



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:26 PM EDT

PDB ID : 1M56 / pdb_00001m56
Title : Structure of cytochrome c oxidase from Rhodobactor sphaeroides (Wild Type)
Authors : Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.
Deposited on : 2002-07-08
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

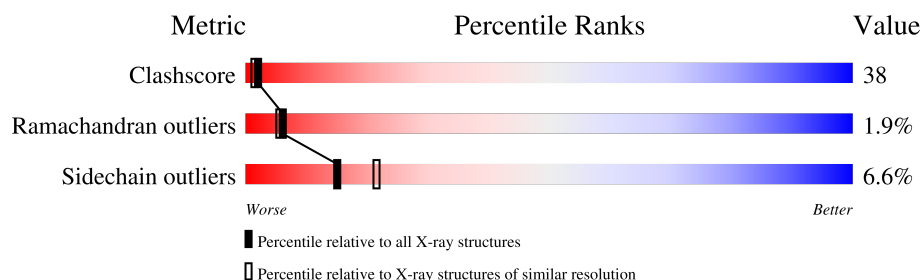
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	28% 45% 20% • •
1	G	566	29% 44% 20% • •
2	B	264	36% 46% 15% • •
2	H	264	37% 41% 19% • •
3	C	266	39% 46% 12% •
3	I	266	37% 48% 14% •
4	D	51	41% 24% 14% • 18%
4	J	51	27% 41% 10% • 18%

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
9	3PE	C	2013	-	-	X	-
9	3PE	D	2011	-	-	X	-
9	3PE	I	3010	-	-	X	-
9	3PE	I	3013	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18934 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 CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4322	2892	684	715	31			
1	G	547	Total	C	N	O	S	0	0	0
			4322	2892	684	715	31			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			
2	H	260	Total	C	N	O	S	0	0	0
			2046	1334	332	374	6			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			
3	I	265	Total	C	N	O	S	0	0	0
			2139	1448	342	337	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			
4	J	42	Total	C	N	O	S	0	0	0
			311	203	52	54	2			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	B	2	Total	Cu	0	0
			2	2		
5	G	1	Total	Cu	0	0
			1	1		
5	H	2	Total	Cu	0	0
			2	2		

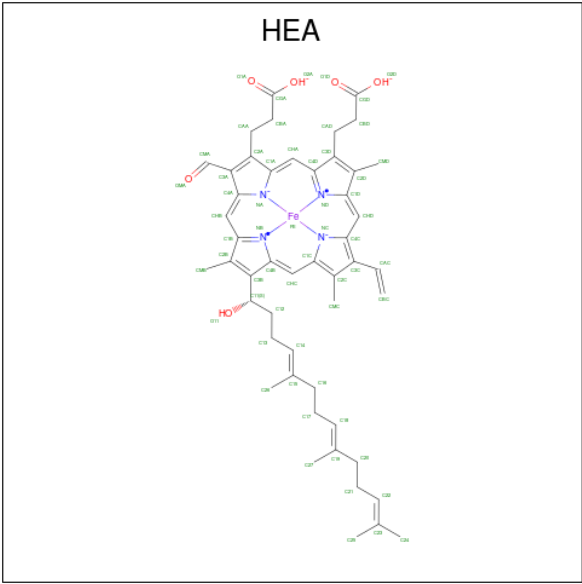
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	G	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

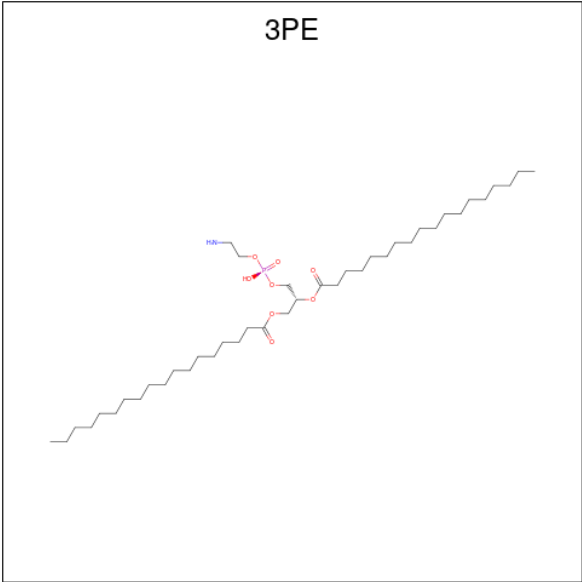
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	G	1	Total	Ca	0	0
			1	1		

- Molecule 8 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	G	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
8	G	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	I	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
9	J	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	101	Total 101	O 101	0	0
10	B	68	Total 68	O 68	0	0
10	C	39	Total 39	O 39	0	0
10	D	12	Total 12	O 12	0	0
10	G	106	Total 106	O 106	0	0
10	H	64	Total 64	O 64	0	0
10	I	38	Total 38	O 38	0	0
10	J	8	Total 8	O 8	0	0

3 Residue-property plots

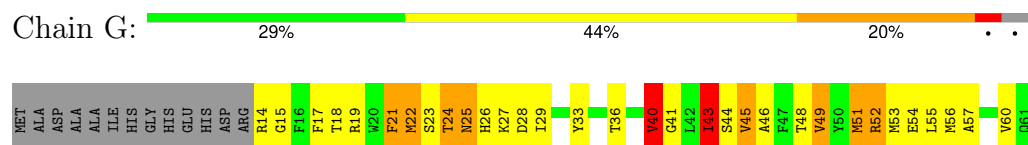
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

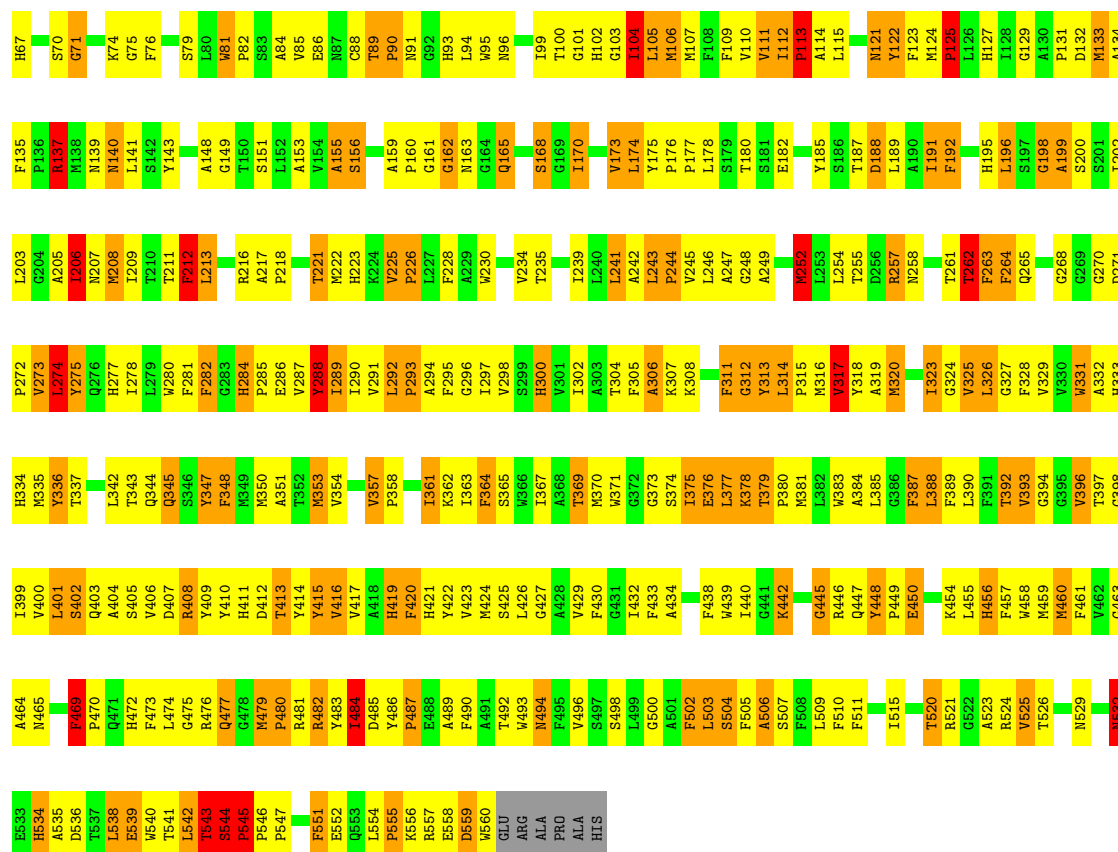
Note EDS was not executed.

• Molecule 1: CYTOCHROME C OXIDASE



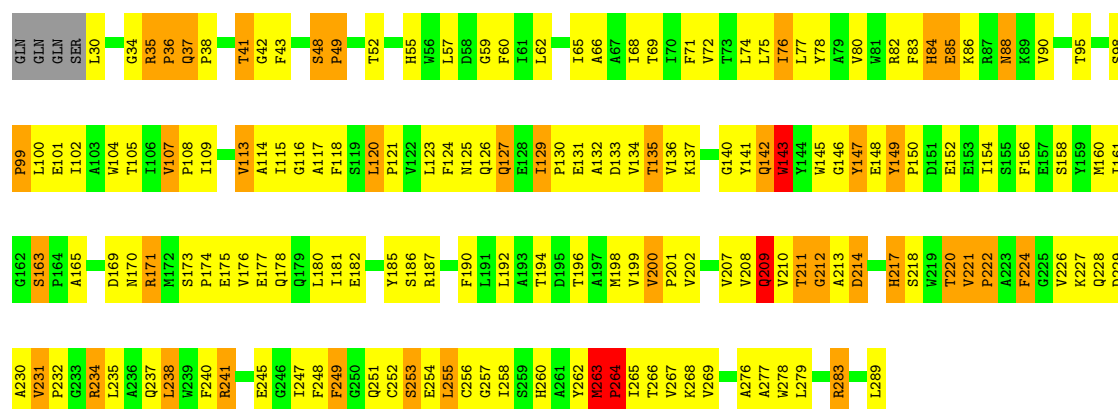
• Molecule 1: CYTOCHROME C OXIDASE



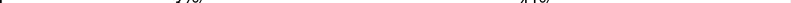


- Molecule 2: CYTOCHROME C OXIDASE

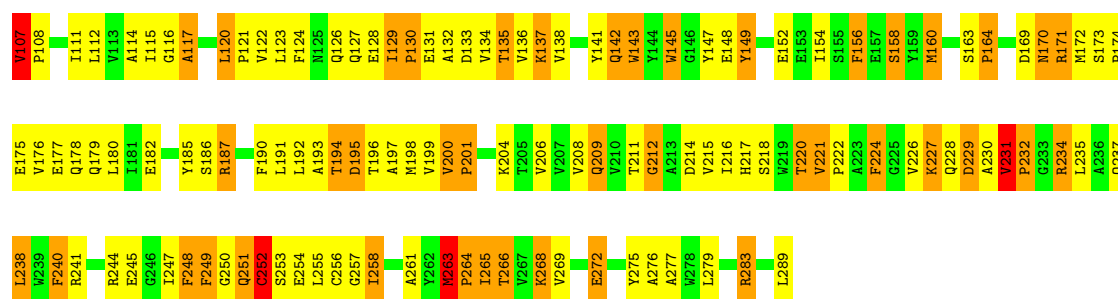
Chain B: 36% 46% 15% 3%



- Molecule 2: CYTOCHROME C OXIDASE

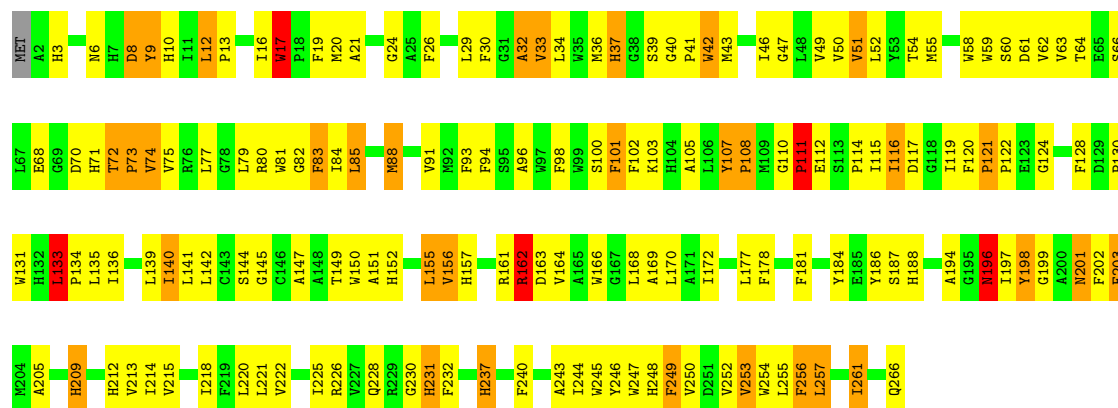
Chain H:  37% 41% 19% 3%





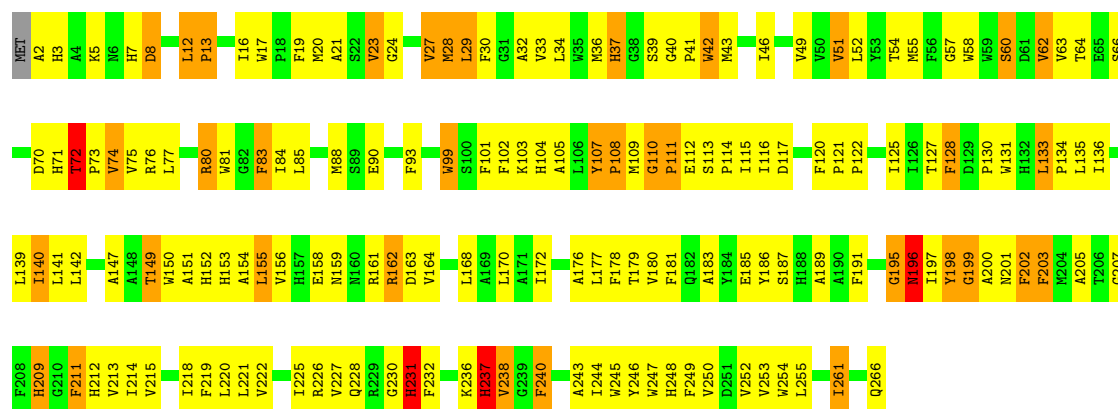
• Molecule 3: CYTOCHROME C OXIDASE

Chain C: 39% 46% 12%



• Molecule 3: CYTOCHROME C OXIDASE

Chain I: 37% 48% 14%



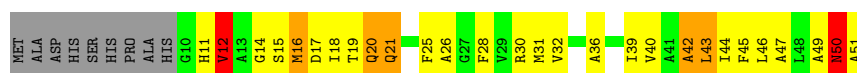
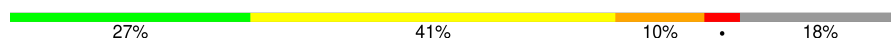
• Molecule 4: CYTOCHROME C OXIDASE

Chain D: 41% 24% 14% 18%



• Molecule 4: CYTOCHROME C OXIDASE

Chain J:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	340.36 Å 340.36 Å 89.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, CU, HEA, MG, CA

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	0.91	5/4482 (0.1%)	2.42	289/6114 (4.7%)
1	G	0.91	3/4482 (0.1%)	2.37	256/6114 (4.2%)
2	B	0.74	0/2105	2.16	83/2879 (2.9%)
2	H	0.74	0/2105	2.17	102/2879 (3.5%)
3	C	0.65	0/2232	1.93	78/3054 (2.6%)
3	I	0.69	0/2232	2.00	77/3054 (2.5%)
4	D	0.67	0/316	2.09	13/428 (3.0%)
4	J	0.68	0/316	2.09	15/428 (3.5%)
All	All	0.81	8/18270 (0.0%)	2.23	913/24950 (3.7%)

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	12
1	G	0	15
2	B	0	6
2	H	0	5
3	C	0	3
3	I	0	2
4	D	0	1
All	All	0	44

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	THR	C-O	7.80	1.34	1.23
1	G	544	SER	N-CA	-7.28	1.35	1.46
1	A	544	SER	N-CA	-7.23	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	THR	CA-C	-6.42	1.44	1.53
1	G	543	THR	CA-C	-6.16	1.44	1.53
1	G	543	THR	N-CA	5.68	1.53	1.45
1	A	543	THR	N-CA	5.10	1.52	1.45
1	A	373	GLY	N-CA	5.03	1.49	1.44

All (913) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	543	THR	CA-C-N	21.62	174.56	121.80
1	G	543	THR	C-N-CA	21.62	174.56	121.80
1	A	420	PHE	CA-CB-CG	19.87	133.67	113.80
1	G	420	PHE	CA-CB-CG	19.21	133.01	113.80
1	G	333	HIS	CA-CB-CG	17.59	131.38	113.80
1	A	544	SER	CA-C-O	-16.87	97.05	120.16
1	A	545	PRO	N-CA-CB	16.14	118.74	103.08
1	A	543	THR	CA-C-N	15.20	158.89	121.80
1	A	543	THR	C-N-CA	15.20	158.89	121.80
1	A	284	HIS	CA-CB-CG	-15.05	98.75	113.80
1	G	284	HIS	CA-CB-CG	-14.87	98.93	113.80
1	G	545	PRO	N-CA-CB	14.72	117.36	103.08
2	B	129	ILE	CA-C-O	13.88	127.34	119.15
1	G	544	SER	CA-C-O	-13.12	102.19	120.16
2	B	129	ILE	N-CA-C	12.88	120.77	107.76
1	A	534	HIS	CA-CB-CG	-12.82	100.98	113.80
3	C	8	ASP	CA-CB-CG	12.79	125.39	112.60
1	G	170	ILE	CB-CA-C	-12.33	99.73	111.44
1	G	165	GLN	OE1-CD-NE2	-12.19	110.41	122.60
2	B	60	PHE	CA-CB-CG	12.13	125.93	113.80
1	A	333	HIS	CA-CB-CG	11.74	125.54	113.80
2	H	129	ILE	N-CA-C	11.73	119.61	107.76
2	B	231	VAL	CA-C-O	11.52	127.22	119.38
1	A	544	SER	N-CA-CB	11.28	130.45	110.37
1	A	257	ARG	NE-CZ-NH1	-11.22	110.28	121.50
1	G	543	THR	N-CA-C	-11.16	95.49	110.55
1	A	175	TYR	CA-CB-CG	10.87	133.47	113.90
2	B	143	TRP	CB-CA-C	10.69	131.70	110.42
4	D	50	ASN	CA-CB-CG	-10.64	101.96	112.60
1	A	544	SER	CA-C-N	10.57	131.27	120.38
1	A	544	SER	C-N-CA	10.57	131.27	120.38
2	H	129	ILE	CA-C-O	10.30	125.23	119.15
1	G	552	GLU	N-CA-C	-10.17	100.15	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	ARG	CD-NE-CZ	10.15	138.61	124.40
2	B	211	THR	CA-C-N	-10.08	115.22	122.18
2	B	211	THR	C-N-CA	-10.08	115.22	122.18
2	B	217	HIS	CA-C-O	-10.04	110.26	121.40
2	H	231	VAL	CA-C-O	10.04	126.20	119.38
1	A	175	TYR	CA-C-O	10.00	131.05	120.25
1	A	15	GLY	N-CA-C	-9.94	100.50	111.93
1	A	545	PRO	CA-N-CD	-9.82	98.25	112.00
2	B	240	PHE	CA-CB-CG	9.80	123.60	113.80
1	A	288	TYR	N-CA-C	-9.70	101.20	113.23
1	A	380	PRO	O-C-N	-9.68	111.11	122.24
1	G	354	VAL	O-C-N	-9.66	112.42	121.89
1	G	465	ASN	CA-CB-CG	-9.64	102.96	112.60
3	I	102	PHE	CA-CB-CG	-9.60	104.20	113.80
3	I	128	PHE	CA-CB-CG	9.60	123.40	113.80
1	G	203	LEU	CA-C-O	9.56	130.86	120.82
2	H	240	PHE	CA-CB-CG	9.54	123.34	113.80
3	C	128	PHE	CA-CB-CG	9.51	123.31	113.80
1	A	420	PHE	CA-C-O	-9.49	108.41	119.61
1	G	545	PRO	CA-N-CD	-9.48	98.73	112.00
2	B	143	TRP	O-C-N	-9.39	110.10	122.59
2	H	251	GLN	OE1-CD-NE2	-9.32	113.28	122.60
1	A	151	SER	CA-C-O	9.26	130.54	120.82
2	H	231	VAL	N-CA-C	9.24	117.96	107.89
2	H	171	ARG	CD-NE-CZ	9.16	137.22	124.40
1	A	436	ILE	CA-C-O	9.09	131.73	121.18
2	H	256	CYS	CA-C-O	-9.08	108.91	118.90
1	G	482	ARG	CD-NE-CZ	9.05	137.07	124.40
3	C	94	PHE	CA-CB-CG	-9.05	104.75	113.80
1	G	348	PHE	O-C-N	-9.04	112.53	122.12
1	G	348	PHE	CA-C-O	8.99	130.09	120.55
2	H	200	VAL	CA-C-N	8.98	129.33	119.90
2	H	200	VAL	C-N-CA	8.98	129.33	119.90
2	B	231	VAL	N-CA-C	8.92	117.62	107.89
4	J	50	ASN	CA-CB-CG	-8.89	103.71	112.60
3	C	9	TYR	CA-C-O	-8.87	112.12	121.87
2	H	107	VAL	CA-CB-CG1	8.86	125.46	110.40
2	H	258	ILE	CB-CA-C	-8.85	99.17	111.65
1	G	199	ALA	CA-C-O	8.85	129.81	120.70
1	A	300	HIS	CA-CB-CG	-8.83	104.97	113.80
2	B	104	TRP	CA-CB-CG	8.81	130.35	113.60
2	H	143	TRP	CB-CA-C	8.80	127.93	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	238	VAL	N-CA-C	8.75	120.54	111.00
3	C	102	PHE	CA-CB-CG	-8.75	105.05	113.80
1	A	532	ASN	CA-C-O	-8.73	111.97	121.31
3	I	8	ASP	CA-CB-CG	8.72	121.33	112.60
1	G	369	THR	CA-CB-OG1	-8.70	96.56	109.60
1	A	545	PRO	CA-C-N	8.66	125.98	119.66
1	A	545	PRO	C-N-CA	8.66	125.98	119.66
1	A	552	GLU	N-CA-C	-8.62	101.83	111.14
2	B	249	PHE	CA-CB-CG	8.62	122.42	113.80
4	D	40	VAL	CA-C-O	-8.61	112.46	121.41
1	G	542	LEU	CA-C-O	-8.60	110.77	121.78
1	A	375	ILE	N-CA-C	8.57	120.62	108.36
1	A	265	GLN	CA-C-O	8.55	127.43	119.99
1	A	411	HIS	CA-CB-CG	-8.55	105.25	113.80
1	G	105	LEU	CA-C-O	8.54	129.79	120.82
1	A	216	ARG	CD-NE-CZ	8.54	136.35	124.40
2	H	224	PHE	CA-CB-CG	-8.51	105.29	113.80
3	I	40	GLY	CA-C-N	8.47	128.60	119.28
3	I	40	GLY	C-N-CA	8.47	128.60	119.28
1	G	479	MET	CA-C-N	8.46	128.98	119.92
1	G	479	MET	C-N-CA	8.46	128.98	119.92
1	G	252	MET	O-C-N	-8.40	113.22	122.12
2	B	171	ARG	CD-NE-CZ	8.39	136.14	124.40
1	A	543	THR	N-CA-C	-8.38	99.80	110.19
1	G	257	ARG	NE-CZ-NH1	-8.36	113.14	121.50
1	G	281	PHE	N-CA-C	-8.36	102.53	112.89
1	G	434	ALA	CA-C-O	-8.34	111.98	120.90
1	G	534	HIS	CA-CB-CG	-8.29	105.51	113.80
2	B	140	GLY	CA-C-O	8.29	128.77	120.98
2	H	283	ARG	CD-NE-CZ	8.29	136.01	124.40
1	A	178	LEU	O-C-N	-8.28	113.15	122.09
3	C	17	TRP	CB-CA-C	8.23	126.39	110.17
1	G	401	LEU	O-C-N	-8.23	113.39	122.12
1	A	96	ASN	CA-C-O	-8.22	111.75	120.63
2	H	60	PHE	CA-CB-CG	8.12	121.92	113.80
2	H	261	ALA	O-C-N	-8.12	110.58	122.43
1	A	81	TRP	CA-C-O	8.09	127.08	119.72
1	G	288	TYR	O-C-N	-8.09	111.30	122.46
1	A	137	ARG	NE-CZ-NH2	8.09	126.48	119.20
1	G	106	MET	CA-C-O	-8.07	112.53	121.00
1	A	521	ARG	NE-CZ-NH2	-8.06	111.94	119.20
2	B	234	ARG	NE-CZ-NH2	-8.06	111.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	162	ARG	N-CA-C	-8.06	102.08	111.03
1	G	502	PHE	CA-CB-CG	8.06	121.86	113.80
2	B	209	GLN	CA-C-O	-8.04	111.76	120.36
2	B	66	ALA	N-CA-C	-8.01	101.63	111.40
2	B	224	PHE	CA-CB-CG	-8.01	105.79	113.80
1	G	446	ARG	NE-CZ-NH2	8.01	126.41	119.20
3	C	83	PHE	CA-CB-CG	-7.98	105.82	113.80
1	A	344	GLN	OE1-CD-NE2	-7.97	114.62	122.60
1	A	347	TYR	N-CA-CB	7.97	121.82	109.94
1	G	472	HIS	N-CA-C	-7.96	102.54	111.14
2	H	217	HIS	CA-C-O	-7.96	112.59	121.51
1	A	397	THR	CA-C-N	7.95	128.97	119.99
1	A	397	THR	C-N-CA	7.95	128.97	119.99
2	H	261	ALA	CA-C-O	7.95	129.29	119.11
1	A	278	ILE	CA-C-O	-7.88	110.50	120.03
1	A	546	PRO	N-CA-C	7.85	118.00	110.47
1	A	303	ALA	CA-C-O	7.84	128.78	120.70
1	A	326	LEU	O-C-N	-7.84	113.21	122.15
2	B	88	ASN	OD1-CG-ND2	-7.81	114.79	122.60
2	H	88	ASN	CA-C-O	-7.79	111.91	120.33
1	A	369	THR	CA-CB-CG2	7.79	123.75	110.50
1	G	534	HIS	CA-C-O	7.79	128.86	119.43
1	A	324	GLY	O-C-N	-7.79	114.62	122.17
1	G	56	MET	CA-C-O	7.76	129.61	121.07
1	A	229	ALA	O-C-N	-7.76	113.90	122.12
2	B	228	GLN	OE1-CD-NE2	-7.76	114.84	122.60
1	G	544	SER	N-CA-C	7.75	126.93	109.81
1	G	93	HIS	CA-CB-CG	-7.74	106.06	113.80
2	H	164	PRO	CA-C-N	7.72	132.96	120.60
2	H	164	PRO	C-N-CA	7.72	132.96	120.60
2	H	195	ASP	CA-CB-CG	7.69	120.29	112.60
2	H	221	VAL	N-CA-CB	7.69	121.97	111.21
1	G	532	ASN	CA-CB-CG	-7.68	104.92	112.60
2	H	107	VAL	CB-CA-C	7.68	125.35	111.36
1	G	465	ASN	OD1-CG-ND2	7.67	130.27	122.60
2	H	251	GLN	CA-C-O	-7.66	110.79	120.14
1	A	212	PHE	CA-CB-CG	7.64	121.44	113.80
2	H	137	LYS	N-CA-CB	7.64	122.45	110.84
2	H	90	VAL	CB-CA-C	-7.63	102.73	110.13
1	G	155	ALA	CA-C-N	7.62	131.26	120.28
1	G	155	ALA	C-N-CA	7.62	131.26	120.28
2	H	89	LYS	CA-C-N	-7.61	116.71	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	89	LYS	C-N-CA	-7.61	116.71	123.33
1	G	389	PHE	N-CA-C	7.60	119.47	111.03
1	G	175	TYR	CA-CB-CG	7.58	127.55	113.90
1	G	156	SER	CA-C-O	7.56	128.64	120.10
1	G	487	PRO	CA-C-O	7.56	134.36	120.60
2	B	283	ARG	CD-NE-CZ	7.56	134.98	124.40
1	A	228	PHE	N-CA-C	-7.55	103.00	111.07
4	D	46	LEU	CA-C-O	7.54	129.37	120.92
1	A	314	LEU	CA-C-O	7.51	126.00	118.79
3	C	198	TYR	CA-C-N	7.50	128.25	120.00
3	C	198	TYR	C-N-CA	7.50	128.25	120.00
1	A	271	ASP	O-C-N	-7.50	116.77	121.27
1	A	326	LEU	CA-C-O	7.49	128.36	120.42
2	H	232	PRO	O-C-N	-7.47	113.74	122.85
1	G	317	VAL	CA-C-O	-7.45	112.53	121.18
1	A	472	HIS	CA-CB-CG	7.45	121.25	113.80
1	A	124	MET	CA-C-N	7.45	126.98	119.24
1	A	124	MET	C-N-CA	7.45	126.98	119.24
3	C	40	GLY	CA-C-N	7.44	127.81	119.32
3	C	40	GLY	C-N-CA	7.44	127.81	119.32
2	B	231	VAL	CB-CA-C	-7.43	102.42	110.37
4	J	42	ALA	CA-C-O	7.42	128.49	120.55
1	G	212	PHE	CA-CB-CG	7.40	121.20	113.80
1	G	228	PHE	CA-CB-CG	-7.40	106.40	113.80
1	A	461	PHE	N-CA-C	-7.39	103.16	111.14
2	B	262	TYR	O-C-N	-7.38	112.77	122.59
1	A	482	ARG	CD-NE-CZ	7.37	134.72	124.40
1	A	420	PHE	O-C-N	7.36	131.90	122.33
1	A	503	LEU	O-C-N	7.36	131.33	122.27
1	A	49	VAL	CB-CA-C	7.36	122.10	112.24
1	G	536	ASP	N-CA-C	7.35	121.83	113.02
1	A	341	SER	CA-C-O	-7.34	113.35	121.87
1	G	300	HIS	CA-CB-CG	-7.34	106.46	113.80
1	A	309	PRO	O-C-N	-7.33	113.58	122.89
1	G	284	HIS	CE1-NE2-CD2	7.33	116.33	109.00
3	I	17	TRP	CB-CA-C	7.32	124.59	110.17
2	B	200	VAL	CA-C-N	7.32	128.98	119.84
2	B	200	VAL	C-N-CA	7.32	128.98	119.84
1	A	508	PHE	CA-CB-CG	-7.30	106.50	113.80
1	A	471	GLN	O-C-N	-7.30	112.88	122.59
1	A	325	VAL	CB-CA-C	-7.29	102.16	112.22
3	C	261	ILE	N-CA-C	7.29	118.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	HIS	N-CA-C	-7.28	103.34	111.71
1	G	305	PHE	N-CA-C	7.27	121.74	113.01
1	A	225	VAL	O-C-N	7.27	129.38	121.10
3	I	12	LEU	N-CA-C	7.27	121.29	110.32
1	G	347	TYR	N-CA-CB	7.26	120.76	109.94
3	I	83	PHE	CA-CB-CG	-7.25	106.55	113.80
2	H	160	MET	CA-C-O	-7.25	113.89	121.87
3	I	70	ASP	CA-C-N	7.25	132.95	122.08
3	I	70	ASP	C-N-CA	7.25	132.95	122.08
1	A	479	MET	CA-C-O	7.24	126.61	119.51
2	B	171	ARG	NE-CZ-NH1	7.24	128.74	121.50
1	A	36	THR	O-C-N	-7.23	114.51	122.03
2	H	104	TRP	CA-CB-CG	7.23	127.33	113.60
2	H	129	ILE	CA-C-N	7.22	128.20	120.11
2	H	129	ILE	C-N-CA	7.22	128.20	120.11
1	A	199	ALA	N-CA-C	-7.21	102.60	111.40
1	A	552	GLU	CA-C-O	7.20	128.12	120.70
1	A	532	ASN	CA-CB-CG	-7.19	105.41	112.60
1	G	312	GLY	O-C-N	-7.19	113.93	122.34
1	A	477	GLN	OE1-CD-NE2	-7.18	115.42	122.60
2	H	231	VAL	O-C-N	-7.17	114.95	121.41
2	H	133	ASP	N-CA-C	-7.16	105.08	114.31
1	A	175	TYR	O-C-N	-7.15	113.42	121.43
1	A	178	LEU	N-CA-C	-7.14	103.43	111.14
1	A	545	PRO	N-CD-CG	7.14	113.91	103.20
1	G	125	PRO	O-C-N	-7.14	113.00	122.64
1	A	479	MET	O-C-N	-7.13	115.11	121.31
1	G	543	THR	CA-C-O	-7.10	113.43	121.81
3	I	205	ALA	CA-C-O	-7.10	113.58	120.90
1	A	305	PHE	N-CA-C	7.09	121.53	113.01
2	H	215	VAL	CA-C-N	-7.09	112.78	122.91
2	H	215	VAL	C-N-CA	-7.09	112.78	122.91
2	B	107	VAL	CA-C-N	7.08	126.91	119.05
2	B	107	VAL	C-N-CA	7.08	126.91	119.05
1	G	387	PHE	O-C-N	-7.07	114.74	122.09
1	G	168	SER	O-C-N	-7.06	113.71	122.68
3	I	231	HIS	CA-CB-CG	7.06	120.86	113.80
1	A	354	VAL	O-C-N	-7.05	114.75	121.87
1	A	369	THR	CA-CB-OG1	-7.05	99.02	109.60
1	A	322	ALA	N-CA-C	-7.05	103.29	110.97
1	G	203	LEU	O-C-N	-7.04	114.81	122.07
2	B	149	TYR	CA-C-N	7.03	127.63	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	149	TYR	C-N-CA	7.03	127.63	119.47
1	G	109	PHE	N-CA-C	7.02	123.48	113.02
1	G	121	ASN	CA-CB-CG	-7.01	105.59	112.60
1	A	413	THR	CA-C-O	-7.01	113.12	121.60
1	G	472	HIS	CA-CB-CG	6.98	120.78	113.80
3	I	17	TRP	CA-C-N	6.96	127.25	119.32
3	I	17	TRP	C-N-CA	6.96	127.25	119.32
1	A	126	LEU	CA-C-O	-6.95	113.46	120.90
3	C	85	LEU	N-CA-C	-6.95	103.47	112.23
1	G	288	TYR	CZ-CE2-CD2	6.94	132.10	119.60
2	B	107	VAL	CA-CB-CG1	6.94	122.20	110.40
1	G	265	GLN	CA-C-N	6.94	127.52	119.47
1	G	265	GLN	C-N-CA	6.94	127.52	119.47
1	G	242	ALA	CA-C-O	-6.93	111.49	119.60
1	G	484	ILE	CA-C-O	6.93	125.54	118.96
3	I	207	GLY	CA-C-O	-6.92	113.32	120.66
1	A	421	HIS	CA-CB-CG	6.92	120.72	113.80
2	B	48	SER	CA-C-N	6.91	126.72	119.05
2	B	48	SER	C-N-CA	6.91	126.72	119.05
1	A	41	GLY	N-CA-C	-6.90	104.14	112.49
2	B	107	VAL	CB-CA-C	6.88	123.88	111.36
1	A	324	GLY	CA-C-N	6.87	130.18	120.42
1	A	324	GLY	C-N-CA	6.87	130.18	120.42
1	G	506	ALA	CA-C-O	6.87	127.78	120.70
2	H	256	CYS	O-C-N	6.87	130.24	122.27
1	A	170	ILE	CB-CA-C	-6.87	104.94	111.05
1	G	545	PRO	N-CA-C	-6.86	102.33	110.70
1	A	168	SER	CB-CA-C	-6.86	99.64	111.30
1	A	185	TYR	CA-CB-CG	6.86	126.24	113.90
1	G	284	HIS	CB-CG-ND1	-6.85	112.42	122.70
3	I	74	VAL	N-CA-CB	6.84	119.33	110.57
1	A	479	MET	CA-C-N	6.83	126.79	120.03
1	A	479	MET	C-N-CA	6.83	126.79	120.03
1	A	454	LYS	O-C-N	6.83	129.93	122.15
1	G	241	LEU	CA-C-O	6.83	126.27	118.97
3	C	74	VAL	N-CA-CB	6.82	119.31	110.57
3	I	72	THR	N-CA-CB	-6.82	100.14	110.03
3	C	6	ASN	CA-CB-CG	6.81	119.41	112.60
1	G	14	ARG	CA-C-N	-6.81	113.63	120.10
1	G	14	ARG	C-N-CA	-6.81	113.63	120.10
1	A	196	LEU	N-CA-CB	-6.81	99.85	110.06
2	H	48	SER	CA-C-N	6.80	126.60	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	48	SER	C-N-CA	6.80	126.60	119.05
1	A	170	ILE	O-C-N	-6.79	116.75	121.98
1	A	49	VAL	N-CA-C	-6.77	103.62	111.00
1	A	239	ILE	O-C-N	-6.77	114.97	121.94
3	C	110	GLY	CA-C-N	6.76	128.30	119.84
3	C	110	GLY	C-N-CA	6.76	128.30	119.84
3	I	211	PHE	CA-C-O	6.76	127.59	120.42
1	A	49	VAL	CA-C-O	6.76	127.94	120.71
3	C	98	PHE	CA-CB-CG	-6.75	107.05	113.80
1	G	413	THR	CA-C-O	-6.75	113.14	121.78
1	A	323	ILE	N-CA-C	6.75	117.25	110.23
2	H	263	MET	N-CA-CB	6.74	122.37	110.37
1	A	392	THR	N-CA-C	-6.74	103.18	111.40
3	C	201	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	529	ASN	OD1-CG-ND2	6.73	129.33	122.60
1	A	288	TYR	CZ-CE2-CD2	6.72	131.70	119.60
1	G	206	ILE	CA-C-O	6.72	128.29	121.17
3	I	28	MET	CA-C-O	-6.71	113.69	121.07
1	A	543	THR	N-CA-CB	-6.71	101.13	110.25
4	J	12	VAL	N-CA-CB	6.70	122.29	111.23
2	B	133	ASP	N-CA-C	-6.70	105.67	114.31
1	G	295	PHE	CA-C-N	6.69	127.36	119.94
1	G	295	PHE	C-N-CA	6.69	127.36	119.94
1	G	469	PHE	N-CA-CB	6.68	118.31	110.42
1	G	170	ILE	N-CA-C	6.68	117.31	111.56
1	A	111	VAL	N-CA-C	6.67	118.27	111.00
1	G	245	VAL	O-C-N	-6.67	115.16	121.90
1	A	202	ILE	O-C-N	-6.67	115.38	121.91
1	G	364	PHE	O-C-N	-6.67	115.09	122.03
4	D	49	ALA	CA-C-O	-6.67	113.48	120.55
4	J	25	PHE	CA-CB-CG	6.66	120.46	113.80
2	B	268	LYS	CA-C-N	-6.65	114.48	123.12
2	B	268	LYS	C-N-CA	-6.65	114.48	123.12
3	I	93	PHE	CA-CB-CG	6.64	120.44	113.80
1	G	81	TRP	CA-C-O	6.63	126.23	119.86
1	G	348	PHE	CA-CB-CG	-6.63	107.17	113.80
2	H	65	ILE	CB-CG1-CD1	6.62	127.70	113.80
1	A	321	VAL	O-C-N	-6.61	115.19	121.87
1	G	545	PRO	N-CD-CG	6.61	113.12	103.20
1	G	274	LEU	N-CA-C	-6.61	104.08	111.28
2	H	90	VAL	O-C-N	6.61	127.78	121.11
3	I	195	GLY	N-CA-C	6.61	128.83	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	216	ARG	CD-NE-CZ	6.60	133.65	124.40
2	H	248	PHE	CA-C-O	-6.60	113.23	120.36
2	B	129	ILE	CA-C-N	6.59	128.07	119.84
2	B	129	ILE	C-N-CA	6.59	128.07	119.84
2	B	113	VAL	CA-C-N	6.58	129.94	120.79
2	B	113	VAL	C-N-CA	6.58	129.94	120.79
2	B	133	ASP	CA-C-O	6.58	126.08	118.77
1	A	120	GLY	O-C-N	-6.58	114.15	122.70
1	G	438	PHE	O-C-N	6.58	129.65	122.15
1	G	345	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	320	MET	CA-CB-CG	-6.56	100.97	114.10
1	G	137	ARG	NE-CZ-NH1	-6.52	114.98	121.50
1	A	226	PRO	CA-C-O	-6.52	113.80	121.95
1	A	93	HIS	CA-C-O	-6.51	112.91	120.20
3	C	29	LEU	CA-C-O	-6.51	112.49	119.97
1	G	66	GLU	CB-CG-CD	6.51	123.66	112.60
3	C	101	PHE	CA-C-O	-6.50	113.92	121.07
1	A	389	PHE	CA-C-O	6.50	127.59	120.90
2	B	90	VAL	O-C-N	6.50	127.26	121.41
2	H	249	PHE	N-CA-C	6.49	120.04	109.59
3	C	116	ILE	N-CA-C	6.49	117.20	108.11
1	A	389	PHE	O-C-N	-6.49	115.03	122.03
1	A	284	HIS	O-C-N	-6.48	113.86	121.32
1	A	135	PHE	CA-C-N	6.47	125.70	118.97
1	A	135	PHE	C-N-CA	6.47	125.70	118.97
1	A	289	ILE	CA-C-O	6.47	127.46	120.47
1	A	315	PRO	O-C-N	-6.47	114.34	122.17
1	A	227	LEU	N-CA-CB	-6.46	100.27	110.28
1	A	259	PHE	CA-CB-CG	-6.46	107.34	113.80
1	A	319	ALA	N-CA-CB	6.46	119.37	110.01
1	A	543	THR	CA-C-O	-6.45	115.24	122.01
3	I	40	GLY	O-C-N	-6.45	115.32	121.77
1	G	71	GLY	N-CA-C	-6.45	103.61	112.25
4	D	30	ARG	NH1-CZ-NH2	6.44	127.67	119.30
1	G	544	SER	CA-C-N	6.44	127.01	120.38
1	G	544	SER	C-N-CA	6.44	127.01	120.38
1	G	288	TYR	N-CA-C	-6.43	104.91	112.89
1	G	552	GLU	CA-CB-CG	6.43	126.96	114.10
3	I	202	PHE	CA-CB-CG	-6.43	107.37	113.80
2	H	171	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	A	261	THR	CA-C-N	-6.41	113.25	122.67
1	A	261	THR	C-N-CA	-6.41	113.25	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	113	PRO	CA-C-N	6.41	131.54	120.58
1	G	113	PRO	C-N-CA	6.41	131.54	120.58
1	A	115	LEU	O-C-N	6.40	130.56	122.23
2	H	149	TYR	CA-C-N	6.40	126.61	119.32
2	H	149	TYR	C-N-CA	6.40	126.61	119.32
3	I	80	ARG	CA-C-O	6.39	127.33	120.55
2	B	76	ILE	O-C-N	6.38	128.86	121.96
3	I	90	GLU	CA-C-O	-6.38	114.13	120.82
1	A	104	ILE	CA-C-O	-6.37	114.32	120.95
3	C	237	HIS	CA-CB-CG	6.37	120.17	113.80
3	I	189	ALA	CA-C-O	-6.37	114.62	121.56
1	A	446	ARG	NE-CZ-NH1	-6.37	115.13	121.50
1	G	554	LEU	CA-C-N	6.37	127.80	119.84
1	G	554	LEU	C-N-CA	6.37	127.80	119.84
3	I	60	SER	CA-C-O	6.36	127.50	120.82
1	A	256	ASP	O-C-N	-6.36	114.14	122.59
1	A	472	HIS	N-CA-C	-6.35	104.36	111.28
1	G	348	PHE	N-CA-C	6.34	118.19	111.28
3	I	40	GLY	N-CA-C	6.34	125.27	112.34
2	B	212	GLY	CA-C-O	-6.34	115.41	121.11
1	A	228	PHE	CA-CB-CG	-6.34	107.46	113.80
3	C	100	SER	CA-CB-OG	-6.33	98.44	111.10
1	A	196	LEU	CB-CA-C	6.33	121.44	110.68
1	G	113	PRO	O-C-N	-6.32	114.97	122.24
2	H	179	GLN	CA-C-O	6.32	127.46	120.63
1	A	436	ILE	O-C-N	-6.32	115.18	121.94
1	A	170	ILE	CA-C-O	6.31	126.42	120.80
2	H	107	VAL	CA-C-N	6.31	126.05	119.05
2	H	107	VAL	C-N-CA	6.31	126.05	119.05
2	H	234	ARG	NH1-CZ-NH2	6.30	127.49	119.30
1	A	419	HIS	CA-CB-CG	6.30	120.10	113.80
1	A	521	ARG	NH1-CZ-NH2	6.30	127.49	119.30
1	G	53	MET	N-CA-C	-6.29	104.11	110.97
1	G	273	VAL	O-C-N	-6.29	115.52	121.87
1	G	392	THR	CA-CB-OG1	-6.29	100.17	109.60
1	G	551	PHE	N-CA-C	6.28	120.33	111.92
1	A	354	VAL	N-CA-C	6.28	118.89	111.05
1	A	343	THR	CA-CB-OG1	6.27	119.00	109.60
2	H	112	LEU	CA-C-O	-6.27	114.19	120.90
1	G	284	HIS	CG-CD2-NE2	-6.26	100.94	107.20
2	B	131	GLU	CA-C-O	-6.26	113.23	120.49
1	A	552	GLU	CA-CB-CG	6.26	126.61	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	297	ILE	CB-CA-C	-6.25	103.70	112.14
3	C	37	HIS	CA-CB-CG	-6.25	107.55	113.80
1	G	536	ASP	N-CA-CB	-6.25	101.41	110.47
3	C	42	TRP	CA-CB-CG	-6.24	101.74	113.60
1	A	159	ALA	CA-C-N	6.24	127.64	119.84
1	A	159	ALA	C-N-CA	6.24	127.64	119.84
1	A	305	PHE	CA-CB-CG	-6.24	107.56	113.80
1	G	15	GLY	N-CA-C	-6.23	104.76	111.93
3	C	10	HIS	CA-C-O	-6.23	114.06	120.54
1	A	348	PHE	CA-CB-CG	-6.22	107.58	113.80
3	I	13	PRO	N-CA-C	-6.21	103.12	110.70
2	B	90	VAL	CB-CA-C	-6.21	103.73	110.37
1	A	434	ALA	N-CA-C	-6.20	104.43	111.07
1	A	81	TRP	CA-C-N	6.20	126.22	119.90
1	A	81	TRP	C-N-CA	6.20	126.22	119.90
1	A	534	HIS	CA-C-O	6.20	126.55	119.18
1	A	505	PHE	N-CA-C	-6.18	104.44	112.23
1	A	245	VAL	CA-C-O	-6.18	113.96	120.57
1	A	162	GLY	CA-C-N	6.18	131.36	122.40
1	A	162	GLY	C-N-CA	6.18	131.36	122.40
2	H	75	LEU	N-CA-C	-6.17	103.16	112.04
1	G	396	VAL	N-CA-CB	-6.17	103.67	110.51
1	G	440	ILE	N-CA-C	6.16	116.90	110.62
2	H	73	THR	CA-C-O	6.16	127.08	120.24
1	A	233	PHE	CA-C-O	6.16	127.04	120.70
1	A	415	TYR	CA-C-O	6.16	126.95	119.38
1	A	484	ILE	N-CA-C	-6.16	106.72	113.43
1	G	196	LEU	O-C-N	-6.16	114.40	122.59
1	G	258	ASN	OD1-CG-ND2	6.16	128.76	122.60
3	C	24	GLY	CA-C-N	6.15	128.52	120.28
3	C	24	GLY	C-N-CA	6.15	128.52	120.28
1	G	107	MET	N-CA-C	6.15	120.04	112.54
3	I	207	GLY	O-C-N	6.15	128.15	122.19
1	G	296	GLY	CA-C-O	-6.14	114.37	121.00
3	C	162	ARG	N-CA-C	-6.14	103.91	111.40
1	G	354	VAL	CA-C-N	6.14	131.61	121.54
1	G	354	VAL	C-N-CA	6.14	131.61	121.54
3	C	116	ILE	CB-CA-C	-6.13	101.55	110.63
1	A	325	VAL	CA-C-O	-6.13	114.36	120.85
2	B	36	PRO	CA-C-O	-6.13	114.57	121.43
2	B	207	VAL	CA-C-O	-6.13	113.91	120.59
3	C	133	LEU	CA-C-N	6.13	125.61	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	133	LEU	C-N-CA	6.13	125.61	119.24
2	H	232	PRO	CB-CA-C	6.12	119.42	111.64
1	A	502	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	153	ALA	CA-C-O	-6.12	114.07	120.55
1	G	226	PRO	CA-C-O	-6.12	109.47	120.60
1	G	383	TRP	O-C-N	-6.11	115.07	122.22
1	G	408	ARG	CD-NE-CZ	6.11	132.95	124.40
1	G	316	MET	CA-C-O	-6.10	113.95	120.42
1	G	555	PRO	N-CA-CB	6.10	109.65	103.25
1	G	371	TRP	O-C-N	-6.10	115.39	122.95
3	C	19	PHE	CA-C-O	6.09	127.21	120.82
1	A	155	ALA	CA-C-O	6.08	127.73	120.92
1	G	206	ILE	N-CA-CB	-6.08	103.44	110.55
1	A	56	MET	CA-C-O	6.07	127.40	120.90
2	B	262	TYR	CA-C-O	6.07	129.19	120.51
1	G	122	TYR	N-CA-C	6.07	117.90	111.28
1	G	40	VAL	O-C-N	-6.07	114.98	122.57
1	G	198	GLY	N-CA-C	-6.07	107.14	114.66
1	A	327	GLY	O-C-N	-6.06	114.82	122.70
1	G	484	ILE	N-CA-C	-6.06	106.83	113.43
1	A	57	ALA	N-CA-C	6.05	119.28	110.14
1	A	59	GLY	CA-C-N	-6.04	115.17	122.90
1	A	59	GLY	C-N-CA	-6.04	115.17	122.90
3	C	108	PRO	N-CA-CB	6.04	108.93	103.19
1	A	265	GLN	CA-C-N	6.04	127.38	119.84
1	A	265	GLN	C-N-CA	6.04	127.38	119.84
4	J	21	GLN	CA-C-O	-6.03	114.48	120.82
1	G	263	PHE	CA-CB-CG	6.03	119.83	113.80
3	I	203	PHE	N-CA-C	6.03	118.81	111.82
1	A	257	ARG	CA-C-O	-6.02	112.66	120.00
1	G	469	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	99	ILE	N-CA-CB	-6.01	102.95	110.47
1	G	353	MET	CA-C-O	6.01	126.88	119.79
1	A	107	MET	N-CA-C	6.00	119.71	112.38
1	A	244	PRO	O-C-N	-6.00	115.03	122.23
1	G	143	TYR	CA-C-O	-5.99	114.20	120.55
1	G	371	TRP	CA-C-O	5.99	127.75	120.92
2	H	133	ASP	CA-C-O	5.99	125.42	118.77
1	A	146	TYR	N-CA-C	-5.98	104.88	111.82
1	A	288	TYR	CA-C-O	-5.98	112.27	119.27
1	G	320	MET	O-C-N	-5.97	115.88	122.09
1	G	313	TYR	CA-C-O	-5.97	114.51	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	446	ARG	CA-C-O	-5.97	113.91	120.24
1	G	244	PRO	O-C-N	-5.96	115.74	122.18
1	A	284	HIS	CA-C-O	5.96	128.33	120.16
1	A	134	ALA	CA-C-N	5.96	130.49	123.16
1	A	134	ALA	C-N-CA	5.96	130.49	123.16
1	A	497	SER	CA-C-O	5.96	127.62	121.07
1	A	115	LEU	CA-C-O	-5.95	113.64	120.24
3	C	32	ALA	N-CA-CB	5.95	118.97	110.16
1	A	493	TRP	N-CA-C	5.95	120.07	112.34
4	D	12	VAL	N-CA-CB	5.95	121.05	111.23
1	A	196	LEU	O-C-N	-5.95	115.82	122.12
1	A	527	ALA	CA-C-O	-5.95	114.79	121.81
2	H	249	PHE	O-C-N	-5.95	115.66	123.21
2	H	227	LYS	CA-C-O	-5.94	113.60	120.31
1	G	122	TYR	O-C-N	-5.93	115.83	122.12
1	G	475	GLY	O-C-N	-5.93	116.26	122.13
3	C	88	MET	N-CA-C	-5.93	104.76	112.23
1	A	263	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	216	ARG	NE-CZ-NH2	-5.92	113.87	119.20
2	H	98	SER	CA-C-O	5.92	124.70	119.08
2	B	258	ILE	CB-CA-C	-5.92	101.58	111.29
1	G	188	ASP	CA-C-O	5.92	126.81	120.24
1	G	257	ARG	CA-C-O	-5.91	112.78	120.00
1	G	213	LEU	N-CA-C	5.91	118.67	111.82
3	I	110	GLY	CA-C-N	5.91	127.22	119.84
3	I	110	GLY	C-N-CA	5.91	127.22	119.84
1	A	419	HIS	CA-C-O	5.90	128.95	120.51
1	A	14	ARG	CA-C-N	-5.90	114.50	120.10
1	A	14	ARG	C-N-CA	-5.90	114.50	120.10
1	G	389	PHE	CA-C-O	5.89	126.97	120.90
2	H	106	ILE	CA-C-O	5.89	127.00	120.46
1	G	302	ILE	CB-CG1-CD1	5.89	126.17	113.80
1	A	295	PHE	CA-C-N	5.89	126.36	119.94
1	A	295	PHE	C-N-CA	5.89	126.36	119.94
1	G	442	LYS	N-CA-CB	5.89	118.71	109.94
2	H	158	SER	CA-C-O	5.88	126.72	120.36
1	G	331	TRP	N-CA-C	5.88	118.47	111.71
1	A	523	ALA	CA-C-O	-5.88	114.22	120.92
1	G	28	ASP	CA-C-O	5.88	125.60	119.14
1	G	230	TRP	CA-C-O	5.87	126.77	120.55
3	I	70	ASP	CA-CB-CG	5.86	118.46	112.60
1	G	415	TYR	CA-C-O	5.86	126.57	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	PHE	CA-C-O	5.86	128.88	120.51
1	G	114	ALA	N-CA-CB	-5.85	101.48	110.20
3	C	93	PHE	CA-CB-CG	5.84	119.64	113.80
3	I	23	VAL	N-CA-C	-5.84	105.39	111.58
1	A	344	GLN	CB-CG-CD	5.84	122.53	112.60
1	A	387	PHE	CA-CB-CG	-5.84	107.96	113.80
1	G	221	THR	CA-C-O	-5.84	114.92	121.81
1	A	413	THR	N-CA-C	-5.83	101.30	109.69
1	A	531	TRP	CA-C-N	-5.82	112.44	122.10
1	A	531	TRP	C-N-CA	-5.82	112.44	122.10
3	C	74	VAL	CB-CA-C	-5.82	104.40	112.02
3	C	257	LEU	N-CA-CB	5.82	118.41	109.91
3	C	121	PRO	CA-C-N	5.81	125.83	119.90
3	C	121	PRO	C-N-CA	5.81	125.83	119.90
1	A	486	TYR	CA-C-O	5.81	125.83	119.91
3	C	93	PHE	CA-C-O	5.81	126.57	120.42
2	B	181	ILE	O-C-N	5.80	127.50	121.87
2	H	220	THR	CA-C-O	5.80	127.66	121.45
1	G	223	HIS	CA-CB-CG	-5.80	108.00	113.80
1	G	413	THR	N-CA-C	-5.79	101.63	110.14
3	I	74	VAL	CB-CA-C	-5.79	104.44	112.02
2	H	216	ILE	O-C-N	-5.78	116.80	122.93
1	A	54	GLU	CB-CG-CD	5.78	122.42	112.60
1	A	210	THR	N-CA-C	-5.78	104.35	111.40
1	A	211	THR	N-CA-C	5.78	118.04	111.11
1	A	473	PHE	O-C-N	-5.77	114.91	122.59
1	G	121	ASN	OD1-CG-ND2	5.76	128.37	122.60
1	G	304	THR	CB-CA-C	-5.76	102.08	110.96
1	A	239	ILE	CA-C-O	5.76	127.46	121.29
3	I	7	HIS	N-CA-C	5.76	118.15	109.23
1	G	257	ARG	CA-C-N	-5.75	112.31	122.26
1	G	257	ARG	C-N-CA	-5.75	112.31	122.26
1	G	545	PRO	CA-C-N	5.75	126.30	120.38
1	G	545	PRO	C-N-CA	5.75	126.30	120.38
3	C	107	TYR	CA-C-N	5.75	126.20	119.99
3	C	107	TYR	C-N-CA	5.75	126.20	119.99
1	G	262	THR	CA-CB-OG1	5.75	118.22	109.60
2	B	127	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	322	ALA	CA-C-O	-5.74	114.97	121.00
2	H	221	VAL	CA-CB-CG2	5.74	120.15	110.40
3	I	3	HIS	CA-CB-CG	-5.74	108.06	113.80
1	G	378	LYS	N-CA-C	-5.73	102.03	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	ALA	N-CA-C	-5.73	104.95	111.14
3	C	41	PRO	CB-CA-C	-5.73	102.67	112.64
1	A	308	LYS	CA-C-O	5.72	124.85	119.13
3	C	68	GLU	CA-C-N	5.72	131.11	120.87
3	C	68	GLU	C-N-CA	5.72	131.11	120.87
1	G	216	ARG	NH1-CZ-NH2	5.72	126.74	119.30
2	H	227	LYS	CB-CA-C	-5.72	100.52	109.72
1	G	33	TYR	CA-CB-CG	5.71	124.18	113.90
1	A	430	PHE	N-CA-C	-5.71	105.20	111.82
2	H	212	GLY	O-C-N	5.71	128.44	123.36
4	J	43	LEU	N-CA-C	-5.70	104.06	111.02
3	C	94	PHE	O-C-N	-5.70	115.26	122.27
1	G	135	PHE	CA-C-N	5.70	124.89	118.97
1	G	135	PHE	C-N-CA	5.70	124.89	118.97
2	B	84	HIS	CA-C-N	5.70	132.42	121.54
2	B	84	HIS	C-N-CA	5.70	132.42	121.54
1	G	192	PHE	CA-CB-CG	5.69	119.49	113.80
1	G	261	THR	N-CA-C	-5.69	101.54	110.36
2	H	84	HIS	O-C-N	-5.69	115.54	122.82
1	A	197	SER	CA-C-O	5.69	126.53	120.10
1	G	458	TRP	CB-CA-C	5.69	119.81	110.88
4	J	32	VAL	CA-C-O	-5.69	115.14	121.17
2	B	258	ILE	CA-C-O	5.69	127.89	120.78
1	A	532	ASN	CA-C-N	5.68	129.69	120.60
1	A	532	ASN	C-N-CA	5.68	129.69	120.60
1	G	503	LEU	CB-CA-C	-5.68	101.19	110.85
1	G	24	THR	N-CA-C	-5.68	106.01	114.64
1	G	255	THR	O-C-N	-5.68	116.22	122.07
1	A	507	SER	CA-C-O	5.67	126.78	120.82
1	A	544	SER	O-C-N	5.67	127.84	121.32
1	A	19	ARG	NE-CZ-NH2	-5.67	114.10	119.20
2	H	128	GLU	CA-C-N	5.66	126.67	122.59
2	H	128	GLU	C-N-CA	5.66	126.67	122.59
1	A	534	HIS	CG-CD2-NE2	-5.66	101.54	107.20
3	I	51	VAL	N-CA-C	5.66	117.07	110.62
1	A	360	GLY	CA-C-O	5.65	126.57	120.75
1	G	140	ASN	CA-C-O	5.65	126.53	120.55
2	H	272	GLU	CA-C-O	-5.64	114.44	120.42
3	C	3	HIS	CA-CB-CG	-5.64	108.16	113.80
1	G	448	TYR	CA-CB-CG	-5.64	103.76	113.90
2	H	201	PRO	N-CA-C	5.63	119.31	110.80
2	H	145	TRP	CA-C-O	-5.62	114.88	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	60	VAL	CA-C-O	-5.62	113.89	120.75
1	G	461	PHE	N-CA-C	-5.62	104.84	110.97
3	C	256	PHE	CB-CA-C	5.62	120.98	110.70
1	A	45	VAL	CA-C-O	-5.61	115.21	121.05
1	G	25	ASN	CA-C-N	5.61	129.58	120.60
1	G	25	ASN	C-N-CA	5.61	129.58	120.60
2	H	200	VAL	CA-C-O	5.61	127.46	119.95
2	B	263	MET	N-CA-CB	5.60	120.34	110.37
2	B	35	ARG	CA-C-N	5.60	125.60	119.89
2	B	35	ARG	C-N-CA	5.60	125.60	119.89
1	G	494	ASN	CA-CB-CG	-5.60	107.00	112.60
3	I	99	TRP	CA-C-O	5.58	126.39	119.97
1	G	420	PHE	CA-C-O	-5.58	112.74	119.49
4	J	20	GLN	N-CA-C	5.58	117.04	111.07
1	G	174	LEU	N-CA-C	5.58	119.27	111.74
2	B	90	VAL	CA-C-N	5.57	125.56	120.21
2	B	90	VAL	C-N-CA	5.57	125.56	120.21
1	A	139	ASN	CB-CG-ND2	5.57	124.75	116.40
1	A	359	THR	CA-CB-OG1	-5.57	101.25	109.60
1	G	336	TYR	N-CA-C	5.56	118.10	111.71
1	A	170	ILE	CA-CB-CG1	5.55	119.84	110.40
2	B	118	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	101	GLY	CA-C-O	5.54	126.02	120.09
2	B	49	PRO	CB-CA-C	-5.54	103.47	112.62
3	C	74	VAL	CA-C-O	-5.54	114.91	121.05
1	G	36	THR	CA-C-N	5.54	126.23	120.03
1	G	36	THR	C-N-CA	5.54	126.23	120.03
1	A	331	TRP	N-CA-C	5.53	119.65	113.01
4	D	28	PHE	CA-C-O	5.53	127.12	120.92
1	G	348	PHE	N-CA-CB	-5.53	101.99	110.12
2	H	212	GLY	CA-C-N	-5.53	109.86	121.80
2	H	212	GLY	C-N-CA	-5.53	109.86	121.80
1	A	382	LEU	O-C-N	-5.53	116.26	122.12
1	G	163	ASN	OD1-CG-ND2	5.52	128.12	122.60
2	H	76	ILE	CB-CA-C	-5.52	102.24	111.29
1	G	439	TRP	CA-CB-CG	5.51	124.07	113.60
1	G	81	TRP	CA-C-N	5.51	125.52	119.90
1	G	81	TRP	C-N-CA	5.51	125.52	119.90
1	G	295	PHE	O-C-N	-5.51	116.36	122.09
1	G	22	MET	CA-C-N	5.50	129.51	121.31
1	G	22	MET	C-N-CA	5.50	129.51	121.31
1	A	520	THR	CA-CB-OG1	-5.50	101.35	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ARG	NH1-CZ-NH2	5.50	126.45	119.30
1	A	376	GLU	OE1-CD-OE2	-5.50	109.70	122.90
3	I	199	GLY	CA-C-O	5.50	126.71	121.05
1	G	101	GLY	O-C-N	-5.50	115.56	122.70
1	G	445	GLY	N-CA-C	-5.49	107.74	115.32
3	C	203	PHE	N-CA-C	5.48	117.34	111.36
1	G	19	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	G	357	VAL	CA-C-N	5.48	126.69	119.84
1	G	357	VAL	C-N-CA	5.48	126.69	119.84
3	I	42	TRP	CA-CB-CG	-5.48	103.19	113.60
1	A	289	ILE	CB-CA-C	-5.47	103.39	112.26
4	D	12	VAL	CG1-CB-CG2	-5.47	98.76	110.80
1	A	469	PHE	CA-CB-CG	-5.47	108.33	113.80
1	G	275	TYR	CB-CA-C	-5.46	102.07	110.81
3	I	237	HIS	CA-CB-CG	5.46	119.26	113.80
1	G	411	HIS	CA-CB-CG	-5.46	108.34	113.80
1	A	457	PHE	CA-CB-CG	-5.46	108.34	113.80
2	B	120	LEU	CA-C-N	5.46	126.66	119.84
2	B	120	LEU	C-N-CA	5.46	126.66	119.84
1	A	184	GLY	O-C-N	5.45	127.59	122.90
1	G	248	GLY	O-C-N	-5.45	116.96	122.19
1	G	264	PHE	CA-CB-CG	-5.45	108.35	113.80
2	B	100	LEU	N-CA-C	5.44	117.92	111.33
2	B	256	CYS	CA-C-O	-5.44	113.06	119.05
3	C	253	VAL	CA-C-O	5.44	126.62	120.85
1	G	502	PHE	CA-C-O	5.44	126.21	119.79
2	H	266	THR	CA-C-O	-5.44	114.28	120.32
1	A	36	THR	CA-CB-CG2	-5.44	101.26	110.50
1	A	142	SER	CA-C-O	-5.44	115.08	120.90
3	C	249	PHE	N-CA-C	-5.44	105.00	111.69
1	G	485	ASP	CB-CG-OD1	5.44	130.91	118.40
1	G	175	TYR	CA-C-N	5.43	125.97	120.38
1	G	175	TYR	C-N-CA	5.43	125.97	120.38
2	H	265	ILE	CA-C-O	-5.43	114.59	120.67
1	G	480	PRO	CB-CA-C	-5.42	104.12	111.12
1	A	262	THR	CA-CB-OG1	5.42	117.73	109.60
2	B	37	GLN	CA-C-O	5.42	123.82	119.59
4	J	43	LEU	CA-C-O	-5.42	115.11	121.07
1	G	417	VAL	CA-C-N	5.42	128.55	120.31
1	G	417	VAL	C-N-CA	5.42	128.55	120.31
3	I	41	PRO	CA-C-N	5.42	127.80	120.38
3	I	41	PRO	C-N-CA	5.42	127.80	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	A	295	PHE	CA-CB-CG	5.42	119.22	113.80
2	H	268	LYS	CA-C-N	-5.42	116.08	123.12
2	H	268	LYS	C-N-CA	-5.42	116.08	123.12
3	I	110	GLY	O-C-N	-5.41	116.36	121.77
3	C	250	VAL	CA-C-N	5.40	127.52	120.28
3	C	250	VAL	C-N-CA	5.40	127.52	120.28
1	G	43	ILE	CA-C-O	-5.40	114.03	120.78
3	C	94	PHE	CA-C-N	5.39	128.04	120.28
3	C	94	PHE	C-N-CA	5.39	128.04	120.28
2	H	194	THR	N-CA-CB	-5.39	102.67	110.70
2	H	221	VAL	CA-C-O	5.38	127.17	119.95
1	A	465	ASN	N-CA-C	-5.38	105.45	112.23
1	A	485	ASP	CA-CB-CG	5.38	117.98	112.60
4	D	39	ILE	CA-C-O	5.37	127.41	121.18
1	A	477	GLN	CA-C-O	5.37	125.84	119.56
1	G	101	GLY	CA-C-O	5.37	129.91	120.57
1	G	500	GLY	CA-C-O	-5.36	115.55	120.80
1	A	275	TYR	N-CA-CB	5.36	117.92	109.94
1	A	244	PRO	CA-C-N	5.35	128.93	120.47
1	A	244	PRO	C-N-CA	5.35	128.93	120.47
1	G	375	ILE	N-CA-C	5.35	116.68	108.71
3	I	200	ALA	N-CA-CB	-5.33	102.12	109.91
3	I	17	TRP	O-C-N	-5.33	115.19	121.32
2	B	264	PRO	CA-CB-CG	-5.33	94.38	104.50
1	G	524	ARG	CA-C-O	-5.32	114.69	120.81
2	B	88	ASN	CA-CB-CG	5.32	117.92	112.60
2	B	220	THR	CA-C-O	5.32	127.75	121.58
3	I	93	PHE	CA-C-O	5.32	126.06	120.42
3	I	191	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	348	PHE	N-CA-CB	-5.31	102.05	110.28
1	A	448	TYR	CA-C-N	5.31	126.48	119.84
1	A	448	TYR	C-N-CA	5.31	126.48	119.84
1	G	535	ALA	N-CA-CB	-5.30	103.41	110.57
1	A	142	SER	CB-CA-C	-5.30	102.33	110.81
3	I	107	TYR	CA-C-N	5.30	125.20	119.85
3	I	107	TYR	C-N-CA	5.30	125.20	119.85
1	G	523	ALA	CB-CA-C	5.29	118.36	109.89
1	A	53	MET	N-CA-C	-5.29	105.41	111.07
3	C	140	ILE	CB-CA-C	-5.29	104.92	112.22
1	A	280	TRP	CA-C-O	5.29	125.92	119.05
1	A	542	LEU	CA-C-O	-5.29	115.44	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	216	ARG	NE-CZ-NH2	-5.28	114.44	119.20
1	A	191	ILE	N-CA-CB	5.28	118.50	110.58
3	C	156	VAL	CB-CA-C	-5.28	103.55	112.16
1	A	48	THR	O-C-N	5.28	129.41	122.33
2	B	163	SER	CA-C-N	5.28	126.44	119.84
2	B	163	SER	C-N-CA	5.28	126.44	119.84
4	D	45	PHE	CA-C-N	5.28	128.74	120.82
4	D	45	PHE	C-N-CA	5.28	128.74	120.82
1	G	292	LEU	O-C-N	-5.27	116.21	120.38
3	I	261	ILE	CA-C-O	-5.27	114.40	120.83
1	G	306	ALA	N-CA-C	-5.27	106.85	113.28
1	A	57	ALA	CA-C-N	5.26	126.42	119.84
1	A	57	ALA	C-N-CA	5.26	126.42	119.84
1	A	171	GLY	N-CA-C	-5.26	99.19	110.66
4	D	35	ALA	CA-C-O	5.26	126.86	121.07
1	G	376	GLU	N-CA-CB	-5.26	101.57	110.46
2	H	135	THR	CA-C-N	-5.26	116.64	122.27
2	H	135	THR	C-N-CA	-5.26	116.64	122.27
1	A	66	GLU	CB-CG-CD	5.25	121.53	112.60
2	H	66	ALA	CA-C-O	5.25	126.11	120.70
1	A	258	ASN	OD1-CG-ND2	5.25	127.85	122.60
3	C	33	VAL	O-C-N	-5.25	116.77	121.91
1	A	408	ARG	CA-C-O	5.24	126.84	121.07
1	G	25	ASN	O-C-N	-5.24	117.25	123.22
1	A	376	GLU	CA-CB-CG	5.24	124.58	114.10
1	G	543	THR	CB-CA-C	5.24	120.19	109.76
1	G	484	ILE	CB-CA-C	-5.24	104.29	110.84
1	A	543	THR	O-C-N	-5.23	115.35	122.36
1	G	311	PHE	CA-C-O	-5.23	114.42	120.49
2	H	252	CYS	N-CA-CB	5.23	119.33	110.49
3	C	12	LEU	N-CA-C	5.23	118.04	110.14
1	G	273	VAL	N-CA-C	5.23	117.59	111.05
1	G	57	ALA	CA-C-N	5.22	126.37	119.84
1	G	57	ALA	C-N-CA	5.22	126.37	119.84
1	G	534	HIS	N-CA-CB	-5.22	102.90	110.47
1	A	28	ASP	CA-C-O	5.22	125.31	119.41
1	A	248	GLY	O-C-N	-5.22	115.92	122.70
3	C	26	PHE	N-CA-C	-5.22	105.28	110.97
3	C	59	TRP	O-C-N	-5.22	115.85	122.27
3	C	119	ILE	CB-CA-C	-5.21	102.47	110.50
1	G	123	PHE	CA-C-O	-5.21	113.68	119.67
2	B	221	VAL	CA-CB-CG1	-5.21	101.54	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	VAL	CB-CA-C	-5.21	103.42	111.08
1	A	554	LEU	N-CA-C	5.21	116.44	109.83
1	G	388	LEU	CA-C-O	-5.21	115.33	120.90
1	A	290	ILE	CA-CB-CG1	-5.20	101.56	110.40
1	A	388	LEU	CA-C-N	5.20	127.70	120.63
1	A	388	LEU	C-N-CA	5.20	127.70	120.63
4	J	30	ARG	NE-CZ-NH1	-5.20	116.30	121.50
3	C	209	HIS	CA-CB-CG	-5.20	108.60	113.80
3	I	62	VAL	CA-C-O	-5.20	115.28	121.05
1	A	249	ALA	O-C-N	-5.19	116.28	122.20
3	I	105	ALA	N-CA-C	-5.19	106.45	112.89
3	I	240	PHE	O-C-N	-5.19	116.62	122.12
1	G	361	ILE	N-CA-C	-5.19	104.92	110.36
1	A	319	ALA	CB-CA-C	-5.18	102.74	110.88
1	A	57	ALA	CB-CA-C	-5.18	101.11	108.88
2	H	170	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	292	LEU	CB-CA-C	5.18	120.37	110.17
1	A	546	PRO	O-C-N	-5.18	118.93	121.31
1	G	51	MET	O-C-N	5.18	127.61	122.12
1	A	400	VAL	CA-CB-CG1	-5.18	101.60	110.40
1	A	230	TRP	N-CA-CB	5.17	117.73	110.12
1	A	546	PRO	CA-C-N	5.17	125.17	119.89
1	A	546	PRO	C-N-CA	5.17	125.17	119.89
1	G	302	ILE	N-CA-C	5.17	115.94	110.72
1	A	381	MET	CA-C-N	-5.16	113.37	120.28
1	A	381	MET	C-N-CA	-5.16	113.37	120.28
3	C	198	TYR	O-C-N	-5.16	116.18	122.11
1	G	377	LEU	CB-CA-C	-5.16	103.69	112.00
3	I	158	GLU	CA-C-O	5.16	124.50	118.77
3	I	27	VAL	O-C-N	-5.16	116.86	121.91
3	I	250	VAL	CA-C-N	5.15	127.44	120.38
3	I	250	VAL	C-N-CA	5.15	127.44	120.38
3	C	205	ALA	CA-C-O	-5.14	115.40	120.70
1	G	21	PHE	CA-CB-CG	-5.14	108.66	113.80
2	H	163	SER	CA-C-N	5.14	126.26	119.84
2	H	163	SER	C-N-CA	5.14	126.26	119.84
1	A	148	ALA	O-C-N	-5.13	116.59	122.08
3	C	111	PRO	CA-C-O	-5.13	111.26	120.60
1	A	468	PHE	N-CA-C	5.13	119.63	113.17
1	A	292	LEU	CA-C-N	5.13	125.16	119.32
1	A	292	LEU	C-N-CA	5.13	125.16	119.32
1	G	367	ILE	N-CA-C	-5.13	105.54	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	104	ILE	O-C-N	-5.12	116.87	121.89
1	G	361	ILE	N-CA-CB	-5.12	104.83	110.51
1	A	167	GLY	CA-C-N	5.12	129.94	122.41
1	A	167	GLY	C-N-CA	5.12	129.94	122.41
3	I	51	VAL	CA-C-N	5.12	127.56	120.29
3	I	51	VAL	C-N-CA	5.12	127.56	120.29
1	A	313	TYR	O-C-N	-5.12	116.70	122.12
1	G	221	THR	N-CA-C	-5.11	103.65	110.55
3	I	198	TYR	CA-C-N	5.11	125.77	119.99
3	I	198	TYR	C-N-CA	5.11	125.77	119.99
1	A	275	TYR	CB-CA-C	-5.11	102.63	110.81
1	G	288	TYR	CG-CD2-CE2	-5.11	113.54	121.20
1	A	238	LEU	O-C-N	-5.10	116.71	122.12
1	A	82	PRO	N-CA-CB	5.10	107.74	103.25
1	G	289	ILE	CB-CA-C	-5.10	104.26	112.16
1	A	52	ARG	CB-CA-C	5.10	120.78	110.38
1	G	320	MET	CA-CB-CG	-5.10	103.91	114.10
2	H	130	PRO	N-CA-C	5.10	118.62	111.33
3	I	19	PHE	CA-C-N	5.09	127.42	120.54
3	I	19	PHE	C-N-CA	5.09	127.42	120.54
1	G	538	LEU	CA-C-O	5.09	125.61	119.61
1	A	357	VAL	CA-C-N	5.09	126.20	119.84
1	A	357	VAL	C-N-CA	5.09	126.20	119.84
1	A	284	HIS	CA-C-N	5.08	124.87	119.28
1	A	284	HIS	C-N-CA	5.08	124.87	119.28
2	H	120	LEU	CA-C-N	5.08	126.19	119.84
2	H	120	LEU	C-N-CA	5.08	126.19	119.84
1	G	19	ARG	NH1-CZ-NH2	5.08	125.91	119.30
1	G	456	HIS	CA-CB-CG	5.08	118.88	113.80
1	A	132	ASP	CA-CB-CG	5.08	117.68	112.60
2	B	41	THR	N-CA-C	-5.08	107.03	114.39
1	A	446	ARG	CB-CA-C	-5.07	103.21	110.62
4	J	26	ALA	CA-C-N	5.07	125.47	119.94
4	J	26	ALA	C-N-CA	5.07	125.47	119.94
3	I	80	ARG	NH1-CZ-NH2	5.07	125.89	119.30
2	B	213	ALA	CA-C-O	-5.07	113.68	119.41
3	C	70	ASP	CA-C-O	5.07	125.80	119.97
1	G	165	GLN	CG-CD-OE1	5.07	130.93	120.80
3	I	29	LEU	N-CA-C	5.07	117.70	111.82
2	B	135	THR	N-CA-C	5.06	116.42	107.61
3	C	50	VAL	N-CA-C	5.06	115.78	110.62
2	B	147	TYR	N-CA-CB	5.06	118.84	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100	LEU	N-CA-C	5.06	117.45	111.33
4	J	50	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	G	503	LEU	O-C-N	5.06	127.92	122.15
2	H	156	PHE	CA-C-O	5.06	126.72	121.36
1	A	214	ASN	CB-CA-C	-5.05	101.22	109.56
2	H	117	ALA	O-C-N	5.05	127.35	122.09
1	A	251	THR	N-CA-C	-5.05	106.62	112.89
3	I	37	HIS	CA-CB-CG	-5.05	108.75	113.80
3	C	6	ASN	OD1-CG-ND2	-5.05	117.55	122.60
3	C	96	ALA	CA-C-N	5.05	127.50	120.63
3	C	96	ALA	C-N-CA	5.05	127.50	120.63
4	D	28	PHE	O-C-N	-5.05	116.30	122.11
3	I	108	PRO	N-CA-CB	5.05	108.03	103.33
1	A	174	LEU	N-CA-C	5.04	118.55	111.74
2	B	95	THR	CB-CA-C	-5.04	101.68	109.80
1	G	257	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	186	SER	CA-C-O	5.04	126.61	121.07
3	I	209	HIS	CA-CB-CG	-5.04	108.76	113.80
1	G	402	SER	N-CA-CB	5.04	117.44	109.94
3	C	61	ASP	CA-C-O	5.04	125.79	120.10
1	G	504	SER	N-CA-C	-5.04	105.89	112.23
1	G	265	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	G	446	ARG	CB-CA-C	-5.03	102.09	110.14
3	I	140	ILE	CB-CA-C	-5.03	105.35	112.14
1	A	547	PRO	N-CA-CB	5.03	107.54	103.32
1	G	225	VAL	CA-C-O	5.03	126.69	119.95
3	C	93	PHE	CA-C-N	5.03	127.95	120.31
3	C	93	PHE	C-N-CA	5.03	127.95	120.31
4	J	49	ALA	CA-C-N	-5.02	114.39	122.08
4	J	49	ALA	C-N-CA	-5.02	114.39	122.08
1	G	526	THR	N-CA-C	-5.02	108.18	114.56
2	H	62	LEU	CB-CA-C	-5.02	102.46	110.79
1	G	388	LEU	O-C-N	5.01	127.30	122.09
2	H	209	GLN	CA-C-O	-5.01	114.97	120.43
3	I	17	TRP	CB-CG-CD2	5.01	133.81	126.80
1	G	450	GLU	CB-CG-CD	5.01	121.11	112.60
2	H	201	PRO	CB-CA-C	-5.00	105.40	111.46
2	B	158	SER	CA-C-O	5.00	125.87	120.32
3	I	199	GLY	CA-C-N	5.00	127.25	120.65
3	I	199	GLY	C-N-CA	5.00	127.25	120.65

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	157	LEU	Mainchain
1	A	202	ILE	Mainchain
1	A	257	ARG	Mainchain
1	A	274	LEU	Mainchain
1	A	538	LEU	Mainchain
1	A	543	THR	Mainchain,Peptide
1	A	544	SER	Mainchain,Peptide
1	A	545	PRO	Mainchain
2	B	142	GLN	Mainchain
2	B	143	TRP	Mainchain
2	B	163	SER	Mainchain
2	B	209	GLN	Mainchain
2	B	253	SER	Mainchain
2	B	263	MET	Mainchain
3	C	162	ARG	Mainchain
3	C	17	TRP	Mainchain
3	C	196	ASN	Mainchain
4	D	49	ALA	Mainchain
1	G	112	ILE	Mainchain
1	G	173	VAL	Mainchain
1	G	234	VAL	Mainchain
1	G	274	LEU	Mainchain
1	G	288	TYR	Mainchain
1	G	317	VAL	Mainchain
1	G	326	LEU	Mainchain
1	G	334	HIS	Mainchain
1	G	343	THR	Mainchain
1	G	416	VAL	Mainchain
1	G	419	HIS	Mainchain
1	G	469	PHE	Mainchain
1	G	543	THR	Peptide
1	G	544	SER	Mainchain,Peptide
2	H	107	VAL	Mainchain
2	H	142	GLN	Mainchain
2	H	229	ASP	Mainchain
2	H	231	VAL	Mainchain
2	H	254	GLU	Mainchain
3	I	196	ASN	Mainchain
3	I	57	GLY	Mainchain

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	4322	0	4238	349	0
1	G	4322	0	4238	353	0
2	B	2046	0	2011	144	0
2	H	2046	0	2011	159	0
3	C	2139	0	2056	165	0
3	I	2139	0	2056	162	0
4	D	311	0	319	28	0
4	J	311	0	319	46	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	120	0	108	25	0
8	G	120	0	108	17	0
9	A	102	0	164	34	0
9	C	153	0	246	48	0
9	D	51	0	82	21	0
9	G	102	0	164	28	0
9	I	153	0	246	51	0
9	J	51	0	82	16	0
10	A	101	0	0	7	0
10	B	68	0	0	4	0
10	C	39	0	0	5	0
10	D	12	0	0	0	0
10	G	106	0	0	8	0
10	H	64	0	0	6	0
10	I	38	0	0	4	0
10	J	8	0	0	2	0
All	All	18934	0	18448	1397	0

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 38.

All (1397) 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)
3:I:8:ASP:HB3	3:I:72:THR:HG21	1.27	1.12
1:A:520:THR:HG22	1:A:521:ARG:HG2	1.32	1.12
9:I:3013:3PE:O14	9:I:3013:3PE:H121	1.51	1.11
9:I:3013:3PE:C3H	9:I:3013:3PE:H2D2	1.78	1.11
9:C:2013:3PE:O14	9:C:2013:3PE:H121	1.48	1.06
1:A:284:HIS:NE2	1:A:288:TYR:HE2	1.53	1.04
9:I:3013:3PE:C2D	9:I:3013:3PE:H3H2	1.88	1.04
3:C:8:ASP:HB3	3:C:72:THR:HG21	1.39	1.03
3:I:161:ARG:HH12	3:I:230:GLY:HA2	1.24	1.01
3:C:161:ARG:HH12	3:C:230:GLY:HA2	1.22	1.01
9:C:2013:3PE:C3H	9:C:2013:3PE:H2D2	1.89	1.01
1:G:543:THR:HG22	1:G:547:PRO:HD3	1.40	1.01
1:G:284:HIS:NE2	1:G:288:TYR:HE2	1.58	1.00
1:G:106:MET:HB3	8:G:1001:HEA:HAC	1.43	0.99
1:A:124:MET:HB3	1:A:125:PRO:HD3	1.39	0.98
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.42	0.98
1:A:390:LEU:HD13	1:A:426:LEU:HB3	1.44	0.98
1:G:345:GLN:HE22	1:G:408:ARG:HH22	1.08	0.98
9:C:2013:3PE:H2D2	9:C:2013:3PE:H3H2	1.41	0.97
1:G:63:MET:HG2	1:G:94:LEU:HD23	1.46	0.97
1:A:543:THR:HG22	1:A:547:PRO:HD3	1.45	0.95
1:G:18:THR:HA	1:G:22:MET:HE3	1.48	0.95
1:A:489:ALA:HB3	2:B:36:PRO:HB2	1.47	0.95
1:G:379:THR:HB	1:G:380:PRO:HD3	1.48	0.94
1:A:379:THR:HB	1:A:380:PRO:HD3	1.48	0.93
1:G:284:HIS:HE2	1:G:288:TYR:HE2	1.15	0.93
1:G:520:THR:HG22	1:G:521:ARG:HG2	1.46	0.93
9:I:3013:3PE:H2D2	9:I:3013:3PE:H3H1	1.50	0.92
3:C:21:ALA:HB2	3:C:54:THR:HG21	1.51	0.92
9:I:3013:3PE:H2D2	9:I:3013:3PE:H3H2	1.43	0.91
1:A:18:THR:HA	1:A:22:MET:HE3	1.53	0.91
1:G:432:ILE:HG21	8:G:1001:HEA:H252	1.50	0.91
3:I:21:ALA:HB2	3:I:54:THR:HG21	1.52	0.91
1:G:133:MET:HE3	1:G:211:THR:HG21	1.50	0.91
9:A:2012:3PE:H2F1	9:D:2011:3PE:H2I2	1.54	0.90
1:G:342:LEU:HD13	2:H:127:GLN:HB2	1.51	0.90
1:G:99:ILE:HD12	8:G:1001:HEA:HBA2	1.55	0.89
9:C:2013:3PE:H3H2	9:C:2013:3PE:C2D	2.02	0.88
1:A:397:THR:HG21	1:A:419:HIS:HB2	1.55	0.88
9:I:3013:3PE:H261	9:I:3013:3PE:H3B1	1.56	0.88
1:A:239:ILE:HG12	1:A:289:ILE:HD13	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:3010:3PE:H3E2	9:I:3010:3PE:H3I3	1.54	0.87
1:A:106:MET:HB3	8:A:1001:HEA:HAC	1.55	0.86
2:H:245:GLU:HA	2:H:269:VAL:HG13	1.57	0.86
1:A:284:HIS:HE2	1:A:288:TYR:HE2	1.17	0.86
1:G:222:MET:H	9:G:3012:3PE:H111	1.38	0.86
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.57	0.86
3:C:161:ARG:NH1	3:C:230:GLY:HA2	1.91	0.85
2:H:211:THR:HG22	2:H:212:GLY:H	1.40	0.85
1:G:397:THR:HG21	1:G:419:HIS:HB2	1.58	0.85
9:C:2013:3PE:O14	9:C:2013:3PE:C12	2.24	0.84
1:A:22:MET:HG2	3:C:16:ILE:HA	1.57	0.84
9:I:3013:3PE:O14	9:I:3013:3PE:C12	2.25	0.84
1:G:350:MET:HA	1:G:353:MET:HE2	1.57	0.84
1:G:489:ALA:HB3	2:H:36:PRO:HB2	1.57	0.84
1:A:133:MET:HE3	1:A:211:THR:HG21	1.59	0.84
1:G:390:LEU:HD13	1:G:426:LEU:HB3	1.59	0.83
3:I:8:ASP:CB	3:I:72:THR:HG21	2.08	0.83
1:G:345:GLN:NE2	1:G:408:ARG:HH22	1.75	0.83
1:A:345:GLN:HE22	1:A:408:ARG:HH22	1.25	0.83
1:G:249:ALA:HB2	1:G:278:ILE:HG22	1.60	0.83
9:C:2010:3PE:H3E2	9:C:2010:3PE:H3I3	1.59	0.83
2:B:245:GLU:HA	2:B:269:VAL:HG13	1.61	0.82
1:A:54:GLU:HG2	1:A:63:MET:HE2	1.63	0.81
3:I:161:ARG:NH1	3:I:230:GLY:HA2	1.94	0.81
2:H:107:VAL:CG1	2:H:108:PRO:HD3	2.10	0.81
3:I:85:LEU:HA	3:I:88:MET:HE2	1.63	0.81
1:A:222:MET:H	9:A:2012:3PE:H111	1.43	0.81
1:A:473:PHE:CD1	2:B:41:THR:HB	2.15	0.81
1:G:25:ASN:HD21	1:G:27:LYS:HZ3	1.26	0.80
3:I:62:VAL:HG11	9:I:3008:3PE:H31	1.63	0.80
3:C:255:LEU:HB3	9:D:2011:3PE:H3I3	1.64	0.79
3:C:8:ASP:CB	3:C:72:THR:HG21	2.12	0.79
1:A:243:LEU:HD22	1:A:282:PHE:CE2	2.18	0.79
2:B:235:LEU:HD21	4:J:11:HIS:HB2	1.66	0.78
1:G:124:MET:HB3	1:G:125:PRO:HD3	1.64	0.78
1:A:432:ILE:CG2	8:A:1001:HEA:H252	2.13	0.78
3:C:133:LEU:H	3:C:134:PRO:HD2	1.48	0.78
1:G:473:PHE:CD1	2:H:41:THR:HB	2.19	0.78
1:A:511:PHE:CZ	1:A:515:ILE:HD11	2.17	0.78
1:A:25:ASN:HD21	1:A:27:LYS:HZ3	1.32	0.78
8:A:1002:HEA:HBC1	8:A:1002:HEA:HMC1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:432:ILE:CG2	8:G:1001:HEA:H252	2.12	0.78
1:A:342:LEU:HD13	2:B:127:GLN:HB2	1.64	0.78
1:G:54:GLU:HG2	1:G:63:MET:HE2	1.64	0.77
1:G:127:HIS:HB3	1:G:226:PRO:HG2	1.66	0.77
1:A:294:ALA:O	1:A:298:VAL:HG23	1.85	0.77
1:G:51:MET:HE3	1:G:99:ILE:HD13	1.65	0.77
3:I:255:LEU:HB3	9:J:3011:3PE:H3I3	1.65	0.77
1:A:529:ASN:OD1	1:A:529:ASN:C	2.26	0.77
3:I:108:PRO:HD2	3:I:117:ASP:HB3	1.66	0.77
1:A:284:HIS:NE2	1:A:288:TYR:CE2	2.46	0.77
3:C:152:HIS:HA	3:C:240:PHE:HE1	1.50	0.77
3:C:111:PRO:HA	4:J:12:VAL:HB	1.67	0.77
9:A:2012:3PE:H2H1	9:C:2010:3PE:H2I3	1.67	0.76
1:A:63:MET:HG2	1:A:94:LEU:HD23	1.67	0.76
2:H:145:TRP:NE1	2:H:263:MET:HE2	2.01	0.76
2:H:226:VAL:HA	10:H:1157:HOH:O	1.85	0.76
1:A:284:HIS:HB3	1:A:285:PRO:HD3	1.66	0.76
9:I:3013:3PE:H261	9:I:3013:3PE:C3B	2.15	0.76
9:A:2009:3PE:H2C2	9:A:2009:3PE:H3A1	1.68	0.76
1:A:442:LYS:O	1:A:546:PRO:HD3	1.86	0.76
3:I:197:ILE:HG13	3:I:198:TYR:H	1.50	0.76
1:G:374:SER:HB2	2:H:85:GLU:HA	1.67	0.76
9:I:3010:3PE:H3I3	9:I:3010:3PE:C3E	2.11	0.75
1:A:243:LEU:HD22	1:A:282:PHE:HE2	1.51	0.75
9:A:2009:3PE:C3E	9:A:2009:3PE:H2E1	2.16	0.75
1:G:22:MET:HG2	3:I:16:ILE:HA	1.69	0.75
9:G:3009:3PE:H2C2	9:G:3009:3PE:H3A1	1.68	0.75
1:G:170:ILE:HD11	1:G:187:THR:OG1	1.87	0.75
3:C:108:PRO:HD2	3:C:117:ASP:HB3	1.69	0.75
9:G:3009:3PE:H3E1	9:G:3009:3PE:H2E1	1.69	0.75
1:G:429:VAL:HG13	8:G:1001:HEA:H273	1.68	0.75
2:H:136:VAL:HG21	2:H:198:MET:HE2	1.68	0.74
3:C:152:HIS:HA	3:C:240:PHE:CE1	2.22	0.74
9:G:3009:3PE:H2E1	9:G:3009:3PE:C3E	2.17	0.74
3:C:80:ARG:O	3:C:84:ILE:HG13	1.87	0.74
2:H:107:VAL:HG13	2:H:108:PRO:HD3	1.68	0.74
1:G:520:THR:CG2	1:G:521:ARG:HG2	2.16	0.73
3:I:220:LEU:HD23	3:I:243:ALA:HB1	1.71	0.73
1:A:137:ARG:HH21	9:A:2009:3PE:H112	1.52	0.73
3:I:8:ASP:H	4:J:16:MET:HE3	1.54	0.73
3:I:152:HIS:HA	3:I:240:PHE:HE1	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2009:3PE:H2E1	9:A:2009:3PE:H3E1	1.71	0.73
1:G:25:ASN:HD21	1:G:27:LYS:NZ	1.87	0.72
3:C:130:PRO:HA	3:C:134:PRO:HG2	1.72	0.72
2:H:191:LEU:O	2:H:264:PRO:HG3	1.88	0.72
2:B:145:TRP:NE1	2:B:263:MET:HE2	2.04	0.72
3:C:42:TRP:O	3:C:46:ILE:HG12	1.90	0.72
3:C:133:LEU:H	3:C:134:PRO:CD	2.03	0.72
2:B:136:VAL:HG21	2:B:198:MET:HE2	1.72	0.71
9:C:2013:3PE:H261	9:C:2013:3PE:H3B1	1.71	0.71
3:I:197:ILE:HG13	3:I:198:TYR:N	2.04	0.71
3:C:58:TRP:O	3:C:62:VAL:HG23	1.91	0.71
1:A:170:ILE:HD11	1:A:187:THR:OG1	1.91	0.71
1:A:314:LEU:HB3	1:A:315:PRO:HD3	1.71	0.71
1:A:350:MET:HA	1:A:353:MET:HE2	1.72	0.71
1:G:127:HIS:HB3	1:G:226:PRO:CG	2.21	0.71
1:G:511:PHE:CZ	1:G:515:ILE:HD11	2.25	0.70
3:I:152:HIS:HA	3:I:240:PHE:CE1	2.26	0.70
3:I:83:PHE:HE1	9:I:3008:3PE:H262	1.54	0.70
3:I:62:VAL:CG1	9:I:3008:3PE:H31	2.21	0.70
3:C:51:VAL:O	3:C:55:MET:HG3	1.92	0.70
1:G:284:HIS:HB3	1:G:285:PRO:HD3	1.74	0.70
9:G:3009:3PE:H111	3:I:12:LEU:HD11	1.74	0.70
3:I:161:ARG:NH2	3:I:232:PHE:H	1.90	0.70
3:I:122:PRO:HG2	3:I:198:TYR:HB2	1.74	0.69
1:G:241:LEU:HD13	9:J:3011:3PE:H2H2	1.75	0.69
1:A:345:GLN:NE2	1:A:408:ARG:HH22	1.90	0.69
1:G:81:TRP:CD2	1:G:82:PRO:HD2	2.27	0.69
2:B:107:VAL:CG1	2:B:108:PRO:HD3	2.22	0.69
3:C:197:ILE:HG13	3:C:198:TYR:H	1.56	0.69
1:A:373:GLY:O	2:B:83:PHE:HB3	1.92	0.69
2:B:147:TYR:CD2	2:B:198:MET:HE3	2.28	0.69
2:B:238:LEU:HD12	2:B:238:LEU:C	2.18	0.69
9:C:2013:3PE:H2D2	9:C:2013:3PE:H3H1	1.74	0.69
1:G:394:GLY:O	1:G:397:THR:HB	1.93	0.69
3:I:248:HIS:O	3:I:252:VAL:HG23	1.93	0.69
9:I:3010:3PE:C3E	9:I:3010:3PE:C3I	2.71	0.69
1:A:99:ILE:CD1	8:A:1001:HEA:HBA2	2.24	0.69
2:B:72:VAL:O	2:B:76:ILE:HG13	1.93	0.68
3:C:62:VAL:CG1	9:C:2008:3PE:H31	2.22	0.68
3:C:73:PRO:HB2	4:D:18:ILE:CD1	2.23	0.68
3:C:161:ARG:NH2	3:C:232:PHE:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:PHE:CE1	3:C:244:ILE:HD11	2.28	0.68
1:G:63:MET:HE1	1:G:95:TRP:HB2	1.75	0.68
1:G:426:LEU:HD21	1:G:464:ALA:HB1	1.75	0.68
3:I:133:LEU:H	3:I:134:PRO:CD	2.06	0.68
1:G:406:VAL:CG2	2:H:57:LEU:HD23	2.24	0.68
3:C:122:PRO:HG2	3:C:198:TYR:HB2	1.75	0.68
1:G:99:ILE:CD1	8:G:1001:HEA:HBA2	2.24	0.68
1:G:486:TYR:CD2	1:G:490:PHE:HB2	2.28	0.68
1:A:400:VAL:HG11	1:A:410:TYR:HE2	1.57	0.68
1:A:543:THR:CG2	1:A:547:PRO:HD3	2.23	0.68
2:H:147:TYR:CD2	2:H:198:MET:HE3	2.28	0.68
2:H:194:THR:HG22	2:H:266:THR:OG1	1.94	0.68
3:I:80:ARG:O	3:I:84:ILE:HG13	1.92	0.68
9:C:2010:3PE:H3I3	9:C:2010:3PE:C3E	2.19	0.68
2:H:211:THR:HG23	2:H:234:ARG:O	1.94	0.68
9:I:3013:3PE:H351	9:I:3013:3PE:C31	2.23	0.68
1:A:543:THR:HG23	1:A:545:PRO:O	1.95	0.68
1:G:91:ASN:C	1:G:91:ASN:OD1	2.36	0.68
1:A:81:TRP:CD2	1:A:82:PRO:HD2	2.29	0.67
2:H:238:LEU:C	2:H:238:LEU:HD12	2.19	0.67
1:G:249:ALA:HB2	1:G:278:ILE:CG2	2.24	0.67
9:G:3012:3PE:H2H1	9:I:3010:3PE:H2I3	1.76	0.67
2:H:175:GLU:O	2:H:178:GLN:HG2	1.94	0.67
4:D:47:ALA:HA	9:D:2011:3PE:H321	1.75	0.67
4:J:47:ALA:HA	9:J:3011:3PE:H321	1.76	0.67
9:G:3012:3PE:H261	4:J:31:MET:SD	2.35	0.67
3:I:133:LEU:H	3:I:134:PRO:HD2	1.59	0.66
1:A:213:LEU:HB2	3:C:81:TRP:CH2	2.31	0.66
3:C:162:ARG:HG3	3:C:163:ASP:N	2.10	0.66
1:G:284:HIS:NE2	1:G:288:TYR:CE2	2.51	0.66
1:G:543:THR:HG23	1:G:545:PRO:O	1.95	0.66
2:H:185:TYR:HE1	2:H:247:ILE:HD13	1.60	0.66
1:A:489:ALA:CB	2:B:36:PRO:HB2	2.25	0.66
2:H:231:VAL:O	2:H:232:PRO:C	2.37	0.66
3:C:73:PRO:HB2	4:D:18:ILE:HD11	1.78	0.66
3:C:62:VAL:HG11	9:C:2008:3PE:H31	1.76	0.66
3:I:120:PHE:HA	3:I:121:PRO:C	2.20	0.66
3:I:130:PRO:HA	3:I:134:PRO:HG2	1.78	0.66
1:G:345:GLN:HE22	1:G:408:ARG:NH2	1.87	0.66
1:G:88:CYS:O	1:G:90:PRO:HD3	1.96	0.65
9:I:3013:3PE:H3H2	9:I:3013:3PE:C2E	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:GLY:O	2:H:83:PHE:HB3	1.96	0.65
1:G:480:PRO:HG2	1:G:483:TYR:CE2	2.32	0.65
2:H:72:VAL:O	2:H:76:ILE:HG13	1.95	0.65
1:A:299:SER:O	1:A:300:HIS:C	2.38	0.65
2:H:43:PHE:CD2	2:H:55:HIS:CD2	2.85	0.65
1:A:357:VAL:HB	1:A:358:PRO:CD	2.26	0.65
9:A:2009:3PE:H2C2	9:A:2009:3PE:H3B2	1.78	0.65
1:G:543:THR:CG2	1:G:547:PRO:HD3	2.20	0.65
1:G:493:TRP:HA	1:G:493:TRP:CE3	2.32	0.65
2:H:30:LEU:HD22	2:H:247:ILE:HD11	1.79	0.65
3:I:73:PRO:HB2	4:J:18:ILE:HD11	1.77	0.65
2:B:175:GLU:O	2:B:178:GLN:HG2	1.97	0.65
9:C:2013:3PE:H351	9:C:2013:3PE:C31	2.27	0.64
1:G:486:TYR:HD2	1:G:490:PHE:HB2	1.63	0.64
1:G:560:TRP:CD1	1:G:560:TRP:C	2.74	0.64
1:A:252:MET:HE3	1:A:264:PHE:HZ	1.63	0.64
1:G:241:LEU:HD13	9:J:3011:3PE:C2H	2.27	0.64
3:I:74:VAL:HG13	4:J:18:ILE:HG12	1.78	0.64
1:G:137:ARG:HH21	9:G:3009:3PE:H112	1.61	0.64
1:A:212:PHE:HE1	1:A:222:MET:HE3	1.62	0.64
1:A:422:TYR:CD2	1:A:426:LEU:HD12	2.33	0.64
2:B:105:THR:O	2:B:109:ILE:HG13	1.98	0.64
9:C:2010:3PE:C3E	9:C:2010:3PE:C3I	2.76	0.64
1:G:18:THR:HA	1:G:22:MET:CE	2.26	0.64
1:A:124:MET:HB3	1:A:125:PRO:CD	2.23	0.63
3:C:101:PHE:CE2	3:C:261:ILE:HG12	2.33	0.63
1:G:221:THR:HG22	9:G:3012:3PE:H121	1.79	0.63
1:A:486:TYR:CD2	1:A:490:PHE:HB2	2.34	0.63
3:I:162:ARG:HG3	3:I:163:ASP:N	2.12	0.63
2:B:263:MET:N	2:B:264:PRO:HD3	2.13	0.63
3:C:52:LEU:HD23	3:C:55:MET:HE2	1.81	0.63
1:A:247:ALA:HB2	9:A:2009:3PE:H3I2	1.80	0.63
1:A:374:SER:HB2	2:B:85:GLU:HA	1.79	0.63
1:A:401:LEU:HD13	8:A:1002:HEA:HBA2	1.79	0.63
2:B:200:VAL:HG13	2:B:201:PRO:HD2	1.79	0.63
3:I:8:ASP:HB3	3:I:72:THR:CG2	2.18	0.63
1:A:199:ALA:O	1:A:200:SER:C	2.41	0.63
1:A:533:GLU:OE1	10:A:2113:HOH:O	2.16	0.63
2:B:71:PHE:O	2:B:75:LEU:HD12	1.99	0.63
1:G:63:MET:CG	1:G:94:LEU:HD23	2.27	0.63
2:H:98:SER:O	2:H:99:PRO:C	2.40	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:220:LEU:HD23	3:C:243:ALA:HB1	1.80	0.62
1:G:247:ALA:HB2	9:G:3009:3PE:H3I2	1.79	0.62
1:G:379:THR:HB	1:G:380:PRO:CD	2.26	0.62
3:I:186:TYR:O	3:I:187:SER:C	2.39	0.62
1:G:447:GLN:HG3	1:G:448:TYR:N	2.13	0.62
3:C:124:GLY:HA2	1:G:557:ARG:HH12	1.64	0.62
2:H:156:PHE:CD2	2:H:196:THR:HG21	2.34	0.62
1:A:397:THR:CG2	1:A:419:HIS:HB2	2.29	0.62
2:B:160:MET:HG3	2:B:264:PRO:HG2	1.81	0.62
1:G:484:ILE:HG12	1:G:484:ILE:O	2.00	0.62
1:A:121:ASN:OD1	1:A:208:MET:HE2	2.00	0.62
1:A:221:THR:HG22	9:A:2012:3PE:H121	1.82	0.62
1:G:91:ASN:ND2	1:G:165:GLN:HE22	1.96	0.62
9:G:3012:3PE:H2F1	9:J:3011:3PE:H2I2	1.82	0.62
3:I:252:VAL:HG12	9:I:3010:3PE:H3H2	1.81	0.62
1:G:397:THR:CG2	1:G:419:HIS:HB2	2.30	0.62
1:A:221:THR:HA	9:A:2012:3PE:H121	1.80	0.62
1:A:429:VAL:HG13	8:A:1001:HEA:H273	1.82	0.62
1:A:445:GLY:HA2	1:A:525:VAL:HG12	1.82	0.62
3:C:231:HIS:O	9:C:2008:3PE:H121	1.99	0.62
2:H:200:VAL:O	2:H:269:VAL:HA	1.99	0.62
3:I:253:VAL:HA	9:I:3010:3PE:H3H1	1.81	0.61
1:A:188:ASP:CG	1:A:257:ARG:HH12	2.08	0.61
1:A:408:ARG:NE	2:B:126:GLN:OE1	2.27	0.61
1:A:539:GLU:HG2	1:A:540:TRP:N	2.14	0.61
3:I:240:PHE:CE1	3:I:244:ILE:HD11	2.35	0.61
1:G:394:GLY:HA3	1:G:423:VAL:HG13	1.83	0.61
1:A:213:LEU:CB	3:C:81:TRP:CH2	2.83	0.61
2:H:211:THR:HG22	2:H:212:GLY:N	2.12	0.61
1:A:135:PHE:HE1	3:C:79:LEU:HD23	1.66	0.61
2:B:145:TRP:CE2	2:B:263:MET:HE2	2.35	0.61
3:C:13:PRO:HG3	10:C:2036:HOH:O	2.00	0.61
3:C:133:LEU:N	3:C:134:PRO:CD	2.60	0.61
3:C:150:TRP:CD1	3:C:150:TRP:C	2.79	0.61
2:B:137:LYS:HZ3	4:J:11:HIS:CD2	2.19	0.61
3:C:85:LEU:HA	3:C:88:MET:HE2	1.83	0.61
1:G:357:VAL:HB	1:G:358:PRO:HD3	1.82	0.61
3:C:112:GLU:HB2	3:C:116:ILE:HB	1.81	0.61
3:C:162:ARG:HG3	3:C:163:ASP:H	1.66	0.61
3:C:214:ILE:O	3:C:218:ILE:HG12	2.01	0.61
8:G:1002:HEA:HHC	8:G:1002:HEA:O11	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:3012:3PE:H3E1	9:J:3011:3PE:H2I3	1.83	0.61
9:I:3013:3PE:C3H	9:I:3013:3PE:C2D	2.54	0.61
1:G:221:THR:HA	9:G:3012:3PE:H121	1.83	0.60
1:G:498:SER:O	1:G:502:PHE:HD2	1.84	0.60
1:A:387:PHE:CD1	1:A:387:PHE:C	2.78	0.60
2:H:263:MET:N	2:H:264:PRO:CD	2.64	0.60
1:A:46:ALA:O	1:A:49:VAL:HG12	2.01	0.60
2:H:160:MET:HB2	2:H:264:PRO:HD2	1.83	0.60
3:I:34:LEU:HB3	3:I:39:SER:OG	2.01	0.60
3:I:249:PHE:O	3:I:253:VAL:HG23	2.02	0.60
2:B:30:LEU:HD22	2:B:247:ILE:HD11	1.81	0.60
3:C:133:LEU:N	3:C:134:PRO:HD2	2.16	0.60
1:G:95:TRP:CZ2	1:G:99:ILE:HD11	2.36	0.60
1:G:243:LEU:HD22	1:G:282:PHE:HE2	1.66	0.60
2:H:145:TRP:CD1	2:H:263:MET:HE2	2.37	0.60
9:A:2009:3PE:H3A1	9:A:2009:3PE:H2A2	1.82	0.60
1:A:480:PRO:HG2	1:A:483:TYR:CE2	2.37	0.60
4:D:18:ILE:O	4:D:18:ILE:HG22	2.02	0.60
1:G:185:TYR:HB3	3:I:37:HIS:CD2	2.37	0.60
2:H:279:LEU:O	2:H:283:ARG:HG2	2.02	0.60
1:A:241:LEU:HD13	9:D:2011:3PE:H2I1	1.83	0.60
1:A:331:TRP:CD1	1:A:331:TRP:C	2.80	0.60
2:B:169:ASP:O	2:B:170:ASN:HB2	2.01	0.60
1:A:206:ILE:HG22	1:A:207:ASN:N	2.16	0.60
1:G:99:ILE:HD12	8:G:1001:HEA:CBA	2.31	0.60
1:A:160:PRO:HG2	1:A:185:TYR:CE1	2.37	0.59
1:G:243:LEU:HD22	1:G:282:PHE:CE2	2.37	0.59
1:G:396:VAL:CG1	2:H:65:ILE:HB	2.32	0.59
1:G:63:MET:CE	1:G:484:ILE:HG13	2.31	0.59
1:G:532:ASN:OD1	1:G:532:ASN:C	2.43	0.59
3:I:151:ALA:O	3:I:164:VAL:HG22	2.02	0.59
1:G:306:ALA:O	1:G:307:LYS:HB2	2.02	0.59
2:H:143:TRP:HZ2	2:H:257:GLY:HA3	1.67	0.59
9:A:2009:3PE:H111	3:C:12:LEU:HD11	1.84	0.59
3:I:73:PRO:HB2	4:J:18:ILE:CD1	2.32	0.59
3:C:8:ASP:H	4:D:16:MET:HE3	1.67	0.59
3:C:141:LEU:O	3:C:142:LEU:C	2.45	0.59
3:I:42:TRP:O	3:I:46:ILE:HG12	2.02	0.59
3:I:133:LEU:N	3:I:134:PRO:CD	2.65	0.59
1:A:472:HIS:O	1:A:476:ARG:HG3	2.02	0.59
9:A:2009:3PE:H2E1	9:A:2009:3PE:H3E2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:ASP:HB3	3:C:72:THR:CG2	2.24	0.59
1:G:374:SER:HA	2:H:83:PHE:O	2.03	0.59
3:I:52:LEU:HD22	9:I:3008:3PE:H3C2	1.85	0.59
3:I:58:TRP:O	3:I:62:VAL:HG23	2.03	0.59
9:A:2009:3PE:H2C2	9:A:2009:3PE:C3A	2.32	0.59
1:G:235:THR:OG1	1:G:293:PRO:HD3	2.03	0.59
1:A:198:GLY:HA2	1:A:243:LEU:HD12	1.84	0.59
2:B:194:THR:HG22	2:B:266:THR:OG1	2.02	0.59
1:G:460:MET:O	1:G:460:MET:HG3	2.02	0.59
1:A:185:TYR:HB3	3:C:37:HIS:CD2	2.38	0.58
1:A:247:ALA:HB2	9:A:2009:3PE:C3I	2.32	0.58
2:B:84:HIS:HD2	2:B:86:LYS:H	1.51	0.58
3:C:155:LEU:HB2	3:C:164:VAL:HG21	1.84	0.58
1:G:489:ALA:CB	2:H:36:PRO:HB2	2.28	0.58
1:A:235:THR:OG1	1:A:293:PRO:HD3	2.03	0.58
3:C:107:TYR:OH	4:D:51:ALA:HA	2.03	0.58
1:G:26:HIS:C	1:G:26:HIS:CD2	2.81	0.58
1:G:112:ILE:N	1:G:113:PRO:CD	2.65	0.58
9:C:2013:3PE:H3H2	9:C:2013:3PE:C2E	2.33	0.58
1:G:63:MET:HE3	1:G:484:ILE:HG13	1.83	0.58
1:G:311:PHE:CD1	1:G:311:PHE:C	2.80	0.58
1:A:432:ILE:HG21	8:A:1001:HEA:H252	1.85	0.58
1:G:282:PHE:CD1	1:G:282:PHE:C	2.79	0.58
3:I:131:TRP:HE3	3:I:135:LEU:HD22	1.68	0.58
1:A:127:HIS:CE1	1:A:300:HIS:CE1	2.91	0.58
1:A:298:VAL:O	1:A:299:SER:C	2.45	0.58
2:B:254:GLU:O	2:B:255:LEU:C	2.46	0.58
2:H:84:HIS:HD2	2:H:86:LYS:H	1.49	0.58
1:A:367:ILE:HA	1:A:370:MET:HE2	1.86	0.58
1:A:520:THR:CG2	1:A:521:ARG:HG2	2.21	0.58
1:G:387:PHE:CD1	1:G:387:PHE:C	2.82	0.58
2:H:134:VAL:HG12	2:H:135:THR:N	2.19	0.58
2:H:220:THR:HB	2:H:227:LYS:HG3	1.84	0.58
1:A:463:GLY:HA2	1:A:503:LEU:HD23	1.85	0.58
1:A:538:LEU:HD21	1:A:560:TRP:CE3	2.39	0.58
1:G:148:ALA:O	1:G:149:GLY:C	2.47	0.58
3:I:30:PHE:CD2	3:I:43:MET:HE1	2.38	0.58
1:A:127:HIS:CE1	1:A:300:HIS:HE1	2.22	0.58
1:A:41:GLY:O	1:A:45:VAL:HB	2.03	0.58
1:A:153:ALA:O	1:A:156:SER:HB3	2.04	0.58
1:A:511:PHE:O	1:A:515:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:O	2:B:283:ARG:HG2	2.03	0.58
3:C:63:VAL:O	3:C:64:THR:C	2.45	0.58
3:C:222:VAL:O	3:C:226:ARG:HG3	2.04	0.58
2:H:147:TYR:CE2	2:H:198:MET:HE3	2.39	0.58
1:A:439:TRP:O	1:A:443:MET:HG3	2.04	0.57
1:A:25:ASN:HD21	1:A:27:LYS:NZ	2.00	0.57
1:A:63:MET:CE	1:A:484:ILE:HG13	2.34	0.57
1:A:63:MET:HE1	1:A:95:TRP:HB2	1.85	0.57
2:B:235:LEU:HD11	4:J:11:HIS:N	2.17	0.57
3:C:184:TYR:O	3:C:187:SER:HB3	2.05	0.57
1:G:409:TYR:CD1	1:G:409:TYR:C	2.81	0.57
1:G:429:VAL:CG1	8:G:1001:HEA:H273	2.35	0.57
1:A:91:ASN:OD1	1:A:91:ASN:C	2.46	0.57
1:A:252:MET:HE3	1:A:264:PHE:CZ	2.39	0.57
1:A:396:VAL:CG1	2:B:65:ILE:HD12	2.34	0.57
1:A:560:TRP:CD1	1:A:560:TRP:C	2.83	0.57
3:C:150:TRP:NE1	3:C:163:ASP:OD1	2.30	0.57
4:D:17:ASP:OD1	4:D:17:ASP:C	2.47	0.57
1:G:112:ILE:N	1:G:113:PRO:HD2	2.20	0.57
1:G:455:LEU:HG	1:G:459:MET:HE2	1.84	0.57
1:A:539:GLU:HG2	1:A:540:TRP:H	1.67	0.57
2:B:185:TYR:HE1	2:B:247:ILE:HD13	1.69	0.57
1:G:426:LEU:CD2	1:G:464:ALA:HB1	2.34	0.57
9:I:3010:3PE:H2I2	4:J:36:ALA:HB1	1.85	0.57
1:A:407:ASP:O	1:A:408:ARG:C	2.47	0.57
2:B:48:SER:HB2	2:B:241:ARG:O	2.03	0.57
1:A:538:LEU:HD21	1:A:560:TRP:HE3	1.69	0.57
1:G:326:LEU:O	1:G:328:PHE:N	2.38	0.57
2:H:143:TRP:CZ2	2:H:257:GLY:HA3	2.40	0.57
1:A:18:THR:HA	1:A:22:MET:CE	2.32	0.57
1:A:456:HIS:CE1	1:A:511:PHE:HB2	2.40	0.57
3:C:42:TRP:CD1	3:C:42:TRP:H	2.16	0.57
1:G:442:LYS:O	1:G:546:PRO:HD3	2.04	0.57
3:C:253:VAL:HA	9:C:2010:3PE:H3H1	1.85	0.57
1:G:410:TYR:O	1:G:413:THR:OG1	2.17	0.57
2:H:197:ALA:HB1	2:H:268:LYS:HG3	1.87	0.57
3:I:199:GLY:O	3:I:203:PHE:HB2	2.05	0.57
1:A:225:VAL:HG12	1:A:226:PRO:O	2.04	0.56
1:A:243:LEU:N	1:A:244:PRO:CD	2.68	0.56
1:G:91:ASN:CG	1:G:165:GLN:HE22	2.13	0.56
2:H:201:PRO:HB2	2:H:204:LYS:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:HIS:C	1:A:26:HIS:CD2	2.83	0.56
9:C:2010:3PE:H381	9:C:2010:3PE:H2B1	1.86	0.56
1:G:408:ARG:NE	2:H:126:GLN:OE1	2.28	0.56
1:A:159:ALA:HB1	1:A:160:PRO:HD2	1.87	0.56
2:B:190:PHE:CD1	2:B:190:PHE:C	2.82	0.56
3:C:133:LEU:O	3:C:136:ILE:HB	2.06	0.56
1:G:273:VAL:HG13	1:G:335:MET:HE1	1.86	0.56
1:G:403:GLN:O	1:G:404:ALA:C	2.47	0.56
1:G:504:SER:O	1:G:507:SER:HB2	2.05	0.56
4:J:36:ALA:O	4:J:40:VAL:HG23	2.05	0.56
2:B:147:TYR:HD2	2:B:198:MET:HE3	1.71	0.56
2:B:211:THR:HG23	2:B:234:ARG:O	2.05	0.56
1:G:332:ALA:HB3	1:G:348:PHE:CG	2.40	0.56
1:G:396:VAL:HG11	2:H:65:ILE:HB	1.86	0.56
2:H:76:ILE:O	2:H:80:VAL:HG23	2.06	0.56
1:A:148:ALA:HB3	1:A:196:LEU:HD13	1.88	0.56
1:G:127:HIS:NE2	1:G:539:GLU:OE1	2.39	0.56
8:G:1002:HEA:HBC1	8:G:1002:HEA:HMC1	1.86	0.56
1:A:95:TRP:HB2	1:A:484:ILE:HG13	1.87	0.56
1:A:241:LEU:HD13	9:D:2011:3PE:C2H	2.35	0.56
1:A:460:MET:O	1:A:460:MET:HG3	2.05	0.56
3:C:30:PHE:CD2	3:C:43:MET:HE1	2.40	0.56
1:G:270:GLY:O	3:I:109:MET:HG3	2.06	0.56
2:B:98:SER:O	2:B:99:PRO:C	2.48	0.56
2:B:235:LEU:HD11	4:J:11:HIS:H	1.71	0.56
3:C:81:TRP:O	3:C:82:GLY:C	2.46	0.56
1:G:63:MET:HE1	1:G:95:TRP:HE3	1.71	0.56
3:I:209:HIS:NE2	3:I:254:TRP:HB2	2.20	0.56
1:G:318:TYR:O	1:G:319:ALA:C	2.49	0.56
9:G:3012:3PE:H3E1	9:J:3011:3PE:H2F1	1.88	0.56
1:A:282:PHE:CD1	1:A:282:PHE:C	2.80	0.56
1:G:225:VAL:HG12	1:G:226:PRO:O	2.06	0.56
2:H:98:SER:HB2	2:H:99:PRO:HD3	1.88	0.56
2:H:106:ILE:O	2:H:107:VAL:C	2.45	0.56
2:H:132:ALA:HB1	2:H:134:VAL:O	2.06	0.56
1:A:127:HIS:HE1	1:A:300:HIS:CE1	2.24	0.55
1:A:394:GLY:HA3	1:A:423:VAL:HG13	1.88	0.55
2:B:200:VAL:O	2:B:269:VAL:HA	2.06	0.55
3:C:83:PHE:HE1	9:C:2008:3PE:H262	1.71	0.55
3:C:248:HIS:O	3:C:252:VAL:HG23	2.05	0.55
3:C:266:GLN:OXT	3:C:266:GLN:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ASN:HD21	1:G:165:GLN:CD	2.14	0.55
1:G:264:PHE:HA	1:G:271:ASP:H	1.71	0.55
3:I:168:LEU:O	3:I:172:ILE:HG13	2.07	0.55
3:I:212:HIS:O	3:I:213:VAL:C	2.48	0.55
1:A:212:PHE:O	1:A:216:ARG:HG3	2.06	0.55
2:B:221:VAL:HB	2:B:224:PHE:HD2	1.70	0.55
1:G:378:LYS:HE2	10:G:3034:HOH:O	2.05	0.55
1:G:483:TYR:OH	2:H:251:GLN:HB3	2.07	0.55
3:I:21:ALA:HB2	3:I:54:THR:CG2	2.31	0.55
1:G:315:PRO:HG2	10:H:1132:HOH:O	2.07	0.55
9:I:3010:3PE:H331	9:I:3010:3PE:H231	1.88	0.55
3:C:74:VAL:HG13	4:D:18:ILE:HG12	1.88	0.55
3:I:133:LEU:HD23	3:I:185:GLU:HG3	1.86	0.55
1:A:125:PRO:O	1:A:126:LEU:C	2.49	0.55
1:A:345:GLN:HE22	1:A:408:ARG:NH2	2.01	0.55
1:A:508:PHE:CE2	1:A:512:LEU:HD11	2.42	0.55
1:G:112:ILE:HD12	10:G:3038:HOH:O	2.05	0.55
9:G:3009:3PE:H2E1	9:G:3009:3PE:H3E2	1.88	0.55
3:C:21:ALA:HB2	3:C:54:THR:CG2	2.30	0.55
3:C:34:LEU:HB3	3:C:39:SER:OG	2.07	0.55
3:C:120:PHE:CD1	3:C:120:PHE:C	2.85	0.55
4:J:18:ILE:HG22	4:J:18:ILE:O	2.06	0.55
1:A:396:VAL:CG1	2:B:65:ILE:HB	2.37	0.55
2:H:145:TRP:CE2	2:H:265:ILE:HD11	2.41	0.55
3:I:222:VAL:HA	3:I:225:ILE:HD12	1.88	0.55
1:A:374:SER:HB3	2:B:88:ASN:O	2.07	0.55
1:A:379:THR:HB	1:A:380:PRO:CD	2.29	0.55
8:A:1002:HEA:O11	8:A:1002:HEA:HHC	2.06	0.55
2:B:98:SER:HB2	2:B:99:PRO:CD	2.37	0.55
2:B:98:SER:HB2	2:B:99:PRO:HD3	1.88	0.55
1:G:357:VAL:HB	1:G:358:PRO:CD	2.37	0.55
2:H:221:VAL:O	2:H:222:PRO:C	2.50	0.55
3:I:155:LEU:HB2	3:I:164:VAL:HG21	1.87	0.55
3:I:228:GLN:HA	3:I:228:GLN:OE1	2.05	0.55
2:H:136:VAL:HG11	2:H:198:MET:CE	2.37	0.55
1:A:17:PHE:O	1:A:21:PHE:HB2	2.07	0.55
1:A:241:LEU:HD13	9:D:2011:3PE:C2I	2.37	0.55
9:A:2009:3PE:H3E1	9:A:2009:3PE:C2E	2.37	0.55
1:G:409:TYR:C	1:G:409:TYR:HD1	2.14	0.55
1:A:49:VAL:O	1:A:50:TYR:C	2.47	0.54
2:B:145:TRP:CE2	2:B:265:ILE:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:ILE:HG13	3:C:198:TYR:N	2.21	0.54
3:C:228:GLN:OE1	3:C:228:GLN:HA	2.07	0.54
1:G:420:PHE:O	1:G:424:MET:HB2	2.07	0.54
2:H:111:ILE:O	2:H:114:ALA:HB3	2.06	0.54
1:A:143:TYR:O	1:A:146:TYR:HB3	2.07	0.54
1:G:284:HIS:O	1:G:287:VAL:HG22	2.07	0.54
1:G:406:VAL:HG23	2:H:57:LEU:HD23	1.88	0.54
3:I:122:PRO:HB2	3:I:125:ILE:HG13	1.89	0.54
1:A:246:LEU:O	1:A:250:ILE:HG12	2.08	0.54
1:A:308:LYS:HD3	1:A:369:THR:O	2.07	0.54
1:A:406:VAL:CG2	2:B:57:LEU:HD23	2.37	0.54
2:B:248:PHE:HE2	2:B:269:VAL:HG12	1.73	0.54
3:C:201:ASN:O	3:C:202:PHE:C	2.49	0.54
1:G:539:GLU:HG2	1:G:540:TRP:H	1.72	0.54
3:I:220:LEU:CD2	3:I:243:ALA:HB1	2.37	0.54
9:A:2012:3PE:C2H	9:C:2010:3PE:H2I3	2.37	0.54
1:G:342:LEU:HD21	2:H:124:PHE:CD1	2.43	0.54
2:H:218:SER:HA	2:H:229:ASP:HA	1.90	0.54
3:C:151:ALA:O	3:C:164:VAL:HG22	2.07	0.54
2:H:263:MET:N	2:H:264:PRO:HD3	2.23	0.54
3:I:42:TRP:H	3:I:42:TRP:CD1	2.20	0.54
3:I:147:ALA:CB	3:I:170:LEU:HD23	2.37	0.54
1:A:406:VAL:HG23	2:B:57:LEU:HD23	1.89	0.54
3:C:226:ARG:HH21	3:C:231:HIS:HB3	1.71	0.54
1:G:105:LEU:O	1:G:110:VAL:HG23	2.07	0.54
3:I:152:HIS:CG	3:I:244:ILE:HD13	2.43	0.54
2:B:78:TYR:CD1	2:B:78:TYR:C	2.85	0.54
2:H:234:ARG:HD3	10:H:1128:HOH:O	2.07	0.54
1:A:115:LEU:HG	1:A:432:ILE:HG12	1.89	0.54
3:C:212:HIS:O	3:C:213:VAL:C	2.51	0.54
1:G:64:CYS:HB2	1:G:67:HIS:CD2	2.43	0.54
1:G:127:HIS:CE1	1:G:300:HIS:CE1	2.95	0.54
2:H:252:CYS:HB2	2:H:263:MET:SD	2.46	0.54
1:A:505:PHE:O	1:A:509:LEU:HG	2.07	0.54
1:G:148:ALA:HB3	1:G:196:LEU:HD13	1.90	0.54
2:H:71:PHE:CD1	2:H:71:PHE:C	2.85	0.54
2:H:173:SER:H	2:H:176:VAL:HB	1.73	0.54
3:I:114:PRO:O	3:I:115:ILE:C	2.48	0.54
1:A:52:ARG:NH1	1:A:498:SER:OG	2.41	0.54
1:A:99:ILE:HD12	8:A:1001:HEA:HBA2	1.90	0.54
1:A:342:LEU:HD21	2:B:124:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:MET:HB3	8:A:1001:HEA:HBC1	1.89	0.54
1:A:541:THR:HG22	1:A:541:THR:O	2.07	0.53
2:H:62:LEU:HA	2:H:65:ILE:HD11	1.90	0.53
1:A:42:LEU:O	1:A:43:ILE:C	2.49	0.53
1:A:426:LEU:CD2	1:A:464:ALA:HB1	2.38	0.53
9:A:2009:3PE:H2C2	9:A:2009:3PE:C3B	2.38	0.53
1:G:247:ALA:HB2	9:G:3009:3PE:C3I	2.37	0.53
1:G:273:VAL:HG13	1:G:335:MET:CE	2.38	0.53
1:G:556:LYS:N	1:G:559:ASP:OD2	2.38	0.53
2:H:220:THR:O	2:H:250:GLY:HA3	2.07	0.53
2:H:289:LEU:HG	2:H:289:LEU:OXT	2.07	0.53
1:A:484:ILE:O	1:A:484:ILE:HG12	2.07	0.53
2:B:152:GLU:HB3	2:B:283:ARG:HH21	1.74	0.53
2:H:145:TRP:CE2	2:H:263:MET:HE2	2.44	0.53
1:A:63:MET:HE1	1:A:95:TRP:HE3	1.73	0.53
3:C:196:ASN:HB2	10:C:2027:HOH:O	2.08	0.53
4:D:18:ILE:HG22	4:D:21:GLN:HB2	1.91	0.53
1:G:17:PHE:O	1:G:21:PHE:HB2	2.08	0.53
1:G:332:ALA:HB3	1:G:348:PHE:CD2	2.42	0.53
2:B:235:LEU:HG	4:J:11:HIS:O	2.09	0.53
1:G:387:PHE:O	1:G:388:LEU:C	2.52	0.53
1:G:41:GLY:O	1:G:45:VAL:HB	2.08	0.53
2:B:161:ILE:HG21	2:B:180:LEU:HD23	1.89	0.53
2:B:220:THR:HB	2:B:227:LYS:HG3	1.90	0.53
1:A:241:LEU:HD13	9:D:2011:3PE:H2H2	1.90	0.53
2:B:147:TYR:CE2	2:B:198:MET:HE3	2.44	0.53
1:G:212:PHE:HE1	1:G:222:MET:HE3	1.73	0.53
1:A:112:ILE:N	1:A:113:PRO:CD	2.72	0.53
2:B:109:ILE:O	2:B:113:VAL:HG23	2.09	0.53
2:B:173:SER:H	2:B:176:VAL:HB	1.74	0.53
3:C:249:PHE:CE1	9:C:2010:3PE:H3I1	2.44	0.53
1:A:256:ASP:N	1:A:261:THR:OG1	2.41	0.53
1:A:370:MET:SD	1:A:385:LEU:HD21	2.49	0.53
1:A:398:GLY:O	1:A:402:SER:N	2.38	0.53
3:C:177:LEU:O	3:C:178:PHE:C	2.52	0.53
1:G:40:VAL:CG1	1:G:105:LEU:HD22	2.39	0.53
1:G:406:VAL:HG22	2:H:57:LEU:HD23	1.90	0.53
2:H:220:THR:OG1	2:H:221:VAL:N	2.41	0.53
1:A:64:CYS:HB2	1:A:67:HIS:CD2	2.45	0.52
1:A:154:VAL:O	1:A:155:ALA:C	2.52	0.52
2:B:43:PHE:CD2	2:B:55:HIS:CD2	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:PHE:HE2	2:B:269:VAL:CG1	2.21	0.52
9:C:2010:3PE:H2I2	4:D:36:ALA:HB1	1.91	0.52
9:G:3009:3PE:H2C2	9:G:3009:3PE:H3B2	1.92	0.52
3:I:103:LYS:HD3	3:I:103:LYS:O	2.08	0.52
3:I:245:TRP:HE1	9:I:3013:3PE:H322	1.74	0.52
4:J:17:ASP:OD2	10:J:1143:HOH:O	2.19	0.52
4:J:20:GLN:NE2	10:J:1130:HOH:O	2.40	0.52
1:A:263:PHE:HE1	3:C:201:ASN:HD22	1.58	0.52
1:A:420:PHE:O	1:A:424:MET:HB2	2.09	0.52
1:A:493:TRP:HA	1:A:493:TRP:CE3	2.43	0.52
2:B:76:ILE:O	2:B:80:VAL:HG23	2.08	0.52
1:G:456:HIS:O	1:G:457:PHE:C	2.53	0.52
3:I:197:ILE:O	3:I:198:TYR:C	2.50	0.52
3:I:245:TRP:NE1	9:I:3013:3PE:H322	2.25	0.52
3:C:249:PHE:HE1	9:C:2010:3PE:H3I1	1.74	0.52
1:A:473:PHE:O	1:A:474:LEU:C	2.49	0.52
2:B:107:VAL:HG13	2:B:108:PRO:HD3	1.90	0.52
3:C:168:LEU:O	3:C:172:ILE:HG13	2.09	0.52
1:G:294:ALA:O	1:G:298:VAL:HG23	2.10	0.52
3:I:136:ILE:HG21	3:I:181:PHE:CE2	2.45	0.52
1:A:432:ILE:O	1:A:436:ILE:HG13	2.09	0.52
1:A:486:TYR:HD2	1:A:490:PHE:HB2	1.73	0.52
2:B:192:LEU:HB3	2:B:249:PHE:CD2	2.45	0.52
3:I:112:GLU:HB2	3:I:116:ILE:HB	1.91	0.52
1:A:415:TYR:CD1	1:A:415:TYR:O	2.63	0.52
1:A:418:ALA:O	1:A:419:HIS:C	2.53	0.52
4:D:50:ASN:O	9:D:2011:3PE:H112	2.09	0.52
1:G:213:LEU:HB3	3:I:81:TRP:CH2	2.44	0.52
2:H:182:GLU:HA	2:H:182:GLU:OE1	2.08	0.52
9:I:3010:3PE:H2B1	9:I:3010:3PE:H381	1.92	0.52
3:C:226:ARG:HB3	3:C:231:HIS:HB2	1.92	0.52
2:H:78:TYR:CD1	2:H:78:TYR:C	2.88	0.52
1:A:63:MET:HE3	1:A:484:ILE:HG13	1.90	0.52
1:A:148:ALA:O	1:A:151:SER:HB2	2.09	0.52
9:A:2009:3PE:H221	3:C:58:TRP:NE1	2.25	0.52
3:C:152:HIS:HB2	3:C:244:ILE:HD13	1.91	0.52
9:C:2013:3PE:H261	9:C:2013:3PE:C3B	2.39	0.52
1:G:52:ARG:HD3	1:G:498:SER:HA	1.91	0.52
1:G:400:VAL:HG11	1:G:410:TYR:HE2	1.75	0.52
1:G:539:GLU:HG2	1:G:540:TRP:N	2.23	0.52
1:A:249:ALA:HB2	1:A:278:ILE:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:THR:O	3:C:73:PRO:C	2.53	0.52
1:G:262:THR:HG22	10:I:3030:HOH:O	2.09	0.52
1:G:331:TRP:CH2	9:I:3010:3PE:H251	2.45	0.52
1:G:433:PHE:HE1	1:G:511:PHE:CZ	2.28	0.52
3:I:130:PRO:HD2	10:I:3038:HOH:O	2.10	0.52
1:A:100:THR:O	1:A:104:ILE:HG13	2.10	0.51
1:A:506:ALA:HA	1:A:509:LEU:HD12	1.93	0.51
1:G:442:LYS:HE2	1:G:539:GLU:O	2.10	0.51
3:I:51:VAL:O	3:I:55:MET:HG3	2.09	0.51
3:I:141:LEU:O	3:I:142:LEU:C	2.53	0.51
3:I:201:ASN:O	3:I:202:PHE:C	2.53	0.51
1:A:262:THR:HG22	10:C:2028:HOH:O	2.10	0.51
1:A:357:VAL:CB	1:A:358:PRO:HD3	2.36	0.51
2:B:156:PHE:CD2	2:B:196:THR:HG21	2.45	0.51
2:B:214:ASP:OD1	2:B:214:ASP:N	2.44	0.51
1:G:29:ILE:HD12	1:G:139:ASN:HD22	1.75	0.51
1:G:71:GLY:HA3	1:G:74:LYS:NZ	2.26	0.51
1:G:112:ILE:HB	1:G:113:PRO:HD3	1.92	0.51
1:G:378:LYS:O	1:G:379:THR:C	2.52	0.51
1:A:141:LEU:O	1:A:141:LEU:HD12	2.11	0.51
1:A:213:LEU:HB3	3:C:81:TRP:HH2	1.75	0.51
1:A:415:TYR:CD1	1:A:415:TYR:C	2.89	0.51
3:C:130:PRO:O	3:C:134:PRO:HB2	2.10	0.51
3:C:212:HIS:HD2	3:C:246:TYR:OH	1.94	0.51
1:G:397:THR:HG21	1:G:419:HIS:CB	2.35	0.51
1:G:445:GLY:HA2	1:G:525:VAL:HG12	1.93	0.51
9:I:3013:3PE:H2B2	9:I:3013:3PE:H3D2	1.93	0.51
1:A:274:LEU:HD22	3:C:103:LYS:HD2	1.91	0.51
2:B:226:VAL:O	2:B:226:VAL:HG23	2.10	0.51
1:A:22:MET:HG2	3:C:16:ILE:CA	2.35	0.51
1:A:63:MET:HE1	1:A:95:TRP:CE3	2.45	0.51
1:A:436:ILE:HD11	8:A:1001:HEA:H251	1.93	0.51
1:A:491:ALA:O	1:A:492:THR:C	2.54	0.51
2:H:258:ILE:O	2:H:258:ILE:HG22	2.11	0.51
3:I:66:SER:HB2	3:I:71:HIS:CE1	2.46	0.51
3:I:152:HIS:CA	3:I:240:PHE:HE1	2.23	0.51
1:A:525:VAL:HG11	1:A:544:SER:HB3	1.93	0.51
3:C:63:VAL:O	3:C:66:SER:N	2.44	0.51
1:G:63:MET:HE1	1:G:95:TRP:CE3	2.45	0.51
1:G:91:ASN:HD21	1:G:165:GLN:NE2	2.09	0.51
1:G:325:VAL:HG22	9:G:3012:3PE:H3D1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:ALA:HB1	3:I:170:LEU:HD23	1.92	0.51
3:I:249:PHE:HE1	9:I:3010:3PE:H3I1	1.76	0.51
1:A:105:LEU:O	1:A:110:VAL:HG23	2.11	0.51
1:G:122:TYR:HD1	1:G:122:TYR:O	1.94	0.51
1:G:127:HIS:CE1	1:G:300:HIS:HE1	2.29	0.51
1:G:422:TYR:CD2	1:G:426:LEU:HD12	2.46	0.51
3:I:107:TYR:OH	4:J:51:ALA:HA	2.11	0.51
3:I:236:LYS:O	3:I:237:HIS:HB3	2.09	0.51
1:G:401:LEU:O	1:G:402:SER:C	2.54	0.51
3:I:133:LEU:HD23	3:I:185:GLU:CG	2.41	0.51
1:A:65:ALA:HB3	1:A:89:THR:HB	1.93	0.51
2:B:134:VAL:HG12	2:B:135:THR:N	2.26	0.51
3:C:152:HIS:O	3:C:156:VAL:HG23	2.11	0.51
1:A:216:ARG:NH1	1:A:220:MET:O	2.36	0.51
1:A:392:THR:O	1:A:393:VAL:C	2.54	0.51
2:B:160:MET:HB2	2:B:264:PRO:HD2	1.93	0.51
3:C:152:HIS:CA	3:C:240:PHE:HE1	2.20	0.51
1:G:24:THR:HG21	3:I:13:PRO:O	2.11	0.51
1:G:416:VAL:O	1:G:419:HIS:N	2.39	0.51
1:A:199:ALA:HA	9:A:2009:3PE:H3D1	1.92	0.50
1:A:450:GLU:O	1:A:454:LYS:HG3	2.11	0.50
2:H:145:TRP:CZ2	2:H:265:ILE:HD11	2.46	0.50
3:I:161:ARG:HH22	3:I:232:PHE:H	1.58	0.50
9:I:3013:3PE:H3H2	9:I:3013:3PE:H2E1	1.92	0.50
4:J:12:VAL:CG1	4:J:15:SER:HB2	2.41	0.50
1:A:74:LYS:H	1:A:74:LYS:HD2	1.76	0.50
2:B:251:GLN:O	2:B:252:CYS:C	2.54	0.50
1:G:63:MET:CE	1:G:95:TRP:HB2	2.42	0.50
1:G:148:ALA:CB	1:G:196:LEU:HD13	2.42	0.50
1:A:74:LYS:H	1:A:74:LYS:CD	2.24	0.50
1:A:347:TYR:CE2	9:D:2011:3PE:H252	2.46	0.50
3:C:161:ARG:HH22	3:C:232:PHE:H	1.59	0.50
1:G:127:HIS:HE1	1:G:300:HIS:CE1	2.29	0.50
1:A:70:SER:C	1:A:71:GLY:O	2.54	0.50
2:B:37:GLN:O	2:B:38:PRO:C	2.51	0.50
1:G:122:TYR:CD1	1:G:122:TYR:C	2.89	0.50
1:G:212:PHE:CD1	1:G:212:PHE:C	2.90	0.50
1:A:311:PHE:CD1	1:A:311:PHE:C	2.90	0.50
1:G:243:LEU:N	1:G:244:PRO:CD	2.74	0.50
1:G:377:LEU:HD21	2:H:80:VAL:HG13	1.94	0.50
3:I:101:PHE:CE2	3:I:261:ILE:HG12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:CD1	3:C:81:TRP:CZ2	2.95	0.50
1:A:394:GLY:O	1:A:397:THR:HB	2.12	0.50
2:B:211:THR:HG22	2:B:212:GLY:N	2.26	0.50
1:G:274:LEU:O	1:G:277:HIS:N	2.45	0.50
1:G:450:GLU:OE2	1:G:454:LYS:HE3	2.12	0.50
2:B:145:TRP:CZ2	2:B:265:ILE:HD11	2.46	0.50
1:G:274:LEU:HD22	3:I:103:LYS:HD2	1.92	0.50
1:G:379:THR:CB	1:G:380:PRO:HD3	2.32	0.50
1:G:427:GLY:O	1:G:430:PHE:HB2	2.11	0.50
2:H:209:GLN:CD	2:H:235:LEU:HD22	2.37	0.50
1:A:137:ARG:NH2	9:A:2009:3PE:H112	2.23	0.50
3:C:124:GLY:CA	1:G:557:ARG:HH12	2.25	0.50
1:A:481:ARG:O	1:A:482:ARG:HB2	2.11	0.49
2:B:62:LEU:HA	2:B:65:ILE:HD11	1.94	0.49
2:H:143:TRP:CD1	2:H:143:TRP:N	2.79	0.49
2:H:221:VAL:HB	2:H:224:PHE:HD2	1.77	0.49
3:I:249:PHE:CE1	9:I:3010:3PE:H3I1	2.47	0.49
4:J:46:LEU:O	4:J:47:ALA:C	2.52	0.49
1:A:52:ARG:HD3	1:A:498:SER:HA	1.93	0.49
2:B:231:VAL:O	2:B:232:PRO:C	2.55	0.49
2:B:278:TRP:NE1	10:B:1026:HOH:O	2.39	0.49
3:C:136:ILE:HG21	3:C:181:PHE:CE2	2.48	0.49
3:C:186:TYR:O	3:C:187:SER:C	2.54	0.49
1:G:121:ASN:OD1	1:G:208:MET:HE2	2.13	0.49
2:H:152:GLU:HB2	2:H:154:ILE:HD12	1.94	0.49
2:H:173:SER:O	2:H:174:PRO:C	2.55	0.49
3:I:155:LEU:O	3:I:155:LEU:HG	2.12	0.49
3:I:227:VAL:HG22	3:I:232:PHE:HD2	1.77	0.49
1:A:427:GLY:O	1:A:430:PHE:HB2	2.13	0.49
1:A:556:LYS:N	1:A:559:ASP:OD2	2.45	0.49
3:C:46:ILE:O	3:C:47:GLY:C	2.54	0.49
1:G:84:ALA:O	1:G:85:VAL:C	2.55	0.49
1:G:379:THR:O	1:G:380:PRO:C	2.53	0.49
1:G:474:LEU:HD11	1:G:494:ASN:ND2	2.27	0.49
3:C:147:ALA:CB	3:C:170:LEU:HD23	2.42	0.49
3:C:221:LEU:O	3:C:225:ILE:HG13	2.11	0.49
1:G:100:THR:O	1:G:104:ILE:HG13	2.12	0.49
2:H:160:MET:HG3	2:H:264:PRO:HG2	1.95	0.49
1:A:300:HIS:H	1:A:300:HIS:CD2	2.31	0.49
3:C:249:PHE:O	3:C:253:VAL:HG23	2.13	0.49
1:G:241:LEU:HD13	9:J:3011:3PE:C2I	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:TYR:HD2	1:G:407:ASP:OD2	1.96	0.49
1:G:477:GLN:NE2	2:H:42:GLY:O	2.46	0.49
1:G:493:TRP:HA	1:G:493:TRP:HE3	1.73	0.49
3:I:152:HIS:HB2	3:I:244:ILE:HD13	1.94	0.49
2:B:141:TYR:O	2:B:142:GLN:C	2.53	0.49
2:H:138:VAL:HG23	2:H:208:VAL:HG13	1.93	0.49
2:B:221:VAL:O	2:B:222:PRO:C	2.55	0.49
1:G:476:ARG:HD3	2:H:41:THR:O	2.12	0.49
2:H:214:ASP:OD1	2:H:214:ASP:N	2.46	0.49
9:A:2012:3PE:H2D1	9:D:2011:3PE:C2I	2.42	0.49
3:C:152:HIS:CG	3:C:244:ILE:HD13	2.48	0.49
1:G:239:ILE:HG12	1:G:289:ILE:HD13	1.94	0.49
2:H:152:GLU:HB2	2:H:154:ILE:CD1	2.43	0.49
3:I:103:LYS:HD3	3:I:103:LYS:C	2.38	0.49
9:I:3010:3PE:C2I	9:I:3013:3PE:H3H1	2.43	0.49
1:A:243:LEU:HD22	1:A:282:PHE:CD2	2.47	0.49
1:G:539:GLU:HA	1:G:542:LEU:HD12	1.95	0.49
9:G:3009:3PE:H2C2	9:G:3009:3PE:C3A	2.40	0.49
3:I:162:ARG:HG3	3:I:163:ASP:H	1.76	0.49
1:A:300:HIS:CD2	1:A:300:HIS:N	2.79	0.49
2:B:71:PHE:CE1	2:B:75:LEU:HD11	2.48	0.49
2:B:142:GLN:HG3	2:B:214:ASP:OD2	2.12	0.49
3:C:74:VAL:HG23	3:C:75:VAL:N	2.27	0.49
3:C:199:GLY:O	3:C:203:PHE:HB2	2.12	0.49
3:I:211:PHE:O	3:I:215:VAL:HG23	2.13	0.49
4:J:42:ALA:O	4:J:43:LEU:C	2.55	0.49
1:A:482:ARG:HD3	2:B:255:LEU:HB2	1.94	0.48
3:C:246:TYR:O	3:C:247:TRP:C	2.55	0.48
1:G:44:SER:HB2	1:G:105:LEU:HB2	1.94	0.48
1:G:91:ASN:ND2	1:G:165:GLN:NE2	2.61	0.48
4:J:11:HIS:O	4:J:12:VAL:HG23	2.12	0.48
1:A:74:LYS:HD2	1:A:74:LYS:N	2.28	0.48
1:A:127:HIS:HB3	1:A:226:PRO:CG	2.29	0.48
2:H:136:VAL:HG11	2:H:198:MET:HE3	1.95	0.48
1:A:54:GLU:HG2	1:A:63:MET:CE	2.40	0.48
1:A:148:ALA:O	1:A:149:GLY:C	2.55	0.48
1:A:396:VAL:HG13	2:B:65:ILE:HB	1.95	0.48
8:A:1001:HEA:H263	8:A:1001:HEA:C12	2.43	0.48
2:B:141:TYR:HE2	2:B:146:GLY:HA3	1.77	0.48
2:B:175:GLU:HA	2:B:178:GLN:NE2	2.28	0.48
2:B:221:VAL:CB	2:B:224:PHE:HD2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:255:LEU:HB3	9:D:2011:3PE:C3I	2.37	0.48
9:C:2013:3PE:H2G2	4:D:37:VAL:HG23	1.95	0.48
1:G:65:ALA:HB3	1:G:89:THR:HB	1.94	0.48
1:A:347:TYR:CE1	1:A:351:ALA:HB2	2.48	0.48
1:A:449:PRO:O	1:A:450:GLU:C	2.55	0.48
2:B:129:ILE:HD13	2:B:237:GLN:HB3	1.95	0.48
1:G:161:GLY:O	1:G:162:GLY:C	2.56	0.48
1:G:449:PRO:O	1:G:450:GLU:C	2.54	0.48
2:H:120:LEU:N	2:H:121:PRO:HD2	2.29	0.48
2:H:152:GLU:HB3	2:H:283:ARG:HH21	1.78	0.48
4:D:18:ILE:CG2	4:D:21:GLN:HB2	2.43	0.48
9:G:3009:3PE:H3E1	9:G:3009:3PE:C2E	2.39	0.48
2:H:192:LEU:HB3	2:H:249:PHE:CD2	2.48	0.48
3:I:32:ALA:O	3:I:36:MET:HG3	2.13	0.48
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.77	0.48
1:A:329:VAL:HB	1:A:347:TYR:OH	2.13	0.48
1:A:455:LEU:HG	1:A:459:MET:HE2	1.96	0.48
2:B:182:GLU:OE1	2:B:182:GLU:HA	2.13	0.48
2:B:263:MET:N	2:B:264:PRO:CD	2.76	0.48
1:G:191:ILE:HG21	1:G:254:LEU:HD13	1.95	0.48
2:H:252:CYS:HB2	2:H:263:MET:HG3	1.94	0.48
1:A:132:ASP:CG	1:A:133:MET:H	2.20	0.48
1:A:314:LEU:CB	1:A:315:PRO:HD3	2.43	0.48
1:A:456:HIS:O	1:A:457:PHE:C	2.57	0.48
1:A:525:VAL:CG1	1:A:544:SER:HB3	2.44	0.48
2:H:158:SER:OG	2:H:194:THR:OG1	2.25	0.48
4:J:18:ILE:HG22	4:J:21:GLN:HB2	1.95	0.48
1:A:81:TRP:CG	1:A:82:PRO:HD2	2.49	0.48
2:H:252:CYS:HB2	2:H:263:MET:CG	2.44	0.48
3:I:214:ILE:O	3:I:218:ILE:HG12	2.14	0.48
3:I:231:HIS:O	9:I:3008:3PE:H121	2.14	0.48
1:A:374:SER:HA	2:B:83:PHE:O	2.14	0.48
2:B:220:THR:OG1	2:B:221:VAL:N	2.47	0.48
3:C:168:LEU:O	3:C:169:ALA:C	2.57	0.48
3:C:209:HIS:NE2	3:C:254:TRP:HB2	2.29	0.48
1:G:396:VAL:HG13	2:H:65:ILE:HG21	1.95	0.48
3:I:120:PHE:CD1	3:I:120:PHE:C	2.92	0.48
1:A:26:HIS:NE2	1:A:27:LYS:HG3	2.29	0.48
1:A:477:GLN:HA	1:A:477:GLN:NE2	2.29	0.48
3:C:253:VAL:HG22	9:C:2010:3PE:H3H1	1.96	0.48
1:G:46:ALA:O	1:G:49:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:VAL:HG11	1:G:290:ILE:HG23	1.96	0.48
1:G:284:HIS:N	1:G:285:PRO:CD	2.77	0.48
3:I:128:PHE:O	3:I:130:PRO:HD3	2.13	0.48
1:A:106:MET:CB	8:A:1001:HEA:HAC	2.36	0.47
1:A:112:ILE:HD12	10:A:2037:HOH:O	2.13	0.47
1:A:556:LYS:HD2	1:A:556:LYS:HA	1.52	0.47
3:C:62:VAL:HG12	9:C:2008:3PE:H31	1.93	0.47
3:C:135:LEU:O	3:C:139:LEU:HG	2.14	0.47
3:C:245:TRP:NE1	9:C:2013:3PE:H322	2.29	0.47
1:G:122:TYR:HD1	1:G:122:TYR:C	2.22	0.47
1:G:397:THR:O	1:G:400:VAL:HB	2.13	0.47
1:G:498:SER:O	1:G:502:PHE:CD2	2.65	0.47
1:G:538:LEU:HD21	1:G:560:TRP:HE3	1.79	0.47
2:H:137:LYS:HB3	2:H:148:GLU:HB2	1.95	0.47
2:H:190:PHE:CD1	2:H:190:PHE:C	2.89	0.47
1:A:137:ARG:NE	9:A:2009:3PE:O14	2.42	0.47
2:B:209:GLN:OE1	4:J:11:HIS:HD2	1.96	0.47
1:G:280:TRP:O	1:G:331:TRP:HB2	2.14	0.47
3:C:74:VAL:O	3:C:77:LEU:N	2.46	0.47
3:C:131:TRP:HE3	3:C:135:LEU:HD22	1.79	0.47
1:G:62:PHE:CE2	1:G:82:PRO:HD3	2.49	0.47
1:G:153:ALA:O	1:G:156:SER:HB3	2.13	0.47
1:G:168:SER:HB3	1:G:170:ILE:CD1	2.44	0.47
2:H:129:ILE:HA	2:H:130:PRO:HD2	1.67	0.47
2:H:248:PHE:HE2	2:H:269:VAL:CG1	2.27	0.47
3:I:74:VAL:CG1	4:J:18:ILE:HG12	2.44	0.47
1:A:285:PRO:O	1:A:289:ILE:HG13	2.14	0.47
1:A:455:LEU:HD23	1:A:510:PHE:CE2	2.49	0.47
1:A:511:PHE:CE1	1:A:515:ILE:HD11	2.48	0.47
8:A:1002:HEA:C22	2:B:68:ILE:HD13	2.44	0.47
2:B:107:VAL:HG12	2:B:108:PRO:HD3	1.97	0.47
2:H:77:LEU:O	2:H:78:TYR:C	2.54	0.47
3:I:20:MET:HE3	3:I:20:MET:HB2	1.61	0.47
2:B:35:ARG:HG2	2:B:36:PRO:O	2.14	0.47
3:C:80:ARG:HH22	9:C:2013:3PE:C11	2.26	0.47
1:G:132:ASP:CG	1:G:133:MET:H	2.21	0.47
1:G:217:ALA:O	1:G:218:PRO:C	2.56	0.47
1:G:414:TYR:OH	10:G:3020:HOH:O	2.20	0.47
1:G:505:PHE:O	1:G:509:LEU:HG	2.14	0.47
1:G:511:PHE:CE1	1:G:515:ILE:HD11	2.49	0.47
1:A:109:PHE:O	1:A:146:TYR:OH	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2012:3PE:H3E1	9:D:2011:3PE:H2I3	1.95	0.47
1:G:456:HIS:CE1	1:G:511:PHE:HB2	2.49	0.47
1:G:551:PHE:CD1	1:G:555:PRO:HD3	2.49	0.47
2:H:248:PHE:HE2	2:H:269:VAL:HG12	1.80	0.47
9:I:3013:3PE:C3H	9:I:3013:3PE:H2E1	2.44	0.47
1:A:66:GLU:OE2	1:A:89:THR:OG1	2.31	0.47
1:A:176:PRO:CB	1:A:177:PRO:HA	2.44	0.47
1:A:424:MET:O	1:A:429:VAL:HG23	2.15	0.47
1:A:447:GLN:HG3	1:A:448:TYR:N	2.30	0.47
1:A:469:PHE:N	1:A:470:PRO:CD	2.76	0.47
1:A:470:PRO:HA	1:A:473:PHE:CD2	2.49	0.47
8:A:1002:HEA:HBC1	8:A:1002:HEA:CMC	2.39	0.47
2:B:137:LYS:HE2	10:B:1072:HOH:O	2.14	0.47
2:B:186:SER:O	2:B:187:ARG:C	2.55	0.47
1:G:43:ILE:O	1:G:44:SER:C	2.57	0.47
1:G:506:ALA:HA	1:G:509:LEU:HD12	1.96	0.47
2:H:164:PRO:HB3	10:H:1122:HOH:O	2.15	0.47
3:I:226:ARG:HE	3:I:231:HIS:CD2	2.32	0.47
1:A:51:MET:HE3	1:A:99:ILE:HD13	1.97	0.47
1:A:91:ASN:ND2	1:A:165:GLN:HE22	2.13	0.47
1:A:403:GLN:O	1:A:404:ALA:C	2.57	0.47
9:A:2012:3PE:H2D1	9:D:2011:3PE:H2I2	1.97	0.47
3:C:147:ALA:HB1	3:C:170:LEU:HD23	1.96	0.47
1:G:48:THR:CG2	1:G:102:HIS:CE1	2.97	0.47
1:G:329:VAL:HB	1:G:347:TYR:OH	2.14	0.47
1:G:370:MET:SD	1:G:385:LEU:HD21	2.54	0.47
1:A:126:LEU:HD23	10:A:2049:HOH:O	2.14	0.47
1:A:135:PHE:CE1	3:C:79:LEU:HD23	2.49	0.47
2:B:152:GLU:HB2	2:B:154:ILE:HD12	1.97	0.47
1:G:86:GLU:O	2:H:171:ARG:NH1	2.48	0.47
1:G:112:ILE:H	1:G:113:PRO:HD2	1.78	0.47
1:G:188:ASP:CG	1:G:257:ARG:HH12	2.22	0.47
1:G:312:GLY:HA2	10:H:1132:HOH:O	2.14	0.47
1:G:344:GLN:O	1:G:348:PHE:HD2	1.98	0.47
1:G:416:VAL:O	1:G:419:HIS:HB3	2.14	0.47
3:I:221:LEU:O	3:I:225:ILE:HG13	2.14	0.47
1:A:368:ALA:O	1:A:369:THR:C	2.56	0.47
2:H:138:VAL:HG23	2:H:208:VAL:CG1	2.45	0.47
1:A:43:ILE:O	1:A:44:SER:C	2.56	0.46
2:B:86:LYS:HE3	10:B:1054:HOH:O	2.15	0.46
2:B:136:VAL:CG2	2:B:198:MET:HE2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TRP:HZ2	2:B:257:GLY:HA3	1.78	0.46
4:D:12:VAL:HG12	4:D:15:SER:HB2	1.97	0.46
1:G:213:LEU:CB	3:I:81:TRP:CH2	2.98	0.46
2:H:200:VAL:N	2:H:268:LYS:O	2.47	0.46
9:A:2009:3PE:H221	3:C:58:TRP:CE2	2.50	0.46
4:D:46:LEU:O	4:D:47:ALA:C	2.57	0.46
1:G:307:LYS:HD2	1:G:374:SER:OG	2.16	0.46
1:G:473:PHE:O	1:G:474:LEU:C	2.58	0.46
1:G:556:LYS:HD2	1:G:556:LYS:HA	1.68	0.46
2:H:172:MET:HE1	2:H:190:PHE:HB2	1.98	0.46
3:I:76:ARG:O	3:I:80:ARG:HG3	2.15	0.46
1:A:212:PHE:CE1	1:A:222:MET:HE3	2.48	0.46
1:A:428:ALA:O	1:A:432:ILE:HG13	2.15	0.46
1:G:85:VAL:HG23	10:G:3116:HOH:O	2.15	0.46
1:G:241:LEU:HD13	9:J:3011:3PE:H2I1	1.96	0.46
1:G:246:LEU:HD22	1:G:282:PHE:CZ	2.50	0.46
2:H:194:THR:HG22	2:H:266:THR:CB	2.45	0.46
1:A:539:GLU:HA	1:A:542:LEU:HD12	1.98	0.46
2:B:209:GLN:CG	2:B:235:LEU:HD22	2.45	0.46
1:G:26:HIS:HD2	1:G:122:TYR:HA	1.80	0.46
1:G:470:PRO:O	1:G:473:PHE:HB2	2.16	0.46
9:G:3012:3PE:H3C1	9:J:3011:3PE:H2I1	1.96	0.46
3:I:72:THR:O	3:I:73:PRO:C	2.58	0.46
4:D:39:ILE:O	4:D:40:VAL:C	2.57	0.46
1:G:27:LYS:HZ3	1:G:27:LYS:HB2	1.79	0.46
1:G:198:GLY:O	1:G:202:ILE:HD12	2.16	0.46
1:G:323:ILE:HG22	1:G:324:GLY:N	2.26	0.46
2:H:234:ARG:NH1	3:I:114:PRO:HG3	2.30	0.46
3:I:23:VAL:O	3:I:24:GLY:C	2.56	0.46
4:J:12:VAL:HG12	4:J:12:VAL:O	2.15	0.46
1:A:497:SER:O	1:A:498:SER:C	2.58	0.46
4:D:50:ASN:O	4:D:51:ALA:C	2.59	0.46
1:G:133:MET:O	1:G:134:ALA:C	2.59	0.46
1:G:312:GLY:O	1:G:313:TYR:C	2.58	0.46
1:G:529:ASN:C	1:G:529:ASN:OD1	2.59	0.46
1:G:538:LEU:HD21	1:G:560:TRP:CE3	2.51	0.46
8:G:1002:HEA:O11	8:G:1002:HEA:CHC	2.64	0.46
1:A:411:HIS:CD2	1:A:412:ASP:HB2	2.51	0.46
1:G:225:VAL:C	1:G:226:PRO:O	2.57	0.46
1:G:264:PHE:HB3	1:G:272:PRO:HA	1.97	0.46
3:I:27:VAL:O	3:I:28:MET:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:CYS:O	1:A:90:PRO:HD3	2.14	0.46
1:G:525:VAL:CG1	1:G:544:SER:HB3	2.46	0.46
2:H:71:PHE:O	2:H:75:LEU:HD12	2.15	0.46
2:H:97:ASN:O	2:H:101:GLU:HG3	2.16	0.46
3:I:196:ASN:HD21	3:I:199:GLY:HA3	1.80	0.46
1:A:280:TRP:O	1:A:331:TRP:HB2	2.16	0.46
3:C:220:LEU:CD2	3:C:243:ALA:HB1	2.46	0.46
1:G:206:ILE:HG22	1:G:207:ASN:N	2.31	0.46
1:G:307:LYS:HA	1:G:534:HIS:CG	2.51	0.46
3:I:172:ILE:CD1	3:I:221:LEU:HA	2.46	0.46
1:A:107:MET:H	1:A:107:MET:HG2	1.45	0.46
1:A:239:ILE:HG12	1:A:289:ILE:CD1	2.38	0.46
1:A:510:PHE:O	1:A:514:VAL:HG23	2.16	0.46
2:B:136:VAL:HG11	2:B:198:MET:HE2	1.98	0.46
3:C:66:SER:HB2	3:C:71:HIS:CE1	2.50	0.46
1:G:199:ALA:HA	9:G:3009:3PE:H3D1	1.97	0.46
1:G:396:VAL:HG11	2:H:65:ILE:HD12	1.97	0.46
4:J:17:ASP:OD1	4:J:17:ASP:C	2.59	0.46
1:A:282:PHE:C	1:A:285:PRO:HD2	2.40	0.45
2:B:211:THR:HG22	2:B:212:GLY:H	1.80	0.45
3:C:114:PRO:O	3:C:115:ILE:C	2.59	0.45
3:C:120:PHE:HA	3:C:121:PRO:C	2.41	0.45
1:A:347:TYR:CD2	9:D:2011:3PE:H252	2.51	0.45
1:A:396:VAL:O	1:A:397:THR:C	2.59	0.45
2:B:59:GLY:HA2	10:B:1016:HOH:O	2.16	0.45
1:G:148:ALA:O	1:G:151:SER:N	2.49	0.45
2:H:136:VAL:CG2	2:H:198:MET:HE2	2.44	0.45
3:I:115:ILE:H	3:I:115:ILE:HG13	1.55	0.45
3:I:209:HIS:CE1	3:I:254:TRP:HB2	2.52	0.45
1:A:357:VAL:CB	1:A:358:PRO:CD	2.91	0.45
1:A:422:TYR:OH	1:A:469:PHE:HD1	1.98	0.45
1:A:426:LEU:HD21	1:A:464:ALA:HB1	1.98	0.45
1:A:469:PHE:N	1:A:470:PRO:HD2	2.31	0.45
9:A:2009:3PE:H3A1	9:A:2009:3PE:C2C	2.41	0.45
1:G:392:THR:O	1:G:393:VAL:C	2.58	0.45
1:G:556:LYS:HB3	1:G:559:ASP:OD1	2.16	0.45
2:H:83:PHE:O	2:H:84:HIS:C	2.57	0.45
1:A:299:SER:O	1:A:302:ILE:N	2.50	0.45
1:A:432:ILE:HG22	8:A:1001:HEA:H252	1.95	0.45
1:G:328:PHE:HA	10:G:3100:HOH:O	2.15	0.45
2:H:251:GLN:O	2:H:252:CYS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:177:LEU:O	3:I:178:PHE:C	2.59	0.45
4:J:47:ALA:CA	9:J:3011:3PE:H321	2.45	0.45
1:A:316:MET:HE3	1:A:316:MET:HB3	1.83	0.45
9:C:2013:3PE:H261	9:C:2013:3PE:H3A2	1.99	0.45
1:G:198:GLY:HA2	1:G:243:LEU:HD12	1.98	0.45
1:G:243:LEU:N	1:G:243:LEU:HD23	2.32	0.45
1:G:384:ALA:O	1:G:388:LEU:HG	2.16	0.45
3:I:20:MET:HG2	3:I:54:THR:OG1	2.16	0.45
3:I:133:LEU:N	3:I:134:PRO:HD2	2.26	0.45
4:J:39:ILE:O	4:J:42:ALA:HB3	2.16	0.45
1:A:26:HIS:HB3	1:A:132:ASP:OD1	2.17	0.45
1:A:44:SER:O	1:A:45:VAL:C	2.59	0.45
1:A:262:THR:HG21	3:C:196:ASN:N	2.31	0.45
1:A:326:LEU:O	1:A:328:PHE:N	2.50	0.45
1:G:137:ARG:NH2	9:G:3009:3PE:H112	2.31	0.45
1:G:479:MET:HA	1:G:480:PRO:HD3	1.82	0.45
3:I:136:ILE:HG21	3:I:181:PHE:HE2	1.81	0.45
4:J:51:ALA:O	9:J:3011:3PE:H122	2.16	0.45
2:B:276:ALA:O	2:B:277:ALA:C	2.57	0.45
1:G:300:HIS:CD2	1:G:300:HIS:N	2.85	0.45
2:H:136:VAL:HG12	2:H:137:LYS:N	2.32	0.45
2:H:195:ASP:OD1	2:H:196:THR:N	2.50	0.45
3:I:74:VAL:HG12	4:J:18:ILE:CG2	2.47	0.45
3:I:85:LEU:HD23	3:I:88:MET:HE2	1.97	0.45
1:A:213:LEU:HD12	3:C:81:TRP:CZ2	2.52	0.45
1:A:225:VAL:HG13	1:A:226:PRO:HD2	1.99	0.45
3:C:52:LEU:HD22	9:C:2008:3PE:H3C2	1.99	0.45
3:C:252:VAL:HG12	9:C:2010:3PE:H3H2	1.98	0.45
1:G:155:ALA:HB1	10:G:3085:HOH:O	2.15	0.45
9:G:3012:3PE:H231	4:J:31:MET:HE1	1.98	0.45
2:H:68:ILE:O	2:H:69:THR:C	2.58	0.45
3:I:135:LEU:O	3:I:139:LEU:HG	2.17	0.45
1:A:163:ASN:HA	3:I:159:ASN:HB3	1.99	0.45
2:B:120:LEU:O	2:B:123:LEU:N	2.47	0.45
3:C:12:LEU:HA	3:C:13:PRO:HD2	1.80	0.45
2:H:134:VAL:CG1	2:H:135:THR:N	2.80	0.45
2:H:176:VAL:O	2:H:180:LEU:HG	2.17	0.45
3:I:176:ALA:O	3:I:179:THR:HB	2.17	0.45
1:A:122:TYR:CD1	1:A:122:TYR:C	2.95	0.45
3:C:245:TRP:HE1	9:C:2013:3PE:H322	1.81	0.45
1:G:350:MET:O	1:G:351:ALA:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:463:GLY:CA	1:G:503:LEU:HD23	2.47	0.45
3:I:122:PRO:HB2	3:I:125:ILE:CG1	2.47	0.45
1:A:45:VAL:HG21	8:A:1001:HEA:H162	1.98	0.44
2:B:171:ARG:O	2:B:176:VAL:HG21	2.17	0.44
2:B:217:HIS:HB2	2:B:230:ALA:HB3	1.98	0.44
4:D:17:ASP:OD1	4:D:18:ILE:N	2.50	0.44
1:G:44:SER:HB2	1:G:105:LEU:CB	2.47	0.44
1:G:192:PHE:CE1	3:I:29:LEU:HD22	2.52	0.44
1:G:424:MET:O	1:G:429:VAL:HG23	2.17	0.44
8:G:1002:HEA:HBC1	8:G:1002:HEA:CMC	2.46	0.44
2:H:114:ALA:O	2:H:115:ILE:C	2.59	0.44
2:H:147:TYR:HD2	2:H:198:MET:HE3	1.78	0.44
3:I:150:TRP:CD1	3:I:150:TRP:C	2.94	0.44
4:J:18:ILE:HG23	4:J:21:GLN:OE1	2.16	0.44
1:A:170:ILE:O	2:B:255:LEU:HD23	2.17	0.44
1:A:212:PHE:CD1	1:A:212:PHE:C	2.94	0.44
1:A:249:ALA:HB2	1:A:278:ILE:HG22	1.98	0.44
1:A:532:ASN:C	1:A:532:ASN:OD1	2.58	0.44
3:C:253:VAL:HG22	9:C:2010:3PE:C3I	2.47	0.44
1:G:257:ARG:HH11	1:G:257:ARG:HD3	1.55	0.44
1:G:262:THR:OG1	1:G:268:GLY:HA3	2.17	0.44
1:G:320:MET:HE2	1:G:362:LYS:HZ3	1.80	0.44
1:G:331:TRP:HH2	9:I:3010:3PE:H251	1.81	0.44
1:A:379:THR:HA	1:A:382:LEU:HD12	1.98	0.44
2:B:129:ILE:HA	2:B:130:PRO:HD2	1.69	0.44
4:D:39:ILE:HD13	9:D:2011:3PE:H2G2	1.98	0.44
1:G:81:TRP:CE3	1:G:82:PRO:HD2	2.52	0.44
1:G:176:PRO:HB2	1:G:177:PRO:HA	1.99	0.44
2:H:122:VAL:O	2:H:126:GLN:HG2	2.18	0.44
2:H:195:ASP:OD1	2:H:196:THR:OG1	2.33	0.44
3:I:127:THR:HG21	3:I:266:GLN:HA	1.99	0.44
1:A:63:MET:HE1	1:A:484:ILE:HG13	2.00	0.44
1:A:341:SER:HB3	1:A:344:GLN:HG3	1.98	0.44
1:G:129:GLY:HA2	1:G:551:PHE:CE2	2.53	0.44
1:G:396:VAL:CG1	2:H:65:ILE:HD12	2.47	0.44
3:I:149:THR:O	3:I:152:HIS:HB3	2.17	0.44
9:A:2012:3PE:C3E	9:D:2011:3PE:H2I3	2.48	0.44
2:B:161:ILE:CD1	2:B:180:LEU:HD23	2.48	0.44
2:B:218:SER:HA	2:B:229:ASP:HA	2.00	0.44
3:C:80:ARG:NH2	9:C:2013:3PE:O13	2.27	0.44
3:C:140:ILE:CD1	3:C:177:LEU:HD23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:SER:HB2	2:H:99:PRO:CD	2.47	0.44
2:H:169:ASP:O	2:H:170:ASN:HB2	2.18	0.44
2:H:228:GLN:HG3	2:H:229:ASP:N	2.29	0.44
9:I:3010:3PE:H362	9:I:3010:3PE:H391	1.63	0.44
1:A:62:PHE:CE2	1:A:82:PRO:HD3	2.53	0.44
1:A:314:LEU:HB3	1:A:315:PRO:CD	2.45	0.44
1:G:168:SER:HB3	1:G:170:ILE:HD11	2.00	0.44
1:G:415:TYR:CD1	1:G:415:TYR:C	2.95	0.44
1:G:422:TYR:OH	1:G:469:PHE:HD1	2.00	0.44
2:H:175:GLU:CD	2:H:175:GLU:H	2.25	0.44
3:I:63:VAL:O	3:I:64:THR:C	2.61	0.44
4:J:40:VAL:O	4:J:44:ILE:HG13	2.17	0.44
1:A:36:THR:O	1:A:40:VAL:HG23	2.18	0.44
1:A:417:VAL:HA	1:A:420:PHE:CE2	2.53	0.44
1:A:477:GLN:NE2	2:B:42:GLY:O	2.51	0.44
9:A:2012:3PE:H3C1	9:D:2011:3PE:H2I1	1.98	0.44
3:C:212:HIS:O	3:C:215:VAL:N	2.50	0.44
1:G:357:VAL:CB	1:G:358:PRO:CD	2.96	0.44
2:H:275:TYR:O	2:H:279:LEU:HG	2.17	0.44
3:I:2:ALA:HB3	3:I:5:LYS:HD3	2.00	0.44
3:I:83:PHE:CE1	9:I:3008:3PE:H262	2.43	0.44
2:B:116:GLY:O	2:B:117:ALA:C	2.60	0.44
2:B:132:ALA:HB1	2:B:134:VAL:O	2.18	0.44
4:D:47:ALA:CA	9:D:2011:3PE:H321	2.46	0.44
1:G:159:ALA:HB1	1:G:160:PRO:HD2	1.99	0.44
1:G:450:GLU:O	1:G:454:LYS:HG3	2.17	0.44
2:H:45:PRO:HB3	2:H:244:ARG:NH2	2.31	0.44
3:I:73:PRO:HD2	4:J:14:GLY:HA2	2.00	0.44
1:A:153:ALA:HB2	1:A:193:ALA:HB1	2.00	0.44
1:A:314:LEU:O	1:A:315:PRO:C	2.60	0.44
1:A:326:LEU:O	1:A:327:GLY:C	2.59	0.44
1:G:63:MET:HE3	1:G:484:ILE:CG1	2.48	0.44
1:G:148:ALA:O	1:G:151:SER:HB2	2.18	0.44
4:J:50:ASN:O	4:J:51:ALA:C	2.61	0.44
1:A:346:SER:O	1:A:350:MET:HG3	2.18	0.43
1:A:380:PRO:HG3	1:A:437:TYR:HB3	1.99	0.43
2:B:71:PHE:CD1	2:B:71:PHE:C	2.96	0.43
1:G:81:TRP:CG	1:G:82:PRO:HD2	2.53	0.43
1:G:398:GLY:O	1:G:402:SER:N	2.38	0.43
1:G:477:GLN:NE2	1:G:477:GLN:HA	2.33	0.43
2:H:186:SER:O	2:H:187:ARG:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:276:ALA:O	2:H:277:ALA:C	2.61	0.43
3:I:212:HIS:HD2	3:I:246:TYR:OH	2.01	0.43
3:I:266:GLN:HG2	3:I:266:GLN:OXT	2.18	0.43
1:A:161:GLY:O	1:A:162:GLY:C	2.60	0.43
1:A:217:ALA:O	1:A:218:PRO:C	2.61	0.43
3:C:33:VAL:O	3:C:34:LEU:C	2.60	0.43
1:G:103:GLY:O	1:G:104:ILE:C	2.58	0.43
1:G:421:HIS:O	1:G:425:SER:N	2.45	0.43
1:G:470:PRO:HA	1:G:473:PHE:CD2	2.53	0.43
3:I:77:LEU:O	3:I:77:LEU:HG	2.18	0.43
3:I:255:LEU:HB3	9:J:3011:3PE:C3I	2.42	0.43
1:A:307:LYS:HA	1:A:534:HIS:CG	2.52	0.43
2:B:176:VAL:O	2:B:177:GLU:C	2.60	0.43
3:C:72:THR:CG2	3:C:73:PRO:N	2.77	0.43
3:C:220:LEU:O	3:C:221:LEU:C	2.59	0.43
1:G:22:MET:CG	3:I:16:ILE:HD12	2.49	0.43
2:H:116:GLY:O	2:H:117:ALA:C	2.60	0.43
2:H:176:VAL:O	2:H:177:GLU:C	2.60	0.43
2:H:206:VAL:HB	2:H:240:PHE:CE1	2.53	0.43
1:A:63:MET:HE3	1:A:484:ILE:CG1	2.48	0.43
1:A:213:LEU:HB3	3:C:81:TRP:CH2	2.50	0.43
1:A:218:PRO:HB3	1:A:557:ARG:HH21	1.84	0.43
1:A:239:ILE:O	1:A:240:LEU:C	2.58	0.43
1:A:498:SER:O	1:A:499:LEU:C	2.57	0.43
1:G:176:PRO:CB	1:G:177:PRO:HA	2.48	0.43
1:G:263:PHE:HE1	3:I:201:ASN:HD22	1.64	0.43
1:G:393:VAL:O	1:G:394:GLY:C	2.61	0.43
1:A:307:LYS:NZ	10:A:2068:HOH:O	2.48	0.43
1:G:48:THR:HG22	1:G:102:HIS:CE1	2.53	0.43
1:G:314:LEU:HB3	1:G:315:PRO:HD3	2.00	0.43
1:G:401:LEU:HD13	8:G:1002:HEA:HBA2	2.00	0.43
1:G:546:PRO:HA	1:G:547:PRO:HD3	1.93	0.43
3:I:104:HIS:HB2	10:I:3022:HOH:O	2.17	0.43
1:A:361:ILE:HD11	2:B:105:THR:OG1	2.18	0.43
2:B:136:VAL:HG11	2:B:198:MET:CE	2.48	0.43
2:B:209:GLN:CD	2:B:235:LEU:HD22	2.44	0.43
4:D:18:ILE:HA	4:D:21:GLN:OE1	2.19	0.43
1:G:239:ILE:HG12	1:G:289:ILE:CD1	2.49	0.43
1:G:401:LEU:CD1	1:G:416:VAL:HG22	2.49	0.43
2:H:156:PHE:HD2	2:H:196:THR:HG21	1.82	0.43
3:I:180:VAL:O	3:I:183:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:16:MET:HG2	4:J:17:ASP:N	2.34	0.43
1:A:63:MET:CE	1:A:95:TRP:HB2	2.49	0.43
1:A:238:LEU:HD22	1:A:328:PHE:CE2	2.54	0.43
1:A:378:LYS:O	1:A:379:THR:C	2.59	0.43
1:A:424:MET:HE2	8:A:1002:HEA:HMD3	1.99	0.43
2:B:289:LEU:HG	2:B:289:LEU:OXT	2.17	0.43
1:G:507:SER:O	1:G:510:PHE:N	2.51	0.43
2:H:98:SER:N	2:H:99:PRO:HD2	2.33	0.43
9:I:3013:3PE:H261	9:I:3013:3PE:C3A	2.48	0.43
1:A:29:ILE:HD12	1:A:139:ASN:HD22	1.83	0.43
2:B:77:LEU:O	2:B:78:TYR:C	2.61	0.43
4:D:18:ILE:HG23	4:D:21:GLN:OE1	2.19	0.43
1:G:74:LYS:H	1:G:74:LYS:CD	2.31	0.43
1:G:329:VAL:HG12	9:J:3011:3PE:H281	2.01	0.43
3:I:52:LEU:HD23	3:I:55:MET:HE2	2.01	0.43
3:I:99:TRP:HD1	3:I:99:TRP:O	2.02	0.43
3:I:133:LEU:O	3:I:136:ILE:HB	2.19	0.43
1:A:40:VAL:O	1:A:40:VAL:HG12	2.18	0.43
9:C:2013:3PE:C3H	9:C:2013:3PE:C2D	2.72	0.43
1:G:274:LEU:O	1:G:275:TYR:C	2.61	0.43
3:I:74:VAL:HG23	3:I:75:VAL:N	2.33	0.43
1:A:70:SER:O	1:A:71:GLY:C	2.60	0.43
1:A:262:THR:O	1:A:262:THR:HG23	2.19	0.43
1:A:420:PHE:HB2	1:A:424:MET:HE2	2.01	0.43
3:C:105:ALA:HB2	10:C:2020:HOH:O	2.18	0.43
2:H:175:GLU:HA	2:H:178:GLN:NE2	2.34	0.43
2:H:185:TYR:CD2	2:H:193:ALA:HB1	2.53	0.43
1:A:271:ASP:O	1:A:272:PRO:C	2.60	0.42
9:A:2009:3PE:H3E1	9:A:2009:3PE:H3B2	1.70	0.42
9:A:2012:3PE:H2I3	3:C:91:VAL:HG11	2.01	0.42
2:B:194:THR:HG22	2:B:266:THR:CB	2.49	0.42
3:C:130:PRO:HD3	3:C:266:GLN:NE2	2.34	0.42
8:G:1002:HEA:HHA	8:G:1002:HEA:HAD2	1.78	0.42
2:H:120:LEU:O	2:H:123:LEU:N	2.52	0.42
3:I:21:ALA:CB	3:I:54:THR:HG21	2.37	0.42
2:B:48:SER:HB2	2:B:49:PRO:HD2	2.01	0.42
3:C:32:ALA:O	3:C:36:MET:HG3	2.19	0.42
1:A:130:ALA:HB2	1:A:215:MET:O	2.18	0.42
1:A:131:PRO:HG2	3:C:9:TYR:CD2	2.54	0.42
1:G:95:TRP:O	1:G:96:ASN:C	2.62	0.42
1:G:191:ILE:HD13	1:G:191:ILE:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:THR:CG2	2:H:266:THR:HB	2.49	0.42
1:A:112:ILE:HB	1:A:113:PRO:HD3	2.00	0.42
1:G:189:LEU:HD23	3:I:33:VAL:HG21	2.02	0.42
1:G:317:VAL:O	1:G:320:MET:HB2	2.20	0.42
1:G:506:ALA:O	1:G:509:LEU:HB2	2.19	0.42
8:G:1002:HEA:C22	2:H:68:ILE:HD13	2.49	0.42
2:H:97:ASN:C	2:H:97:ASN:OD1	2.62	0.42
3:I:219:PHE:HE1	9:I:3008:3PE:H342	1.84	0.42
1:A:188:ASP:OD1	1:A:257:ARG:NH1	2.41	0.42
1:A:284:HIS:N	1:A:285:PRO:CD	2.83	0.42
3:C:13:PRO:HD2	10:C:2018:HOH:O	2.19	0.42
4:D:45:PHE:CD1	4:D:45:PHE:C	2.96	0.42
1:G:188:ASP:O	1:G:189:LEU:C	2.62	0.42
1:G:493:TRP:CZ3	1:G:496:VAL:HG21	2.54	0.42
1:G:525:VAL:HG11	1:G:544:SER:HB3	2.02	0.42
3:I:80:ARG:HH12	9:I:3013:3PE:H111	1.83	0.42
1:A:91:ASN:HD21	1:A:165:GLN:CD	2.27	0.42
2:B:173:SER:O	2:B:174:PRO:C	2.60	0.42
3:C:17:TRP:O	3:C:20:MET:HB3	2.19	0.42
3:C:226:ARG:HH22	9:C:2008:3PE:C12	2.32	0.42
3:C:256:PHE:O	3:C:257:LEU:C	2.62	0.42
9:C:2010:3PE:H322	9:D:2011:3PE:O32	2.20	0.42
1:G:246:LEU:O	1:G:246:LEU:HG	2.19	0.42
1:G:481:ARG:O	1:G:482:ARG:HB2	2.19	0.42
1:G:511:PHE:O	1:G:515:ILE:HG13	2.19	0.42
8:G:1001:HEA:HMA	8:G:1001:HEA:HAA1	1.81	0.42
2:H:129:ILE:HD13	2:H:237:GLN:HB3	2.02	0.42
2:H:211:THR:O	2:H:230:ALA:HB1	2.19	0.42
3:I:238:VAL:HB	9:I:3008:3PE:O14	2.20	0.42
9:I:3010:3PE:H322	9:J:3011:3PE:O32	2.19	0.42
4:J:50:ASN:O	9:J:3011:3PE:H112	2.19	0.42
1:A:26:HIS:HD2	1:A:122:TYR:HA	1.84	0.42
1:A:122:TYR:C	1:A:122:TYR:HD1	2.28	0.42
1:A:201:SER:HB3	1:A:239:ILE:HG21	2.01	0.42
2:B:175:GLU:O	2:B:176:VAL:C	2.61	0.42
9:C:2010:3PE:H3E2	9:C:2010:3PE:C3I	2.37	0.42
9:C:2010:3PE:H2A1	9:D:2011:3PE:H2E1	2.02	0.42
1:G:284:HIS:H	1:G:285:PRO:CD	2.32	0.42
1:G:375:ILE:HD12	2:H:80:VAL:HA	2.02	0.42
10:G:3036:HOH:O	3:I:109:MET:HG2	2.18	0.42
1:A:71:GLY:CA	1:A:74:LYS:HD3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:O	1:A:470:PRO:HD2	2.20	0.42
1:A:498:SER:O	1:A:502:PHE:HD2	2.03	0.42
8:A:1002:HEA:H252	2:B:108:PRO:HB3	2.02	0.42
2:B:252:CYS:HB2	2:B:263:MET:HG3	2.02	0.42
4:D:43:LEU:HD23	4:D:43:LEU:HA	1.72	0.42
1:G:48:THR:HG21	1:G:102:HIS:CE1	2.54	0.42
9:G:3009:3PE:H392	9:G:3009:3PE:H291	2.00	0.42
2:H:220:THR:HB	2:H:227:LYS:CG	2.49	0.42
3:I:80:ARG:HH12	9:I:3013:3PE:C11	2.33	0.42
3:I:83:PHE:CE1	9:I:3008:3PE:H241	2.55	0.42
3:I:152:HIS:O	3:I:156:VAL:HG23	2.20	0.42
1:A:149:GLY:O	1:A:150:THR:C	2.62	0.42
1:A:191:ILE:HD13	1:A:191:ILE:HA	1.68	0.42
2:B:120:LEU:N	2:B:121:PRO:HD2	2.34	0.42
2:B:137:LYS:NZ	4:J:11:HIS:CD2	2.88	0.42
1:G:337:THR:HA	10:H:1069:HOH:O	2.20	0.42
1:G:376:GLU:CG	1:G:378:LYS:HZ3	2.33	0.42
1:G:442:LYS:HD2	1:G:442:LYS:HA	1.91	0.42
3:I:153:HIS:O	3:I:154:ALA:C	2.62	0.42
8:A:1002:HEA:O11	8:A:1002:HEA:CHC	2.68	0.42
2:B:143:TRP:CD1	2:B:143:TRP:N	2.84	0.42
1:G:205:ALA:O	1:G:209:ILE:HG13	2.20	0.42
1:G:286:GLU:O	1:G:290:ILE:HG13	2.20	0.42
3:I:110:GLY:H	3:I:113:SER:HG	1.66	0.42
3:I:172:ILE:HD13	3:I:221:LEU:HA	2.01	0.42
1:A:22:MET:CG	3:C:16:ILE:HD12	2.49	0.41
9:A:2012:3PE:C2I	3:C:91:VAL:HG11	2.50	0.41
2:B:211:THR:OG1	2:B:235:LEU:HD23	2.20	0.41
3:C:107:TYR:HH	4:D:51:ALA:HA	1.85	0.41
1:G:52:ARG:CD	1:G:498:SER:HA	2.50	0.41
1:G:396:VAL:O	1:G:397:THR:C	2.62	0.41
1:G:406:VAL:HG12	1:G:410:TYR:CE2	2.55	0.41
3:I:120:PHE:CA	3:I:121:PRO:C	2.91	0.41
9:I:3013:3PE:H3B1	9:I:3013:3PE:C26	2.39	0.41
1:A:74:LYS:CD	1:A:74:LYS:N	2.82	0.41
1:A:481:ARG:O	10:A:2021:HOH:O	2.21	0.41
3:C:133:LEU:HD12	3:C:133:LEU:HA	1.98	0.41
9:C:2010:3PE:H231	9:C:2010:3PE:C33	2.50	0.41
1:G:284:HIS:CB	1:G:285:PRO:HD3	2.49	0.41
3:I:72:THR:CG2	3:I:73:PRO:N	2.77	0.41
1:A:222:MET:HE2	1:A:230:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:PHE:O	1:A:470:PRO:C	2.63	0.41
2:B:101:GLU:O	2:B:102:ILE:C	2.63	0.41
3:C:46:ILE:O	3:C:49:VAL:N	2.53	0.41
3:C:103:LYS:HD3	3:C:103:LYS:C	2.45	0.41
3:C:226:ARG:HE	3:C:231:HIS:CD2	2.38	0.41
9:C:2013:3PE:H3D2	9:C:2013:3PE:C2B	2.51	0.41
4:D:36:ALA:O	4:D:40:VAL:HG23	2.21	0.41
1:G:178:LEU:HD12	10:G:3028:HOH:O	2.20	0.41
1:G:199:ALA:O	1:G:200:SER:C	2.62	0.41
2:H:141:TYR:O	2:H:142:GLN:C	2.62	0.41
2:H:231:VAL:HB	2:H:234:ARG:HB2	2.01	0.41
2:B:98:SER:CB	2:B:99:PRO:CD	2.98	0.41
2:B:137:LYS:HD2	4:J:11:HIS:NE2	2.35	0.41
3:C:91:VAL:HG22	9:C:2010:3PE:H3I2	2.02	0.41
3:C:136:ILE:HG21	3:C:181:PHE:HE2	1.84	0.41
2:H:136:VAL:HG11	2:H:147:TYR:HD2	1.85	0.41
1:A:106:MET:HG3	8:A:1001:HEA:C3C	2.50	0.41
1:A:314:LEU:O	1:A:317:VAL:N	2.53	0.41
1:A:400:VAL:CG1	1:A:410:TYR:HE2	2.31	0.41
1:A:539:GLU:CG	1:A:540:TRP:N	2.82	0.41
10:A:2040:HOH:O	2:B:143:TRP:HH2	2.02	0.41
3:C:155:LEU:HB2	3:C:164:VAL:CG2	2.50	0.41
3:C:172:ILE:HD13	3:C:221:LEU:HA	2.02	0.41
1:G:202:ILE:HD11	1:G:243:LEU:HB2	2.01	0.41
1:G:225:VAL:O	1:G:226:PRO:C	2.63	0.41
1:G:252:MET:HE3	1:G:264:PHE:HZ	1.86	0.41
1:G:273:VAL:O	1:G:274:LEU:C	2.60	0.41
1:G:463:GLY:HA2	1:G:503:LEU:HD23	2.01	0.41
2:H:289:LEU:OXT	2:H:289:LEU:CG	2.68	0.41
3:I:110:GLY:O	3:I:112:GLU:N	2.53	0.41
3:I:253:VAL:HG22	9:I:3010:3PE:H3I1	2.02	0.41
1:A:81:TRP:CE3	1:A:82:PRO:HD2	2.56	0.41
1:A:95:TRP:O	1:A:96:ASN:C	2.63	0.41
1:A:189:LEU:HD21	3:C:30:PHE:CD1	2.55	0.41
1:A:424:MET:CE	8:A:1002:HEA:HMD3	2.51	0.41
2:B:35:ARG:HG3	2:B:36:PRO:HD2	2.02	0.41
4:D:51:ALA:O	9:D:2011:3PE:H122	2.21	0.41
1:G:115:LEU:HG	1:G:432:ILE:HG12	2.03	0.41
1:G:482:ARG:HH21	8:G:1001:HEA:CGD	2.33	0.41
2:H:62:LEU:HD12	2:H:65:ILE:HD11	2.03	0.41
2:H:107:VAL:HG12	2:H:108:PRO:HD3	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:238:LEU:C	2:H:238:LEU:CD1	2.90	0.41
9:I:3010:3PE:H382	9:I:3010:3PE:H3B2	1.85	0.41
1:A:131:PRO:HG2	3:C:9:TYR:HD2	1.85	0.41
1:A:295:PHE:HB3	1:A:362:LYS:HE2	2.02	0.41
1:A:382:LEU:HD11	1:A:454:LYS:HE2	2.03	0.41
1:G:396:VAL:HG12	1:G:397:THR:N	2.29	0.41
1:G:469:PHE:N	1:G:470:PRO:CD	2.84	0.41
1:G:558:GLU:O	1:G:560:TRP:N	2.53	0.41
1:A:318:TYR:HD1	1:A:318:TYR:HA	1.71	0.41
1:A:493:TRP:CE3	1:A:496:VAL:HG21	2.55	0.41
9:A:2012:3PE:H2I3	9:C:2010:3PE:H2F1	2.02	0.41
2:B:208:VAL:HG12	2:B:210:VAL:HG23	2.03	0.41
9:C:2013:3PE:H3H2	9:C:2013:3PE:H2E1	2.01	0.41
1:G:140:ASN:O	1:G:141:LEU:C	2.63	0.41
9:G:3009:3PE:H3E1	9:G:3009:3PE:H3B2	1.67	0.41
9:G:3012:3PE:H231	4:J:31:MET:CE	2.50	0.41
2:H:106:ILE:O	2:H:107:VAL:O	2.38	0.41
2:H:185:TYR:CE1	2:H:247:ILE:HD13	2.49	0.41
1:A:38:GLY:HA2	8:A:1001:HEA:H22	2.02	0.41
1:A:133:MET:HE3	1:A:211:THR:CG2	2.40	0.41
1:A:213:LEU:HD13	3:C:81:TRP:CZ2	2.55	0.41
1:A:393:VAL:O	1:A:394:GLY:C	2.62	0.41
1:A:433:PHE:HA	1:A:436:ILE:HD12	2.03	0.41
2:B:75:LEU:O	2:B:76:ILE:C	2.64	0.41
2:B:161:ILE:HD12	2:B:180:LEU:HD23	2.03	0.41
3:C:144:SER:O	3:C:145:GLY:C	2.64	0.41
3:C:187:SER:HG	3:C:188:HIS:CE1	2.31	0.41
9:C:2010:3PE:H2I2	4:D:36:ALA:CB	2.49	0.41
1:G:26:HIS:HB3	1:G:132:ASP:OD1	2.19	0.41
1:G:75:GLY:O	1:G:76:PHE:C	2.64	0.41
1:G:243:LEU:N	1:G:244:PRO:HD2	2.35	0.41
1:G:308:LYS:HD3	1:G:369:THR:O	2.21	0.41
1:G:361:ILE:HD11	2:H:105:THR:OG1	2.21	0.41
1:G:381:MET:O	1:G:381:MET:HG3	2.21	0.41
9:G:3009:3PE:H221	3:I:58:TRP:CE2	2.56	0.41
3:I:246:TYR:O	3:I:247:TRP:C	2.63	0.41
3:I:253:VAL:HG22	9:I:3010:3PE:C3I	2.51	0.41
4:J:12:VAL:HG12	4:J:15:SER:HB2	2.03	0.41
1:A:47:PHE:HB3	1:A:98:MET:HE3	2.03	0.41
1:A:63:MET:HE3	1:A:484:ILE:HD11	2.03	0.41
1:A:88:CYS:C	2:B:171:ARG:HH11	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:O	1:A:467:THR:C	2.62	0.41
9:C:2013:3PE:H3D2	9:C:2013:3PE:H2B2	2.02	0.41
1:G:314:LEU:CB	1:G:315:PRO:HD3	2.51	0.41
3:I:81:TRP:NE1	4:J:28:PHE:CE2	2.88	0.41
9:I:3010:3PE:H2I2	4:J:36:ALA:CB	2.51	0.41
1:A:260:GLY:O	3:C:194:ALA:HB1	2.21	0.40
2:B:114:ALA:O	2:B:115:ILE:C	2.61	0.40
3:C:20:MET:HE3	3:C:20:MET:HB2	1.91	0.40
3:C:240:PHE:CD1	3:C:244:ILE:HD11	2.56	0.40
1:G:29:ILE:HD12	1:G:139:ASN:ND2	2.37	0.40
1:G:173:VAL:O	1:G:174:LEU:HB2	2.21	0.40
1:G:357:VAL:N	1:G:358:PRO:HD2	2.36	0.40
1:A:201:SER:HB3	1:A:239:ILE:CG2	2.51	0.40
2:B:148:GLU:O	2:B:150:PRO:HD3	2.21	0.40
2:B:254:GLU:H	2:B:260:HIS:HE1	1.69	0.40
3:C:84:ILE:HG23	9:C:2013:3PE:H272	2.04	0.40
1:G:493:TRP:CE3	1:G:496:VAL:HG21	2.57	0.40
2:H:98:SER:CB	2:H:99:PRO:CD	2.99	0.40
2:H:175:GLU:O	2:H:176:VAL:C	2.64	0.40
9:I:3010:3PE:H231	9:I:3010:3PE:C33	2.50	0.40
9:I:3013:3PE:H3D2	9:I:3013:3PE:C2B	2.51	0.40
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.91	0.40
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.96	0.40
1:G:180:THR:HA	1:G:257:ARG:CG	2.52	0.40
2:H:71:PHE:CE1	2:H:75:LEU:HD11	2.56	0.40
2:H:131:GLU:H	2:H:131:GLU:CD	2.29	0.40
1:A:136:PRO:HA	10:A:2052:HOH:O	2.21	0.40
1:A:547:PRO:HD2	1:A:550:THR:HG22	2.03	0.40
8:A:1001:HEA:HAA1	8:A:1001:HEA:HMA	1.70	0.40
8:A:1001:HEA:HHC	8:A:1001:HEA:H11	1.81	0.40
2:H:234:ARG:HH12	3:I:114:PRO:HG3	1.86	0.40
3:I:113:SER:HA	3:I:114:PRO:HA	1.82	0.40
4:J:45:PHE:CD1	4:J:45:PHE:C	2.98	0.40
1:A:323:ILE:HG22	1:A:324:GLY:N	2.34	0.40
1:A:381:MET:O	1:A:382:LEU:C	2.60	0.40
1:A:476:ARG:HD3	2:B:41:THR:O	2.21	0.40
2:B:165:ALA:HB2	10:I:3042:HOH:O	2.20	0.40
3:C:111:PRO:HA	4:J:12:VAL:CB	2.44	0.40
3:C:135:LEU:HD12	3:C:135:LEU:HA	1.83	0.40
1:G:74:LYS:HD2	1:G:74:LYS:N	2.36	0.40
1:G:292:LEU:HD23	1:G:292:LEU:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:364:PHE:O	1:G:365:SER:C	2.63	0.40
1:G:396:VAL:O	1:G:399:ILE:N	2.54	0.40
1:G:541:THR:O	1:G:541:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	545/566 (96%)	479 (88%)	54 (10%)	12 (2%)	5	4
1	G	545/566 (96%)	466 (86%)	67 (12%)	12 (2%)	5	4
2	B	258/264 (98%)	222 (86%)	32 (12%)	4 (2%)	7	7
2	H	258/264 (98%)	220 (85%)	33 (13%)	5 (2%)	6	5
3	C	263/266 (99%)	229 (87%)	30 (11%)	4 (2%)	8	8
3	I	263/266 (99%)	234 (89%)	25 (10%)	4 (2%)	8	8
4	D	40/51 (78%)	37 (92%)	2 (5%)	1 (2%)	4	3
4	J	40/51 (78%)	32 (80%)	7 (18%)	1 (2%)	4	3
All	All	2212/2294 (96%)	1919 (87%)	250 (11%)	43 (2%)	6	5

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	SER
3	C	111	PRO
1	G	327	GLY
1	G	544	SER
2	H	264	PRO
3	I	111	PRO
4	J	12	VAL

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Mol	Chain	Res	Type
1	A	487	PRO
1	A	492	THR
4	D	12	VAL
1	G	162	GLY
1	G	487	PRO
1	G	492	THR
1	G	545	PRO
1	G	559	ASP
3	I	195	GLY
1	A	58	PRO
1	A	256	ASP
1	A	419	HIS
2	H	252	CYS
2	H	255	LEU
1	A	71	GLY
1	A	106	MET
1	A	327	GLY
1	A	545	PRO
2	B	85	GLU
2	B	255	LEU
1	G	90	PRO
1	G	405	SER
2	H	45	PRO
2	H	187	ARG
3	I	237	HIS
2	B	99	PRO
3	C	237	HIS
1	A	131	PRO
3	C	73	PRO
1	G	393	VAL
3	I	133	LEU
1	G	43	ILE
1	G	323	ILE
2	B	34	GLY
3	C	133	LEU
1	A	90	PRO

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	446/459 (97%)	415 (93%)	31 (7%)	14	19
1	G	446/459 (97%)	405 (91%)	41 (9%)	8	11
2	B	216/220 (98%)	202 (94%)	14 (6%)	15	22
2	H	216/220 (98%)	207 (96%)	9 (4%)	26	40
3	C	215/216 (100%)	206 (96%)	9 (4%)	26	40
3	I	215/216 (100%)	206 (96%)	9 (4%)	26	40
4	D	30/37 (81%)	26 (87%)	4 (13%)	4	4
4	J	30/37 (81%)	27 (90%)	3 (10%)	7	9
All	All	1814/1864 (97%)	1694 (93%)	120 (7%)	15	21

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	24	THR
1	A	45	VAL
1	A	52	ARG
1	A	55	LEU
1	A	70	SER
1	A	79	SER
1	A	89	THR
1	A	133	MET
1	A	137	ARG
1	A	151	SER
1	A	182	GLU
1	A	191	ILE
1	A	195	HIS
1	A	206	ILE
1	A	208	MET
1	A	212	PHE
1	A	243	LEU
1	A	251	THR
1	A	262	THR
1	A	282	PHE
1	A	310	ILE
1	A	355	ILE
1	A	412	ASP

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Mol	Chain	Res	Type
1	A	460	MET
1	A	477	GLN
1	A	484	ILE
1	A	520	THR
1	A	525	VAL
1	A	529	ASN
1	A	539	GLU
2	B	52	THR
2	B	69	THR
2	B	74	LEU
2	B	125	ASN
2	B	149	TYR
2	B	199	VAL
2	B	214	ASP
2	B	222	PRO
2	B	238	LEU
2	B	241	ARG
2	B	253	SER
2	B	263	MET
2	B	264	PRO
2	B	267	VAL
3	C	51	VAL
3	C	60	SER
3	C	72	THR
3	C	149	THR
3	C	155	LEU
3	C	157	HIS
3	C	166	TRP
3	C	196	ASN
3	C	231	HIS
4	D	15	SER
4	D	16	MET
4	D	29	VAL
4	D	50	ASN
1	G	23	SER
1	G	40	VAL
1	G	45	VAL
1	G	49	VAL
1	G	52	ARG
1	G	55	LEU
1	G	70	SER
1	G	79	SER

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Mol	Chain	Res	Type
1	G	89	THR
1	G	104	ILE
1	G	111	VAL
1	G	113	PRO
1	G	125	PRO
1	G	131	PRO
1	G	133	MET
1	G	137	ARG
1	G	182	GLU
1	G	191	ILE
1	G	195	HIS
1	G	206	ILE
1	G	208	MET
1	G	212	PHE
1	G	243	LEU
1	G	252	MET
1	G	262	THR
1	G	274	LEU
1	G	282	PHE
1	G	291	VAL
1	G	293	PRO
1	G	314	LEU
1	G	325	VAL
1	G	363	ILE
1	G	379	THR
1	G	412	ASP
1	G	460	MET
1	G	477	GLN
1	G	484	ILE
1	G	520	THR
1	G	525	VAL
1	G	532	ASN
1	G	539	GLU
2	H	35	ARG
2	H	76	ILE
2	H	149	TYR
2	H	199	VAL
2	H	238	LEU
2	H	241	ARG
2	H	253	SER
2	H	263	MET
2	H	272	GLU

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Mol	Chain	Res	Type
3	I	49	VAL
3	I	60	SER
3	I	72	THR
3	I	111	PRO
3	I	140	ILE
3	I	149	THR
3	I	155	LEU
3	I	196	ASN
3	I	231	HIS
4	J	16	MET
4	J	19	THR
4	J	50	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	26	HIS
1	A	345	GLN
1	A	494	ASN
2	B	55	HIS
2	B	84	HIS
2	B	127	GLN
2	B	170	ASN
2	B	178	GLN
2	B	209	GLN
2	B	237	GLN
2	B	251	GLN
3	C	37	HIS
3	C	132	HIS
3	C	152	HIS
3	C	153	HIS
3	C	159	ASN
3	C	201	ASN
3	C	212	HIS
3	C	231	HIS
1	G	25	ASN
1	G	26	HIS
1	G	91	ASN
1	G	96	ASN
1	G	163	ASN
1	G	165	GLN

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Mol	Chain	Res	Type
1	G	345	GLN
1	G	403	GLN
1	G	494	ASN
1	G	534	HIS
2	H	53	GLN
2	H	55	HIS
2	H	84	HIS
2	H	88	ASN
2	H	127	GLN
2	H	170	ASN
2	H	178	GLN
2	H	209	GLN
2	H	237	GLN
3	I	37	HIS
3	I	153	HIS
3	I	159	ASN
3	I	201	ASN
3	I	212	HIS
3	I	231	HIS
4	J	11	HIS

5.3.3 RNA [i](#)

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 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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
9	3PE	C	2010	-	50,50,50	1.61	3 (6%)	53,55,55	1.00	3 (5%)
8	HEA	G	1002	1	67,67,67	1.31	10 (14%)	81,103,103	2.21	28 (34%)
9	3PE	C	2013	-	50,50,50	1.60	3 (6%)	53,55,55	1.13	3 (5%)
9	3PE	I	3013	-	50,50,50	1.55	4 (8%)	53,55,55	1.09	4 (7%)
8	HEA	G	1001	1	67,67,67	1.21	7 (10%)	81,103,103	1.99	24 (29%)
9	3PE	A	2009	-	50,50,50	1.53	2 (4%)	53,55,55	1.02	3 (5%)
9	3PE	A	2012	-	50,50,50	1.60	3 (6%)	53,55,55	1.08	5 (9%)
9	3PE	G	3012	-	50,50,50	1.59	3 (6%)	53,55,55	1.12	4 (7%)
8	HEA	A	1002	1	67,67,67	1.31	9 (13%)	81,103,103	1.92	19 (23%)
9	3PE	I	3008	-	50,50,50	1.55	2 (4%)	53,55,55	1.16	4 (7%)
9	3PE	C	2008	-	50,50,50	1.59	2 (4%)	53,55,55	1.19	5 (9%)
9	3PE	J	3011	-	50,50,50	1.55	2 (4%)	53,55,55	1.32	4 (7%)
9	3PE	G	3009	-	50,50,50	1.56	2 (4%)	53,55,55	1.02	1 (1%)
9	3PE	I	3010	-	50,50,50	1.61	2 (4%)	53,55,55	0.98	3 (5%)
9	3PE	D	2011	-	50,50,50	1.55	2 (4%)	53,55,55	1.29	4 (7%)
8	HEA	A	1001	1	67,67,67	1.36	8 (11%)	81,103,103	2.09	21 (25%)

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
9	3PE	C	2010	-	-	29/54/54/54	-
8	HEA	G	1002	1	-	5/36/76/76	-
9	3PE	C	2013	-	-	27/54/54/54	-
9	3PE	I	3013	-	-	27/54/54/54	-
8	HEA	G	1001	1	-	13/36/76/76	-
9	3PE	A	2009	-	-	31/54/54/54	-
9	3PE	A	2012	-	-	23/54/54/54	-
9	3PE	G	3012	-	-	24/54/54/54	-
8	HEA	A	1002	1	-	10/36/76/76	-
9	3PE	I	3008	-	-	34/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	3PE	C	2008	-	-	34/54/54/54	-
9	3PE	J	3011	-	-	25/54/54/54	-
9	3PE	G	3009	-	-	27/54/54/54	-
9	3PE	I	3010	-	-	24/54/54/54	-
9	3PE	D	2011	-	-	22/54/54/54	-
8	HEA	A	1001	1	-	17/36/76/76	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	2013	3PE	O21-C21	7.68	1.56	1.34
9	C	2010	3PE	O31-C31	7.67	1.55	1.33
9	G	3009	3PE	O21-C21	7.51	1.55	1.34
9	C	2008	3PE	O31-C31	7.49	1.55	1.33
9	C	2008	3PE	O21-C21	7.49	1.55	1.34
9	I	3010	3PE	O31-C31	7.49	1.55	1.33
9	J	3011	3PE	O21-C21	7.46	1.55	1.34
9	A	2012	3PE	O31-C31	7.46	1.55	1.33
9	I	3010	3PE	O21-C21	7.45	1.55	1.34
9	I	3008	3PE	O31-C31	7.45	1.55	1.33
9	G	3012	3PE	O31-C31	7.42	1.55	1.33
9	D	2011	3PE	O21-C21	7.37	1.55	1.34
9	C	2010	3PE	O21-C21	7.25	1.54	1.34
9	A	2009	3PE	O21-C21	7.24	1.54	1.34
9	G	3012	3PE	O21-C21	7.23	1.54	1.34
9	I	3013	3PE	O21-C21	7.19	1.54	1.34
9	A	2012	3PE	O21-C21	7.10	1.54	1.34
9	I	3013	3PE	O31-C31	7.08	1.54	1.33
9	C	2013	3PE	O31-C31	7.06	1.53	1.33
9	A	2009	3PE	O31-C31	7.03	1.53	1.33
9	I	3008	3PE	O21-C21	7.01	1.54	1.34
9	D	2011	3PE	O31-C31	6.91	1.53	1.33
9	J	3011	3PE	O31-C31	6.80	1.53	1.33
9	G	3009	3PE	O31-C31	6.80	1.53	1.33
8	A	1002	HEA	CMA-C3A	3.58	1.53	1.45
8	A	1001	HEA	CAC-C3C	-3.20	1.38	1.47
8	A	1001	HEA	C16-C15	-3.18	1.44	1.51
8	A	1002	HEA	CAC-C3C	-3.17	1.38	1.47
8	A	1001	HEA	FE-NB	3.16	2.04	1.94
8	G	1002	HEA	C11-C3B	-3.10	1.47	1.51
8	A	1001	HEA	FE-ND	-3.06	1.85	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1002	HEA	FE-ND	-3.05	1.85	1.94
8	G	1002	HEA	C4D-ND	-3.03	1.32	1.38
8	G	1001	HEA	CMA-C3A	2.98	1.52	1.45
8	G	1002	HEA	C4C-NC	-2.98	1.34	1.39
8	G	1001	HEA	C1D-ND	-2.76	1.35	1.40
8	G	1001	HEA	CAC-C3C	-2.75	1.40	1.47
8	A	1002	HEA	C1A-NA	-2.71	1.34	1.39
8	A	1001	HEA	C4C-NC	-2.66	1.34	1.39
9	A	2012	3PE	O21-C2	-2.65	1.40	1.46
8	G	1002	HEA	CAC-C3C	-2.52	1.40	1.47
8	A	1001	HEA	O11-C11	2.48	1.48	1.42
8	A	1002	HEA	FE-NB	2.47	2.02	1.94
8	G	1002	HEA	C1D-ND	-2.39	1.36	1.40
8	G	1002	HEA	C3A-C2A	-2.38	1.31	1.37
8	A	1001	HEA	O2A-CGA	-2.37	1.23	1.30
8	G	1001	HEA	FE-ND	-2.34	1.87	1.94
8	G	1002	HEA	CMA-C3A	2.31	1.50	1.45
9	G	3012	3PE	O21-C2	-2.29	1.41	1.46
8	A	1002	HEA	C1D-ND	-2.28	1.36	1.40
8	G	1001	HEA	FE-NB	2.23	2.01	1.94
9	I	3013	3PE	O32-C31	2.21	1.29	1.22
8	G	1002	HEA	CAA-C2A	2.20	1.57	1.51
9	C	2013	3PE	O21-C2	-2.19	1.41	1.46
9	I	3013	3PE	O21-C2	-2.18	1.41	1.46
8	A	1002	HEA	C4C-NC	-2.12	1.35	1.39
9	C	2010	3PE	O21-C2	-2.11	1.41	1.46
8	G	1001	HEA	C4D-ND	-2.11	1.34	1.38
8	G	1002	HEA	C3C-C2C	-2.11	1.34	1.41
8	A	1001	HEA	CMA-C3A	2.10	1.50	1.45
8	A	1002	HEA	O2A-CGA	-2.09	1.23	1.30
8	A	1002	HEA	C4D-ND	-2.08	1.34	1.38
8	G	1001	HEA	C16-C15	-2.04	1.47	1.51
8	G	1002	HEA	FE-ND	-2.02	1.88	1.94

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	HEA	C13-C14-C15	-7.31	110.89	127.62
8	A	1001	HEA	CAA-C2A-C1A	6.36	137.78	124.85
8	G	1001	HEA	C13-C14-C15	-5.66	114.68	127.62
9	J	3011	3PE	C2-O21-C21	-5.62	104.36	117.80
8	A	1002	HEA	C12-C11-C3B	5.44	120.62	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1002	HEA	C17-C18-C19	-5.37	115.34	127.62
8	G	1001	HEA	CAA-C2A-C1A	5.25	135.52	124.85
8	G	1002	HEA	OMA-CMA-C3A	-5.04	114.24	125.62
9	G	3009	3PE	C3-C2-C1	-4.99	100.15	111.78
8	G	1002	HEA	CHA-C4D-ND	4.93	129.73	124.42
8	G	1002	HEA	CMB-C2B-C3B	-4.93	120.75	130.28
8	A	1001	HEA	C3C-C4C-NC	4.87	113.90	109.80
9	C	2008	3PE	C2-O21-C21	-4.71	106.53	117.80
8	A	1002	HEA	C3C-C4C-NC	4.64	113.70	109.80
9	D	2011	3PE	C2-O21-C21	-4.63	106.72	117.80
8	A	1001	HEA	C26-C15-C14	-4.60	111.81	123.63
8	G	1002	HEA	C12-C11-C3B	4.46	119.09	112.12
8	G	1001	HEA	C17-C18-C19	-4.45	117.43	127.62
8	G	1002	HEA	C27-C19-C20	4.35	122.78	115.23
8	G	1001	HEA	O1D-CGD-CBD	-4.32	109.41	123.09
8	G	1002	HEA	CHA-C4D-C3D	-4.28	118.53	124.77
8	G	1002	HEA	CHC-C4B-NB	4.27	129.64	124.37
9	C	2013	3PE	C2-O21-C21	-4.25	107.63	117.80
9	J	3011	3PE	C3-C2-C1	-4.17	102.06	111.78
8	A	1001	HEA	C17-C18-C19	-4.14	118.15	127.62
8	A	1001	HEA	C3B-C4B-NB	4.13	114.58	109.84
9	A	2009	3PE	C3-C2-C1	-4.05	102.34	111.78
8	G	1002	HEA	CMB-C2B-C1B	4.05	131.36	125.03
8	A	1002	HEA	O11-C11-C3B	-4.03	103.87	111.26
9	D	2011	3PE	C3-C2-C1	-4.00	102.46	111.78
8	G	1001	HEA	C4B-NB-C1B	-3.98	100.50	105.21
8	A	1001	HEA	C4B-NB-C1B	-3.94	100.54	105.21
9	I	3008	3PE	O21-C2-C3	-3.91	94.31	108.34
8	G	1001	HEA	CBA-CAA-C2A	3.80	123.03	112.53
9	I	3008	3PE	C2-O21-C21	-3.73	108.86	117.80
8	G	1002	HEA	CMD-C2D-C1D	3.73	130.86	125.03
9	I	3013	3PE	C2-O21-C21	-3.72	108.89	117.80
8	G	1002	HEA	CHB-C1B-NB	-3.71	120.43	124.42
8	G	1002	HEA	C17-C18-C19	-3.69	119.18	127.62
8	A	1002	HEA	O2D-CGD-CBD	3.62	125.45	114.00
8	G	1002	HEA	C1C-CHC-C4B	-3.58	117.83	126.25
8	G	1001	HEA	C3B-C4B-NB	3.56	113.93	109.84
8	A	1001	HEA	C26-C15-C16	3.54	121.38	115.23
8	G	1001	HEA	C12-C11-C3B	3.51	117.61	112.12
9	G	3012	3PE	O21-C21-O22	3.48	131.83	123.70
9	G	3012	3PE	C3-C2-C1	-3.47	103.70	111.78
8	G	1001	HEA	C3C-C4C-NC	3.35	112.62	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1001	HEA	C4C-NC-C1C	-3.35	100.36	105.82
8	A	1002	HEA	C13-C14-C15	-3.34	119.98	127.62
8	G	1002	HEA	C3C-C4C-NC	3.34	112.61	109.80
8	A	1001	HEA	CMC-C2C-C1C	3.29	130.43	125.42
8	G	1002	HEA	CBD-CAD-C3D	3.27	121.56	112.53
8	A	1002	HEA	C2A-C1A-NA	3.24	113.45	110.32
9	C	2008	3PE	C3-O31-C31	-3.21	105.37	117.12
8	A	1001	HEA	O2D-CGD-CBD	3.14	123.91	114.00
9	A	2012	3PE	O21-C21-O22	3.12	131.00	123.70
9	C	2010	3PE	C3-C2-C1	-3.10	104.56	111.78
9	C	2010	3PE	O31-C3-C2	3.10	117.32	108.40
8	G	1001	HEA	C16-C15-C14	3.09	128.11	121.17
9	C	2013	3PE	C3-O31-C31	-3.02	106.08	117.12
8	G	1001	HEA	C27-C19-C20	2.99	120.41	115.23
9	C	2008	3PE	O21-C2-C3	-2.97	97.70	108.34
9	I	3008	3PE	O31-C3-C2	2.96	116.94	108.40
9	G	3012	3PE	O21-C2-C1	2.91	118.80	108.34
8	A	1001	HEA	C25-C23-C24	-2.91	107.88	114.59
8	G	1001	HEA	C2B-C1B-NB	2.90	113.25	109.90
8	A	1002	HEA	O1A-CGA-CBA	-2.82	114.15	123.09
8	A	1002	HEA	C4B-NB-C1B	-2.81	101.88	105.21
8	A	1002	HEA	CMD-C2D-C1D	2.78	129.38	125.03
8	G	1001	HEA	O2D-CGD-O1D	2.78	130.49	123.33
8	A	1001	HEA	C2C-C1C-NC	2.78	114.59	110.14
9	A	2012	3PE	C3-C2-C1	-2.74	105.39	111.78
9	D	2011	3PE	P-O13-C11	-2.72	108.29	121.26
8	A	1001	HEA	C13-C12-C11	2.72	118.73	114.39
8	G	1002	HEA	C27-C19-C18	-2.70	116.69	123.63
8	G	1002	HEA	C13-C14-C15	-2.70	121.45	127.62
8	A	1002	HEA	C3D-C4D-ND	2.69	112.95	110.35
9	I	3008	3PE	C3-O31-C31	-2.67	107.35	117.12
8	G	1002	HEA	C1A-CHA-C4D	-2.66	120.36	126.02
8	A	1002	HEA	O1D-CGD-CBD	-2.66	114.65	123.09
8	G	1002	HEA	C4A-C3A-C2A	2.66	109.12	106.81
8	G	1001	HEA	C2A-C1A-NA	2.64	112.87	110.32
8	A	1002	HEA	CBD-CAD-C3D	2.64	119.82	112.53
9	I	3010	3PE	C2-O21-C21	-2.62	111.54	117.80
8	G	1001	HEA	C4C-NC-C1C	-2.60	101.58	105.82
8	A	1001	HEA	C2B-C1B-NB	2.59	112.90	109.90
9	I	3013	3PE	C23-C22-C21	-2.59	104.19	113.69
8	A	1002	HEA	C3B-C4B-NB	2.59	112.82	109.84
9	A	2012	3PE	C3-O31-C31	-2.58	107.69	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1001	HEA	C24-C23-C22	2.57	130.37	122.66
8	G	1002	HEA	C2A-C1A-NA	2.57	112.80	110.32
9	A	2009	3PE	O21-C2-C3	-2.55	99.20	108.34
8	G	1002	HEA	CHC-C4B-C3B	-2.55	119.37	125.80
8	A	1001	HEA	C16-C15-C14	2.51	126.81	121.17
8	A	1002	HEA	C2B-C1B-NB	2.49	112.78	109.90
8	A	1002	HEA	C4C-NC-C1C	-2.46	101.81	105.82
8	G	1002	HEA	CHB-C1B-C2B	2.46	128.91	125.03
8	G	1001	HEA	C2C-C1C-NC	2.44	114.05	110.14
9	J	3011	3PE	P-O11-C1	-2.40	107.59	121.35
9	I	3010	3PE	C3-O31-C31	-2.37	108.46	117.12
9	C	2013	3PE	O31-C31-C32	2.36	119.02	111.83
8	G	1002	HEA	C26-C15-C16	-2.34	111.16	115.23
9	J	3011	3PE	P-O13-C11	-2.33	110.17	121.26
8	A	1002	HEA	CHB-C1B-NB	-2.32	121.93	124.42
8	G	1001	HEA	C26-C15-C16	-2.31	111.22	115.23
9	I	3010	3PE	C3-C2-C1	-2.30	106.43	111.78
9	C	2008	3PE	O13-C11-C12	-2.29	100.78	109.17
8	G	1002	HEA	CAA-CBA-CGA	2.27	119.67	113.67
9	D	2011	3PE	P-O11-C1	-2.26	108.39	121.35
8	A	1002	HEA	C2C-C1C-NC	2.25	113.75	110.14
8	G	1002	HEA	CHB-C4A-C3A	2.22	128.96	125.21
8	G	1001	HEA	C21-C22-C23	-2.22	120.25	127.64
8	A	1001	HEA	C1D-C2D-C3D	-2.20	104.66	106.98
9	A	2009	3PE	C3-O31-C31	-2.20	109.08	117.12
9	A	2012	3PE	O21-C2-C1	2.19	116.21	108.34
9	A	2012	3PE	C2E-C2D-C2C	-2.18	103.37	114.37
9	I	3013	3PE	C2B-C2A-C29	-2.16	103.46	114.37
8	G	1002	HEA	CAD-C3D-C2D	2.16	131.91	127.87
8	A	1002	HEA	C4C-C3C-C2C	-2.15	104.63	107.30
8	G	1002	HEA	CHC-C1C-C2C	-2.14	121.20	127.43
8	G	1002	HEA	O2A-CGA-O1A	-2.14	117.82	123.33
8	A	1001	HEA	C12-C11-C3B	2.12	115.44	112.12
8	G	1002	HEA	CBA-CAA-C2A	2.11	118.37	112.53
8	G	1001	HEA	C1D-C2D-C3D	-2.11	104.76	106.98
8	A	1001	HEA	O11-C11-C3B	-2.10	107.42	111.26
8	A	1001	HEA	CHC-C4B-C3B	-2.09	120.53	125.80
9	C	2010	3PE	C2-O21-C21	-2.09	112.80	117.80
8	G	1001	HEA	CHA-C1A-NA	-2.08	122.19	124.45
8	G	1001	HEA	O2A-CGA-O1A	-2.07	118.01	123.33
9	C	2008	3PE	P-O13-C11	-2.05	111.51	121.26
8	G	1001	HEA	CHC-C1C-C2C	-2.04	121.51	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	3013	3PE	O32-C31-C32	-2.03	115.85	123.78
8	A	1001	HEA	C21-C20-C19	2.03	119.90	113.19
9	G	3012	3PE	O21-C21-C22	-2.02	107.11	111.48
8	G	1001	HEA	CAA-CBA-CGA	2.01	119.01	113.67

There are no chirality outliers.

All (372) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C2A-C3A-CMA-OMA
8	A	1001	HEA	C2C-C3C-CAC-CBC
8	A	1001	HEA	C4C-C3C-CAC-CBC
8	A	1001	HEA	C11-C12-C13-C14
8	A	1002	HEA	C2A-C3A-CMA-OMA
8	A	1002	HEA	C4A-C3A-CMA-OMA
8	G	1001	HEA	C3B-C11-C12-C13
8	G	1001	HEA	C11-C12-C13-C14
9	A	2009	3PE	C1-O11-P-O13
9	A	2009	3PE	C11-O13-P-O11
9	A	2009	3PE	C11-O13-P-O12
9	A	2009	3PE	C11-O13-P-O14
9	A	2009	3PE	O13-C11-C12-N
9	A	2012	3PE	C1-O11-P-O13
9	A	2012	3PE	C1-O11-P-O14
9	A	2012	3PE	O13-C11-C12-N
9	A	2012	3PE	O11-C1-C2-O21
9	C	2008	3PE	C1-O11-P-O12
9	C	2008	3PE	C1-O11-P-O13
9	C	2008	3PE	C1-O11-P-O14
9	C	2008	3PE	O13-C11-C12-N
9	C	2010	3PE	C1-O11-P-O12
9	C	2010	3PE	C1-O11-P-O13
9	C	2010	3PE	C1-O11-P-O14
9	C	2010	3PE	C11-O13-P-O11
9	C	2010	3PE	C11-O13-P-O12
9	C	2010	3PE	O13-C11-C12-N
9	C	2013	3PE	C1-O11-P-O13
9	C	2013	3PE	C11-O13-P-O11
9	C	2013	3PE	C11-O13-P-O12
9	C	2013	3PE	C12-C11-O13-P
9	C	2013	3PE	C22-C21-O21-C2
9	D	2011	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
9	D	2011	3PE	C11-O13-P-O12
9	D	2011	3PE	C11-O13-P-O14
9	G	3009	3PE	C1-O11-P-O12
9	G	3009	3PE	C1-O11-P-O13
9	G	3009	3PE	C11-O13-P-O11
9	G	3009	3PE	C11-O13-P-O12
9	G	3009	3PE	C11-O13-P-O14
9	G	3009	3PE	O13-C11-C12-N
9	G	3012	3PE	C1-O11-P-O12
9	G	3012	3PE	C1-O11-P-O13
9	G	3012	3PE	C1-O11-P-O14
9	G	3012	3PE	O13-C11-C12-N
9	G	3012	3PE	O11-C1-C2-O21
9	I	3008	3PE	C1-O11-P-O12
9	I	3008	3PE	C1-O11-P-O13
9	I	3008	3PE	C1-O11-P-O14
9	I	3008	3PE	O13-C11-C12-N
9	I	3010	3PE	C1-O11-P-O12
9	I	3010	3PE	C1-O11-P-O13
9	I	3010	3PE	O13-C11-C12-N
9	I	3013	3PE	C1-O11-P-O13
9	I	3013	3PE	C11-O13-P-O11
9	I	3013	3PE	C11-O13-P-O12
9	I	3013	3PE	C12-C11-O13-P
9	I	3013	3PE	C22-C21-O21-C2
9	J	3011	3PE	C11-O13-P-O11
9	J	3011	3PE	C11-O13-P-O12
9	J	3011	3PE	C11-O13-P-O14
9	C	2013	3PE	O22-C21-O21-C2
8	A	1001	HEA	C3A-C2A-CAA-CBA
9	C	2008	3PE	O32-C31-O31-C3
9	I	3008	3PE	O32-C31-O31-C3
8	A	1001	HEA	C1A-C2A-CAA-CBA
9	I	3013	3PE	O22-C21-O21-C2
9	I	3008	3PE	C32-C31-O31-C3
9	C	2008	3PE	C32-C31-O31-C3
8	A	1001	HEA	C27-C19-C20-C21
8	G	1001	HEA	C27-C19-C20-C21
8	A	1001	HEA	C18-C19-C20-C21
8	G	1001	HEA	C18-C19-C20-C21
9	C	2013	3PE	C32-C33-C34-C35
9	I	3013	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
9	A	2009	3PE	C3B-C3C-C3D-C3E
9	G	3009	3PE	C3B-C3C-C3D-C3E
8	G	1001	HEA	C1A-C2A-CAA-CBA
9	C	2010	3PE	C38-C39-C3A-C3B
9	I	3010	3PE	C38-C39-C3A-C3B
9	A	2012	3PE	C31-C32-C33-C34
9	D	2011	3PE	C31-C32-C33-C34
9	J	3011	3PE	C31-C32-C33-C34
9	G	3012	3PE	C31-C32-C33-C34
9	A	2009	3PE	C31-C32-C33-C34
9	J	3011	3PE	C21-C22-C23-C24
9	J	3011	3PE	C28-C29-C2A-C2B
8	G	1001	HEA	C3A-C2A-CAA-CBA
9	D	2011	3PE	C21-C22-C23-C24
9	G	3009	3PE	C31-C32-C33-C34
9	I	3013	3PE	C25-C26-C27-C28
9	I	3010	3PE	C36-C37-C38-C39
9	A	2009	3PE	C24-C25-C26-C27
9	I	3008	3PE	C26-C27-C28-C29
9	G	3009	3PE	C3D-C3E-C3F-C3G
9	A	2012	3PE	C28-C29-C2A-C2B
9	C	2010	3PE	C36-C37-C38-C39
9	C	2013	3PE	C39-C3A-C3B-C3C
9	C	2013	3PE	C22-C23-C24-C25
8	G	1001	HEA	C4C-C3C-CAC-CBC
9	A	2012	3PE	C36-C37-C38-C39
9	A	2009	3PE	C3D-C3E-C3F-C3G
9	C	2008	3PE	C26-C27-C28-C29
9	D	2011	3PE	C26-C27-C28-C29
9	G	3012	3PE	C36-C37-C38-C39
9	I	3013	3PE	C39-C3A-C3B-C3C
9	C	2013	3PE	C3D-C3E-C3F-C3G
9	I	3013	3PE	C3D-C3E-C3F-C3G
9	G	3012	3PE	C26-C27-C28-C29
9	I	3013	3PE	C33-C34-C35-C36
9	I	3013	3PE	C22-C23-C24-C25
9	A	2012	3PE	C26-C27-C28-C29
9	C	2008	3PE	C24-C25-C26-C27
9	C	2013	3PE	C33-C34-C35-C36
9	J	3011	3PE	C2B-C2C-C2D-C2E
9	C	2008	3PE	C32-C33-C34-C35
9	C	2008	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
9	G	3009	3PE	C29-C2A-C2B-C2C
9	J	3011	3PE	C26-C27-C28-C29
9	A	2009	3PE	C36-C37-C38-C39
9	D	2011	3PE	C28-C29-C2A-C2B
9	G	3009	3PE	C24-C25-C26-C27
9	I	3008	3PE	C3A-C3B-C3C-C3D
9	A	2009	3PE	C22-C21-O21-C2
9	I	3008	3PE	C32-C33-C34-C35
9	C	2008	3PE	C23-C24-C25-C26
9	C	2013	3PE	C2C-C2D-C2E-C2F
9	D	2011	3PE	C2B-C2C-C2D-C2E
9	G	3012	3PE	C28-C29-C2A-C2B
9	D	2011	3PE	C29-C2A-C2B-C2C
9	I	3013	3PE	C2C-C2D-C2E-C2F
9	G	3009	3PE	C39-C3A-C3B-C3C
9	A	2009	3PE	C39-C3A-C3B-C3C
9	G	3009	3PE	C38-C39-C3A-C3B
9	G	3009	3PE	C3E-C3F-C3G-C3H
9	I	3008	3PE	C24-C25-C26-C27
9	A	2012	3PE	C38-C39-C3A-C3B
9	A	2012	3PE	C3C-C3D-C3E-C3F
9	I	3008	3PE	C23-C24-C25-C26
9	A	2009	3PE	C38-C39-C3A-C3B
9	G	3009	3PE	C36-C37-C38-C39
9	A	2012	3PE	C27-C28-C29-C2A
9	C	2013	3PE	C25-C26-C27-C28
9	C	2010	3PE	C22-C23-C24-C25
9	C	2008	3PE	C2D-C2E-C2F-C2G
9	A	2009	3PE	C3E-C3F-C3G-C3H
9	C	2008	3PE	C2A-C2B-C2C-C2D
9	C	2008	3PE	C29-C2A-C2B-C2C
9	I	3013	3PE	C3C-C3D-C3E-C3F
9	A	2009	3PE	C29-C2A-C2B-C2C
9	I	3008	3PE	C36-C37-C38-C39
9	C	2013	3PE	C3C-C3D-C3E-C3F
9	I	3008	3PE	C29-C2A-C2B-C2C
9	G	3012	3PE	C27-C28-C29-C2A
9	C	2008	3PE	C27-C28-C29-C2A
9	G	3012	3PE	C38-C39-C3A-C3B
9	C	2010	3PE	C2C-C2D-C2E-C2F
9	I	3013	3PE	O11-C1-C2-C3
9	A	2009	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
9	I	3008	3PE	C2A-C2B-C2C-C2D
9	I	3013	3PE	C36-C37-C38-C39
9	C	2010	3PE	C1-C2-C3-O31
9	I	3010	3PE	C1-C2-C3-O31
9	I	3013	3PE	C38-C39-C3A-C3B
9	A	2012	3PE	C3E-C3F-C3G-C3H
9	C	2013	3PE	C3A-C3B-C3C-C3D
9	C	2010	3PE	C23-C24-C25-C26
9	J	3011	3PE	C27-C28-C29-C2A
9	C	2010	3PE	C21-C22-C23-C24
9	C	2013	3PE	C36-C37-C38-C39
9	G	3009	3PE	C2E-C2F-C2G-C2H
9	J	3011	3PE	C29-C2A-C2B-C2C
9	C	2008	3PE	C36-C37-C38-C39
9	C	2013	3PE	O11-C1-C2-O21
9	C	2008	3PE	C38-C39-C3A-C3B
9	D	2011	3PE	C27-C28-C29-C2A
9	D	2011	3PE	C2F-C2G-C2H-C2I
9	C	2013	3PE	C38-C39-C3A-C3B
9	I	3008	3PE	C39-C3A-C3B-C3C
9	I	3008	3PE	C2F-C2G-C2H-C2I
8	A	1001	HEA	C3B-C11-C12-C13
9	A	2012	3PE	C24-C25-C26-C27
9	I	3008	3PE	C38-C39-C3A-C3B
9	G	3012	3PE	C24-C25-C26-C27
9	I	3008	3PE	C34-C35-C36-C37
9	I	3013	3PE	C3E-C3F-C3G-C3H
9	J	3011	3PE	C39-C3A-C3B-C3C
9	J	3011	3PE	C2F-C2G-C2H-C2I
9	C	2013	3PE	C3E-C3F-C3G-C3H
9	G	3012	3PE	C29-C2A-C2B-C2C
9	I	3008	3PE	C37-C38-C39-C3A
9	A	2012	3PE	O11-C1-C2-C3
9	C	2013	3PE	O11-C1-C2-C3
9	C	2008	3PE	C2F-C2G-C2H-C2I
9	C	2008	3PE	C37-C38-C39-C3A
9	I	3008	3PE	C2D-C2E-C2F-C2G
9	D	2011	3PE	C32-C31-O31-C3
9	A	2009	3PE	C2E-C2F-C2G-C2H
9	C	2008	3PE	C21-C22-C23-C24
9	C	2010	3PE	C26-C27-C28-C29
9	G	3012	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
9	I	3013	3PE	C1-C2-C3-O31
9	D	2011	3PE	C33-C34-C35-C36
9	D	2011	3PE	C36-C37-C38-C39
9	C	2008	3PE	O11-C1-C2-O21
9	I	3013	3PE	O11-C1-C2-O21
9	A	2009	3PE	C3C-C3D-C3E-C3F
9	A	2012	3PE	C22-C23-C24-C25
9	G	3012	3PE	C3C-C3D-C3E-C3F
9	C	2008	3PE	O21-C2-C3-O31
9	C	2013	3PE	O21-C2-C3-O31
9	I	3008	3PE	O21-C2-C3-O31
9	I	3010	3PE	O21-C2-C3-O31
9	I	3013	3PE	O21-C2-C3-O31
9	G	3009	3PE	C3C-C3D-C3E-C3F
9	I	3013	3PE	C3A-C3B-C3C-C3D
9	G	3012	3PE	C22-C23-C24-C25
9	I	3010	3PE	C28-C29-C2A-C2B
9	I	3010	3PE	C3D-C3E-C3F-C3G
9	I	3010	3PE	C2C-C2D-C2E-C2F
9	I	3013	3PE	C26-C27-C28-C29
9	I	3008	3PE	C21-C22-C23-C24
9	A	2009	3PE	C2B-C2C-C2D-C2E
9	G	3009	3PE	C2B-C2C-C2D-C2E
9	C	2008	3PE	O11-C1-C2-C3
9	G	3012	3PE	O11-C1-C2-C3
9	I	3008	3PE	O11-C1-C2-C3
9	I	3008	3PE	C27-C28-C29-C2A
9	C	2010	3PE	C2F-C2G-C2H-C2I
9	A	2012	3PE	C29-C2A-C2B-C2C
9	C	2013	3PE	C37-C38-C39-C3A
9	G	3009	3PE	C2F-C2G-C2H-C2I
9	I	3010	3PE	C21-C22-C23-C24
9	D	2011	3PE	O32-C31-O31-C3
9	A	2009	3PE	C1-C2-C3-O31
9	A	2012	3PE	C1-C2-C3-O31
9	C	2013	3PE	C1-C2-C3-O31
8	A	1001	HEA	O11-C11-C12-C13
8	G	1001	HEA	O11-C11-C12-C13
9	A	2012	3PE	C12-C11-O13-P
9	G	3012	3PE	C12-C11-O13-P
9	C	2008	3PE	C39-C3A-C3B-C3C
9	C	2010	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
9	C	2010	3PE	C25-C26-C27-C28
9	G	3012	3PE	C3E-C3F-C3G-C3H
9	A	2012	3PE	C23-C24-C25-C26
9	G	3009	3PE	C25-C26-C27-C28
9	J	3011	3PE	C37-C38-C39-C3A
9	C	2008	3PE	C3D-C3E-C3F-C3G
9	C	2010	3PE	C3D-C3E-C3F-C3G
9	I	3010	3PE	C26-C27-C28-C29
9	I	3008	3PE	C2E-C2F-C2G-C2H
9	I	3008	3PE	O11-C1-C2-O21
9	C	2008	3PE	C22-C21-O21-C2
9	C	2008	3PE	C34-C35-C36-C37
9	D	2011	3PE	C39-C3A-C3B-C3C
8	A	1001	HEA	C4A-C3A-CMA-OMA
9	I	3008	3PE	C3D-C3E-C3F-C3G
9	C	2008	3PE	C1-C2-C3-O31
9	I	3008	3PE	C1-C2-C3-O31
9	J	3011	3PE	C1-C2-C3-O31
9	D	2011	3PE	C24-C25-C26-C27
8	A	1001	HEA	O11-C11-C3B-C2B
8	G	1001	HEA	O11-C11-C3B-C2B
9	A	2009	3PE	C1-O11-P-O12
9	A	2012	3PE	C1-O11-P-O12
9	C	2010	3PE	C11-O13-P-O14
9	C	2013	3PE	C1-O11-P-O14
9	I	3010	3PE	C11-O13-P-O11
9	I	3013	3PE	C1-O11-P-O14
9	J	3011	3PE	C36-C37-C38-C39
8	G	1001	HEA	C2C-C3C-CAC-CBC
9	C	2010	3PE	C22-C21-O21-C2
9	A	2009	3PE	C2F-C2G-C2H-C2I
9	I	3010	3PE	C2F-C2G-C2H-C2I
9	G	3012	3PE	C21-C22-C23-C24
9	I	3013	3PE	C3F-C3G-C3H-C3I
9	A	2009	3PE	C25-C26-C27-C28
9	C	2008	3PE	O22-C21-O21-C2
9	C	2010	3PE	O22-C21-O21-C2
9	C	2013	3PE	C26-C27-C28-C29
9	I	3010	3PE	C22-C23-C24-C25
9	C	2013	3PE	C24-C25-C26-C27
9	I	3013	3PE	C28-C29-C2A-C2B
9	C	2013	3PE	C3F-C3G-C3H-C3I

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Mol	Chain	Res	Type	Atoms
9	C	2010	3PE	C28-C29-C2A-C2B
9	I	3010	3PE	C3E-C3F-C3G-C3H
9	J	3011	3PE	C3B-C3C-C3D-C3E
9	I	3013	3PE	C24-C25-C26-C27
9	G	3012	3PE	C23-C24-C25-C26
9	A	2009	3PE	C27-C28-C29-C2A
9	J	3011	3PE	C33-C34-C35-C36
9	I	3008	3PE	C22-C23-C24-C25
8	A	1001	HEA	C26-C15-C16-C17
9	G	3009	3PE	C23-C24-C25-C26
9	I	3008	3PE	C35-C36-C37-C38
9	C	2010	3PE	C2D-C2E-C2F-C2G
9	I	3008	3PE	O22-C21-O21-C2
8	G	1002	HEA	CAD-CBD-CGD-O2D
9	C	2008	3PE	C33-C34-C35-C36
8	A	1002	HEA	CAD-CBD-CGD-O1D
9	I	3010	3PE	C23-C24-C25-C26
8	A	1002	HEA	CAD-CBD-CGD-O2D
8	G	1002	HEA	CAD-CBD-CGD-O1D
9	C	2008	3PE	C2E-C2F-C2G-C2H
8	G	1002	HEA	CAA-CBA-CGA-O1A
9	G	3009	3PE	O22-C21-O21-C2
9	A	2012	3PE	C21-C22-C23-C24
9	G	3012	3PE	C2E-C2F-C2G-C2H
8	G	1002	HEA	CAA-CBA-CGA-O2A
8	A	1002	HEA	C20-C21-C22-C23
8	A	1002	HEA	C26-C15-C16-C17
9	G	3009	3PE	C22-C21-O21-C2
8	A	1001	HEA	CAA-CBA-CGA-O2A
8	A	1002	HEA	CAA-CBA-CGA-O2A
9	C	2010	3PE	C3F-C3G-C3H-C3I
9	I	3008	3PE	C22-C21-O21-C2
9	G	3009	3PE	C3F-C3G-C3H-C3I
9	C	2008	3PE	C35-C36-C37-C38
9	C	2010	3PE	C3A-C3B-C3C-C3D
8	A	1002	HEA	CAA-CBA-CGA-O1A
8	G	1001	HEA	CAA-CBA-CGA-O2A
9	I	3010	3PE	C33-C34-C35-C36
9	D	2011	3PE	C3A-C3B-C3C-C3D
9	C	2008	3PE	C3-C2-O21-C21
9	I	3010	3PE	C2D-C2E-C2F-C2G
8	A	1001	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
9	J	3011	3PE	O32-C31-O31-C3
9	D	2011	3PE	C1-C2-C3-O31
8	G	1001	HEA	CAA-CBA-CGA-O1A
9	J	3011	3PE	C32-C31-O31-C3
9	I	3008	3PE	C2B-C2C-C2D-C2E
9	C	2010	3PE	O31-C31-C32-C33
9	I	3010	3PE	O31-C31-C32-C33
9	J	3011	3PE	O21-C2-C3-O31
9	A	2009	3PE	C23-C24-C25-C26
9	A	2009	3PE	C21-C22-C23-C24
9	D	2011	3PE	C3D-C3E-C3F-C3G
9	I	3010	3PE	C35-C36-C37-C38
8	A	1002	HEA	C3B-C11-C12-C13
8	G	1002	HEA	C3B-C11-C12-C13
9	J	3011	3PE	C3F-C3G-C3H-C3I
9	A	2009	3PE	O31-C31-C32-C33
8	A	1001	HEA	C14-C15-C16-C17
9	A	2012	3PE	O21-C21-C22-C23
9	G	3009	3PE	O31-C31-C32-C33
9	C	2010	3PE	O21-C21-C22-C23
9	A	2009	3PE	O21-C2-C3-O31
9	C	2008	3PE	C28-C29-C2A-C2B
9	G	3012	3PE	O21-C21-C22-C23
9	A	2009	3PE	C3A-C3B-C3C-C3D
9	I	3008	3PE	C3-C2-O21-C21
9	D	2011	3PE	C37-C38-C39-C3A
9	J	3011	3PE	C2A-C2B-C2C-C2D
9	C	2010	3PE	O32-C31-C32-C33
9	I	3010	3PE	C3F-C3G-C3H-C3I
9	J	3011	3PE	C2C-C2D-C2E-C2F
9	J	3011	3PE	O21-C21-C22-C23
8	A	1002	HEA	O11-C11-C12-C13
9	A	2009	3PE	O32-C31-C32-C33
9	I	3010	3PE	O32-C31-C32-C33
9	G	3009	3PE	O32-C31-C32-C33
9	G	3012	3PE	O22-C21-C22-C23
9	C	2010	3PE	O22-C21-C22-C23
9	I	3010	3PE	O21-C21-C22-C23
9	A	2012	3PE	O22-C21-C22-C23
9	A	2009	3PE	C22-C23-C24-C25
8	A	1001	HEA	O11-C11-C3B-C4B
8	G	1001	HEA	O11-C11-C3B-C4B

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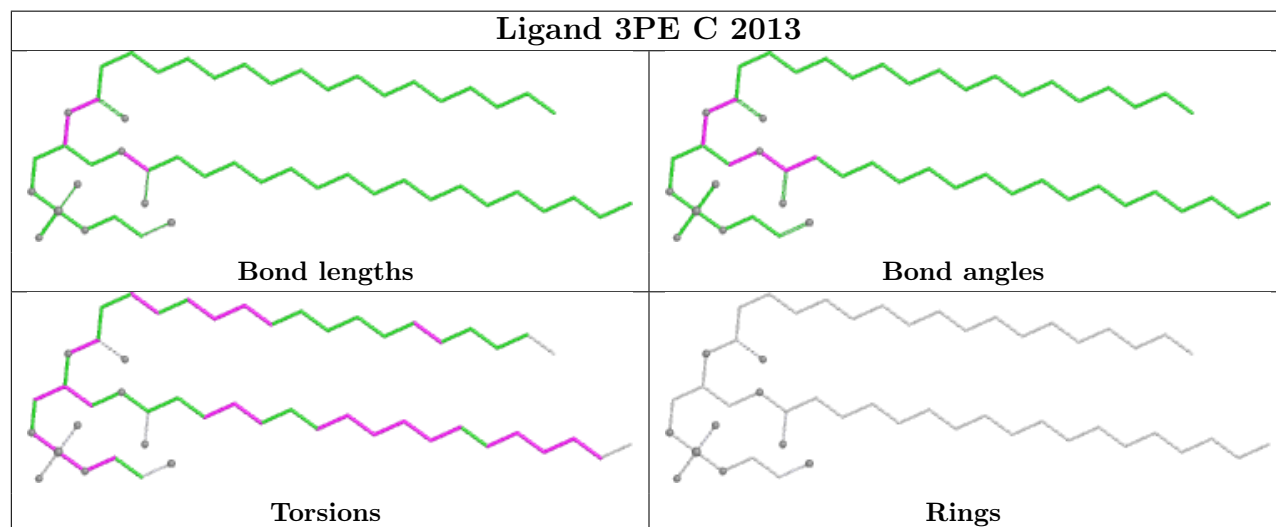
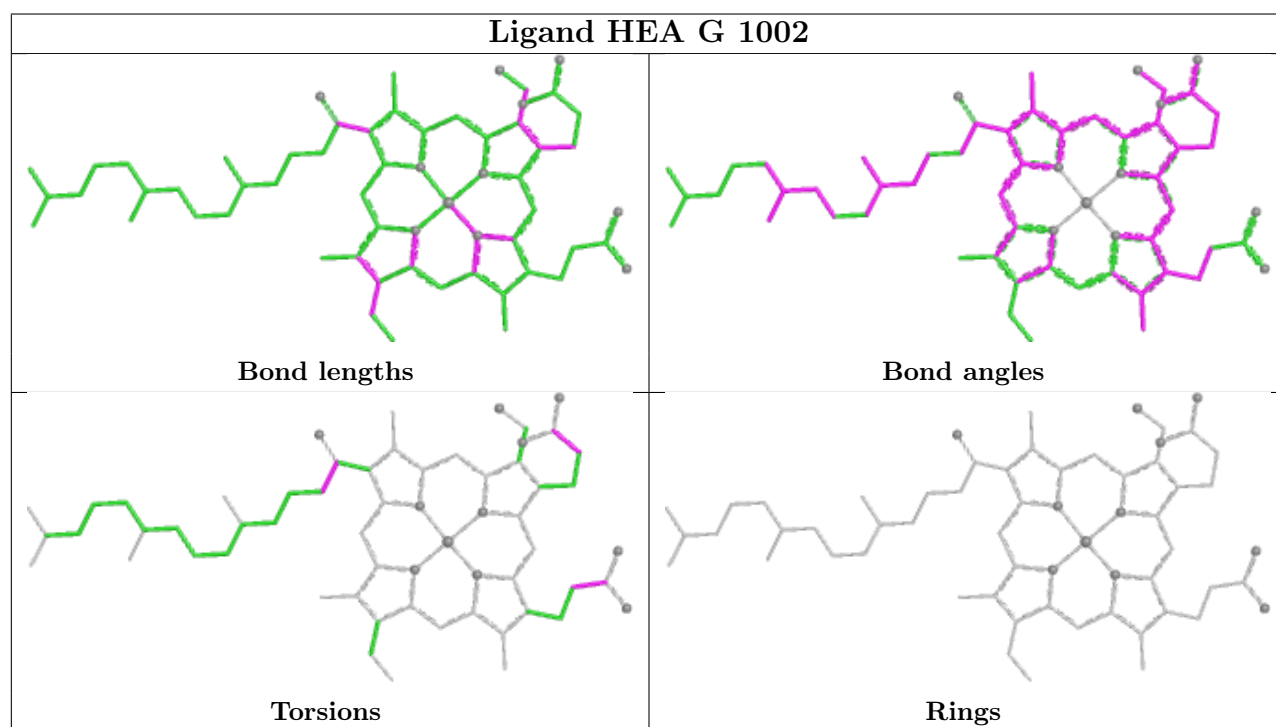
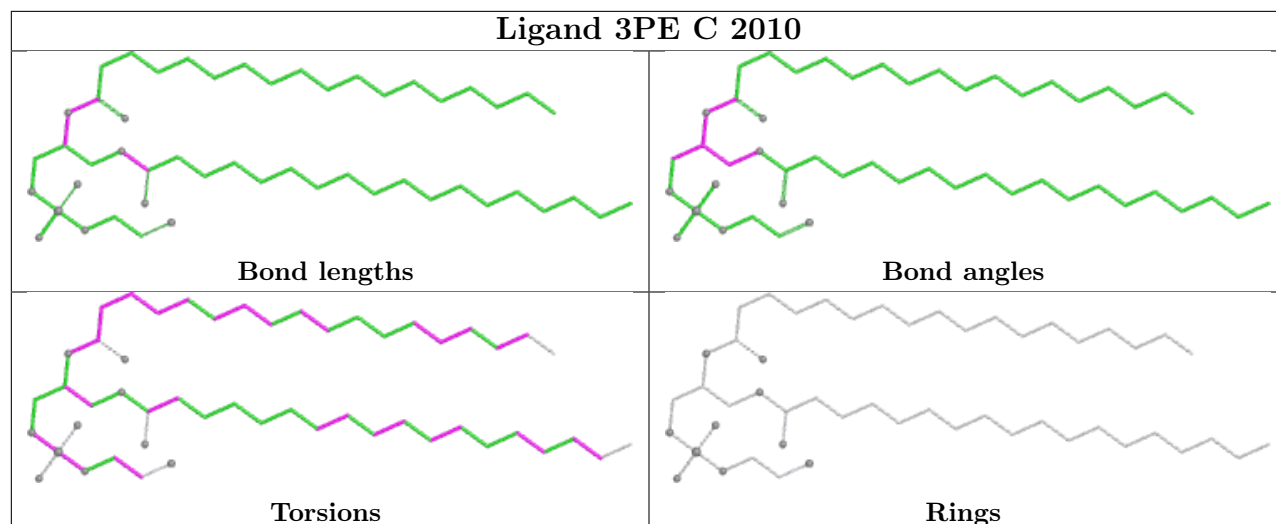
Mol	Chain	Res	Type	Atoms
9	D	2011	3PE	O21-C21-C22-C23
9	G	3009	3PE	C37-C38-C39-C3A
9	J	3011	3PE	C3A-C3B-C3C-C3D

There are no ring outliers.

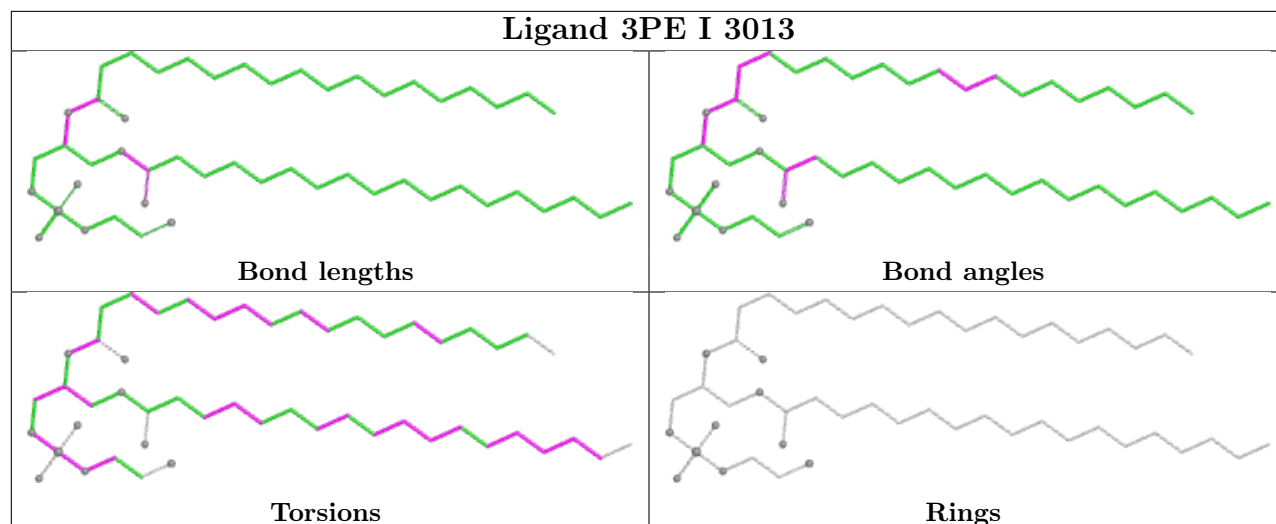
16 monomers are involved in 223 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2010	3PE	20	0
8	G	1002	HEA	7	0
9	C	2013	3PE	21	0
9	I	3013	3PE	22	0
8	G	1001	HEA	10	0
9	A	2009	3PE	20	0
9	A	2012	3PE	14	0
9	G	3012	3PE	12	0
8	A	1002	HEA	9	0
9	I	3008	3PE	9	0
9	C	2008	3PE	7	0
9	J	3011	3PE	16	0
9	G	3009	3PE	16	0
9	I	3010	3PE	21	0
9	D	2011	3PE	21	0
8	A	1001	HEA	16	0

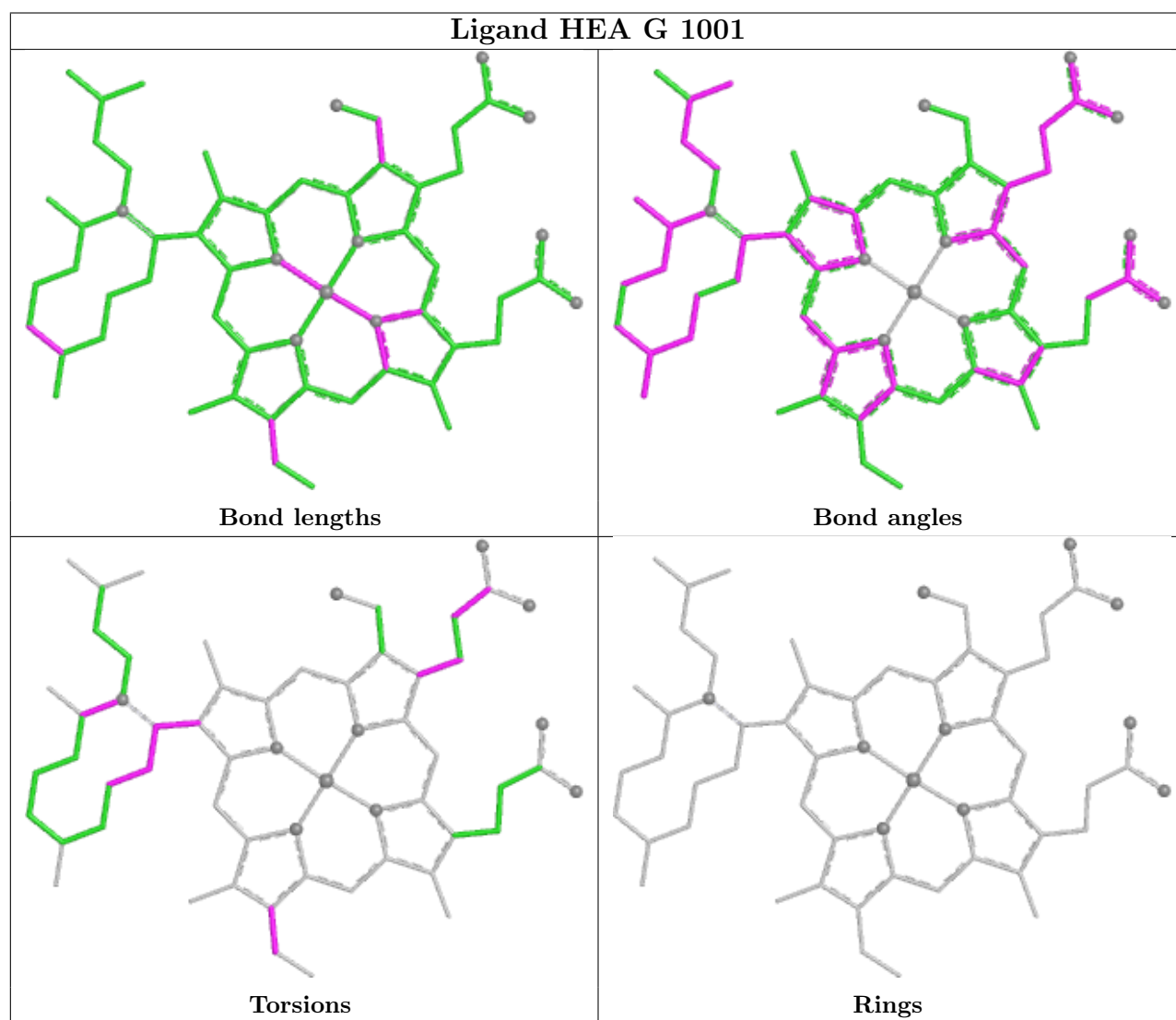
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

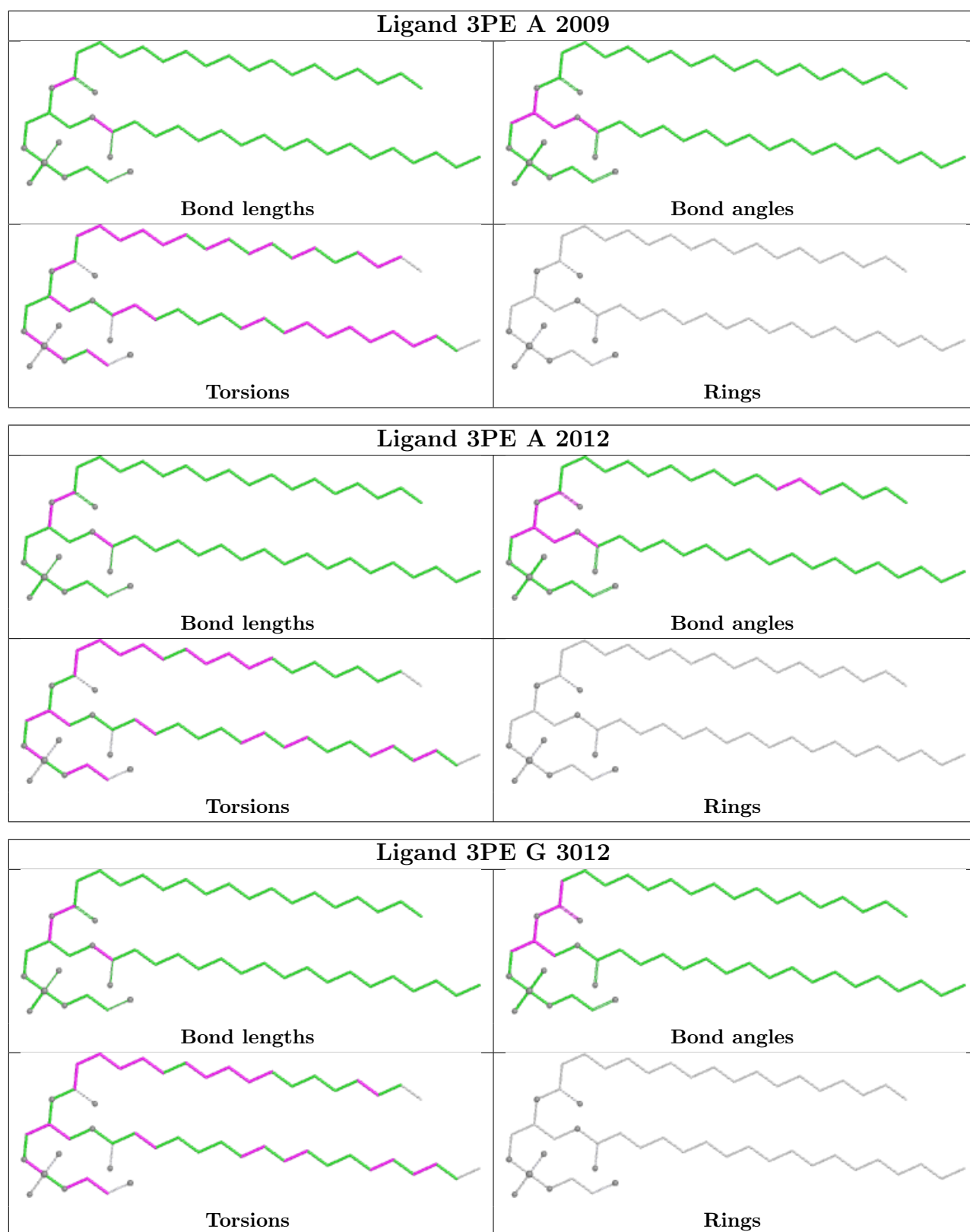


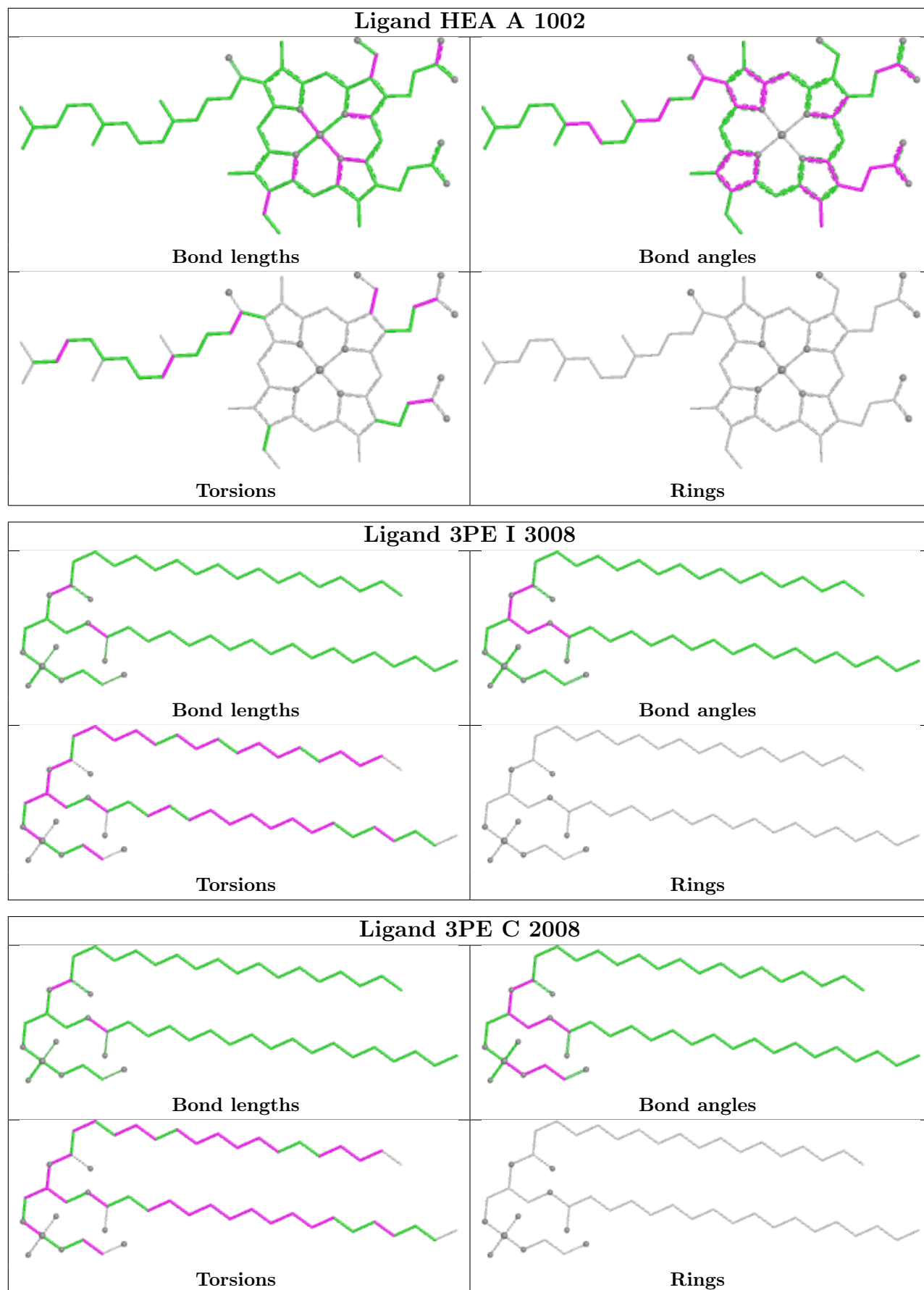
Ligand 3PE I 3013



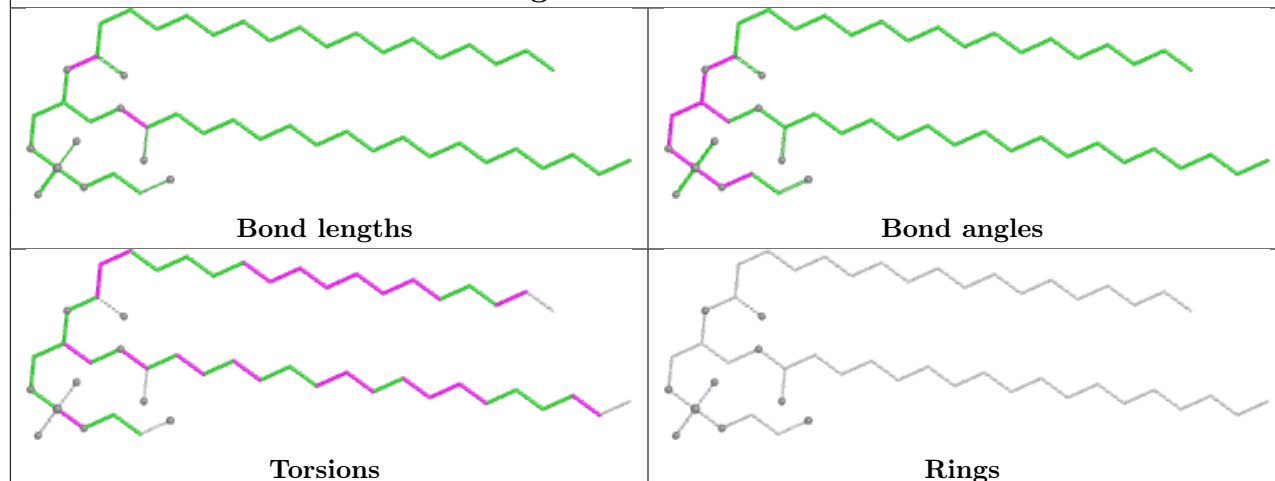
Ligand HEA G 1001



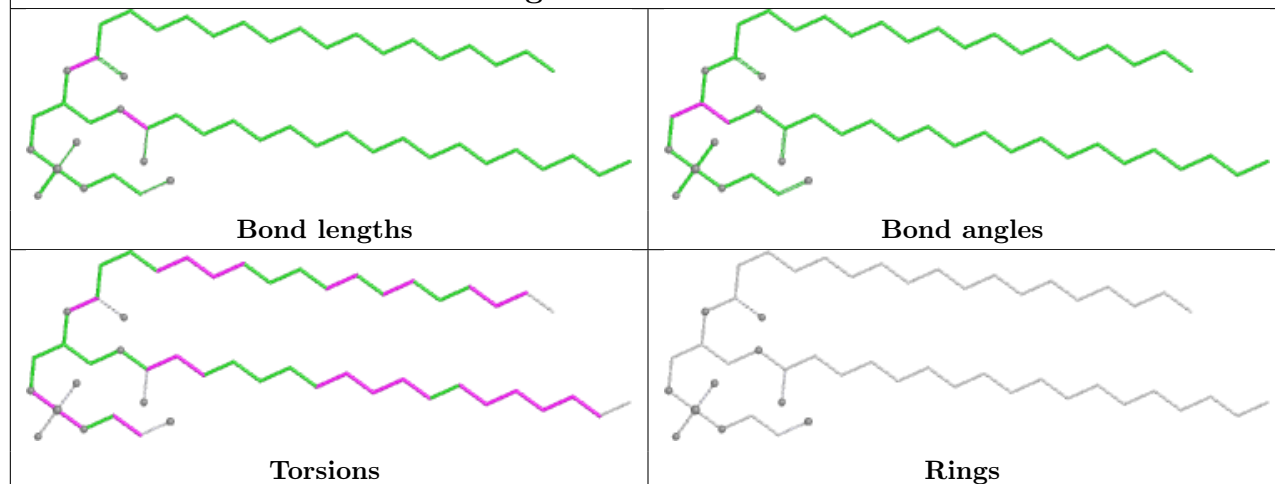




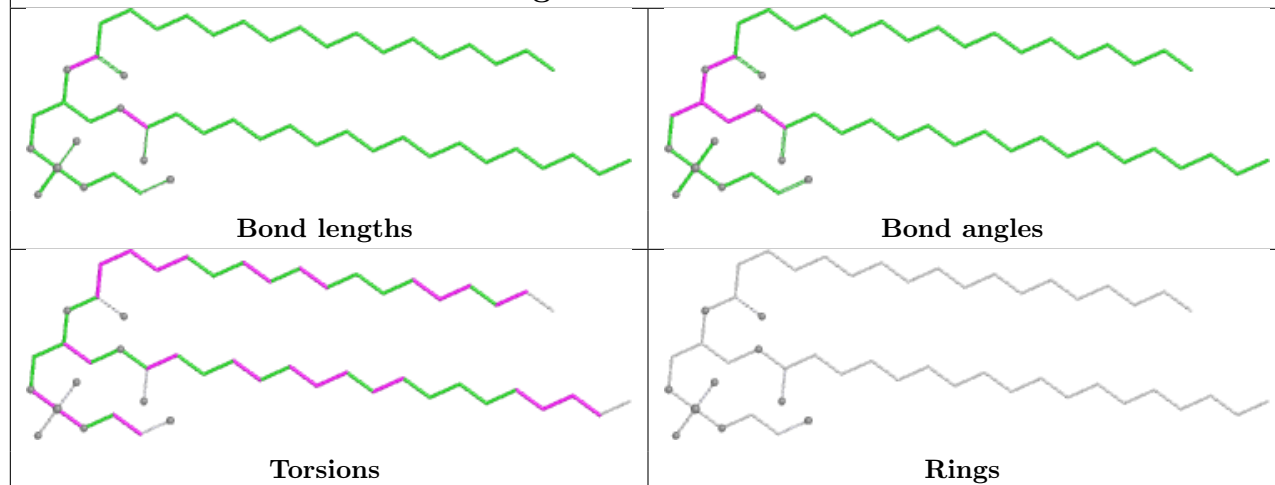
Ligand 3PE J 3011

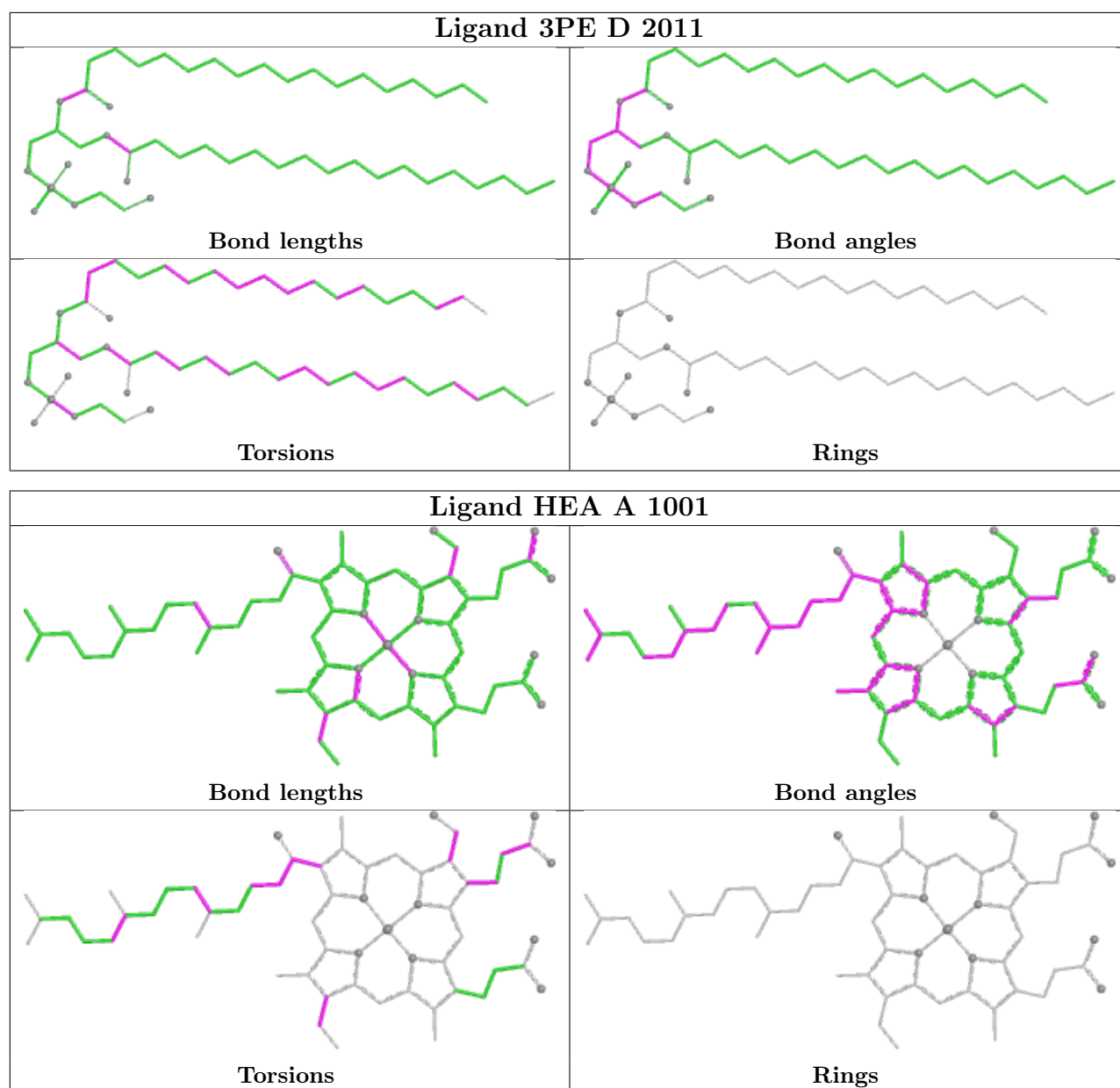


Ligand 3PE G 3009



Ligand 3PE I 3010





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.