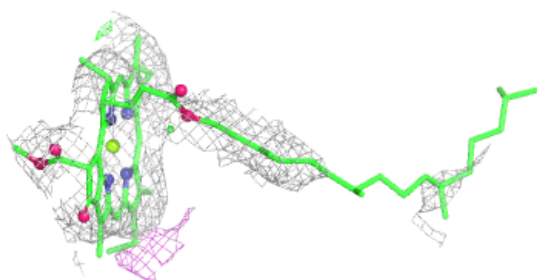
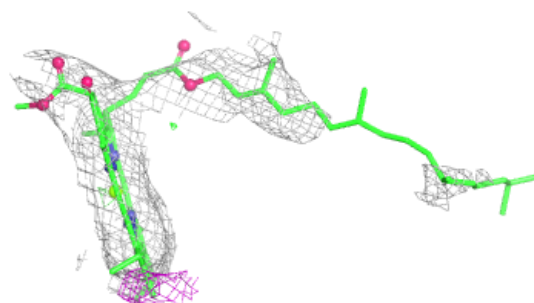
Electron density around CLA b 2524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



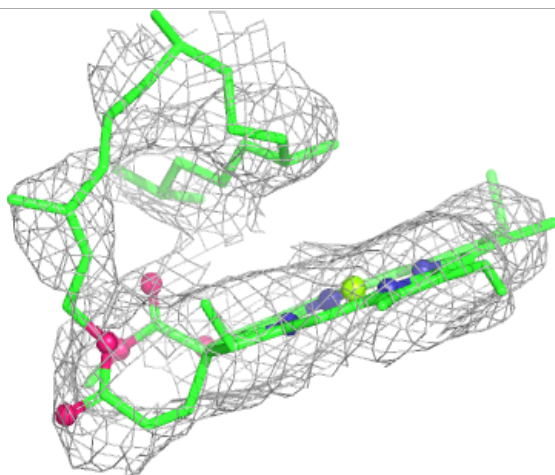
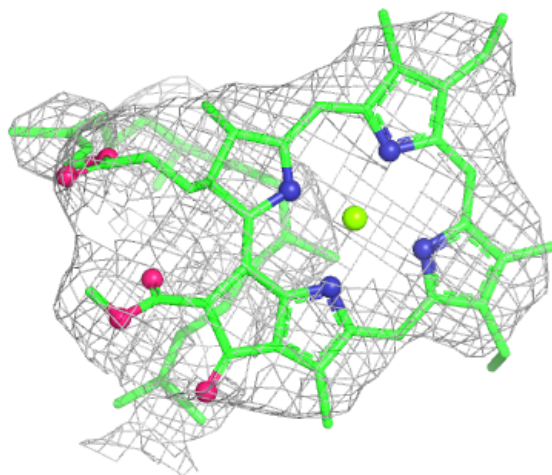
Electron density around CLA b 2518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



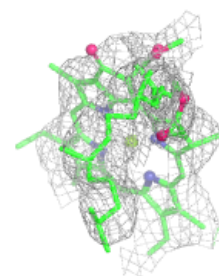
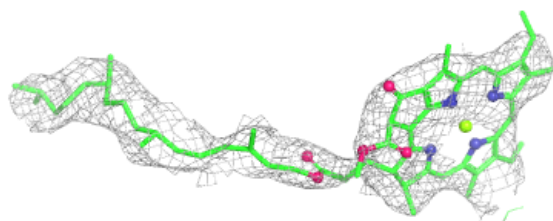
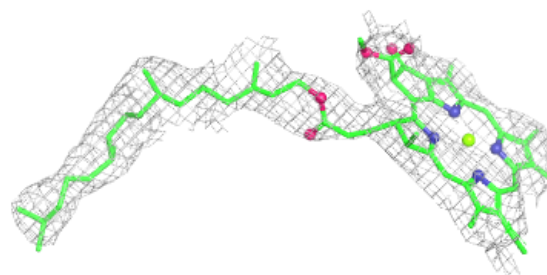
Electron density around CLA b 2512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

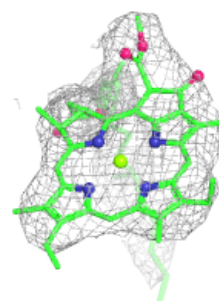
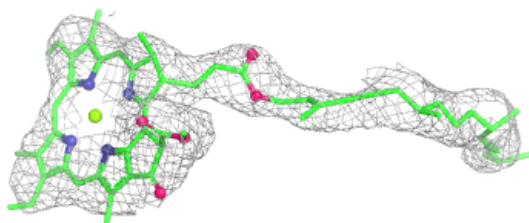
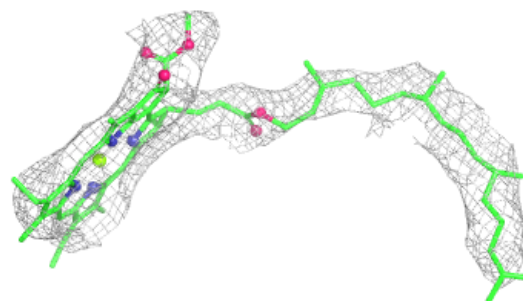


Electron density around CLA A 348:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

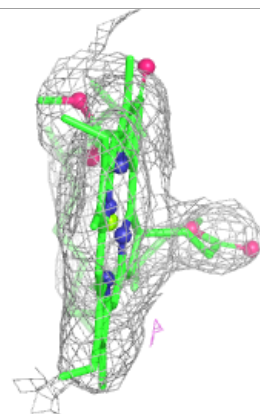
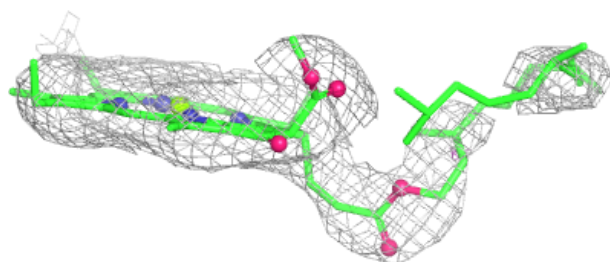
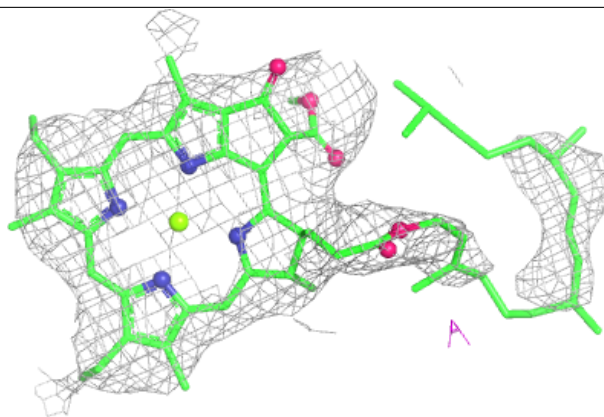
**Electron density around CLA d 2354:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

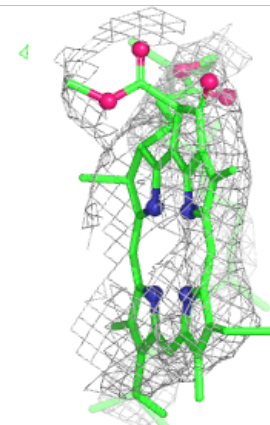
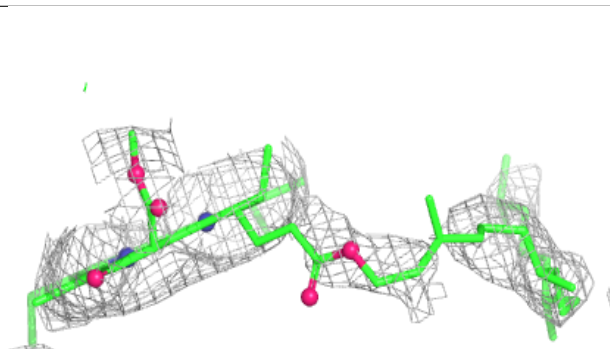
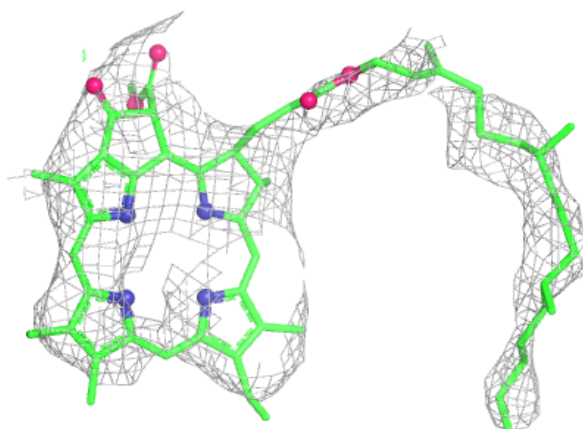


Electron density around CLA B 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

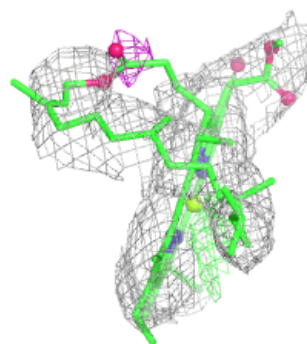
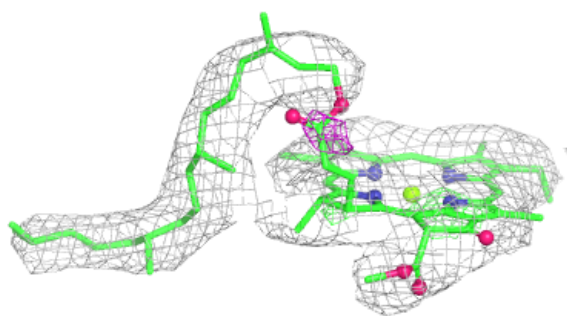
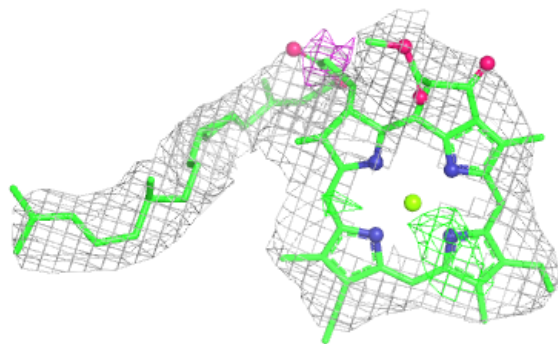
**Electron density around PHO A 351:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

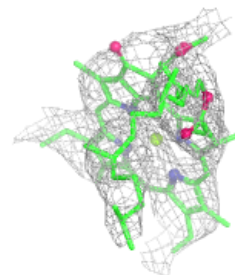
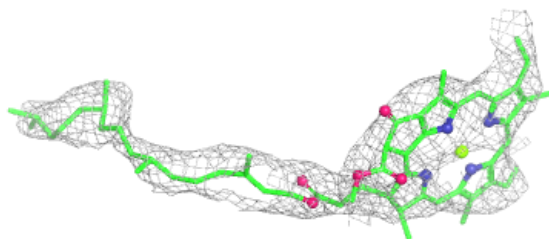
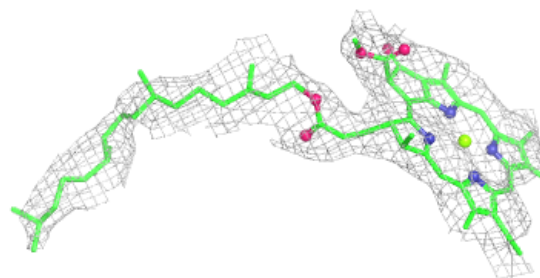


Electron density around CLA d 2355:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

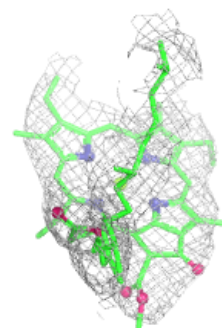
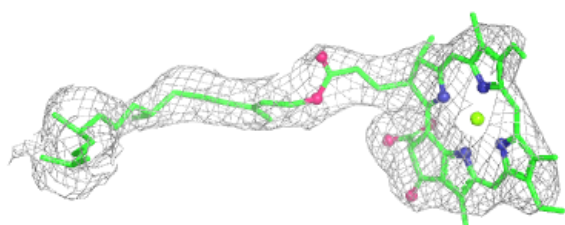
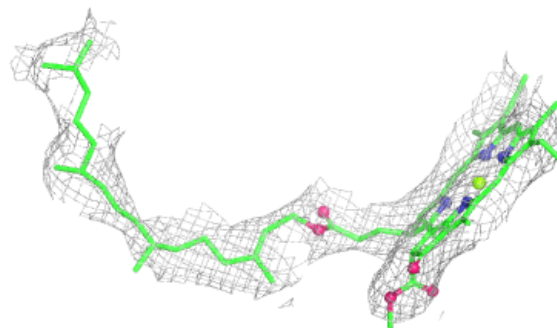
**Electron density around CLA a 2348:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

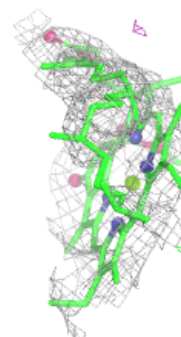
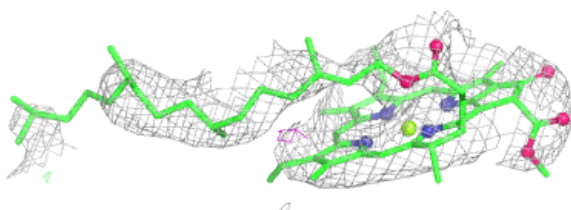
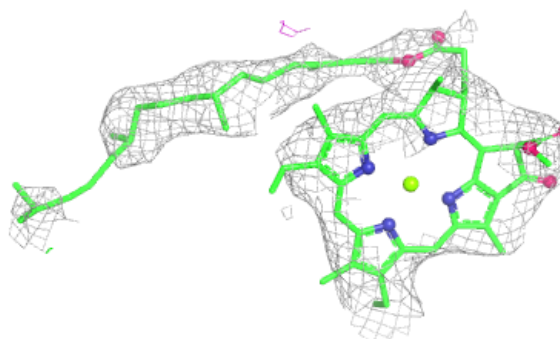


Electron density around CLA D 354:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

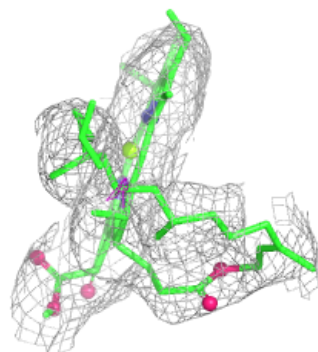
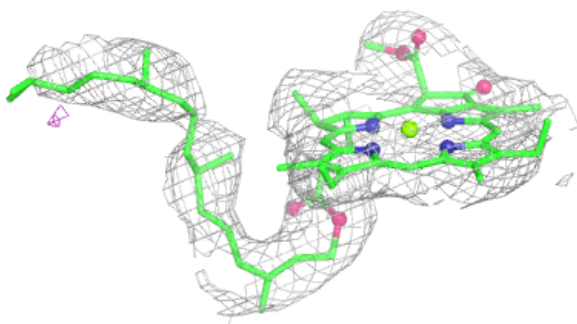
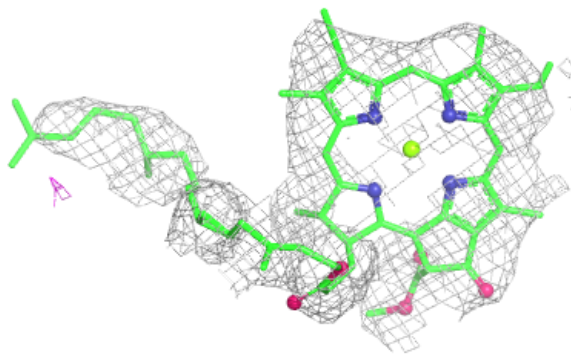
**Electron density around CLA C 479:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



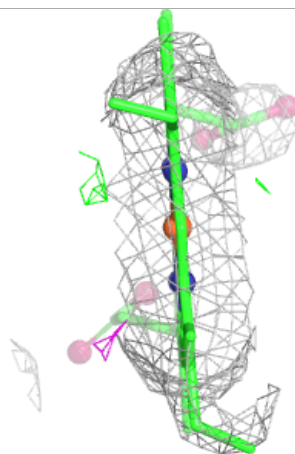
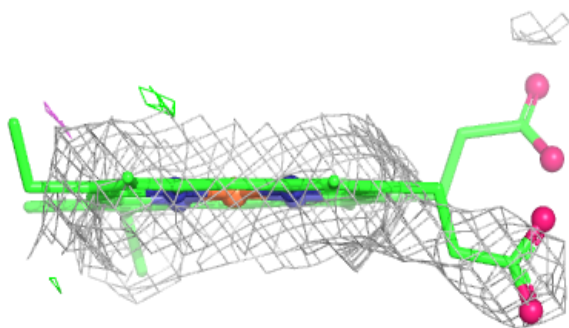
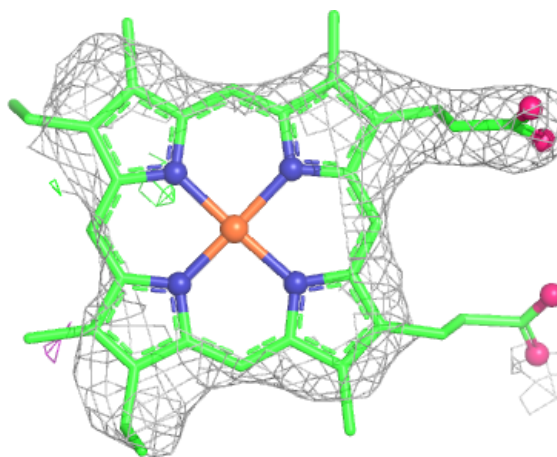
Electron density around CLA A 349:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



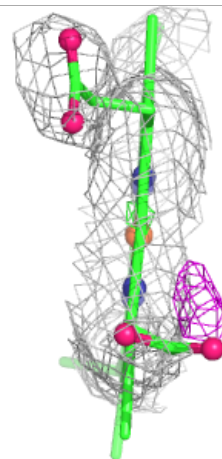
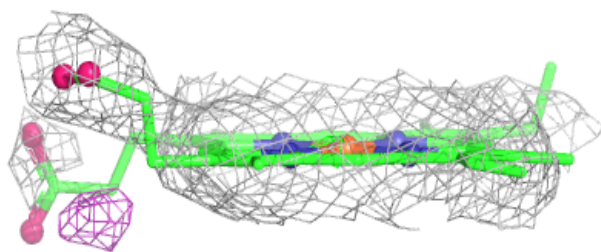
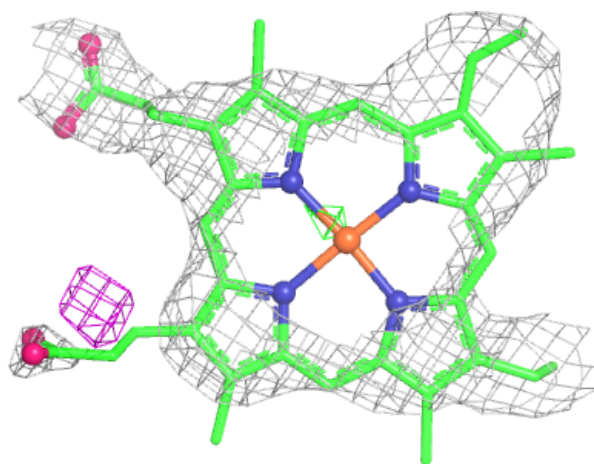
Electron density around HEC E 84:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



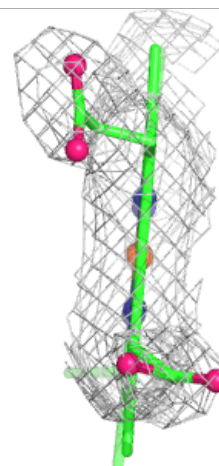
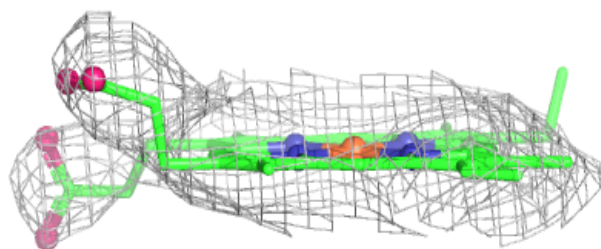
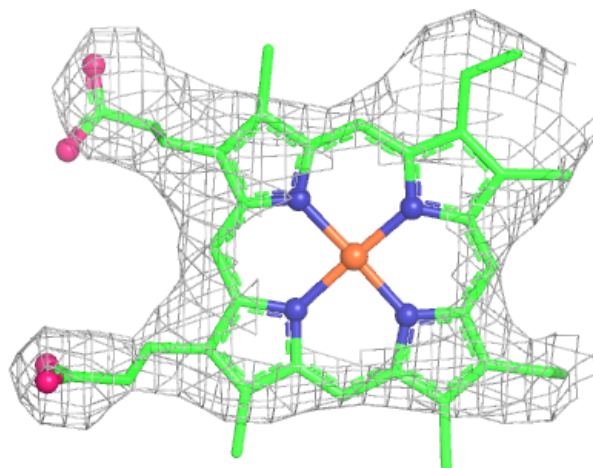
Electron density around HEC V 138:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC v 2138:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.