



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:42 AM JST

PDB ID : 5IY5 / pdb_00005iy5
Title : Electron transfer complex of cytochrome c and cytochrome c oxidase at 2.0 angstrom resolution
Authors : Shimada, S.; Baba, J.; Aoe, S.; Shimada, A.; Yamashita, E.; Tsukihara, T.
Deposited on : 2016-03-24
Resolution : 2.00 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:

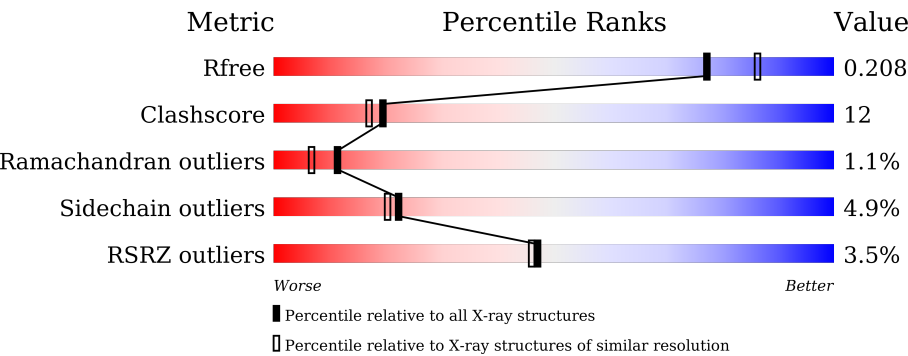
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	514	80%18%.
1	N	514	84%14%.
2	B	227	2% 71%23%5%
2	O	227	79%15%5%
3	C	259	2% 79%20%.
3	P	259	2% 85%14%.

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	
14	1	105	
14	2	105	

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
17	NA	P	302	-	-	-	X
26	CDL	G	101	-	-	X	-
26	CDL	T	101	-	-	X	-
27	UNL	C	310	-	-	X	-
27	UNL	N	601	-	-	X	-
27	UNL	P	308	-	-	X	-
27	UNL	P	310	-	-	X	-
28	PSC	V	101	-	-	X	-
31	HEC	1	201	X	-	-	-
31	HEC	2	201	X	-	-	-
9	SAC	I	1	-	X	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 34765 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 subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	11	0
			4084	2731	628	685	40			
1	N	514	Total	C	N	O	S	0	8	0
			4065	2717	627	683	38			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	2	0
			1836	1192	283	343	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	6	0
			2149	1437	343	355	14			
3	P	259	Total	C	N	O	S	0	5	0
			2143	1433	342	354	14			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	199	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			
14	2	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ACE	-	acetylation	UNP P00004
2	0	ACE	-	acetylation	UNP P00004

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Cu 1 1	0	0
15	N	1	Total Cu 1 1	0	0

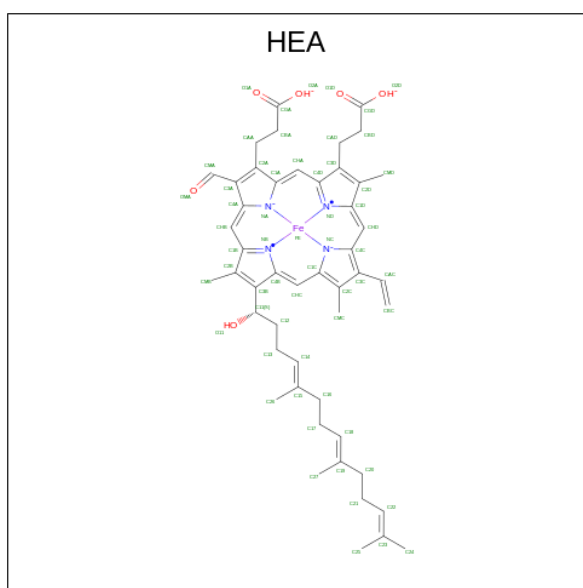
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Mg 1 1	0	0
16	N	1	Total Mg 1 1	0	0

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

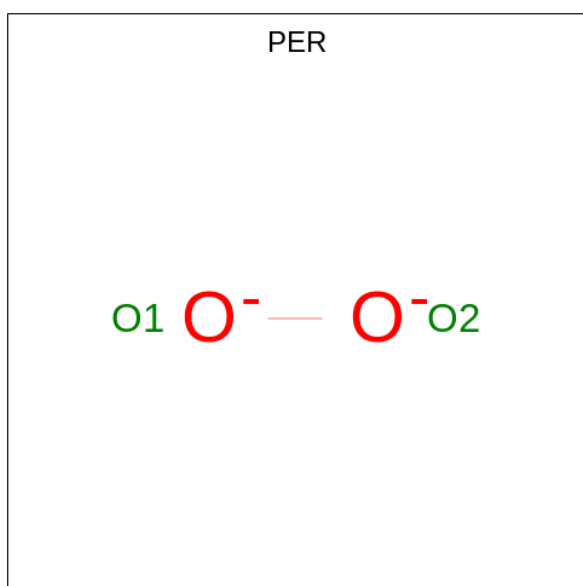
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



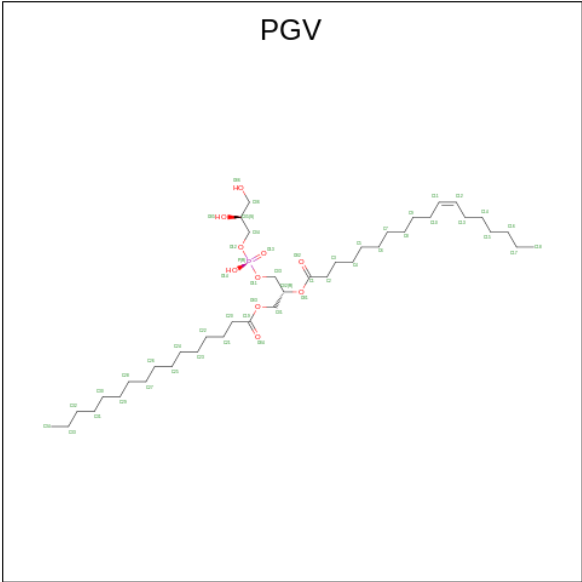
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



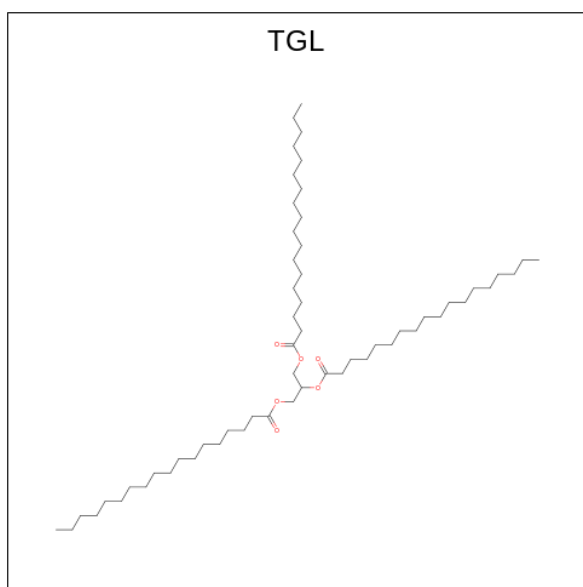
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		
19	N	1	Total	O	0	0
			2	2		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



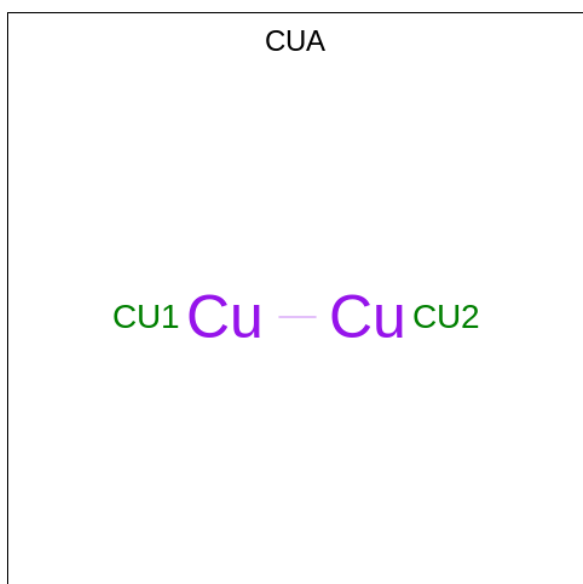
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



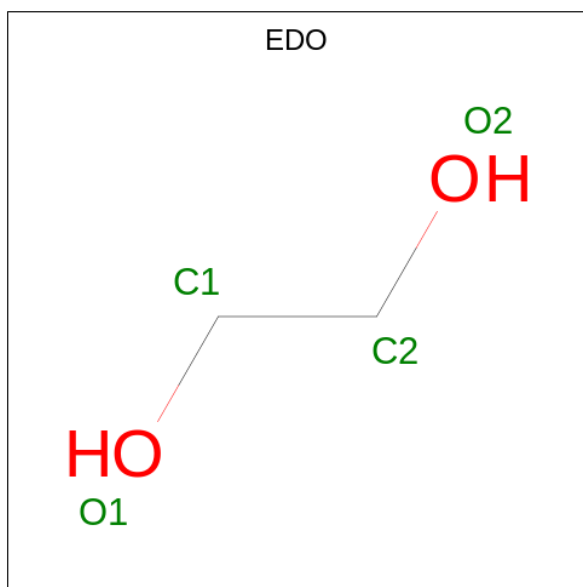
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



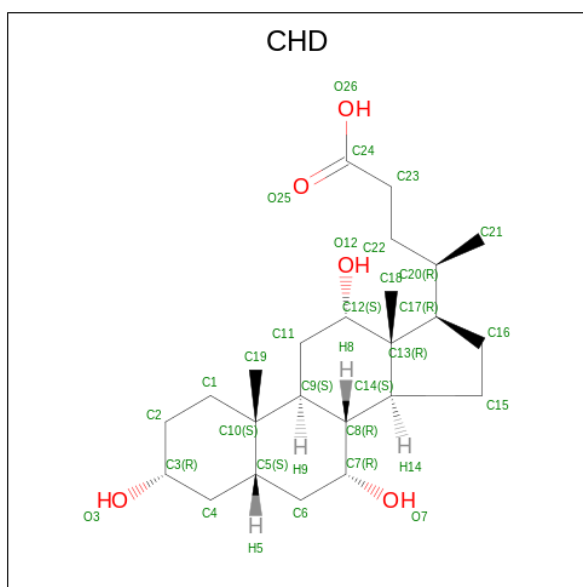
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



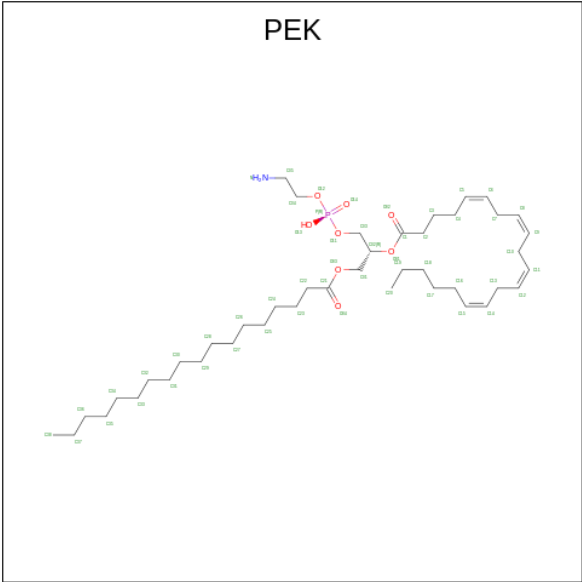
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	F	1	Total C O 4 2 2	0	0
23	G	1	Total C O 4 2 2	0	0
23	I	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	S	1	Total C O 4 2 2	0	0

- Molecule 24 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



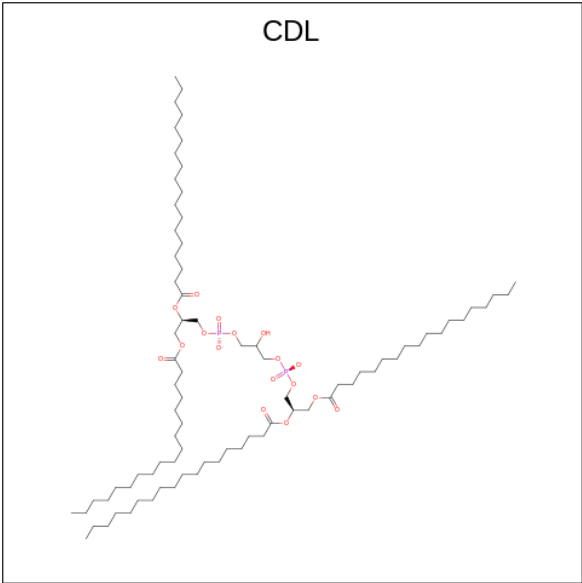
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	G	1	Total C O 29 24 5	0	0
24	J	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	T	1	Total C O 29 24 5	0	0
24	W	1	Total C O 29 24 5	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		

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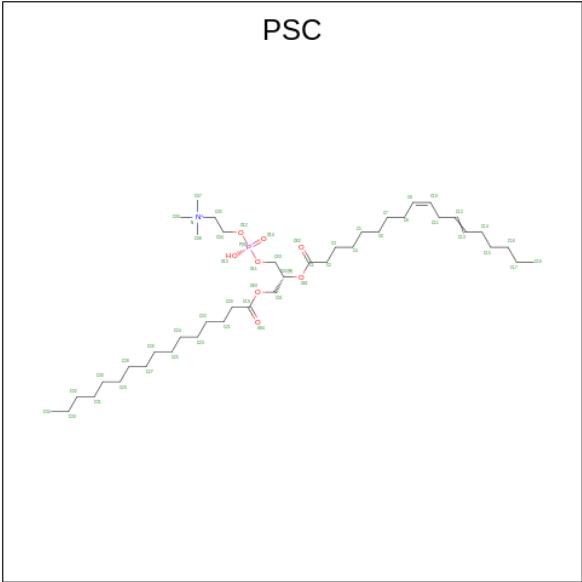
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	C	3	Total	C	0	0
			42	42		
27	J	1	Total	C	0	0
			10	10		
27	L	1	Total	C	0	0
			10	10		
27	N	4	Total	C	0	0
			63	63		
27	P	3	Total	C	0	0
			43	43		
27	T	1	Total	C	0	0
			18	18		
27	W	1	Total	C	0	0
			9	9		
27	Y	1	Total	C	0	0
			10	10		

- Molecule 28 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

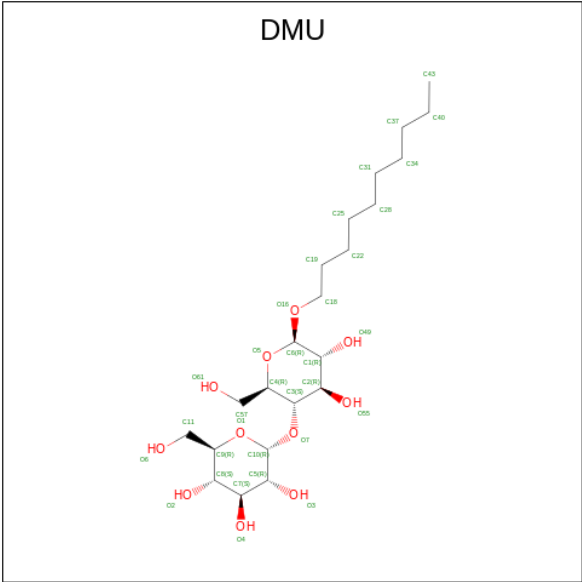


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	V	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

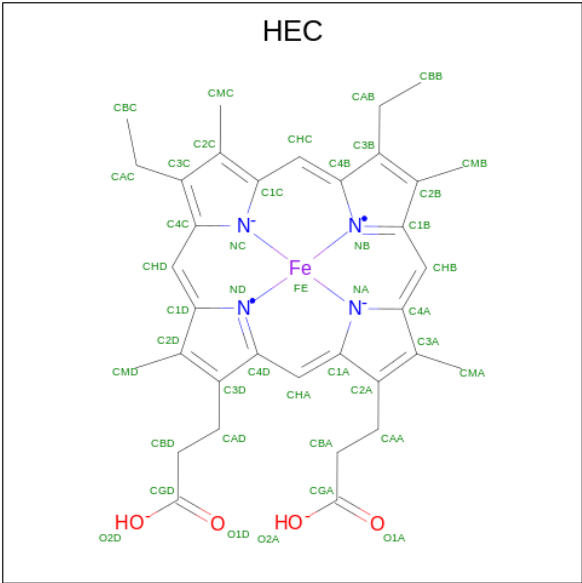
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	1	Total	Zn	0	0
			1	1		
29	S	1	Total	Zn	0	0
			1	1		

- Molecule 30 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	M	1	Total	C	O		0	0
			33	22	11			
30	Z	1	Total	C	O		0	0
			33	22	11			

- Molecule 31 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	2	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	252	Total O 252 252	0	0
32	B	193	Total O 193 193	0	0
32	C	137	Total O 137 137	0	0
32	D	122	Total O 122 122	0	0
32	E	119	Total O 119 119	0	0
32	F	97	Total O 97 97	0	0
32	G	60	Total O 60 60	0	0
32	H	76	Total O 76 76	0	0
32	I	49	Total O 49 49	0	0
32	J	30	Total O 30 30	0	0
32	K	29	Total O 29 29	0	0
32	L	33	Total O 33 33	0	0
32	M	26	Total O 26 26	0	0
32	N	229	Total O 229 229	0	0
32	O	141	Total O 141 141	0	0
32	P	110	Total O 110 110	0	0
32	Q	99	Total O 99 99	0	0
32	R	83	Total O 83 83	0	0
32	S	95	Total O 95 95	0	0
32	T	41	Total O 41 41	0	0
32	U	54	Total O 54 54	0	0

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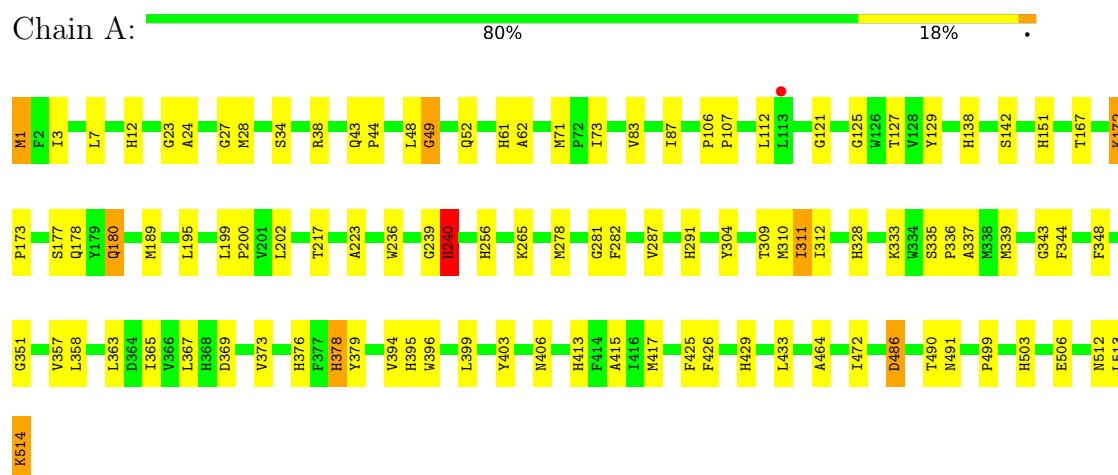
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	V	17	Total 17	O 17	0	0
32	W	10	Total 10	O 10	0	0
32	X	17	Total 17	O 17	0	0
32	Y	21	Total 21	O 21	0	0
32	Z	16	Total 16	O 16	0	0
32	1	53	Total 53	O 53	0	0
32	2	28	Total 28	O 28	0	0

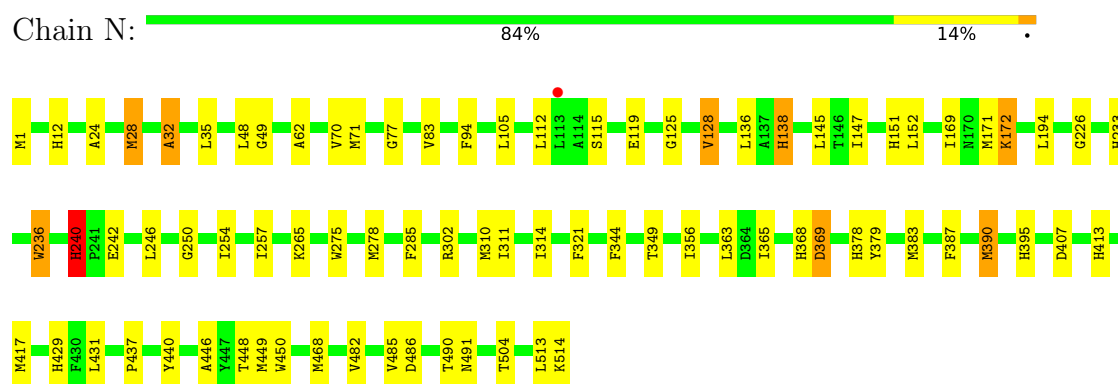
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

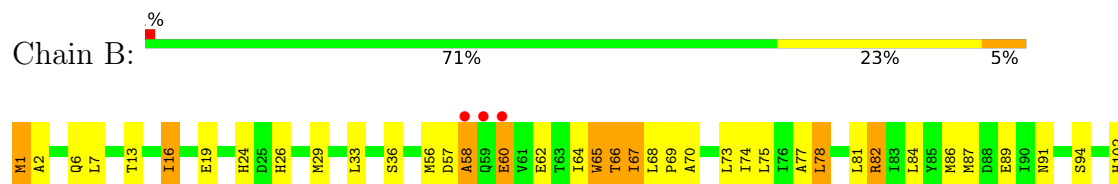
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

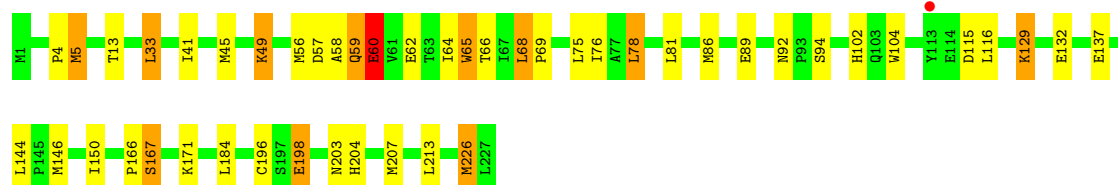
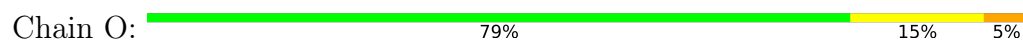


• Molecule 2: Cytochrome c oxidase subunit 2

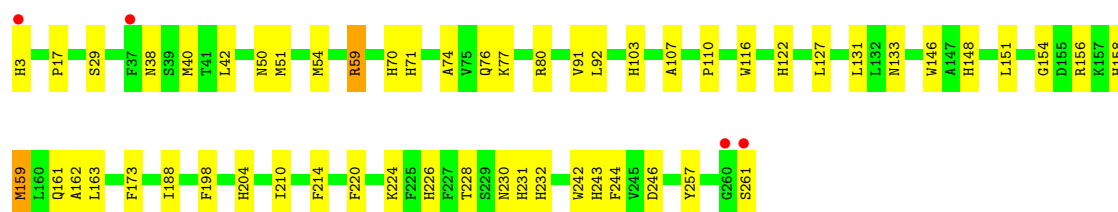
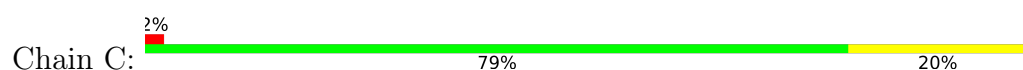




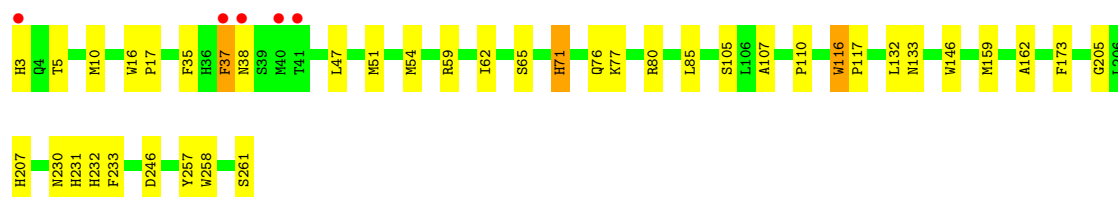
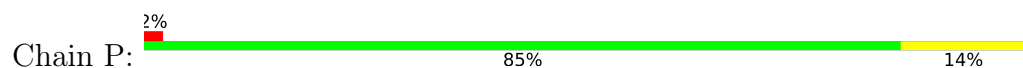
• Molecule 2: Cytochrome c oxidase subunit 2



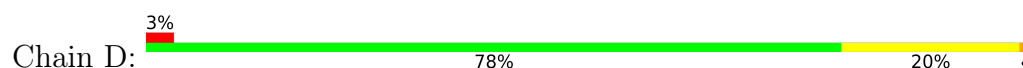
• Molecule 3: Cytochrome c oxidase subunit 3



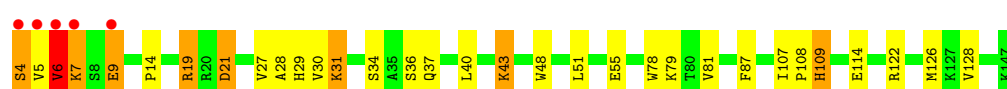
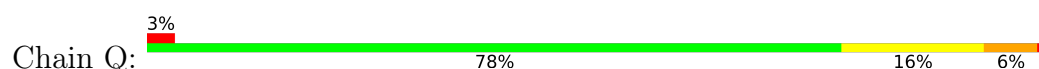
• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:  90% 9%



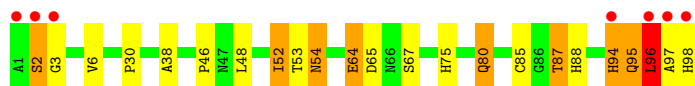
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:  88% 12%



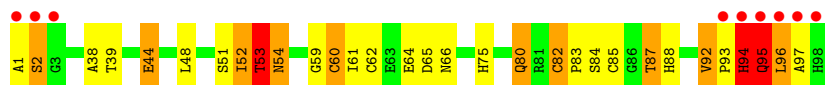
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:  7% 77% 14% 8%



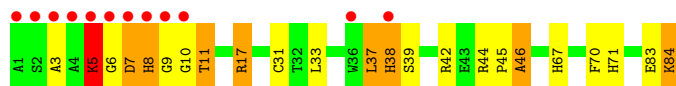
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:  9% 68% 18% 10%



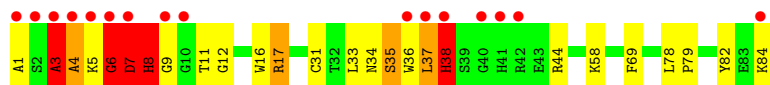
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:  14% 73% 17% 10%



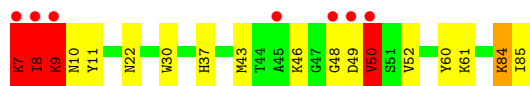
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:  19% 69% 20% 5% 6%

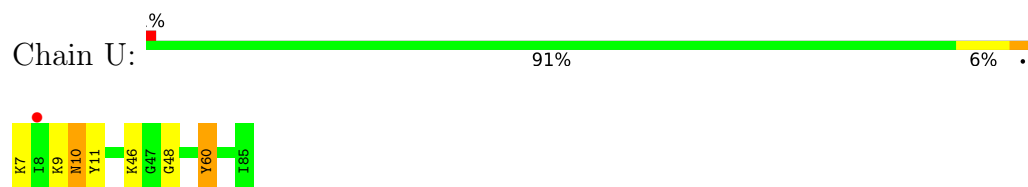


- Molecule 8: Cytochrome c oxidase subunit 6B1

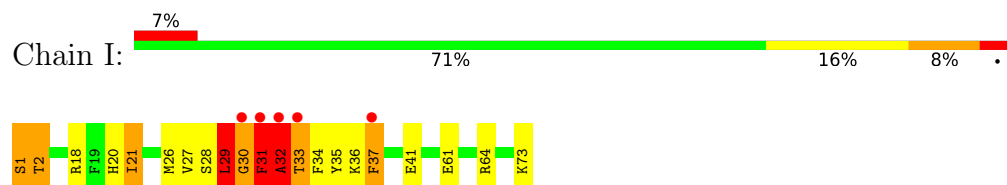
Chain H:  9% 77% 16% 5%



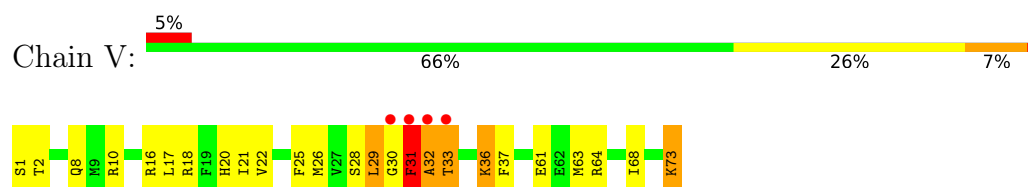
- Molecule 8: Cytochrome c oxidase subunit 6B1



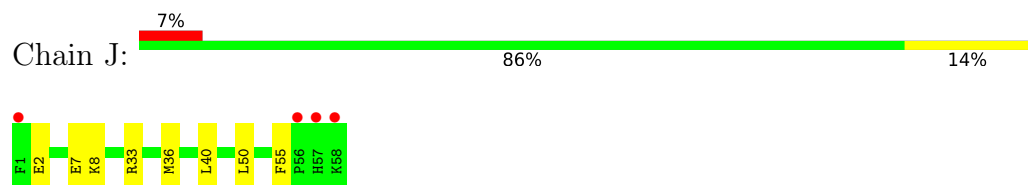
- Molecule 9: Cytochrome c oxidase subunit 6C



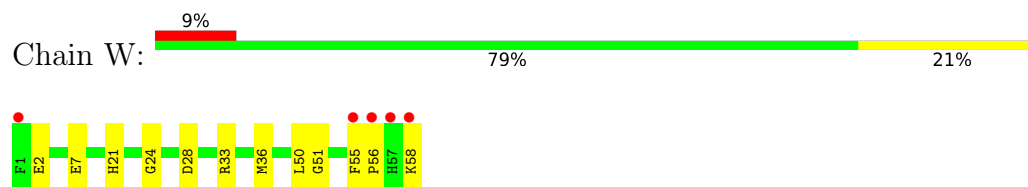
- Molecule 9: Cytochrome c oxidase subunit 6C



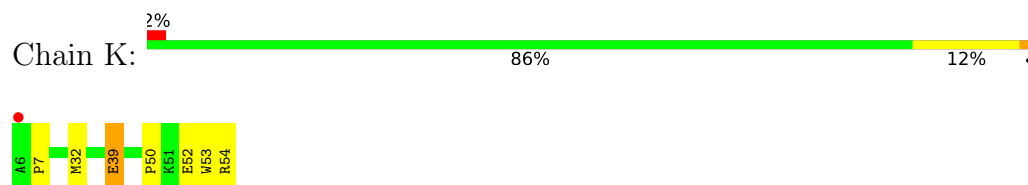
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



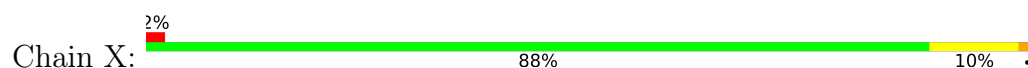
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

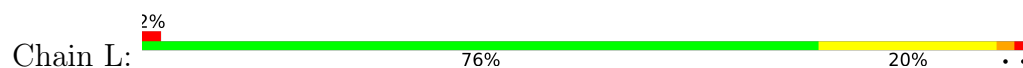


- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

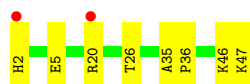
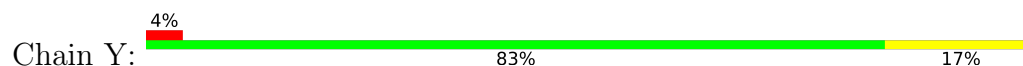




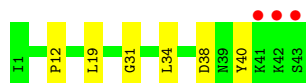
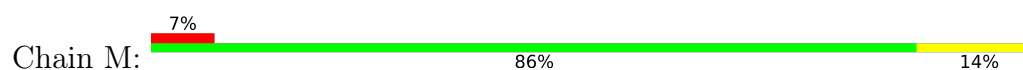
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



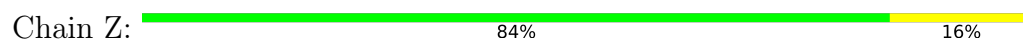
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



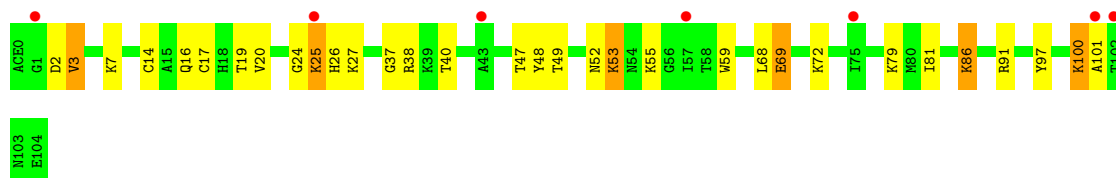
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



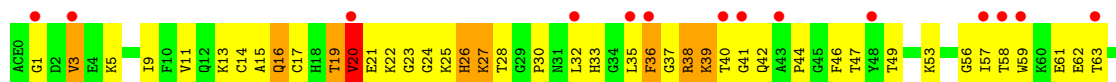
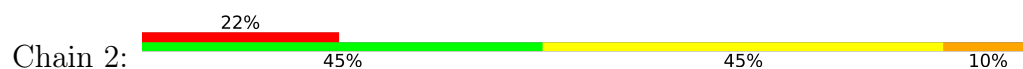
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

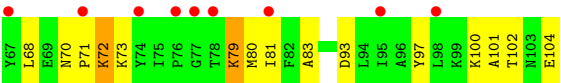


- Molecule 14: Cytochrome c



- Molecule 14: Cytochrome c





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.29Å 183.87Å 148.93Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.00) 99.4 (40.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.167 , 0.207 0.168 , 0.208	Depositor DCC
R_{free} test set	19991 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34765	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TGL, CUA, CU, EDO, HEC, ACE, PSC, CHD, HEA, MG, UNL, ZN, CDL, PEK, SAC, NA, TPO, PGV, DMU, FME, PER

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	1.66	45/4244 (1.1%)	1.27	13/5793 (0.2%)
1	N	1.50	29/4214 (0.7%)	1.22	18/5754 (0.3%)
2	B	1.55	13/1878 (0.7%)	1.28	6/2558 (0.2%)
2	O	1.29	6/1860 (0.3%)	1.16	4/2534 (0.2%)
3	C	1.53	20/2247 (0.9%)	1.13	8/3070 (0.3%)
3	P	1.42	9/2238 (0.4%)	1.08	3/3058 (0.1%)
4	D	1.48	6/1229 (0.5%)	1.29	7/1658 (0.4%)
4	Q	1.31	6/1240 (0.5%)	1.18	3/1672 (0.2%)
5	E	1.36	1/871 (0.1%)	1.12	0/1182
5	R	1.27	2/871 (0.2%)	1.15	0/1182
6	F	1.53	6/765 (0.8%)	1.32	5/1038 (0.5%)
6	S	1.55	8/765 (1.0%)	1.58	14/1038 (1.3%)
7	G	1.50	3/690 (0.4%)	1.20	1/937 (0.1%)
7	T	1.56	6/690 (0.9%)	1.29	6/937 (0.6%)
8	H	1.56	6/682 (0.9%)	1.45	6/921 (0.7%)
8	U	1.24	0/682	1.19	0/921
9	I	1.36	2/605 (0.3%)	1.37	4/802 (0.5%)
9	V	1.13	1/605 (0.2%)	1.18	1/802 (0.1%)
10	J	1.22	0/471	1.14	2/636 (0.3%)
10	W	1.14	1/471 (0.2%)	1.13	3/636 (0.5%)
11	K	1.35	0/398	1.17	1/546 (0.2%)
11	X	1.11	0/398	1.17	1/546 (0.2%)
12	L	1.45	2/393 (0.5%)	1.13	0/526
12	Y	1.29	0/393	1.20	0/526
13	M	1.25	0/345	1.23	1/470 (0.2%)
13	Z	1.25	2/345 (0.6%)	1.29	0/470
14	1	1.00	0/840	1.16	5/1120 (0.4%)
14	2	0.98	0/840	1.14	1/1120 (0.1%)
All	All	1.44	174/31270 (0.6%)	1.22	113/42453 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	S	0	2
8	H	0	2
9	V	0	2
All	All	0	8

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	83	VAL	CA-CB	12.01	1.60	1.54
1	A	378	HIS	ND1-CE1	10.96	1.43	1.32
8	H	8	ILE	N-CA	10.40	1.59	1.46
1	A	61	HIS	ND1-CE1	10.00	1.42	1.32
1	A	378	HIS	CG-CD2	9.73	1.46	1.35
1	A	61	HIS	CG-CD2	9.66	1.46	1.35
8	H	9	LYS	C-O	9.46	1.35	1.24
2	O	198	GLU	C-O	7.96	1.33	1.23
2	B	194	GLY	C-O	7.95	1.31	1.23
3	C	70	HIS	ND1-CE1	7.86	1.40	1.32
9	I	29	LEU	CA-C	-7.82	1.43	1.52
1	A	49	GLY	C-O	7.63	1.34	1.23
8	H	8	ILE	CA-C	7.62	1.62	1.52
3	P	232	HIS	ND1-CE1	7.55	1.40	1.32
7	T	7	ASP	N-CA	7.52	1.55	1.46
1	A	429	HIS	ND1-CE1	7.38	1.40	1.32
2	B	198	GLU	C-O	7.36	1.32	1.23
12	L	2	HIS	CG-CD2	7.21	1.43	1.35
1	N	12	HIS	CG-CD2	7.20	1.43	1.35
1	N	395	HIS	CG-CD2	7.10	1.43	1.35
3	C	148	HIS	CG-CD2	7.07	1.43	1.35
6	S	61	ILE	C-N	7.04	1.43	1.34
3	C	232	HIS	ND1-CE1	6.83	1.39	1.32
3	P	132	LEU	CA-C	6.82	1.61	1.52
8	H	8	ILE	C-O	6.77	1.32	1.24
1	A	351	GLY	CA-C	6.76	1.59	1.52
1	N	233	HIS	CG-CD2	6.75	1.43	1.35
6	F	94	HIS	CB-CG	6.74	1.59	1.50
2	O	204	HIS	CG-CD2	6.68	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	232	HIS	CG-CD2	6.67	1.43	1.35
1	N	49	GLY	C-O	6.65	1.30	1.23
6	S	60	CYS	C-O	6.65	1.31	1.24
1	A	12	HIS	CE1-NE2	6.61	1.39	1.32
3	C	214	PHE	CA-C	6.57	1.61	1.52
2	B	26	HIS	CE1-NE2	6.55	1.39	1.32
9	V	31	PHE	CA-C	6.55	1.61	1.52
6	F	2	SER	N-CA	6.51	1.54	1.46
1	A	291	HIS	CE1-NE2	6.47	1.39	1.32
2	B	24	HIS	ND1-CE1	6.42	1.39	1.32
1	N	378	HIS	CG-CD2	6.38	1.42	1.35
2	B	148	MET	SD-CE	6.37	1.95	1.79
1	N	378	HIS	CE1-NE2	6.34	1.38	1.32
7	G	67	HIS	ND1-CE1	6.32	1.38	1.32
6	F	2	SER	CA-C	6.29	1.61	1.52
3	C	92	LEU	N-CA	6.29	1.54	1.46
3	C	232	HIS	CG-CD2	6.23	1.42	1.35
2	B	123	ILE	N-CA	6.22	1.54	1.46
6	S	82	CYS	C-N	-6.21	1.27	1.34
13	Z	6	ALA	C-O	6.19	1.31	1.23
1	N	395	HIS	CE1-NE2	6.16	1.38	1.32
1	A	121	GLY	N-CA	6.13	1.51	1.45
1	A	256	HIS	CG-CD2	6.07	1.42	1.35
6	F	94	HIS	CG-CD2	6.06	1.42	1.35
3	P	3	HIS	CG-CD2	6.06	1.42	1.35
6	F	88	HIS	CG-CD2	6.05	1.42	1.35
1	A	491	ASN	CA-CB	6.05	1.59	1.53
1	N	390	MET	N-CA	6.03	1.53	1.46
8	H	7	LYS	C-N	6.02	1.41	1.33
3	C	226	HIS	CG-CD2	5.99	1.42	1.35
1	N	147	ILE	CA-CB	5.96	1.61	1.54
9	I	32	ALA	CA-C	-5.96	1.44	1.52
4	Q	29	HIS	CG-CD2	5.95	1.42	1.35
1	A	12	HIS	CG-CD2	5.95	1.42	1.35
7	T	3	ALA	CA-C	5.94	1.60	1.52
3	C	59	ARG	N-CA	5.94	1.53	1.46
3	P	116	TRP	CD2-CE2	5.91	1.51	1.41
7	T	8	HIS	N-CA	5.91	1.53	1.46
4	Q	30	VAL	CA-CB	5.88	1.60	1.53
3	C	103	HIS	N-CA	5.87	1.53	1.46
4	Q	29	HIS	CE1-NE2	5.87	1.38	1.32
1	A	413	HIS	CG-ND1	-5.86	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	32	ALA	N-CA	5.86	1.53	1.46
4	D	114	GLU	CA-C	5.84	1.60	1.52
6	S	62	CYS	N-CA	5.83	1.53	1.46
7	T	17	ARG	CD-NE	-5.79	1.38	1.46
3	C	243	HIS	CE1-NE2	5.74	1.38	1.32
1	N	151	HIS	ND1-CE1	5.73	1.38	1.32
1	A	376	HIS	ND1-CE1	5.72	1.38	1.32
5	R	63	SER	N-CA	5.70	1.53	1.46
1	A	378	HIS	CE1-NE2	5.70	1.38	1.32
1	A	287	VAL	N-CA	5.69	1.51	1.46
1	A	200	PRO	CA-CB	5.69	1.61	1.53
2	O	102	HIS	ND1-CE1	5.69	1.38	1.32
3	P	116	TRP	CA-C	-5.68	1.46	1.53
1	A	376	HIS	CE1-NE2	5.66	1.38	1.32
5	R	51	ALA	N-CA	5.64	1.53	1.46
1	N	429	HIS	CG-CD2	5.63	1.42	1.35
1	A	503	HIS	CE1-NE2	5.62	1.38	1.32
1	N	491	ASN	CA-CB	5.60	1.58	1.53
2	B	155	SER	C-O	5.57	1.29	1.23
1	N	395	HIS	ND1-CE1	5.57	1.38	1.32
1	A	395	HIS	CG-CD2	5.55	1.42	1.35
3	C	70	HIS	CG-CD2	5.54	1.42	1.35
2	O	102	HIS	CG-CD2	5.53	1.42	1.35
1	N	482	VAL	CA-CB	5.51	1.59	1.54
1	N	236	TRP	CD2-CE2	5.50	1.50	1.41
3	C	242	TRP	NE1-CE2	-5.49	1.31	1.37
7	G	71	HIS	CG-CD2	5.49	1.41	1.35
1	A	357	VAL	CA-CB	5.48	1.60	1.54
3	C	204	HIS	CE1-NE2	5.47	1.38	1.32
1	N	128	VAL	N-CA	5.47	1.53	1.46
5	E	81	ILE	N-CA	5.46	1.52	1.46
1	N	77	GLY	N-CA	5.46	1.53	1.45
1	A	358	LEU	N-CA	5.44	1.53	1.46
1	A	512	ASN	N-CA	5.44	1.52	1.45
3	C	71	HIS	ND1-CE1	5.42	1.38	1.32
2	B	24	HIS	CG-CD2	5.42	1.41	1.35
1	A	151	HIS	ND1-CE1	5.42	1.38	1.32
1	A	195	LEU	CA-C	-5.41	1.46	1.52
1	N	275	TRP	CD2-CE2	5.40	1.50	1.41
3	P	71	HIS	CG-CD2	5.40	1.41	1.35
3	C	231	HIS	ND1-CE1	5.40	1.38	1.32
1	A	223	ALA	CA-C	5.40	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	HIS	CG-CD2	5.38	1.41	1.35
1	N	446	ALA	CA-C	5.37	1.60	1.52
12	L	26	THR	CA-CB	5.35	1.61	1.53
4	D	115	TRP	CD2-CE2	5.35	1.50	1.41
4	D	119	GLN	N-CA	5.34	1.52	1.46
4	Q	36	SER	CA-C	5.34	1.59	1.52
3	P	231	HIS	CG-CD2	5.33	1.41	1.35
1	N	233	HIS	CE1-NE2	5.32	1.37	1.32
6	S	60	CYS	C-N	5.32	1.39	1.33
8	H	9	LYS	CG-CD	5.31	1.68	1.52
2	B	212	GLU	N-CA	-5.30	1.40	1.46
13	Z	5	PRO	CA-CB	5.30	1.61	1.53
4	D	90	GLY	N-CA	5.30	1.52	1.45
1	N	151	HIS	CG-CD2	5.29	1.41	1.35
1	A	503	HIS	CG-CD2	5.29	1.41	1.35
1	N	226	GLY	C-O	5.28	1.28	1.23
3	C	116	TRP	CD2-CE2	5.27	1.50	1.41
7	G	67	HIS	CG-CD2	5.26	1.41	1.35
4	Q	40	LEU	CA-C	5.26	1.59	1.52
1	A	396	TRP	CD2-CE2	5.24	1.50	1.41
3	C	162	ALA	CA-C	5.23	1.59	1.52
1	A	83	VAL	C-O	-5.23	1.20	1.24
1	A	379	TYR	N-CA	5.23	1.52	1.46
3	C	243	HIS	CG-CD2	5.23	1.41	1.35
2	B	65	TRP	CD2-CE2	5.22	1.50	1.41
6	F	67	SER	CA-C	5.21	1.59	1.52
1	A	403	TYR	N-CA	5.21	1.52	1.45
6	S	88	HIS	CG-CD2	5.20	1.41	1.35
1	A	256	HIS	CE1-NE2	5.20	1.37	1.32
6	S	2	SER	N-CA	5.20	1.51	1.46
1	A	328	HIS	CE1-NE2	5.19	1.37	1.32
2	B	167	SER	CB-OG	-5.18	1.31	1.42
7	T	3	ALA	N-CA	5.18	1.52	1.46
1	N	138	HIS	ND1-CE1	5.18	1.37	1.32
4	D	65	LYS	CA-C	5.17	1.59	1.52
2	O	102	HIS	CE1-NE2	5.15	1.37	1.32
4	D	107	ILE	CA-C	5.13	1.58	1.52
1	N	171	MET	N-CA	5.13	1.52	1.46
1	A	291	HIS	ND1-CE1	5.11	1.37	1.32
1	A	379	TYR	CA-C	5.11	1.59	1.52
2	O	204	HIS	CE1-NE2	5.11	1.37	1.32
1	A	27	GLY	CA-C	5.10	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	94	PHE	CA-C	5.10	1.58	1.52
3	C	148	HIS	ND1-CE1	5.09	1.37	1.32
1	A	167	THR	N-CA	5.09	1.52	1.46
4	Q	109	HIS	CG-CD2	5.09	1.41	1.35
6	S	61	ILE	CA-CB	5.09	1.59	1.53
10	W	21	HIS	CG-CD2	5.07	1.41	1.35
1	A	311	ILE	N-CA	-5.07	1.40	1.46
3	P	207	HIS	N-CA	5.05	1.52	1.46
1	A	426	PHE	C-O	-5.04	1.19	1.24
1	A	142	SER	N-CA	5.04	1.52	1.46
1	A	506	GLU	C-O	-5.03	1.18	1.24
1	A	486	ASP	CG-OD1	5.03	1.34	1.25
2	B	220	GLU	N-CA	5.03	1.52	1.46
2	B	161	HIS	CE1-NE2	5.02	1.37	1.32
1	A	12	HIS	CB-CG	5.01	1.57	1.50
7	T	7	ASP	CA-C	5.01	1.59	1.52
1	N	429	HIS	ND1-CE1	5.01	1.37	1.32
3	C	158	HIS	CG-ND1	-5.00	1.32	1.38
1	N	349	THR	C-O	5.00	1.29	1.24

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	82	CYS	CA-C-N	-11.55	108.50	119.82
6	S	82	CYS	C-N-CA	-11.55	108.50	119.82
8	H	9	LYS	CA-CB-CG	-11.23	91.63	114.10
9	I	29	LEU	N-CA-C	-10.64	99.65	111.14
8	H	9	LYS	O-C-N	8.69	134.15	122.59
6	S	92	VAL	CA-C-N	-8.39	110.94	119.92
6	S	92	VAL	C-N-CA	-8.39	110.94	119.92
1	A	71	MET	CG-SD-CE	-8.38	82.46	100.90
6	F	3	GLY	N-CA-C	-8.18	99.27	110.80
14	1	3	VAL	N-CA-C	8.12	118.89	110.36
6	S	60	CYS	O-C-N	8.02	132.73	123.27
1	A	172	LYS	CA-C-N	-7.92	113.88	119.66
1	A	172	LYS	C-N-CA	-7.92	113.88	119.66
3	C	91	VAL	N-CA-C	-7.79	103.21	110.53
6	S	60	CYS	CA-C-N	-7.71	112.84	122.48
6	S	60	CYS	C-N-CA	-7.71	112.84	122.48
2	B	82	ARG	NE-CZ-NH2	7.63	126.07	119.20
8	H	8	ILE	CG1-CB-CG2	7.36	132.77	110.70
3	P	37	PHE	N-CA-C	-7.12	102.18	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	8	ILE	CA-C-O	7.10	129.65	120.78
9	I	31	PHE	N-CA-C	-7.00	95.88	110.80
1	N	105	LEU	CA-C-N	-6.94	113.23	120.38
1	N	105	LEU	C-N-CA	-6.94	113.23	120.38
1	N	240	HIS	N-CA-CB	6.76	118.40	110.42
1	A	373	VAL	N-CA-C	-6.72	103.67	111.00
8	H	9	LYS	CB-CG-CD	-6.69	95.91	111.30
2	B	167	SER	CB-CA-C	-6.67	99.34	110.68
6	S	82	CYS	O-C-N	6.52	127.25	121.18
6	S	59	GLY	CA-C-O	-6.52	114.62	120.75
1	N	169	ILE	CB-CA-C	-6.46	103.59	112.24
1	N	172	LYS	CA-C-N	-6.42	113.77	120.38
1	N	172	LYS	C-N-CA	-6.42	113.77	120.38
4	D	105	GLY	CA-C-N	6.41	127.85	119.84
4	D	105	GLY	C-N-CA	6.41	127.85	119.84
7	T	17	ARG	CB-CG-CD	-6.39	96.61	111.30
6	S	53	THR	CB-CA-C	-6.37	97.75	110.42
4	D	102	TYR	CA-C-N	-6.34	116.68	123.08
4	D	102	TYR	C-N-CA	-6.34	116.68	123.08
1	A	240	HIS	CA-CB-CG	-6.31	107.49	113.80
7	T	7	ASP	N-CA-C	6.30	124.22	110.80
9	V	32	ALA	N-CA-C	-6.29	105.66	113.15
14	2	20	VAL	N-CA-C	6.29	117.22	111.81
1	A	49	GLY	N-CA-C	-6.24	98.39	113.18
7	G	17	ARG	CB-CG-CD	-6.18	97.09	111.30
10	W	55	PHE	CA-C-N	6.17	127.56	119.84
10	W	55	PHE	C-N-CA	6.17	127.56	119.84
8	H	8	ILE	N-CA-CB	-6.08	101.19	111.23
11	K	39	GLU	CB-CA-C	-6.08	100.62	110.77
2	B	78	LEU	CA-C-N	-6.04	112.78	119.19
2	B	78	LEU	C-N-CA	-6.04	112.78	119.19
6	F	2	SER	N-CA-C	6.02	123.63	110.80
3	C	163	LEU	N-CA-C	-5.95	104.87	111.36
1	N	125	GLY	N-CA-C	-5.93	105.21	112.68
14	1	101	ALA	N-CA-C	5.86	118.45	111.71
2	B	67	ILE	N-CA-C	5.86	116.64	110.72
6	S	2	SER	N-CA-C	5.85	115.22	108.49
1	N	28	MET	N-CA-C	-5.83	104.52	111.69
3	C	198	PHE	N-CA-C	5.77	117.65	111.36
10	W	51	GLY	N-CA-C	-5.75	105.83	112.73
7	T	12	GLY	N-CA-C	5.74	129.95	113.30
4	D	19	ARG	NE-CZ-NH2	5.73	124.36	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	CA-CB-CG	-5.73	108.07	113.80
4	D	71	MET	N-CA-C	-5.71	105.81	112.89
3	P	35	PHE	N-CA-C	5.64	117.43	111.28
1	N	119	GLU	CB-CA-C	-5.63	110.06	116.54
1	A	199	LEU	CA-C-N	-5.61	113.11	119.28
1	A	199	LEU	C-N-CA	-5.61	113.11	119.28
1	N	49	GLY	N-CA-C	-5.58	102.49	111.59
10	J	55	PHE	CA-C-N	-5.55	113.52	120.51
10	J	55	PHE	C-N-CA	-5.55	113.52	120.51
3	C	228	THR	N-CA-C	-5.53	102.27	110.46
1	A	348	PHE	N-CA-C	-5.52	105.27	111.28
3	P	85	LEU	N-CA-C	-5.51	105.36	111.36
1	N	448	THR	N-CA-C	5.46	116.91	111.07
9	I	29	LEU	CB-CA-C	-5.45	102.28	110.90
1	A	189	MET	CA-CB-CG	-5.43	103.23	114.10
3	C	107	ALA	CA-C-N	-5.43	114.17	119.76
3	C	107	ALA	C-N-CA	-5.43	114.17	119.76
1	A	125	GLY	N-CA-C	-5.40	105.63	112.65
1	N	70	VAL	N-CA-C	5.38	115.59	110.42
9	I	21	ILE	CG1-CB-CG2	-5.37	94.60	110.70
7	T	58	LYS	CA-C-N	-5.37	114.39	119.76
7	T	58	LYS	C-N-CA	-5.37	114.39	119.76
4	Q	14	PRO	CA-C-N	-5.35	113.83	122.82
4	Q	14	PRO	C-N-CA	-5.35	113.83	122.82
2	B	58	ALA	N-CA-C	5.30	119.39	113.02
1	N	71	MET	CG-SD-CE	-5.30	89.23	100.90
6	F	64	GLU	CA-C-N	-5.30	115.70	125.02
6	F	64	GLU	C-N-CA	-5.30	115.70	125.02
1	N	314	ILE	CA-C-N	-5.25	113.63	119.19
1	N	314	ILE	C-N-CA	-5.25	113.63	119.19
4	D	20	ARG	NE-CZ-NH2	-5.24	114.49	119.20
2	O	65	TRP	CB-CA-C	5.22	119.67	110.37
13	M	31	GLY	N-CA-C	-5.21	106.48	112.73
2	O	64	ILE	CA-C-N	-5.21	113.60	122.56
2	O	64	ILE	C-N-CA	-5.21	113.60	122.56
1	N	407	ASP	N-CA-C	5.17	116.92	111.28
14	1	2	ASP	CA-C-N	5.14	127.23	120.60
14	1	2	ASP	C-N-CA	5.14	127.23	120.60
3	C	74	ALA	N-CA-C	-5.12	105.78	111.36
6	S	39	THR	N-CA-C	-5.10	101.96	109.86
4	Q	9	GLU	CA-C-O	5.09	127.80	120.51
3	C	244	PHE	N-CA-C	-5.08	105.64	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	38	ILE	N-CA-C	-5.07	102.96	109.30
6	S	66	ASN	N-CA-C	-5.07	102.89	110.23
1	A	202	LEU	N-CA-C	-5.05	105.77	111.28
1	N	257	ILE	N-CA-C	5.05	115.27	110.42
2	O	5	MET	N-CA-C	5.04	118.70	112.24
6	F	96	LEU	N-CA-C	5.04	121.53	110.80
6	S	95	GLN	N-CA-C	-5.03	100.10	110.80
7	T	6	GLY	N-CA-C	5.01	125.06	113.18
1	A	52	GLN	N-CA-C	-5.01	105.47	111.03
14	1	3	VAL	CB-CA-C	-5.00	105.47	111.88

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	8	ILE	Peptide
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
6	S	94	HIS	Peptide
6	S	95	GLN	Peptide
9	V	32	ALA	Peptide
9	V	33	THR	Peptide

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	4084	0	4069	69	0
1	N	4065	0	4046	50	0
2	B	1836	0	1843	47	0
2	O	1824	0	1833	43	0
3	C	2149	0	2075	26	0
3	P	2143	0	2067	32	0
4	D	1195	0	1183	19	0
4	Q	1203	0	1196	30	0
5	E	852	0	845	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	852	0	845	6	0
6	F	748	0	728	25	0
6	S	748	0	729	26	0
7	G	675	0	643	22	0
7	T	675	0	644	29	0
8	H	662	0	623	37	0
8	U	662	0	623	8	0
9	I	601	0	613	40	0
9	V	601	0	613	21	0
10	J	460	0	459	7	0
10	W	460	0	459	13	0
11	K	384	0	366	5	0
11	X	384	0	366	8	0
12	L	380	0	380	13	0
12	Y	380	0	380	6	0
13	M	335	0	352	1	0
13	Z	335	0	352	4	0
14	1	826	0	849	27	0
14	2	826	0	848	40	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	129	0	88	10	0
18	N	129	0	88	9	0
19	A	2	0	0	0	0
19	N	2	0	0	1	0
20	A	102	0	152	9	0
20	C	102	0	152	14	0
20	N	51	0	76	1	0
20	P	102	0	152	10	0
21	B	63	0	110	6	0
21	D	63	0	110	13	0
21	L	63	0	110	20	0
21	N	63	0	110	2	0
21	Q	63	0	110	10	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	4	0	6	0	0
23	C	4	0	6	0	0
23	E	4	0	6	1	0
23	F	4	0	6	0	0
23	G	4	0	6	0	0
23	I	4	0	6	0	0
23	N	8	0	12	0	0
23	S	4	0	6	0	0
24	C	58	0	78	4	0
24	G	29	0	39	0	0
24	J	29	0	38	5	0
24	P	58	0	78	2	0
24	T	29	0	39	1	0
24	W	29	0	37	5	0
25	C	53	0	77	7	0
25	P	53	0	77	3	0
26	C	100	0	156	15	0
26	G	100	0	156	23	0
26	P	100	0	156	12	0
26	T	100	0	156	24	0
27	C	42	0	0	4	0
27	J	10	0	0	1	0
27	L	10	0	0	1	0
27	N	63	0	0	2	0
27	P	43	0	0	6	0
27	T	18	0	0	1	0
27	W	9	0	0	1	0
27	Y	10	0	0	1	0
28	E	52	0	80	19	0
28	V	52	0	80	21	0
29	F	1	0	0	0	0
29	S	1	0	0	1	0
30	M	33	0	42	1	0
30	Z	33	0	42	1	0
31	1	43	0	31	4	0
31	2	43	0	30	4	0
32	1	53	0	0	7	0
32	2	28	0	0	7	0
32	A	252	0	0	19	0
32	B	193	0	0	6	0
32	C	137	0	0	8	0
32	D	122	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	E	119	0	0	6	0
32	F	97	0	0	2	2
32	G	60	0	0	11	0
32	H	76	0	0	7	0
32	I	49	0	0	5	0
32	J	30	0	0	3	0
32	K	29	0	0	1	0
32	L	33	0	0	1	0
32	M	26	0	0	2	0
32	N	229	0	0	6	0
32	O	141	0	0	3	0
32	P	110	0	0	9	0
32	Q	99	0	0	7	0
32	R	83	0	0	1	0
32	S	95	0	0	5	0
32	T	41	0	0	3	0
32	U	54	0	0	4	2
32	V	17	0	0	2	0
32	W	10	0	0	0	0
32	X	17	0	0	3	0
32	Y	21	0	0	0	0
32	Z	16	0	0	0	0
All	All	34765	0	32733	753	2

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 12.

All (753) 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)
14:1:17:CYS:SG	31:1:201:HEC:CAC	2.06	1.41
27:C:310:UNL:C4	27:C:310:UNL:C6	1.76	1.36
32:A:927:HOH:O	26:T:101:CDL:H412	1.17	1.28
5:E:79:LYS:HE3	32:E:387:HOH:O	1.31	1.24
27:W:102:UNL:C5	27:W:102:UNL:C4	2.17	1.23
1:A:486:ASP:OD2	4:D:19:ARG:HD2	1.32	1.21
19:N:607:PER:O2	19:N:607:PER:O1	1.54	1.21
9:I:29:LEU:O	9:I:32:ALA:N	1.71	1.20
32:P:475:HOH:O	10:W:58:LYS:HE2	1.38	1.20
24:J:101:CHD:H212	32:J:221:HOH:O	1.41	1.17
28:V:101:PSC:H343	28:V:101:PSC:H12	1.22	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E:201:PSC:H221	28:E:201:PSC:C01	1.79	1.13
32:C:526:HOH:O	26:G:101:CDL:H551	0.98	1.12
9:I:29:LEU:O	9:I:32:ALA:CA	1.98	1.12
2:O:226:MET:HA	2:O:226:MET:HE3	1.28	1.12
32:A:927:HOH:O	26:T:101:CDL:C40	1.97	1.12
28:E:201:PSC:H221	28:E:201:PSC:O03	1.37	1.10
26:P:306:CDL:OB3	32:P:401:HOH:O	1.65	1.10
14:I:17:CYS:SG	31:I:201:HEC:HAC	1.78	1.09
8:H:7:LYS:O	8:H:8:ILE:CG2	2.01	1.09
21:L:101:TGL:OC1	21:L:101:TGL:HC41	1.29	1.08
26:G:101:CDL:CB2	32:G:244:HOH:O	2.00	1.07
6:F:94:HIS:HB2	6:F:96:LEU:HB2	1.09	1.06
8:H:7:LYS:O	8:H:8:ILE:HB	1.47	1.06
27:P:310:UNL:C5	27:P:310:UNL:C4	2.33	1.06
27:C:310:UNL:C6	27:C:310:UNL:C5	2.33	1.06
2:B:220:GLU:OE2	32:B:401:HOH:O	1.73	1.05
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.36	1.05
9:I:26:MET:O	9:I:30:GLY:CA	2.05	1.05
8:H:7:LYS:O	8:H:8:ILE:CB	2.05	1.04
28:E:201:PSC:H343	28:E:201:PSC:H12	1.40	1.04
20:A:607:PGV:H22	32:A:701:HOH:O	1.57	1.04
27:L:102:UNL:C4	27:L:102:UNL:C10	2.35	1.04
3:C:133:ASN:ND2	32:C:402:HOH:O	1.89	1.04
28:V:101:PSC:H22	32:V:212:HOH:O	1.58	1.03
9:V:29:LEU:O	9:V:31:PHE:N	1.91	1.03
4:D:6:VAL:HG21	4:D:31:LYS:NZ	1.75	1.01
21:D:201:TGL:H231	21:D:201:TGL:HA91	1.40	1.00
9:I:26:MET:O	9:I:30:GLY:HA3	1.61	1.00
9:I:31:PHE:CZ	9:I:32:ALA:O	2.15	1.00
10:W:33:ARG:HG2	24:W:101:CHD:H152	1.42	0.99
8:H:9:LYS:N	8:H:9:LYS:HD3	1.49	0.98
6:F:85:CYS:SG	6:F:87:THR:HG23	2.02	0.98
26:C:306:CDL:O1	32:C:401:HOH:O	1.83	0.97
8:H:7:LYS:O	8:H:8:ILE:HG22	1.62	0.97
8:H:8:ILE:N	32:H:101:HOH:O	1.94	0.96
2:O:226:MET:HA	2:O:226:MET:CE	1.96	0.96
25:C:303:PEK:H161	25:C:303:PEK:H11	1.47	0.94
7:G:11:TPO:O	32:G:201:HOH:O	1.87	0.94
3:P:133:ASN:ND2	32:P:402:HOH:O	2.02	0.93
2:B:29:MET:HG3	9:I:31:PHE:HZ	1.33	0.92
32:A:927:HOH:O	26:T:101:CDL:C41	1.82	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:101:CDL:HB21	32:G:244:HOH:O	1.62	0.91
3:P:37:PHE:CE1	10:W:58:LYS:HG3	2.05	0.91
6:F:30:PRO:O	6:F:96:LEU:HD21	1.70	0.91
26:P:306:CDL:H1	32:P:403:HOH:O	1.70	0.91
9:I:29:LEU:O	9:I:32:ALA:CB	2.19	0.90
1:N:514:LYS:HE2	32:S:258:HOH:O	1.70	0.90
32:P:493:HOH:O	6:S:1:ALA:HB1	1.67	0.90
21:L:101:TGL:OC1	21:L:101:TGL:CC4	2.16	0.90
4:Q:21:ASP:HB2	32:Q:301:HOH:O	1.72	0.90
2:O:58:ALA:O	2:O:62:GLU:HG3	1.71	0.90
6:F:75:HIS:H	6:F:80:GLN:HE22	1.19	0.89
7:G:5:LYS:HA	1:N:278[B]:MET:HE1	1.55	0.88
6:S:85:CYS:SG	6:S:87:THR:HG23	2.13	0.88
14:2:81:ILE:HD12	32:2:328:HOH:O	1.74	0.87
26:G:101:CDL:H522	26:G:101:CDL:H241	1.55	0.87
12:L:2:HIS:CD2	12:L:3:TYR:H	1.93	0.87
21:B:301:TGL:H121	21:B:301:TGL:H302	1.56	0.87
9:I:29:LEU:O	9:I:32:ALA:HB2	1.75	0.86
9:I:30:GLY:O	9:I:31:PHE:C	2.16	0.86
20:P:305:PGV:H062	32:U:103:HOH:O	1.76	0.86
12:L:20:ARG:HH21	21:L:101:TGL:HC52	1.39	0.86
3:P:37:PHE:CD1	10:W:58:LYS:HG3	2.11	0.85
27:Y:101:UNL:C5	27:Y:101:UNL:C4	2.54	0.85
6:F:30:PRO:O	6:F:96:LEU:CD2	2.24	0.85
1:A:282:PHE:HA	7:T:4:ALA:CB	2.07	0.84
26:G:101:CDL:H111	26:G:101:CDL:HA21	1.57	0.84
26:G:101:CDL:HB22	32:G:244:HOH:O	1.70	0.84
9:I:33:THR:HG22	9:I:37:PHE:HB3	1.57	0.84
28:E:201:PSC:O03	28:E:201:PSC:C22	2.23	0.84
6:F:94:HIS:CB	6:F:96:LEU:HB2	2.02	0.84
8:H:84:LYS:HA	8:H:84:LYS:HZ3	1.42	0.83
27:C:310:UNL:C4	27:C:310:UNL:C5	2.56	0.83
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.43	0.83
20:P:304:PGV:H151	20:P:304:PGV:H11	1.58	0.83
6:F:94:HIS:HB2	6:F:96:LEU:CB	2.02	0.83
2:B:16:ILE:HD13	32:B:549:HOH:O	1.79	0.82
4:D:6:VAL:HG21	4:D:31:LYS:HZ1	1.40	0.82
9:I:26:MET:O	9:I:30:GLY:N	2.12	0.81
6:S:75:HIS:H	6:S:80:GLN:HE22	1.23	0.81
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.61	0.81
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:205:GLY:HA3	25:P:303:PEK:H161	1.63	0.81
4:Q:31:LYS:HE3	32:Q:376:HOH:O	1.80	0.81
20:A:607:PGV:H211	32:M:216:HOH:O	1.80	0.80
8:U:46:LYS:HE3	32:U:143:HOH:O	1.80	0.80
4:Q:21:ASP:CG	32:Q:301:HOH:O	2.23	0.80
14:2:20:VAL:HG12	14:2:102:THR:HG22	1.64	0.80
2:B:81:LEU:HD12	26:T:101:CDL:H351	1.64	0.80
6:S:64:GLU:O	6:S:65:ASP:HB2	1.81	0.79
32:N:737:HOH:O	21:Q:201:TGL:HB32	1.83	0.79
28:V:101:PSC:H291	28:V:101:PSC:H331	1.65	0.79
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.79
24:P:307:CHD:H231	32:P:504:HOH:O	1.83	0.79
20:A:608:PGV:H343	25:C:303:PEK:H383	1.65	0.78
21:L:101:TGL:H312	21:L:101:TGL:C36	2.13	0.78
12:L:2:HIS:HD2	12:L:3:TYR:H	1.30	0.78
14:2:3:VAL:HG13	14:2:97:TYR:HA	1.65	0.78
20:P:305:PGV:C06	32:U:103:HOH:O	2.31	0.78
32:N:725:HOH:O	3:P:77:LYS:HE3	1.83	0.78
7:G:6:GLY:O	7:G:7:ASP:HB2	1.83	0.78
1:A:417[B]:MET:HE3	32:A:921:HOH:O	1.82	0.77
27:J:102:UNL:C10	27:J:102:UNL:C6	2.62	0.77
12:L:24:MET:HG3	32:L:223:HOH:O	1.83	0.77
2:B:29:MET:HG3	9:I:31:PHE:CZ	2.17	0.77
1:N:417:MET:HE3	32:N:928:HOH:O	1.83	0.77
4:Q:21:ASP:CB	32:Q:301:HOH:O	2.29	0.77
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.67	0.77
12:L:20:ARG:NH2	21:L:101:TGL:HC52	1.99	0.77
14:2:70:ASN:HB3	14:2:73:LYS:HB3	1.67	0.76
6:F:94:HIS:HD2	6:F:97:ALA:H	1.33	0.76
1:A:28:MET:CE	18:A:604[B]:HEA:H271	2.15	0.76
14:2:21:GLU:OE2	14:2:24:GLY:HA3	1.86	0.76
8:H:8:ILE:C	8:H:9:LYS:HD3	2.11	0.76
14:2:19:THR:HG23	14:2:27:LYS:HD2	1.67	0.76
9:I:29:LEU:C	9:I:32:ALA:H	1.94	0.75
7:G:38:HIS:NE2	26:G:101:CDL:H122	2.01	0.75
9:I:31:PHE:CE1	9:I:32:ALA:O	2.38	0.75
9:V:10:ARG:HD3	28:V:101:PSC:H063	1.67	0.75
2:B:58:ALA:O	2:B:62:GLU:HG3	1.87	0.75
14:1:81:ILE:CG2	32:1:346:HOH:O	2.34	0.74
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.03	0.74
6:F:94:HIS:O	32:F:201:HOH:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.69	0.74
8:H:7:LYS:C	32:H:101:HOH:O	2.26	0.74
28:E:201:PSC:H12	28:E:201:PSC:C34	2.14	0.73
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.69	0.73
9:V:31:PHE:C	9:V:31:PHE:CD1	2.66	0.73
2:O:56:MET:HB3	28:V:101:PSC:H211	1.70	0.73
9:I:2:THR:N	32:I:201:HOH:O	1.94	0.73
26:P:306:CDL:H521	26:P:306:CDL:OB9	1.87	0.73
14:1:17:CYS:SG	31:1:201:HEC:C3C	2.75	0.73
2:B:19:GLU:OE2	2:B:82:ARG:NH1	2.22	0.72
8:H:43:MET:CE	8:H:49:ASP:H	2.02	0.72
9:I:31:PHE:CD2	9:I:32:ALA:N	2.57	0.72
28:E:201:PSC:H221	28:E:201:PSC:H011	1.71	0.72
14:2:71:PRO:HD2	14:2:83:ALA:O	1.89	0.72
1:A:28:MET:CE	18:A:604[B]:HEA:C27	2.68	0.72
2:O:57:ASP:H	28:V:101:PSC:H202	1.55	0.71
8:H:84:LYS:HZ2	8:H:85:ILE:H	1.36	0.71
4:Q:87:PHE:HB2	32:X:113:HOH:O	1.90	0.71
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.53	0.71
28:E:201:PSC:H343	28:E:201:PSC:C12	2.18	0.71
9:I:30:GLY:C	9:I:32:ALA:N	2.38	0.71
20:A:608:PGV:H183	25:C:303:PEK:H322	1.72	0.70
26:G:101:CDL:H271	27:N:601:UNL:C17	2.21	0.70
28:V:101:PSC:H343	28:V:101:PSC:C12	2.13	0.70
14:1:17:CYS:SG	31:1:201:HEC:CBC	2.76	0.70
2:B:66:THR:HG22	2:B:67:ILE:HD13	1.72	0.70
14:2:16:GLN:H	14:2:16:GLN:HE21	1.38	0.70
4:D:6:VAL:HG21	4:D:31:LYS:HZ2	1.53	0.70
1:A:278[B]:MET:HE1	7:T:6:GLY:H	1.57	0.69
4:Q:19[B]:ARG:HD3	4:Q:21:ASP:OD1	1.92	0.69
3:P:37:PHE:HE1	10:W:58:LYS:HG3	1.57	0.69
14:2:32:LEU:HD22	14:2:35:LEU:HD22	1.74	0.69
2:O:226:MET:HE3	2:O:226:MET:CA	2.18	0.69
4:Q:28:ALA:O	4:Q:31:LYS:HD2	1.93	0.69
9:I:31:PHE:O	9:I:34:PHE:N	2.18	0.69
21:D:201:TGL:H122	21:D:201:TGL:HB81	1.75	0.68
7:T:34:ASN:O	7:T:38:HIS:HB3	1.92	0.68
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.19	0.68
20:A:608:PGV:H343	25:C:303:PEK:C38	2.23	0.68
2:B:57:ASP:H	28:E:201:PSC:H211	1.58	0.68
1:A:239:GLY:CA	32:A:900:HOH:O	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:60:CYS:HG	29:S:101:ZN:ZN	1.05	0.68
12:L:14:SER:H	21:L:101:TGL:HC31	1.60	0.67
1:A:304:TYR:HD1	26:T:101:CDL:HB32	1.59	0.67
2:O:116:LEU:HD11	2:O:226:MET:CG	2.24	0.67
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.76	0.67
26:T:101:CDL:H271	27:T:102:UNL:C17	2.24	0.67
28:V:101:PSC:H072	32:V:201:HOH:O	1.94	0.67
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.77	0.67
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.77	0.67
7:T:38:HIS:CD2	7:T:38:HIS:O	2.48	0.67
21:B:301:TGL:H211	21:B:301:TGL:H342	1.76	0.66
6:F:64:GLU:O	6:F:65:ASP:HB2	1.95	0.66
8:H:84:LYS:HA	8:H:84:LYS:NZ	2.09	0.66
1:N:28:MET:CE	18:N:605[B]:HEA:H271	2.25	0.66
26:C:306:CDL:H522	26:C:306:CDL:OB9	1.96	0.66
9:V:73:LYS:HB3	9:V:73:LYS:NZ	2.08	0.66
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.77	0.66
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.94	0.66
26:T:101:CDL:H382	26:T:101:CDL:H152	1.78	0.66
2:B:64:ILE:HG22	32:B:554:HOH:O	1.95	0.66
14:1:86:LYS:HE3	14:1:86:LYS:HA	1.77	0.66
1:N:145:LEU:HD11	27:P:310:UNL:C6	2.26	0.66
1:A:172:LYS:HZ1	7:T:9:GLY:HA3	1.60	0.65
32:A:927:HOH:O	26:T:101:CDL:H401	1.76	0.65
1:N:28:MET:HE1	18:N:605[B]:HEA:H271	1.78	0.65
1:A:339:MET:HE2	32:D:392:HOH:O	1.97	0.65
28:V:101:PSC:C28	28:V:101:PSC:H322	2.27	0.65
4:D:100:LYS:NZ	32:D:301:HOH:O	2.21	0.65
4:Q:4:SER:N	4:Q:31:LYS:H	1.95	0.65
7:G:45:PRO:O	7:G:46:ALA:CB	2.44	0.65
12:L:25:MET:HG2	21:L:101:TGL:HA62	1.78	0.65
6:F:94:HIS:O	6:F:95:GLN:HB3	1.94	0.64
14:1:19:THR:HG23	14:1:27:LYS:HD2	1.79	0.64
14:2:26:HIS:CD2	14:2:26:HIS:H	2.15	0.64
3:P:51[B]:MET:HE1	20:P:304:PGV:H172	1.78	0.64
28:V:101:PSC:P	28:V:101:PSC:H012	2.37	0.64
1:A:239:GLY:HA3	32:A:900:HOH:O	1.98	0.64
9:I:33:THR:HG22	9:I:37:PHE:CB	2.27	0.64
8:U:9:LYS:O	8:U:10:ASN:HB2	1.97	0.64
4:D:109:HIS:HD2	32:D:355:HOH:O	1.80	0.64
31:2:201:HEC:HBC1	32:2:317:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.06	0.64
21:D:201:TGL:HA91	21:D:201:TGL:C23	2.17	0.63
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.31	0.63
7:T:7:ASP:O	7:T:8:HIS:HB2	1.97	0.63
9:I:73:LYS:HD3	9:I:73:LYS:N	2.12	0.63
3:P:80[B]:ARG:HH22	27:P:308:UNL:C1	2.10	0.63
3:C:220:PHE:HB2	26:C:306:CDL:H711	1.81	0.63
7:T:17:ARG:HD3	32:T:205:HOH:O	1.98	0.63
31:2:201:HEC:CBC	32:2:317:HOH:O	2.46	0.63
20:C:305:PGV:C06	8:H:22:ASN:HD22	2.12	0.63
5:R:44:GLU:OE1	32:R:201:HOH:O	2.15	0.63
1:N:28:MET:CE	18:N:605[B]:HEA:C27	2.77	0.63
21:N:608:TGL:HA72	21:N:608:TGL:H221	1.79	0.63
6:S:94:HIS:O	6:S:95:GLN:HB2	1.99	0.63
2:B:57:ASP:H	28:E:201:PSC:C21	2.11	0.62
6:F:96:LEU:C	6:F:98:HIS:H	2.07	0.62
1:N:310:MET:HE1	2:O:76:ILE:HG21	1.81	0.62
2:B:68:LEU:HD23	28:E:201:PSC:H171	1.80	0.62
3:C:51[A]:MET:SD	26:C:306:CDL:H612	2.38	0.62
14:2:30:PRO:HD3	14:2:46:PHE:CE2	2.33	0.62
32:A:892:HOH:O	12:L:2:HIS:HE1	1.81	0.62
21:L:101:TGL:C23	21:L:101:TGL:HA92	2.29	0.62
1:A:112:LEU:C	1:A:112:LEU:HD23	2.24	0.62
4:Q:9:GLU:HA	4:Q:9:GLU:OE1	2.00	0.62
4:Q:43:LYS:HE3	4:Q:55:GLU:OE1	1.98	0.62
14:1:7:LYS:HG3	14:1:97:TYR:CE1	2.35	0.62
14:2:16:GLN:H	14:2:16:GLN:NE2	1.96	0.62
28:V:101:PSC:H322	28:V:101:PSC:H281	1.82	0.62
32:B:554:HOH:O	28:E:201:PSC:H151	2.00	0.62
26:G:101:CDL:C27	27:N:601:UNL:C17	2.76	0.62
9:I:30:GLY:O	9:I:32:ALA:N	2.32	0.62
8:H:84:LYS:NZ	8:H:85:ILE:H	1.97	0.61
2:O:57:ASP:N	28:V:101:PSC:H202	2.15	0.61
26:G:101:CDL:H142	26:G:101:CDL:OB2	1.99	0.61
2:O:116:LEU:CD1	2:O:226:MET:CG	2.79	0.61
2:O:198:GLU:OE2	32:O:401:HOH:O	2.16	0.61
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.30	0.61
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.46	0.61
26:T:101:CDL:H322	26:T:101:CDL:OA7	1.99	0.61
14:2:22:LYS:HA	14:2:33:HIS:HB2	1.82	0.61
7:T:37:LEU:O	7:T:38:HIS:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:33:ARG:HG2	24:W:101:CHD:C15	2.25	0.61
2:B:86:MET:O	2:B:89:GLU:HG2	2.00	0.61
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.83	0.61
7:G:38:HIS:NE2	26:G:101:CDL:H362	2.16	0.60
20:N:612:PGV:H61	3:P:54:MET:HG2	1.83	0.60
2:B:145:PRO:HG2	2:B:148:MET:HE2	1.82	0.60
7:G:84:LYS:N	32:G:203:HOH:O	2.19	0.60
14:2:5:LYS:HD3	14:2:93:ASP:OD2	2.02	0.60
1:A:28:MET:HE1	18:A:604[B]:HEA:C27	2.31	0.60
3:C:3:HIS:HA	32:C:410:HOH:O	2.01	0.60
10:J:7:GLU:HG3	32:J:220:HOH:O	2.01	0.60
1:N:486:ASP:OD2	4:Q:19[A]:ARG:NE	2.34	0.60
26:T:101:CDL:CA5	26:T:101:CDL:H311	2.31	0.60
26:P:306:CDL:H262	26:P:306:CDL:H222	1.84	0.60
7:G:7:ASP:O	7:G:8:HIS:HB2	2.02	0.60
1:N:468:MET:HE1	18:N:605[B]:HEA:H22	1.84	0.60
1:A:28:MET:HE1	18:A:604[B]:HEA:H271	1.84	0.59
1:A:310:MET:CE	2:B:77:ALA:HB2	2.31	0.59
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.83	0.59
20:P:304:PGV:H11	20:P:304:PGV:C15	2.27	0.59
26:G:101:CDL:HB32	26:G:101:CDL:H201	1.84	0.59
21:Q:201:TGL:HB32	21:Q:201:TGL:HG2	1.83	0.59
9:I:30:GLY:C	9:I:32:ALA:H	2.09	0.59
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.33	0.59
7:G:9:GLY:HA3	1:N:172:LYS:HZ1	1.68	0.59
7:G:17:ARG:HD3	32:G:208:HOH:O	2.01	0.59
8:H:9:LYS:HB3	32:H:102:HOH:O	2.03	0.59
3:C:224:LYS:HE3	26:C:306:CDL:HB32	1.85	0.59
26:G:101:CDL:H371	2:O:81:LEU:HD12	1.85	0.59
3:C:210:ILE:HG12	20:C:304:PGV:H132	1.85	0.58
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.33	0.58
1:A:282:PHE:HZ	26:T:101:CDL:H752	1.68	0.58
1:N:28:MET:HE1	18:N:605[B]:HEA:C27	2.33	0.58
1:A:278[B]:MET:CE	7:T:5:LYS:HB3	2.33	0.58
21:L:101:TGL:HA92	21:L:101:TGL:H231	1.85	0.58
2:B:84:LEU:HA	2:B:87:MET:HE2	1.85	0.58
32:P:493:HOH:O	6:S:1:ALA:CB	2.35	0.58
26:T:101:CDL:OB4	26:T:101:CDL:H1	2.03	0.58
20:C:305:PGV:H061	8:H:22:ASN:ND2	2.18	0.57
9:I:31:PHE:HE1	9:I:35:TYR:CB	2.17	0.57
2:B:56:MET:HA	28:E:201:PSC:H212	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:201:TGL:HG32	21:D:201:TGL:OB1	2.04	0.57
9:I:28:SER:O	9:I:31:PHE:HD2	1.88	0.57
1:A:304:TYR:CD1	26:T:101:CDL:HB32	2.40	0.57
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.86	0.57
1:A:278[B]:MET:SD	7:T:5:LYS:HB3	2.45	0.57
25:C:303:PEK:H161	25:C:303:PEK:C11	2.28	0.57
20:C:304:PGV:H12	26:C:306:CDL:H622	1.86	0.57
11:X:24:PHE:O	11:X:28:VAL:HG12	2.05	0.57
3:C:54:MET:HE1	20:C:304:PGV:H141	1.86	0.57
32:A:858:HOH:O	6:F:96:LEU:CD1	2.53	0.56
6:F:85:CYS:SG	6:F:87:THR:CG2	2.87	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.04	0.56
4:Q:27:VAL:HG21	4:Q:31:LYS:HE2	1.87	0.56
21:Q:201:TGL:HC21	21:Q:201:TGL:HG11	1.88	0.56
14:1:52:ASN:HD22	14:1:52:ASN:C	2.14	0.56
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.87	0.56
8:H:8:ILE:C	8:H:9:LYS:O	2.46	0.56
8:H:9:LYS:N	8:H:9:LYS:CD	2.41	0.56
1:N:28:MET:HE2	18:N:605[B]:HEA:H273	1.88	0.56
1:A:514:LYS:HE2	32:F:237:HOH:O	2.06	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
6:S:82:CYS:C	6:S:84:SER:N	2.63	0.56
24:C:307:CHD:H41	24:C:307:CHD:O7	2.06	0.55
3:P:10:MET:HA	3:P:10:MET:HE2	1.87	0.55
7:T:7:ASP:CG	7:T:8:HIS:N	2.63	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.89	0.55
14:1:48:TYR:HB2	14:1:53:LYS:HG3	1.87	0.55
1:A:406:ASN:HD21	20:A:607:PGV:H31	1.71	0.55
21:Q:201:TGL:HG11	21:Q:201:TGL:CC2	2.36	0.55
1:A:514:LYS:HA	6:F:38:ALA:CB	2.35	0.55
4:D:121:LYS:HE2	11:K:52:GLU:OE2	2.07	0.55
26:G:101:CDL:H111	26:G:101:CDL:CA2	2.32	0.55
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.39	0.55
6:S:64:GLU:O	6:S:65:ASP:CB	2.48	0.55
4:Q:109:HIS:HD2	32:Q:371:HOH:O	1.89	0.55
21:D:201:TGL:CA3	32:D:392:HOH:O	2.54	0.55
6:F:94:HIS:CD2	6:F:97:ALA:H	2.19	0.55
8:H:43:MET:HE3	8:H:49:ASP:H	1.72	0.55
9:I:33:THR:HA	9:I:36:LYS:HB3	1.89	0.55
24:P:301:CHD:H12	24:P:301:CHD:H212	1.88	0.55
21:D:201:TGL:HA31	32:D:392:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:33:THR:O	9:I:34:PHE:C	2.49	0.54
28:E:201:PSC:H072	32:I:221:HOH:O	2.07	0.54
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.07	0.54
26:G:101:CDL:O1	32:G:202:HOH:O	2.18	0.54
6:S:60:CYS:SG	6:S:85:CYS:SG	3.05	0.54
31:2:201:HEC:HBC2	31:2:201:HEC:HHD	1.88	0.54
1:A:365:ILE:HD11	32:A:899:HOH:O	2.06	0.54
6:S:53:THR:CG2	32:S:292:HOH:O	2.55	0.54
14:1:19:THR:CG2	14:1:27:LYS:HD2	2.37	0.54
32:A:858:HOH:O	6:F:96:LEU:HD11	2.07	0.54
6:F:94:HIS:CG	6:F:95:GLN:N	2.75	0.54
9:V:17:LEU:CD2	28:V:101:PSC:H271	2.38	0.54
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.43	0.54
8:U:9:LYS:O	8:U:10:ASN:CB	2.55	0.54
32:A:911:HOH:O	26:T:101:CDL:H131	2.07	0.54
2:B:57:ASP:H	28:E:201:PSC:C20	2.21	0.54
9:V:31:PHE:CD1	9:V:31:PHE:O	2.60	0.54
11:X:54:ARG:CG	11:X:54:ARG:NH2	2.64	0.54
4:Q:9:GLU:HB3	32:S:275:HOH:O	2.07	0.53
14:1:55:LYS:NZ	32:1:302:HOH:O	2.40	0.53
1:A:177:SER:H	1:A:180:GLN:HE21	1.56	0.53
1:A:312[A]:ILE:HD12	32:A:763:HOH:O	2.07	0.53
1:N:379:TYR:O	1:N:383[A]:MET:HB2	2.08	0.53
2:O:59:GLN:O	2:O:60:GLU:HG3	2.09	0.53
23:E:202:EDO:H22	32:E:391:HOH:O	2.08	0.53
14:1:49:THR:HG23	14:1:79:LYS:HD3	1.90	0.53
8:H:49:ASP:O	8:H:50:VAL:HB	2.09	0.53
21:Q:201:TGL:H352	9:V:16:ARG:HE	1.73	0.53
9:V:17:LEU:HD21	28:V:101:PSC:H271	1.90	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.49	0.53
4:Q:28:ALA:O	4:Q:31:LYS:CD	2.56	0.53
32:N:737:HOH:O	21:Q:201:TGL:HG2	2.08	0.53
1:N:240:HIS:C	1:N:240:HIS:CD2	2.86	0.53
28:V:101:PSC:H291	28:V:101:PSC:C33	2.32	0.53
2:B:33:LEU:HD11	9:I:29:LEU:HD13	1.91	0.52
2:B:57:ASP:N	28:E:201:PSC:H211	2.24	0.52
8:H:7:LYS:CA	8:H:7:LYS:HE3	2.39	0.52
26:T:101:CDL:H132	26:T:101:CDL:H342	1.91	0.52
1:A:513:LEU:O	1:A:514:LYS:CB	2.55	0.52
1:N:365:ILE:HD11	32:N:863:HOH:O	2.08	0.52
6:S:85:CYS:SG	6:S:87:THR:CG2	2.94	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:LYS:O	8:U:10:ASN:ND2	2.40	0.52
14:1:16:GLN:CB	32:1:338:HOH:O	2.58	0.52
9:I:31:PHE:HE1	9:I:35:TYR:H	1.57	0.52
21:L:101:TGL:H231	21:L:101:TGL:CA9	2.39	0.52
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.92	0.52
7:T:31:CYS:SG	26:T:101:CDL:H551	2.49	0.52
11:X:54:ARG:HH21	11:X:54:ARG:CB	2.23	0.52
8:H:43:MET:HE2	8:H:49:ASP:H	1.72	0.52
7:G:31:CYS:SG	26:G:101:CDL:H512	2.50	0.52
8:H:7:LYS:C	8:H:8:ILE:HG22	2.34	0.52
2:O:13:THR:OG1	2:O:167:SER:HB2	2.09	0.52
5:E:78:HIS:HD2	32:E:364:HOH:O	1.91	0.51
21:L:101:TGL:C36	21:L:101:TGL:C31	2.88	0.51
3:C:161[B]:GLN:HG2	24:C:307:CHD:O7	2.10	0.51
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.92	0.51
3:P:5:THR:HG21	6:S:96:LEU:HD13	1.92	0.51
14:2:62:GLU:HG2	14:2:63:THR:HG23	1.92	0.51
3:C:156:ARG:HE	24:C:307:CHD:C24	2.23	0.51
26:C:306:CDL:H262	26:C:306:CDL:H381	1.91	0.51
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.41	0.51
27:P:310:UNL:C4	27:P:310:UNL:C6	2.89	0.51
8:U:7:LYS:HE3	8:U:10:ASN:HD21	1.74	0.51
10:J:2:GLU:HG2	32:J:209:HOH:O	2.11	0.51
1:N:24:ALA:HA	18:N:605[A]:HEA:H22	1.93	0.51
26:P:306:CDL:H162	26:P:306:CDL:H201	1.93	0.51
14:2:36:PHE:CE2	14:2:61:GLU:HG3	2.46	0.51
9:I:29:LEU:O	9:I:32:ALA:HA	2.05	0.51
1:A:343:GLY:HA2	21:D:201:TGL:H201	1.93	0.51
8:H:10:ASN:N	32:H:102:HOH:O	1.98	0.51
1:A:28:MET:HE2	18:A:604[B]:HEA:H273	1.92	0.51
32:A:950:HOH:O	14:1:81:ILE:HG21	2.10	0.51
14:2:30:PRO:HD3	14:2:46:PHE:CZ	2.46	0.51
9:I:1:SAC:CB	9:I:1:SAC:H2A1	2.40	0.50
26:G:101:CDL:H372	2:O:78:LEU:HD12	1.94	0.50
8:H:7:LYS:HE3	8:H:7:LYS:HA	1.93	0.50
4:D:107:ILE:HD11	4:D:111:PHE:CB	2.42	0.50
4:D:118:LYS:HB3	11:K:53:TRP:HB3	1.94	0.50
24:J:101:CHD:H61	24:J:101:CHD:H21	1.94	0.50
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.45	0.50
20:C:305:PGV:H061	8:H:22:ASN:HD22	1.76	0.50
26:T:101:CDL:H791	26:T:101:CDL:H832	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:306:CDL:HB21	10:J:8:LYS:HD2	1.92	0.50
14:2:3:VAL:O	14:2:97:TYR:HB2	2.11	0.50
20:C:305:PGV:H11	3:P:258:TRP:HH2	1.76	0.50
1:N:514:LYS:HA	6:S:38:ALA:CB	2.41	0.50
2:O:137:GLU:OE1	4:Q:122:ARG:NH1	2.37	0.50
3:P:59:ARG:HG3	26:P:306:CDL:HA22	1.92	0.50
14:2:9:ILE:O	14:2:13:LYS:HG2	2.11	0.50
14:2:42:GLN:O	14:2:44:PRO:HD3	2.11	0.50
2:O:56:MET:CB	28:V:101:PSC:H211	2.41	0.50
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.94	0.50
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.11	0.50
1:A:49:GLY:HA3	32:A:908:HOH:O	2.10	0.50
14:1:72:LYS:HD2	32:1:334:HOH:O	2.12	0.50
20:C:304:PGV:H172	26:C:306:CDL:H631	1.93	0.49
21:L:101:TGL:C31	21:L:101:TGL:H362	2.42	0.49
14:2:3:VAL:HG11	14:2:100:LYS:HD2	1.94	0.49
6:F:46:PRO:O	6:F:48:LEU:HD22	2.12	0.49
1:A:28:MET:HE2	18:A:604[B]:HEA:C27	2.41	0.49
7:G:5:LYS:HA	1:N:278[B]:MET:CE	2.34	0.49
2:O:58:ALA:O	2:O:62:GLU:CG	2.53	0.49
2:B:70:ALA:HB1	26:T:101:CDL:H441	1.95	0.49
26:C:306:CDL:OB9	26:C:306:CDL:HB4	2.11	0.49
8:H:43:MET:HE3	8:H:49:ASP:N	2.28	0.49
8:H:46:LYS:HE2	8:H:46:LYS:HA	1.94	0.49
6:S:44:GLU:H	6:S:44:GLU:CD	2.19	0.49
2:O:116:LEU:CD1	2:O:226:MET:HG3	2.42	0.49
10:W:36:MET:HB3	24:W:101:CHD:C18	2.42	0.49
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.48	0.49
6:F:52:ILE:HA	6:F:94:HIS:HB3	1.94	0.49
4:D:34:SER:H	4:D:37:GLN:NE2	2.11	0.49
14:2:13:LYS:HE3	32:2:311:HOH:O	2.13	0.49
1:A:333:LYS:HE2	32:M:212:HOH:O	2.11	0.49
14:1:16:GLN:HB3	32:1:338:HOH:O	2.12	0.49
8:H:9:LYS:N	32:H:101:HOH:O	2.18	0.48
9:V:33:THR:O	9:V:36:LYS:N	2.46	0.48
14:1:47:THR:HB	32:1:332:HOH:O	2.12	0.48
1:A:24:ALA:HB2	18:A:604[B]:HEA:H253	1.95	0.48
2:B:148:MET:HE3	2:B:148:MET:HB3	1.69	0.48
28:E:201:PSC:H222	28:E:201:PSC:H21	1.95	0.48
9:I:31:PHE:CE2	9:I:32:ALA:O	2.64	0.48
1:A:417[A]:MET:HE2	1:A:464:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:72:LYS:NZ	14:2:83:ALA:HA	2.29	0.48
21:B:301:TGL:H301	21:B:301:TGL:HA72	1.96	0.48
6:S:82:CYS:C	6:S:84:SER:H	2.21	0.48
2:B:86:MET:HB3	32:B:536:HOH:O	2.14	0.48
26:G:101:CDL:H402	26:G:101:CDL:H172	1.95	0.48
10:W:36:MET:HG2	24:W:101:CHD:H183	1.94	0.48
7:T:31:CYS:SG	26:T:101:CDL:H532	2.54	0.48
4:D:63:LYS:HG2	4:D:64:PHE:CE2	2.49	0.48
9:I:33:THR:O	9:I:36:LYS:N	2.47	0.48
1:N:485:VAL:HG22	13:Z:1:ILE:HG13	1.95	0.48
1:A:309:THR:HG22	18:A:605:HEA:HMB2	1.96	0.47
14:2:32:LEU:O	14:2:102:THR:HB	2.13	0.47
7:G:11:TPO:HG22	32:G:210:HOH:O	2.13	0.47
3:P:246:ASP:HB2	32:P:485:HOH:O	2.13	0.47
12:Y:47:LYS:OXT	12:Y:47:LYS:HD2	2.14	0.47
9:I:61:GLU:OE1	9:I:64:ARG:NE	2.40	0.47
21:L:101:TGL:H312	21:L:101:TGL:H363	1.92	0.47
2:B:145:PRO:HG2	2:B:148:MET:CE	2.43	0.47
3:P:107:ALA:HB2	20:P:305:PGV:H031	1.96	0.47
1:A:278[B]:MET:HE3	7:T:5:LYS:HB3	1.95	0.47
2:B:129[A]:LYS:NZ	2:B:132:GLU:OE1	2.43	0.47
8:H:9:LYS:HG3	8:H:11:TYR:H	1.80	0.47
6:S:53:THR:HG22	32:S:292:HOH:O	2.14	0.47
7:G:10:GLY:N	32:G:205:HOH:O	2.47	0.47
7:G:37:LEU:HD23	26:G:101:CDL:H381	1.96	0.47
9:I:33:THR:HA	9:I:36:LYS:HE3	1.95	0.47
1:N:437:PRO:HG2	1:N:440:TYR:CZ	2.49	0.47
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.47
3:P:37:PHE:CE2	27:P:310:UNL:C1	2.98	0.47
4:Q:78:TRP:N	21:Q:201:TGL:HB22	2.30	0.47
21:Q:201:TGL:H362	9:V:20:HIS:CE1	2.49	0.47
7:T:3:ALA:O	32:T:201:HOH:O	2.20	0.47
28:V:101:PSC:O02	28:V:101:PSC:H011	2.15	0.47
14:2:68:LEU:HD21	31:2:201:HEC:HMB2	1.96	0.47
26:C:306:CDL:HB21	10:J:8:LYS:CD	2.45	0.47
4:D:68:PHE:HA	4:D:71:MET:HE3	1.97	0.47
4:D:86:MET:HE3	21:D:201:TGL:H311	1.95	0.47
20:P:304:PGV:C15	20:P:304:PGV:C11	2.92	0.47
7:T:44:ARG:HD2	7:T:82:TYR:CE1	2.50	0.47
14:1:3:VAL:HG13	14:1:97:TYR:HA	1.97	0.47
14:2:16:GLN:NE2	14:2:16:GLN:N	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:49:THR:O	14:2:53:LYS:HB2	2.14	0.47
8:H:52:VAL:HG11	8:U:48:GLY:HA3	1.97	0.46
4:Q:19[B]:ARG:CD	4:Q:21:ASP:OD1	2.61	0.46
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.98	0.46
21:D:201:TGL:HA32	32:D:392:HOH:O	2.16	0.46
2:O:33:LEU:HD12	9:V:28:SER:HB3	1.96	0.46
20:P:304:PGV:H151	20:P:304:PGV:C11	2.37	0.46
14:1:3:VAL:HG21	14:1:100:LYS:HE2	1.97	0.46
3:C:76:GLN:NE2	3:C:80[A]:ARG:HH21	2.13	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.50	0.46
3:C:131:LEU:HD11	26:G:101:CDL:H552	1.96	0.46
3:C:133:ASN:HB3	3:C:173:PHE:CE2	2.50	0.46
26:G:101:CDL:H212	1:N:311:ILE:CD1	2.44	0.46
20:C:305:PGV:H321	7:T:1:ALA:HB2	1.96	0.46
3:P:16:TRP:N	3:P:17:PRO:CD	2.78	0.46
14:2:11:VAL:HA	14:2:15:ALA:HB2	1.96	0.46
1:N:310:MET:HE3	1:N:356:ILE:HG23	1.96	0.46
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.79	0.46
6:S:51:SER:O	6:S:94:HIS:N	2.49	0.46
21:D:201:TGL:OB1	21:D:201:TGL:CG3	2.64	0.46
28:E:201:PSC:C22	28:E:201:PSC:H011	2.44	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.46
26:C:306:CDL:O1	26:C:306:CDL:OA3	2.34	0.46
9:I:29:LEU:O	9:I:30:GLY:C	2.59	0.46
9:V:31:PHE:C	9:V:33:THR:N	2.74	0.46
32:A:911:HOH:O	26:T:101:CDL:H151	2.15	0.46
1:N:112:LEU:HD23	1:N:112:LEU:C	2.40	0.46
1:A:310:MET:HB3	2:B:73:LEU:HD22	1.97	0.46
12:L:46:LYS:O	12:L:47:LYS:HB2	2.15	0.46
2:B:13:THR:HG21	2:B:192:TYR:CZ	2.51	0.45
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.87	0.45
21:B:301:TGL:H101	21:B:301:TGL:HA62	1.98	0.45
9:I:31:PHE:C	9:I:31:PHE:CD2	2.87	0.45
20:P:305:PGV:H041	32:U:103:HOH:O	2.15	0.45
5:E:90:ARG:HD3	32:E:370:HOH:O	2.16	0.45
9:I:31:PHE:HE1	9:I:35:TYR:HB3	1.81	0.45
12:L:20:ARG:HH22	21:L:101:TGL:HC72	1.82	0.45
1:N:28:MET:HE2	18:N:605[B]:HEA:C27	2.43	0.45
11:X:44:PRO:HG3	32:X:115:HOH:O	2.15	0.45
1:A:217:THR:HG22	3:C:188:ILE:HG12	1.99	0.45
1:A:399:LEU:O	1:A:499:PRO:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:46:LYS:HG2	32:E:333:HOH:O	2.16	0.45
21:L:101:TGL:H312	21:L:101:TGL:H362	1.93	0.45
21:D:201:TGL:H362	9:I:20:HIS:CE1	2.51	0.45
1:N:368:HIS:CD2	1:N:369:ASP:HB2	2.51	0.45
28:V:101:PSC:H12	28:V:101:PSC:C34	2.16	0.45
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.98	0.45
1:A:311:ILE:CD1	26:T:101:CDL:H201	2.47	0.45
1:A:378:HIS:CG	1:A:425:PHE:CE1	3.05	0.45
20:A:607:PGV:C2	32:A:701:HOH:O	2.35	0.45
2:B:129[A]:LYS:NZ	32:B:407:HOH:O	2.49	0.45
24:C:301:CHD:O7	20:C:305:PGV:H42	2.17	0.45
6:F:53:THR:OG1	6:F:54:ASN:N	2.43	0.45
1:N:250:GLY:O	1:N:254:ILE:HG12	2.17	0.45
2:O:116:LEU:HD11	2:O:226:MET:HG3	1.98	0.45
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.51	0.45
9:V:33:THR:HA	9:V:37:PHE:HD2	1.82	0.45
1:A:240:HIS:C	1:A:240:HIS:CD2	2.94	0.45
5:E:6:GLU:O	28:E:201:PSC:H081	2.17	0.45
7:G:45:PRO:O	7:G:46:ALA:HB3	2.17	0.45
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.99	0.45
14:1:40:THR:HG22	14:1:59:TRP:CE2	2.52	0.45
1:N:344:PHE:CD1	1:N:344:PHE:C	2.96	0.44
7:T:37:LEU:O	7:T:38:HIS:HB2	2.16	0.44
20:C:305:PGV:H032	32:C:502:HOH:O	2.17	0.44
14:1:16:GLN:HB2	32:1:338:HOH:O	2.17	0.44
14:1:25:LYS:HZ3	14:1:26:HIS:H	1.64	0.44
1:N:321:PHE:CE2	28:V:101:PSC:H162	2.53	0.44
3:P:173:PHE:CD1	3:P:173:PHE:C	2.95	0.44
14:2:11:VAL:O	14:2:15:ALA:HB3	2.18	0.44
1:A:281:GLY:C	7:T:4:ALA:HB1	2.43	0.44
28:E:201:PSC:H041	32:I:221:HOH:O	2.18	0.44
6:S:53:THR:HG23	32:S:292:HOH:O	2.17	0.44
2:B:58:ALA:O	2:B:62:GLU:CG	2.61	0.44
21:L:101:TGL:HC22	21:L:101:TGL:HC81	2.00	0.44
2:O:144:LEU:HD22	2:O:150:ILE:HD13	1.99	0.44
1:A:281:GLY:O	7:T:4:ALA:HB1	2.18	0.44
2:O:129:LYS:HE2	32:O:516:HOH:O	2.18	0.44
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.18	0.44
26:P:306:CDL:H471	26:P:306:CDL:H441	1.80	0.44
21:Q:201:TGL:HA91	21:Q:201:TGL:H231	1.99	0.44
5:R:12:ASP:OD2	5:R:44:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:4:PRO:HG2	32:X:115:HOH:O	2.17	0.44
2:O:146:MET:HA	2:O:213:LEU:HD12	2.00	0.43
3:P:62:ILE:CD1	26:P:306:CDL:H522	2.48	0.43
1:A:367:LEU:HD21	1:A:433:LEU:HD23	2.01	0.43
20:A:608:PGV:H311	25:C:303:PEK:H382	2.00	0.43
8:H:37:HIS:HD2	32:H:127:HOH:O	2.00	0.43
3:P:37:PHE:HE1	10:W:58:LYS:CG	2.27	0.43
3:P:116:TRP:HA	3:P:117:PRO:C	2.43	0.43
20:C:305:PGV:C06	8:H:22:ASN:ND2	2.76	0.43
26:C:306:CDL:C19	26:C:306:CDL:H602	2.49	0.43
5:E:41:LEU:HA	32:I:228:HOH:O	2.17	0.43
10:J:33:ARG:HG2	24:J:101:CHD:H151	1.99	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.18	0.43
21:N:608:TGL:H221	21:N:608:TGL:CA7	2.47	0.43
26:T:101:CDL:H241	26:T:101:CDL:H542	2.00	0.43
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.75	0.43
3:C:210:ILE:HD13	20:C:304:PGV:H302	1.99	0.43
14:2:35:LEU:O	14:2:37:GLY:N	2.52	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.99	0.43
5:E:79:LYS:HD2	32:E:412:HOH:O	2.19	0.43
10:J:40:LEU:HD12	24:J:101:CHD:H183	2.01	0.43
20:P:304:PGV:H282	20:P:304:PGV:H312	1.86	0.43
4:Q:114:GLU:HG3	11:X:51:LYS:HE3	2.01	0.43
9:V:18:ARG:NH2	28:V:101:PSC:C7	2.82	0.43
1:N:136[A]:LEU:HD11	32:2:328:HOH:O	2.18	0.43
2:O:150:ILE:HD12	2:O:184:LEU:HD22	2.01	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.43
21:L:101:TGL:H261	21:L:101:TGL:H232	1.67	0.43
9:V:29:LEU:O	9:V:31:PHE:CA	2.65	0.43
14:1:100:LYS:HB3	14:1:100:LYS:HE3	1.73	0.43
25:C:303:PEK:H041	7:G:70:PHE:HB2	2.01	0.43
4:D:34:SER:H	4:D:37:GLN:HE21	1.67	0.43
1:N:302:ARG:HH11	1:N:302:ARG:HD2	1.70	0.43
1:N:390:MET:HE1	1:N:468:MET:SD	2.59	0.43
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.43
25:P:303:PEK:H71	25:P:303:PEK:H31	2.00	0.43
3:C:77:LYS:NZ	32:C:408:HOH:O	2.52	0.42
9:I:2:THR:CA	32:I:201:HOH:O	2.59	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42
1:A:1:FME:HE3	12:L:3:TYR:HE1	1.83	0.42
2:B:7:LEU:HD11	21:B:301:TGL:H152	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:92:ASN:N	2:O:92:ASN:HD22	2.18	0.42
4:Q:78:TRP:CE2	4:Q:79:LYS:HG3	2.54	0.42
14:2:26:HIS:ND1	14:2:46:PHE:HB2	2.33	0.42
14:2:58:THR:HG22	14:2:59:TRP:N	2.34	0.42
2:B:19:GLU:CD	2:B:82:ARG:NH1	2.77	0.42
3:C:151:LEU:HB2	3:C:159:MET:HG3	2.00	0.42
26:G:101:CDL:HA22	32:G:244:HOH:O	2.19	0.42
2:B:68:LEU:HB3	2:B:69:PRO:HD3	2.02	0.42
2:B:74:ILE:HG12	26:T:101:CDL:H402	2.02	0.42
6:S:96:LEU:O	6:S:97:ALA:HB3	2.19	0.42
26:T:101:CDL:H152	26:T:101:CDL:H362	2.00	0.42
2:O:86:MET:HE3	2:O:86:MET:HB2	1.70	0.42
26:P:306:CDL:HB22	26:P:306:CDL:OB6	2.20	0.42
4:Q:19[A]:ARG:HG2	32:Q:385:HOH:O	2.19	0.42
4:Q:81:VAL:HG11	21:Q:201:TGL:HB62	2.02	0.42
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.01	0.42
6:S:52:ILE:CG2	6:S:96:LEU:HB2	2.50	0.42
9:V:29:LEU:C	9:V:31:PHE:N	2.70	0.42
10:W:24:GLY:N	10:W:28:ASP:OD2	2.50	0.42
14:2:38:ARG:NH2	14:2:38:ARG:HB2	2.35	0.42
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.42
6:F:94:HIS:HD2	6:F:97:ALA:N	2.11	0.42
6:F:94:HIS:CG	6:F:95:GLN:H	2.38	0.42
9:I:27:VAL:O	9:I:31:PHE:N	2.49	0.42
1:N:48:LEU:O	13:Z:41:LYS:HE2	2.20	0.42
2:O:57:ASP:O	2:O:60:GLU:OE2	2.38	0.42
8:U:9:LYS:HG3	8:U:11:TYR:H	1.84	0.42
9:V:25:PHE:O	9:V:29:LEU:HB2	2.20	0.42
4:D:107:ILE:HD11	4:D:111:PHE:HB2	2.01	0.42
3:P:37:PHE:HD1	10:W:58:LYS:HG3	1.71	0.42
26:P:306:CDL:H612	26:P:306:CDL:H642	1.65	0.42
6:S:54:ASN:HD22	6:S:54:ASN:H	1.66	0.42
14:2:16:GLN:NE2	32:2:303:HOH:O	2.51	0.42
14:2:49:THR:CG2	14:2:79:LYS:HG2	2.50	0.42
1:A:309:THR:CG2	18:A:605:HEA:HMB2	2.50	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.42
8:H:43:MET:CE	8:H:49:ASP:N	2.77	0.42
3:P:257:TYR:O	3:P:261:SER:HB3	2.20	0.42
25:P:303:PEK:H221	7:T:69:PHE:CD1	2.54	0.42
26:P:306:CDL:HA21	26:P:306:CDL:CB5	2.49	0.42
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.47	0.42
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.18	0.42
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.79	0.42
8:H:46:LYS:C	8:H:48:GLY:H	2.27	0.42
30:M:101:DMU:H30	30:M:101:DMU:O1	2.19	0.42
1:N:242:GLU:O	1:N:246:LEU:HG	2.20	0.42
3:P:76:GLN:HE21	3:P:233:PHE:HB2	1.84	0.42
9:V:22:VAL:O	9:V:26:MET:HG2	2.20	0.42
1:A:472:ILE:HG21	21:L:101:TGL:HA91	2.02	0.42
5:E:7:THR:OG1	5:E:10:GLU:HG3	2.20	0.42
11:K:50:PRO:HD2	32:K:105:HOH:O	2.19	0.42
10:W:36:MET:HE2	10:W:36:MET:HB2	1.88	0.42
14:1:86:LYS:HE3	14:1:86:LYS:CA	2.45	0.42
2:B:91:ASN:OD1	2:B:183:THR:HG21	2.20	0.41
2:B:162:SER:HB3	2:B:197:SER:C	2.45	0.41
3:C:122:HIS:CE1	32:C:498:HOH:O	2.73	0.41
14:2:97:TYR:CE1	14:2:101:ALA:HB2	2.55	0.41
1:A:3:ILE:HG12	1:A:7:LEU:HD22	2.02	0.41
20:C:305:PGV:H161	32:T:241:HOH:O	2.21	0.41
2:O:129:LYS:HB3	2:O:129:LYS:HE3	1.61	0.41
3:P:105:SER:HA	3:P:116:TRP:CE3	2.56	0.41
3:P:146:TRP:HB2	7:T:16:TRP:HB3	2.02	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.87	0.41
2:B:94:SER:HB2	2:B:148:MET:HE3	2.01	0.41
11:K:32:MET:O	11:K:32:MET:HG2	2.19	0.41
12:L:2:HIS:HD2	12:L:3:TYR:N	2.08	0.41
2:O:49:LYS:HE3	32:O:437:HOH:O	2.20	0.41
7:T:3:ALA:O	7:T:4:ALA:CB	2.68	0.41
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.84	0.41
3:C:257:TYR:O	3:C:261:SER:HB3	2.21	0.41
7:G:31:CYS:SG	26:G:101:CDL:H532	2.61	0.41
26:P:306:CDL:CA2	32:P:403:HOH:O	2.67	0.41
14:2:59:TRP:HA	14:2:59:TRP:CE3	2.56	0.41
8:H:7:LYS:N	32:H:101:HOH:O	2.53	0.41
1:N:278[B]:MET:HE3	1:N:278[B]:MET:HB3	1.87	0.41
2:O:78:LEU:HD12	2:O:78:LEU:HA	1.84	0.41
4:Q:107:ILE:HB	4:Q:108:PRO:CD	2.51	0.41
10:W:36:MET:HB3	24:W:101:CHD:H183	2.02	0.41
1:A:48:LEU:HB2	32:A:721:HOH:O	2.20	0.41
2:B:200:CYS:SG	2:B:204:HIS:HA	2.61	0.41
10:J:36:MET:HG2	24:J:101:CHD:H162	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:383[A]:MET:O	1:N:387:PHE:HB2	2.21	0.41
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.56	0.41
26:C:306:CDL:H602	26:C:306:CDL:H201	2.02	0.41
1:N:136[B]:LEU:HD11	32:N:925:HOH:O	2.21	0.41
5:R:20:ASN:O	5:R:21:LYS:C	2.63	0.41
21:L:101:TGL:H291	21:L:101:TGL:H122	1.71	0.41
1:N:236:TRP:CH2	18:N:606:HEA:HBD1	2.56	0.41
24:T:103:CHD:H12	24:T:103:CHD:H212	2.02	0.41
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.41
3:C:246:ASP:HB2	32:C:477:HOH:O	2.20	0.41
2:O:116:LEU:HD13	2:O:226:MET:CG	2.51	0.41
30:Z:101:DMU:H15	30:Z:101:DMU:H9	1.98	0.41
14:2:16:GLN:HG3	32:2:316:HOH:O	2.21	0.41
1:A:127:THR:HB	1:A:129:TYR:CE1	2.56	0.41
2:B:36:SER:HB3	21:B:301:TGL:C13	2.51	0.41
1:A:236:TRP:CH2	18:A:605:HEA:HBD1	2.56	0.40
1:A:335:SER:HB2	1:A:336:PRO:HD2	2.03	0.40
1:A:415:ALA:HB1	21:D:201:TGL:H121	2.03	0.40
3:C:59:ARG:HG3	26:C:306:CDL:H512	2.03	0.40
14:1:69:GLU:HG3	14:1:91:ARG:CZ	2.50	0.40
14:2:104:GLU:OE1	14:2:104:GLU:HA	2.21	0.40
2:O:68:LEU:CD2	28:V:101:PSC:H172	2.50	0.40
6:S:92:VAL:O	6:S:93:PRO:C	2.64	0.40
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.03	0.40
8:U:60:TYR:CD1	8:U:60:TYR:C	2.99	0.40
1:A:278[B]:MET:HE1	7:T:6:GLY:N	2.29	0.40
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.40
1:A:344:PHE:CD1	1:A:344:PHE:C	2.99	0.40
3:C:29:SER:HB2	27:C:310:UNL:C4	2.51	0.40
4:D:11:TYR:CD1	4:D:11:TYR:C	2.99	0.40
7:G:10:GLY:HA3	32:G:205:HOH:O	2.21	0.40
12:L:25:MET:HG2	21:L:101:TGL:CA6	2.48	0.40
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.83	0.40
3:P:80[B]:ARG:NH2	27:P:308:UNL:C1	2.81	0.40
4:Q:31:LYS:HG3	32:Q:399:HOH:O	2.21	0.40
6:S:82:CYS:O	6:S:83:PRO:C	2.63	0.40
14:1:68:LEU:HD23	14:1:68:LEU:HA	1.89	0.40
14:2:3:VAL:CG1	14:2:97:TYR:HA	2.45	0.40
20:A:607:PGV:H231	13:M:12:PRO:HG3	2.03	0.40
4:D:112:GLU:HB3	32:D:363:HOH:O	2.21	0.40
7:G:37:LEU:C	7:G:39:SER:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:35:SER:C	7:T:37:LEU:H	2.29	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:266:HOH:O	32:U:148:HOH:O[1_455]	2.11	0.09
32:F:276:HOH:O	32:U:141:HOH:O[1_455]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	520/514 (101%)	504 (97%)	16 (3%)	0	100	100
2	B	227/227 (100%)	217 (96%)	9 (4%)	1 (0%)	30	27
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	30	27
3	C	263/259 (102%)	259 (98%)	4 (2%)	0	100	100
3	P	262/259 (101%)	256 (98%)	5 (2%)	1 (0%)	30	27
4	D	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
4	Q	143/144 (99%)	136 (95%)	5 (4%)	2 (1%)	9	4
5	E	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	5	2
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	1
7	G	81/84 (96%)	65 (80%)	10 (12%)	6 (7%)	1	0
7	T	81/84 (96%)	64 (79%)	10 (12%)	7 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	77/79 (98%)	70 (91%)	4 (5%)	3 (4%)	2	1
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	9	5
9	I	71/73 (97%)	67 (94%)	1 (1%)	3 (4%)	2	0
9	V	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	4	1
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	55 (98%)	0	1 (2%)	6	3
11	K	47/49 (96%)	47 (100%)	0	0	100	100
11	X	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
12	L	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
14	1	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	6	3
14	2	103/105 (98%)	81 (79%)	15 (15%)	7 (7%)	1	0
All	All	3744/3768 (99%)	3557 (95%)	145 (4%)	42 (1%)	11	7

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	96	LEU
7	G	3	ALA
7	G	7	ASP
7	G	8	HIS
7	G	46	ALA
8	H	8	ILE
8	H	9	LYS
8	H	50	VAL
9	I	2	THR
9	I	32	ALA
3	P	38	ASN
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	38	HIS
8	U	10	ASN

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Mol	Chain	Res	Type
9	V	30	GLY
10	W	56	PRO
14	2	25	LYS
14	2	36	PHE
14	2	39	LYS
2	B	60	GLU
7	G	5	LYS
2	O	60	GLU
6	S	94	HIS
7	T	3	ALA
14	1	24	GLY
7	G	38	HIS
6	S	95	GLN
7	T	37	LEU
14	2	56	GLY
4	Q	5	VAL
7	T	6	GLY
9	V	29	LEU
4	Q	6	VAL
14	1	37	GLY
14	2	1	GLY
9	I	30	GLY
14	2	23	GLY
14	2	41	GLY

5.3.2 Protein sidechains ⓘ

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	437/426 (103%)	430 (98%)	7 (2%)	55	62
1	N	433/426 (102%)	425 (98%)	8 (2%)	51	58
2	B	212/210 (101%)	205 (97%)	7 (3%)	33	34
2	O	210/210 (100%)	193 (92%)	17 (8%)	11	7
3	C	230/224 (103%)	224 (97%)	6 (3%)	40	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	229/224 (102%)	226 (99%)	3 (1%)	61	68
4	D	128/128 (100%)	122 (95%)	6 (5%)	23	22
4	Q	129/128 (101%)	120 (93%)	9 (7%)	14	10
5	E	92/92 (100%)	90 (98%)	2 (2%)	45	50
5	R	92/92 (100%)	89 (97%)	3 (3%)	33	34
6	F	81/81 (100%)	76 (94%)	5 (6%)	16	13
6	S	81/81 (100%)	73 (90%)	8 (10%)	7	4
7	G	67/67 (100%)	61 (91%)	6 (9%)	9	6
7	T	67/67 (100%)	62 (92%)	5 (8%)	12	9
8	H	71/71 (100%)	64 (90%)	7 (10%)	7	4
8	U	71/71 (100%)	70 (99%)	1 (1%)	59	66
9	I	57/57 (100%)	50 (88%)	7 (12%)	4	3
9	V	57/57 (100%)	51 (90%)	6 (10%)	6	4
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	54
10	W	49/49 (100%)	46 (94%)	3 (6%)	17	14
11	K	39/39 (100%)	37 (95%)	2 (5%)	21	19
11	X	39/39 (100%)	38 (97%)	1 (3%)	40	44
12	L	39/39 (100%)	35 (90%)	4 (10%)	7	4
12	Y	39/39 (100%)	36 (92%)	3 (8%)	12	8
13	M	37/37 (100%)	33 (89%)	4 (11%)	6	3
13	Z	37/37 (100%)	35 (95%)	2 (5%)	20	17
14	1	86/86 (100%)	78 (91%)	8 (9%)	8	5
14	2	86/86 (100%)	69 (80%)	17 (20%)	1	0
All	All	3244/3212 (101%)	3086 (95%)	158 (5%)	22	20

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	138	HIS
1	A	178	GLN
1	A	180	GLN
1	A	363	LEU
1	A	369	ASP

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Mol	Chain	Res	Type
1	A	514	LYS
2	B	16	ILE
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	171	LYS
3	C	17	PRO
3	C	38	ASN
3	C	40	MET
3	C	127	LEU
3	C	159	MET
3	C	230	ASN
4	D	5	VAL
4	D	7	LYS
4	D	8	SER
4	D	51	LEU
4	D	58	GLU
4	D	107	ILE
5	E	5	HIS
5	E	90	ARG
6	F	52	ILE
6	F	54	ASN
6	F	80	GLN
6	F	87	THR
6	F	95	GLN
7	G	5	LYS
7	G	33	LEU
7	G	37	LEU
7	G	42	ARG
7	G	83	GLU
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	50	VAL
8	H	60	TYR
8	H	61	LYS
8	H	84	LYS
9	I	18	ARG
9	I	21	ILE

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Mol	Chain	Res	Type
9	I	29	LEU
9	I	31	PHE
9	I	33	THR
9	I	37	PHE
9	I	41	GLU
10	J	50	LEU
11	K	7	PRO
11	K	54	ARG
12	L	2	HIS
12	L	4	GLU
12	L	5	GLU
12	L	26	THR
13	M	19	LEU
13	M	34	LEU
13	M	38	ASP
13	M	40	TYR
1	N	35	LEU
1	N	115	SER
1	N	128	VAL
1	N	138	HIS
1	N	152	LEU
1	N	363	LEU
1	N	369	ASP
1	N	504	THR
2	O	33	LEU
2	O	49	LYS
2	O	59	GLN
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	89	GLU
2	O	94	SER
2	O	115	ASP
2	O	129	LYS
2	O	166	PRO
2	O	167	SER
2	O	171	LYS
2	O	226	MET
3	P	110	PRO

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Mol	Chain	Res	Type
3	P	159	MET
3	P	230	ASN
4	Q	4	SER
4	Q	6	VAL
4	Q	7	LYS
4	Q	19[A]	ARG
4	Q	19[B]	ARG
4	Q	21	ASP
4	Q	31	LYS
4	Q	43	LYS
4	Q	51	LEU
5	R	6	GLU
5	R	80	GLU
5	R	109	VAL
6	S	2	SER
6	S	44	GLU
6	S	48	LEU
6	S	52	ILE
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
6	S	87	THR
7	T	33	LEU
7	T	35	SER
7	T	36	TRP
7	T	38	HIS
7	T	84	LYS
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	21	ILE
9	V	31	PHE
9	V	36	LYS
9	V	73	LYS
10	W	2	GLU
10	W	7	GLU
10	W	50	LEU
11	X	54	ARG
12	Y	2	HIS
12	Y	5	GLU
12	Y	20	ARG
13	Z	34	LEU

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Mol	Chain	Res	Type
13	Z	43	SER
14	1	14	CYS
14	1	20	VAL
14	1	25	LYS
14	1	38	ARG
14	1	53	LYS
14	1	69	GLU
14	1	86	LYS
14	1	100	LYS
14	2	3	VAL
14	2	14	CYS
14	2	16	GLN
14	2	17	CYS
14	2	19	THR
14	2	20	VAL
14	2	26	HIS
14	2	27	LYS
14	2	28	THR
14	2	38	ARG
14	2	39	LYS
14	2	40	THR
14	2	47	THR
14	2	57	ILE
14	2	72	LYS
14	2	79	LYS
14	2	80	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	10	GLN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN

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Mol	Chain	Res	Type
4	D	109	HIS
4	D	119	GLN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
6	F	94	HIS
6	F	95	GLN
6	F	98	HIS
7	G	8	HIS
8	H	22	ASN
9	I	20	HIS
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
12	L	2	HIS
1	N	4	ASN
1	N	55	ASN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
1	N	422	ASN
1	N	503	HIS
1	N	512	ASN
2	O	10	GLN
2	O	92	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
3	P	161	GLN
3	P	222	GLN
4	Q	37	GLN
4	Q	76	ASN
4	Q	101	HIS
4	Q	119	GLN
5	R	78	HIS
5	R	94	ASN
6	S	54	ASN

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Mol	Chain	Res	Type
6	S	80	GLN
7	T	8	HIS
7	T	38	HIS
8	U	10	ASN
8	U	12	GLN
8	U	31	GLN
8	U	37	HIS
9	V	20	HIS
9	V	53	ASN
10	W	29	ASN
14	1	33	HIS
14	1	103	ASN
14	2	16	GLN
14	2	26	HIS
14	2	54	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
7	TPO	T	11	7	8,10,11	2.15	2 (25%)	10,14,16	1.27	1 (10%)
2	FME	O	1	2	8,9,10	0.83	0	7,9,11	0.96	0
9	SAC	I	1	9	7,8,9	2.23	2 (28%)	8,9,11	2.36	3 (37%)
2	FME	B	1	2	8,9,10	2.62	3 (37%)	7,9,11	8.29	5 (71%)
7	TPO	G	11	7	8,10,11	1.80	2 (25%)	10,14,16	1.05	0
1	FME	A	1	1	8,9,10	1.47	1 (12%)	7,9,11	5.60	5 (71%)
1	FME	N	1	1	8,9,10	0.82	0	7,9,11	6.36	5 (71%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	V	1	9	7,8,9	2.50	2 (28%)	8,9,11	1.76	3 (37%)

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
7	TPO	T	11	7	-	6/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	6/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	4/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	2/7/8/10	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	5.44	1.54	1.46
9	V	1	SAC	OAC-C1A	4.88	1.34	1.23
9	I	1	SAC	OAC-C1A	4.72	1.33	1.23
9	V	1	SAC	CA-N	4.17	1.52	1.46
2	B	1	FME	O1-CN	-3.92	1.10	1.22
1	A	1	FME	CA-N	3.68	1.51	1.46
7	T	11	TPO	P-O1P	3.58	1.62	1.50
7	T	11	TPO	P-OG1	3.35	1.65	1.59
9	I	1	SAC	CA-N	3.20	1.50	1.46
7	G	11	TPO	P-O1P	3.13	1.60	1.50
7	G	11	TPO	P-OG1	3.10	1.65	1.59
2	B	1	FME	CB-CA	2.66	1.58	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.68	91.02	122.82
1	N	1	FME	CA-N-CN	-15.59	98.84	122.82
1	A	1	FME	CA-N-CN	-13.93	101.39	122.82
2	B	1	FME	O1-CN-N	5.84	140.65	125.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	CA-N-C1A	4.65	131.72	123.15
1	N	1	FME	CE-SD-CG	3.93	113.91	100.40
9	I	1	SAC	C2A-C1A-N	3.44	121.92	116.10
2	B	1	FME	C-CA-N	3.13	115.39	109.73
1	A	1	FME	CE-SD-CG	3.08	111.00	100.40
1	N	1	FME	O1-CN-N	2.92	132.96	125.27
1	N	1	FME	C-CA-N	-2.85	104.58	109.73
7	T	11	TPO	P-OG1-CB	2.58	131.00	123.21
1	A	1	FME	CG-CB-CA	-2.55	105.87	112.95
9	V	1	SAC	C2A-C1A-N	2.54	120.40	116.10
9	V	1	SAC	CA-N-C1A	2.51	127.78	123.15
1	N	1	FME	CG-CB-CA	-2.42	106.21	112.95
9	V	1	SAC	C-CA-N	2.31	113.91	109.73
1	A	1	FME	O1-CN-N	2.20	131.07	125.27
2	B	1	FME	O-C-CA	-2.15	119.13	124.78
2	B	1	FME	CG-CB-CA	-2.07	107.21	112.95
9	I	1	SAC	OAC-C1A-N	-2.02	118.25	121.95
1	A	1	FME	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	CB-CA-N-C1A
9	I	1	SAC	O-C-CA-CB
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	CA-CB-OG1-P
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
1	N	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
9	I	1	SAC	N-CA-CB-OG
1	A	1	FME	CB-CG-SD-CE
7	G	11	TPO	N-CA-CB-CG2
7	T	11	TPO	CB-OG1-P-O1P
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O3P
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1	SAC	1	0
2	B	1	FME	2	0
7	G	11	TPO	2	0
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 10 are monoatomic and 15 are unknown - leaving 51 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	EDO	S	102	-	3,3,3	0.64	0	2,2,2	0.79	0
26	CDL	G	101	-	99,99,99	1.44	12 (12%)	105,111,111	1.35	13 (12%)
25	PEK	P	303	-	52,52,52	0.99	3 (5%)	55,57,57	0.96	2 (3%)
31	HEC	2	201	14	50,50,50	1.77	9 (18%)	68,82,82	1.62	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DMU	M	101	-	34,34,34	0.74	0	45,45,45	1.77	9 (20%)
23	EDO	N	614	-	3,3,3	0.41	0	2,2,2	0.47	0
20	PGV	N	612	-	50,50,50	0.85	1 (2%)	53,56,56	1.21	4 (7%)
30	DMU	Z	101	-	34,34,34	0.75	1 (2%)	45,45,45	1.07	5 (11%)
24	CHD	G	102	-	32,32,32	1.13	2 (6%)	51,51,51	1.99	13 (25%)
18	HEA	N	605[B]	-	66,67,67	1.92	21 (31%)	78,103,103	1.88	20 (25%)
19	PER	N	607	15,18	1,1,1	1.16	0	-		
24	CHD	C	307	-	32,32,32	0.91	1 (3%)	51,51,51	3.50	25 (49%)
20	PGV	C	305	-	50,50,50	1.40	3 (6%)	53,56,56	1.42	7 (13%)
26	CDL	C	306	-	99,99,99	1.39	12 (12%)	105,111,111	1.41	10 (9%)
24	CHD	P	301	-	32,32,32	1.09	2 (6%)	51,51,51	1.85	13 (25%)
19	PER	A	606	15,18	1,1,1	0.72	0	-		
23	EDO	E	202	-	3,3,3	0.50	0	2,2,2	0.73	0
18	HEA	A	605	1,19	66,67,67	2.08	23 (34%)	78,103,103	1.74	23 (29%)
26	CDL	T	101	-	99,99,99	1.43	12 (12%)	105,111,111	1.48	15 (14%)
23	EDO	C	311	-	3,3,3	0.61	0	2,2,2	0.29	0
22	CUA	O	301	2	0,1,1	-	-	-		
24	CHD	P	307	-	32,32,32	0.64	0	51,51,51	2.37	19 (37%)
21	TGL	D	201	-	62,62,62	1.39	6 (9%)	65,65,65	1.51	8 (12%)
20	PGV	P	305	-	50,50,50	1.29	2 (4%)	53,56,56	1.39	6 (11%)
20	PGV	C	304	-	50,50,50	0.80	2 (4%)	53,56,56	1.33	7 (13%)
18	HEA	N	606	1,19	66,67,67	2.18	23 (34%)	78,103,103	1.59	17 (21%)
24	CHD	T	103	-	32,32,32	1.25	4 (12%)	51,51,51	2.01	18 (35%)
20	PGV	A	608	-	50,50,50	1.06	4 (8%)	53,56,56	1.28	6 (11%)
28	PSC	V	101	-	51,51,51	1.21	3 (5%)	57,59,59	1.31	5 (8%)
31	HEC	1	201	14	50,50,50	1.69	8 (16%)	68,82,82	1.98	17 (25%)
21	TGL	B	301	-	62,62,62	1.45	8 (12%)	65,65,65	1.87	13 (20%)
23	EDO	I	101	-	3,3,3	0.63	0	2,2,2	0.28	0
23	EDO	N	613	-	3,3,3	0.57	0	2,2,2	0.37	0
24	CHD	C	301	-	32,32,32	1.31	4 (12%)	51,51,51	1.76	10 (19%)
22	CUA	B	302	2	0,1,1	-	-	-		
23	EDO	G	103	-	3,3,3	0.84	0	2,2,2	0.68	0
18	HEA	A	604[A]	-	66,67,67	1.81	22 (33%)	78,103,103	1.91	21 (26%)
24	CHD	W	101	-	32,32,32	0.92	2 (6%)	51,51,51	3.13	23 (45%)
23	EDO	B	303	-	3,3,3	0.78	0	2,2,2	0.48	0
20	PGV	P	304	-	50,50,50	0.82	2 (4%)	53,56,56	1.17	6 (11%)
21	TGL	Q	201	-	62,62,62	1.40	6 (9%)	65,65,65	1.29	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	C	303	-	52,52,52	0.96	2 (3%)	55,57,57	1.20	5 (9%)
21	TGL	L	101	-	62,62,62	1.56	6 (9%)	65,65,65	1.58	14 (21%)
20	PGV	A	607	-	50,50,50	1.12	2 (4%)	53,56,56	1.05	5 (9%)
21	TGL	N	608	-	62,62,62	1.48	8 (12%)	65,65,65	2.09	14 (21%)
26	CDL	P	306	-	99,99,99	1.41	12 (12%)	105,111,111	1.22	10 (9%)
24	CHD	J	101	-	32,32,32	0.89	1 (3%)	51,51,51	2.13	15 (29%)
18	HEA	N	605[A]	-	66,67,67	1.92	21 (31%)	78,103,103	1.86	18 (23%)
28	PSC	E	201	-	51,51,51	1.32	3 (5%)	57,59,59	1.51	9 (15%)
23	EDO	F	102	-	3,3,3	0.45	0	2,2,2	0.54	0
18	HEA	A	604[B]	-	66,67,67	1.80	21 (31%)	78,103,103	1.86	21 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	EDO	S	102	-	-	0/1/1/1	-
26	CDL	G	101	-	-	58/110/110/110	-
31	HEC	2	201	14	1/1/3/7	10/14/54/54	-
25	PEK	P	303	-	-	20/56/56/56	-
30	DMU	M	101	-	-	6/19/59/59	0/2/2/2
23	EDO	N	614	-	-	1/1/1/1	-
20	PGV	N	612	-	-	9/55/55/55	-
30	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
24	CHD	G	102	-	-	3/9/74/74	0/4/4/4
18	HEA	N	605[B]	-	-	8/36/76/76	-
24	CHD	C	307	-	-	8/9/74/74	0/4/4/4
20	PGV	C	305	-	-	30/55/55/55	-
26	CDL	C	306	-	-	62/110/110/110	-
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
23	EDO	E	202	-	-	1/1/1/1	-
18	HEA	A	605	1,19	-	7/36/76/76	-
26	CDL	T	101	-	-	61/110/110/110	-
23	EDO	C	311	-	-	1/1/1/1	-
24	CHD	P	307	-	-	5/9/74/74	1/4/4/4
21	TGL	D	201	-	-	38/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	305	-	-	31/55/55/55	-
20	PGV	C	304	-	-	19/55/55/55	-
18	HEA	N	606	1,19	-	6/36/76/76	-
24	CHD	T	103	-	-	2/9/74/74	0/4/4/4
20	PGV	A	608	-	-	12/55/55/55	-
28	PSC	V	101	-	-	35/55/55/55	-
31	HEC	1	201	14	1/1/3/7	3/14/54/54	-
21	TGL	B	301	-	-	33/65/65/65	-
23	EDO	I	101	-	-	0/1/1/1	-
23	EDO	N	613	-	-	0/1/1/1	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
23	EDO	G	103	-	-	0/1/1/1	-
18	HEA	A	604[A]	-	-	5/36/76/76	-
24	CHD	W	101	-	-	8/9/74/74	0/4/4/4
23	EDO	B	303	-	-	1/1/1/1	-
20	PGV	P	304	-	-	12/55/55/55	-
21	TGL	Q	201	-	-	35/65/65/65	-
25	PEK	C	303	-	-	20/56/56/56	-
21	TGL	L	101	-	-	46/65/65/65	-
20	PGV	A	607	-	-	30/55/55/55	-
21	TGL	N	608	-	-	34/65/65/65	-
26	CDL	P	306	-	-	67/110/110/110	-
24	CHD	J	101	-	-	7/9/74/74	0/4/4/4
18	HEA	N	605[A]	-	-	6/36/76/76	-
28	PSC	E	201	-	-	36/55/55/55	-
23	EDO	F	102	-	-	0/1/1/1	-
18	HEA	A	604[B]	-	-	6/36/76/76	-

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	101	TGL	OG2-CB1	7.00	1.54	1.34
31	2	201	HEC	FE-NB	5.90	2.13	1.94
20	C	305	PGV	O01-C1	5.88	1.50	1.34
21	L	101	TGL	OG3-CC1	5.77	1.50	1.33
28	E	201	PSC	O01-C1	5.63	1.50	1.34
28	V	101	PSC	O01-C1	5.60	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	101	CDL	OB6-CB5	5.47	1.49	1.34
18	A	605	HEA	FE-NB	5.42	2.11	1.94
21	N	608	TGL	OG2-CB1	5.40	1.49	1.34
31	2	201	HEC	FE-NC	5.36	2.13	1.95
26	C	306	CDL	OB8-CB7	5.36	1.49	1.33
20	P	305	PGV	O03-C19	5.29	1.48	1.33
21	N	608	TGL	OG1-CA1	5.28	1.48	1.33
26	T	101	CDL	OB6-CB5	5.28	1.49	1.34
21	D	201	TGL	OG1-CA1	5.22	1.48	1.33
26	C	306	CDL	OA6-CA5	5.21	1.49	1.34
20	C	305	PGV	O03-C19	5.19	1.48	1.33
20	P	305	PGV	O01-C1	5.16	1.48	1.34
21	B	301	TGL	OG3-CC1	5.15	1.48	1.33
21	Q	201	TGL	OG2-CB1	5.13	1.48	1.34
26	P	306	CDL	OA8-CA7	5.11	1.48	1.33
18	A	605	HEA	FE-NA	5.07	2.12	1.95
26	T	101	CDL	OA8-CA7	5.07	1.48	1.33
26	T	101	CDL	OA6-CA5	5.07	1.48	1.34
20	A	607	PGV	O03-C19	5.05	1.48	1.33
21	N	608	TGL	OG3-CC1	5.04	1.48	1.33
18	N	606	HEA	FE-ND	5.04	2.10	1.94
26	G	101	CDL	OB8-CB7	5.03	1.48	1.33
21	Q	201	TGL	OG3-CC1	5.02	1.48	1.33
21	D	201	TGL	OG2-CB1	5.02	1.48	1.34
26	P	306	CDL	OA6-CA5	5.01	1.48	1.34
31	1	201	HEC	FE-NB	5.00	2.10	1.94
18	N	606	HEA	FE-NC	4.98	2.12	1.95
26	C	306	CDL	OA8-CA7	4.94	1.47	1.33
21	B	301	TGL	OG1-CA1	4.93	1.47	1.33
26	P	306	CDL	OB8-CB7	4.92	1.47	1.33
31	1	201	HEC	FE-NC	4.91	2.11	1.95
21	Q	201	TGL	OG1-CA1	4.88	1.47	1.33
18	N	606	HEA	CHA-C1A	4.77	1.47	1.38
26	G	101	CDL	OA8-CA7	4.77	1.47	1.33
21	L	101	TGL	OG1-CA1	4.76	1.47	1.33
18	A	605	HEA	FE-ND	4.69	2.09	1.94
21	D	201	TGL	OG3-CC1	4.69	1.47	1.33
28	E	201	PSC	O03-C19	4.69	1.47	1.33
26	P	306	CDL	OB6-CB5	4.68	1.47	1.34
26	T	101	CDL	OB8-CB7	4.66	1.46	1.33
26	G	101	CDL	OA6-CA5	4.59	1.47	1.34
20	N	612	PGV	O03-C19	4.55	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	605	HEA	C4A-NA	-4.42	1.31	1.39
25	P	303	PEK	O01-C1	4.40	1.46	1.34
18	A	605	HEA	CHC-C4B	4.38	1.47	1.38
18	N	606	HEA	C4D-C3D	-4.35	1.37	1.45
18	N	605[A]	HEA	FE-NB	4.33	2.08	1.94
18	N	605[B]	HEA	FE-NB	4.33	2.08	1.94
25	C	303	PEK	O01-C1	4.33	1.46	1.34
21	B	301	TGL	OG2-CB1	4.30	1.46	1.34
18	N	605[A]	HEA	FE-NA	4.27	2.09	1.95
18	N	605[B]	HEA	FE-NA	4.27	2.09	1.95
20	A	607	PGV	O01-C1	4.24	1.46	1.34
18	N	606	HEA	C1D-ND	-4.13	1.33	1.40
31	1	201	HEC	CBC-CAC	-3.98	1.33	1.51
18	N	606	HEA	CHC-C1C	3.95	1.48	1.39
20	A	608	PGV	O03-C19	3.94	1.44	1.33
18	N	605[A]	HEA	FE-NC	3.90	2.08	1.95
18	N	605[B]	HEA	FE-NC	3.90	2.08	1.95
31	2	201	HEC	CBB-CAB	-3.89	1.34	1.51
21	B	301	TGL	OC1-CC1	-3.88	1.11	1.22
31	2	201	HEC	CBC-CAC	-3.86	1.34	1.51
18	A	605	HEA	CHA-C1A	3.81	1.45	1.38
31	1	201	HEC	CBB-CAB	-3.81	1.34	1.51
28	V	101	PSC	O03-C19	3.79	1.44	1.33
18	N	606	HEA	FE-NA	3.78	2.08	1.95
26	C	306	CDL	OB6-CB5	3.77	1.44	1.34
28	E	201	PSC	C13-C12	3.74	1.53	1.31
28	V	101	PSC	C13-C12	3.71	1.53	1.31
18	A	604[A]	HEA	C4D-C3D	-3.63	1.38	1.45
18	A	604[B]	HEA	C4D-C3D	-3.63	1.38	1.45
18	N	606	HEA	CHD-C1D	3.62	1.45	1.38
18	A	604[A]	HEA	C1D-ND	-3.59	1.34	1.40
18	A	604[B]	HEA	C1D-ND	-3.59	1.34	1.40
18	N	605[A]	HEA	CHA-C1A	3.57	1.45	1.38
18	N	605[B]	HEA	CHA-C1A	3.57	1.45	1.38
18	A	605	HEA	C1A-NA	-3.46	1.33	1.39
26	P	306	CDL	C59-C58	-3.43	1.32	1.51
24	G	102	CHD	C4-C3	3.36	1.58	1.51
25	P	303	PEK	O03-C21	3.33	1.43	1.33
18	A	604[A]	HEA	C3A-C4A	-3.32	1.40	1.46
18	A	604[B]	HEA	C3A-C4A	-3.32	1.40	1.46
21	L	101	TGL	C20-CA9	-3.30	1.33	1.51
18	N	605[A]	HEA	C4A-NA	-3.29	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	605[B]	HEA	C4A-NA	-3.29	1.33	1.39
31	1	201	HEC	C4B-NB	-3.26	1.34	1.40
18	N	605[A]	HEA	CHC-C4B	3.25	1.45	1.38
18	N	605[B]	HEA	CHC-C4B	3.25	1.45	1.38
18	N	606	HEA	CHB-C4A	3.25	1.44	1.38
18	N	605[A]	HEA	C1A-C2A	-3.23	1.39	1.45
18	N	605[B]	HEA	C1A-C2A	-3.23	1.39	1.45
26	C	306	CDL	C59-C58	-3.22	1.33	1.51
20	P	304	PGV	O01-C1	3.17	1.43	1.34
26	P	306	CDL	C82-C81	-3.16	1.33	1.51
18	N	605[A]	HEA	C3A-C4A	-3.16	1.40	1.46
18	N	605[B]	HEA	C3A-C4A	-3.16	1.40	1.46
26	T	101	CDL	C59-C58	-3.15	1.33	1.51
18	N	606	HEA	O11-C11	3.11	1.49	1.42
21	N	608	TGL	C20-CA9	-3.11	1.34	1.51
21	L	101	TGL	C10-CB9	-3.11	1.34	1.51
26	C	306	CDL	C79-C78	-3.10	1.34	1.51
20	C	304	PGV	O03-C19	3.09	1.42	1.33
26	C	306	CDL	C62-C61	-3.09	1.34	1.51
26	C	306	CDL	C19-C18	-3.08	1.34	1.51
18	A	604[A]	HEA	CHA-C1A	3.07	1.44	1.38
18	A	604[B]	HEA	CHA-C1A	3.07	1.44	1.38
18	N	606	HEA	C4A-NA	-3.07	1.33	1.39
21	Q	201	TGL	C15-CC9	-3.06	1.34	1.51
26	G	101	CDL	C42-C41	-3.05	1.34	1.51
24	T	103	CHD	C4-C3	3.04	1.57	1.51
26	P	306	CDL	C79-C78	-3.04	1.34	1.51
26	T	101	CDL	C19-C18	-3.03	1.34	1.51
26	G	101	CDL	C22-C21	-3.03	1.34	1.51
18	A	605	HEA	CHC-C1C	3.03	1.46	1.39
26	G	101	CDL	C62-C61	-3.01	1.34	1.51
21	D	201	TGL	C10-CB9	-3.00	1.34	1.51
26	C	306	CDL	C82-C81	-2.99	1.34	1.51
26	C	306	CDL	C22-C21	-2.99	1.34	1.51
26	P	306	CDL	C19-C18	-2.99	1.34	1.51
25	C	303	PEK	O03-C21	2.99	1.42	1.33
18	N	605[A]	HEA	C1D-ND	-2.99	1.35	1.40
18	N	605[B]	HEA	C1D-ND	-2.99	1.35	1.40
21	D	201	TGL	C15-CC9	-2.98	1.34	1.51
26	T	101	CDL	C62-C61	-2.97	1.34	1.51
26	P	306	CDL	C62-C61	-2.95	1.35	1.51
21	N	608	TGL	C15-CC9	-2.94	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	605[A]	HEA	C4B-NB	-2.94	1.35	1.40
18	N	605[B]	HEA	C4B-NB	-2.94	1.35	1.40
26	P	306	CDL	C39-C38	-2.94	1.35	1.51
26	C	306	CDL	C42-C41	-2.94	1.35	1.51
26	P	306	CDL	C22-C21	-2.93	1.35	1.51
26	P	306	CDL	C42-C41	-2.93	1.35	1.51
18	N	605[A]	HEA	CHB-C1B	2.93	1.45	1.39
18	N	605[B]	HEA	CHB-C1B	2.93	1.45	1.39
26	T	101	CDL	C39-C38	-2.92	1.35	1.51
21	B	301	TGL	C15-CC9	-2.92	1.35	1.51
21	Q	201	TGL	C10-CB9	-2.92	1.35	1.51
26	G	101	CDL	C19-C18	-2.92	1.35	1.51
26	G	101	CDL	C39-C38	-2.91	1.35	1.51
21	B	301	TGL	C20-CA9	-2.91	1.35	1.51
26	T	101	CDL	C82-C81	-2.90	1.35	1.51
26	G	101	CDL	C82-C81	-2.88	1.35	1.51
18	A	605	HEA	C1D-ND	-2.88	1.35	1.40
20	P	304	PGV	O03-C19	2.84	1.41	1.33
18	N	606	HEA	CHD-C4C	2.83	1.45	1.39
24	G	102	CHD	C13-C14	-2.83	1.50	1.55
18	N	605[A]	HEA	FE-ND	2.82	2.03	1.94
18	N	605[B]	HEA	FE-ND	2.82	2.03	1.94
26	G	101	CDL	C79-C78	-2.82	1.35	1.51
26	G	101	CDL	C59-C58	-2.82	1.35	1.51
24	T	103	CHD	O26-C24	-2.82	1.21	1.30
18	N	605[A]	HEA	CHC-C1C	2.80	1.45	1.39
18	N	605[B]	HEA	CHC-C1C	2.80	1.45	1.39
18	N	606	HEA	FE-NB	2.80	2.03	1.94
26	T	101	CDL	C22-C21	-2.80	1.35	1.51
18	A	605	HEA	CMC-C2C	2.79	1.56	1.50
21	N	608	TGL	C10-CB9	-2.79	1.35	1.51
18	A	605	HEA	C1B-NB	-2.78	1.33	1.38
26	T	101	CDL	C42-C41	-2.77	1.36	1.51
20	A	608	PGV	O01-C1	2.77	1.42	1.34
21	D	201	TGL	C20-CA9	-2.77	1.36	1.51
18	N	605[A]	HEA	O11-C11	2.76	1.48	1.42
18	N	605[B]	HEA	O11-C11	2.76	1.48	1.42
18	N	605[A]	HEA	CHB-C4A	2.76	1.43	1.38
18	N	605[B]	HEA	CHB-C4A	2.76	1.43	1.38
18	N	605[A]	HEA	CHA-C4D	2.74	1.45	1.39
18	N	605[B]	HEA	CHA-C4D	2.74	1.45	1.39
24	C	301	CHD	C8-C7	2.73	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	604[A]	HEA	FE-ND	2.72	2.03	1.94
18	A	604[B]	HEA	FE-ND	2.72	2.03	1.94
18	A	604[A]	HEA	CHD-C1D	2.72	1.44	1.38
18	A	604[B]	HEA	CHD-C1D	2.72	1.44	1.38
26	T	101	CDL	C79-C78	-2.71	1.36	1.51
21	L	101	TGL	C15-CC9	-2.70	1.36	1.51
18	A	604[A]	HEA	CHC-C4B	2.67	1.44	1.38
18	A	604[B]	HEA	CHC-C4B	2.67	1.44	1.38
18	N	606	HEA	C3B-C2B	2.67	1.40	1.34
18	A	604[A]	HEA	C4C-NC	-2.66	1.34	1.39
18	A	604[B]	HEA	C4C-NC	-2.66	1.34	1.39
31	2	201	HEC	C4B-C3B	2.66	1.49	1.45
24	P	301	CHD	C18-C13	2.64	1.58	1.54
26	C	306	CDL	C39-C38	-2.64	1.36	1.51
18	N	605[A]	HEA	C3B-C2B	2.62	1.40	1.34
18	N	605[B]	HEA	C3B-C2B	2.62	1.40	1.34
18	N	606	HEA	C1C-NC	-2.61	1.34	1.39
18	N	606	HEA	C3A-C4A	-2.60	1.41	1.46
18	A	604[A]	HEA	C4A-NA	-2.58	1.34	1.39
18	A	604[B]	HEA	C4A-NA	-2.58	1.34	1.39
18	A	605	HEA	FE-NC	2.57	2.03	1.95
24	P	301	CHD	C8-C7	2.57	1.57	1.53
18	A	604[A]	HEA	CHA-C4D	2.55	1.45	1.39
18	A	604[B]	HEA	CHA-C4D	2.55	1.45	1.39
30	Z	101	DMU	O16-C6	2.54	1.44	1.40
24	C	301	CHD	C11-C9	2.52	1.57	1.53
18	N	606	HEA	C4C-NC	-2.50	1.34	1.39
18	N	606	HEA	C1A-C2A	-2.50	1.40	1.45
18	A	605	HEA	C3B-C2B	2.50	1.40	1.34
21	Q	201	TGL	C20-CA9	-2.50	1.37	1.51
21	B	301	TGL	C10-CB9	-2.50	1.37	1.51
18	A	605	HEA	CBA-CAA	2.49	1.59	1.52
31	1	201	HEC	C1D-C2D	2.48	1.49	1.44
24	C	301	CHD	C16-C17	2.48	1.59	1.54
18	A	605	HEA	C18-C19	2.45	1.38	1.33
18	A	604[A]	HEA	CMA-C3A	2.45	1.50	1.45
18	A	604[B]	HEA	CMA-C3A	2.45	1.50	1.45
24	T	103	CHD	C11-C9	2.44	1.57	1.53
18	N	606	HEA	C4B-C3B	-2.44	1.40	1.44
20	C	305	PGV	C01-C02	2.41	1.58	1.50
18	A	604[A]	HEA	C1B-C2B	-2.41	1.39	1.44
18	A	604[B]	HEA	C1B-C2B	-2.41	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	605[A]	HEA	C4C-NC	-2.40	1.35	1.39
18	N	605[B]	HEA	C4C-NC	-2.40	1.35	1.39
21	N	608	TGL	OC1-CC1	-2.39	1.15	1.22
18	A	604[A]	HEA	FE-NB	2.36	2.02	1.94
18	A	604[B]	HEA	FE-NB	2.36	2.02	1.94
18	N	605[A]	HEA	CMB-C2B	2.35	1.55	1.50
18	N	605[B]	HEA	CMB-C2B	2.35	1.55	1.50
31	2	201	HEC	C1D-ND	-2.34	1.36	1.40
18	A	604[A]	HEA	C3B-C2B	2.31	1.40	1.34
18	A	604[B]	HEA	C3B-C2B	2.31	1.40	1.34
20	A	608	PGV	O03-C01	2.31	1.50	1.45
18	N	605[A]	HEA	CHD-C4C	2.31	1.44	1.39
18	N	605[B]	HEA	CHD-C4C	2.31	1.44	1.39
18	A	605	HEA	C4B-NB	-2.29	1.36	1.40
18	A	605	HEA	C4C-NC	-2.29	1.35	1.39
18	A	604[A]	HEA	C4B-C3B	-2.29	1.40	1.44
18	A	604[B]	HEA	C4B-C3B	-2.29	1.40	1.44
18	N	605[A]	HEA	CHD-C1D	2.28	1.43	1.38
18	N	605[B]	HEA	CHD-C1D	2.28	1.43	1.38
25	P	303	PEK	O03-C01	-2.27	1.40	1.45
18	N	606	HEA	C18-C19	2.27	1.38	1.33
24	W	101	CHD	C20-C17	2.23	1.58	1.54
18	A	605	HEA	CHB-C4A	2.22	1.42	1.38
18	A	605	HEA	C4D-C3D	-2.22	1.41	1.45
20	C	304	PGV	O01-C1	2.22	1.40	1.34
18	N	606	HEA	CMA-C3A	2.21	1.49	1.45
18	A	604[A]	HEA	C22-C23	2.21	1.38	1.32
18	A	604[A]	HEA	CHC-C1C	2.20	1.44	1.39
18	A	604[B]	HEA	CHC-C1C	2.20	1.44	1.39
20	A	608	PGV	O01-C02	-2.19	1.41	1.46
24	C	301	CHD	C18-C13	2.18	1.57	1.54
18	N	606	HEA	CAA-C2A	2.18	1.56	1.51
31	1	201	HEC	FE-NA	2.17	2.02	1.95
18	A	604[A]	HEA	FE-NA	2.15	2.02	1.95
18	A	604[B]	HEA	FE-NA	2.15	2.02	1.95
31	2	201	HEC	C1D-C2D	2.13	1.48	1.44
31	1	201	HEC	CHD-C1D	2.12	1.42	1.38
18	N	606	HEA	C1B-NB	-2.12	1.34	1.38
18	A	604[A]	HEA	C1D-C2D	-2.11	1.40	1.44
18	A	604[B]	HEA	C1D-C2D	-2.11	1.40	1.44
24	T	103	CHD	C23-C24	2.10	1.55	1.50
18	A	605	HEA	C4B-C3B	-2.08	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	604[A]	HEA	C14-C15	2.08	1.38	1.33
18	A	604[B]	HEA	C14-C15	2.08	1.38	1.33
18	A	605	HEA	CHD-C1D	2.08	1.42	1.38
21	N	608	TGL	OG2-CG2	2.07	1.51	1.46
24	J	101	CHD	C2-C3	2.07	1.56	1.51
24	C	307	CHD	C11-C12	2.07	1.56	1.53
18	A	604[A]	HEA	C1B-NB	-2.06	1.34	1.38
18	A	604[B]	HEA	C1B-NB	-2.06	1.34	1.38
21	B	301	TGL	OG1-CG1	-2.05	1.40	1.45
18	A	605	HEA	C16-C15	2.05	1.55	1.51
24	W	101	CHD	C13-C17	2.05	1.59	1.55
31	2	201	HEC	C4B-NB	-2.02	1.36	1.40
18	A	605	HEA	C1B-C2B	-2.02	1.40	1.44
18	A	604[A]	HEA	CMC-C2C	2.02	1.55	1.50
18	A	604[B]	HEA	CMC-C2C	2.02	1.55	1.50
31	2	201	HEC	C4D-C3D	2.01	1.48	1.45

All (470) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	307	CHD	C10-C9-C8	10.37	122.96	111.82
24	W	101	CHD	C17-C13-C12	9.83	126.64	117.67
24	C	307	CHD	C6-C5-C4	-7.51	102.55	111.19
24	W	101	CHD	C13-C17-C20	7.48	128.43	119.50
24	C	307	CHD	C4-C5-C10	7.22	120.33	112.66
24	G	102	CHD	C6-C7-C8	6.79	118.73	111.48
21	B	301	TGL	CG2-OG2-CB1	6.74	134.38	117.79
31	1	201	HEC	C4B-NB-C1B	6.74	112.03	105.07
21	N	608	TGL	CG2-OG2-CB1	6.60	134.03	117.79
21	D	201	TGL	OG2-CB1-CB2	6.52	125.56	111.50
28	E	201	PSC	O01-C1-C2	6.43	125.35	111.50
24	C	307	CHD	C15-C14-C8	6.42	127.30	118.33
24	C	307	CHD	C19-C10-C1	-6.40	97.94	108.26
24	W	101	CHD	C15-C14-C8	6.24	127.05	118.33
24	C	307	CHD	C11-C9-C8	-6.05	102.02	110.88
26	T	101	CDL	OB6-CB5-C51	5.97	124.36	111.50
21	N	608	TGL	OG3-CC1-CC2	5.87	130.33	111.91
24	P	307	CHD	C9-C10-C5	5.85	116.79	108.58
24	W	101	CHD	C1-C10-C5	5.81	116.36	107.77
21	L	101	TGL	OG2-CB1-CB2	5.79	123.98	111.50
24	C	307	CHD	C11-C12-C13	5.77	117.16	111.24
21	B	301	TGL	CG3-OG3-CC1	5.76	138.47	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	301	CHD	C15-C14-C13	5.69	109.13	103.55
24	C	307	CHD	C6-C7-C8	-5.65	105.45	111.48
26	C	306	CDL	CB4-OB6-CB5	-5.63	103.92	117.79
24	P	307	CHD	C10-C9-C8	5.61	117.84	111.82
24	G	102	CHD	C6-C5-C4	-5.56	104.78	111.19
24	J	101	CHD	C13-C17-C20	5.56	126.13	119.50
24	T	103	CHD	C18-C13-C12	-5.54	103.42	109.07
18	N	605[A]	HEA	C13-C12-C11	-5.53	106.05	114.35
18	N	605[B]	HEA	C13-C12-C11	-5.53	106.05	114.35
21	B	301	TGL	OG2-CG2-CG1	5.49	128.27	108.40
26	G	101	CDL	OB6-CB5-C51	5.47	123.30	111.50
20	P	305	PGV	O01-C1-C2	5.46	123.26	111.50
24	W	101	CHD	C17-C13-C14	-5.43	94.62	100.09
24	P	307	CHD	C9-C11-C12	-5.33	107.27	114.30
21	B	301	TGL	OG2-CB1-CB2	5.28	122.89	111.50
24	W	101	CHD	C14-C8-C7	5.27	118.80	111.81
26	T	101	CDL	OA6-CA5-C11	5.24	122.80	111.50
24	W	101	CHD	C14-C8-C9	-5.22	102.55	109.71
24	J	101	CHD	C22-C20-C17	5.22	121.07	110.28
24	C	307	CHD	C11-C9-C10	5.22	119.11	113.73
21	N	608	TGL	OG1-CA1-CA2	5.19	128.20	111.91
18	N	605[A]	HEA	C3C-C4C-NC	5.19	113.44	110.25
18	N	605[B]	HEA	C3C-C4C-NC	5.19	113.44	110.25
18	A	604[A]	HEA	C13-C12-C11	-5.16	106.60	114.35
18	A	604[B]	HEA	C13-C12-C11	-5.16	106.60	114.35
21	N	608	TGL	OG2-CB1-CB2	5.10	122.50	111.50
20	C	305	PGV	O01-C1-C2	5.10	122.49	111.50
28	V	101	PSC	O01-C1-C2	5.07	122.42	111.50
20	P	305	PGV	O03-C19-C20	5.03	127.70	111.91
24	W	101	CHD	C6-C5-C4	-4.84	105.61	111.19
18	N	606	HEA	CAD-CBD-CGD	-4.78	103.33	113.60
18	A	605	HEA	C13-C12-C11	-4.76	107.20	114.35
26	C	306	CDL	OA6-CA5-C11	4.74	121.72	111.50
24	C	301	CHD	C21-C20-C22	-4.72	102.96	110.36
18	A	604[A]	HEA	CAA-CBA-CGA	-4.71	103.47	113.60
18	A	604[B]	HEA	CAA-CBA-CGA	-4.71	103.47	113.60
24	P	301	CHD	C15-C14-C13	4.69	108.15	103.55
31	2	201	HEC	C4B-NB-C1B	4.64	109.86	105.07
20	N	612	PGV	O03-C19-C20	4.51	126.07	111.91
30	M	101	DMU	C18-O16-C6	-4.51	106.37	113.84
18	N	605[A]	HEA	C3A-C2A-C1A	-4.50	102.78	107.08
18	N	605[B]	HEA	C3A-C2A-C1A	-4.50	102.78	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	608	TGL	OG3-CC1-OC1	-4.45	112.36	123.59
24	P	307	CHD	C14-C8-C9	-4.39	103.69	109.71
31	1	201	HEC	CHC-C4B-NB	4.36	129.75	124.37
21	N	608	TGL	CG3-OG3-CC1	4.32	133.13	117.12
30	M	101	DMU	O2-C8-C9	-4.29	98.63	109.30
31	1	201	HEC	CBC-CAC-C3C	4.26	124.18	112.43
24	W	101	CHD	C18-C13-C12	-4.24	104.75	109.07
24	C	307	CHD	C21-C20-C22	-4.17	103.83	110.36
31	2	201	HEC	CHC-C4B-NB	4.16	129.51	124.37
18	N	605[A]	HEA	C20-C21-C22	-4.13	98.32	111.88
24	P	307	CHD	C16-C17-C13	4.12	107.59	103.55
31	1	201	HEC	CHA-C4D-ND	4.10	128.87	124.42
18	A	605	HEA	CAD-CBD-CGD	-4.09	104.80	113.60
31	1	201	HEC	C3B-C4B-NB	-4.07	105.64	110.17
24	P	307	CHD	C4-C5-C10	4.06	116.97	112.66
26	G	101	CDL	OA6-CA5-C11	4.04	120.22	111.50
30	M	101	DMU	O1-C9-C11	4.02	116.42	106.44
18	A	604[A]	HEA	C27-C19-C20	4.01	122.03	115.27
26	T	101	CDL	CA4-OA6-CA5	4.00	127.65	117.79
21	N	608	TGL	OG1-CA1-OA1	-3.99	113.52	123.59
24	W	101	CHD	C6-C7-C8	3.98	115.73	111.48
24	P	307	CHD	C14-C8-C7	3.98	117.08	111.81
28	V	101	PSC	C21-C20-C19	-3.96	99.21	113.62
24	C	307	CHD	C14-C8-C9	-3.96	104.28	109.71
24	C	307	CHD	C15-C14-C13	3.95	107.43	103.55
24	J	101	CHD	C16-C17-C20	3.95	118.26	112.15
20	N	612	PGV	O03-C19-O04	-3.92	113.69	123.59
21	L	101	TGL	OG3-CC1-CC2	3.92	124.22	111.91
30	M	101	DMU	O3-C5-C7	3.92	119.40	110.35
24	T	103	CHD	C13-C17-C20	-3.90	114.84	119.50
26	C	306	CDL	OB8-CB7-C71	3.86	124.01	111.91
20	C	305	PGV	O03-C19-C20	3.85	123.98	111.91
31	1	201	HEC	C4C-NC-C1C	3.83	109.10	105.35
18	N	605[A]	HEA	C2A-C1A-NA	3.82	114.04	110.32
18	N	605[B]	HEA	C2A-C1A-NA	3.82	114.04	110.32
24	J	101	CHD	C17-C13-C14	-3.81	96.25	100.09
24	W	101	CHD	C1-C10-C9	-3.79	105.39	111.35
21	B	301	TGL	OG1-CA1-CA2	3.79	123.80	111.91
18	A	604[B]	HEA	C27-C19-C20	3.76	121.60	115.27
26	P	306	CDL	OB8-CB7-C71	3.76	123.70	111.91
31	1	201	HEC	CHB-C1B-NB	3.73	128.47	124.42
24	C	307	CHD	C21-C20-C17	3.73	118.63	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	102	CHD	O12-C12-C13	-3.72	104.74	111.03
24	J	101	CHD	C15-C14-C13	3.72	107.20	103.55
24	C	307	CHD	C1-C2-C3	3.72	115.24	110.47
24	P	307	CHD	C15-C14-C8	3.70	123.50	118.33
18	A	605	HEA	CHD-C1D-ND	-3.68	119.83	124.37
24	J	101	CHD	C14-C8-C7	3.67	116.67	111.81
25	C	303	PEK	O03-C21-O04	-3.65	114.39	123.59
24	P	301	CHD	C9-C11-C12	-3.63	109.50	114.30
20	A	608	PGV	O03-C19-O04	-3.63	114.44	123.59
21	N	608	TGL	OG2-CG2-CG3	3.61	121.47	108.40
20	A	608	PGV	O01-C1-O02	-3.60	115.01	123.70
20	C	305	PGV	C01-O03-C19	3.59	130.41	117.12
18	A	604[A]	HEA	C13-C14-C15	-3.58	119.04	127.66
18	A	604[B]	HEA	C13-C14-C15	-3.58	119.04	127.66
26	T	101	CDL	OA8-CA7-C31	3.58	123.14	111.91
21	N	608	TGL	CG3-CG2-CG1	-3.57	103.36	111.79
20	A	608	PGV	O01-C1-C2	3.57	119.19	111.50
21	Q	201	TGL	OG1-CA1-CA2	3.55	123.04	111.91
21	Q	201	TGL	OG3-CC1-CC2	3.53	123.00	111.91
20	C	304	PGV	O01-C1-O02	-3.53	115.17	123.70
24	P	301	CHD	C13-C14-C8	-3.53	110.23	114.74
25	C	303	PEK	O03-C01-C02	-3.53	98.17	108.43
24	C	307	CHD	C14-C8-C7	3.52	116.48	111.81
18	A	604[A]	HEA	C3C-C4C-NC	3.52	112.42	110.25
18	A	604[B]	HEA	C3C-C4C-NC	3.52	112.42	110.25
20	C	304	PGV	O03-C19-O04	-3.52	114.71	123.59
24	C	307	CHD	C9-C10-C5	3.51	113.50	108.58
24	W	101	CHD	C10-C9-C8	3.50	115.58	111.82
24	G	102	CHD	C18-C13-C12	-3.50	105.51	109.07
24	P	301	CHD	C22-C23-C24	-3.48	103.26	112.51
18	A	604[A]	HEA	O2A-CGA-CBA	3.47	125.19	114.03
18	A	604[B]	HEA	O2A-CGA-CBA	3.47	125.19	114.03
18	A	605	HEA	CMB-C2B-C1B	3.47	130.33	125.04
18	N	606	HEA	O1A-CGA-CBA	-3.47	111.93	123.08
31	2	201	HEC	C4C-NC-C1C	3.46	108.73	105.35
24	J	101	CHD	C4-C3-C2	3.45	114.67	110.55
18	A	604[A]	HEA	C26-C15-C16	-3.42	109.51	115.27
18	A	604[B]	HEA	C26-C15-C16	-3.42	109.51	115.27
24	T	103	CHD	O26-C24-O25	-3.37	114.89	123.30
24	W	101	CHD	C4-C5-C10	3.37	116.24	112.66
24	T	103	CHD	C15-C14-C13	3.37	106.85	103.55
21	L	101	TGL	CG2-OG2-CB1	3.36	126.07	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	303	PEK	C2-C3-C4	3.36	119.21	113.23
24	P	307	CHD	C1-C10-C9	-3.35	106.09	111.35
24	P	307	CHD	O7-C7-C8	3.34	116.89	109.43
24	W	101	CHD	C6-C5-C10	3.33	116.19	112.66
18	A	604[A]	HEA	C21-C20-C19	3.31	123.87	112.98
25	C	303	PEK	C01-O03-C21	3.31	129.37	117.12
18	A	604[A]	HEA	C20-C19-C18	-3.29	114.45	121.12
24	T	103	CHD	C4-C3-C2	3.28	114.47	110.55
21	B	301	TGL	OG3-CC1-CC2	3.28	122.20	111.91
20	P	304	PGV	O01-C1-C2	3.28	118.56	111.50
31	1	201	HEC	CHA-C4D-C3D	-3.28	120.03	124.84
18	N	605[A]	HEA	O2D-CGD-CBD	3.27	124.54	114.03
18	N	605[B]	HEA	O2D-CGD-CBD	3.27	124.54	114.03
21	N	608	TGL	OG3-CG3-CG2	3.27	117.95	108.43
26	P	306	CDL	OA6-CA5-C11	3.26	118.54	111.50
21	D	201	TGL	OG3-CC1-CC2	3.25	122.11	111.91
24	T	103	CHD	C9-C8-C7	3.24	115.75	111.88
20	C	305	PGV	C02-O01-C1	3.23	125.75	117.79
18	A	604[A]	HEA	C3C-C2C-C1C	-3.22	103.28	107.16
18	A	604[B]	HEA	C3C-C2C-C1C	-3.22	103.28	107.16
18	N	606	HEA	C27-C19-C20	3.21	120.68	115.27
24	G	102	CHD	C13-C17-C20	-3.20	115.67	119.50
26	G	101	CDL	CB6-OB8-CB7	3.20	128.98	117.12
21	D	201	TGL	OG1-CG1-CG2	3.20	117.75	108.43
24	J	101	CHD	C10-C9-C8	3.18	115.23	111.82
21	Q	201	TGL	OG2-CB1-CB2	3.18	118.34	111.50
21	D	201	TGL	OG1-CA1-CA2	3.17	121.86	111.91
21	N	608	TGL	OG2-CG2-CG1	3.17	119.86	108.40
18	N	605[A]	HEA	CAD-CBD-CGD	-3.16	106.79	113.60
18	N	605[B]	HEA	CAD-CBD-CGD	-3.16	106.79	113.60
18	N	605[A]	HEA	C3D-C4D-ND	3.16	113.42	110.36
18	N	605[B]	HEA	C3D-C4D-ND	3.16	113.42	110.36
26	C	306	CDL	CA6-OA8-CA7	3.15	128.77	117.12
31	2	201	HEC	C3B-C4B-NB	-3.14	106.67	110.17
30	M	101	DMU	O3-C5-C10	-3.14	102.43	110.05
24	C	301	CHD	C17-C13-C14	-3.13	96.94	100.09
31	2	201	HEC	CBC-CAC-C3C	3.11	121.01	112.43
24	P	301	CHD	C17-C13-C14	-3.10	96.96	100.09
18	N	606	HEA	C20-C19-C18	-3.10	114.84	121.12
24	P	301	CHD	C1-C10-C5	3.09	112.34	107.77
24	J	101	CHD	C1-C2-C3	3.08	114.41	110.47
24	P	301	CHD	C6-C7-C8	3.05	114.74	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	301	CHD	C5-C4-C3	-3.04	108.30	112.76
21	Q	201	TGL	OG1-CG1-CG2	3.03	117.25	108.43
20	A	608	PGV	O03-C19-C20	3.03	121.41	111.91
26	T	101	CDL	OA8-CA6-CA4	3.02	117.22	108.43
18	N	606	HEA	C2B-C1B-NB	3.02	113.50	109.88
18	A	605	HEA	O2A-CGA-CBA	3.02	123.72	114.03
18	N	605[B]	HEA	C27-C19-C20	3.01	120.34	115.27
28	E	201	PSC	O01-C1-O02	-3.00	116.45	123.70
18	N	605[A]	HEA	CAA-CBA-CGA	-3.00	107.15	113.60
18	N	605[B]	HEA	CAA-CBA-CGA	-3.00	107.15	113.60
24	J	101	CHD	C9-C11-C12	-3.00	110.34	114.30
31	1	201	HEC	CBD-CAD-C3D	-2.99	104.33	112.63
25	P	303	PEK	O01-C1-C2	2.99	117.94	111.50
21	L	101	TGL	CG3-OG3-CC1	2.98	128.15	117.12
25	C	303	PEK	O01-C1-C2	2.98	117.92	111.50
24	P	301	CHD	C11-C12-C13	2.97	114.30	111.24
31	2	201	HEC	C4A-NA-C1A	2.97	108.26	105.35
20	C	304	PGV	O01-C1-C2	2.97	117.90	111.50
24	C	301	CHD	C11-C9-C8	2.97	115.22	110.88
18	N	605[A]	HEA	CHB-C1B-NB	2.95	127.62	124.42
18	N	605[B]	HEA	CHB-C1B-NB	2.95	127.62	124.42
26	P	306	CDL	OB6-CB5-C51	2.93	117.82	111.50
24	P	307	CHD	O7-C7-C6	-2.90	102.74	109.94
18	A	605	HEA	C3D-C4D-ND	2.90	113.17	110.36
26	C	306	CDL	C52-C51-CB5	-2.88	103.14	113.62
24	C	307	CHD	C18-C13-C12	2.88	112.00	109.07
21	D	201	TGL	OG2-CB1-OB1	-2.88	116.74	123.70
21	L	101	TGL	OB1-CB1-CB2	-2.86	112.56	123.73
21	L	101	TGL	OG1-CG1-CG2	2.86	116.76	108.43
26	T	101	CDL	OB8-CB6-CB4	2.86	116.75	108.43
18	N	606	HEA	C1B-C2B-C3B	-2.83	103.42	106.80
24	T	103	CHD	O3-C3-C2	-2.81	103.00	110.16
24	C	307	CHD	C16-C17-C13	2.81	106.31	103.55
20	A	607	PGV	O03-C19-C20	2.81	120.72	111.91
28	V	101	PSC	C28-C27-C26	-2.80	100.20	114.42
31	1	201	HEC	C3C-C4C-NC	-2.80	107.02	110.15
18	A	604[A]	HEA	C2C-C1C-NC	2.79	114.33	110.08
18	A	604[B]	HEA	C2C-C1C-NC	2.79	114.33	110.08
31	1	201	HEC	CHD-C1D-ND	2.78	127.80	124.37
21	L	101	TGL	OG1-CA1-CA2	2.78	120.63	111.91
26	C	306	CDL	OB6-CB5-C51	2.78	117.48	111.50
26	P	306	CDL	OA8-CA7-C31	2.77	120.60	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	301	TGL	OB1-CB1-CB2	-2.76	112.96	123.73
26	G	101	CDL	OB8-CB7-C71	2.76	120.56	111.91
24	J	101	CHD	C1-C10-C5	2.76	111.84	107.77
26	G	101	CDL	OA6-CA5-OA7	-2.75	117.05	123.70
18	N	605[A]	HEA	C16-C15-C14	-2.75	115.55	121.12
18	N	605[B]	HEA	C16-C15-C14	-2.75	115.55	121.12
28	E	201	PSC	C28-C27-C26	-2.75	100.47	114.42
24	J	101	CHD	C13-C14-C8	-2.75	111.23	114.74
20	A	607	PGV	C01-O03-C19	2.71	127.17	117.12
18	A	605	HEA	CBC-CAC-C3C	-2.71	114.14	127.62
24	T	103	CHD	C14-C13-C12	2.71	109.92	107.40
31	2	201	HEC	CMD-C2D-C1D	2.70	129.16	125.04
18	N	606	HEA	C3C-C4C-NC	2.70	111.91	110.25
24	W	101	CHD	C11-C12-C13	2.69	114.01	111.24
30	M	101	DMU	C10-C5-C7	-2.69	104.39	110.00
18	A	605	HEA	C3C-C4C-NC	2.69	111.90	110.25
18	A	605	HEA	CMB-C2B-C3B	-2.68	125.23	130.34
24	G	102	CHD	C1-C2-C3	2.68	113.91	110.47
18	A	605	HEA	C3A-C2A-C1A	-2.68	104.52	107.08
24	J	101	CHD	C15-C14-C8	2.68	122.07	118.33
18	A	604[A]	HEA	C1A-CHA-C4D	-2.67	120.29	126.06
18	A	604[B]	HEA	C1A-CHA-C4D	-2.67	120.29	126.06
21	N	608	TGL	OB1-CB1-CB2	-2.66	113.35	123.73
28	E	201	PSC	O03-C19-C20	2.65	120.24	111.91
18	A	605	HEA	CAA-C2A-C1A	2.65	129.90	124.89
24	P	307	CHD	C4-C3-C2	2.65	113.72	110.55
31	2	201	HEC	CBB-CAB-C3B	2.64	119.72	112.43
18	A	605	HEA	C2B-C1B-NB	2.64	113.04	109.88
24	T	103	CHD	C6-C5-C4	-2.63	108.16	111.19
31	1	201	HEC	O2A-CGA-CBA	2.63	122.49	114.03
26	C	306	CDL	OA8-CA7-C31	2.63	120.17	111.91
24	T	103	CHD	C22-C23-C24	-2.63	105.53	112.51
20	C	304	PGV	O03-C19-C20	2.63	120.15	111.91
24	C	301	CHD	C11-C12-C13	2.62	113.94	111.24
18	A	605	HEA	CHB-C1B-NB	-2.62	121.57	124.42
31	1	201	HEC	CMD-C2D-C1D	2.62	129.03	125.04
20	C	304	PGV	C27-C26-C25	-2.61	101.17	114.42
21	Q	201	TGL	OG3-CC1-OC1	-2.61	117.01	123.59
24	C	307	CHD	O7-C7-C8	2.61	115.25	109.43
18	N	605[A]	HEA	CHB-C1B-C2B	-2.60	120.91	124.98
18	N	605[B]	HEA	CHB-C1B-C2B	-2.60	120.91	124.98
20	P	305	PGV	O03-C19-O04	-2.60	117.02	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	CDL	CB6-CB4-CB3	-2.60	105.64	111.79
21	Q	201	TGL	OG1-CA1-OA1	-2.60	117.04	123.59
26	G	101	CDL	CB4-OB6-CB5	2.59	124.17	117.79
24	G	102	CHD	C1-C10-C9	-2.58	107.30	111.35
18	A	604[A]	HEA	CHA-C4D-C3D	-2.57	121.06	124.84
18	A	604[B]	HEA	CHA-C4D-C3D	-2.57	121.06	124.84
18	N	605[A]	HEA	C26-C15-C16	2.57	119.59	115.27
18	N	605[B]	HEA	C26-C15-C16	2.57	119.59	115.27
26	G	101	CDL	OA8-CA7-C31	2.57	119.96	111.91
24	W	101	CHD	C2-C1-C10	2.57	117.18	112.78
24	W	101	CHD	O7-C7-C6	-2.56	103.59	109.94
21	L	101	TGL	C11-C10-CB9	2.56	127.43	114.42
24	T	103	CHD	O12-C12-C11	-2.56	103.91	109.12
24	T	103	CHD	C9-C10-C5	2.55	112.17	108.58
26	G	101	CDL	C83-C82-C81	2.55	127.36	114.42
31	2	201	HEC	CHD-C1D-ND	2.54	127.51	124.37
28	E	201	PSC	C31-C30-C29	-2.54	101.54	114.42
18	N	605[B]	HEA	C17-C18-C19	2.53	133.76	127.66
31	2	201	HEC	CHA-C4D-ND	2.53	127.17	124.42
20	P	304	PGV	O03-C19-O04	-2.52	117.23	123.59
24	W	101	CHD	C9-C10-C5	2.51	112.11	108.58
18	A	604[B]	HEA	C20-C19-C18	-2.51	116.03	121.12
18	N	606	HEA	CHA-C4D-C3D	-2.50	121.16	124.84
24	C	301	CHD	C16-C15-C14	-2.50	100.18	105.13
31	1	201	HEC	CBB-CAB-C3B	2.50	119.31	112.43
30	Z	101	DMU	O1-C9-C11	2.50	112.64	106.44
24	P	307	CHD	C19-C10-C5	-2.49	106.14	110.36
18	A	605	HEA	C2D-C1D-ND	2.49	112.79	109.84
18	N	605[A]	HEA	C2D-C1D-ND	2.49	112.79	109.84
18	N	605[B]	HEA	C2D-C1D-ND	2.49	112.79	109.84
24	C	301	CHD	C18-C13-C12	2.49	111.60	109.07
18	A	604[A]	HEA	CHA-C4D-ND	2.49	127.12	124.42
18	A	604[B]	HEA	CHA-C4D-ND	2.49	127.12	124.42
24	G	102	CHD	C19-C10-C1	-2.48	104.26	108.26
20	P	305	PGV	O03-C01-C02	2.48	115.66	108.43
20	A	608	PGV	O14-P-O13	2.47	124.45	112.24
20	P	304	PGV	O14-P-O13	2.47	124.45	112.24
18	N	606	HEA	C16-C15-C14	2.47	126.11	121.12
18	N	606	HEA	CMB-C2B-C1B	2.47	128.79	125.04
24	P	307	CHD	C22-C23-C24	-2.46	105.97	112.51
18	A	605	HEA	CAA-CBA-CGA	-2.46	108.31	113.60
18	N	606	HEA	CHC-C4B-NB	2.45	127.40	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	307	CHD	C15-C14-C13	2.45	105.96	103.55
18	A	605	HEA	O2D-CGD-CBD	2.45	121.89	114.03
31	I	201	HEC	C4C-CHD-C1D	-2.44	120.55	126.34
20	A	607	PGV	O01-C1-C2	2.43	116.74	111.50
24	T	103	CHD	C1-C10-C5	2.42	111.35	107.77
26	G	101	CDL	OB8-CB7-OB9	-2.42	117.49	123.59
21	L	101	TGL	OG2-CG2-CG3	2.42	117.16	108.40
18	A	604[B]	HEA	C17-C18-C19	-2.42	121.84	127.66
30	M	101	DMU	O1-C9-C8	-2.42	105.30	109.69
24	T	103	CHD	C5-C4-C3	-2.41	109.22	112.76
24	P	301	CHD	C13-C17-C20	-2.40	116.63	119.50
26	P	306	CDL	OB8-CB7-OB9	-2.40	117.55	123.59
18	A	605	HEA	O1A-CGA-CBA	-2.39	115.39	123.08
18	A	604[A]	HEA	C3A-C2A-C1A	-2.39	104.79	107.08
18	A	604[B]	HEA	C3A-C2A-C1A	-2.39	104.79	107.08
26	T	101	CDL	C82-C81-C80	2.39	126.56	114.42
21	N	608	TGL	OG1-CG1-CG2	2.39	115.39	108.43
18	A	604[A]	HEA	CHA-C1A-C2A	-2.38	121.07	124.94
18	A	604[B]	HEA	CHA-C1A-C2A	-2.38	121.07	124.94
28	E	201	PSC	O01-C02-C03	2.38	117.03	108.40
18	N	605[A]	HEA	O1D-CGD-CBD	-2.38	115.44	123.08
18	N	605[B]	HEA	O1D-CGD-CBD	-2.38	115.44	123.08
20	N	612	PGV	O01-C1-O02	-2.37	117.97	123.70
21	Q	201	TGL	C11-C10-CB9	2.37	126.44	114.42
24	C	307	CHD	C9-C11-C12	-2.36	111.19	114.30
24	C	307	CHD	O12-C12-C13	-2.36	107.05	111.03
20	C	305	PGV	O03-C01-C02	2.36	115.29	108.43
24	C	301	CHD	C16-C17-C13	2.35	105.86	103.55
20	P	304	PGV	C02-O01-C1	2.35	123.57	117.79
18	N	606	HEA	CAA-CBA-CGA	-2.35	108.55	113.60
26	T	101	CDL	OB8-CB7-OB9	-2.34	117.67	123.59
30	Z	101	DMU	O5-C4-C57	2.34	112.26	106.44
20	A	607	PGV	C5-C4-C3	-2.34	102.53	114.42
18	N	605[A]	HEA	CHA-C1A-C2A	-2.34	121.14	124.94
18	N	605[B]	HEA	CHA-C1A-C2A	-2.34	121.14	124.94
25	C	303	PEK	O13-P-O14	2.34	123.79	112.24
24	W	101	CHD	C18-C13-C17	2.33	114.86	111.21
20	P	304	PGV	O01-C1-O02	-2.33	118.06	123.70
30	M	101	DMU	O4-C7-C8	-2.33	104.97	110.35
26	P	306	CDL	C56-C55-C54	-2.33	102.62	114.42
26	P	306	CDL	CA6-OA8-CA7	2.32	125.72	117.12
24	G	102	CHD	C2-C1-C10	2.32	116.76	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	M	101	DMU	O4-C7-C5	2.31	115.69	110.35
31	2	201	HEC	CHA-C4D-C3D	-2.31	121.44	124.84
31	2	201	HEC	CAD-C3D-C4D	2.31	128.69	124.66
24	W	101	CHD	C14-C13-C12	-2.30	105.26	107.40
28	V	101	PSC	C25-C24-C23	-2.30	102.75	114.42
21	B	301	TGL	OG3-CC1-OC1	-2.30	117.80	123.59
24	P	307	CHD	C23-C22-C20	-2.30	110.33	114.52
20	A	608	PGV	O03-C01-C02	2.29	115.11	108.43
26	P	306	CDL	OB8-CB6-CB4	-2.29	101.76	108.43
24	G	102	CHD	O7-C7-C6	-2.29	104.26	109.94
18	N	605[B]	HEA	C25-C23-C24	2.29	119.66	114.60
18	A	605	HEA	O1D-CGD-CBD	-2.29	115.73	123.08
18	A	605	HEA	CMC-C2C-C3C	2.28	132.12	126.59
26	P	306	CDL	C54-C53-C52	-2.28	102.86	114.42
31	1	201	HEC	O2A-CGA-O1A	-2.27	117.65	123.30
30	Z	101	DMU	C1-C2-C3	2.26	114.84	109.68
21	D	201	TGL	OG3-CG3-CG2	2.26	115.00	108.43
24	T	103	CHD	C6-C7-C8	2.26	113.89	111.48
18	N	606	HEA	O2D-CGD-CBD	2.26	121.28	114.03
26	G	101	CDL	C60-C59-C58	2.25	125.86	114.42
24	P	301	CHD	C18-C13-C14	2.25	114.73	111.21
21	L	101	TGL	CA5-CA4-CA3	-2.25	103.00	114.42
24	P	301	CHD	C14-C13-C12	-2.25	105.31	107.40
31	1	201	HEC	C4A-CHB-C1B	-2.25	121.21	126.06
28	E	201	PSC	C02-O01-C1	2.24	123.32	117.79
21	L	101	TGL	CC4-CC3-CC2	-2.24	105.14	113.19
26	T	101	CDL	OA6-CA5-OA7	-2.24	118.29	123.70
18	A	605	HEA	C1B-C2B-C3B	-2.24	104.13	106.80
24	C	307	CHD	C16-C17-C20	2.23	115.60	112.15
18	A	604[A]	HEA	O1A-CGA-CBA	-2.23	115.93	123.08
18	A	604[B]	HEA	O1A-CGA-CBA	-2.23	115.93	123.08
24	J	101	CHD	C11-C12-C13	2.22	113.52	111.24
21	D	201	TGL	C21-C20-CA9	2.21	125.66	114.42
24	W	101	CHD	C9-C11-C12	-2.20	111.39	114.30
21	Q	201	TGL	C21-C20-CA9	2.20	125.60	114.42
24	P	307	CHD	C21-C20-C22	-2.20	106.91	110.36
24	W	101	CHD	C19-C10-C5	-2.20	106.63	110.36
21	B	301	TGL	OG1-CA1-OA1	-2.20	118.04	123.59
20	P	305	PGV	O01-C1-O02	-2.20	118.39	123.70
18	N	605[A]	HEA	C21-C20-C19	2.19	120.19	112.98
20	C	305	PGV	O01-C02-C01	2.19	116.34	108.40
24	C	307	CHD	C2-C1-C10	2.19	116.53	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	605	HEA	CAD-C3D-C2D	2.19	131.95	127.88
21	L	101	TGL	OG3-CG3-CG2	2.18	114.79	108.43
18	A	604[A]	HEA	CHA-C1A-NA	2.18	126.80	124.44
18	A	604[B]	HEA	CHA-C1A-NA	2.18	126.80	124.44
24	C	301	CHD	C13-C14-C8	-2.18	111.96	114.74
26	C	306	CDL	C83-C82-C81	2.17	125.44	114.42
20	P	304	PGV	C22-C21-C20	-2.17	105.39	113.19
20	P	305	PGV	O04-C19-C20	-2.17	115.27	123.73
26	C	306	CDL	C39-C38-C37	2.16	125.40	114.42
28	V	101	PSC	C29-C28-C27	-2.16	103.47	114.42
31	2	201	HEC	CHA-C1A-NA	2.16	126.77	124.44
24	C	307	CHD	C5-C4-C3	2.16	115.92	112.76
24	P	307	CHD	C5-C4-C3	-2.16	109.59	112.76
24	C	307	CHD	C23-C22-C20	-2.15	110.58	114.52
20	C	304	PGV	C03-C02-C01	-2.15	106.70	111.79
28	E	201	PSC	C21-C20-C19	-2.15	105.80	113.62
26	C	306	CDL	C40-C39-C38	2.14	125.28	114.42
24	G	102	CHD	C18-C13-C14	2.14	114.55	111.21
30	Z	101	DMU	C7-C8-C9	2.13	114.05	110.24
18	A	604[A]	HEA	CMB-C2B-C3B	-2.13	126.28	130.34
18	A	604[B]	HEA	CMB-C2B-C3B	-2.13	126.28	130.34
24	T	103	CHD	C1-C10-C9	-2.13	108.00	111.35
26	P	306	CDL	C82-C81-C80	2.13	125.24	114.42
26	T	101	CDL	C83-C82-C81	2.13	125.23	114.42
18	N	606	HEA	C16-C17-C18	2.13	118.88	111.88
26	T	101	CDL	OB7-CB5-C51	-2.13	115.44	123.73
18	A	605	HEA	CBA-CAA-C2A	-2.13	106.72	112.63
18	N	606	HEA	O1D-CGD-CBD	-2.13	116.25	123.08
24	P	301	CHD	C14-C8-C7	-2.12	108.99	111.81
24	T	103	CHD	C13-C14-C8	-2.12	112.03	114.74
26	T	101	CDL	OA6-CA4-CA6	2.12	116.08	108.40
24	P	307	CHD	O3-C3-C4	-2.12	105.63	109.85
26	G	101	CDL	CA6-OA8-CA7	2.11	124.95	117.12
20	A	607	PGV	C8-C9-C10	-2.11	104.58	113.79
26	G	101	CDL	C82-C81-C80	2.11	125.15	114.42
24	P	301	CHD	O26-C24-O25	-2.11	118.05	123.30
24	J	101	CHD	C14-C8-C9	-2.10	106.82	109.71
21	N	608	TGL	C10-CB9-CB8	2.10	125.10	114.42
18	N	606	HEA	O2A-CGA-CBA	2.10	120.77	114.03
18	A	605	HEA	C1D-C2D-C3D	-2.10	104.75	106.96
28	E	201	PSC	C03-C02-C01	-2.09	106.86	111.79
24	T	103	CHD	C19-C10-C1	-2.08	104.91	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	301	TGL	C10-CB9-CB8	2.08	124.98	114.42
20	N	612	PGV	O01-C1-C2	2.08	115.98	111.50
20	C	305	PGV	C21-C20-C19	2.07	121.14	113.62
21	L	101	TGL	C16-C15-CC9	2.07	124.91	114.42
18	A	604[A]	HEA	CHC-C1C-C2C	-2.06	121.41	127.24
18	A	604[B]	HEA	CHC-C1C-C2C	-2.06	121.41	127.24
20	C	304	PGV	O14-P-O13	2.06	122.42	112.24
31	2	201	HEC	CAB-C3B-C4B	2.06	127.48	124.81
21	L	101	TGL	OC1-CC1-CC2	-2.05	115.73	123.73
18	A	604[B]	HEA	C21-C22-C23	-2.05	120.74	127.75
21	Q	201	TGL	OG2-CB1-OB1	-2.05	118.75	123.70
18	N	606	HEA	CAD-C3D-C2D	2.05	131.69	127.88
26	G	101	CDL	C80-C79-C78	2.05	124.83	114.42
24	W	101	CHD	O26-C24-C23	2.05	120.61	114.03
26	T	101	CDL	C79-C78-C77	2.04	124.80	114.42
24	G	102	CHD	C4-C3-C2	2.04	112.99	110.55
21	B	301	TGL	C16-C15-CC9	2.04	124.79	114.42
18	A	604[A]	HEA	C16-C17-C18	2.04	118.57	111.88
21	D	201	TGL	C16-C15-CC9	2.03	124.74	114.42
21	B	301	TGL	CA3-CA2-CA1	-2.03	106.24	113.62
26	T	101	CDL	C63-C62-C61	2.02	124.70	114.42
21	B	301	TGL	C15-CC9-CC8	2.02	124.66	114.42
18	N	605[B]	HEA	C21-C22-C23	-2.02	120.86	127.75
18	N	605[A]	HEA	CHA-C4D-C3D	-2.01	121.88	124.84
18	N	605[B]	HEA	CHA-C4D-C3D	-2.01	121.88	124.84
24	G	102	CHD	C15-C14-C13	2.01	105.52	103.55
31	2	201	HEC	CHB-C1B-NB	2.01	126.60	124.42
30	Z	101	DMU	O55-C2-C1	-2.00	105.72	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	1	201	HEC	NA
31	2	201	HEC	NA

All (790) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	604[A]	HEA	C2A-C3A-CMA-OMA
18	A	604[B]	HEA	C2A-C3A-CMA-OMA
18	A	605	HEA	C2A-C3A-CMA-OMA
18	N	605[A]	HEA	C2A-C3A-CMA-OMA

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Mol	Chain	Res	Type	Atoms
18	N	605[B]	HEA	C2A-C3A-CMA-OMA
18	N	605[B]	HEA	C16-C17-C18-C19
18	N	605[B]	HEA	C19-C20-C21-C22
20	C	305	PGV	C04-O12-P-O13
20	C	305	PGV	O01-C02-C03-O11
20	P	305	PGV	C03-O11-P-O12
20	P	305	PGV	C03-O11-P-O13
20	P	305	PGV	C03-O11-P-O14
20	P	305	PGV	O01-C02-C03-O11
20	P	305	PGV	O12-C04-C05-C06
20	P	305	PGV	C04-C05-C06-O06
21	B	301	TGL	OB1-CB1-OG2-CG2
21	B	301	TGL	OG1-CG1-CG2-OG2
21	D	201	TGL	OG1-CG1-CG2-OG2
21	D	201	TGL	CC2-CC1-OG3-CG3
21	D	201	TGL	OC1-CC1-OG3-CG3
21	L	101	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
21	N	608	TGL	OB1-CB1-OG2-CG2
21	N	608	TGL	OG1-CG1-CG2-OG2
21	N	608	TGL	CC2-CC1-OG3-CG3
21	N	608	TGL	OC1-CC1-OG3-CG3
21	Q	201	TGL	CB2-CB1-OG2-CG2
21	Q	201	TGL	OB1-CB1-OG2-CG2
24	J	101	CHD	C13-C17-C20-C22
24	J	101	CHD	C16-C17-C20-C21
24	W	101	CHD	C13-C17-C20-C22
24	W	101	CHD	C16-C17-C20-C21
24	W	101	CHD	C16-C17-C20-C22
26	C	306	CDL	CA2-C1-CB2-OB2
26	C	306	CDL	CA3-OA5-PA1-OA3
26	C	306	CDL	CA3-OA5-PA1-OA4
26	C	306	CDL	OA7-CA5-OA6-CA4
26	C	306	CDL	CB3-OB5-PB2-OB2
26	C	306	CDL	C51-CB5-OB6-CB4
26	G	101	CDL	CA2-OA2-PA1-OA3
26	G	101	CDL	CA2-OA2-PA1-OA4
26	G	101	CDL	C11-CA5-OA6-CA4
26	G	101	CDL	CB3-OB5-PB2-OB2
26	P	306	CDL	CB2-OB2-PB2-OB3
26	P	306	CDL	CB2-OB2-PB2-OB4
26	P	306	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	CB3-OB5-PB2-OB4
26	T	101	CDL	CA2-OA2-PA1-OA3
26	T	101	CDL	CA3-OA5-PA1-OA3
26	T	101	CDL	CA3-OA5-PA1-OA4
26	T	101	CDL	C11-CA5-OA6-CA4
26	T	101	CDL	OA9-CA7-OA8-CA6
26	T	101	CDL	C31-CA7-OA8-CA6
26	T	101	CDL	C1-CB2-OB2-PB2
26	T	101	CDL	CB3-OB5-PB2-OB3
28	E	201	PSC	C03-O11-P-O13
28	E	201	PSC	C04-O12-P-O13
28	E	201	PSC	C04-O12-P-O14
28	E	201	PSC	O12-C04-C05-N
28	E	201	PSC	C2-C1-O01-C02
28	E	201	PSC	C9-C10-C11-C12
28	V	101	PSC	C03-O11-P-O12
28	V	101	PSC	C03-O11-P-O13
28	V	101	PSC	C03-O11-P-O14
28	V	101	PSC	C2-C1-O01-C02
28	V	101	PSC	C11-C12-C13-C14
31	1	201	HEC	C2C-C3C-CAC-CBC
21	Q	201	TGL	OC1-CC1-OG3-CG3
28	V	101	PSC	O04-C19-O03-C01
21	Q	201	TGL	CC2-CC1-OG3-CG3
24	J	101	CHD	C16-C17-C20-C22
31	1	201	HEC	C4C-C3C-CAC-CBC
26	C	306	CDL	OB7-CB5-OB6-CB4
28	E	201	PSC	O02-C1-O01-C02
28	V	101	PSC	O02-C1-O01-C02
28	V	101	PSC	C20-C19-O03-C01
21	N	608	TGL	CB2-CB1-OG2-CG2
26	C	306	CDL	C11-CA5-OA6-CA4
24	J	101	CHD	C20-C22-C23-C24
26	P	306	CDL	C61-C62-C63-C64
20	A	607	PGV	C20-C19-O03-C01
26	T	101	CDL	C71-CB7-OB8-CB6
20	A	607	PGV	C10-C11-C12-C13
20	C	304	PGV	C10-C11-C12-C13
25	C	303	PEK	C13-C14-C15-C16
26	T	101	CDL	C79-C80-C81-C82
26	G	101	CDL	OA7-CA5-OA6-CA4
26	T	101	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
20	A	607	PGV	O04-C19-O03-C01
20	P	305	PGV	O12-C04-C05-O05
26	C	306	CDL	O1-C1-CB2-OB2
26	G	101	CDL	O1-C1-CA2-OA2
28	E	201	PSC	C20-C19-O03-C01
20	P	305	PGV	C2-C1-O01-C02
21	B	301	TGL	CB2-CB1-OG2-CG2
26	T	101	CDL	C22-C23-C24-C25
28	V	101	PSC	C26-C27-C28-C29
20	P	304	PGV	C28-C29-C30-C31
21	D	201	TGL	CA9-C20-C21-C22
30	Z	101	DMU	C19-C22-C25-C28
21	B	301	TGL	C15-C16-C17-C18
24	W	101	CHD	C17-C20-C22-C23
26	P	306	CDL	C58-C59-C60-C61
26	G	101	CDL	CB4-CB3-OB5-PB2
26	T	101	CDL	OB9-CB7-OB8-CB6
28	E	201	PSC	O04-C19-O03-C01
31	2	201	HEC	C2A-CAA-CBA-CGA
21	L	101	TGL	C12-C13-C14-C29
18	A	604[A]	HEA	C19-C20-C21-C22
18	A	604[B]	HEA	C19-C20-C21-C22
18	N	605[B]	HEA	C15-C16-C17-C18
26	T	101	CDL	C51-CB5-OB6-CB4
26	T	101	CDL	C17-C18-C19-C20
28	E	201	PSC	C04-C05-N-C06
21	B	301	TGL	CC2-CC1-OG3-CG3
31	2	201	HEC	C2C-C3C-CAC-CBC
28	E	201	PSC	C6-C7-C8-C9
20	C	305	PGV	C1-C2-C3-C4
30	M	101	DMU	O6-C11-C9-O1
24	C	307	CHD	C17-C20-C22-C23
26	T	101	CDL	O1-C1-CB2-OB2
28	V	101	PSC	C29-C30-C31-C32
20	P	305	PGV	O02-C1-O01-C02
21	L	101	TGL	C23-C24-C25-C26
21	B	301	TGL	OC1-CC1-OG3-CG3
24	P	307	CHD	C17-C20-C22-C23
24	C	307	CHD	C21-C20-C22-C23
21	N	608	TGL	CA1-CA2-CA3-CA4
26	T	101	CDL	CB7-C71-C72-C73
21	L	101	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
24	J	101	CHD	C13-C17-C20-C21
21	B	301	TGL	CB1-CB2-CB3-CB4
21	D	201	TGL	CC1-CC2-CC3-CC4
26	C	306	CDL	CB7-C71-C72-C73
26	G	101	CDL	CB5-C51-C52-C53
26	P	306	CDL	CA7-C31-C32-C33
21	L	101	TGL	CA2-CA1-OG1-CG1
24	P	307	CHD	C21-C20-C22-C23
21	D	201	TGL	CB1-CB2-CB3-CB4
28	V	101	PSC	C19-C20-C21-C22
30	M	101	DMU	O6-C11-C9-C8
21	N	608	TGL	C10-C11-C12-C13
24	W	101	CHD	C21-C20-C22-C23
21	L	101	TGL	CA9-C20-C21-C22
26	T	101	CDL	OB7-CB5-OB6-CB4
24	W	101	CHD	C13-C17-C20-C21
31	2	201	HEC	C4C-C3C-CAC-CBC
26	T	101	CDL	CA5-C11-C12-C13
20	A	608	PGV	C10-C11-C12-C13
25	P	303	PEK	C7-C8-C9-C10
28	E	201	PSC	C11-C10-C9-C8
20	A	607	PGV	C03-O11-P-O12
20	C	305	PGV	C04-O12-P-O11
20	P	305	PGV	C04-O12-P-O11
26	C	306	CDL	CA3-OA5-PA1-OA2
26	G	101	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	CA3-OA5-PA1-OA2
26	P	306	CDL	CB2-OB2-PB2-OB5
26	P	306	CDL	CB3-OB5-PB2-OB2
26	T	101	CDL	CA3-OA5-PA1-OA2
26	T	101	CDL	CB3-OB5-PB2-OB2
28	E	201	PSC	C03-O11-P-O12
28	E	201	PSC	C04-O12-P-O11
21	Q	201	TGL	C20-C21-C22-C23
26	G	101	CDL	CB2-C1-CA2-OA2
26	T	101	CDL	CA2-C1-CB2-OB2
30	Z	101	DMU	O16-C18-C19-C22
20	N	612	PGV	C26-C27-C28-C29
28	E	201	PSC	C04-C05-N-C07
28	E	201	PSC	C04-C05-N-C08
21	D	201	TGL	CB9-C10-C11-C12
21	Q	201	TGL	CC9-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C59-C60-C61-C62
28	V	101	PSC	C4-C5-C6-C7
20	A	607	PGV	C20-C21-C22-C23
21	D	201	TGL	C17-C18-C19-C33
21	D	201	TGL	C18-C19-C33-C34
21	Q	201	TGL	CB9-C10-C11-C12
21	Q	201	TGL	C13-C14-C29-C30
25	P	303	PEK	C26-C27-C28-C29
26	C	306	CDL	C59-C60-C61-C62
26	T	101	CDL	C31-C32-C33-C34
20	P	305	PGV	C20-C21-C22-C23
21	N	608	TGL	CA5-CA6-CA7-CA8
26	G	101	CDL	C72-C73-C74-C75
26	P	306	CDL	C21-C22-C23-C24
21	D	201	TGL	CG3-CG2-OG2-CB1
21	B	301	TGL	CC4-CC5-CC6-CC7
21	Q	201	TGL	CA7-CA8-CA9-C20
21	Q	201	TGL	CB7-CB8-CB9-C10
26	G	101	CDL	C42-C43-C44-C45
26	G	101	CDL	C76-C77-C78-C79
26	P	306	CDL	C37-C38-C39-C40
20	P	305	PGV	C5-C6-C7-C8
21	D	201	TGL	C23-C24-C25-C26
21	L	101	TGL	CC3-CC4-CC5-CC6
25	C	303	PEK	C28-C29-C30-C31
26	C	306	CDL	C12-C13-C14-C15
26	C	306	CDL	C20-C21-C22-C23
26	G	101	CDL	C12-C13-C14-C15
26	P	306	CDL	C56-C57-C58-C59
26	T	101	CDL	C58-C59-C60-C61
20	P	305	PGV	C6-C7-C8-C9
21	B	301	TGL	C11-C10-CB9-CB8
21	B	301	TGL	C22-C23-C24-C25
21	L	101	TGL	CB7-CB8-CB9-C10
21	L	101	TGL	C19-C33-C34-C35
21	Q	201	TGL	CC3-CC4-CC5-CC6
21	Q	201	TGL	C17-C18-C19-C33
26	C	306	CDL	C82-C83-C84-C85
26	T	101	CDL	C38-C39-C40-C41
21	L	101	TGL	CC1-CC2-CC3-CC4
25	C	303	PEK	C21-C22-C23-C24
20	P	304	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	P	305	PGV	C30-C31-C32-C33
21	B	301	TGL	CA4-CA5-CA6-CA7
21	N	608	TGL	CC6-CC7-CC8-CC9
26	P	306	CDL	C62-C63-C64-C65
28	E	201	PSC	C27-C28-C29-C30
21	L	101	TGL	OA1-CA1-OG1-CG1
21	N	608	TGL	CC4-CC5-CC6-CC7
26	C	306	CDL	C76-C77-C78-C79
26	G	101	CDL	C19-C20-C21-C22
26	G	101	CDL	C61-C62-C63-C64
26	P	306	CDL	C40-C41-C42-C43
26	P	306	CDL	C81-C82-C83-C84
21	L	101	TGL	CB3-CB4-CB5-CB6
21	L	101	TGL	C21-C22-C23-C24
21	N	608	TGL	CB7-CB8-CB9-C10
21	N	608	TGL	CC5-CC6-CC7-CC8
21	Q	201	TGL	C10-C11-C12-C13
25	P	303	PEK	C28-C29-C30-C31
26	C	306	CDL	C13-C14-C15-C16
26	C	306	CDL	C31-C32-C33-C34
26	C	306	CDL	C63-C64-C65-C66
26	P	306	CDL	C73-C74-C75-C76
21	N	608	TGL	C23-C24-C25-C26
21	Q	201	TGL	CB6-CB7-CB8-CB9
26	C	306	CDL	C21-C22-C23-C24
26	P	306	CDL	C43-C44-C45-C46
26	T	101	CDL	C40-C41-C42-C43
30	M	101	DMU	C22-C25-C28-C31
20	A	607	PGV	O02-C1-O01-C02
26	P	306	CDL	OB7-CB5-OB6-CB4
26	P	306	CDL	C51-CB5-OB6-CB4
26	C	306	CDL	C81-C82-C83-C84
28	V	101	PSC	C14-C15-C16-C17
28	E	201	PSC	C1-C2-C3-C4
20	C	305	PGV	C28-C29-C30-C31
20	N	612	PGV	C29-C30-C31-C32
20	P	304	PGV	C25-C26-C27-C28
21	L	101	TGL	CB4-CB5-CB6-CB7
21	L	101	TGL	CC4-CC5-CC6-CC7
21	N	608	TGL	CA3-CA4-CA5-CA6
21	N	608	TGL	C11-C12-C13-C14
21	Q	201	TGL	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	C17-C18-C19-C20
26	T	101	CDL	C82-C83-C84-C85
28	V	101	PSC	C2-C3-C4-C5
20	C	304	PGV	C29-C30-C31-C32
21	B	301	TGL	CA9-C20-C21-C22
21	N	608	TGL	CA2-CA3-CA4-CA5
21	Q	201	TGL	CA4-CA5-CA6-CA7
25	C	303	PEK	C34-C35-C36-C37
26	C	306	CDL	C71-C72-C73-C74
26	G	101	CDL	C82-C83-C84-C85
20	A	607	PGV	C14-C15-C16-C17
20	A	607	PGV	C27-C28-C29-C30
20	C	304	PGV	C24-C25-C26-C27
21	Q	201	TGL	CC5-CC6-CC7-CC8
20	C	304	PGV	C14-C15-C16-C17
21	B	301	TGL	CB9-C10-C11-C12
21	N	608	TGL	C12-C13-C14-C29
21	Q	201	TGL	C23-C24-C25-C26
20	A	607	PGV	C23-C24-C25-C26
21	B	301	TGL	CB7-CB8-CB9-C10
21	B	301	TGL	C20-C21-C22-C23
21	L	101	TGL	CB6-CB7-CB8-CB9
20	A	607	PGV	C29-C30-C31-C32
20	C	305	PGV	C2-C3-C4-C5
20	C	305	PGV	C6-C7-C8-C9
26	C	306	CDL	C22-C23-C24-C25
26	T	101	CDL	C59-C60-C61-C62
21	D	201	TGL	C21-C22-C23-C24
26	T	101	CDL	C52-C53-C54-C55
20	P	305	PGV	C23-C24-C25-C26
21	N	608	TGL	C13-C14-C29-C30
20	C	305	PGV	C19-C20-C21-C22
26	T	101	CDL	CA7-C31-C32-C33
20	A	607	PGV	C2-C1-O01-C02
20	P	305	PGV	C26-C27-C28-C29
26	P	306	CDL	C80-C81-C82-C83
20	P	305	PGV	O05-C05-C06-O06
25	C	303	PEK	C16-C17-C18-C19
26	G	101	CDL	C14-C15-C16-C17
26	P	306	CDL	C51-C52-C53-C54
21	Q	201	TGL	CB2-CB3-CB4-CB5
26	P	306	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
21	D	201	TGL	CA6-CA7-CA8-CA9
26	C	306	CDL	C43-C44-C45-C46
26	P	306	CDL	C35-C36-C37-C38
23	E	202	EDO	O1-C1-C2-O2
20	C	305	PGV	C7-C8-C9-C10
20	C	305	PGV	C23-C24-C25-C26
28	V	101	PSC	C30-C31-C32-C33
21	L	101	TGL	CB1-CB2-CB3-CB4
21	D	201	TGL	C21-C20-CA9-CA8
26	P	306	CDL	C41-C42-C43-C44
20	C	305	PGV	C14-C15-C16-C17
21	L	101	TGL	CB2-CB3-CB4-CB5
26	G	101	CDL	C11-C12-C13-C14
26	T	101	CDL	C57-C58-C59-C60
20	C	305	PGV	C11-C10-C9-C8
26	C	306	CDL	C71-CB7-OB8-CB6
25	P	303	PEK	C23-C24-C25-C26
26	C	306	CDL	C33-C34-C35-C36
26	T	101	CDL	C71-C72-C73-C74
20	C	304	PGV	C30-C31-C32-C33
26	P	306	CDL	C79-C80-C81-C82
28	V	101	PSC	C5-C6-C7-C8
28	V	101	PSC	C28-C29-C30-C31
26	C	306	CDL	C38-C39-C40-C41
26	P	306	CDL	C23-C24-C25-C26
26	C	306	CDL	C31-CA7-OA8-CA6
26	G	101	CDL	C71-CB7-OB8-CB6
18	A	604[B]	HEA	C15-C16-C17-C18
20	N	612	PGV	C13-C14-C15-C16
26	T	101	CDL	C20-C21-C22-C23
26	G	101	CDL	C51-CB5-OB6-CB4
26	P	306	CDL	C76-C77-C78-C79
20	C	305	PGV	C24-C25-C26-C27
26	T	101	CDL	OB6-CB4-CB6-OB8
26	T	101	CDL	C60-C61-C62-C63
20	P	304	PGV	C29-C30-C31-C32
26	T	101	CDL	C37-C38-C39-C40
20	P	305	PGV	C11-C10-C9-C8
20	P	304	PGV	C1-C2-C3-C4
20	P	304	PGV	C27-C28-C29-C30
21	L	101	TGL	C22-C23-C24-C25
26	C	306	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	C41-C42-C43-C44
26	T	101	CDL	C56-C57-C58-C59
21	B	301	TGL	CC7-CC8-CC9-C15
26	C	306	CDL	OA9-CA7-OA8-CA6
26	G	101	CDL	OB7-CB5-OB6-CB4
26	C	306	CDL	C14-C15-C16-C17
20	A	607	PGV	C22-C23-C24-C25
21	L	101	TGL	C11-C12-C13-C14
26	C	306	CDL	C56-C57-C58-C59
20	A	607	PGV	C02-C03-O11-P
26	C	306	CDL	C1-CA2-OA2-PA1
20	P	304	PGV	C22-C23-C24-C25
20	C	304	PGV	C7-C8-C9-C10
21	D	201	TGL	CC6-CC7-CC8-CC9
25	P	303	PEK	C1-C2-C3-C4
26	C	306	CDL	CA7-C31-C32-C33
26	P	306	CDL	CB7-C71-C72-C73
28	E	201	PSC	C19-C20-C21-C22
28	E	201	PSC	C22-C23-C24-C25
21	L	101	TGL	CA1-CA2-CA3-CA4
26	G	101	CDL	C52-C53-C54-C55
26	T	101	CDL	C63-C64-C65-C66
26	G	101	CDL	CA2-C1-CB2-OB2
20	A	608	PGV	C13-C14-C15-C16
30	M	101	DMU	C25-C28-C31-C34
28	E	201	PSC	C26-C27-C28-C29
20	A	607	PGV	C25-C26-C27-C28
21	N	608	TGL	C29-C30-C31-C32
21	Q	201	TGL	C21-C22-C23-C24
20	P	305	PGV	C24-C25-C26-C27
21	B	301	TGL	OG1-CG1-CG2-CG3
21	N	608	TGL	CG1-CG2-CG3-OG3
21	Q	201	TGL	OG1-CG1-CG2-CG3
26	P	306	CDL	CA3-CA4-CA6-OA8
26	T	101	CDL	CA3-CA4-CA6-OA8
26	T	101	CDL	CB3-CB4-CB6-OB8
28	E	201	PSC	O03-C01-C02-C03
28	E	201	PSC	C2-C3-C4-C5
28	E	201	PSC	C24-C25-C26-C27
25	C	303	PEK	C7-C8-C9-C10
20	P	305	PGV	C31-C32-C33-C34
21	D	201	TGL	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
21	N	608	TGL	C25-C26-C27-C28
21	N	608	TGL	C14-C29-C30-C31
20	C	305	PGV	C25-C26-C27-C28
26	C	306	CDL	C83-C84-C85-C86
26	G	101	CDL	C44-C45-C46-C47
20	C	304	PGV	C27-C28-C29-C30
26	P	306	CDL	C38-C39-C40-C41
26	P	306	CDL	C78-C79-C80-C81
21	B	301	TGL	CB5-CB6-CB7-CB8
21	N	608	TGL	CC2-CC3-CC4-CC5
26	G	101	CDL	C58-C59-C60-C61
30	M	101	DMU	C34-C37-C40-C43
21	B	301	TGL	CA2-CA1-OG1-CG1
20	N	612	PGV	C4-C5-C6-C7
20	P	305	PGV	C15-C16-C17-C18
25	C	303	PEK	C17-C18-C19-C20
28	E	201	PSC	C01-C02-O01-C1
28	V	101	PSC	C01-C02-O01-C1
26	P	306	CDL	C13-C14-C15-C16
20	C	304	PGV	C15-C16-C17-C18
28	V	101	PSC	C21-C22-C23-C24
26	C	306	CDL	OB5-CB3-CB4-OB6
20	C	304	PGV	C26-C27-C28-C29
21	D	201	TGL	CA5-CA6-CA7-CA8
28	V	101	PSC	C15-C16-C17-C18
26	C	306	CDL	OB9-CB7-OB8-CB6
20	C	305	PGV	C27-C28-C29-C30
25	C	303	PEK	C15-C16-C17-C18
26	P	306	CDL	C11-CA5-OA6-CA4
21	Q	201	TGL	CC7-CC8-CC9-C15
26	P	306	CDL	C31-C32-C33-C34
21	N	608	TGL	OG2-CG2-CG3-OG3
26	G	101	CDL	OB6-CB4-CB6-OB8
28	E	201	PSC	C28-C29-C30-C31
26	G	101	CDL	OB9-CB7-OB8-CB6
20	C	304	PGV	C13-C14-C15-C16
21	N	608	TGL	CA7-CA8-CA9-C20
26	G	101	CDL	C60-C61-C62-C63
20	A	607	PGV	C31-C32-C33-C34
20	C	304	PGV	C31-C32-C33-C34
26	T	101	CDL	C64-C65-C66-C67
20	A	607	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
20	N	612	PGV	C14-C15-C16-C17
28	E	201	PSC	C31-C32-C33-C34
28	V	101	PSC	C27-C28-C29-C30
20	N	612	PGV	C12-C13-C14-C15
25	C	303	PEK	C4-C5-C6-C7
21	N	608	TGL	C16-C17-C18-C19
26	C	306	CDL	C53-C54-C55-C56
20	P	305	PGV	C01-C02-C03-O11
26	C	306	CDL	OB5-CB3-CB4-CB6
26	G	101	CDL	OB5-CB3-CB4-CB6
21	D	201	TGL	CA3-CA4-CA5-CA6
21	Q	201	TGL	C11-C12-C13-C14
25	P	303	PEK	C27-C28-C29-C30
25	C	303	PEK	O12-C04-C05-N
25	P	303	PEK	C16-C17-C18-C19
28	V	101	PSC	C25-C26-C27-C28
26	P	306	CDL	C63-C64-C65-C66
21	D	201	TGL	CC3-CC4-CC5-CC6
26	P	306	CDL	O1-C1-CA2-OA2
21	B	301	TGL	OA1-CA1-OG1-CG1
21	L	101	TGL	C24-C25-C26-C27
26	T	101	CDL	C55-C56-C57-C58
21	L	101	TGL	C21-C20-CA9-CA8
26	C	306	CDL	C34-C35-C36-C37
28	E	201	PSC	C23-C24-C25-C26
20	P	304	PGV	C02-C03-O11-P
28	V	101	PSC	C02-C03-O11-P
20	P	305	PGV	C22-C23-C24-C25
21	B	301	TGL	CA5-CA6-CA7-CA8
21	B	301	TGL	CB3-CB4-CB5-CB6
25	C	303	PEK	C32-C33-C34-C35
21	D	201	TGL	OG1-CG1-CG2-CG3
21	L	101	TGL	OG1-CG1-CG2-CG3
21	N	608	TGL	OG1-CG1-CG2-CG3
26	P	306	CDL	CB3-CB4-CB6-OB8
21	B	301	TGL	C11-C12-C13-C14
21	L	101	TGL	C29-C30-C31-C32
26	G	101	CDL	CA7-C31-C32-C33
20	N	612	PGV	C10-C11-C12-C13
25	P	303	PEK	C4-C5-C6-C7
20	N	612	PGV	C31-C32-C33-C34
21	L	101	TGL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C75-C76-C77-C78
26	T	101	CDL	C41-C42-C43-C44
21	N	608	TGL	CB4-CB5-CB6-CB7
26	P	306	CDL	C15-C16-C17-C18
28	V	101	PSC	C20-C21-C22-C23
21	L	101	TGL	C13-C14-C29-C30
26	G	101	CDL	C37-C38-C39-C40
21	B	301	TGL	CA3-CA4-CA5-CA6
26	C	306	CDL	CB4-CB6-OB8-CB7
20	A	608	PGV	C31-C32-C33-C34
26	C	306	CDL	C35-C36-C37-C38
18	N	606	HEA	C2A-C3A-CMA-OMA
28	E	201	PSC	C10-C11-C12-C13
28	V	101	PSC	C9-C10-C11-C12
26	G	101	CDL	C23-C24-C25-C26
20	C	305	PGV	O05-C05-C06-O06
21	N	608	TGL	CB1-CB2-CB3-CB4
21	B	301	TGL	C24-C25-C26-C27
21	Q	201	TGL	OG1-CA1-CA2-CA3
21	Q	201	TGL	C19-C33-C34-C35
21	L	101	TGL	OG2-CG2-CG3-OG3
21	Q	201	TGL	OG1-CG1-CG2-OG2
26	P	306	CDL	OB6-CB4-CB6-OB8
28	E	201	PSC	O03-C01-C02-O01
21	D	201	TGL	C11-C12-C13-C14
25	P	303	PEK	C33-C34-C35-C36
25	C	303	PEK	C26-C27-C28-C29
26	C	306	CDL	C79-C80-C81-C82
26	P	306	CDL	C74-C75-C76-C77
30	Z	101	DMU	C18-C19-C22-C25
26	P	306	CDL	C60-C61-C62-C63
21	L	101	TGL	C11-C10-CB9-CB8
20	C	305	PGV	C01-C02-C03-O11
24	G	102	CHD	C17-C20-C22-C23
21	D	201	TGL	C11-C10-CB9-CB8
21	L	101	TGL	C10-C11-C12-C13
25	C	303	PEK	C10-C11-C12-C13
26	P	306	CDL	C57-C58-C59-C60
20	C	304	PGV	C12-C13-C14-C15
26	P	306	CDL	OA7-CA5-OA6-CA4
28	E	201	PSC	C4-C5-C6-C7
20	A	607	PGV	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
21	D	201	TGL	CG1-CG2-CG3-OG3
26	T	101	CDL	CB4-CB3-OB5-PB2
20	A	607	PGV	C15-C16-C17-C18
26	G	101	CDL	OB5-CB3-CB4-OB6
28	V	101	PSC	O01-C02-C03-O11
24	C	307	CHD	C20-C22-C23-C24
21	Q	201	TGL	CA2-CA3-CA4-CA5
26	T	101	CDL	C54-C55-C56-C57
20	P	304	PGV	C11-C12-C13-C14
26	P	306	CDL	CB2-C1-CA2-OA2
20	P	304	PGV	C7-C8-C9-C10
26	P	306	CDL	C75-C76-C77-C78
20	A	607	PGV	O03-C01-C02-O01
26	C	306	CDL	OB6-CB4-CB6-OB8
26	C	306	CDL	C60-C61-C62-C63
26	P	306	CDL	C34-C35-C36-C37
26	C	306	CDL	C16-C17-C18-C19
26	T	101	CDL	C14-C15-C16-C17
21	D	201	TGL	C25-C26-C27-C28
26	C	306	CDL	C61-C62-C63-C64
21	B	301	TGL	CB6-CB7-CB8-CB9
25	P	303	PEK	C10-C11-C12-C13
21	L	101	TGL	CA4-CA5-CA6-CA7
21	L	101	TGL	C16-C15-CC9-CC8
26	P	306	CDL	C17-C18-C19-C20
20	C	305	PGV	C3-C4-C5-C6
21	L	101	TGL	C17-C18-C19-C33
26	T	101	CDL	C78-C79-C80-C81
20	A	608	PGV	C12-C13-C14-C15
26	G	101	CDL	CB2-OB2-PB2-OB5
21	D	201	TGL	CA2-CA3-CA4-CA5
30	M	101	DMU	C19-C22-C25-C28
20	P	305	PGV	C02-C03-O11-P
26	P	306	CDL	CA4-CA3-OA5-PA1
25	C	303	PEK	C33-C34-C35-C36
26	C	306	CDL	C36-C37-C38-C39
20	A	607	PGV	C03-O11-P-O13
20	C	305	PGV	C04-O12-P-O14
20	P	305	PGV	C04-O12-P-O13
26	C	306	CDL	CB3-OB5-PB2-OB3
26	G	101	CDL	CA3-OA5-PA1-OA3
26	G	101	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
26	G	101	CDL	CB3-OB5-PB2-OB4
26	P	306	CDL	CA2-OA2-PA1-OA3
26	T	101	CDL	CB3-OB5-PB2-OB4
26	G	101	CDL	C77-C78-C79-C80
25	P	303	PEK	C22-C21-O03-C01
28	V	101	PSC	C01-C02-C03-O11
26	G	101	CDL	C32-C31-CA7-OA8
31	2	201	HEC	C3D-CAD-CBD-CGD
24	C	307	CHD	C16-C17-C20-C21
26	G	101	CDL	C16-C17-C18-C19
28	E	201	PSC	C05-C04-O12-P
28	E	201	PSC	C3-C4-C5-C6
21	L	101	TGL	CA2-CA3-CA4-CA5
20	A	608	PGV	C27-C28-C29-C30
21	B	301	TGL	CA6-CA7-CA8-CA9
25	C	303	PEK	C23-C24-C25-C26
26	G	101	CDL	O1-C1-CB2-OB2
26	G	101	CDL	C59-C60-C61-C62
18	A	604[A]	HEA	C4A-C3A-CMA-OMA
18	A	604[B]	HEA	C4A-C3A-CMA-OMA
18	A	605	HEA	C4A-C3A-CMA-OMA
18	N	605[A]	HEA	C4A-C3A-CMA-OMA
18	N	605[B]	HEA	C4A-C3A-CMA-OMA
18	N	606	HEA	C4A-C3A-CMA-OMA
26	G	101	CDL	CB3-CB4-CB6-OB8
21	D	201	TGL	OG2-CG2-CG3-OG3
26	P	306	CDL	OA6-CA4-CA6-OA8
26	T	101	CDL	OA6-CA4-CA6-OA8
28	V	101	PSC	O03-C01-C02-O01
26	P	306	CDL	C12-C13-C14-C15
21	Q	201	TGL	C14-C29-C30-C31
20	C	304	PGV	C02-C03-O11-P
25	P	303	PEK	C17-C18-C19-C20
21	D	201	TGL	C20-C21-C22-C23
20	C	304	PGV	C25-C26-C27-C28
20	P	305	PGV	C21-C22-C23-C24
20	P	305	PGV	C27-C28-C29-C30
25	P	303	PEK	C21-C22-C23-C24
21	D	201	TGL	C10-C11-C12-C13
21	N	608	TGL	CC7-CC8-CC9-C15
31	2	201	HEC	C1A-C2A-CAA-CBA
28	E	201	PSC	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
20	A	607	PGV	C21-C22-C23-C24
25	C	303	PEK	C24-C25-C26-C27
21	B	301	TGL	CG1-CG2-OG2-CB1
20	A	607	PGV	C01-C02-C03-O11
24	P	307	CHD	C20-C22-C23-C24
18	N	606	HEA	C11-C12-C13-C14
20	C	304	PGV	C1-C2-C3-C4
21	Q	201	TGL	CA5-CA6-CA7-CA8
26	P	306	CDL	CB4-CB6-OB8-CB7
20	A	608	PGV	C02-C01-O03-C19
20	C	305	PGV	C31-C32-C33-C34
21	B	301	TGL	C21-C22-C23-C24
21	L	101	TGL	OG1-CG1-CG2-OG2
20	A	607	PGV	C04-O12-P-O11
20	C	305	PGV	C03-O11-P-O12
26	P	306	CDL	CA3-OA5-PA1-OA2
26	T	101	CDL	CB2-OB2-PB2-OB5
21	B	301	TGL	CG1-CG2-CG3-OG3
21	L	101	TGL	CG1-CG2-CG3-OG3
26	C	306	CDL	CA3-CA4-CA6-OA8
26	T	101	CDL	C12-C13-C14-C15
26	C	306	CDL	C75-C76-C77-C78
25	P	303	PEK	C35-C36-C37-C38
28	E	201	PSC	C14-C15-C16-C17
26	C	306	CDL	C44-C45-C46-C47
20	C	304	PGV	C05-C04-O12-P
20	A	607	PGV	O01-C1-C2-C3
18	A	605	HEA	CAA-CBA-CGA-O1A
26	G	101	CDL	C81-C82-C83-C84
20	P	304	PGV	C11-C10-C9-C8
20	C	305	PGV	C10-C11-C12-C13
24	C	301	CHD	C22-C23-C24-O25
24	P	301	CHD	C22-C23-C24-O26
21	Q	201	TGL	CB3-CB4-CB5-CB6
18	N	605[A]	HEA	C19-C20-C21-C22
21	D	201	TGL	CC5-CC6-CC7-CC8
20	A	607	PGV	C11-C10-C9-C8
21	L	101	TGL	C16-C17-C18-C19
26	T	101	CDL	O1-C1-CA2-OA2
24	C	307	CHD	C22-C23-C24-O25
24	C	307	CHD	C22-C23-C24-O26
24	P	307	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C1-CB2-OB2-PB2
26	T	101	CDL	C1-CA2-OA2-PA1
18	A	604[A]	HEA	CAD-CBD-CGD-O1D
18	A	604[B]	HEA	CAD-CBD-CGD-O1D
24	P	301	CHD	C22-C23-C24-O25
31	2	201	HEC	CAA-CBA-CGA-O2A
21	L	101	TGL	CC2-CC3-CC4-CC5
20	P	304	PGV	C31-C32-C33-C34
21	D	201	TGL	CC7-CC8-CC9-C15
21	L	101	TGL	CC5-CC6-CC7-CC8
26	T	101	CDL	C53-C54-C55-C56
18	A	605	HEA	CAD-CBD-CGD-O1D
24	J	101	CHD	C22-C23-C24-O25
31	2	201	HEC	CAA-CBA-CGA-O1A
31	2	201	HEC	C3A-C2A-CAA-CBA
21	N	608	TGL	CG1-CG2-OG2-CB1
20	C	305	PGV	C15-C16-C17-C18
28	V	101	PSC	C3-C4-C5-C6
20	A	607	PGV	C9-C10-C11-C12
21	N	608	TGL	C11-C10-CB9-CB8
25	C	303	PEK	C6-C7-C8-C9
25	C	303	PEK	C9-C10-C11-C12
20	P	305	PGV	C25-C26-C27-C28
26	C	306	CDL	C1-CB2-OB2-PB2
20	A	607	PGV	O05-C05-C06-O06
20	A	607	PGV	C7-C8-C9-C10
20	P	305	PGV	C9-C10-C11-C12
26	C	306	CDL	C52-C53-C54-C55
18	A	605	HEA	CAA-CBA-CGA-O2A
18	N	606	HEA	CAD-CBD-CGD-O1D
21	D	201	TGL	C33-C34-C35-C36
26	G	101	CDL	C31-C32-C33-C34
21	D	201	TGL	OB1-CB1-OG2-CG2
24	G	102	CHD	C22-C23-C24-O25
18	A	604[A]	HEA	CAD-CBD-CGD-O2D
18	A	604[B]	HEA	CAD-CBD-CGD-O2D
18	A	605	HEA	CAD-CBD-CGD-O2D
24	J	101	CHD	C22-C23-C24-O26
24	P	307	CHD	C22-C23-C24-O25
21	L	101	TGL	CB9-C10-C11-C12
26	G	101	CDL	C51-C52-C53-C54
25	P	303	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C73-C74-C75-C76
18	N	605[A]	HEA	CAD-CBD-CGD-O1D
18	N	605[B]	HEA	CAD-CBD-CGD-O1D
21	L	101	TGL	C14-C29-C30-C31
26	C	306	CDL	C74-C75-C76-C77
18	N	606	HEA	CAD-CBD-CGD-O2D
26	P	306	CDL	CA5-C11-C12-C13
24	C	301	CHD	C22-C23-C24-O26
24	T	103	CHD	C22-C23-C24-O26
25	P	303	PEK	C29-C30-C31-C32
28	E	201	PSC	C7-C8-C9-C10
26	P	306	CDL	C42-C43-C44-C45
26	P	306	CDL	C84-C85-C86-C87
24	G	102	CHD	C22-C23-C24-O26
26	T	101	CDL	OB5-CB3-CB4-CB6
26	P	306	CDL	C77-C78-C79-C80
21	L	101	TGL	OG1-CA1-CA2-CA3
26	G	101	CDL	C52-C51-CB5-OB6
21	N	608	TGL	CB9-C10-C11-C12
20	C	305	PGV	C05-C04-O12-P
20	A	608	PGV	C14-C15-C16-C17
21	D	201	TGL	C24-C25-C26-C27
18	N	606	HEA	C2D-C3D-CAD-CBD
21	B	301	TGL	C12-C13-C14-C29
31	2	201	HEC	C2B-C3B-CAB-CBB
21	Q	201	TGL	C24-C25-C26-C27
20	C	304	PGV	C11-C12-C13-C14
21	D	201	TGL	CA1-CA2-CA3-CA4
30	Z	101	DMU	C31-C34-C37-C40
28	V	101	PSC	C24-C25-C26-C27
28	V	101	PSC	C11-C10-C9-C8
26	P	306	CDL	C24-C25-C26-C27
24	W	101	CHD	C22-C23-C24-O26
20	P	305	PGV	C13-C14-C15-C16
21	D	201	TGL	CC4-CC5-CC6-CC7
26	T	101	CDL	C35-C36-C37-C38
26	P	306	CDL	C19-C20-C21-C22
26	T	101	CDL	C32-C31-CA7-OA8
25	P	303	PEK	C30-C31-C32-C33
25	P	303	PEK	O04-C21-O03-C01
20	C	304	PGV	C9-C10-C11-C12
25	C	303	PEK	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	CB3-CB4-CB6-OB8
21	Q	201	TGL	OA1-CA1-CA2-CA3
20	A	607	PGV	O01-C02-C03-O11
24	T	103	CHD	C22-C23-C24-O25
26	G	101	CDL	C84-C85-C86-C87
21	D	201	TGL	OG3-CC1-CC2-CC3
23	N	614	EDO	O1-C1-C2-O2
21	Q	201	TGL	CC6-CC7-CC8-CC9
26	C	306	CDL	C77-C78-C79-C80
20	C	305	PGV	O12-C04-C05-O05
20	A	608	PGV	C4-C5-C6-C7
26	G	101	CDL	C62-C63-C64-C65
26	P	306	CDL	C32-C31-CA7-OA8
28	V	101	PSC	C22-C23-C24-C25
26	G	101	CDL	C39-C40-C41-C42
20	P	305	PGV	C1-C2-C3-C4
25	P	303	PEK	C15-C16-C17-C18
20	A	608	PGV	O03-C19-C20-C21
18	N	605[A]	HEA	CAD-CBD-CGD-O2D
18	N	605[B]	HEA	CAD-CBD-CGD-O2D
24	W	101	CHD	C22-C23-C24-O25
21	L	101	TGL	OG2-CB1-CB2-CB3
21	L	101	TGL	C25-C26-C27-C28
21	N	608	TGL	CA9-C20-C21-C22
26	P	306	CDL	C22-C23-C24-C25
20	C	305	PGV	C04-C05-C06-O06
21	B	301	TGL	C16-C15-CC9-CC8
20	C	305	PGV	O12-C04-C05-C06
21	B	301	TGL	CC6-CC7-CC8-CC9
26	T	101	CDL	C32-C31-CA7-OA9
28	V	101	PSC	C7-C8-C9-C10
28	V	101	PSC	O03-C01-C02-C03
26	P	306	CDL	C72-C73-C74-C75
24	C	307	CHD	C13-C17-C20-C21
21	D	201	TGL	OC1-CC1-CC2-CC3
18	A	605	HEA	C26-C15-C16-C17
26	P	306	CDL	C32-C31-CA7-OA9
20	A	607	PGV	C04-O12-P-O13
26	C	306	CDL	CB2-OB2-PB2-OB3
26	C	306	CDL	CB3-OB5-PB2-OB4
26	P	306	CDL	CA2-OA2-PA1-OA4
28	V	101	PSC	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
31	2	201	HEC	C4B-C3B-CAB-CBB
23	B	303	EDO	O1-C1-C2-O2
23	C	311	EDO	O1-C1-C2-O2
18	N	605[A]	HEA	CAA-CBA-CGA-O2A
18	N	605[B]	HEA	CAA-CBA-CGA-O2A
21	L	101	TGL	OB1-CB1-CB2-CB3
26	P	306	CDL	OB9-CB7-OB8-CB6
26	G	101	CDL	C55-C56-C57-C58
26	G	101	CDL	C79-C80-C81-C82
20	A	608	PGV	C19-C20-C21-C22
26	T	101	CDL	C12-C11-CA5-OA6
21	Q	201	TGL	C15-C16-C17-C18
26	G	101	CDL	C21-C22-C23-C24
24	C	307	CHD	C16-C17-C20-C22
26	T	101	CDL	C19-C20-C21-C22
20	C	305	PGV	O01-C1-C2-C3
26	C	306	CDL	C52-C51-CB5-OB6
26	G	101	CDL	C80-C81-C82-C83
20	C	304	PGV	C28-C29-C30-C31
20	N	612	PGV	O03-C19-C20-C21
21	Q	201	TGL	C25-C26-C27-C28
20	A	608	PGV	C11-C10-C9-C8
25	P	303	PEK	C25-C26-C27-C28
26	T	101	CDL	C12-C11-CA5-OA7
31	1	201	HEC	CAA-CBA-CGA-O1A
20	A	608	PGV	C9-C10-C11-C12
20	C	305	PGV	C9-C10-C11-C12
25	C	303	PEK	C22-C23-C24-C25
20	C	305	PGV	O02-C1-C2-C3
21	D	201	TGL	OG1-CA1-CA2-CA3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	P	307	CHD	C1-C10-C2-C3-C4-C5

38 monomers are involved in 250 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	G	101	CDL	23	0
25	P	303	PEK	3	0
31	2	201	HEC	4	0

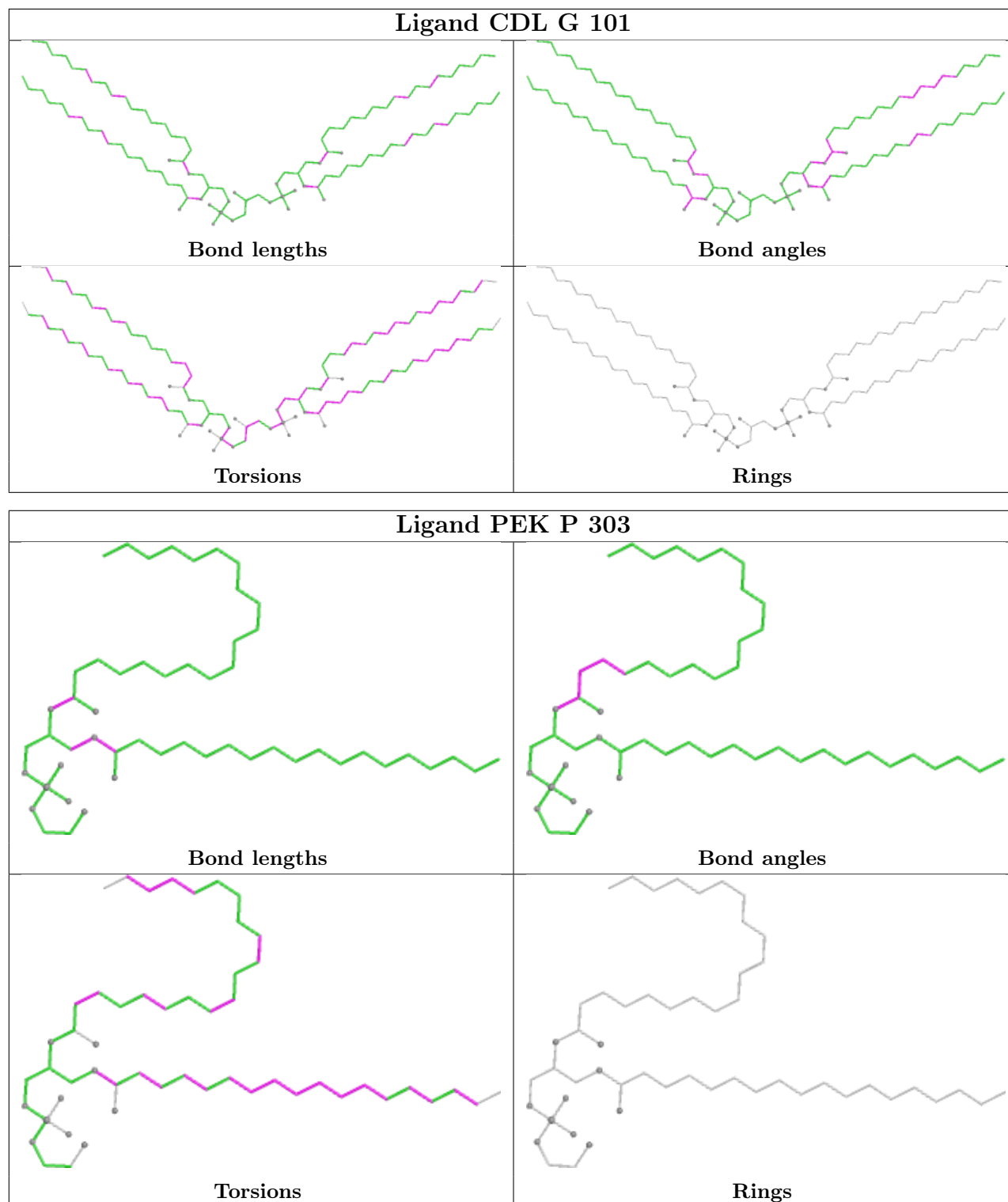
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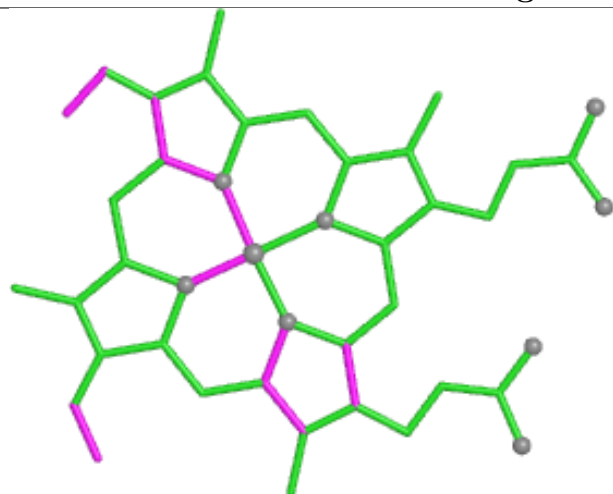
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	M	101	DMU	1	0
20	N	612	PGV	1	0
30	Z	101	DMU	1	0
18	N	605[B]	HEA	7	0
19	N	607	PER	1	0
24	C	307	CHD	3	0
20	C	305	PGV	9	0
26	C	306	CDL	15	0
24	P	301	CHD	1	0
23	E	202	EDO	1	0
18	A	605	HEA	3	0
26	T	101	CDL	24	0
24	P	307	CHD	1	0
21	D	201	TGL	13	0
20	P	305	PGV	4	0
20	C	304	PGV	5	0
18	N	606	HEA	1	0
24	T	103	CHD	1	0
20	A	608	PGV	4	0
28	V	101	PSC	21	0
31	I	201	HEC	4	0
21	B	301	TGL	6	0
24	C	301	CHD	1	0
24	W	101	CHD	5	0
20	P	304	PGV	6	0
21	Q	201	TGL	10	0
25	C	303	PEK	7	0
21	L	101	TGL	20	0
20	A	607	PGV	5	0
21	N	608	TGL	2	0
26	P	306	CDL	12	0
24	J	101	CHD	5	0
18	N	605[A]	HEA	1	0
28	E	201	PSC	19	0
18	A	604[B]	HEA	7	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

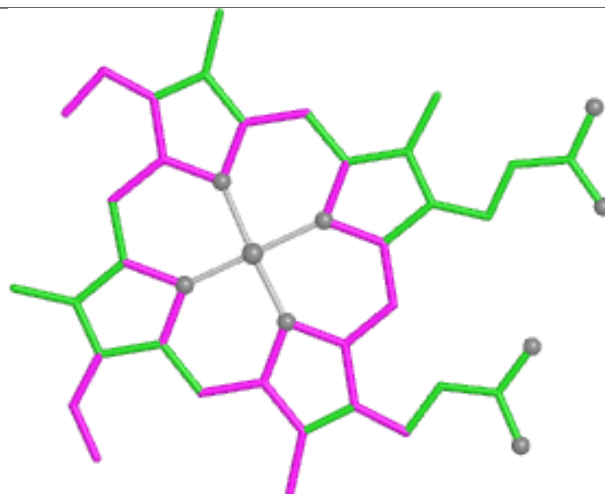
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



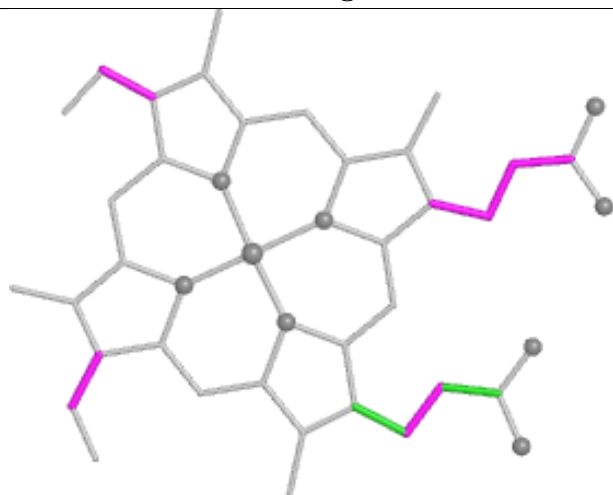
Ligand HEC 2 201



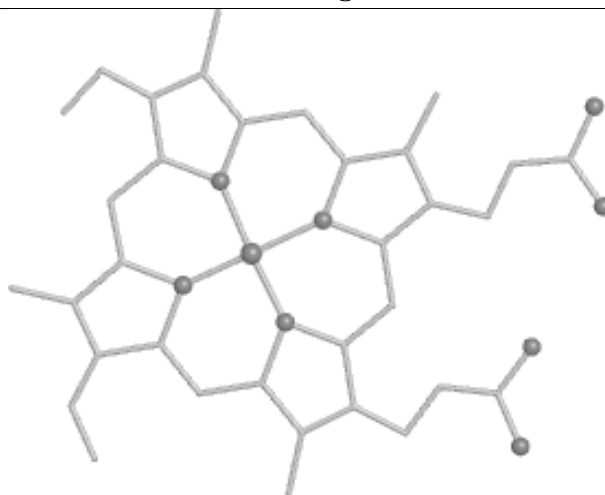
Bond lengths



Bond angles

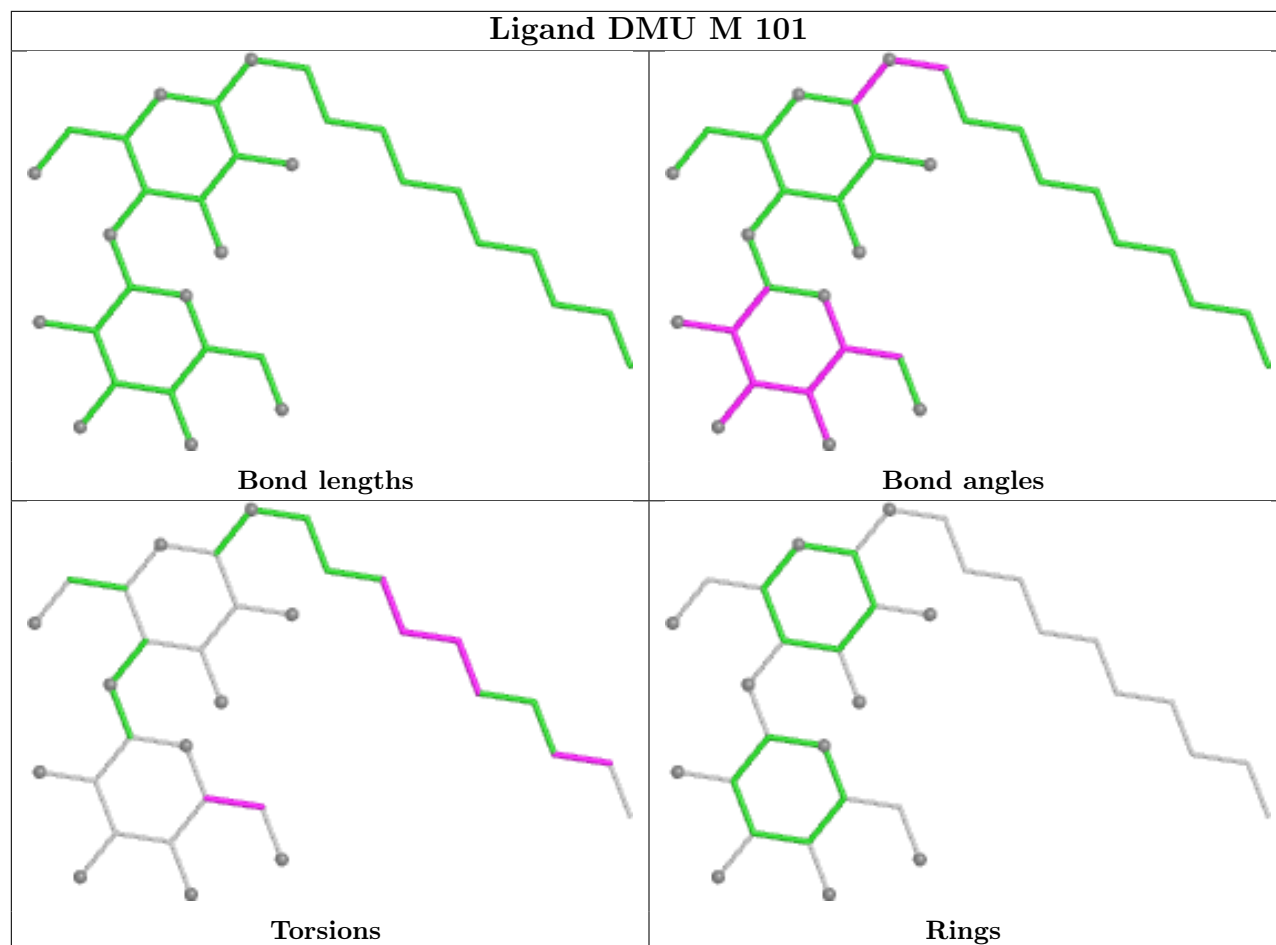


Torsions

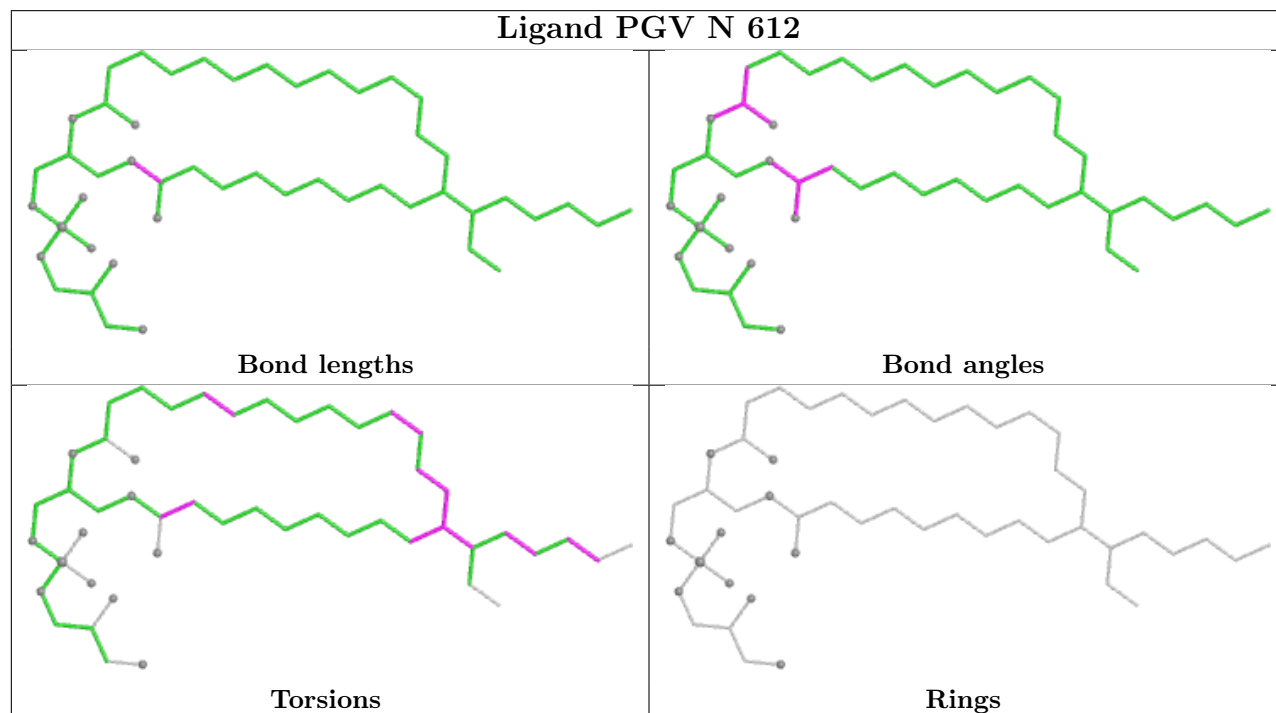


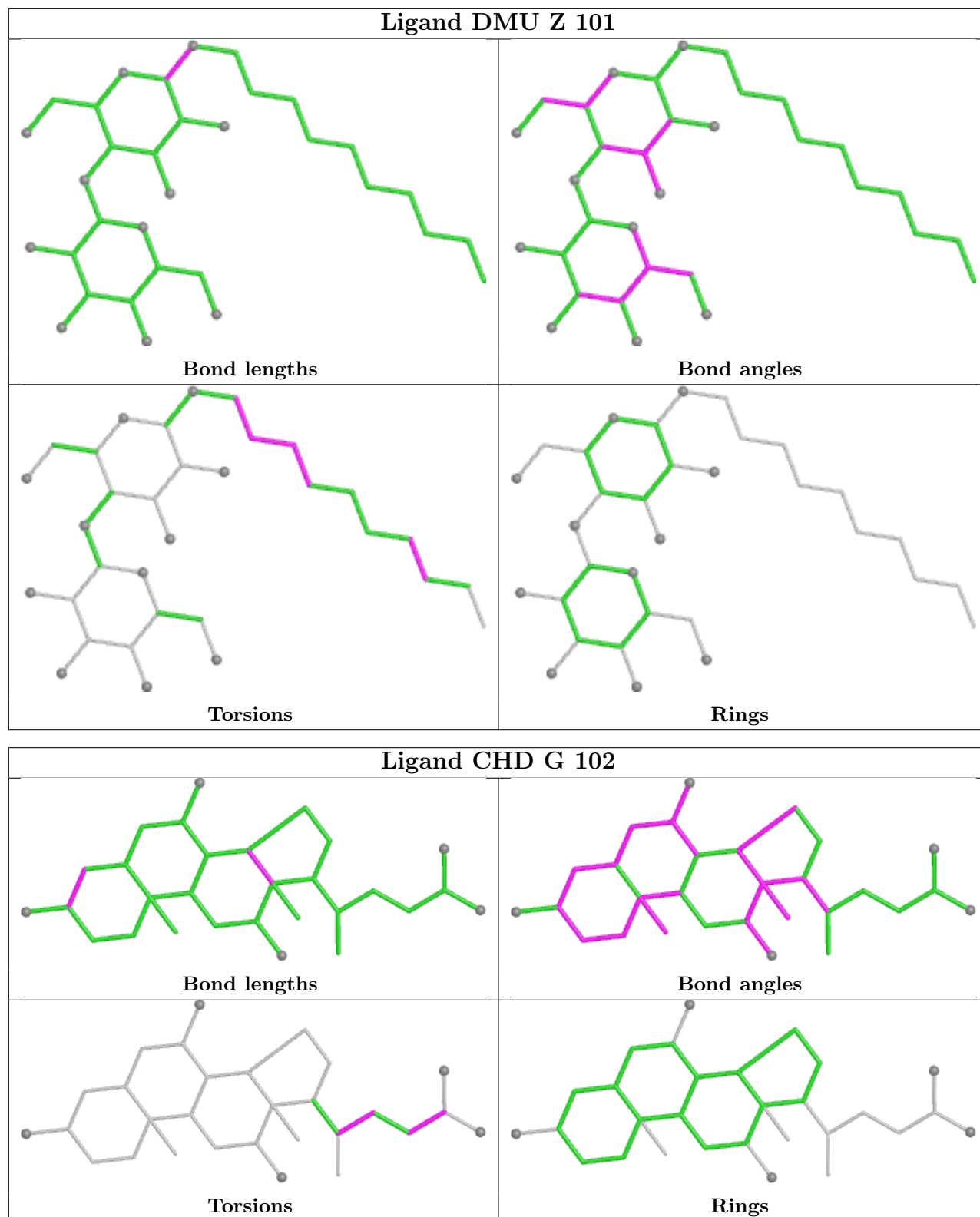
Rings

Ligand DMU M 101

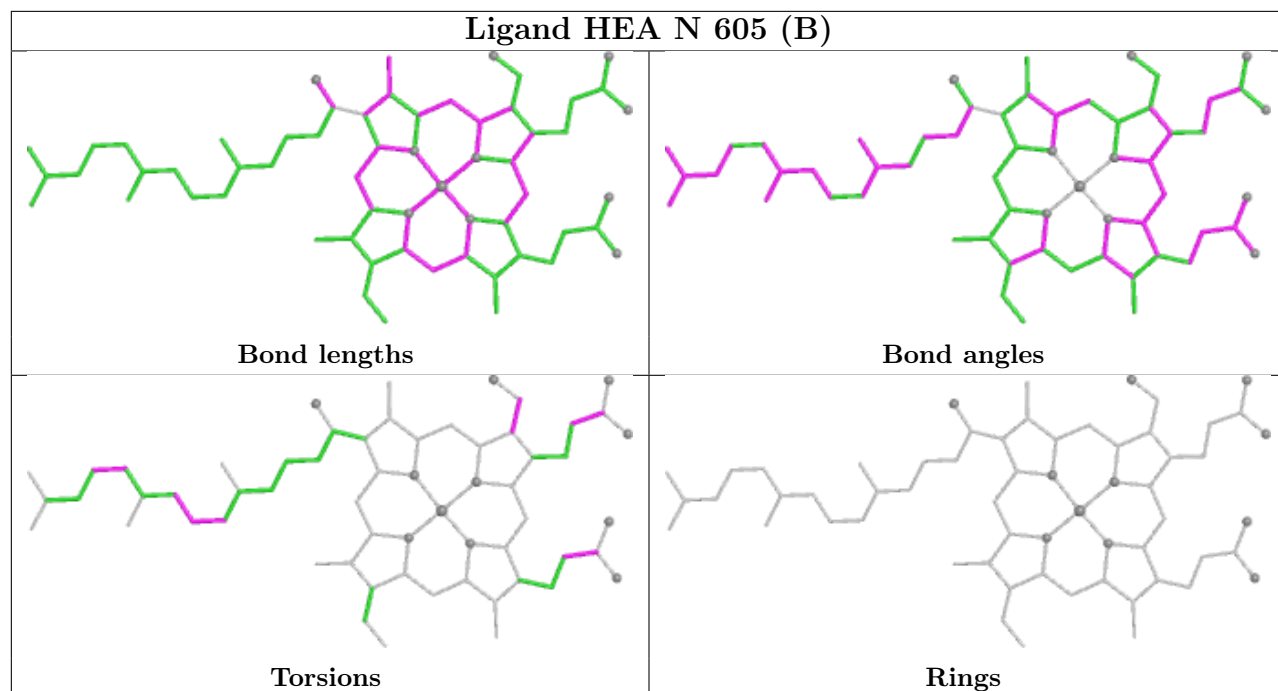


Ligand PGV N 612

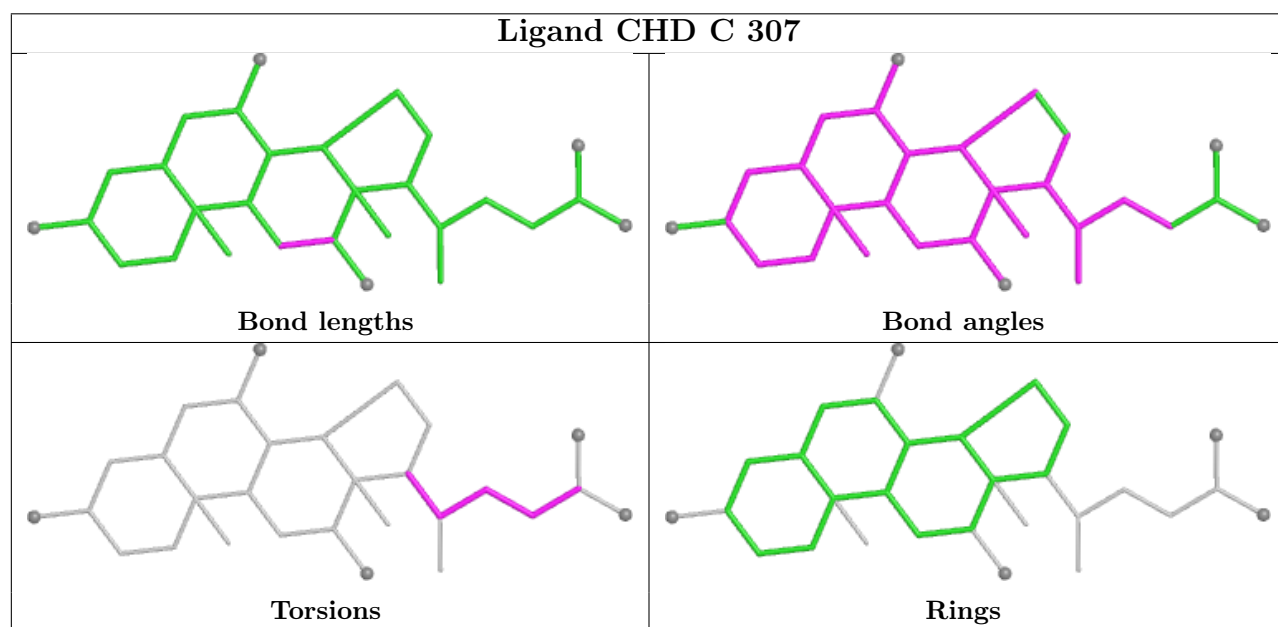


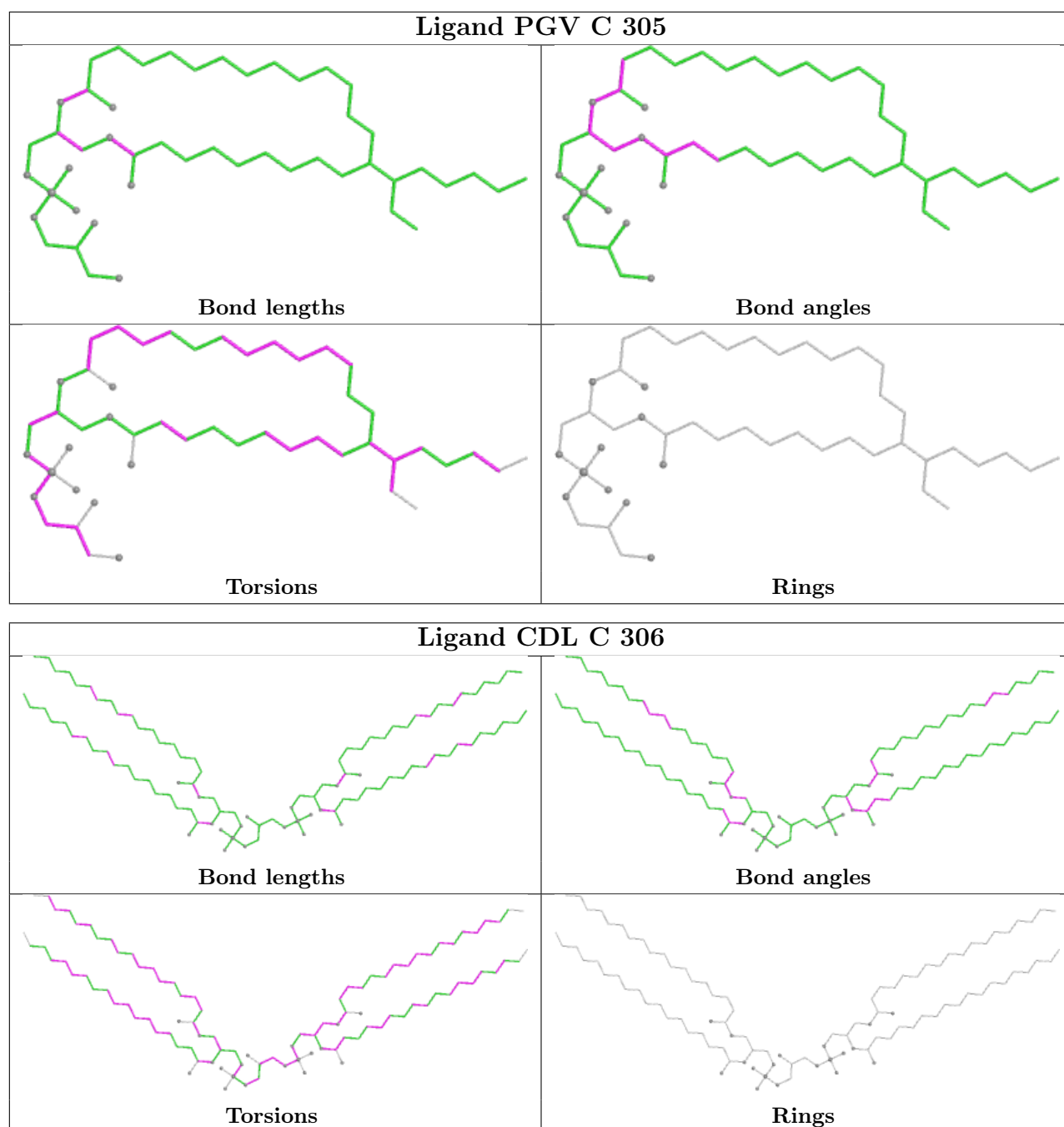


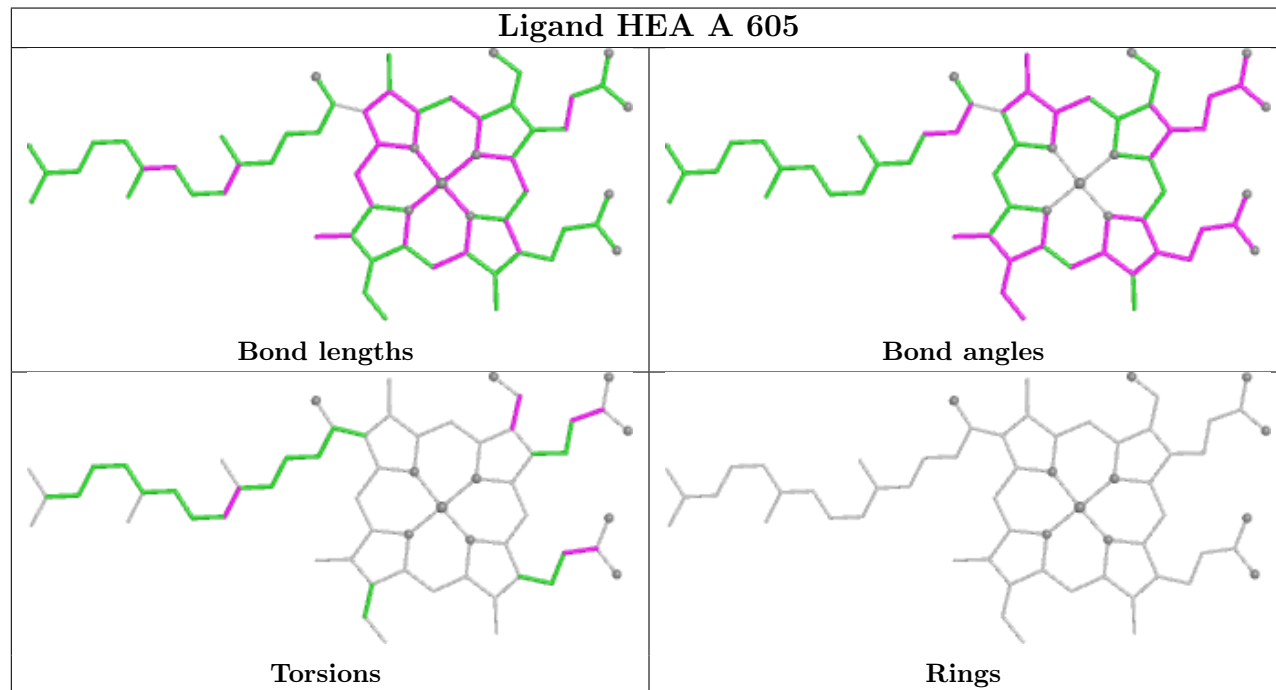
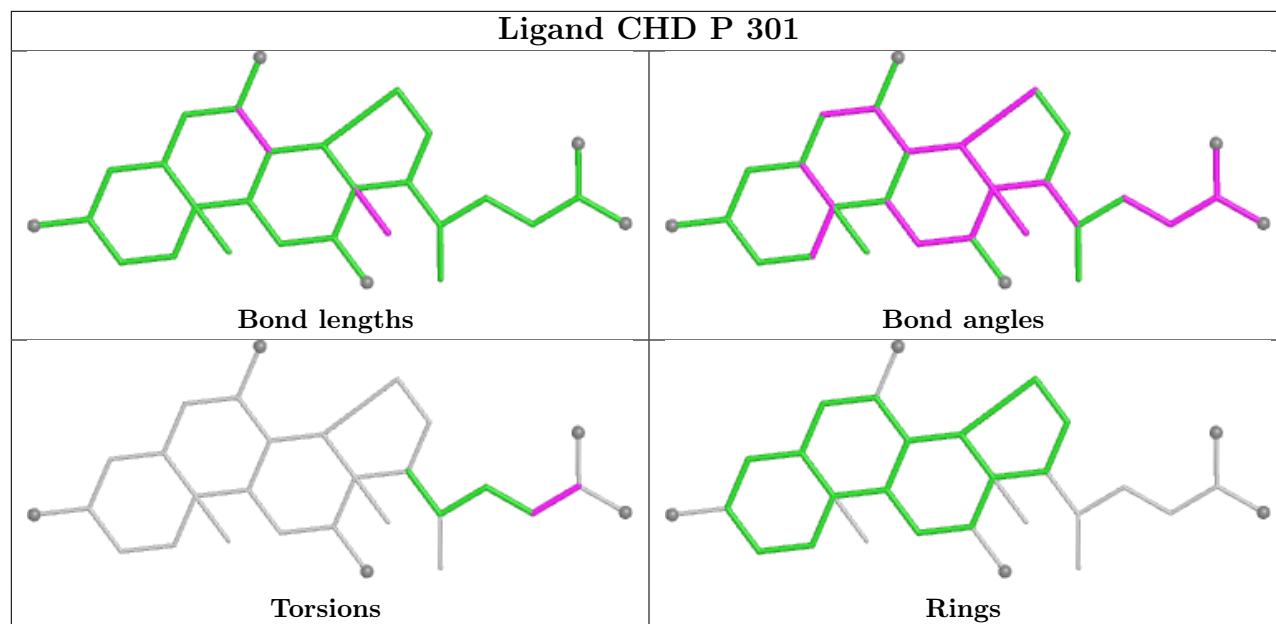
Ligand HEA N 605 (B)

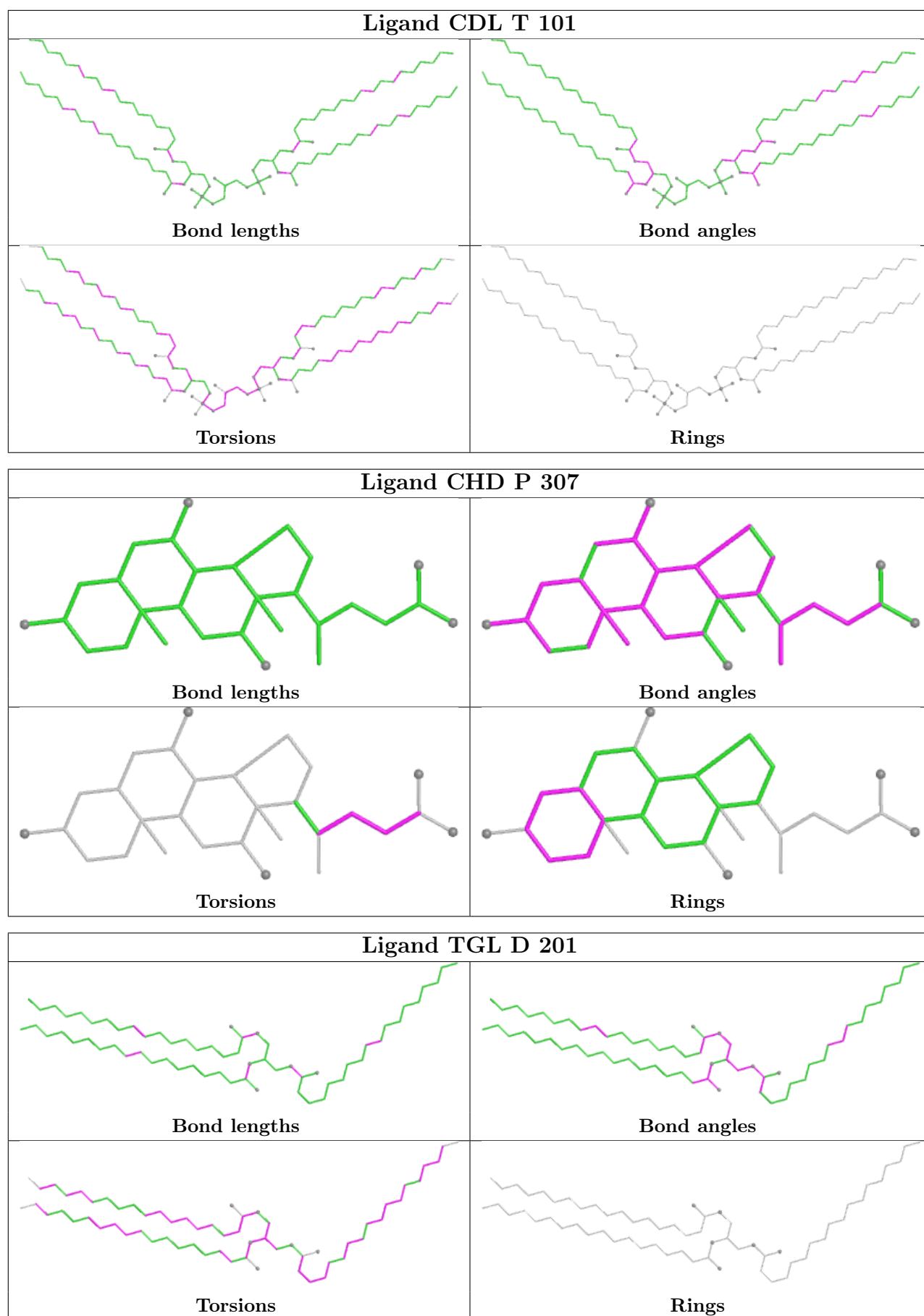


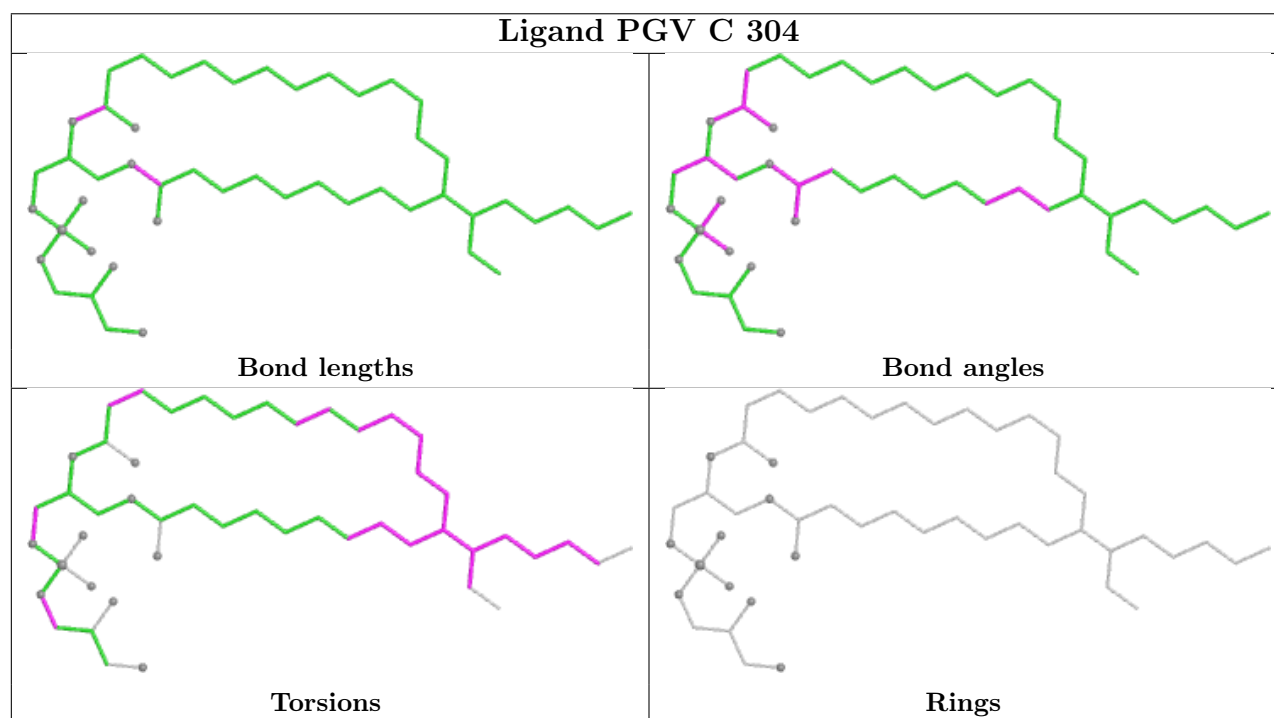
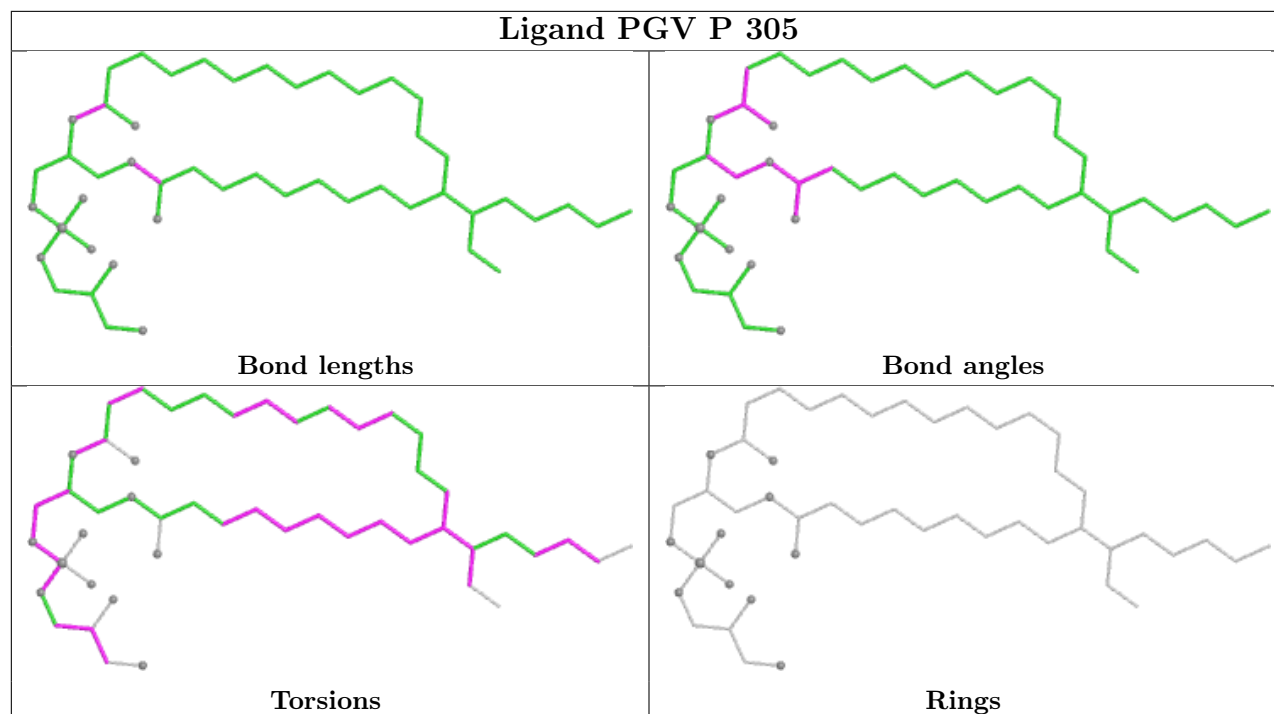
Ligand CHD C 307

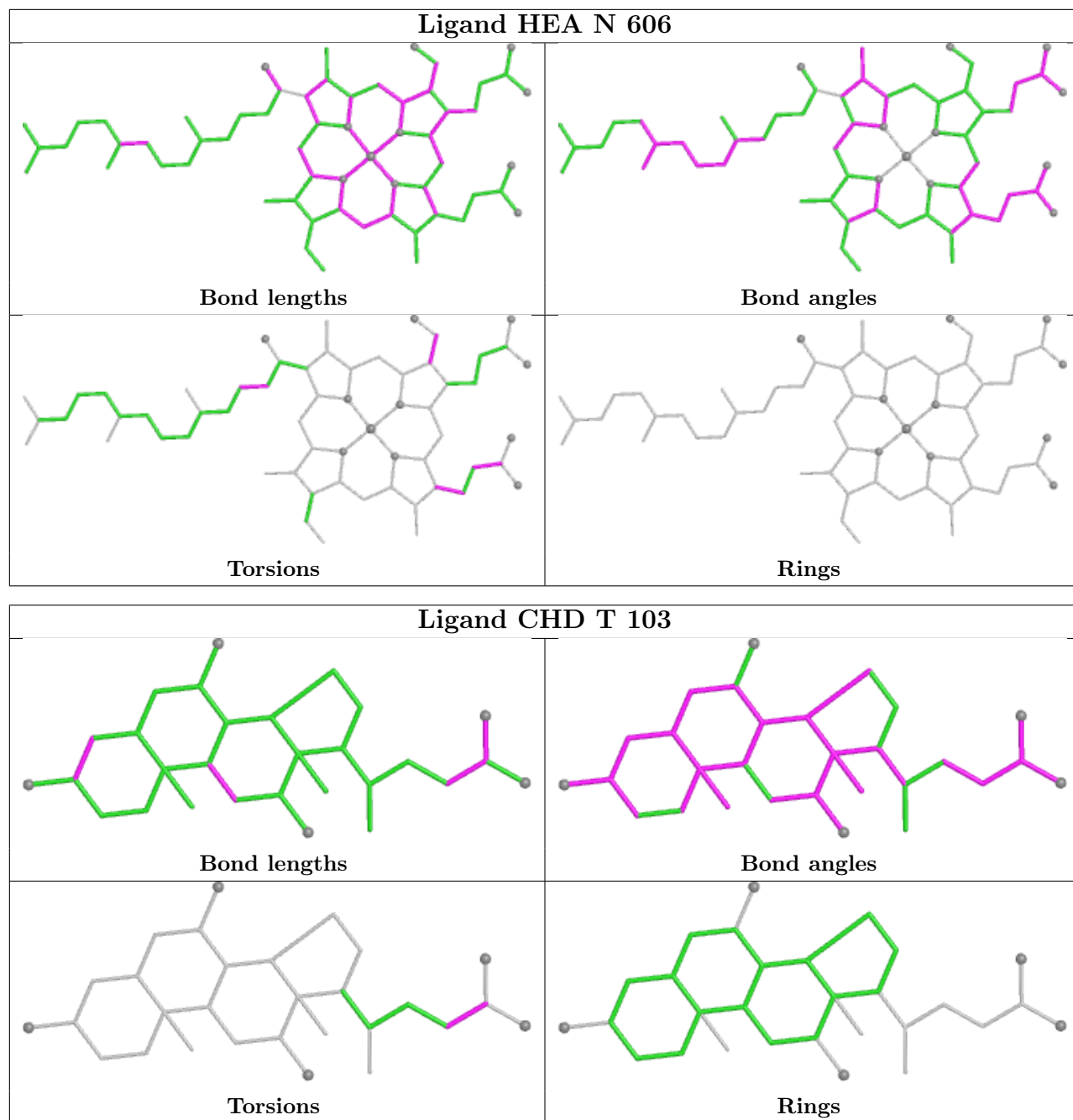


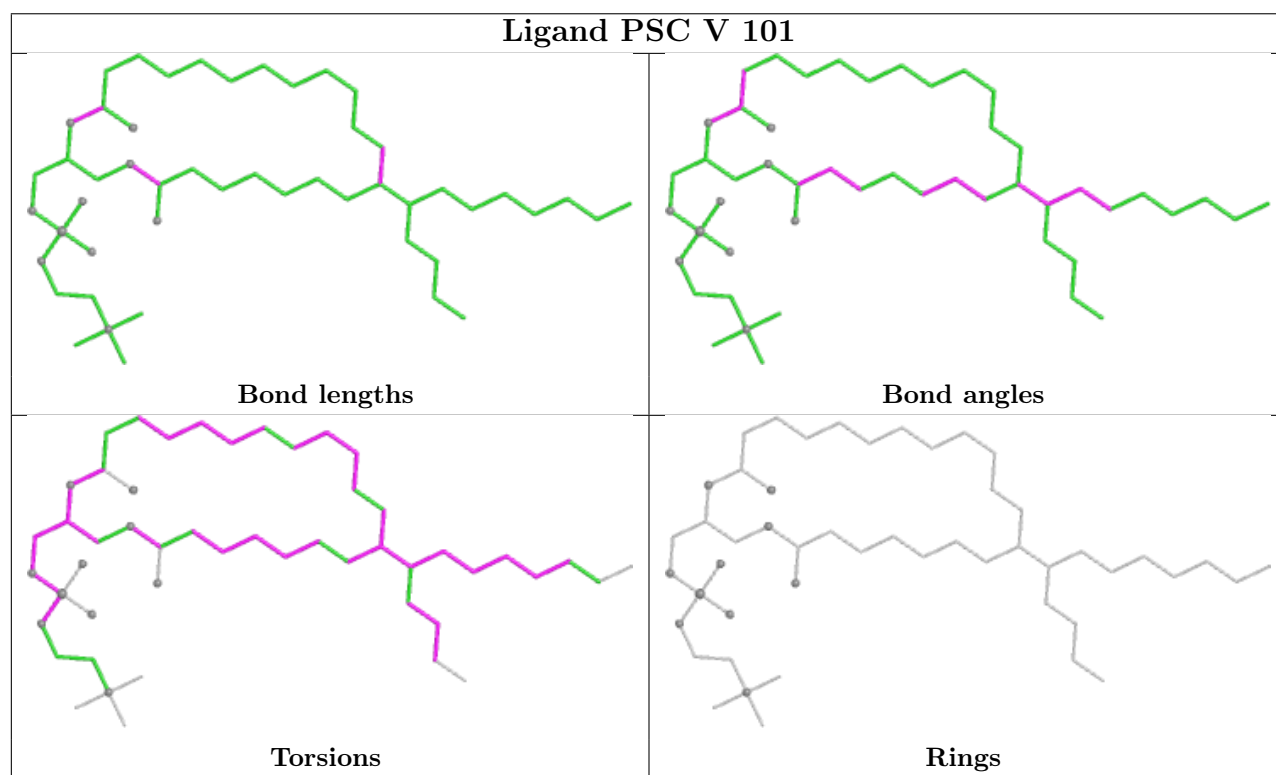
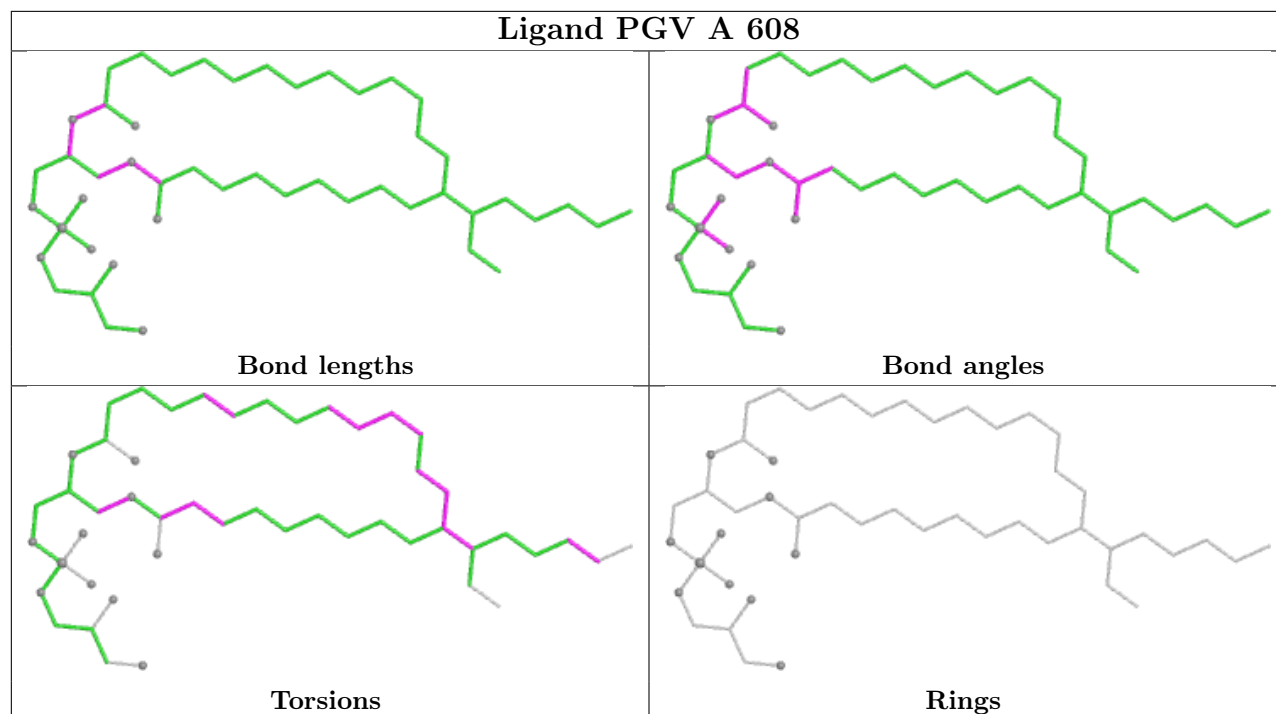




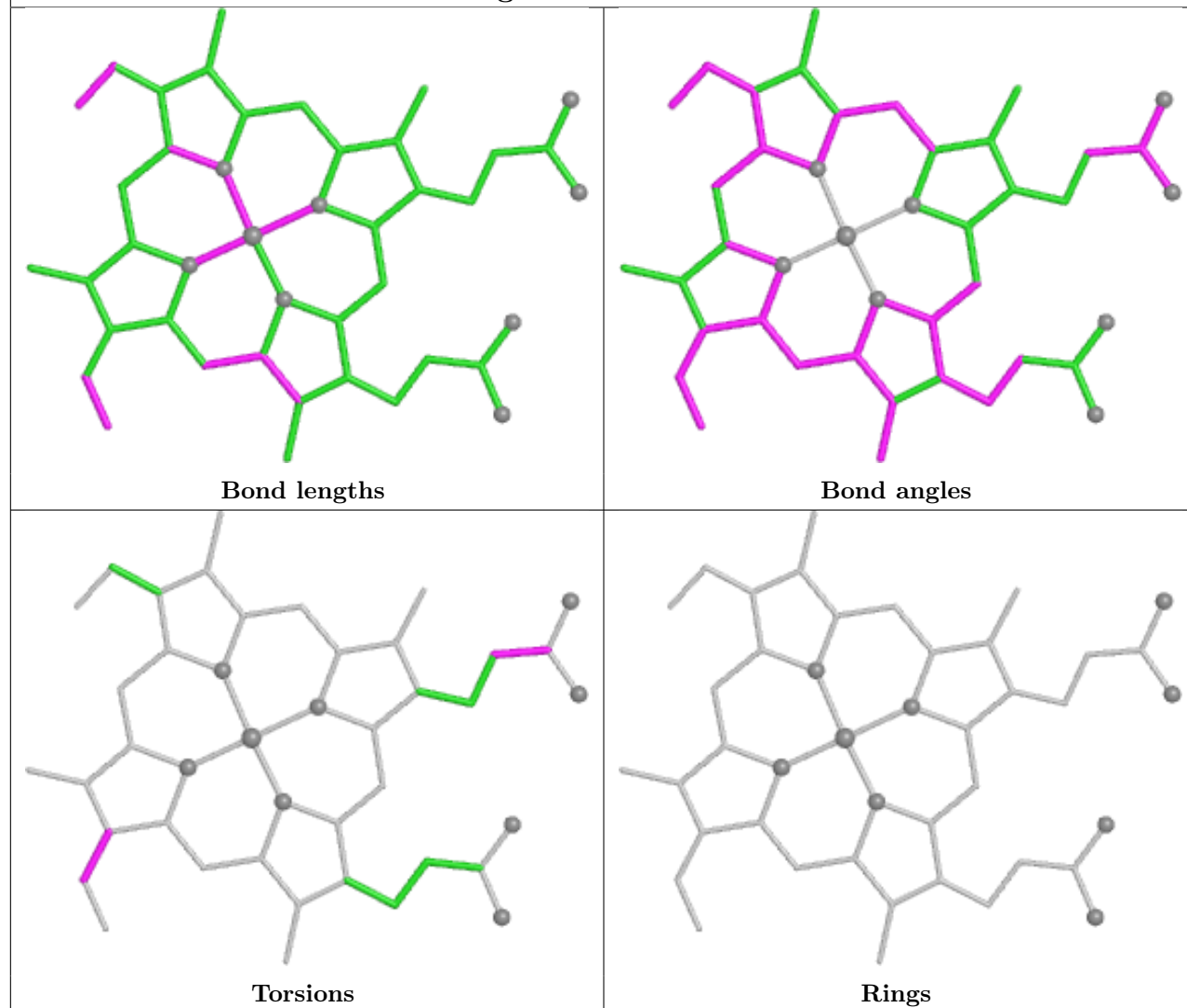




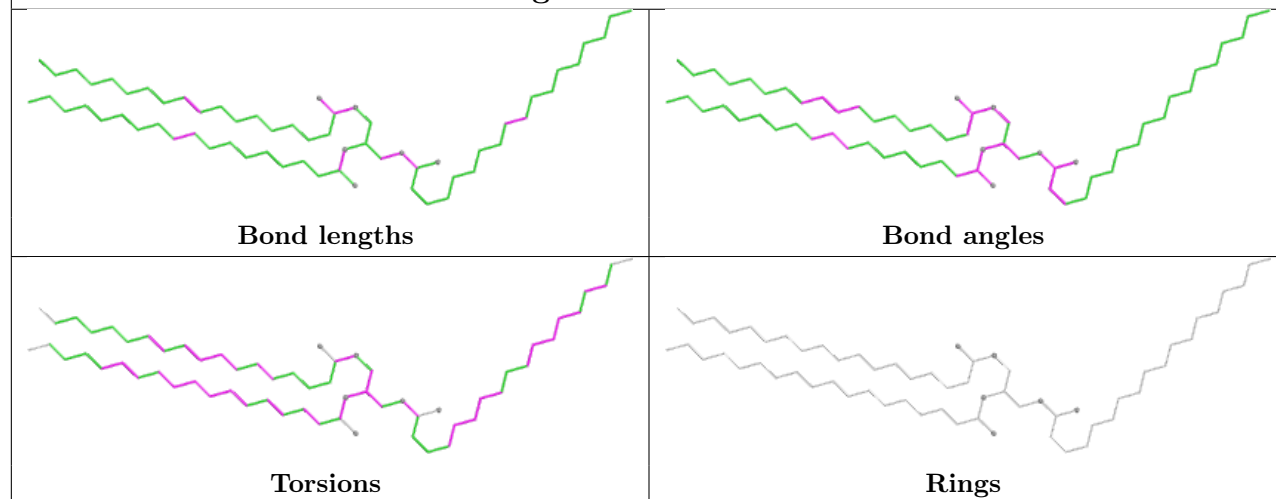


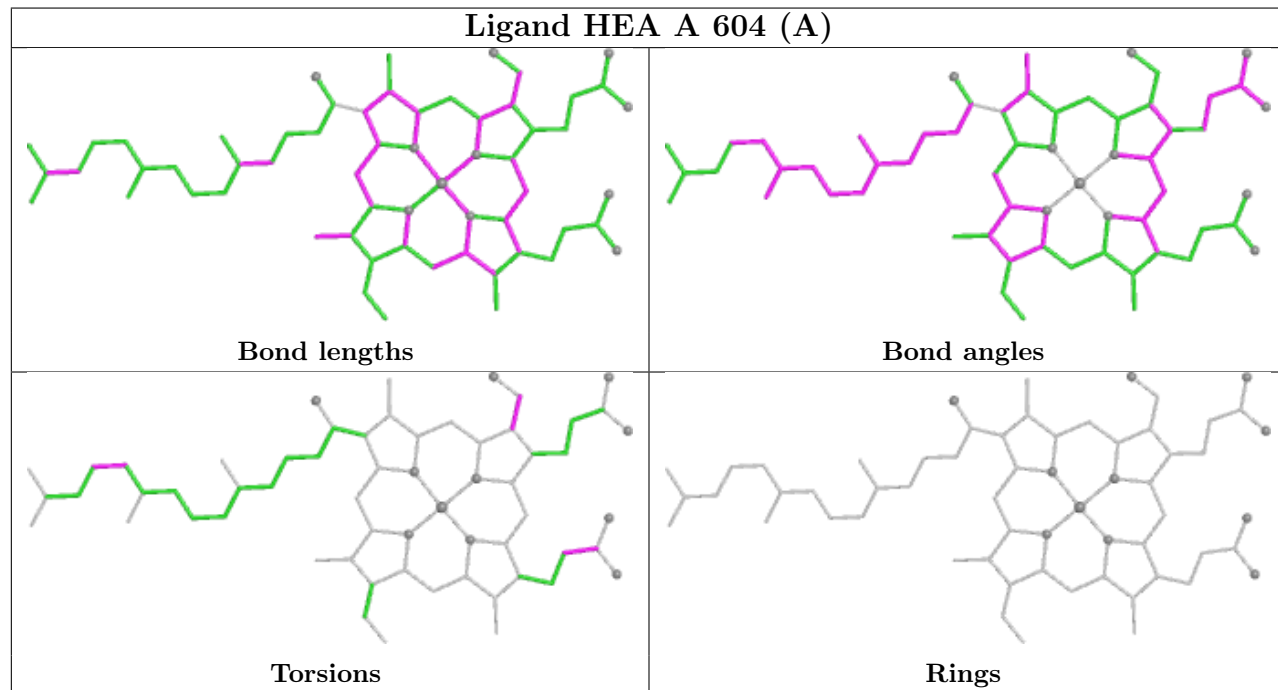
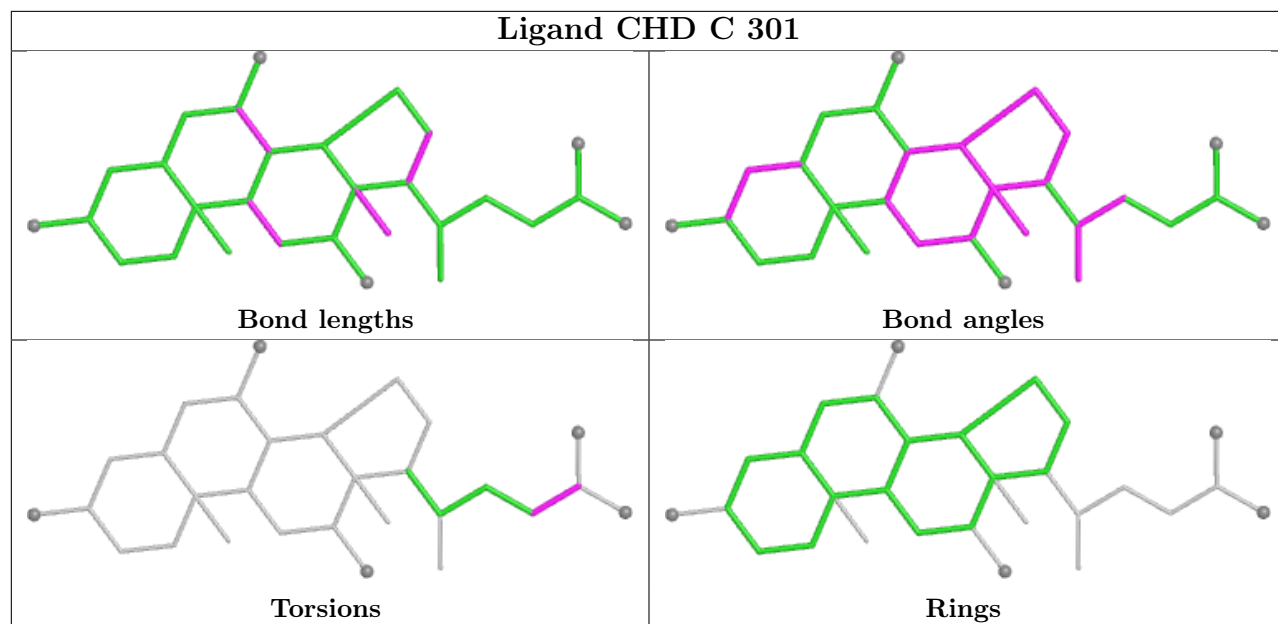


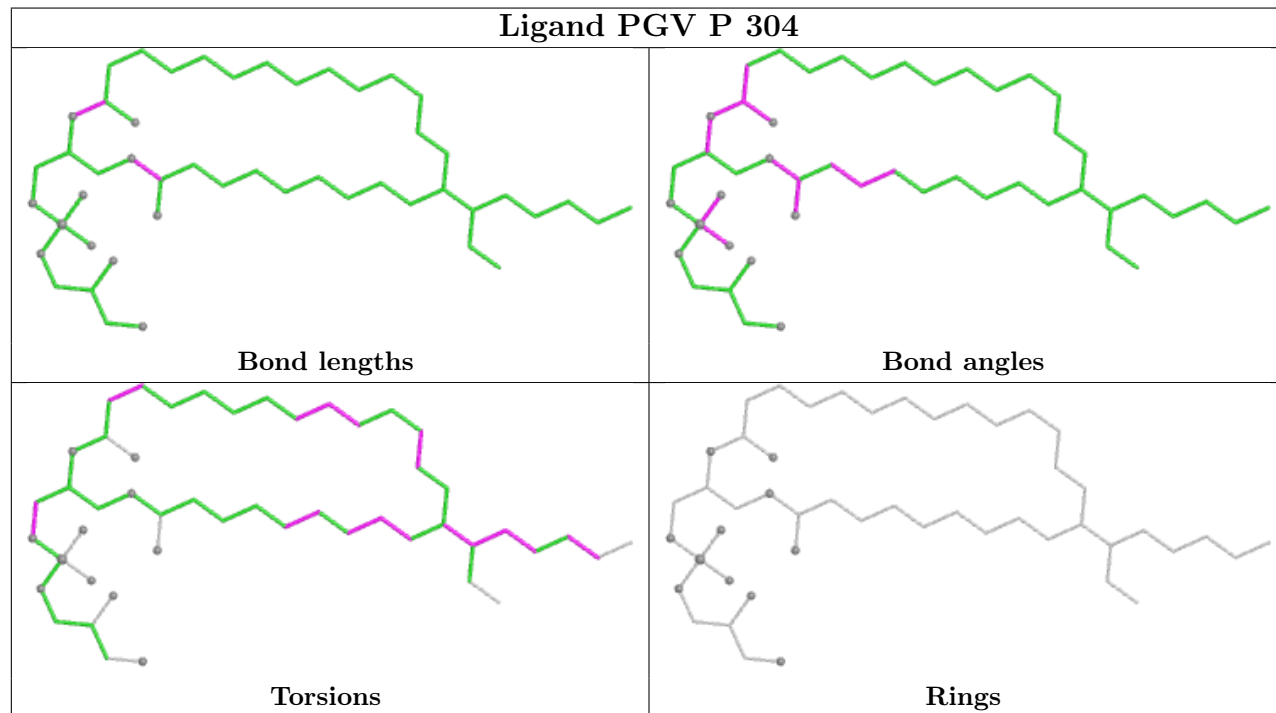
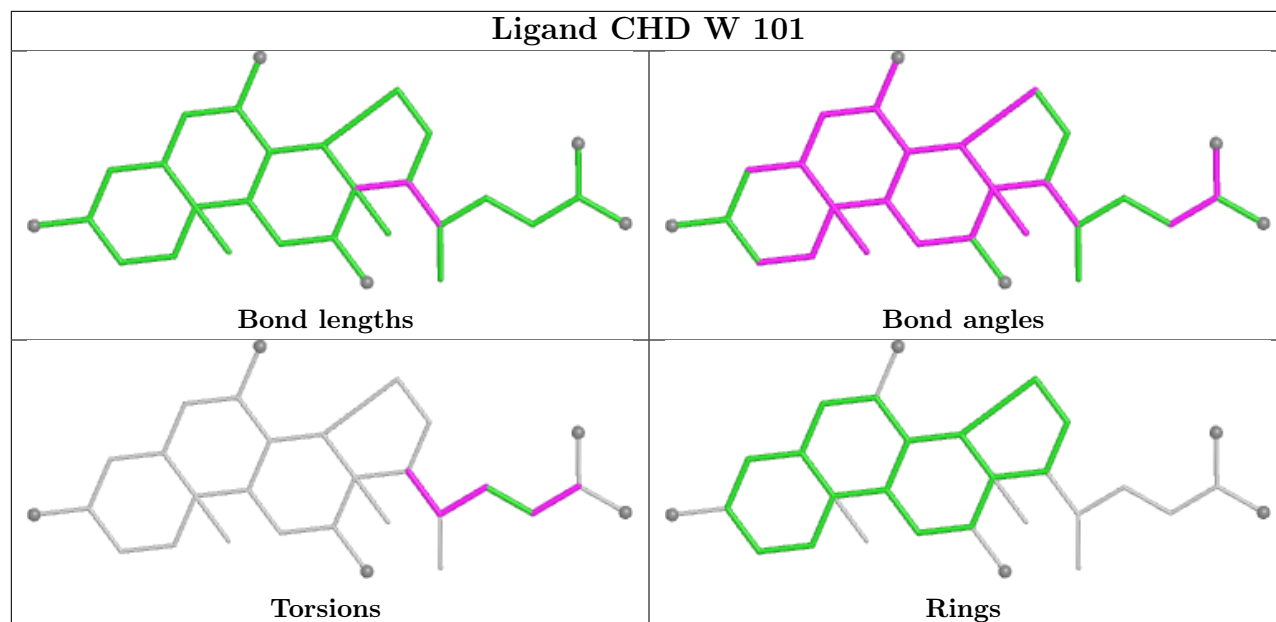
Ligand HEC 1 201

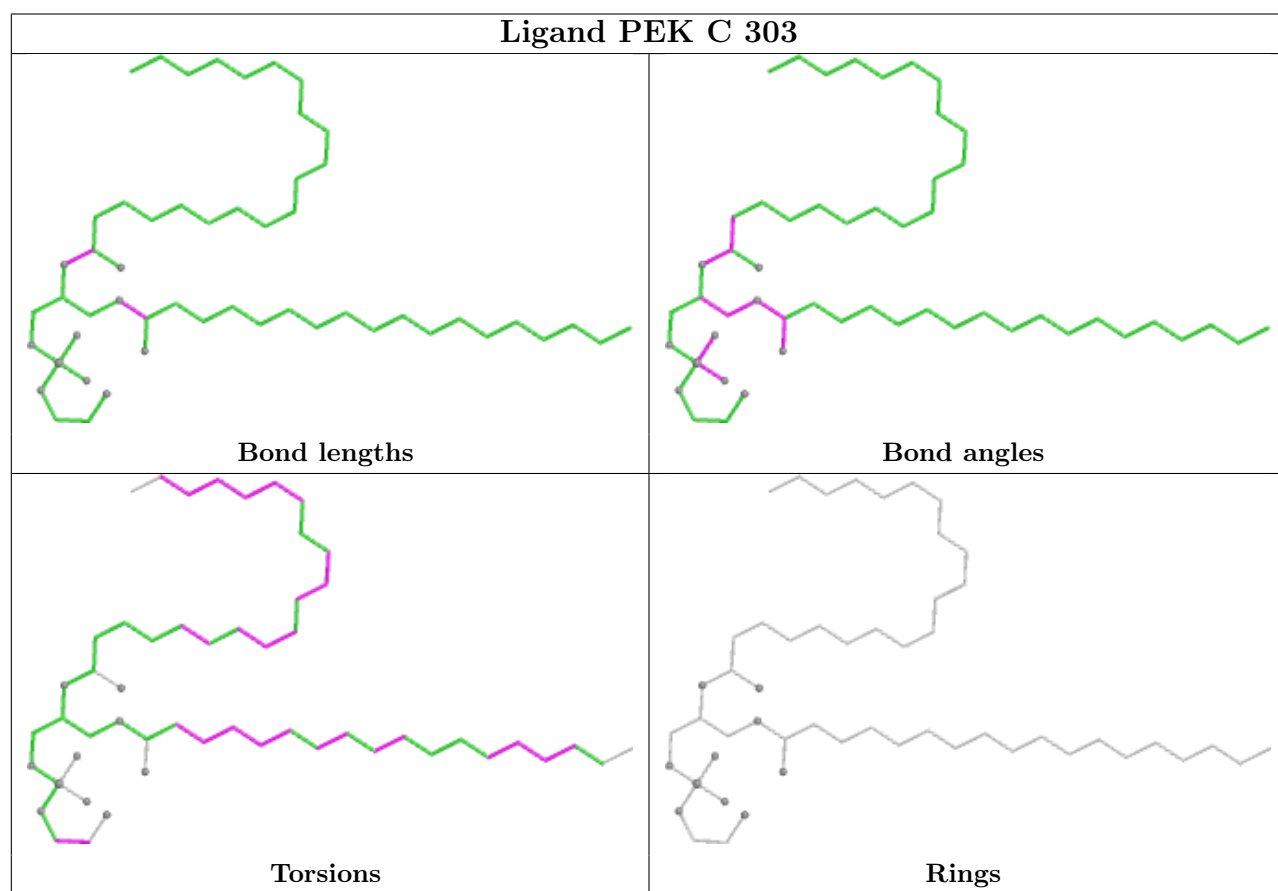
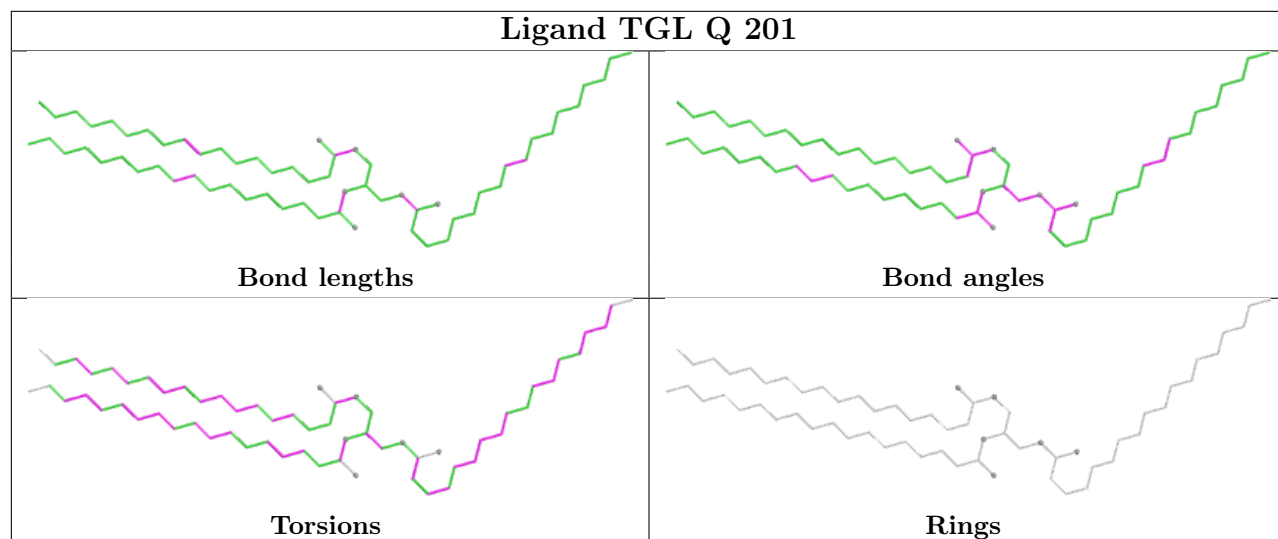


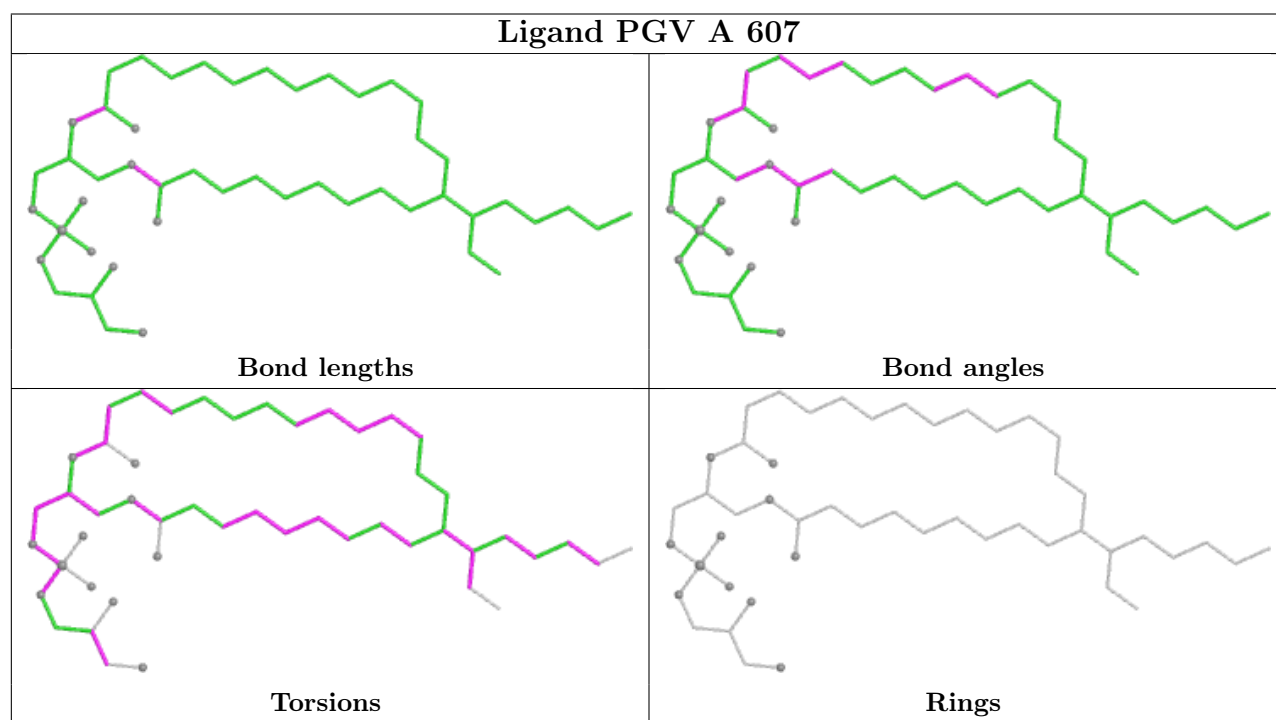
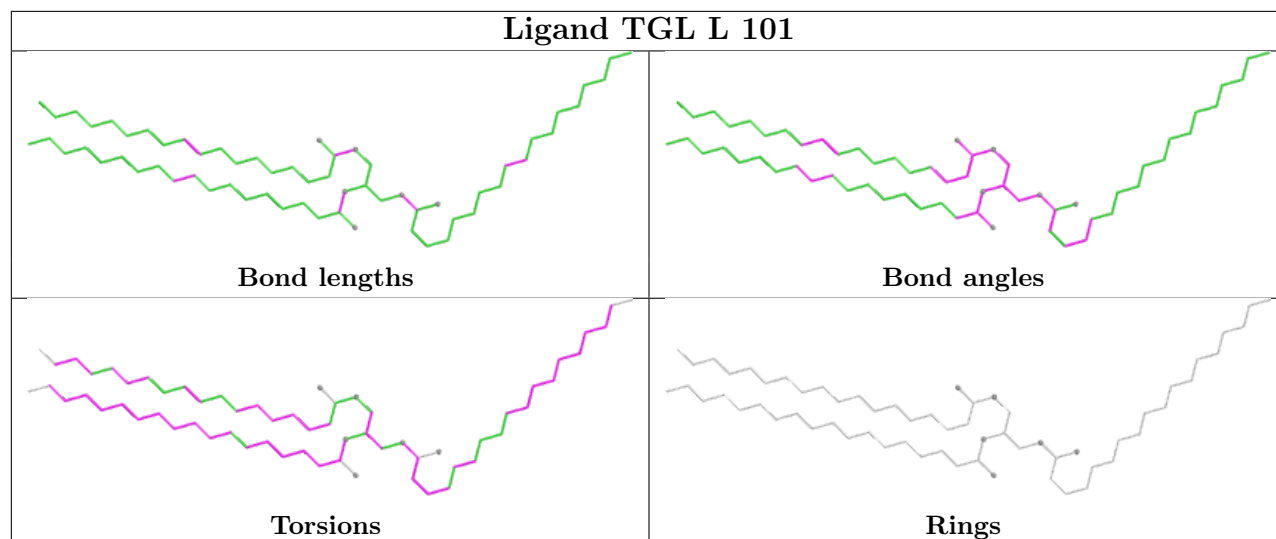
Ligand TGL B 301

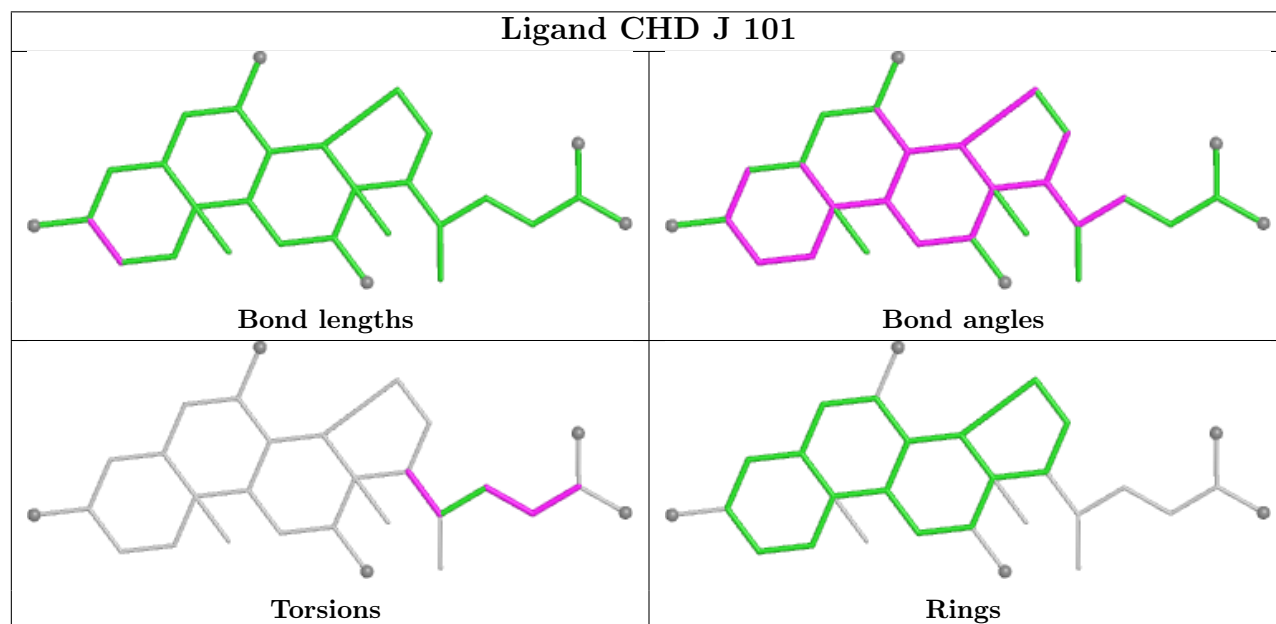
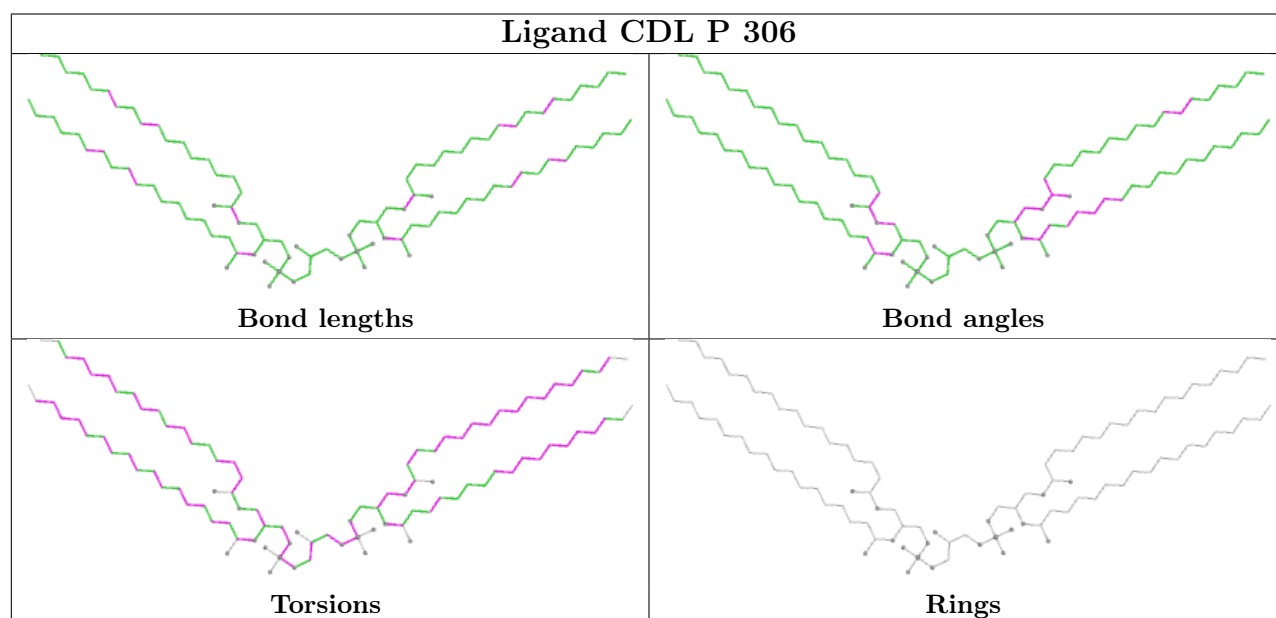
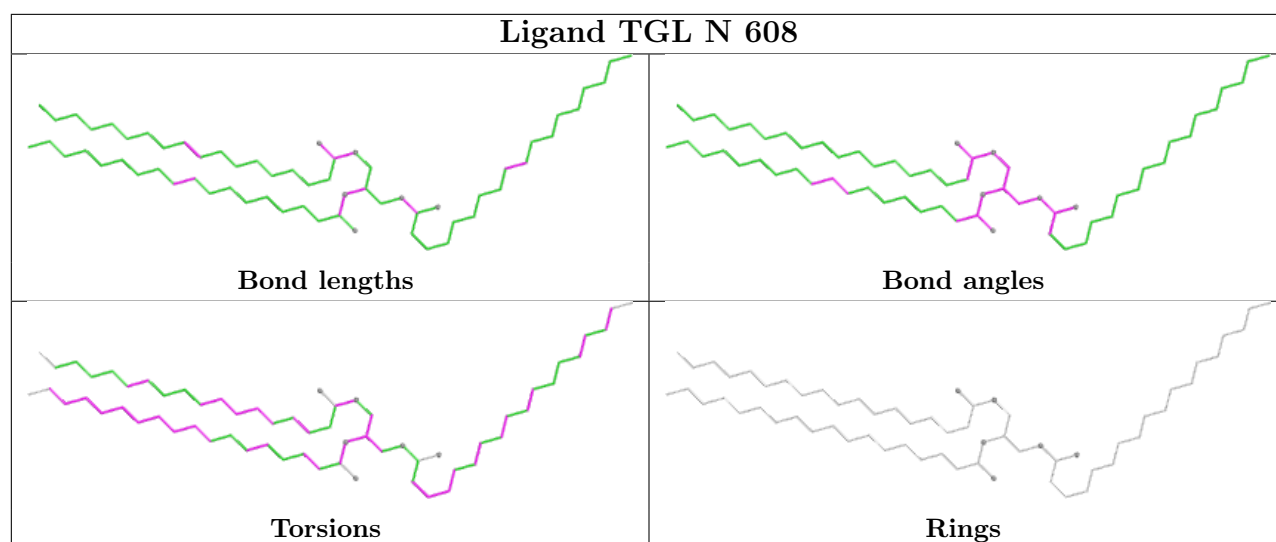


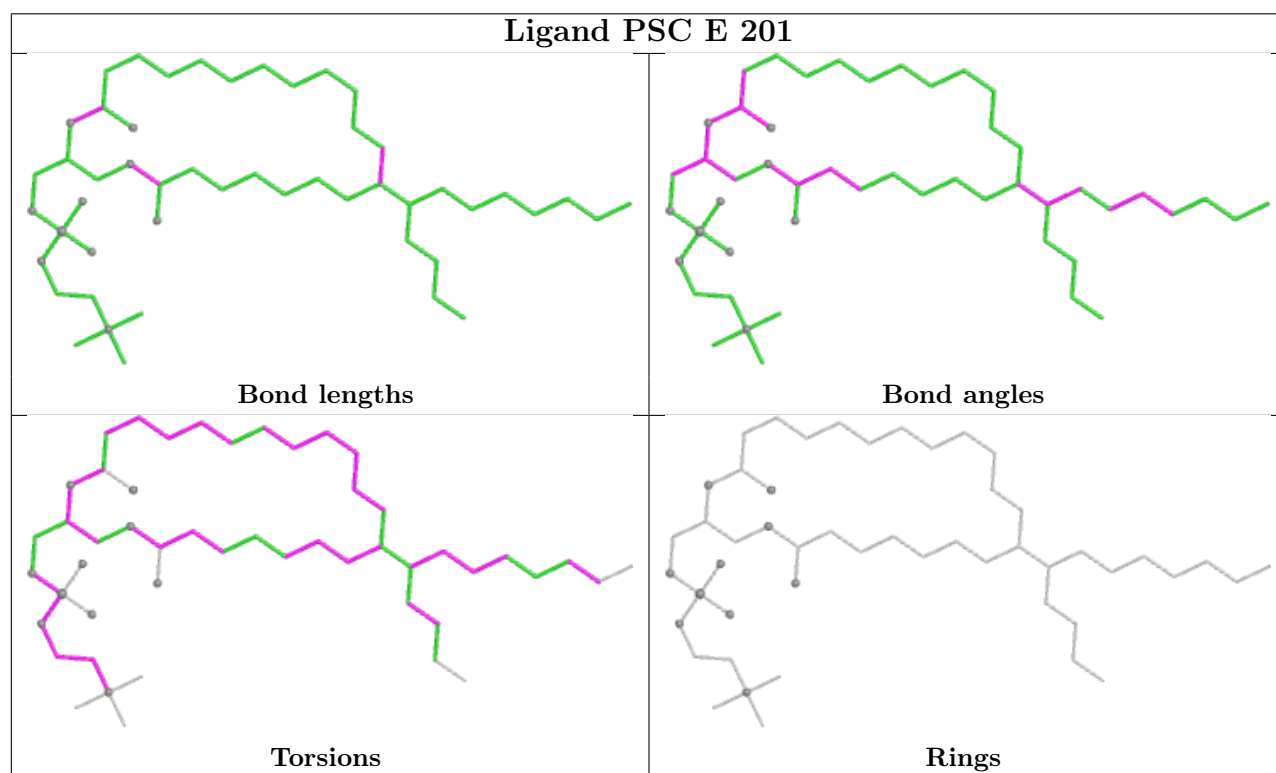
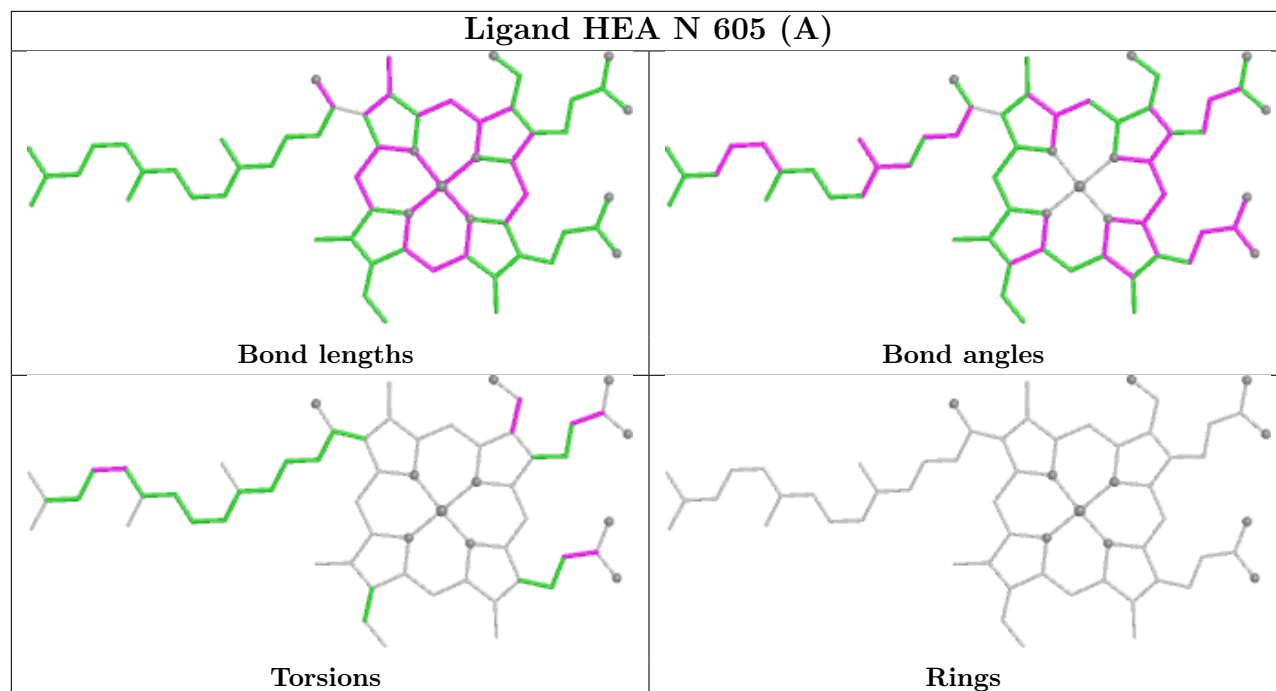


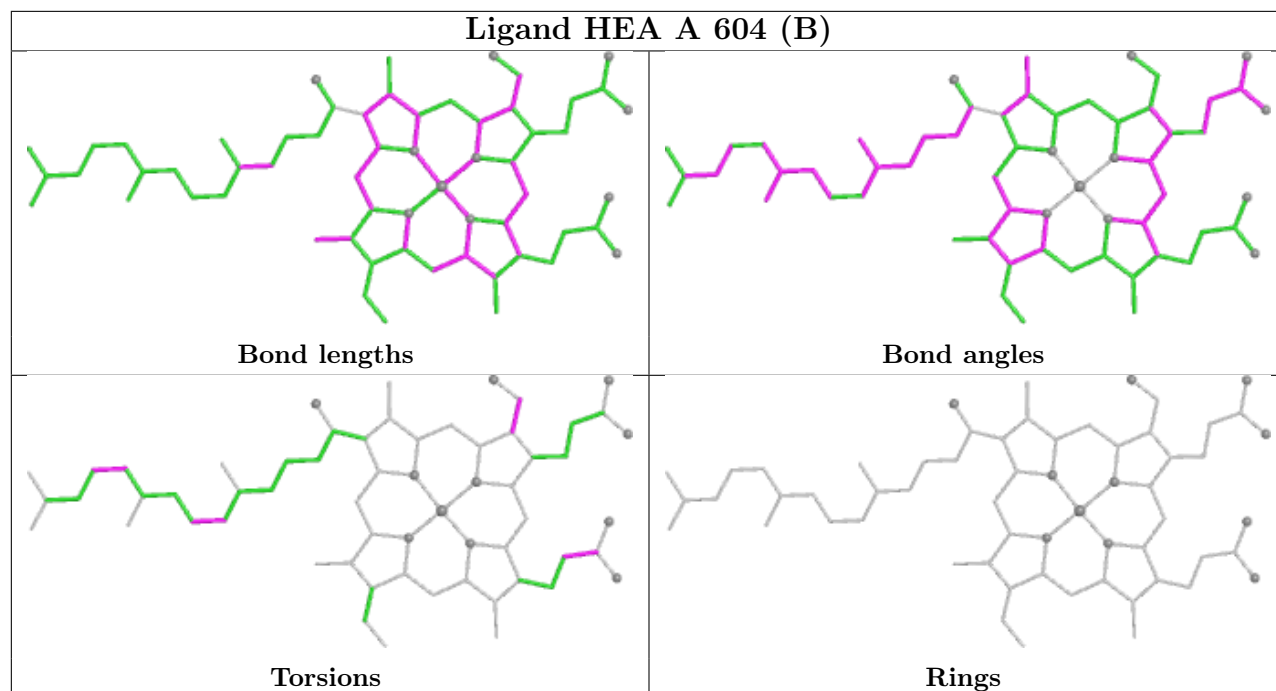












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.76	1 (0%)	91 90	11, 30, 39, 74	11 (2%)
1	N	513/514 (99%)	-0.58	1 (0%)	91 90	18, 36, 48, 71	8 (1%)
2	B	226/227 (99%)	-0.49	3 (1%)	75 74	15, 35, 59, 109	2 (0%)
2	O	226/227 (99%)	-0.07	1 (0%)	88 88	34, 49, 78, 98	0
3	C	259/259 (100%)	-0.52	4 (1%)	72 71	16, 35, 48, 83	6 (2%)
3	P	259/259 (100%)	-0.38	5 (1%)	66 66	17, 38, 52, 87	5 (1%)
4	D	144/144 (100%)	-0.34	4 (2%)	55 54	30, 38, 63, 144	0
4	Q	144/144 (100%)	-0.01	5 (3%)	47 46	22, 50, 81, 139	1 (0%)
5	E	105/105 (100%)	-0.52	0	100 100	30, 38, 62, 134	0
5	R	105/105 (100%)	-0.62	0	100 100	33, 41, 62, 123	0
6	F	98/98 (100%)	-0.14	7 (7%)	22 20	30, 40, 95, 141	0
6	S	98/98 (100%)	0.14	9 (9%)	14 13	32, 45, 106, 141	0
7	G	83/84 (98%)	0.39	12 (14%)	6 5	34, 44, 116, 138	0
7	T	83/84 (98%)	0.49	16 (19%)	3 3	31, 47, 111, 136	0
8	H	79/79 (100%)	-0.05	7 (8%)	15 14	33, 43, 90, 106	0
8	U	79/79 (100%)	-0.10	1 (1%)	75 74	38, 49, 69, 137	0
9	I	72/73 (98%)	-0.05	5 (6%)	23 21	33, 46, 66, 79	0
9	V	72/73 (98%)	0.38	4 (5%)	30 29	36, 63, 85, 111	0
10	J	58/58 (100%)	-0.04	4 (6%)	23 21	36, 46, 75, 135	0
10	W	58/58 (100%)	0.08	5 (8%)	16 15	39, 53, 84, 144	0
11	K	49/49 (100%)	-0.24	1 (2%)	65 64	35, 42, 58, 70	0
11	X	49/49 (100%)	0.06	1 (2%)	65 64	47, 58, 77, 78	0
12	L	46/46 (100%)	-0.46	1 (2%)	62 61	30, 38, 59, 104	0
12	Y	46/46 (100%)	-0.24	2 (4%)	40 39	36, 46, 69, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	-0.18	3 (6%) 22 21	32, 40, 79, 127	0
13	Z	43/43 (100%)	-0.11	0 100 100	36, 50, 81, 108	0
14	1	104/105 (99%)	0.77	7 (6%) 24 22	45, 90, 118, 125	0
14	2	104/105 (99%)	1.33	23 (22%) 2 2	67, 115, 139, 147	0
All	All	3758/3768 (99%)	-0.26	132 (3%) 47 46	11, 40, 98, 147	33 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	9.7
6	F	1	ALA	7.8
7	G	3	ALA	6.8
8	H	8	ILE	6.5
4	Q	5	VAL	6.4
4	Q	6	VAL	6.0
6	S	93	PRO	5.5
8	U	8	ILE	5.4
7	G	9	GLY	5.4
6	S	96	LEU	5.1
7	T	36	TRP	5.0
3	C	37	PHE	4.9
9	V	30	GLY	4.8
7	G	4	ALA	4.8
6	F	97	ALA	4.8
1	N	113[A]	LEU	4.8
4	D	5	VAL	4.7
7	T	3	ALA	4.7
1	A	113[A]	LEU	4.7
7	G	36	TRP	4.6
7	G	5	LYS	4.5
7	T	9	GLY	4.4
2	B	58	ALA	4.3
6	S	94	HIS	4.1
7	G	2	SER	4.1
9	V	32	ALA	4.0
6	F	94	HIS	4.0
9	V	31	PHE	3.9
6	F	96	LEU	3.9
6	F	3	GLY	3.8
7	T	4	ALA	3.7
7	T	37	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
7	G	6	GLY	3.7
9	I	30	GLY	3.6
7	T	10	GLY	3.5
4	Q	4	SER	3.5
9	I	31	PHE	3.4
14	2	57	ILE	3.4
3	P	3	HIS	3.4
6	F	98	HIS	3.3
10	W	57	HIS	3.3
7	T	5	LYS	3.3
10	W	1	PHE	3.3
14	2	59	TRP	3.2
3	C	261	SER	3.2
7	T	6	GLY	3.2
14	2	35	LEU	3.1
9	V	33	THR	3.1
2	O	113	TYR	3.1
9	I	33	THR	3.1
7	T	2	SER	3.1
6	S	97	ALA	3.1
4	D	6	VAL	3.1
14	2	36	PHE	3.0
7	G	1	ALA	3.0
14	2	43	ALA	3.0
14	2	58	THR	3.0
14	2	1	GLY	2.9
14	2	81	ILE	2.9
7	T	7	ASP	2.9
8	H	49	ASP	2.9
6	F	2	SER	2.9
14	2	77	GLY	2.9
8	H	48	GLY	2.8
4	D	7	LYS	2.8
3	C	260	GLY	2.7
14	2	74	TYR	2.7
6	S	98	HIS	2.7
10	J	57	HIS	2.7
10	J	1	PHE	2.6
4	Q	7	LYS	2.6
9	I	37	PHE	2.6
6	S	2	SER	2.6
3	P	37	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
10	W	58	LYS	2.6
13	M	43	SER	2.6
14	1	75	ILE	2.5
3	P	40	MET	2.5
6	S	3	GLY	2.5
8	H	45	ALA	2.5
14	1	101	ALA	2.5
8	H	9	LYS	2.5
12	Y	20	ARG	2.5
14	1	102	THR	2.4
11	X	6	ALA	2.4
14	2	32	LEU	2.4
14	2	78	THR	2.4
13	M	41	LYS	2.4
14	2	98	LEU	2.4
7	G	7	ASP	2.4
14	2	20	VAL	2.4
7	T	1	ALA	2.3
8	H	7	LYS	2.3
11	K	6	ALA	2.3
7	G	10	GLY	2.3
7	T	42	ARG	2.3
13	M	42	LYS	2.3
3	P	41	THR	2.3
10	J	56	PRO	2.3
12	Y	2	HIS	2.3
8	H	50	VAL	2.3
10	W	56	PRO	2.3
7	T	40	GLY	2.2
10	W	55	PHE	2.2
14	2	40	THR	2.2
14	2	63	THR	2.2
14	2	76	PRO	2.2
14	2	95	ILE	2.2
2	B	60	GLU	2.2
7	T	38	HIS	2.2
14	2	71	PRO	2.2
7	T	41	HIS	2.2
4	D	8	SER	2.2
14	2	48	TYR	2.2
3	P	38	ASN	2.2
14	1	25	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	Q	9	GLU	2.1
2	B	59	GLN	2.1
14	1	1	GLY	2.1
9	I	32	ALA	2.1
14	2	67	TYR	2.1
12	L	2	HIS	2.1
14	1	43	ALA	2.1
6	S	95	GLN	2.1
14	2	41	GLY	2.1
14	1	57	ILE	2.1
14	2	3	VAL	2.1
7	G	8	HIS	2.0
7	T	84	LYS	2.0
3	C	3	HIS	2.0
7	G	38	HIS	2.0
10	J	58	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.51	0.18	131,137,150,153	0
9	SAC	I	1	9/10	0.60	0.15	98,106,110,119	0
7	TPO	G	11	11/12	0.62	0.17	81,97,160,160	0
7	TPO	T	11	11/12	0.76	0.21	85,109,117,125	0
1	FME	A	1	10/11	0.89	0.13	40,52,71,88	0
1	FME	N	1	10/11	0.92	0.11	43,61,73,95	0
2	FME	B	1	10/11	0.97	0.08	30,35,39,51	0
2	FME	O	1	10/11	0.97	0.08	49,56,65,78	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	NA	C	302	1/1	0.62	0.40	59,59,59,59	0
17	NA	P	302	1/1	0.72	0.42	57,57,57,57	0
20	PGV	C	305	51/51	0.76	0.21	55,80,122,138	0
24	CHD	W	101	29/29	0.77	0.21	73,114,126,130	0
20	PGV	P	305	51/51	0.78	0.19	54,86,135,150	0
27	UNL	P	309	16/-	0.78	0.25	70,79,89,95	0
26	CDL	T	101	100/100	0.80	0.21	61,95,153,161	0
24	CHD	C	307	29/29	0.81	0.19	73,85,93,99	0
20	PGV	A	607	51/51	0.82	0.19	44,84,151,159	0
26	CDL	G	101	100/100	0.82	0.21	58,103,158,163	0
21	TGL	D	201	63/63	0.83	0.19	47,70,101,105	0
26	CDL	P	306	100/100	0.84	0.19	49,97,149,159	0
21	TGL	Q	201	63/63	0.84	0.22	52,82,104,109	0
27	UNL	C	308	18/-	0.84	0.19	55,66,77,81	0
27	UNL	C	309	17/-	0.84	0.21	60,71,87,90	0
21	TGL	N	608	63/63	0.84	0.18	51,73,104,115	0
28	PSC	E	201	52/52	0.84	0.18	50,79,162,163	0
28	PSC	V	101	52/52	0.84	0.18	49,77,145,166	0
27	UNL	J	102	10/-	0.85	0.30	61,65,77,92	0
21	TGL	L	101	63/63	0.85	0.21	45,70,98,107	0
24	CHD	P	307	29/29	0.86	0.13	71,80,88,95	0
27	UNL	Y	101	10/-	0.86	0.24	69,76,86,94	0
27	UNL	C	310	7/-	0.86	0.29	41,64,76,83	0
24	CHD	J	101	29/29	0.86	0.15	61,75,106,109	0
27	UNL	N	609	16/-	0.87	0.20	54,59,79,85	0
27	UNL	N	610	18/-	0.87	0.17	51,59,69,70	0
27	UNL	L	102	10/-	0.87	0.25	61,75,82,86	0
30	DMU	Z	101	33/33	0.87	0.11	55,76,107,113	0
23	EDO	E	202	4/4	0.88	0.12	57,61,68,79	0
27	UNL	T	102	18/-	0.88	0.19	47,66,85,92	0
27	UNL	W	102	9/-	0.88	0.24	59,62,79,82	0
27	UNL	N	601	17/-	0.88	0.18	52,60,83,85	0
26	CDL	C	306	100/100	0.88	0.17	51,86,124,152	0
21	TGL	B	301	63/63	0.88	0.18	33,68,103,114	0
27	UNL	N	611	12/-	0.88	0.19	48,56,68,69	0
27	UNL	P	308	20/-	0.89	0.16	58,64,72,73	0
23	EDO	I	101	4/4	0.90	0.17	55,59,63,72	0

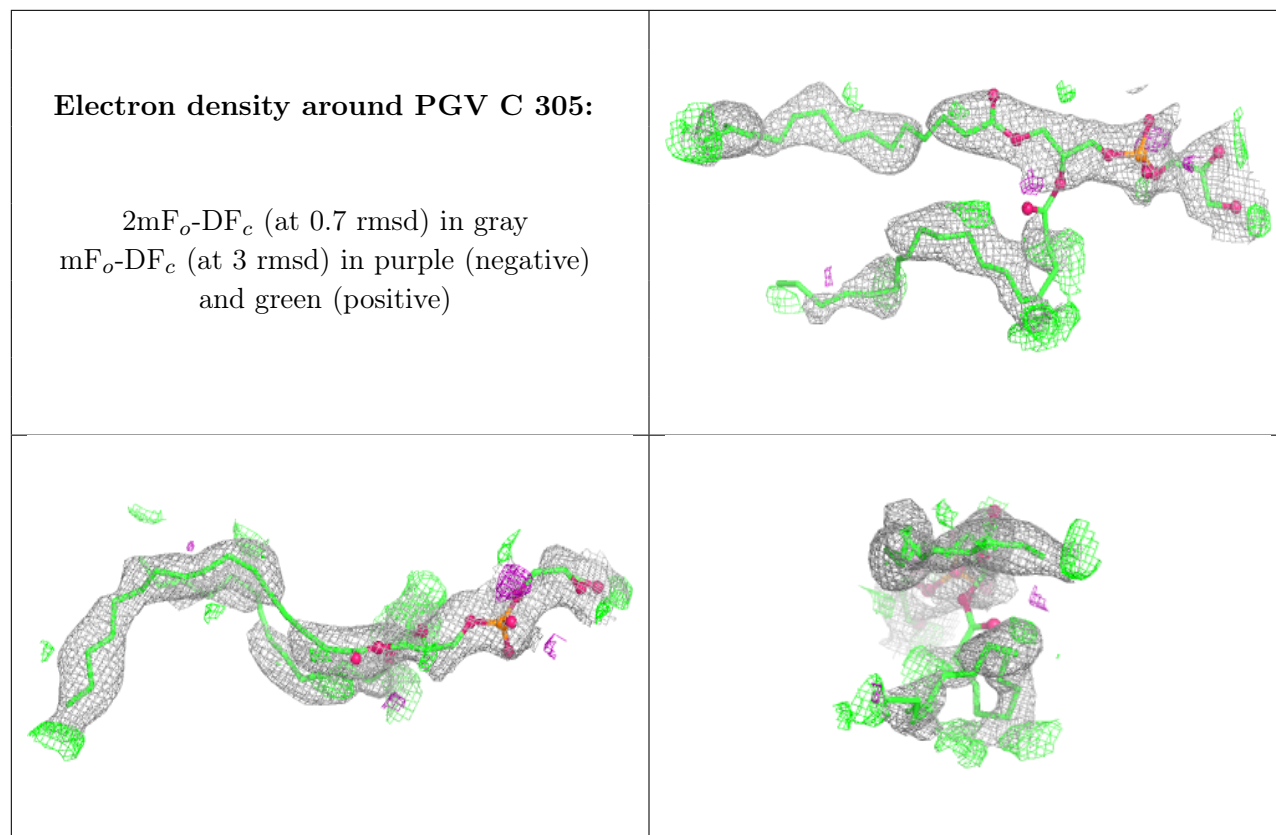
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	UNL	P	310	7/-	0.91	0.23	53,60,76,88	0
24	CHD	P	301	29/29	0.93	0.09	40,45,52,55	0
24	CHD	C	301	29/29	0.94	0.07	34,40,48,53	0
31	HEC	2	201	43/43	0.94	0.12	79,101,135,149	0
25	PEK	C	303	53/53	0.95	0.12	34,48,88,97	0
23	EDO	N	614	4/4	0.95	0.11	56,59,63,85	0
30	DMU	M	101	33/33	0.95	0.08	40,46,62,65	0
24	CHD	T	103	29/29	0.95	0.07	30,36,42,53	0
23	EDO	S	102	4/4	0.95	0.10	44,45,46,53	0
16	MG	A	602	1/1	0.96	0.08	36,36,36,36	0
23	EDO	G	103	4/4	0.96	0.10	37,39,49,51	0
16	MG	N	603	1/1	0.96	0.07	42,42,42,42	0
24	CHD	G	102	29/29	0.96	0.07	35,38,43,52	0
23	EDO	C	311	4/4	0.96	0.09	48,51,51,52	0
31	HEC	1	201	43/43	0.96	0.10	57,81,94,99	0
25	PEK	P	303	53/53	0.96	0.11	39,53,94,101	0
20	PGV	P	304	51/51	0.97	0.09	30,46,73,76	0
20	PGV	C	304	51/51	0.97	0.09	31,38,95,103	0
20	PGV	A	608	51/51	0.97	0.09	29,41,68,74	0
23	EDO	B	303	4/4	0.98	0.05	30,31,33,36	0
20	PGV	N	612	51/51	0.98	0.08	33,43,70,80	0
23	EDO	N	613	4/4	0.98	0.06	38,38,39,41	0
19	PER	N	607	2/2	0.98	0.10	36,36,36,48	0
23	EDO	F	102	4/4	0.98	0.07	45,47,49,49	0
19	PER	A	606	2/2	0.99	0.09	40,40,40,54	0
17	NA	N	604	1/1	0.99	0.03	45,45,45,45	0
17	NA	A	603	1/1	0.99	0.07	31,31,31,31	0
18	HEA	A	604[A]	60/60	0.99	0.06	23,28,38,40	9
18	HEA	A	604[B]	60/60	0.99	0.06	23,28,35,40	9
22	CUA	O	301	2/2	0.99	0.04	42,42,42,43	0
29	ZN	S	101	1/1	0.99	0.05	37,37,37,37	0
18	HEA	A	605	60/60	0.99	0.04	22,26,33,39	0
18	HEA	N	605[A]	60/60	0.99	0.06	32,38,47,50	9
18	HEA	N	605[B]	60/60	0.99	0.06	32,38,44,47	9
18	HEA	N	606	60/60	0.99	0.05	27,33,41,47	0
15	CU	A	601	1/1	1.00	0.01	29,29,29,29	0
15	CU	N	602	1/1	1.00	0.01	35,35,35,35	0
29	ZN	F	101	1/1	1.00	0.01	36,36,36,36	0
22	CUA	B	302	2/2	1.00	0.01	27,27,27,29	0

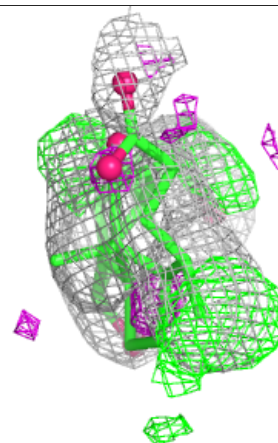
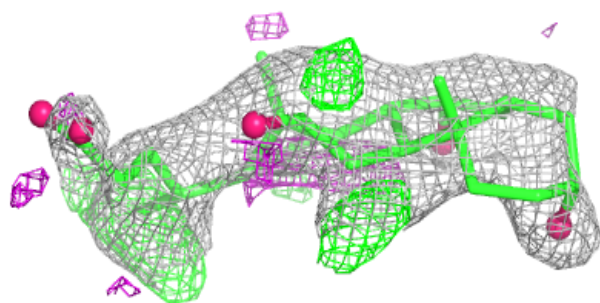
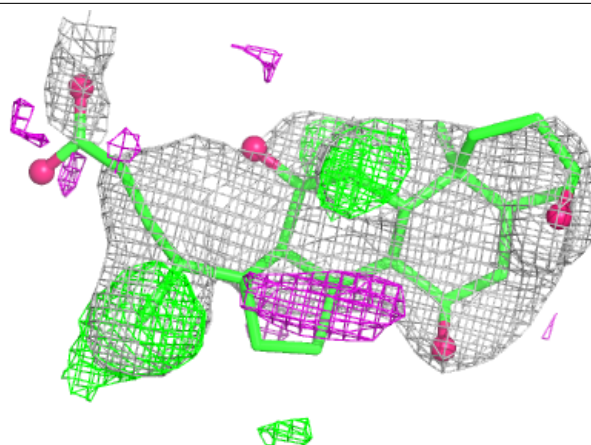
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

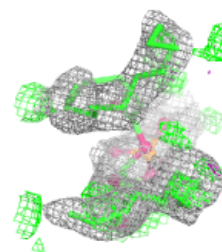
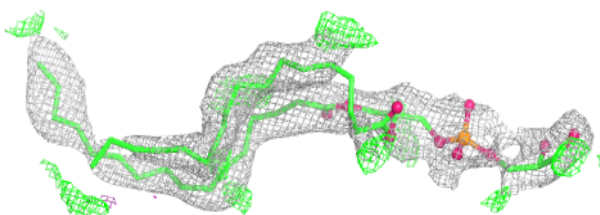
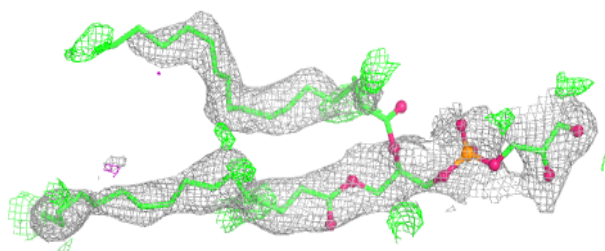


Electron density around CHD W 101:

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

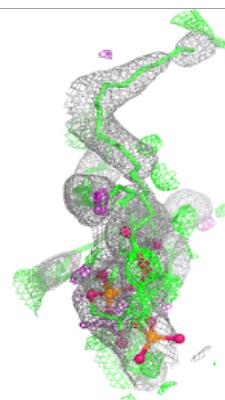
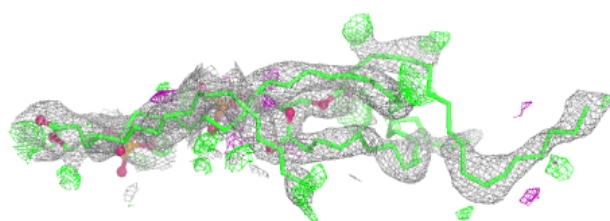
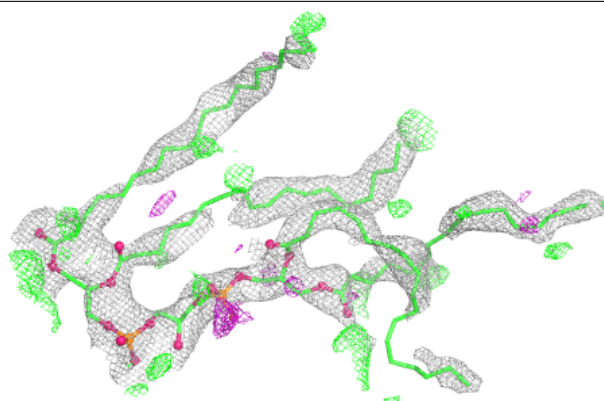
**Electron density around PGV P 305:**

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

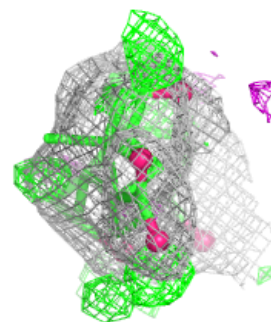
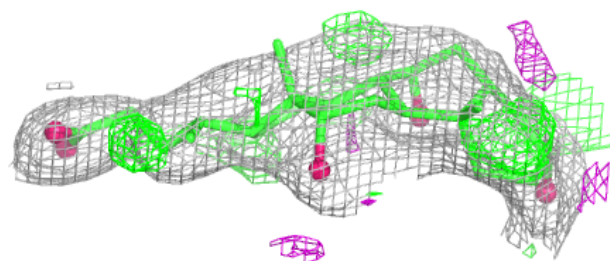
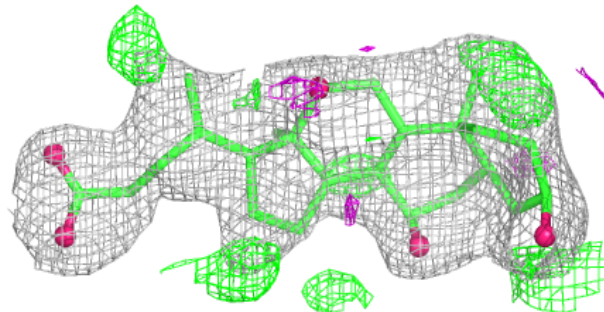


Electron density around CDL T 101:

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

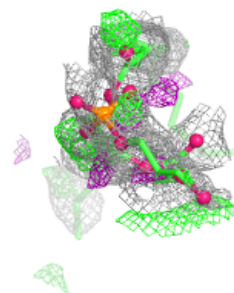
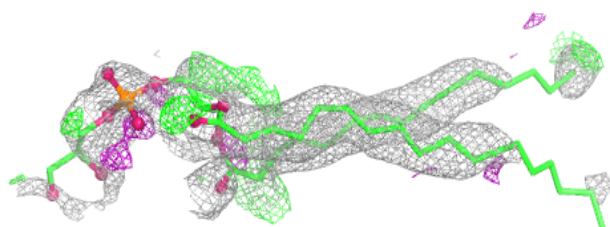
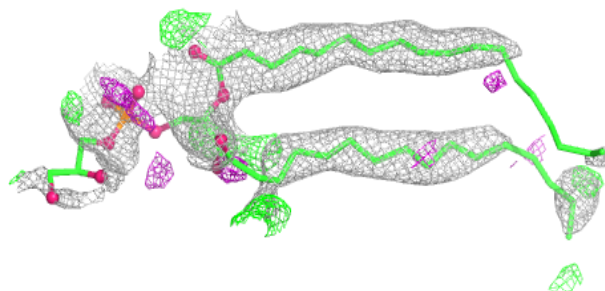
**Electron density around CHD C 307:**

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

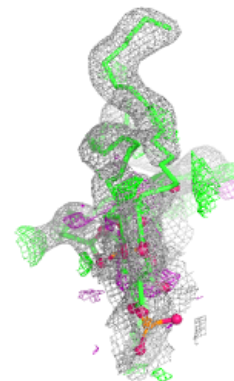
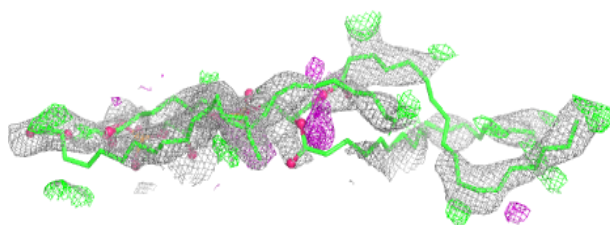
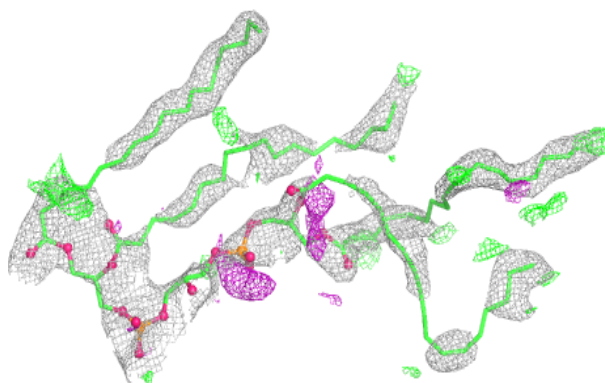


Electron density around PGV A 607:

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

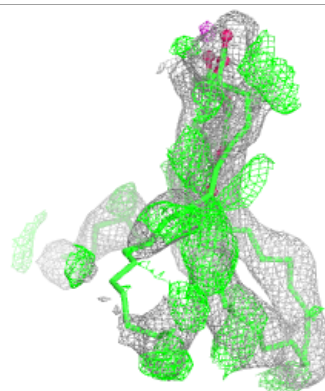
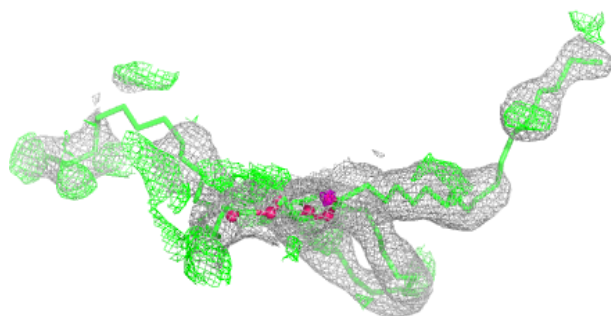
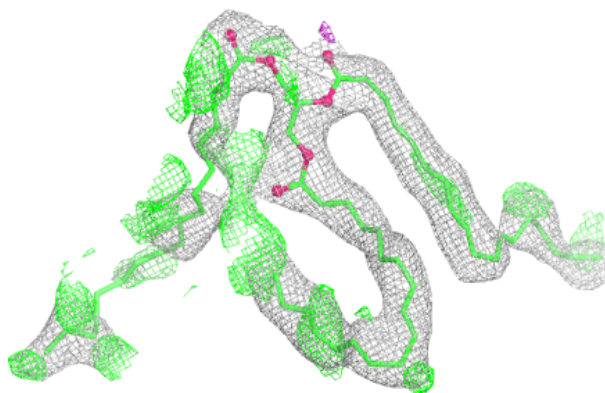
**Electron density around CDL G 101:**

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

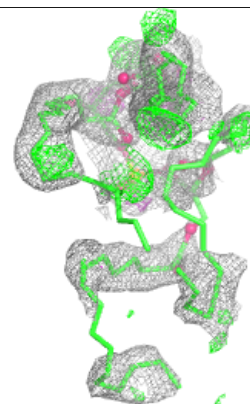
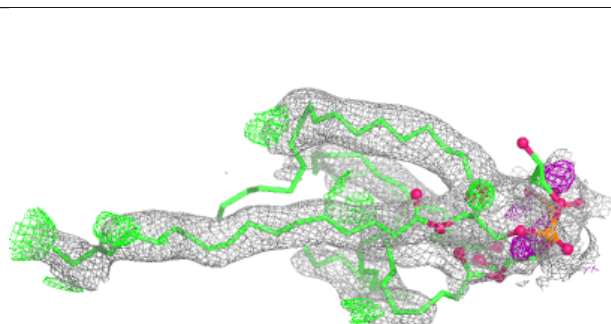
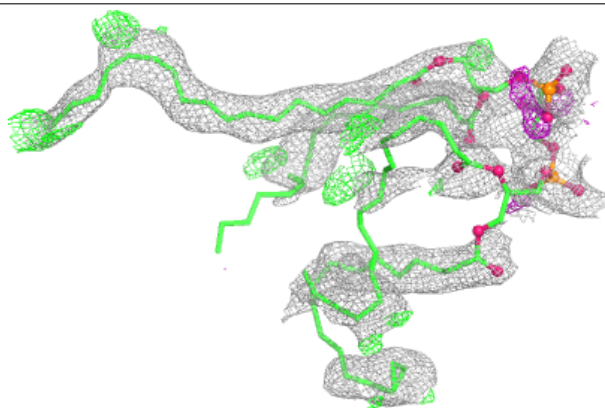


Electron density around TGL D 201:

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

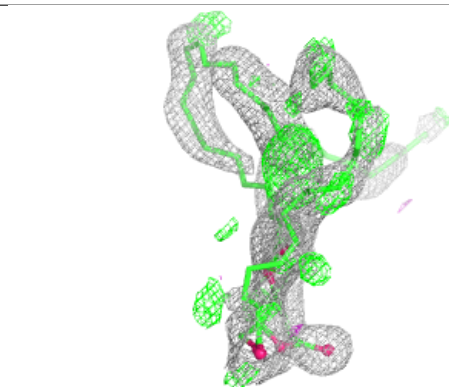
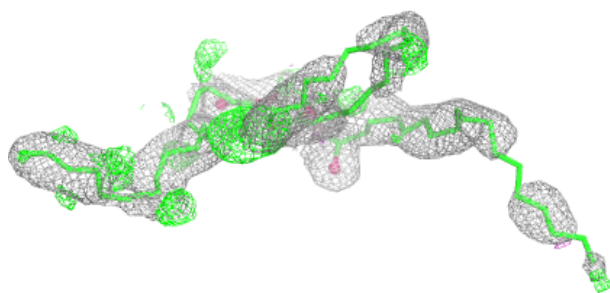
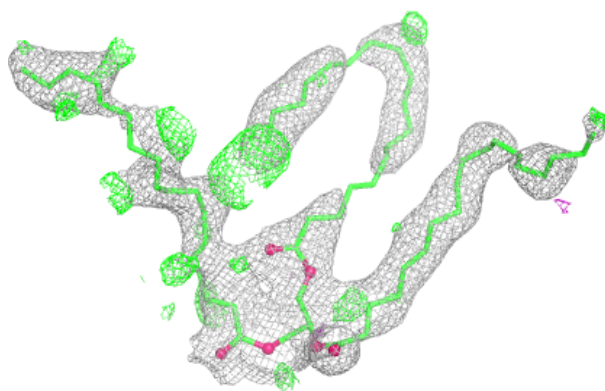
**Electron density around CDL P 306:**

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

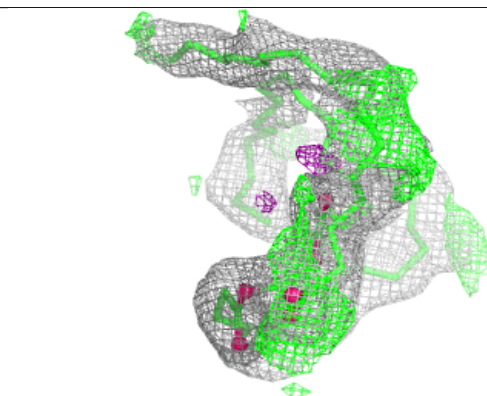
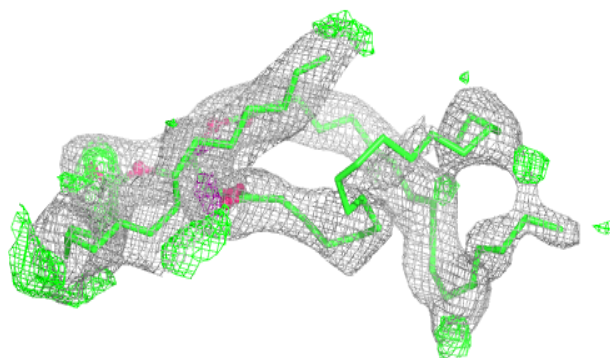
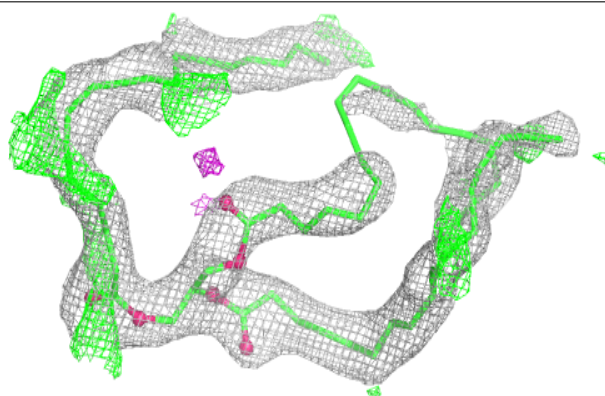


Electron density around TGL Q 201:

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

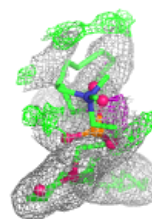
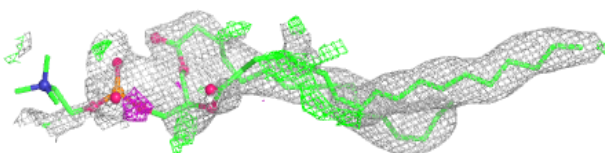
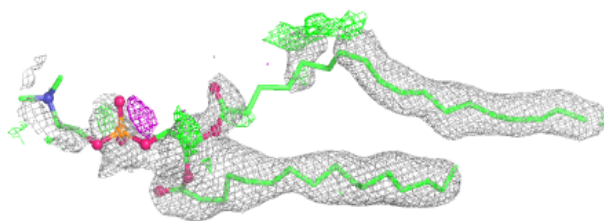
**Electron density around TGL N 608:**

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

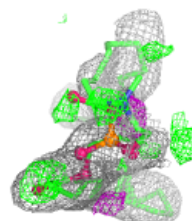
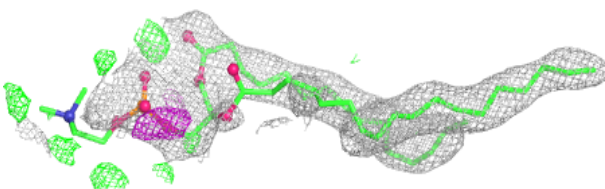
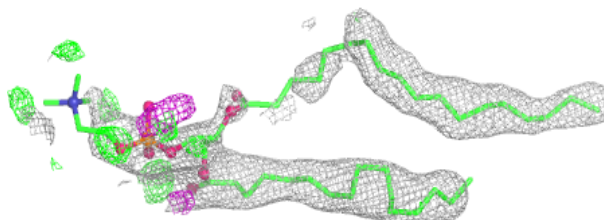


Electron density around PSC E 201:

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

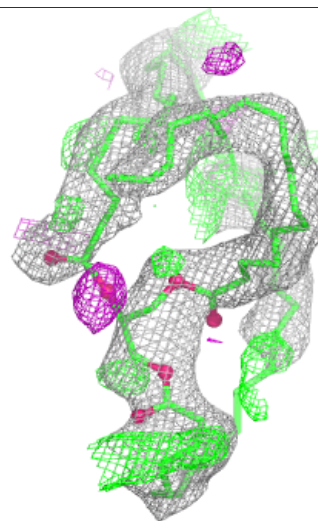
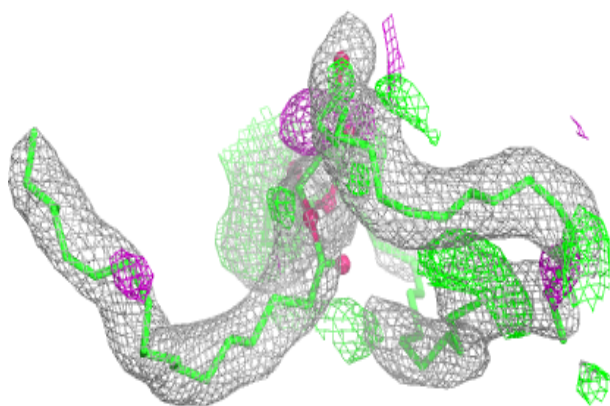
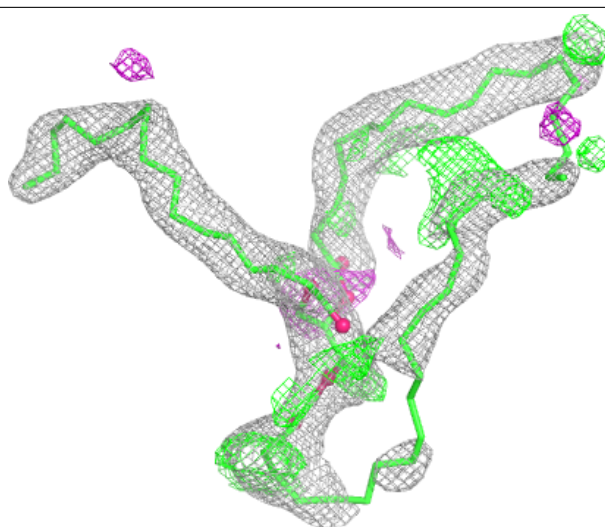
**Electron density around PSC V 101:**

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



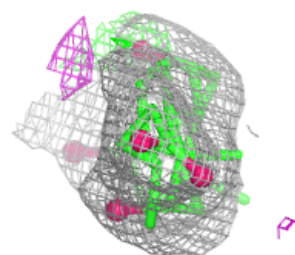
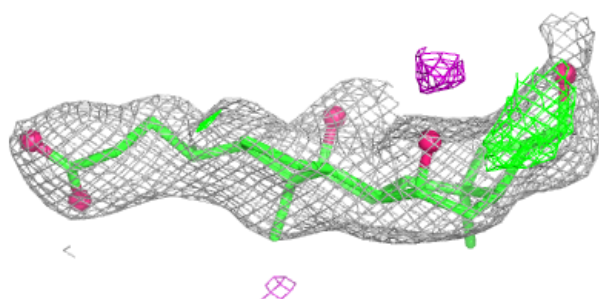
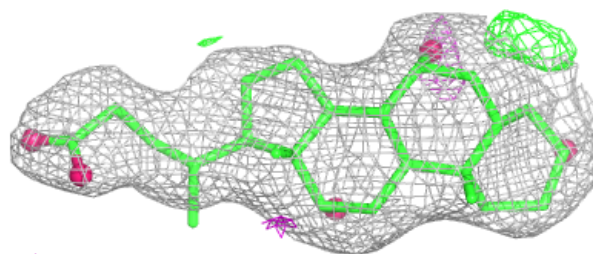
Electron density around TGL L 101:

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

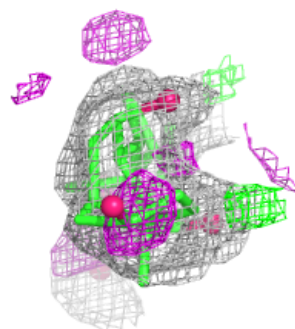
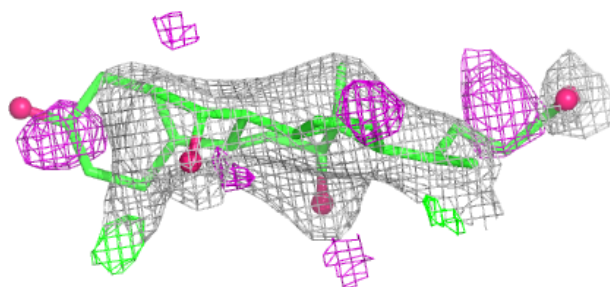
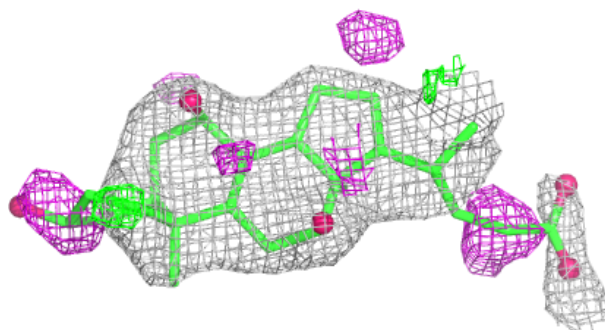


Electron density around CHD P 307:

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

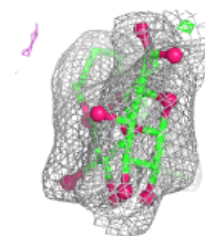
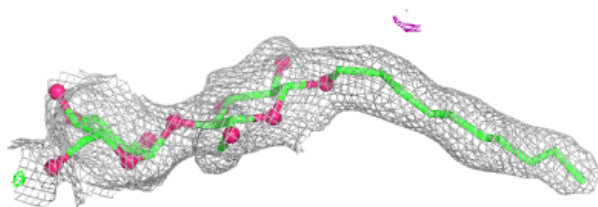
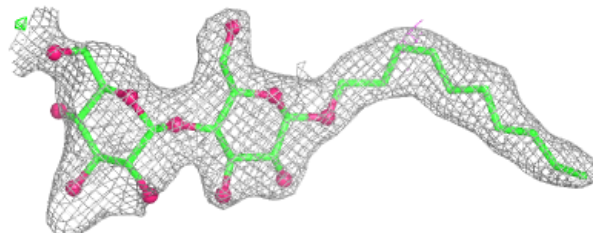
**Electron density around CHD J 101:**

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

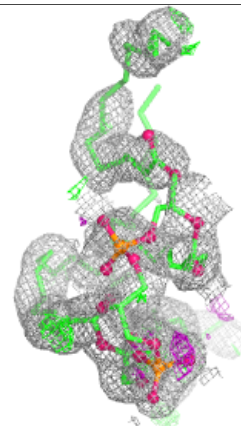
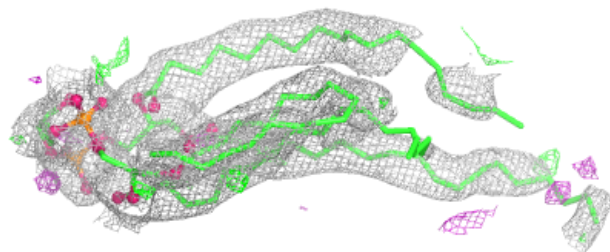
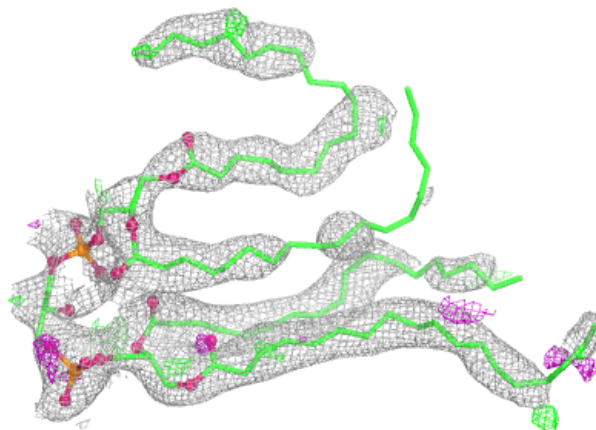


Electron density around DMU Z 101:

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

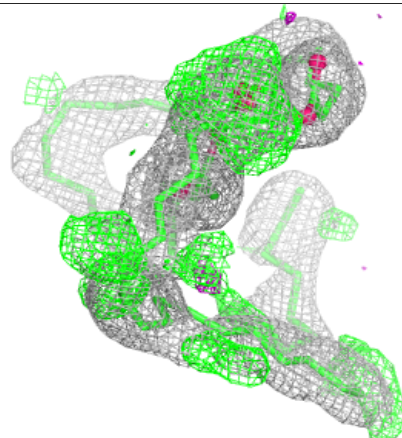
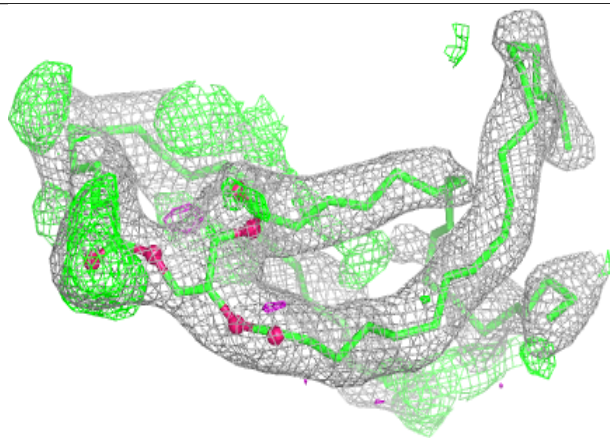
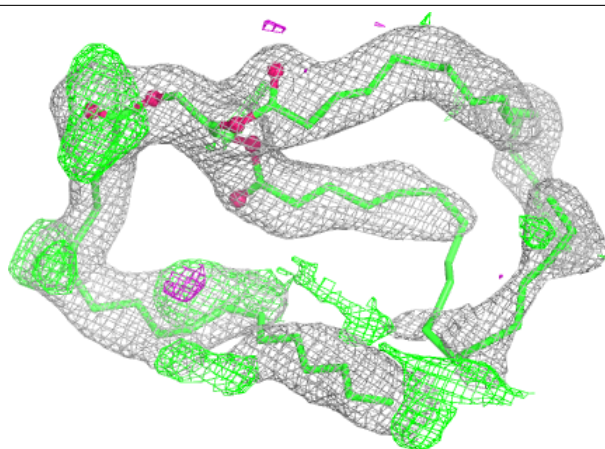
**Electron density around CDL C 306:**

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

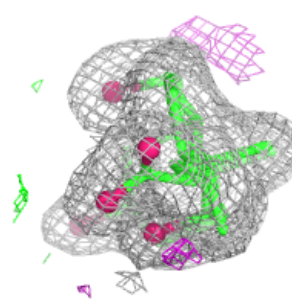
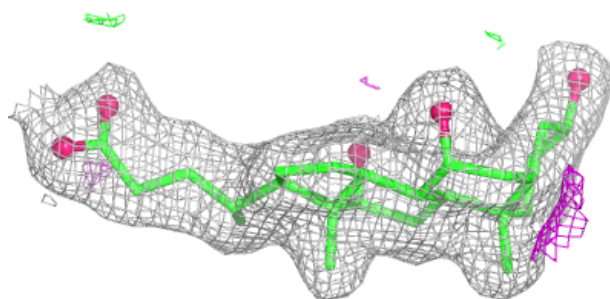
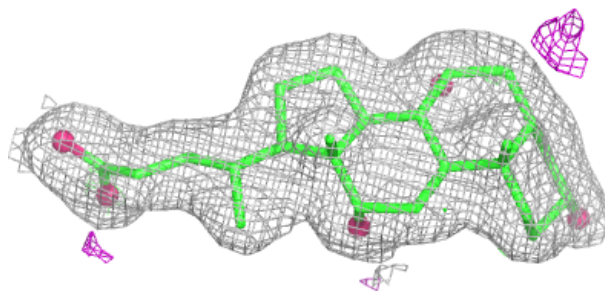


Electron density around TGL B 301:

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

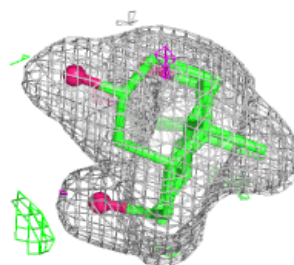
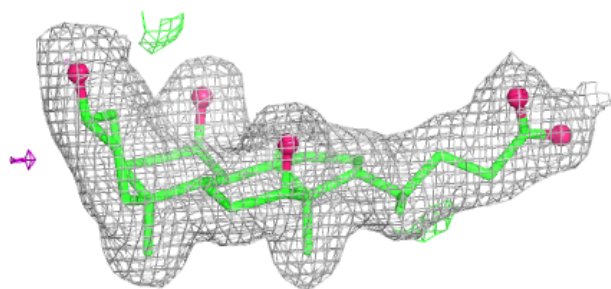
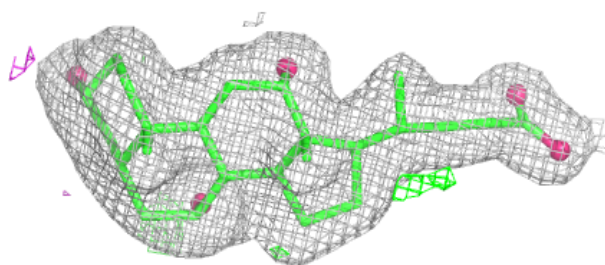
**Electron density around CHD P 301:**

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

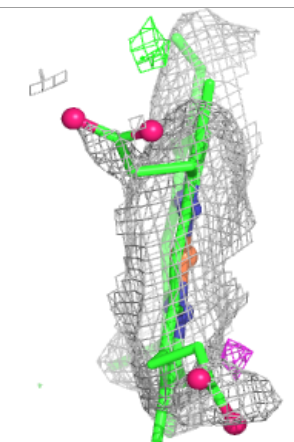
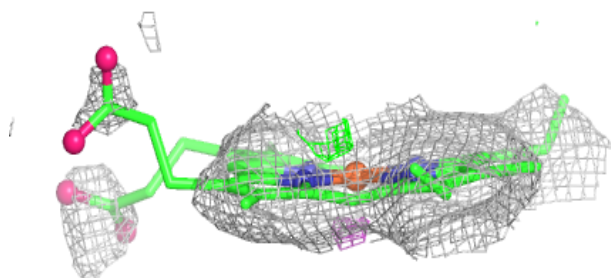
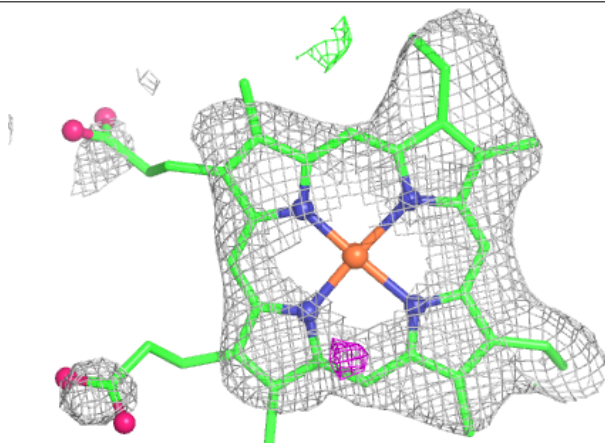


Electron density around CHD C 301:

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

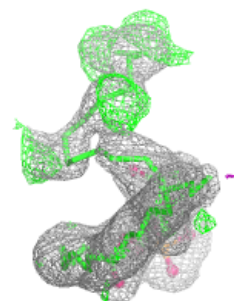
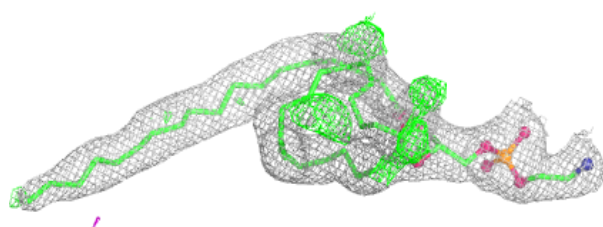
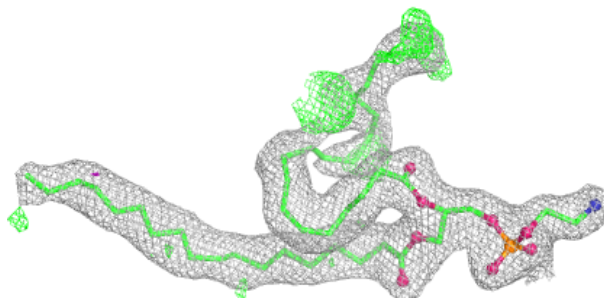
**Electron density around HEC 2 201:**

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

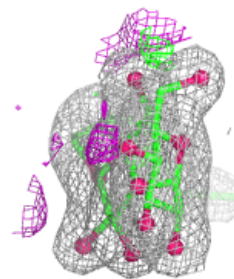
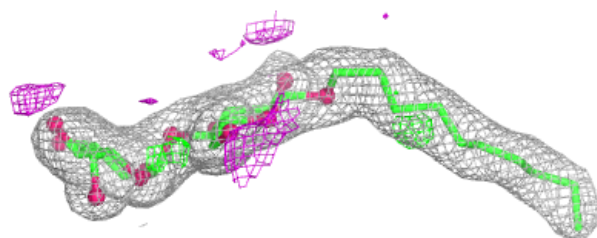
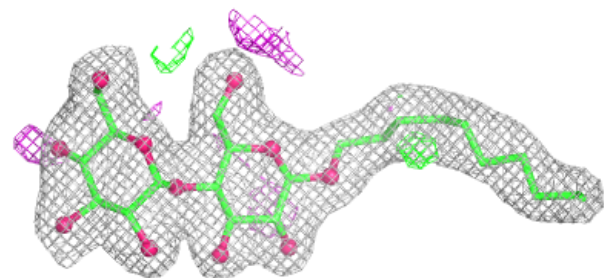


Electron density around PEK C 303:

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

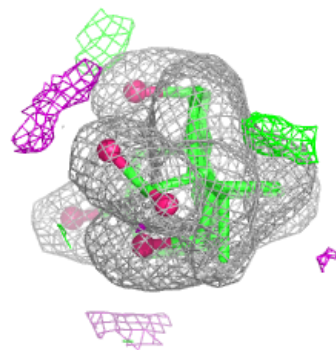
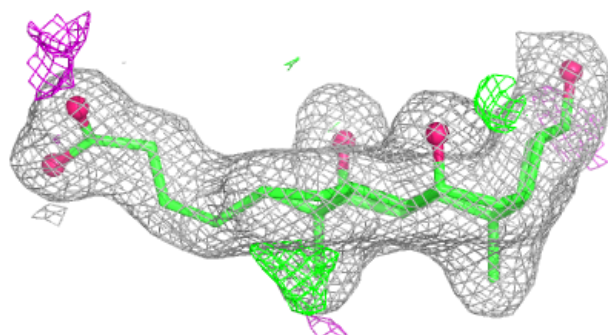
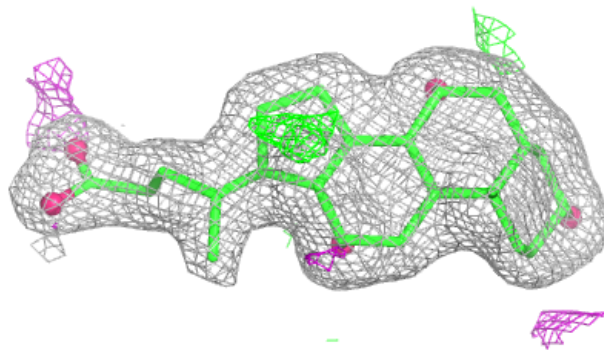
**Electron density around DMU M 101:**

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

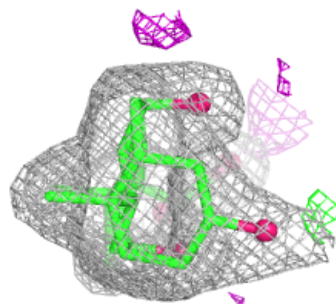
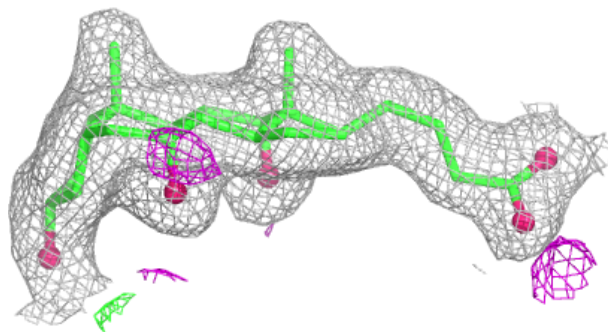
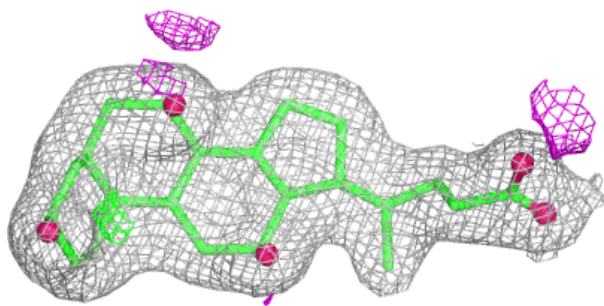


Electron density around CHD T 103:

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

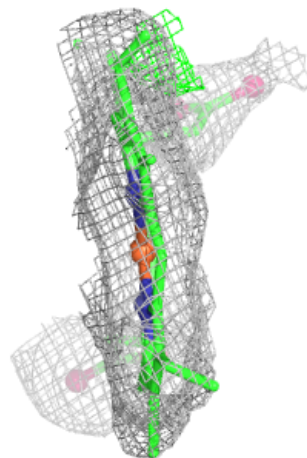
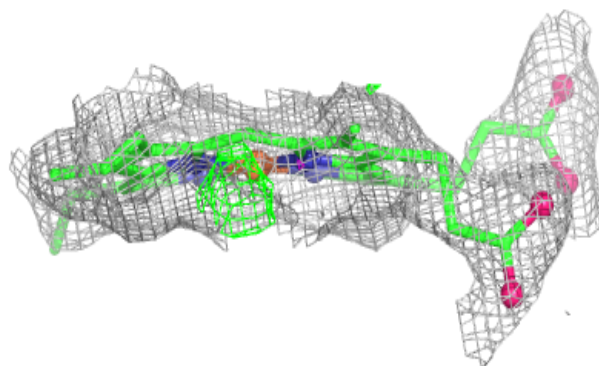
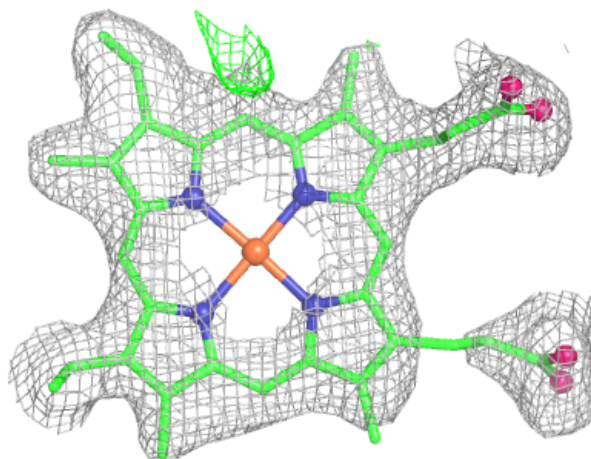
**Electron density around CHD G 102:**

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



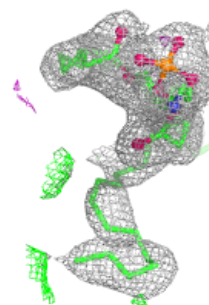
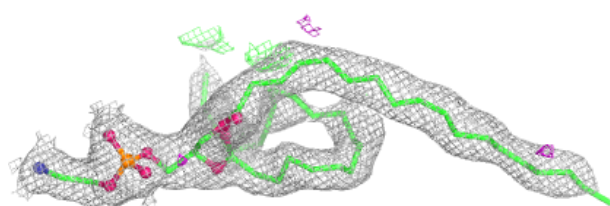
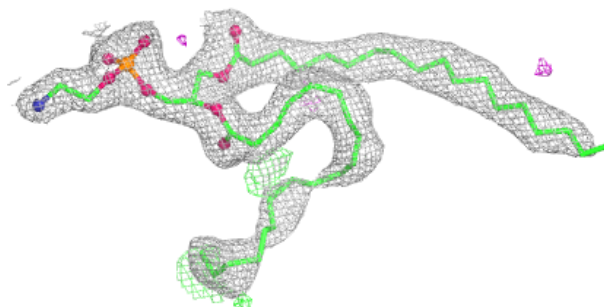
Electron density around HEC 1 201:

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

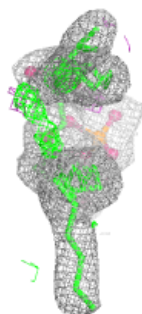
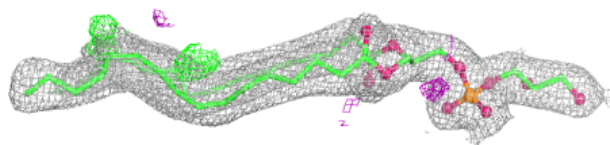
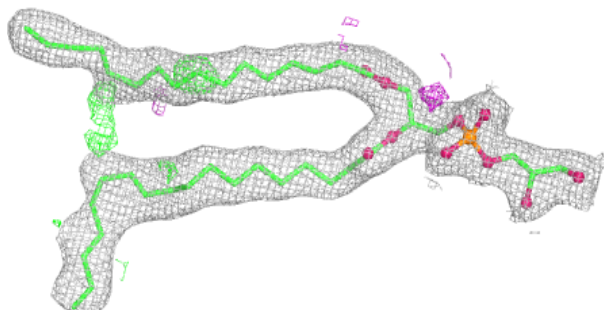


Electron density around PEK P 303:

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

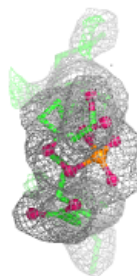
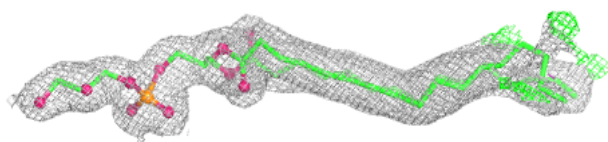
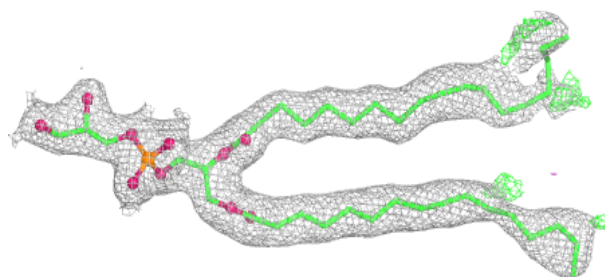
**Electron density around PGV P 304:**

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

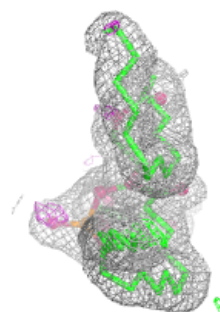
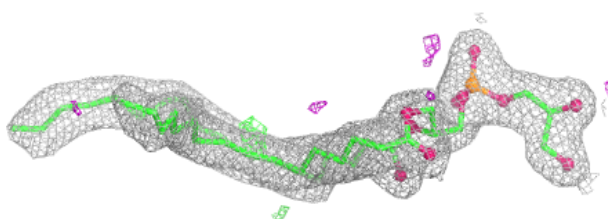
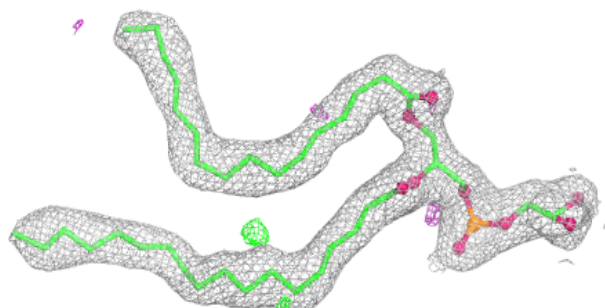


Electron density around PGV C 304:

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

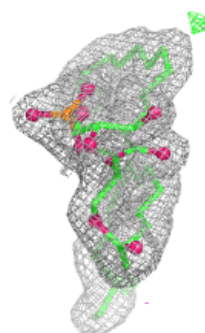
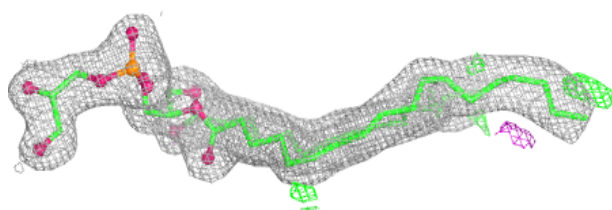
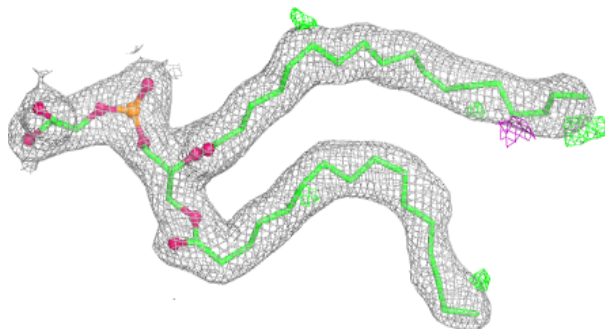
**Electron density around PGV A 608:**

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

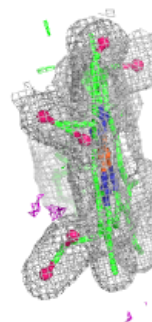
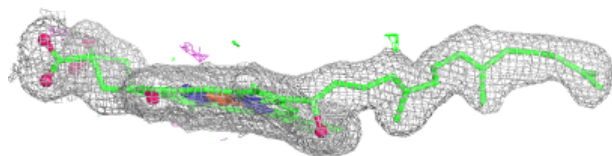
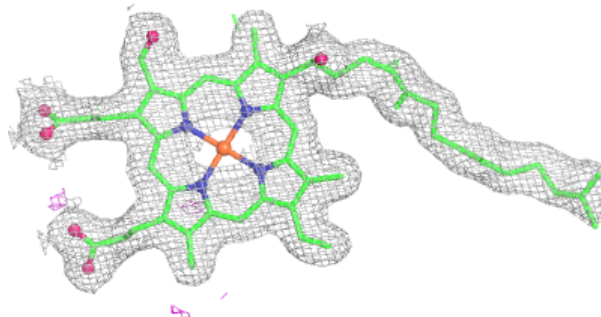


Electron density around PGV N 612:

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

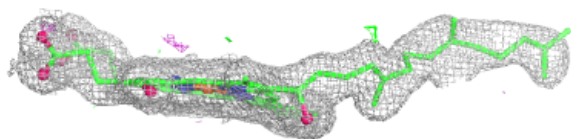
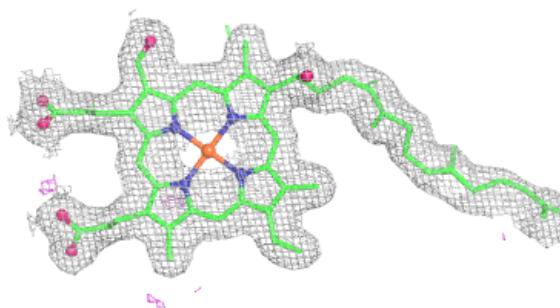
**Electron density around HEA A 604 (A):**

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

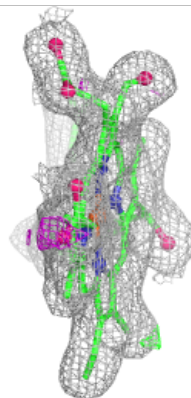
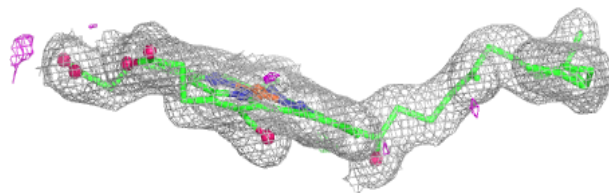
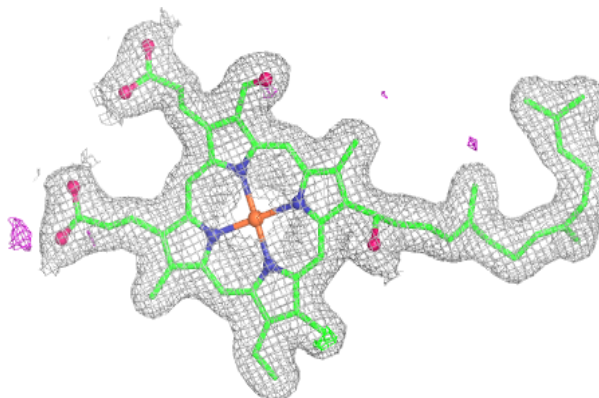


Electron density around HEA A 604 (B):

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

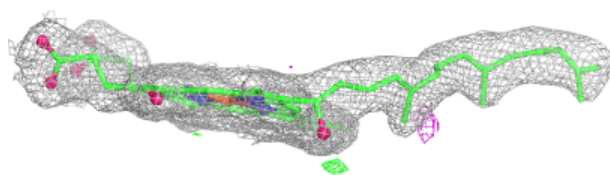
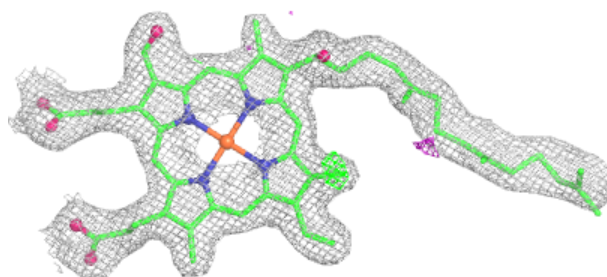
**Electron density around HEA A 605:**

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

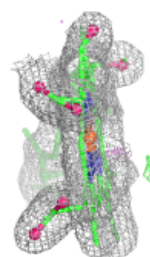
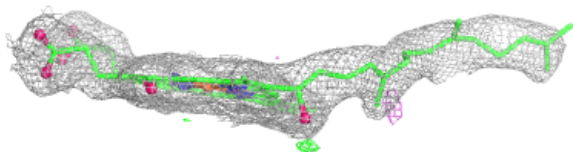
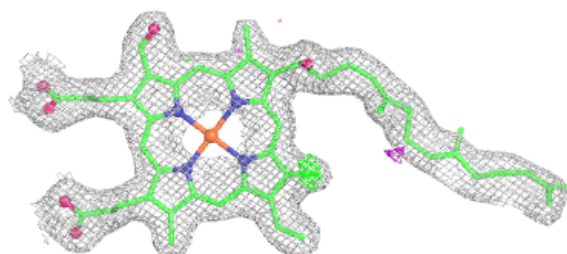


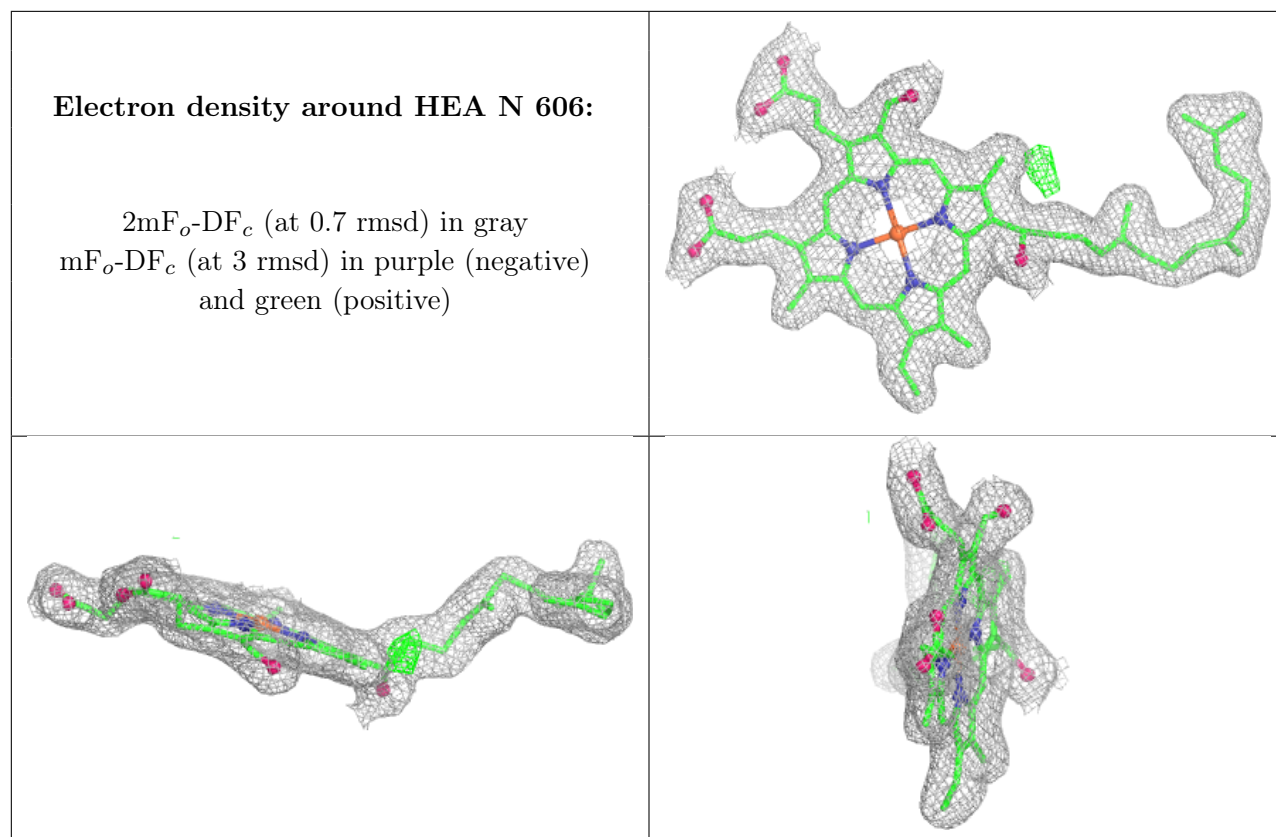
Electron density around HEA N 605 (A):

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

**Electron density around HEA N 605 (B):**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.