Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 08:38 PM EDT

PDB ID	:	3H1H
Title	:	Cytochrome bc1 complex from chicken
Authors	:	Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.; Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on	:	2009-04-12
Resolution	:	3.16 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:

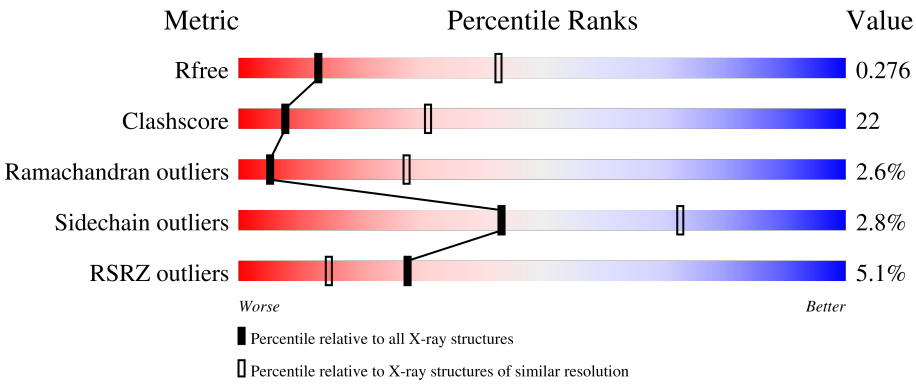
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	446	% 61% 35% • •
1	N	446	% 59% 37% • •
2	B	441	3% 49% 42% • 5%
2	O	441	% 49% 41% 5% •
3	C	380	68% 31% •

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Mol	Chain	Length	Quality of chain
3	P	380	%, 63%, 35%
4	D	241	%, 64%, 35%
4	Q	241	4%, 65%, 34%
5	E	196	39%, 53%, 41%, 5%
5	R	196	18%, 60%, 37%
6	F	110	65%, 25%, 8%
6	S	110	5%, 57%, 33%, 8%
7	G	81	%, 60%, 35%
7	T	81	11%, 57%, 37%
8	H	77	3%, 64%, 27%, 9%
8	U	77	21%, 56%, 31%, 13%
9	I	47	15%, 51%, 43%
9	V	47	17%, 36%, 57%, 6%
10	J	61	7%, 85%, 10%, 5%
10	W	61	3%, 82%, 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	UNL	A	3231	-	-	-	X
13	UQ	P	3002	-	-	-	X
14	CDL	Q	3003	-	-	-	X
15	PEE	C	2008	-	-	-	X
15	PEE	N	3008	-	X	-	-
15	PEE	R	3005	-	-	-	X
18	BOG	D	2091	-	-	-	X
18	BOG	P	2010	-	-	-	X
18	BOG	Q	3091	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 32608 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 UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3442	2157	606	658	21	0	0	0
1	N	442	3437	2154	605	657	21	0	0	0

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	421	3141	1974	545	613	9	0	0	0
2	O	422	3147	1977	546	614	10	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	380	3017	2022	478	505	12	0	0	0
3	P	379	3012	2019	477	504	12	0	0	0

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1898	1212	327	347	12	0	0	0
4	Q	241	1898	1212	327	347	12	0	0	0

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1513	952	263	292	6	0	0	0
5	R	196	1509	950	263	290	6	0	0	0

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	891	570	159	159	3	0	0	0
6	S	101	891	570	159	159	3	0	0	0

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	G	80	672	437	119	116	0	0	0
7	T	79	662	432	117	113	0	0	0

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	70	574	350	105	114	5	0	0	0
8	U	67	553	338	103	107	5	0	0	0

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	46	287	171	58	56	2	0	0	0
9	V	44	278	167	56	53	2	0	0	1

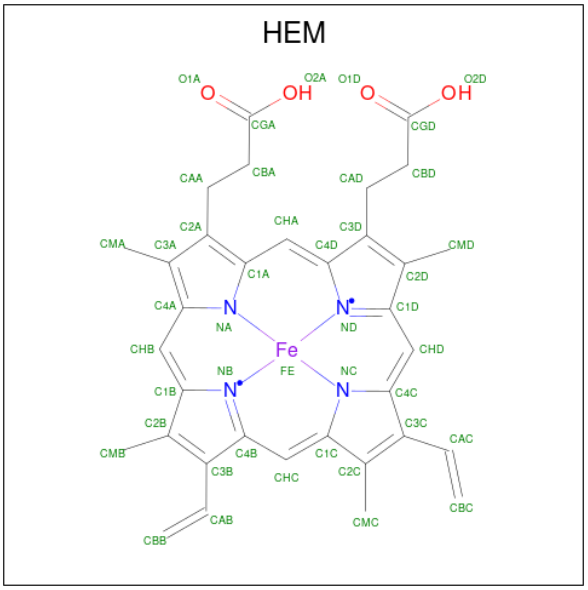
- Molecule 10 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	61	497	321	87	89	0	0	0
			Total	C	N	O			
10	W	60	479	311	86	82	0	0	1

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	3	3	3	0	0
			Total	O		
11	C	2	2	2	0	0
			Total	O		
11	N	3	3	3	0	0
			Total	O		
11	P	1	1	1	0	0

- Molecule 12 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		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0

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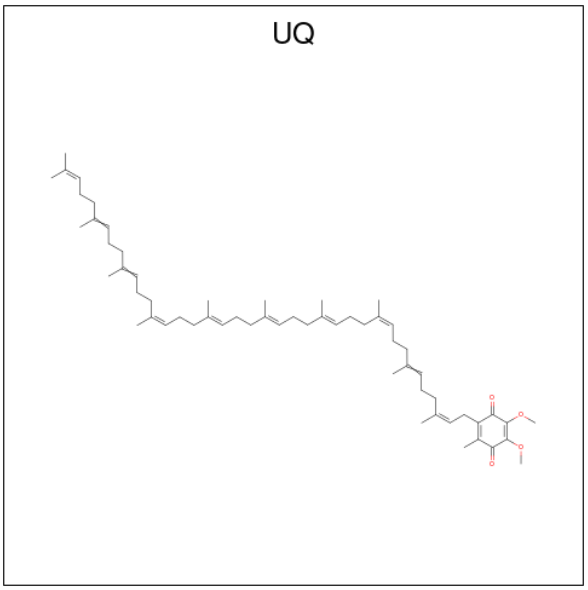
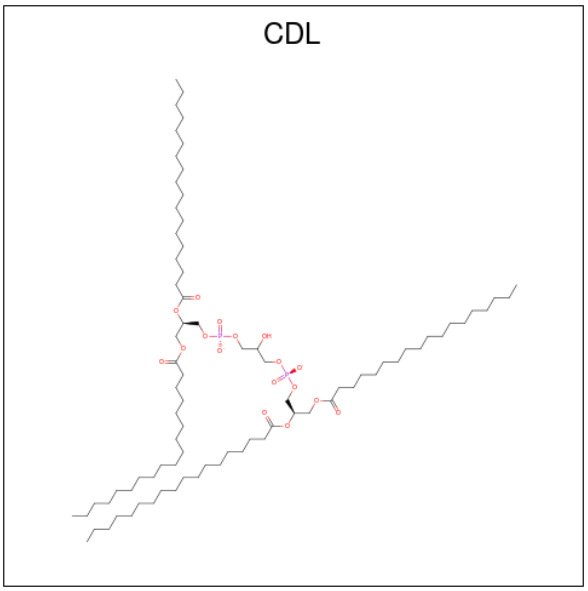
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	P	1	43	34	1	4	4	0	0

- Molecule 13 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



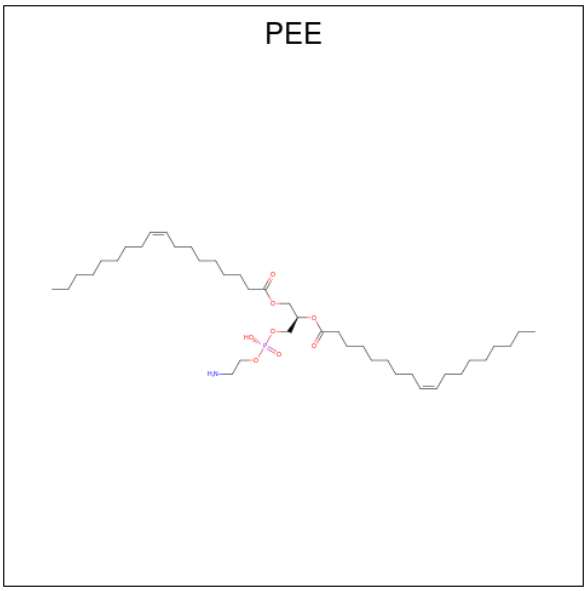
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	O				
13	C	1	19	15	4			0	0
			Total	C	O				
13	P	1	19	15	4			0	0

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



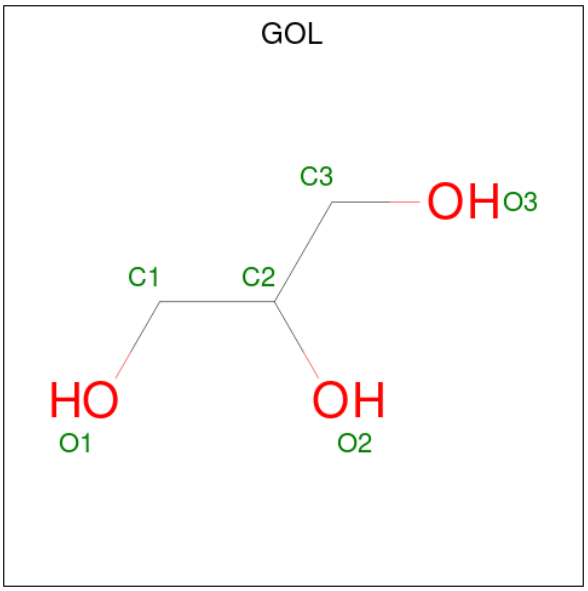
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
14	C	1	40	21	17	2	0	0
			Total	C	O	P		
14	D	1	42	23	17	2	0	0
			Total	C	O	P		
14	P	1	40	21	17	2	0	0
			Total	C	O	P		
14	Q	1	42	23	17	2	0	0

- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



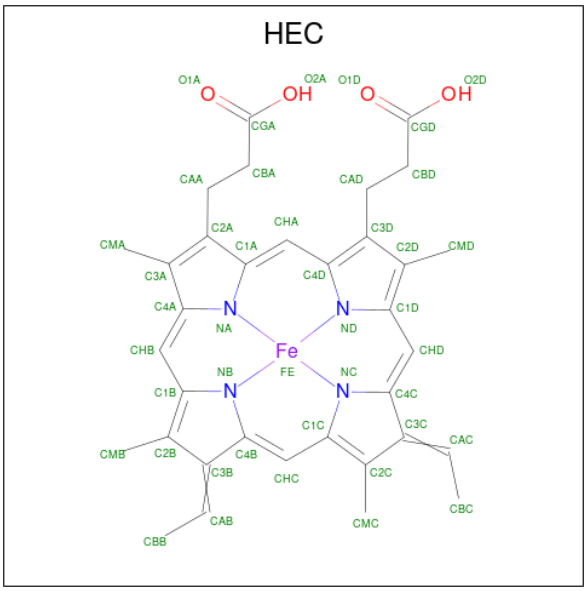
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C N O P 49 39 1 8 1	0	0
15	C	1	Total C O P 21 12 8 1	0	0
15	E	1	Total C N O P 50 40 1 8 1	0	0
15	N	1	Total O P 5 4 1	0	0
15	P	1	Total C N O P 49 39 1 8 1	0	0
15	R	1	Total C N O P 50 40 1 8 1	0	0

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



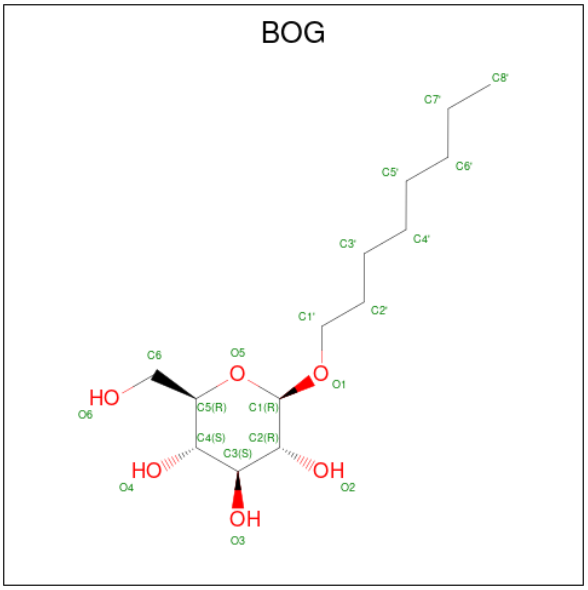
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 6 3 3	0	0
16	P	1	Total C O 6 3 3	0	0

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
17	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
17	Q	1	43	34	1	4	4	0	0

- Molecule 18 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	D	1	20	14	6	0	0
			Total	C	O		
18	D	1	13	7	6	0	0

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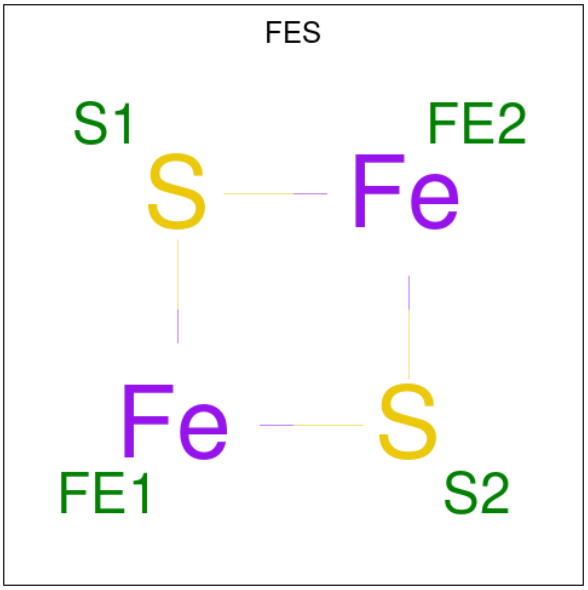
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	P	1	12	6	6	0	0
			Total	C	O		
18	Q	1	20	14	6	0	0
			Total	C	O		
18	Q	1	13	7	6	0	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
19	E	1	4	2	2	0	0
			Total	Fe	S		
19	R	1	4	2	2	0	0

- Molecule 20 is water.

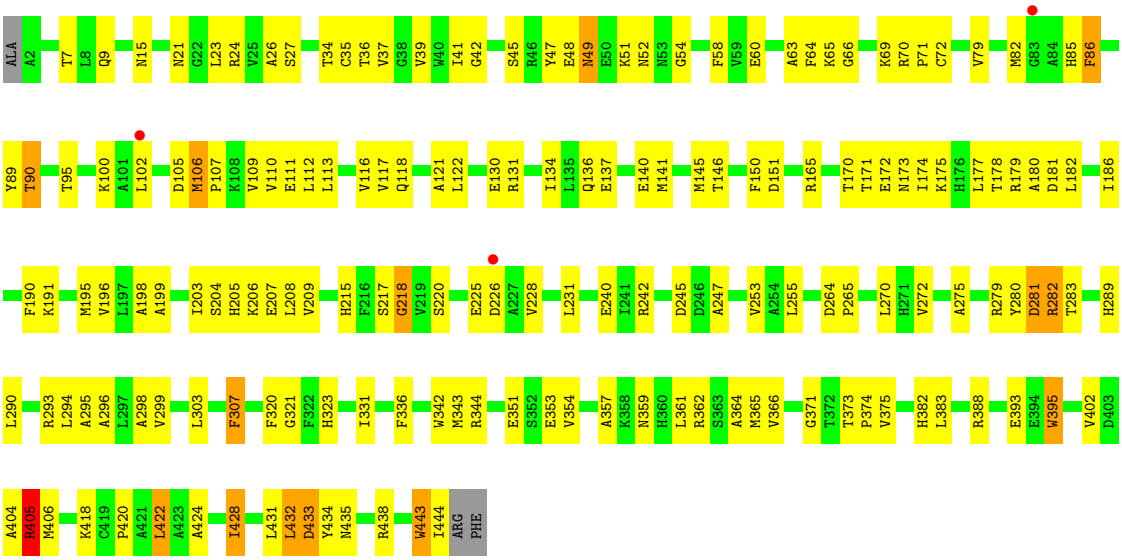
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
20	C	8	8	8	0	0
			Total	O		
20	E	1	1	1	0	0
			Total	O		
20	P	9	9	9	0	0
			Total	O		
20	R	1	1	1	0	0

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.

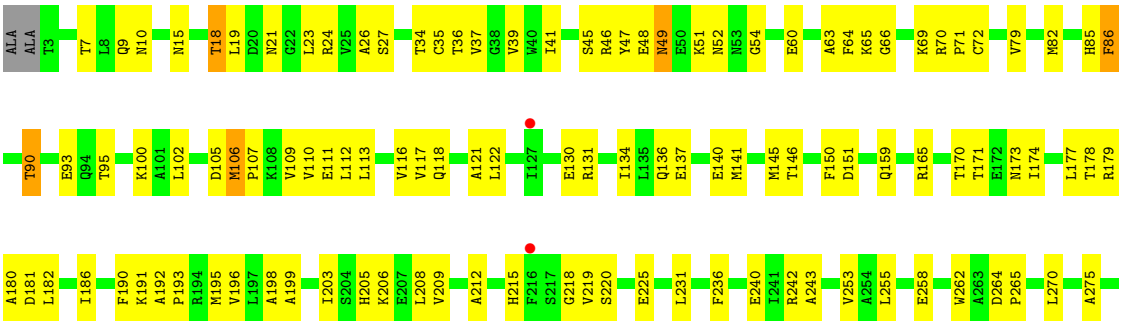
• Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

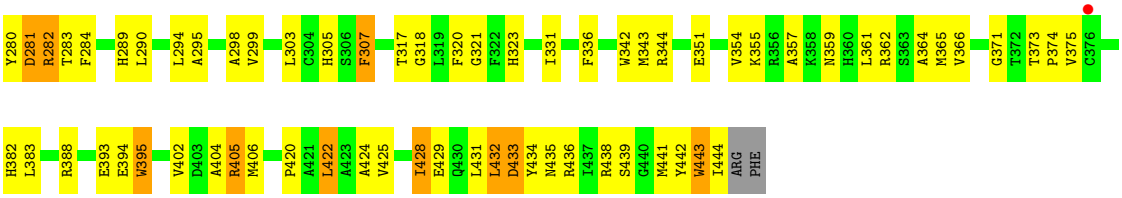
Chain A:



• Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

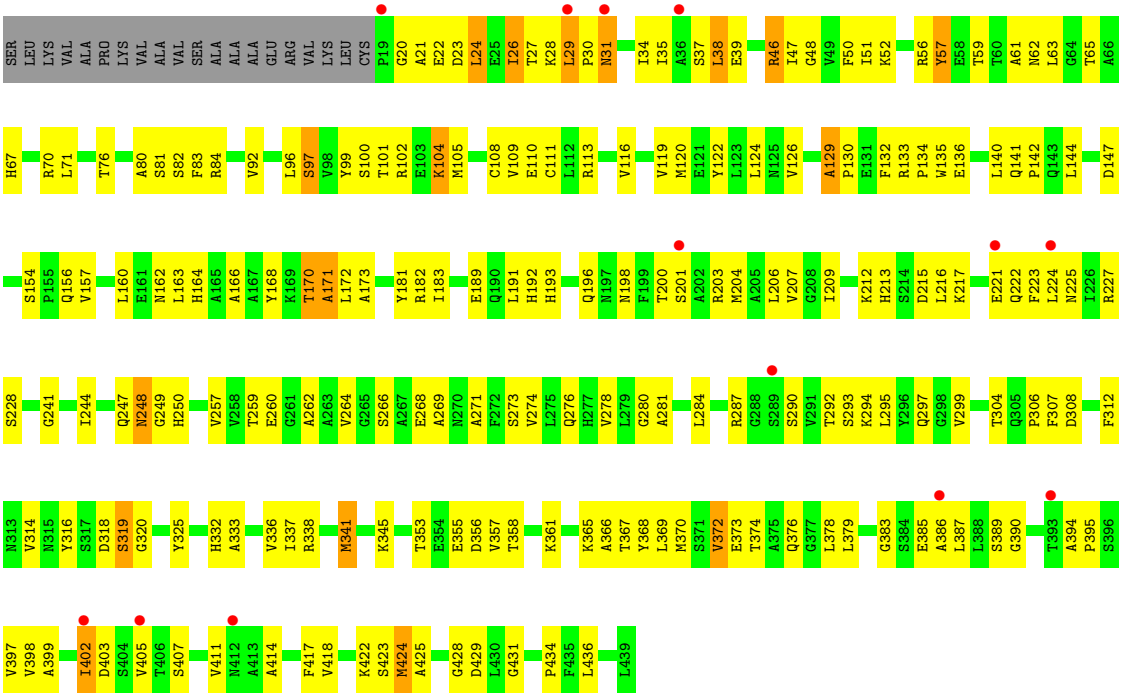
Chain N:





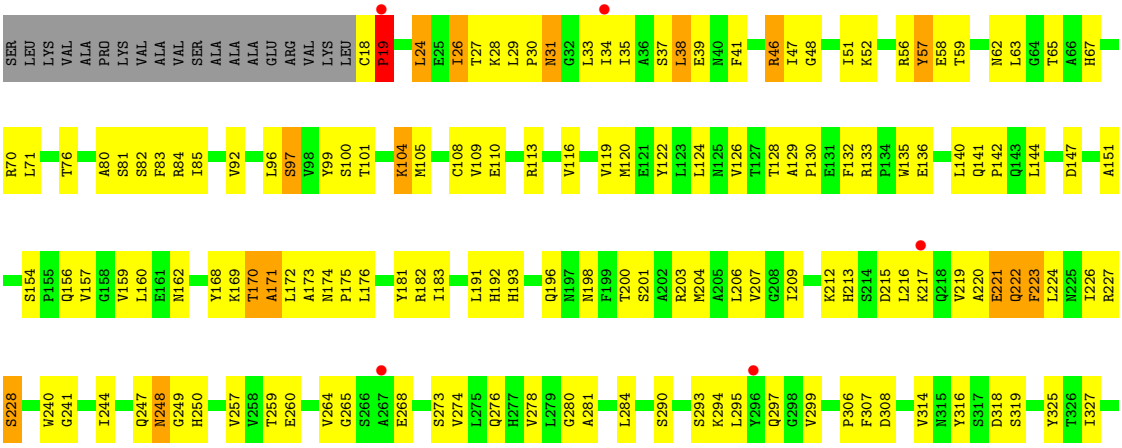
• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL

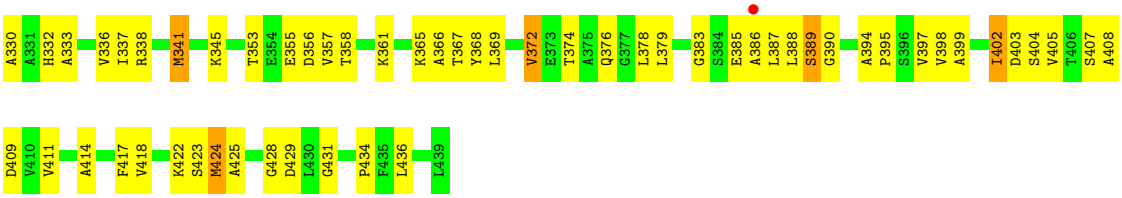
Chain B:



• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL

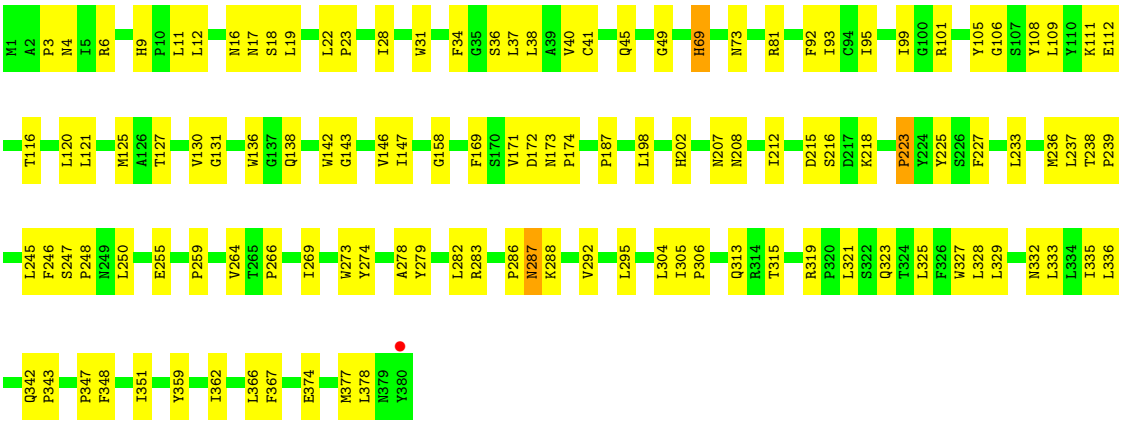
Chain O:





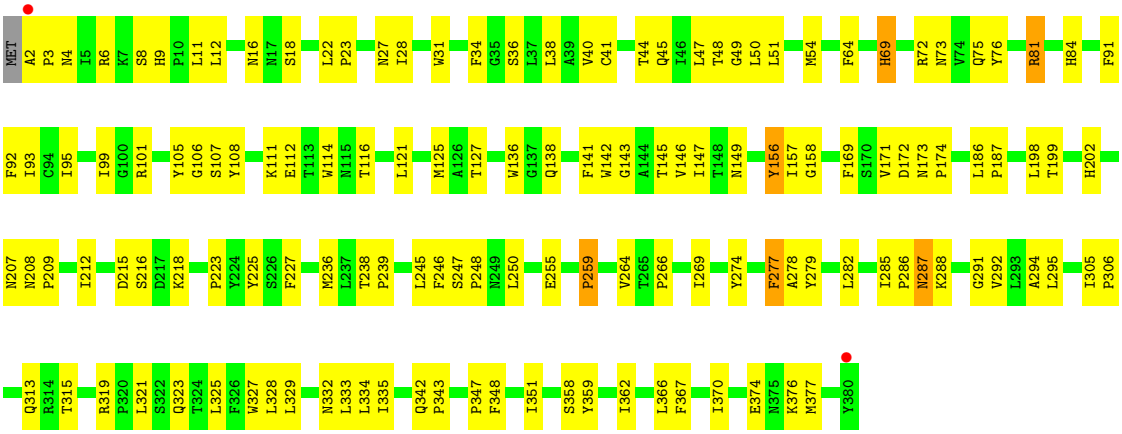
• Molecule 3: Cytochrome b

Chain C:



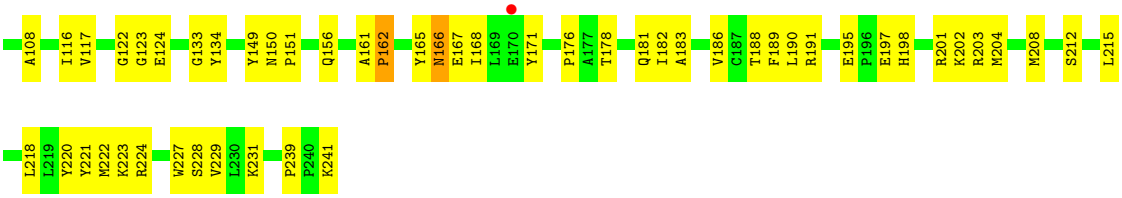
• Molecule 3: Cytochrome b

Chain P:



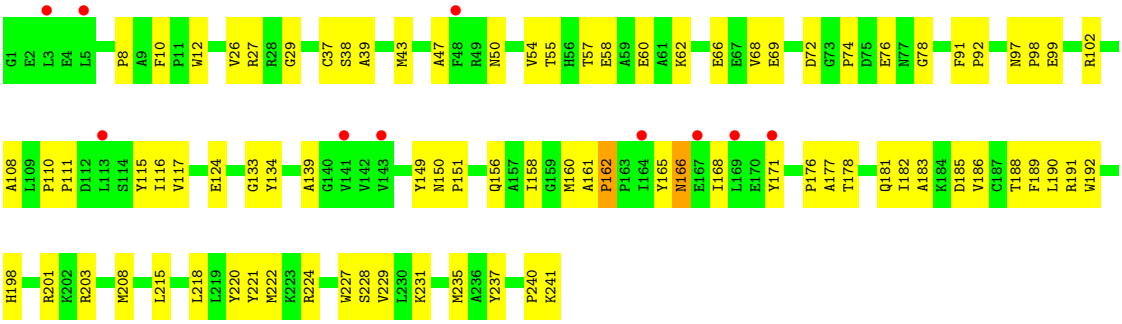
• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

Chain D:



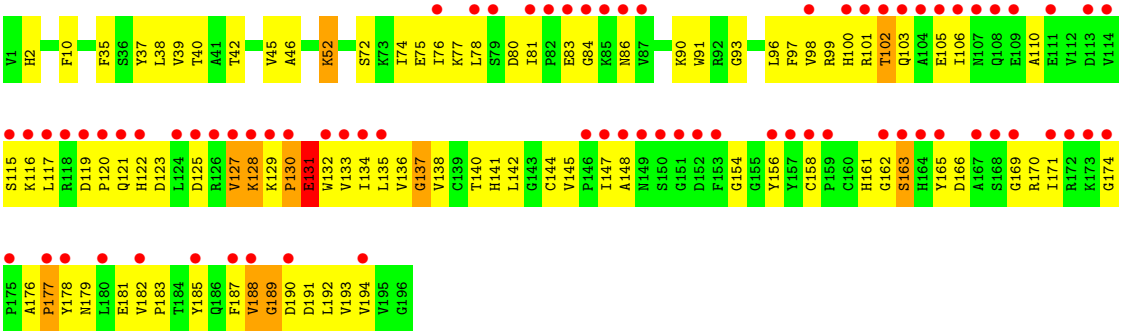
• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

Chain Q:



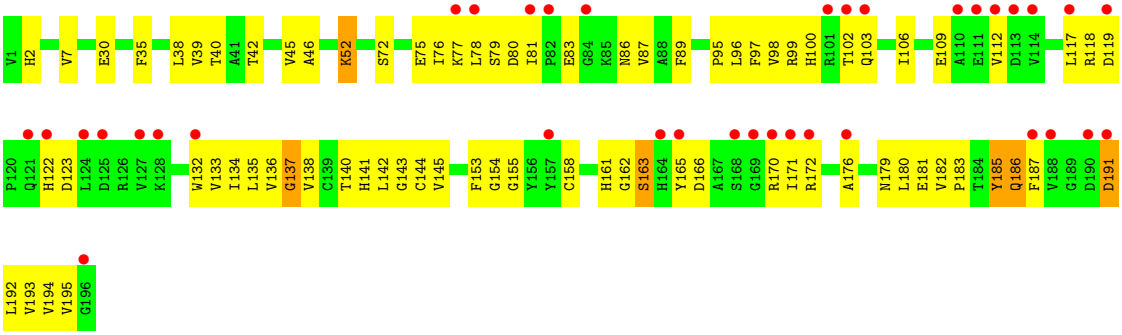
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:

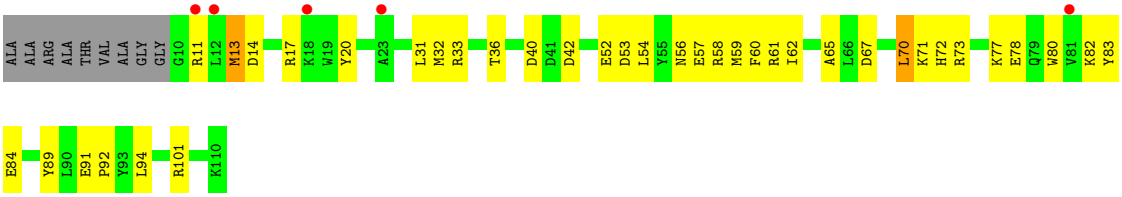


• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN

Chain F:

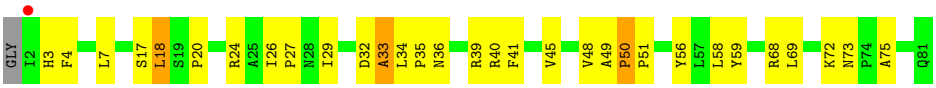
• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN

Chain S:



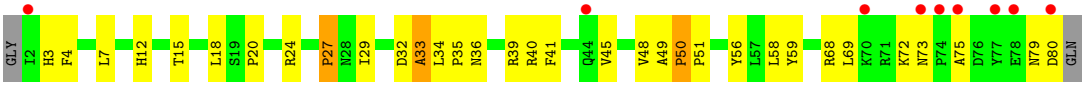
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain G:



• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain T:

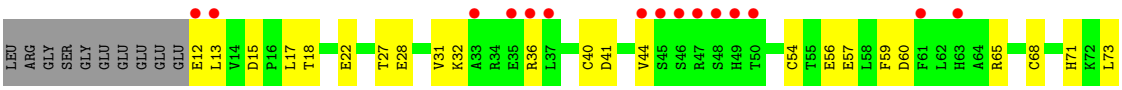


• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN

Chain H:

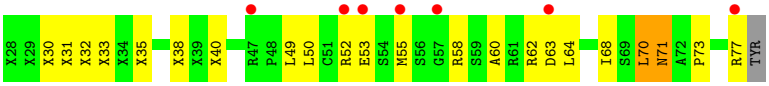
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN

Chain U:



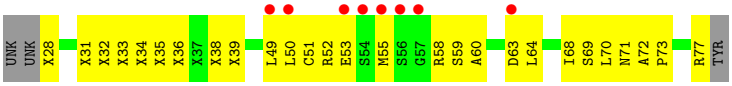
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



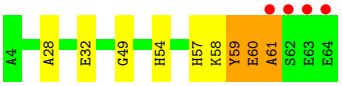
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



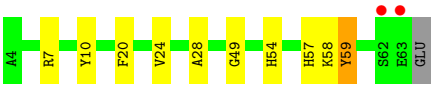
• Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN

Chain J:



• Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	169.59Å 182.52Å 240.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.16 69.31 – 3.16	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-3.16) 96.9 (69.31-3.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.291 0.236 , 0.276	Depositor DCC
R_{free} test set	2453 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	75.4	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	32608	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CDL, UNL, FES, HEC, UQ, GOL, BOG, HEM, PEE

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	0.48	0/3513	0.67	0/4760
1	N	0.46	0/3508	0.66	0/4753
2	B	0.41	0/3196	0.64	0/4334
2	O	0.44	0/3202	0.67	1/4343 (0.0%)
3	C	0.54	0/3119	0.69	0/4270
3	P	0.48	0/3114	0.65	0/4263
4	D	0.48	0/1956	0.66	1/2658 (0.0%)
4	Q	0.39	0/1956	0.63	1/2658 (0.0%)
5	E	0.40	0/1547	0.60	0/2103
5	R	0.39	0/1543	0.61	1/2098 (0.0%)
6	F	0.54	0/911	0.66	0/1219
6	S	0.44	0/911	0.62	0/1219
7	G	0.53	0/694	0.69	1/941 (0.1%)
7	T	0.46	0/684	0.66	1/929 (0.1%)
8	H	0.48	0/582	0.65	0/779
8	U	0.36	0/561	0.59	0/751
9	I	0.45	0/218	0.66	0/293
9	V	0.43	0/218	0.65	0/293
10	J	0.46	0/508	0.62	0/682
10	W	0.41	0/490	0.59	0/660
All	All	0.46	0/32431	0.65	6/44006 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	18	LEU	CA-CB-CG	5.82	128.69	115.30
4	D	133	GLY	N-CA-C	5.71	127.39	113.10
4	Q	133	GLY	N-CA-C	5.44	126.69	113.10
7	G	18	LEU	CA-CB-CG	5.37	127.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	143	GLY	N-CA-C	5.11	125.88	113.10
2	O	226	ILE	N-CA-C	-5.00	97.49	111.00

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	3442	0	3354	153	0
1	N	3437	0	3349	155	0
2	B	3141	0	3142	215	0
2	O	3147	0	3146	215	0
3	C	3017	0	3063	108	0
3	P	3012	0	3058	126	0
4	D	1898	0	1846	71	0
4	Q	1898	0	1846	75	0
5	E	1513	0	1478	94	0
5	R	1509	0	1474	87	0
6	F	891	0	893	25	0
6	S	891	0	893	35	0
7	G	672	0	653	31	0
7	T	662	0	645	33	0
8	H	574	0	548	18	0
8	U	553	0	535	25	0
9	I	287	0	250	40	0
9	V	278	0	253	38	0
10	J	497	0	490	8	0
10	W	479	0	478	9	0
11	A	3	0	0	0	0
11	C	2	0	0	0	0
11	N	3	0	0	0	0
11	P	1	0	0	0	0
12	C	86	0	60	6	0
12	P	86	0	60	8	0
13	C	19	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	P	19	0	17	4	0
14	C	40	0	24	2	0
14	D	42	0	28	2	0
14	P	40	0	24	2	0
14	Q	42	0	28	3	0
15	C	70	0	85	2	0
15	E	50	0	77	1	0
15	N	5	0	0	0	0
15	P	49	0	72	2	0
15	R	50	0	77	0	0
16	C	6	0	8	0	0
16	P	6	0	8	0	0
17	D	43	0	30	3	0
17	Q	43	0	30	1	0
18	D	33	0	39	1	0
18	P	12	0	11	1	0
18	Q	33	0	39	0	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	2	0
20	R	1	0	0	0	0
All	All	32608	0	32128	1415	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 22.

All (1415) 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)
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.40	1.04
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.07	1.02
1:N:10:ASN:HD21	2:O:18:CYS:HB3	1.23	1.01
9:I:32:UNK:N	9:I:73:PRO:HG2	1.75	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.27	0.99
2:B:353:THR:HG22	2:B:355:GLU:H	1.27	0.98
2:O:353:THR:HG22	2:O:355:GLU:H	1.26	0.97
1:N:178:THR:HG22	1:N:180:ALA:H	1.26	0.97
9:I:33:UNK:HG2	9:I:73:PRO:CB	1.95	0.96
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.48	0.95
3:P:238:THR:HB	3:P:239:PRO:HD3	1.48	0.95
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.50	0.94
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.93
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.31	0.92
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.69	0.91
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.89
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.53	0.89
2:O:219:VAL:O	2:O:223:PHE:HB2	1.73	0.89
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.53	0.88
3:C:238:THR:HB	3:C:239:PRO:HD3	1.55	0.88
2:B:76:THR:HG22	2:B:82:SER:H	1.39	0.88
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.39	0.88
5:E:127:VAL:HG12	5:E:128:LYS:H	1.38	0.87
2:O:27:THR:HG22	2:O:28:LYS:H	1.37	0.86
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.91	0.86
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.57	0.86
2:O:76:THR:HG22	2:O:82:SER:H	1.39	0.86
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.55	0.85
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.55	0.85
2:B:24:LEU:HD12	2:B:37:SER:O	1.76	0.85
2:B:47:ILE:HD13	2:B:120:MET:CE	2.07	0.85
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.02	0.84
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.42	0.84
2:O:248:ASN:HD22	2:O:249:GLY:N	1.75	0.83
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.59	0.83
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.60	0.83
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.42	0.83
2:O:46:ARG:NH2	2:O:376:GLN:HG3	1.94	0.83
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.60	0.83
2:O:221:GLU:HG3	2:O:222:GLN:H	1.42	0.83
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.60	0.83
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.60	0.83
2:B:23:ASP:O	2:B:24:LEU:HB3	1.76	0.82
9:I:38:UNK:C	9:I:40:UNK:H	1.89	0.82
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.43	0.82
2:B:248:ASN:HD22	2:B:249:GLY:N	1.76	0.82
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.60	0.82
4:D:231:LYS:O	6:F:71:LYS:HE3	1.79	0.82
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.59	0.82
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.63	0.81
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.81	0.81
2:O:154:SER:O	2:O:157:VAL:HG12	1.81	0.80
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.64	0.80
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.64	0.79
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.61	0.79
2:O:27:THR:HG22	2:O:28:LYS:N	1.97	0.79
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.97	0.79
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.64	0.79
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.81	0.79
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.79
2:O:24:LEU:HD12	2:O:37:SER:O	1.83	0.78
2:O:47:ILE:HD13	2:O:120:MET:CE	2.13	0.78
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.66	0.78
5:E:101:ARG:HA	5:E:105:GLU:OE1	1.84	0.78
1:N:105:ASP:O	1:N:109:VAL:HG23	1.85	0.78
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.66	0.77
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.66	0.77
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.67	0.77
2:B:76:THR:CG2	2:B:82:SER:H	1.97	0.77
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.84	0.77
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.66	0.76
1:N:49:ASN:ND2	1:N:51:LYS:H	1.83	0.76
2:B:274:VAL:O	2:B:278:VAL:HG23	1.86	0.76
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.67	0.76
9:I:70:LEU:HD23	9:I:71:ASN:H	1.50	0.76
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.16	0.76
2:O:76:THR:CG2	2:O:82:SER:H	2.00	0.75
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.67	0.75
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.66	0.75
2:B:27:THR:HG22	2:B:28:LYS:N	2.02	0.75
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.68	0.75
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.68	0.74
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.54	0.74
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.67	0.74
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.17	0.74
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.50	0.74
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.54	0.74
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.69	0.74
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.74
2:B:27:THR:HG22	2:B:28:LYS:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.52	0.73
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.23	0.73
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.02	0.73
1:A:49:ASN:ND2	1:A:51:LYS:H	1.85	0.73
2:O:422:LYS:O	2:O:436:LEU:HD21	1.88	0.73
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.71	0.73
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.69	0.73
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.24	0.73
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.71	0.73
1:A:23:LEU:HD23	1:A:24:ARG:N	2.03	0.73
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.18	0.73
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.54	0.72
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.69	0.72
2:O:274:VAL:O	2:O:278:VAL:HG23	1.89	0.72
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.72	0.72
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.29	0.72
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.71	0.72
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.18	0.72
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.55	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.90	0.71
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.20	0.71
3:C:9:HIS:HD2	3:C:12:LEU:H	1.38	0.71
3:P:22:LEU:HD21	13:P:3002:UQ:HM32	1.70	0.71
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.70	0.71
4:D:222:MET:HE1	5:E:40:THR:HG23	1.71	0.71
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.23	0.71
7:G:29:ILE:O	7:G:33:ALA:HB3	1.91	0.71
1:A:140:GLU:OE2	9:I:50:LEU:N	2.19	0.71
3:C:236:MET:O	3:C:239:PRO:HD2	1.91	0.70
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.21	0.70
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.73	0.70
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.73	0.70
9:V:31:UNK:C	9:V:73:PRO:HG2	2.21	0.70
3:C:169:PHE:HE1	5:R:72:SER:HA	1.57	0.70
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.07	0.70
1:N:281:ASP:O	1:N:283:THR:N	2.24	0.70
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.71	0.70
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.26	0.70
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.26	0.70
1:A:130:GLU:O	1:A:134:ILE:HG13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:HD2	3:P:12:LEU:H	1.40	0.69
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.74	0.69
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.73	0.69
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.22	0.69
1:A:281:ASP:O	1:A:283:THR:N	2.26	0.69
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.75	0.69
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.56	0.69
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.87	0.69
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.56	0.69
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.75	0.69
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.74	0.69
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.28	0.68
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.56	0.68
2:B:399:ALA:O	2:B:402:ILE:HG22	1.94	0.68
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.29	0.68
1:N:112:LEU:O	1:N:116:VAL:HG23	1.94	0.68
7:T:29:ILE:O	7:T:33:ALA:HB3	1.93	0.68
2:B:31:ASN:HD22	2:B:31:ASN:N	1.90	0.67
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.76	0.67
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.74	0.67
1:A:178:THR:HB	1:A:181:ASP:OD1	1.94	0.67
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.26	0.67
1:N:130:GLU:O	1:N:134:ILE:HG13	1.94	0.67
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.74	0.67
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.56	0.67
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.76	0.67
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.57	0.67
2:B:248:ASN:HD22	2:B:248:ASN:C	1.94	0.67
8:U:18:THR:O	8:U:22:GLU:HG3	1.94	0.67
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.28	0.67
2:B:422:LYS:O	2:B:436:LEU:HD21	1.95	0.67
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.76	0.67
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.77	0.67
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.30	0.67
5:E:78:LEU:HD12	5:E:190:ASP:O	1.95	0.67
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.77	0.66
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.25	0.66
3:P:199:THR:HA	18:P:2010:BOG:O1	1.95	0.66
7:T:41:PHE:O	7:T:45:VAL:HG23	1.94	0.66
2:B:76:THR:HG22	2:B:81:SER:HA	1.78	0.66
3:C:286:PRO:O	3:C:287:ASN:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.29	0.66
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.26	0.66
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.11	0.66
5:R:102:THR:O	5:R:106:ILE:HG13	1.95	0.66
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.77	0.66
2:O:248:ASN:HD22	2:O:248:ASN:C	1.94	0.66
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.77	0.66
3:P:121:LEU:O	3:P:125:MET:HG3	1.96	0.66
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.76	0.65
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.76	0.65
2:O:27:THR:CG2	2:O:28:LYS:H	2.08	0.65
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.31	0.65
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.32	0.65
10:W:49:GLY:N	10:W:54:HIS:ND1	2.45	0.65
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.11	0.65
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.96	0.65
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.31	0.65
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.24	0.65
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.78	0.65
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.26	0.65
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.31	0.65
1:N:23:LEU:HD23	1:N:24:ARG:N	2.11	0.65
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.61	0.65
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.79	0.64
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.79	0.64
1:N:382:HIS:HB3	1:N:388:ARG:O	1.97	0.64
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.62	0.64
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.32	0.64
5:R:136:VAL:HG21	5:R:181:GLU:OE1	1.97	0.64
5:E:101:ARG:HG2	5:E:105:GLU:OE2	1.98	0.64
2:O:273:SER:O	2:O:276:GLN:HB3	1.98	0.64
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.23	0.64
1:N:402:VAL:HG22	1:N:406:MET:CE	2.28	0.64
3:P:207:ASN:ND2	3:P:208:ASN:H	1.96	0.64
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.63	0.64
10:J:49:GLY:N	10:J:54:HIS:ND1	2.46	0.64
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.33	0.64
5:R:186:GLN:O	5:R:193:VAL:HG23	1.98	0.64
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.16	0.63
1:A:105:ASP:O	1:A:109:VAL:HG23	1.97	0.63
3:C:278:ALA:HB1	3:C:295:LEU:HD12	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:57:THR:HB	4:D:60:GLU:HG3	1.81	0.63
2:O:399:ALA:O	2:O:402:ILE:HG22	1.97	0.63
2:B:341:MET:CE	2:B:417:PHE:HE2	2.05	0.63
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.19	0.63
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.63	0.63
3:P:105:TYR:HA	3:P:315:THR:HG22	1.80	0.63
1:A:36:THR:HG21	1:A:373:THR:HA	1.81	0.63
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.81	0.63
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.81	0.63
3:P:138:GLN:HA	3:P:138:GLN:OE1	1.99	0.63
1:A:191:LYS:CA	1:A:195:MET:HE2	2.29	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.35	0.62
2:O:76:THR:HG22	2:O:81:SER:HA	1.82	0.62
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.82	0.62
5:R:118:ARG:NH1	5:R:118:ARG:HB2	2.15	0.62
7:G:41:PHE:O	7:G:45:VAL:HG23	1.98	0.62
2:B:122:TYR:O	2:B:126:VAL:HG23	2.00	0.62
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.62
3:C:105:TYR:HA	3:C:315:THR:HG22	1.80	0.62
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.27	0.62
1:A:240:GLU:OE1	1:A:434:TYR:HB2	1.99	0.62
2:B:76:THR:HG22	2:B:82:SER:N	2.12	0.62
1:N:165:ARG:HH11	1:N:165:ARG:HG3	1.65	0.62
1:A:112:LEU:O	1:A:116:VAL:HG23	2.00	0.62
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.35	0.62
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.82	0.62
8:H:18:THR:O	8:H:22:GLU:HG3	1.99	0.61
2:O:361:LYS:O	2:O:365:LYS:HG3	1.99	0.61
1:A:371:GLY:O	1:A:375:VAL:HG23	2.00	0.61
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.30	0.61
4:D:62:LYS:O	4:D:66:GLU:HG3	2.00	0.61
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.35	0.61
2:O:341:MET:CE	2:O:417:PHE:HE2	2.11	0.61
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.81	0.61
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.80	0.61
8:H:12:GLU:HG2	8:H:13:LEU:N	2.15	0.61
1:N:371:GLY:O	1:N:375:VAL:HG23	2.00	0.61
5:E:72:SER:HA	3:P:169:PHE:HE1	1.64	0.61
2:O:353:THR:HB	2:O:356:ASP:OD1	2.00	0.61
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.83	0.61
5:E:137:GLY:O	5:E:145:VAL:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.82	0.61
1:N:359:ASN:HD22	2:O:92:VAL:HA	1.65	0.61
6:S:13:MET:O	6:S:17:ARG:HG3	2.01	0.61
2:B:332:HIS:O	2:B:336:VAL:HG23	2.01	0.61
9:I:31:UNK:C	9:I:73:PRO:HG2	2.30	0.61
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.03	0.61
3:P:236:MET:O	3:P:239:PRO:HD2	2.01	0.61
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.01	0.61
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.36	0.60
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.01	0.60
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.60
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.65	0.60
8:U:12:GLU:HG2	8:U:13:LEU:H	1.66	0.60
1:A:281:ASP:OD1	9:I:33:UNK:HB2	2.02	0.60
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.30	0.60
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.83	0.60
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.83	0.60
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.01	0.60
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.34	0.60
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.83	0.60
2:O:46:ARG:HH22	2:O:376:GLN:HG3	1.67	0.60
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.84	0.60
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.37	0.60
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.66	0.60
2:B:333:ALA:O	2:B:337:ILE:HG13	2.01	0.60
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.33	0.60
1:A:178:THR:HG22	1:A:180:ALA:N	2.09	0.60
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.36	0.60
4:D:171:TYR:OH	4:D:182:ILE:HA	2.01	0.60
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.60
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.60
1:N:63:ALA:O	1:N:116:VAL:HG13	2.02	0.60
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.20	0.60
2:B:31:ASN:H	2:B:31:ASN:ND2	2.00	0.60
1:A:402:VAL:HG22	1:A:406:MET:CE	2.31	0.59
1:N:131:ARG:NH2	1:N:177:LEU:O	2.35	0.59
3:P:286:PRO:O	3:P:287:ASN:HB2	2.02	0.59
1:A:280:TYR:CG	1:A:281:ASP:N	2.70	0.59
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.84	0.59
1:A:402:VAL:HA	1:A:406:MET:CE	2.32	0.59
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.32	0.59
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.85	0.59
2:O:402:ILE:C	2:O:402:ILE:HD13	2.23	0.59
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.82	0.59
2:B:223:PHE:O	2:B:225:ASN:HB2	2.03	0.59
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.32	0.59
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.85	0.59
2:O:76:THR:HG22	2:O:82:SER:N	2.12	0.59
2:O:122:TYR:O	2:O:126:VAL:HG23	2.03	0.59
2:B:294:LYS:HE3	2:B:356:ASP:OD2	2.03	0.59
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.83	0.59
1:N:15:ASN:O	1:N:26:ALA:HA	2.02	0.59
2:O:372:VAL:HG12	2:O:372:VAL:O	2.01	0.59
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.02	0.59
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.83	0.59
1:N:255:LEU:HD12	1:N:422:LEU:HB2	1.84	0.59
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.33	0.59
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.84	0.59
3:C:143:GLY:O	3:C:147:ILE:HG12	2.02	0.59
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.67	0.59
2:B:264:VAL:HG23	2:B:316:TYR:C	2.23	0.59
2:O:294:LYS:HE3	2:O:356:ASP:OD2	2.02	0.59
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.16	0.59
1:N:170:THR:HG22	1:N:171:THR:N	2.18	0.58
2:O:333:ALA:O	2:O:337:ILE:HG13	2.03	0.58
2:O:345:LYS:HG2	2:O:418:VAL:HG13	1.85	0.58
7:T:72:LYS:HG2	8:U:56:GLU:OE2	2.02	0.58
2:B:100:SER:HB2	2:B:105:MET:HG2	1.85	0.58
3:C:9:HIS:CD2	3:C:12:LEU:H	2.20	0.58
3:C:279:TYR:CE2	3:C:283:ARG:HD3	2.39	0.58
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.16	0.58
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.68	0.58
2:B:361:LYS:O	2:B:365:LYS:HG3	2.02	0.58
1:N:136:GLN:OE1	9:V:50:LEU:HD13	2.03	0.58
2:B:96:LEU:HD12	2:B:97:SER:N	2.19	0.58
5:E:136:VAL:O	5:E:138:VAL:N	2.31	0.58
5:E:141:HIS:O	5:E:142:LEU:HD23	2.04	0.58
1:N:36:THR:HG21	1:N:373:THR:HA	1.85	0.58
1:A:382:HIS:HB3	1:A:388:ARG:O	2.03	0.58
2:B:372:VAL:HG12	2:B:372:VAL:O	2.03	0.58
3:C:45:GLN:CB	12:C:501:HEM:HAB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.86	0.58
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.37	0.58
9:V:33:UNK:HA	9:V:73:PRO:HG3	1.86	0.58
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.86	0.58
2:O:99:TYR:HE1	2:O:108:CYS:SG	2.27	0.58
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.85	0.58
2:O:248:ASN:ND2	2:O:250:HIS:H	2.01	0.58
5:E:127:VAL:HG12	5:E:128:LYS:N	2.15	0.58
4:Q:139:ALA:HB2	8:U:41:ASP:HA	1.86	0.58
3:C:34:PHE:HB2	20:C:381:HOH:O	2.04	0.58
2:O:27:THR:CG2	2:O:28:LYS:N	2.67	0.58
2:O:52:LYS:O	2:O:203:ARG:NH2	2.37	0.58
5:E:84:GLY:N	5:E:102:THR:HG23	2.19	0.57
3:P:9:HIS:CD2	3:P:12:LEU:H	2.22	0.57
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.86	0.57
1:N:106:MET:O	1:N:110:VAL:HG23	2.04	0.57
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.39	0.57
2:O:100:SER:CB	2:O:105:MET:HG2	2.34	0.57
2:O:332:HIS:O	2:O:336:VAL:HG23	2.03	0.57
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.39	0.57
1:A:137:GLU:O	1:A:141:MET:HG3	2.04	0.57
2:B:31:ASN:HD22	2:B:31:ASN:H	1.52	0.57
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.85	0.57
2:B:290:SER:O	2:B:297:GLN:HG2	2.04	0.57
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.86	0.57
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.18	0.57
2:O:338:ARG:HG3	2:O:338:ARG:NH1	2.19	0.57
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.86	0.57
5:E:190:ASP:C	5:E:192:LEU:H	2.07	0.57
2:B:353:THR:HB	2:B:356:ASP:OD1	2.04	0.57
1:N:90:THR:HB	1:N:95:THR:HG23	1.86	0.57
2:O:147:ASP:OD1	9:V:68:ILE:HD11	2.05	0.57
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.39	0.57
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.53	0.57
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.86	0.57
2:B:402:ILE:HD13	2:B:402:ILE:C	2.24	0.57
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.04	0.57
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.86	0.57
2:O:47:ILE:HG22	2:O:48:GLY:N	2.19	0.57
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.87	0.57
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:CG2	2:B:28:LYS:H	2.18	0.57
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.87	0.57
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.35	0.57
5:E:147:ILE:O	5:E:156:TYR:HA	2.05	0.57
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.20	0.57
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.87	0.57
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.69	0.57
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.34	0.56
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.05	0.56
2:B:38:LEU:C	2:B:38:LEU:HD12	2.24	0.56
2:B:46:ARG:HG3	2:B:379:LEU:HD22	1.87	0.56
3:P:215:ASP:HA	3:P:218:LYS:HE2	1.87	0.56
12:P:502:HEM:HBD1	20:P:386:HOH:O	2.04	0.56
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.21	0.56
2:B:35:ILE:O	2:B:213:HIS:HE1	1.87	0.56
1:N:182:LEU:O	1:N:186:ILE:HG13	2.05	0.56
2:O:306:PRO:HB3	9:V:52:ARG:N	2.21	0.56
3:P:238:THR:HB	3:P:239:PRO:CD	2.30	0.56
2:B:31:ASN:N	2:B:31:ASN:ND2	2.53	0.56
2:B:248:ASN:ND2	2:B:250:HIS:H	2.03	0.56
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.05	0.56
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.34	0.56
1:N:240:GLU:OE1	1:N:434:TYR:HB2	2.04	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.56
5:R:122:HIS:CD2	5:R:123:ASP:H	2.24	0.56
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.86	0.56
1:N:402:VAL:HA	1:N:406:MET:CE	2.35	0.56
3:P:216:SER:HB3	6:S:59:MET:CE	2.35	0.56
4:Q:139:ALA:CB	8:U:41:ASP:HA	2.35	0.56
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.86	0.56
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.40	0.56
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.88	0.56
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.36	0.56
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.35	0.56
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.88	0.56
3:C:37:LEU:O	3:C:41:CYS:HB2	2.05	0.56
3:C:245:LEU:O	4:D:201:ARG:HD3	2.06	0.56
3:P:142:TRP:O	3:P:146:VAL:HG23	2.05	0.56
2:B:385:GLU:O	2:B:387:LEU:N	2.39	0.56
3:C:377:MET:HE2	6:F:20:TYR:CG	2.41	0.56
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:338:ARG:O	2:O:341:MET:HB2	2.06	0.56
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.36	0.56
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.41	0.56
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.06	0.56
2:B:100:SER:CB	2:B:105:MET:HG2	2.36	0.56
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.88	0.56
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.53	0.56
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.20	0.55
2:O:192:HIS:O	2:O:196:GLN:HG3	2.06	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.41	0.55
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.41	0.55
1:A:15:ASN:O	1:A:26:ALA:HA	2.04	0.55
3:C:286:PRO:O	3:C:287:ASN:CB	2.55	0.55
2:O:403:ASP:O	2:O:405:VAL:N	2.38	0.55
8:U:65:ARG:O	8:U:68:CYS:HB3	2.06	0.55
3:C:9:HIS:CD2	3:C:11:LEU:H	2.24	0.55
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.24	0.55
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.55
13:P:3002:UQ:C8	13:P:3002:UQ:HM51	2.37	0.55
2:B:27:THR:CG2	2:B:28:LYS:N	2.70	0.55
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.87	0.55
1:N:362:ARG:O	1:N:365:MET:HG2	2.07	0.55
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.89	0.55
1:A:402:VAL:HA	1:A:406:MET:HE1	1.89	0.55
2:B:345:LYS:HG2	2:B:418:VAL:CG1	2.36	0.55
1:N:140:GLU:OE2	9:V:50:LEU:N	2.37	0.55
1:A:90:THR:HB	1:A:95:THR:HG23	1.88	0.55
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.89	0.55
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.21	0.55
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.37	0.55
5:E:76:ILE:O	5:E:193:VAL:HG12	2.07	0.55
3:P:138:GLN:HB2	3:P:255:GLU:O	2.06	0.55
3:P:245:LEU:O	4:Q:201:ARG:CD	2.55	0.55
9:V:34:UNK:N	9:V:35:UNK:N	2.54	0.55
2:B:52:LYS:O	2:B:203:ARG:NH2	2.40	0.55
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.88	0.55
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.35	0.55
3:P:34:PHE:HB2	20:P:381:HOH:O	2.06	0.55
3:P:101:ARG:C	3:P:101:ARG:HD2	2.28	0.55
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.71	0.55
4:Q:218:LEU:HD11	5:R:42:THR:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:373:THR:N	1:N:374:PRO:HD2	2.22	0.54
2:O:57:TYR:CD1	2:O:57:TYR:N	2.74	0.54
2:O:290:SER:O	2:O:297:GLN:HG2	2.07	0.54
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.35	0.54
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.88	0.54
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.89	0.54
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.89	0.54
4:Q:161:ALA:O	4:Q:162:PRO:C	2.45	0.54
4:Q:220:TYR:CZ	4:Q:224:ARG:HD3	2.42	0.54
9:V:69:SER:HB2	9:V:72:ALA:HB3	1.89	0.54
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.43	0.54
2:B:47:ILE:HG22	2:B:48:GLY:N	2.23	0.54
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.72	0.54
6:S:17:ARG:HH11	6:S:17:ARG:HG2	1.72	0.54
1:A:170:THR:HG22	1:A:171:THR:N	2.23	0.54
3:P:9:HIS:CD2	3:P:11:LEU:H	2.25	0.54
3:P:112:GLU:O	3:P:116:THR:HG23	2.08	0.54
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.07	0.54
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.42	0.54
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.34	0.54
3:C:22:LEU:HD21	13:C:2002:UQ:HM32	1.89	0.54
3:C:169:PHE:CE1	5:R:72:SER:HA	2.39	0.54
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.89	0.54
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.90	0.54
3:C:245:LEU:O	4:D:201:ARG:CD	2.55	0.54
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.48	0.54
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.23	0.54
2:O:100:SER:HB2	2:O:105:MET:HG2	1.90	0.54
2:O:385:GLU:O	2:O:387:LEU:N	2.41	0.54
3:P:173:ASN:N	3:P:174:PRO:HD2	2.22	0.54
3:C:207:ASN:ND2	3:C:208:ASN:H	2.05	0.54
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.42	0.54
1:N:295:ALA:O	1:N:298:ALA:HB3	2.07	0.54
2:O:407:SER:O	2:O:411:VAL:HG23	2.08	0.54
3:C:142:TRP:O	3:C:146:VAL:HG23	2.07	0.54
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.54
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.54
1:A:131:ARG:NH2	1:A:177:LEU:O	2.41	0.54
1:A:255:LEU:HD12	1:A:422:LEU:HB2	1.90	0.54
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.26	0.54
3:P:329:LEU:O	3:P:332:ASN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.91	0.54
8:U:73:LEU:HD12	8:U:73:LEU:O	2.08	0.54
2:B:57:TYR:HE2	2:B:203:ARG:HH22	1.45	0.54
2:B:402:ILE:HG23	2:B:403:ASP:N	2.23	0.54
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.43	0.54
1:N:209:VAL:O	1:N:212:ALA:HB3	2.08	0.54
5:R:76:ILE:O	5:R:193:VAL:HG12	2.08	0.54
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.91	0.54
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.43	0.53
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.38	0.53
2:B:318:ASP:O	2:B:319:SER:HB2	2.08	0.53
1:N:178:THR:HG22	1:N:180:ALA:N	2.09	0.53
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.90	0.53
6:S:91:GLU:HB3	6:S:92:PRO:HD3	1.91	0.53
13:C:2002:UQ:C8	13:C:2002:UQ:HM51	2.38	0.53
4:D:47:ALA:H	4:D:50:ASN:ND2	1.96	0.53
5:E:116:LYS:HD2	5:E:116:LYS:N	2.23	0.53
2:O:46:ARG:HG3	2:O:379:LEU:HD22	1.90	0.53
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.43	0.53
2:O:57:TYR:HE2	2:O:203:ARG:HH22	1.48	0.53
1:A:182:LEU:O	1:A:186:ILE:HG13	2.07	0.53
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.43	0.53
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.23	0.53
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.90	0.53
2:B:96:LEU:H	9:I:70:LEU:HD22	1.74	0.53
2:B:345:LYS:HG2	2:B:418:VAL:HG13	1.91	0.53
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.34	0.53
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.43	0.53
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.90	0.53
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.44	0.53
9:V:69:SER:CB	9:V:72:ALA:HB3	2.39	0.53
1:A:136:GLN:OE1	9:I:50:LEU:HD12	2.08	0.53
2:B:28:LYS:O	2:B:29:LEU:O	2.27	0.53
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.22	0.53
5:E:117:LEU:HD23	5:E:121:GLN:H	1.73	0.53
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.53
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.24	0.53
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.39	0.53
1:A:165:ARG:HG3	1:A:165:ARG:HH11	1.74	0.53
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.91	0.53
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:TYR:HE1	2:B:108:CYS:SG	2.32	0.53
2:B:268:GLU:O	2:B:271:ALA:HB3	2.09	0.53
3:C:92:PHE:O	3:C:95:ILE:HG22	2.08	0.53
1:N:191:LYS:CA	1:N:195:MET:HE2	2.39	0.53
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.24	0.53
2:O:424:MET:HG2	2:O:425:ALA:N	2.24	0.53
3:P:143:GLY:O	3:P:147:ILE:HG12	2.09	0.53
3:P:156:TYR:CD2	3:P:156:TYR:N	2.75	0.53
6:F:94:LEU:HD12	6:F:94:LEU:O	2.08	0.53
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.74	0.52
2:B:357:VAL:O	2:B:361:LYS:HG3	2.09	0.52
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.10	0.52
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.52
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.44	0.52
2:O:140:LEU:C	2:O:142:PRO:HD2	2.28	0.52
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.39	0.52
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.43	0.52
2:B:140:LEU:C	2:B:142:PRO:HD2	2.30	0.52
3:C:121:LEU:O	3:C:125:MET:HG3	2.08	0.52
5:R:136:VAL:O	5:R:138:VAL:N	2.38	0.52
10:W:59:TYR:N	10:W:59:TYR:CD1	2.76	0.52
5:E:117:LEU:HD23	5:E:119:ASP:O	2.10	0.52
3:P:92:PHE:O	3:P:95:ILE:HG22	2.08	0.52
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.91	0.52
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.28	0.52
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.92	0.52
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.92	0.52
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.74	0.52
3:P:49:GLY:C	12:P:501:HEM:HAC	2.30	0.52
3:P:347:PRO:O	3:P:351:ILE:HG13	2.09	0.52
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.92	0.52
3:C:99:ILE:HD11	3:C:121:LEU:HD22	1.91	0.52
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.44	0.52
2:O:67:HIS:O	2:O:70:ARG:HB3	2.10	0.52
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.45	0.52
3:P:278:ALA:HB1	3:P:295:LEU:HD12	1.91	0.52
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.43	0.52
1:A:359:ASN:HD22	2:B:92:VAL:HA	1.74	0.52
3:C:101:ARG:HD2	3:C:101:ARG:C	2.30	0.52
3:C:215:ASP:HA	3:C:218:LYS:HE2	1.90	0.52
4:D:68:VAL:HG12	4:D:69:GLU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:VAL:HA	1:N:196:VAL:O	2.10	0.52
1:A:191:LYS:N	1:A:195:MET:HE2	2.25	0.52
2:B:170:THR:O	2:B:172:LEU:N	2.43	0.52
4:D:161:ALA:O	4:D:162:PRO:C	2.48	0.52
7:G:36:ASN:O	7:G:40:ARG:HG3	2.10	0.52
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.45	0.52
3:P:202:HIS:NE2	13:P:3002:UQ:O4	2.38	0.52
1:A:362:ARG:O	1:A:365:MET:HG2	2.09	0.52
2:B:57:TYR:N	2:B:57:TYR:CD1	2.77	0.52
6:F:32:MET:O	6:F:33:ARG:C	2.49	0.52
1:N:137:GLU:O	1:N:141:MET:HG3	2.09	0.52
4:Q:12:TRP:CZ2	4:Q:124:GLU:HB2	2.44	0.52
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.92	0.52
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.92	0.52
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.12	0.52
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.09	0.52
2:B:338:ARG:O	2:B:341:MET:HB2	2.10	0.51
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.10	0.51
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.92	0.51
2:O:341:MET:CE	2:O:341:MET:HA	2.40	0.51
1:A:404:ALA:O	1:A:406:MET:N	2.43	0.51
3:P:282:LEU:HD12	3:P:291:GLY:O	2.10	0.51
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.91	0.51
8:U:40:CYS:O	8:U:44:VAL:HG23	2.10	0.51
1:A:307:PHE:CD1	1:A:307:PHE:C	2.83	0.51
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.51
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.51
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.93	0.51
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.25	0.51
3:P:377:MET:HE2	6:S:20:TYR:CG	2.45	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
2:O:38:LEU:HD12	2:O:38:LEU:C	2.31	0.51
2:B:22:GLU:HG3	2:B:23:ASP:H	1.74	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.43	0.51
2:O:414:ALA:O	2:O:418:VAL:HG23	2.11	0.51
4:D:102:ARG:HA	4:D:108:ALA:O	2.10	0.51
4:D:167:GLU:HG3	8:H:13:LEU:HD23	1.91	0.51
5:E:52:LYS:C	5:E:52:LYS:HD3	2.30	0.51
8:H:65:ARG:O	8:H:68:CYS:HB3	2.10	0.51
2:O:156:GLN:HE22	9:V:77:ARG:C	2.14	0.51
2:O:170:THR:O	2:O:172:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:318:ASP:O	2:O:319:SER:HB2	2.11	0.51
2:O:341:MET:HA	2:O:341:MET:HE2	1.92	0.51
2:B:38:LEU:HD12	2:B:39:GLU:N	2.26	0.51
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.75	0.51
2:B:307:PHE:CD1	2:B:308:ASP:N	2.79	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.11	0.51
3:C:173:ASN:N	3:C:174:PRO:HD2	2.26	0.51
1:N:10:ASN:ND2	2:O:19:PRO:HD2	2.26	0.51
1:N:178:THR:CG2	1:N:179:ARG:N	2.73	0.51
2:O:46:ARG:HG3	2:O:46:ARG:O	2.10	0.51
8:H:40:CYS:O	8:H:44:VAL:HG23	2.10	0.51
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.45	0.51
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.93	0.51
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.40	0.51
1:N:106:MET:O	1:N:106:MET:HE2	2.10	0.51
1:N:295:ALA:O	1:N:299:VAL:HG23	2.10	0.51
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.42	0.51
3:P:31:TRP:CZ3	15:P:3007:PEE:H20	2.46	0.51
14:P:3004:CDL:HA32	7:T:40:ARG:HB3	1.92	0.51
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	1.92	0.51
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.92	0.51
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.93	0.51
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.93	0.51
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.45	0.51
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.26	0.51
3:C:246:PHE:C	3:C:248:PRO:HD3	2.31	0.51
3:P:332:ASN:ND2	3:P:358:SER:OG	2.42	0.51
1:A:121:ALA:O	1:A:122:LEU:HB2	2.11	0.50
5:E:130:PRO:C	5:E:132:TRP:H	2.14	0.50
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.30	0.50
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.75	0.50
4:Q:47:ALA:O	4:Q:50:ASN:HB2	2.11	0.50
2:B:273:SER:O	2:B:276:GLN:HB3	2.11	0.50
3:C:138:GLN:HB2	3:C:255:GLU:O	2.11	0.50
4:D:168:ILE:HG12	4:D:168:ILE:O	2.10	0.50
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.46	0.50
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.32	0.50
1:N:26:ALA:O	1:N:198:ALA:HA	2.12	0.50
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.46	0.50
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.46	0.50
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.93	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.26	0.50
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.94	0.50
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.76	0.50
2:B:141:GLN:N	2:B:142:PRO:HD2	2.27	0.50
6:F:53:ASP:OD1	6:F:54:LEU:N	2.44	0.50
1:N:255:LEU:CD1	1:N:422:LEU:HB2	2.40	0.50
3:P:48:THR:HG1	3:P:84:HIS:HD1	1.57	0.50
3:P:105:TYR:CA	3:P:315:THR:HG22	2.41	0.50
5:R:81:ILE:HD13	5:R:98:VAL:O	2.11	0.50
5:R:162:GLY:O	5:R:163:SER:C	2.50	0.50
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.94	0.50
2:B:414:ALA:O	2:B:418:VAL:HG23	2.12	0.50
3:C:105:TYR:CA	3:C:315:THR:HG22	2.41	0.50
1:N:255:LEU:O	1:N:321:GLY:HA3	2.12	0.50
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.34	0.50
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.12	0.50
9:V:64:LEU:HD12	9:V:77:ARG:O	2.12	0.50
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.93	0.50
1:A:343:MET:HB3	1:A:444:ILE:HA	1.94	0.50
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.75	0.50
2:O:141:GLN:N	2:O:142:PRO:HD2	2.26	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.91	0.50
2:B:341:MET:CE	2:B:341:MET:HA	2.42	0.50
3:C:31:TRP:NE1	15:C:2007:PEE:O4	2.45	0.50
3:C:347:PRO:O	3:C:351:ILE:HG13	2.12	0.50
5:E:72:SER:HA	3:P:169:PHE:CE1	2.46	0.50
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.42	0.50
10:J:59:TYR:CD1	10:J:59:TYR:N	2.79	0.50
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.47	0.50
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.12	0.50
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.12	0.50
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.93	0.50
1:N:317:THR:HG23	1:N:318:GLY:N	2.27	0.50
17:Q:501:HEC:HBB3	17:Q:501:HEC:HMB1	1.94	0.50
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.41	0.50
1:A:106:MET:O	1:A:110:VAL:HG23	2.11	0.49
1:A:255:LEU:O	1:A:321:GLY:HA3	2.11	0.49
3:C:28:ILE:HD11	3:C:225:TYR:CZ	2.47	0.49
4:D:183:ALA:O	4:D:186:VAL:HG12	2.11	0.49
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.77	0.49
2:B:46:ARG:HG3	2:B:46:ARG:O	2.11	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.49
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.45	0.49
1:N:178:THR:HB	1:N:181:ASP:OD1	2.12	0.49
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.47	0.49
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.94	0.49
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.12	0.49
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.46	0.49
5:E:84:GLY:N	5:E:100:HIS:O	2.43	0.49
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.46	0.49
2:O:206:LEU:O	2:O:206:LEU:HG	2.12	0.49
1:A:63:ALA:O	1:A:116:VAL:HG13	2.12	0.49
2:B:353:THR:HG22	2:B:355:GLU:N	2.10	0.49
5:E:84:GLY:CA	5:E:102:THR:HG23	2.42	0.49
9:I:70:LEU:HG	9:I:71:ASN:N	2.26	0.49
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.27	0.49
5:R:52:LYS:HD3	5:R:52:LYS:C	2.33	0.49
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.95	0.49
2:B:280:GLY:HA3	2:B:293:SER:OG	2.12	0.49
3:C:31:TRP:CZ3	15:C:2007:PEE:H20	2.48	0.49
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.43	0.49
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.27	0.49
3:P:45:GLN:CB	12:P:501:HEM:HAB	2.43	0.49
3:P:247:SER:OG	3:P:250:LEU:HB2	2.13	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
1:A:49:ASN:HD21	1:A:51:LYS:H	1.59	0.49
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.95	0.49
3:C:238:THR:HB	3:C:239:PRO:CD	2.36	0.49
5:E:127:VAL:O	5:E:128:LYS:HB2	2.13	0.49
1:N:165:ARG:HG3	1:N:165:ARG:NH1	2.26	0.49
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.12	0.49
2:O:56:ARG:NH1	2:O:171:ALA:HB1	2.27	0.49
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.48	0.49
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.48	0.49
4:Q:227:TRP:O	4:Q:228:SER:C	2.51	0.49
6:S:71:LYS:O	6:S:72:HIS:HB2	2.13	0.49
2:B:248:ASN:C	2:B:248:ASN:ND2	2.64	0.49
1:N:173:ASN:O	1:N:177:LEU:HG	2.13	0.49
3:P:319:ARG:O	3:P:323:GLN:HG3	2.13	0.49
14:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.42	0.49
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.24	0.49
3:C:112:GLU:O	3:C:116:THR:HG23	2.12	0.49
14:D:2003:CDL:H721	14:D:2003:CDL:HA62	1.93	0.49
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.48	0.49
5:R:137:GLY:O	5:R:145:VAL:HG13	2.12	0.49
1:A:23:LEU:HD23	1:A:23:LEU:C	2.33	0.49
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.76	0.49
2:B:200:THR:OG1	2:B:203:ARG:HG3	2.13	0.49
3:C:49:GLY:C	12:C:501:HEM:HAC	2.33	0.49
4:D:37:CYS:O	4:D:39:ALA:N	2.44	0.49
1:N:121:ALA:O	1:N:122:LEU:HB2	2.12	0.49
2:O:129:ALA:N	2:O:130:PRO:CD	2.76	0.49
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.45	0.49
9:V:32:UNK:O	9:V:33:UNK:C	2.61	0.49
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.48	0.49
1:N:354:VAL:HG23	1:N:355:LYS:N	2.28	0.49
2:O:96:LEU:HD12	2:O:97:SER:N	2.28	0.49
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.48	0.49
3:P:246:PHE:C	3:P:248:PRO:HD3	2.33	0.49
3:P:292:VAL:O	3:P:295:LEU:HB3	2.13	0.49
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.94	0.48
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.43	0.48
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.48	0.48
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.46	0.48
14:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.27	0.48
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.77	0.48
9:V:51:CYS:HB2	9:V:53:GLU:OE1	2.13	0.48
1:A:279:ARG:HH22	9:I:30:UNK:C	2.26	0.48
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.95	0.48
14:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.28	0.48
7:G:3:HIS:O	7:G:7:LEU:HG	2.12	0.48
1:N:307:PHE:CD1	1:N:307:PHE:C	2.85	0.48
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.94	0.48
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.48
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.95	0.48
3:P:286:PRO:O	3:P:287:ASN:CB	2.61	0.48
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.13	0.48
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.47	0.48
1:N:361:LEU:O	1:N:364:ALA:HB3	2.14	0.48
3:P:342:GLN:HB3	3:P:343:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.78	0.48
9:V:70:LEU:HD23	9:V:71:ASN:H	1.78	0.48
2:B:129:ALA:N	2:B:130:PRO:CD	2.77	0.48
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.78	0.48
4:D:47:ALA:HA	4:D:90:TYR:HA	1.95	0.48
1:A:178:THR:CG2	1:A:179:ARG:N	2.76	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.14	0.48
2:B:312:PHE:HE1	9:I:62:ARG:O	1.96	0.48
3:C:319:ARG:O	3:C:323:GLN:HG3	2.13	0.48
5:E:163:SER:HA	5:E:174:GLY:HA3	1.95	0.48
3:P:28:ILE:HD11	3:P:225:TYR:CZ	2.48	0.48
4:Q:178:THR:CG2	8:U:15:ASP:HA	2.43	0.48
1:A:39:VAL:HA	1:A:196:VAL:O	2.13	0.48
1:A:295:ALA:O	1:A:299:VAL:HG23	2.14	0.48
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.16	0.48
1:N:191:LYS:C	1:N:193:PRO:HD2	2.34	0.48
2:O:374:THR:HG22	2:O:376:GLN:H	1.79	0.48
4:Q:116:ILE:CG2	4:Q:190:LEU:HD13	2.43	0.48
3:C:233:LEU:O	3:C:237:LEU:HB2	2.12	0.48
5:E:102:THR:C	5:E:103:GLN:HG3	2.34	0.48
1:N:280:TYR:CG	1:N:281:ASP:N	2.81	0.48
2:O:221:GLU:HG3	2:O:222:GLN:N	2.21	0.48
2:O:248:ASN:C	2:O:248:ASN:ND2	2.64	0.48
3:P:319:ARG:HD2	3:P:374:GLU:OE2	2.14	0.48
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.44	0.48
4:D:37:CYS:C	4:D:39:ALA:N	2.67	0.48
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.96	0.48
4:D:150:ASN:O	4:D:156:GLN:HA	2.13	0.48
4:D:227:TRP:O	4:D:228:SER:C	2.51	0.48
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.44	0.48
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.95	0.48
10:W:57:HIS:ND1	10:W:58:LYS:N	2.62	0.48
1:N:170:THR:HG22	1:N:171:THR:H	1.78	0.48
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.95	0.47
4:D:37:CYS:C	4:D:39:ALA:H	2.16	0.47
9:I:55:MET:O	9:I:58:ARG:HG2	2.13	0.47
1:N:402:VAL:HA	1:N:406:MET:HE1	1.96	0.47
2:O:353:THR:HG22	2:O:355:GLU:N	2.09	0.47
3:P:377:MET:HE2	6:S:20:TYR:CD1	2.49	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.96	0.47
2:B:259:THR:HG22	2:B:260:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLU:C	2:B:387:LEU:H	2.17	0.47
2:B:403:ASP:O	2:B:405:VAL:N	2.44	0.47
14:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.14	0.47
5:E:35:PHE:O	5:E:38:LEU:HB3	2.15	0.47
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.96	0.47
3:P:146:VAL:HG21	3:P:269:ILE:HG21	1.95	0.47
1:A:240:GLU:HA	1:A:422:LEU:O	2.14	0.47
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.49	0.47
5:E:119:ASP:O	5:E:121:GLN:N	2.47	0.47
9:I:49:LEU:O	9:I:50:LEU:HD23	2.15	0.47
7:T:3:HIS:O	7:T:7:LEU:HG	2.13	0.47
7:T:68:ARG:NH2	7:T:69:LEU:HD21	2.29	0.47
2:B:306:PRO:HA	9:I:52:ARG:CG	2.45	0.47
2:B:374:THR:HG22	2:B:376:GLN:H	1.79	0.47
5:E:165:TYR:HA	5:E:170:ARG:O	2.15	0.47
2:O:38:LEU:HD12	2:O:39:GLU:N	2.29	0.47
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.39	0.47
1:A:170:THR:HB	1:A:173:ASN:HB2	1.96	0.47
3:C:36:SER:O	3:C:40:VAL:HG23	2.14	0.47
5:E:188:VAL:HG12	5:E:188:VAL:O	2.14	0.47
9:I:70:LEU:CD2	9:I:71:ASN:N	2.78	0.47
1:N:23:LEU:HD23	1:N:23:LEU:C	2.35	0.47
1:N:79:VAL:O	1:N:82:MET:HG2	2.14	0.47
1:N:438:ARG:HG3	1:N:438:ARG:HH11	1.80	0.47
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.95	0.47
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.54	0.47
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.45	0.47
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.78	0.47
4:D:116:ILE:CG2	4:D:190:LEU:HD13	2.43	0.47
9:V:70:LEU:HD23	9:V:71:ASN:N	2.30	0.47
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.82	0.47
3:C:92:PHE:O	3:C:93:ILE:C	2.50	0.47
4:D:122:GLY:O	4:D:123:GLY:C	2.53	0.47
7:G:68:ARG:NH2	7:G:69:LEU:HD21	2.29	0.47
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.32	0.47
3:P:92:PHE:O	3:P:93:ILE:C	2.52	0.47
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.50	0.47
5:R:96:LEU:HD12	5:R:135:LEU:O	2.14	0.47
5:R:153:PHE:O	5:R:155:GLY:N	2.48	0.47
7:T:36:ASN:O	7:T:40:ARG:HG3	2.14	0.47
2:B:206:LEU:O	2:B:216:LEU:HD21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.50	0.47
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.47	0.47
10:W:20:PHE:O	10:W:24:VAL:HG23	2.15	0.47
1:A:106:MET:O	1:A:106:MET:HE2	2.15	0.47
2:B:292:THR:HG22	2:B:292:THR:O	2.15	0.47
1:N:219:VAL:HG12	1:N:220:SER:N	2.30	0.47
3:P:44:THR:O	3:P:48:THR:HG23	2.15	0.47
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.50	0.47
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.96	0.47
5:R:79:SER:OG	5:R:191:ASP:HB2	2.15	0.47
3:C:22:LEU:HD12	3:C:23:PRO:N	2.29	0.47
4:D:47:ALA:O	4:D:50:ASN:HB2	2.14	0.47
1:N:47:TYR:CE2	1:N:231:LEU:HD11	2.49	0.47
1:N:49:ASN:HD21	1:N:51:LYS:H	1.57	0.47
1:N:253:VAL:O	1:N:323:HIS:HA	2.14	0.47
2:O:31:ASN:N	2:O:31:ASN:HD22	2.13	0.47
2:O:31:ASN:N	2:O:31:ASN:ND2	2.63	0.47
3:P:18:SER:HA	3:P:22:LEU:HD22	1.96	0.47
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.50	0.47
2:B:28:LYS:O	2:B:28:LYS:HG2	2.14	0.46
3:C:292:VAL:O	3:C:295:LEU:HB3	2.15	0.46
4:D:17:PRO:O	4:D:202:LYS:HD3	2.14	0.46
4:D:220:TYR:O	4:D:224:ARG:HG2	2.15	0.46
5:E:140:THR:O	5:E:177:PRO:HD2	2.15	0.46
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.79	0.46
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.97	0.46
2:O:345:LYS:HG2	2:O:418:VAL:HG11	1.97	0.46
3:P:141:PHE:HE1	3:P:171:VAL:O	1.97	0.46
3:C:335:ILE:HD13	7:G:58:LEU:HD23	1.96	0.46
1:N:205:HIS:O	1:N:208:LEU:HB3	2.14	0.46
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.46
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.84	0.46
8:U:15:ASP:O	8:U:17:LEU:N	2.49	0.46
3:C:146:VAL:HG21	3:C:269:ILE:HG21	1.96	0.46
5:E:162:GLY:O	5:E:163:SER:C	2.53	0.46
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.79	0.46
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.75	0.46
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.15	0.46
4:D:57:THR:HG22	4:D:58:GLU:N	2.30	0.46
2:O:33:LEU:HD12	2:O:204:MET:O	2.15	0.46
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:179:ASN:O	5:R:180:LEU:C	2.54	0.46
1:A:255:LEU:CD1	1:A:422:LEU:HB2	2.46	0.46
2:B:424:MET:HG2	2:B:425:ALA:N	2.30	0.46
3:C:202:HIS:NE2	13:C:2002:UQ:O4	2.46	0.46
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.96	0.46
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.16	0.46
5:R:163:SER:OG	5:R:176:ALA:HB2	2.16	0.46
1:A:27:SER:HA	1:A:199:ALA:O	2.15	0.46
2:B:206:LEU:HG	2:B:206:LEU:O	2.15	0.46
2:B:370:MET:O	2:B:373:GLU:HG3	2.15	0.46
4:D:239:PRO:HG2	4:D:241:LYS:HB2	1.97	0.46
8:H:15:ASP:O	8:H:17:LEU:N	2.48	0.46
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.15	0.46
1:A:289:HIS:CD2	2:B:83:PHE:HD1	2.32	0.46
2:B:366:ALA:O	2:B:369:LEU:N	2.49	0.46
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.51	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
9:I:38:UNK:O	9:I:40:UNK:N	2.47	0.46
5:R:165:TYR:HA	5:R:170:ARG:O	2.15	0.46
1:A:64:PHE:C	1:A:66:GLY:H	2.20	0.46
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.98	0.46
5:E:131:GLU:CD	5:E:131:GLU:H	2.18	0.46
5:R:185:TYR:O	5:R:186:GLN:HB3	2.16	0.46
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.97	0.46
3:C:216:SER:HB3	6:F:59:MET:CE	2.46	0.46
5:E:133:VAL:O	5:E:133:VAL:HG13	2.15	0.46
5:R:181:GLU:HG2	5:R:182:VAL:N	2.30	0.46
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.98	0.46
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.56	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.50	0.46
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.37	0.46
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.46	0.46
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.51	0.46
2:O:307:PHE:HD1	2:O:308:ASP:N	2.14	0.46
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.57	0.45
1:A:217:SER:O	1:A:218:GLY:C	2.54	0.45
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.42	0.45
2:B:135:TRP:O	2:B:136:GLU:C	2.53	0.45
5:E:96:LEU:HD12	5:E:135:LEU:O	2.16	0.45
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.56	0.45
2:O:57:TYR:N	2:O:57:TYR:HD1	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.46	0.45
2:O:355:GLU:O	2:O:358:THR:N	2.49	0.45
2:O:385:GLU:C	2:O:387:LEU:H	2.19	0.45
2:O:422:LYS:C	2:O:436:LEU:HD21	2.36	0.45
4:Q:181:GLN:HE21	4:Q:185:ASP:CG	2.19	0.45
5:R:185:TYR:N	5:R:185:TYR:CD2	2.85	0.45
7:T:79:ASN:O	7:T:80:ASP:HB2	2.16	0.45
1:A:48:GLU:HB3	1:A:52:ASN:OD1	2.16	0.45
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.98	0.45
5:E:52:LYS:NZ	10:J:32:GLU:OE1	2.42	0.45
1:N:34:THR:HA	1:N:102:LEU:HA	1.97	0.45
1:N:436:ARG:HD2	1:N:436:ARG:HA	1.77	0.45
2:O:198:ASN:O	2:O:203:ARG:HD3	2.16	0.45
2:O:327:ILE:HD11	9:V:58:ARG:O	2.16	0.45
1:A:52:ASN:OD1	1:A:52:ASN:C	2.55	0.45
1:A:245:ASP:OD1	1:A:247:ALA:HB3	2.16	0.45
2:B:26:ILE:HG23	2:B:26:ILE:O	2.16	0.45
2:B:57:TYR:HE2	2:B:203:ARG:NH2	2.09	0.45
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.99	0.45
3:C:273:TRP:CG	3:C:274:TYR:N	2.84	0.45
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.96	0.45
4:D:208:MET:SD	4:D:208:MET:C	2.95	0.45
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.98	0.45
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.98	0.45
8:H:28:GLU:O	8:H:32:LYS:HG3	2.16	0.45
1:N:64:PHE:C	1:N:66:GLY:H	2.20	0.45
1:A:146:THR:O	1:A:150:PHE:HD1	1.98	0.45
4:D:57:THR:HG22	4:D:59:ALA:H	1.81	0.45
1:N:48:GLU:HB3	1:N:52:ASN:OD1	2.16	0.45
2:B:306:PRO:HB3	9:I:52:ARG:N	2.31	0.45
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.84	0.45
1:N:48:GLU:CD	1:N:54:GLY:H	2.20	0.45
2:O:56:ARG:NH2	2:O:318:ASP:OD2	2.50	0.45
9:V:38:UNK:O	9:V:39:UNK:CB	2.63	0.45
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.84	0.45
8:H:10:GLU:O	8:H:11:GLU:HG3	2.17	0.45
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.52	0.45
5:R:106:ILE:O	5:R:109:GLU:HB3	2.17	0.45
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.98	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.78	0.45
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.17	0.45
3:P:238:THR:CB	3:P:239:PRO:HD3	2.34	0.45
3:P:376:LYS:O	6:S:17:ARG:NH1	2.50	0.45
6:S:94:LEU:O	6:S:94:LEU:HD12	2.17	0.45
7:T:56:TYR:O	7:T:59:TYR:HB3	2.16	0.45
1:A:191:LYS:C	1:A:195:MET:HE2	2.37	0.45
2:B:47:ILE:HD13	2:B:120:MET:SD	2.56	0.45
3:C:28:ILE:CD1	13:C:2002:UQ:HM21	2.47	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.15	0.45
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.51	0.45
2:O:341:MET:CE	2:O:417:PHE:CE2	2.98	0.45
3:P:99:ILE:HD11	3:P:121:LEU:HD22	1.98	0.45
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.32	0.45
2:B:110:GLU:O	2:B:111:CYS:HB3	2.17	0.45
2:B:290:SER:C	2:B:297:GLN:HE21	2.20	0.45
3:C:287:ASN:O	3:C:288:LYS:C	2.55	0.45
8:H:73:LEU:HD12	8:H:73:LEU:O	2.17	0.45
3:P:72:ARG:HH11	3:P:72:ARG:HG2	1.82	0.45
5:R:133:VAL:O	5:R:133:VAL:HG13	2.16	0.45
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.31	0.45
4:D:195:GLU:HG3	4:D:195:GLU:O	2.17	0.45
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.99	0.45
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.99	0.45
9:I:70:LEU:CG	9:I:71:ASN:N	2.78	0.45
1:N:10:ASN:ND2	2:O:18:CYS:HB3	2.08	0.45
1:N:106:MET:N	1:N:107:PRO:HD2	2.32	0.45
2:O:57:TYR:HE2	2:O:203:ARG:NH2	2.11	0.45
3:P:107:SER:OG	12:P:502:HEM:O1D	2.32	0.45
4:Q:37:CYS:C	4:Q:39:ALA:H	2.20	0.45
1:A:48:GLU:CD	1:A:54:GLY:H	2.21	0.44
2:B:162:ASN:O	2:B:244:ILE:HD12	2.17	0.44
1:N:106:MET:HE2	1:N:110:VAL:CG2	2.47	0.44
1:N:106:MET:HE2	1:N:110:VAL:HG23	1.99	0.44
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.82	0.44
2:O:290:SER:C	2:O:297:GLN:HE21	2.20	0.44
4:Q:178:THR:HG21	8:U:15:ASP:HA	1.99	0.44
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.47	0.44
5:E:181:GLU:HG2	5:E:182:VAL:N	2.31	0.44
7:G:29:ILE:HA	7:G:33:ALA:HB3	1.99	0.44
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.99	0.44
2:O:96:LEU:HD13	2:O:109:VAL:CG1	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.52	0.44
2:B:50:PHE:C	2:B:51:ILE:HG13	2.37	0.44
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.17	0.44
3:C:187:PRO:HG2	12:C:501:HEM:HMC3	2.00	0.44
5:E:106:ILE:O	5:E:106:ILE:HG22	2.17	0.44
6:F:71:LYS:O	6:F:72:HIS:HB2	2.16	0.44
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.44
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.99	0.44
5:R:153:PHE:C	5:R:155:GLY:H	2.20	0.44
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.30	0.44
4:D:151:PRO:HA	4:D:156:GLN:HG3	1.97	0.44
1:N:18:THR:HG23	1:N:24:ARG:CG	2.48	0.44
1:N:270:LEU:HD23	1:N:270:LEU:HA	1.81	0.44
2:O:221:GLU:C	2:O:223:PHE:H	2.20	0.44
3:P:223:PRO:O	3:P:227:PHE:HB2	2.17	0.44
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	2.00	0.44
5:R:141:HIS:HB3	19:R:501:FES:S2	2.58	0.44
2:B:56:ARG:NH1	2:B:171:ALA:HB1	2.32	0.44
5:R:136:VAL:HG12	5:R:138:VAL:HG23	1.99	0.44
1:A:253:VAL:O	1:A:323:HIS:HA	2.17	0.44
2:B:366:ALA:O	2:B:367:THR:C	2.55	0.44
4:D:224:ARG:HH21	7:G:26:ILE:HA	1.81	0.44
8:H:59:PHE:O	8:H:60:ASP:C	2.55	0.44
2:O:200:THR:OG1	2:O:203:ARG:HG3	2.17	0.44
2:O:209:ILE:HD11	2:O:378:LEU:HG	2.00	0.44
3:P:81:ARG:O	3:P:81:ARG:HD3	2.18	0.44
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	3.00	0.44
2:B:22:GLU:HG3	2:B:23:ASP:N	2.32	0.44
5:E:102:THR:O	5:E:103:GLN:HG3	2.17	0.44
5:E:161:HIS:HB2	19:E:501:FES:S1	2.58	0.44
1:N:23:LEU:HA	1:N:192:ALA:O	2.17	0.44
2:O:19:PRO:HG3	2:O:41:PHE:CD2	2.52	0.44
1:A:373:THR:N	1:A:374:PRO:HD2	2.31	0.44
2:B:368:TYR:O	2:B:372:VAL:HG23	2.18	0.44
1:A:7:THR:HG21	2:B:113:ARG:CD	2.44	0.44
1:A:79:VAL:O	1:A:82:MET:HG2	2.17	0.44
2:B:63:LEU:O	2:B:182:ARG:NE	2.43	0.44
2:B:76:THR:HG22	2:B:81:SER:CA	2.45	0.44
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.98	0.44
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.18	0.44
4:D:116:ILE:HG21	4:D:190:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:239:PRO:C	4:D:241:LYS:H	2.20	0.44
8:H:17:LEU:HD13	8:H:73:LEU:CD2	2.47	0.44
2:O:33:LEU:HD21	2:O:224:LEU:HD12	2.00	0.44
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.18	0.44
2:O:101:THR:HG23	2:O:104:LYS:HE3	2.00	0.44
2:O:276:GLN:HG2	2:O:281:ALA:HB2	2.00	0.44
3:P:282:LEU:HD12	3:P:291:GLY:C	2.38	0.44
5:R:185:TYR:N	5:R:185:TYR:HD2	2.16	0.44
1:A:418:LYS:O	1:A:420:PRO:HD3	2.18	0.43
3:C:378:LEU:HD22	6:F:33:ARG:HG3	2.01	0.43
7:G:56:TYR:O	7:G:59:TYR:HB3	2.18	0.43
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.47	0.43
3:P:45:GLN:HB3	12:P:501:HEM:HAB	2.00	0.43
3:P:216:SER:HB3	6:S:59:MET:HE1	2.00	0.43
3:P:287:ASN:O	3:P:288:LYS:C	2.55	0.43
1:A:289:HIS:O	1:A:290:LEU:C	2.57	0.43
2:B:67:HIS:O	2:B:70:ARG:HB3	2.18	0.43
2:B:156:GLN:HE22	9:I:77:ARG:C	2.21	0.43
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.99	0.43
5:E:189:GLY:O	5:E:192:LEU:O	2.35	0.43
2:O:385:GLU:C	2:O:387:LEU:N	2.72	0.43
1:A:47:TYR:CE2	1:A:231:LEU:HD11	2.54	0.43
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.50	0.43
2:B:379:LEU:O	2:B:379:LEU:HG	2.18	0.43
4:D:208:MET:O	4:D:212:SER:HB2	2.18	0.43
2:O:174:ASN:HA	2:O:175:PRO:HD2	1.85	0.43
2:O:280:GLY:HA3	2:O:293:SER:OG	2.18	0.43
3:P:36:SER:O	3:P:40:VAL:HG23	2.19	0.43
6:S:40:ASP:OD1	6:S:40:ASP:C	2.57	0.43
9:V:32:UNK:N	9:V:73:PRO:HG2	2.32	0.43
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.73	0.43
2:O:151:ALA:O	2:O:157:VAL:HG11	2.19	0.43
2:O:366:ALA:O	2:O:367:THR:C	2.57	0.43
14:Q:3003:CDL:H721	14:Q:3003:CDL:HA62	1.99	0.43
1:A:295:ALA:O	1:A:298:ALA:HB3	2.18	0.43
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.47	0.43
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.99	0.43
3:C:362:ILE:HA	3:C:366:LEU:HB2	2.01	0.43
17:D:501:HEC:HMB1	17:D:501:HEC:HBB3	2.00	0.43
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.82	0.43
3:P:31:TRP:NE1	15:P:3007:PEE:O4	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:50:LEU:O	3:P:54:MET:HG3	2.17	0.43
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.32	0.43
5:R:155:GLY:HA3	5:R:165:TYR:O	2.18	0.43
1:A:272:VAL:O	1:A:275:ALA:HB3	2.18	0.43
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.43
3:C:304:LEU:O	3:C:305:ILE:C	2.57	0.43
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.19	0.43
3:P:142:TRP:CD1	3:P:266:PRO:HD3	2.53	0.43
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.18	0.43
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.90	0.43
1:A:361:LEU:O	1:A:364:ALA:HB3	2.17	0.43
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.40	0.43
1:N:240:GLU:HA	1:N:422:LEU:O	2.18	0.43
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.83	0.43
2:O:295:LEU:O	2:O:299:VAL:HG23	2.19	0.43
3:P:2:ALA:HB3	3:P:8:SER:HB3	2.00	0.43
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.32	0.43
4:Q:220:TYR:CE2	14:Q:3003:CDL:H722	2.54	0.43
1:A:41:ILE:HG22	1:A:42:GLY:N	2.34	0.43
1:A:140:GLU:HG2	9:I:50:LEU:HG	1.99	0.43
2:B:57:TYR:N	2:B:57:TYR:HD1	2.16	0.43
2:B:207:VAL:HG21	2:B:383:GLY:HA2	2.01	0.43
3:C:313:GLN:HE21	6:F:36:THR:CB	2.31	0.43
5:E:101:ARG:HG2	5:E:105:GLU:CD	2.38	0.43
6:F:52:GLU:HG3	6:F:56:ASN:ND2	2.34	0.43
2:O:207:VAL:HG21	2:O:383:GLY:HA2	2.00	0.43
3:P:38:LEU:HD23	3:P:38:LEU:HA	1.86	0.43
3:P:285:ILE:HD12	3:P:294:ALA:HB2	2.00	0.43
4:Q:208:MET:SD	4:Q:208:MET:C	2.97	0.43
3:C:273:TRP:CD2	3:C:274:TYR:N	2.87	0.43
4:D:223:LYS:HD3	4:D:223:LYS:C	2.38	0.43
1:N:18:THR:HG23	1:N:24:ARG:HG3	2.00	0.43
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.83	0.43
1:N:433:ASP:OD1	1:N:435:ASN:HB2	2.18	0.43
2:O:135:TRP:O	2:O:136:GLU:C	2.57	0.43
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.52	0.43
3:P:172:ASP:C	3:P:174:PRO:HD2	2.39	0.43
3:P:313:GLN:HE21	6:S:36:THR:CB	2.32	0.43
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.46	0.43
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.34	0.43
5:R:77:LYS:HA	5:R:192:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:135:LEU:CD2	5:R:182:VAL:HG22	2.49	0.43
3:C:247:SER:OG	3:C:250:LEU:HB2	2.19	0.43
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.54	0.43
4:D:165:TYR:O	4:D:166:ASN:C	2.57	0.43
10:J:57:HIS:ND1	10:J:58:LYS:N	2.67	0.43
2:O:264:VAL:HG12	2:O:265:GLY:N	2.34	0.43
3:P:22:LEU:HD12	3:P:23:PRO:N	2.34	0.43
3:P:41:CYS:SG	3:P:91:PHE:HA	2.58	0.43
3:P:198:LEU:HD21	12:P:502:HEM:CMA	2.49	0.43
3:P:279:TYR:O	3:P:282:LEU:HB3	2.18	0.43
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.19	0.43
7:T:50:PRO:HB2	7:T:51:PRO:HD2	1.99	0.43
1:A:178:THR:O	1:A:179:ARG:C	2.58	0.42
2:B:209:ILE:HD11	2:B:378:LEU:HG	2.01	0.42
5:E:130:PRO:O	5:E:132:TRP:N	2.52	0.42
1:N:27:SER:HA	1:N:199:ALA:O	2.19	0.42
2:O:124:LEU:HD23	2:O:124:LEU:C	2.39	0.42
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.54	0.42
5:R:134:ILE:HB	5:R:185:TYR:CE1	2.54	0.42
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.19	0.42
3:C:329:LEU:O	3:C:332:ASN:HB3	2.20	0.42
1:N:106:MET:CE	1:N:110:VAL:HG21	2.49	0.42
3:P:325:LEU:HD12	3:P:325:LEU:HA	1.77	0.42
13:P:3002:UQ:HM51	13:P:3002:UQ:H8	2.01	0.42
7:T:29:ILE:HA	7:T:33:ALA:HB3	2.00	0.42
8:U:27:THR:O	8:U:31:VAL:HG23	2.19	0.42
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.35	0.42
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.39	0.42
3:C:336:LEU:HD23	3:C:336:LEU:HA	1.86	0.42
13:C:2002:UQ:HM51	13:C:2002:UQ:H8	2.01	0.42
4:D:178:THR:HG21	8:H:15:ASP:HA	2.00	0.42
1:N:404:ALA:O	1:N:406:MET:N	2.53	0.42
3:P:145:THR:O	3:P:149:ASN:HB2	2.20	0.42
6:S:70:LEU:HD12	6:S:70:LEU:O	2.19	0.42
1:A:45:SER:HA	1:A:48:GLU:CD	2.39	0.42
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.54	0.42
2:O:96:LEU:HB3	9:V:70:LEU:HD22	2.01	0.42
2:O:162:ASN:O	2:O:244:ILE:HD12	2.19	0.42
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.54	0.42
2:O:357:VAL:O	2:O:361:LYS:HG3	2.19	0.42
3:P:362:ILE:HA	3:P:366:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.01	0.42
2:B:163:LEU:O	2:B:166:ALA:N	2.49	0.42
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.42
1:N:289:HIS:O	1:N:290:LEU:C	2.58	0.42
2:O:206:LEU:HG	2:O:216:LEU:HD11	2.01	0.42
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.02	0.42
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.42
8:U:28:GLU:O	8:U:32:LYS:HG3	2.19	0.42
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.42	0.42
2:B:355:GLU:O	2:B:358:THR:N	2.52	0.42
3:C:377:MET:CE	6:F:20:TYR:HB2	2.50	0.42
2:O:341:MET:HE2	2:O:341:MET:CA	2.49	0.42
1:A:365:MET:HG3	1:A:366:VAL:N	2.35	0.42
2:B:341:MET:CE	2:B:417:PHE:CE2	2.93	0.42
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.98	0.42
2:O:26:ILE:HG23	2:O:26:ILE:O	2.19	0.42
2:O:257:VAL:HG22	2:O:424:MET:HG3	2.02	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.88	0.42
3:P:377:MET:CE	6:S:20:TYR:HB2	2.50	0.42
5:R:99:ARG:HB3	5:R:133:VAL:HG12	2.02	0.42
7:T:34:LEU:HB2	7:T:35:PRO:HD3	2.02	0.42
1:A:281:ASP:OD2	9:I:33:UNK:HB2	2.18	0.42
2:B:51:ILE:CG2	2:B:52:LYS:N	2.82	0.42
2:B:341:MET:HA	2:B:341:MET:HE2	2.02	0.42
3:C:245:LEU:O	4:D:201:ARG:HD2	2.19	0.42
1:N:394:GLU:O	1:N:395:TRP:C	2.58	0.42
5:R:141:HIS:O	5:R:142:LEU:HD23	2.19	0.42
6:S:52:GLU:HG3	6:S:56:ASN:ND2	2.35	0.42
1:A:106:MET:HE2	1:A:110:VAL:HG23	2.02	0.42
1:A:228:VAL:O	1:A:228:VAL:HG13	2.20	0.42
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.46	0.42
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.55	0.42
2:B:266:SER:HB3	2:B:269:ALA:HB2	2.01	0.42
7:G:29:ILE:HA	7:G:33:ALA:CB	2.50	0.42
2:O:221:GLU:O	2:O:223:PHE:N	2.51	0.42
2:O:306:PRO:HB3	9:V:52:ARG:H	1.85	0.42
3:P:186:LEU:O	3:P:187:PRO:C	2.58	0.42
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.50	0.42
1:A:402:VAL:HG22	1:A:406:MET:HE2	2.01	0.42
3:C:279:TYR:O	3:C:282:LEU:HB3	2.19	0.42
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.55	0.42
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.42
5:E:190:ASP:C	5:E:192:LEU:N	2.72	0.42
2:O:259:THR:O	2:O:260:GLU:C	2.56	0.42
2:O:268:GLU:O	2:O:268:GLU:HG2	2.20	0.42
2:O:314:VAL:HG22	9:V:63:ASP:N	2.34	0.42
2:O:366:ALA:O	2:O:369:LEU:N	2.52	0.42
2:O:408:ALA:O	2:O:409:ASP:C	2.57	0.42
3:P:187:PRO:HG2	12:P:501:HEM:HMC3	2.00	0.42
4:Q:165:TYR:O	4:Q:166:ASN:C	2.58	0.42
1:A:205:HIS:O	1:A:208:LEU:HB3	2.20	0.41
2:B:192:HIS:O	2:B:196:GLN:HG3	2.19	0.41
2:B:264:VAL:HG23	2:B:316:TYR:O	2.20	0.41
2:B:385:GLU:C	2:B:387:LEU:N	2.72	0.41
5:E:37:TYR:CE2	15:E:2005:PEE:H10	2.56	0.41
5:E:177:PRO:HG2	5:E:178:TYR:H	1.85	0.41
1:N:146:THR:O	1:N:150:PHE:HD1	2.03	0.41
1:N:219:VAL:CG1	1:N:220:SER:N	2.83	0.41
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.47	0.41
1:N:365:MET:HG3	1:N:366:VAL:N	2.35	0.41
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.46	0.41
2:O:176:LEU:HD12	2:O:176:LEU:O	2.20	0.41
5:R:35:PHE:O	5:R:38:LEU:HB3	2.19	0.41
5:R:76:ILE:HD13	5:R:89:PHE:CD1	2.54	0.41
8:U:59:PHE:O	8:U:60:ASP:C	2.58	0.41
1:A:21:ASN:OD1	1:A:21:ASN:N	2.54	0.41
2:B:29:LEU:HB3	2:B:30:PRO:HD2	2.02	0.41
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.87	0.41
14:C:2004:CDL:HA32	7:G:40:ARG:HB3	2.02	0.41
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.20	0.41
2:O:35:ILE:O	2:O:213:HIS:HE1	2.03	0.41
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.02	0.41
3:C:223:PRO:O	3:C:227:PHE:HB2	2.20	0.41
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.30	0.41
3:P:245:LEU:HD23	3:P:245:LEU:HA	1.90	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.75	0.41
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.50	0.41
5:R:97:PHE:O	5:R:134:ILE:HA	2.20	0.41
6:S:32:MET:O	6:S:33:ARG:C	2.58	0.41
6:S:67:ASP:HA	6:S:70:LEU:HD23	2.02	0.41
1:A:191:LYS:O	1:A:195:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.44	0.41
2:B:345:LYS:HG2	2:B:418:VAL:HG11	2.02	0.41
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.21	0.41
2:O:85:ILE:HA	2:O:122:TYR:CD2	2.56	0.41
8:U:15:ASP:C	8:U:17:LEU:N	2.74	0.41
1:A:58:PHE:HZ	1:A:131:ARG:HB2	1.86	0.41
1:A:220:SER:HB2	1:A:225:GLU:HB2	2.03	0.41
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.41	0.41
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.84	0.41
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.55	0.41
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.51	0.41
3:P:64:PHE:CD2	3:P:259:PRO:HG3	2.56	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.55	0.41
6:S:70:LEU:HD12	6:S:70:LEU:C	2.41	0.41
1:A:89:TYR:CD1	1:A:89:TYR:C	2.94	0.41
1:A:172:GLU:O	1:A:175:LYS:N	2.51	0.41
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.55	0.41
2:B:222:GLN:O	2:B:222:GLN:CG	2.68	0.41
2:B:280:GLY:HA3	2:B:293:SER:HG	1.86	0.41
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.21	0.41
4:D:102:ARG:HG2	4:D:102:ARG:NH1	2.36	0.41
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.56	0.41
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.21	0.41
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.56	0.41
4:Q:37:CYS:O	4:Q:39:ALA:N	2.54	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.93	0.41
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.84	0.41
9:V:70:LEU:HD21	9:V:71:ASN:OD1	2.20	0.41
1:A:34:THR:HA	1:A:102:LEU:HA	2.02	0.41
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.85	0.41
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.55	0.41
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.88	0.41
4:D:204:MET:HE3	18:D:2009:BOG:H1'1	2.02	0.41
5:E:77:LYS:HA	5:E:192:LEU:HD23	2.01	0.41
8:H:15:ASP:C	8:H:17:LEU:N	2.74	0.41
1:N:191:LYS:N	1:N:195:MET:HE2	2.36	0.41
9:V:33:UNK:N	9:V:73:PRO:CG	2.83	0.41
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.35	0.41
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.55	0.41
2:B:307:PHE:HD1	2:B:308:ASP:N	2.19	0.41
5:E:97:PHE:O	5:E:134:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.03	0.41
1:N:206:LYS:H	1:N:206:LYS:HD2	1.86	0.41
2:O:47:ILE:CG2	2:O:48:GLY:N	2.84	0.41
2:O:56:ARG:HA	2:O:171:ALA:O	2.20	0.41
2:O:169:LYS:HG3	2:O:240:TRP:HB2	2.01	0.41
1:A:106:MET:HE2	1:A:110:VAL:CG2	2.50	0.41
1:A:280:TYR:CD2	1:A:281:ASP:N	2.88	0.41
1:A:404:ALA:O	1:A:405:ARG:C	2.59	0.41
2:B:56:ARG:HA	2:B:171:ALA:O	2.21	0.41
2:B:59:THR:O	2:B:61:ALA:N	2.53	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.91	0.41
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.56	0.41
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.85	0.41
4:D:28:ARG:O	4:D:31:GLN:N	2.54	0.41
4:D:40:CYS:SG	17:D:501:HEC:HMC1	2.61	0.41
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.56	0.41
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.51	0.41
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.41
1:N:351:GLU:O	1:N:354:VAL:HG22	2.21	0.41
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.41	0.41
3:P:47:LEU:HD12	3:P:47:LEU:HA	1.93	0.41
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	2.03	0.41
4:Q:37:CYS:C	4:Q:39:ALA:N	2.74	0.41
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.35	0.41
5:R:122:HIS:HA	5:R:170:ARG:NH1	2.36	0.41
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.51	0.41
6:S:67:ASP:CG	6:S:71:LYS:HZ3	2.24	0.41
8:U:17:LEU:HD13	8:U:73:LEU:CD2	2.48	0.41
1:A:47:TYR:CZ	1:A:231:LEU:HD11	2.56	0.41
1:A:351:GLU:O	1:A:354:VAL:HG22	2.21	0.41
2:B:23:ASP:O	2:B:24:LEU:CB	2.56	0.41
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.56	0.41
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.38	0.41
4:D:215:LEU:HD13	5:E:46:ALA:HB3	2.03	0.41
5:E:141:HIS:HB2	5:E:176:ALA:HB2	2.03	0.41
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.84	0.41
1:N:281:ASP:C	1:N:283:THR:H	2.24	0.41
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.51	0.41
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.39	0.41
10:W:10:TYR:CD2	10:W:10:TYR:C	2.94	0.41
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:246:PHE:O	3:C:248:PRO:HD3	2.21	0.40
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.52	0.40
1:N:7:THR:HG21	2:O:113:ARG:CD	2.47	0.40
1:N:439:SER:C	1:N:441:MET:H	2.24	0.40
6:S:82:LYS:O	6:S:83:TYR:C	2.58	0.40
9:V:33:UNK:N	9:V:73:PRO:HG2	2.36	0.40
1:A:106:MET:N	1:A:107:PRO:HD2	2.36	0.40
9:I:38:UNK:C	9:I:40:UNK:N	2.64	0.40
1:N:159:GLN:NE2	5:R:7:VAL:HG11	2.37	0.40
1:N:439:SER:HA	1:N:442:TYR:CE2	2.56	0.40
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.55	0.40
3:P:23:PRO:HG2	7:T:3:HIS:HB3	2.03	0.40
3:P:92:PHE:CA	3:P:95:ILE:HG22	2.49	0.40
6:S:57:GLU:O	6:S:61:ARG:HG3	2.21	0.40
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.51	0.40
1:A:204:SER:HB3	1:A:207:GLU:HB2	2.03	0.40
1:A:293:ARG:CD	1:A:344:ARG:CZ	3.00	0.40
2:B:198:ASN:HA	2:B:203:ARG:NH1	2.37	0.40
2:B:209:ILE:HD12	2:B:379:LEU:HB2	2.03	0.40
3:C:22:LEU:HD12	3:C:23:PRO:HD2	2.03	0.40
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.50	0.40
17:D:501:HEC:HMC1	17:D:501:HEC:HBC3	2.04	0.40
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.03	0.40
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.45	0.40
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.61	0.40
1:N:134:ILE:HG21	1:N:174:ILE:CD1	2.50	0.40
1:N:220:SER:HB2	1:N:225:GLU:HB2	2.03	0.40
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.21	0.40
3:P:75:GLN:O	3:P:76:TYR:HB2	2.21	0.40
5:R:83:GLU:HA	5:R:100:HIS:CB	2.49	0.40
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.88	0.40
1:A:296:ALA:O	1:A:299:VAL:N	2.55	0.40
2:B:51:ILE:HG22	2:B:52:LYS:N	2.37	0.40
2:B:56:ARG:NH2	2:B:318:ASP:OD2	2.55	0.40
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.78	0.40
3:C:130:VAL:HG23	3:C:131:GLY:N	2.37	0.40
4:D:26:VAL:HG12	4:D:55:THR:HG21	2.03	0.40
5:E:52:LYS:C	5:E:52:LYS:CD	2.89	0.40
5:E:101:ARG:HD2	5:E:105:GLU:HB3	2.03	0.40
1:N:45:SER:HA	1:N:48:GLU:CD	2.41	0.40
2:O:368:TYR:O	2:O:372:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:388:LEU:O	2:O:389:SER:HB2	2.21	0.40
5:R:30:GLU:HB2	10:W:7:ARG:HG3	2.03	0.40
2:B:62:ASN:O	2:B:65:THR:CG2	2.64	0.40
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.51	0.40
3:C:172:ASP:C	3:C:174:PRO:HD2	2.42	0.40
5:E:130:PRO:C	5:E:132:TRP:N	2.75	0.40
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.03	0.40
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.85	0.40
2:O:227:ARG:HB3	2:O:228:SER:H	1.42	0.40
3:P:51:LEU:HA	3:P:51:LEU:HD23	1.88	0.40
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.57	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	441/446 (99%)	384 (87%)	48 (11%)	9 (2%)	7	34
1	N	440/446 (99%)	385 (88%)	45 (10%)	10 (2%)	6	31
2	B	419/441 (95%)	350 (84%)	51 (12%)	18 (4%)	2	17
2	O	420/441 (95%)	359 (86%)	46 (11%)	15 (4%)	3	20
3	C	378/380 (100%)	346 (92%)	25 (7%)	7 (2%)	8	36
3	P	377/380 (99%)	336 (89%)	33 (9%)	8 (2%)	7	33
4	D	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	9	38
4	Q	239/241 (99%)	216 (90%)	17 (7%)	6 (2%)	5	29
5	E	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	1	4
5	R	194/196 (99%)	162 (84%)	27 (14%)	5 (3%)	5	28
6	F	99/110 (90%)	93 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	99/110 (90%)	89 (90%)	10 (10%)	0	100	100
7	G	78/81 (96%)	65 (83%)	11 (14%)	2 (3%)	5	28
7	T	77/81 (95%)	65 (84%)	10 (13%)	2 (3%)	5	28
8	H	68/77 (88%)	59 (87%)	9 (13%)	0	100	100
8	U	65/77 (84%)	53 (82%)	12 (18%)	0	100	100
9	I	29/47 (62%)	26 (90%)	3 (10%)	0	100	100
9	V	29/47 (62%)	23 (79%)	6 (21%)	0	100	100
10	J	59/61 (97%)	53 (90%)	5 (8%)	1 (2%)	9	38
10	W	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
All	All	4002/4160 (96%)	3481 (87%)	418 (10%)	103 (3%)	5	28

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	224	LEU
2	B	227	ARG
3	C	287	ASN
5	E	115	SER
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
5	E	191	ASP
1	N	282	ARG
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
1	A	71	PRO
1	A	218	GLY
1	A	405	ARG
1	A	433	ASP
2	B	21	ALA
2	B	201	SER

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Mol	Chain	Res	Type
2	B	221	GLU
2	B	372	VAL
2	B	386	ALA
2	B	389	SER
5	E	102	THR
5	E	127	VAL
5	E	131	GLU
5	E	137	GLY
2	O	24	LEU
2	O	201	SER
2	O	221	GLU
2	O	222	GLN
2	O	372	VAL
2	O	386	ALA
2	O	389	SER
3	P	274	TYR
5	R	137	GLY
5	R	154	GLY
5	R	163	SER
7	T	33	ALA
2	B	24	LEU
2	B	46	ARG
3	C	3	PRO
4	D	166	ASN
5	E	80	ASP
5	E	120	PRO
5	E	177	PRO
7	G	33	ALA
1	N	72	CYS
2	O	46	ARG
2	O	330	ALA
3	P	111	LYS
4	Q	166	ASN
4	Q	177	ALA
5	R	186	GLN
5	R	191	ASP
7	T	50	PRO
1	A	65	LYS
1	A	72	CYS
1	A	145	MET
2	B	189	GLU
3	C	111	LYS

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Mol	Chain	Res	Type
5	E	123	ASP
5	E	154	GLY
1	N	65	LYS
1	N	71	PRO
1	N	145	MET
1	N	262	TRP
1	N	405	ARG
3	P	156	TYR
3	P	264	VAL
2	B	319	SER
3	C	17	ASN
4	D	38	SER
4	D	176	PRO
7	G	50	PRO
10	J	61	ALA
2	O	404	SER
3	P	158	GLY
4	Q	38	SER
4	Q	176	PRO
4	Q	198	HIS
2	B	431	GLY
3	C	19	LEU
5	E	189	GLY
3	P	3	PRO
2	B	20	GLY
5	E	188	VAL
1	N	428	ILE
2	B	129	ALA
4	Q	162	PRO
3	C	158	GLY
3	C	264	VAL
1	N	218	GLY
3	P	157	ILE
1	A	428	ILE
4	D	162	PRO
2	O	431	GLY

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	365/368 (99%)	353 (97%)	12 (3%)	38	69
1	N	365/368 (99%)	352 (96%)	13 (4%)	35	67
2	B	332/347 (96%)	319 (96%)	13 (4%)	32	64
2	O	333/347 (96%)	319 (96%)	14 (4%)	30	62
3	C	328/329 (100%)	323 (98%)	5 (2%)	65	84
3	P	328/329 (100%)	322 (98%)	6 (2%)	59	81
4	D	200/200 (100%)	197 (98%)	3 (2%)	65	84
4	Q	200/200 (100%)	197 (98%)	3 (2%)	65	84
5	E	166/166 (100%)	163 (98%)	3 (2%)	59	81
5	R	165/166 (99%)	162 (98%)	3 (2%)	59	81
6	F	93/96 (97%)	90 (97%)	3 (3%)	39	70
6	S	93/96 (97%)	88 (95%)	5 (5%)	22	55
7	G	71/71 (100%)	69 (97%)	2 (3%)	43	73
7	T	70/71 (99%)	68 (97%)	2 (3%)	42	72
8	H	65/71 (92%)	64 (98%)	1 (2%)	65	84
8	U	63/71 (89%)	62 (98%)	1 (2%)	62	83
9	I	23/26 (88%)	21 (91%)	2 (9%)	10	34
9	V	23/26 (88%)	22 (96%)	1 (4%)	29	62
10	J	49/49 (100%)	47 (96%)	2 (4%)	30	63
10	W	47/49 (96%)	46 (98%)	1 (2%)	53	78
All	All	3379/3446 (98%)	3284 (97%)	95 (3%)	43	73

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	86	PHE
1	A	90	THR
1	A	106	MET
1	A	226	ASP
1	A	281	ASP
1	A	307	PHE
1	A	395	TRP

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Mol	Chain	Res	Type
1	A	405	ARG
1	A	422	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	38	LEU
2	B	57	TYR
2	B	97	SER
2	B	104	LYS
2	B	170	THR
2	B	193	HIS
2	B	228	SER
2	B	248	ASN
2	B	304	THR
2	B	341	MET
2	B	402	ILE
2	B	424	MET
3	C	69	HIS
3	C	81	ARG
3	C	223	PRO
3	C	259	PRO
3	C	367	PHE
4	D	43	MET
4	D	72	ASP
4	D	203	ARG
5	E	52	LYS
5	E	131	GLU
5	E	185	TYR
6	F	58	ARG
6	F	70	LEU
6	F	78	GLU
7	G	4	PHE
7	G	17	SER
8	H	71	HIS
9	I	70	LEU
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	18	THR
1	N	49	ASN
1	N	86	PHE
1	N	90	THR

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Mol	Chain	Res	Type
1	N	106	MET
1	N	281	ASP
1	N	307	PHE
1	N	395	TRP
1	N	405	ARG
1	N	420	PRO
1	N	422	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	38	LEU
2	O	57	TYR
2	O	59	THR
2	O	97	SER
2	O	104	LYS
2	O	170	THR
2	O	193	HIS
2	O	223	PHE
2	O	248	ASN
2	O	341	MET
2	O	402	ILE
2	O	424	MET
3	P	69	HIS
3	P	81	ARG
3	P	259	PRO
3	P	277	PHE
3	P	334	LEU
3	P	367	PHE
4	Q	43	MET
4	Q	72	ASP
4	Q	203	ARG
5	R	52	LYS
5	R	80	ASP
5	R	185	TYR
6	S	13	MET
6	S	58	ARG
6	S	70	LEU
6	S	78	GLU
6	S	84	GLU
7	T	4	PHE
7	T	27	PRO

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Mol	Chain	Res	Type
8	U	71	HIS
9	V	59	SER
10	W	59	TYR

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	10	ASN
1	A	49	ASN
1	A	85	HIS
1	A	274	ASN
1	A	289	HIS
1	A	301	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	329	GLN
2	B	343	GLN
3	C	9	HIS
3	C	17	ASN
3	C	73	ASN
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
5	E	3	ASN
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
6	F	56	ASN
7	G	6	ASN
7	G	23	GLN

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Mol	Chain	Res	Type
7	G	73	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	329	GLN
2	O	343	GLN
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
5	R	57	GLN
5	R	122	HIS
5	R	164	HIS
6	S	72	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	71	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 9 are unknown - leaving 27 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	$\#\|Z\| > 2$
15	PEE	N	3008	-	4,4,50	3.83	4 (100%)	6,6,55	0.66	0
15	PEE	C	2008	-	20,20,50	1.87	6 (30%)	23,25,55	0.68	0
17	HEC	D	501	4	32,50,50	2.94	6 (18%)	30,82,82	2.29	4 (13%)
15	PEE	R	3005	-	49,49,50	1.56	10 (20%)	52,54,55	0.88	3 (5%)
15	PEE	C	2007	-	48,48,50	1.47	6 (12%)	51,53,55	0.82	3 (5%)
18	BOG	Q	3091	-	13,13,20	1.42	3 (23%)	18,18,25	1.12	2 (11%)
12	HEM	C	501	3	42,50,50	1.65	6 (14%)	46,82,82	1.89	13 (28%)
12	HEM	P	501	3	42,50,50	1.54	6 (14%)	46,82,82	1.53	10 (21%)
19	FES	E	501	5	0,4,4	-	-	-		
13	UQ	P	3002	-	19,19,63	2.63	10 (52%)	24,26,79	1.33	3 (12%)
14	CDL	C	2004	-	39,39,99	1.24	2 (5%)	45,51,111	1.16	3 (6%)
19	FES	R	501	5	0,4,4	-	-	-		
16	GOL	P	3011	-	5,5,5	1.32	1 (20%)	5,5,5	0.55	0
18	BOG	D	2091	-	13,13,20	1.40	3 (23%)	18,18,25	1.20	2 (11%)
15	PEE	P	3007	-	48,48,50	1.40	5 (10%)	51,53,55	0.77	2 (3%)
15	PEE	E	2005	-	49,49,50	1.61	11 (22%)	52,54,55	0.89	3 (5%)
14	CDL	P	3004	-	39,39,99	1.21	3 (7%)	45,51,111	1.19	4 (8%)
17	HEC	Q	501	4	32,50,50	2.11	4 (12%)	30,82,82	2.25	3 (10%)
16	GOL	C	2011	-	5,5,5	1.22	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	HEM	C	502	3	42,50,50	2.17	12 (28%)	46,82,82	2.22	13 (28%)
13	UQ	C	2002	-	19,19,63	2.73	11 (57%)	24,26,79	1.29	3 (12%)
12	HEM	P	502	3	42,50,50	1.63	6 (14%)	46,82,82	1.83	10 (21%)
18	BOG	P	2010	-	12,12,20	1.40	3 (25%)	17,17,25	0.62	0
14	CDL	D	2003	-	41,41,99	1.18	2 (4%)	47,53,111	1.09	4 (8%)
18	BOG	D	2009	-	20,20,20	1.00	1 (5%)	25,25,25	0.94	1 (4%)
14	CDL	Q	3003	-	41,41,99	1.16	1 (2%)	47,53,111	1.08	4 (8%)
18	BOG	Q	3009	-	20,20,20	0.95	1 (5%)	25,25,25	0.96	1 (4%)

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
15	PEE	C	2008	-	-	8/24/24/54	-
17	HEC	D	501	4	-	4/10/54/54	-
15	PEE	R	3005	-	-	28/53/53/54	-
15	PEE	C	2007	-	-	29/52/52/54	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
12	HEM	C	501	3	-	5/12/54/54	-
12	HEM	P	501	3	-	5/12/54/54	-
19	FES	E	501	5	-	-	0/1/1/1
13	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
14	CDL	C	2004	-	-	23/49/49/110	-
19	FES	R	501	5	-	-	0/1/1/1
16	GOL	P	3011	-	-	3/4/4/4	-
18	BOG	D	2091	-	-	0/4/24/31	0/1/1/1
15	PEE	P	3007	-	-	28/52/52/54	-
15	PEE	E	2005	-	-	28/53/53/54	-
14	CDL	P	3004	-	-	21/49/49/110	-
17	HEC	Q	501	4	-	4/10/54/54	-
16	GOL	C	2011	-	-	4/4/4/4	-
12	HEM	C	502	3	-	6/12/54/54	-
13	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
12	HEM	P	502	3	-	7/12/54/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	D	2003	-	-	27/51/51/110	-
18	BOG	D	2009	-	-	8/11/31/31	0/1/1/1
14	CDL	Q	3003	-	-	28/51/51/110	-
18	BOG	Q	3009	-	-	8/11/31/31	0/1/1/1

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	501	HEC	C3C-C2C	-10.98	1.28	1.40
17	D	501	HEC	C2B-C3B	-10.13	1.29	1.40
17	Q	501	HEC	C2B-C3B	-7.38	1.32	1.40
17	Q	501	HEC	C3C-C2C	-6.85	1.33	1.40
12	C	502	HEM	C3C-C2C	-6.39	1.31	1.40
15	N	3008	PEE	P-O1P	5.23	1.62	1.50
13	P	3002	UQ	C7-C6	5.04	1.60	1.51
13	C	2002	UQ	C7-C6	5.01	1.60	1.51
12	C	502	HEM	C3C-C4C	4.97	1.48	1.41
13	C	2002	UQ	C6-C5	4.95	1.44	1.35
13	P	3002	UQ	C6-C5	4.68	1.43	1.35
12	P	501	HEM	CBC-CAC	4.40	1.56	1.29
12	P	502	HEM	CBB-CAB	4.38	1.51	1.30
12	C	501	HEM	CBC-CAC	4.33	1.56	1.29
15	C	2007	PEE	C39-C38	4.29	1.56	1.31
13	C	2002	UQ	C6-C1	4.26	1.58	1.46
15	P	3007	PEE	C39-C38	4.21	1.55	1.31
15	R	3005	PEE	C39-C38	4.17	1.55	1.31
15	E	2005	PEE	C39-C38	4.13	1.55	1.31
12	C	502	HEM	CBB-CAB	4.08	1.50	1.30
13	P	3002	UQ	C6-C1	3.83	1.57	1.46
12	P	502	HEM	C3C-CAC	-3.70	1.38	1.47
15	N	3008	PEE	P-O4P	3.69	1.65	1.54
15	E	2005	PEE	O3-C30	3.65	1.44	1.33
13	C	2002	UQ	O3-C3	3.63	1.45	1.36
15	R	3005	PEE	O2-C10	3.63	1.44	1.34
12	P	502	HEM	CBC-CAC	3.61	1.51	1.29
12	C	501	HEM	CBB-CAB	3.61	1.47	1.30
17	D	501	HEC	C2A-C1A	3.60	1.50	1.42
12	P	501	HEM	CBB-CAB	3.59	1.47	1.30
15	E	2005	PEE	O2-C10	3.56	1.44	1.34
12	P	501	HEM	CAB-C3B	-3.48	1.38	1.47
15	C	2008	PEE	O3-C30	3.46	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	3008	PEE	P-O3P	3.38	1.64	1.54
15	R	3005	PEE	O3-C30	3.37	1.43	1.33
15	C	2007	PEE	O3-C30	3.35	1.43	1.33
13	P	3002	UQ	O3-C3	3.34	1.44	1.36
15	R	3005	PEE	P-O1P	3.33	1.62	1.50
15	C	2008	PEE	O2-C10	3.32	1.43	1.34
15	P	3007	PEE	O3-C30	3.28	1.42	1.33
15	C	2008	PEE	P-O1P	3.27	1.62	1.50
12	C	502	HEM	C4D-C3D	3.26	1.50	1.45
12	C	502	HEM	C3C-CAC	-3.25	1.39	1.47
12	C	502	HEM	C2C-C1C	3.24	1.49	1.42
15	P	3007	PEE	C22-C21	-3.23	1.35	1.51
15	E	2005	PEE	P-O1P	3.23	1.62	1.50
15	R	3005	PEE	C22-C21	-3.21	1.35	1.51
15	E	2005	PEE	C22-C21	-3.17	1.36	1.51
15	C	2007	PEE	P-O1P	3.15	1.61	1.50
12	C	501	HEM	CAB-C3B	-3.12	1.39	1.47
12	P	502	HEM	CAB-C3B	-3.05	1.39	1.47
12	C	502	HEM	CBC-CAC	3.05	1.48	1.29
15	C	2007	PEE	C22-C21	-2.98	1.37	1.51
13	C	2002	UQ	O2-C2	2.97	1.43	1.36
12	P	501	HEM	C3C-CAC	-2.95	1.40	1.47
15	P	3007	PEE	O2-C10	2.94	1.42	1.34
15	C	2007	PEE	O2-C10	2.91	1.42	1.34
15	E	2005	PEE	C31-C30	2.89	1.59	1.50
15	P	3007	PEE	P-O1P	2.86	1.60	1.50
13	C	2002	UQ	C3-C4	2.86	1.57	1.48
12	P	501	HEM	C3C-C2C	-2.86	1.36	1.40
13	C	2002	UQ	C2-C1	2.85	1.57	1.48
12	C	501	HEM	C3C-C4C	2.84	1.45	1.41
12	C	502	HEM	C3B-C4B	2.84	1.50	1.44
17	D	501	HEC	C3A-C4A	2.81	1.48	1.42
13	P	3002	UQ	O2-C2	2.80	1.43	1.36
13	P	3002	UQ	C2-C1	2.80	1.56	1.48
13	P	3002	UQ	C7-C8	2.80	1.55	1.50
12	C	502	HEM	CAB-C3B	-2.76	1.40	1.47
13	C	2002	UQ	CM5-C5	2.75	1.56	1.50
13	C	2002	UQ	C7-C8	2.73	1.54	1.50
13	P	3002	UQ	C5-C4	2.70	1.56	1.47
13	P	3002	UQ	CM5-C5	2.66	1.56	1.50
12	C	502	HEM	C1A-CHA	-2.66	1.33	1.41
18	D	2091	BOG	C4-C5	2.59	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C1B-C2B	2.58	1.49	1.44
12	C	501	HEM	C3C-C2C	-2.58	1.36	1.40
18	Q	3091	BOG	C4-C5	2.56	1.58	1.53
13	P	3002	UQ	C3-C4	2.55	1.56	1.48
15	R	3005	PEE	C31-C30	2.54	1.58	1.50
13	C	2002	UQ	C5-C4	2.54	1.55	1.47
12	C	501	HEM	C3C-CAC	-2.53	1.41	1.47
12	P	502	HEM	C3C-C2C	-2.52	1.37	1.40
17	Q	501	HEC	C4D-CHA	-2.51	1.34	1.41
15	N	3008	PEE	P-O2P	2.50	1.61	1.54
15	R	3005	PEE	C11-C10	2.50	1.58	1.50
18	P	2010	BOG	C4-C5	2.49	1.58	1.53
18	Q	3091	BOG	O5-C1	2.48	1.48	1.41
18	D	2091	BOG	O5-C1	2.46	1.48	1.41
15	E	2005	PEE	C3-C2	2.39	1.58	1.50
18	P	2010	BOG	C1-C2	2.38	1.57	1.52
15	E	2005	PEE	C11-C10	2.36	1.57	1.50
18	D	2009	BOG	O5-C1	2.35	1.47	1.41
14	D	2003	CDL	O1-C1	2.34	1.50	1.43
12	P	501	HEM	CHD-C1D	-2.33	1.34	1.40
12	C	502	HEM	C3D-C2D	-2.33	1.31	1.36
14	P	3004	CDL	O1-C1	2.32	1.50	1.43
15	E	2005	PEE	C1-C2	2.28	1.57	1.50
15	C	2008	PEE	C1-C2	2.28	1.57	1.50
12	P	502	HEM	C3B-C4B	2.27	1.49	1.44
17	D	501	HEC	C1D-CHD	-2.27	1.34	1.41
17	Q	501	HEC	C2A-C1A	2.26	1.47	1.42
15	C	2008	PEE	C11-C10	2.26	1.57	1.50
18	Q	3009	BOG	O5-C1	2.25	1.47	1.41
15	R	3005	PEE	C3-C2	2.25	1.57	1.50
14	Q	3003	CDL	O1-C1	2.23	1.49	1.43
14	C	2004	CDL	O1-C1	2.23	1.49	1.43
15	C	2008	PEE	C3-C2	2.21	1.57	1.50
15	E	2005	PEE	P-O4P	2.21	1.68	1.59
15	R	3005	PEE	O2-C2	2.15	1.51	1.46
15	E	2005	PEE	O2-C2	2.14	1.51	1.46
14	P	3004	CDL	OB2-CB2	-2.11	1.36	1.44
13	C	2002	UQ	C8-C9	2.10	1.37	1.33
15	R	3005	PEE	C1-C2	2.10	1.57	1.50
17	D	501	HEC	C1B-CHB	-2.09	1.35	1.41
18	P	2010	BOG	O5-C1	2.09	1.48	1.42
14	D	2003	CDL	OA6-CA5	2.08	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	3091	BOG	C1-C2	2.07	1.58	1.52
14	P	3004	CDL	OB8-CB7	2.03	1.39	1.33
16	P	3011	GOL	O2-C2	2.02	1.49	1.43
14	C	2004	CDL	OA6-CA4	-2.01	1.41	1.46
18	D	2091	BOG	C1-C2	2.00	1.58	1.52
15	C	2007	PEE	C3-C2	2.00	1.57	1.50

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	D	501	HEC	CBB-CAB-C3B	-8.33	107.99	127.49
17	Q	501	HEC	CBC-CAC-C3C	-7.11	110.84	127.49
17	Q	501	HEC	CBB-CAB-C3B	-7.03	111.03	127.49
12	C	502	HEM	C3B-C2B-C1B	-6.48	101.54	106.41
17	D	501	HEC	CBC-CAC-C3C	-5.87	113.75	127.49
12	C	502	HEM	C4C-CHD-C1D	5.74	130.13	122.56
17	Q	501	HEC	CBA-CAA-C2A	4.77	120.41	112.55
12	P	502	HEM	CAD-C3D-C4D	4.75	132.97	124.70
12	C	502	HEM	CAD-C3D-C4D	4.74	132.97	124.70
12	C	502	HEM	C2B-C1B-NB	4.49	115.00	109.84
13	C	2002	UQ	C8-C7-C6	4.38	122.88	112.08
12	C	501	HEM	C3B-C2B-C1B	-4.34	103.15	106.41
13	P	3002	UQ	C8-C7-C6	4.34	122.76	112.08
18	D	2091	BOG	C1'-O1-C1	4.15	119.56	113.26
12	P	501	HEM	C4B-CHC-C1C	4.10	127.97	122.56
12	C	501	HEM	CMA-C3A-C4A	-4.00	122.59	128.46
18	Q	3009	BOG	C1'-O1-C1	3.83	120.22	113.68
18	D	2009	BOG	C1'-O1-C1	3.78	120.13	113.68
12	C	501	HEM	C4B-CHC-C1C	3.74	127.49	122.56
12	C	501	HEM	CMB-C2B-C1B	3.72	130.85	125.03
14	P	3004	CDL	CB4-OB6-CB5	-3.65	109.06	117.80
12	C	501	HEM	CAD-C3D-C4D	3.61	130.98	124.70
17	D	501	HEC	CBA-CAA-C2A	3.56	118.42	112.55
12	C	501	HEM	CAD-C3D-C2D	-3.54	121.23	127.87
12	C	502	HEM	CHD-C1D-ND	-3.50	120.67	124.44
12	P	502	HEM	C4B-CHC-C1C	3.48	127.15	122.56
14	C	2004	CDL	CA4-OA6-CA5	-3.48	109.47	117.80
18	Q	3091	BOG	C1'-O1-C1	3.45	118.50	113.26
14	C	2004	CDL	CB4-OB6-CB5	-3.43	109.58	117.80
12	P	501	HEM	C2C-C3C-C4C	-3.38	104.54	106.90
12	C	502	HEM	CAD-C3D-C2D	-3.38	121.54	127.87
12	P	502	HEM	C2B-C1B-NB	3.35	113.69	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	502	HEM	C3B-C2B-C1B	-3.35	103.89	106.41
12	P	502	HEM	C4C-CHD-C1D	3.35	126.98	122.56
12	C	501	HEM	C3B-C4B-NB	3.28	111.83	109.47
12	P	502	HEM	CAD-C3D-C2D	-3.27	121.75	127.87
12	P	502	HEM	CMB-C2B-C1B	3.21	130.06	125.03
14	P	3004	CDL	CA4-OA6-CA5	-3.21	110.12	117.80
12	C	502	HEM	C2D-C1D-ND	3.06	113.44	109.90
13	P	3002	UQ	C7-C6-C1	-3.00	115.03	118.52
12	P	502	HEM	CBA-CAA-C2A	2.97	117.53	112.54
12	C	501	HEM	CMA-C3A-C2A	2.91	130.43	124.94
15	C	2007	PEE	C22-C21-C20	2.91	127.86	113.86
15	E	2005	PEE	C22-C21-C20	2.87	127.66	113.86
12	P	502	HEM	C3B-C4B-NB	2.86	111.53	109.47
12	C	502	HEM	C3B-C4B-NB	2.83	111.50	109.47
15	R	3005	PEE	C22-C21-C20	2.82	127.43	113.86
12	C	502	HEM	CMB-C2B-C1B	2.80	129.41	125.03
12	P	501	HEM	CAD-C3D-C4D	2.79	129.57	124.70
12	C	502	HEM	CMD-C2D-C1D	2.78	129.38	125.03
13	C	2002	UQ	C7-C6-C1	-2.78	115.28	118.52
15	P	3007	PEE	C22-C21-C20	2.76	127.13	113.86
12	P	501	HEM	CMB-C2B-C1B	2.71	129.28	125.03
15	C	2007	PEE	C23-C22-C21	2.68	127.93	114.37
12	C	501	HEM	C2B-C1B-NB	2.64	112.88	109.84
12	P	501	HEM	C4A-C3A-C2A	-2.62	105.17	107.00
12	P	501	HEM	CAD-C3D-C2D	-2.60	122.99	127.87
15	P	3007	PEE	C23-C22-C21	2.59	127.48	114.37
12	C	502	HEM	C4D-ND-C1D	-2.59	102.14	105.21
18	Q	3091	BOG	O1-C1-C2	2.58	111.12	108.14
14	D	2003	CDL	CB4-OB6-CB5	-2.57	111.65	117.80
15	E	2005	PEE	C23-C22-C21	2.54	127.19	114.37
14	Q	3003	CDL	CB4-OB6-CB5	-2.53	111.75	117.80
15	R	3005	PEE	C23-C22-C21	2.38	126.39	114.37
14	P	3004	CDL	OB6-CB4-CB3	2.35	116.77	108.34
18	D	2091	BOG	O1-C1-C2	2.34	110.84	108.14
14	D	2003	CDL	CA6-CA4-CA3	-2.34	106.33	111.78
15	R	3005	PEE	O3-C3-C2	2.29	115.01	108.40
12	P	501	HEM	C2B-C1B-NB	2.27	112.45	109.84
13	P	3002	UQ	C10-C9-C8	-2.26	117.82	123.63
14	Q	3003	CDL	CA6-CA4-CA3	-2.24	106.56	111.78
12	C	502	HEM	CHA-C4D-ND	-2.24	121.60	124.37
14	Q	3003	CDL	CA4-OA6-CA5	-2.20	112.52	117.80
12	C	501	HEM	CBB-CAB-C3B	-2.20	116.54	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	502	HEM	C2D-C1D-ND	2.20	112.44	109.90
15	E	2005	PEE	O3-C3-C2	2.19	114.70	108.40
12	P	501	HEM	CBB-CAB-C3B	-2.17	116.66	127.53
14	P	3004	CDL	CA6-CA4-CA3	-2.15	106.78	111.78
14	D	2003	CDL	CA6-OA8-CA7	-2.13	111.81	117.08
17	D	501	HEC	CAA-C2A-C3A	-2.13	121.14	127.25
12	C	502	HEM	C3D-C4D-ND	2.12	112.49	110.17
12	C	501	HEM	C2C-C3C-C4C	-2.11	105.42	106.90
14	Q	3003	CDL	CA6-OA8-CA7	-2.10	111.89	117.08
13	C	2002	UQ	C10-C9-C8	-2.10	118.24	123.63
12	C	501	HEM	CBD-CAD-C3D	2.06	118.23	112.53
15	C	2007	PEE	O3-C3-C2	2.06	114.32	108.40
12	P	501	HEM	C3B-C4B-NB	2.05	110.94	109.47
14	C	2004	CDL	OB6-CB4-CB3	2.04	115.65	108.34
12	C	501	HEM	CHD-C1D-C2D	-2.03	121.82	125.03
14	D	2003	CDL	CA4-OA6-CA5	-2.03	112.95	117.80
12	P	501	HEM	C3B-C2B-C1B	-2.00	104.91	106.41

There are no chirality outliers.

All (286) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	501	HEM	C2B-C3B-CAB-CBB
12	C	501	HEM	C4B-C3B-CAB-CBB
12	P	501	HEM	C2B-C3B-CAB-CBB
12	P	501	HEM	C4B-C3B-CAB-CBB
13	C	2002	UQ	C1-C6-C7-C8
13	C	2002	UQ	C5-C6-C7-C8
13	C	2002	UQ	C12-C11-C9-C8
13	P	3002	UQ	C1-C6-C7-C8
13	P	3002	UQ	C5-C6-C7-C8
13	P	3002	UQ	C12-C11-C9-C8
14	C	2004	CDL	O1-C1-CA2-OA2
14	C	2004	CDL	CA3-OA5-PA1-OA2
14	C	2004	CDL	CA3-OA5-PA1-OA3
14	C	2004	CDL	CA3-OA5-PA1-OA4
14	C	2004	CDL	C51-CB5-OB6-CB4
14	D	2003	CDL	CB2-OB2-PB2-OB4
14	D	2003	CDL	CB2-OB2-PB2-OB5
14	D	2003	CDL	CB3-OB5-PB2-OB4
14	P	3004	CDL	O1-C1-CA2-OA2
14	P	3004	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
14	P	3004	CDL	CA3-OA5-PA1-OA3
14	P	3004	CDL	CA3-OA5-PA1-OA4
14	P	3004	CDL	C51-CB5-OB6-CB4
14	Q	3003	CDL	CB2-OB2-PB2-OB4
14	Q	3003	CDL	CB2-OB2-PB2-OB5
14	Q	3003	CDL	CB3-OB5-PB2-OB4
15	C	2007	PEE	O4P-C4-C5-N
15	C	2007	PEE	C1-O3P-P-O2P
15	C	2007	PEE	C1-O3P-P-O4P
15	C	2007	PEE	C4-O4P-P-O1P
15	C	2007	PEE	C4-O4P-P-O2P
15	C	2007	PEE	C4-O4P-P-O3P
15	C	2008	PEE	C4-O4P-P-O1P
15	C	2008	PEE	C4-O4P-P-O2P
15	C	2008	PEE	C4-O4P-P-O3P
15	E	2005	PEE	C11-C10-O2-C2
15	E	2005	PEE	C4-O4P-P-O2P
15	E	2005	PEE	C4-O4P-P-O3P
15	P	3007	PEE	O4P-C4-C5-N
15	P	3007	PEE	C1-O3P-P-O2P
15	P	3007	PEE	C1-O3P-P-O4P
15	P	3007	PEE	C4-O4P-P-O1P
15	P	3007	PEE	C4-O4P-P-O2P
15	P	3007	PEE	C4-O4P-P-O3P
15	R	3005	PEE	C11-C10-O2-C2
15	R	3005	PEE	C4-O4P-P-O2P
15	R	3005	PEE	C4-O4P-P-O3P
16	C	2011	GOL	O1-C1-C2-C3
16	C	2011	GOL	C1-C2-C3-O3
16	P	3011	GOL	C1-C2-C3-O3
17	D	501	HEC	C1A-C2A-CAA-CBA
17	D	501	HEC	C3A-C2A-CAA-CBA
17	Q	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
14	P	3004	CDL	C31-CA7-OA8-CA6
14	C	2004	CDL	OB9-CB7-OB8-CB6
14	P	3004	CDL	OB9-CB7-OB8-CB6
15	E	2005	PEE	O5-C30-O3-C3
15	R	3005	PEE	O5-C30-O3-C3
14	C	2004	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
14	D	2003	CDL	C31-CA7-OA8-CA6
14	Q	3003	CDL	C31-CA7-OA8-CA6
14	C	2004	CDL	OB7-CB5-OB6-CB4
14	P	3004	CDL	OB7-CB5-OB6-CB4
15	E	2005	PEE	O4-C10-O2-C2
15	R	3005	PEE	O4-C10-O2-C2
15	R	3005	PEE	C31-C30-O3-C3
14	C	2004	CDL	OA9-CA7-OA8-CA6
14	P	3004	CDL	OA9-CA7-OA8-CA6
14	C	2004	CDL	C71-CB7-OB8-CB6
14	P	3004	CDL	C71-CB7-OB8-CB6
15	E	2005	PEE	C31-C30-O3-C3
18	Q	3091	BOG	C4-C5-C6-O6
14	D	2003	CDL	OA9-CA7-OA8-CA6
14	Q	3003	CDL	OA9-CA7-OA8-CA6
18	Q	3091	BOG	O5-C5-C6-O6
14	D	2003	CDL	C71-CB7-OB8-CB6
14	Q	3003	CDL	C71-CB7-OB8-CB6
15	C	2007	PEE	C17-C18-C19-C20
18	D	2009	BOG	C4-C5-C6-O6
14	D	2003	CDL	OB9-CB7-OB8-CB6
14	Q	3003	CDL	OB9-CB7-OB8-CB6
14	D	2003	CDL	CB7-C71-C72-C73
14	Q	3003	CDL	CB7-C71-C72-C73
14	Q	3003	CDL	O1-C1-CA2-OA2
18	D	2009	BOG	O1-C1'-C2'-C3'
15	P	3007	PEE	C17-C18-C19-C20
18	Q	3009	BOG	O1-C1'-C2'-C3'
14	C	2004	CDL	CB2-C1-CA2-OA2
14	P	3004	CDL	CB2-C1-CA2-OA2
14	C	2004	CDL	C11-CA5-OA6-CA4
14	P	3004	CDL	C11-CA5-OA6-CA4
14	C	2004	CDL	OA7-CA5-OA6-CA4
18	D	2009	BOG	C2-C1-O1-C1'
18	Q	3009	BOG	C2-C1-O1-C1'
14	D	2003	CDL	O1-C1-CA2-OA2
18	D	2009	BOG	O5-C5-C6-O6
14	P	3004	CDL	OA7-CA5-OA6-CA4
16	C	2011	GOL	O1-C1-C2-O2
16	C	2011	GOL	O2-C2-C3-O3
16	P	3011	GOL	O2-C2-C3-O3
15	C	2007	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	C41-C42-C43-C44
15	R	3005	PEE	C34-C35-C36-C37
15	E	2005	PEE	C34-C35-C36-C37
18	D	2009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
18	D	2009	BOG	C1'-C2'-C3'-C4'
18	Q	3009	BOG	C1'-C2'-C3'-C4'
14	D	2003	CDL	C51-CB5-OB6-CB4
14	Q	3003	CDL	C51-CB5-OB6-CB4
12	C	502	HEM	C4D-C3D-CAD-CBD
14	Q	3003	CDL	OB7-CB5-OB6-CB4
15	C	2007	PEE	C15-C16-C17-C18
15	C	2007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C15-C16-C17-C18
15	P	3007	PEE	C35-C36-C37-C38
15	C	2007	PEE	C10-C11-C12-C13
15	P	3007	PEE	C31-C32-C33-C34
15	C	2007	PEE	C31-C32-C33-C34
15	R	3005	PEE	C20-C21-C22-C23
15	E	2005	PEE	C35-C36-C37-C38
15	R	3005	PEE	C35-C36-C37-C38
15	R	3005	PEE	C42-C43-C44-C45
14	D	2003	CDL	OB7-CB5-OB6-CB4
15	E	2005	PEE	C42-C43-C44-C45
15	E	2005	PEE	C39-C40-C41-C42
15	R	3005	PEE	C39-C40-C41-C42
15	R	3005	PEE	O3P-C1-C2-C3
15	E	2005	PEE	C20-C21-C22-C23
15	C	2008	PEE	C11-C10-O2-C2
15	R	3005	PEE	C23-C24-C25-C26
12	P	502	HEM	C4D-C3D-CAD-CBD
15	C	2007	PEE	C42-C43-C44-C45
15	P	3007	PEE	C42-C43-C44-C45
15	E	2005	PEE	C23-C24-C25-C26
15	P	3007	PEE	C10-C11-C12-C13
18	Q	3009	BOG	C4-C5-C6-O6
14	D	2003	CDL	OB5-CB3-CB4-OB6
14	Q	3003	CDL	OB5-CB3-CB4-OB6
15	E	2005	PEE	O3P-C1-C2-O2
15	C	2007	PEE	C43-C44-C45-C46
15	P	3007	PEE	C43-C44-C45-C46
15	E	2005	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
15	C	2007	PEE	C11-C12-C13-C14
14	Q	3003	CDL	C71-C72-C73-C74
15	P	3007	PEE	C11-C12-C13-C14
14	D	2003	CDL	OA5-CA3-CA4-CA6
14	Q	3003	CDL	OA5-CA3-CA4-CA6
15	E	2005	PEE	O3P-C1-C2-C3
14	D	2003	CDL	C71-C72-C73-C74
15	P	3007	PEE	C40-C41-C42-C43
13	C	2002	UQ	C12-C11-C9-C10
13	P	3002	UQ	C12-C11-C9-C10
14	C	2004	CDL	CA3-CA4-CA6-OA8
14	P	3004	CDL	CA3-CA4-CA6-OA8
15	R	3005	PEE	C40-C41-C42-C43
18	D	2009	BOG	C4'-C5'-C6'-C7'
15	P	3007	PEE	C14-C15-C16-C17
15	R	3005	PEE	C21-C22-C23-C24
14	C	2004	CDL	OB5-CB3-CB4-OB6
14	P	3004	CDL	OB5-CB3-CB4-OB6
14	Q	3003	CDL	OA5-CA3-CA4-OA6
15	C	2007	PEE	O3P-C1-C2-O2
15	P	3007	PEE	O3P-C1-C2-O2
15	R	3005	PEE	O3P-C1-C2-O2
14	C	2004	CDL	OA6-CA4-CA6-OA8
14	P	3004	CDL	OA6-CA4-CA6-OA8
15	E	2005	PEE	C10-C11-C12-C13
15	R	3005	PEE	C10-C11-C12-C13
15	E	2005	PEE	C21-C22-C23-C24
15	C	2007	PEE	C40-C41-C42-C43
16	P	3011	GOL	O1-C1-C2-O2
18	Q	3009	BOG	O5-C5-C6-O6
15	E	2005	PEE	C31-C32-C33-C34
15	C	2008	PEE	O3P-C1-C2-C3
18	D	2009	BOG	C2'-C3'-C4'-C5'
15	C	2007	PEE	C12-C13-C14-C15
15	E	2005	PEE	C33-C34-C35-C36
15	R	3005	PEE	C31-C32-C33-C34
15	R	3005	PEE	C33-C34-C35-C36
15	R	3005	PEE	C30-C31-C32-C33
15	C	2008	PEE	O4-C10-O2-C2
14	D	2003	CDL	OA5-CA3-CA4-OA6
15	C	2008	PEE	O3P-C1-C2-O2
15	P	3007	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
15	C	2007	PEE	C14-C15-C16-C17
14	P	3004	CDL	OB5-CB3-CB4-CB6
15	E	2005	PEE	C41-C42-C43-C44
18	Q	3009	BOG	C4'-C5'-C6'-C7'
15	R	3005	PEE	C22-C23-C24-C25
15	E	2005	PEE	C14-C15-C16-C17
14	C	2004	CDL	CB3-OB5-PB2-OB2
14	C	2004	CDL	CB3-OB5-PB2-OB4
14	D	2003	CDL	CA3-OA5-PA1-OA2
14	D	2003	CDL	CA3-OA5-PA1-OA3
14	D	2003	CDL	CA3-OA5-PA1-OA4
14	D	2003	CDL	CB3-OB5-PB2-OB2
14	D	2003	CDL	CB3-OB5-PB2-OB3
14	P	3004	CDL	CB3-OB5-PB2-OB2
14	P	3004	CDL	CB3-OB5-PB2-OB4
14	Q	3003	CDL	CA3-OA5-PA1-OA2
14	Q	3003	CDL	CA3-OA5-PA1-OA3
14	Q	3003	CDL	CA3-OA5-PA1-OA4
14	Q	3003	CDL	CB3-OB5-PB2-OB2
14	Q	3003	CDL	CB3-OB5-PB2-OB3
15	C	2008	PEE	C1-O3P-P-O1P
15	E	2005	PEE	C30-C31-C32-C33
15	E	2005	PEE	C19-C20-C21-C22
18	Q	3009	BOG	C2'-C3'-C4'-C5'
15	R	3005	PEE	C14-C15-C16-C17
15	E	2005	PEE	C43-C44-C45-C46
14	D	2003	CDL	OB5-CB3-CB4-CB6
14	Q	3003	CDL	OB5-CB3-CB4-CB6
15	R	3005	PEE	C41-C42-C43-C44
15	P	3007	PEE	O4-C10-O2-C2
15	C	2007	PEE	O2-C2-C3-O3
15	P	3007	PEE	C20-C21-C22-C23
15	P	3007	PEE	C11-C10-O2-C2
15	P	3007	PEE	C19-C20-C21-C22
15	C	2007	PEE	C20-C21-C22-C23
15	R	3005	PEE	C43-C44-C45-C46
15	E	2005	PEE	C22-C23-C24-C25
14	C	2004	CDL	OB5-CB3-CB4-CB6
14	D	2003	CDL	OA6-CA4-CA6-OA8
14	Q	3003	CDL	OA6-CA4-CA6-OA8
15	P	3007	PEE	O2-C2-C3-O3
14	C	2004	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
14	P	3004	CDL	C1-CB2-OB2-PB2
15	C	2007	PEE	C19-C20-C21-C22
15	R	3005	PEE	C19-C20-C21-C22
12	C	502	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAD-CBD-CGD-O1D
15	E	2005	PEE	C1-C2-O2-C10
15	R	3005	PEE	C1-C2-O2-C10
15	E	2005	PEE	C11-C12-C13-C14
12	C	502	HEM	CAA-CBA-CGA-O2A
12	P	502	HEM	CAA-CBA-CGA-O2A
14	D	2003	CDL	C1-CA2-OA2-PA1
14	Q	3003	CDL	C1-CA2-OA2-PA1
12	P	502	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	CAA-CBA-CGA-O1A
17	Q	501	HEC	CAA-CBA-CGA-O2A
14	C	2004	CDL	C1-CB2-OB2-PB2
15	C	2007	PEE	O4-C10-O2-C2
15	C	2007	PEE	C38-C39-C40-C41
12	C	501	HEM	CAA-CBA-CGA-O2A
15	R	3005	PEE	C11-C12-C13-C14
17	Q	501	HEC	CAA-CBA-CGA-O1A
15	P	3007	PEE	C38-C39-C40-C41
15	R	3005	PEE	C38-C39-C40-C41
12	P	501	HEM	CAA-CBA-CGA-O2A
14	Q	3003	CDL	CB5-C51-C52-C53
12	C	501	HEM	CAA-CBA-CGA-O1A
15	P	3007	PEE	C16-C17-C18-C19
17	D	501	HEC	CAA-CBA-CGA-O2A
14	P	3004	CDL	OB6-CB4-CB6-OB8
12	P	501	HEM	CAA-CBA-CGA-O1A
15	E	2005	PEE	C38-C39-C40-C41
14	C	2004	CDL	C12-C11-CA5-OA6
14	Q	3003	CDL	CB4-CB3-OB5-PB2
15	C	2007	PEE	C16-C17-C18-C19
15	C	2007	PEE	C11-C10-O2-C2
15	P	3007	PEE	O2-C10-C11-C12
15	C	2007	PEE	C33-C34-C35-C36
12	P	502	HEM	C2A-CAA-CBA-CGA
15	C	2007	PEE	O2-C10-C11-C12
14	D	2003	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
14	D	2003	CDL	CA3-CA4-CA6-OA8
14	Q	3003	CDL	CA3-CA4-CA6-OA8
14	D	2003	CDL	C72-C71-CB7-OB8
14	Q	3003	CDL	C72-C71-CB7-OB8
17	D	501	HEC	CAA-CBA-CGA-O1A
15	P	3007	PEE	O4-C10-C11-C12
15	C	2007	PEE	O4-C10-C11-C12
12	C	501	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAD-CBD-CGD-O2D
14	Q	3003	CDL	C72-C71-CB7-OB9
14	C	2004	CDL	OB6-CB4-CB6-OB8
12	C	502	HEM	C2B-C3B-CAB-CBB
12	P	502	HEM	C2B-C3B-CAB-CBB
14	D	2003	CDL	C72-C71-CB7-OB9

There are no ring outliers.

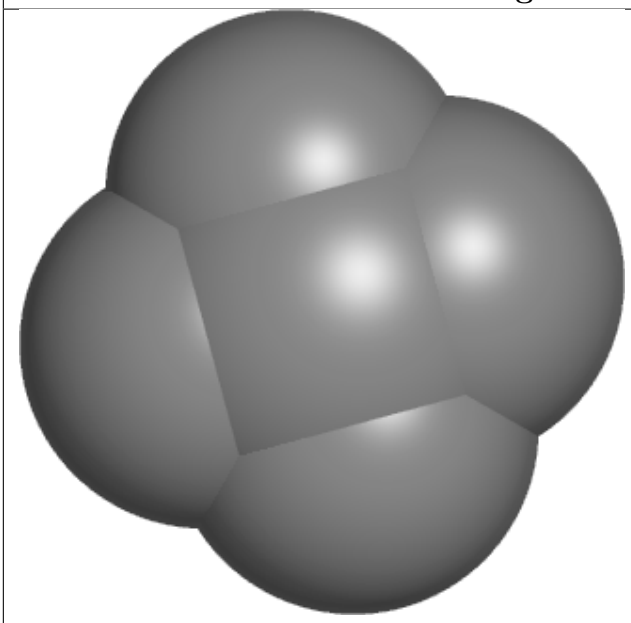
19 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	501	HEC	3	0
15	C	2007	PEE	2	0
12	C	501	HEM	5	0
12	P	501	HEM	5	0
19	E	501	FES	2	0
13	P	3002	UQ	4	0
14	C	2004	CDL	2	0
19	R	501	FES	2	0
15	P	3007	PEE	2	0
15	E	2005	PEE	1	0
14	P	3004	CDL	2	0
17	Q	501	HEC	1	0
12	C	502	HEM	1	0
13	C	2002	UQ	5	0
12	P	502	HEM	3	0
18	P	2010	BOG	1	0
14	D	2003	CDL	2	0
18	D	2009	BOG	1	0
14	Q	3003	CDL	3	0

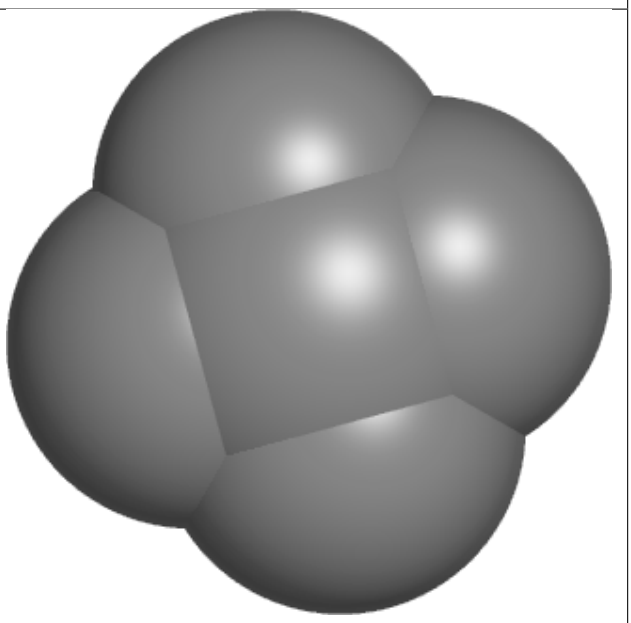
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

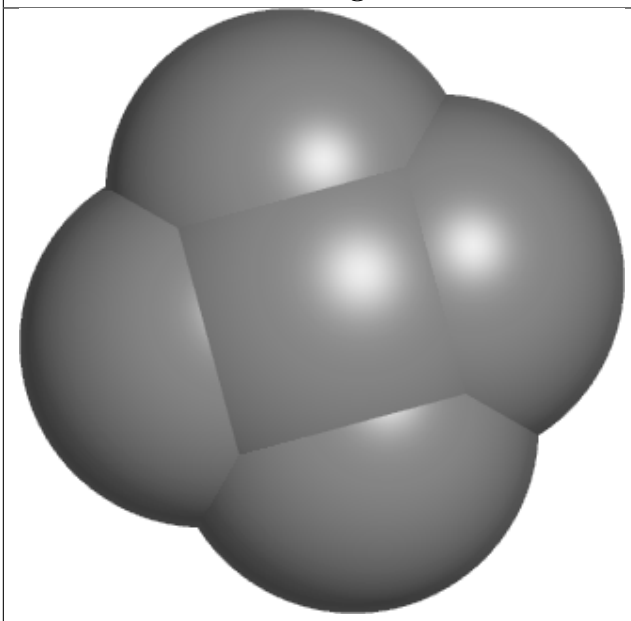
Ligand PEE N 3008



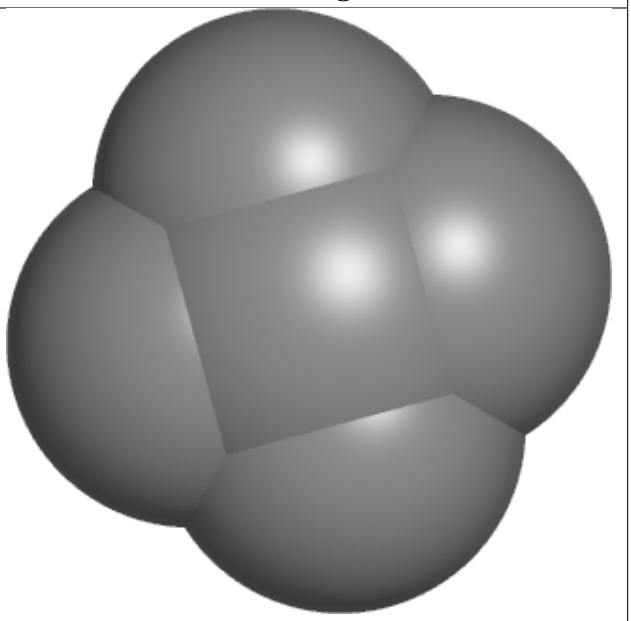
Bond lengths



Bond angles

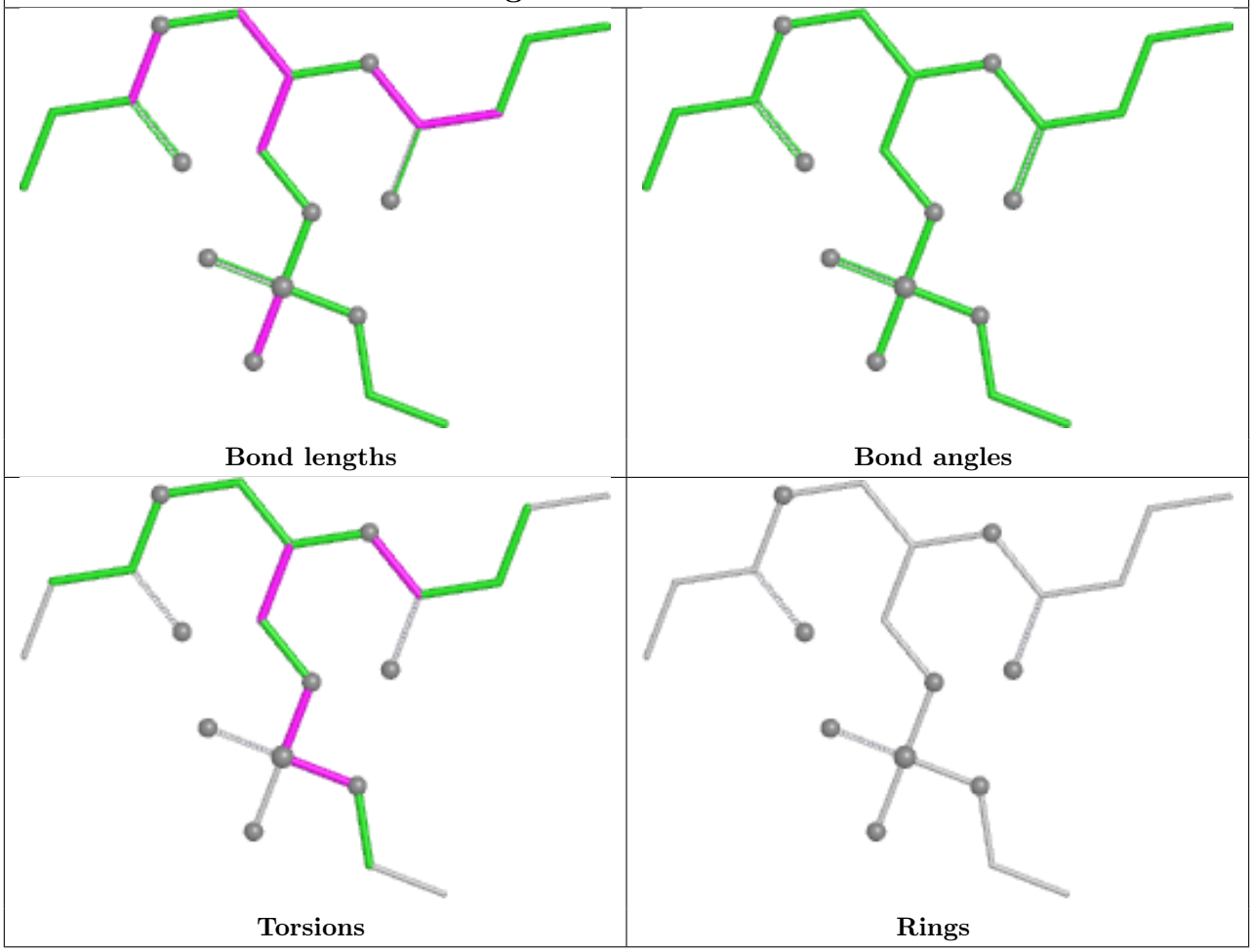


Torsions

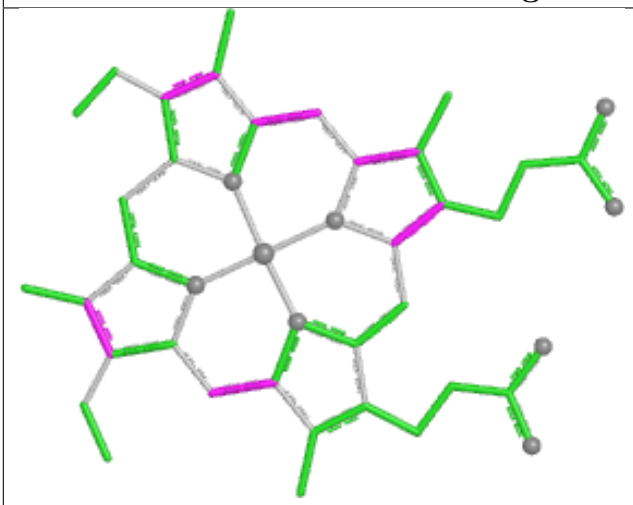


Rings

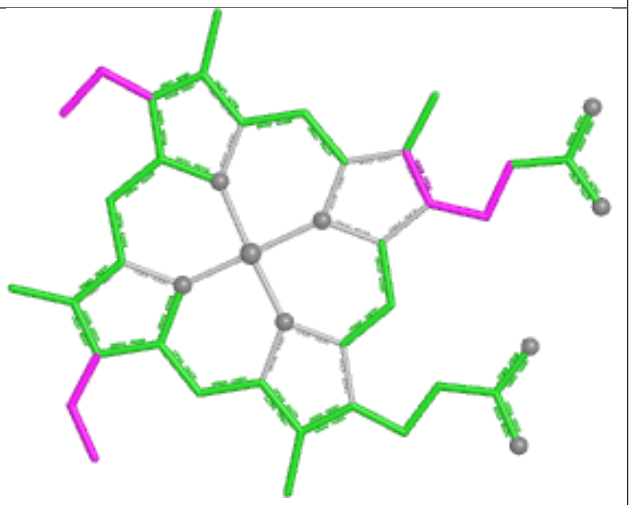
Ligand PEE C 2008



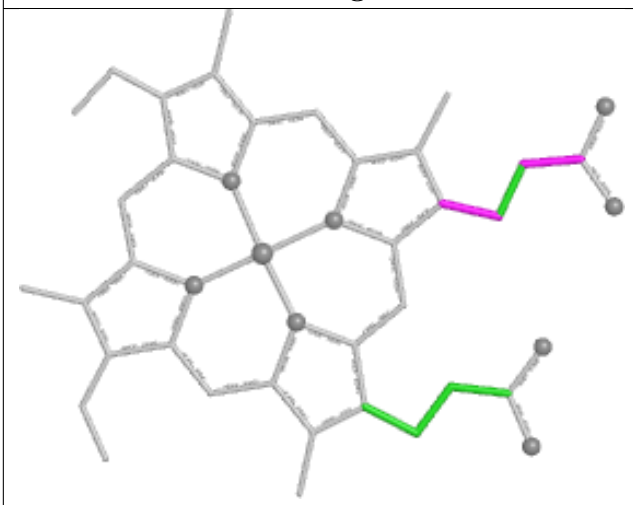
Ligand HEC D 501



Bond lengths



Bond angles



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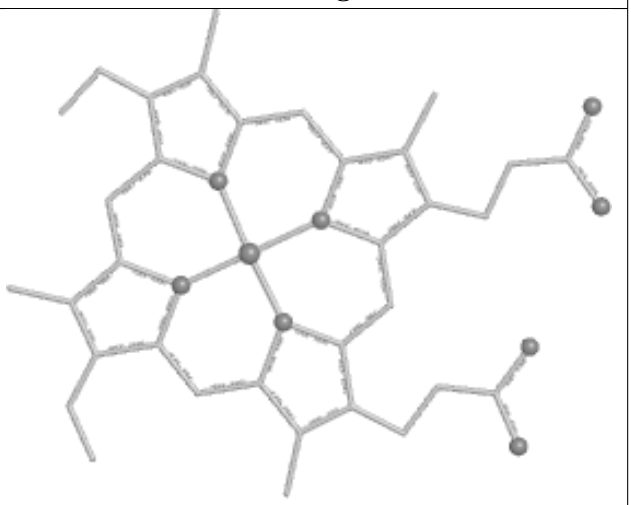
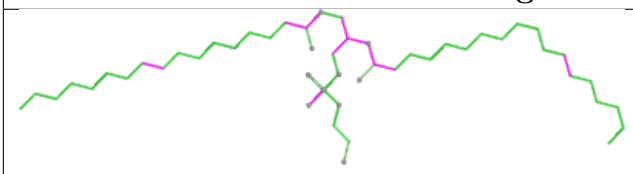
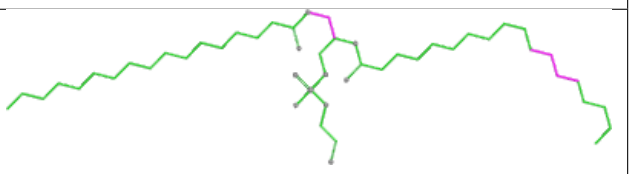


Rings

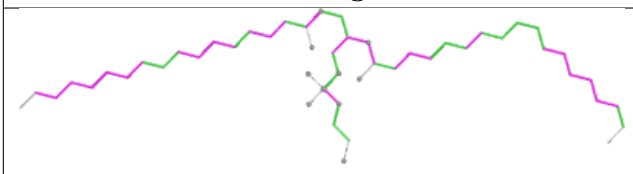
Ligand PEE R 3005



Bond lengths



Bond angles



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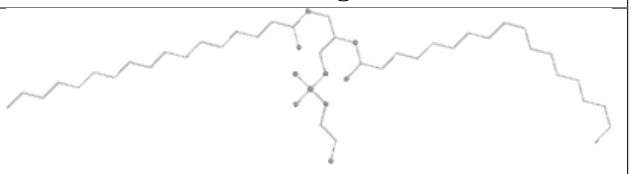
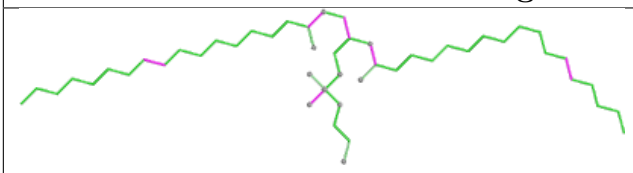


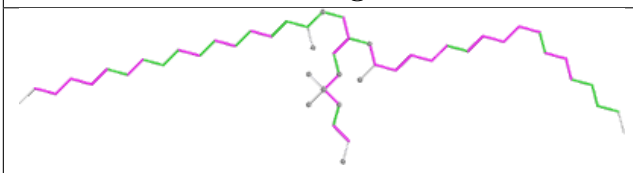
Rings

Ligand PEE C 2007



Bond lengths

Bond angles



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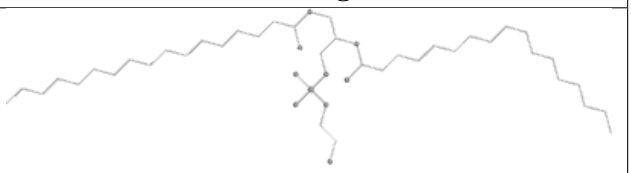
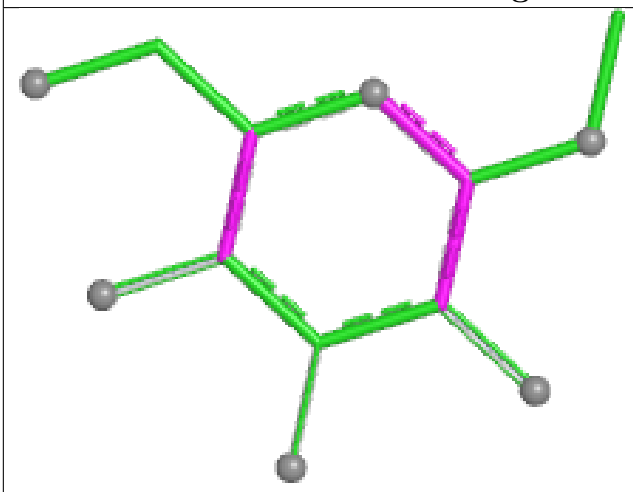


Rings

Ligand BOG Q 3091



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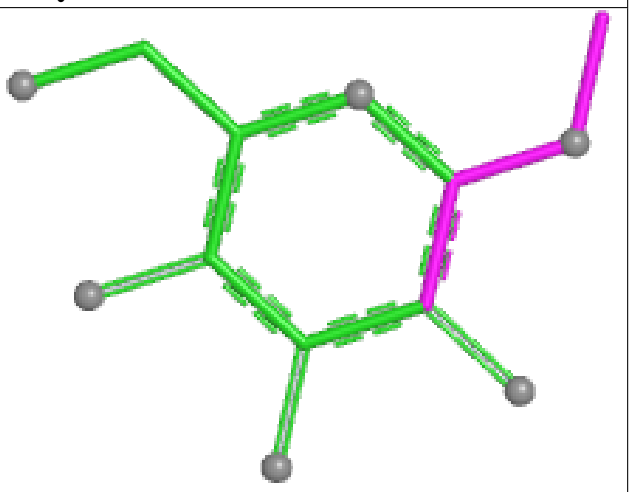

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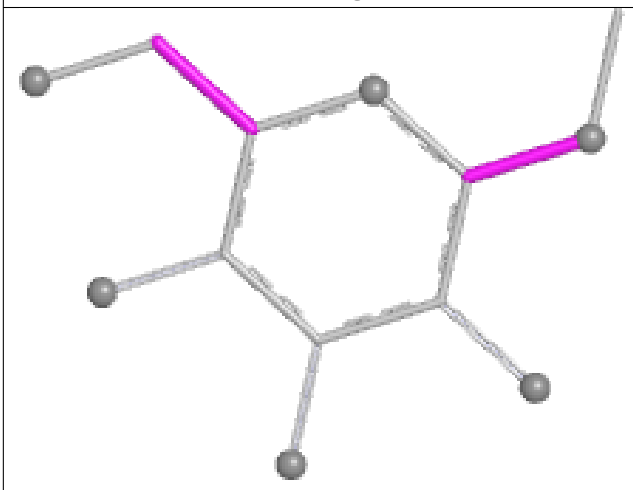
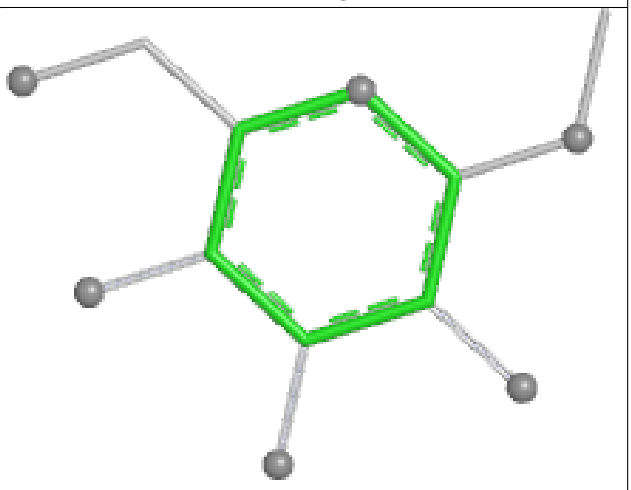
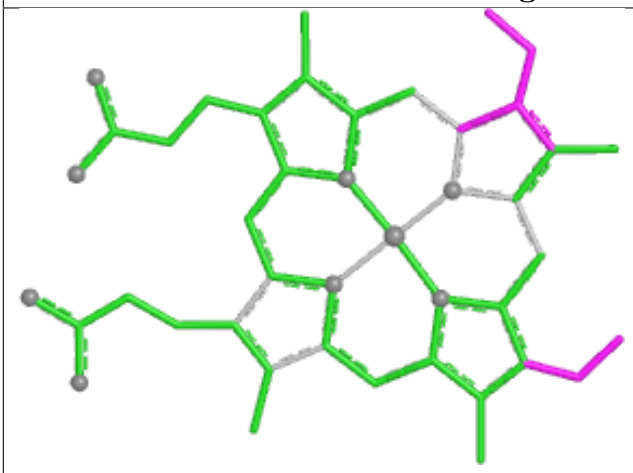


Torsions



Rings

Ligand HEM C 501



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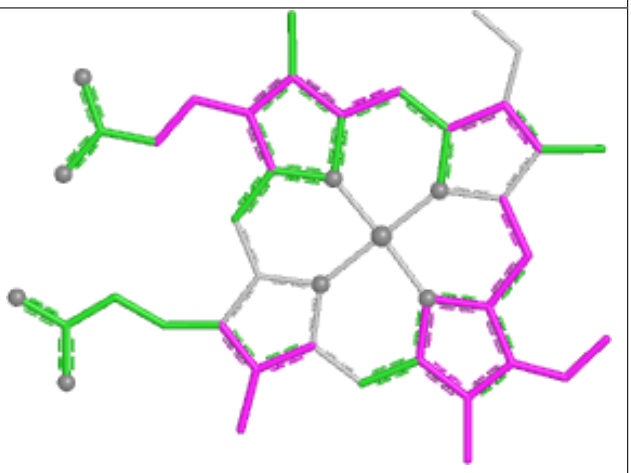

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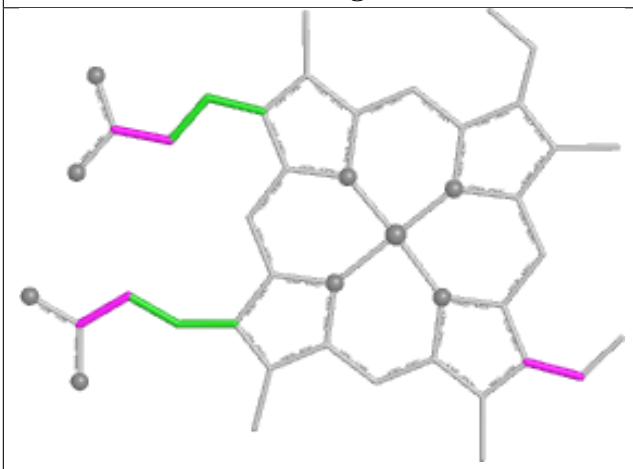

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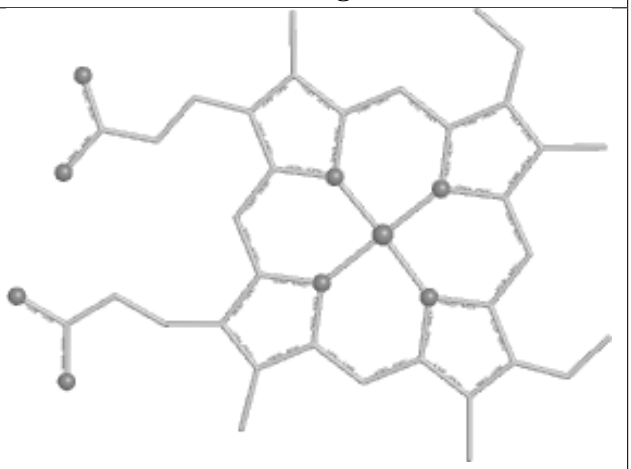

Rings

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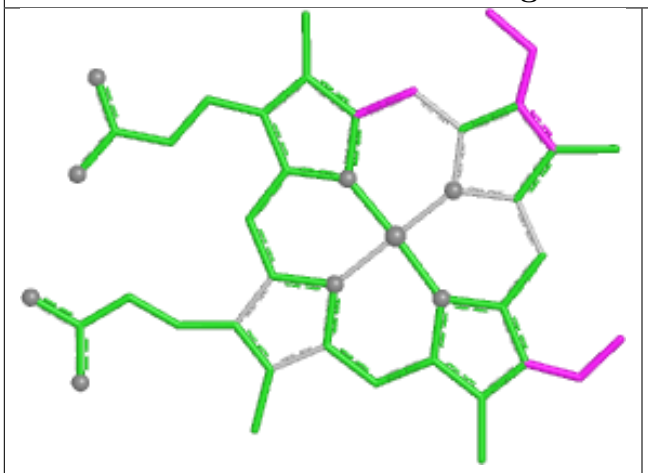

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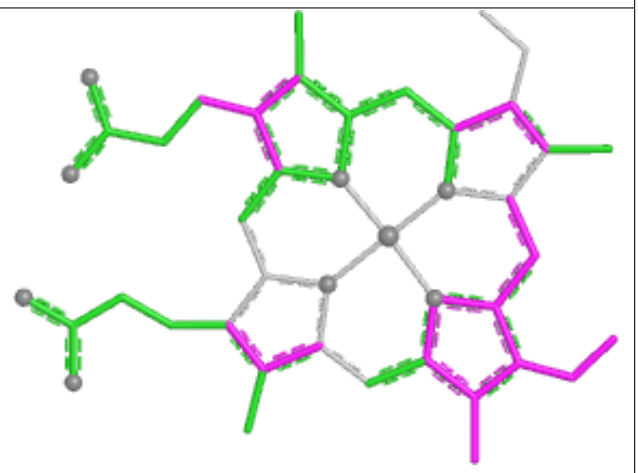

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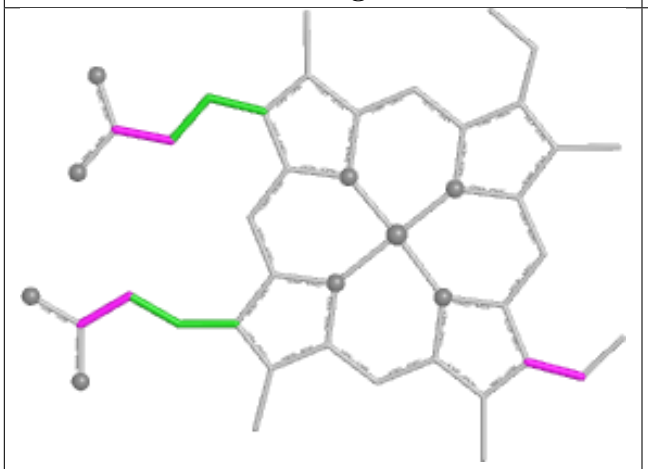

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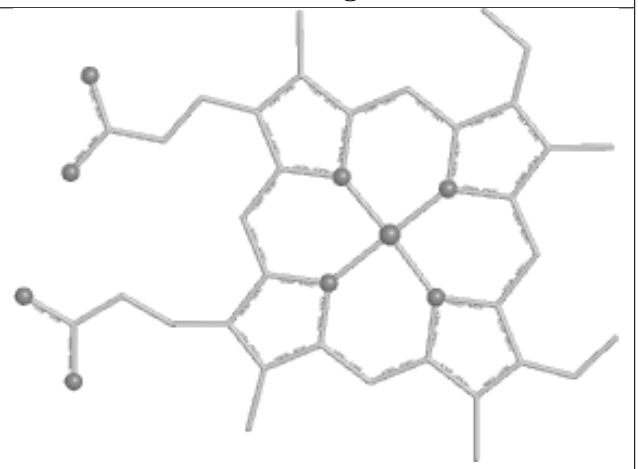
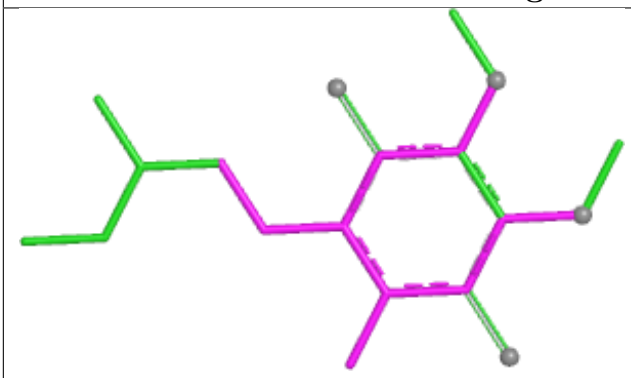


Rings

Ligand UQ P 3002



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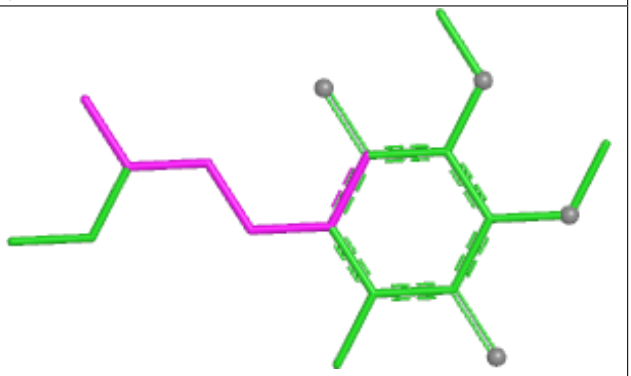

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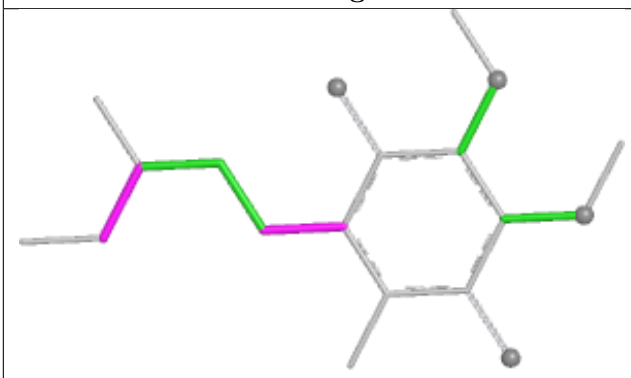

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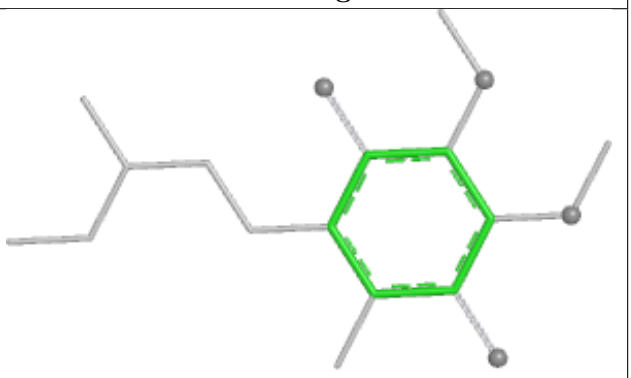
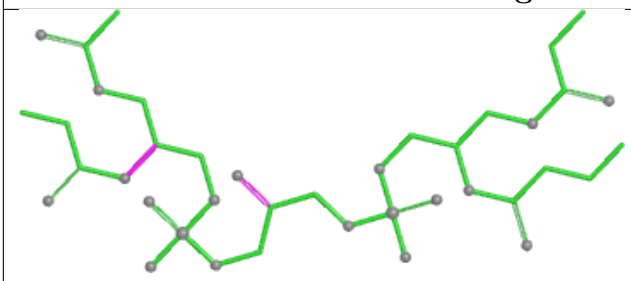


Rings

Ligand CDL C 2004



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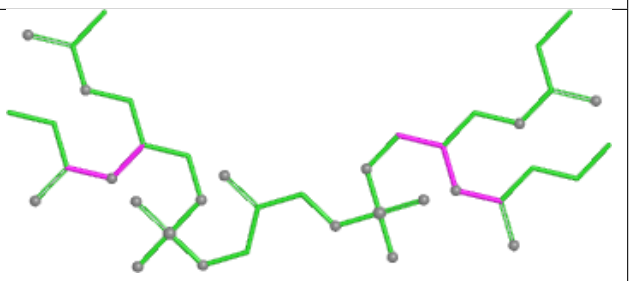

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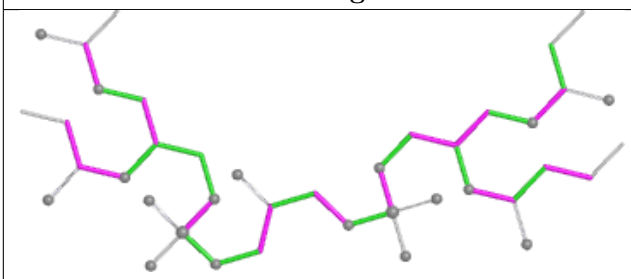

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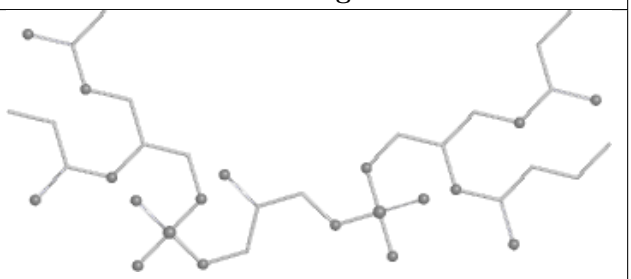
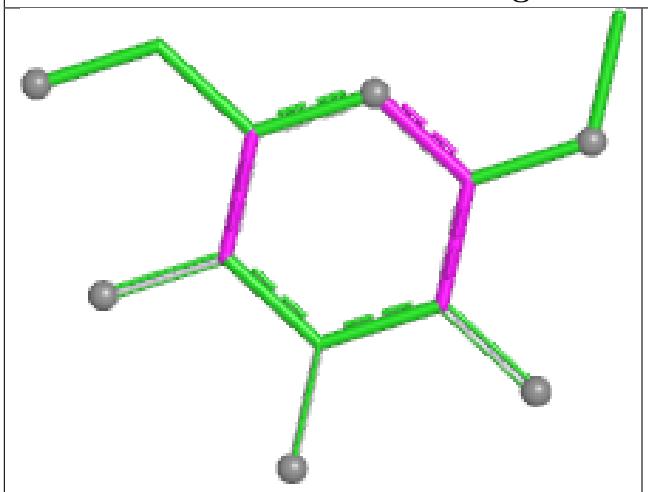


Rings

Ligand BOG D 2091



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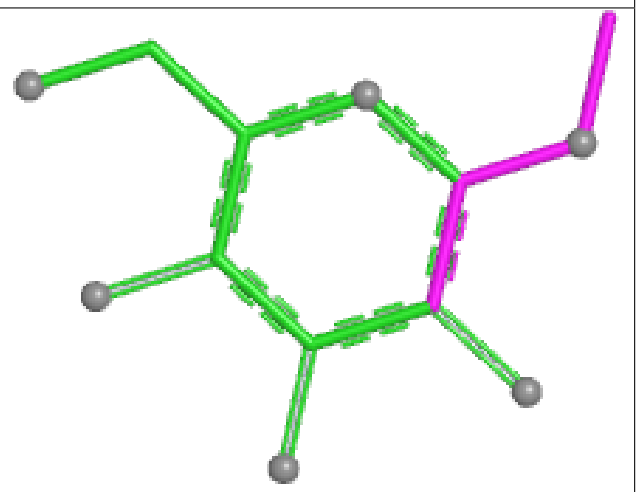

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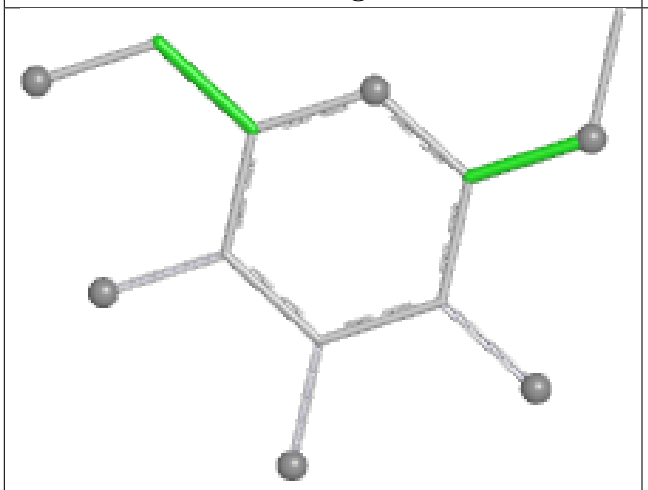

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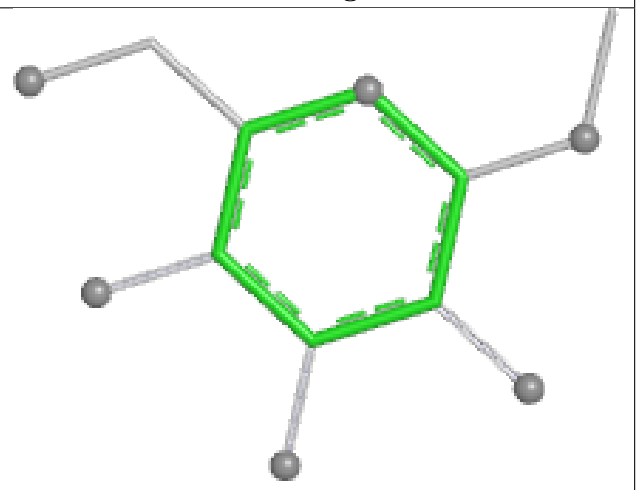

Rings

Ligand PEE P 3007

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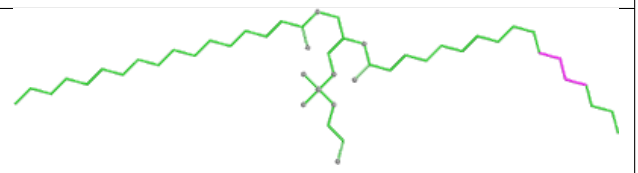

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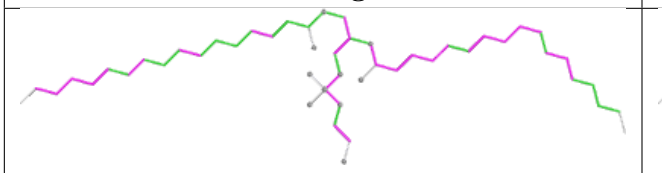

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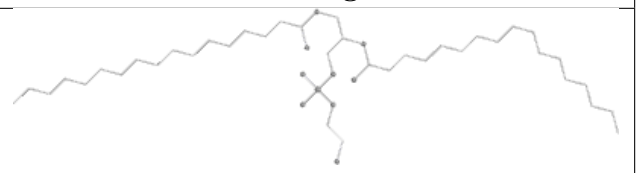
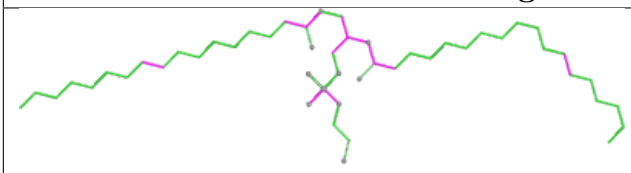


Rings

Ligand PEE E 2005



Bond lengths

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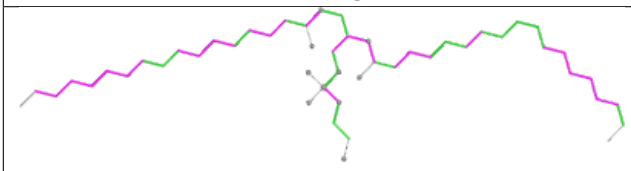

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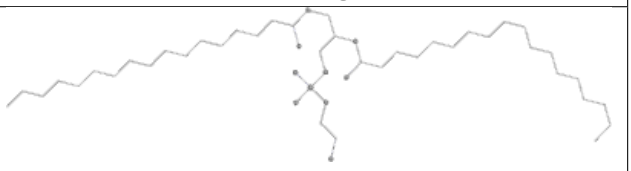
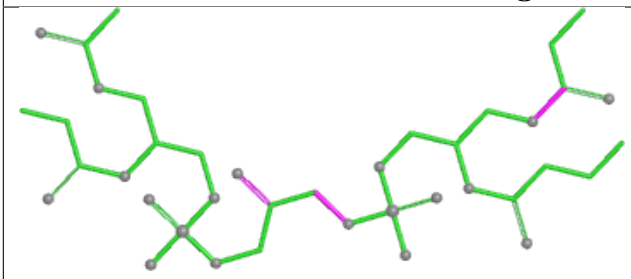


Rings

Ligand CDL P 3004



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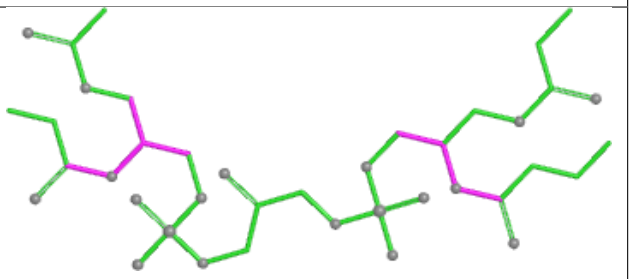

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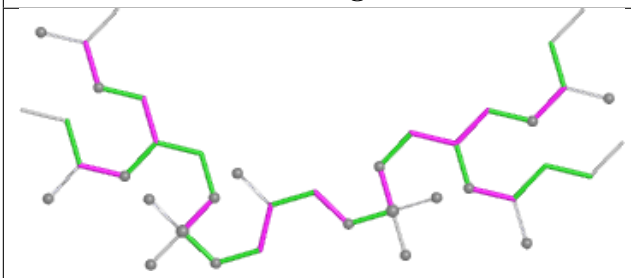

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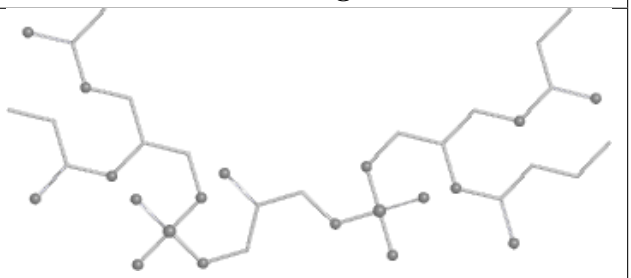
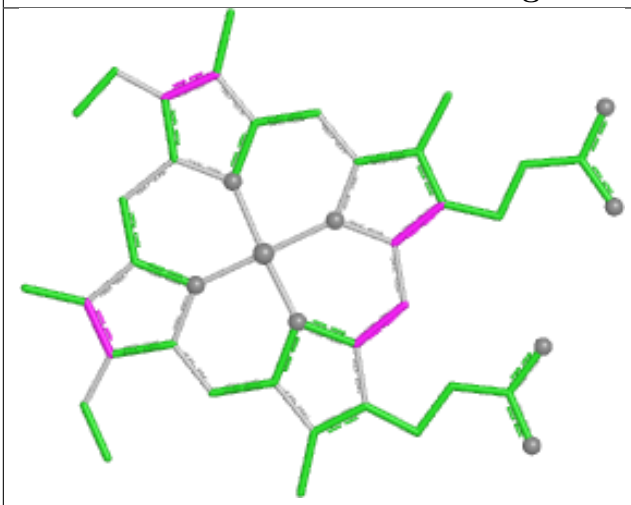


Rings

Ligand HEC Q 501



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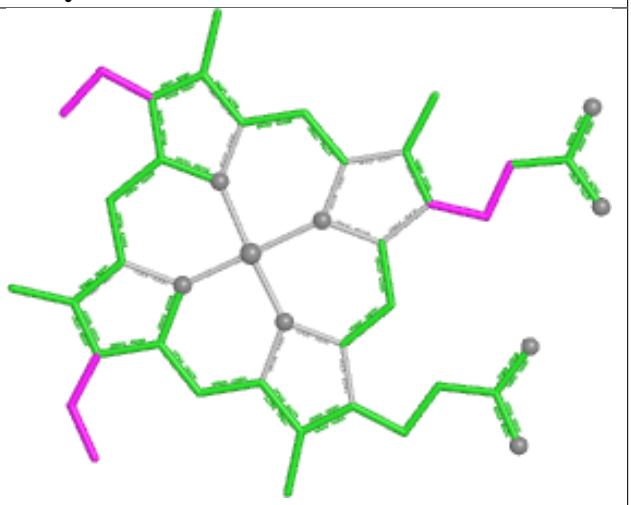

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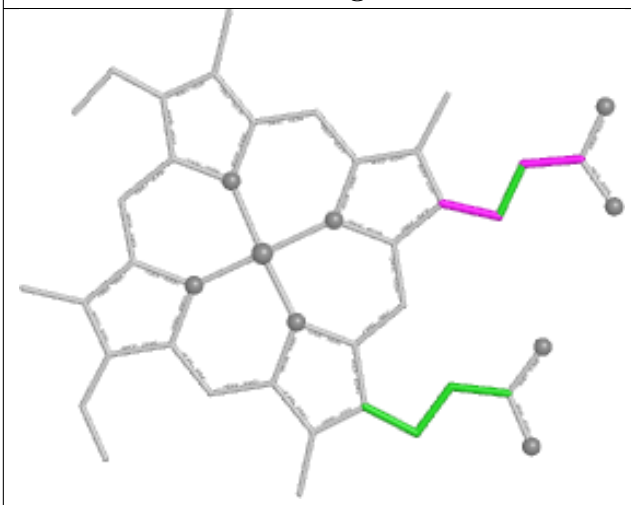

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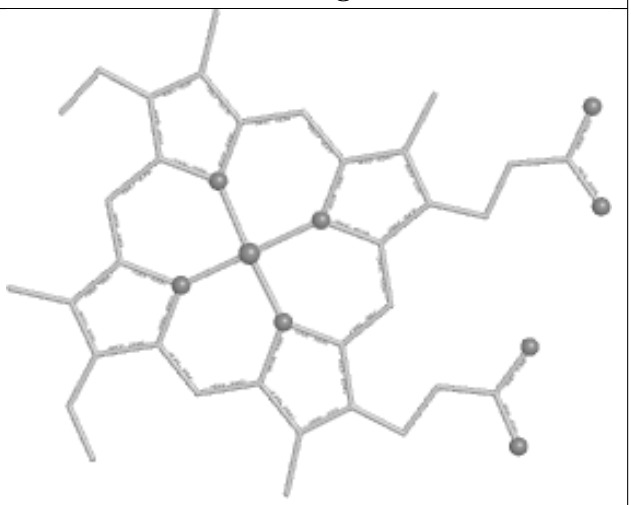
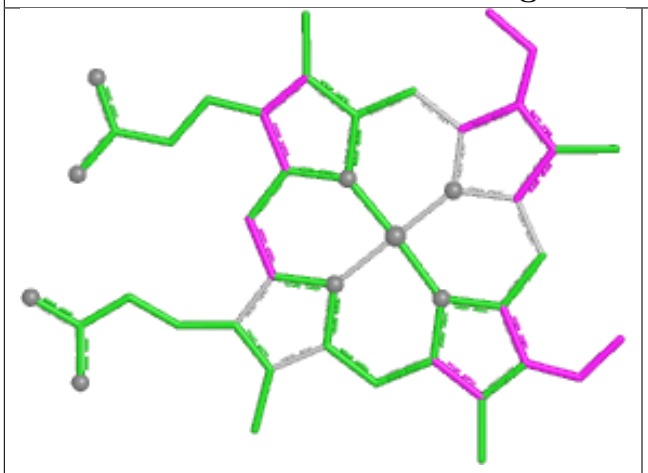


Rings

Ligand HEM C 502



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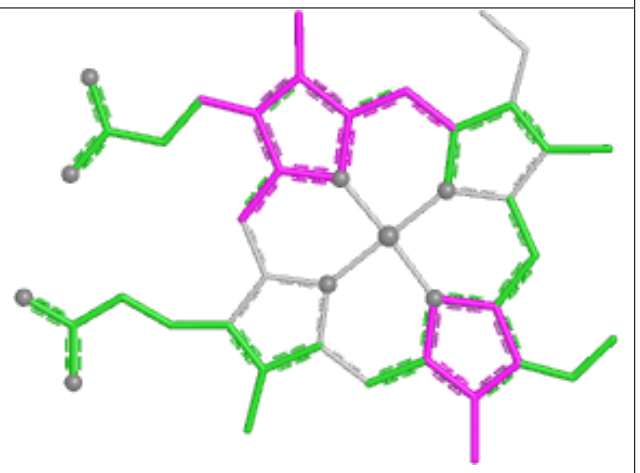

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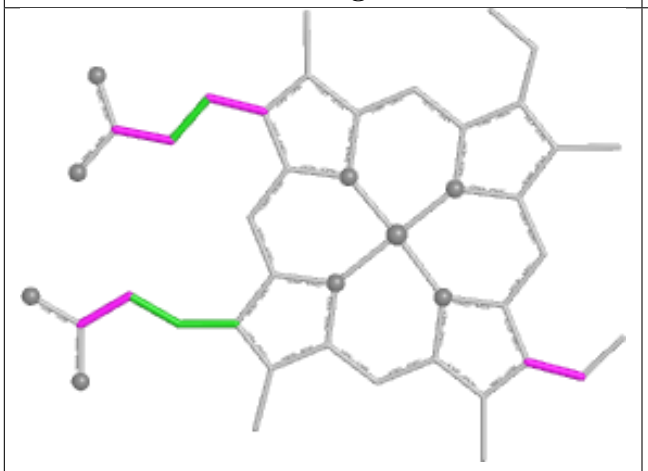

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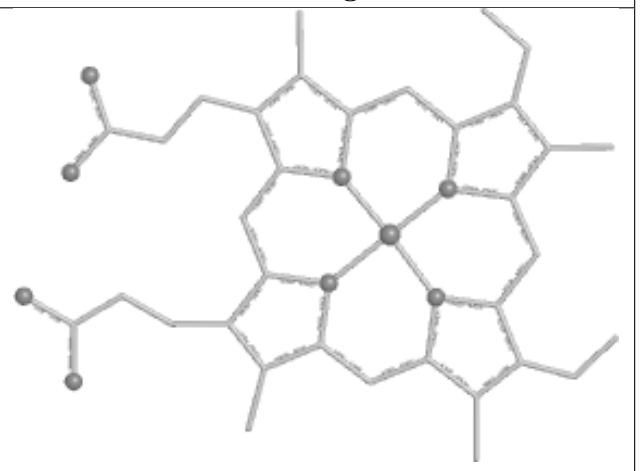
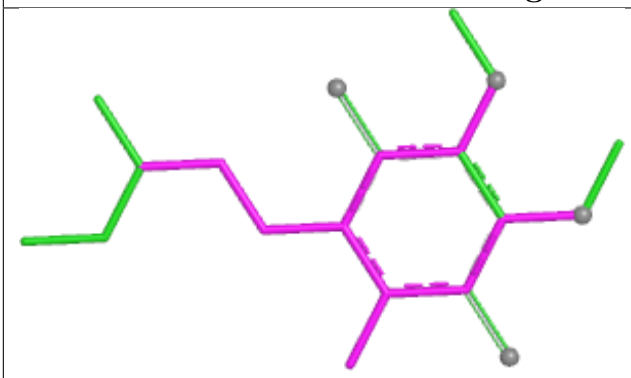


Rings

Ligand UQ C 2002



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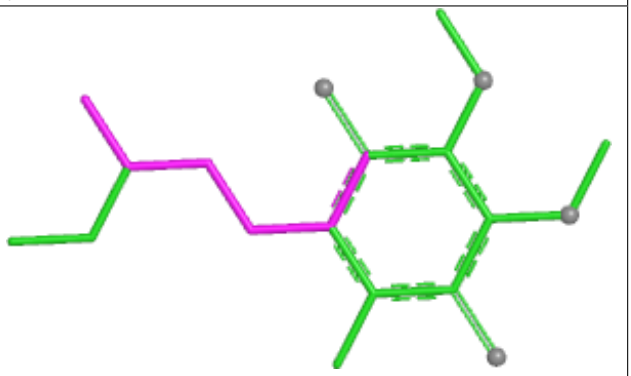

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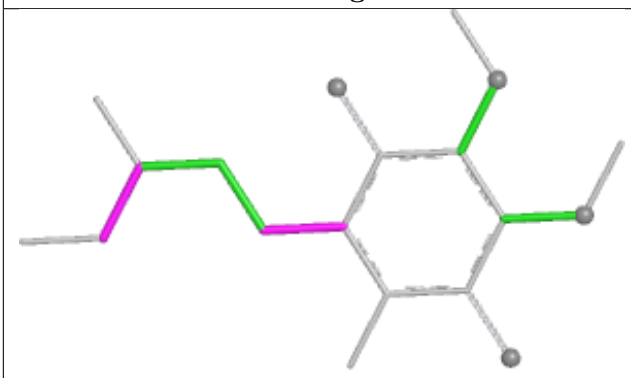

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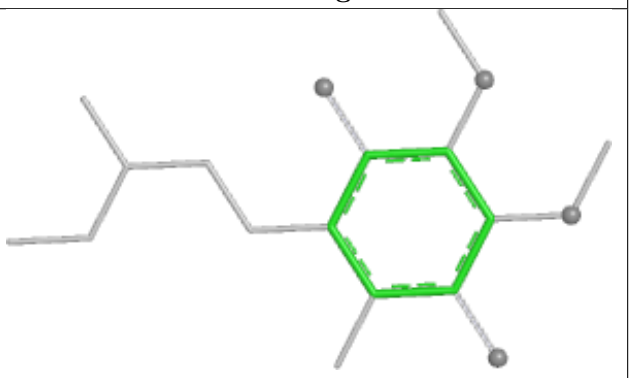
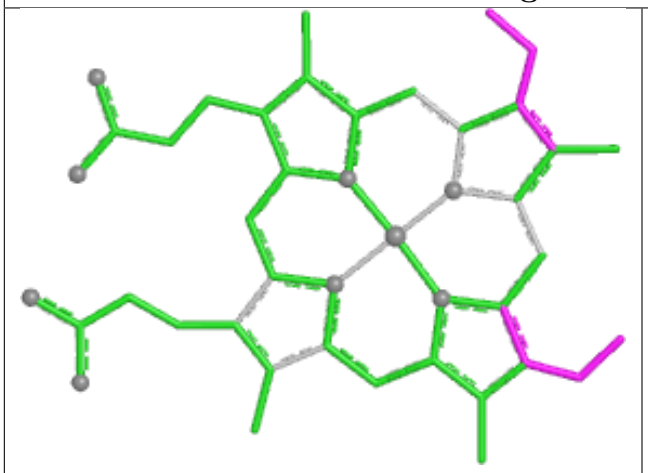


Rings

Ligand HEM P 502



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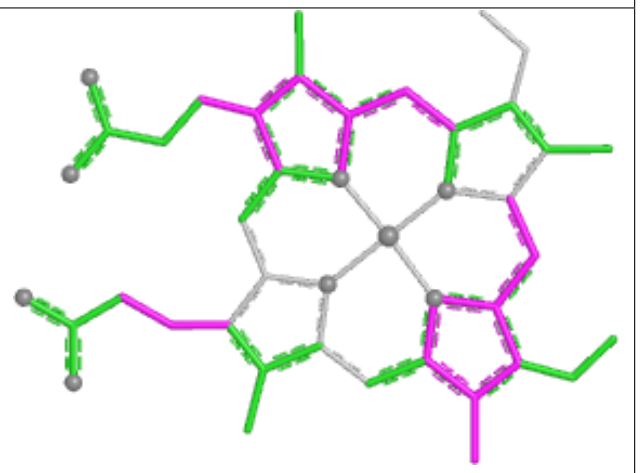
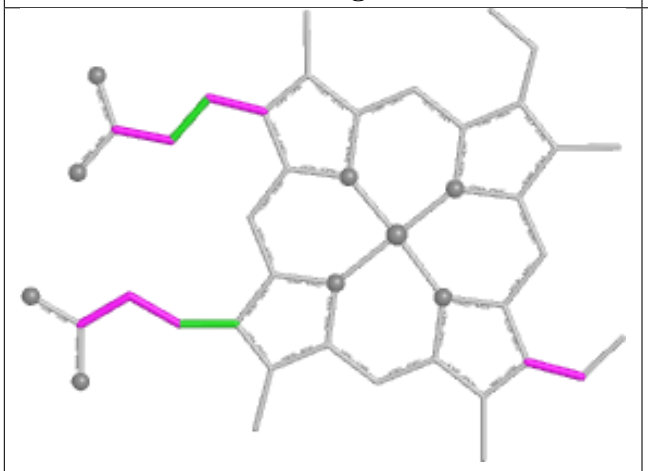


Bond angles



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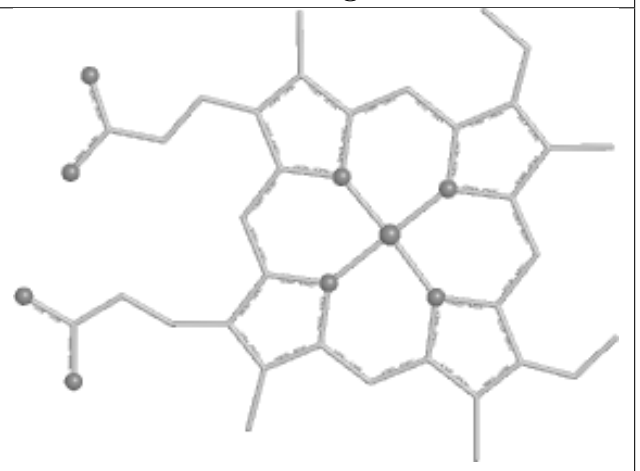
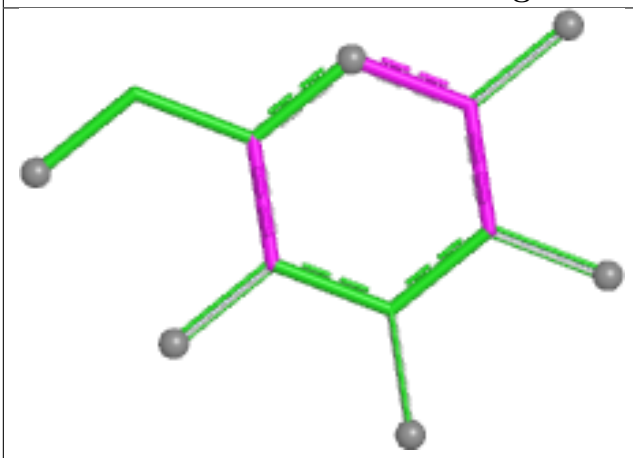


Rings

Ligand BOG P 2010



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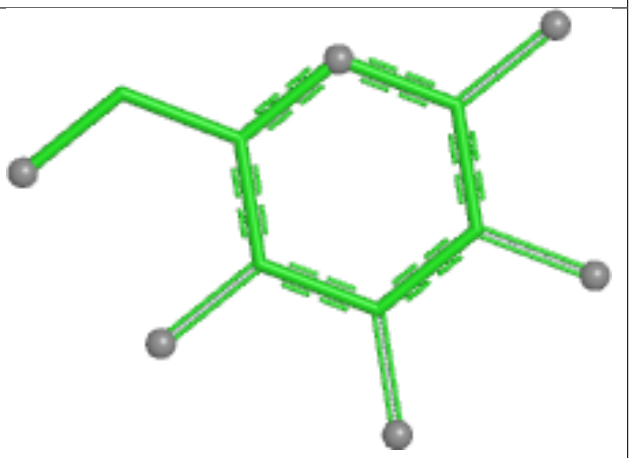
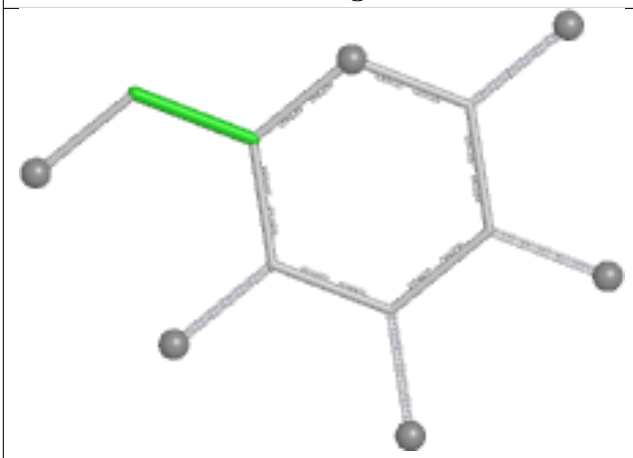
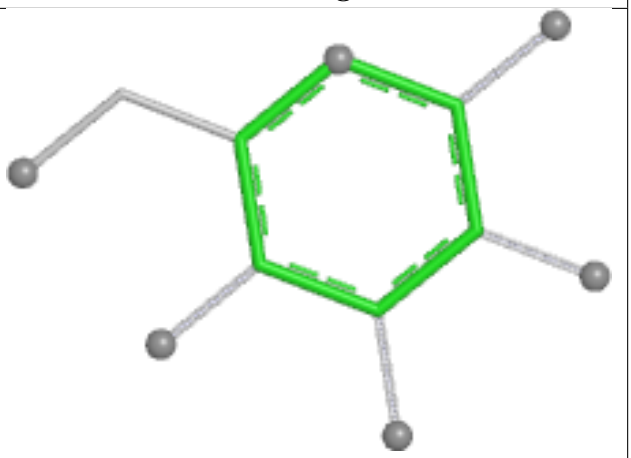


Bond angles

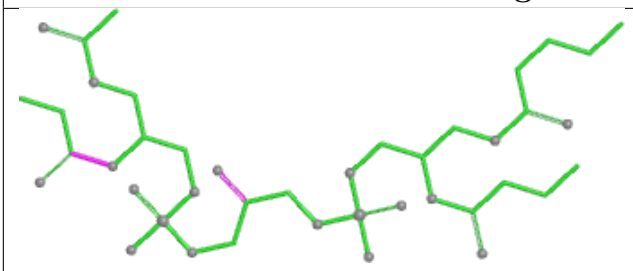


Torsions

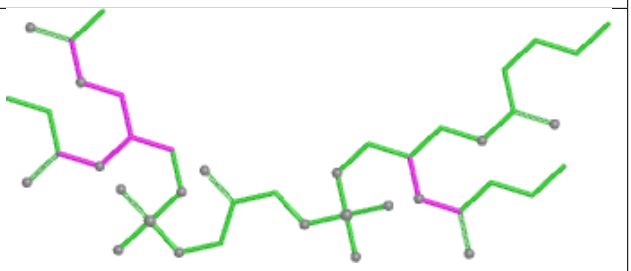


Rings

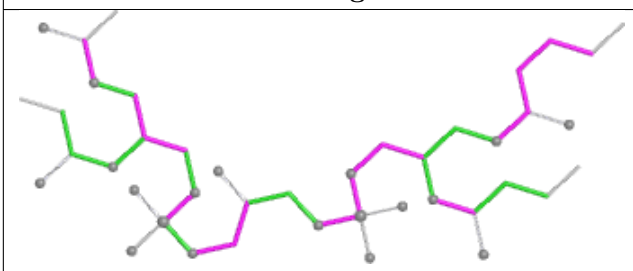
Ligand CDL D 2003



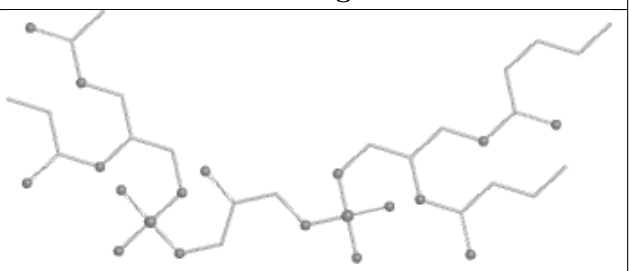
Bond lengths



Bond angles

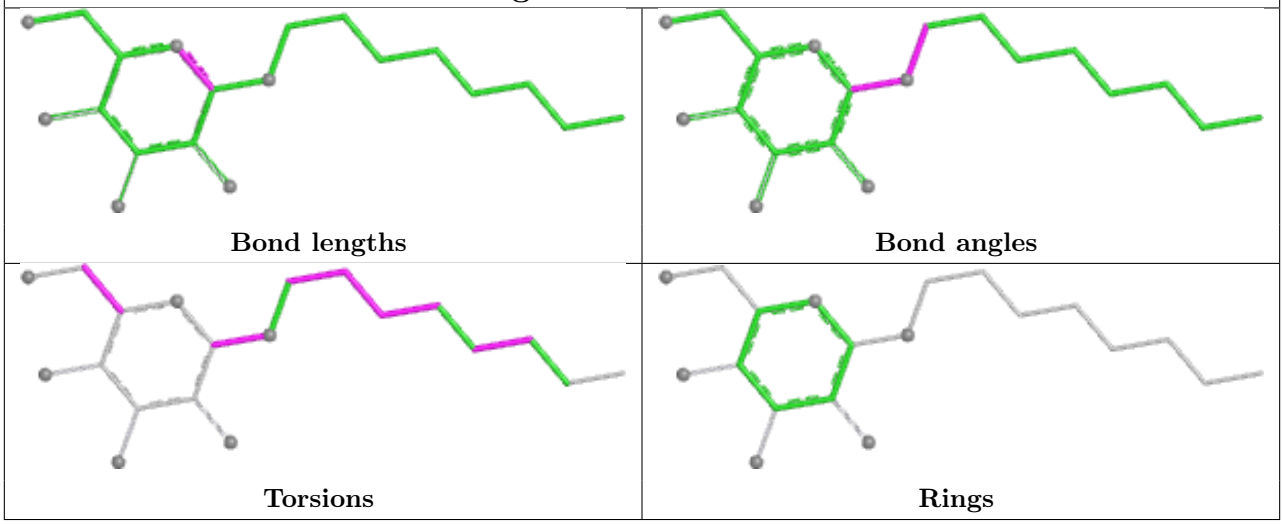


Torsions

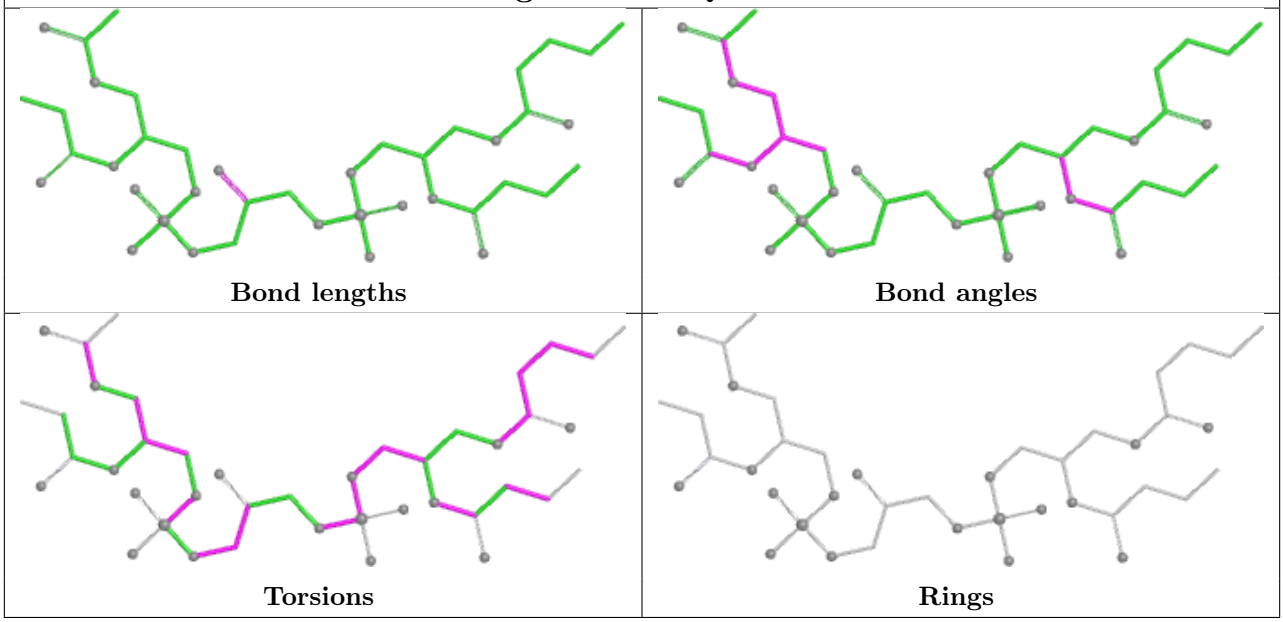


Rings

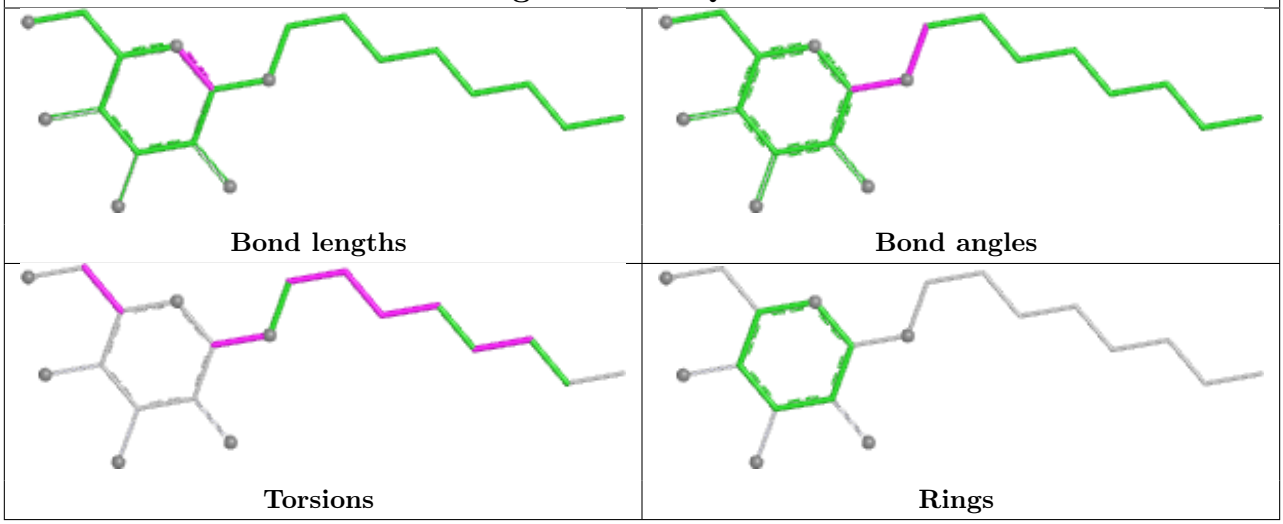
Ligand BOG D 2009



Ligand CDL Q 3003



Ligand BOG Q 3009



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	443/446 (99%)	0.08	3 (0%)	87	81	38, 72, 106, 123	0
1	N	442/446 (99%)	0.16	3 (0%)	87	81	41, 79, 111, 121	0
2	B	421/441 (95%)	0.48	13 (3%)	49	32	59, 90, 133, 158	0
2	O	422/441 (95%)	0.24	6 (1%)	75	63	49, 86, 120, 149	0
3	C	380/380 (100%)	-0.06	1 (0%)	94	92	25, 46, 88, 131	0
3	P	379/380 (99%)	0.01	2 (0%)	91	86	34, 70, 102, 127	0
4	D	241/241 (100%)	-0.09	2 (0%)	86	78	38, 51, 105, 124	0
4	Q	241/241 (100%)	0.28	10 (4%)	37	22	55, 88, 124, 142	0
5	E	196/196 (100%)	1.68	76 (38%)	0	0	42, 150, 175, 178	125 (63%)
5	R	196/196 (100%)	0.94	36 (18%)	1	0	51, 104, 148, 162	127 (64%)
6	F	101/110 (91%)	-0.09	0	100	100	32, 53, 74, 109	0
6	S	101/110 (91%)	0.39	5 (4%)	28	15	56, 79, 121, 145	0
7	G	80/81 (98%)	0.11	1 (1%)	77	66	37, 63, 111, 120	0
7	T	79/81 (97%)	0.65	9 (11%)	5	3	54, 99, 162, 174	0
8	H	70/77 (90%)	0.07	2 (2%)	51	35	44, 73, 98, 145	0
8	U	67/77 (87%)	1.41	16 (23%)	0	0	110, 132, 150, 155	0
9	I	31/47 (65%)	1.32	7 (22%)	0	0	80, 125, 161, 162	0
9	V	31/47 (65%)	1.37	8 (25%)	0	0	81, 114, 162, 165	0
10	J	61/61 (100%)	0.14	4 (6%)	18	10	51, 66, 113, 156	0
10	W	60/61 (98%)	0.14	2 (3%)	46	29	66, 86, 130, 135	0
All	All	4042/4160 (97%)	0.31	206 (5%)	28	15	25, 77, 143, 178	252 (6%)

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	157	TYR	11.6
5	E	163	SER	7.0
9	V	63	ASP	6.9
5	E	85	LYS	6.8
5	E	152	ASP	6.7
5	E	171	ILE	6.7
5	E	165	TYR	6.5
5	E	173	LYS	6.2
5	E	158	CYS	6.1
8	H	9	GLU	6.1
5	E	109	GLU	6.0
5	R	112	VAL	5.8
5	E	129	LYS	5.8
5	E	117	LEU	5.7
5	E	174	GLY	5.7
8	U	13	LEU	5.6
7	T	77	TYR	5.6
5	E	124	LEU	5.5
10	J	63	GLU	5.5
5	E	106	ILE	5.3
3	C	380	TYR	5.3
9	I	63	ASP	5.2
5	E	84	GLY	5.1
5	E	156	TYR	5.1
8	U	37	LEU	4.9
5	E	172	ARG	4.9
5	E	167	ALA	4.8
5	R	81	ILE	4.7
5	R	122	HIS	4.7
5	E	107	ASN	4.6
2	B	19	PRO	4.6
5	E	79	SER	4.6
5	E	169	GLY	4.5
5	E	105	GLU	4.5
5	E	177	PRO	4.5
10	J	62	SER	4.5
9	V	56	SER	4.4
5	R	113	ASP	4.4
5	E	134	ILE	4.3
5	E	119	ASP	4.2
5	E	164	HIS	4.2
5	E	108	GLN	4.2
5	R	124	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
5	E	168	SER	4.2
5	E	120	PRO	4.2
5	E	125	ASP	4.1
5	E	86	ASN	4.0
5	R	172	ARG	4.0
5	E	83	GLU	4.0
5	E	102	THR	4.0
5	R	84	GLY	3.9
2	O	19	PRO	3.9
9	I	52	ARG	3.9
8	H	10	GLU	3.9
5	R	102	THR	3.8
5	E	115	SER	3.8
8	U	12	GLU	3.8
5	E	121	GLN	3.7
1	N	216	PHE	3.6
5	R	196	GLY	3.6
5	E	190	ASP	3.6
5	E	147	ILE	3.6
5	E	98	VAL	3.5
5	E	180	LEU	3.5
5	E	130	PRO	3.5
5	R	110	ALA	3.5
8	U	78	LYS	3.4
5	E	159	PRO	3.4
5	E	187	PHE	3.4
2	O	386	ALA	3.4
10	W	62	SER	3.4
5	E	118	ARG	3.4
5	E	100	HIS	3.3
7	T	80	ASP	3.3
5	E	185	TYR	3.3
4	Q	169	LEU	3.2
7	G	2	ILE	3.2
5	R	164	HIS	3.2
5	R	169	GLY	3.1
8	U	50	THR	3.1
7	T	75	ALA	3.1
5	E	188	VAL	3.1
5	E	81	ILE	3.1
5	E	135	LEU	3.1
5	E	178	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
5	E	116	LYS	3.1
5	E	104	ALA	3.1
5	E	194	VAL	3.0
5	E	162	GLY	3.0
5	R	171	ILE	3.0
5	R	111	GLU	3.0
6	S	11	ARG	3.0
5	E	103	GLN	3.0
9	I	77	ARG	3.0
5	R	101	ARG	3.0
2	B	224	LEU	3.0
4	Q	143	VAL	2.9
5	R	114	VAL	2.9
9	I	55	MET	2.9
5	E	128	LYS	2.9
2	B	36	ALA	2.8
9	V	55	MET	2.8
5	E	148	ALA	2.8
1	N	376	CYS	2.8
5	E	101	ARG	2.8
8	U	44	VAL	2.8
4	D	1	GLY	2.8
5	R	119	ASP	2.8
7	T	78	GLU	2.8
4	Q	164	ILE	2.7
7	T	2	ILE	2.7
9	V	53	GLU	2.7
8	U	49	HIS	2.7
5	R	103	GLN	2.7
5	R	165	TYR	2.7
6	S	12	LEU	2.7
5	R	82	PRO	2.7
10	J	64	GLU	2.7
1	A	102	LEU	2.7
9	I	47	ARG	2.6
10	J	61	ALA	2.6
5	E	114	VAL	2.6
5	E	175	PRO	2.6
5	R	170	ARG	2.6
5	R	128	LYS	2.6
5	R	191	ASP	2.6
2	B	405	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	29	LEU	2.6
5	E	153	PHE	2.6
5	E	151	GLY	2.6
7	T	74	PRO	2.6
6	S	81	VAL	2.5
9	V	54	SER	2.5
5	E	146	PRO	2.5
5	R	190	ASP	2.5
9	V	57	GLY	2.5
5	E	87	VAL	2.5
5	E	133	VAL	2.5
5	R	168	SER	2.5
5	E	113	ASP	2.5
5	R	117	LEU	2.5
1	A	83	GLY	2.5
5	R	125	ASP	2.5
2	B	221	GLU	2.5
5	E	122	HIS	2.5
2	B	201	SER	2.4
2	O	217	LYS	2.4
5	E	82	PRO	2.4
8	U	46	SER	2.4
4	Q	141	VAL	2.4
5	R	188	VAL	2.4
9	V	50	LEU	2.4
2	B	393	THR	2.4
6	S	18	LYS	2.4
8	U	33	ALA	2.3
5	R	121	GLN	2.3
3	P	2	ALA	2.3
8	U	48	SER	2.3
9	V	49	LEU	2.3
4	Q	48	PHE	2.3
8	U	36	ARG	2.3
8	U	45	SER	2.3
5	E	182	VAL	2.3
5	R	157	TYR	2.3
2	B	289	SER	2.2
8	U	35	GLU	2.2
2	B	412	ASN	2.2
9	I	57	GLY	2.2
5	R	77	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	402	ILE	2.2
1	A	226	ASP	2.2
3	P	380	TYR	2.2
4	Q	167	GLU	2.2
2	O	34	ILE	2.2
5	R	176	ALA	2.2
7	T	44	GLN	2.2
5	R	127	VAL	2.2
4	D	170	GLU	2.2
5	E	149	ASN	2.2
10	W	63	GLU	2.2
5	E	132	TRP	2.1
8	U	61	PHE	2.1
5	E	127	VAL	2.1
2	B	31	ASN	2.1
8	U	63	HIS	2.1
5	E	150	SER	2.1
5	R	132	TRP	2.1
5	E	126	ARG	2.1
7	T	70	LYS	2.1
4	Q	3	LEU	2.1
5	E	111	GLU	2.1
1	N	127	ILE	2.1
5	R	78	LEU	2.1
5	R	187	PHE	2.0
8	U	47	ARG	2.0
2	B	386	ALA	2.0
2	O	267	ALA	2.0
2	O	296	TYR	2.0
5	E	76	ILE	2.0
5	E	78	LEU	2.0
9	I	53	GLU	2.0
4	Q	171	TYR	2.0
4	Q	5	LEU	2.0
6	S	23	ALA	2.0
7	T	73	ASN	2.0
4	Q	113	LEU	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
18	BOG	D	2091	13/20	0.33	0.84	185,187,187,187	0
18	BOG	Q	3091	13/20	0.47	0.60	195,196,196,196	0
11	UNL	A	3231	1/-	0.52	0.65	91,91,91,91	0
18	BOG	P	2010	12/20	0.62	0.43	155,156,157,158	0
15	PEE	C	2008	21/51	0.67	0.47	150,154,158,159	0
13	UQ	P	3002	19/63	0.69	0.59	121,130,133,133	0
15	PEE	N	3008	5/51	0.72	0.28	117,118,119,119	0
14	CDL	Q	3003	42/100	0.77	0.48	134,150,157,158	0
11	UNL	P	3286	1/-	0.77	0.37	55,55,55,55	0
15	PEE	R	3005	50/51	0.80	0.42	87,109,125,125	0
11	UNL	N	3290	1/-	0.80	0.47	53,53,53,53	0
11	UNL	N	4231	1/-	0.81	0.55	67,67,67,67	0
15	PEE	E	2005	50/51	0.83	0.45	72,96,104,105	0
13	UQ	C	2002	19/63	0.83	0.39	82,84,86,86	0
15	PEE	P	3007	49/51	0.85	0.48	65,94,110,112	0
14	CDL	D	2003	42/100	0.86	0.39	97,106,116,117	0
11	UNL	C	3287	1/-	0.86	0.95	88,88,88,88	0
14	CDL	P	3004	40/100	0.87	0.39	107,115,122,124	0
11	UNL	A	3289	1/-	0.88	0.69	38,38,38,38	0
15	PEE	C	2007	49/51	0.91	0.36	42,65,85,87	0
16	GOL	C	2011	6/6	0.92	0.31	70,71,72,75	0
14	CDL	C	2004	40/100	0.93	0.33	69,86,100,102	0
16	GOL	P	3011	6/6	0.93	0.30	86,87,88,89	0
18	BOG	Q	3009	20/20	0.93	0.31	82,93,95,95	0
18	BOG	D	2009	20/20	0.93	0.25	52,70,74,76	0
11	UNL	C	3288	1/-	0.94	0.55	84,84,84,84	0
19	FES	E	501	4/4	0.94	0.13	161,162,162,162	4
11	UNL	A	3284	1/-	0.95	0.40	28,28,28,28	0
11	UNL	N	3291	1/-	0.96	0.34	37,37,37,37	0
17	HEC	Q	501	43/43	0.97	0.25	70,75,81,84	0
12	HEM	C	502	43/43	0.98	0.29	23,30,38,44	0
12	HEM	P	501	43/43	0.98	0.27	48,52,61,66	0

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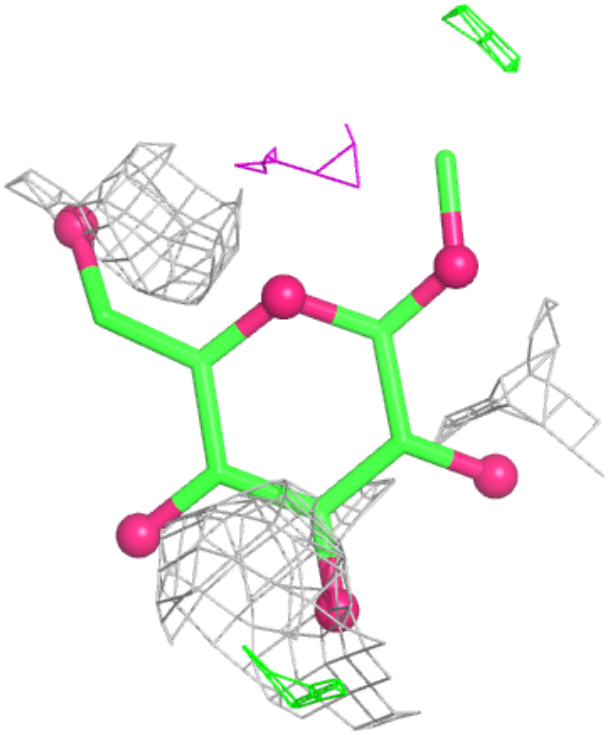
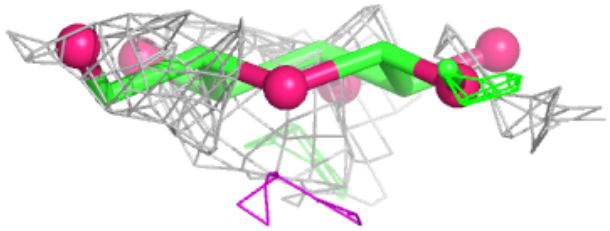
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	HEM	P	502	43/43	0.98	0.27	43,50,60,65	0
12	HEM	C	501	43/43	0.98	0.26	30,36,47,53	0
19	FES	R	501	4/4	0.98	0.09	92,94,94,95	4
17	HEC	D	501	43/43	0.99	0.22	35,40,48,52	0

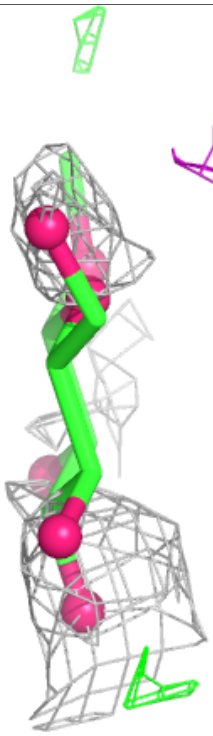
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG D 2091:

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

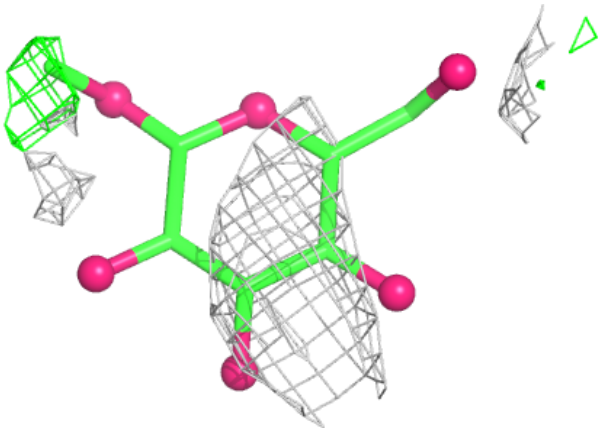


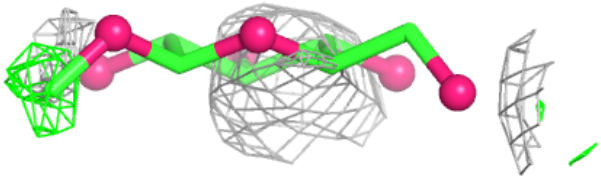


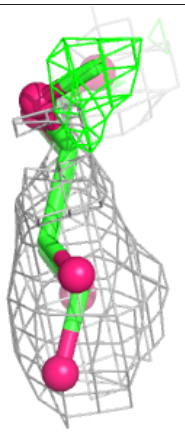


Electron density around BOG Q 3091:

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

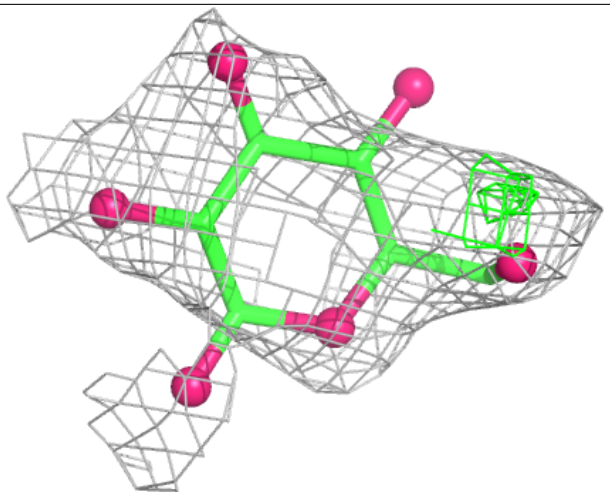


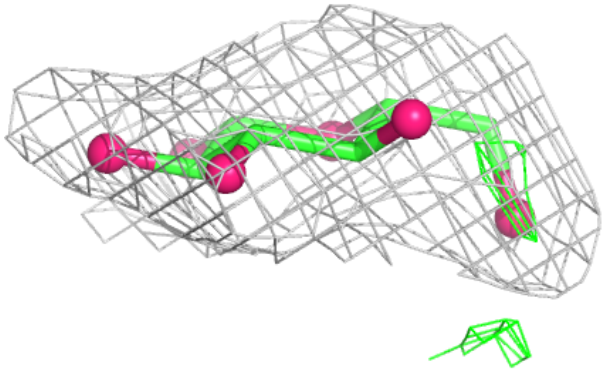


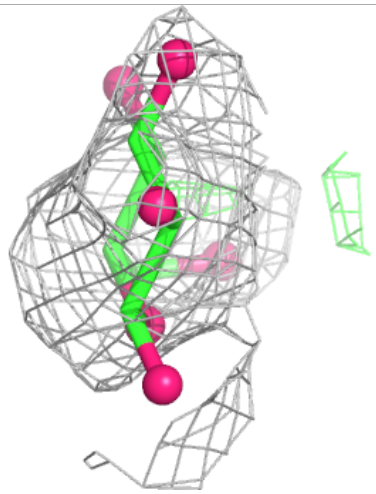


Electron density around BOG P 2010:

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

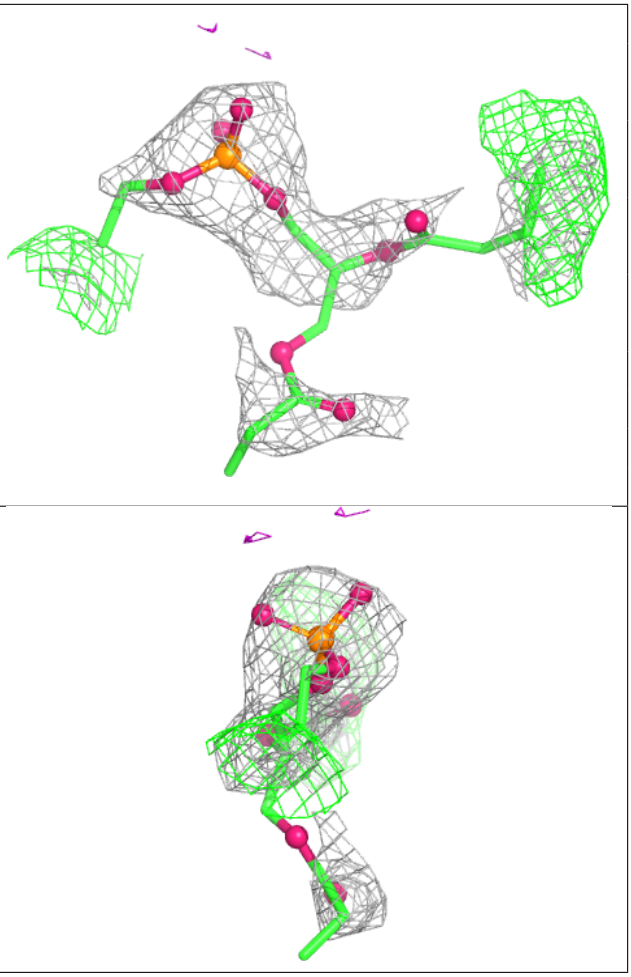






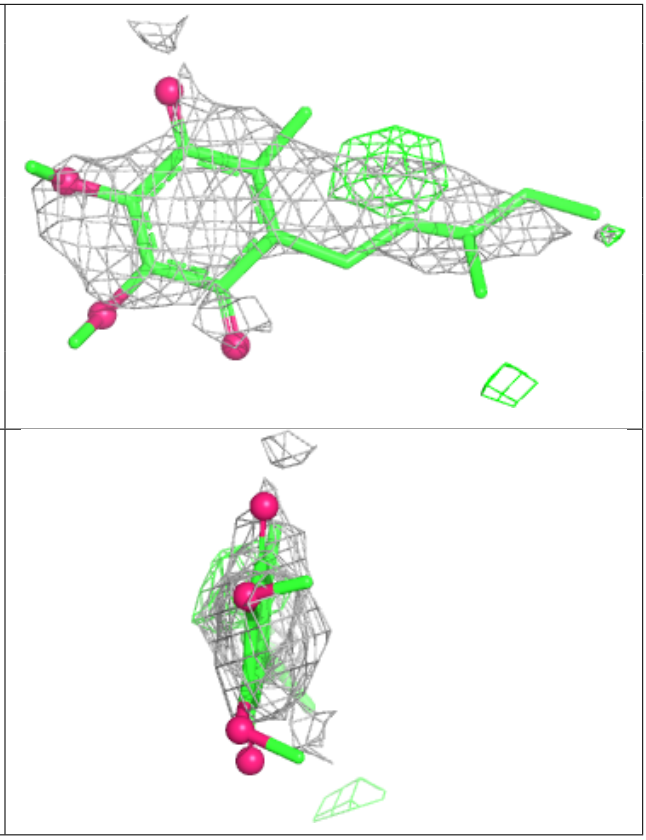
Electron density around PEE C 2008:

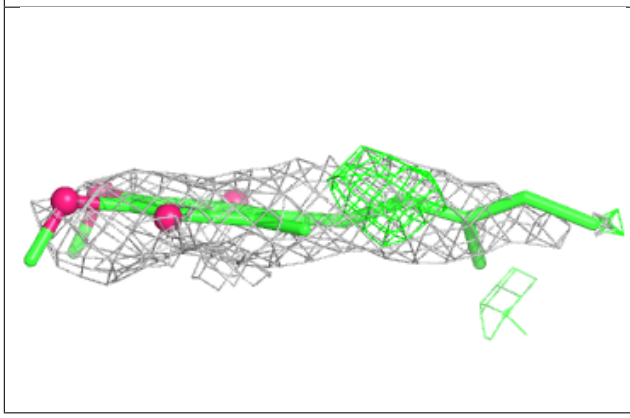
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UQ P 3002:

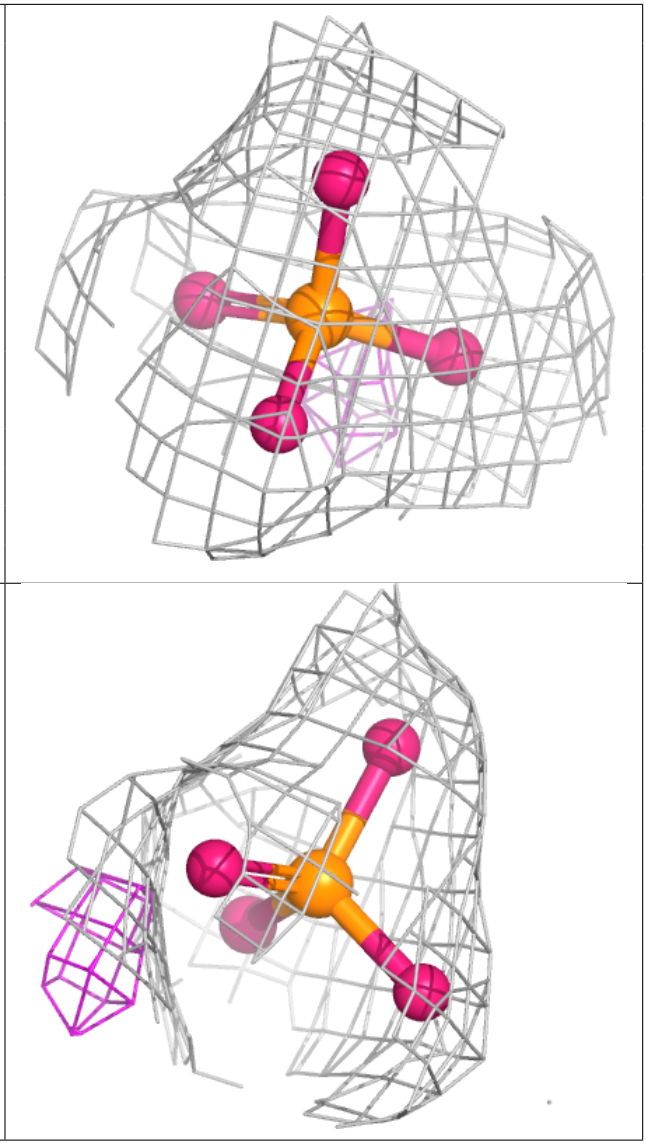
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





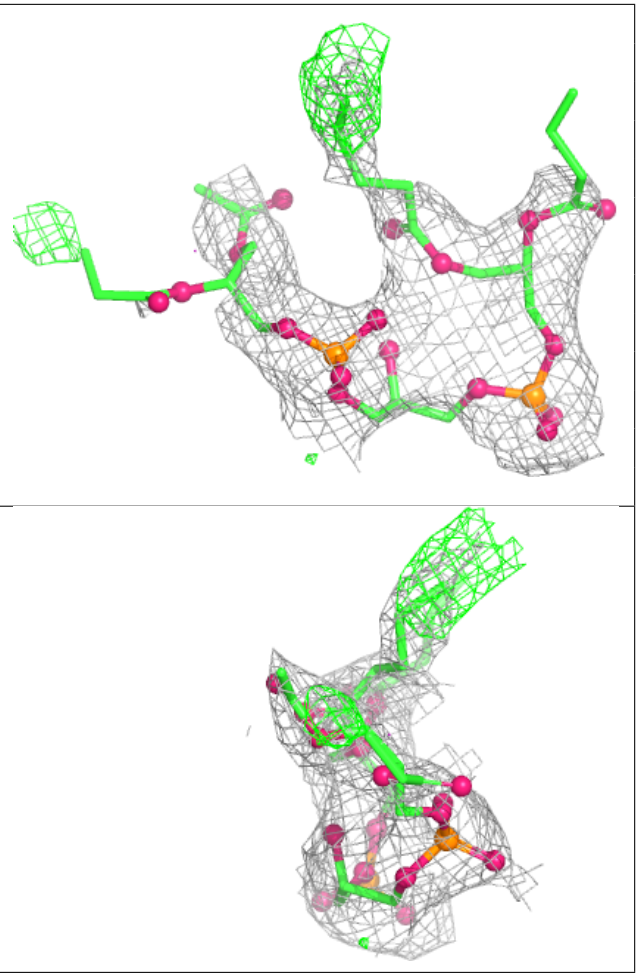
Electron density around PEE N 3008:

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



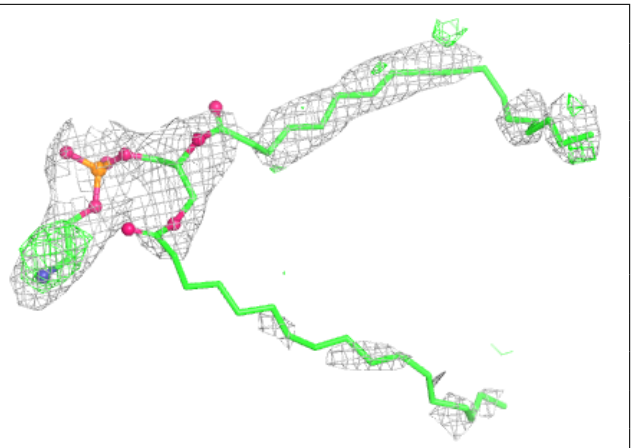
Electron density around CDL Q 3003:

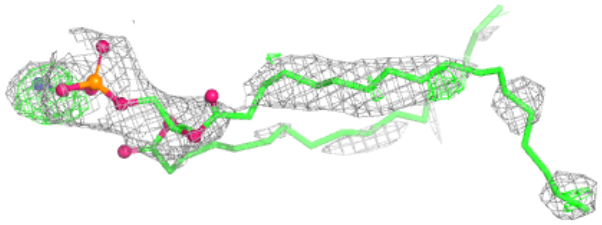
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

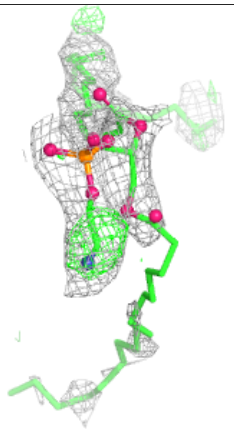


Electron density around PEE R 3005:

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

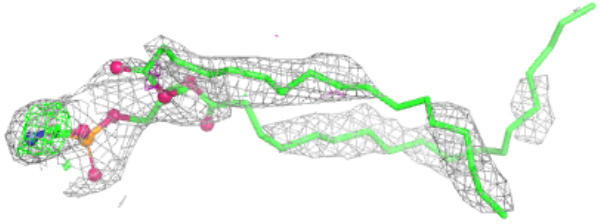






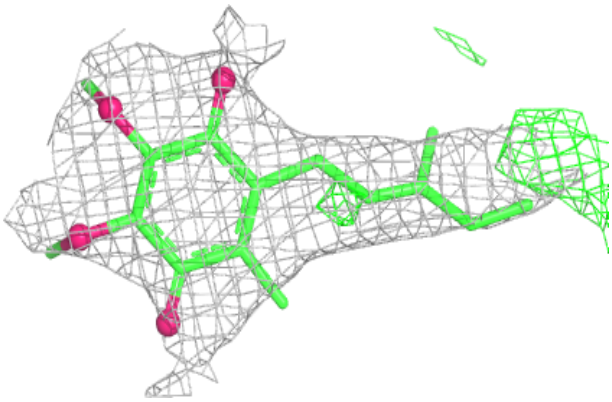
Electron density around PEE E 2005:

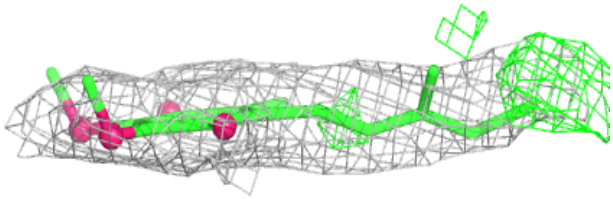
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

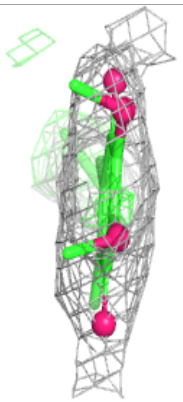


Electron density around UQ C 2002:

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

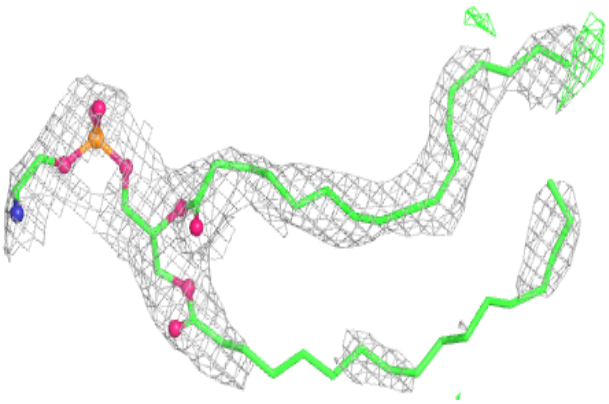


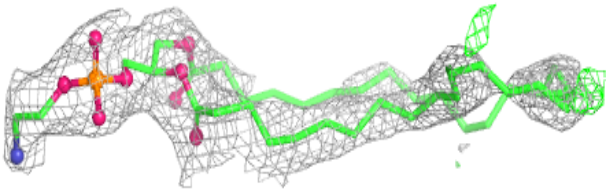




Electron density around PEE P 3007:

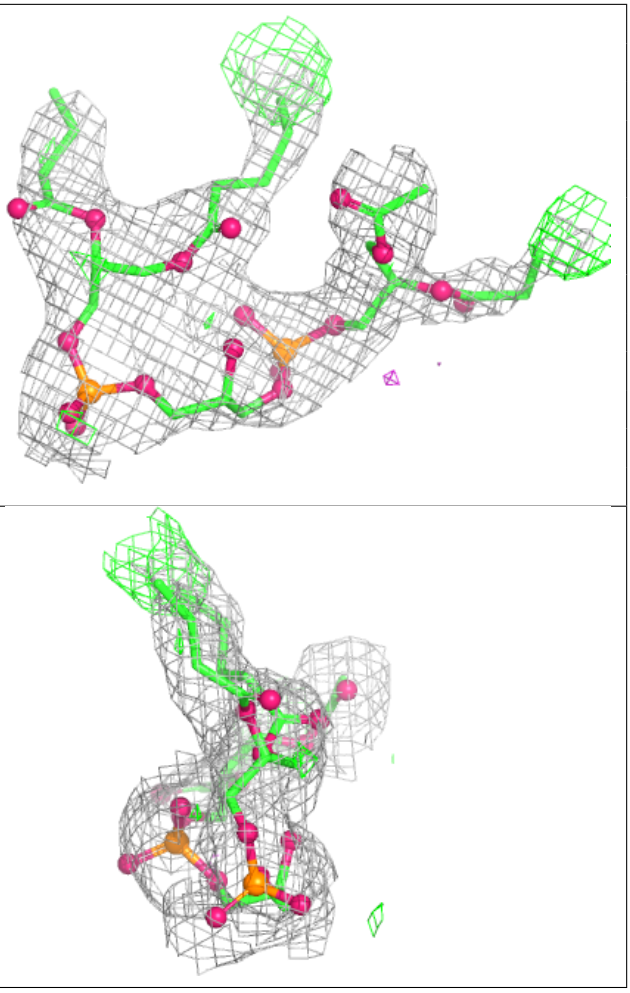
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





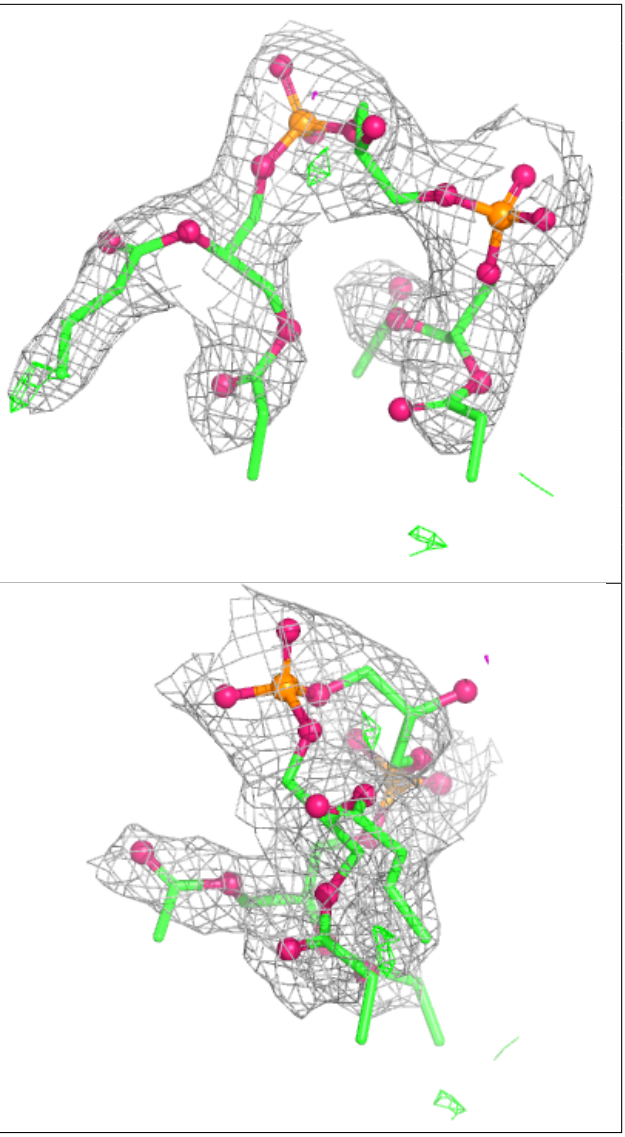
Electron density around CDL D 2003:

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



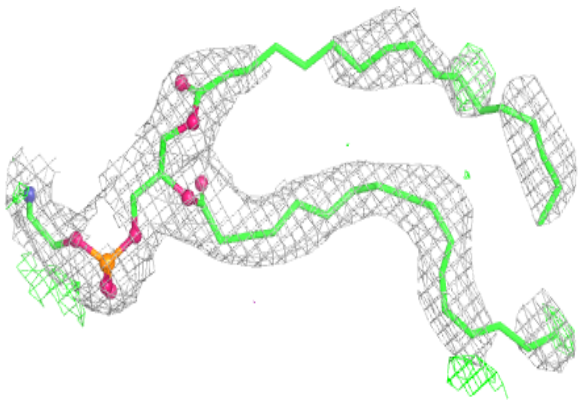
Electron density around CDL P 3004:

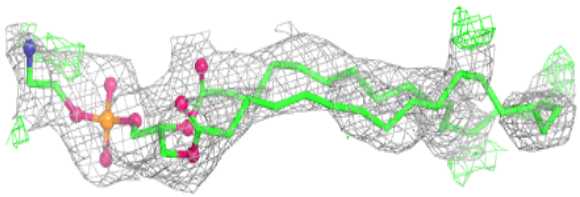
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

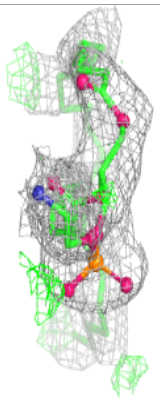


Electron density around PEE C 2007:

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

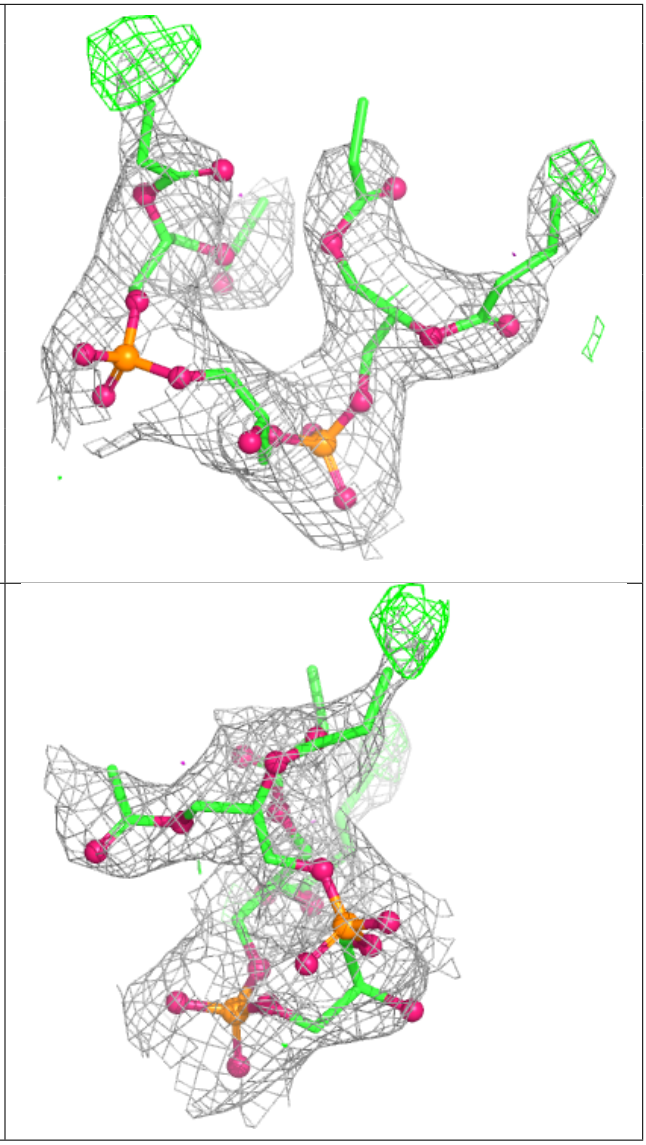






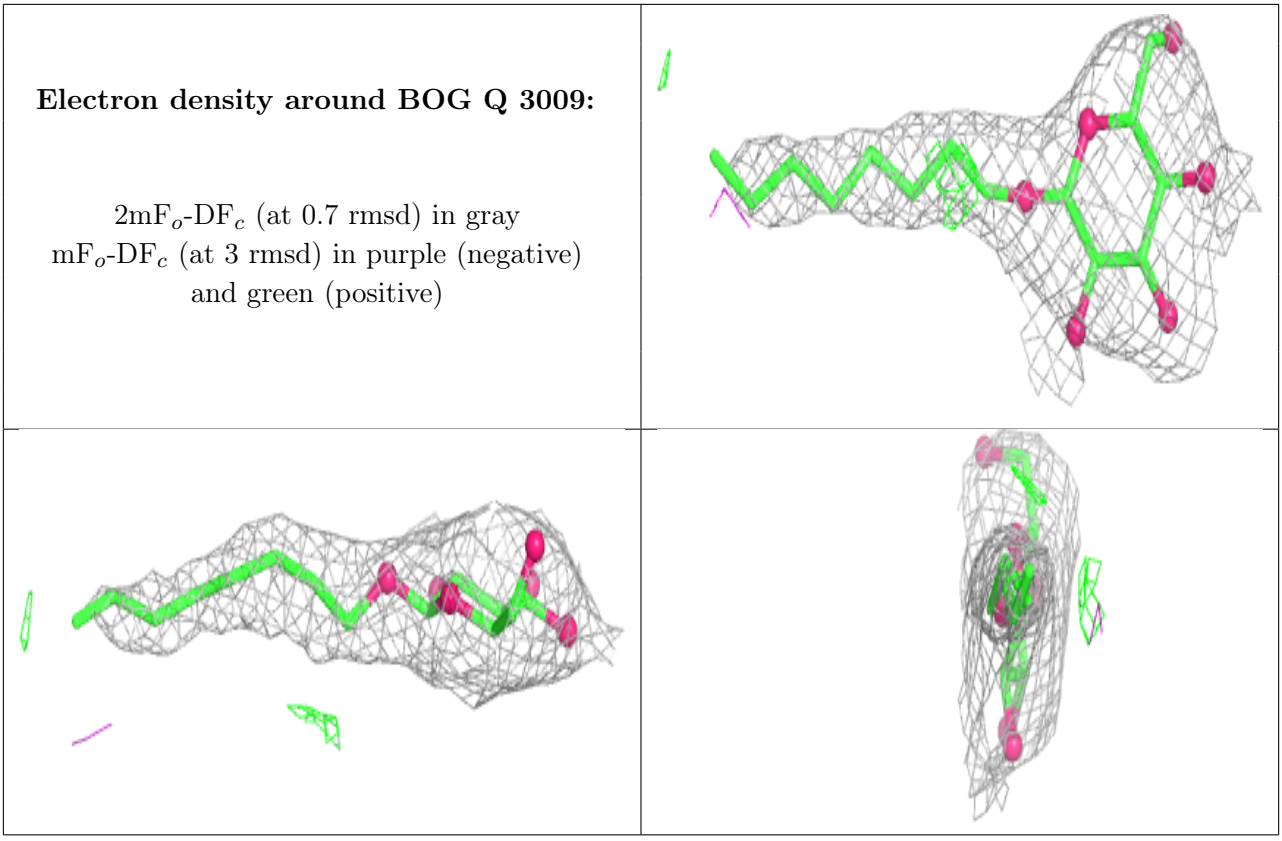
Electron density around CDL C 2004:

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



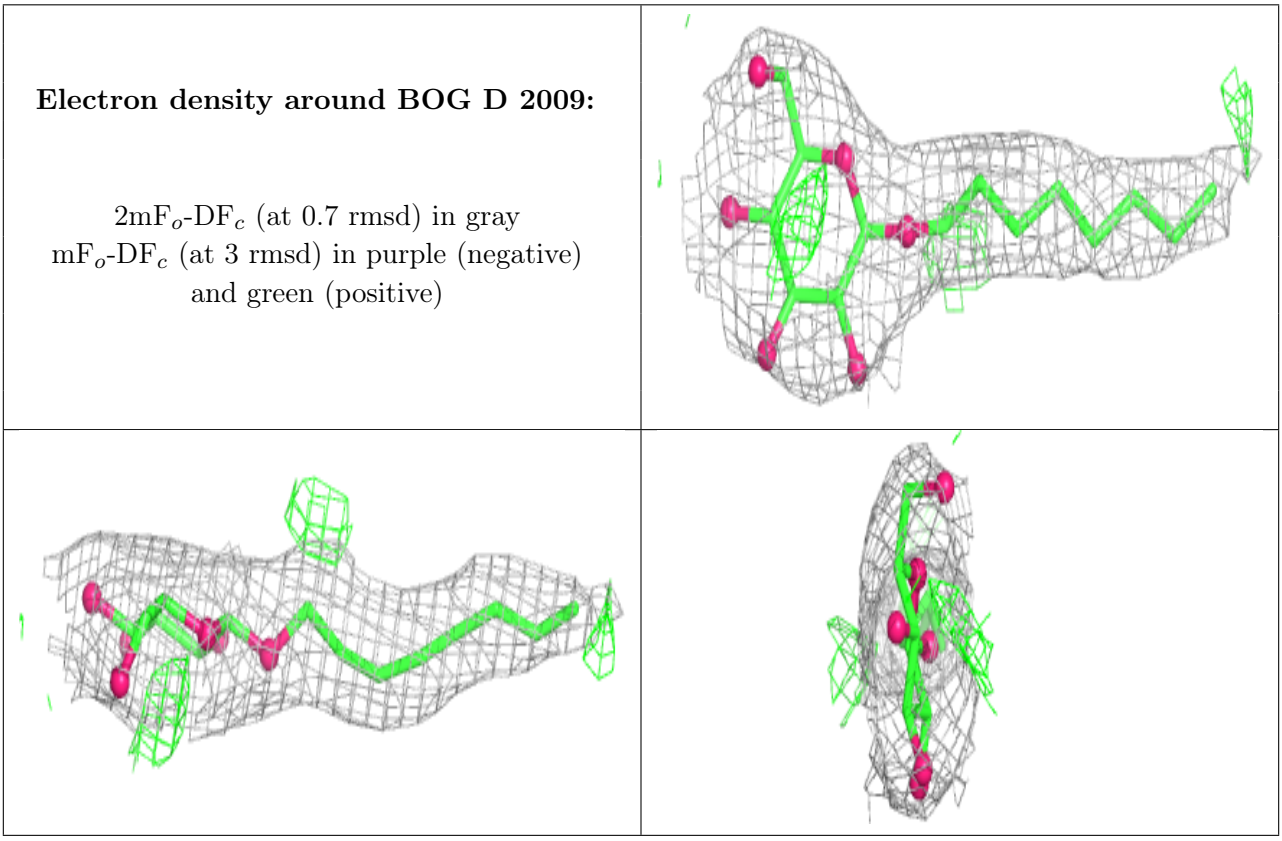
Electron density around BOG Q 3009:

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



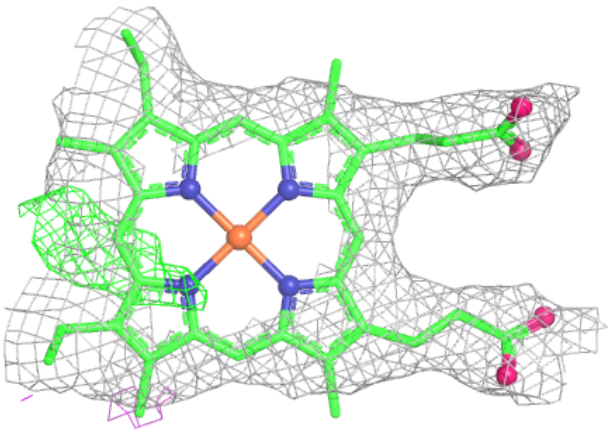
Electron density around BOG D 2009:

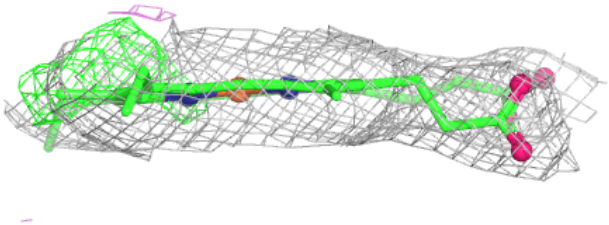
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

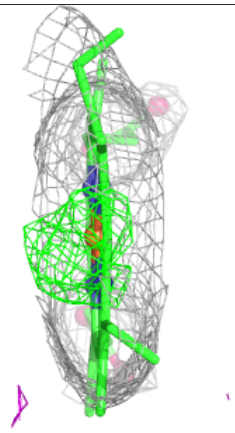


Electron density around HEC Q 501:

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

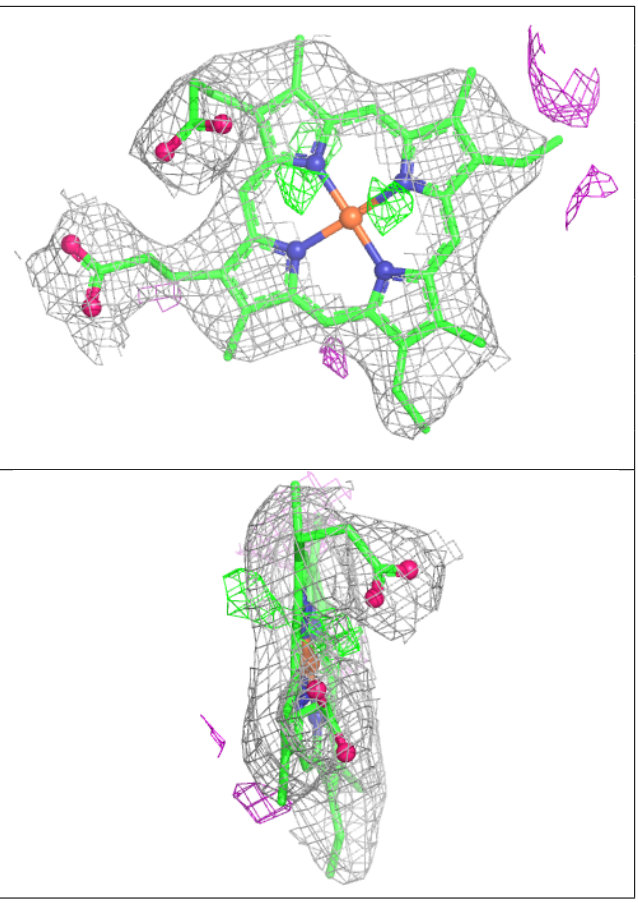






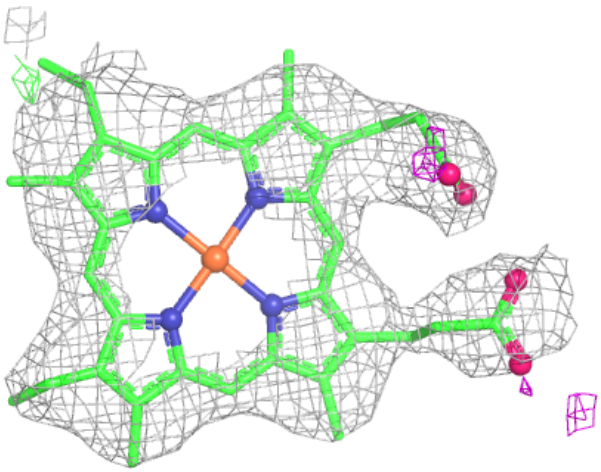
Electron density around HEM C 502:

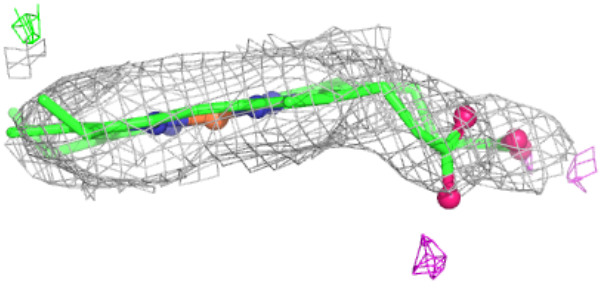
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

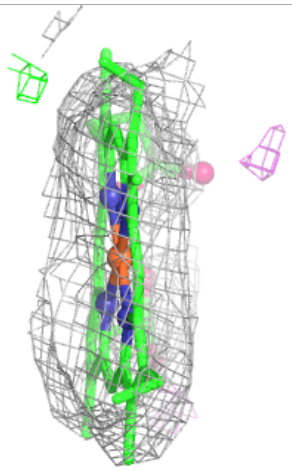


Electron density around HEM P 501:

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

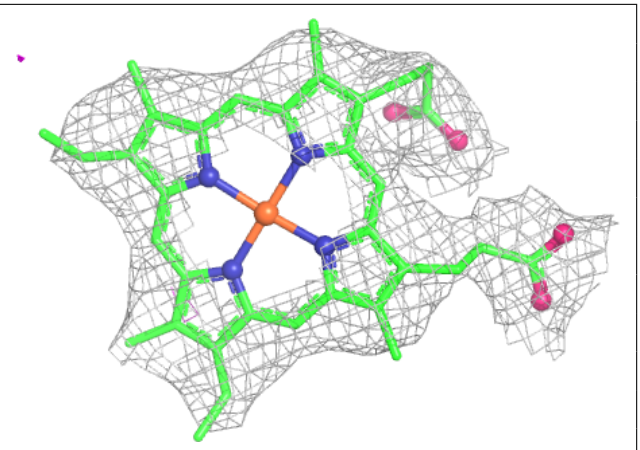


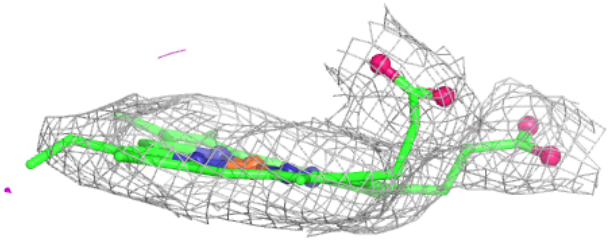


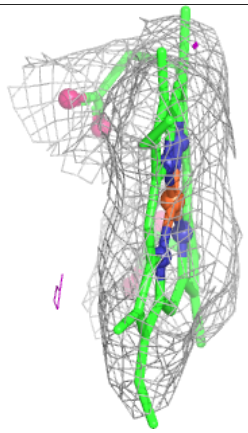


Electron density around HEM P 502:

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

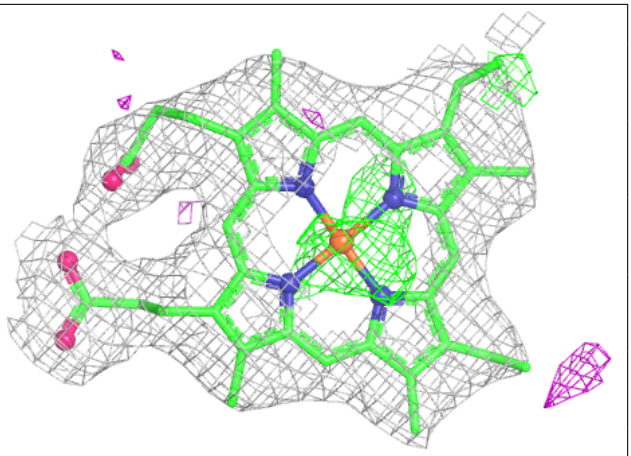


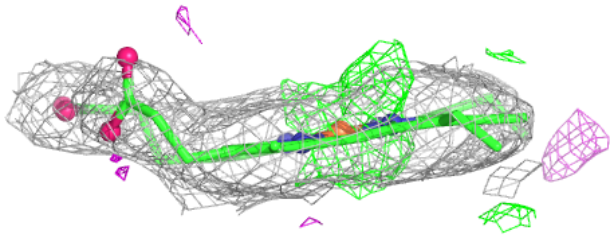


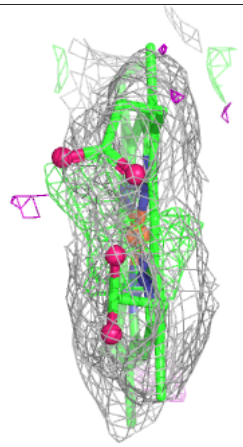


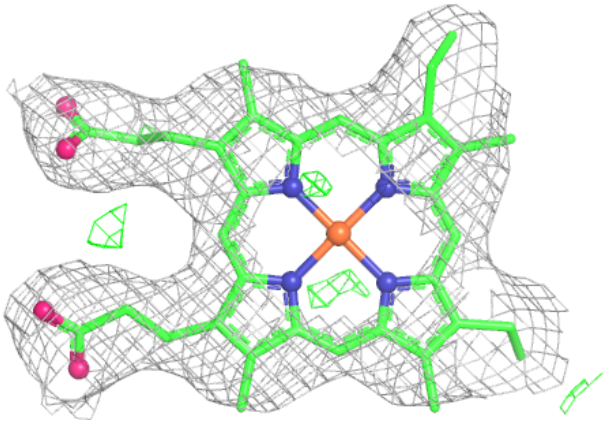
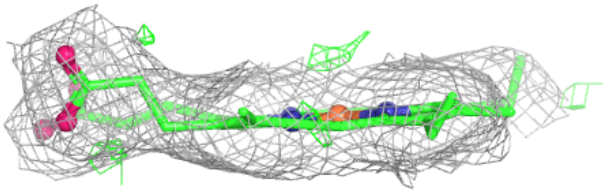
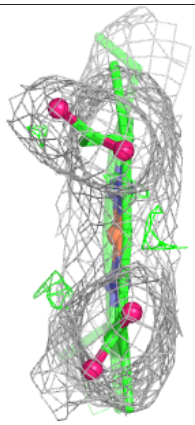
Electron density around HEM C 501:

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







Electron density around HEC 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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.