Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 07:05 AM EDT

PDB ID	:	2QJP
Title	:	Crystal structure of wild type rhodobacter sphaeroides with stigmatellin and antimycin inhibited
Authors	:	Esser, L.; Xia, D.
Deposited on	:	2007-07-08
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

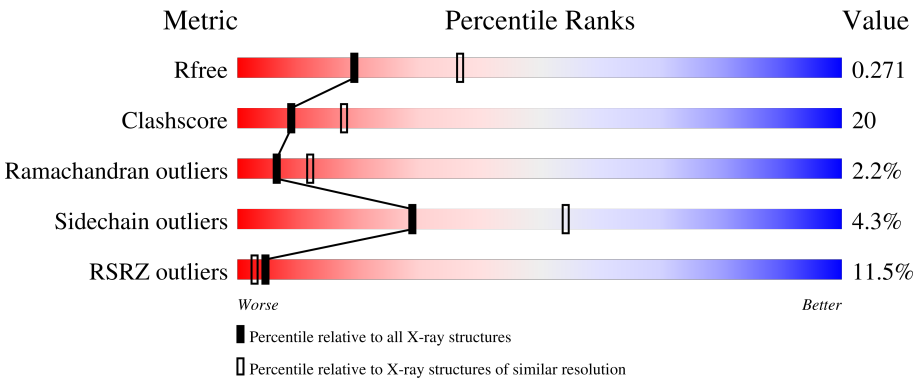
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	428	6% 65% 32% ·
1	D	428	6% 63% 35% ·
1	G	428	4% 64% 34% ·
1	J	428	4% 69% 29% ·
2	B	256	14% 61% 36% ·

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Mol	Chain	Length	Quality of chain
2	E	256	22% 58% 38% •
2	H	256	14% 54% 42% •
2	K	256	19% 61% 35% •
3	C	179	14% 60% 35% 5%
3	F	179	23% 54% 41% 5%
3	I	179	12% 58% 39% •
3	L	179	23% 56% 37% 6%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28227 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 b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	428	3435	2319	545	556	15	0	0	0
1	D	428	3435	2319	545	556	15	0	0	0
1	G	428	3435	2319	545	556	15	0	0	0
1	J	428	3435	2319	545	556	15	0	0	0

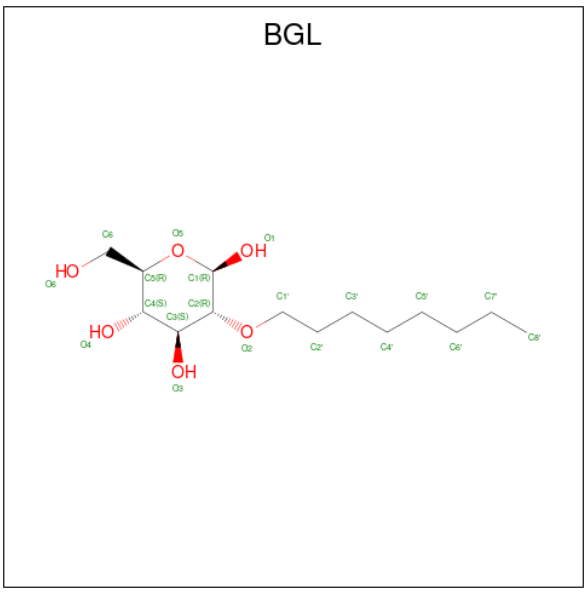
- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	256	1953	1240	326	374	13	0	0	0
2	E	256	1953	1240	326	374	13	0	0	0
2	H	256	1953	1240	326	374	13	0	0	0
2	K	256	1953	1240	326	374	13	0	0	0

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

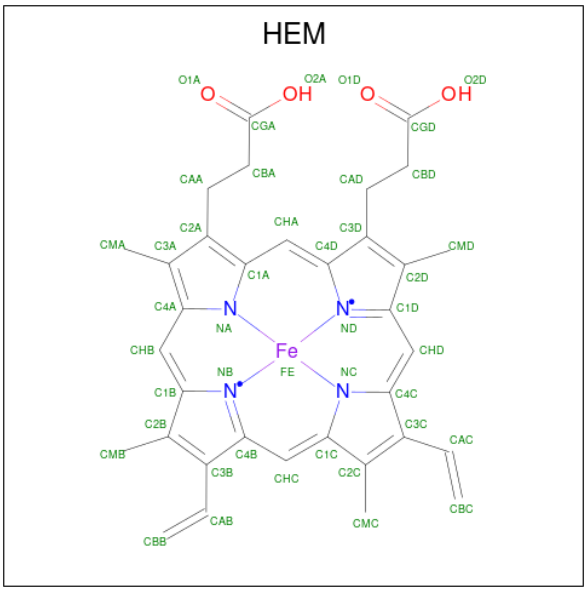
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	179	1341	845	237	253	6	0	0	0
3	F	179	1341	845	237	253	6	0	0	0
3	I	179	1341	845	237	253	6	0	0	0
3	L	179	1341	845	237	253	6	0	0	0

- Molecule 4 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	20	14	6	0	0
			Total	C	O		
4	E	1	20	14	6	0	0
			Total	C	O		
4	G	1	20	14	6	0	0
			Total	C	O		
4	J	1	20	14	6	0	0

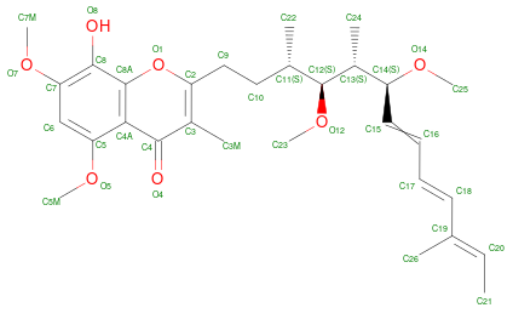
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	G	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	G	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	H	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	J	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	J	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	K	1	43	34	1	4	4	0	0

- Molecule 6 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).

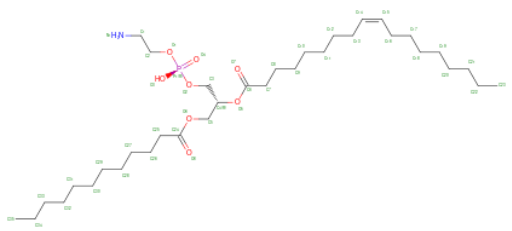
SMA



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	37	30	7	0	0
			Total	C	O		
6	D	1	37	30	7	0	0
			Total	C	O		
6	G	1	37	30	7	0	0
			Total	C	O		
6	J	1	37	30	7	0	0

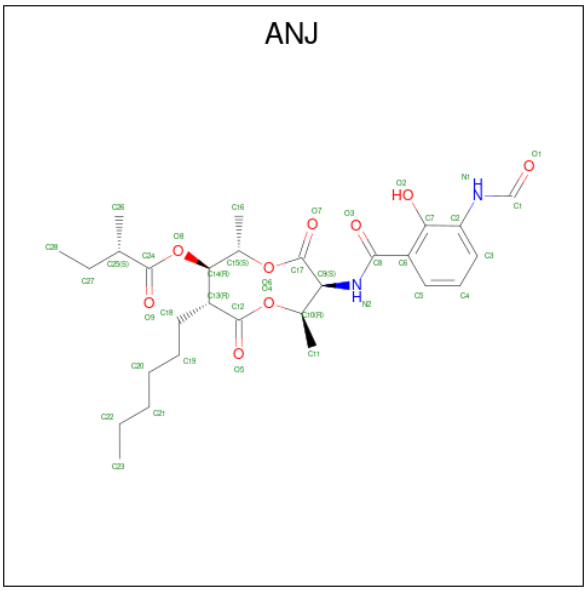
- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: $C_{35}H_{68}NO_8P$).

LOP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	45	35	1	8	1	0	0
7	D	1	45	35	1	8	1	0	0
7	G	1	45	35	1	8	1	0	0
7	J	1	45	35	1	8	1	0	0

- Molecule 8 is (2R,3S,6S,7R,8R)-3-{[3-(FORMYLAMINO)-2-HYDROXYBENZOYL]AMINO}-8-HEXYL-2,6-DIMETHYL-4,9-DIOXO-1,5-DIOXONAN-7-YL (2S)-2-METHYLBUTANOATE (three-letter code: ANJ) (formula: $C_{28}H_{40}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	39	28	2	9	0	0
8	D	1	39	28	2	9	0	0
8	G	1	39	28	2	9	0	0
8	J	1	39	28	2	9	0	0

- Molecule 9 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
9	B	1	1	1	0	0

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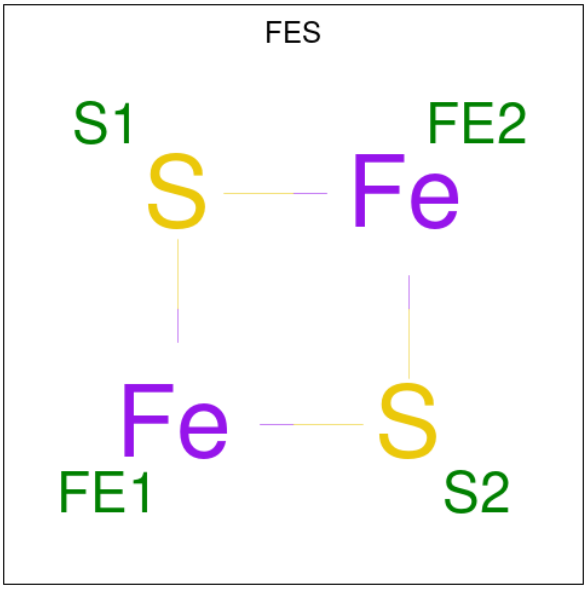
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total Sr 1 1	0	0
9	G	1	Total Sr 1 1	0	0
9	H	1	Total Sr 1 1	0	0
9	J	1	Total Sr 1 1	0	0
9	K	1	Total Sr 1 1	0	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Fe S 4 2 2	0	0
10	F	1	Total Fe S 4 2 2	0	0
10	I	1	Total Fe S 4 2 2	0	0
10	L	1	Total Fe S 4 2 2	0	0

- Molecule 11 is water.

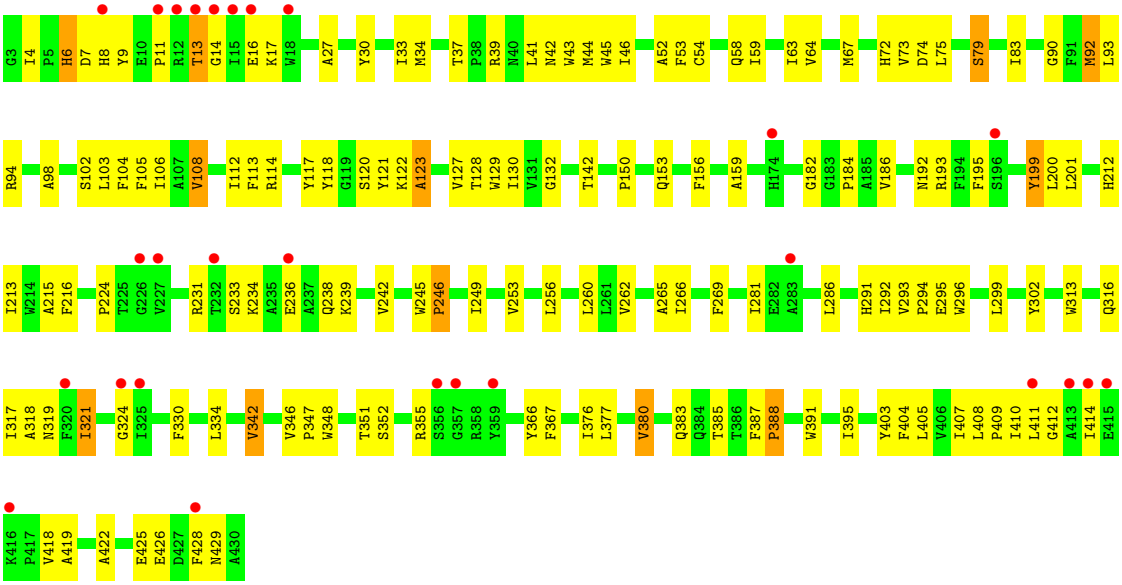
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	36	36	36	0	0
			Total	O		
11	B	7	7	7	0	0
			Total	O		
11	C	13	13	13	0	0
			Total	O		
11	D	41	41	41	0	0
			Total	O		
11	E	3	3	3	0	0
			Total	O		
11	F	13	13	13	0	0
			Total	O		
11	G	41	41	41	0	0
			Total	O		
11	H	4	4	4	0	0
			Total	O		
11	I	14	14	14	0	0
			Total	O		
11	J	23	23	23	0	0
			Total	O		
11	K	3	3	3	0	0
			Total	O		
11	L	11	11	11	0	0

3 Residue-property plots (i)

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.

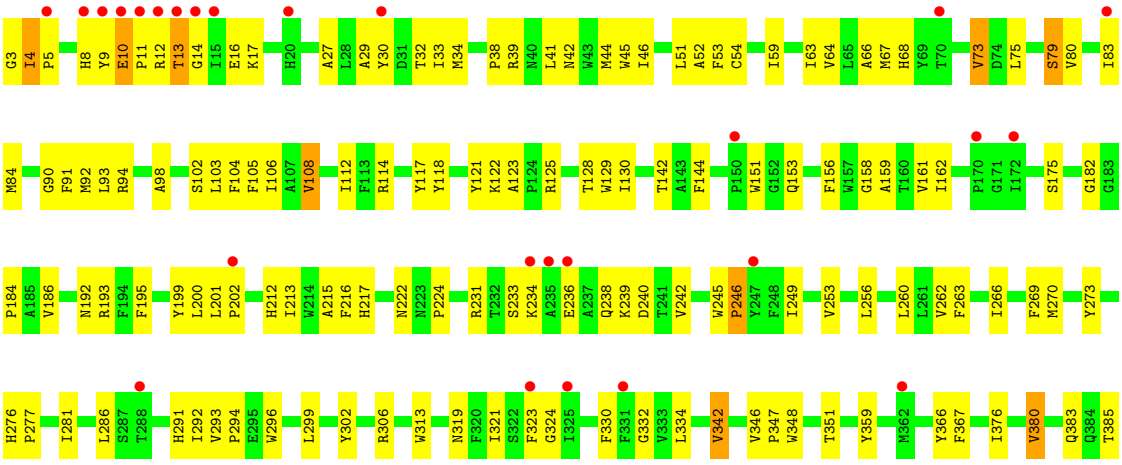
• Molecule 1: Cytochrome b

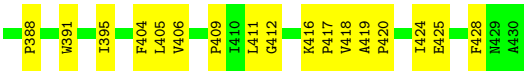
Chain A: 6% 65% 32%



• Molecule 1: Cytochrome b

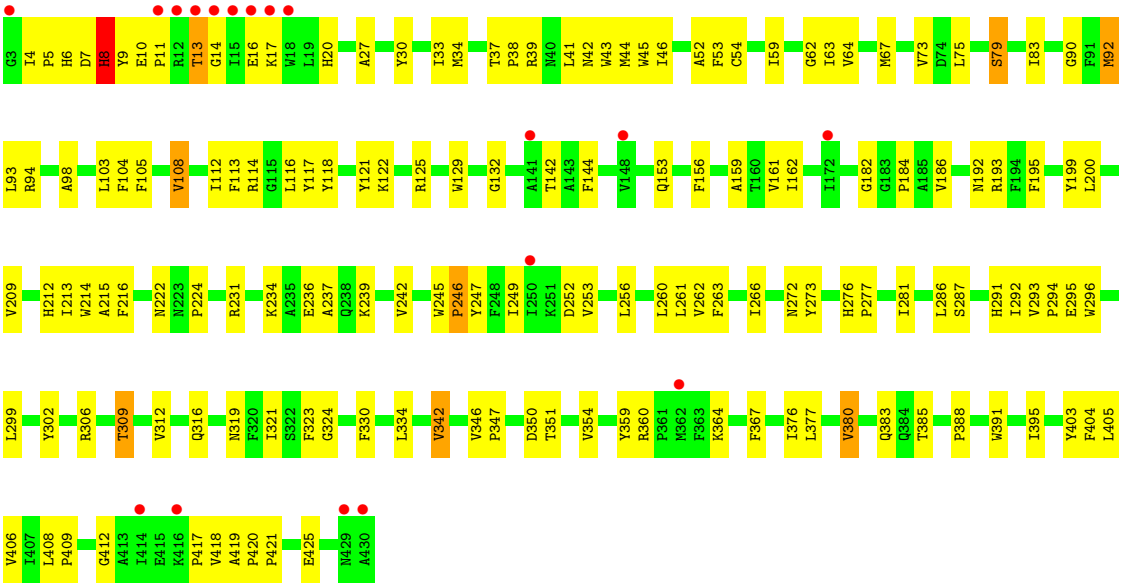
Chain D: 6% 63% 35%





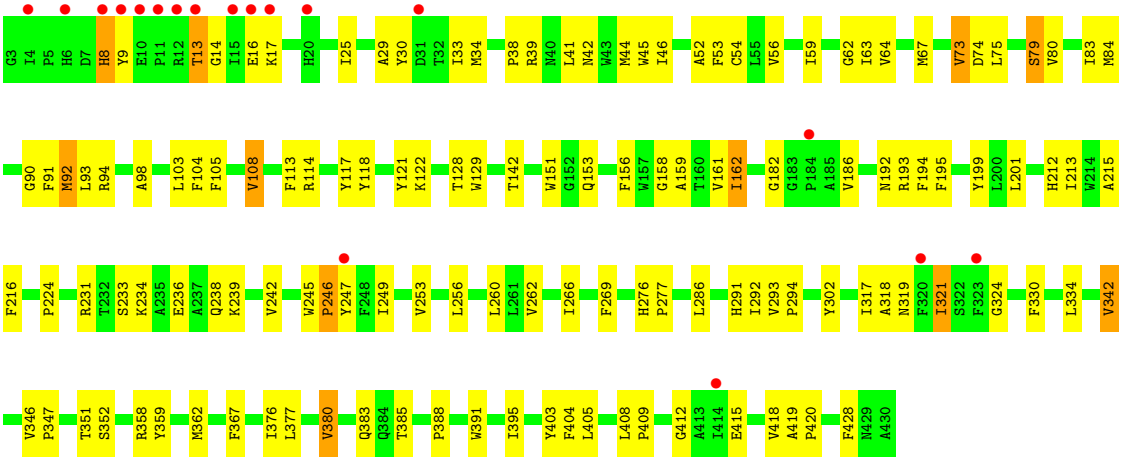
- Molecule 1: Cytochrome b

Chain G:



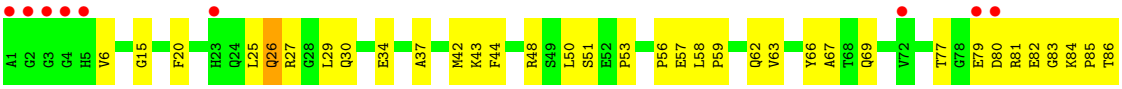
- Molecule 1: Cytochrome b

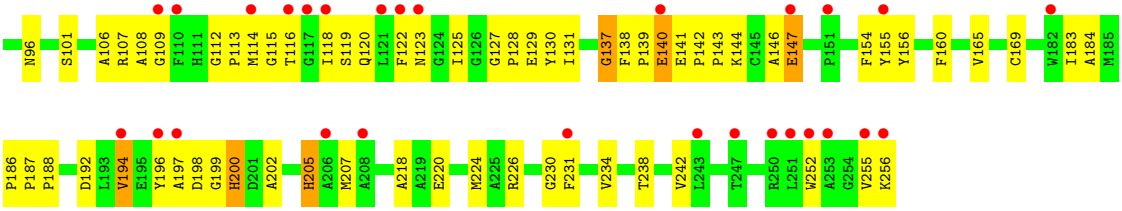
Chain J:



- Molecule 2: Cytochrome c1

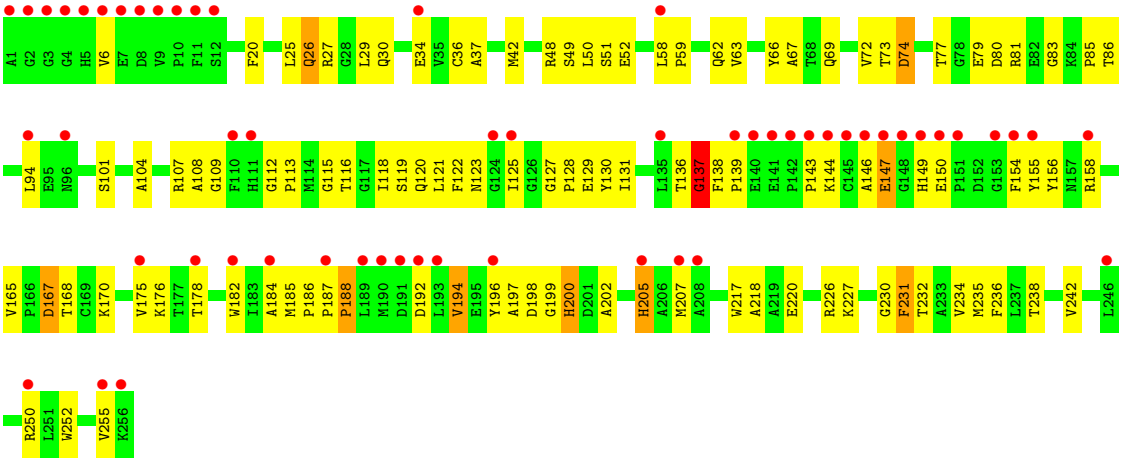
Chain B:





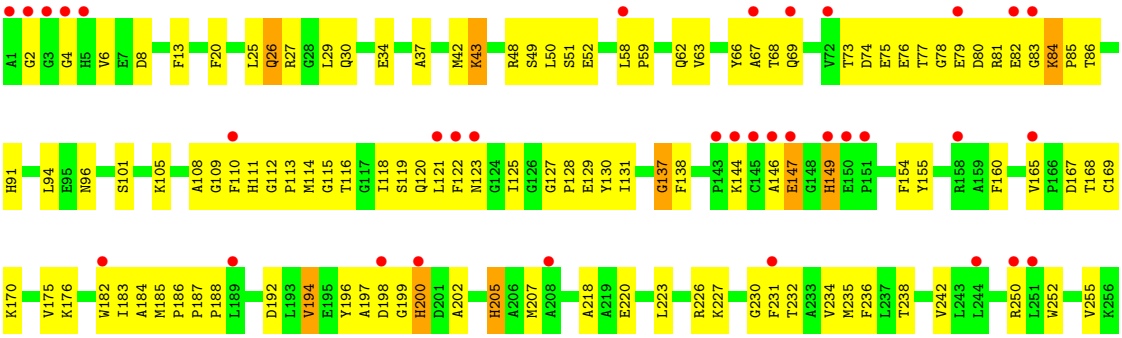
- Molecule 2: Cytochrome c1

Chain E:



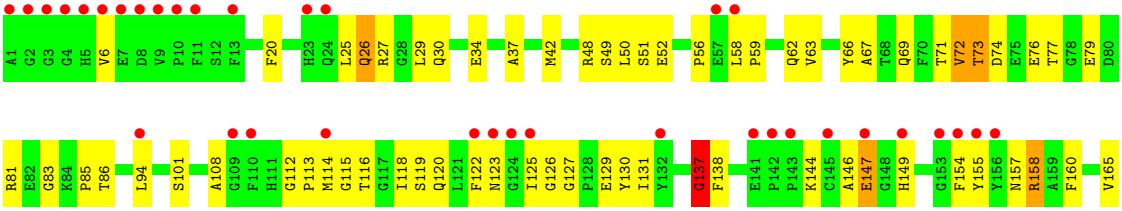
- Molecule 2: Cytochrome c1

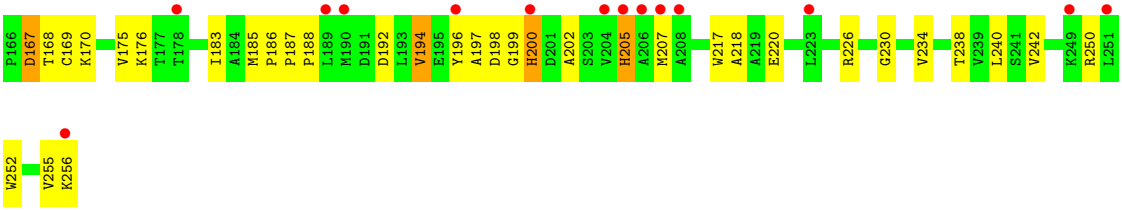
Chain H:



- Molecule 2: Cytochrome c1

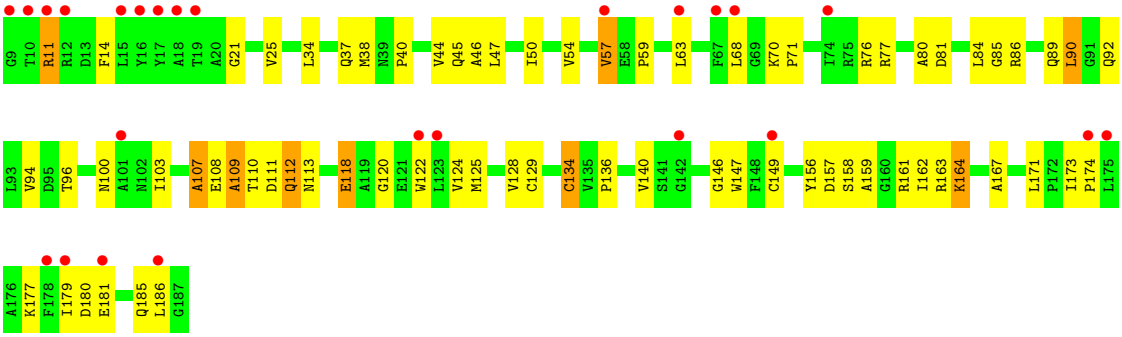
Chain K:





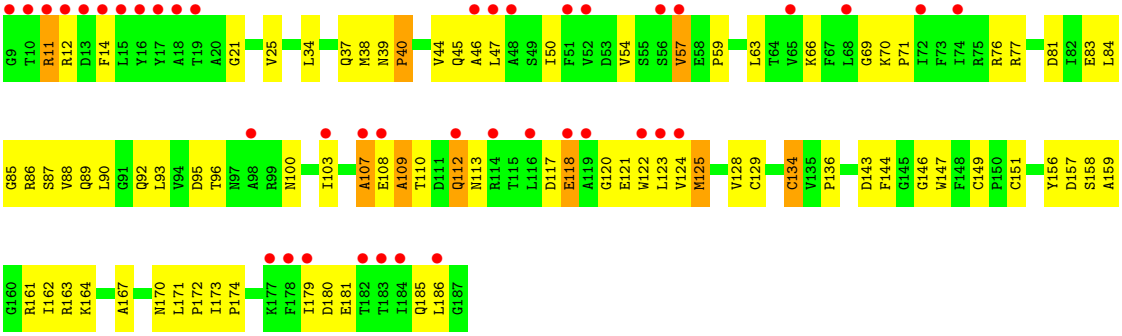
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C:



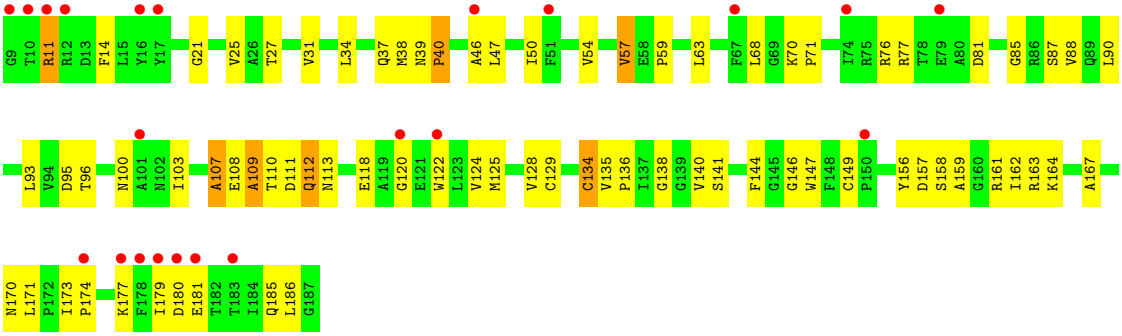
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain F:



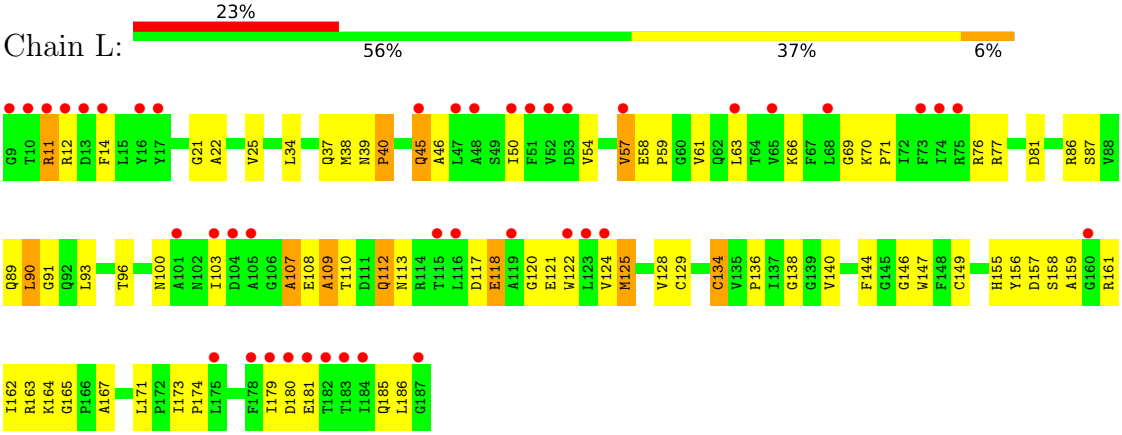
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain I:



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.06Å 146.52Å 141.00Å 90.00° 110.21° 90.00°	Depositor
Resolution (Å)	17.98 – 2.60 47.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (17.98-2.60) 97.7 (47.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.277 0.257 , 0.271	Depositor DCC
R_{free} test set	5654 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28227	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3332e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BGL, SR, ANJ, HEM, LOP, FES, SMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.36	0/3565	0.64	0/4891
1	D	0.35	0/3565	0.63	0/4891
1	G	0.35	0/3565	0.64	0/4891
1	J	0.36	0/3565	0.65	0/4891
2	B	0.32	0/2010	0.64	1/2733 (0.0%)
2	E	0.31	0/2010	0.64	1/2733 (0.0%)
2	H	0.32	0/2010	0.65	1/2733 (0.0%)
2	K	0.31	0/2010	0.65	1/2733 (0.0%)
3	C	0.32	0/1371	0.69	0/1868
3	F	0.31	0/1371	0.68	1/1868 (0.1%)
3	I	0.32	0/1371	0.70	0/1868
3	L	0.31	0/1371	0.67	0/1868
All	All	0.34	0/27784	0.65	5/37968 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	137	GLY	N-CA-C	5.84	127.71	113.10
2	K	137	GLY	N-CA-C	5.55	126.98	113.10
2	E	137	GLY	N-CA-C	5.54	126.94	113.10
2	B	137	GLY	N-CA-C	5.51	126.87	113.10
3	F	47	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3435	0	3420	134	0
1	D	3435	0	3420	144	0
1	G	3435	0	3420	131	0
1	J	3435	0	3420	119	0
2	B	1953	0	1848	87	0
2	E	1953	0	1848	115	0
2	H	1953	0	1848	113	0
2	K	1953	0	1848	91	0
3	C	1341	0	1307	52	0
3	F	1341	0	1307	71	0
3	I	1341	0	1307	64	0
3	L	1341	0	1307	70	0
4	A	20	0	28	3	0
4	E	20	0	28	2	0
4	G	20	0	28	1	0
4	J	20	0	28	1	0
5	A	86	0	60	9	0
5	B	43	0	30	5	0
5	D	86	0	60	10	0
5	E	43	0	30	5	0
5	G	86	0	60	7	0
5	H	43	0	30	4	0
5	J	86	0	60	5	0
5	K	43	0	30	1	0
6	A	37	0	42	2	0
6	D	37	0	42	3	0
6	G	37	0	42	1	0
6	J	37	0	42	3	0
7	A	45	0	67	2	0
7	D	45	0	67	4	0
7	G	45	0	67	5	0
7	J	45	0	67	5	0
8	A	39	0	39	9	0
8	D	39	0	39	12	0
8	G	39	0	39	6	0
8	J	39	0	39	10	0
9	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
10	C	4	0	0	0	0
10	F	4	0	0	0	0
10	I	4	0	0	0	0
10	L	4	0	0	0	0
11	A	36	0	0	2	0
11	B	7	0	0	3	0
11	C	13	0	0	0	0
11	D	41	0	0	4	0
11	E	3	0	0	0	0
11	F	13	0	0	2	0
11	G	41	0	0	3	0
11	H	4	0	0	0	0
11	I	14	0	0	0	0
11	J	23	0	0	1	0
11	K	3	0	0	1	0
11	L	11	0	0	1	0
All	All	28227	0	27364	1123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1123) 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)
1:D:213:ILE:HD11	8:D:504:ANJ:H14	1.39	1.05
1:J:213:ILE:HD11	8:J:505:ANJ:H14	1.40	1.04
1:A:317:ILE:O	1:A:321:ILE:HG22	1.60	1.02
1:A:213:ILE:HD11	8:A:504:ANJ:H14	1.39	1.01
1:J:317:ILE:O	1:J:321:ILE:HG22	1.62	1.00
1:D:4:ILE:HD12	1:D:4:ILE:H	1.22	0.99
1:A:195:PHE:HE2	1:D:195:PHE:HE2	1.08	0.99
1:G:195:PHE:HE2	1:J:195:PHE:HE2	1.11	0.98
3:C:47:LEU:HG	3:C:68:LEU:HD21	1.44	0.97
1:G:213:ILE:HD11	8:G:505:ANJ:H14	1.47	0.95
2:B:144:LYS:O	2:B:147:GLU:HG2	1.68	0.93
1:D:142:THR:HG21	5:D:502:HEM:HBB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77:THR:HG22	2:H:79:GLU:HB2	1.51	0.91
1:G:142:THR:HG21	5:G:502:HEM:HBB2	1.54	0.90
2:H:144:LYS:O	2:H:147:GLU:HG2	1.72	0.89
5:A:502:HEM:HMC1	5:A:502:HEM:HBC2	1.55	0.89
1:J:8:HIS:H	1:J:8:HIS:CD2	1.89	0.87
2:E:42:MET:HE1	2:E:218:ALA:HB1	1.58	0.85
1:D:213:ILE:CD1	8:D:504:ANJ:H14	2.05	0.85
1:A:4:ILE:HD12	1:A:4:ILE:H	1.41	0.84
1:A:142:THR:HG21	5:A:502:HEM:HBB2	1.58	0.83
1:J:213:ILE:CD1	8:J:505:ANJ:H14	2.09	0.83
2:K:42:MET:HE1	2:K:218:ALA:HB1	1.60	0.83
3:C:179:ILE:HD11	3:C:185:GLN:HE21	1.44	0.83
1:G:213:ILE:CD1	8:G:505:ANJ:H14	2.08	0.83
1:G:236:GLU:HA	1:G:239:LYS:HG3	1.60	0.82
3:F:179:ILE:HD11	3:F:185:GLN:HE21	1.44	0.82
2:H:42:MET:HE1	2:H:218:ALA:HB1	1.60	0.82
2:B:42:MET:HE1	2:B:218:ALA:HB1	1.62	0.82
3:I:179:ILE:HD11	3:I:185:GLN:HE21	1.44	0.82
1:J:8:HIS:H	1:J:8:HIS:HD2	1.25	0.81
1:J:29:ALA:HA	8:J:505:ANJ:H233	1.63	0.81
1:A:195:PHE:HE2	1:D:195:PHE:CE2	1.97	0.81
1:A:213:ILE:CD1	8:A:504:ANJ:H14	2.11	0.81
3:L:112:GLN:H	3:L:112:GLN:NE2	1.79	0.81
3:L:179:ILE:HD11	3:L:185:GLN:HE21	1.44	0.80
2:E:236:PHE:HE2	3:F:25:VAL:HG12	1.47	0.80
3:F:112:GLN:H	3:F:112:GLN:NE2	1.78	0.80
2:H:74:ASP:HB2	2:H:81:ARG:HD3	1.64	0.80
2:H:86:THR:HG22	3:I:46:ALA:HB1	1.61	0.80
1:J:142:THR:HG21	5:J:502:HEM:HBB2	1.61	0.80
1:A:195:PHE:CE2	1:D:195:PHE:HE2	1.98	0.80
3:C:107:ALA:HB1	3:C:113:ASN:ND2	1.97	0.79
2:K:49:SER:HA	2:K:52:GLU:HG3	1.65	0.79
2:K:137:GLY:HA2	2:K:158:ARG:NH1	1.98	0.79
1:D:29:ALA:HB1	8:D:504:ANJ:H231	1.66	0.78
3:I:112:GLN:H	3:I:112:GLN:NE2	1.81	0.78
3:I:107:ALA:HB1	3:I:113:ASN:ND2	1.98	0.78
1:J:321:ILE:HG12	1:J:321:ILE:O	1.82	0.78
1:G:5:PRO:HB2	1:G:234:LYS:HA	1.62	0.78
3:L:89:GLN:HE21	3:L:89:GLN:HA	1.49	0.78
2:K:108:ALA:HA	2:K:125:ILE:HG22	1.66	0.78
1:A:321:ILE:HG12	1:A:321:ILE:O	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:GLN:H	3:C:112:GLN:NE2	1.82	0.77
2:K:138:PHE:CD2	2:K:187:PRO:HG3	2.19	0.77
2:H:86:THR:CG2	3:I:46:ALA:HB1	2.15	0.76
1:G:281:ILE:HA	11:G:535:HOH:O	1.86	0.75
1:G:52:ALA:HB2	8:G:505:ANJ:H163	1.68	0.75
1:D:383:GLN:HE22	2:E:115:GLY:HA3	1.50	0.75
1:A:46:ILE:HG22	8:A:504:ANJ:H1	1.70	0.74
1:G:184:PRO:O	3:L:70:LYS:HE3	1.88	0.74
2:H:138:PHE:CD2	2:H:187:PRO:HG3	2.23	0.73
2:K:51:SER:OG	2:K:63:VAL:HG21	1.88	0.73
3:L:100:ASN:HB3	3:L:103:ILE:HG12	1.70	0.73
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.53	0.73
2:B:51:SER:OG	2:B:63:VAL:HG21	1.89	0.73
1:G:38:PRO:HG2	1:G:41:LEU:HD21	1.71	0.73
1:A:13:THR:HB	1:A:16:GLU:HB2	1.71	0.73
2:E:149:HIS:CE1	2:E:168:THR:HG21	2.23	0.72
2:E:128:PRO:HG2	2:E:129:GLU:OE1	1.90	0.72
1:D:13:THR:HB	1:D:16:GLU:HB2	1.71	0.72
1:D:103:LEU:HD13	7:D:503:LOP:H202	1.72	0.72
8:D:504:ANJ:O6	8:D:504:ANJ:C12	2.38	0.72
8:J:505:ANJ:O6	8:J:505:ANJ:C12	2.37	0.72
1:A:383:GLN:HE22	2:B:115:GLY:HA3	1.54	0.72
3:C:100:ASN:HB3	3:C:103:ILE:HG12	1.71	0.72
2:E:108:ALA:HA	2:E:125:ILE:HG22	1.71	0.72
3:F:100:ASN:HB3	3:F:103:ILE:HG12	1.71	0.72
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.02	0.72
2:E:49:SER:HA	2:E:52:GLU:HG3	1.72	0.72
1:G:13:THR:HB	1:G:16:GLU:HB2	1.71	0.71
1:A:13:THR:HG22	1:A:14:GLY:N	2.05	0.71
2:E:108:ALA:HA	2:E:125:ILE:O	1.89	0.71
3:I:100:ASN:HB3	3:I:103:ILE:HG12	1.70	0.71
1:D:332:GLY:HA3	11:D:539:HOH:O	1.90	0.71
1:J:39:ARG:HG2	1:J:242:VAL:HG13	1.73	0.71
1:D:39:ARG:HG2	1:D:242:VAL:HG13	1.72	0.71
1:J:13:THR:HG22	1:J:14:GLY:N	2.06	0.71
1:G:195:PHE:HE2	1:J:195:PHE:CE2	2.03	0.71
1:G:383:GLN:HE22	2:H:115:GLY:HA3	1.54	0.71
1:D:13:THR:HG22	1:D:14:GLY:N	2.05	0.71
3:L:89:GLN:HA	3:L:89:GLN:NE2	2.06	0.71
2:H:236:PHE:HE2	3:I:25:VAL:HG12	1.56	0.70
1:J:113:PHE:HB3	7:J:504:LOP:H272	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:HB2	8:A:504:ANJ:C16	2.20	0.70
1:D:13:THR:HG22	1:D:14:GLY:H	1.56	0.70
1:G:9:TYR:HB2	1:G:30:TYR:CD2	2.27	0.70
2:H:77:THR:C	2:H:79:GLU:H	1.94	0.70
1:A:281:ILE:HA	11:A:527:HOH:O	1.91	0.70
3:C:71:PRO:HB3	1:D:286:LEU:HD22	1.74	0.70
1:G:13:THR:HG22	1:G:14:GLY:N	2.06	0.70
1:J:13:THR:HG22	1:J:14:GLY:H	1.57	0.70
1:A:13:THR:HG22	1:A:14:GLY:H	1.57	0.70
1:D:330:PHE:CE2	1:D:334:LEU:HD11	2.27	0.70
1:G:39:ARG:HG2	1:G:242:VAL:HG13	1.73	0.70
2:K:72:VAL:HG12	2:K:73:THR:H	1.57	0.70
1:A:39:ARG:HG2	1:A:242:VAL:HG13	1.72	0.69
1:A:193:ARG:HH11	3:F:38:MET:HE2	1.57	0.69
1:G:309:THR:HG22	3:L:165:GLY:C	2.11	0.69
3:L:179:ILE:HD11	3:L:185:GLN:NE2	2.07	0.69
1:J:13:THR:HB	1:J:16:GLU:HB2	1.72	0.69
8:A:504:ANJ:C12	8:A:504:ANJ:O6	2.40	0.69
8:G:505:ANJ:C12	8:G:505:ANJ:O6	2.41	0.69
1:J:128:THR:HG21	5:J:501:HEM:HBD1	1.73	0.69
1:D:105:PHE:HA	1:D:108:VAL:HG23	1.74	0.69
2:E:167:ASP:HA	2:E:170:LYS:HE3	1.73	0.69
2:H:146:ALA:HA	2:H:149:HIS:HD2	1.56	0.69
1:A:330:PHE:CE2	1:A:334:LEU:HD11	2.28	0.69
3:I:179:ILE:HD11	3:I:185:GLN:NE2	2.07	0.69
2:K:72:VAL:HG12	2:K:73:THR:N	2.08	0.69
1:J:9:TYR:HB2	1:J:30:TYR:CD2	2.27	0.69
1:D:10:GLU:HG2	1:D:12:ARG:NH2	2.07	0.68
2:K:59:PRO:HD2	2:K:62:GLN:NE2	2.09	0.68
3:C:179:ILE:HD11	3:C:185:GLN:NE2	2.07	0.68
3:F:179:ILE:HD11	3:F:185:GLN:NE2	2.07	0.68
1:G:105:PHE:HA	1:G:108:VAL:HG22	1.76	0.68
3:L:66:LYS:HE2	3:L:69:GLY:HA2	1.74	0.68
2:H:59:PRO:HD2	2:H:62:GLN:NE2	2.09	0.68
1:A:52:ALA:HB2	8:A:504:ANJ:H163	1.76	0.68
3:C:107:ALA:HB1	3:C:113:ASN:HD21	1.57	0.68
1:J:330:PHE:CE2	1:J:334:LEU:HD11	2.28	0.68
3:L:107:ALA:HB1	3:L:113:ASN:ND2	2.09	0.68
2:E:236:PHE:CE2	3:F:25:VAL:HG12	2.29	0.67
1:A:123:ALA:O	1:A:355:ARG:NH1	2.28	0.67
1:D:33:ILE:HD11	8:D:504:ANJ:H212	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PHE:CD1	1:D:162:ILE:HD12	2.30	0.67
1:G:286:LEU:HD22	3:L:71:PRO:HB3	1.76	0.67
2:H:74:ASP:HB3	2:H:77:THR:HB	1.75	0.67
3:I:107:ALA:HB1	3:I:113:ASN:HD21	1.58	0.67
1:G:63:ILE:N	5:G:502:HEM:HBC2	2.10	0.67
2:B:59:PRO:HD2	2:B:62:GLN:NE2	2.09	0.67
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.77	0.67
5:D:502:HEM:HBC2	5:D:502:HEM:HHD	1.75	0.67
1:A:184:PRO:O	3:F:70:LYS:HE3	1.94	0.67
2:H:51:SER:OG	2:H:63:VAL:HG21	1.94	0.67
1:G:13:THR:HG22	1:G:14:GLY:H	1.57	0.66
1:J:103:LEU:HD13	7:J:504:LOP:H202	1.77	0.66
1:D:240:ASP:HB3	1:D:424:ILE:HD12	1.78	0.66
2:H:232:THR:HG22	2:H:236:PHE:HE1	1.59	0.66
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.28	0.66
2:K:77:THR:C	2:K:79:GLU:H	1.99	0.66
2:E:250:ARG:HD3	3:F:12:ARG:HB2	1.77	0.66
3:F:123:LEU:HD21	3:F:125:MET:HE1	1.77	0.66
1:G:351:THR:OG1	1:G:412:GLY:HA3	1.96	0.66
2:H:108:ALA:HA	2:H:125:ILE:HG22	1.78	0.66
1:J:30:TYR:CE1	1:J:34:MET:HG3	2.31	0.66
1:D:125:ARG:NE	1:D:222:ASN:HB2	2.10	0.66
3:C:80:ALA:O	3:C:84:LEU:HD13	1.96	0.66
2:B:140:GLU:CD	2:B:140:GLU:H	2.00	0.66
1:D:30:TYR:CE1	1:D:34:MET:HG3	2.30	0.66
1:D:319:ASN:OD1	1:D:324:GLY:HA2	1.96	0.66
2:E:59:PRO:HD2	2:E:62:GLN:NE2	2.08	0.66
3:L:40:PRO:HB2	3:L:45:GLN:HE21	1.61	0.66
1:A:105:PHE:HA	1:A:108:VAL:HG22	1.77	0.65
1:J:62:GLY:O	5:J:502:HEM:HBC2	1.96	0.65
1:G:113:PHE:HB3	7:G:504:LOP:H271	1.77	0.65
1:G:330:PHE:CE2	1:G:334:LEU:HD11	2.30	0.65
2:H:184:ALA:HB3	5:H:301:HEM:HBD1	1.79	0.65
3:I:71:PRO:HB3	1:J:286:LEU:HD22	1.78	0.65
1:J:403:TYR:CE2	1:J:408:LEU:HD11	2.31	0.65
2:K:86:THR:HG22	3:L:46:ALA:HB1	1.77	0.65
2:B:29:LEU:HD22	2:B:50:LEU:HD22	1.79	0.65
2:E:144:LYS:HD2	2:E:147:GLU:OE2	1.96	0.65
1:G:319:ASN:OD1	1:G:324:GLY:HA2	1.96	0.65
1:A:30:TYR:CE1	1:A:34:MET:HG3	2.31	0.65
1:G:30:TYR:CE1	1:G:34:MET:HG3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.30	0.65
1:A:239:LYS:HE2	1:A:425:GLU:OE2	1.96	0.64
2:H:128:PRO:HG2	2:H:129:GLU:OE1	1.97	0.64
1:A:236:GLU:HA	1:A:239:LYS:HD3	1.79	0.64
2:K:29:LEU:HD22	2:K:50:LEU:HD22	1.80	0.64
2:B:77:THR:C	2:B:79:GLU:H	2.00	0.64
1:G:103:LEU:HD13	7:G:504:LOP:H202	1.80	0.64
2:K:147:GLU:HA	2:K:147:GLU:OE1	1.98	0.64
4:A:431:BGL:H5	2:B:15:GLY:H	1.62	0.64
2:E:144:LYS:O	2:E:147:GLU:HG2	1.98	0.64
2:B:108:ALA:HA	2:B:125:ILE:O	1.97	0.64
2:K:149:HIS:CE1	2:K:168:THR:HG21	2.32	0.64
3:L:89:GLN:HE21	3:L:89:GLN:CA	2.09	0.64
3:L:89:GLN:C	3:L:91:GLY:H	2.01	0.64
2:E:230:GLY:O	2:E:234:VAL:HG23	1.99	0.63
1:G:52:ALA:HB2	8:G:505:ANJ:C16	2.28	0.63
3:I:90:LEU:HD11	3:I:108:GLU:HB3	1.80	0.63
2:K:77:THR:HG22	2:K:79:GLU:HB2	1.79	0.63
3:L:90:LEU:HG	3:L:90:LEU:O	1.98	0.63
2:B:42:MET:CE	2:B:218:ALA:HB1	2.28	0.63
2:E:42:MET:CE	2:E:218:ALA:HB1	2.28	0.63
3:F:118:GLU:CD	3:F:118:GLU:N	2.51	0.63
1:J:62:GLY:C	5:J:502:HEM:HBC2	2.19	0.63
2:E:138:PHE:CE2	2:E:187:PRO:HA	2.33	0.63
2:E:139:PRO:HG3	2:E:158:ARG:NE	2.14	0.63
2:B:77:THR:HG22	2:B:79:GLU:HB2	1.79	0.63
2:K:74:ASP:HB2	2:K:81:ARG:HD3	1.80	0.63
3:L:136:PRO:HB2	3:L:147:TRP:HB3	1.81	0.63
2:B:138:PHE:CD1	2:B:187:PRO:HG3	2.33	0.63
2:K:42:MET:CE	2:K:218:ALA:HB1	2.28	0.63
2:E:29:LEU:HD22	2:E:50:LEU:HD22	1.80	0.62
2:H:113:PRO:HD3	2:H:119:SER:HB2	1.81	0.62
2:H:77:THR:CG2	2:H:79:GLU:HB2	2.28	0.62
3:I:136:PRO:HB2	3:I:147:TRP:HB3	1.81	0.62
3:F:136:PRO:HB2	3:F:147:TRP:HB3	1.81	0.62
2:E:137:GLY:O	2:E:139:PRO:HD3	1.99	0.62
1:J:84:MET:HE2	11:K:303:HOH:O	1.99	0.62
2:B:113:PRO:HD3	2:B:119:SER:HB2	1.81	0.62
2:H:29:LEU:HD22	2:H:50:LEU:HD22	1.79	0.62
2:H:27:ARG:HD2	2:H:196:TYR:CZ	2.35	0.62
2:K:230:GLY:O	2:K:234:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:77:THR:C	2:E:79:GLU:H	2.03	0.62
3:F:125:MET:SD	3:F:171:LEU:HD12	2.40	0.62
2:H:42:MET:CE	2:H:218:ALA:HB1	2.28	0.62
3:F:107:ALA:HB1	3:F:113:ASN:ND2	2.15	0.62
2:E:29:LEU:HD12	2:E:29:LEU:O	2.00	0.61
2:B:184:ALA:HB3	5:B:301:HEM:CBD	2.30	0.61
3:C:136:PRO:HB2	3:C:147:TRP:HB3	1.81	0.61
2:E:113:PRO:HD3	2:E:119:SER:HB2	1.81	0.61
1:J:52:ALA:HB2	8:J:505:ANJ:C16	2.30	0.61
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.35	0.61
1:A:41:LEU:HD23	1:A:224:PRO:HD3	1.82	0.61
1:J:64:VAL:HG11	1:J:93:LEU:HD13	1.82	0.61
1:G:132:GLY:HA3	5:G:501:HEM:HBC2	1.83	0.61
1:J:318:ALA:HA	1:J:321:ILE:CG2	2.30	0.61
1:J:319:ASN:OD1	1:J:324:GLY:HA2	2.00	0.61
1:D:13:THR:O	1:D:17:LYS:HG3	2.00	0.61
1:J:46:ILE:HG22	8:J:505:ANJ:H1	1.83	0.61
2:B:230:GLY:O	2:B:234:VAL:HG23	2.00	0.61
1:D:64:VAL:O	1:D:67:MET:HB2	2.00	0.61
2:K:29:LEU:HD12	2:K:29:LEU:O	2.00	0.61
1:J:362:MET:CE	1:J:415:GLU:HA	2.31	0.61
2:B:29:LEU:HD12	2:B:29:LEU:O	2.01	0.61
1:A:64:VAL:HG11	1:A:93:LEU:HD13	1.81	0.60
1:J:64:VAL:O	1:J:67:MET:HB2	2.01	0.60
1:A:319:ASN:OD1	1:A:324:GLY:HA2	2.00	0.60
2:H:230:GLY:O	2:H:234:VAL:HG23	2.02	0.60
1:D:32:THR:HG23	1:D:217:HIS:HE1	1.65	0.60
2:H:4:GLY:O	2:H:111:HIS:HD2	1.83	0.60
2:H:183:ILE:HG23	2:H:185:MET:H	1.65	0.60
2:K:113:PRO:HD3	2:K:119:SER:HB2	1.81	0.60
1:A:318:ALA:HA	1:A:321:ILE:CG2	2.31	0.60
1:G:39:ARG:HH12	2:H:255:VAL:CG1	2.15	0.60
1:G:64:VAL:O	1:G:67:MET:HB2	2.01	0.60
2:K:160:PHE:CD2	2:K:183:ILE:HB	2.37	0.60
1:D:4:ILE:H	1:D:4:ILE:CD1	1.97	0.60
1:G:262:VAL:HG13	4:G:431:BGL:H8'1	1.84	0.60
1:D:64:VAL:HG11	1:D:93:LEU:HD13	1.83	0.60
1:D:236:GLU:HA	1:D:239:LYS:HG3	1.83	0.60
3:L:90:LEU:HD21	3:L:108:GLU:CD	2.21	0.60
2:E:184:ALA:HB3	5:E:301:HEM:HBD2	1.84	0.60
2:H:29:LEU:O	2:H:29:LEU:HD12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:140:VAL:HG12	3:L:140:VAL:O	2.02	0.60
3:C:90:LEU:HD11	3:C:108:GLU:HB3	1.83	0.60
2:K:250:ARG:HD3	3:L:12:ARG:HB2	1.84	0.60
2:H:86:THR:HG22	3:I:46:ALA:CB	2.32	0.59
2:K:250:ARG:HH12	3:L:11:ARG:CD	2.14	0.59
1:A:64:VAL:O	1:A:67:MET:HB2	2.02	0.59
1:A:4:ILE:HD12	1:A:4:ILE:N	2.15	0.59
1:G:64:VAL:HG11	1:G:93:LEU:HD13	1.83	0.59
1:D:52:ALA:HB2	8:D:504:ANJ:C16	2.33	0.59
6:J:503:SMA:H39	6:J:503:SMA:H33	1.84	0.59
2:E:66:TYR:CE1	2:E:69:GLN:NE2	2.71	0.59
8:A:504:ANJ:O6	8:A:504:ANJ:O4	2.21	0.58
1:G:54:CYS:SG	1:G:103:LEU:HG	2.43	0.58
2:E:42:MET:HE1	2:E:218:ALA:CB	2.32	0.58
2:K:74:ASP:HB3	2:K:77:THR:HB	1.85	0.58
1:A:286:LEU:HD22	3:F:71:PRO:HB3	1.85	0.58
1:D:236:GLU:HA	1:D:239:LYS:CD	2.33	0.58
1:D:269:PHE:HB3	4:E:257:BGL:H1'2	1.85	0.58
1:G:193:ARG:HH11	3:L:38:MET:HE2	1.69	0.58
1:J:38:PRO:HG2	1:J:41:LEU:HD21	1.85	0.58
1:D:9:TYR:HB2	1:D:30:TYR:CD2	2.38	0.58
1:D:144:PHE:HE2	6:D:2:SMA:H43	1.69	0.58
1:D:273:TYR:HE1	2:E:120:GLN:HB2	1.67	0.58
3:F:86:ARG:HG2	3:F:112:GLN:OE1	2.03	0.58
1:G:39:ARG:HH12	2:H:255:VAL:HG12	1.69	0.58
8:G:505:ANJ:O6	8:G:505:ANJ:O4	2.22	0.58
1:J:362:MET:HE3	1:J:415:GLU:HG3	1.86	0.58
2:K:250:ARG:HH12	3:L:11:ARG:HD3	1.69	0.58
1:A:54:CYS:SG	1:A:103:LEU:HG	2.43	0.58
1:J:54:CYS:SG	1:J:103:LEU:HG	2.44	0.58
1:D:9:TYR:HE1	1:D:11:PRO:HG3	1.70	0.57
1:G:62:GLY:C	5:G:502:HEM:HBC2	2.24	0.57
2:K:66:TYR:O	2:K:69:GLN:HG2	2.04	0.57
1:A:105:PHE:HA	1:A:108:VAL:CG2	2.34	0.57
1:J:9:TYR:HB2	1:J:30:TYR:CG	2.39	0.57
2:K:149:HIS:ND1	2:K:168:THR:HG21	2.19	0.57
1:D:125:ARG:CZ	1:D:222:ASN:HB2	2.35	0.57
8:D:504:ANJ:O6	8:D:504:ANJ:O4	2.21	0.57
2:H:96:ASN:O	5:H:301:HEM:HAD1	2.04	0.57
1:G:405:LEU:O	1:G:409:PRO:HG2	2.04	0.57
2:B:140:GLU:CD	2:B:140:GLU:N	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PRO:HG2	1:D:41:LEU:HD21	1.86	0.57
8:J:505:ANJ:O6	8:J:505:ANJ:O4	2.21	0.57
2:K:205:HIS:ND1	2:K:205:HIS:C	2.59	0.57
3:L:124:VAL:O	3:L:173:ILE:HG23	2.05	0.57
2:E:149:HIS:CD2	2:E:168:THR:HG21	2.40	0.56
3:L:89:GLN:O	3:L:91:GLY:N	2.37	0.56
1:A:33:ILE:O	1:A:33:ILE:HG22	2.05	0.56
1:D:54:CYS:SG	1:D:103:LEU:HG	2.45	0.56
2:E:20:PHE:HB3	2:E:25:LEU:HD11	1.86	0.56
2:H:205:HIS:ND1	2:H:205:HIS:C	2.59	0.56
1:G:33:ILE:HG22	1:G:33:ILE:O	2.05	0.56
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.87	0.56
3:I:124:VAL:O	3:I:173:ILE:HG23	2.05	0.56
1:D:52:ALA:HB2	8:D:504:ANJ:H163	1.87	0.56
2:E:77:THR:HG22	2:E:79:GLU:HB2	1.87	0.56
1:G:13:THR:O	1:G:17:LYS:HG3	2.04	0.56
3:I:77:ARG:HB3	3:I:81:ASP:HB2	1.88	0.56
2:B:77:THR:CG2	2:B:79:GLU:HB2	2.36	0.56
2:E:27:ARG:HD2	2:E:196:TYR:CZ	2.41	0.56
1:G:125:ARG:NE	1:G:222:ASN:HB2	2.20	0.56
1:A:295:GLU:OE2	6:A:1:SMA:H10	2.06	0.56
1:D:33:ILE:O	1:D:33:ILE:HG22	2.06	0.56
1:J:33:ILE:HG22	1:J:33:ILE:O	2.06	0.56
2:E:205:HIS:ND1	2:E:205:HIS:C	2.58	0.56
1:D:359:TYR:CD2	1:D:420:PRO:HB3	2.41	0.56
1:D:391:TRP:O	1:D:395:ILE:HG13	2.06	0.56
3:F:89:GLN:HB2	3:F:92:GLN:OE1	2.05	0.55
3:I:85:GLY:HA3	3:I:111:ASP:OD2	2.06	0.55
3:L:125:MET:SD	3:L:171:LEU:HD12	2.45	0.55
2:B:128:PRO:HG2	2:B:129:GLU:OE1	2.06	0.55
3:C:77:ARG:HB3	3:C:81:ASP:HB2	1.87	0.55
1:D:294:PRO:HG2	1:D:302:TYR:CG	2.41	0.55
2:H:232:THR:HG22	2:H:236:PHE:CE1	2.41	0.55
3:C:124:VAL:O	3:C:173:ILE:HG23	2.06	0.55
3:L:86:ARG:HG2	3:L:112:GLN:OE1	2.06	0.55
2:B:205:HIS:ND1	2:B:205:HIS:C	2.59	0.55
3:C:90:LEU:HD21	3:C:108:GLU:OE2	2.06	0.55
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.87	0.55
3:F:85:GLY:O	3:F:88:VAL:HG23	2.07	0.55
1:G:239:LYS:HE2	1:G:425:GLU:OE2	2.06	0.55
3:L:77:ARG:HB3	3:L:81:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:GLY:O	1:D:162:ILE:HG13	2.06	0.55
1:D:236:GLU:HA	1:D:239:LYS:CG	2.37	0.55
1:J:294:PRO:HG2	1:J:302:TYR:CG	2.42	0.55
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.40	0.55
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.40	0.55
3:C:70:LYS:HE3	1:D:184:PRO:O	2.06	0.55
2:H:74:ASP:HB2	2:H:81:ARG:CD	2.35	0.55
2:H:250:ARG:HH12	3:I:11:ARG:HD3	1.70	0.55
1:A:418:VAL:HG12	1:A:419:ALA:N	2.22	0.55
2:B:20:PHE:HB3	2:B:25:LEU:HD11	1.87	0.55
2:E:227:LYS:HE2	4:E:257:BGL:O1	2.06	0.55
3:F:124:VAL:O	3:F:173:ILE:HG23	2.06	0.55
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.70	0.55
2:B:160:PHE:CD2	2:B:183:ILE:HB	2.41	0.54
2:B:184:ALA:HB3	5:B:301:HEM:HBD1	1.88	0.54
3:F:90:LEU:HD12	3:F:93:LEU:HD12	1.89	0.54
1:J:161:VAL:HG11	6:J:503:SMA:O5	2.07	0.54
2:K:194:VAL:HB	2:K:207:MET:CE	2.37	0.54
1:A:269:PHE:HB3	4:A:431:BGL:H1'2	1.87	0.54
1:G:39:ARG:NH1	2:H:255:VAL:HG12	2.21	0.54
2:H:184:ALA:HB3	5:H:301:HEM:CBD	2.37	0.54
1:J:391:TRP:O	1:J:395:ILE:HG13	2.07	0.54
1:A:72:HIS:HE1	1:A:74:ASP:OD2	1.91	0.54
1:A:39:ARG:HH12	2:B:255:VAL:CG1	2.20	0.54
1:A:121:TYR:CE1	1:A:122:LYS:HG3	2.42	0.54
3:F:144:PHE:N	3:F:144:PHE:CD1	2.76	0.54
1:A:118:TYR:OH	7:A:503:LOP:H32	2.07	0.54
2:E:147:GLU:OE1	2:E:147:GLU:HA	2.06	0.54
1:A:294:PRO:HG2	1:A:302:TYR:CG	2.43	0.54
3:C:37:GLN:NE2	3:C:38:MET:HG3	2.23	0.54
3:F:77:ARG:HB3	3:F:81:ASP:HB2	1.88	0.54
1:J:234:LYS:O	1:J:238:GLN:HG3	2.08	0.54
2:H:81:ARG:CZ	2:H:84:LYS:HE2	2.38	0.54
1:D:39:ARG:HD3	1:D:428:PHE:CD2	2.43	0.54
1:D:46:ILE:HG22	8:D:504:ANJ:H1	1.90	0.54
2:E:149:HIS:CG	2:E:168:THR:HG21	2.43	0.54
3:F:110:THR:OG1	3:F:113:ASN:HB2	2.08	0.54
3:C:21:GLY:O	3:C:25:VAL:HG23	2.08	0.54
2:E:51:SER:OG	2:E:63:VAL:HG21	2.08	0.54
3:F:21:GLY:O	3:F:25:VAL:HG23	2.08	0.54
1:A:113:PHE:HB3	7:A:503:LOP:H272	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:VAL:HG11	6:D:2:SMA:O5	2.08	0.53
2:E:194:VAL:HB	2:E:207:MET:CE	2.38	0.53
2:H:77:THR:C	2:H:79:GLU:N	2.61	0.53
2:H:81:ARG:HG3	2:H:81:ARG:HH11	1.73	0.53
2:B:192:ASP:HA	2:B:202:ALA:HB3	1.91	0.53
2:K:192:ASP:HA	2:K:202:ALA:HB3	1.91	0.53
1:D:263:PHE:HD1	7:D:503:LOP:H221	1.73	0.53
2:E:66:TYR:CD1	2:E:69:GLN:NE2	2.77	0.53
2:E:165:VAL:HG13	2:E:182:TRP:CZ3	2.43	0.53
3:I:37:GLN:NE2	3:I:38:MET:HG3	2.23	0.53
1:G:294:PRO:HG2	1:G:302:TYR:CG	2.44	0.53
3:L:37:GLN:NE2	3:L:38:MET:HG3	2.22	0.53
1:A:391:TRP:O	1:A:395:ILE:HG13	2.08	0.53
2:E:104:ALA:O	2:E:127:GLY:HA3	2.09	0.53
3:F:37:GLN:NE2	3:F:38:MET:HG3	2.24	0.53
3:I:21:GLY:O	3:I:25:VAL:HG23	2.09	0.53
3:I:70:LYS:HB2	3:I:70:LYS:NZ	2.23	0.53
1:D:130:ILE:HD11	1:D:348:TRP:HH2	1.73	0.53
1:J:358:ARG:HH21	7:J:504:LOP:H21	1.73	0.53
5:J:501:HEM:CMA	8:J:505:ANJ:O7	2.57	0.53
3:L:110:THR:OG1	3:L:113:ASN:HB2	2.08	0.53
2:E:86:THR:HG22	3:F:46:ALA:HB1	1.90	0.53
2:E:194:VAL:HB	2:E:207:MET:HE3	1.91	0.53
1:G:359:TYR:CZ	1:G:421:PRO:HD3	2.44	0.53
1:G:391:TRP:O	1:G:395:ILE:HG13	2.09	0.53
2:B:238:THR:O	2:B:242:VAL:HG23	2.09	0.53
1:D:103:LEU:HB2	7:D:503:LOP:H222	1.90	0.53
2:E:155:TYR:CZ	2:E:186:PRO:HB3	2.44	0.53
2:H:194:VAL:HB	2:H:207:MET:CE	2.38	0.53
1:J:362:MET:HE1	1:J:415:GLU:HA	1.91	0.53
3:C:85:GLY:HA3	3:C:111:ASP:OD2	2.09	0.52
2:H:66:TYR:O	2:H:69:GLN:HG2	2.09	0.52
2:H:250:ARG:HH12	3:I:11:ARG:CD	2.22	0.52
2:K:155:TYR:CZ	2:K:186:PRO:HB3	2.44	0.52
2:B:127:GLY:O	2:B:131:ILE:HG13	2.09	0.52
2:E:238:THR:O	2:E:242:VAL:HG23	2.09	0.52
1:G:256:LEU:O	1:G:260:LEU:HG	2.08	0.52
3:L:107:ALA:HB1	3:L:113:ASN:HD21	1.75	0.52
2:E:192:ASP:HA	2:E:202:ALA:HB3	1.91	0.52
2:H:127:GLY:O	2:H:131:ILE:HG13	2.09	0.52
2:H:155:TYR:CZ	2:H:186:PRO:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:138:GLY:O	3:I:141:SER:OG	2.24	0.52
1:A:403:TYR:CE2	1:A:408:LEU:HD11	2.44	0.52
2:B:194:VAL:HB	2:B:207:MET:CE	2.39	0.52
2:H:68:THR:HG23	2:H:82:GLU:OE2	2.10	0.52
1:D:75:LEU:O	1:D:79:SER:HB3	2.09	0.52
2:K:238:THR:O	2:K:242:VAL:HG23	2.09	0.52
1:A:256:LEU:O	1:A:260:LEU:HG	2.09	0.52
1:G:212:HIS:O	1:G:215:ALA:HB3	2.10	0.52
2:H:238:THR:O	2:H:242:VAL:HG23	2.09	0.52
3:I:34:LEU:O	3:I:37:GLN:HG3	2.10	0.52
1:J:269:PHE:HB3	4:J:431:BGL:H1'2	1.92	0.52
3:F:66:LYS:HE3	3:F:69:GLY:HA2	1.92	0.52
2:K:59:PRO:HD2	2:K:62:GLN:HE21	1.75	0.52
2:E:143:PRO:HG3	2:E:178:THR:HG21	1.92	0.52
3:L:21:GLY:O	3:L:25:VAL:HG23	2.09	0.52
3:F:172:PRO:HG3	11:F:213:HOH:O	2.10	0.51
1:G:4:ILE:HD12	1:G:4:ILE:H	1.75	0.51
3:L:34:LEU:O	3:L:37:GLN:HG3	2.10	0.51
3:C:34:LEU:O	3:C:37:GLN:HG3	2.10	0.51
3:F:34:LEU:O	3:F:37:GLN:HG3	2.10	0.51
2:H:192:ASP:HA	2:H:202:ALA:HB3	1.91	0.51
1:A:59:ILE:O	1:A:63:ILE:HG13	2.11	0.51
3:C:163:ARG:O	3:C:164:LYS:HB2	2.08	0.51
1:D:83:ILE:O	1:D:90:GLY:HA3	2.11	0.51
6:D:2:SMA:H39	6:D:2:SMA:H33	1.93	0.51
1:G:249:ILE:O	1:G:253:VAL:HG23	2.10	0.51
1:J:52:ALA:HB2	8:J:505:ANJ:H163	1.92	0.51
2:K:127:GLY:O	2:K:131:ILE:HG13	2.10	0.51
2:E:127:GLY:O	2:E:131:ILE:HG13	2.10	0.51
1:G:263:PHE:HD1	7:G:504:LOP:H221	1.75	0.51
1:J:249:ILE:O	1:J:253:VAL:HG23	2.11	0.51
2:B:53:PRO:HA	2:B:57:GLU:CD	2.31	0.51
2:B:96:ASN:O	5:B:301:HEM:HAD1	2.11	0.51
1:G:42:ASN:OD1	1:G:44:MET:HB2	2.11	0.51
1:J:256:LEU:O	1:J:260:LEU:HG	2.10	0.51
2:K:144:LYS:O	2:K:147:GLU:HG2	2.10	0.51
1:A:39:ARG:NH1	2:B:255:VAL:CG1	2.73	0.51
1:D:256:LEU:O	1:D:260:LEU:HG	2.10	0.51
2:E:165:VAL:HG13	2:E:182:TRP:HZ3	1.76	0.51
1:G:44:MET:HE3	7:G:504:LOP:H92	1.90	0.51
1:G:59:ILE:O	1:G:63:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:ASN:OD1	1:J:44:MET:HB2	2.11	0.51
1:J:75:LEU:O	1:J:79:SER:HB3	2.11	0.51
1:A:249:ILE:O	1:A:253:VAL:HG23	2.11	0.51
1:A:351:THR:OG1	1:A:412:GLY:HA3	2.11	0.51
1:D:128:THR:HG21	5:D:501:HEM:HBD1	1.93	0.51
2:H:43:LYS:HE3	2:H:91:HIS:CE1	2.46	0.51
2:H:66:TYR:CE1	2:H:69:GLN:NE2	2.79	0.51
1:A:200:LEU:HD22	1:D:63:ILE:HD13	1.92	0.51
2:B:77:THR:C	2:B:79:GLU:N	2.63	0.51
3:C:47:LEU:HG	3:C:68:LEU:CD2	2.29	0.51
3:C:90:LEU:HD21	3:C:108:GLU:CD	2.31	0.51
3:F:44:VAL:O	3:F:46:ALA:N	2.44	0.51
1:G:403:TYR:O	1:G:408:LEU:HG	2.11	0.51
3:C:125:MET:SD	3:C:171:LEU:HD12	2.50	0.51
1:A:39:ARG:NH1	2:B:255:VAL:HG12	2.26	0.51
1:A:408:LEU:HB2	1:A:409:PRO:HD3	1.92	0.51
1:A:428:PHE:CZ	2:B:256:LYS:HB2	2.45	0.51
3:F:87:SER:O	3:F:87:SER:OG	2.28	0.51
1:A:407:ILE:HG22	1:A:411:LEU:HD12	1.93	0.50
2:B:59:PRO:HD2	2:B:62:GLN:HE21	1.76	0.50
2:B:224:MET:HB2	11:B:307:HOH:O	2.09	0.50
1:D:42:ASN:OD1	1:D:44:MET:HB2	2.11	0.50
1:D:45:TRP:CZ3	1:D:224:PRO:HG3	2.46	0.50
1:D:182:GLY:HA3	1:D:193:ARG:NH2	2.26	0.50
1:D:281:ILE:HD11	2:E:107:ARG:HH12	1.75	0.50
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.11	0.50
2:K:73:THR:HG22	2:K:73:THR:O	2.11	0.50
2:B:155:TYR:CZ	2:B:186:PRO:HB3	2.45	0.50
1:D:249:ILE:O	1:D:253:VAL:HG23	2.11	0.50
3:I:125:MET:SD	3:I:171:LEU:HD12	2.51	0.50
1:D:212:HIS:O	1:D:215:ALA:HB3	2.11	0.50
1:G:13:THR:CG2	1:G:14:GLY:N	2.75	0.50
1:J:92:MET:CE	2:K:226:ARG:HG3	2.41	0.50
1:J:292:ILE:O	1:J:293:VAL:HG23	2.12	0.50
1:A:366:TYR:CD2	1:A:411:LEU:HD11	2.47	0.50
2:H:42:MET:HE1	2:H:218:ALA:CB	2.36	0.50
1:A:182:GLY:HA3	1:A:193:ARG:NH2	2.27	0.50
1:D:73:VAL:HG12	1:D:151:TRP:CE2	2.46	0.50
2:H:30:GLN:HG2	2:H:34:GLU:OE2	2.12	0.50
2:H:165:VAL:HG12	2:H:169:CYS:HB2	1.93	0.50
2:K:42:MET:HE1	2:K:218:ALA:CB	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HH12	2:B:255:VAL:HG12	1.76	0.50
2:E:74:ASP:HB3	2:E:77:THR:HB	1.94	0.50
2:E:250:ARG:CD	3:F:12:ARG:HG3	2.42	0.50
1:J:39:ARG:HH12	2:K:255:VAL:HG12	1.77	0.50
2:K:42:MET:HE2	2:K:101:SER:HA	1.94	0.50
2:K:183:ILE:HG12	2:K:185:MET:H	1.76	0.50
3:L:90:LEU:O	3:L:90:LEU:CG	2.59	0.50
1:D:13:THR:CG2	1:D:14:GLY:N	2.74	0.50
1:D:418:VAL:CG1	1:D:419:ALA:N	2.75	0.50
1:J:83:ILE:O	1:J:90:GLY:HA3	2.12	0.50
1:J:158:GLY:O	1:J:162:ILE:HG13	2.12	0.50
1:J:359:TYR:CD2	1:J:420:PRO:HB3	2.47	0.50
3:L:89:GLN:C	3:L:91:GLY:N	2.65	0.50
1:A:102:SER:O	1:A:106:ILE:HG13	2.11	0.50
1:J:182:GLY:HA3	1:J:193:ARG:NH2	2.26	0.50
1:D:53:PHE:CE2	1:D:260:LEU:HD21	2.47	0.50
2:E:30:GLN:HG2	2:E:34:GLU:OE2	2.12	0.50
1:G:44:MET:CE	7:G:504:LOP:H92	2.42	0.50
2:H:67:ALA:O	2:H:83:GLY:HA3	2.10	0.50
1:J:212:HIS:O	1:J:215:ALA:HB3	2.12	0.49
1:A:234:LYS:O	1:A:238:GLN:HG3	2.12	0.49
1:G:75:LEU:O	1:G:79:SER:HB3	2.12	0.49
1:J:53:PHE:CE2	1:J:260:LEU:HD21	2.47	0.49
2:K:30:GLN:HG2	2:K:34:GLU:OE2	2.12	0.49
1:A:114:ARG:C	1:A:114:ARG:HD2	2.33	0.49
1:A:346:VAL:CG1	1:A:347:PRO:HD3	2.42	0.49
2:E:143:PRO:HG3	2:E:178:THR:CG2	2.41	0.49
1:G:4:ILE:HD12	1:G:4:ILE:N	2.27	0.49
1:A:75:LEU:O	1:A:79:SER:HB3	2.12	0.49
1:A:212:HIS:O	1:A:215:ALA:HB3	2.11	0.49
1:D:342:VAL:HG13	1:D:404:PHE:CB	2.43	0.49
2:H:26:GLN:HG3	2:H:58:LEU:HD21	1.95	0.49
2:K:138:PHE:HD2	2:K:187:PRO:HG3	1.73	0.49
1:A:128:THR:HG21	5:A:501:HEM:HBD1	1.93	0.49
2:B:26:GLN:HG3	2:B:58:LEU:HD21	1.94	0.49
2:B:30:GLN:HG2	2:B:34:GLU:OE2	2.12	0.49
2:B:165:VAL:HG12	2:B:169:CYS:HB2	1.95	0.49
1:D:59:ILE:O	1:D:63:ILE:HG13	2.13	0.49
1:D:239:LYS:HE2	1:D:425:GLU:OE2	2.12	0.49
2:H:112:GLY:O	2:H:119:SER:HB3	2.13	0.49
1:A:313:TRP:HA	1:A:316:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:GLN:HG3	2:E:58:LEU:HD21	1.95	0.49
1:G:83:ILE:O	1:G:90:GLY:HA3	2.13	0.49
1:A:42:ASN:OD1	1:A:44:MET:HB2	2.12	0.49
2:B:183:ILE:HG13	5:B:301:HEM:O2D	2.13	0.49
1:G:53:PHE:CE2	1:G:260:LEU:HD21	2.47	0.49
1:G:182:GLY:HA3	1:G:193:ARG:NH2	2.27	0.49
2:H:27:ARG:HD2	2:H:196:TYR:CE2	2.48	0.49
2:H:94:LEU:HD22	5:H:301:HEM:HAC	1.95	0.49
2:K:26:GLN:HG3	2:K:58:LEU:HD21	1.95	0.49
1:A:127:VAL:N	11:A:515:HOH:O	2.43	0.49
2:E:42:MET:HE2	2:E:101:SER:HA	1.95	0.49
1:G:144:PHE:CD1	1:G:162:ILE:HD12	2.47	0.49
1:A:6:HIS:C	1:A:6:HIS:CD2	2.84	0.49
1:A:58:GLN:CB	5:A:502:HEM:HAB	2.42	0.49
3:C:89:GLN:O	3:C:92:GLN:N	2.23	0.49
2:E:149:HIS:NE2	2:E:168:THR:HG21	2.27	0.49
1:J:9:TYR:N	1:J:30:TYR:CE2	2.81	0.49
1:J:92:MET:HE3	2:K:226:ARG:HG3	1.95	0.49
1:A:112:ILE:HG12	5:A:501:HEM:HAC	1.94	0.49
1:D:114:ARG:HD2	1:D:114:ARG:C	2.34	0.49
3:I:71:PRO:HG3	3:I:135:VAL:CG2	2.43	0.49
3:L:162:ILE:HD13	3:L:167:ALA:HB3	1.95	0.49
1:D:292:ILE:O	1:D:293:VAL:HG23	2.12	0.48
3:I:96:THR:O	3:I:109:ALA:N	2.37	0.48
1:J:39:ARG:NH1	2:K:255:VAL:HG12	2.27	0.48
2:E:59:PRO:HD2	2:E:62:GLN:HE21	1.75	0.48
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.26	0.48
1:J:122:LYS:NZ	1:J:352:SER:O	2.46	0.48
2:K:72:VAL:CG1	2:K:73:THR:H	2.26	0.48
1:J:13:THR:CG2	1:J:14:GLY:H	2.25	0.48
2:K:112:GLY:O	2:K:119:SER:HB3	2.14	0.48
2:B:116:THR:HG22	2:B:118:ILE:HG13	1.95	0.48
2:B:42:MET:HE2	2:B:101:SER:HA	1.94	0.48
1:D:376:ILE:O	1:D:380:VAL:HG22	2.14	0.48
1:G:114:ARG:HD2	1:G:114:ARG:C	2.33	0.48
1:J:342:VAL:HG13	1:J:404:PHE:CB	2.43	0.48
1:J:383:GLN:HE22	2:K:115:GLY:HA3	1.78	0.48
1:A:292:ILE:O	1:A:293:VAL:HG23	2.14	0.48
1:A:342:VAL:HG13	1:A:404:PHE:CB	2.44	0.48
1:G:292:ILE:O	1:G:293:VAL:HG23	2.14	0.48
1:J:114:ARG:HD2	1:J:114:ARG:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TRP:O	1:A:46:ILE:HG13	2.14	0.48
5:D:502:HEM:HHD	5:D:502:HEM:CBC	2.42	0.48
2:E:77:THR:C	2:E:79:GLU:N	2.67	0.48
2:E:143:PRO:HD3	2:E:156:TYR:CD2	2.48	0.48
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.96	0.48
2:E:112:GLY:O	2:E:119:SER:HB3	2.14	0.48
3:F:156:TYR:HA	3:F:161:ARG:O	2.14	0.48
1:G:121:TYR:HB3	1:G:129:TRP:CE3	2.49	0.48
1:G:295:GLU:OE1	1:G:295:GLU:N	2.47	0.48
2:H:59:PRO:HD2	2:H:62:GLN:HE21	1.76	0.48
1:J:121:TYR:HB3	1:J:129:TRP:CE3	2.49	0.48
1:J:194:PHE:CE1	6:J:503:SMA:H28	2.49	0.48
1:A:53:PHE:CE2	1:A:260:LEU:HD21	2.48	0.48
2:B:194:VAL:HB	2:B:207:MET:HE3	1.95	0.48
3:C:96:THR:O	3:C:109:ALA:N	2.36	0.48
2:H:199:GLY:O	2:H:200:HIS:O	2.32	0.48
1:J:13:THR:CG2	1:J:14:GLY:N	2.75	0.48
2:B:112:GLY:O	2:B:119:SER:HB3	2.13	0.48
3:C:86:ARG:HG2	3:C:112:GLN:OE1	2.14	0.48
2:E:116:THR:HG22	2:E:118:ILE:HG13	1.96	0.48
1:G:45:TRP:CZ3	1:G:224:PRO:HG3	2.49	0.48
1:G:92:MET:CE	2:H:226:ARG:HG3	2.44	0.48
2:H:223:LEU:CD2	2:H:227:LYS:HD2	2.43	0.48
1:J:105:PHE:HA	1:J:108:VAL:CG2	2.44	0.48
1:A:13:THR:CG2	1:A:14:GLY:N	2.74	0.47
1:A:83:ILE:O	1:A:90:GLY:HA3	2.14	0.47
1:G:13:THR:CG2	1:G:14:GLY:H	2.25	0.47
1:G:272:ASN:ND2	2:H:105:LYS:HD2	2.28	0.47
1:G:346:VAL:CG1	1:G:347:PRO:HD3	2.43	0.47
2:K:194:VAL:HB	2:K:207:MET:HE3	1.95	0.47
1:A:13:THR:CG2	1:A:14:GLY:H	2.25	0.47
1:A:45:TRP:CZ3	1:A:224:PRO:HG3	2.48	0.47
2:B:42:MET:HE1	2:B:218:ALA:CB	2.39	0.47
1:D:51:LEU:HD13	5:D:501:HEM:C3B	2.48	0.47
3:F:143:ASP:HB2	3:F:144:PHE:CE1	2.49	0.47
1:G:209:VAL:CG2	5:G:501:HEM:HBB2	2.44	0.47
2:H:116:THR:HG22	2:H:118:ILE:HG13	1.95	0.47
2:H:119:SER:O	2:H:123:ASN:HB2	2.15	0.47
1:J:45:TRP:CZ3	1:J:224:PRO:HG3	2.49	0.47
1:J:376:ILE:O	1:J:380:VAL:HG22	2.14	0.47
2:B:119:SER:O	2:B:123:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:ILE:HD13	3:C:167:ALA:HB3	1.96	0.47
2:E:67:ALA:O	2:E:83:GLY:HA3	2.15	0.47
1:J:8:HIS:CD2	1:J:8:HIS:N	2.66	0.47
1:A:422:ALA:HB3	1:A:426:GLU:OE1	2.13	0.47
2:K:138:PHE:CE1	2:K:157:ASN:ND2	2.82	0.47
1:J:346:VAL:CG1	1:J:347:PRO:HD3	2.45	0.47
2:K:199:GLY:O	2:K:200:HIS:O	2.32	0.47
1:G:418:VAL:HG12	1:G:419:ALA:N	2.30	0.47
2:H:199:GLY:O	2:H:200:HIS:C	2.53	0.47
3:I:162:ILE:HD13	3:I:167:ALA:HB3	1.96	0.47
1:A:46:ILE:HD12	1:A:46:ILE:C	2.35	0.47
1:A:67:MET:HG2	1:D:193:ARG:HA	1.96	0.47
2:B:6:VAL:HG11	2:B:130:TYR:HA	1.97	0.47
2:B:77:THR:HG22	2:B:79:GLU:CB	2.44	0.47
3:C:44:VAL:C	3:C:46:ALA:H	2.18	0.47
3:C:177:LYS:HE2	3:C:185:GLN:NE2	2.28	0.47
1:D:91:PHE:HE2	1:D:92:MET:CE	2.26	0.47
5:D:501:HEM:CMA	8:D:504:ANJ:O7	2.62	0.47
2:E:119:SER:O	2:E:123:ASN:HB2	2.15	0.47
2:E:136:THR:O	2:E:138:PHE:N	2.43	0.47
2:E:199:GLY:O	2:E:200:HIS:O	2.32	0.47
3:F:92:GLN:HG2	11:F:207:HOH:O	2.14	0.47
1:G:8:HIS:N	1:G:8:HIS:CD2	2.80	0.47
1:G:112:ILE:HG12	5:G:501:HEM:HAC	1.97	0.47
1:G:376:ILE:O	1:G:380:VAL:HG22	2.14	0.47
2:H:160:PHE:CE2	2:H:183:ILE:HG13	2.49	0.47
3:I:156:TYR:HA	3:I:161:ARG:O	2.14	0.47
1:J:44:MET:CE	7:J:504:LOP:H92	2.45	0.47
2:K:72:VAL:CG1	2:K:73:THR:N	2.77	0.47
2:K:77:THR:C	2:K:79:GLU:N	2.67	0.47
2:K:113:PRO:O	2:K:114:MET:HB2	2.14	0.47
2:K:116:THR:HG22	2:K:118:ILE:HG13	1.95	0.47
1:G:406:VAL:O	1:G:409:PRO:HD2	2.15	0.47
2:H:113:PRO:O	2:H:114:MET:HB2	2.15	0.47
1:D:91:PHE:CE2	1:D:92:MET:HE2	2.49	0.47
2:E:48:ARG:HB3	2:E:85:PRO:O	2.15	0.47
1:D:121:TYR:HB3	1:D:129:TRP:CE3	2.49	0.47
1:D:313:TRP:CD1	1:D:313:TRP:N	2.82	0.47
3:F:128:VAL:O	3:F:129:CYS:C	2.54	0.47
1:J:39:ARG:NH1	2:K:255:VAL:CG1	2.78	0.47
1:J:91:PHE:CE2	1:J:92:MET:HE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:67:ALA:O	2:K:83:GLY:HA3	2.15	0.47
3:C:179:ILE:O	3:C:180:ASP:HB3	2.15	0.46
1:D:39:ARG:HD3	1:D:428:PHE:HD2	1.80	0.46
1:D:91:PHE:CE2	1:D:92:MET:CE	2.98	0.46
1:D:202:PRO:HG2	5:D:502:HEM:HMC3	1.97	0.46
1:D:346:VAL:CG1	1:D:347:PRO:HD3	2.45	0.46
3:I:164:LYS:HG3	11:J:524:HOH:O	2.14	0.46
1:J:59:ILE:O	1:J:63:ILE:HG13	2.15	0.46
3:L:156:TYR:HA	3:L:161:ARG:O	2.15	0.46
3:L:163:ARG:O	3:L:164:LYS:HB2	2.15	0.46
3:C:156:TYR:HA	3:C:161:ARG:O	2.15	0.46
2:E:77:THR:CG2	2:E:79:GLU:HB2	2.45	0.46
2:E:120:GLN:C	2:E:122:PHE:N	2.69	0.46
3:F:54:VAL:HG13	3:F:57:VAL:HG21	1.97	0.46
3:F:179:ILE:O	3:F:180:ASP:HB3	2.16	0.46
2:H:81:ARG:HG3	2:H:81:ARG:NH1	2.30	0.46
3:L:110:THR:O	3:L:113:ASN:N	2.47	0.46
2:B:43:LYS:HD2	2:B:44:PHE:CE2	2.50	0.46
2:B:66:TYR:CE1	2:B:69:GLN:NE2	2.83	0.46
1:D:405:LEU:O	1:D:409:PRO:HG2	2.15	0.46
2:E:154:PHE:HB3	2:E:182:TRP:HB3	1.98	0.46
1:G:122:LYS:NZ	1:G:354:VAL:O	2.45	0.46
2:H:165:VAL:HG21	2:H:176:LYS:CD	2.46	0.46
3:I:118:GLU:C	3:I:120:GLY:N	2.69	0.46
2:K:6:VAL:HG11	2:K:130:TYR:HA	1.98	0.46
3:L:50:ILE:HD11	3:L:186:LEU:HD12	1.98	0.46
2:B:199:GLY:O	2:B:200:HIS:O	2.33	0.46
1:D:13:THR:CG2	1:D:14:GLY:H	2.25	0.46
2:E:81:ARG:HG3	2:E:81:ARG:HH11	1.80	0.46
1:G:342:VAL:HG13	1:G:404:PHE:CB	2.45	0.46
2:H:42:MET:HE2	2:H:101:SER:HA	1.96	0.46
3:I:54:VAL:HG13	3:I:57:VAL:HG21	1.97	0.46
3:I:128:VAL:O	3:I:129:CYS:C	2.54	0.46
1:J:236:GLU:O	1:J:239:LYS:HB2	2.15	0.46
3:L:118:GLU:C	3:L:120:GLY:H	2.18	0.46
1:A:376:ILE:O	1:A:380:VAL:HG22	2.16	0.46
2:B:120:GLN:C	2:B:122:PHE:N	2.69	0.46
2:E:250:ARG:HH22	3:F:11:ARG:HD3	1.80	0.46
3:F:162:ILE:HD13	3:F:167:ALA:HB3	1.96	0.46
1:A:122:LYS:O	1:A:123:ALA:C	2.52	0.46
3:C:157:ASP:C	3:C:159:ALA:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:77:THR:HG22	2:E:79:GLU:CB	2.46	0.46
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.50	0.46
1:D:346:VAL:HG12	1:D:347:PRO:HD3	1.98	0.46
1:G:346:VAL:HG12	1:G:347:PRO:HD3	1.97	0.46
1:G:360:ARG:O	1:G:364:LYS:HG3	2.15	0.46
2:H:6:VAL:HG11	2:H:130:TYR:HA	1.97	0.46
3:I:11:ARG:CB	3:I:11:ARG:HH11	2.29	0.46
3:L:118:GLU:C	3:L:120:GLY:N	2.68	0.46
3:L:157:ASP:HB2	11:L:210:HOH:O	2.15	0.46
1:A:245:TRP:CE3	1:A:246:PRO:HA	2.51	0.46
1:D:9:TYR:CE1	1:D:11:PRO:HG3	2.50	0.46
1:D:273:TYR:CE2	2:E:121:LEU:HD13	2.51	0.46
3:F:96:THR:O	3:F:109:ALA:N	2.36	0.46
1:J:46:ILE:HD12	1:J:46:ILE:C	2.36	0.46
3:C:11:ARG:CB	3:C:11:ARG:HH11	2.28	0.46
1:D:213:ILE:HD12	8:D:504:ANJ:O9	2.16	0.46
2:E:231:PHE:HD1	2:E:231:PHE:O	1.98	0.46
1:G:46:ILE:C	1:G:46:ILE:HD12	2.37	0.46
1:G:156:PHE:CE1	1:G:186:VAL:HG12	2.51	0.46
2:H:149:HIS:CD2	2:H:168:THR:OG1	2.69	0.46
2:K:119:SER:O	2:K:123:ASN:HB2	2.15	0.46
2:K:199:GLY:O	2:K:200:HIS:C	2.54	0.46
3:L:11:ARG:HH11	3:L:11:ARG:CB	2.29	0.46
3:L:179:ILE:O	3:L:180:ASP:HB3	2.16	0.46
3:C:94:VAL:HG23	3:C:162:ILE:O	2.15	0.46
2:E:138:PHE:CD2	2:E:187:PRO:HA	2.51	0.46
2:E:184:ALA:HB3	5:E:301:HEM:CBD	2.44	0.46
1:G:245:TRP:CE3	1:G:246:PRO:HA	2.51	0.46
3:C:146:GLY:HA3	3:C:156:TYR:O	2.15	0.45
1:D:291:HIS:O	1:D:293:VAL:HG23	2.17	0.45
3:F:50:ILE:HD11	3:F:186:LEU:HD12	1.98	0.45
3:F:112:GLN:H	3:F:112:GLN:CD	2.20	0.45
3:L:155:HIS:CD2	3:L:164:LYS:HD3	2.51	0.45
1:D:102:SER:O	1:D:106:ILE:HG13	2.17	0.45
3:F:163:ARG:O	3:F:164:LYS:HB2	2.16	0.45
2:H:86:THR:HG21	3:I:46:ALA:HB1	1.98	0.45
3:I:157:ASP:C	3:I:159:ALA:H	2.19	0.45
1:J:156:PHE:O	1:J:159:ALA:HB3	2.16	0.45
2:K:149:HIS:CD2	2:K:149:HIS:N	2.85	0.45
2:K:165:VAL:HG12	2:K:169:CYS:HB2	1.98	0.45
3:L:144:PHE:N	3:L:144:PHE:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:CG2	8:A:504:ANJ:H1	2.44	0.45
2:B:226:ARG:NH2	11:B:308:HOH:O	2.49	0.45
3:C:54:VAL:HG13	3:C:57:VAL:HG21	1.97	0.45
2:E:6:VAL:HG11	2:E:130:TYR:HA	1.98	0.45
3:F:107:ALA:HB1	3:F:113:ASN:HD21	1.81	0.45
1:A:265:ALA:HB1	4:A:431:BGL:H5'2	1.98	0.45
1:A:291:HIS:O	1:A:293:VAL:HG23	2.16	0.45
2:B:48:ARG:HB3	2:B:85:PRO:O	2.16	0.45
2:B:67:ALA:O	2:B:83:GLY:HA3	2.17	0.45
1:D:144:PHE:CE1	1:D:162:ILE:HD12	2.51	0.45
3:F:11:ARG:CB	3:F:11:ARG:HH11	2.29	0.45
3:F:157:ASP:C	3:F:159:ALA:H	2.20	0.45
2:H:48:ARG:HB3	2:H:85:PRO:O	2.16	0.45
2:H:155:TYR:N	2:H:155:TYR:CD1	2.85	0.45
3:I:93:LEU:HD12	3:I:109:ALA:HB3	1.98	0.45
1:D:245:TRP:CE3	1:D:246:PRO:HA	2.51	0.45
1:D:351:THR:OG1	1:D:412:GLY:HA3	2.16	0.45
2:H:194:VAL:HB	2:H:207:MET:HE3	1.98	0.45
2:K:48:ARG:HB3	2:K:85:PRO:O	2.16	0.45
1:D:46:ILE:C	1:D:46:ILE:HD12	2.37	0.45
3:F:118:GLU:C	3:F:120:GLY:N	2.70	0.45
2:H:236:PHE:CE2	3:I:25:VAL:HG12	2.45	0.45
3:I:144:PHE:CD1	3:I:144:PHE:N	2.85	0.45
3:L:128:VAL:O	3:L:129:CYS:C	2.53	0.45
3:F:83:GLU:O	3:F:84:LEU:C	2.55	0.45
3:F:146:GLY:HA3	3:F:156:TYR:O	2.16	0.45
2:K:86:THR:HG22	3:L:46:ALA:CB	2.46	0.45
3:L:96:THR:O	3:L:109:ALA:N	2.37	0.45
2:B:143:PRO:HD3	2:B:156:TYR:CD2	2.52	0.45
2:E:74:ASP:CB	2:E:77:THR:HB	2.47	0.45
2:E:149:HIS:ND1	2:E:168:THR:HG21	2.31	0.45
3:F:44:VAL:C	3:F:46:ALA:H	2.20	0.45
3:F:108:GLU:O	3:F:110:THR:N	2.44	0.45
2:H:49:SER:HA	2:H:52:GLU:OE1	2.17	0.45
2:B:199:GLY:O	2:B:200:HIS:C	2.55	0.45
3:C:50:ILE:HD11	3:C:186:LEU:HD12	1.98	0.45
1:G:291:HIS:O	1:G:293:VAL:HG23	2.17	0.45
3:I:50:ILE:HD11	3:I:186:LEU:HD12	1.97	0.45
2:K:120:GLN:C	2:K:122:PHE:N	2.69	0.45
1:A:4:ILE:H	1:A:4:ILE:CD1	2.16	0.45
1:A:63:ILE:HD13	1:D:200:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ILE:O	1:D:321:ILE:HG22	2.17	0.45
1:G:156:PHE:O	1:G:159:ALA:HB3	2.17	0.45
1:G:406:VAL:C	1:G:409:PRO:HD2	2.38	0.45
1:A:156:PHE:CE1	1:A:186:VAL:HG12	2.52	0.44
1:D:9:TYR:HB2	1:D:30:TYR:CG	2.52	0.44
2:E:77:THR:HG22	2:E:79:GLU:CG	2.47	0.44
2:E:175:VAL:HG12	2:E:176:LYS:N	2.32	0.44
2:H:170:LYS:HA	2:H:176:LYS:HA	1.99	0.44
3:L:157:ASP:C	3:L:159:ALA:H	2.19	0.44
2:B:155:TYR:N	2:B:155:TYR:CD1	2.85	0.44
2:E:250:ARG:HH12	3:F:11:ARG:CD	2.30	0.44
1:J:346:VAL:HG12	1:J:347:PRO:HD3	1.99	0.44
2:K:86:THR:CG2	3:L:46:ALA:HB1	2.45	0.44
2:B:27:ARG:HD2	2:B:196:TYR:CZ	2.52	0.44
3:C:128:VAL:O	3:C:129:CYS:C	2.54	0.44
1:D:292:ILE:O	1:D:293:VAL:CG2	2.65	0.44
2:H:120:GLN:C	2:H:122:PHE:H	2.20	0.44
3:L:54:VAL:HG13	3:L:57:VAL:HG21	1.98	0.44
3:I:71:PRO:HG3	3:I:135:VAL:HG21	1.99	0.44
1:J:156:PHE:CE1	1:J:186:VAL:HG12	2.53	0.44
3:C:112:GLN:H	3:C:112:GLN:HE21	1.61	0.44
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.48	0.44
2:H:8:ASP:OD1	2:H:110:PHE:HZ	2.01	0.44
3:I:179:ILE:O	3:I:180:ASP:HB3	2.16	0.44
1:A:236:GLU:HA	1:A:239:LYS:CD	2.47	0.44
1:A:39:ARG:HG2	1:A:242:VAL:CG1	2.45	0.44
2:K:59:PRO:CD	2:K:62:GLN:NE2	2.80	0.44
1:A:156:PHE:O	1:A:159:ALA:HB3	2.18	0.44
1:D:376:ILE:O	1:D:380:VAL:CG2	2.66	0.44
2:E:155:TYR:CD1	2:E:155:TYR:N	2.86	0.44
1:J:201:LEU:HD23	1:J:201:LEU:HA	1.76	0.44
1:J:245:TRP:CE3	1:J:246:PRO:HA	2.51	0.44
1:J:292:ILE:O	1:J:293:VAL:CG2	2.66	0.44
1:D:51:LEU:HB3	5:D:501:HEM:HMB1	2.00	0.44
1:G:312:VAL:O	1:G:316:GLN:HG3	2.18	0.44
2:H:73:THR:HG23	2:H:78:GLY:O	2.18	0.44
2:H:154:PHE:C	2:H:155:TYR:CD1	2.92	0.44
1:J:262:VAL:O	1:J:266:ILE:HG12	2.18	0.44
1:J:405:LEU:O	1:J:409:PRO:HG2	2.18	0.44
1:A:387:PHE:CZ	1:A:388:PRO:HB3	2.53	0.43
1:A:418:VAL:CG1	1:A:419:ALA:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:GLN:C	2:B:122:PHE:H	2.21	0.43
2:B:154:PHE:C	2:B:155:TYR:CD1	2.91	0.43
3:I:112:GLN:NE2	3:I:112:GLN:N	2.60	0.43
3:L:109:ALA:O	3:L:161:ARG:NH1	2.44	0.43
3:L:117:ASP:OD2	3:L:121:GLU:HB3	2.17	0.43
1:A:41:LEU:HD22	1:A:45:TRP:CD1	2.53	0.43
3:C:134:CYS:HB2	3:C:149:CYS:SG	2.59	0.43
1:D:112:ILE:HG12	5:D:501:HEM:HAC	2.00	0.43
1:D:406:VAL:O	1:D:409:PRO:HD2	2.18	0.43
1:G:209:VAL:HG22	5:G:501:HEM:HBB2	2.00	0.43
1:A:52:ALA:HB2	8:A:504:ANJ:H161	1.98	0.43
2:B:48:ARG:HG3	2:B:48:ARG:HH11	1.82	0.43
1:G:377:LEU:HA	1:G:380:VAL:HG23	2.01	0.43
1:G:418:VAL:CG1	1:G:419:ALA:N	2.81	0.43
3:L:134:CYS:HB2	3:L:149:CYS:SG	2.58	0.43
1:A:9:TYR:HB2	1:A:30:TYR:CD2	2.52	0.43
3:C:44:VAL:O	3:C:46:ALA:N	2.52	0.43
2:E:170:LYS:HA	2:E:175:VAL:O	2.17	0.43
2:H:76:GLU:O	2:H:77:THR:C	2.55	0.43
3:I:177:LYS:HE3	3:I:179:ILE:CD1	2.49	0.43
1:J:13:THR:O	1:J:17:LYS:HG3	2.18	0.43
2:K:120:GLN:C	2:K:122:PHE:H	2.20	0.43
2:K:155:TYR:CD1	2:K:155:TYR:N	2.86	0.43
3:L:146:GLY:HA3	3:L:156:TYR:O	2.17	0.43
2:B:86:THR:HG22	3:C:46:ALA:HB1	2.00	0.43
2:E:154:PHE:C	2:E:155:TYR:CD1	2.92	0.43
3:F:118:GLU:C	3:F:120:GLY:H	2.20	0.43
3:F:134:CYS:HB2	3:F:149:CYS:SG	2.59	0.43
3:F:157:ASP:OD2	3:F:161:ARG:HB2	2.19	0.43
2:H:120:GLN:C	2:H:122:PHE:N	2.69	0.43
2:H:165:VAL:HG21	2:H:176:LYS:HD3	1.99	0.43
3:I:118:GLU:CD	3:I:118:GLU:N	2.71	0.43
2:K:71:THR:HG22	2:K:71:THR:O	2.18	0.43
1:A:37:THR:HG22	1:A:41:LEU:HD11	1.99	0.43
1:A:153:GLN:HA	1:A:153:GLN:OE1	2.19	0.43
1:A:193:ARG:HA	1:D:67:MET:HG2	2.00	0.43
3:L:138:GLY:HA2	3:L:147:TRP:CD1	2.54	0.43
1:A:403:TYR:O	1:A:408:LEU:HG	2.18	0.43
2:B:81:ARG:NH1	2:B:84:LYS:HG3	2.34	0.43
2:B:194:VAL:HG12	2:B:194:VAL:O	2.19	0.43
3:C:157:ASP:OD2	3:C:161:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:LEU:HA	1:D:201:LEU:HD23	1.76	0.43
2:E:73:THR:HA	2:E:79:GLU:O	2.18	0.43
2:E:197:ALA:C	2:E:199:GLY:H	2.22	0.43
3:I:118:GLU:C	3:I:120:GLY:H	2.20	0.43
3:I:157:ASP:OD2	3:I:161:ARG:HB2	2.19	0.43
1:J:213:ILE:HA	1:J:216:PHE:CE2	2.54	0.43
1:A:39:ARG:HD3	1:A:428:PHE:CD2	2.54	0.43
2:B:66:TYR:O	2:B:69:GLN:HG2	2.18	0.43
3:C:59:PRO:HA	3:C:76:ARG:HB3	2.00	0.43
2:E:48:ARG:HG3	2:E:48:ARG:HH11	1.84	0.43
2:E:250:ARG:HD2	3:F:12:ARG:HG3	2.00	0.43
3:F:117:ASP:OD2	3:F:121:GLU:HB2	2.18	0.43
1:G:262:VAL:O	1:G:266:ILE:HG12	2.19	0.43
1:J:376:ILE:O	1:J:380:VAL:CG2	2.66	0.43
2:K:154:PHE:C	2:K:155:TYR:CD1	2.92	0.43
3:L:157:ASP:OD2	3:L:161:ARG:HB2	2.19	0.43
2:E:120:GLN:C	2:E:122:PHE:H	2.20	0.43
2:E:199:GLY:O	2:E:200:HIS:C	2.57	0.43
1:G:118:TYR:CD1	1:G:224:PRO:HA	2.54	0.43
2:K:94:LEU:HD22	5:K:301:HEM:HAC	1.99	0.43
2:K:197:ALA:C	2:K:199:GLY:H	2.22	0.43
1:D:66:ALA:HB2	5:D:502:HEM:CBC	2.48	0.43
2:E:36:CYS:N	5:E:301:HEM:HAB	2.33	0.43
2:E:150:GLU:HG2	2:E:182:TRP:HE1	1.83	0.43
2:H:6:VAL:HG21	2:H:109:GLY:HA3	2.00	0.43
3:I:162:ILE:CD1	3:I:167:ALA:HB3	2.49	0.43
3:I:163:ARG:O	3:I:164:LYS:HB2	2.17	0.43
1:J:39:ARG:HG2	1:J:242:VAL:CG1	2.47	0.43
1:J:44:MET:HE3	7:J:504:LOP:H92	2.01	0.43
1:J:92:MET:HE2	1:J:92:MET:CA	2.49	0.43
3:L:54:VAL:HG11	3:L:122:TRP:CZ3	2.54	0.43
1:D:156:PHE:O	1:D:159:ALA:HB3	2.18	0.42
2:E:185:MET:HB2	5:E:301:HEM:C1D	2.53	0.42
3:F:54:VAL:HG12	3:F:54:VAL:O	2.19	0.42
3:F:110:THR:O	3:F:113:ASN:N	2.51	0.42
2:H:81:ARG:NH1	2:H:82:GLU:O	2.52	0.42
3:I:54:VAL:HG11	3:I:122:TRP:CZ3	2.54	0.42
1:J:153:GLN:OE1	1:J:153:GLN:HA	2.19	0.42
2:K:240:LEU:HD13	3:L:22:ALA:HB3	2.01	0.42
2:B:56:PRO:HD2	11:B:304:HOH:O	2.18	0.42
2:B:197:ALA:C	2:B:199:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:MET:HE2	1:D:193:ARG:HH11	1.84	0.42
3:C:118:GLU:C	3:C:120:GLY:H	2.21	0.42
1:D:262:VAL:O	1:D:266:ILE:HG12	2.19	0.42
2:E:49:SER:HA	2:E:52:GLU:CG	2.45	0.42
2:E:94:LEU:HD22	5:E:301:HEM:HAC	2.01	0.42
1:G:247:TYR:HB3	2:H:252:TRP:CZ2	2.55	0.42
1:G:292:ILE:O	1:G:293:VAL:CG2	2.67	0.42
1:G:296:TRP:HA	1:G:299:LEU:HG	2.01	0.42
2:H:146:ALA:O	2:H:147:GLU:C	2.57	0.42
3:I:54:VAL:O	3:I:54:VAL:HG12	2.20	0.42
2:B:146:ALA:O	2:B:147:GLU:C	2.57	0.42
1:D:117:TYR:HB2	1:D:367:PHE:CZ	2.55	0.42
2:E:146:ALA:O	2:E:147:GLU:C	2.58	0.42
1:J:291:HIS:O	1:J:293:VAL:HG23	2.18	0.42
1:A:262:VAL:O	1:A:266:ILE:HG12	2.19	0.42
2:B:114:MET:HG2	2:B:114:MET:O	2.18	0.42
1:D:39:ARG:HH12	2:E:255:VAL:CG1	2.33	0.42
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.88	0.42
2:E:72:VAL:O	2:E:80:ASP:HA	2.19	0.42
1:G:5:PRO:HB2	1:G:234:LYS:CA	2.41	0.42
1:G:43:TRP:O	1:G:46:ILE:HG13	2.19	0.42
1:G:161:VAL:HG11	6:G:503:SMA:O5	2.19	0.42
1:G:214:TRP:CH2	1:J:25:ILE:HA	2.54	0.42
1:G:273:TYR:CE2	2:H:121:LEU:HD13	2.54	0.42
3:I:59:PRO:HA	3:I:76:ARG:HB3	2.01	0.42
1:J:92:MET:HE2	1:J:92:MET:HA	2.01	0.42
3:L:59:PRO:HA	3:L:76:ARG:HB3	2.00	0.42
3:L:108:GLU:O	3:L:110:THR:N	2.44	0.42
3:L:162:ILE:CD1	3:L:167:ALA:HB3	2.49	0.42
1:A:425:GLU:O	1:A:429:ASN:ND2	2.53	0.42
1:D:122:LYS:O	1:D:123:ALA:C	2.58	0.42
2:E:139:PRO:HG3	2:E:158:ARG:CZ	2.48	0.42
2:H:13:PHE:O	2:H:227:LYS:NZ	2.53	0.42
3:I:140:VAL:HG12	3:I:140:VAL:O	2.20	0.42
1:A:120:SER:HB3	5:A:501:HEM:HAD2	2.02	0.42
1:A:292:ILE:O	1:A:293:VAL:CG2	2.68	0.42
3:C:118:GLU:C	3:C:120:GLY:N	2.71	0.42
3:C:162:ILE:CD1	3:C:167:ALA:HB3	2.49	0.42
2:E:165:VAL:HG21	2:E:176:LYS:HD3	2.01	0.42
2:E:232:THR:HG22	2:E:236:PHE:HE1	1.84	0.42
2:H:197:ALA:C	2:H:199:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:CZ	5:A:502:HEM:HBC1	2.55	0.42
2:B:59:PRO:CD	2:B:62:GLN:NE2	2.81	0.42
1:D:4:ILE:HG22	1:D:5:PRO:CD	2.50	0.42
3:F:95:ASP:OD2	3:F:170:ASN:ND2	2.52	0.42
3:F:123:LEU:HG	3:F:125:MET:HE2	2.02	0.42
1:G:6:HIS:ND1	1:G:6:HIS:C	2.72	0.42
1:G:153:GLN:OE1	1:G:153:GLN:HA	2.19	0.42
3:L:54:VAL:HG12	3:L:54:VAL:O	2.19	0.42
1:A:296:TRP:HA	1:A:299:LEU:HG	2.00	0.42
1:A:317:ILE:C	1:A:321:ILE:HG22	2.36	0.42
1:D:27:ALA:O	1:D:30:TYR:HB3	2.20	0.42
2:E:182:TRP:N	2:E:182:TRP:CE3	2.88	0.42
3:F:57:VAL:HG22	3:F:63:LEU:HD13	2.02	0.42
1:G:276:HIS:HA	1:G:277:PRO:HD3	1.91	0.42
2:K:27:ARG:HD2	2:K:196:TYR:CZ	2.54	0.42
1:A:132:GLY:HA3	5:A:501:HEM:HBC2	2.01	0.42
2:B:106:ALA:O	2:B:107:ARG:HD3	2.19	0.42
3:C:54:VAL:HG11	3:C:122:TRP:CZ3	2.54	0.42
1:D:118:TYR:CD1	1:D:224:PRO:HA	2.55	0.42
1:D:234:LYS:O	1:D:238:GLN:HG3	2.19	0.42
1:D:276:HIS:HA	1:D:277:PRO:HD3	1.92	0.42
1:D:416:LYS:HA	1:D:417:PRO:HD2	1.85	0.42
3:F:59:PRO:HA	3:F:76:ARG:HB3	2.01	0.42
1:G:4:ILE:CG2	1:G:237:ALA:HB1	2.50	0.42
1:G:10:GLU:HA	1:G:11:PRO:HD3	1.91	0.42
1:G:37:THR:CG2	1:G:41:LEU:HD11	2.49	0.42
3:I:146:GLY:HA3	3:I:156:TYR:O	2.20	0.42
1:J:377:LEU:HA	1:J:380:VAL:HG23	2.02	0.42
1:A:130:ILE:HD11	1:A:348:TRP:CH2	2.43	0.42
1:D:39:ARG:HG2	1:D:242:VAL:CG1	2.46	0.42
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.55	0.42
2:E:20:PHE:CB	2:E:25:LEU:HD11	2.49	0.42
3:F:54:VAL:HG11	3:F:122:TRP:CZ3	2.54	0.42
1:G:8:HIS:O	1:G:30:TYR:CE2	2.72	0.42
1:G:213:ILE:HA	1:G:216:PHE:CE2	2.55	0.42
2:H:59:PRO:CD	2:H:62:GLN:NE2	2.81	0.42
2:H:154:PHE:HB3	2:H:182:TRP:HB3	2.01	0.42
2:H:170:LYS:HA	2:H:175:VAL:O	2.19	0.42
1:J:362:MET:HE3	1:J:415:GLU:HA	2.00	0.42
1:J:408:LEU:HB2	1:J:409:PRO:HD3	2.01	0.42
1:A:92:MET:HA	1:A:92:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:NH1	3:F:38:MET:HB3	2.35	0.41
2:B:77:THR:O	2:B:79:GLU:N	2.53	0.41
1:G:11:PRO:HG2	1:G:20:HIS:CG	2.55	0.41
2:H:20:PHE:CB	2:H:25:LEU:HD11	2.50	0.41
1:J:118:TYR:CD1	1:J:224:PRO:HA	2.54	0.41
2:K:167:ASP:HA	2:K:170:LYS:HE3	2.02	0.41
1:A:150:PRO:HG3	5:A:502:HEM:O2D	2.19	0.41
3:C:110:THR:OG1	3:C:113:ASN:HB2	2.20	0.41
1:D:39:ARG:NH1	2:E:255:VAL:HG12	2.35	0.41
2:E:231:PHE:HE1	2:E:235:MET:CE	2.33	0.41
1:G:200:LEU:HD22	1:J:63:ILE:HD13	2.02	0.41
1:G:321:ILE:O	1:G:321:ILE:HG22	2.18	0.41
1:G:376:ILE:O	1:G:380:VAL:CG2	2.68	0.41
3:I:47:LEU:HG	3:I:68:LEU:HD21	2.02	0.41
1:J:93:LEU:HD23	1:J:93:LEU:HA	1.87	0.41
2:K:20:PHE:CB	2:K:25:LEU:HD11	2.49	0.41
1:A:118:TYR:CD1	1:A:224:PRO:HA	2.55	0.41
1:A:122:LYS:NZ	1:A:352:SER:O	2.53	0.41
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.55	0.41
1:A:239:LYS:HE2	1:A:425:GLU:CD	2.40	0.41
1:A:410:ILE:HG22	1:A:414:ILE:HD12	2.01	0.41
1:D:3:GLY:N	1:D:4:ILE:HD12	2.35	0.41
1:D:4:ILE:HG22	1:D:5:PRO:HD2	2.02	0.41
2:E:59:PRO:CD	2:E:62:GLN:NE2	2.80	0.41
1:G:122:LYS:HE2	1:G:350:ASP:CG	2.41	0.41
2:H:77:THR:O	2:H:79:GLU:N	2.50	0.41
1:J:117:TYR:HB2	1:J:367:PHE:CZ	2.55	0.41
1:J:317:ILE:C	1:J:321:ILE:HG22	2.36	0.41
2:K:252:TRP:O	2:K:255:VAL:HG23	2.20	0.41
3:L:93:LEU:HD13	3:L:109:ALA:HB3	2.01	0.41
1:A:376:ILE:O	1:A:380:VAL:CG2	2.69	0.41
2:B:43:LYS:HD2	2:B:44:PHE:CZ	2.56	0.41
1:D:153:GLN:OE1	1:D:153:GLN:HA	2.19	0.41
1:D:236:GLU:HA	1:D:239:LYS:HD3	2.02	0.41
3:I:134:CYS:HB2	3:I:149:CYS:SG	2.60	0.41
2:K:146:ALA:O	2:K:147:GLU:C	2.58	0.41
1:A:11:PRO:O	1:A:17:LYS:NZ	2.54	0.41
6:A:1:SMA:H4	3:F:151:CYS:HB3	2.02	0.41
2:B:231:PHE:CD1	2:B:231:PHE:C	2.93	0.41
1:D:323:PHE:CD1	1:D:323:PHE:N	2.88	0.41
1:D:366:TYR:HD2	1:D:411:LEU:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:162:ILE:CD1	3:F:167:ALA:HB3	2.50	0.41
1:J:73:VAL:HG12	1:J:151:TRP:CE2	2.56	0.41
1:A:405:LEU:O	1:A:409:PRO:HG2	2.21	0.41
3:C:54:VAL:HG12	3:C:54:VAL:O	2.19	0.41
1:D:156:PHE:CE1	1:D:186:VAL:HG12	2.54	0.41
2:H:48:ARG:HG3	2:H:48:ARG:HH11	1.85	0.41
1:A:233:SER:OG	1:A:236:GLU:HG2	2.21	0.41
1:D:296:TRP:HA	1:D:299:LEU:HG	2.02	0.41
1:G:117:TYR:HB2	1:G:367:PHE:CZ	2.56	0.41
2:H:42:MET:CE	2:H:218:ALA:CB	2.97	0.41
2:K:126:GLY:HA2	2:K:129:GLU:OE1	2.21	0.41
2:B:139:PRO:HG3	2:B:156:TYR:HD2	1.86	0.41
2:B:184:ALA:HB3	5:B:301:HEM:HBD2	2.01	0.41
3:C:57:VAL:HG22	3:C:63:LEU:HD13	2.03	0.41
1:D:39:ARG:NH1	2:E:255:VAL:CG1	2.84	0.41
3:I:57:VAL:HG22	3:I:63:LEU:HD13	2.02	0.41
3:I:95:ASP:OD2	3:I:170:ASN:ND2	2.54	0.41
1:J:236:GLU:HA	1:J:239:LYS:HG3	2.03	0.41
2:B:252:TRP:O	2:B:255:VAL:HG23	2.21	0.41
1:D:321:ILE:O	1:D:321:ILE:CG2	2.69	0.41
1:D:406:VAL:C	1:D:409:PRO:HD2	2.41	0.41
2:E:20:PHE:CZ	2:E:217:TRP:HA	2.56	0.41
3:F:83:GLU:OE2	3:F:87:SER:HB3	2.21	0.41
1:G:291:HIS:HE1	2:H:2:GLY:N	2.19	0.41
1:G:323:PHE:N	1:G:323:PHE:CD1	2.89	0.41
1:G:359:TYR:CD2	1:G:420:PRO:HB3	2.56	0.41
1:G:403:TYR:CE2	1:G:408:LEU:HD11	2.55	0.41
2:H:194:VAL:HB	2:H:207:MET:HE2	2.03	0.41
3:I:110:THR:OG1	3:I:113:ASN:HB2	2.20	0.41
2:K:26:GLN:NE2	2:K:56:PRO:O	2.54	0.41
1:A:27:ALA:O	1:A:30:TYR:HB3	2.21	0.41
1:D:41:LEU:CD1	8:D:504:ANJ:H3	2.51	0.41
1:D:233:SER:OG	1:D:236:GLU:HG2	2.20	0.41
2:E:109:GLY:N	2:E:125:ILE:O	2.52	0.41
2:H:252:TRP:O	2:H:255:VAL:HG23	2.21	0.41
2:K:175:VAL:HG12	2:K:176:LYS:N	2.36	0.41
2:E:232:THR:HG22	2:E:236:PHE:CE1	2.55	0.40
1:G:27:ALA:O	1:G:30:TYR:HB3	2.21	0.40
1:G:125:ARG:HD2	11:G:517:HOH:O	2.20	0.40
2:H:183:ILE:HG23	2:H:185:MET:N	2.32	0.40
1:J:80:VAL:O	1:J:84:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:HB2	1:A:367:PHE:CZ	2.56	0.40
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.76	0.40
2:B:81:ARG:NH1	2:B:82:GLU:O	2.53	0.40
1:D:306:ARG:HG3	11:D:540:HOH:O	2.20	0.40
1:D:366:TYR:CD2	1:D:411:LEU:HD11	2.55	0.40
2:E:252:TRP:O	2:E:255:VAL:HG23	2.21	0.40
1:G:39:ARG:HG2	1:G:242:VAL:CG1	2.46	0.40
3:I:177:LYS:HE3	3:I:179:ILE:HD11	2.03	0.40
1:J:233:SER:OG	1:J:236:GLU:HG2	2.21	0.40
2:K:48:ARG:HG3	2:K:48:ARG:HH11	1.85	0.40
2:B:77:THR:HG22	2:B:79:GLU:CG	2.51	0.40
1:D:80:VAL:O	1:D:84:MET:HG2	2.21	0.40
1:D:118:TYR:OH	7:D:503:LOP:H32	2.21	0.40
2:E:127:GLY:N	2:E:128:PRO:HD2	2.36	0.40
1:G:272:ASN:HD21	2:H:105:LYS:HD2	1.85	0.40
1:G:309:THR:HG22	3:L:165:GLY:CA	2.50	0.40
3:I:39:ASN:O	3:I:40:PRO:C	2.59	0.40
3:I:112:GLN:H	3:I:112:GLN:HE21	1.61	0.40
3:I:135:VAL:HA	3:I:136:PRO:HD2	1.92	0.40
1:J:247:TYR:HB3	2:K:252:TRP:CZ2	2.55	0.40
1:J:276:HIS:HA	1:J:277:PRO:HD3	1.92	0.40
2:K:59:PRO:CD	2:K:62:GLN:HE21	2.35	0.40
2:B:109:GLY:N	2:B:125:ILE:O	2.49	0.40
1:D:270:MET:C	11:D:532:HOH:O	2.60	0.40
2:E:231:PHE:HE1	2:E:235:MET:SD	2.44	0.40
1:G:92:MET:HA	1:G:92:MET:HE2	2.03	0.40
1:G:116:LEU:HA	1:G:121:TYR:HE2	1.87	0.40
2:H:129:GLU:OE1	2:H:129:GLU:N	2.48	0.40
2:H:194:VAL:O	2:H:194:VAL:HG12	2.21	0.40
2:H:235:MET:O	2:H:236:PHE:C	2.60	0.40
3:I:27:THR:O	3:I:31:VAL:HG23	2.22	0.40
1:J:56:VAL:HG23	8:J:505:ANJ:H281	2.03	0.40
1:J:418:VAL:HG12	1:J:419:ALA:N	2.36	0.40
1:A:377:LEU:HA	1:A:380:VAL:HG23	2.03	0.40
2:B:141:GLU:HA	2:B:142:PRO:HD3	1.84	0.40
1:D:68:HIS:ND1	11:D:507:HOH:O	2.37	0.40
3:F:39:ASN:O	3:F:40:PRO:C	2.59	0.40
3:F:162:ILE:HG22	3:F:170:ASN:OD1	2.22	0.40
1:G:306:ARG:NH1	11:G:542:HOH:O	2.39	0.40
3:I:110:THR:O	3:I:113:ASN:N	2.55	0.40
1:J:245:TRP:HE3	1:J:249:ILE:HG13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:20:PHE:CZ	2:K:217:TRP:HA	2.56	0.40
3:L:39:ASN:O	3:L:40:PRO:C	2.60	0.40
3:L:57:VAL:HG22	3:L:63:LEU:HD13	2.02	0.40
3:L:58:GLU:O	3:L:61:VAL:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/428 (100%)	398 (93%)	24 (6%)	4 (1%)	17	35
1	D	426/428 (100%)	402 (94%)	21 (5%)	3 (1%)	22	43
1	G	426/428 (100%)	400 (94%)	22 (5%)	4 (1%)	17	35
1	J	426/428 (100%)	397 (93%)	26 (6%)	3 (1%)	22	43
2	B	254/256 (99%)	227 (89%)	21 (8%)	6 (2%)	6	10
2	E	254/256 (99%)	229 (90%)	18 (7%)	7 (3%)	5	7
2	H	254/256 (99%)	225 (89%)	21 (8%)	8 (3%)	4	6
2	K	254/256 (99%)	229 (90%)	18 (7%)	7 (3%)	5	7
3	C	177/179 (99%)	143 (81%)	23 (13%)	11 (6%)	1	1
3	F	177/179 (99%)	144 (81%)	25 (14%)	8 (4%)	2	3
3	I	177/179 (99%)	144 (81%)	26 (15%)	7 (4%)	3	3
3	L	177/179 (99%)	142 (80%)	26 (15%)	9 (5%)	2	2
All	All	3428/3452 (99%)	3080 (90%)	271 (8%)	77 (2%)	6	12

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	137	GLY
2	B	147	GLU
2	B	200	HIS
3	C	109	ALA
2	E	137	GLY
2	E	147	GLU
2	E	200	HIS
3	F	109	ALA
1	G	8	HIS
2	H	137	GLY
2	H	147	GLU
2	H	200	HIS
3	I	109	ALA
2	K	137	GLY
2	K	147	GLU
2	K	200	HIS
3	L	90	LEU
3	L	109	ALA
3	C	57	VAL
3	C	158	SER
3	C	181	GLU
2	E	37	ALA
3	F	45	GLN
3	F	57	VAL
3	F	158	SER
3	F	181	GLU
2	H	37	ALA
3	I	57	VAL
3	I	158	SER
3	I	181	GLU
2	K	37	ALA
2	K	72	VAL
3	L	57	VAL
3	L	158	SER
3	L	181	GLU
1	A	13	THR
2	B	37	ALA
2	B	198	ASP
3	C	45	GLN
3	C	90	LEU
3	C	134	CYS
1	D	13	THR
2	E	74	ASP

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Mol	Chain	Res	Type
2	E	198	ASP
3	F	134	CYS
1	G	13	THR
2	H	188	PRO
2	H	198	ASP
1	J	13	THR
2	K	198	ASP
3	L	134	CYS
2	B	188	PRO
3	C	107	ALA
3	F	107	ALA
1	G	73	VAL
2	H	75	GLU
3	I	134	CYS
3	L	45	GLN
3	L	107	ALA
1	A	73	VAL
1	A	98	ALA
3	C	164	LYS
1	D	98	ALA
1	G	98	ALA
3	I	107	ALA
1	D	73	VAL
2	E	188	PRO
2	H	43	LYS
1	J	98	ALA
2	K	188	PRO
1	A	123	ALA
3	I	40	PRO
3	L	40	PRO
3	C	40	PRO
3	C	140	VAL
3	F	40	PRO
1	J	73	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/353 (100%)	336 (95%)	17 (5%)	25	49
1	D	353/353 (100%)	337 (96%)	16 (4%)	27	52
1	G	353/353 (100%)	334 (95%)	19 (5%)	22	44
1	J	353/353 (100%)	336 (95%)	17 (5%)	25	49
2	B	203/203 (100%)	198 (98%)	5 (2%)	47	73
2	E	203/203 (100%)	197 (97%)	6 (3%)	41	67
2	H	203/203 (100%)	195 (96%)	8 (4%)	32	58
2	K	203/203 (100%)	196 (97%)	7 (3%)	37	63
3	C	138/138 (100%)	133 (96%)	5 (4%)	35	61
3	F	138/138 (100%)	132 (96%)	6 (4%)	29	54
3	I	138/138 (100%)	132 (96%)	6 (4%)	29	54
3	L	138/138 (100%)	131 (95%)	7 (5%)	24	46
All	All	2776/2776 (100%)	2657 (96%)	119 (4%)	29	54

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	7	ASP
1	A	8	HIS
1	A	79	SER
1	A	92	MET
1	A	94	ARG
1	A	104	PHE
1	A	108	VAL
1	A	192	ASN
1	A	199	TYR
1	A	231	ARG
1	A	246	PRO
1	A	321	ILE
1	A	342	VAL
1	A	380	VAL
1	A	385	THR
1	A	388	PRO
2	B	26	GLN
2	B	80	ASP
2	B	140	GLU
2	B	194	VAL
2	B	205	HIS

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Mol	Chain	Res	Type
3	C	11	ARG
3	C	14	PHE
3	C	112	GLN
3	C	118	GLU
3	C	174	PRO
1	D	4	ILE
1	D	8	HIS
1	D	10	GLU
1	D	79	SER
1	D	94	ARG
1	D	104	PHE
1	D	108	VAL
1	D	175	SER
1	D	192	ASN
1	D	199	TYR
1	D	231	ARG
1	D	246	PRO
1	D	342	VAL
1	D	380	VAL
1	D	385	THR
1	D	388	PRO
2	E	26	GLN
2	E	167	ASP
2	E	188	PRO
2	E	194	VAL
2	E	205	HIS
2	E	231	PHE
3	F	11	ARG
3	F	14	PHE
3	F	112	GLN
3	F	118	GLU
3	F	125	MET
3	F	174	PRO
1	G	7	ASP
1	G	8	HIS
1	G	79	SER
1	G	92	MET
1	G	94	ARG
1	G	104	PHE
1	G	108	VAL
1	G	192	ASN
1	G	199	TYR

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Mol	Chain	Res	Type
1	G	231	ARG
1	G	246	PRO
1	G	252	ASP
1	G	287	SER
1	G	309	THR
1	G	342	VAL
1	G	380	VAL
1	G	385	THR
1	G	388	PRO
1	G	417	PRO
2	H	26	GLN
2	H	80	ASP
2	H	84	LYS
2	H	149	HIS
2	H	167	ASP
2	H	194	VAL
2	H	205	HIS
2	H	231	PHE
3	I	11	ARG
3	I	14	PHE
3	I	87	SER
3	I	88	VAL
3	I	112	GLN
3	I	174	PRO
1	J	8	HIS
1	J	74	ASP
1	J	79	SER
1	J	92	MET
1	J	94	ARG
1	J	104	PHE
1	J	108	VAL
1	J	162	ILE
1	J	192	ASN
1	J	199	TYR
1	J	231	ARG
1	J	246	PRO
1	J	321	ILE
1	J	342	VAL
1	J	380	VAL
1	J	385	THR
1	J	388	PRO
2	K	26	GLN

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Mol	Chain	Res	Type
2	K	73	THR
2	K	76	GLU
2	K	158	ARG
2	K	167	ASP
2	K	194	VAL
2	K	205	HIS
3	L	11	ARG
3	L	14	PHE
3	L	87	SER
3	L	112	GLN
3	L	118	GLU
3	L	125	MET
3	L	174	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	8	HIS
1	A	217	HIS
1	A	238	GLN
1	A	383	GLN
1	A	429	ASN
2	B	22	GLN
2	B	26	GLN
2	B	62	GLN
2	B	69	GLN
2	B	111	HIS
2	B	228	GLN
3	C	36	ASN
3	C	39	ASN
3	C	112	GLN
3	C	113	ASN
3	C	185	GLN
1	D	217	HIS
1	D	291	HIS
1	D	383	GLN
2	E	22	GLN
2	E	26	GLN
2	E	62	GLN
2	E	69	GLN
2	E	111	HIS

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Mol	Chain	Res	Type
2	E	149	HIS
2	E	228	GLN
3	F	36	ASN
3	F	39	ASN
3	F	89	GLN
3	F	112	GLN
3	F	113	ASN
3	F	185	GLN
1	G	8	HIS
1	G	217	HIS
1	G	272	ASN
1	G	291	HIS
1	G	383	GLN
1	G	429	ASN
2	H	22	GLN
2	H	26	GLN
2	H	62	GLN
2	H	69	GLN
2	H	111	HIS
2	H	149	HIS
2	H	228	GLN
3	I	36	ASN
3	I	39	ASN
3	I	89	GLN
3	I	112	GLN
3	I	113	ASN
3	I	185	GLN
1	J	8	HIS
1	J	217	HIS
1	J	383	GLN
1	J	429	ASN
2	K	22	GLN
2	K	26	GLN
2	K	62	GLN
2	K	69	GLN
2	K	111	HIS
2	K	149	HIS
2	K	228	GLN
3	L	36	ASN
3	L	39	ASN
3	L	45	GLN
3	L	89	GLN

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Mol	Chain	Res	Type
3	L	112	GLN
3	L	113	ASN
3	L	185	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
5	HEM	A	502	1	41,50,50	1.33	4 (9%)	45,82,82	1.14	2 (4%)
4	BGL	G	431	-	20,20,20	0.86	1 (5%)	24,25,25	1.10	2 (8%)
4	BGL	A	431	-	20,20,20	1.06	1 (5%)	24,25,25	0.72	0
8	ANJ	D	504	-	40,40,40	1.81	11 (27%)	36,54,54	1.91	7 (19%)
5	HEM	D	502	1	41,50,50	1.44	5 (12%)	45,82,82	1.14	4 (8%)
6	SMA	A	1	-	38,38,38	2.28	9 (23%)	48,52,52	1.96	9 (18%)
7	LOP	G	504	-	44,44,44	0.60	0	47,49,49	1.30	6 (12%)
8	ANJ	J	505	-	40,40,40	1.82	11 (27%)	36,54,54	1.68	9 (25%)
5	HEM	J	502	1	41,50,50	1.42	5 (12%)	45,82,82	1.10	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	LOP	D	503	-	44,44,44	0.56	0	47,49,49	1.28	8 (17%)
5	HEM	G	501	1	41,50,50	1.45	5 (12%)	45,82,82	1.05	2 (4%)
5	HEM	H	301	2	41,50,50	1.49	5 (12%)	45,82,82	1.09	2 (4%)
5	HEM	B	301	2	41,50,50	1.44	4 (9%)	45,82,82	1.09	2 (4%)
5	HEM	K	301	2	41,50,50	1.42	4 (9%)	45,82,82	1.08	2 (4%)
10	FES	I	200	3	0,4,4	-	-	-		
10	FES	L	200	3	0,4,4	-	-	-		
7	LOP	A	503	-	44,44,44	0.58	0	47,49,49	1.32	8 (17%)
10	FES	F	200	3	0,4,4	-	-	-		
4	BGL	J	431	-	20,20,20	0.97	1 (5%)	24,25,25	0.79	0
5	HEM	G	502	1	41,50,50	1.43	5 (12%)	45,82,82	1.04	1 (2%)
6	SMA	D	2	-	38,38,38	2.26	8 (21%)	48,52,52	1.79	11 (22%)
6	SMA	J	503	-	38,38,38	2.16	7 (18%)	48,52,52	1.74	8 (16%)
6	SMA	G	503	-	38,38,38	2.34	8 (21%)	48,52,52	1.83	8 (16%)
5	HEM	J	501	1	41,50,50	1.40	4 (9%)	45,82,82	1.06	1 (2%)
5	HEM	A	501	1	41,50,50	1.49	4 (9%)	45,82,82	1.01	1 (2%)
10	FES	C	200	3	0,4,4	-	-	-		
5	HEM	D	501	1	41,50,50	1.47	5 (12%)	45,82,82	1.06	2 (4%)
4	BGL	E	257	-	20,20,20	0.89	1 (5%)	24,25,25	1.14	2 (8%)
8	ANJ	G	505	-	40,40,40	1.79	9 (22%)	36,54,54	1.77	6 (16%)
7	LOP	J	504	-	44,44,44	0.56	0	47,49,49	1.39	9 (19%)
5	HEM	E	301	2	41,50,50	1.43	5 (12%)	45,82,82	1.06	1 (2%)
8	ANJ	A	504	-	40,40,40	1.79	9 (22%)	36,54,54	1.81	8 (22%)

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
5	HEM	A	502	1	-	6/12/54/54	-
4	BGL	G	431	-	-	0/11/31/31	0/1/1/1
4	BGL	A	431	-	-	0/11/31/31	0/1/1/1
8	ANJ	D	504	-	-	6/40/55/55	0/1/2/2
5	HEM	D	502	1	-	6/12/54/54	-
6	SMA	A	1	-	-	4/34/34/34	0/2/2/2
7	LOP	G	504	-	-	10/48/48/48	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ANJ	J	505	-	-	6/40/55/55	0/1/2/2
5	HEM	J	502	1	-	6/12/54/54	-
7	LOP	D	503	-	-	13/48/48/48	-
5	HEM	G	501	1	-	4/12/54/54	-
5	HEM	H	301	2	-	7/12/54/54	-
5	HEM	B	301	2	-	5/12/54/54	-
5	HEM	K	301	2	-	6/12/54/54	-
10	FES	I	200	3	-	-	0/1/1/1
10	FES	L	200	3	-	-	0/1/1/1
7	LOP	A	503	-	-	12/48/48/48	-
10	FES	F	200	3	-	-	0/1/1/1
4	BGL	J	431	-	-	0/11/31/31	0/1/1/1
5	HEM	G	502	1	-	7/12/54/54	-
6	SMA	D	2	-	-	5/34/34/34	0/2/2/2
6	SMA	J	503	-	-	5/34/34/34	0/2/2/2
6	SMA	G	503	-	-	5/34/34/34	0/2/2/2
5	HEM	J	501	1	-	3/12/54/54	-
5	HEM	A	501	1	-	2/12/54/54	-
10	FES	C	200	3	-	-	0/1/1/1
5	HEM	D	501	1	-	4/12/54/54	-
4	BGL	E	257	-	-	0/11/31/31	0/1/1/1
8	ANJ	G	505	-	-	4/40/55/55	0/1/2/2
7	LOP	J	504	-	-	7/48/48/48	-
5	HEM	E	301	2	-	8/12/54/54	-
8	ANJ	A	504	-	-	2/40/55/55	0/1/2/2

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	503	SMA	O5-C5	7.56	1.49	1.37
6	A	1	SMA	O5-C5	7.52	1.49	1.37
6	G	503	SMA	O7-C7	7.42	1.49	1.37
6	D	2	SMA	O5-C5	7.40	1.48	1.37
6	A	1	SMA	O7-C7	7.18	1.48	1.37
6	D	2	SMA	O7-C7	7.07	1.48	1.37
6	J	503	SMA	O7-C7	6.95	1.48	1.37
6	J	503	SMA	O5-C5	6.87	1.48	1.37
5	A	501	HEM	CBB-CAB	4.81	1.54	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	HEM	CBB-CAB	4.65	1.53	1.30
5	E	301	HEM	CBB-CAB	4.65	1.53	1.30
5	K	301	HEM	CBB-CAB	4.63	1.53	1.30
5	D	501	HEM	CBB-CAB	4.61	1.53	1.30
5	A	502	HEM	CBB-CAB	4.60	1.53	1.30
5	J	502	HEM	CBB-CAB	4.60	1.53	1.30
5	D	502	HEM	CBB-CAB	4.54	1.52	1.30
5	H	301	HEM	CBB-CAB	4.51	1.52	1.30
5	G	501	HEM	CBB-CAB	4.51	1.52	1.30
5	J	501	HEM	CBB-CAB	4.49	1.52	1.30
5	G	502	HEM	CBB-CAB	4.48	1.52	1.30
6	D	2	SMA	O8-C8	4.29	1.46	1.37
5	H	301	HEM	C3C-CAC	-4.29	1.39	1.47
6	J	503	SMA	O8-C8	4.19	1.46	1.37
6	A	1	SMA	O1-C2	4.14	1.41	1.36
6	G	503	SMA	O1-C2	4.08	1.41	1.36
6	G	503	SMA	O8-C8	3.97	1.46	1.37
5	B	301	HEM	C3C-CAC	-3.92	1.39	1.47
5	G	502	HEM	C3C-CAC	-3.90	1.39	1.47
8	G	505	ANJ	C5-C6	3.86	1.46	1.39
8	J	505	ANJ	O4-C10	3.85	1.52	1.46
5	D	501	HEM	C3C-CAC	-3.84	1.39	1.47
8	D	504	ANJ	C5-C6	3.84	1.46	1.39
5	A	501	HEM	C3C-CAC	-3.83	1.40	1.47
8	A	504	ANJ	O4-C12	3.81	1.43	1.34
8	A	504	ANJ	O4-C10	3.79	1.52	1.46
8	J	505	ANJ	O8-C14	3.79	1.50	1.44
5	G	501	HEM	C3C-CAC	-3.77	1.40	1.47
8	A	504	ANJ	C5-C6	3.75	1.45	1.39
8	G	505	ANJ	C2-N1	3.73	1.47	1.41
6	A	1	SMA	O8-C8	3.73	1.45	1.37
8	G	505	ANJ	O4-C12	3.72	1.43	1.34
8	D	504	ANJ	O8-C14	3.67	1.50	1.44
8	D	504	ANJ	O4-C10	3.64	1.52	1.46
8	A	504	ANJ	C10-C9	3.62	1.62	1.53
5	B	301	HEM	CBC-CAC	3.61	1.53	1.29
5	E	301	HEM	CBC-CAC	3.60	1.53	1.29
8	G	505	ANJ	C10-C9	3.60	1.62	1.53
5	J	501	HEM	CBC-CAC	3.60	1.53	1.29
8	J	505	ANJ	C5-C6	3.60	1.45	1.39
5	H	301	HEM	CBC-CAC	3.59	1.53	1.29
5	K	301	HEM	CBC-CAC	3.57	1.53	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	301	HEM	C3C-CAC	-3.56	1.40	1.47
5	D	502	HEM	CBC-CAC	3.55	1.52	1.29
5	A	501	HEM	CBC-CAC	3.48	1.52	1.29
5	D	501	HEM	CBC-CAC	3.47	1.52	1.29
5	G	501	HEM	CBC-CAC	3.46	1.52	1.29
8	J	505	ANJ	C10-C9	3.44	1.61	1.53
6	D	2	SMA	C3-C4	-3.43	1.40	1.48
8	D	504	ANJ	C10-C9	3.43	1.61	1.53
5	E	301	HEM	C3C-CAC	-3.43	1.40	1.47
8	J	505	ANJ	C2-N1	3.41	1.46	1.41
5	A	502	HEM	CBC-CAC	3.39	1.51	1.29
8	J	505	ANJ	O4-C12	3.38	1.42	1.34
8	D	504	ANJ	O4-C12	3.36	1.42	1.34
5	J	502	HEM	CBC-CAC	3.33	1.51	1.29
6	A	1	SMA	C3-C4	-3.32	1.40	1.48
5	J	502	HEM	C3C-CAC	-3.27	1.41	1.47
8	G	505	ANJ	O4-C10	3.26	1.51	1.46
8	D	504	ANJ	C2-N1	3.26	1.46	1.41
6	G	503	SMA	C3-C4	-3.25	1.41	1.48
5	J	502	HEM	C3C-C2C	-3.24	1.35	1.40
8	A	504	ANJ	C2-N1	3.20	1.46	1.41
4	A	431	BGL	C1-C2	3.18	1.55	1.52
8	A	504	ANJ	O8-C14	3.16	1.49	1.44
5	J	501	HEM	C3C-CAC	-3.15	1.41	1.47
5	G	502	HEM	CBC-CAC	3.12	1.50	1.29
4	J	431	BGL	C1-C2	3.10	1.55	1.52
5	D	502	HEM	C3C-C2C	-3.09	1.36	1.40
6	J	503	SMA	C3-C4	-3.08	1.41	1.48
6	D	2	SMA	O1-C2	3.08	1.40	1.36
5	E	301	HEM	CAB-C3B	-2.98	1.39	1.47
5	A	502	HEM	C3C-CAC	-2.96	1.41	1.47
6	J	503	SMA	O1-C2	2.95	1.40	1.36
8	J	505	ANJ	C4-C3	2.94	1.45	1.38
8	A	504	ANJ	C4-C3	2.90	1.45	1.38
8	A	504	ANJ	C26-C25	2.89	1.62	1.52
5	A	501	HEM	C3C-C2C	-2.85	1.36	1.40
5	G	502	HEM	C3C-C2C	-2.82	1.36	1.40
5	D	502	HEM	CAB-C3B	-2.67	1.40	1.47
8	G	505	ANJ	C4-C3	2.65	1.44	1.38
8	D	504	ANJ	C4-C3	2.65	1.44	1.38
8	G	505	ANJ	C1-N1	2.62	1.37	1.34
5	D	501	HEM	C3C-C2C	-2.59	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	505	ANJ	O8-C14	2.58	1.48	1.44
5	G	502	HEM	CAB-C3B	-2.56	1.40	1.47
8	D	504	ANJ	C1-N1	2.54	1.37	1.34
6	G	503	SMA	C20-C19	2.52	1.35	1.33
4	G	431	BGL	C1-C2	2.50	1.54	1.52
5	G	501	HEM	C3C-C2C	-2.50	1.36	1.40
6	D	2	SMA	C20-C19	2.49	1.35	1.33
8	G	505	ANJ	C26-C25	2.49	1.61	1.52
5	K	301	HEM	CAB-C3B	-2.44	1.40	1.47
5	H	301	HEM	CAB-C3B	-2.43	1.40	1.47
5	A	502	HEM	CAB-C3B	-2.43	1.40	1.47
6	J	503	SMA	C4A-C4	-2.38	1.40	1.46
4	E	257	BGL	C1-C2	2.37	1.54	1.52
5	J	501	HEM	CAB-C3B	-2.36	1.41	1.47
8	D	504	ANJ	C26-C25	2.36	1.60	1.52
5	J	502	HEM	CAB-C3B	-2.34	1.41	1.47
8	J	505	ANJ	C26-C25	2.34	1.60	1.52
6	D	2	SMA	C4A-C4	-2.31	1.40	1.46
5	D	501	HEM	CAB-C3B	-2.31	1.41	1.47
6	G	503	SMA	C4A-C4	-2.26	1.40	1.46
5	B	301	HEM	CAB-C3B	-2.25	1.41	1.47
8	J	505	ANJ	C13-C14	2.24	1.57	1.53
6	J	503	SMA	C7-C8	-2.23	1.37	1.40
8	J	505	ANJ	C1-N1	2.22	1.37	1.34
5	G	501	HEM	CAB-C3B	-2.22	1.41	1.47
8	J	505	ANJ	C13-C12	2.22	1.55	1.51
5	H	301	HEM	C3C-C2C	-2.20	1.37	1.40
6	G	503	SMA	O12-C12	2.18	1.48	1.42
8	D	504	ANJ	C13-C12	2.17	1.55	1.51
6	A	1	SMA	C3-C2	2.15	1.38	1.34
5	E	301	HEM	C3C-C2C	-2.14	1.37	1.40
5	D	502	HEM	C3C-CAC	-2.12	1.43	1.47
6	A	1	SMA	C4A-C4	-2.11	1.41	1.46
6	D	2	SMA	C7-C8	-2.11	1.37	1.40
6	A	1	SMA	O12-C12	2.08	1.47	1.42
8	D	504	ANJ	C13-C14	2.06	1.57	1.53
6	A	1	SMA	C20-C19	2.04	1.35	1.33
8	A	504	ANJ	C13-C14	2.02	1.57	1.53

All (124) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1	SMA	O7-C7-C8	7.45	122.06	114.54
8	G	505	ANJ	O6-C17-C9	-5.49	101.65	110.28
8	A	504	ANJ	O6-C17-C9	-5.45	101.70	110.28
8	D	504	ANJ	C19-C18-C13	-5.34	104.68	114.28
8	D	504	ANJ	O6-C17-C9	-5.09	102.27	110.28
8	J	505	ANJ	O6-C17-C9	-4.95	102.49	110.28
8	G	505	ANJ	O6-C17-O7	4.72	130.03	124.08
8	A	504	ANJ	O6-C17-O7	4.70	130.00	124.08
6	G	503	SMA	O7-C7-C8	4.53	119.11	114.54
6	D	2	SMA	C9-C2-C3	-4.53	120.45	127.07
6	J	503	SMA	O7-C7-C8	4.44	119.03	114.54
8	D	504	ANJ	O6-C17-O7	4.41	129.64	124.08
6	G	503	SMA	O1-C2-C9	4.40	119.92	110.58
8	J	505	ANJ	O6-C17-O7	4.32	129.52	124.08
6	D	2	SMA	O1-C2-C9	4.31	119.72	110.58
6	G	503	SMA	C9-C2-C3	-4.28	120.81	127.07
6	D	2	SMA	O7-C7-C8	4.27	118.85	114.54
6	A	1	SMA	O1-C2-C9	4.08	119.23	110.58
6	J	503	SMA	O1-C2-C9	4.03	119.12	110.58
6	J	503	SMA	C9-C2-C3	-3.82	121.48	127.07
6	A	1	SMA	C9-C2-C3	-3.80	121.51	127.07
7	G	504	LOP	C19-C18-C17	-3.79	95.16	114.42
6	D	2	SMA	O5-C5-C4A	3.76	121.09	115.85
6	J	503	SMA	C5M-O5-C5	-3.76	111.86	117.53
6	J	503	SMA	O5-C5-C4A	3.66	120.95	115.85
8	D	504	ANJ	C5-C6-C7	-3.65	115.15	118.74
7	J	504	LOP	C19-C18-C17	-3.65	95.90	114.42
6	G	503	SMA	O5-C5-C4A	3.56	120.81	115.85
5	G	502	HEM	CBB-CAB-C3B	-3.52	110.13	127.62
8	J	505	ANJ	C5-C6-C7	-3.47	115.33	118.74
5	A	502	HEM	CBB-CAB-C3B	-3.45	110.48	127.62
8	A	504	ANJ	C5-C6-C7	-3.43	115.37	118.74
5	H	301	HEM	CBB-CAB-C3B	-3.42	110.60	127.62
5	D	502	HEM	CBB-CAB-C3B	-3.42	110.60	127.62
6	A	1	SMA	O7-C7-C6	-3.42	118.24	124.12
5	B	301	HEM	CBB-CAB-C3B	-3.38	110.79	127.62
6	A	1	SMA	C9-C10-C11	-3.38	108.35	114.52
4	G	431	BGL	C1'-O2-C2	-3.37	106.28	114.32
5	E	301	HEM	CBB-CAB-C3B	-3.37	110.83	127.62
5	J	502	HEM	CBB-CAB-C3B	-3.36	110.89	127.62
5	K	301	HEM	CBB-CAB-C3B	-3.36	110.89	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	257	BGL	C1'-O2-C2	-3.35	106.33	114.32
6	G	503	SMA	C5M-O5-C5	-3.32	112.51	117.53
7	D	503	LOP	C19-C18-C17	-3.30	97.69	114.42
5	D	501	HEM	CBB-CAB-C3B	-3.29	111.25	127.62
6	G	503	SMA	C16-C17-C18	-3.28	116.49	124.67
5	J	501	HEM	CBB-CAB-C3B	-3.27	111.33	127.62
8	G	505	ANJ	C5-C6-C7	-3.23	115.57	118.74
5	G	501	HEM	CBB-CAB-C3B	-3.20	111.72	127.62
6	D	2	SMA	C5M-O5-C5	-3.14	112.79	117.53
8	G	505	ANJ	C6-C8-N2	3.12	122.58	116.80
5	A	501	HEM	CBB-CAB-C3B	-3.11	112.14	127.62
7	A	503	LOP	C19-C18-C17	-3.11	98.65	114.42
6	A	1	SMA	C5M-O5-C5	-2.98	113.04	117.53
7	G	504	LOP	O5-C6-C7	2.95	117.86	111.50
7	J	504	LOP	C21-C20-C19	-2.91	99.64	114.42
7	A	503	LOP	O6-C24-C25	2.91	121.03	111.91
6	A	1	SMA	O5-C5-C4A	2.86	119.83	115.85
8	A	504	ANJ	C6-C8-N2	2.85	122.08	116.80
6	D	2	SMA	C7M-O7-C7	-2.82	113.28	117.53
6	J	503	SMA	C9-C10-C11	-2.80	109.40	114.52
6	G	503	SMA	C9-C10-C11	-2.79	109.43	114.52
8	G	505	ANJ	O3-C8-N2	-2.78	117.34	122.45
7	D	503	LOP	C29-C28-C27	-2.75	100.45	114.42
8	D	504	ANJ	O3-C8-N2	-2.73	117.42	122.45
7	J	504	LOP	C9-C8-C7	-2.67	103.58	113.19
7	G	504	LOP	C21-C20-C19	-2.67	100.88	114.42
6	J	503	SMA	C7M-O7-C7	-2.67	113.50	117.53
7	D	503	LOP	C9-C8-C7	-2.66	103.64	113.19
6	D	2	SMA	C9-C10-C11	-2.65	109.68	114.52
8	A	504	ANJ	O3-C8-N2	-2.63	117.61	122.45
8	D	504	ANJ	C6-C8-N2	2.61	121.64	116.80
7	G	504	LOP	C17-C16-C15	-2.58	97.63	112.43
7	D	503	LOP	C21-C20-C19	-2.57	101.37	114.42
7	J	504	LOP	C17-C16-C15	-2.54	97.86	112.43
7	J	504	LOP	O6-C24-C25	2.50	119.74	111.91
7	A	503	LOP	C27-C26-C25	-2.48	104.28	113.19
5	D	502	HEM	CBA-CAA-C2A	-2.45	108.44	112.62
6	D	2	SMA	C16-C17-C18	-2.43	118.59	124.67
5	J	502	HEM	C4B-CHC-C1C	2.43	125.76	122.56
7	J	504	LOP	O5-C6-C7	2.42	116.73	111.50
7	A	503	LOP	C21-C20-C19	-2.41	102.19	114.42
7	A	503	LOP	O5-C6-C7	2.40	116.68	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1	SMA	C7M-O7-C7	-2.39	113.91	117.53
6	D	2	SMA	C14-C15-C16	-2.39	120.93	125.61
7	A	503	LOP	C9-C8-C7	-2.34	104.78	113.19
7	A	503	LOP	C17-C16-C15	-2.33	99.11	112.43
5	H	301	HEM	C4C-CHD-C1D	2.29	125.57	122.56
8	A	504	ANJ	O1-C1-N1	2.28	128.71	125.80
5	A	502	HEM	CMC-C2C-C3C	2.27	128.93	124.68
8	J	505	ANJ	O3-C8-N2	-2.26	118.29	122.45
5	J	502	HEM	CBA-CAA-C2A	-2.25	108.78	112.62
7	D	503	LOP	C31-C30-C29	-2.25	103.00	114.42
8	D	504	ANJ	O1-C1-N1	2.25	128.66	125.80
7	D	503	LOP	C17-C16-C15	-2.25	99.57	112.43
8	J	505	ANJ	C20-C19-C18	-2.24	105.70	113.62
5	G	501	HEM	C4B-CHC-C1C	2.24	125.51	122.56
5	D	502	HEM	C4B-CHC-C1C	2.24	125.51	122.56
6	G	503	SMA	C7M-O7-C7	-2.22	114.18	117.53
5	B	301	HEM	C4C-CHD-C1D	2.22	125.48	122.56
8	G	505	ANJ	O1-C1-N1	2.19	128.59	125.80
7	A	503	LOP	C29-C28-C27	-2.19	103.32	114.42
6	J	503	SMA	O5-C5-C6	-2.18	120.37	124.12
8	J	505	ANJ	C6-C8-N2	2.18	120.84	116.80
5	D	501	HEM	C4B-CHC-C1C	2.17	125.43	122.56
5	K	301	HEM	C4C-CHD-C1D	2.17	125.42	122.56
8	A	504	ANJ	C20-C19-C18	-2.17	105.96	113.62
8	J	505	ANJ	C3-C2-C7	2.15	121.19	119.79
7	J	504	LOP	C29-C28-C27	-2.15	103.51	114.42
4	E	257	BGL	C3'-C2'-C1'	-2.14	104.03	113.49
8	A	504	ANJ	C14-O8-C24	2.12	121.42	117.78
7	D	503	LOP	O6-C24-C25	2.12	118.55	111.91
6	D	2	SMA	C6-C5-C4A	-2.11	118.16	121.86
7	J	504	LOP	C31-C30-C29	-2.09	103.80	114.42
7	G	504	LOP	P1-O1-C2	-2.07	111.39	121.59
8	J	505	ANJ	O1-C1-N1	2.07	128.44	125.80
7	J	504	LOP	C27-C26-C25	-2.05	105.81	113.19
5	D	502	HEM	C2C-C3C-C4C	-2.04	105.47	106.90
6	A	1	SMA	O1-C8A-C8	2.04	119.65	116.42
8	J	505	ANJ	O6-C15-C16	2.03	110.47	106.63
4	G	431	BGL	C3'-C2'-C1'	-2.02	104.52	113.49
7	D	503	LOP	C27-C26-C25	-2.02	105.94	113.19
7	G	504	LOP	C27-C26-C25	-2.01	105.97	113.19
6	D	2	SMA	O5-C5-C6	-2.00	120.67	124.12

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	HEM	C2B-C3B-CAB-CBB
5	A	502	HEM	C4B-C3B-CAB-CBB
5	D	502	HEM	C2B-C3B-CAB-CBB
5	D	502	HEM	C4B-C3B-CAB-CBB
5	G	502	HEM	C2B-C3B-CAB-CBB
5	G	502	HEM	C4B-C3B-CAB-CBB
5	J	502	HEM	C2B-C3B-CAB-CBB
7	A	503	LOP	C2-O1-P1-O3
7	D	503	LOP	C2-O1-P1-O2
7	D	503	LOP	C2-O1-P1-O3
7	D	503	LOP	C2-O1-P1-O4
7	G	504	LOP	C2-O1-P1-O4
7	G	504	LOP	C3-O2-P1-O4
8	A	504	ANJ	C16-C15-O6-C17
8	D	504	ANJ	C16-C15-O6-C17
8	G	505	ANJ	C16-C15-O6-C17
8	J	505	ANJ	C16-C15-O6-C17
5	B	301	HEM	C3D-CAD-CBD-CGD
6	A	1	SMA	C6-C7-O7-C7M
8	D	504	ANJ	C26-C25-C27-C28
8	J	505	ANJ	C26-C25-C27-C28
6	J	503	SMA	C6-C5-O5-C5M
5	H	301	HEM	C3D-CAD-CBD-CGD
7	A	503	LOP	C2-O1-P1-O2
7	J	504	LOP	C2-O1-P1-O2
6	A	1	SMA	C8-C7-O7-C7M
6	J	503	SMA	C4A-C5-O5-C5M
6	D	2	SMA	C9-C10-C11-C22
8	D	504	ANJ	C24-C25-C27-C28
8	J	505	ANJ	C24-C25-C27-C28
5	E	301	HEM	C2B-C3B-CAB-CBB
5	J	502	HEM	C4B-C3B-CAB-CBB
5	E	301	HEM	C4D-C3D-CAD-CBD
8	J	505	ANJ	O9-C24-C25-C27
8	D	504	ANJ	O8-C24-C25-C27
8	J	505	ANJ	O8-C24-C25-C27
5	E	301	HEM	C2D-C3D-CAD-CBD
5	H	301	HEM	C4D-C3D-CAD-CBD
6	D	2	SMA	C4A-C5-O5-C5M
7	A	503	LOP	O2-C3-C4-O5
8	G	505	ANJ	C26-C25-C27-C28
6	G	503	SMA	C9-C10-C11-C22

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Mol	Chain	Res	Type	Atoms
6	J	503	SMA	C9-C10-C11-C22
6	G	503	SMA	C11-C10-C9-C2
6	D	2	SMA	C6-C5-O5-C5M
7	D	503	LOP	O2-C3-C4-C5
6	D	2	SMA	C15-C14-O14-C25
6	J	503	SMA	C15-C14-O14-C25
8	G	505	ANJ	C24-C25-C27-C28
7	G	504	LOP	C3-O2-P1-O1
8	D	504	ANJ	O9-C24-C25-C27
7	D	503	LOP	O5-C4-C5-O6
6	G	503	SMA	C6-C5-O5-C5M
5	B	301	HEM	C2B-C3B-CAB-CBB
5	D	501	HEM	C2B-C3B-CAB-CBB
5	G	501	HEM	C2B-C3B-CAB-CBB
5	H	301	HEM	C2B-C3B-CAB-CBB
5	J	501	HEM	C2B-C3B-CAB-CBB
5	K	301	HEM	C2B-C3B-CAB-CBB
7	D	503	LOP	C3-C4-C5-O6
7	D	503	LOP	O2-C3-C4-O5
7	J	504	LOP	O6-C24-C25-C26
6	J	503	SMA	C13-C14-O14-C25
7	G	504	LOP	C2-O1-P1-O2
6	G	503	SMA	C4A-C5-O5-C5M
7	A	503	LOP	C2-O1-P1-O4
7	D	503	LOP	C3-O2-P1-O3
7	J	504	LOP	C2-O1-P1-O4
7	A	503	LOP	O2-C3-C4-C5
7	G	504	LOP	O2-C3-C4-C5
7	G	504	LOP	O2-C3-C4-O5
6	G	503	SMA	C15-C14-O14-C25
5	H	301	HEM	C2D-C3D-CAD-CBD
5	G	502	HEM	C3D-CAD-CBD-CGD
7	A	503	LOP	C3-C4-C5-O6
5	G	501	HEM	CAA-CBA-CGA-O2A
5	D	501	HEM	C4B-C3B-CAB-CBB
5	E	301	HEM	C4B-C3B-CAB-CBB
5	G	501	HEM	C4B-C3B-CAB-CBB
5	A	502	HEM	CAD-CBD-CGD-O1D
5	D	502	HEM	CAD-CBD-CGD-O2D
5	A	501	HEM	CAA-CBA-CGA-O2A
5	D	502	HEM	CAD-CBD-CGD-O1D
5	J	501	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
7	G	504	LOP	C14-C15-C16-C17
6	A	1	SMA	C15-C14-O14-C25
5	D	502	HEM	CAA-CBA-CGA-O1A
7	A	503	LOP	O6-C24-C25-C26
5	A	502	HEM	CAD-CBD-CGD-O2D
5	B	301	HEM	CAA-CBA-CGA-O2A
5	E	301	HEM	CAA-CBA-CGA-O1A
5	J	501	HEM	CAA-CBA-CGA-O2A
5	A	501	HEM	CAA-CBA-CGA-O1A
5	D	501	HEM	CAA-CBA-CGA-O2A
5	G	502	HEM	CAD-CBD-CGD-O1D
7	D	503	LOP	C14-C15-C16-C17
6	D	2	SMA	C13-C14-O14-C25
5	D	501	HEM	CAA-CBA-CGA-O1A
5	D	502	HEM	CAA-CBA-CGA-O2A
5	J	502	HEM	CAA-CBA-CGA-O1A
5	A	502	HEM	CAA-CBA-CGA-O1A
5	G	501	HEM	CAA-CBA-CGA-O1A
5	G	502	HEM	CAD-CBD-CGD-O2D
5	B	301	HEM	CAA-CBA-CGA-O1A
5	G	502	HEM	CAA-CBA-CGA-O1A
5	G	502	HEM	CAA-CBA-CGA-O2A
7	A	503	LOP	O5-C4-C5-O6
5	E	301	HEM	CAA-CBA-CGA-O2A
6	A	1	SMA	C9-C10-C11-C22
5	A	502	HEM	CAA-CBA-CGA-O2A
7	G	504	LOP	C12-C13-C14-C15
5	E	301	HEM	CAD-CBD-CGD-O2D
5	J	502	HEM	CAA-CBA-CGA-O2A
7	J	504	LOP	C14-C15-C16-C17
7	A	503	LOP	C14-C15-C16-C17
5	J	502	HEM	CAD-CBD-CGD-O1D
5	J	502	HEM	CAD-CBD-CGD-O2D
7	D	503	LOP	C12-C13-C14-C15
5	H	301	HEM	CAA-CBA-CGA-O2A
5	E	301	HEM	CAD-CBD-CGD-O1D
5	K	301	HEM	CAA-CBA-CGA-O2A
5	B	301	HEM	C4B-C3B-CAB-CBB
5	H	301	HEM	C4B-C3B-CAB-CBB
5	K	301	HEM	C4B-C3B-CAB-CBB
5	K	301	HEM	CAA-CBA-CGA-O1A
7	A	503	LOP	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
7	J	504	LOP	C12-C13-C14-C15
5	H	301	HEM	CAA-CBA-CGA-O1A
5	K	301	HEM	CAD-CBD-CGD-O2D
8	A	504	ANJ	C14-C15-O6-C17
8	D	504	ANJ	C14-C15-O6-C17
8	G	505	ANJ	C14-C15-O6-C17
8	J	505	ANJ	C14-C15-O6-C17
7	A	503	LOP	O5-C6-C7-C8
7	G	504	LOP	C3-C4-C5-O6
7	D	503	LOP	C3-O2-P1-O4
7	A	503	LOP	O7-C6-C7-C8
5	K	301	HEM	CAD-CBD-CGD-O1D
7	J	504	LOP	O5-C6-C7-C8
7	J	504	LOP	O8-C24-C25-C26
7	D	503	LOP	O5-C6-C7-C8
7	G	504	LOP	O6-C24-C25-C26
7	D	503	LOP	O7-C6-C7-C8

There are no ring outliers.

28 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	HEM	5	0
4	G	431	BGL	1	0
4	A	431	BGL	3	0
8	D	504	ANJ	12	0
5	D	502	HEM	5	0
6	A	1	SMA	2	0
7	G	504	LOP	5	0
8	J	505	ANJ	10	0
5	J	502	HEM	3	0
7	D	503	LOP	4	0
5	G	501	HEM	4	0
5	H	301	HEM	4	0
5	B	301	HEM	5	0
5	K	301	HEM	1	0
7	A	503	LOP	2	0
4	J	431	BGL	1	0
5	G	502	HEM	3	0
6	D	2	SMA	3	0
6	J	503	SMA	3	0
6	G	503	SMA	1	0

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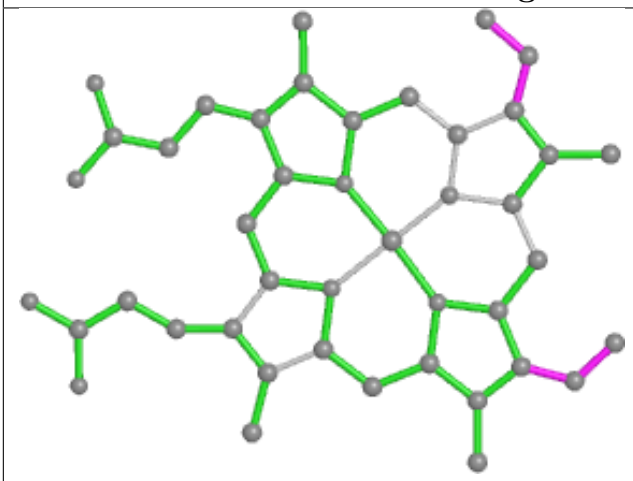
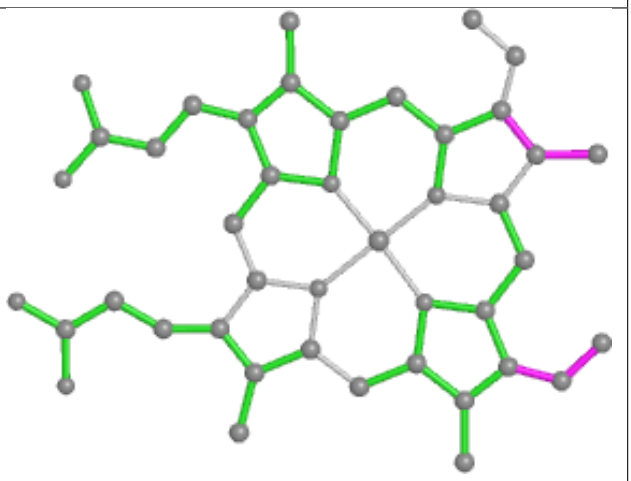
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	501	HEM	2	0
5	A	501	HEM	4	0
5	D	501	HEM	5	0
4	E	257	BGL	2	0
8	G	505	ANJ	6	0
7	J	504	LOP	5	0
5	E	301	HEM	5	0
8	A	504	ANJ	9	0

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 then 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.

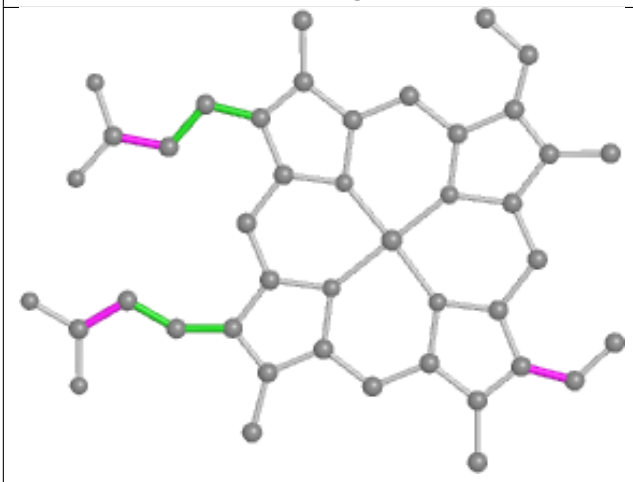
Ligand HEM A 502



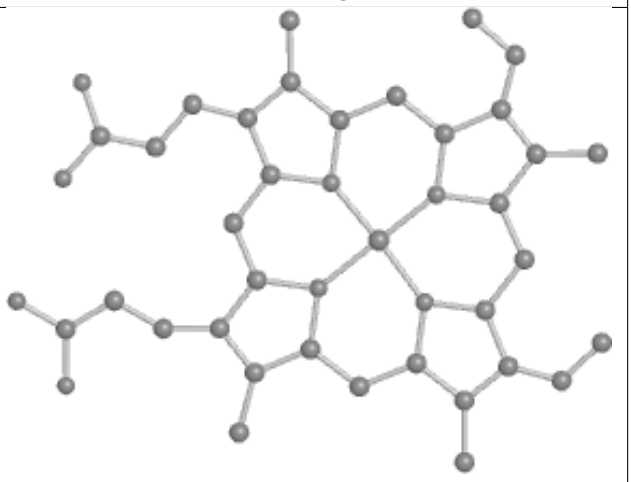
Bond lengths



Bond angles

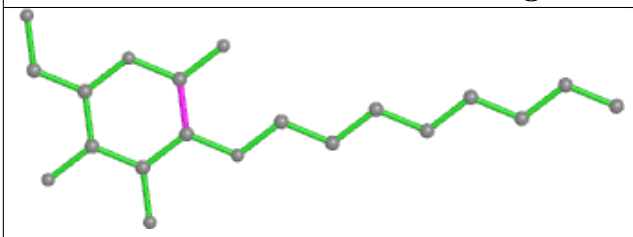


Torsions

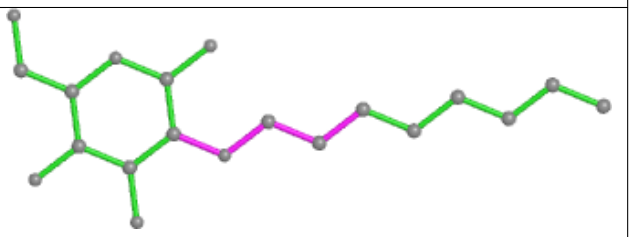


Rings

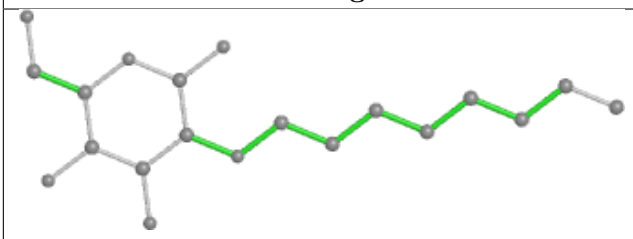
Ligand BGL G 431



Bond lengths

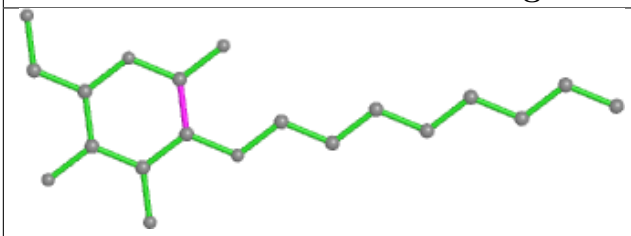
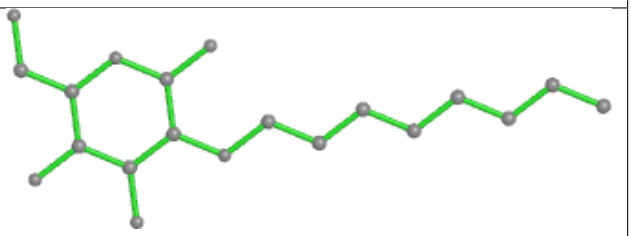
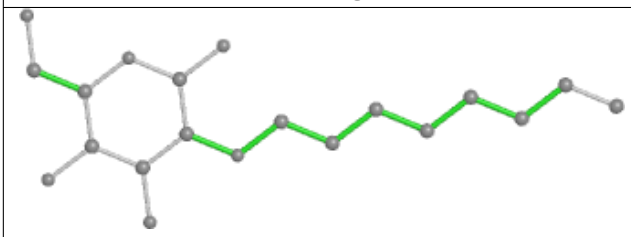
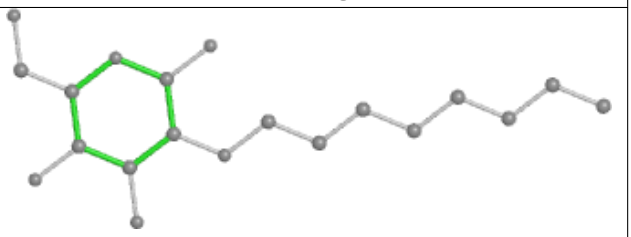


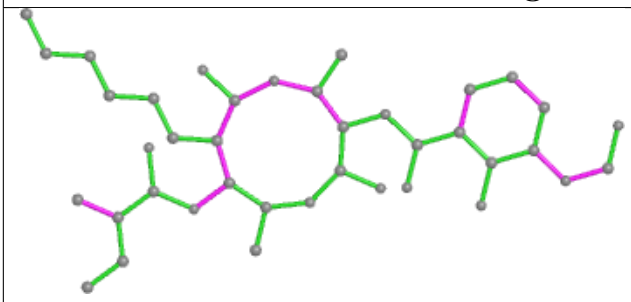
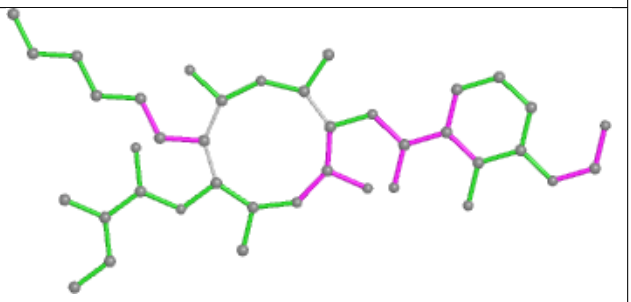
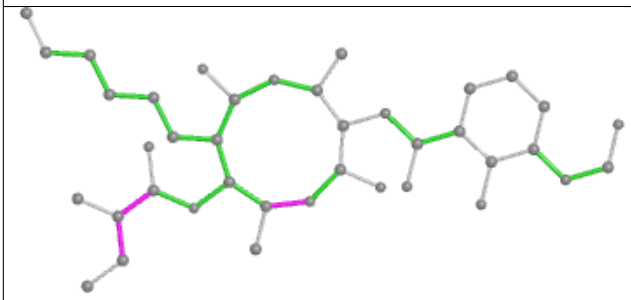
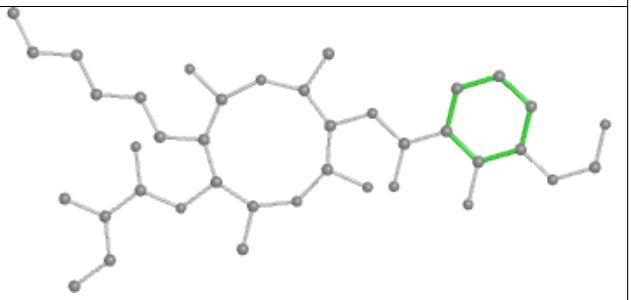
Bond angles



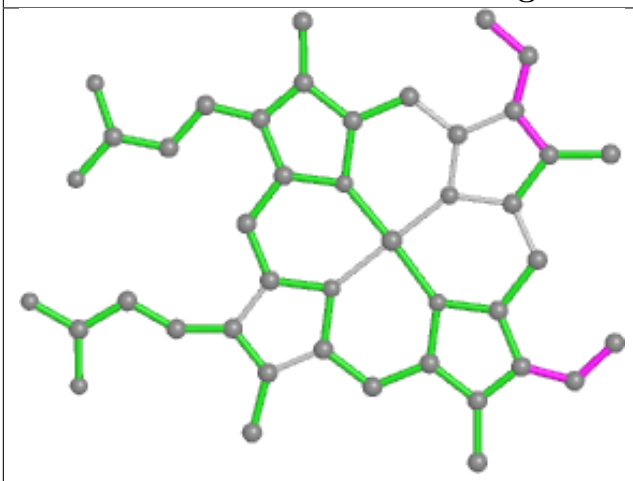
Torsions

Rings

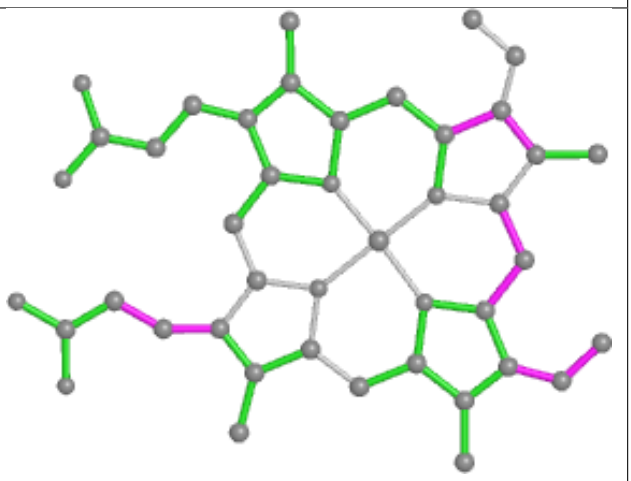
Ligand BGL A 431	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANJ D 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

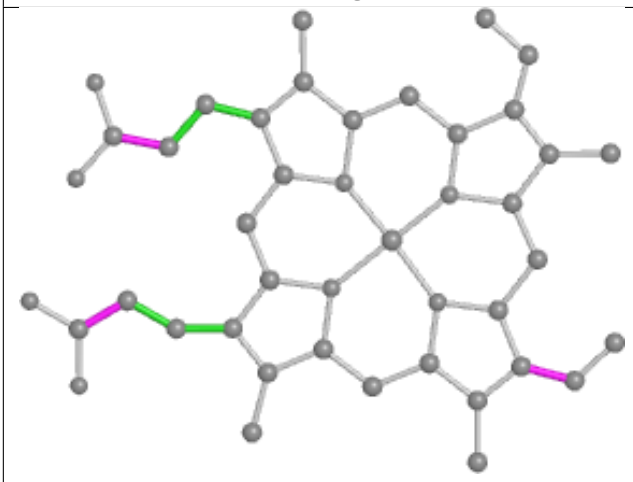
Ligand HEM D 502



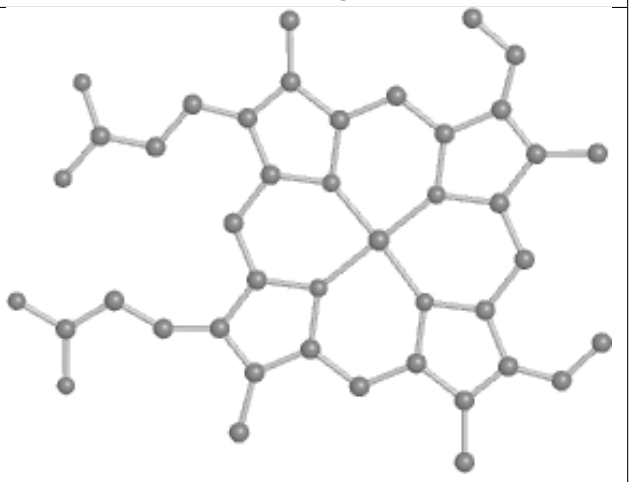
Bond lengths



Bond angles

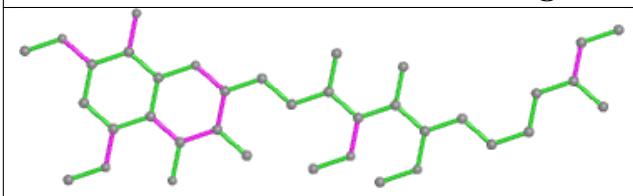


Torsions



Rings

Ligand SMA A 1



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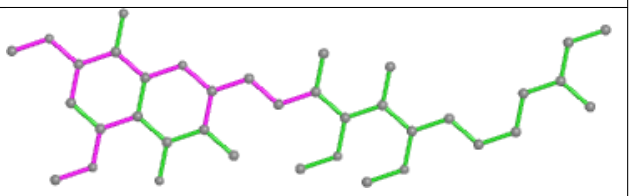
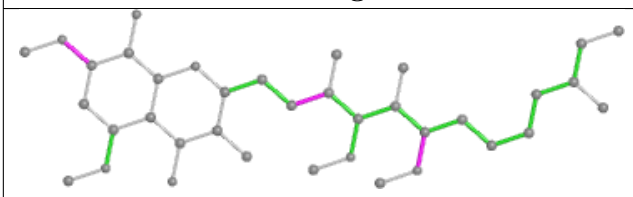


Bond angles



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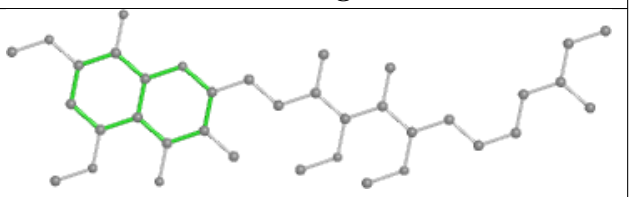
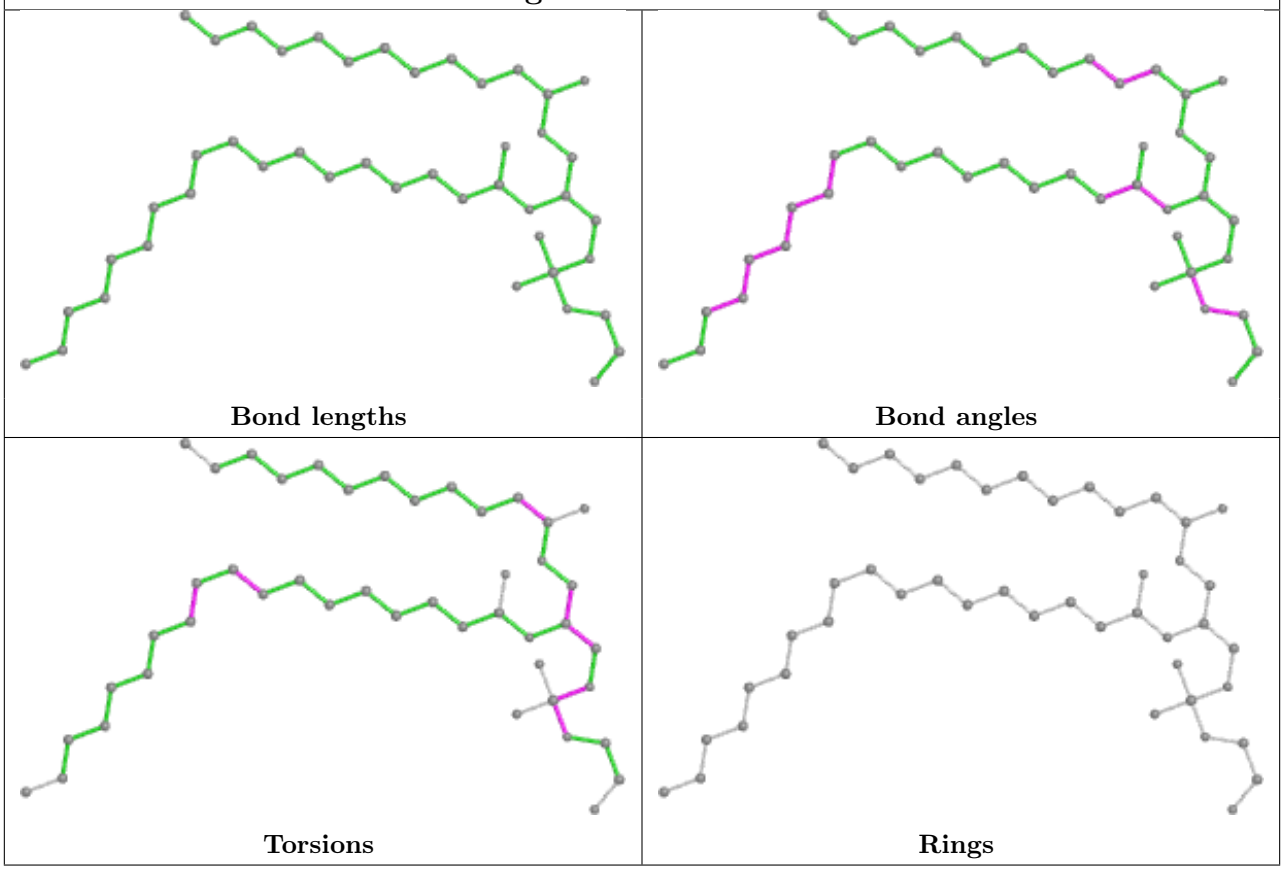
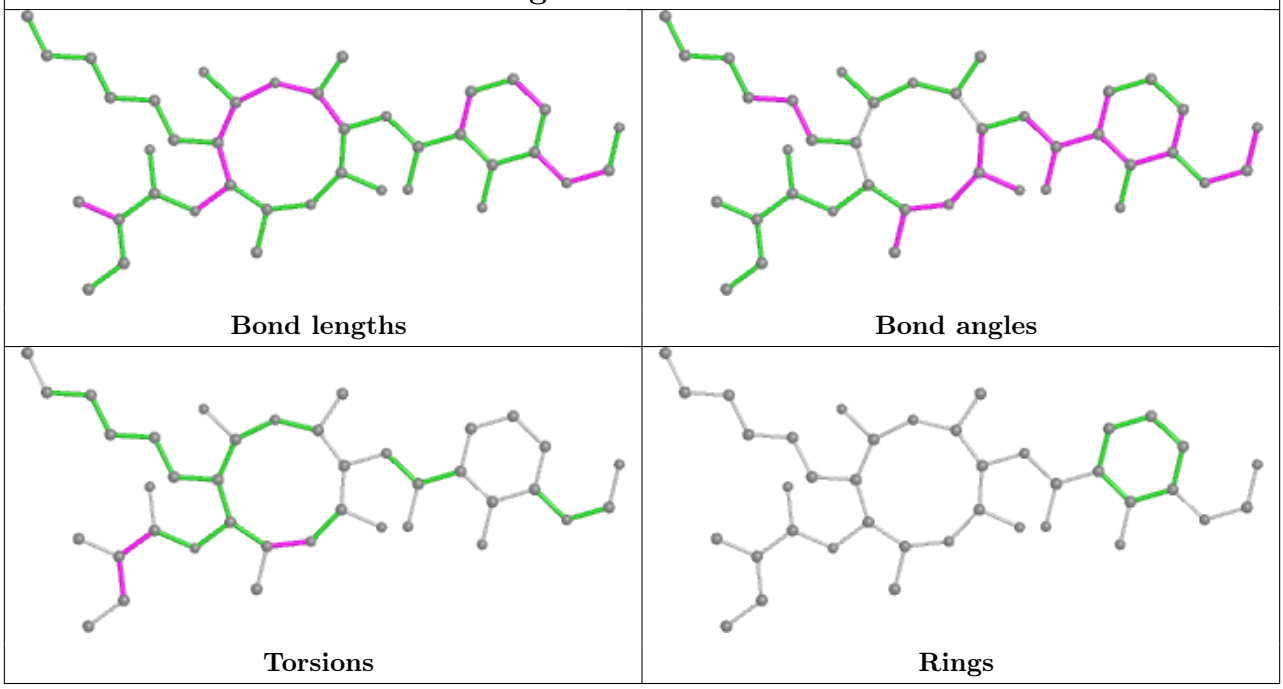


Rings

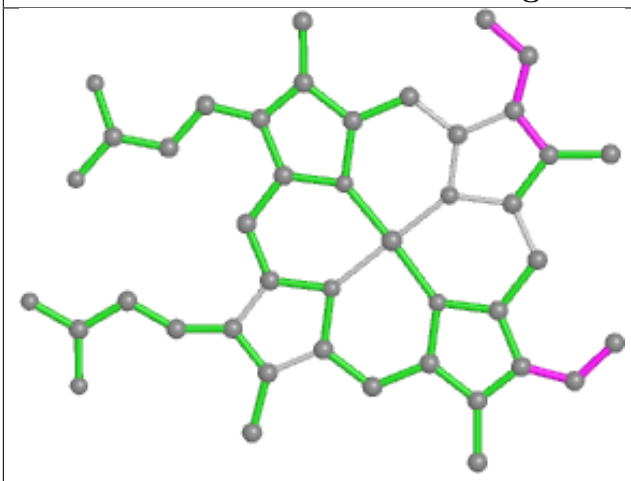
Ligand LOP G 504



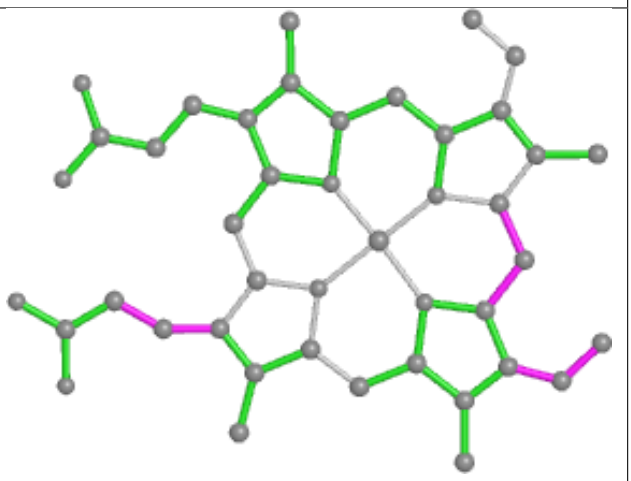
Ligand ANJ J 505



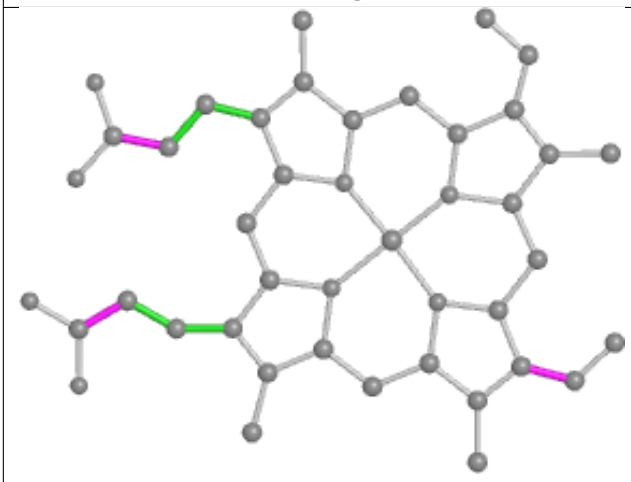
Ligand HEM J 502



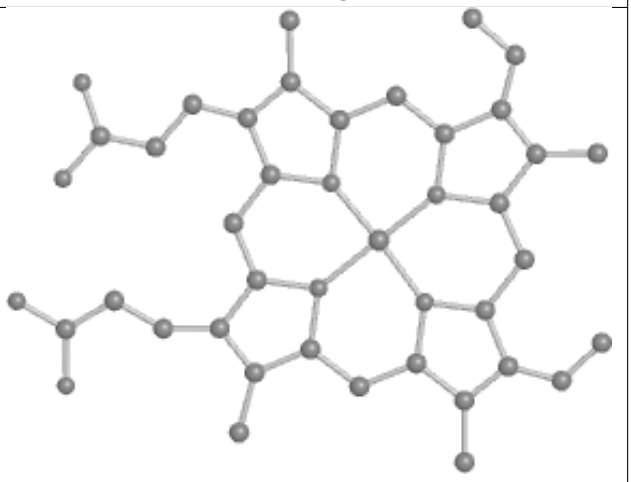
Bond lengths



Bond angles

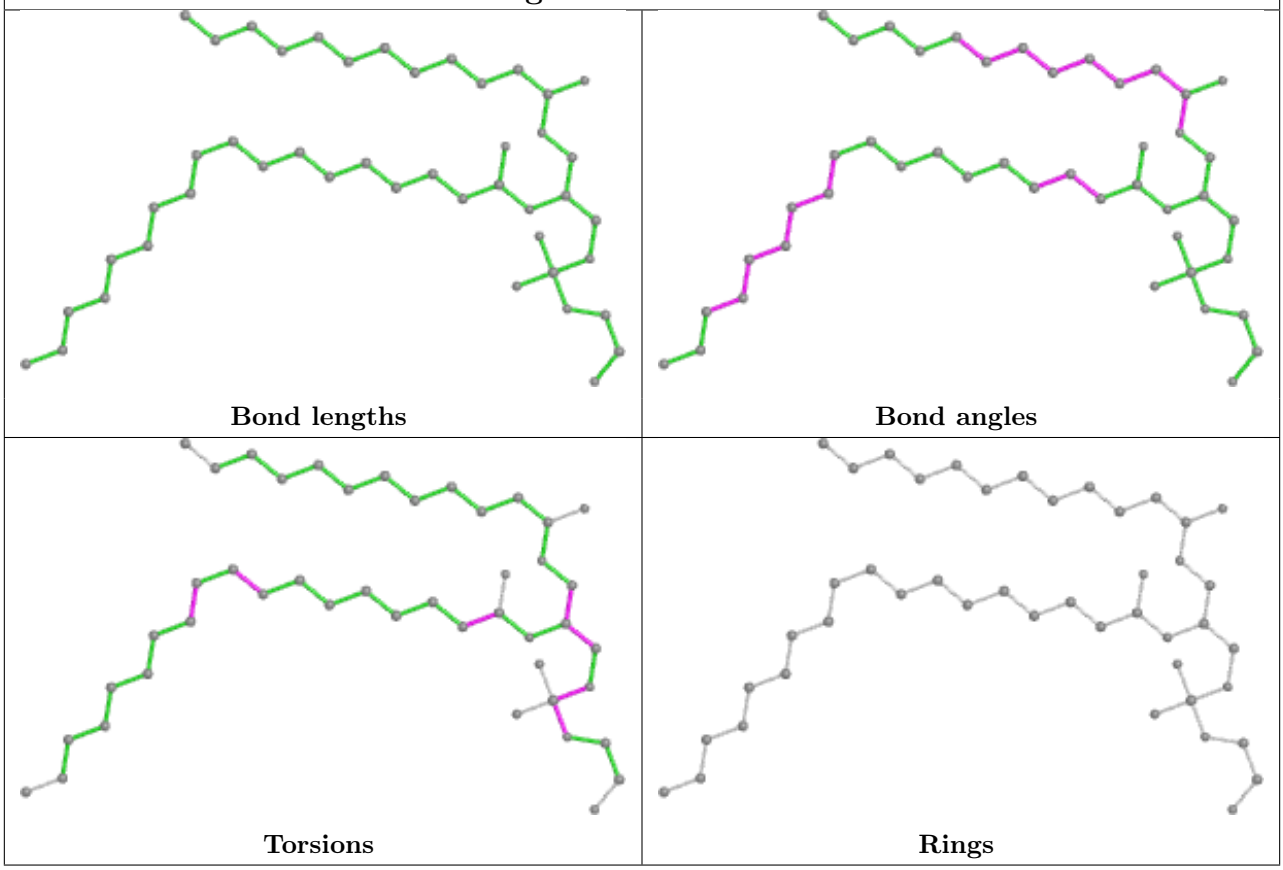


Torsions

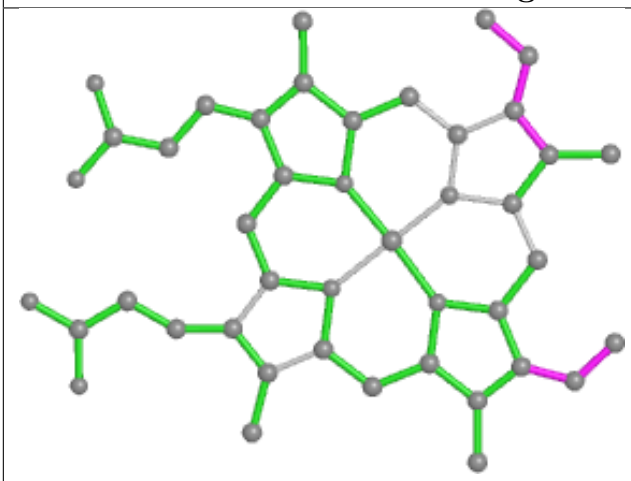


Rings

Ligand LOP D 503



Ligand HEM G 501



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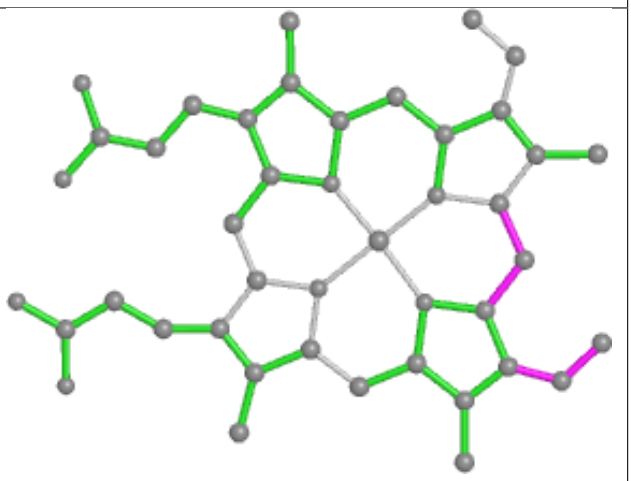
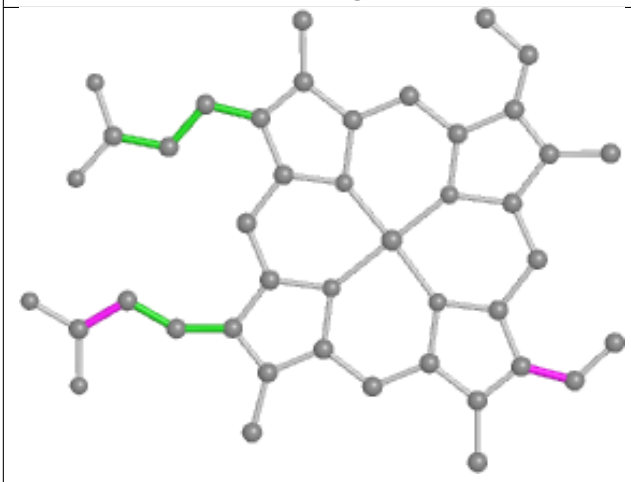
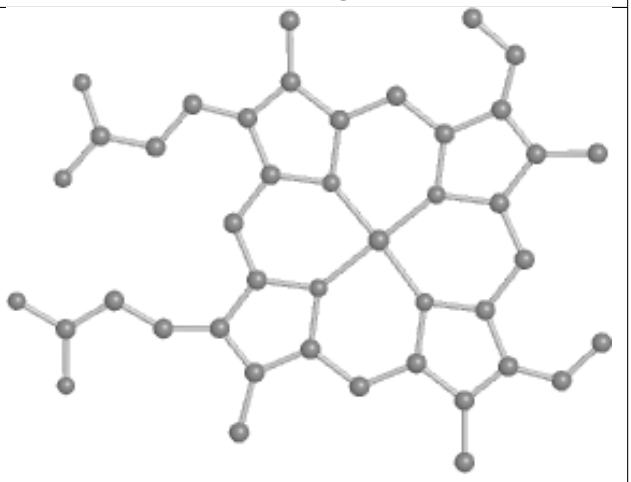


Bond angles

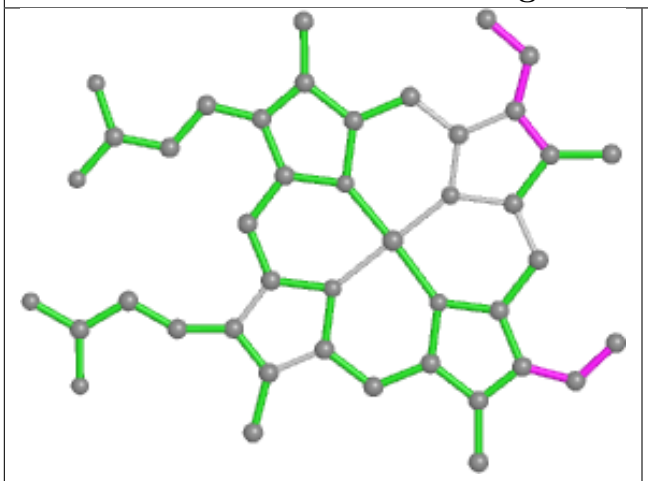


Torsions



Rings

Ligand HEM H 301



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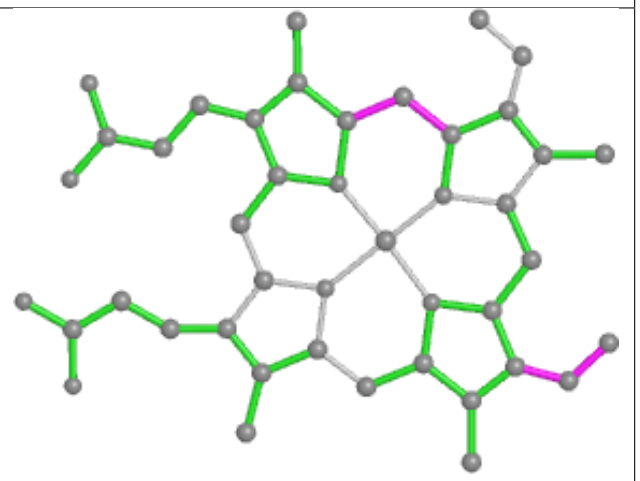

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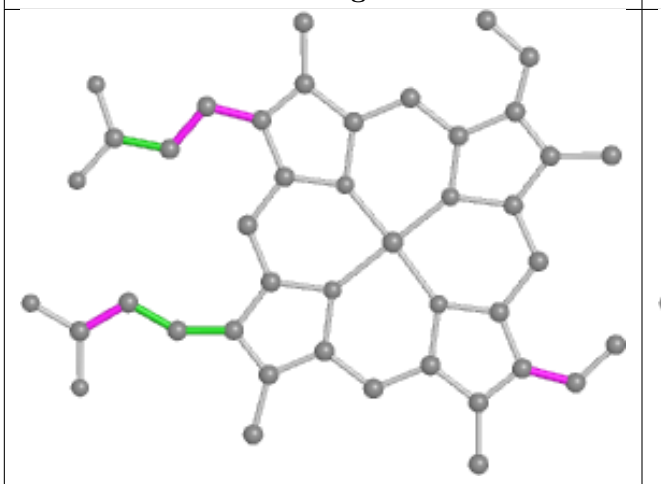

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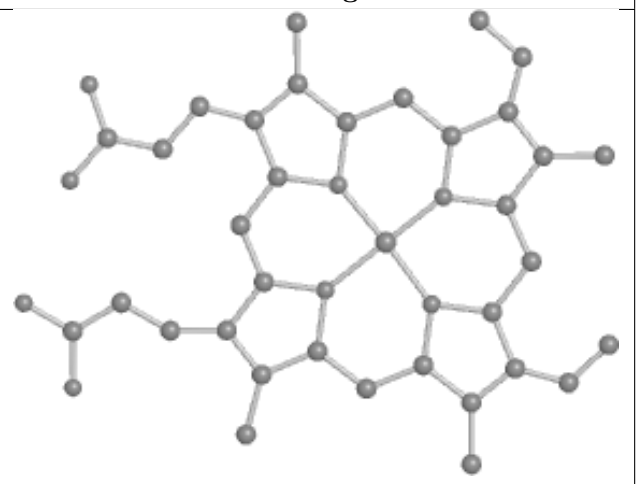
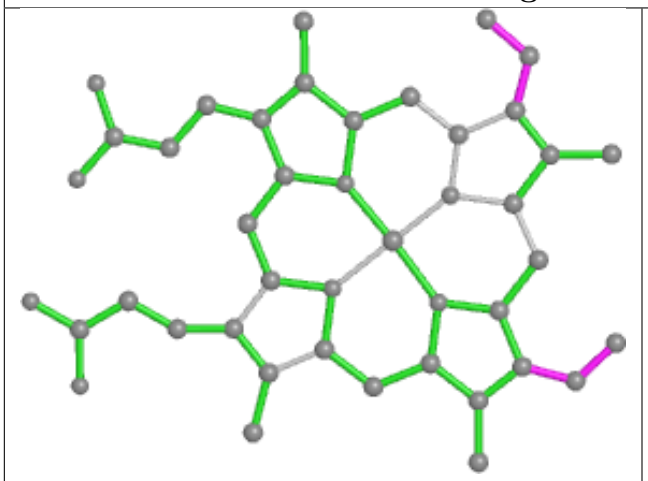


Rings

Ligand HEM B 301



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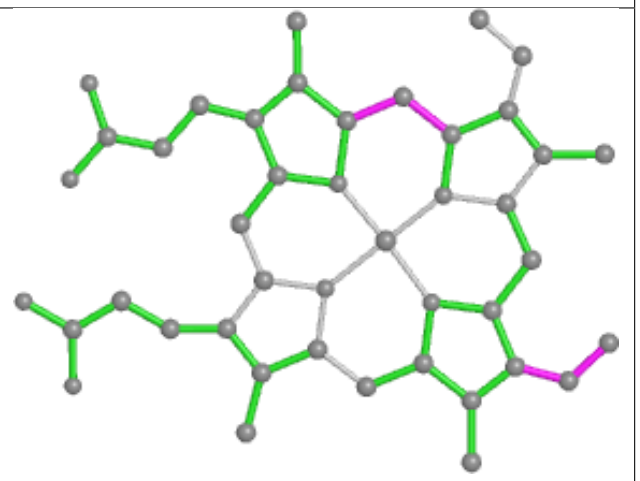

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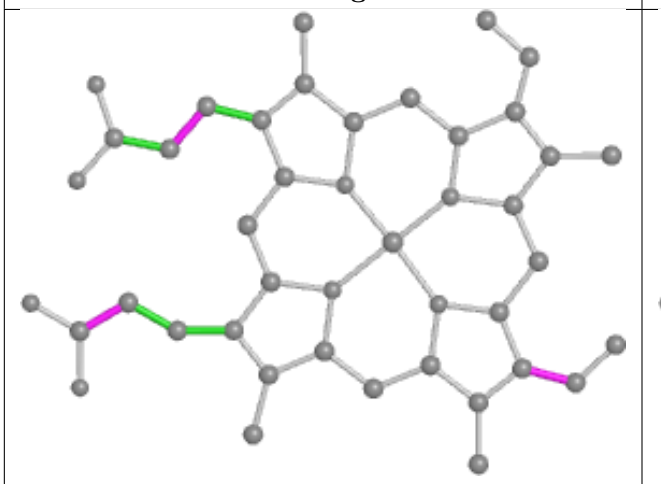

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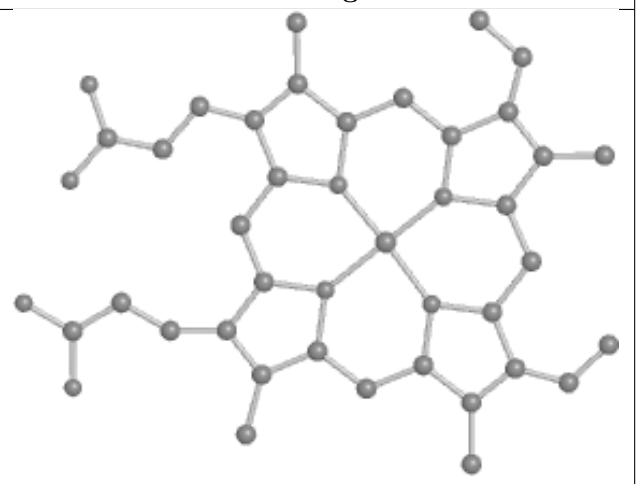
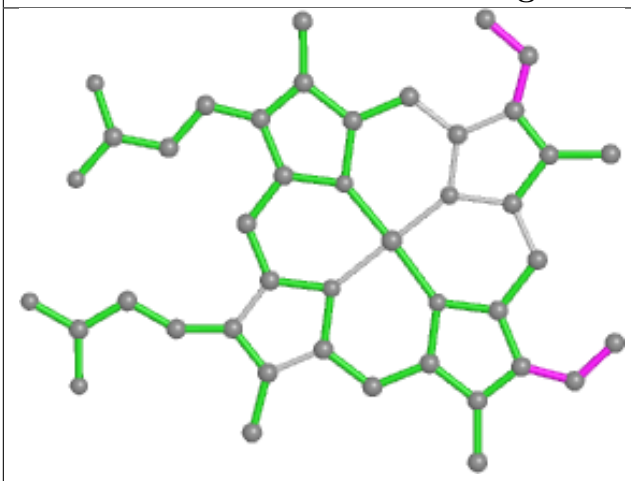


Rings

Ligand HEM K 301



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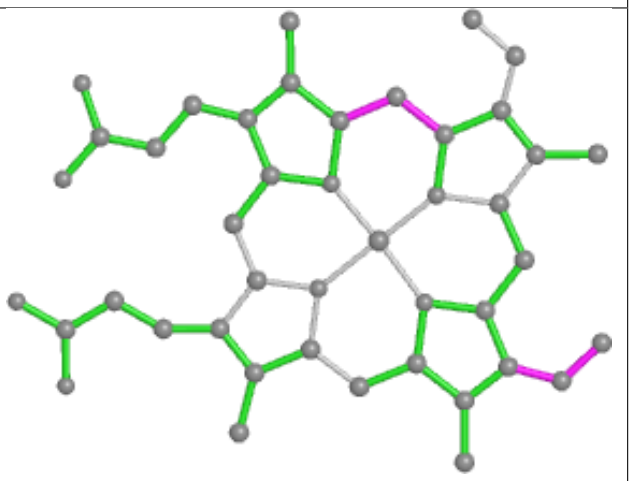
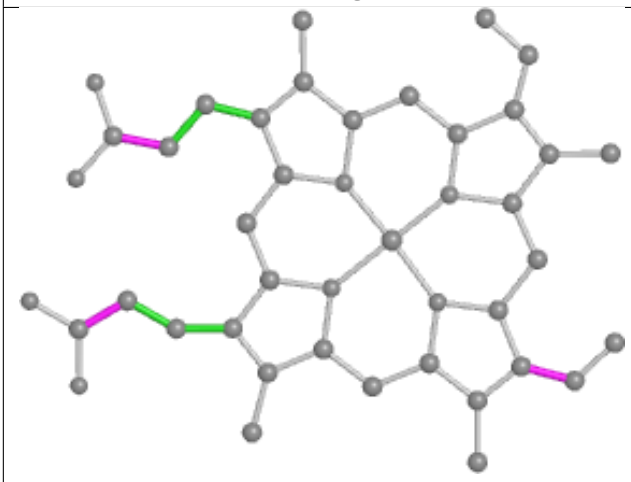


Bond angles



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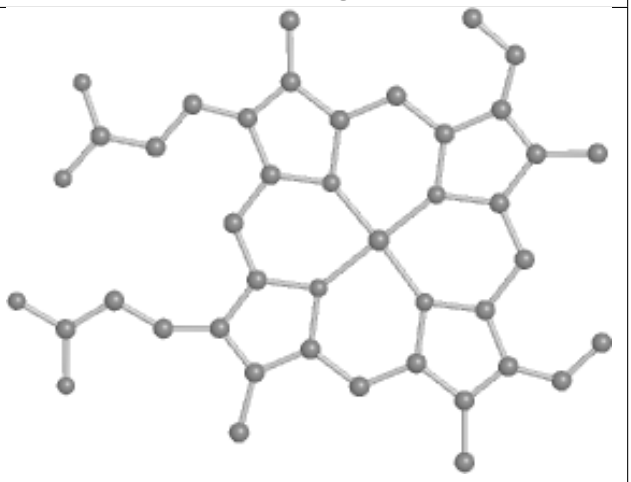
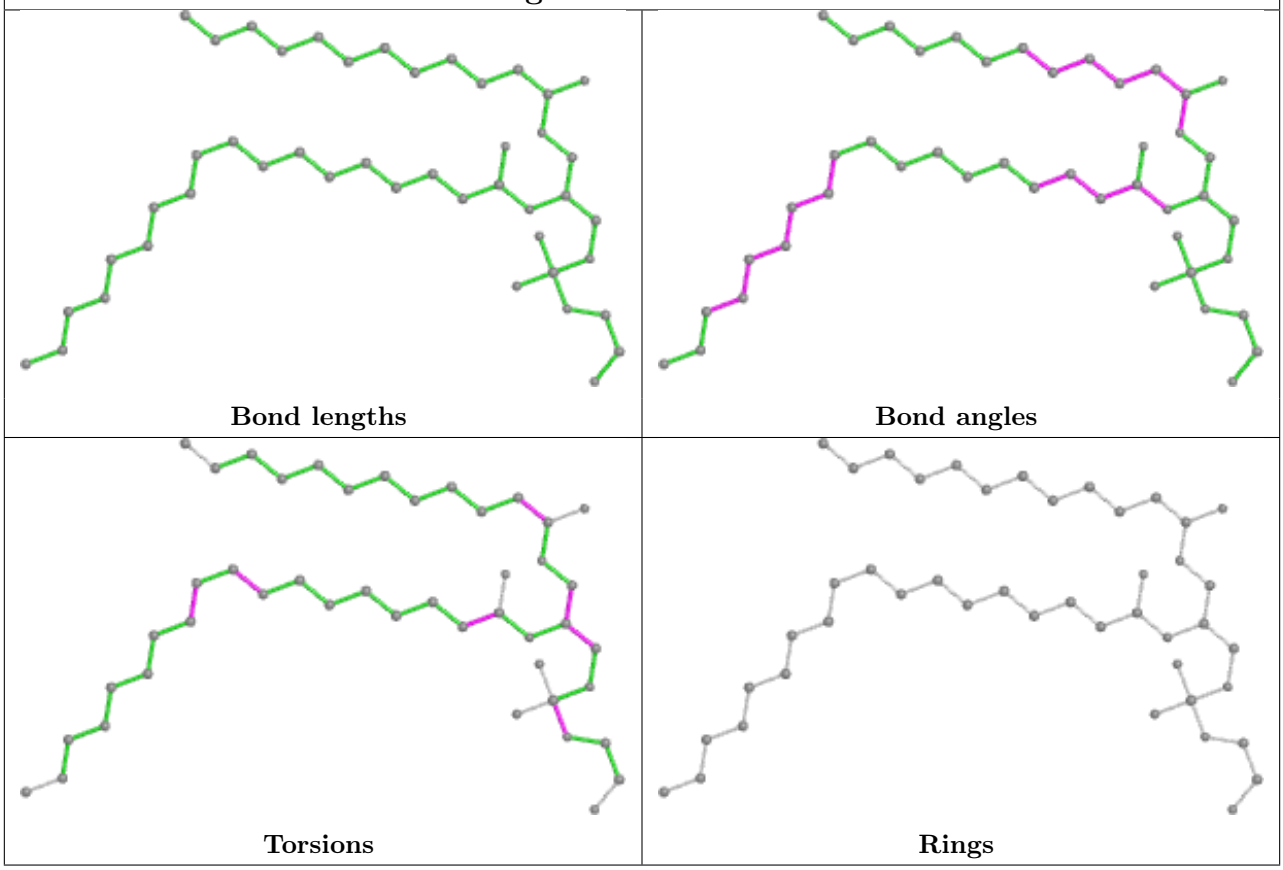
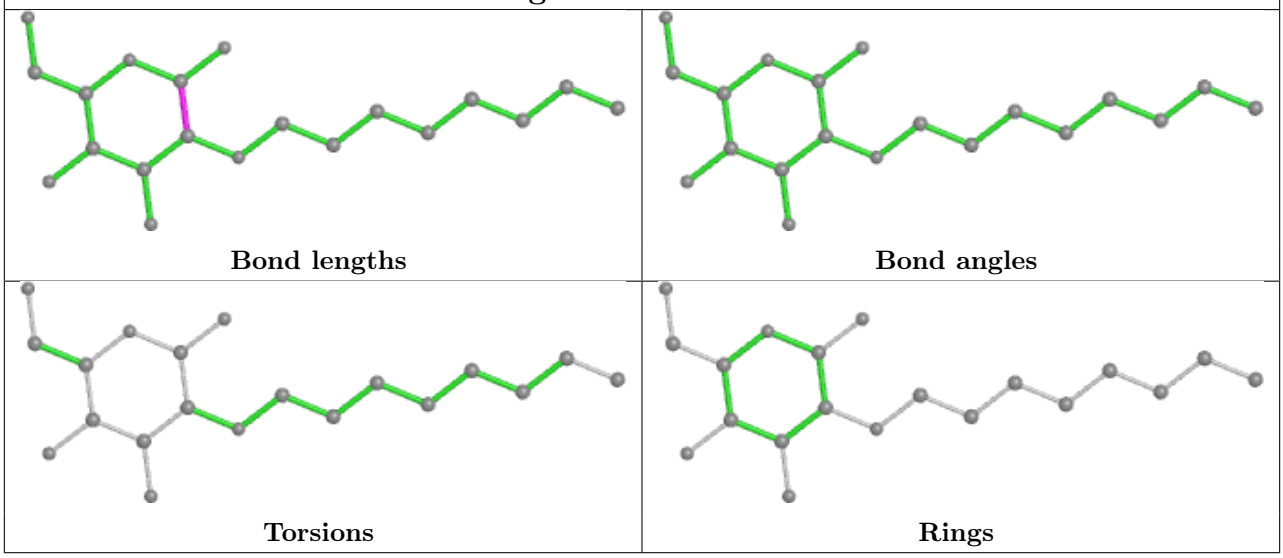


Rings

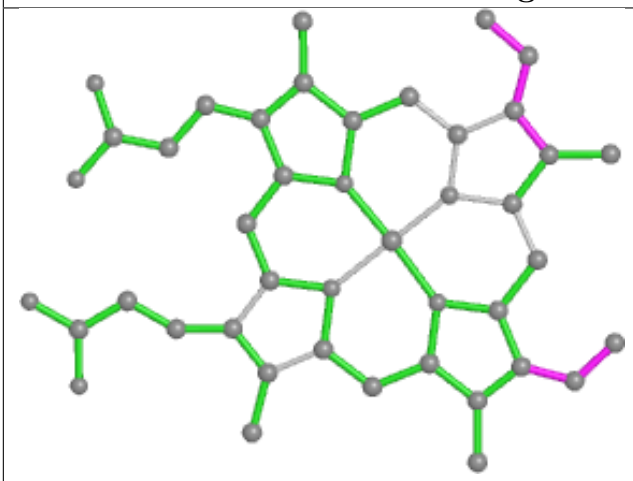
Ligand LOP A 503



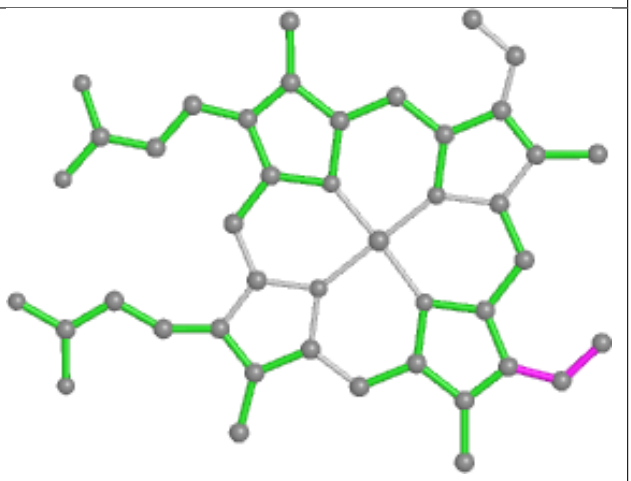
Ligand BGL J 431



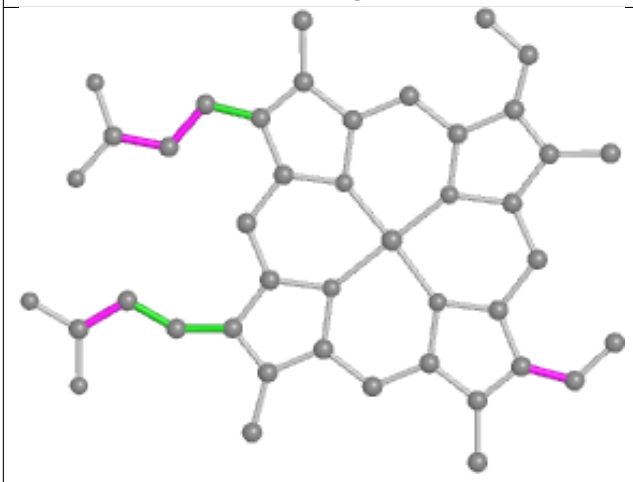
Ligand HEM G 502



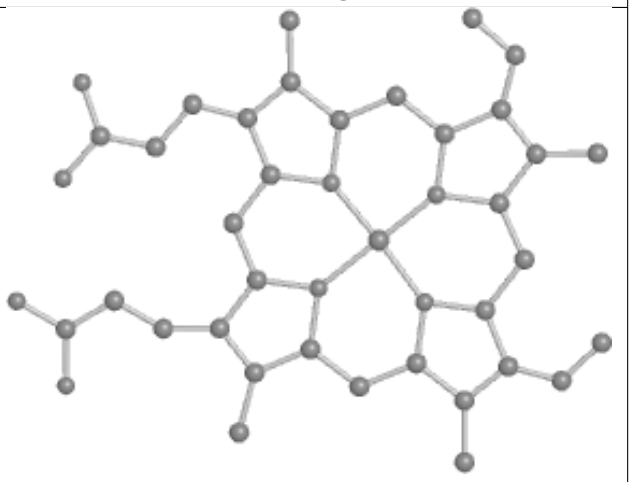
Bond lengths



Bond angles

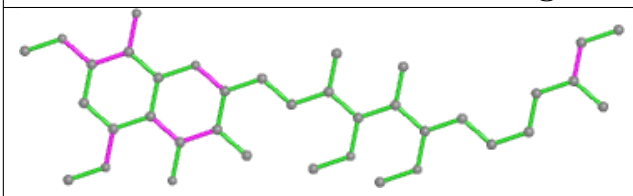


Torsions

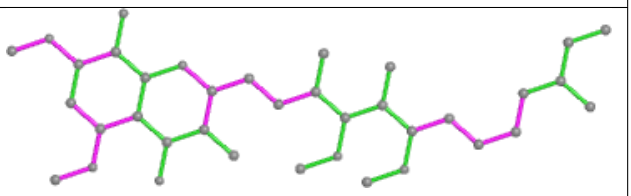


Rings

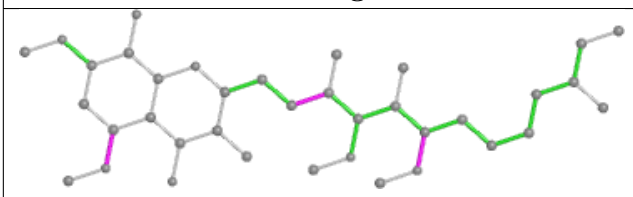
Ligand SMA D 2



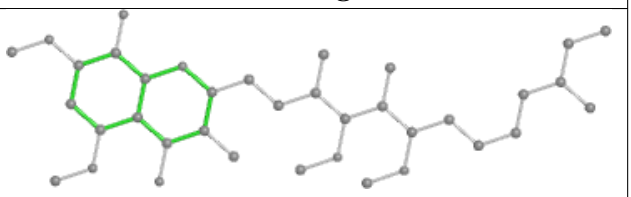
Bond lengths



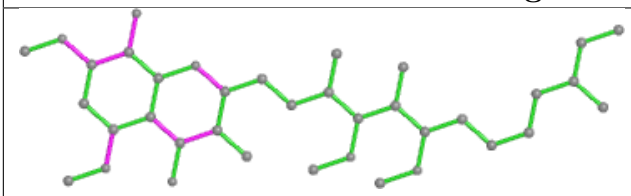
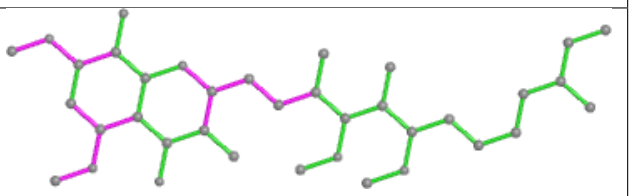
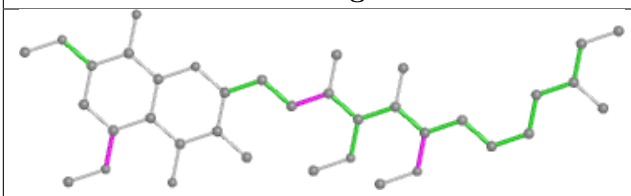
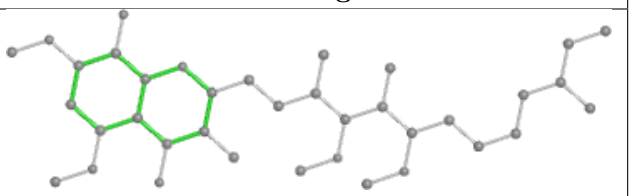
Bond angles

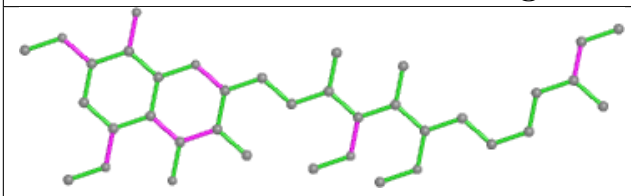
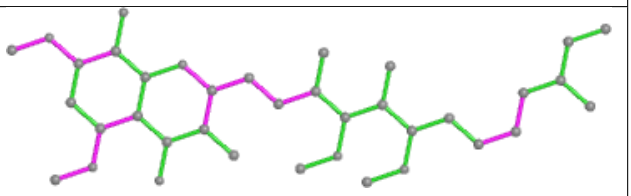
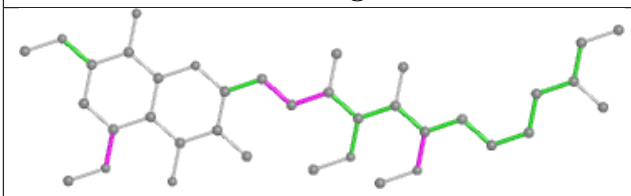
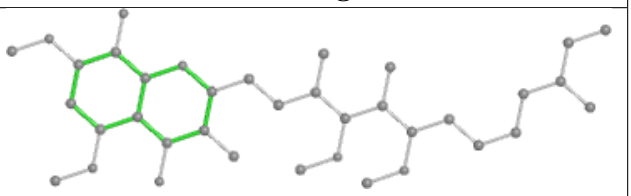


Torsions

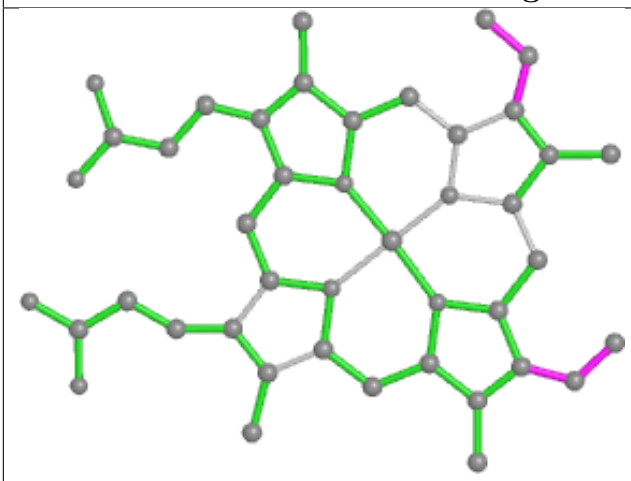


Rings

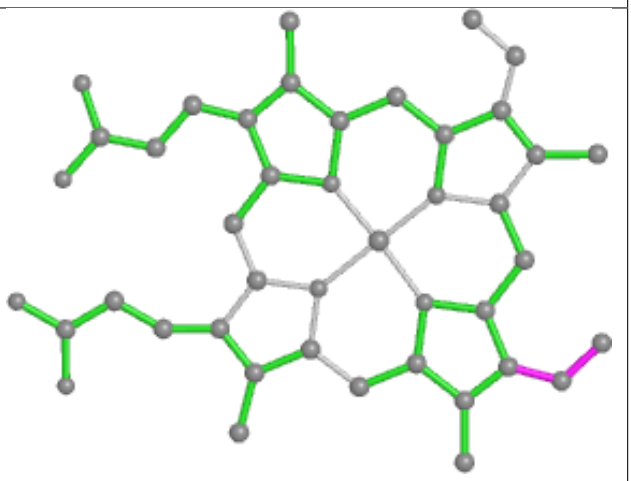
Ligand SMA J 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SMA G 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

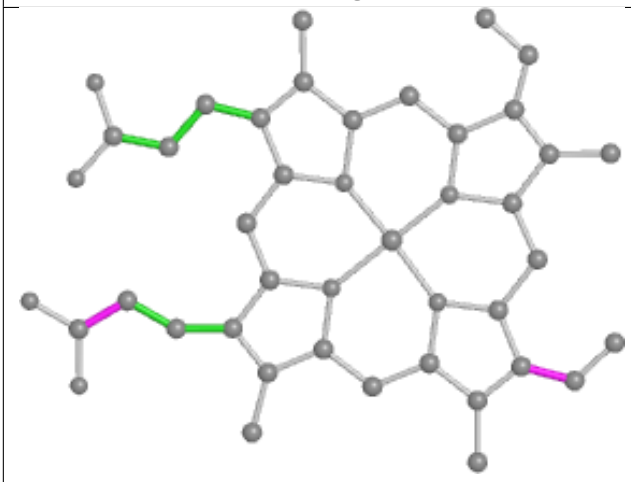
Ligand HEM J 501



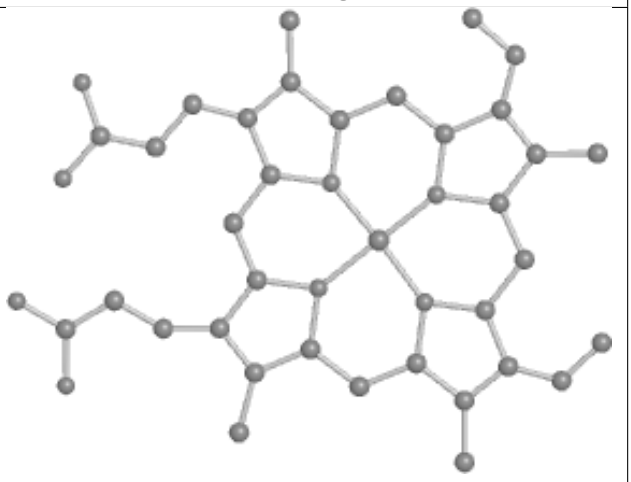
Bond lengths



Bond angles

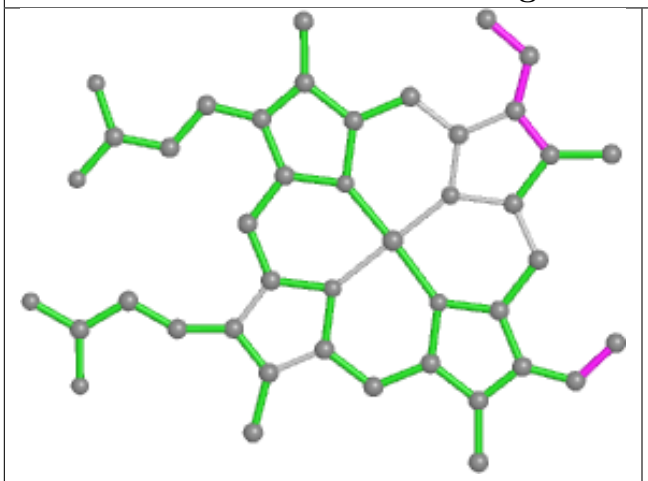


Torsions

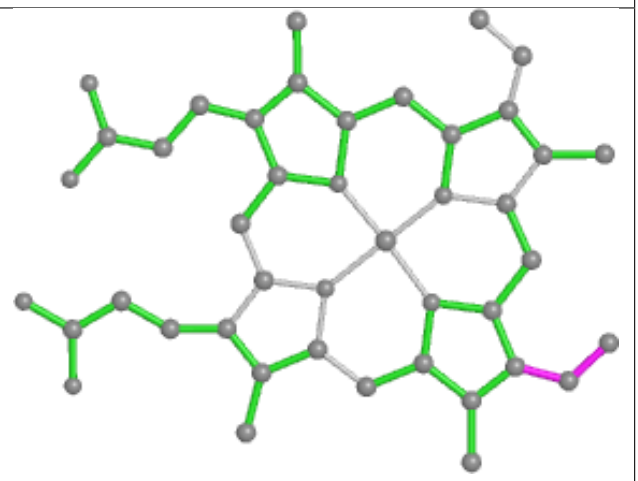


Rings

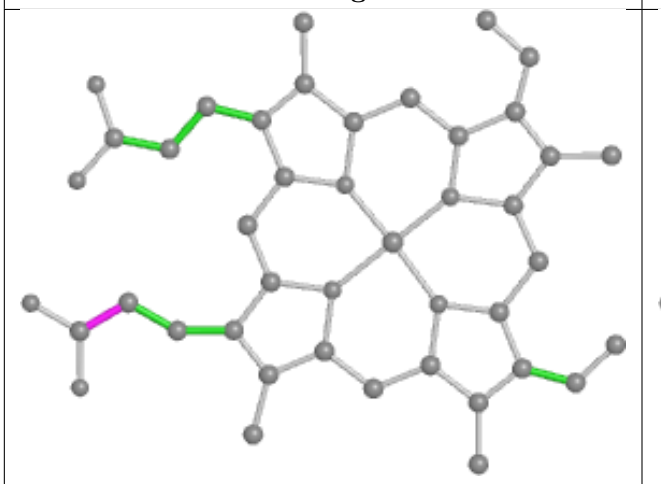
Ligand HEM A 501



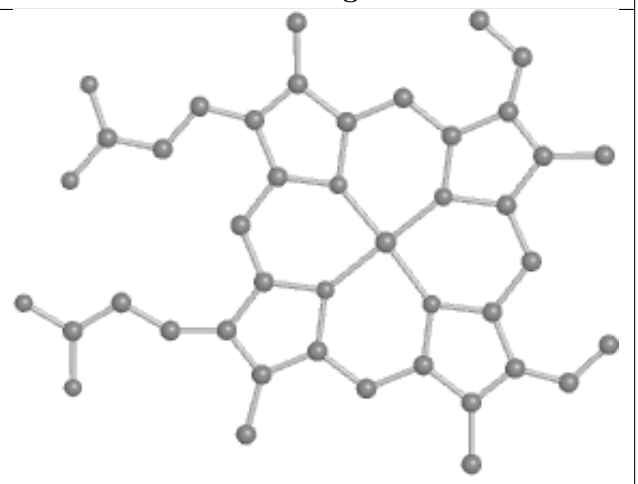
Bond lengths



Bond angles

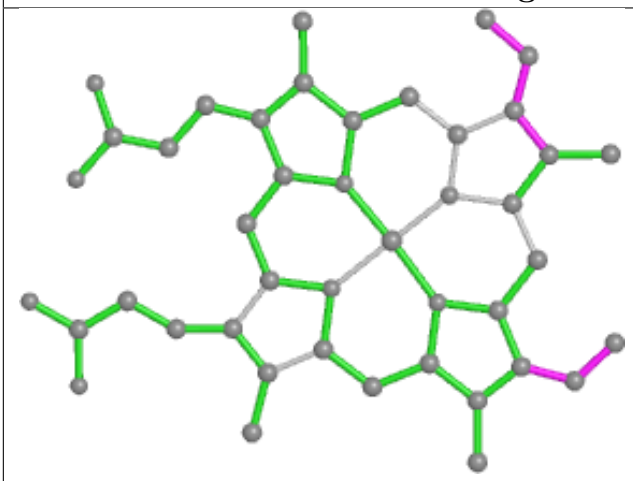


Torsions

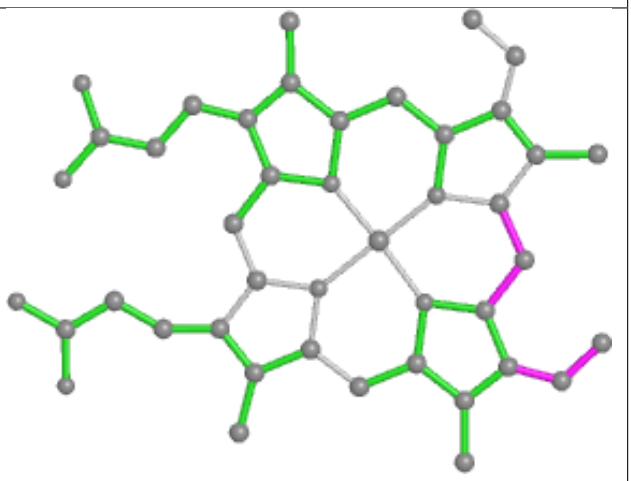


Rings

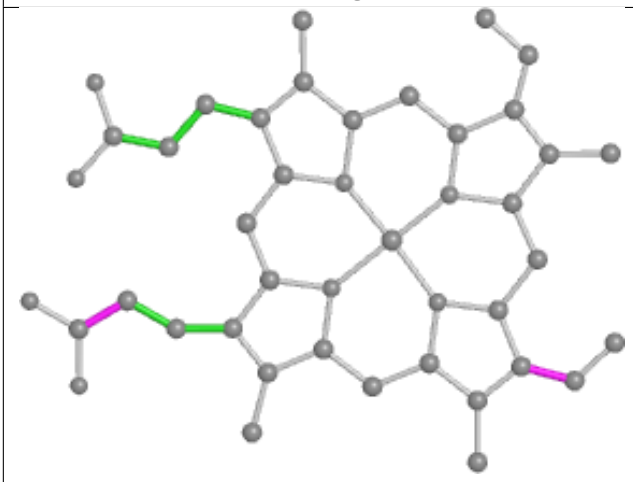
Ligand HEM D 501



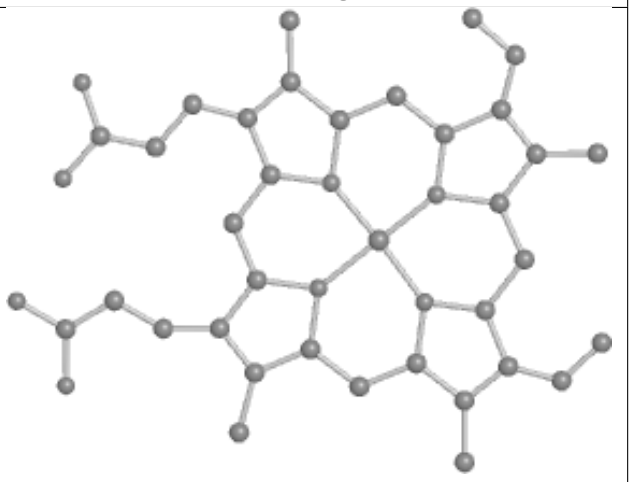
Bond lengths



Bond angles

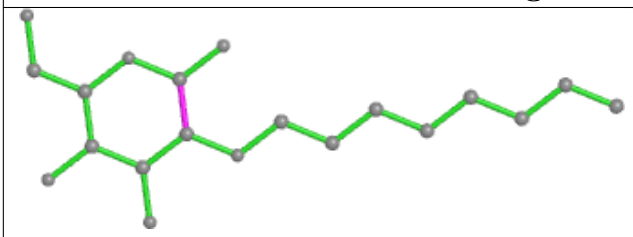


Torsions

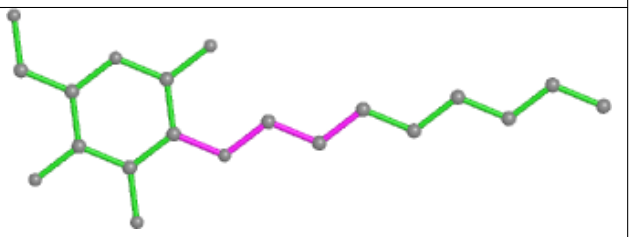


Rings

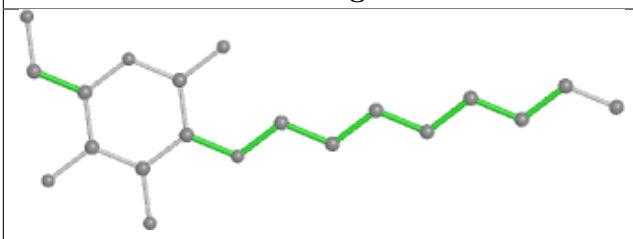
Ligand BGL E 257



Bond lengths



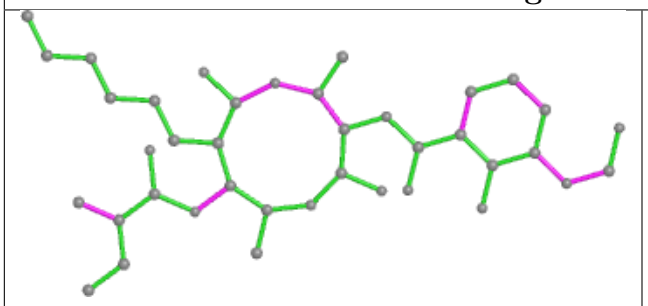
Bond angles



Torsions

Rings

Ligand ANJ G 505



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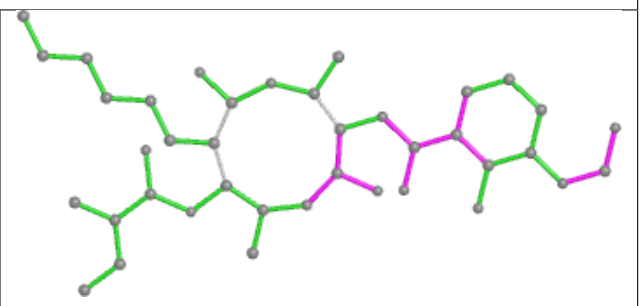
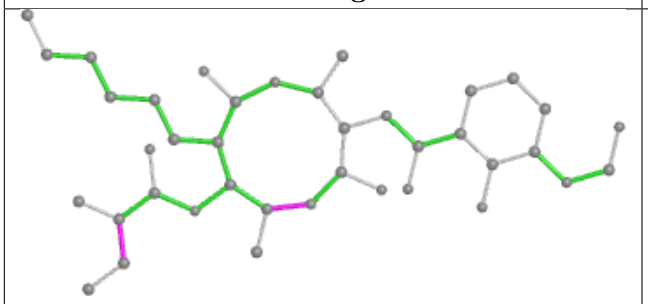
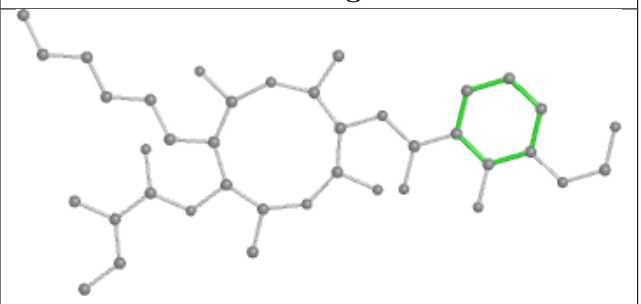


Bond angles

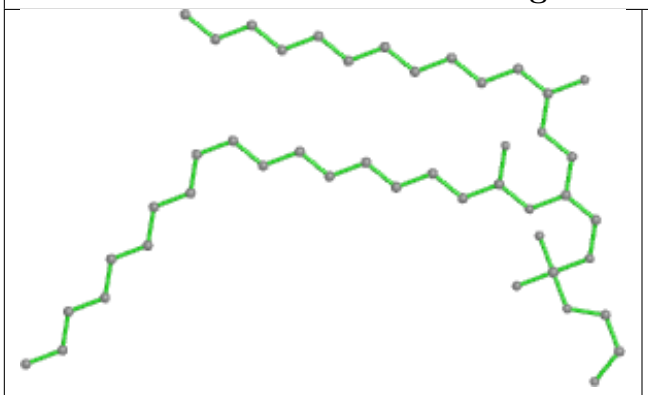


Torsions

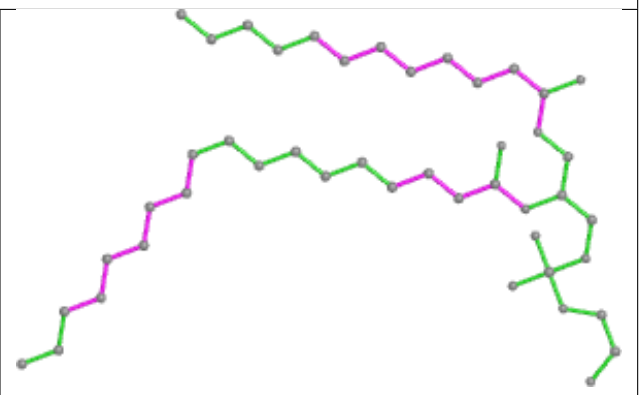


Rings

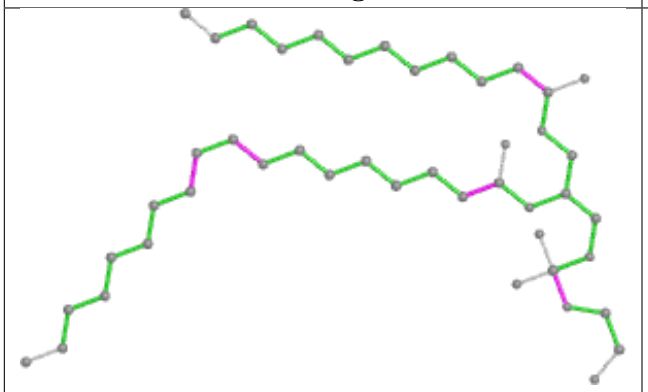
Ligand LOP J 504



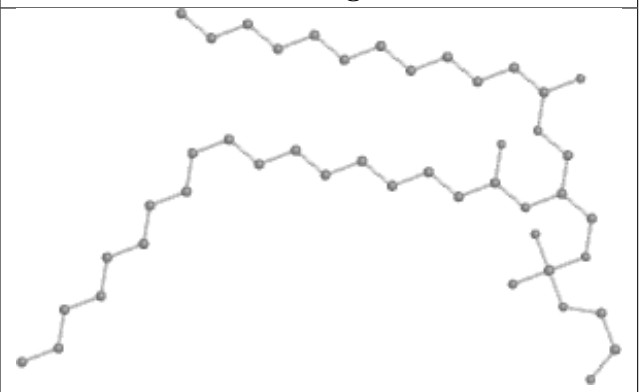
Bond lengths



Bond angles

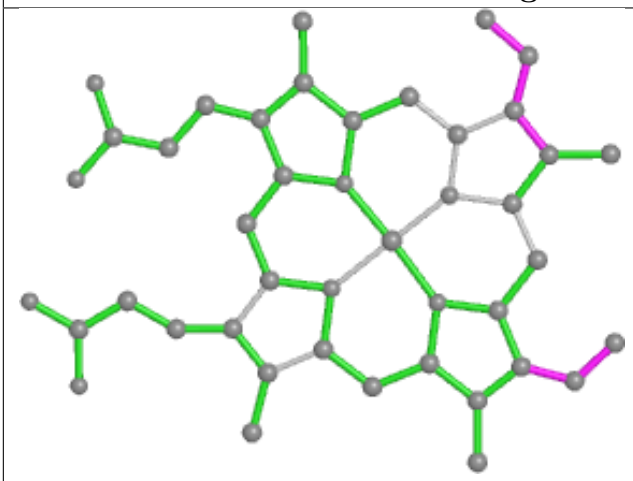


Torsions



Rings

Ligand HEM E 301



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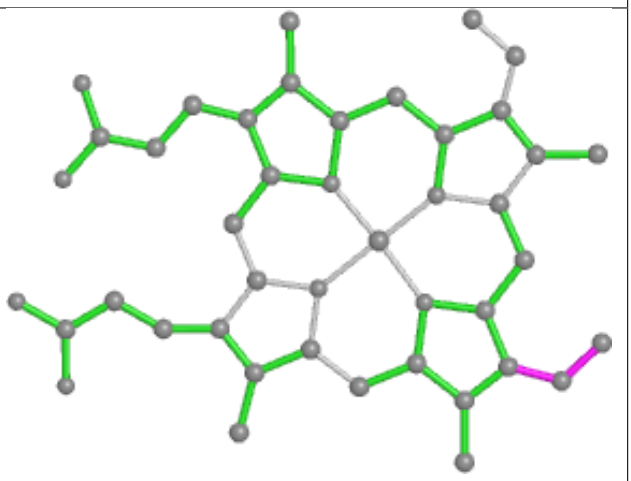
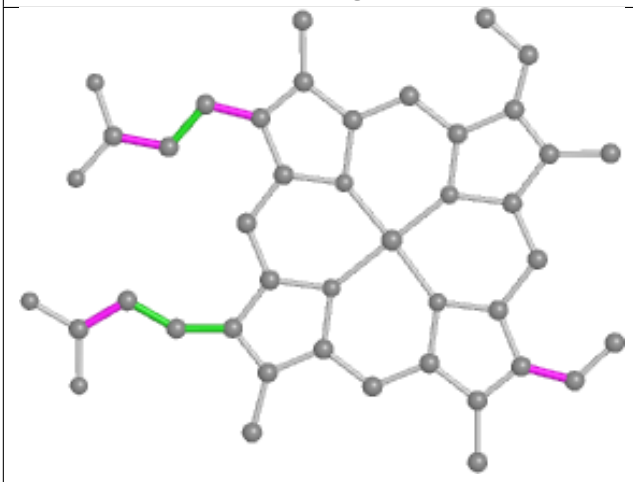
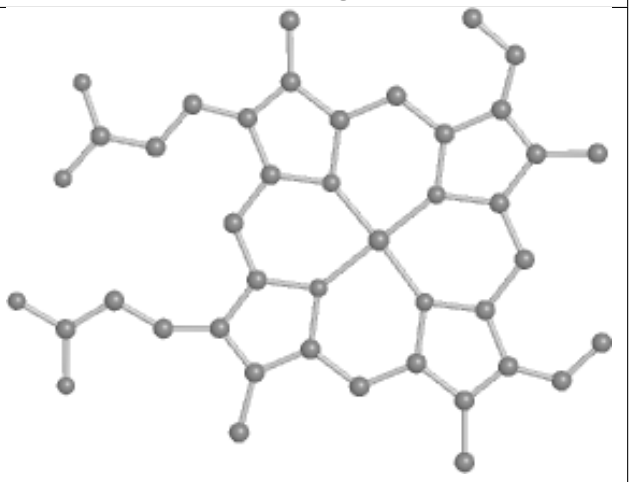


Bond angles

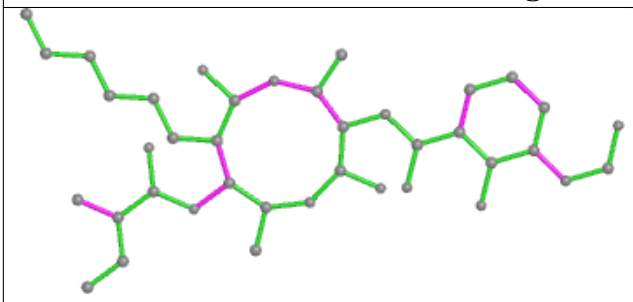


Torsions

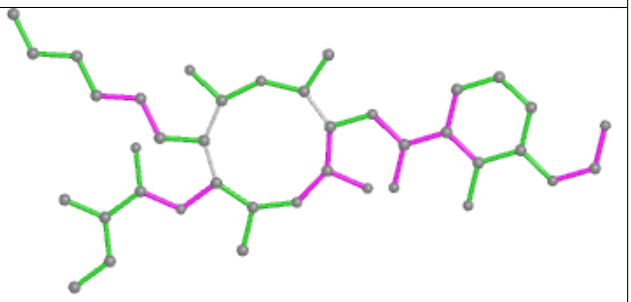


Rings

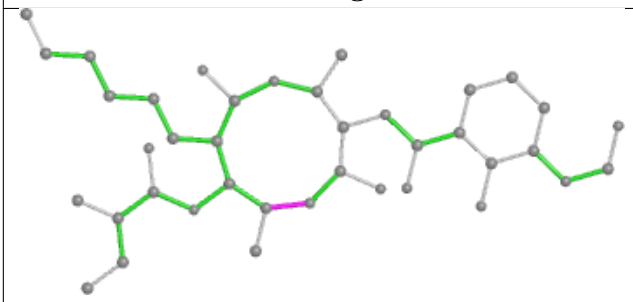
Ligand ANJ A 504



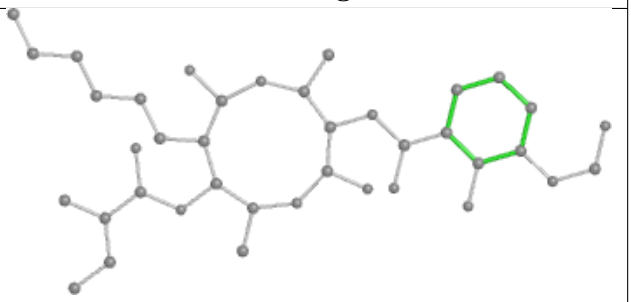
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	428/428 (100%)	0.66	27 (6%)	20	15	42, 63, 104, 129	0
1	D	428/428 (100%)	0.57	26 (6%)	21	16	43, 62, 100, 128	0
1	G	428/428 (100%)	0.57	18 (4%)	36	29	43, 64, 104, 128	0
1	J	428/428 (100%)	0.50	18 (4%)	36	29	43, 62, 100, 126	0
2	B	256/256 (100%)	0.92	37 (14%)	2	1	55, 89, 125, 149	0
2	E	256/256 (100%)	1.27	56 (21%)	0	0	65, 93, 128, 148	0
2	H	256/256 (100%)	0.88	35 (13%)	3	1	57, 90, 126, 151	0
2	K	256/256 (100%)	1.01	49 (19%)	1	0	62, 91, 127, 150	0
3	C	179/179 (100%)	0.99	25 (13%)	2	1	49, 82, 123, 155	0
3	F	179/179 (100%)	1.20	41 (22%)	0	0	49, 84, 124, 155	0
3	I	179/179 (100%)	0.93	22 (12%)	4	2	50, 83, 125, 156	0
3	L	179/179 (100%)	1.19	42 (23%)	0	0	52, 85, 124, 156	0
All	All	3452/3452 (100%)	0.81	396 (11%)	4	3	42, 75, 122, 156	0

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2	GLY	12.6
2	K	4	GLY	12.5
2	B	2	GLY	11.5
2	K	3	GLY	11.3
3	I	9	GLY	11.3
3	F	10	THR	10.9
3	C	9	GLY	10.8
2	K	1	ALA	10.8
2	E	4	GLY	10.0
3	F	11	ARG	10.0
3	F	12	ARG	9.8

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Mol	Chain	Res	Type	RSRZ
3	C	12	ARG	9.7
3	L	12	ARG	9.6
3	I	10	THR	9.0
2	E	1	ALA	8.4
2	H	2	GLY	8.4
2	B	1	ALA	8.4
2	K	110	PHE	8.1
3	L	10	THR	8.0
2	H	1	ALA	8.0
2	K	6	VAL	7.9
3	C	11	ARG	7.8
3	L	52	VAL	7.5
3	C	16	TYR	7.5
3	I	179	ILE	7.4
3	C	10	THR	7.4
2	H	4	GLY	7.4
3	C	179	ILE	7.3
2	K	122	PHE	6.9
2	K	5	HIS	6.8
3	L	11	ARG	6.6
2	H	3	GLY	6.5
2	E	150	GLU	6.4
2	E	143	PRO	6.4
3	F	184	ILE	6.4
1	J	9	TYR	6.3
2	E	5	HIS	6.2
2	E	187	PRO	6.1
3	L	179	ILE	5.9
2	E	9	VAL	5.8
3	L	184	ILE	5.8
3	F	14	PHE	5.7
3	L	123	LEU	5.7
3	F	9	GLY	5.6
1	D	9	TYR	5.5
2	K	124	GLY	5.5
2	E	144	LYS	5.4
3	L	178	PHE	5.4
2	E	7	GLU	5.4
3	L	9	GLY	5.3
1	G	12	ARG	5.2
3	L	116	LEU	5.1
3	I	46	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
3	I	178	PHE	5.1
1	D	13	THR	5.1
2	E	3	GLY	5.0
1	A	414	ILE	5.0
3	C	15	LEU	5.0
1	A	12	ARG	4.9
2	E	124	GLY	4.9
2	H	5	HIS	4.9
2	B	5	HIS	4.8
1	D	8	HIS	4.8
3	F	13	ASP	4.8
2	K	7	GLU	4.8
2	E	142	PRO	4.7
1	A	13	THR	4.7
2	E	149	HIS	4.7
2	H	251	LEU	4.7
3	F	179	ILE	4.7
1	A	15	ILE	4.6
1	J	11	PRO	4.6
3	L	182	THR	4.6
3	I	181	GLU	4.5
1	D	15	ILE	4.5
3	F	116	LEU	4.5
2	K	143	PRO	4.5
2	B	122	PHE	4.4
3	F	47	LEU	4.4
2	B	250	ARG	4.3
2	B	110	PHE	4.3
1	D	11	PRO	4.3
1	J	10	GLU	4.3
3	L	48	ALA	4.3
2	E	11	PHE	4.2
2	K	132	TYR	4.2
2	E	145	CYS	4.2
1	D	12	ARG	4.2
2	H	147	GLU	4.2
2	E	147	GLU	4.2
2	B	206	ALA	4.2
3	L	183	THR	4.2
1	J	12	ARG	4.2
3	F	17	TYR	4.1
3	F	51	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
3	L	17	TYR	4.1
3	I	183	THR	4.1
3	I	11	ARG	4.0
2	E	193	LEU	4.0
3	F	124	VAL	4.0
2	B	182	TRP	4.0
2	E	208	ALA	4.0
3	L	14	PHE	3.9
1	G	362	MET	3.9
3	L	181	GLU	3.9
3	F	18	ALA	3.9
2	K	204	VAL	3.9
3	F	123	LEU	3.9
3	F	103	ILE	3.9
1	G	414	ILE	3.9
2	K	109	GLY	3.8
2	E	111	HIS	3.8
2	H	72	VAL	3.8
3	L	124	VAL	3.8
3	I	12	ARG	3.8
1	G	17	LYS	3.8
1	G	416	LYS	3.8
3	L	187	GLY	3.8
3	C	181	GLU	3.7
2	E	58	LEU	3.7
2	E	155	TYR	3.7
3	L	103	ILE	3.7
1	A	11	PRO	3.7
3	L	68	LEU	3.7
1	D	10	GLU	3.7
2	B	116	THR	3.7
2	H	82	GLU	3.7
1	G	250	ILE	3.7
2	E	182	TRP	3.6
3	C	122	TRP	3.6
2	E	10	PRO	3.6
2	B	252	TRP	3.6
2	E	96	ASN	3.6
1	J	16	GLU	3.6
1	G	11	PRO	3.6
1	A	18	TRP	3.5
3	L	13	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	256	LYS	3.5
3	F	52	VAL	3.5
2	E	158	ARG	3.5
2	B	251	LEU	3.5
2	H	121	LEU	3.5
3	L	47	LEU	3.5
3	I	17	TYR	3.4
2	E	151	PRO	3.4
2	H	198	ASP	3.4
1	D	170	PRO	3.4
2	K	8	ASP	3.4
1	A	232	THR	3.4
1	J	8	HIS	3.4
2	E	34	GLU	3.4
2	K	11	PHE	3.4
2	E	178	THR	3.4
1	D	20	HIS	3.4
1	A	357	GLY	3.4
3	I	67	PHE	3.4
1	G	18	TRP	3.4
2	K	9	VAL	3.4
1	A	14	GLY	3.4
1	G	3	GLY	3.4
1	D	323	PHE	3.3
3	C	123	LEU	3.3
3	F	183	THR	3.3
2	H	83	GLY	3.3
2	B	121	LEU	3.3
3	F	182	THR	3.3
1	A	416	LYS	3.3
2	K	196	TYR	3.3
1	A	8	HIS	3.3
3	C	18	ALA	3.3
2	E	189	LEU	3.3
2	E	94	LEU	3.3
2	B	243	LEU	3.2
2	H	151	PRO	3.2
2	E	6	VAL	3.2
2	K	2	GLY	3.2
1	A	413	ALA	3.2
2	B	4	GLY	3.2
1	D	235	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	122	TRP	3.2
3	F	178	PHE	3.2
1	G	15	ILE	3.2
3	F	56	SER	3.2
3	F	16	TYR	3.2
3	L	74	ILE	3.2
1	D	14	GLY	3.2
3	L	63	LEU	3.2
3	C	101	ALA	3.1
2	E	146	ALA	3.1
2	K	114	MET	3.1
2	E	139	PRO	3.1
1	A	415	GLU	3.1
1	D	247	TYR	3.1
1	J	247	TYR	3.1
2	B	114	MET	3.1
2	E	207	MET	3.1
2	H	182	TRP	3.1
3	L	122	TRP	3.1
1	G	429	ASN	3.1
2	H	123	ASN	3.0
2	E	255	VAL	3.0
1	A	16	GLU	3.0
2	K	208	ALA	3.0
3	F	15	LEU	3.0
2	E	110	PHE	3.0
2	B	255	VAL	3.0
3	C	178	PHE	3.0
2	B	151	PRO	3.0
2	K	256	LYS	3.0
3	I	174	PRO	3.0
3	L	73	PHE	2.9
2	E	184	ALA	2.9
1	D	362	MET	2.9
3	L	16	TYR	2.9
2	K	142	PRO	2.9
3	F	98	ALA	2.9
2	H	110	PHE	2.9
2	B	79	GLU	2.9
3	I	16	TYR	2.9
2	H	149	HIS	2.8
3	C	68	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	247	THR	2.8
2	K	58	LEU	2.8
3	I	120	GLY	2.8
1	A	324	GLY	2.8
1	D	234	LYS	2.8
2	H	79	GLU	2.8
2	E	8	ASP	2.8
2	E	246	LEU	2.8
2	H	122	PHE	2.8
3	C	175	LEU	2.8
3	F	114	ARG	2.7
2	H	165	VAL	2.7
2	E	196	TYR	2.7
2	K	123	ASN	2.7
3	C	63	LEU	2.7
1	A	428	PHE	2.7
3	C	57	VAL	2.7
2	K	147	GLU	2.7
2	E	191	ASP	2.7
2	K	10	PRO	2.6
1	J	20	HIS	2.6
2	H	189	LEU	2.6
1	A	320	PHE	2.6
2	E	141	GLU	2.6
2	K	155	TYR	2.6
2	E	153	GLY	2.6
3	C	19	THR	2.6
2	H	67	ALA	2.6
3	L	104	ASP	2.6
1	G	430	ALA	2.6
1	A	174	HIS	2.6
2	E	205	HIS	2.6
2	E	135	LEU	2.6
3	F	48	ALA	2.6
1	G	13	THR	2.6
2	H	250	ARG	2.6
2	K	200	HIS	2.6
3	I	101	ALA	2.6
2	H	69	GLN	2.6
3	F	112	GLN	2.6
3	L	57	VAL	2.6
3	I	177	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	14	GLY	2.6
3	C	67	PHE	2.6
1	A	411	LEU	2.6
3	F	186	LEU	2.6
3	C	174	PRO	2.5
2	B	253	ALA	2.5
2	B	72	VAL	2.5
3	F	68	LEU	2.5
2	E	154	PHE	2.5
1	A	196	SER	2.5
2	B	196	TYR	2.5
1	J	184	PRO	2.5
3	L	50	ILE	2.5
3	I	79	GLU	2.5
1	A	325	ILE	2.5
1	J	13	THR	2.5
2	H	145	CYS	2.5
3	I	122	TRP	2.5
2	E	125	ILE	2.5
2	E	148	GLY	2.5
1	J	17	LYS	2.5
2	H	231	PHE	2.5
1	D	70	THR	2.5
2	K	205	HIS	2.5
1	D	30	TYR	2.5
2	H	146	ALA	2.4
2	H	244	LEU	2.4
1	G	16	GLU	2.4
3	F	74	ILE	2.4
3	L	75	ARG	2.4
1	J	31	ASP	2.4
2	K	13	PHE	2.4
2	K	189	LEU	2.4
1	A	356	SER	2.4
3	L	105	ALA	2.4
1	J	4	ILE	2.4
1	J	414	ILE	2.4
3	L	51	PHE	2.4
2	H	200	HIS	2.4
2	K	145	CYS	2.4
2	K	251	LEU	2.4
2	H	150	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	5	PRO	2.4
3	I	74	ILE	2.4
3	F	65	VAL	2.4
3	I	150	PRO	2.4
1	D	288	THR	2.4
2	K	153	GLY	2.4
1	G	148	VAL	2.4
3	L	101	ALA	2.3
3	F	118	GLU	2.3
2	E	190	MET	2.3
3	C	17	TYR	2.3
3	C	74	ILE	2.3
3	F	57	VAL	2.3
2	H	58	LEU	2.3
3	F	177	LYS	2.3
1	D	202	PRO	2.3
2	E	256	LYS	2.3
1	D	83	ILE	2.3
2	H	143	PRO	2.3
2	E	12	SER	2.3
2	K	190	MET	2.3
1	A	359	TYR	2.3
1	J	15	ILE	2.3
3	L	53	ASP	2.3
2	K	249	LYS	2.3
2	B	23	HIS	2.2
2	K	94	LEU	2.2
2	B	197	ALA	2.2
2	K	178	THR	2.2
2	H	144	LYS	2.2
2	H	158	ARG	2.2
2	H	208	ALA	2.2
3	C	142	GLY	2.2
2	B	140	GLU	2.2
3	F	72	ILE	2.2
3	L	175	LEU	2.2
1	D	236	GLU	2.2
3	L	45	GLN	2.2
2	K	156	TYR	2.2
3	I	51	PHE	2.2
2	B	80	ASP	2.2
2	K	154	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	186	LEU	2.2
2	B	117	GLY	2.2
2	K	223	LEU	2.1
3	C	149	CYS	2.1
1	A	236	GLU	2.1
1	G	172	ILE	2.1
2	B	155	TYR	2.1
3	L	180	ASP	2.1
2	E	250	ARG	2.1
2	K	207	MET	2.1
2	B	231	PHE	2.1
1	D	172	ILE	2.1
2	E	140	GLU	2.1
2	K	57	GLU	2.1
3	F	108	GLU	2.1
3	F	119	ALA	2.1
1	J	323	PHE	2.1
2	B	118	ILE	2.1
2	E	192	ASP	2.1
2	K	141	GLU	2.1
1	D	325	ILE	2.1
2	E	175	VAL	2.1
3	L	65	VAL	2.1
1	G	141	ALA	2.1
2	B	123	ASN	2.1
3	F	19	THR	2.1
1	A	226	GLY	2.1
2	B	3	GLY	2.1
1	D	150	PRO	2.1
1	A	283	ALA	2.1
2	K	206	ALA	2.1
2	B	147	GLU	2.1
2	K	125	ILE	2.1
3	L	119	ALA	2.1
3	L	115	THR	2.1
1	D	331	PHE	2.1
1	J	320	PHE	2.1
1	A	227	VAL	2.0
2	K	24	GLN	2.0
3	F	46	ALA	2.0
3	F	107	ALA	2.0
2	B	109	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	208	ALA	2.0
3	L	160	GLY	2.0
1	J	6	HIS	2.0
2	B	194	VAL	2.0
3	I	180	ASP	2.0
2	K	23	HIS	2.0
2	K	149	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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	SR	E	258	1/1	0.75	0.08	126,126,126,126	0
9	SR	H	257	1/1	0.75	0.09	117,117,117,117	0
4	BGL	J	431	20/20	0.76	0.37	95,96,100,101	0
4	BGL	G	431	20/20	0.79	0.37	97,99,102,102	0
4	BGL	A	431	20/20	0.82	0.33	89,92,93,93	0
7	LOP	J	504	45/45	0.84	0.28	81,84,95,97	0
4	BGL	E	257	20/20	0.84	0.36	101,101,102,102	0
7	LOP	G	504	45/45	0.84	0.23	70,87,96,98	0
7	LOP	A	503	45/45	0.86	0.23	79,99,105,107	0
9	SR	J	432	1/1	0.86	0.30	114,114,114,114	0
9	SR	K	257	1/1	0.87	0.04	144,144,144,144	0
9	SR	G	432	1/1	0.88	0.26	135,135,135,135	0
7	LOP	D	503	45/45	0.88	0.24	75,88,94,94	0
8	ANJ	D	504	39/39	0.92	0.21	49,66,79,82	0
8	ANJ	G	505	39/39	0.92	0.25	69,72,79,81	0
8	ANJ	J	505	39/39	0.92	0.21	51,67,82,85	0

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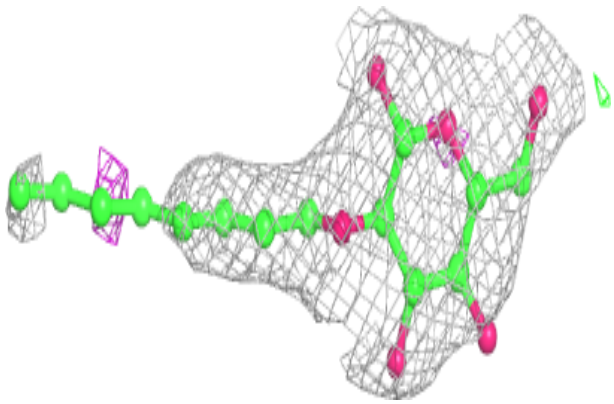
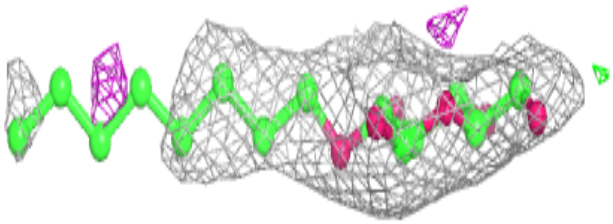
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SMA	J	503	37/37	0.92	0.24	45,50,56,56	0
9	SR	B	257	1/1	0.93	0.07	126,126,126,126	0
8	ANJ	A	504	39/39	0.93	0.24	70,74,77,78	0
6	SMA	D	2	37/37	0.93	0.25	47,53,62,64	0
6	SMA	G	503	37/37	0.94	0.22	51,58,60,62	0
6	SMA	A	1	37/37	0.94	0.23	46,55,58,58	0
5	HEM	K	301	43/43	0.95	0.21	73,79,80,81	0
5	HEM	D	501	43/43	0.96	0.19	60,61,62,64	0
5	HEM	D	502	43/43	0.96	0.23	34,42,45,46	0
5	HEM	E	301	43/43	0.96	0.21	74,80,81,81	0
5	HEM	G	502	43/43	0.96	0.24	47,52,54,54	0
5	HEM	H	301	43/43	0.96	0.22	66,70,71,72	0
5	HEM	A	501	43/43	0.96	0.19	61,64,70,73	0
5	HEM	A	502	43/43	0.96	0.24	43,47,51,52	0
5	HEM	B	301	43/43	0.96	0.22	61,65,67,69	0
5	HEM	J	501	43/43	0.97	0.19	55,56,57,58	0
5	HEM	J	502	43/43	0.97	0.22	36,43,47,48	0
5	HEM	G	501	43/43	0.97	0.23	55,59,63,65	0
10	FES	C	200	4/4	0.97	0.19	54,54,54,54	0
10	FES	F	200	4/4	0.98	0.18	55,55,55,55	0
10	FES	I	200	4/4	0.98	0.21	53,53,54,54	0
10	FES	L	200	4/4	0.98	0.22	56,57,57,57	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 BGL J 431:

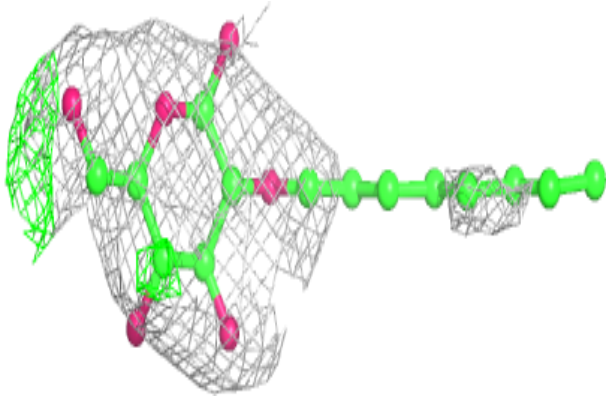
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

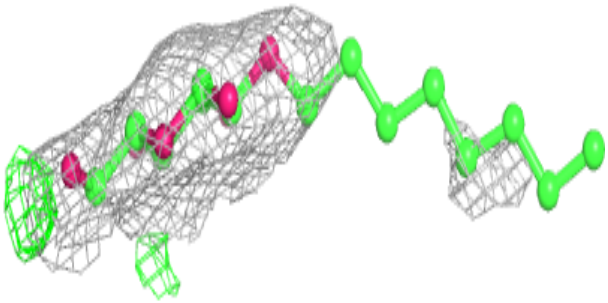


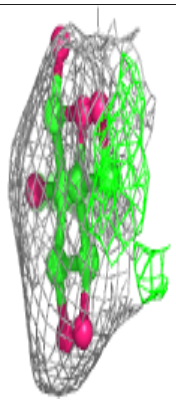


Electron density around BGL G 431:

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

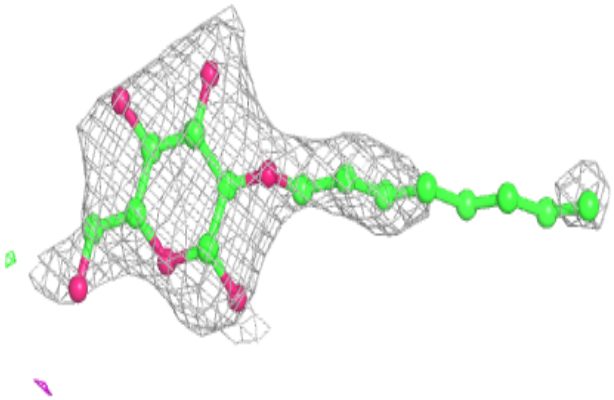


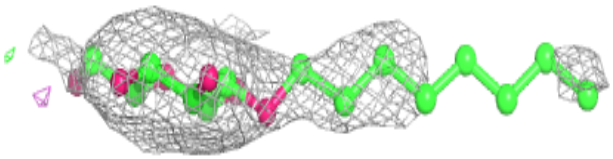


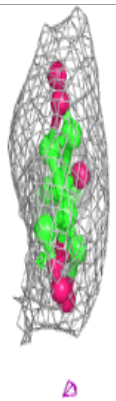


Electron density around BGL A 431:

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

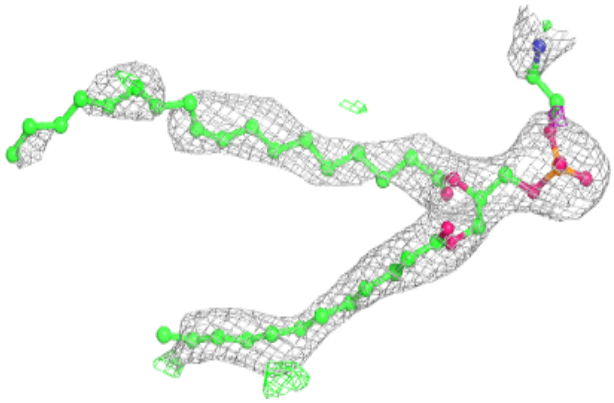


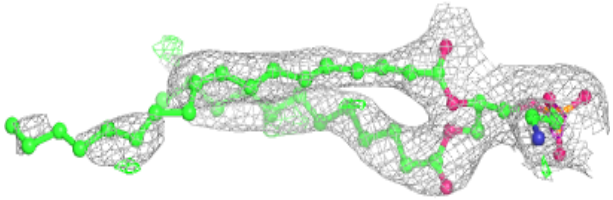


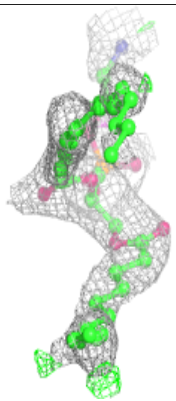


Electron density around LOP J 504:

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

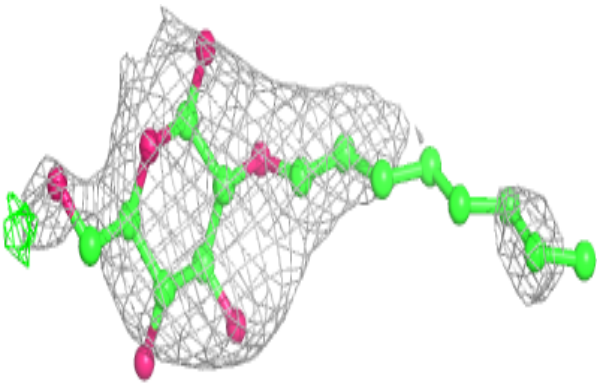


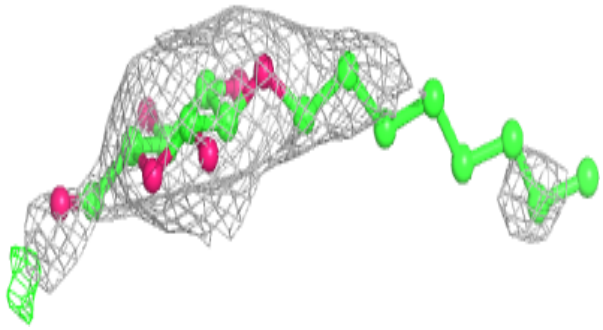


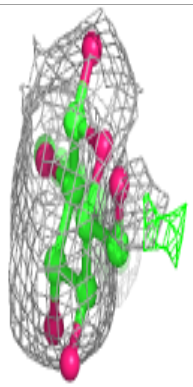


Electron density around BGL E 257:

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

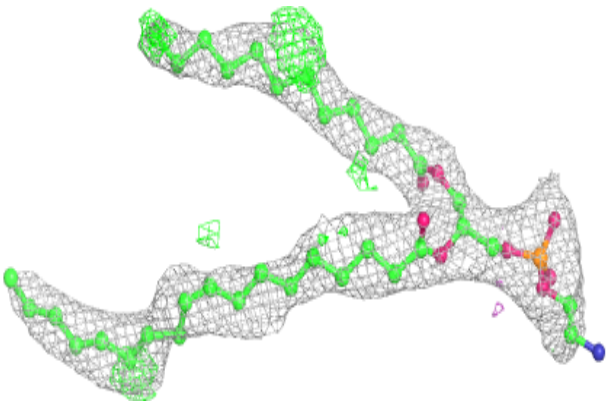


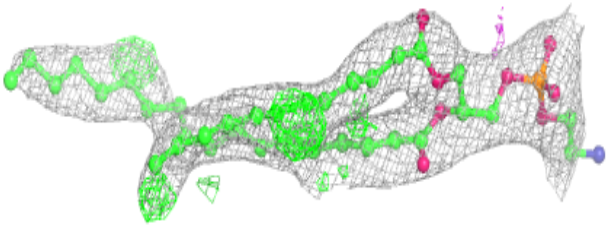


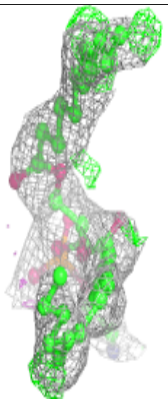


Electron density around LOP G 504:

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

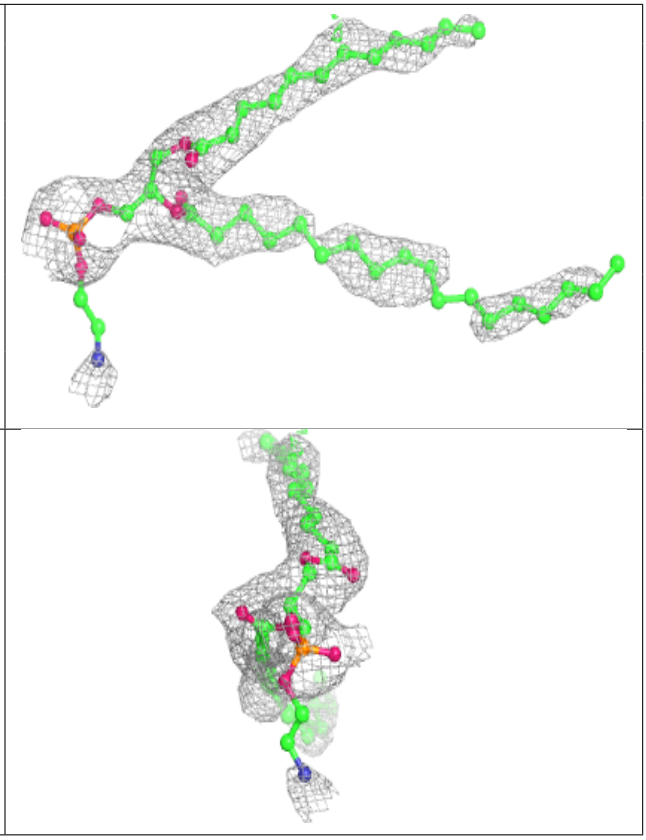






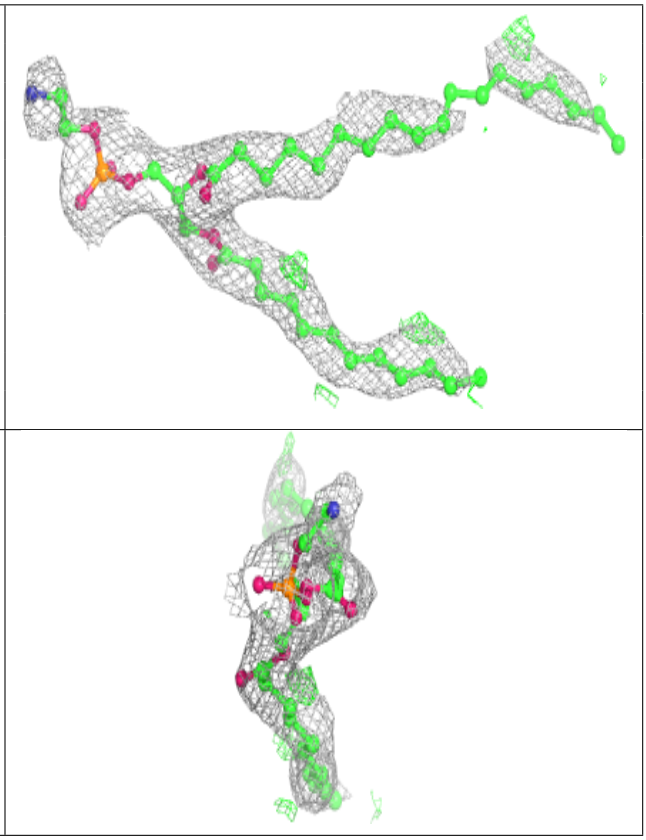
Electron density around LOP A 503:

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



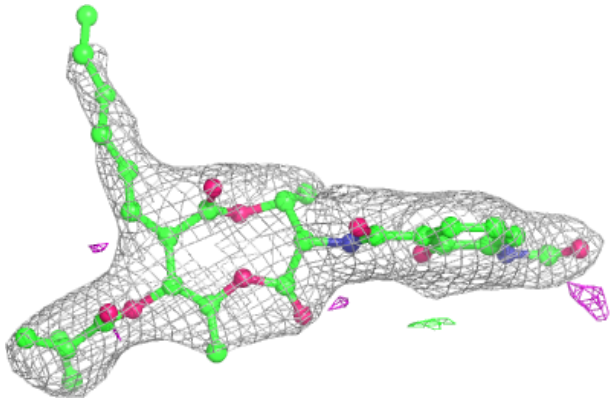
Electron density around LOP D 503:

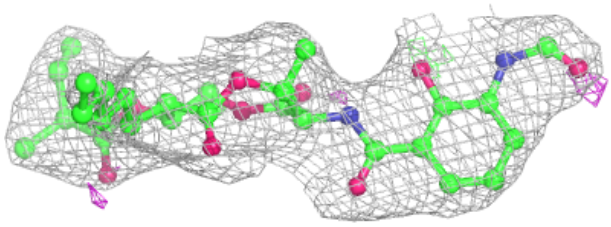
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

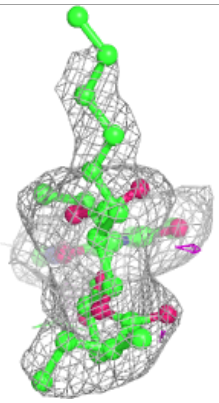


Electron density around ANJ D 504:

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

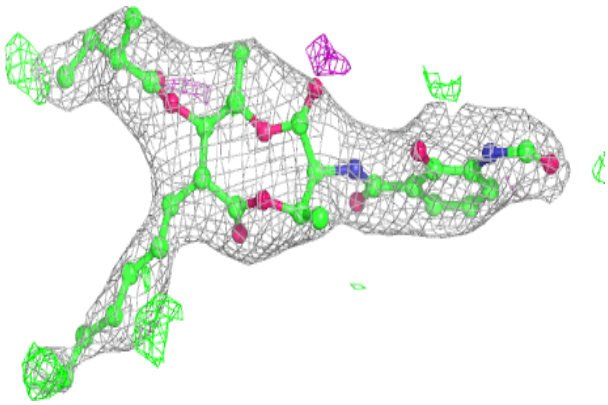


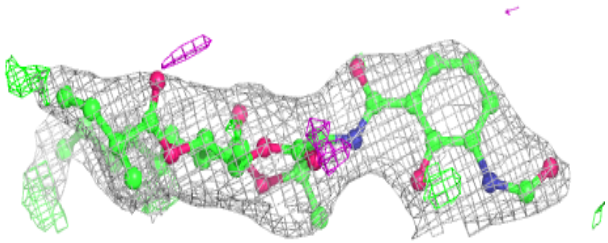


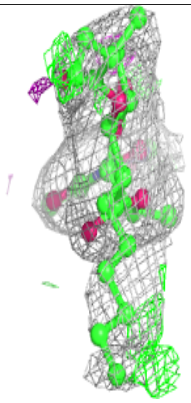


Electron density around ANJ G 505:

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

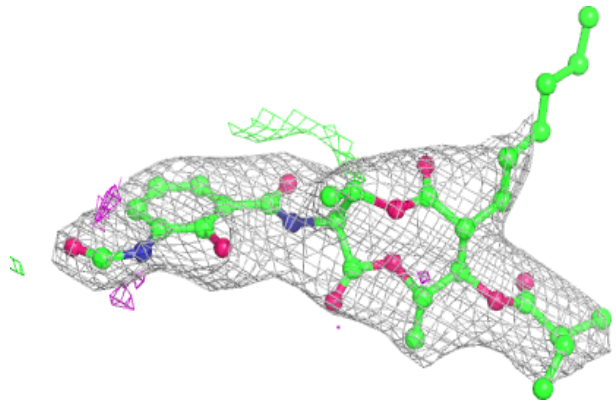


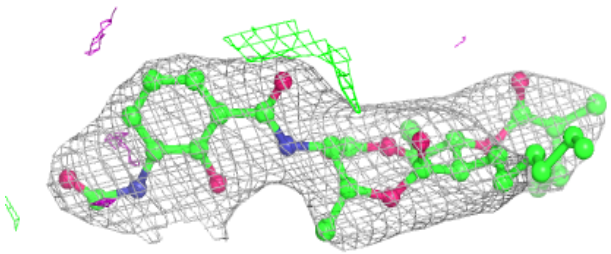


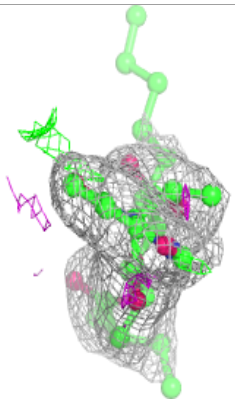


Electron density around ANJ J 505:

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

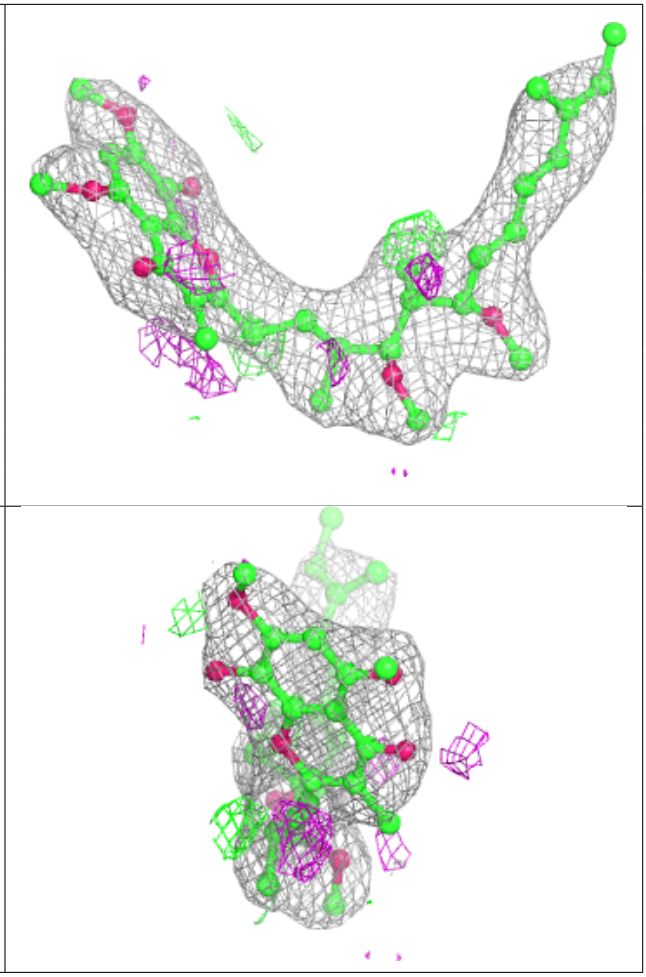






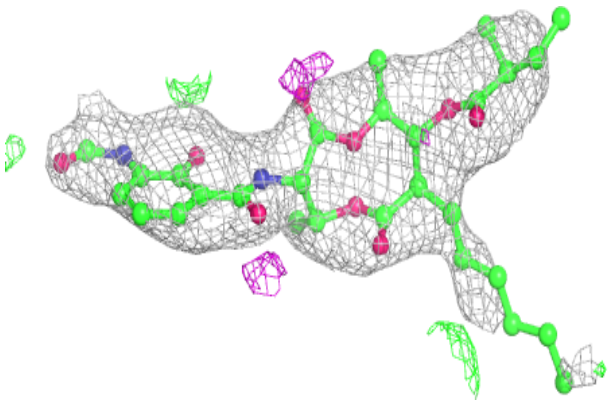
Electron density around SMA J 503:

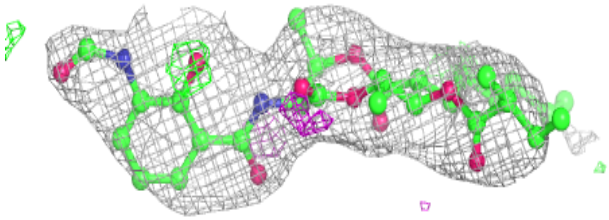
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

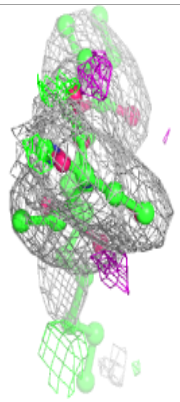


Electron density around ANJ A 504:

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

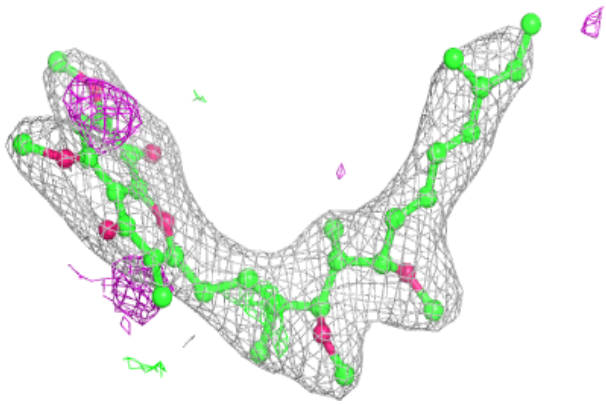


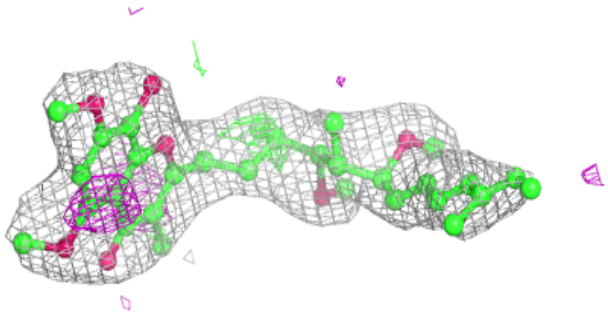


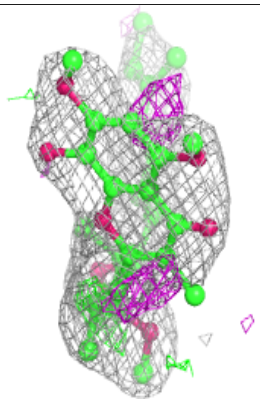


Electron density around SMA D 2:

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

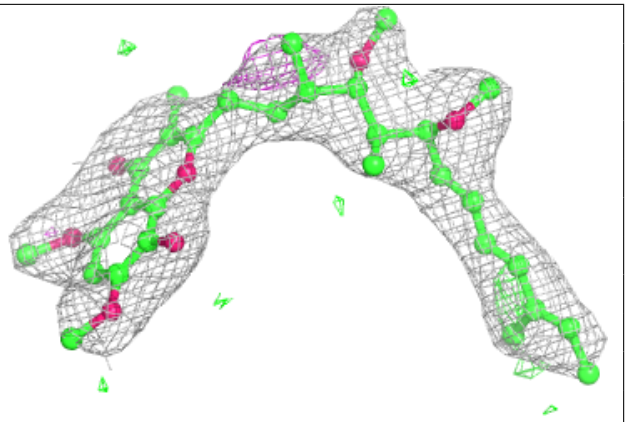


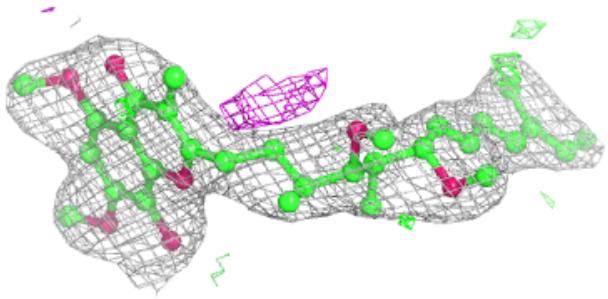


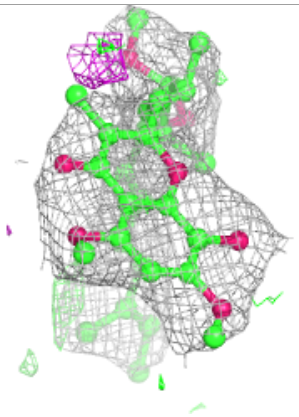


Electron density around SMA G 503:

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

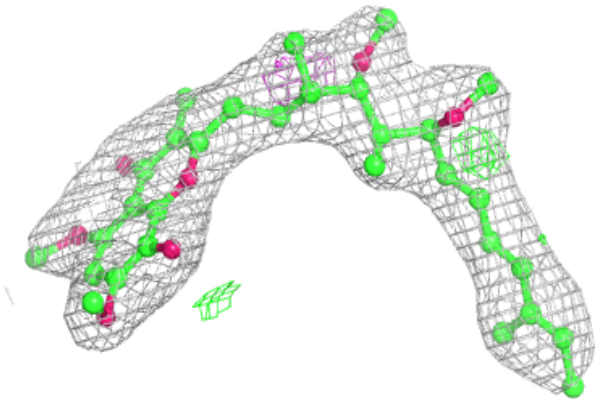


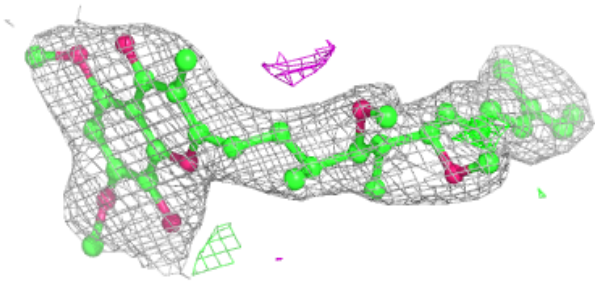


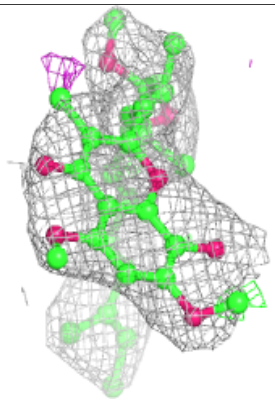


Electron density around SMA A 1:

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

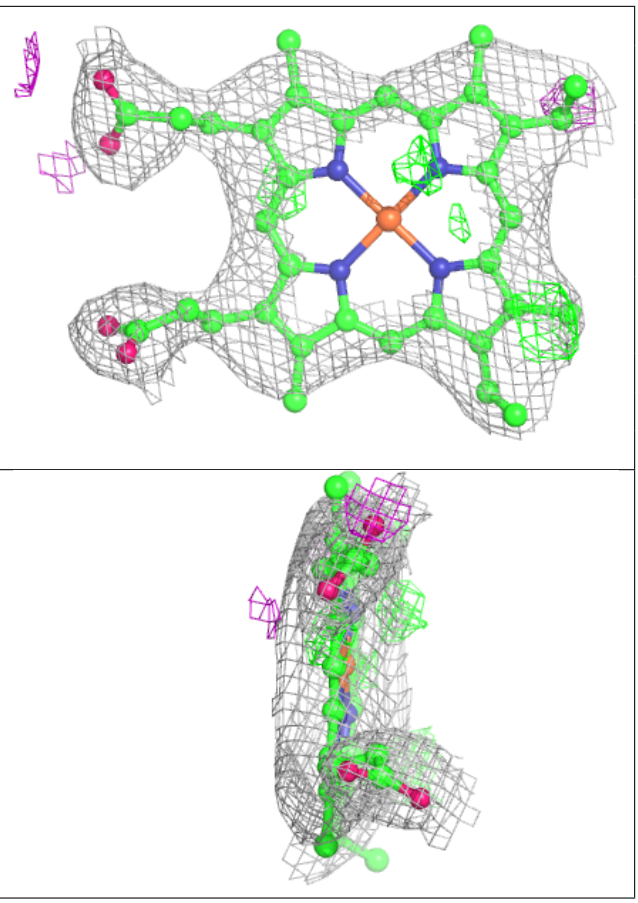






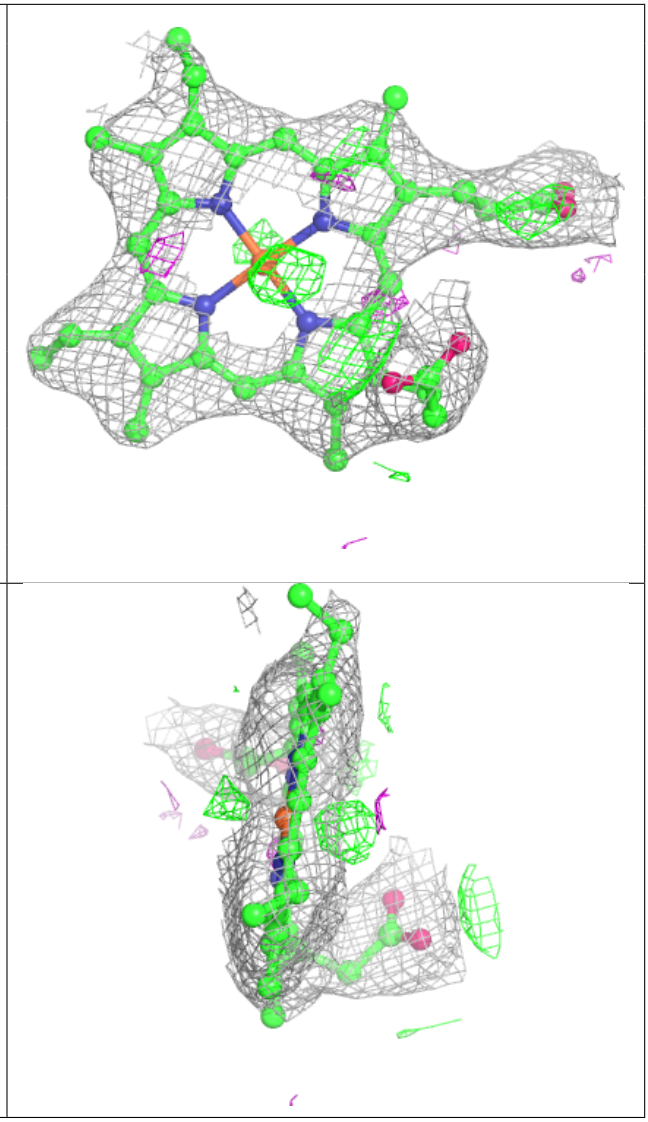
Electron density around HEM K 301:

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



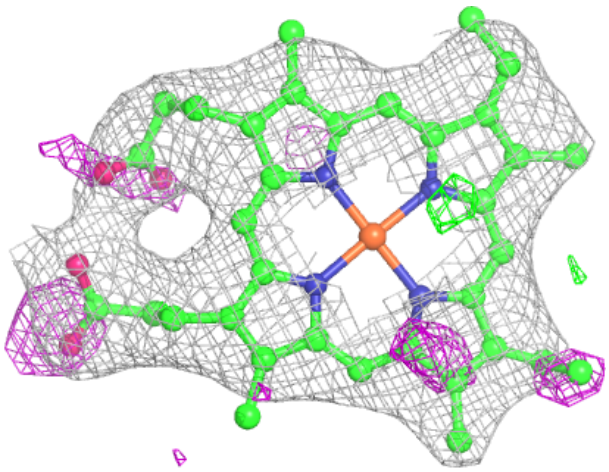
Electron density around HEM D 501:

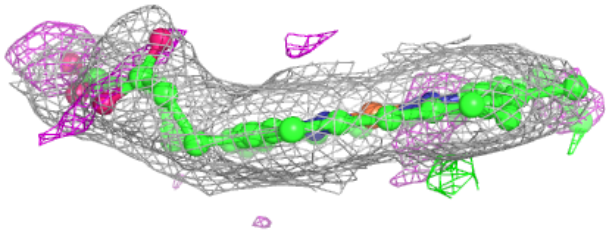
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

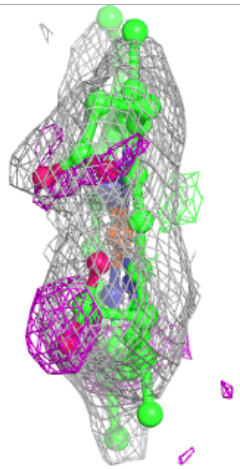


Electron density around HEM D 502:

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

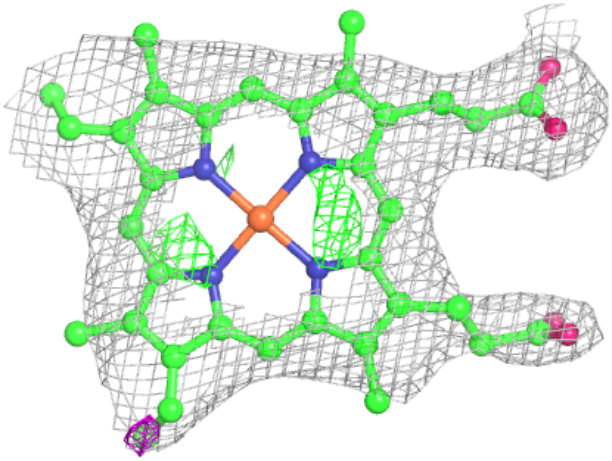


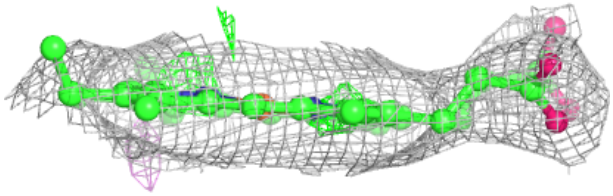


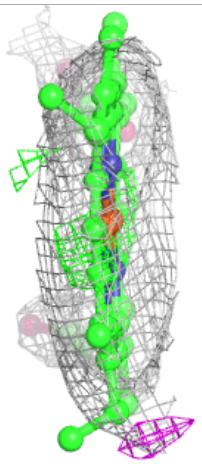


Electron density around HEM E 301:

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

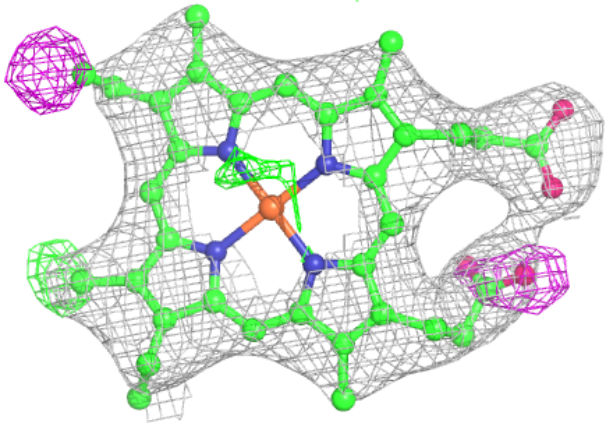


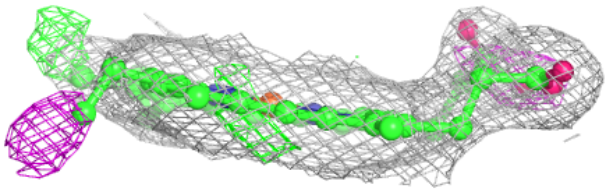


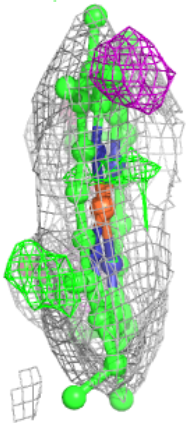


Electron density around HEM G 502:

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

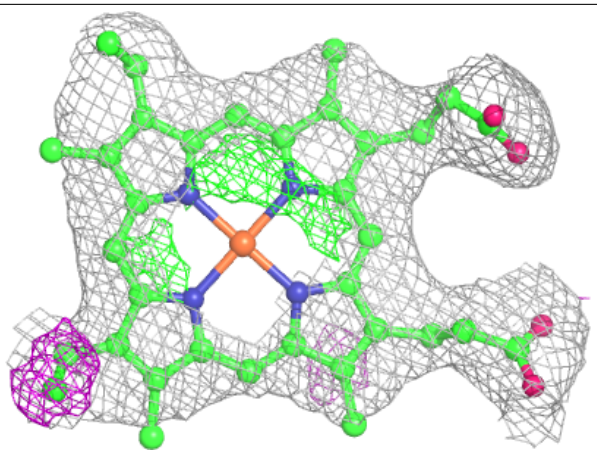


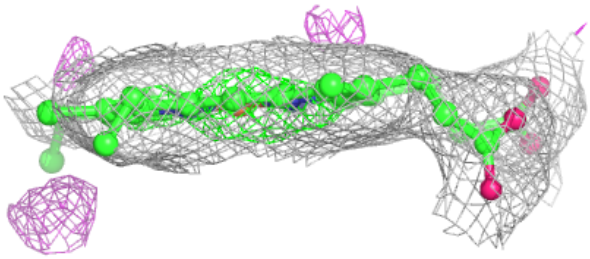


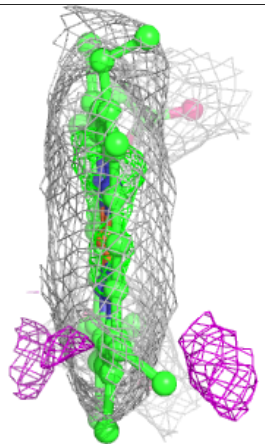


Electron density around HEM H 301:

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

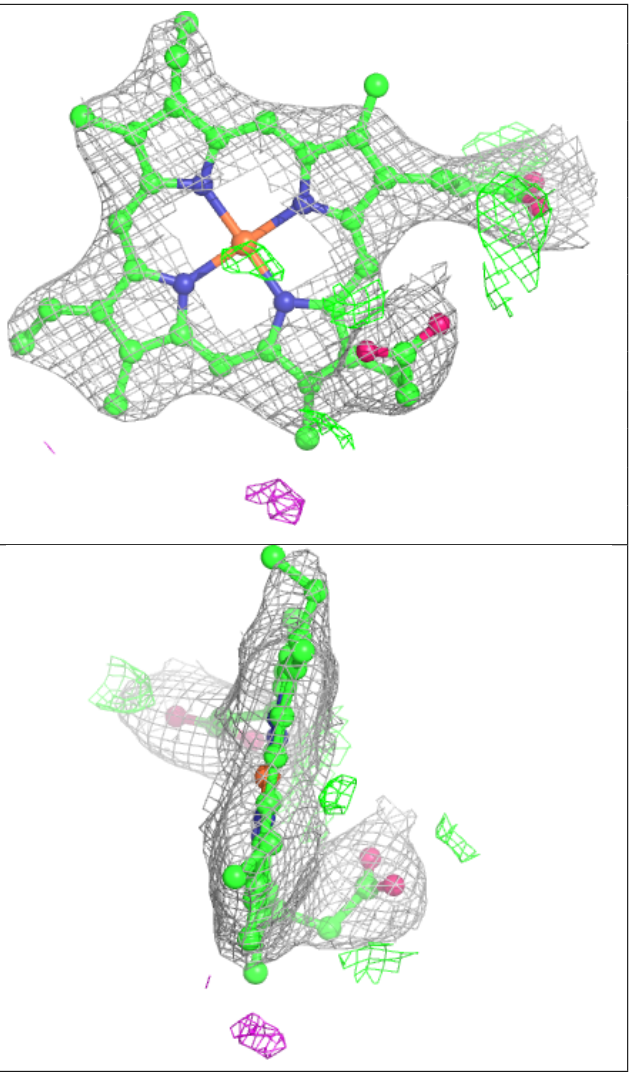






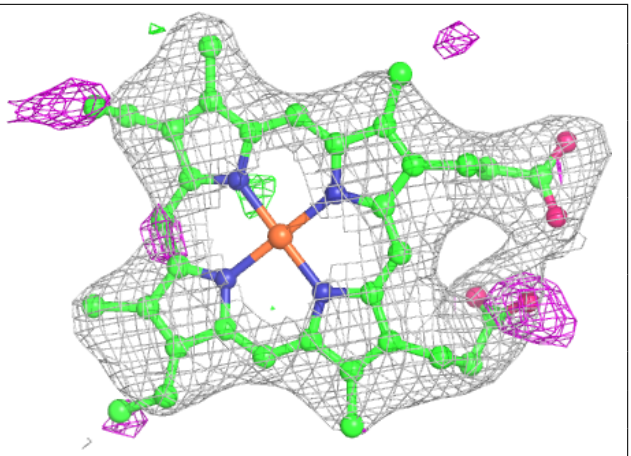
Electron density around HEM A 501:

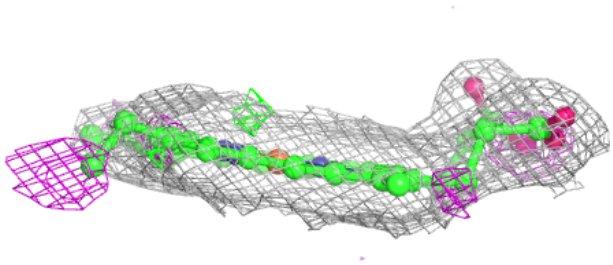
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

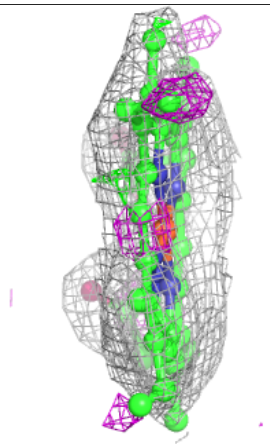


Electron density around HEM A 502:

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

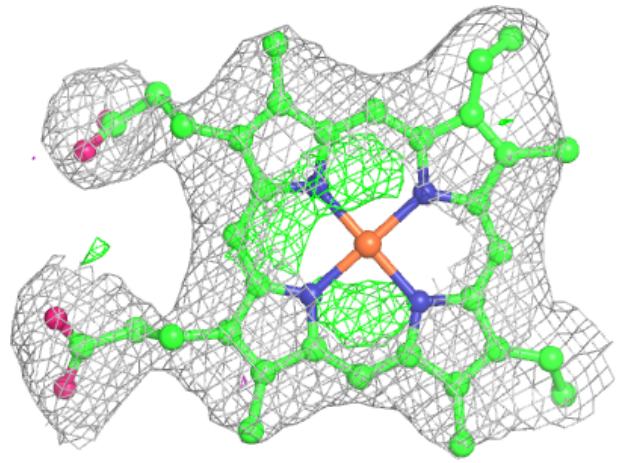


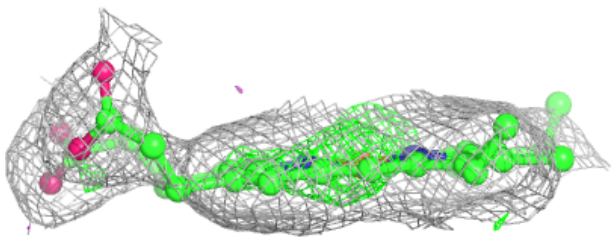


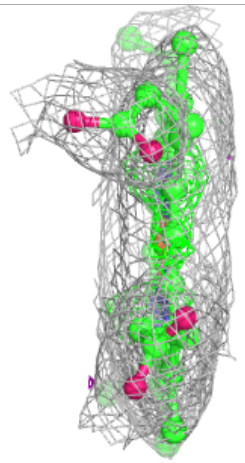


Electron density around HEM B 301:

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

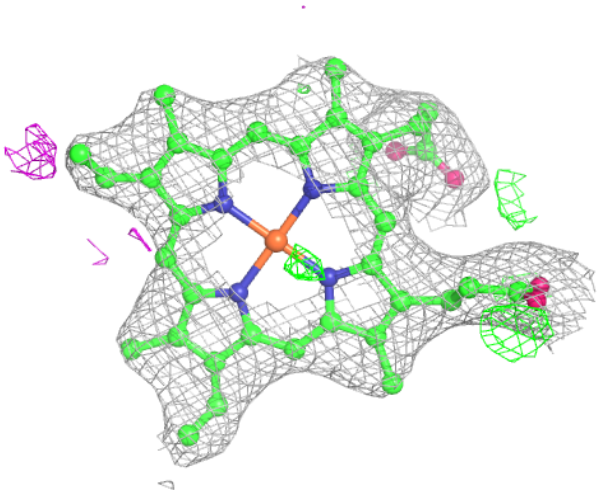


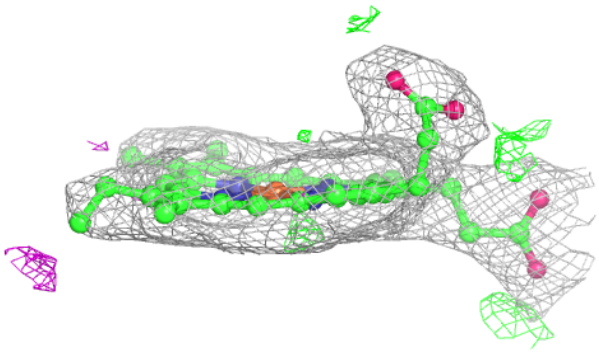


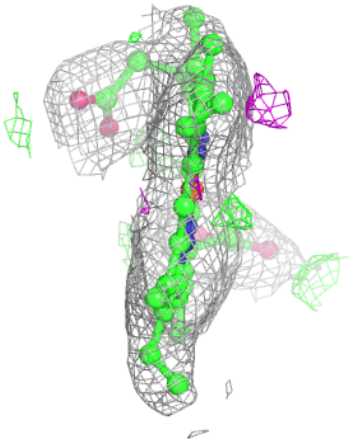


Electron density around HEM J 501:

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

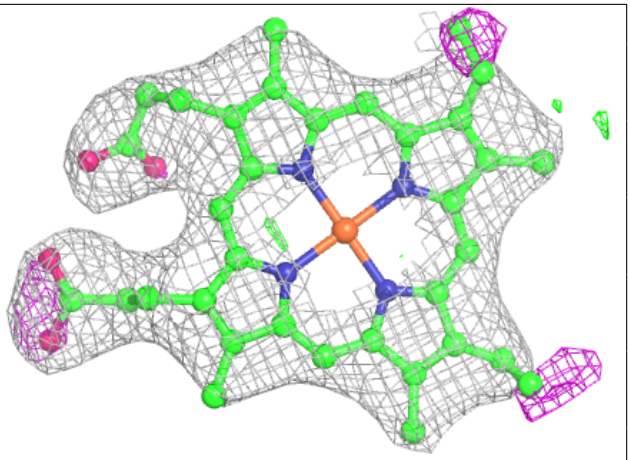


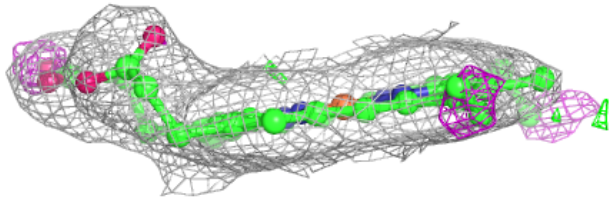


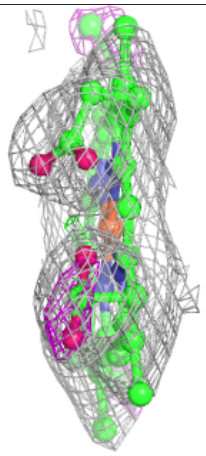


Electron density around HEM J 502:

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

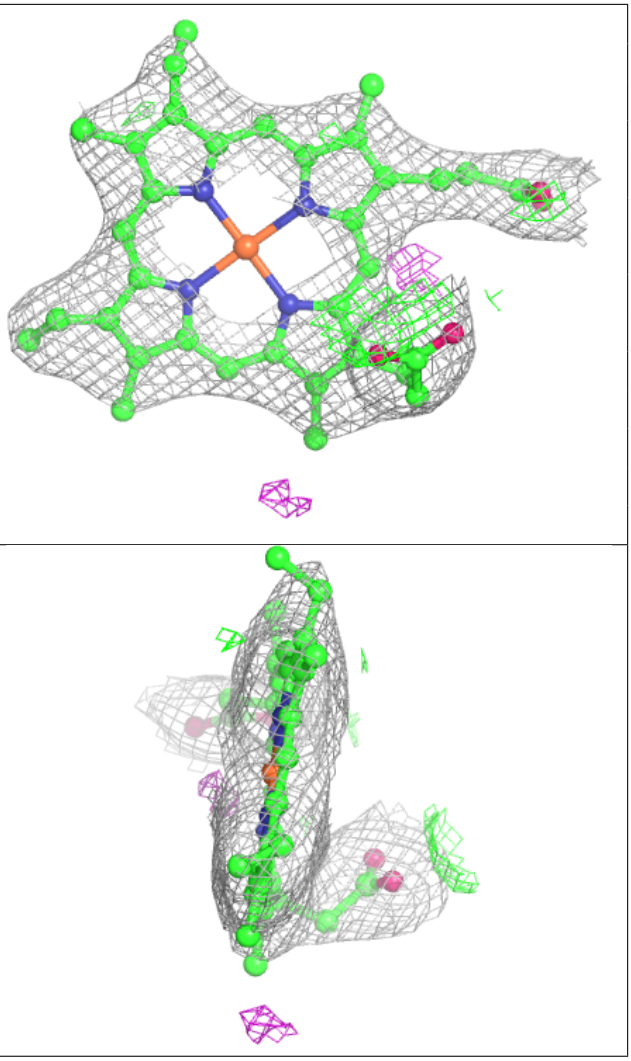






Electron density around HEM G 501:

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.