Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 12:08 AM EDT

PDB ID	:	3L75
Title	:	Cytochrome BC1 complex from chicken with fenamidone bound
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-28
Resolution	:	2.79 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

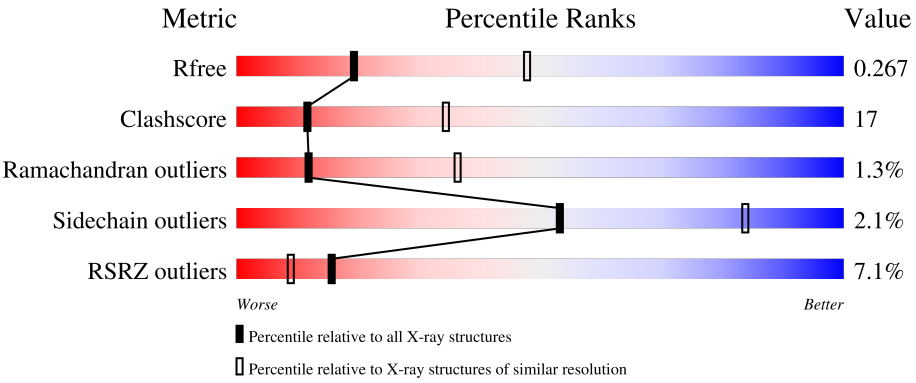
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	2% 65% 31%
1	N	446	4% 67% 29%
2	B	441	4% 55% 38% 5%
2	O	441	3% 55% 39%
3	C	380	80% 20%

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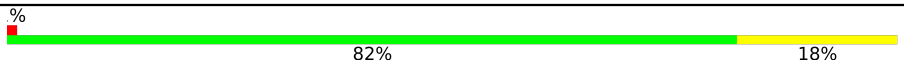
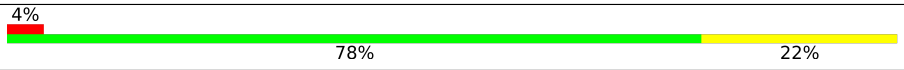
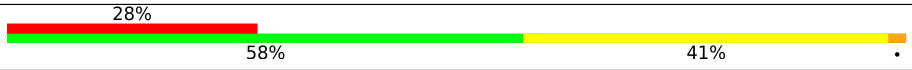
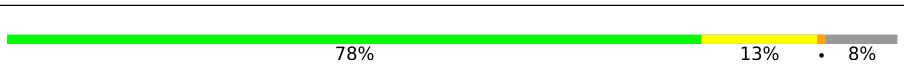
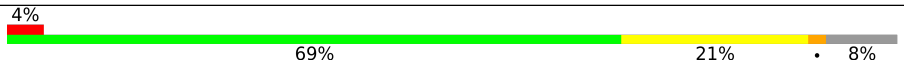
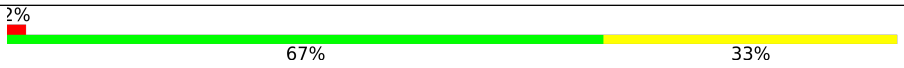
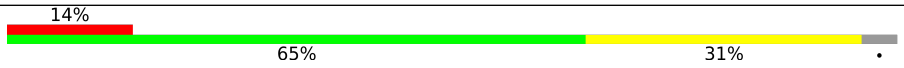
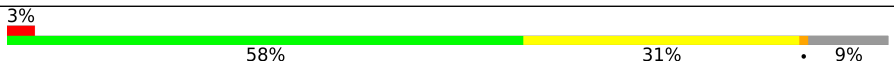
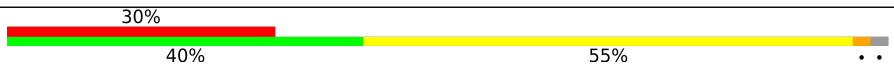
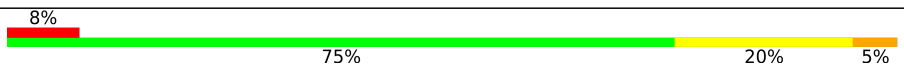
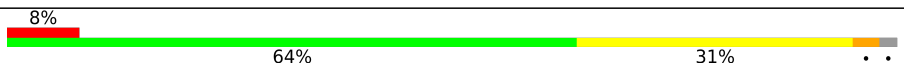
Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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	PEE	N	3008	-	X	-	-
12	UNL	C	2046	-	-	-	X
17	BOG	D	2091	-	-	-	X
17	BOG	P	2010	-	-	-	X
17	BOG	Q	3091	-	-	-	X
20	FES	R	501	-	-	X	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 32691 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 MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

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

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

- Molecule 3 is a protein called CYTOCHROME B.

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

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

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

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1512	952	262	292	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	78	Total	C	N	O	0	0	0
			654	428	116	110			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

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

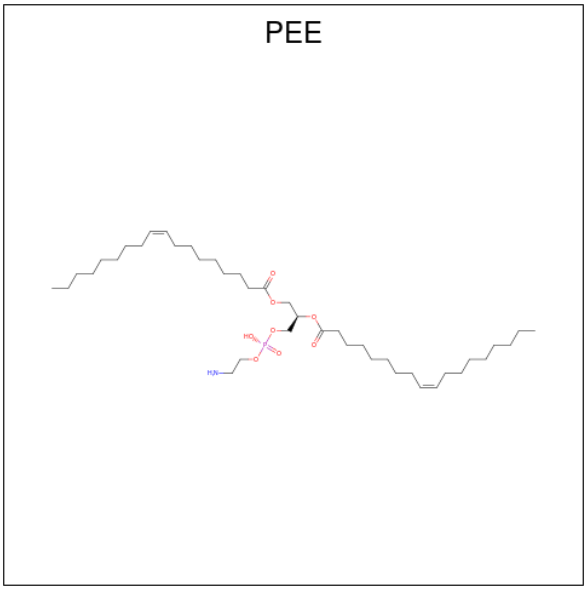
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			288	172	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			278	167	56	53	2			

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

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

- Molecule 11 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
11	A	1	Total C O P 21 12 8 1	0	0
11	C	1	Total C N O P 50 40 1 8 1	0	0
11	C	1	Total C N O P 48 38 1 8 1	0	0
11	N	1	Total O P 5 4 1	0	0
11	P	1	Total C N O P 50 40 1 8 1	0	0
11	P	1	Total C N O P 48 38 1 8 1	0	0

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total O 1 1	0	0

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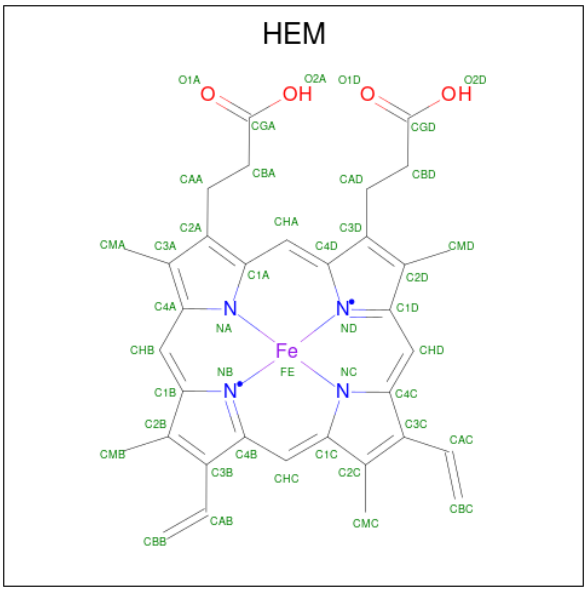
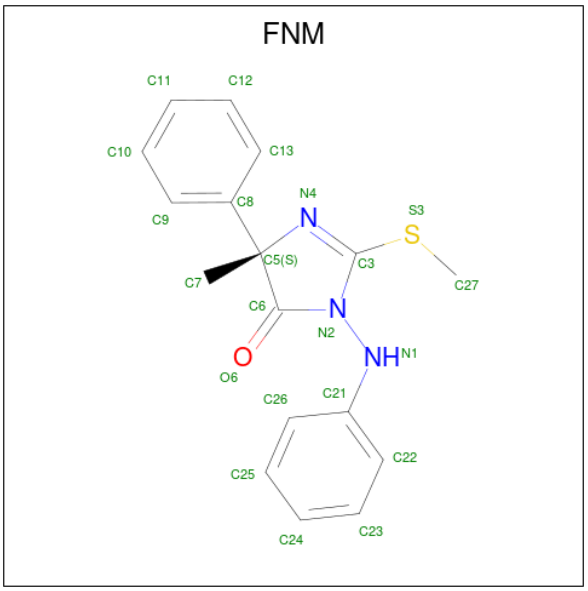
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	3	Total O 5 5	0	0
12	D	1	Total O 2 2	0	0
12	P	5	Total O 7 7	0	0
12	R	1	Total O 1 1	0	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



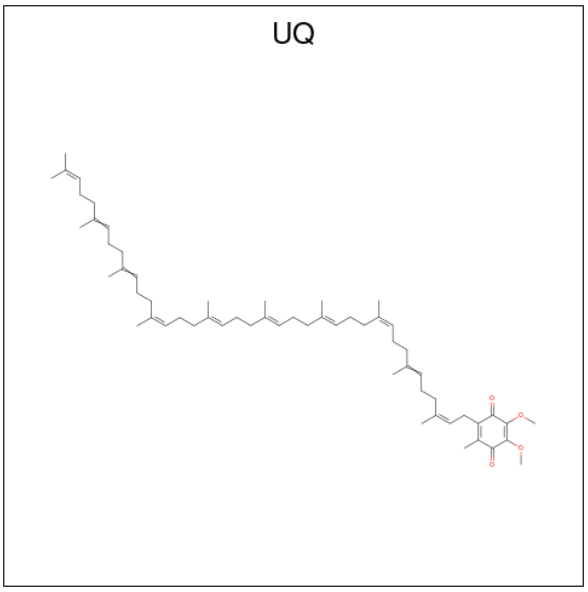
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 14 is (5S)-5-methyl-2-(methylsulfanyl)-5-phenyl-3-(phenylamino)-3,5-dihydro-4H-imidazol-4-one (three-letter code: FNM) (formula: $C_{17}H_{17}N_3OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	S	0	0
			22	17	3	1	1		
14	P	1	Total	C	N	O	S	0	0
			22	17	3	1	1		

- Molecule 15 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
15	C	1	Total	C	O		0	0
			19	15	4			

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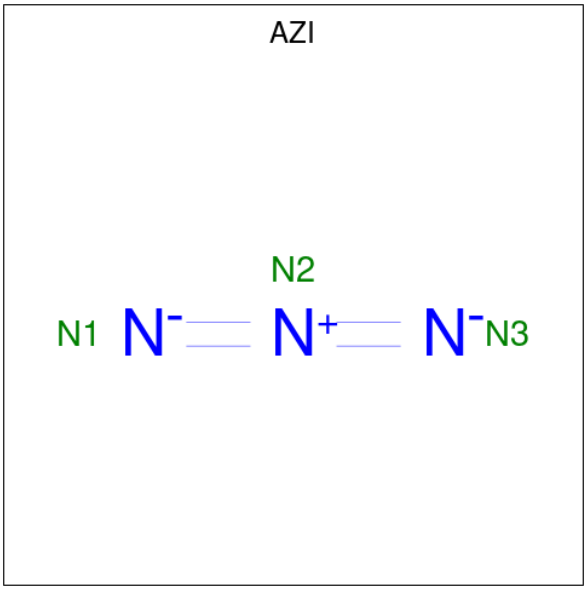
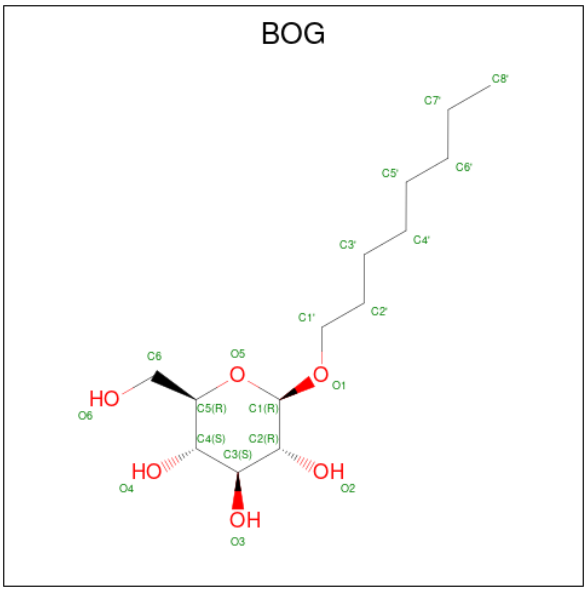
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	P	1	Total C O 19 15 4	0	0

- Molecule 16 is AZIDE ION (three-letter code: AZI) (formula: N_3).



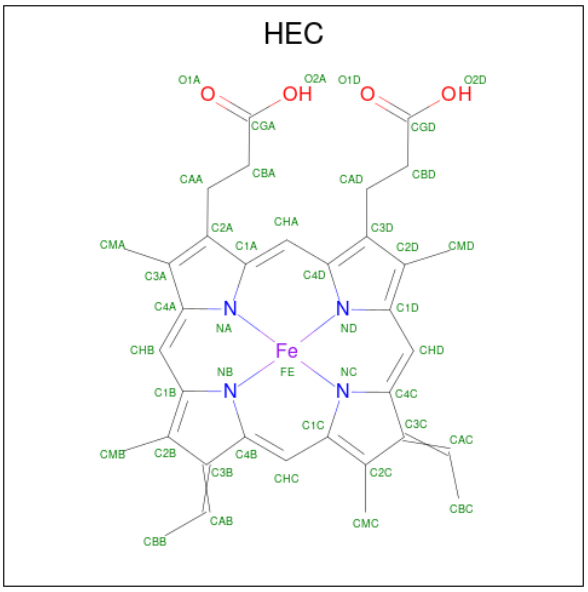
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total N 3 3	0	0
16	P	1	Total N 3 3	0	0

- Molecule 17 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



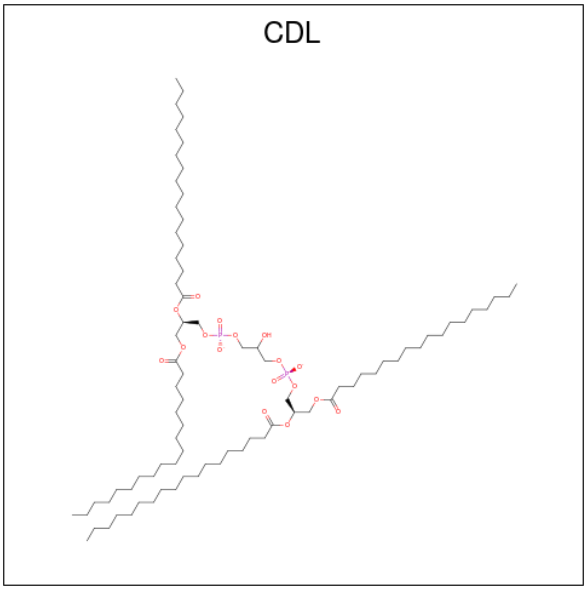
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total C O 12 10 2	0	0
17	D	1	Total C O 20 14 6	0	0
17	D	1	Total C O 20 14 6	0	0
17	P	1	Total C O 19 13 6	0	0
17	Q	1	Total C O 20 14 6	0	0
17	Q	1	Total C O 20 14 6	0	0

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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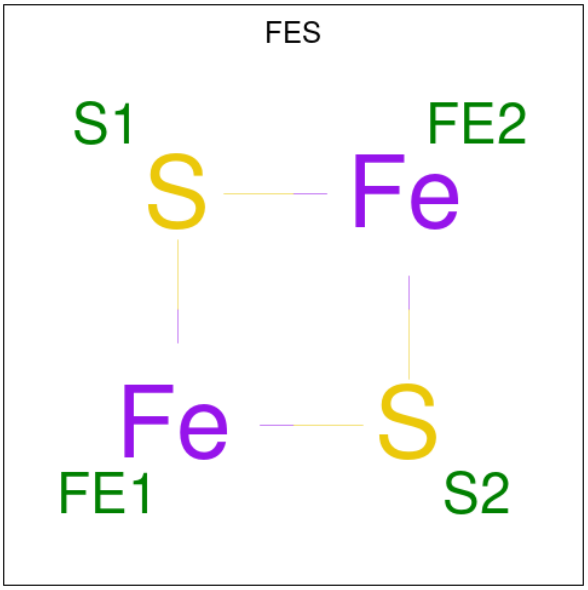
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	Q	1	Total C O P 42 23 17 2	0	0
19	T	1	Total C O P 40 21 17 2	0	0

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 21 is water.

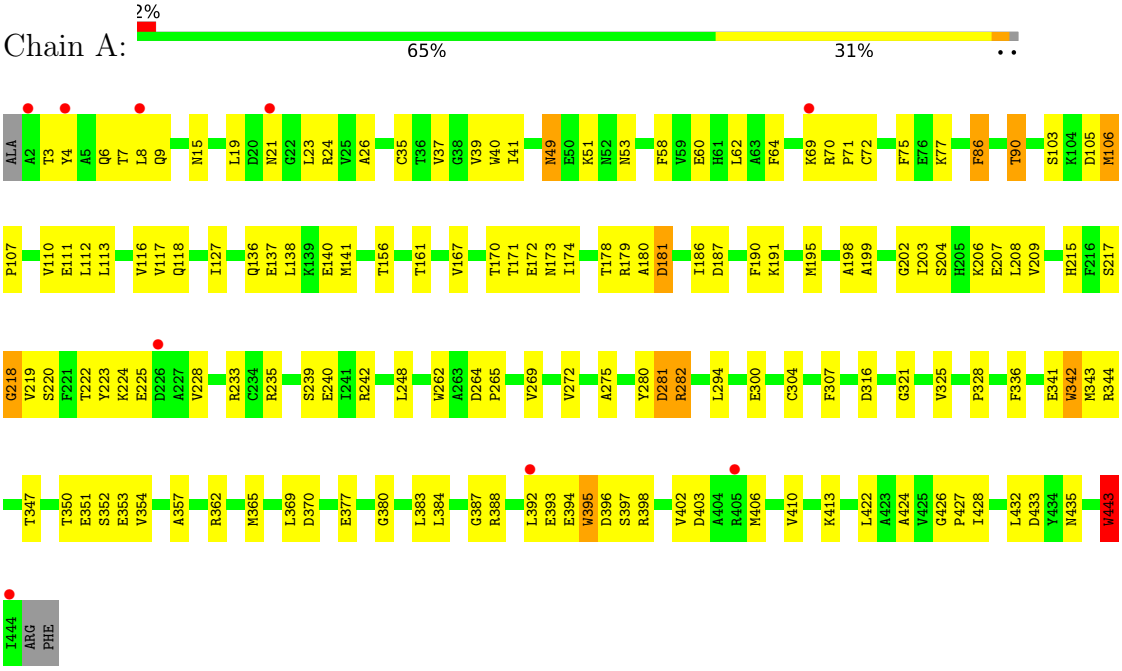
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	2	Total O 2 2	0	0
21	C	9	Total O 9 9	0	0
21	E	3	Total O 3 3	0	0
21	P	10	Total O 10 10	0	0
21	R	4	Total O 4 4	0	0

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.

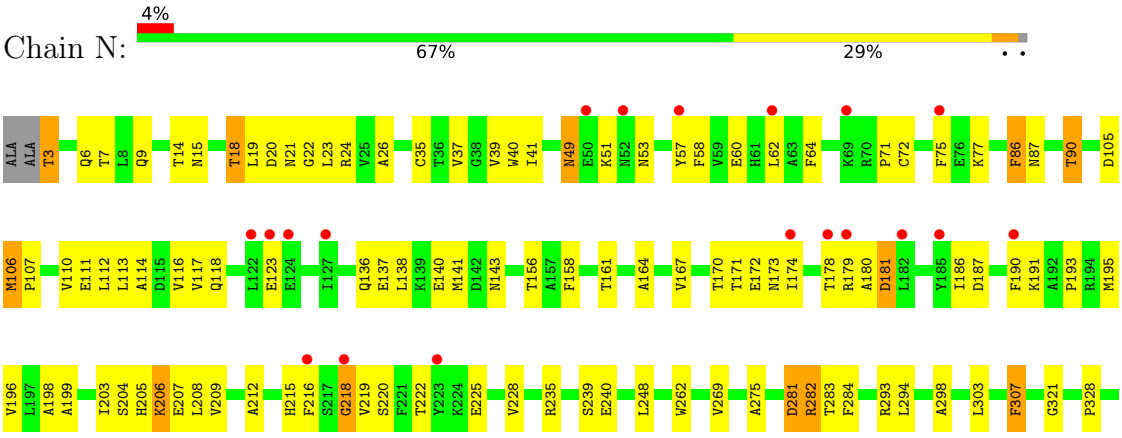
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

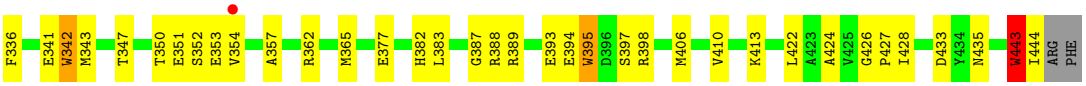
Chain A:



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

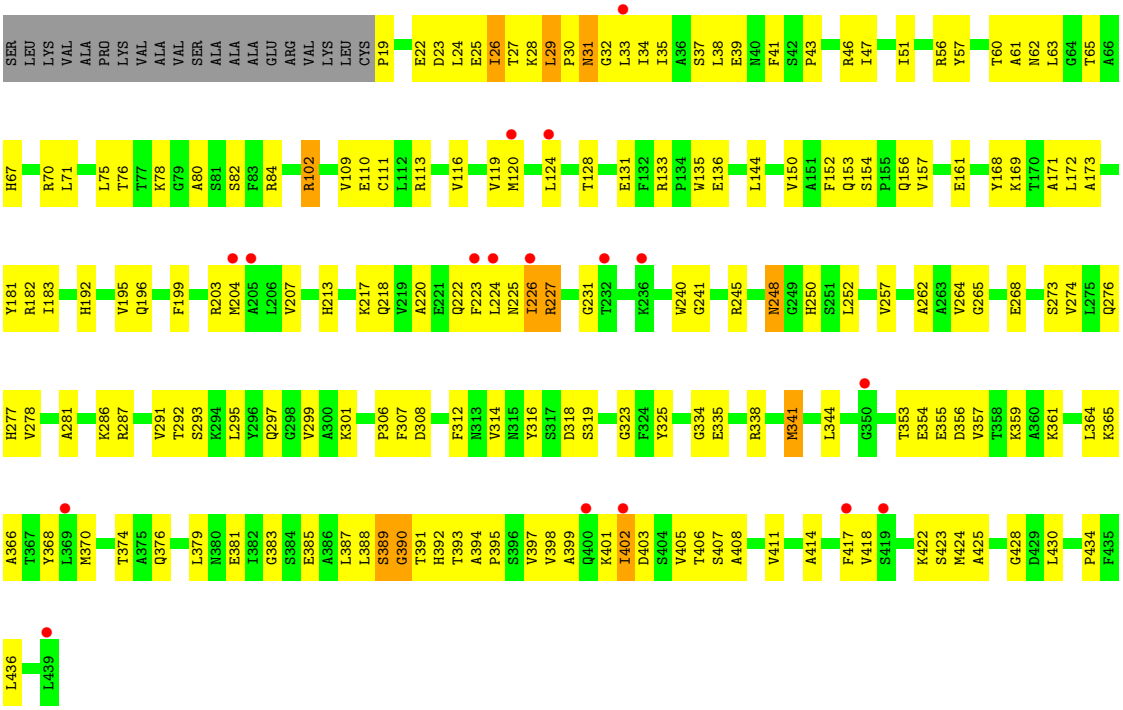
Chain N:





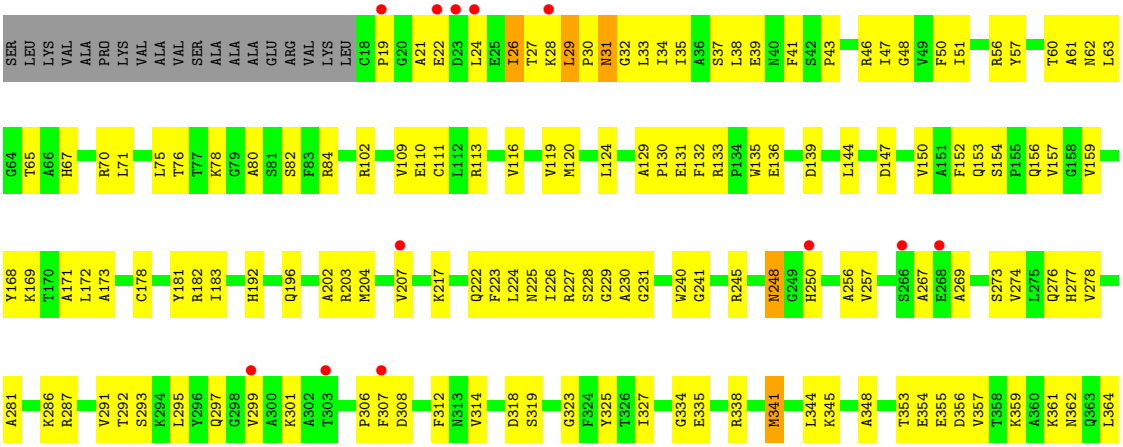
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

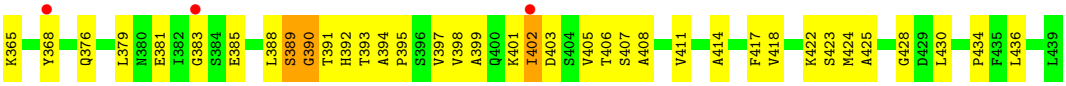
Chain B:



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

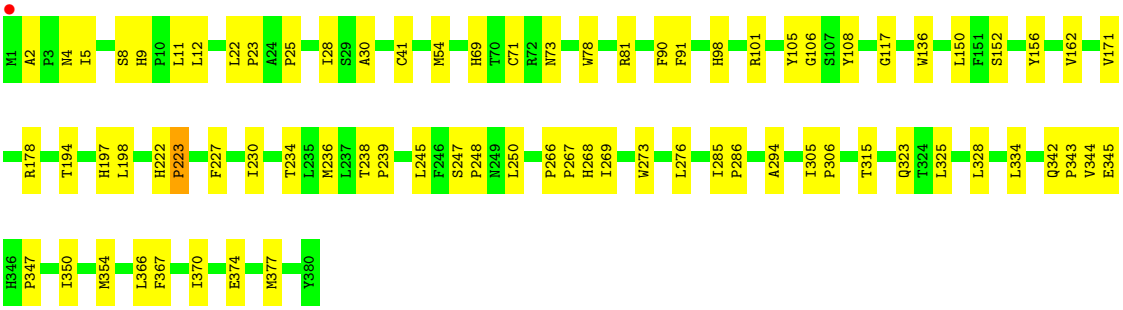
Chain O:





• Molecule 3: CYTOCHROME B

Chain C:

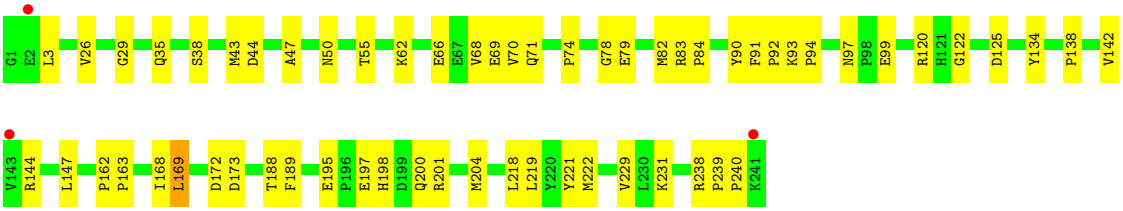


• Molecule 3: CYTOCHROME B

Chain P:

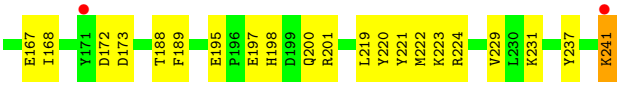
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:

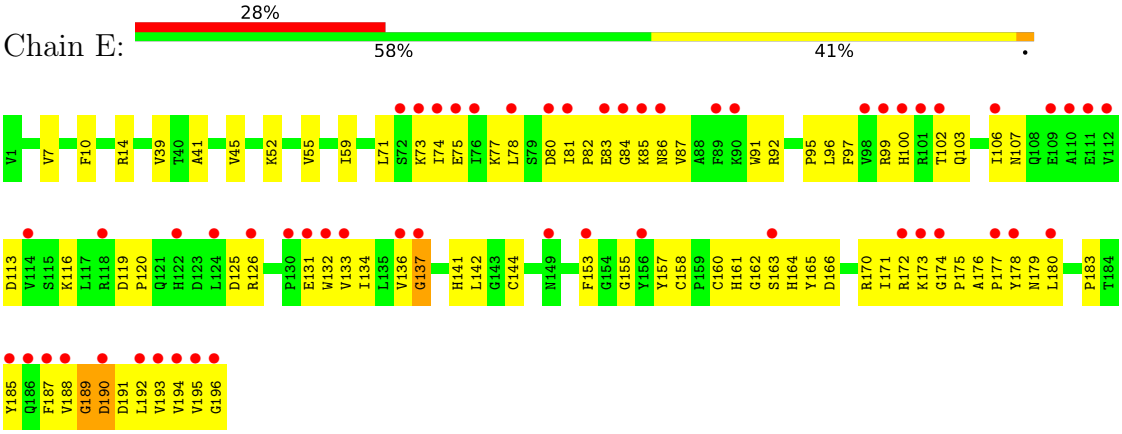


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

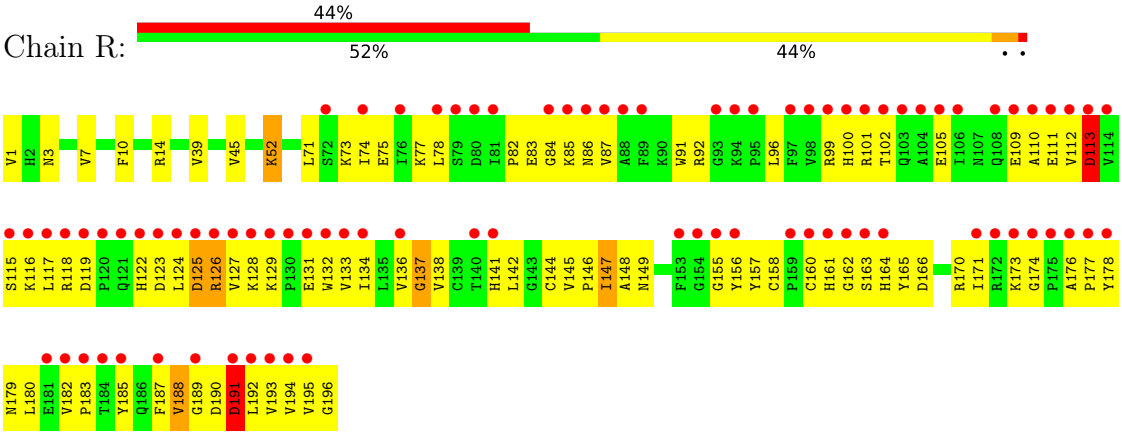
Chain Q:



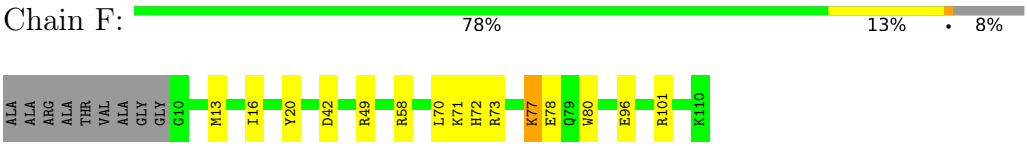
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



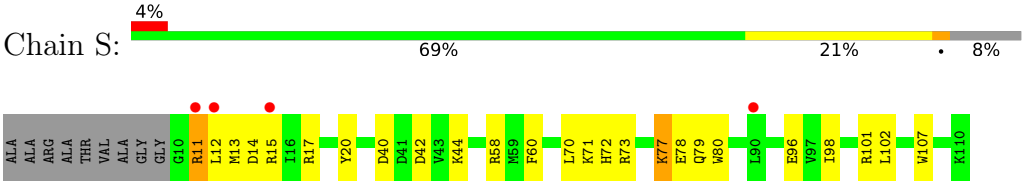
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



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

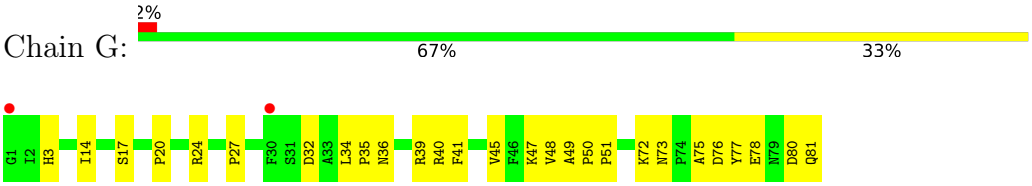


• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



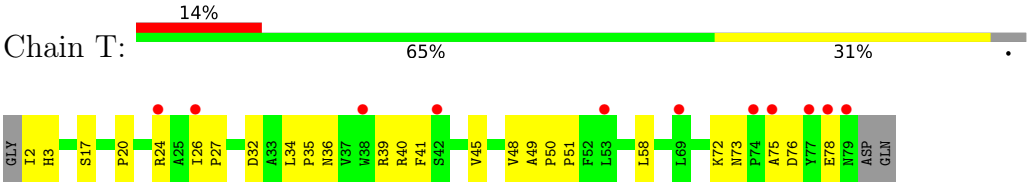
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G:



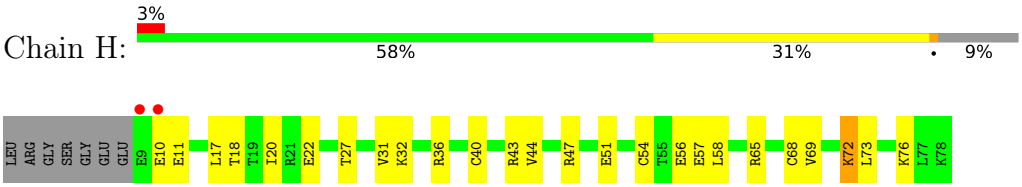
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T:



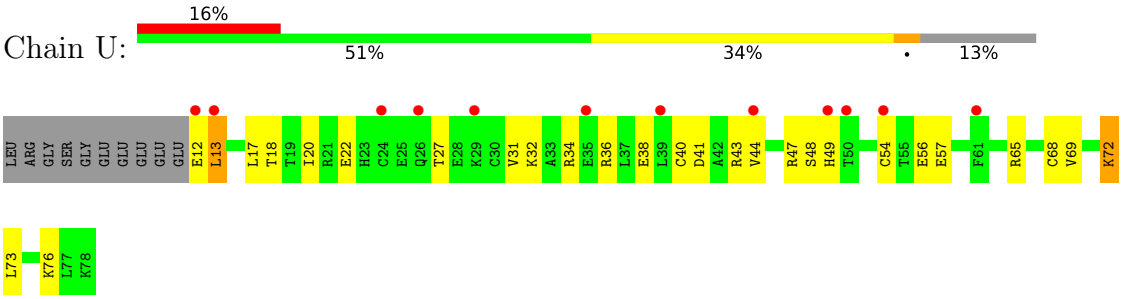
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H:



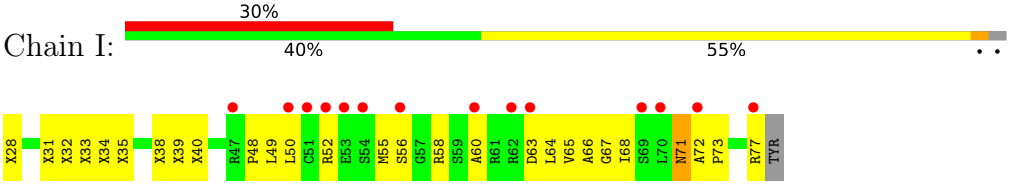
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:



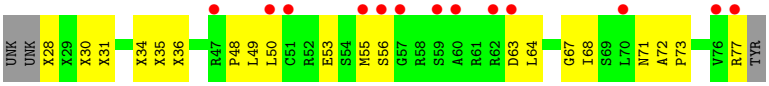
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I:



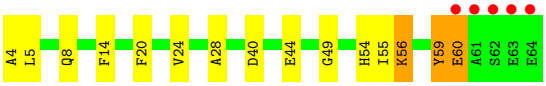
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain V:



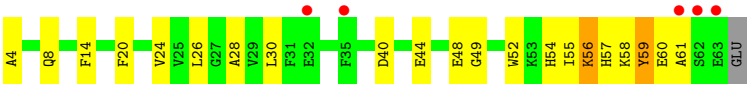
• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:



• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 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	172.28Å 182.14Å 241.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.78 – 2.79 58.78 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.6 (58.78-2.79) 97.3 (58.78-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.275 0.235 , 0.267	Depositor DCC
R_{free} test set	3613 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32691	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, UQ, CDL, FES, PEE, UNL, HEC, HEM, BOG, FNM

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	0.43	0/3511	0.63	0/4757
1	N	0.42	0/3508	0.63	0/4753
2	B	0.37	0/3196	0.60	0/4334
2	O	0.38	0/3202	0.62	1/4343 (0.0%)
3	C	0.52	0/3119	0.65	0/4270
3	P	0.46	0/3114	0.63	0/4263
4	D	0.47	0/1956	0.63	0/2658
4	Q	0.39	0/1956	0.60	0/2658
5	E	0.37	0/1547	0.59	0/2103
5	R	0.35	0/1545	0.57	0/2098
6	F	0.51	0/911	0.65	0/1219
6	S	0.42	0/911	0.61	0/1219
7	G	0.49	0/698	0.66	0/946
7	T	0.44	0/676	0.65	0/918
8	H	0.43	0/582	0.59	0/779
8	U	0.31	0/561	0.55	0/751
9	I	0.36	0/218	0.61	0/293
9	V	0.36	0/218	0.58	0/293
10	J	0.43	0/508	0.59	0/682
10	W	0.42	0/490	0.57	0/660
All	All	0.43	0/32427	0.62	1/43997 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	227	ARG	N-CA-C	5.48	125.81	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	3440	0	3353	135	0
1	N	3437	0	3349	137	0
2	B	3141	0	3142	187	0
2	O	3147	0	3146	178	0
3	C	3017	0	3063	69	0
3	P	3012	0	3058	60	0
4	D	1898	0	1846	48	0
4	Q	1898	0	1846	47	0
5	E	1513	0	1478	67	0
5	R	1512	0	1476	95	0
6	F	891	0	893	15	0
6	S	891	0	893	22	0
7	G	676	0	659	26	0
7	T	654	0	641	24	0
8	H	574	0	548	17	0
8	U	553	0	535	23	0
9	I	288	0	254	42	0
9	V	278	0	252	31	0
10	J	497	0	490	11	0
10	W	479	0	478	14	0
11	A	21	0	13	1	0
11	C	98	0	147	0	0
11	N	5	0	0	0	0
11	P	98	0	147	1	0
12	A	1	0	0	0	0
12	C	5	0	0	0	0
12	D	2	0	0	0	0
12	P	7	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	5	0
13	P	86	0	60	5	0
14	C	22	0	17	2	0
14	P	22	0	17	1	0
15	C	19	0	17	4	0
15	P	19	0	17	3	0
16	C	3	0	0	0	0
16	P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	12	0	18	0	0
17	D	40	0	56	2	0
17	P	19	0	24	1	0
17	Q	40	0	56	1	0
18	D	43	0	30	3	0
18	Q	43	0	30	1	0
19	D	42	0	28	2	0
19	G	40	0	24	1	0
19	Q	42	0	28	3	0
19	T	40	0	24	1	0
20	E	4	0	0	1	0
20	R	4	0	0	2	0
21	A	2	0	0	0	0
21	C	9	0	0	1	0
21	E	3	0	0	0	0
21	P	10	0	0	1	0
21	R	4	0	0	0	0
All	All	32691	0	32213	1132	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 17.

All (1132) 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:353:THR:HG22	2:O:355:GLU:H	1.16	1.11
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.33	1.07
2:B:353:THR:HG22	2:B:355:GLU:H	1.20	1.06
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.38	1.03
1:N:178:THR:HG22	1:N:180:ALA:H	1.22	1.02
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.62	1.00
1:A:343:MET:O	1:A:347:THR:HG22	1.62	1.00
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.24	0.99
1:N:343:MET:O	1:N:347:THR:HG22	1.63	0.98
2:B:76:THR:HG22	2:B:82:SER:H	1.25	0.97
4:D:47:ALA:H	4:D:50:ASN:HD22	1.11	0.95
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.47	0.95
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.49	0.94
1:N:206:LYS:H	1:N:206:LYS:HD2	1.32	0.94
1:A:344:ARG:NH1	1:A:344:ARG:HB2	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.49	0.93
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.49	0.91
1:N:206:LYS:H	1:N:206:LYS:CD	1.84	0.91
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.56	0.88
1:A:178:THR:HB	1:A:181:ASP:OD1	1.74	0.87
9:I:71:ASN:HD22	9:I:71:ASN:H	1.19	0.87
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.55	0.87
1:N:178:THR:HB	1:N:181:ASP:OD1	1.75	0.85
2:B:27:THR:HG22	2:B:28:LYS:H	1.39	0.85
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.74	0.85
9:I:32:UNK:N	9:I:73:PRO:HG2	1.93	0.83
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.44	0.83
9:I:64:LEU:HD12	9:I:77:ARG:O	1.78	0.83
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.59	0.83
1:N:282:ARG:HH21	9:V:36:UNK:CB	1.91	0.82
4:D:47:ALA:H	4:D:50:ASN:ND2	1.76	0.82
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.62	0.82
5:R:101:ARG:HH22	5:R:127:VAL:HG11	1.45	0.81
2:O:76:THR:HG22	2:O:82:SER:H	1.43	0.81
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.44	0.81
5:E:134:ILE:HB	5:E:185:TYR:CE2	2.15	0.81
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.61	0.81
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.45	0.80
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.64	0.80
1:N:22:GLY:O	1:N:193:PRO:HA	1.82	0.80
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.64	0.80
5:R:188:VAL:HG11	5:R:192:LEU:HD12	1.62	0.80
1:N:205:HIS:HB3	1:N:206:LYS:NZ	1.97	0.80
2:B:153:GLN:HE22	9:I:34:UNK:CG	1.95	0.79
9:I:71:ASN:HD22	9:I:71:ASN:N	1.79	0.79
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.45	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.46	0.79
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.63	0.78
2:B:153:GLN:HE22	9:I:34:UNK:HG2	1.48	0.78
1:A:281:ASP:CG	9:I:33:UNK:HB1	2.03	0.78
2:O:192:HIS:O	2:O:196:GLN:HG3	1.83	0.78
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.64	0.77
2:O:62:ASN:O	2:O:65:THR:HG22	1.83	0.77
2:B:22:GLU:HG2	2:B:39:GLU:HB3	1.66	0.77
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.02	0.76
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.66	0.76
1:N:49:ASN:HD22	1:N:51:LYS:H	1.32	0.76
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.66	0.76
1:N:362:ARG:O	1:N:365:MET:HG2	1.86	0.75
3:P:238:THR:HB	3:P:239:PRO:HD3	1.69	0.75
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.53	0.74
10:W:40:ASP:O	10:W:44:GLU:HG3	1.87	0.74
3:C:30:ALA:HB1	19:D:2003:CDL:H111	1.69	0.74
2:B:27:THR:HG22	2:B:28:LYS:N	2.01	0.74
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.01	0.74
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.23	0.73
2:B:47:ILE:HD13	2:B:120:MET:CE	2.18	0.73
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.73
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.06	0.73
2:B:76:THR:HG22	2:B:82:SER:N	2.03	0.73
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.18	0.73
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.18	0.73
3:P:247:SER:OG	3:P:250:LEU:HB2	1.89	0.72
2:B:227:ARG:HA	2:B:227:ARG:NE	2.04	0.72
1:A:362:ARG:O	1:A:365:MET:HG2	1.89	0.72
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.04	0.72
1:N:49:ASN:ND2	1:N:51:LYS:H	1.86	0.72
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.71	0.72
7:T:73:ASN:HB3	7:T:76:ASP:OD2	1.89	0.71
2:O:76:THR:HG22	2:O:82:SER:HB2	1.72	0.71
1:A:49:ASN:HD22	1:A:51:LYS:H	1.38	0.71
3:C:238:THR:HB	3:C:239:PRO:HD3	1.73	0.71
8:U:47:ARG:HD3	8:U:48:SER:H	1.54	0.71
2:O:297:GLN:O	2:O:301:LYS:HG3	1.91	0.71
3:P:9:HIS:HD2	3:P:12:LEU:H	1.37	0.71
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.31	0.71
10:J:40:ASP:O	10:J:44:GLU:HG3	1.90	0.70
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.26	0.70
1:A:178:THR:HG22	1:A:180:ALA:N	2.03	0.70
2:O:376:GLN:HE22	9:V:77:ARG:NH2	1.89	0.70
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.55	0.70
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.22	0.70
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.91	0.70
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.73	0.70
3:C:328:LEU:HD23	7:G:51:PRO:HB3	1.72	0.70
2:O:47:ILE:HD13	2:O:120:MET:CE	2.21	0.69
2:O:248:ASN:HD22	2:O:248:ASN:C	1.95	0.69
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.73	0.69
3:C:269:ILE:HD12	5:R:160:CYS:SG	2.33	0.69
3:P:30:ALA:HB1	19:Q:3003:CDL:H111	1.75	0.69
5:R:101:ARG:HG2	5:R:105:GLU:OE1	1.93	0.69
2:B:248:ASN:C	2:B:248:ASN:HD22	1.96	0.69
7:G:73:ASN:HB3	7:G:76:ASP:OD2	1.92	0.69
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.58	0.69
2:B:153:GLN:NE2	9:I:34:UNK:HG1	2.09	0.68
8:U:27:THR:O	8:U:31:VAL:HG23	1.93	0.68
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.58	0.68
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.34	0.68
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.58	0.68
1:N:187:ASP:O	1:N:191:LYS:HE3	1.94	0.68
3:C:9:HIS:HD2	3:C:12:LEU:H	1.41	0.68
3:P:101:ARG:C	3:P:101:ARG:HD2	2.14	0.68
2:B:192:HIS:O	2:B:196:GLN:HG3	1.94	0.67
2:O:27:THR:HG22	2:O:28:LYS:N	2.07	0.67
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.56	0.67
2:B:297:GLN:O	2:B:301:LYS:HG3	1.93	0.67
8:U:47:ARG:HG3	8:U:49:HIS:H	1.59	0.67
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.75	0.67
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.77	0.67
1:N:178:THR:HG22	1:N:180:ALA:N	2.03	0.67
2:B:156:GLN:HE22	9:I:77:ARG:C	1.98	0.67
1:A:350:THR:HG22	1:A:352:SER:H	1.59	0.67
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.59	0.67
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.10	0.67
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.77	0.66
5:R:129:LYS:HB3	5:R:131:GLU:OE1	1.95	0.66
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.77	0.66
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.66
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.78	0.66
2:O:407:SER:O	2:O:411:VAL:HG23	1.95	0.66
2:B:264:VAL:HG23	2:B:316:TYR:C	2.16	0.66
2:O:154:SER:O	2:O:157:VAL:HG12	1.96	0.66
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.78	0.66
2:O:399:ALA:O	2:O:402:ILE:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:LEU:O	1:N:21:ASN:N	2.29	0.66
3:C:344:VAL:O	3:C:345:GLU:HG3	1.95	0.65
9:I:28:UNK:HA	9:I:72:ALA:HB2	1.77	0.65
4:Q:241:LYS:HE3	4:Q:241:LYS:HA	1.78	0.65
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.77	0.65
5:E:163:SER:OG	5:E:175:PRO:HD2	1.96	0.65
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.26	0.65
2:B:381:GLU:OE1	2:B:381:GLU:HA	1.96	0.65
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.78	0.65
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.78	0.65
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.60	0.65
9:I:31:UNK:C	9:I:73:PRO:HG2	2.27	0.65
5:R:147:ILE:HG22	5:R:148:ALA:N	2.12	0.65
5:R:10:PHE:O	5:R:14:ARG:HG3	1.96	0.64
1:A:222:THR:OG1	1:A:225:GLU:HG3	1.96	0.64
2:O:31:ASN:ND2	2:O:33:LEU:H	1.94	0.64
2:O:381:GLU:HA	2:O:381:GLU:OE1	1.97	0.64
1:N:350:THR:HG22	1:N:352:SER:H	1.61	0.64
5:R:116:LYS:HA	5:R:116:LYS:HE2	1.79	0.64
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.11	0.64
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.32	0.64
1:N:106:MET:HE1	1:N:107:PRO:HA	1.79	0.64
1:N:21:ASN:HB2	1:N:218:GLY:O	1.97	0.64
2:B:27:THR:HG21	2:B:217:LYS:HE3	1.81	0.63
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.63	0.63
1:N:222:THR:OG1	1:N:225:GLU:HG3	1.98	0.63
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.32	0.63
3:P:269:ILE:HG23	14:P:3001:FNM:H23	1.81	0.63
1:A:49:ASN:ND2	1:A:51:LYS:H	1.96	0.63
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.81	0.63
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.63
3:P:273:TRP:HA	3:P:276:LEU:HD12	1.79	0.63
1:A:350:THR:HB	1:A:353:GLU:HG3	1.81	0.63
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.80	0.63
1:N:49:ASN:HD22	1:N:49:ASN:C	2.02	0.63
1:A:77:LYS:HE3	2:B:359:LYS:NZ	2.14	0.63
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.14	0.63
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.81	0.63
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.79	0.63
9:I:71:ASN:N	9:I:71:ASN:ND2	2.40	0.63
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.80	0.62
5:R:164:HIS:HB2	5:R:173:LYS:HB3	1.80	0.62
1:A:187:ASP:O	1:A:191:LYS:HE3	1.98	0.62
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.00	0.62
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.00	0.62
2:B:389:SER:O	2:B:391:THR:HG23	1.99	0.62
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.64	0.62
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.40	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.34	0.62
5:R:142:LEU:HD12	5:R:161:HIS:CE1	2.35	0.62
7:T:41:PHE:O	7:T:45:VAL:HG23	1.99	0.62
5:R:190:ASP:O	5:R:191:ASP:HB2	2.00	0.62
2:B:31:ASN:ND2	2:B:33:LEU:H	1.98	0.62
1:N:205:HIS:HB3	1:N:206:LYS:HZ1	1.65	0.62
2:B:113:ARG:O	2:B:116:VAL:HG23	2.00	0.61
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.65	0.61
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.81	0.61
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.30	0.61
5:E:171:ILE:HG12	5:E:176:ALA:O	2.00	0.61
7:G:41:PHE:O	7:G:45:VAL:HG23	2.00	0.61
1:N:77:LYS:HE3	2:O:359:LYS:NZ	2.15	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.36	0.61
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.63	0.61
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.66	0.61
5:R:82:PRO:HD2	5:R:85:LYS:CD	2.30	0.61
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.00	0.61
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.35	0.61
2:O:388:LEU:O	2:O:389:SER:HB3	1.99	0.61
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.82	0.61
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.61
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.35	0.61
8:H:27:THR:O	8:H:31:VAL:HG23	2.01	0.60
3:P:347:PRO:O	3:P:350:ILE:HG22	2.01	0.60
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.16	0.60
8:H:40:CYS:O	8:H:44:VAL:HG23	2.02	0.60
9:V:34:UNK:N	9:V:35:UNK:N	2.48	0.60
2:B:38:LEU:HD12	2:B:39:GLU:N	2.17	0.60
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.24	0.60
4:D:47:ALA:N	4:D:50:ASN:HD22	1.92	0.60
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.81	0.60
5:R:188:VAL:HB	5:R:192:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LEU:O	2:B:389:SER:HB3	2.02	0.60
1:A:7:THR:HG21	2:B:113:ARG:CD	2.31	0.60
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.32	0.60
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.82	0.60
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.84	0.60
2:O:124:LEU:HD21	2:O:223:PHE:HB3	1.82	0.60
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.83	0.59
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.84	0.59
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.85	0.59
1:A:106:MET:HE1	1:A:107:PRO:HA	1.85	0.59
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.70	0.59
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.83	0.59
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.44	0.59
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.68	0.59
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.17	0.59
2:B:399:ALA:O	2:B:402:ILE:HG22	2.03	0.59
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.38	0.59
4:Q:241:LYS:OXT	4:Q:241:LYS:HG3	2.03	0.59
2:B:226:ILE:O	2:B:226:ILE:HG23	2.02	0.59
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.38	0.59
9:V:31:UNK:C	9:V:73:PRO:HG2	2.32	0.59
2:O:38:LEU:HD12	2:O:39:GLU:N	2.17	0.59
2:O:353:THR:HG22	2:O:354:GLU:N	2.18	0.59
1:A:170:THR:HG22	1:A:171:THR:N	2.18	0.59
2:O:335:GLU:HA	2:O:338:ARG:HH12	1.68	0.59
2:O:385:GLU:OE1	2:O:392:HIS:HA	2.02	0.59
3:C:269:ILE:HG23	14:C:2001:FNM:H23	1.83	0.59
2:O:306:PRO:HG2	9:V:50:LEU:O	2.03	0.59
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.91	0.58
2:B:43:PRO:O	2:B:113:ARG:HG3	2.03	0.58
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.85	0.58
1:N:350:THR:HB	1:N:353:GLU:HG3	1.85	0.58
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.85	0.58
3:C:41:CYS:SG	3:C:90:PHE:CD2	2.96	0.58
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.33	0.58
2:O:353:THR:HG22	2:O:355:GLU:N	2.01	0.58
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.44	0.58
5:E:160:CYS:SG	3:P:269:ILE:HD12	2.44	0.58
7:G:72:LYS:HG2	8:H:56:GLU:OE2	2.03	0.58
1:N:205:HIS:HB3	1:N:206:LYS:HZ2	1.68	0.58
3:P:328:LEU:HD23	7:T:51:PRO:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:30:UNK:HG3	9:V:31:UNK:N	2.18	0.58
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.34	0.58
5:R:122:HIS:O	5:R:125:ASP:HB2	2.04	0.58
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.85	0.58
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.86	0.58
2:O:402:ILE:C	2:O:402:ILE:HD13	2.24	0.58
4:D:200:GLN:NE2	17:D:2091:BOG:H5	2.19	0.58
1:N:383:LEU:O	1:N:387:GLY:HA2	2.03	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.39	0.58
5:R:82:PRO:HD2	5:R:85:LYS:HD2	1.86	0.58
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.03	0.57
5:E:77:LYS:HE2	5:E:80:ASP:OD2	2.04	0.57
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.37	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.33	0.57
10:W:55:ILE:CG2	10:W:59:TYR:HE1	2.16	0.57
2:B:353:THR:HG22	2:B:354:GLU:N	2.18	0.57
10:J:55:ILE:CG2	10:J:59:TYR:HE1	2.17	0.57
7:T:72:LYS:HG2	8:U:56:GLU:CD	2.24	0.57
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.37	0.57
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.86	0.57
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.28	0.57
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.39	0.57
6:S:11:ARG:O	6:S:15:ARG:HG3	2.05	0.57
3:C:245:LEU:O	4:D:201:ARG:HD2	2.04	0.57
5:E:103:GLN:O	5:E:107:ASN:ND2	2.37	0.57
1:N:206:LYS:HD2	1:N:206:LYS:N	2.13	0.57
2:B:292:THR:HG22	2:B:292:THR:O	2.05	0.57
2:O:338:ARG:HB2	2:O:338:ARG:HH11	1.70	0.57
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.87	0.57
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.18	0.57
2:B:414:ALA:O	2:B:418:VAL:HG23	2.05	0.57
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.87	0.57
2:B:407:SER:O	2:B:411:VAL:HG23	2.05	0.57
3:C:247:SER:OG	3:C:250:LEU:HB2	2.05	0.57
1:A:49:ASN:HD22	1:A:49:ASN:C	2.08	0.56
2:B:385:GLU:OE1	2:B:392:HIS:HA	2.04	0.56
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.87	0.56
10:W:4:ALA:O	10:W:8:GLN:HG3	2.05	0.56
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.87	0.56
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:THR:HG21	1:N:235:ARG:H	1.70	0.56
1:A:219:VAL:HG12	1:A:220:SER:N	2.20	0.56
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.70	0.56
2:B:402:ILE:HD13	2:B:402:ILE:C	2.26	0.56
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.45	0.56
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.32	0.56
5:R:126:ARG:HB3	5:R:182:VAL:HG21	1.88	0.56
1:A:15:ASN:O	1:A:26:ALA:HA	2.05	0.56
2:O:389:SER:O	2:O:391:THR:HG23	2.05	0.56
2:B:341:MET:CE	2:B:417:PHE:HE2	2.17	0.56
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.88	0.56
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.87	0.56
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.41	0.56
2:O:414:ALA:O	2:O:418:VAL:HG23	2.06	0.56
2:B:76:THR:HG22	2:B:82:SER:HB2	1.88	0.56
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.87	0.56
1:N:347:THR:HG21	1:N:444:ILE:C	2.26	0.56
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.40	0.56
1:N:170:THR:HG22	1:N:171:THR:N	2.21	0.56
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.71	0.56
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.87	0.55
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	1.88	0.55
19:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.39	0.55
2:O:308:ASP:OD2	9:V:56:SER:HA	2.05	0.55
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.88	0.55
1:A:350:THR:HG22	1:A:351:GLU:N	2.21	0.55
2:B:27:THR:CG2	2:B:28:LYS:H	2.14	0.55
2:B:338:ARG:HH11	2:B:338:ARG:HB2	1.72	0.55
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.89	0.55
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.54	0.55
2:O:341:MET:CE	2:O:417:PHE:HE2	2.17	0.55
7:T:48:VAL:O	7:T:51:PRO:HD2	2.05	0.55
2:B:124:LEU:HD21	2:B:223:PHE:HB3	1.88	0.55
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.42	0.55
9:I:38:UNK:O	9:I:39:UNK:C	2.55	0.55
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.72	0.55
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.41	0.55
5:E:85:LYS:HG2	5:E:86:ASN:N	2.22	0.55
5:R:52:LYS:HD3	5:R:52:LYS:C	2.27	0.55
5:R:131:GLU:CD	5:R:131:GLU:H	2.10	0.55
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:501:HEC:HMC1	18:D:501:HEC:HBC3	1.89	0.55
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.42	0.55
3:P:270:LYS:O	3:P:270:LYS:HG3	2.07	0.55
5:R:74:ILE:HD11	5:R:96:LEU:HD23	1.88	0.55
5:R:85:LYS:HG2	5:R:86:ASN:N	2.21	0.55
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.89	0.55
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.71	0.55
1:N:15:ASN:O	1:N:26:ALA:HA	2.07	0.55
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.37	0.55
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.88	0.55
1:A:4:TYR:HE2	1:A:396:ASP:OD2	1.90	0.55
3:C:101:ARG:HD2	3:C:101:ARG:C	2.26	0.55
1:N:106:MET:HE2	1:N:110:VAL:CG2	2.36	0.55
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.42	0.55
2:O:150:VAL:O	2:O:153:GLN:HG3	2.07	0.55
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.42	0.55
1:N:350:THR:HG22	1:N:351:GLU:N	2.22	0.55
5:R:128:LYS:O	5:R:129:LYS:HG3	2.07	0.55
1:A:106:MET:N	1:A:107:PRO:HD2	2.22	0.54
7:G:48:VAL:O	7:G:51:PRO:HD2	2.07	0.54
1:N:398:ARG:HH11	1:N:398:ARG:HG2	1.72	0.54
5:R:126:ARG:H	5:R:126:ARG:HD3	1.72	0.54
2:B:368:TYR:HE1	2:B:381:GLU:OE2	1.90	0.54
1:N:191:LYS:C	1:N:195:MET:HE2	2.28	0.54
5:R:137:GLY:O	5:R:145:VAL:HG22	2.07	0.54
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.08	0.54
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.43	0.54
2:O:292:THR:HG22	2:O:292:THR:O	2.08	0.54
2:O:368:TYR:HE1	2:O:381:GLU:OE2	1.91	0.54
5:R:122:HIS:HB3	5:R:125:ASP:OD1	2.08	0.54
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.89	0.54
5:E:119:ASP:OD2	5:E:179:ASN:ND2	2.40	0.54
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.23	0.54
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.90	0.54
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.37	0.54
9:I:71:ASN:H	9:I:71:ASN:ND2	1.94	0.54
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.22	0.54
2:B:335:GLU:HA	2:B:338:ARG:HH12	1.72	0.54
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.89	0.54
8:U:47:ARG:CD	8:U:48:SER:H	2.21	0.54
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.36	0.54
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.43	0.54
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.37	0.54
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.54
1:A:239:SER:HB2	7:G:17:SER:O	2.08	0.54
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.38	0.54
5:E:177:PRO:HB2	5:E:178:TYR:CD1	2.43	0.54
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.54	0.54
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.73	0.54
4:Q:195:GLU:HG3	4:Q:198:HIS:HB2	1.89	0.54
2:B:150:VAL:O	2:B:153:GLN:HG3	2.08	0.54
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.28	0.54
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.43	0.53
2:B:156:GLN:NE2	9:I:77:ARG:C	2.60	0.53
2:B:227:ARG:HA	2:B:227:ARG:HE	1.72	0.53
1:N:106:MET:N	1:N:107:PRO:HD2	2.23	0.53
3:P:9:HIS:CD2	3:P:11:LEU:H	2.26	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.42	0.53
5:R:115:SER:O	5:R:116:LYS:HG2	2.08	0.53
3:C:78:TRP:CD2	4:D:197:GLU:HG3	2.44	0.53
2:O:248:ASN:ND2	2:O:250:HIS:H	2.06	0.53
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.89	0.53
5:E:165:TYR:HA	5:E:170:ARG:O	2.08	0.53
5:R:134:ILE:HD11	5:R:193:VAL:HG21	1.89	0.53
2:B:46:ARG:HH11	2:B:110:GLU:HG3	1.73	0.53
1:N:53:ASN:H	1:N:173:ASN:ND2	2.07	0.53
8:U:12:GLU:O	8:U:13:LEU:HB2	2.08	0.53
1:N:90:THR:O	1:N:167:VAL:HG11	2.09	0.53
1:N:106:MET:HE2	1:N:110:VAL:HG23	1.89	0.53
2:O:46:ARG:HH11	2:O:110:GLU:HG3	1.72	0.53
3:P:198:LEU:HD13	15:P:3002:UQ:HM53	1.91	0.53
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.91	0.53
2:O:76:THR:HG22	2:O:82:SER:CB	2.38	0.53
2:O:353:THR:HB	2:O:356:ASP:CG	2.29	0.53
3:C:273:TRP:HA	3:C:276:LEU:HD12	1.90	0.53
19:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.42	0.53
8:U:40:CYS:O	8:U:44:VAL:HG23	2.07	0.53
1:A:383:LEU:O	1:A:387:GLY:HA2	2.09	0.52
2:B:306:PRO:HA	9:I:52:ARG:CG	2.38	0.52
3:P:376:LYS:O	6:S:17:ARG:NH1	2.40	0.52
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HE2	1:A:110:VAL:HG23	1.90	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.73	0.52
2:B:128:THR:HG21	2:B:224:LEU:HD23	1.92	0.52
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.39	0.52
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.38	0.52
2:B:78:LYS:HA	2:B:131:GLU:OE2	2.09	0.52
8:H:65:ARG:O	8:H:69:VAL:HG23	2.10	0.52
1:N:170:THR:HG22	1:N:172:GLU:H	1.74	0.52
2:O:31:ASN:HD22	2:O:32:GLY:N	2.07	0.52
2:O:46:ARG:HD2	2:O:110:GLU:OE2	2.09	0.52
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.90	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
5:R:190:ASP:O	5:R:191:ASP:CB	2.58	0.52
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.91	0.52
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.74	0.52
3:C:347:PRO:O	3:C:350:ILE:HG22	2.09	0.52
1:N:112:LEU:O	1:N:116:VAL:HG23	2.09	0.52
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.44	0.52
11:A:2008:PEE:H13	3:C:222:HIS:HE1	1.73	0.52
3:C:150:LEU:HD23	5:R:142:LEU:HD21	1.92	0.52
5:E:113:ASP:OD1	5:E:116:LYS:HG2	2.10	0.52
9:I:49:LEU:O	9:I:50:LEU:HD23	2.10	0.52
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.44	0.52
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.17	0.52
5:E:83:GLU:HG2	5:E:102:THR:HA	1.92	0.52
9:I:64:LEU:HA	9:I:77:ARG:O	2.10	0.52
4:Q:97:ASN:OD1	4:Q:99:GLU:HB2	2.10	0.52
2:B:353:THR:HB	2:B:356:ASP:CG	2.30	0.52
2:O:203:ARG:HD2	2:O:230:ALA:O	2.10	0.52
2:O:273:SER:O	2:O:276:GLN:HB3	2.10	0.52
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.10	0.52
2:B:264:VAL:HG23	2:B:316:TYR:O	2.10	0.52
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.10	0.52
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.92	0.52
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.10	0.51
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.74	0.51
1:N:206:LYS:H	1:N:206:LYS:CE	2.23	0.51
2:O:335:GLU:HA	2:O:338:ARG:NH1	2.24	0.51
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.92	0.51
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.45	0.51
2:B:307:PHE:CD1	2:B:308:ASP:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ASP:O	2:B:319:SER:HB2	2.09	0.51
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.46	0.51
1:N:387:GLY:O	1:N:388:ARG:HB3	2.09	0.51
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.25	0.51
3:P:344:VAL:O	3:P:345:GLU:HG3	2.09	0.51
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.46	0.51
1:A:106:MET:HE2	1:A:110:VAL:CG2	2.40	0.51
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.78	0.51
3:C:9:HIS:CD2	3:C:11:LEU:H	2.28	0.51
8:H:43:ARG:O	8:H:47:ARG:HG3	2.10	0.51
1:A:344:ARG:HB2	1:A:344:ARG:CZ	2.40	0.51
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.45	0.51
8:U:65:ARG:O	8:U:68:CYS:HB3	2.09	0.51
2:B:248:ASN:ND2	2:B:250:HIS:H	2.08	0.51
5:E:74:ILE:HD11	5:E:96:LEU:HD23	1.92	0.51
1:A:106:MET:HG3	1:A:203:ILE:HG21	1.93	0.51
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.41	0.51
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.11	0.51
2:B:361:LYS:O	2:B:365:LYS:HG3	2.10	0.51
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.45	0.51
10:W:49:GLY:N	10:W:54:HIS:ND1	2.59	0.51
2:B:27:THR:CG2	2:B:28:LYS:N	2.72	0.51
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.31	0.51
5:E:133:VAL:HG13	5:E:133:VAL:O	2.11	0.51
2:O:287:ARG:HD3	9:V:53:GLU:HG2	1.92	0.51
5:R:83:GLU:HG2	5:R:102:THR:CG2	2.23	0.51
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.92	0.51
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.93	0.51
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.50	0.51
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.93	0.51
2:B:274:VAL:O	2:B:278:VAL:HG23	2.11	0.51
2:O:308:ASP:OD2	9:V:55:MET:O	2.29	0.51
2:O:422:LYS:O	2:O:436:LEU:HD21	2.11	0.51
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.11	0.51
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.93	0.50
2:B:31:ASN:HD22	2:B:32:GLY:N	2.08	0.50
1:N:206:LYS:HA	1:N:209:VAL:CG1	2.41	0.50
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.93	0.50
10:J:4:ALA:O	10:J:8:GLN:HG3	2.11	0.50
1:N:106:MET:CE	1:N:110:VAL:HG21	2.41	0.50
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:84:GLY:N	5:R:100:HIS:O	2.44	0.50
1:A:21:ASN:HB3	1:A:219:VAL:HG22	1.92	0.50
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.93	0.50
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.10	0.50
2:B:225:ASN:O	2:B:226:ILE:C	2.48	0.50
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.78	0.50
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.46	0.50
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.41	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.26	0.50
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.93	0.50
5:R:116:LYS:O	5:R:117:LEU:HD23	2.11	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.93	0.50
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.46	0.50
5:E:52:LYS:C	5:E:52:LYS:HD3	2.31	0.50
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.50
5:E:190:ASP:CG	5:E:191:ASP:H	2.15	0.50
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.46	0.50
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.93	0.50
3:P:98:HIS:CD2	13:P:502:HEM:NC	2.79	0.50
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.94	0.50
2:B:273:SER:O	2:B:276:GLN:HB3	2.11	0.50
1:A:380:GLY:O	1:A:384:LEU:HB2	2.12	0.50
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.47	0.50
2:B:308:ASP:OD2	9:I:56:SER:HA	2.11	0.50
2:O:26:ILE:HG12	2:O:26:ILE:O	2.11	0.50
3:P:377:MET:HE1	6:S:20:TYR:CD1	2.47	0.50
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.46	0.50
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.94	0.50
2:B:424:MET:HG2	2:B:425:ALA:N	2.27	0.50
1:N:209:VAL:O	1:N:212:ALA:HB3	2.11	0.50
2:O:361:LYS:O	2:O:365:LYS:HG3	2.11	0.50
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.27	0.50
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.92	0.49
1:A:23:LEU:HD23	1:A:24:ARG:N	2.26	0.49
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.93	0.49
1:N:410:VAL:O	1:N:413:LYS:HB3	2.11	0.49
2:O:225:ASN:O	2:O:226:ILE:C	2.50	0.49
2:O:307:PHE:CD1	2:O:308:ASP:N	2.80	0.49
5:R:101:ARG:HB3	5:R:105:GLU:HB2	1.93	0.49
5:R:109:GLU:C	5:R:111:GLU:H	2.15	0.49
1:N:219:VAL:HG12	1:N:220:SER:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.93	0.49
9:V:67:GLY:O	9:V:68:ILE:HD13	2.13	0.49
9:I:67:GLY:O	9:I:68:ILE:HD13	2.12	0.49
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.47	0.49
3:P:156:TYR:CD2	3:P:156:TYR:N	2.79	0.49
5:R:82:PRO:HD2	5:R:85:LYS:HD3	1.94	0.49
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.47	0.49
1:A:138:LEU:HD11	1:A:174:ILE:HD12	1.95	0.49
1:A:156:THR:HA	5:E:7:VAL:HG21	1.93	0.49
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.12	0.49
1:N:138:LEU:HD11	1:N:174:ILE:HD12	1.95	0.49
1:N:156:THR:HA	5:R:7:VAL:HG21	1.94	0.49
2:O:274:VAL:O	2:O:278:VAL:HG23	2.13	0.49
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.94	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
2:O:113:ARG:O	2:O:116:VAL:HG23	2.12	0.49
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.94	0.49
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.13	0.49
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.43	0.49
2:B:262:ALA:HB2	2:B:268:GLU:HG2	1.94	0.49
1:A:217:SER:O	1:A:218:GLY:C	2.51	0.49
1:A:281:ASP:OD1	9:I:33:UNK:HB1	2.13	0.49
2:B:102:ARG:HH22	2:B:161:GLU:HA	1.76	0.49
2:B:257:VAL:O	2:B:323:GLY:HA3	2.13	0.49
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.47	0.49
4:D:47:ALA:HA	4:D:90:TYR:HA	1.95	0.49
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.95	0.49
8:H:72:LYS:HD2	8:H:72:LYS:N	2.27	0.49
1:N:178:THR:CG2	1:N:179:ARG:N	2.75	0.49
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.78	0.49
5:R:77:LYS:HA	5:R:191:ASP:O	2.13	0.49
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.48	0.49
1:A:106:MET:CE	1:A:110:VAL:HG21	2.43	0.48
2:B:335:GLU:HA	2:B:338:ARG:NH1	2.28	0.48
2:B:389:SER:O	2:B:391:THR:N	2.46	0.48
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.94	0.48
4:D:231:LYS:O	6:F:71:LYS:HE3	2.13	0.48
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.48
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.43	0.48
10:W:14:PHE:N	10:W:14:PHE:CD2	2.80	0.48
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.94	0.48
3:P:90:PHE:CZ	3:P:236:MET:HB3	2.48	0.48
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.48	0.48
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.94	0.48
2:B:60:THR:HG23	2:B:61:ALA:N	2.29	0.48
2:B:402:ILE:HG23	2:B:403:ASP:N	2.28	0.48
3:C:41:CYS:HG	3:C:90:PHE:HD2	1.61	0.48
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.95	0.48
1:N:49:ASN:HD22	1:N:51:LYS:N	2.05	0.48
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.48
2:O:318:ASP:O	2:O:319:SER:HB2	2.13	0.48
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.94	0.48
5:R:101:ARG:HH22	5:R:127:VAL:CG1	2.19	0.48
2:B:110:GLU:O	2:B:111:CYS:HB3	2.13	0.48
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.94	0.48
1:N:49:ASN:ND2	1:N:49:ASN:C	2.66	0.48
2:O:248:ASN:HD22	2:O:250:HIS:H	1.61	0.48
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.94	0.48
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.96	0.48
1:A:75:PHE:HZ	1:A:86:PHE:HE2	1.61	0.48
3:C:54:MET:HG2	3:P:178:ARG:HA	1.95	0.48
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.96	0.48
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.78	0.48
2:B:422:LYS:O	2:B:436:LEU:HD21	2.14	0.48
1:N:26:ALA:O	1:N:198:ALA:HA	2.14	0.48
2:O:78:LYS:HA	2:O:131:GLU:OE2	2.14	0.48
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.94	0.48
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.78	0.48
1:A:351:GLU:O	1:A:354:VAL:HG22	2.13	0.48
5:E:82:PRO:HD2	5:E:85:LYS:HD3	1.95	0.48
5:E:134:ILE:HD11	5:E:193:VAL:HG21	1.96	0.48
8:H:32:LYS:O	8:H:36:ARG:HG3	2.14	0.48
1:N:206:LYS:CA	1:N:209:VAL:HG12	2.43	0.48
2:O:67:HIS:O	2:O:70:ARG:HB3	2.14	0.48
2:O:76:THR:HG22	2:O:82:SER:N	2.20	0.48
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.26	0.48
3:P:2:ALA:CB	3:P:8:SER:HB3	2.40	0.48
10:W:20:PHE:O	10:W:24:VAL:HG23	2.14	0.48
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.96	0.48
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.43	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:71:CYS:SG	3:P:81:ARG:HD2	2.54	0.48
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.14	0.48
15:P:3002:UQ:C8	15:P:3002:UQ:HM51	2.44	0.48
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.14	0.48
19:Q:3003:CDL:H511	7:T:26:ILE:HG21	1.96	0.48
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.43	0.48
3:C:323:GLN:OE1	7:G:47:LYS:HD3	2.14	0.48
15:C:2002:UQ:C8	15:C:2002:UQ:HM51	2.44	0.48
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.94	0.48
5:E:41:ALA:O	5:E:45:VAL:HG23	2.14	0.48
7:G:40:ARG:HD2	19:G:2004:CDL:OA4	2.13	0.48
1:N:394:GLU:O	1:N:397:SER:HB3	2.13	0.48
3:P:34:PHE:HB2	21:P:381:HOH:O	2.13	0.48
6:S:98:ILE:O	6:S:102:LEU:HG	2.14	0.48
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.44	0.47
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.13	0.47
2:O:156:GLN:HE22	9:V:77:ARG:C	2.17	0.47
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	1.95	0.47
9:V:28:UNK:HA	9:V:72:ALA:HB2	1.94	0.47
1:A:233:ARG:HH12	1:A:316:ASP:HB2	1.80	0.47
2:B:248:ASN:C	2:B:248:ASN:ND2	2.67	0.47
1:N:21:ASN:CB	1:N:219:VAL:HA	2.44	0.47
1:N:239:SER:HB2	7:T:17:SER:O	2.14	0.47
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.49	0.47
5:R:165:TYR:HA	5:R:170:ARG:O	2.14	0.47
1:A:136:GLN:O	1:A:140:GLU:HG3	2.13	0.47
2:B:60:THR:CG2	2:B:61:ALA:N	2.76	0.47
2:B:76:THR:CG2	2:B:82:SER:HB2	2.45	0.47
8:H:18:THR:O	8:H:22:GLU:HG3	2.14	0.47
1:N:53:ASN:N	1:N:173:ASN:ND2	2.62	0.47
2:O:341:MET:CE	2:O:341:MET:HA	2.44	0.47
2:O:353:THR:CG2	2:O:354:GLU:N	2.77	0.47
5:R:147:ILE:HG22	5:R:148:ALA:H	1.78	0.47
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.97	0.47
1:N:77:LYS:HE3	2:O:359:LYS:HZ1	1.79	0.47
2:O:295:LEU:O	2:O:299:VAL:HG23	2.14	0.47
3:P:78:TRP:CD2	4:Q:197:GLU:HG3	2.49	0.47
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.97	0.47
7:T:36:ASN:O	7:T:40:ARG:HG3	2.14	0.47
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.96	0.47
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLU:O	1:A:397:SER:HB3	2.15	0.47
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.96	0.47
5:E:155:GLY:HA3	5:E:166:ASP:C	2.35	0.47
2:O:338:ARG:HB2	2:O:338:ARG:NH1	2.28	0.47
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.49	0.47
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.97	0.47
1:A:307:PHE:CD1	1:A:307:PHE:C	2.88	0.47
1:A:387:GLY:O	1:A:388:ARG:HB3	2.13	0.47
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.30	0.47
2:B:406:THR:OG1	2:B:408:ALA:HB3	2.15	0.47
4:D:70:VAL:HG21	4:D:83:ARG:NH1	2.28	0.47
5:E:102:THR:O	5:E:106:ILE:HG13	2.14	0.47
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.49	0.47
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.50	0.47
6:F:78:GLU:H	6:F:78:GLU:CD	2.17	0.47
1:N:75:PHE:HZ	1:N:86:PHE:HE2	1.61	0.47
1:N:443:TRP:O	1:N:444:ILE:CB	2.63	0.47
2:O:76:THR:HG23	2:O:136:GLU:CD	2.35	0.47
2:O:202:ALA:HB3	2:O:229:GLY:O	2.14	0.47
5:R:78:LEU:HD13	5:R:132:TRP:CE2	2.50	0.47
8:U:65:ARG:O	8:U:69:VAL:HG23	2.15	0.47
1:A:269:VAL:HG22	1:A:406:MET:HE2	1.97	0.47
2:B:46:ARG:HG3	2:B:110:GLU:HG2	1.96	0.47
4:D:71:GLN:HG3	4:D:82:MET:HE2	1.97	0.47
1:A:350:THR:CG2	1:A:351:GLU:N	2.77	0.47
2:B:341:MET:CE	2:B:341:MET:HA	2.45	0.47
2:B:353:THR:CG2	2:B:354:GLU:N	2.78	0.47
3:C:156:TYR:N	3:C:156:TYR:CD2	2.81	0.47
4:Q:43:MET:HE3	4:Q:189:PHE:CZ	2.50	0.47
4:Q:167:GLU:CG	8:U:13:LEU:HD13	2.45	0.47
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.50	0.47
2:B:312:PHE:CE2	2:B:314:VAL:HG23	2.50	0.47
3:C:269:ILE:HG22	3:C:269:ILE:O	2.14	0.47
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.97	0.47
10:J:49:GLY:N	10:J:54:HIS:ND1	2.63	0.47
13:P:502:HEM:HMC2	13:P:502:HEM:HBC2	1.97	0.47
5:R:113:ASP:OD2	5:R:116:LYS:HG3	2.14	0.47
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.50	0.47
2:B:26:ILE:HG12	2:B:26:ILE:O	2.16	0.46
3:C:152:SER:HB3	3:C:162:VAL:HG21	1.96	0.46
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:307:PHE:CD1	1:N:307:PHE:C	2.89	0.46
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.96	0.46
9:V:64:LEU:HD12	9:V:77:ARG:C	2.36	0.46
1:A:21:ASN:HA	1:A:219:VAL:HG13	1.98	0.46
1:A:240:GLU:HA	1:A:422:LEU:O	2.14	0.46
1:A:304:CYS:HB2	1:A:325:VAL:O	2.15	0.46
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.97	0.46
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.48	0.46
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.97	0.46
8:H:65:ARG:O	8:H:68:CYS:HB3	2.16	0.46
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.50	0.46
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.95	0.46
2:O:338:ARG:HH11	2:O:338:ARG:CB	2.28	0.46
4:Q:200:GLN:NE2	17:Q:3091:BOG:H3	2.29	0.46
5:R:118:ARG:HB2	5:R:171:ILE:CG2	2.45	0.46
1:A:103:SER:HB3	1:A:202:GLY:O	2.15	0.46
2:O:393:THR:HG23	2:O:397:VAL:HB	1.97	0.46
5:R:101:ARG:NH2	5:R:127:VAL:HG11	2.22	0.46
1:A:410:VAL:O	1:A:413:LYS:HB3	2.15	0.46
2:O:27:THR:CG2	2:O:28:LYS:H	2.21	0.46
2:O:76:THR:CG2	2:O:82:SER:HB2	2.43	0.46
6:S:78:GLU:CD	6:S:78:GLU:H	2.19	0.46
7:T:75:ALA:HA	7:T:78:GLU:HG3	1.97	0.46
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.97	0.46
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.95	0.46
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.97	0.46
2:O:19:PRO:HB3	2:O:41:PHE:CE2	2.50	0.46
2:O:424:MET:HG2	2:O:425:ALA:N	2.30	0.46
8:U:72:LYS:N	8:U:72:LYS:HD2	2.29	0.46
1:A:178:THR:CG2	1:A:179:ARG:N	2.79	0.46
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.97	0.46
3:C:268:HIS:HB3	21:C:1288:HOH:O	2.14	0.46
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.15	0.46
2:O:31:ASN:HD22	2:O:31:ASN:C	2.19	0.46
5:R:78:LEU:HB3	5:R:132:TRP:CH2	2.50	0.46
5:R:146:PRO:HB2	5:R:156:TYR:HB3	1.97	0.46
8:H:54:CYS:HA	8:H:57:GLU:OE2	2.16	0.46
1:N:19:LEU:C	1:N:21:ASN:H	2.19	0.46
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.46
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.16	0.46
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:382:HIS:HB3	1:N:388:ARG:O	2.16	0.46
1:A:49:ASN:HD22	1:A:51:LYS:N	2.08	0.46
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.98	0.46
3:C:198:LEU:HD21	13:C:502:HEM:CMA	2.45	0.46
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.97	0.46
2:O:327:ILE:HG22	9:V:55:MET:CE	2.46	0.46
3:P:269:ILE:O	3:P:269:ILE:HG22	2.14	0.46
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.97	0.46
8:U:32:LYS:O	8:U:36:ARG:HG3	2.16	0.46
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.49	0.46
2:B:393:THR:HG23	2:B:397:VAL:HB	1.97	0.46
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.98	0.46
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.51	0.46
2:O:353:THR:HB	2:O:356:ASP:OD1	2.16	0.46
6:S:96:GLU:OE2	6:S:96:GLU:HA	2.16	0.46
1:A:106:MET:HE2	1:A:106:MET:O	2.16	0.45
4:D:195:GLU:HG3	4:D:198:HIS:HB2	1.97	0.45
1:N:7:THR:HG21	2:O:113:ARG:CD	2.44	0.45
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.97	0.45
1:N:351:GLU:O	1:N:354:VAL:HG22	2.16	0.45
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.50	0.45
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.15	0.45
18:Q:501:HEC:HBC3	18:Q:501:HEC:HMC1	1.98	0.45
5:R:126:ARG:NH2	5:R:170:ARG:HG3	2.30	0.45
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.30	0.45
9:V:31:UNK:O	9:V:73:PRO:HG2	2.16	0.45
1:A:280:TYR:CG	1:A:281:ASP:N	2.84	0.45
4:D:97:ASN:OD1	4:D:99:GLU:HB2	2.16	0.45
5:E:73:LYS:HB3	5:E:195:VAL:O	2.16	0.45
2:O:402:ILE:HG23	2:O:403:ASP:H	1.81	0.45
3:P:17:ASN:HB2	17:P:2010:BOG:O3	2.15	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.16	0.45
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.46	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.34	0.45
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.98	0.45
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.52	0.45
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.47	0.45
2:O:291:VAL:C	2:O:293:SER:H	2.19	0.45
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.51	0.45
5:R:134:ILE:CD1	5:R:193:VAL:HG21	2.46	0.45
1:A:4:TYR:CE2	1:A:396:ASP:OD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG22	2:B:82:SER:CB	2.46	0.45
1:N:23:LEU:HD23	1:N:24:ARG:N	2.31	0.45
1:N:294:LEU:HB2	1:N:341:GLU:HG3	1.99	0.45
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.17	0.45
1:N:350:THR:HG22	1:N:352:SER:N	2.31	0.45
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.46	0.45
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.98	0.45
1:A:49:ASN:ND2	1:A:49:ASN:C	2.69	0.45
2:B:116:VAL:O	2:B:120:MET:HB2	2.16	0.45
2:B:218:GLN:O	2:B:222:GLN:HG3	2.16	0.45
2:B:353:THR:HB	2:B:356:ASP:OD1	2.16	0.45
2:O:248:ASN:C	2:O:248:ASN:ND2	2.67	0.45
5:R:71:LEU:HD13	5:R:92:ARG:HD3	1.98	0.45
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.16	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.17	0.45
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.17	0.45
2:B:195:VAL:O	2:B:199:PHE:HB2	2.16	0.45
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.99	0.45
2:B:338:ARG:HB2	2:B:338:ARG:NH1	2.31	0.45
2:B:357:VAL:O	2:B:361:LYS:HG3	2.16	0.45
4:D:238:ARG:HD2	7:G:14:ILE:HD12	1.97	0.45
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.97	0.45
2:B:24:LEU:HG	2:B:24:LEU:O	2.17	0.45
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.52	0.45
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.99	0.45
8:H:10:GLU:HB2	8:H:11:GLU:OE2	2.16	0.45
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.32	0.45
2:O:397:VAL:O	2:O:401:LYS:HG2	2.16	0.45
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.47	0.45
1:A:370:ASP:O	2:B:374:THR:HG22	2.17	0.45
2:B:46:ARG:HE	2:B:376:GLN:HA	1.82	0.45
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.97	0.45
1:N:136:GLN:O	1:N:140:GLU:HG3	2.17	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.45
3:C:198:LEU:HD21	13:C:502:HEM:C3A	2.52	0.45
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.47	0.45
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.99	0.45
1:N:161:THR:HG21	1:N:235:ARG:N	2.32	0.45
2:O:116:VAL:O	2:O:120:MET:HB2	2.17	0.45
5:R:147:ILE:CG2	5:R:148:ALA:N	2.80	0.45
1:A:242:ARG:O	7:G:14:ILE:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:HIS:O	2:B:70:ARG:HB3	2.16	0.44
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.53	0.44
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.47	0.44
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.99	0.44
1:A:3:THR:OG1	1:A:6:GLN:HG3	2.17	0.44
2:B:389:SER:O	2:B:390:GLY:C	2.56	0.44
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.17	0.44
4:D:62:LYS:O	4:D:66:GLU:HG3	2.17	0.44
5:E:10:PHE:O	5:E:14:ARG:HG3	2.17	0.44
1:A:170:THR:CG2	1:A:171:THR:N	2.81	0.44
2:O:62:ASN:O	2:O:65:THR:CG2	2.62	0.44
2:O:406:THR:OG1	2:O:408:ALA:HB3	2.17	0.44
3:P:358:SER:O	3:P:362:ILE:HG13	2.18	0.44
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.53	0.44
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.81	0.44
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.31	0.44
3:C:305:ILE:HB	3:C:306:PRO:HD3	2.00	0.44
7:G:24:ARG:HB2	7:G:27:PRO:HB3	2.00	0.44
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.46	0.44
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.44
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.37	0.44
5:R:133:VAL:HG13	5:R:133:VAL:O	2.17	0.44
2:B:248:ASN:HD22	2:B:250:HIS:H	1.65	0.44
1:N:350:THR:CG2	1:N:351:GLU:N	2.80	0.44
2:O:60:THR:CG2	2:O:61:ALA:N	2.80	0.44
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.82	0.44
1:A:23:LEU:HD23	1:A:23:LEU:C	2.38	0.44
2:B:312:PHE:CZ	2:B:314:VAL:CG2	3.01	0.44
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.98	0.44
1:N:106:MET:HE3	1:N:208:LEU:HA	1.98	0.44
2:O:110:GLU:O	2:O:111:CYS:HB3	2.17	0.44
1:A:53:ASN:H	1:A:173:ASN:ND2	2.16	0.44
1:A:281:ASP:OD1	1:A:281:ASP:C	2.55	0.44
2:B:19:PRO:HB2	2:B:41:PHE:CE1	2.52	0.44
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.52	0.44
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.99	0.44
5:R:109:GLU:HB3	5:R:123:ASP:HB2	2.00	0.44
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.53	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.99	0.44
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:80:ASP:O	7:G:81:GLN:OXT	2.36	0.44
8:H:11:GLU:CD	8:H:11:GLU:H	2.20	0.44
1:N:191:LYS:CA	1:N:195:MET:HE2	2.48	0.44
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.48	0.44
4:Q:95:TYR:HA	4:Q:96:PRO:HD3	1.85	0.44
5:R:177:PRO:HB2	5:R:178:TYR:CE1	2.53	0.44
1:A:191:LYS:C	1:A:195:MET:HE2	2.37	0.44
4:D:43:MET:HE3	4:D:189:PHE:CZ	2.53	0.44
4:D:120:ARG:HH21	18:D:501:HEC:CGA	2.31	0.44
5:R:124:LEU:HA	5:R:127:VAL:CG2	2.48	0.44
5:R:163:SER:HA	5:R:174:GLY:HA3	2.00	0.44
7:T:40:ARG:HD2	19:T:3004:CDL:OA4	2.18	0.44
2:B:218:GLN:HG2	2:B:222:GLN:OE1	2.18	0.43
1:N:143:ASN:ND2	9:V:48:PRO:HD2	2.27	0.43
2:O:24:LEU:O	2:O:24:LEU:HG	2.18	0.43
2:O:276:GLN:HG2	2:O:281:ALA:HB2	2.00	0.43
3:P:25:PRO:HB2	3:P:28:ILE:HG23	2.00	0.43
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.17	0.43
2:B:291:VAL:C	2:B:293:SER:H	2.21	0.43
2:B:402:ILE:HG23	2:B:403:ASP:H	1.81	0.43
4:D:3:LEU:HD11	7:G:72:LYS:HE3	2.00	0.43
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.53	0.43
9:I:32:UNK:N	9:I:73:PRO:CG	2.74	0.43
2:O:60:THR:HG23	2:O:61:ALA:N	2.33	0.43
2:O:389:SER:O	2:O:391:THR:N	2.51	0.43
3:P:101:ARG:NH2	13:P:502:HEM:HBD2	2.32	0.43
5:R:146:PRO:CB	5:R:156:TYR:HB3	2.48	0.43
6:S:71:LYS:O	6:S:72:HIS:HB2	2.18	0.43
1:A:272:VAL:O	1:A:275:ALA:HB3	2.18	0.43
5:E:185:TYR:CB	5:E:195:VAL:HG22	2.47	0.43
6:F:96:GLU:HA	6:F:96:GLU:OE2	2.18	0.43
7:G:75:ALA:HA	7:G:78:GLU:HG3	1.99	0.43
5:R:193:VAL:HG13	5:R:193:VAL:O	2.18	0.43
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.89	0.43
3:C:178:ARG:HA	3:P:54:MET:HG2	1.99	0.43
4:D:138:PRO:HB3	8:H:58:LEU:HD22	2.00	0.43
5:E:74:ILE:HD11	5:E:96:LEU:CD2	2.48	0.43
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.43
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.51	0.43
2:B:397:VAL:O	2:B:401:LYS:HG2	2.18	0.43
5:E:193:VAL:O	5:E:193:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:58:ARG:HA	9:I:58:ARG:HD3	1.90	0.43
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.48	0.43
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.43
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.99	0.43
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.01	0.43
2:B:366:ALA:O	2:B:370:MET:HG3	2.19	0.43
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.54	0.43
4:D:35:GLN:NE2	4:D:169:LEU:HD12	2.34	0.43
10:J:20:PHE:O	10:J:24:VAL:HG23	2.19	0.43
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.47	0.43
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	2.00	0.43
5:R:109:GLU:C	5:R:111:GLU:N	2.72	0.43
5:R:136:VAL:O	5:R:138:VAL:N	2.43	0.43
1:A:350:THR:HG22	1:A:352:SER:N	2.28	0.43
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.43
3:C:105:TYR:O	3:C:315:THR:HG22	2.18	0.43
3:C:234:THR:HG21	4:D:219:LEU:HD12	2.01	0.43
3:C:344:VAL:C	3:C:345:GLU:HG3	2.37	0.43
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.18	0.43
1:N:206:LYS:O	1:N:209:VAL:HG12	2.17	0.43
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.99	0.43
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.18	0.43
5:R:112:VAL:O	5:R:113:ASP:O	2.36	0.43
5:R:155:GLY:HA3	5:R:166:ASP:C	2.39	0.43
8:U:17:LEU:HD13	8:U:73:LEU:HD22	2.00	0.43
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.49	0.43
1:A:240:GLU:CD	1:A:242:ARG:HE	2.21	0.43
3:C:117:GLY:O	13:C:502:HEM:HMC3	2.19	0.43
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.00	0.43
1:N:240:GLU:HA	1:N:422:LEU:O	2.19	0.43
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.00	0.43
5:R:161:HIS:HB2	20:R:501:FES:S1	2.58	0.43
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.54	0.43
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.19	0.43
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.01	0.43
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.43
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.34	0.43
1:N:39:VAL:HA	1:N:196:VAL:O	2.19	0.43
5:R:71:LEU:HD13	5:R:92:ARG:NH1	2.34	0.43
1:A:62:LEU:HD11	1:A:127:ILE:HG12	2.00	0.42
5:E:55:VAL:O	5:E:59:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:PHE:CE2	5:E:137:GLY:HA3	2.54	0.42
5:E:161:HIS:HB2	20:E:501:FES:S1	2.59	0.42
2:O:402:ILE:O	2:O:405:VAL:HG23	2.19	0.42
2:B:394:ALA:HB3	2:B:397:VAL:HG23	2.01	0.42
3:C:247:SER:N	3:C:248:PRO:HD3	2.34	0.42
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	2.00	0.42
2:O:47:ILE:HG22	2:O:48:GLY:N	2.34	0.42
2:O:312:PHE:CE2	2:O:314:VAL:HG23	2.54	0.42
2:O:399:ALA:C	2:O:402:ILE:HG22	2.39	0.42
5:R:85:LYS:O	5:R:99:ARG:HG3	2.20	0.42
2:B:399:ALA:CA	2:B:402:ILE:HG22	2.50	0.42
7:G:77:TYR:O	8:H:47:ARG:NH1	2.52	0.42
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.01	0.42
1:A:328:PRO:HB3	1:A:427:PRO:HB2	2.02	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.76	0.42
5:E:126:ARG:HG2	5:E:126:ARG:HH11	1.85	0.42
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.82	0.42
10:J:14:PHE:CD2	10:J:14:PHE:N	2.85	0.42
2:O:389:SER:O	2:O:390:GLY:C	2.58	0.42
9:V:28:UNK:CB	9:V:71:ASN:ND2	2.83	0.42
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.27	0.42
2:B:28:LYS:O	2:B:28:LYS:HG2	2.18	0.42
5:E:134:ILE:CD1	5:E:193:VAL:HG21	2.50	0.42
9:I:65:VAL:HG12	9:I:66:ALA:N	2.34	0.42
2:O:245:ARG:HB3	2:O:430:LEU:CD1	2.49	0.42
3:P:350:ILE:O	3:P:354:MET:HG2	2.19	0.42
7:T:24:ARG:HB2	7:T:27:PRO:HB3	2.01	0.42
8:U:18:THR:O	8:U:22:GLU:HG3	2.19	0.42
5:E:191:ASP:OD1	5:E:191:ASP:O	2.38	0.42
7:G:45:VAL:O	7:G:49:ALA:HB3	2.19	0.42
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.55	0.42
1:N:137:GLU:O	1:N:141:MET:HG3	2.20	0.42
2:O:24:LEU:HD12	2:O:37:SER:O	2.18	0.42
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.54	0.42
6:S:40:ASP:O	6:S:44:LYS:HG3	2.18	0.42
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.54	0.42
2:O:129:ALA:N	2:O:130:PRO:CD	2.83	0.42
2:O:395:PRO:HA	2:O:398:VAL:HG12	2.00	0.42
3:P:198:LEU:HD21	13:P:502:HEM:CMA	2.49	0.42
8:U:34:ARG:O	8:U:38:GLU:HG3	2.20	0.42
2:B:84:ARG:HD2	6:S:107:TRP:HZ3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:269:ILE:CG2	14:C:2001:FNM:H23	2.48	0.42
3:C:285:ILE:HA	3:C:286:PRO:HD2	1.92	0.42
18:D:501:HEC:HAD1	18:D:501:HEC:HMD1	1.83	0.42
5:E:189:GLY:O	5:E:192:LEU:N	2.52	0.42
1:N:206:LYS:CD	1:N:206:LYS:N	2.64	0.42
2:O:357:VAL:O	2:O:361:LYS:HG3	2.20	0.42
7:T:72:LYS:HE3	8:U:56:GLU:HB2	2.02	0.42
10:W:52:TRP:O	10:W:56:LYS:HB2	2.19	0.42
1:A:106:MET:HE3	1:A:208:LEU:HA	2.02	0.42
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.80	0.42
2:B:385:GLU:C	2:B:387:LEU:H	2.23	0.42
4:D:68:VAL:HG12	4:D:69:GLU:N	2.35	0.42
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.54	0.42
5:E:163:SER:HA	5:E:174:GLY:HA3	2.01	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.53	0.42
2:O:257:VAL:O	2:O:323:GLY:HA3	2.19	0.42
6:S:12:LEU:HB3	6:S:13:MET:CE	2.50	0.42
7:T:72:LYS:CG	8:U:56:GLU:OE2	2.51	0.42
1:A:161:THR:HG21	1:A:235:ARG:H	1.83	0.42
2:B:26:ILE:HA	2:B:35:ILE:O	2.19	0.42
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.55	0.42
6:F:71:LYS:O	6:F:72:HIS:HB2	2.20	0.42
9:I:38:UNK:O	9:I:40:UNK:N	2.52	0.42
1:N:158:PHE:O	1:N:164:ALA:HB2	2.20	0.42
4:Q:79:GLU:OE2	4:Q:79:GLU:HA	2.20	0.42
5:R:73:LYS:HB3	5:R:195:VAL:O	2.20	0.42
6:S:77:LYS:HG2	6:S:77:LYS:O	2.19	0.42
5:E:189:GLY:O	5:E:190:ASP:C	2.59	0.41
1:N:123:GLU:OE1	1:N:123:GLU:HA	2.20	0.41
1:N:170:THR:CG2	1:N:171:THR:N	2.83	0.41
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.84	0.41
2:B:22:GLU:HG3	2:B:23:ASP:H	1.84	0.41
1:A:228:VAL:O	1:A:228:VAL:HG13	2.20	0.41
2:B:395:PRO:HA	2:B:398:VAL:HG12	2.02	0.41
3:C:194:THR:O	3:C:197:HIS:HB3	2.21	0.41
2:O:63:LEU:HB2	2:O:182:ARG:HD3	2.02	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.75	0.41
4:Q:195:GLU:HG3	4:Q:195:GLU:O	2.20	0.41
5:R:73:LYS:HG2	5:R:196:GLY:HA3	2.01	0.41
10:W:48:GLU:HA	10:W:54:HIS:CE1	2.55	0.41
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.82	0.41
2:B:295:LEU:O	2:B:299:VAL:HG23	2.20	0.41
1:N:105:ASP:O	1:N:106:MET:C	2.59	0.41
1:N:284:PHE:CE2	9:V:71:ASN:O	2.73	0.41
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.03	0.41
5:R:141:HIS:HB3	20:R:501:FES:S2	2.61	0.41
5:R:176:ALA:HA	5:R:177:PRO:HD2	1.95	0.41
1:A:90:THR:O	1:A:167:VAL:HG11	2.21	0.41
1:A:233:ARG:NH1	1:A:316:ASP:HB2	2.34	0.41
1:A:294:LEU:HB2	1:A:341:GLU:HG3	2.02	0.41
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.51	0.41
2:B:398:VAL:HG13	2:B:399:ALA:N	2.35	0.41
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.84	0.41
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.02	0.41
1:N:62:LEU:C	1:N:64:PHE:H	2.23	0.41
1:N:140:GLU:CG	9:V:50:LEU:HD12	2.49	0.41
2:O:34:ILE:HD13	2:O:390:GLY:CA	2.51	0.41
5:R:75:GLU:HG2	5:R:194:VAL:HG22	2.02	0.41
1:A:316:ASP:OD1	1:A:316:ASP:N	2.51	0.41
4:D:38:SER:O	4:D:94:PRO:HG3	2.20	0.41
4:D:142:VAL:O	4:D:142:VAL:HG23	2.21	0.41
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.54	0.41
2:O:132:PHE:HB2	2:O:192:HIS:CE1	2.56	0.41
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.47	0.41
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	2.03	0.41
1:A:105:ASP:O	1:A:106:MET:C	2.59	0.41
2:B:306:PRO:HA	9:I:52:ARG:HG2	2.02	0.41
2:O:178:CYS:SG	2:O:183:ILE:HD13	2.61	0.41
2:O:359:LYS:O	2:O:362:ASN:HB2	2.21	0.41
10:W:60:GLU:C	10:W:60:GLU:CD	2.79	0.41
4:D:204:MET:HG2	17:D:2009:BOG:H5	2.02	0.41
5:E:85:LYS:O	5:E:99:ARG:HG3	2.21	0.41
5:E:185:TYR:HB3	5:E:195:VAL:HG22	2.02	0.41
6:F:13:MET:CE	6:F:16:ILE:HD12	2.51	0.41
1:A:191:LYS:CA	1:A:195:MET:HE2	2.51	0.41
1:A:281:ASP:OD2	9:I:33:UNK:HB1	2.20	0.41
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.03	0.41
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.03	0.41
2:B:84:ARG:HD2	6:S:107:TRP:CZ3	2.56	0.41
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.36	0.41
3:C:223:PRO:HB2	3:C:227:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:162:PRO:HA	4:D:163:PRO:HD2	2.01	0.41
1:N:14:THR:OG1	1:N:389:ARG:HG2	2.21	0.41
1:N:228:VAL:O	1:N:228:VAL:HG13	2.21	0.41
2:O:50:PHE:C	2:O:51:ILE:HG13	2.41	0.41
2:O:57:TYR:CD1	2:O:57:TYR:N	2.89	0.41
2:O:147:ASP:O	2:O:150:VAL:HG22	2.20	0.41
2:O:222:GLN:O	2:O:223:PHE:HD2	2.04	0.41
2:O:345:LYS:O	2:O:348:ALA:N	2.52	0.41
3:P:31:TRP:CH2	11:P:3007:PEE:H20	2.55	0.41
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.34	0.41
2:B:31:ASN:HD22	2:B:31:ASN:C	2.23	0.41
4:D:74:PRO:HA	4:D:79:GLU:O	2.20	0.41
5:E:71:LEU:HD13	5:E:92:ARG:HD3	2.02	0.41
8:H:51:GLU:HA	8:H:51:GLU:OE1	2.20	0.41
1:N:18:THR:HG23	1:N:24:ARG:HG3	2.02	0.41
1:N:57:TYR:HA	1:N:90:THR:HG21	2.03	0.41
1:N:328:PRO:HB3	1:N:427:PRO:HB2	2.03	0.41
10:W:26:LEU:O	10:W:30:LEU:HG	2.20	0.41
1:A:219:VAL:CG1	1:A:220:SER:N	2.84	0.40
2:B:38:LEU:HD12	2:B:39:GLU:H	1.85	0.40
2:B:109:VAL:HG21	2:B:119:VAL:HG12	2.02	0.40
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.85	0.40
10:J:5:LEU:HD23	10:J:5:LEU:HA	1.95	0.40
6:S:79:GLN:HE21	6:S:79:GLN:HB3	1.68	0.40
10:W:56:LYS:HE2	10:W:56:LYS:HB3	1.86	0.40
3:C:350:ILE:O	3:C:354:MET:HG2	2.21	0.40
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.03	0.40
4:D:218:LEU:CD2	5:E:39:VAL:HG13	2.51	0.40
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	2.03	0.40
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.21	0.40
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.57	0.40
5:E:84:GLY:N	5:E:100:HIS:O	2.47	0.40
5:E:153:PHE:CD2	5:E:172:ARG:NH1	2.89	0.40
2:O:256:ALA:HB2	2:O:325:TYR:CD1	2.57	0.40
2:O:267:ALA:C	2:O:269:ALA:H	2.24	0.40
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.51	0.40
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.93	0.40
1:N:293:ARG:HE	1:N:293:ARG:HB3	1.71	0.40
2:O:31:ASN:ND2	2:O:31:ASN:C	2.74	0.40
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.36	0.40
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:GLN:HB3	3:C:343:PRO:HD2	2.04	0.40
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.03	0.40
4:D:122:GLY:O	4:D:125:ASP:HB2	2.22	0.40
7:G:41:PHE:O	7:G:45:VAL:CG2	2.67	0.40
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.85	0.40
2:O:21:ALA:O	2:O:22:GLU:HB2	2.21	0.40
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.22	0.40
5:R:147:ILE:HG13	5:R:157:TYR:O	2.22	0.40
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.56	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%)	412 (93%)	23 (5%)	6 (1%)	11 34
1	N	440/446 (99%)	411 (93%)	22 (5%)	7 (2%)	9 31
2	B	419/441 (95%)	374 (89%)	35 (8%)	10 (2%)	6 20
2	O	420/441 (95%)	372 (89%)	41 (10%)	7 (2%)	9 29
3	C	378/380 (100%)	364 (96%)	14 (4%)	0	100 100
3	P	377/380 (99%)	360 (96%)	17 (4%)	0	100 100
4	D	239/241 (99%)	228 (95%)	11 (5%)	0	100 100
4	Q	239/241 (99%)	224 (94%)	15 (6%)	0	100 100
5	E	194/196 (99%)	170 (88%)	18 (9%)	6 (3%)	4 14
5	R	192/196 (98%)	156 (81%)	28 (15%)	8 (4%)	3 9
6	F	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	15 44
6	S	99/110 (90%)	91 (92%)	6 (6%)	2 (2%)	7 24
7	G	79/81 (98%)	69 (87%)	10 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	T	76/81 (94%)	68 (90%)	8 (10%)	0	100 100
8	H	68/77 (88%)	62 (91%)	6 (9%)	0	100 100
8	U	65/77 (84%)	60 (92%)	4 (6%)	1 (2%)	10 33
9	I	29/47 (62%)	26 (90%)	2 (7%)	1 (3%)	3 13
9	V	29/47 (62%)	24 (83%)	5 (17%)	0	100 100
10	J	59/61 (97%)	55 (93%)	3 (5%)	1 (2%)	9 29
10	W	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	3 13
All	All	4000/4160 (96%)	3673 (92%)	275 (7%)	52 (1%)	12 36

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
2	B	26	ILE
2	B	226	ILE
2	B	227	ARG
2	B	389	SER
5	E	188	VAL
5	E	190	ASP
1	N	20	ASP
1	N	282	ARG
2	O	26	ILE
2	O	228	SER
2	O	389	SER
5	R	113	ASP
5	R	191	ASP
8	U	13	LEU
1	A	218	GLY
2	B	171	ALA
2	B	390	GLY
5	E	137	GLY
1	N	218	GLY
2	O	171	ALA
2	O	390	GLY
5	R	137	GLY
5	R	147	ILE
5	R	189	GLY
1	A	72	CYS
1	A	443	TRP
6	F	77	LYS

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Mol	Chain	Res	Type
1	N	72	CYS
1	N	262	TRP
1	N	443	TRP
5	R	149	ASN
1	A	262	TRP
5	R	110	ALA
6	S	77	LYS
10	W	56	LYS
2	B	29	LEU
5	E	141	HIS
10	J	56	LYS
6	S	11	ARG
10	W	61	ALA
2	B	220	ALA
2	B	231	GLY
2	O	29	LEU
5	E	189	GLY
1	A	71	PRO
2	B	265	GLY
5	E	120	PRO
2	O	231	GLY
9	I	48	PRO
1	N	71	PRO
5	R	188	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	355 (97%)	10 (3%)	44	78
1	N	365/368 (99%)	351 (96%)	14 (4%)	33	67
2	B	332/347 (96%)	327 (98%)	5 (2%)	65	89
2	O	333/347 (96%)	327 (98%)	6 (2%)	59	86
3	C	328/329 (100%)	323 (98%)	5 (2%)	65	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	328/329 (100%)	323 (98%)	5 (2%)	65	89
4	D	200/200 (100%)	197 (98%)	3 (2%)	65	89
4	Q	200/200 (100%)	197 (98%)	3 (2%)	65	89
5	E	166/166 (100%)	165 (99%)	1 (1%)	86	96
5	R	165/166 (99%)	159 (96%)	6 (4%)	35	69
6	F	93/96 (97%)	91 (98%)	2 (2%)	52	83
6	S	93/96 (97%)	90 (97%)	3 (3%)	39	73
7	G	71/71 (100%)	71 (100%)	0	100	100
7	T	69/71 (97%)	68 (99%)	1 (1%)	67	90
8	H	65/71 (92%)	64 (98%)	1 (2%)	65	89
8	U	63/71 (89%)	62 (98%)	1 (2%)	62	88
9	I	23/26 (88%)	22 (96%)	1 (4%)	29	62
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	47 (96%)	2 (4%)	30	64
10	W	47/49 (96%)	46 (98%)	1 (2%)	53	84
All	All	3378/3446 (98%)	3308 (98%)	70 (2%)	53	84

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	90	THR
1	A	106	MET
1	A	181	ASP
1	A	281	ASP
1	A	342	TRP
1	A	395	TRP
1	A	443	TRP
2	B	31	ASN
2	B	102	ARG
2	B	248	ASN
2	B	341	MET
2	B	402	ILE
3	C	5	ILE
3	C	91	PHE

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Mol	Chain	Res	Type
3	C	223	PRO
3	C	334	LEU
3	C	367	PHE
4	D	169	LEU
4	D	172	ASP
4	D	173	ASP
5	E	125	ASP
6	F	58	ARG
6	F	70	LEU
8	H	72	LYS
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	90	THR
1	N	106	MET
1	N	181	ASP
1	N	206	LYS
1	N	281	ASP
1	N	307	PHE
1	N	342	TRP
1	N	395	TRP
1	N	443	TRP
2	O	31	ASN
2	O	102	ARG
2	O	139	ASP
2	O	248	ASN
2	O	341	MET
2	O	402	ILE
3	P	5	ILE
3	P	91	PHE
3	P	223	PRO
3	P	334	LEU
3	P	367	PHE
4	Q	172	ASP
4	Q	173	ASP
4	Q	241	LYS
5	R	52	LYS

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Mol	Chain	Res	Type
5	R	113	ASP
5	R	125	ASP
5	R	126	ARG
5	R	187	PHE
5	R	191	ASP
6	S	14	ASP
6	S	58	ARG
6	S	70	LEU
7	T	2	ILE
8	U	72	LYS
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	118	GLN
1	A	126	GLN
1	A	147	ASN
1	A	173	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	192	HIS
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	376	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	332	ASN
3	C	342	GLN

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Mol	Chain	Res	Type
4	D	35	GLN
4	D	50	ASN
4	D	71	GLN
4	D	148	HIS
4	D	200	GLN
5	E	3	ASN
5	E	57	GLN
5	E	164	HIS
5	E	186	GLN
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	79	ASN
8	H	71	HIS
8	H	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	126	GLN
1	N	143	ASN
1	N	147	ASN
1	N	173	ASN
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	192	HIS
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	376	GLN
3	P	9	HIS
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN

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Mol	Chain	Res	Type
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	71	GLN
4	Q	148	HIS
4	Q	200	GLN
5	R	3	ASN
5	R	57	GLN
5	R	164	HIS
6	S	79	GLN
7	T	44	GLN
7	T	79	ASN
8	U	71	HIS
8	U	75	ASN
10	W	8	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 41 ligands modelled in this entry, 11 are unknown - leaving 30 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	$\#\|Z\|>2$
11	PEE	N	3008	-	4,4,50	3.54	4 (100%)	6,6,55	0.60	0
13	HEM	P	501	3	41,50,50	1.52	7 (17%)	45,82,82	1.58	10 (22%)
11	PEE	C	2005	-	49,49,50	1.45	9 (18%)	52,54,55	0.83	2 (3%)
19	CDL	Q	3003	-	41,41,99	1.19	2 (4%)	47,53,111	1.05	4 (8%)
16	AZI	P	3011	-	0,2,2	-	-	0,1,1	-	-
20	FES	E	501	5	0,4,4	-	-	-		
19	CDL	D	2003	-	41,41,99	1.14	1 (2%)	47,53,111	1.04	3 (6%)
19	CDL	T	3004	-	39,39,99	1.22	3 (7%)	45,51,111	1.07	1 (2%)
11	PEE	P	3005	-	49,49,50	1.44	9 (18%)	52,54,55	0.84	3 (5%)
15	UQ	P	3002	-	19,19,63	2.50	10 (52%)	23,26,79	1.08	2 (8%)
15	UQ	C	2002	-	19,19,63	2.67	10 (52%)	23,26,79	1.12	2 (8%)
16	AZI	C	2011	-	0,2,2	-	-	0,1,1	-	-
17	BOG	Q	3009	-	20,20,20	0.95	1 (5%)	25,25,25	0.84	1 (4%)
13	HEM	P	502	3	41,50,50	1.61	5 (12%)	45,82,82	1.50	9 (20%)
14	FNM	C	2001	-	23,24,24	1.81	3 (13%)	25,34,34	1.88	4 (16%)
18	HEC	Q	501	4	32,50,50	1.99	2 (6%)	24,82,82	1.61	3 (12%)
17	BOG	P	2010	-	18,18,20	1.10	2 (11%)	22,22,25	0.56	0
13	HEM	C	502	3	41,50,50	1.70	8 (19%)	45,82,82	1.78	14 (31%)
17	BOG	D	2091	-	20,20,20	1.13	3 (15%)	25,25,25	0.99	1 (4%)
11	PEE	C	2007	-	47,47,50	1.28	6 (12%)	50,52,55	0.81	3 (6%)
14	FNM	P	3001	-	23,24,24	1.85	3 (13%)	25,34,34	1.72	2 (8%)
11	PEE	A	2008	-	20,20,50	1.70	4 (20%)	23,25,55	0.63	0
18	HEC	D	501	4	32,50,50	1.59	3 (9%)	24,82,82	1.50	2 (8%)
17	BOG	D	2009	-	20,20,20	0.99	1 (5%)	25,25,25	0.92	1 (4%)
13	HEM	C	501	3	41,50,50	1.47	5 (12%)	45,82,82	1.71	12 (26%)
20	FES	R	501	5	0,4,4	-	-	-		
17	BOG	C	3010	-	11,11,20	1.07	2 (18%)	10,11,25	0.93	1 (10%)
17	BOG	Q	3091	-	20,20,20	1.15	2 (10%)	25,25,25	0.89	1 (4%)
11	PEE	P	3007	-	47,47,50	1.34	5 (10%)	50,52,55	0.78	2 (4%)
19	CDL	G	2004	-	39,39,99	1.21	4 (10%)	45,51,111	1.07	2 (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
13	HEM	P	501	3	-	2/12/54/54	-
11	PEE	C	2005	-	-	28/53/53/54	-
19	CDL	Q	3003	-	-	25/51/51/110	-
20	FES	E	501	5	-	-	0/1/1/1
19	CDL	D	2003	-	-	26/51/51/110	-
19	CDL	T	3004	-	-	23/49/49/110	-
11	PEE	P	3005	-	-	29/53/53/54	-
15	UQ	P	3002	-	-	2/11/35/87	0/1/1/1
15	UQ	C	2002	-	-	3/11/35/87	0/1/1/1
17	BOG	Q	3009	-	-	6/11/31/31	0/1/1/1
13	HEM	P	502	3	-	6/12/54/54	-
14	FNM	C	2001	-	-	2/12/31/31	0/3/3/3
18	HEC	Q	501	4	-	4/10/54/54	-
17	BOG	P	2010	-	-	1/6/26/31	0/1/1/1
13	HEM	C	502	3	-	6/12/54/54	-
17	BOG	D	2091	-	-	6/11/31/31	0/1/1/1
11	PEE	C	2007	-	-	24/51/51/54	-
14	FNM	P	3001	-	-	2/12/31/31	0/3/3/3
11	PEE	A	2008	-	-	12/24/24/54	-
18	HEC	D	501	4	-	4/10/54/54	-
17	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
13	HEM	C	501	3	-	2/12/54/54	-
20	FES	R	501	5	-	-	0/1/1/1
17	BOG	C	3010	-	-	5/9/9/31	-
17	BOG	Q	3091	-	-	4/11/31/31	0/1/1/1
11	PEE	P	3007	-	-	25/51/51/54	-
19	CDL	G	2004	-	-	21/49/49/110	-

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	501	HEC	C2B-C3B	-6.88	1.33	1.40
14	C	2001	FNM	C3-N4	6.85	1.34	1.28
18	Q	501	HEC	C3C-C2C	-6.81	1.33	1.40
14	P	3001	FNM	C3-N4	6.46	1.33	1.28
15	C	2002	UQ	C7-C6	5.67	1.60	1.51
15	P	3002	UQ	C7-C6	5.51	1.60	1.51
13	P	502	HEM	CBB-CAB	5.15	1.55	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2002	UQ	C6-C5	5.00	1.44	1.35
11	N	3008	PEE	P-O1P	4.75	1.62	1.50
18	D	501	HEC	C3C-C2C	-4.69	1.35	1.40
15	P	3002	UQ	C6-C5	4.63	1.43	1.35
13	C	502	HEM	CBB-CAB	4.54	1.52	1.30
13	P	501	HEM	CBB-CAB	4.49	1.52	1.30
13	C	502	HEM	C4D-C3D	4.47	1.52	1.45
18	D	501	HEC	C2B-C3B	-4.46	1.36	1.40
11	C	2007	PEE	C39-C38	4.14	1.55	1.31
11	P	3007	PEE	C39-C38	4.11	1.55	1.31
11	P	3005	PEE	C39-C38	4.09	1.55	1.31
11	C	2005	PEE	C39-C38	4.07	1.55	1.31
13	C	501	HEM	CBB-CAB	4.04	1.50	1.30
13	P	502	HEM	C4D-C3D	3.94	1.51	1.45
15	C	2002	UQ	C6-C1	3.83	1.57	1.46
13	C	501	HEM	CAB-C3B	-3.75	1.37	1.47
15	P	3002	UQ	C6-C1	3.62	1.56	1.46
11	N	3008	PEE	P-O4P	3.50	1.65	1.54
13	C	501	HEM	C3C-CAC	-3.45	1.40	1.47
13	P	502	HEM	CBC-CAC	3.38	1.51	1.29
13	P	501	HEM	CAB-C3B	-3.38	1.38	1.47
13	P	501	HEM	CBC-CAC	3.32	1.51	1.29
13	C	502	HEM	C3C-CAC	-3.31	1.41	1.47
11	C	2005	PEE	O2-C10	3.29	1.43	1.34
11	P	3005	PEE	O2-C10	3.25	1.43	1.34
11	A	2008	PEE	O3-C30	3.25	1.42	1.33
11	C	2005	PEE	O3-C30	3.16	1.42	1.33
11	C	2005	PEE	P-O1P	3.15	1.62	1.50
11	A	2008	PEE	O2-C10	3.11	1.43	1.34
11	P	3005	PEE	P-O1P	3.10	1.61	1.50
15	C	2002	UQ	O3-C3	3.07	1.44	1.36
11	P	3007	PEE	C21-C22	-3.06	1.34	1.51
13	P	501	HEM	C3C-CAC	-3.06	1.41	1.47
11	A	2008	PEE	P-O1P	3.02	1.61	1.50
11	P	3007	PEE	O3-C30	3.01	1.42	1.33
11	N	3008	PEE	P-O3P	3.01	1.63	1.54
13	C	501	HEM	CBC-CAC	2.99	1.49	1.29
13	C	502	HEM	CAB-C3B	-2.97	1.39	1.47
13	C	502	HEM	CBC-CAC	2.96	1.48	1.29
11	C	2007	PEE	C21-C22	-2.95	1.35	1.51
11	P	3007	PEE	P-O1P	2.94	1.61	1.50
11	P	3005	PEE	O3-C30	2.92	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2002	UQ	CM5-C5	2.88	1.56	1.50
11	P	3005	PEE	C21-C22	-2.88	1.35	1.51
11	C	2005	PEE	C21-C22	-2.86	1.35	1.51
15	C	2002	UQ	O2-C2	2.86	1.43	1.36
11	C	2007	PEE	P-O1P	2.85	1.61	1.50
13	C	502	HEM	C4A-NA	2.84	1.42	1.36
15	C	2002	UQ	C2-C1	2.83	1.57	1.48
14	P	3001	FNM	C3-N2	-2.81	1.33	1.38
15	P	3002	UQ	C7-C8	2.81	1.54	1.50
11	P	3007	PEE	O2-C10	2.79	1.42	1.34
15	P	3002	UQ	O3-C3	2.79	1.43	1.36
14	C	2001	FNM	C3-N2	-2.75	1.33	1.38
15	P	3002	UQ	CM5-C5	2.67	1.56	1.50
11	C	2007	PEE	O3-C30	2.65	1.41	1.33
13	C	502	HEM	C3B-C4B	2.63	1.50	1.44
15	C	2002	UQ	C5-C4	2.62	1.56	1.47
13	P	502	HEM	C3C-CAC	-2.60	1.42	1.47
13	P	501	HEM	C3C-C2C	-2.59	1.36	1.40
13	P	502	HEM	CAB-C3B	-2.57	1.40	1.47
17	D	2091	BOG	O5-C1	2.50	1.48	1.41
17	C	3010	BOG	C2-C1	2.50	1.57	1.50
17	Q	3091	BOG	C4-C5	2.50	1.58	1.53
11	N	3008	PEE	P-O2P	2.49	1.62	1.54
15	P	3002	UQ	C2-C1	2.49	1.56	1.48
11	C	2007	PEE	O2-C10	2.47	1.41	1.34
17	Q	3091	BOG	O5-C1	2.47	1.48	1.41
14	P	3001	FNM	C26-C21	2.47	1.43	1.39
19	T	3004	CDL	O1-C1	2.45	1.50	1.43
11	C	2005	PEE	C31-C30	2.43	1.57	1.50
17	D	2091	BOG	C4-C5	2.42	1.58	1.53
15	P	3002	UQ	O2-C2	2.41	1.42	1.36
15	C	2002	UQ	C7-C8	2.41	1.54	1.50
14	C	2001	FNM	C6-N2	-2.40	1.35	1.38
19	G	2004	CDL	CA3-CA4	2.37	1.58	1.50
17	C	3010	BOG	O5-C1	2.34	1.45	1.40
13	C	501	HEM	C3C-C2C	-2.33	1.37	1.40
15	P	3002	UQ	C5-C4	2.32	1.55	1.47
15	C	2002	UQ	C3-C4	2.32	1.55	1.48
11	P	3005	PEE	C11-C10	2.30	1.57	1.50
13	P	501	HEM	CHD-C1D	-2.29	1.34	1.41
11	P	3005	PEE	C3-C2	2.29	1.57	1.50
17	P	2010	BOG	C4-C5	2.29	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	2009	BOG	O5-C1	2.28	1.47	1.41
19	T	3004	CDL	CA3-CA4	2.28	1.57	1.50
19	G	2004	CDL	O1-C1	2.24	1.50	1.43
11	P	3005	PEE	C31-C30	2.20	1.57	1.50
17	Q	3009	BOG	O5-C1	2.20	1.47	1.41
15	P	3002	UQ	C3-C4	2.19	1.55	1.48
11	C	2005	PEE	C11-C10	2.19	1.57	1.50
19	Q	3003	CDL	O1-C1	2.18	1.49	1.43
11	C	2005	PEE	C1-C2	2.18	1.57	1.50
11	P	3005	PEE	C1-C2	2.16	1.57	1.50
17	P	2010	BOG	C1-C2	2.14	1.57	1.52
11	C	2005	PEE	C3-C2	2.12	1.57	1.50
11	A	2008	PEE	C3-C2	2.10	1.57	1.50
18	D	501	HEC	C2A-C1A	2.09	1.47	1.42
19	Q	3003	CDL	OA2-CA2	-2.09	1.36	1.44
13	P	501	HEM	C4A-NA	2.08	1.40	1.36
11	C	2007	PEE	C3-C2	2.08	1.57	1.50
19	G	2004	CDL	CB3-CB4	2.07	1.57	1.50
19	G	2004	CDL	OA6-CA5	2.06	1.40	1.34
19	T	3004	CDL	OA8-CA6	-2.03	1.40	1.45
17	D	2091	BOG	C1-C2	2.01	1.58	1.52
13	C	502	HEM	C1A-CHA	-2.00	1.35	1.41
19	D	2003	CDL	O1-C1	2.00	1.49	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	2001	FNM	C27-S3-C3	7.67	110.67	100.40
14	P	3001	FNM	C27-S3-C3	6.90	109.64	100.40
18	D	501	HEC	CBA-CAA-C2A	5.51	121.89	112.60
13	C	502	HEM	CAD-C3D-C4D	5.48	134.23	124.66
18	Q	501	HEC	CBA-CAA-C2A	5.47	121.83	112.60
13	P	502	HEM	CAD-C3D-C4D	4.34	132.25	124.66
17	D	2091	BOG	C1'-O1-C1	3.93	120.36	113.84
13	C	501	HEM	C3B-C2B-C1B	-3.91	103.59	106.49
14	P	3001	FNM	C21-N1-N2	3.74	123.42	116.23
13	P	501	HEM	C3B-C2B-C1B	-3.69	103.75	106.49
14	C	2001	FNM	C21-N1-N2	3.66	123.27	116.23
13	C	501	HEM	C4A-C3A-C2A	-3.43	104.61	107.00
13	P	501	HEM	C4B-CHC-C1C	3.43	127.08	122.56
13	C	501	HEM	C4B-CHC-C1C	3.40	127.05	122.56
17	D	2009	BOG	C1'-O1-C1	3.40	119.48	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	502	HEM	C2C-C3C-C4C	-3.36	104.55	106.90
13	C	501	HEM	C2D-C1D-ND	3.23	113.76	109.88
13	C	502	HEM	C4D-ND-C1D	-3.23	101.74	105.07
19	T	3004	CDL	CB4-OB6-CB5	-3.19	109.94	117.79
13	C	501	HEM	CAD-C3D-C4D	3.17	130.21	124.66
17	Q	3091	BOG	C1'-O1-C1	3.17	119.10	113.84
13	P	502	HEM	C4B-CHC-C1C	3.17	126.74	122.56
15	C	2002	UQ	C8-C7-C6	3.15	120.53	112.05
19	G	2004	CDL	CB4-OB6-CB5	-3.13	110.08	117.79
11	P	3005	PEE	C22-C21-C20	3.11	127.33	113.79
11	C	2007	PEE	C22-C21-C20	3.07	127.15	113.79
11	C	2005	PEE	C22-C21-C20	3.06	127.12	113.79
11	P	3007	PEE	C22-C21-C20	3.04	127.03	113.79
13	C	502	HEM	C3D-C4D-ND	3.01	113.52	110.17
13	P	501	HEM	C4A-C3A-C2A	-2.97	104.93	107.00
15	P	3002	UQ	C8-C7-C6	2.94	119.98	112.05
17	Q	3009	BOG	C1'-O1-C1	2.93	118.70	113.84
13	C	501	HEM	CAD-C3D-C2D	-2.91	122.45	127.88
13	P	501	HEM	CAD-C3D-C4D	2.79	129.54	124.66
13	C	502	HEM	C4D-C3D-C2D	-2.75	102.89	106.90
13	C	502	HEM	C2C-C3C-C4C	-2.75	104.98	106.90
13	P	501	HEM	C2D-C1D-ND	2.75	113.17	109.88
13	C	502	HEM	CAD-C3D-C2D	-2.71	122.83	127.88
13	P	501	HEM	C4C-CHD-C1D	2.67	126.09	122.56
13	P	502	HEM	CAD-C3D-C2D	-2.65	122.95	127.88
13	C	502	HEM	C4C-CHD-C1D	2.62	126.01	122.56
19	D	2003	CDL	CB4-OB6-CB5	-2.54	111.54	117.79
18	Q	501	HEC	CMC-C2C-C3C	-2.52	122.86	125.82
13	P	502	HEM	C2D-C1D-ND	2.51	112.89	109.88
13	C	502	HEM	CMA-C3A-C4A	-2.49	124.63	128.46
13	P	502	HEM	C4C-CHD-C1D	2.48	125.83	122.56
13	C	501	HEM	C4D-ND-C1D	-2.47	102.53	105.07
13	C	502	HEM	C2D-C1D-ND	2.46	112.83	109.88
11	C	2005	PEE	C21-C22-C23	2.46	126.91	114.42
19	Q	3003	CDL	CB4-OB6-CB5	-2.46	111.74	117.79
11	P	3005	PEE	C21-C22-C23	2.42	126.71	114.42
13	C	501	HEM	C2C-C3C-C4C	-2.38	105.23	106.90
14	C	2001	FNM	O6-C6-C5	2.38	128.42	126.03
13	P	501	HEM	C2C-C3C-C4C	-2.38	105.24	106.90
11	C	2007	PEE	C21-C22-C23	2.36	126.42	114.42
13	C	502	HEM	CMC-C2C-C3C	2.35	129.08	124.68
15	C	2002	UQ	C7-C6-C1	-2.34	115.66	118.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	2001	FNM	C5-C6-N2	-2.34	105.64	107.77
19	D	2003	CDL	CA6-OA8-CA7	-2.33	111.24	117.10
11	P	3007	PEE	C21-C22-C23	2.26	125.87	114.42
17	C	3010	BOG	C1'-O1-C1	2.24	118.91	114.00
13	C	502	HEM	CMA-C3A-C2A	2.23	129.15	124.94
13	C	501	HEM	CHD-C1D-C2D	-2.22	121.50	124.98
13	C	501	HEM	CBD-CAD-C3D	2.22	118.81	112.63
19	Q	3003	CDL	CA6-OA8-CA7	-2.22	111.52	117.10
15	P	3002	UQ	C7-C6-C1	-2.21	115.81	118.48
13	C	501	HEM	C2B-C1B-NB	2.19	112.44	109.84
19	Q	3003	CDL	CA4-OA6-CA5	-2.19	112.40	117.79
19	G	2004	CDL	CA4-OA6-CA5	-2.16	112.46	117.79
13	C	502	HEM	C4B-CHC-C1C	2.16	125.41	122.56
13	P	501	HEM	C4D-ND-C1D	-2.16	102.85	105.07
13	P	502	HEM	C4A-C3A-C2A	-2.14	105.50	107.00
13	P	502	HEM	CBA-CAA-C2A	2.14	116.27	112.62
19	D	2003	CDL	CA6-CA4-CA3	-2.14	106.73	111.79
13	C	502	HEM	C2B-C1B-NB	2.11	112.33	109.84
18	Q	501	HEC	CAA-C2A-C3A	-2.10	121.22	127.25
13	C	502	HEM	CHA-C4D-ND	-2.09	121.79	124.38
13	P	501	HEM	C2B-C1B-NB	2.07	112.29	109.84
18	D	501	HEC	CAA-C2A-C3A	-2.05	121.35	127.25
13	P	502	HEM	C2B-C1B-NB	2.05	112.26	109.84
13	C	501	HEM	CMB-C2B-C1B	2.04	128.15	125.04
11	C	2007	PEE	O3-C3-C2	2.04	114.38	108.43
19	Q	3003	CDL	CA6-CA4-CA3	-2.03	106.99	111.79
11	P	3005	PEE	O3-C3-C2	2.03	114.34	108.43
13	P	501	HEM	CAD-C3D-C2D	-2.01	124.13	127.88

There are no chirality outliers.

All (272) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	C1-O3P-P-O1P
11	C	2005	PEE	C11-C10-O2-C2
11	C	2005	PEE	C4-O4P-P-O2P
11	C	2005	PEE	C4-O4P-P-O1P
11	P	3005	PEE	C11-C10-O2-C2
11	P	3005	PEE	C4-O4P-P-O2P
11	P	3005	PEE	C4-O4P-P-O1P
11	P	3007	PEE	C17-C18-C19-C20
14	P	3001	FNM	N4-C5-C8-C13

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Mol	Chain	Res	Type	Atoms
15	C	2002	UQ	C1-C6-C7-C8
15	C	2002	UQ	C5-C6-C7-C8
15	C	2002	UQ	C12-C11-C9-C10
15	P	3002	UQ	C1-C6-C7-C8
15	P	3002	UQ	C5-C6-C7-C8
17	D	2091	BOG	O5-C1-O1-C1'
17	Q	3009	BOG	C2-C1-O1-C1'
17	Q	3091	BOG	C2-C1-O1-C1'
18	D	501	HEC	C1A-C2A-CAA-CBA
18	D	501	HEC	C3A-C2A-CAA-CBA
18	Q	501	HEC	C1A-C2A-CAA-CBA
18	Q	501	HEC	C3A-C2A-CAA-CBA
19	D	2003	CDL	CB2-C1-CA2-OA2
19	D	2003	CDL	CA2-OA2-PA1-OA3
19	D	2003	CDL	CA2-OA2-PA1-OA4
19	D	2003	CDL	CB2-OB2-PB2-OB3
19	D	2003	CDL	CB2-OB2-PB2-OB5
19	G	2004	CDL	O1-C1-CA2-OA2
19	G	2004	CDL	CA3-OA5-PA1-OA3
19	Q	3003	CDL	CA2-OA2-PA1-OA4
19	Q	3003	CDL	CB2-OB2-PB2-OB3
19	T	3004	CDL	O1-C1-CA2-OA2
19	T	3004	CDL	CA3-OA5-PA1-OA3
11	P	3005	PEE	O5-C30-O3-C3
19	D	2003	CDL	C31-CA7-OA8-CA6
19	Q	3003	CDL	C31-CA7-OA8-CA6
11	C	2005	PEE	O5-C30-O3-C3
19	G	2004	CDL	OB9-CB7-OB8-CB6
19	T	3004	CDL	OB9-CB7-OB8-CB6
11	C	2005	PEE	O4-C10-O2-C2
11	P	3005	PEE	O4-C10-O2-C2
19	G	2004	CDL	OB7-CB5-OB6-CB4
19	T	3004	CDL	OB7-CB5-OB6-CB4
11	C	2005	PEE	C31-C30-O3-C3
11	P	3005	PEE	C31-C30-O3-C3
19	T	3004	CDL	C51-CB5-OB6-CB4
19	G	2004	CDL	C71-CB7-OB8-CB6
19	T	3004	CDL	C71-CB7-OB8-CB6
19	D	2003	CDL	OA9-CA7-OA8-CA6
11	C	2007	PEE	C17-C18-C19-C20
17	D	2009	BOG	C4-C5-C6-O6
19	D	2003	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
19	Q	3003	CDL	O1-C1-CA2-OA2
19	Q	3003	CDL	OA9-CA7-OA8-CA6
19	G	2004	CDL	C51-CB5-OB6-CB4
17	D	2091	BOG	O5-C5-C6-O6
17	Q	3091	BOG	O5-C1-O1-C1'
19	G	2004	CDL	CB2-C1-CA2-OA2
19	Q	3003	CDL	CB2-C1-CA2-OA2
19	T	3004	CDL	CB2-C1-CA2-OA2
19	D	2003	CDL	C71-CB7-OB8-CB6
19	Q	3003	CDL	C71-CB7-OB8-CB6
17	D	2091	BOG	C4-C5-C6-O6
17	D	2009	BOG	O5-C5-C6-O6
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
17	Q	3009	BOG	O1-C1'-C2'-C3'
19	Q	3003	CDL	OB9-CB7-OB8-CB6
17	Q	3009	BOG	O5-C1-O1-C1'
19	D	2003	CDL	OB9-CB7-OB8-CB6
11	A	2008	PEE	C1-O3P-P-O4P
11	C	2005	PEE	C4-O4P-P-O3P
11	P	3005	PEE	C4-O4P-P-O3P
19	D	2003	CDL	CA2-OA2-PA1-OA5
19	Q	3003	CDL	CA2-OA2-PA1-OA5
19	Q	3003	CDL	CB2-OB2-PB2-OB5
11	P	3007	PEE	C12-C13-C14-C15
11	C	2005	PEE	C33-C34-C35-C36
11	P	3005	PEE	C33-C34-C35-C36
19	D	2003	CDL	CB7-C71-C72-C73
17	C	3010	BOG	C3'-C4'-C5'-C6'
11	P	3005	PEE	C10-C11-C12-C13
19	Q	3003	CDL	CB7-C71-C72-C73
11	C	2007	PEE	C12-C13-C14-C15
19	T	3004	CDL	OA7-CA5-OA6-CA4
19	G	2004	CDL	C11-CA5-OA6-CA4
19	T	3004	CDL	C11-CA5-OA6-CA4
11	C	2005	PEE	C14-C15-C16-C17
11	C	2007	PEE	C10-C11-C12-C13
11	P	3005	PEE	C30-C31-C32-C33
11	P	3007	PEE	C10-C11-C12-C13
11	P	3005	PEE	C14-C15-C16-C17
17	D	2009	BOG	C3'-C4'-C5'-C6'
11	C	2005	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	C	2005	PEE	C30-C31-C32-C33
17	C	3010	BOG	C2'-C1'-O1-C1
17	D	2091	BOG	C2'-C1'-O1-C1
19	G	2004	CDL	OA7-CA5-OA6-CA4
17	P	2010	BOG	C3'-C4'-C5'-C6'
11	P	3007	PEE	C40-C41-C42-C43
19	G	2004	CDL	CB5-C51-C52-C53
19	T	3004	CDL	CB5-C51-C52-C53
11	C	2007	PEE	C34-C35-C36-C37
11	P	3007	PEE	C34-C35-C36-C37
11	C	2007	PEE	C40-C41-C42-C43
17	Q	3009	BOG	C2'-C3'-C4'-C5'
11	P	3007	PEE	C11-C12-C13-C14
11	C	2005	PEE	C19-C20-C21-C22
11	P	3005	PEE	C19-C20-C21-C22
11	P	3007	PEE	C39-C40-C41-C42
11	A	2008	PEE	O4-C10-O2-C2
11	A	2008	PEE	C31-C30-O3-C3
17	C	3010	BOG	C4'-C5'-C6'-C7'
11	P	3007	PEE	C14-C15-C16-C17
11	P	3005	PEE	C40-C41-C42-C43
17	D	2009	BOG	C2'-C3'-C4'-C5'
11	A	2008	PEE	C11-C10-O2-C2
11	C	2007	PEE	C21-C22-C23-C24
11	C	2007	PEE	C11-C12-C13-C14
11	P	3005	PEE	C11-C12-C13-C14
11	P	3007	PEE	C21-C22-C23-C24
11	C	2007	PEE	C39-C40-C41-C42
11	P	3005	PEE	C37-C38-C39-C40
11	C	2005	PEE	C11-C12-C13-C14
13	C	502	HEM	C4D-C3D-CAD-CBD
13	P	502	HEM	C4D-C3D-CAD-CBD
19	G	2004	CDL	CA3-OA5-PA1-OA2
19	T	3004	CDL	CA3-OA5-PA1-OA2
11	A	2008	PEE	O3P-C1-C2-C3
11	C	2005	PEE	C40-C41-C42-C43
11	P	3007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C32-C33-C34-C35
11	A	2008	PEE	O5-C30-O3-C3
11	C	2007	PEE	C14-C15-C16-C17
19	G	2004	CDL	CA3-CA4-CA6-OA8
19	T	3004	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
11	C	2005	PEE	C17-C18-C19-C20
11	P	3005	PEE	C17-C18-C19-C20
11	C	2007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C15-C16-C17-C18
19	Q	3003	CDL	C71-C72-C73-C74
11	C	2007	PEE	C32-C33-C34-C35
19	D	2003	CDL	C71-C72-C73-C74
11	P	3005	PEE	O3P-C1-C2-O2
17	Q	3009	BOG	C1'-C2'-C3'-C4'
11	P	3005	PEE	C20-C21-C22-C23
11	C	2005	PEE	C20-C21-C22-C23
14	C	2001	FNM	N4-C5-C8-C9
14	C	2001	FNM	N4-C5-C8-C13
14	P	3001	FNM	N4-C5-C8-C9
11	P	3005	PEE	O3P-C1-C2-C3
11	P	3007	PEE	O4P-C4-C5-N
19	D	2003	CDL	CA3-OA5-PA1-OA2
19	G	2004	CDL	CA2-OA2-PA1-OA5
19	Q	3003	CDL	CA3-OA5-PA1-OA2
19	T	3004	CDL	CA2-OA2-PA1-OA5
11	C	2005	PEE	O3P-C1-C2-O2
19	G	2004	CDL	OB5-CB3-CB4-OB6
17	Q	3091	BOG	C3'-C4'-C5'-C6'
11	C	2005	PEE	C12-C13-C14-C15
19	D	2003	CDL	OA6-CA4-CA6-OA8
19	Q	3003	CDL	OA6-CA4-CA6-OA8
11	C	2005	PEE	C37-C38-C39-C40
17	D	2091	BOG	C1'-C2'-C3'-C4'
17	Q	3091	BOG	O1-C1'-C2'-C3'
11	P	3005	PEE	C12-C13-C14-C15
17	C	3010	BOG	O1-C1'-C2'-C3'
13	P	502	HEM	C2D-C3D-CAD-CBD
11	C	2005	PEE	O3P-C1-C2-C3
11	A	2008	PEE	O3P-C1-C2-O2
11	C	2005	PEE	C21-C22-C23-C24
19	D	2003	CDL	CB5-C51-C52-C53
19	Q	3003	CDL	CB5-C51-C52-C53
11	P	3007	PEE	C43-C44-C45-C46
11	P	3005	PEE	C21-C22-C23-C24
19	D	2003	CDL	CA3-OA5-PA1-OA4
19	G	2004	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
19	G	2004	CDL	CA3-OA5-PA1-OA4
19	G	2004	CDL	CB2-OB2-PB2-OB3
19	G	2004	CDL	CB3-OB5-PB2-OB4
19	Q	3003	CDL	CA2-OA2-PA1-OA3
19	Q	3003	CDL	CA3-OA5-PA1-OA4
19	T	3004	CDL	CA3-OA5-PA1-OA4
19	T	3004	CDL	CB2-OB2-PB2-OB3
19	T	3004	CDL	CB3-OB5-PB2-OB4
11	C	2005	PEE	C35-C36-C37-C38
11	P	3005	PEE	C35-C36-C37-C38
19	Q	3003	CDL	OB7-CB5-OB6-CB4
19	Q	3003	CDL	OB5-CB3-CB4-OB6
19	T	3004	CDL	OB5-CB3-CB4-OB6
19	Q	3003	CDL	C51-CB5-OB6-CB4
19	G	2004	CDL	OA6-CA4-CA6-OA8
19	T	3004	CDL	OA6-CA4-CA6-OA8
11	C	2007	PEE	C33-C34-C35-C36
11	C	2007	PEE	C43-C44-C45-C46
11	P	3005	PEE	C15-C16-C17-C18
13	C	502	HEM	C2D-C3D-CAD-CBD
11	A	2008	PEE	O5-C30-C31-C32
19	T	3004	CDL	C1-CB2-OB2-PB2
19	D	2003	CDL	OB7-CB5-OB6-CB4
17	Q	3009	BOG	C3'-C4'-C5'-C6'
11	C	2005	PEE	C15-C16-C17-C18
13	P	502	HEM	CAA-CBA-CGA-O2A
11	P	3007	PEE	C33-C34-C35-C36
19	D	2003	CDL	OB5-CB3-CB4-OB6
11	P	3005	PEE	C42-C43-C44-C45
13	P	502	HEM	CAA-CBA-CGA-O1A
19	G	2004	CDL	C1-CB2-OB2-PB2
11	C	2005	PEE	C13-C14-C15-C16
11	P	3005	PEE	C13-C14-C15-C16
13	C	502	HEM	CAA-CBA-CGA-O1A
11	C	2007	PEE	C19-C20-C21-C22
13	C	502	HEM	CAA-CBA-CGA-O2A
11	C	2007	PEE	C31-C32-C33-C34
17	C	3010	BOG	C1'-C2'-C3'-C4'
11	C	2005	PEE	C1-C2-O2-C10
11	P	3005	PEE	C1-C2-O2-C10
11	A	2008	PEE	O3-C30-C31-C32
19	D	2003	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
19	Q	3003	CDL	C12-C11-CA5-OA6
19	T	3004	CDL	CB3-OB5-PB2-OB2
13	P	502	HEM	CAD-CBD-CGD-O1D
11	P	3007	PEE	C31-C32-C33-C34
13	C	501	HEM	CAA-CBA-CGA-O1A
13	C	501	HEM	CAA-CBA-CGA-O2A
11	C	2005	PEE	C42-C43-C44-C45
13	P	502	HEM	CAD-CBD-CGD-O2D
18	D	501	HEC	CAD-CBD-CGD-O2D
19	D	2003	CDL	C51-CB5-OB6-CB4
11	P	3005	PEE	C36-C37-C38-C39
13	C	502	HEM	CAD-CBD-CGD-O2D
18	Q	501	HEC	CAD-CBD-CGD-O2D
19	G	2004	CDL	OB5-CB3-CB4-CB6
13	P	501	HEM	CAA-CBA-CGA-O1A
11	C	2007	PEE	C18-C19-C20-C21
13	C	502	HEM	CAD-CBD-CGD-O1D
13	P	501	HEM	CAA-CBA-CGA-O2A
11	C	2007	PEE	C16-C17-C18-C19
11	C	2007	PEE	O2-C10-C11-C12
11	P	3007	PEE	O2-C10-C11-C12
11	P	3007	PEE	C18-C19-C20-C21
11	P	3007	PEE	C16-C17-C18-C19
11	C	2005	PEE	C36-C37-C38-C39
11	C	2007	PEE	C38-C39-C40-C41
11	P	3005	PEE	C38-C39-C40-C41
11	P	3007	PEE	C38-C39-C40-C41
19	D	2003	CDL	CA3-CA4-CA6-OA8
19	Q	3003	CDL	CA3-CA4-CA6-OA8
11	P	3007	PEE	O3-C30-C31-C32
18	D	501	HEC	CAD-CBD-CGD-O1D
18	Q	501	HEC	CAD-CBD-CGD-O1D
11	P	3007	PEE	C19-C20-C21-C22
19	D	2003	CDL	OB5-CB3-CB4-CB6
19	Q	3003	CDL	OB5-CB3-CB4-CB6
19	T	3004	CDL	OB5-CB3-CB4-CB6
11	C	2007	PEE	O3-C30-C31-C32
11	C	2005	PEE	C38-C39-C40-C41
19	D	2003	CDL	C72-C71-CB7-OB8
11	C	2007	PEE	O4-C10-C11-C12
19	T	3004	CDL	C31-CA7-OA8-CA6
19	T	3004	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	O4-C10-C11-C12
11	P	3007	PEE	O5-C30-C31-C32
17	D	2091	BOG	C2'-C3'-C4'-C5'
11	C	2007	PEE	O5-C30-C31-C32
11	A	2008	PEE	O2-C10-C11-C12
19	Q	3003	CDL	C72-C71-CB7-OB8
11	P	3005	PEE	C22-C23-C24-C25
11	A	2008	PEE	O4-C10-C11-C12
19	D	2003	CDL	C72-C71-CB7-OB9
19	D	2003	CDL	C52-C51-CB5-OB6
19	Q	3003	CDL	C52-C51-CB5-OB6

There are no ring outliers.

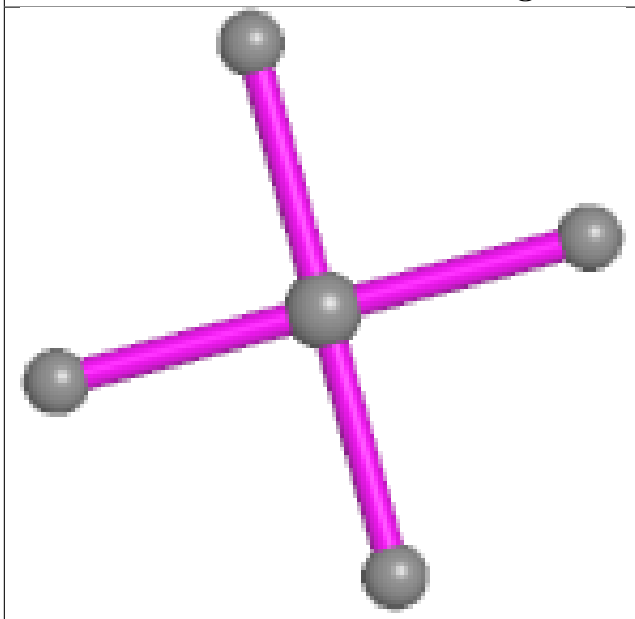
22 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	501	HEM	1	0
19	Q	3003	CDL	3	0
20	E	501	FES	1	0
19	D	2003	CDL	2	0
19	T	3004	CDL	1	0
15	P	3002	UQ	3	0
15	C	2002	UQ	4	0
13	P	502	HEM	4	0
14	C	2001	FNM	2	0
18	Q	501	HEC	1	0
17	P	2010	BOG	1	0
13	C	502	HEM	4	0
17	D	2091	BOG	1	0
14	P	3001	FNM	1	0
11	A	2008	PEE	1	0
18	D	501	HEC	3	0
17	D	2009	BOG	1	0
13	C	501	HEM	1	0
20	R	501	FES	2	0
17	Q	3091	BOG	1	0
11	P	3007	PEE	1	0
19	G	2004	CDL	1	0

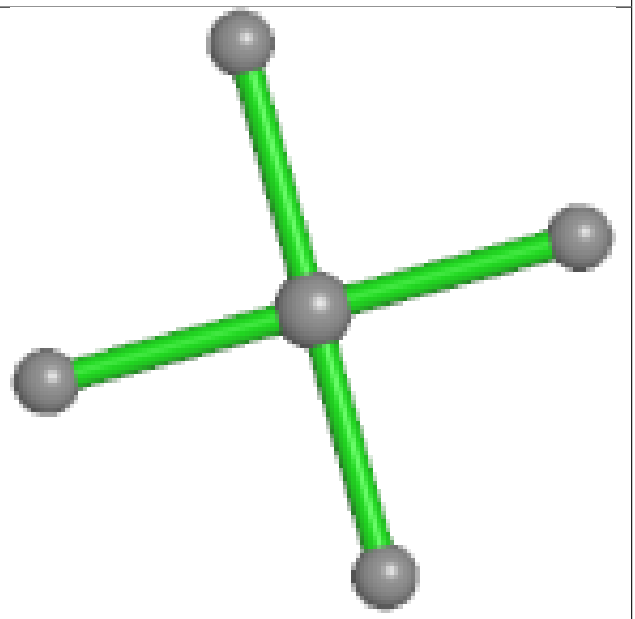
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

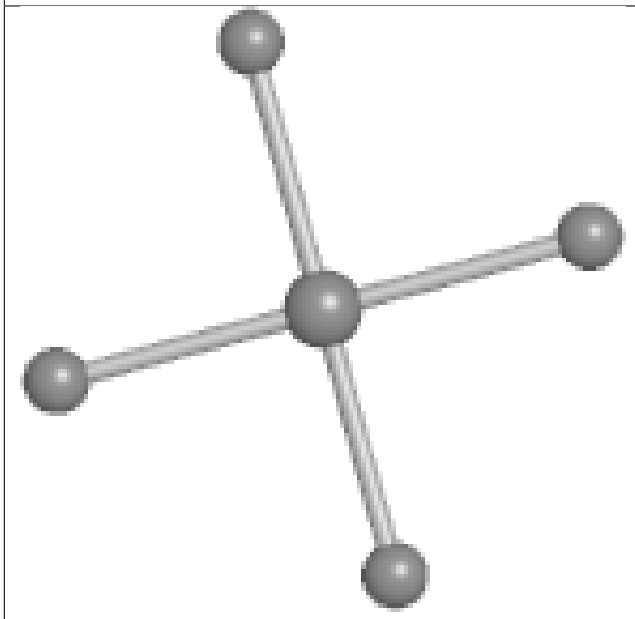
Ligand PEE N 3008



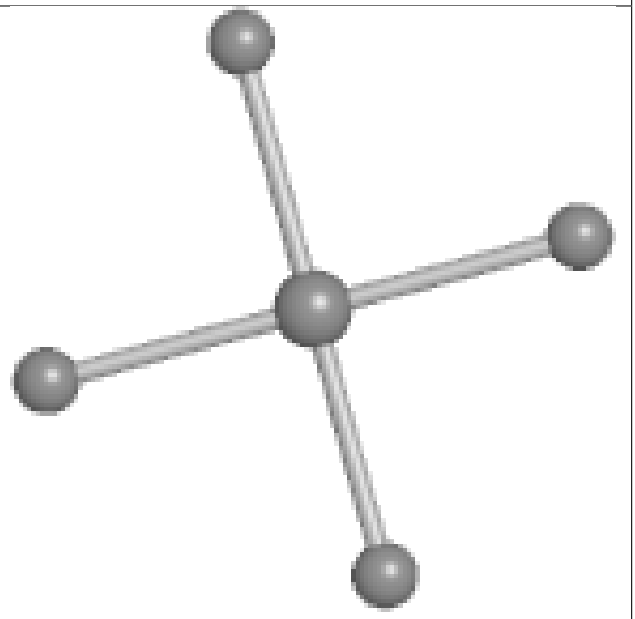
Bond lengths



Bond angles

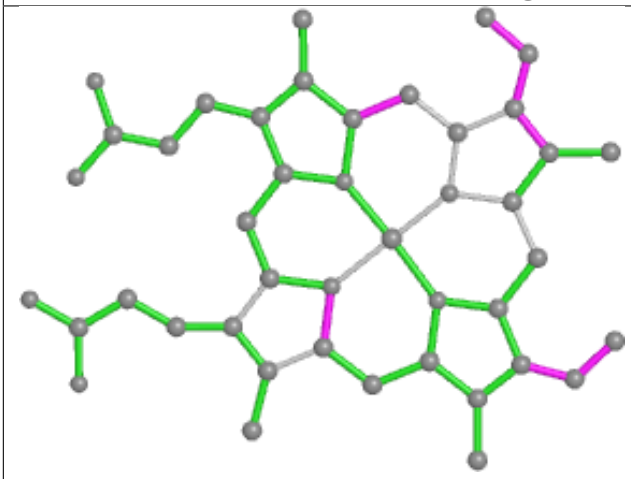


Torsions

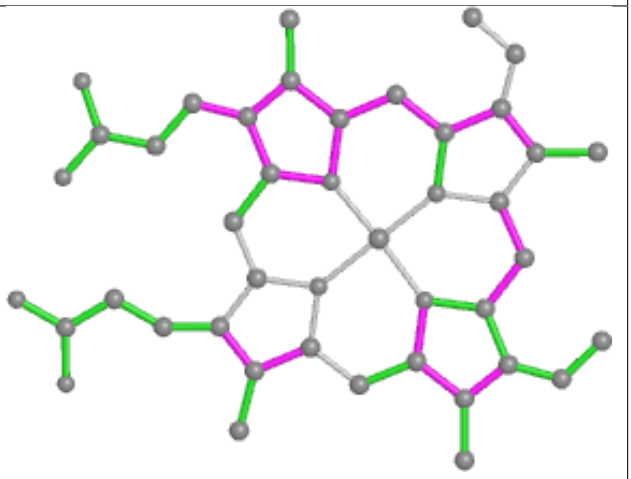


Rings

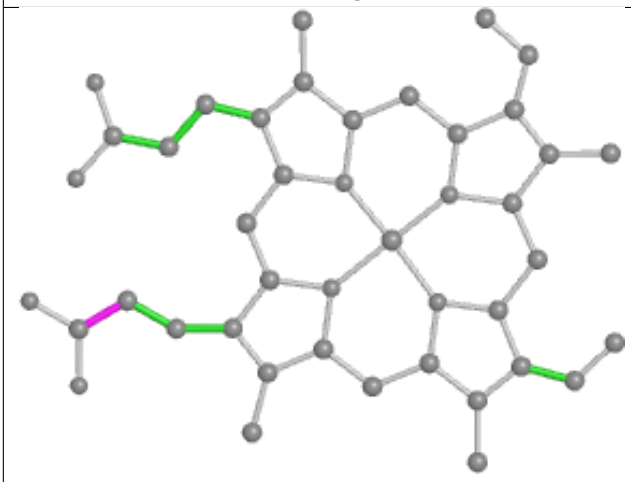
Ligand HEM P 501



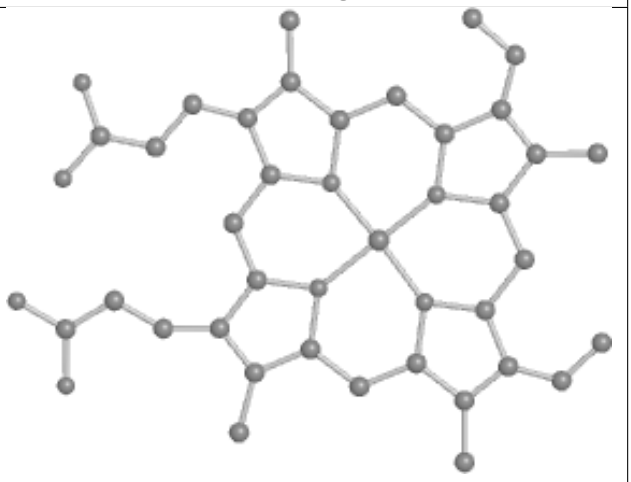
Bond lengths



Bond angles

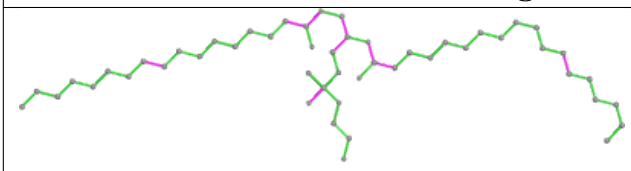


Torsions

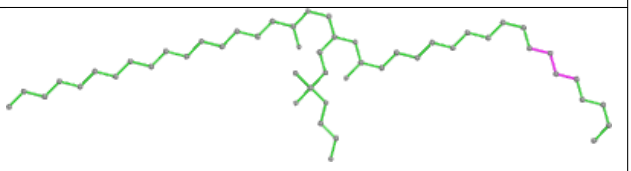


Rings

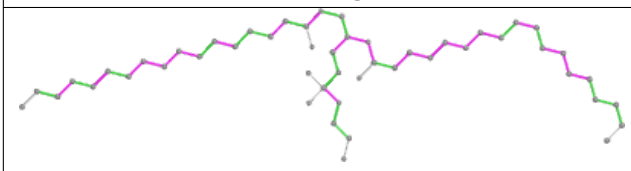
Ligand PEE C 2005



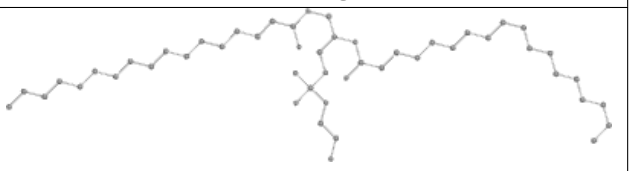
Bond lengths



Bond angles

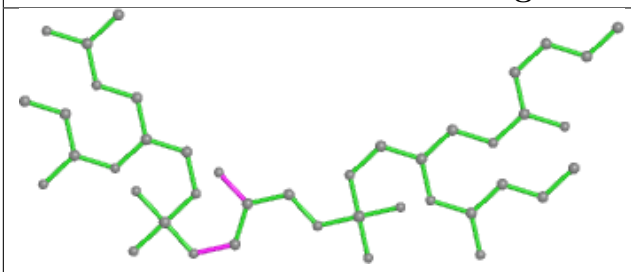


Torsions

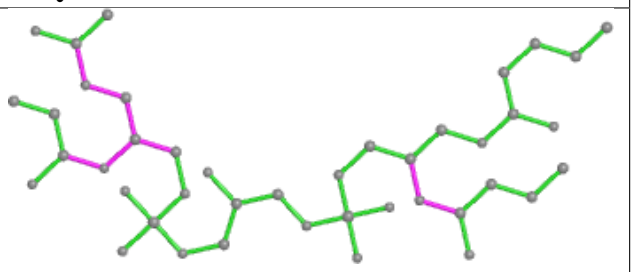


Rings

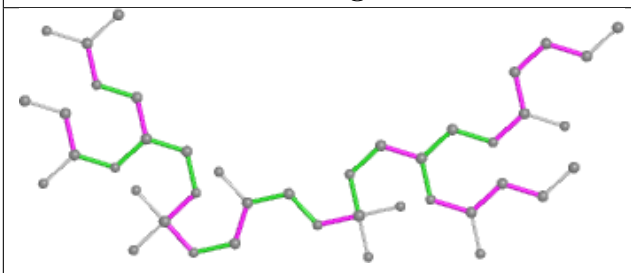
Ligand CDL Q 3003



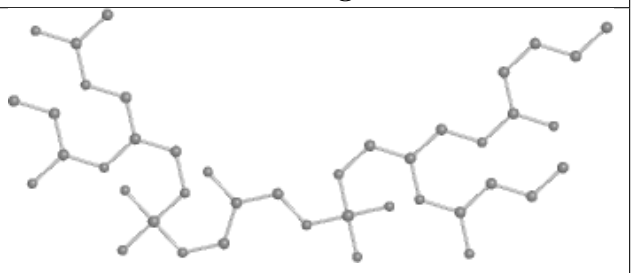
Bond lengths



Bond angles

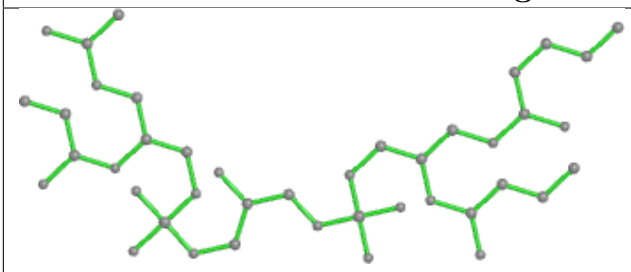


Torsions

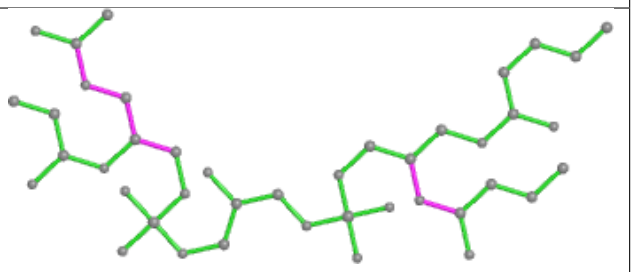


Rings

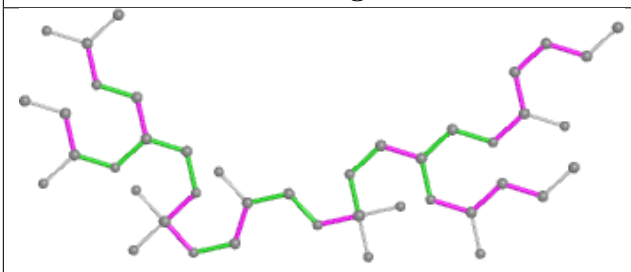
Ligand CDL D 2003



Bond lengths



Bond angles



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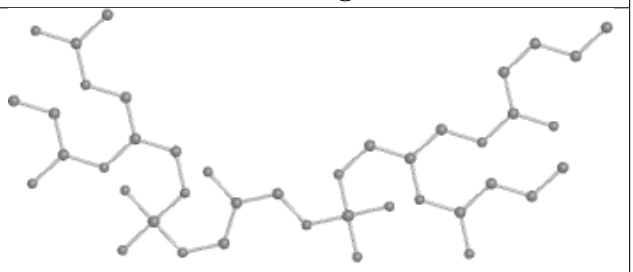
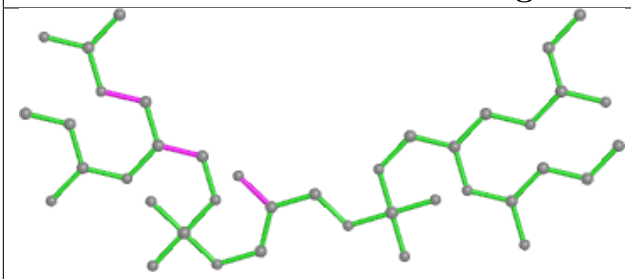


Rings

Ligand CDL T 3004



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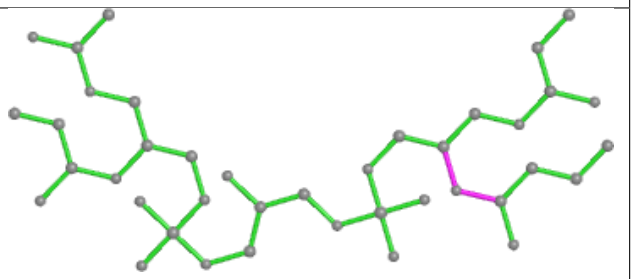
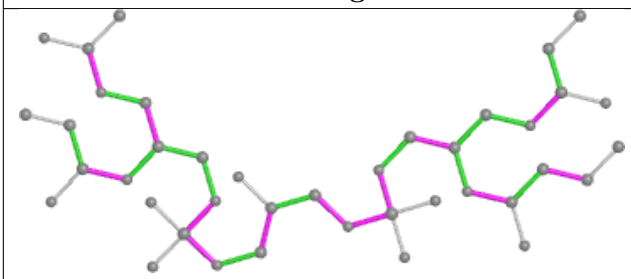


Bond angles



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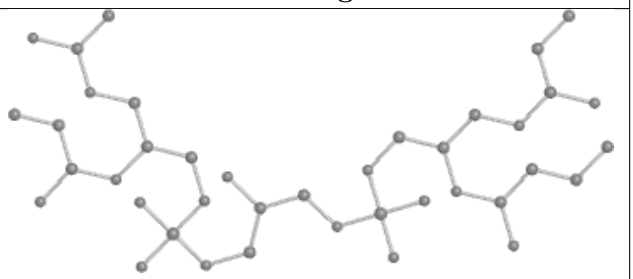
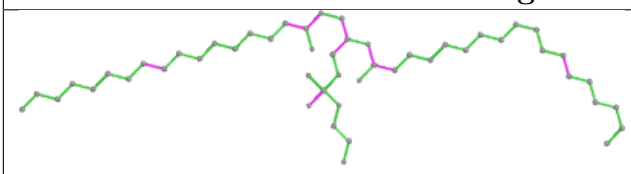
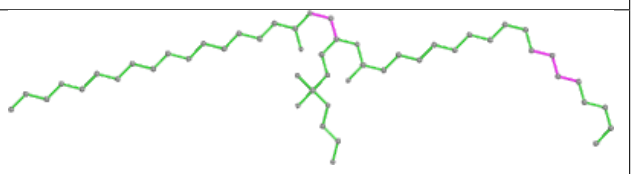


Rings

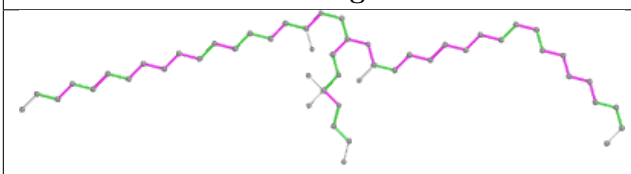
Ligand PEE P 3005



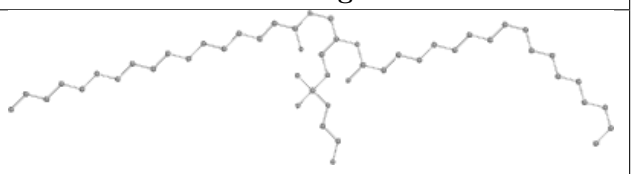
Bond lengths



Bond angles

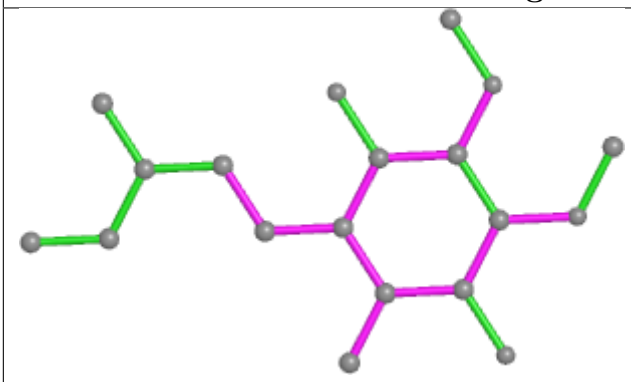


Torsions

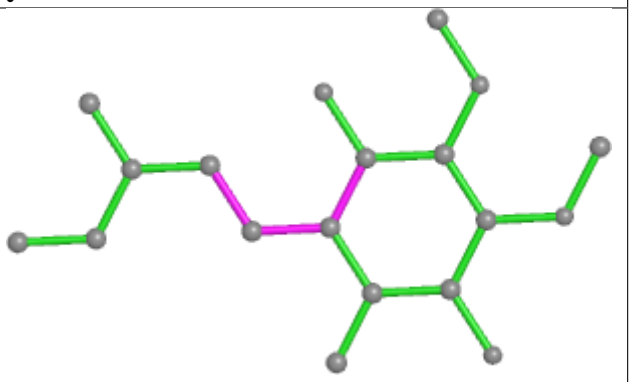


Rings

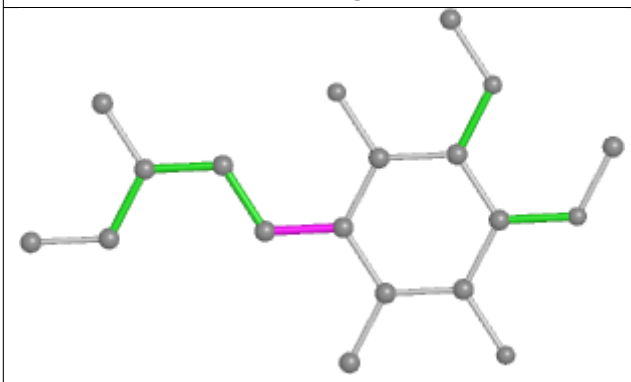
Ligand UQ P 3002



Bond lengths



Bond angles



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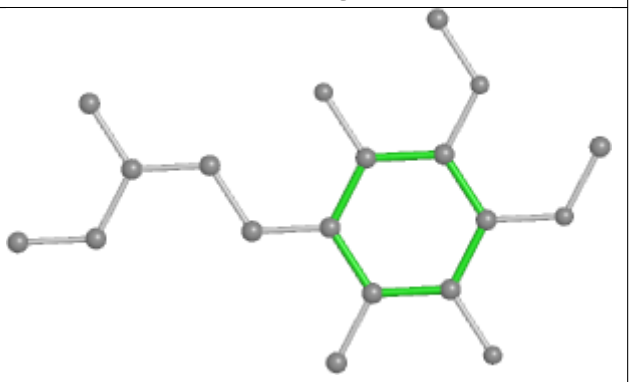
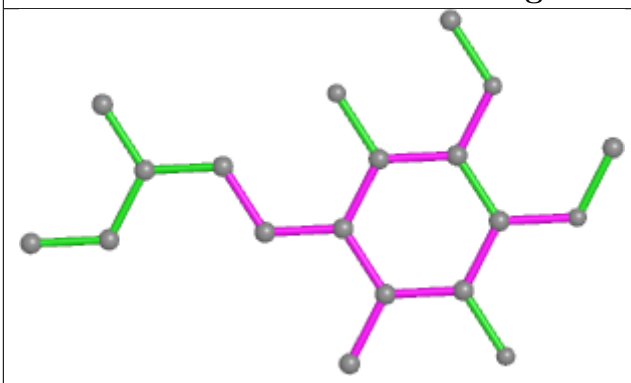


Rings

Ligand UQ C 2002



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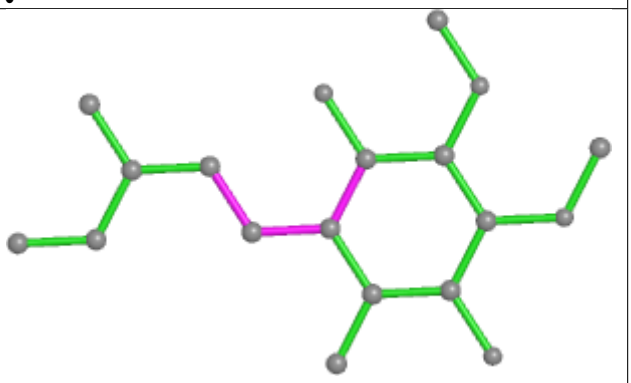
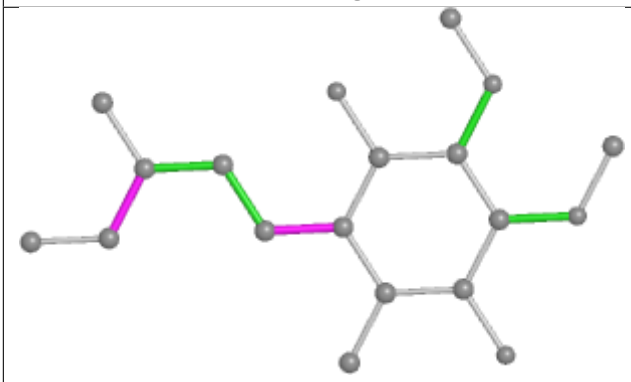


Bond angles



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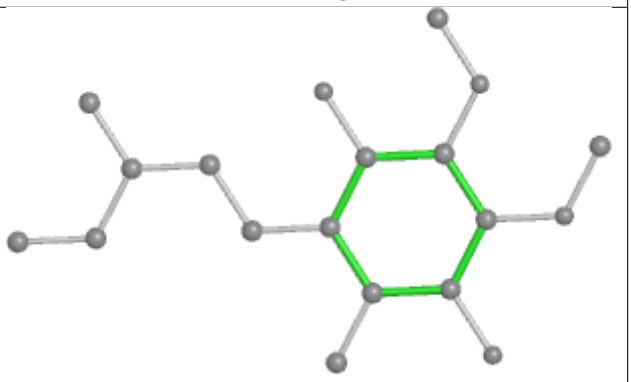
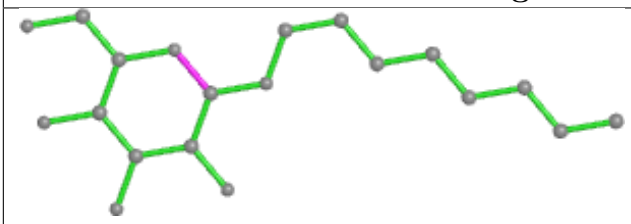


Rings

Ligand BOG Q 3009



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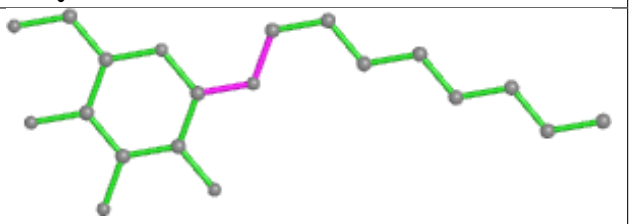
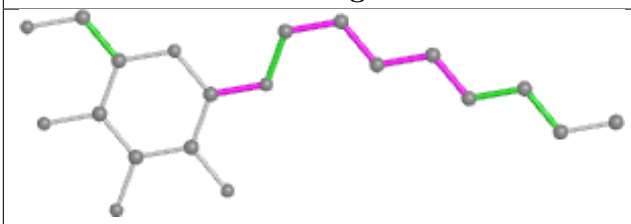


Bond angles



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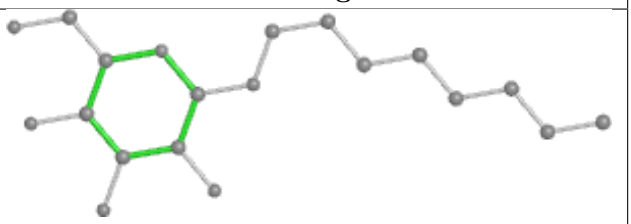
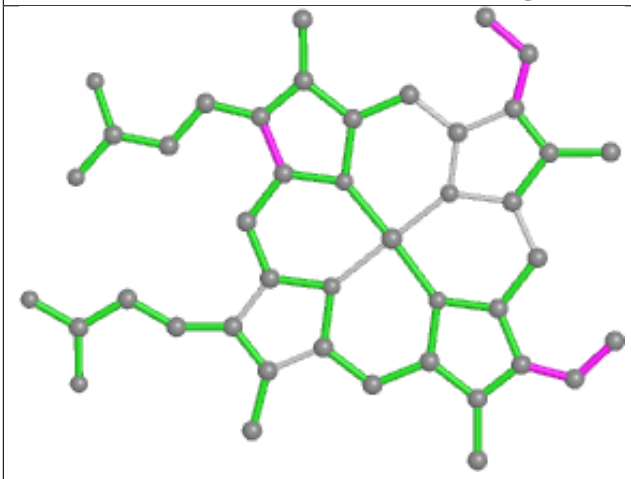


Rings

Ligand HEM P 502



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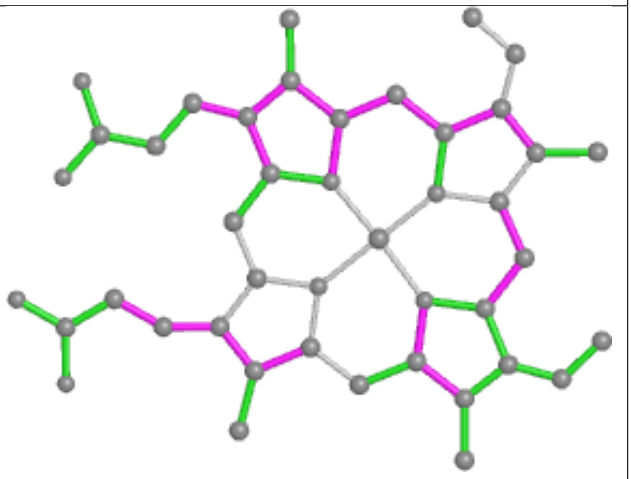
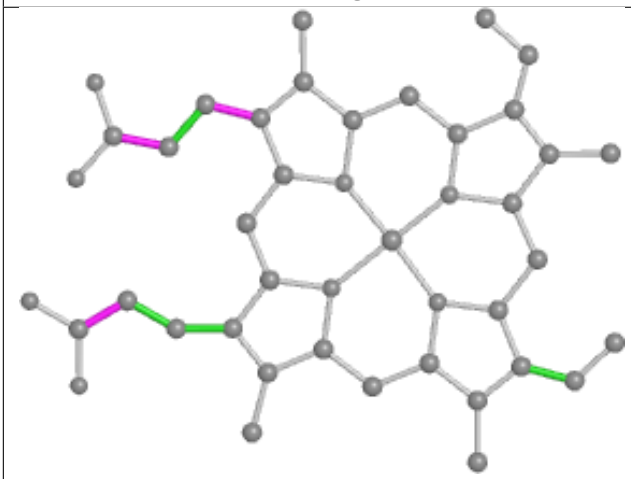


Bond angles



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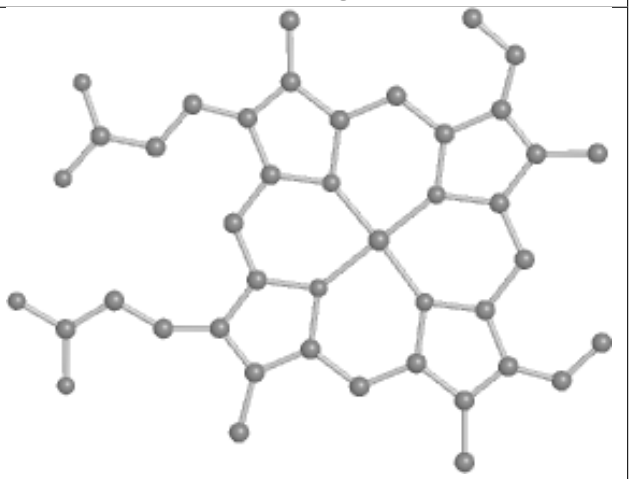
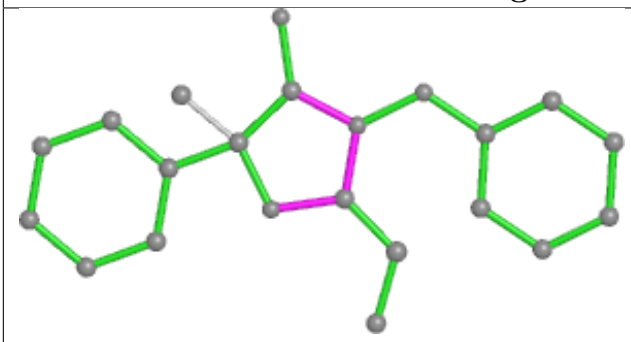


Rings

Ligand FNM C 2001



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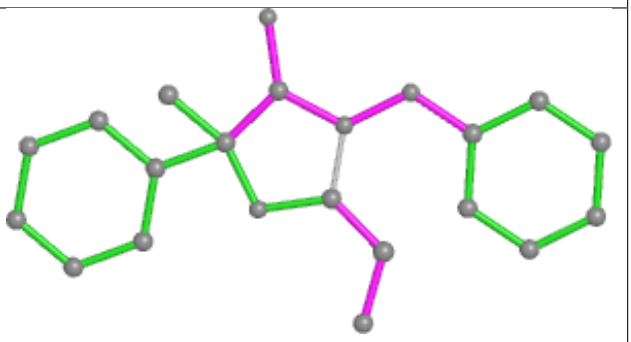
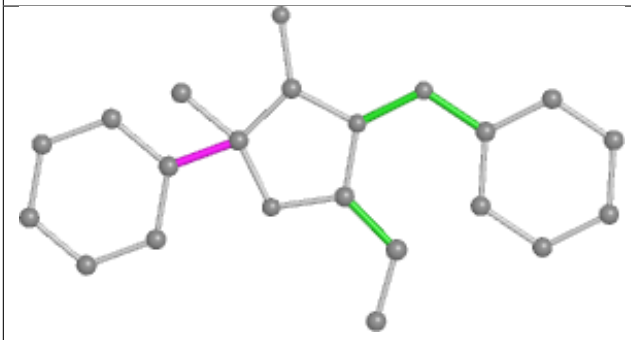


Bond angles



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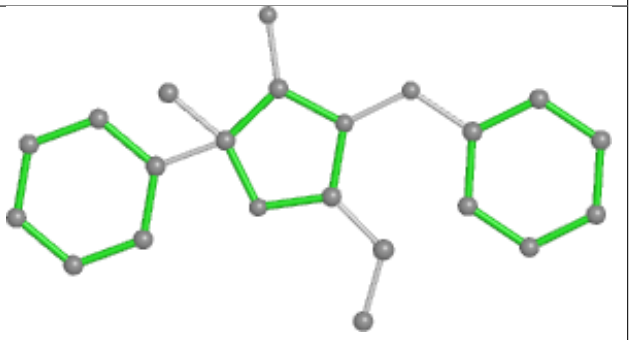
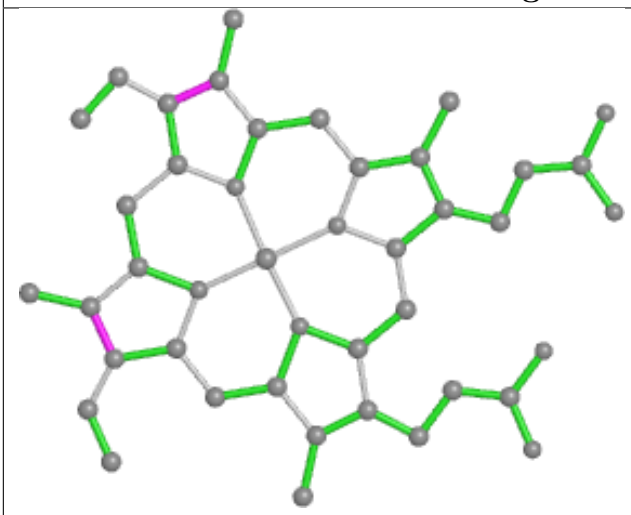


Rings

Ligand HEC Q 501



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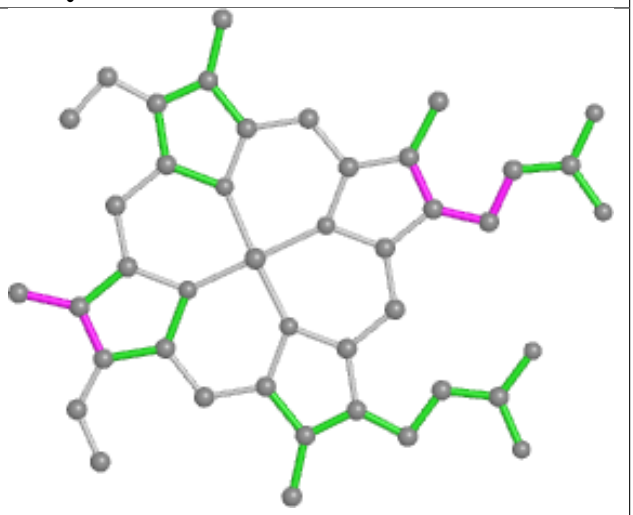

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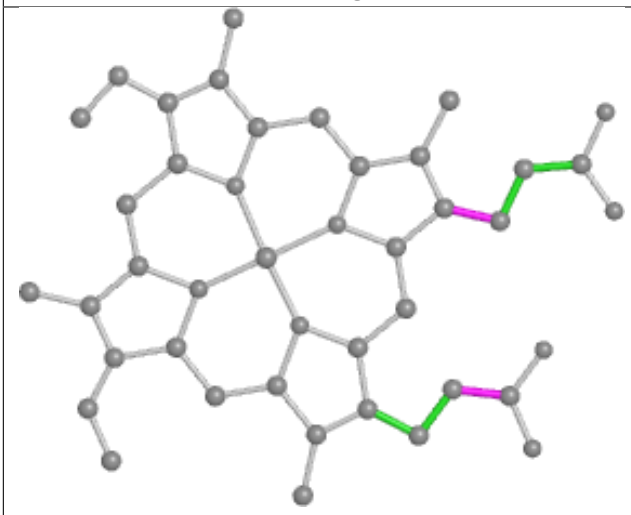

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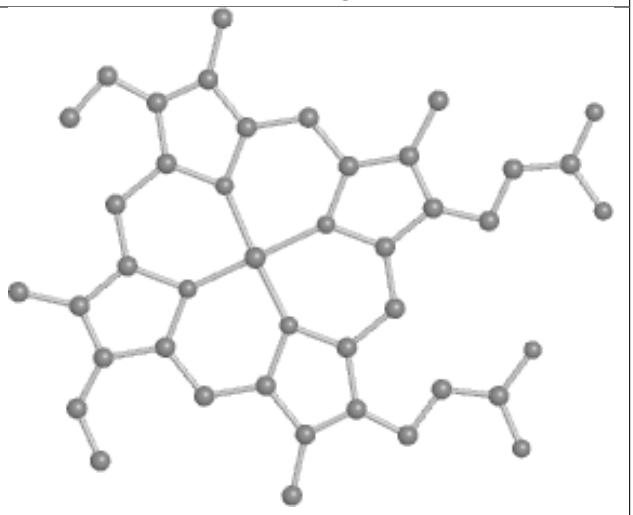
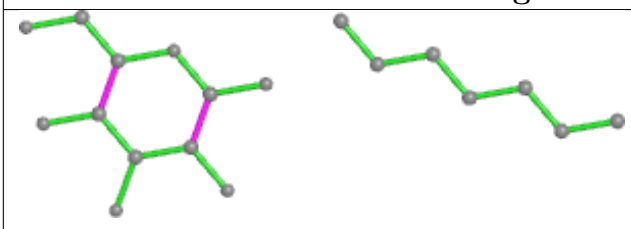


Rings

Ligand BOG P 2010



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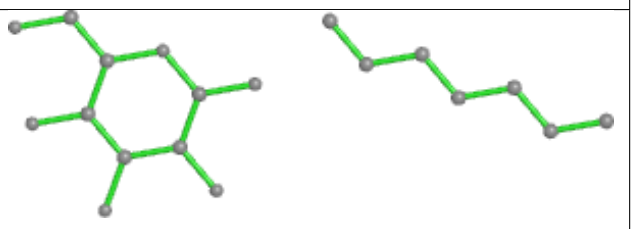
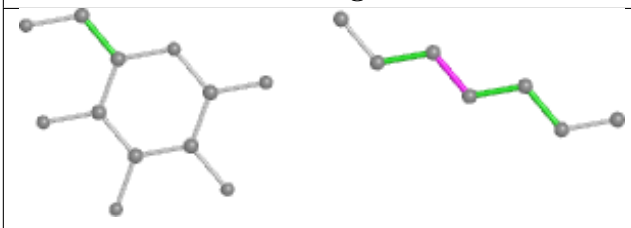


Bond angles



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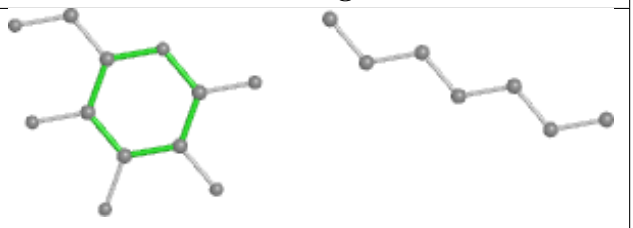
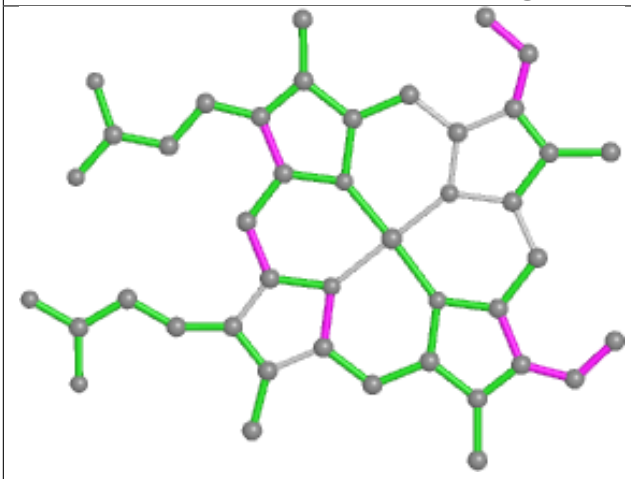


Rings

Ligand HEM C 502



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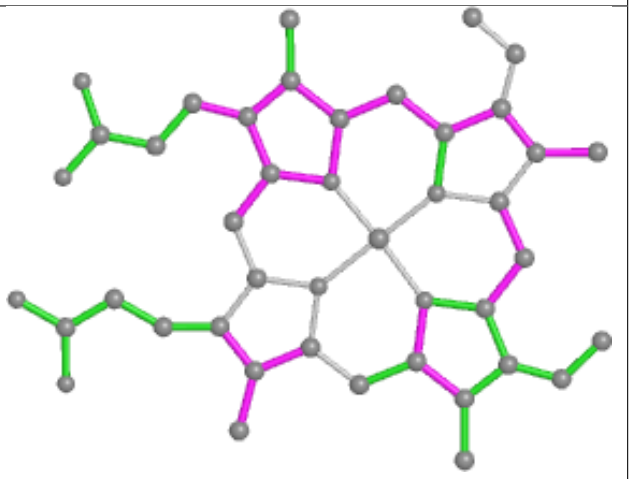
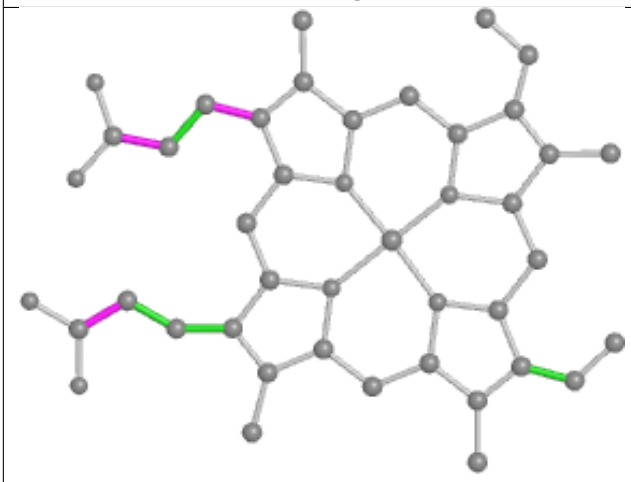


Bond angles



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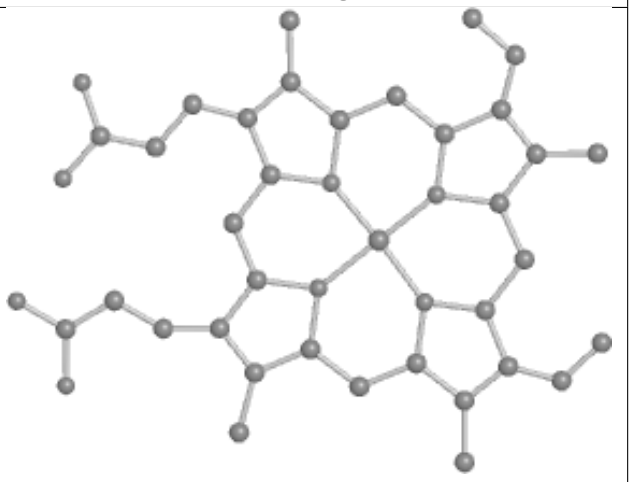
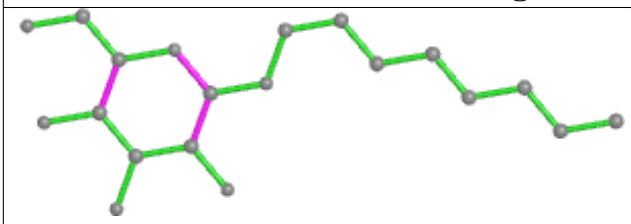


Rings

Ligand BOG D 2091



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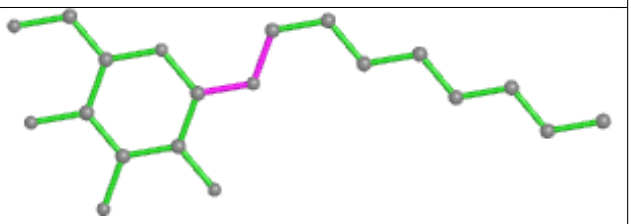
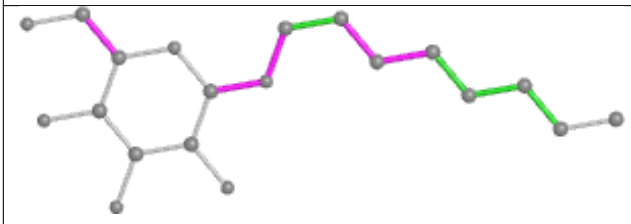


Bond angles



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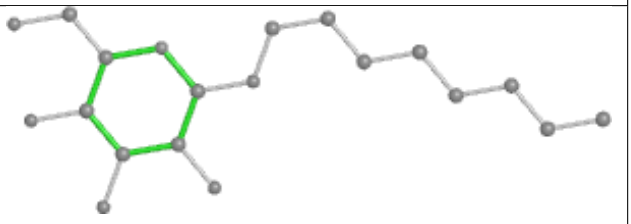
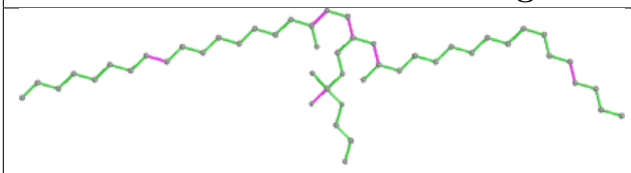


Rings

Ligand PEE C 2007



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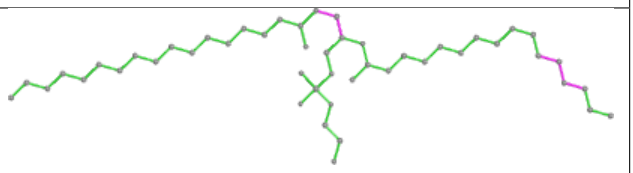
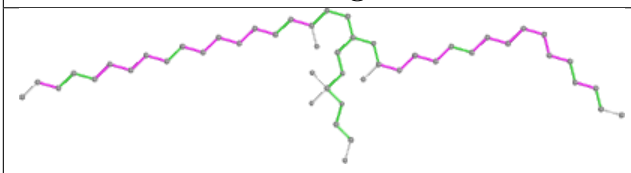


Bond angles



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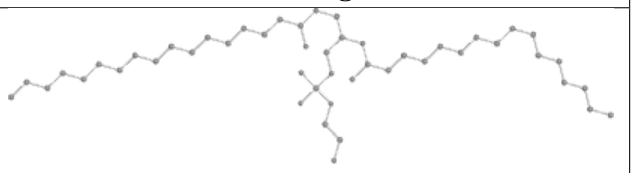
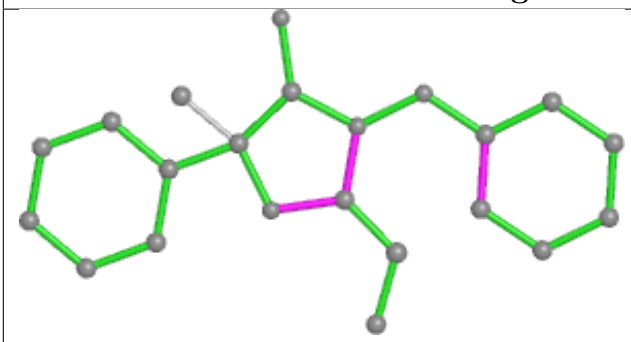


Rings

Ligand FNM P 3001



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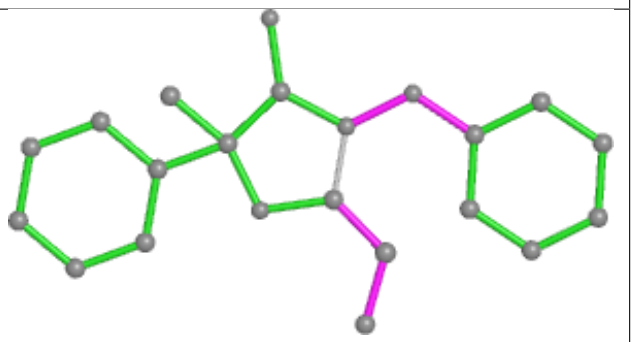
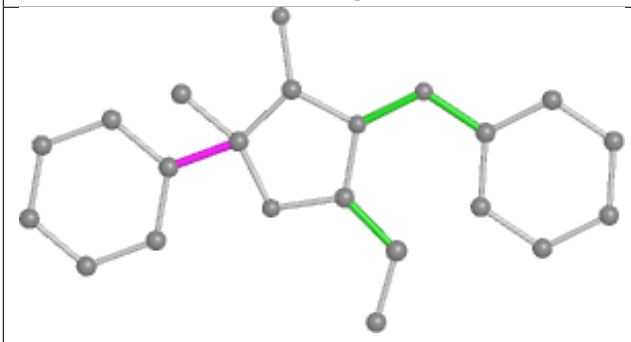
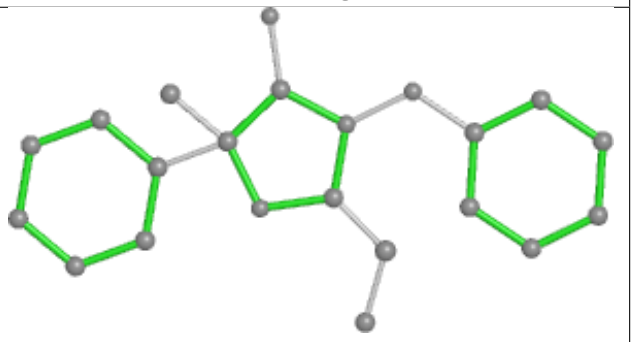


Bond angles

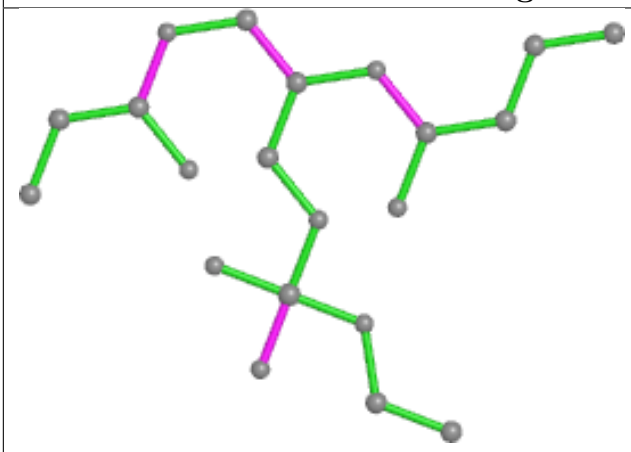


Torsions



Rings

Ligand PEE A 2008



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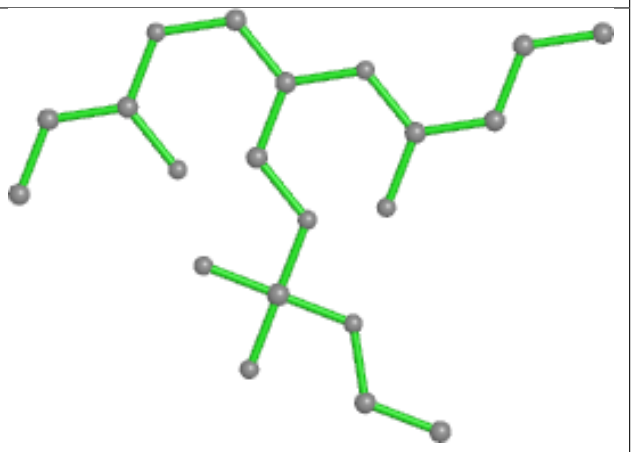
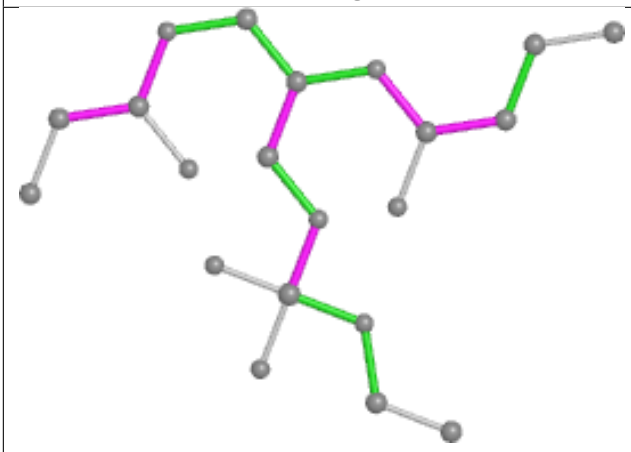


Bond angles



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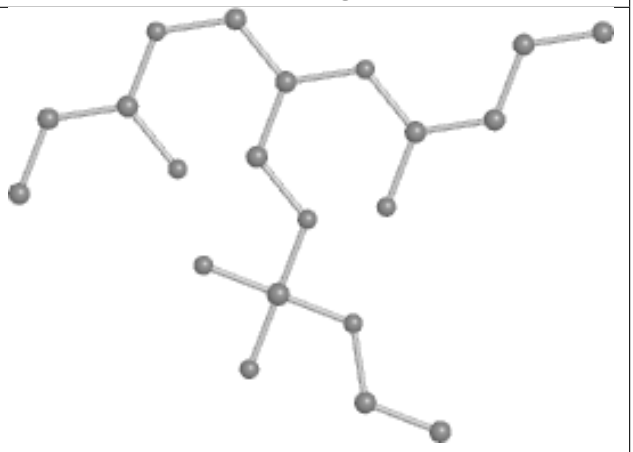
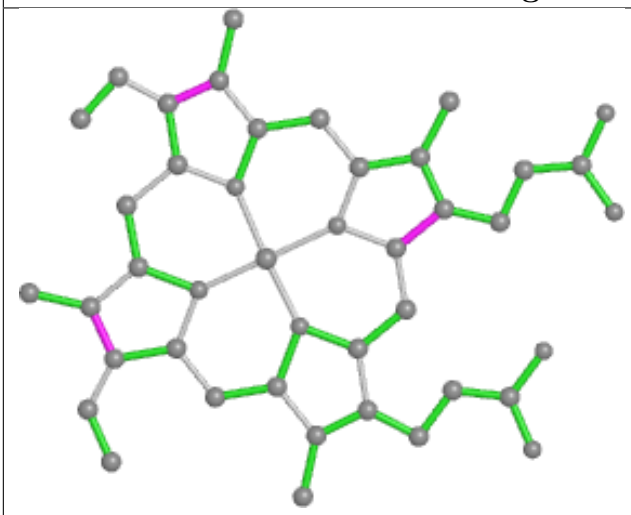


Rings

Ligand HEC D 501



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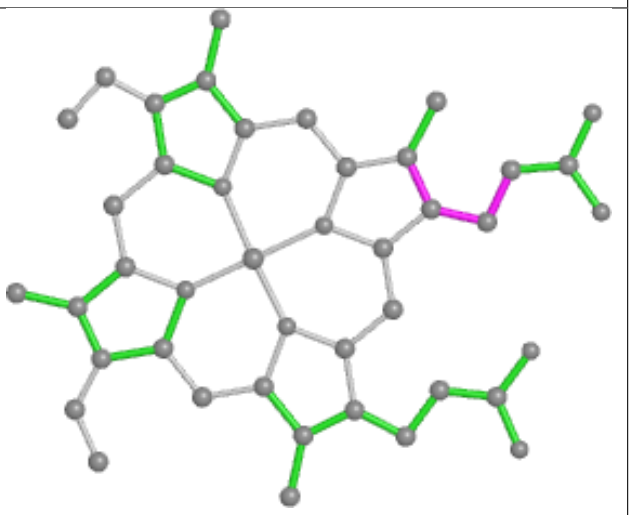
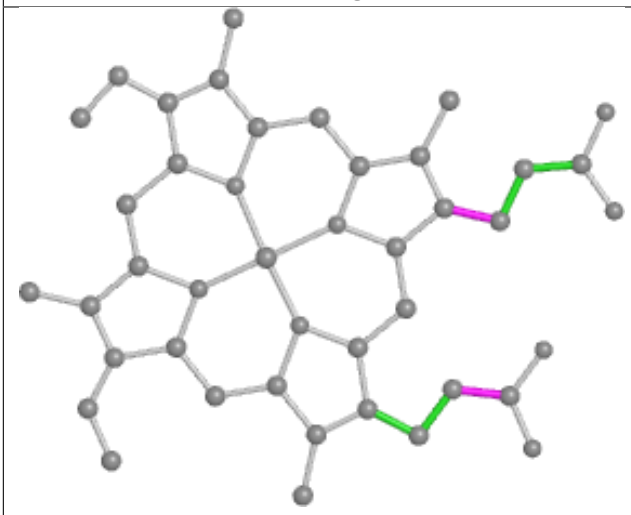


Bond angles



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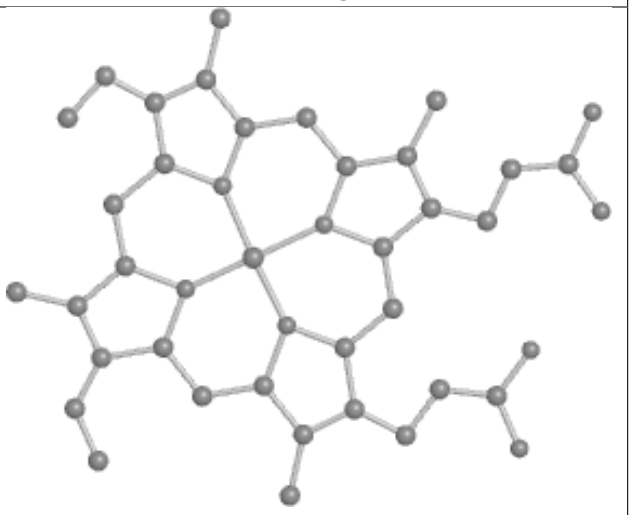
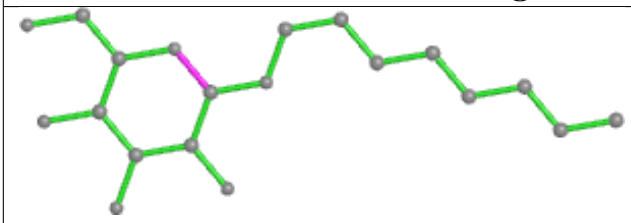


Rings

Ligand BOG D 2009



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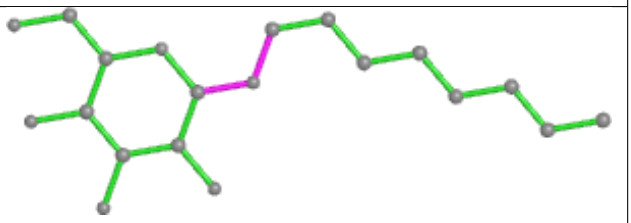
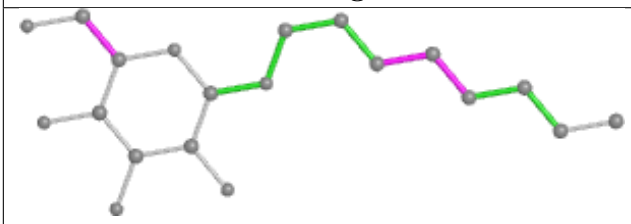


Bond angles



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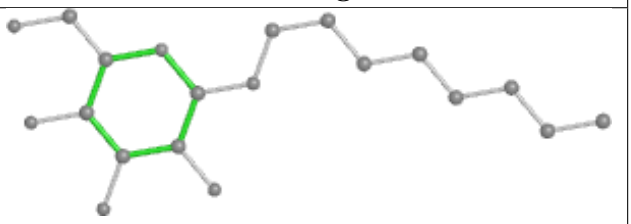
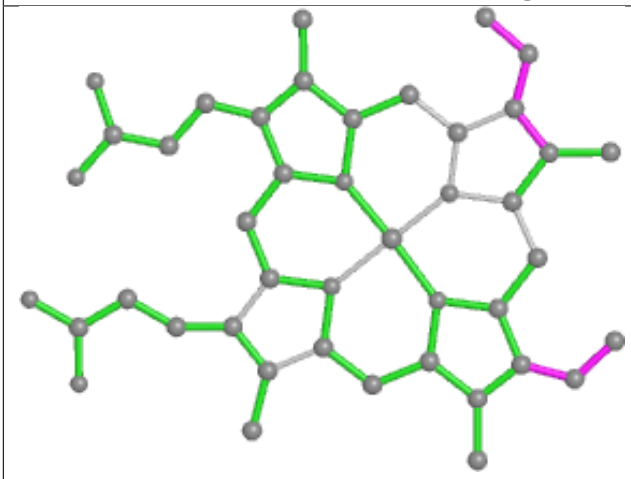
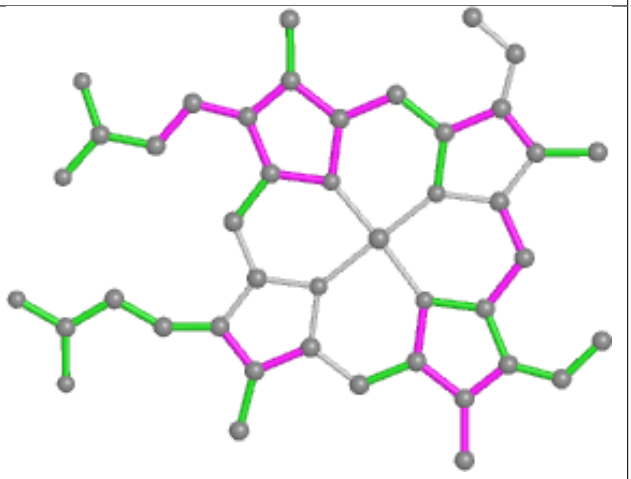


Rings

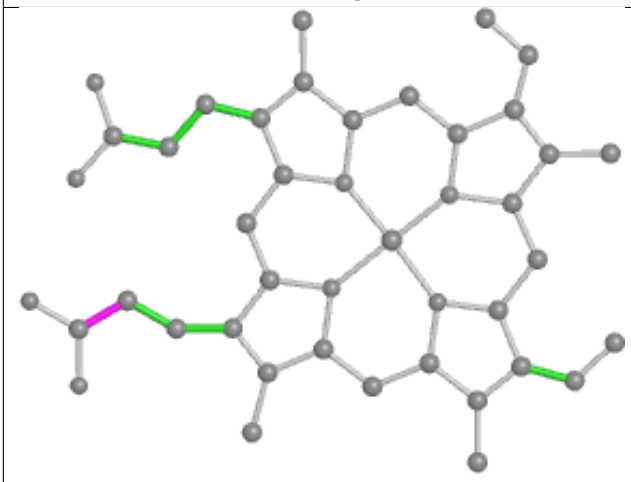
Ligand HEM C 501



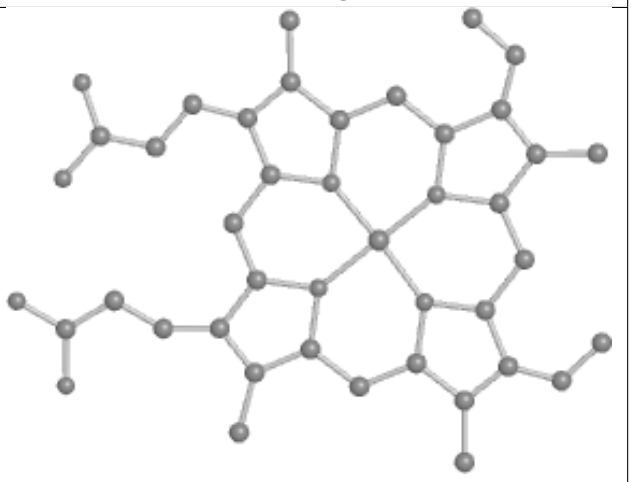
Bond lengths



Bond angles

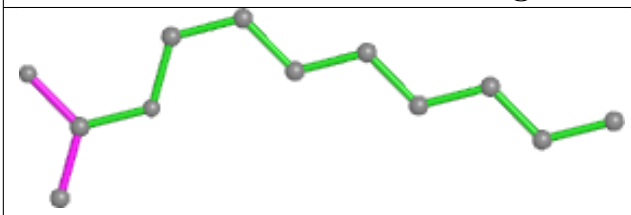


Torsions

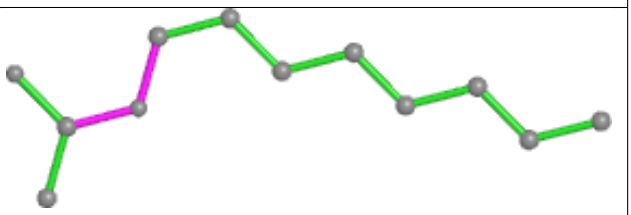


Rings

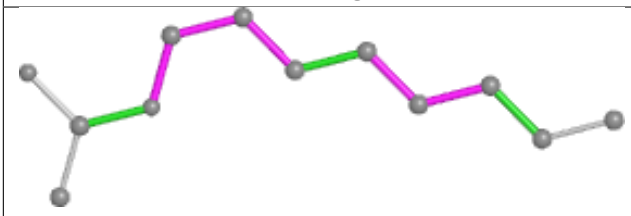
Ligand BOG C 3010



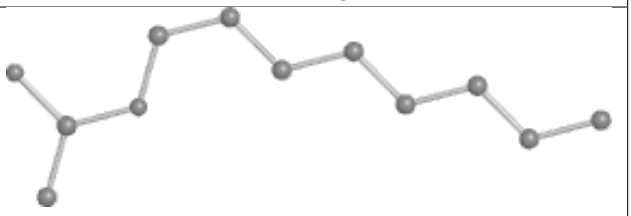
Bond lengths



Bond angles

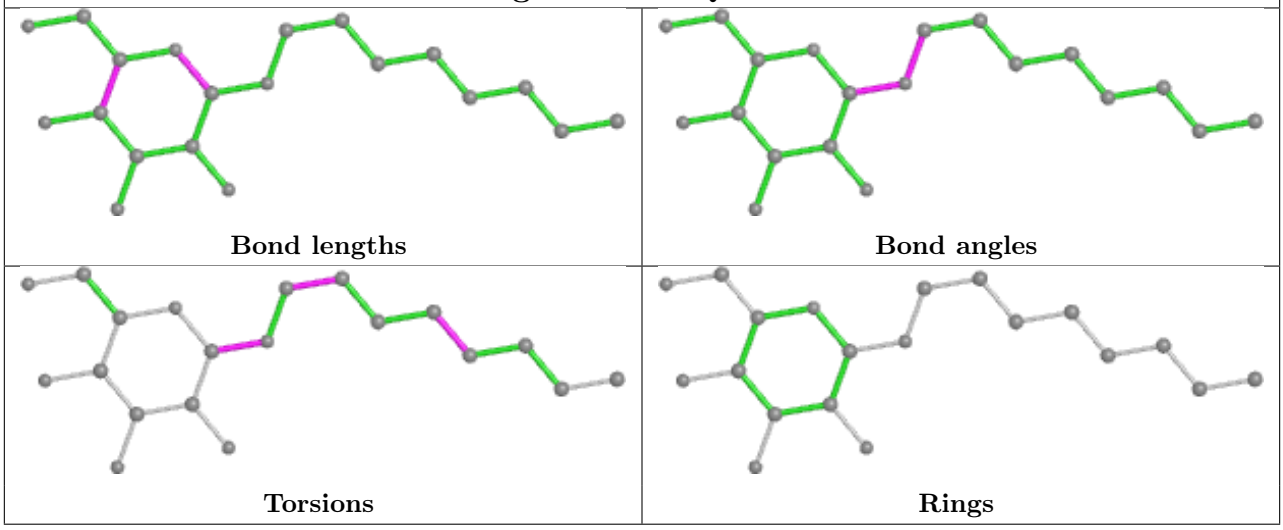


Torsions

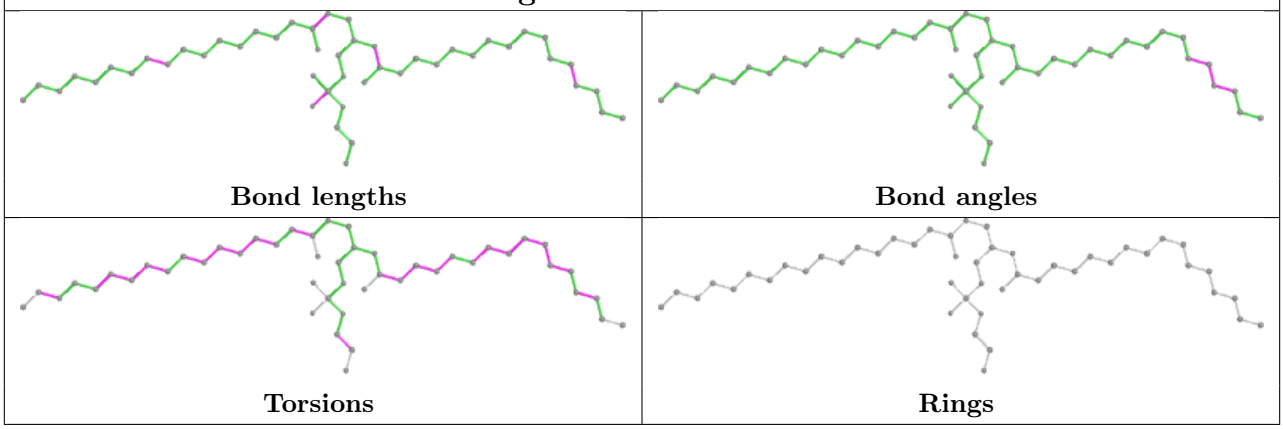


Rings

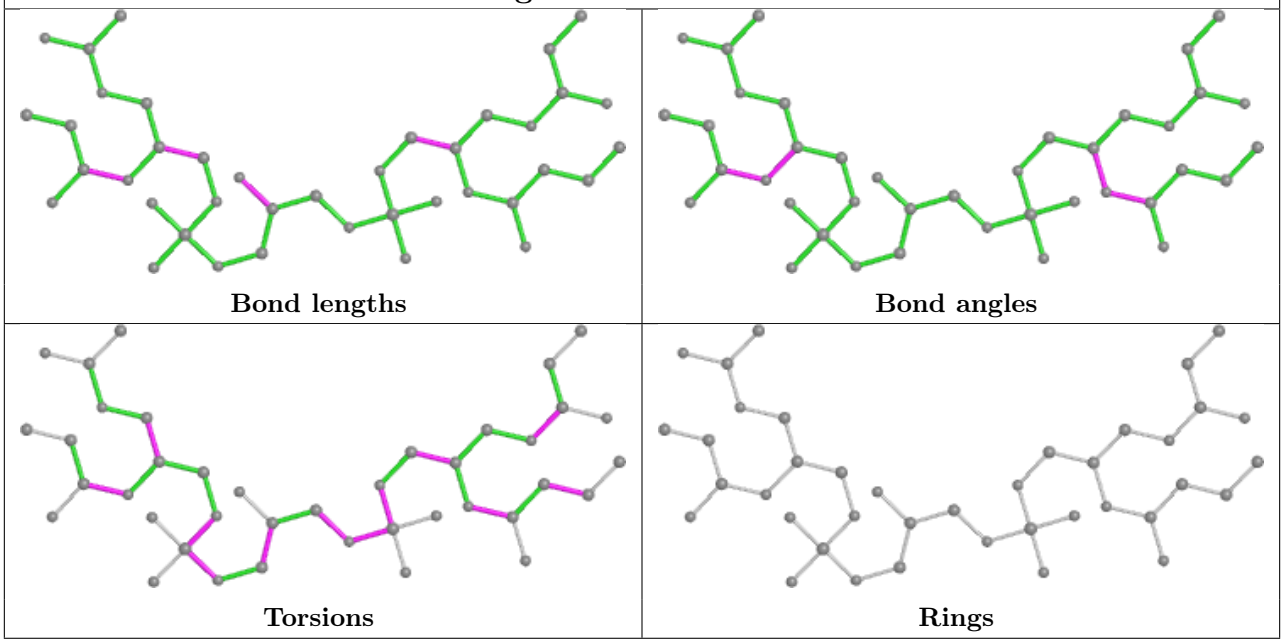
Ligand BOG Q 3091



Ligand PEE P 3007



Ligand CDL G 2004



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.12	9 (2%) 65 56	29, 61, 87, 104	0
1	N	442/446 (99%)	0.30	20 (4%) 33 23	39, 69, 95, 104	0
2	B	421/441 (95%)	0.39	17 (4%) 38 28	50, 78, 116, 141	0
2	O	422/441 (95%)	0.26	15 (3%) 42 32	37, 74, 106, 120	0
3	C	380/380 (100%)	0.17	1 (0%) 94 93	21, 39, 73, 109	0
3	P	379/380 (99%)	0.19	4 (1%) 80 75	30, 62, 84, 96	0
4	D	241/241 (100%)	0.00	3 (1%) 79 73	30, 42, 78, 94	0
4	Q	241/241 (100%)	0.23	9 (3%) 41 31	50, 69, 99, 119	0
5	E	196/196 (100%)	1.13	55 (28%) 0 0	38, 88, 118, 125	0
5	R	196/196 (100%)	2.48	86 (43%) 0 0	42, 112, 159, 163	127 (64%)
6	F	101/110 (91%)	-0.16	0 100 100	29, 42, 60, 96	0
6	S	101/110 (91%)	0.25	4 (3%) 38 28	55, 68, 111, 135	0
7	G	81/81 (100%)	0.29	2 (2%) 57 47	32, 52, 93, 108	0
7	T	78/81 (96%)	0.77	11 (14%) 2 1	48, 82, 144, 161	0
8	H	70/77 (90%)	0.16	2 (2%) 51 41	39, 59, 84, 123	0
8	U	67/77 (87%)	1.09	12 (17%) 1 1	96, 115, 133, 140	0
9	I	31/47 (65%)	2.09	14 (45%) 0 0	81, 105, 125, 126	0
9	V	31/47 (65%)	2.03	13 (41%) 0 0	69, 109, 142, 145	0
10	J	61/61 (100%)	0.40	5 (8%) 11 6	44, 60, 92, 130	0
10	W	60/61 (98%)	1.01	5 (8%) 11 6	56, 77, 99, 111	0
All	All	4042/4160 (97%)	0.43	287 (7%) 16 9	21, 65, 116, 163	127 (3%)

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	193	VAL	14.1
5	R	133	VAL	13.8
5	R	195	VAL	13.6
10	W	62	SER	11.6
5	R	132	TRP	11.3
5	R	114	VAL	11.0
5	R	130	PRO	10.9
10	W	63	GLU	10.9
5	R	127	VAL	8.8
5	R	98	VAL	8.2
5	R	109	GLU	8.2
5	R	115	SER	7.9
7	T	77	TYR	7.6
5	R	79	SER	7.6
5	R	99	ARG	7.5
5	R	87	VAL	7.5
9	V	63	ASP	7.3
7	G	1	GLY	7.1
5	E	133	VAL	6.9
5	R	192	LEU	6.9
5	R	80	ASP	6.8
5	R	175	PRO	6.6
5	R	191	ASP	6.6
8	H	9	GLU	6.5
5	R	116	LYS	6.5
5	R	131	GLU	6.4
5	R	117	LEU	6.4
2	O	23	ASP	6.0
5	R	185	TYR	6.0
5	R	93	GLY	6.0
2	B	226	ILE	5.9
4	D	241	LYS	5.7
1	A	2	ALA	5.6
5	R	194	VAL	5.6
2	B	236	LYS	5.6
5	R	160	CYS	5.6
5	R	176	ALA	5.5
5	R	106	ILE	5.5
5	R	100	HIS	5.5
5	R	162	GLY	5.5
5	R	112	VAL	5.5
7	T	78	GLU	5.4
5	R	174	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
5	R	81	ILE	5.2
3	C	1	MET	5.1
5	R	172	ARG	5.1
5	R	177	PRO	5.1
5	R	86	ASN	5.1
1	N	218	GLY	5.1
5	R	184	THR	5.0
5	R	74	ILE	5.0
5	R	108	GLN	5.0
5	R	119	ASP	4.9
2	O	19	PRO	4.9
5	R	113	ASP	4.9
8	H	10	GLU	4.9
5	R	163	SER	4.9
5	R	78	LEU	4.8
5	R	183	PRO	4.8
9	V	77	ARG	4.7
5	R	164	HIS	4.6
5	E	195	VAL	4.6
5	E	74	ILE	4.6
5	R	76	ILE	4.6
5	R	120	PRO	4.6
5	E	188	VAL	4.5
5	E	132	TRP	4.5
5	R	89	PHE	4.5
5	R	128	LYS	4.4
9	I	47	ARG	4.3
9	I	51	CYS	4.3
10	J	64	GLU	4.3
5	R	118	ARG	4.2
5	R	153	PHE	4.2
10	J	63	GLU	4.2
2	B	402	ILE	4.2
5	E	81	ILE	4.1
4	Q	139	ALA	4.1
2	O	299	VAL	4.0
6	S	15	ARG	4.0
5	R	110	ALA	4.0
5	R	122	HIS	4.0
10	W	61	ALA	4.0
5	R	173	LYS	3.9
8	U	49	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
5	R	134	ILE	3.9
5	R	104	ALA	3.9
7	T	74	PRO	3.9
5	E	76	ILE	3.8
5	E	80	ASP	3.8
5	R	189	GLY	3.8
9	I	50	LEU	3.7
8	U	44	VAL	3.7
5	R	126	ARG	3.7
1	A	69	LYS	3.7
5	E	109	GLU	3.7
9	I	63	ASP	3.7
5	R	105	GLU	3.6
5	R	123	ASP	3.6
5	E	101	ARG	3.6
2	O	24	LEU	3.6
8	U	13	LEU	3.6
5	E	187	PHE	3.6
4	Q	143	VAL	3.5
5	R	94	LYS	3.5
9	V	50	LEU	3.5
5	E	114	VAL	3.5
5	E	110	ALA	3.5
5	E	85	LYS	3.5
9	V	76	VAL	3.5
5	E	122	HIS	3.4
7	T	79	ASN	3.4
5	E	89	PHE	3.4
4	Q	241	LYS	3.4
5	E	178	TYR	3.4
9	I	53	GLU	3.4
5	E	98	VAL	3.4
5	R	155	GLY	3.4
1	N	122	LEU	3.3
9	V	70	LEU	3.3
5	R	102	THR	3.3
5	E	106	ILE	3.3
5	R	136	VAL	3.3
5	E	186	GLN	3.3
5	E	174	GLY	3.3
5	R	95	PRO	3.3
9	V	59	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	4	TYR	3.2
3	P	156	TYR	3.2
5	E	194	VAL	3.2
5	R	178	TYR	3.2
5	E	185	TYR	3.2
2	B	124	LEU	3.2
3	P	373	LEU	3.2
5	R	159	PRO	3.2
8	U	54	CYS	3.2
1	N	182	LEU	3.1
5	R	129	LYS	3.1
5	E	100	HIS	3.1
9	V	62	ARG	3.1
5	E	112	VAL	3.1
5	E	86	ASN	3.1
2	B	224	LEU	3.1
5	E	131	GLU	3.0
7	T	75	ALA	3.0
2	O	368	TYR	3.0
5	E	118	ARG	3.0
5	E	193	VAL	3.0
9	I	77	ARG	3.0
5	R	121	GLN	3.0
5	R	156	TYR	3.0
9	I	60	ALA	3.0
5	E	111	GLU	3.0
5	R	111	GLU	3.0
6	S	12	LEU	2.9
1	A	226	ASP	2.9
9	I	62	ARG	2.9
5	E	84	GLY	2.9
5	E	99	ARG	2.9
2	O	402	ILE	2.8
1	N	75	PHE	2.8
5	E	192	LEU	2.8
2	B	232	THR	2.8
6	S	11	ARG	2.8
2	B	205	ALA	2.8
5	R	72	SER	2.8
2	B	439	LEU	2.8
5	E	156	TYR	2.8
5	R	182	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
9	V	60	ALA	2.8
10	J	61	ALA	2.8
2	B	33	LEU	2.8
2	O	207	VAL	2.8
2	B	400	GLN	2.8
4	Q	9	ALA	2.7
6	S	90	LEU	2.7
2	O	383	GLY	2.7
5	R	84	GLY	2.7
5	E	83	GLU	2.7
5	R	187	PHE	2.7
1	N	127	ILE	2.7
9	V	57	GLY	2.7
5	E	75	GLU	2.7
5	E	72	SER	2.7
5	E	177	PRO	2.7
5	E	149	ASN	2.7
5	R	171	ILE	2.7
2	B	223	PHE	2.6
8	U	26	GLN	2.6
7	T	26	ILE	2.6
1	N	124	GLU	2.6
2	B	204	MET	2.6
5	R	124	LEU	2.6
9	V	55	MET	2.6
1	A	444	ILE	2.6
5	E	130	PRO	2.6
7	T	24	ARG	2.6
1	A	392	LEU	2.6
4	Q	145	GLU	2.6
4	D	143	VAL	2.6
8	U	24	CYS	2.6
2	O	266	SER	2.5
2	O	22	GLU	2.5
5	R	140	THR	2.5
9	I	54	SER	2.5
10	J	62	SER	2.5
5	E	124	LEU	2.5
1	N	216	PHE	2.5
2	B	417	PHE	2.5
4	D	2	GLU	2.5
1	N	190	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
5	E	153	PHE	2.5
5	R	125	ASP	2.5
2	O	268	GLU	2.4
5	E	78	LEU	2.4
5	E	180	LEU	2.4
9	I	70	LEU	2.4
1	A	21	ASN	2.4
5	R	161	HIS	2.4
1	N	62	LEU	2.4
1	N	174	ILE	2.4
8	U	61	PHE	2.4
4	Q	141	VAL	2.4
5	E	126	ARG	2.4
3	P	346	HIS	2.4
4	Q	147	LEU	2.4
9	I	72	ALA	2.4
5	E	137	GLY	2.4
2	O	28	LYS	2.4
5	E	102	THR	2.3
1	N	50	GLU	2.3
2	O	307	PHE	2.3
10	W	35	PHE	2.3
1	N	223	TYR	2.3
4	Q	138	PRO	2.3
4	Q	171	TYR	2.3
5	R	88	ALA	2.3
9	I	52	ARG	2.3
7	T	69	LEU	2.3
1	N	178	THR	2.3
5	R	154	GLY	2.2
5	E	163	SER	2.2
1	A	8	LEU	2.2
5	R	85	LYS	2.2
5	E	136	VAL	2.2
5	R	103	GLN	2.2
2	B	120	MET	2.2
8	U	50	THR	2.2
5	E	190	ASP	2.2
9	V	47	ARG	2.2
1	N	57	TYR	2.2
5	R	181	GLU	2.2
1	N	354	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
7	T	53	LEU	2.2
8	U	12	GLU	2.2
5	E	73	LYS	2.2
10	W	32	GLU	2.2
9	I	69	SER	2.2
5	R	97	PHE	2.2
1	N	185	TYR	2.1
5	E	172	ARG	2.1
2	B	419	SER	2.1
8	U	35	GLU	2.1
1	A	405	ARG	2.1
8	U	39	LEU	2.1
1	N	69	LYS	2.1
10	J	60	GLU	2.1
1	N	52	ASN	2.1
5	E	90	LYS	2.1
2	B	350	GLY	2.1
7	T	38	TRP	2.1
5	R	101	ARG	2.1
7	G	30	PHE	2.1
9	V	56	SER	2.1
1	N	179	ARG	2.1
2	O	303	THR	2.1
1	N	123	GLU	2.1
3	P	345	GLU	2.1
2	O	250	HIS	2.1
8	U	29	LYS	2.1
9	V	51	CYS	2.1
2	B	369	LEU	2.0
5	R	141	HIS	2.0
5	E	173	LYS	2.0
5	E	196	GLY	2.0
9	I	56	SER	2.0
7	T	42	SER	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	BOG	D	2091	20/20	0.26	0.60	177,189,190,190	0
17	BOG	Q	3091	20/20	0.29	0.63	178,186,187,187	0
17	BOG	P	2010	19/20	0.59	0.47	102,183,184,184	0
12	UNL	P	3048	2/-	0.62	0.25	92,92,92,95	0
12	UNL	C	2046	2/-	0.76	0.50	87,87,87,91	0
12	UNL	D	2012	2/-	0.76	0.32	59,59,59,60	0
12	UNL	P	3047	1/-	0.78	0.27	47,47,47,47	0
16	AZI	C	2011	3/3	0.82	0.50	68,68,69,71	0
12	UNL	P	3046	2/-	0.83	0.73	85,85,85,85	0
11	PEE	P	3005	50/51	0.83	0.31	74,100,105,105	0
11	PEE	C	2005	50/51	0.83	0.32	83,93,101,104	0
15	UQ	C	2002	19/63	0.84	0.33	85,87,89,89	0
15	UQ	P	3002	19/63	0.84	0.39	138,141,143,143	0
12	UNL	P	3014	1/-	0.84	0.32	55,55,55,55	0
19	CDL	Q	3003	42/100	0.84	0.25	119,124,137,138	0
19	CDL	D	2003	42/100	0.87	0.20	81,93,97,98	0
17	BOG	C	3010	12/20	0.87	0.35	94,96,97,98	0
19	CDL	T	3004	40/100	0.87	0.21	94,97,106,107	0
11	PEE	A	2008	21/51	0.88	0.23	95,113,116,118	0
12	UNL	C	2048	2/-	0.89	0.41	62,62,62,63	0
17	BOG	D	2009	20/20	0.90	0.20	56,63,65,67	0
17	BOG	Q	3009	20/20	0.90	0.20	71,79,81,82	0
19	CDL	G	2004	40/100	0.91	0.22	60,70,85,86	0
16	AZI	P	3011	3/3	0.91	0.50	74,74,76,77	0
11	PEE	P	3007	48/51	0.91	0.36	76,90,105,106	0
12	UNL	A	3015	1/-	0.92	0.21	48,48,48,48	0
12	UNL	P	3013	1/-	0.92	0.28	56,56,56,56	0
12	UNL	R	3012	1/-	0.94	0.18	38,38,38,38	0
11	PEE	C	2007	48/51	0.95	0.23	41,52,81,82	0
11	PEE	N	3008	5/51	0.95	0.15	88,88,89,89	0
14	FNM	P	3001	22/22	0.96	0.22	49,53,59,62	0
18	HEC	Q	501	43/43	0.96	0.19	47,55,64,66	0

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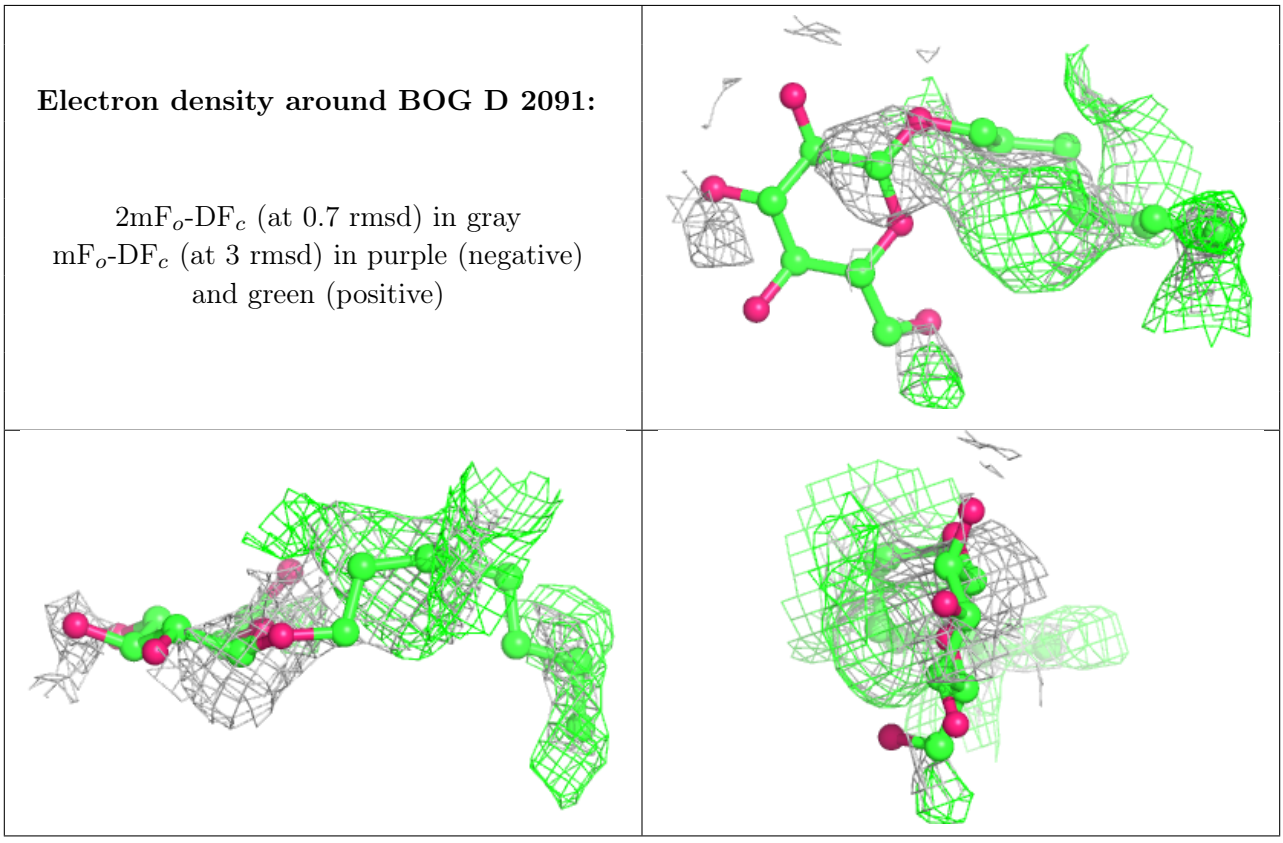
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	UNL	C	2047	1/-	0.96	0.34	34,34,34,34	0
20	FES	R	501	4/4	0.96	0.17	106,106,106,107	4
13	HEM	P	502	43/43	0.98	0.17	34,40,55,62	0
18	HEC	D	501	43/43	0.98	0.18	23,30,35,37	0
14	FNM	C	2001	22/22	0.98	0.18	38,40,42,44	0
20	FES	E	501	4/4	0.98	0.11	83,84,85,86	0
13	HEM	P	501	43/43	0.98	0.21	40,43,54,58	0
13	HEM	C	501	43/43	0.99	0.22	23,31,38,43	0
13	HEM	C	502	43/43	0.99	0.19	23,26,33,39	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.

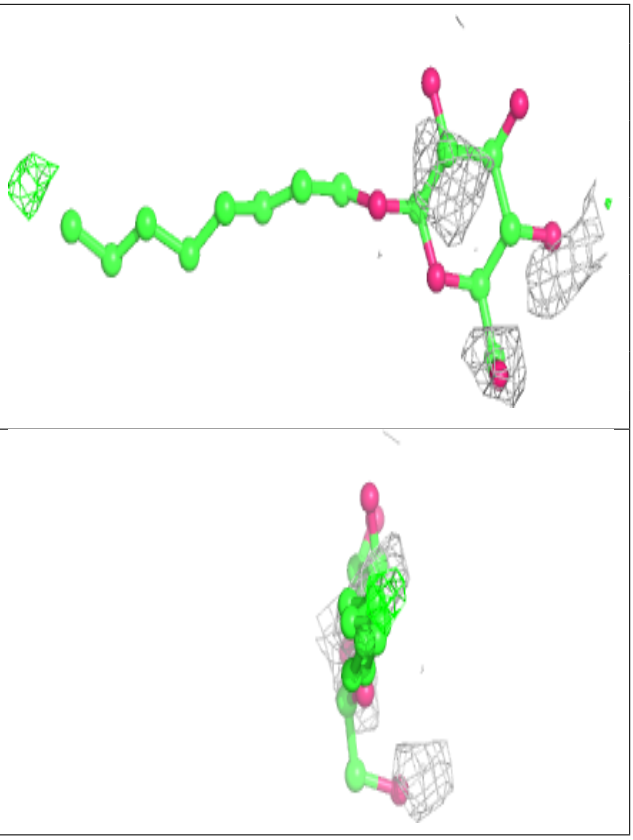
Electron density around BOG D 2091:

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



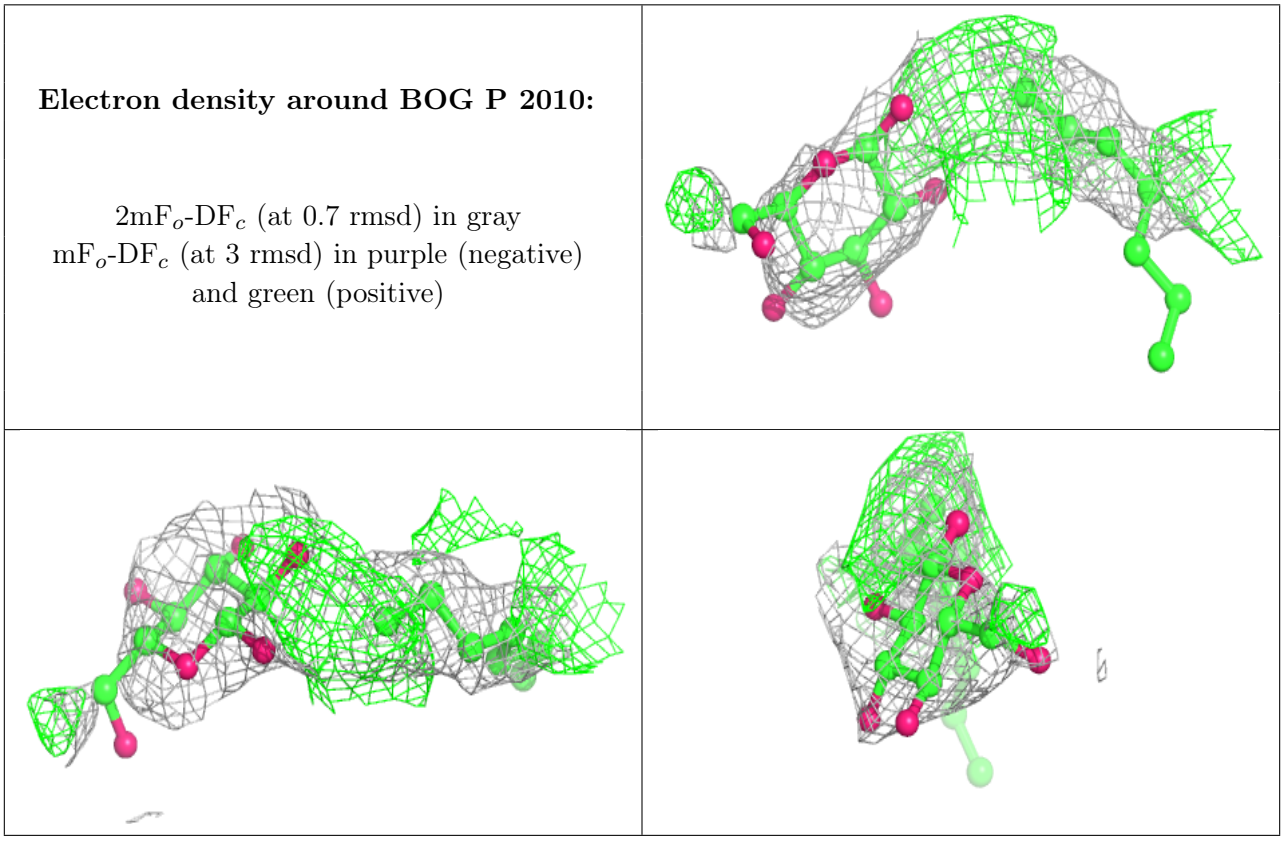
Electron density around BOG Q 3091:

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



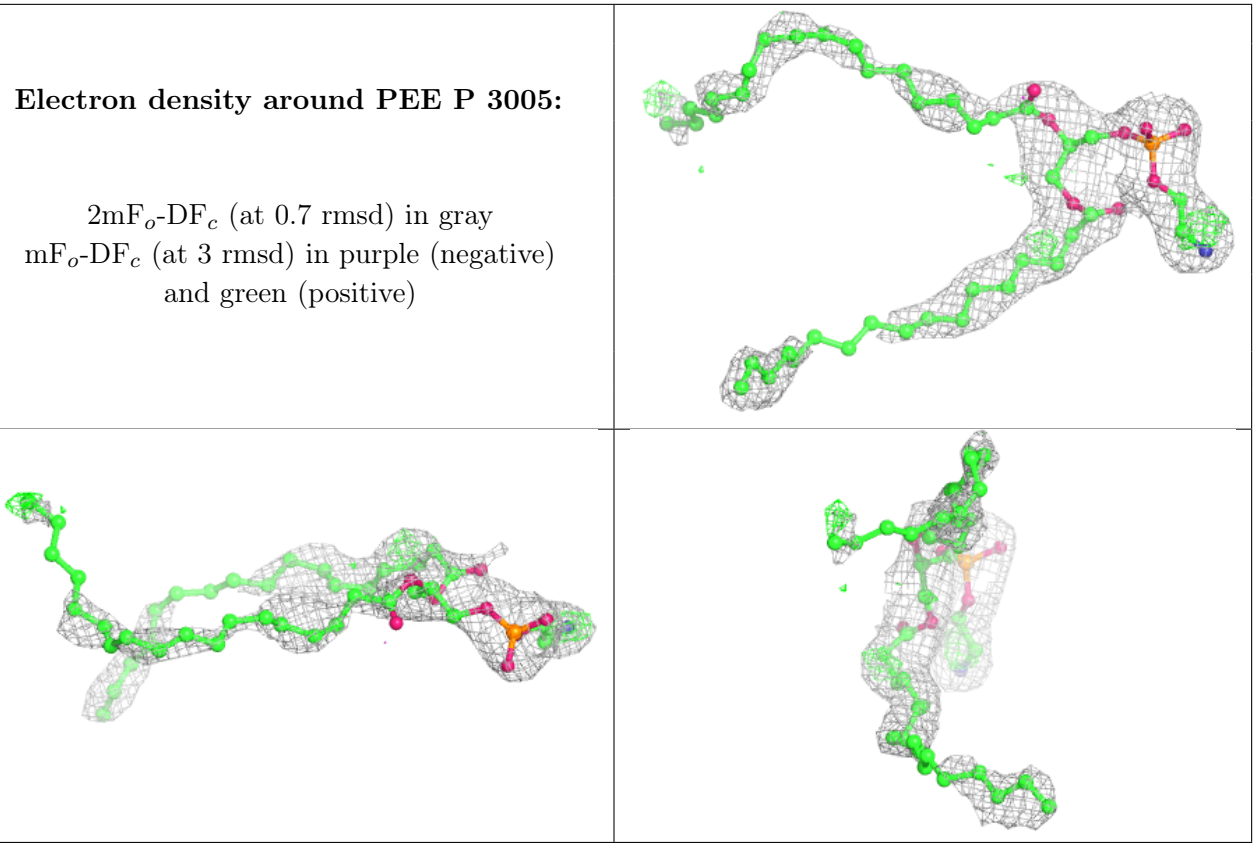
Electron density around BOG P 2010:

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



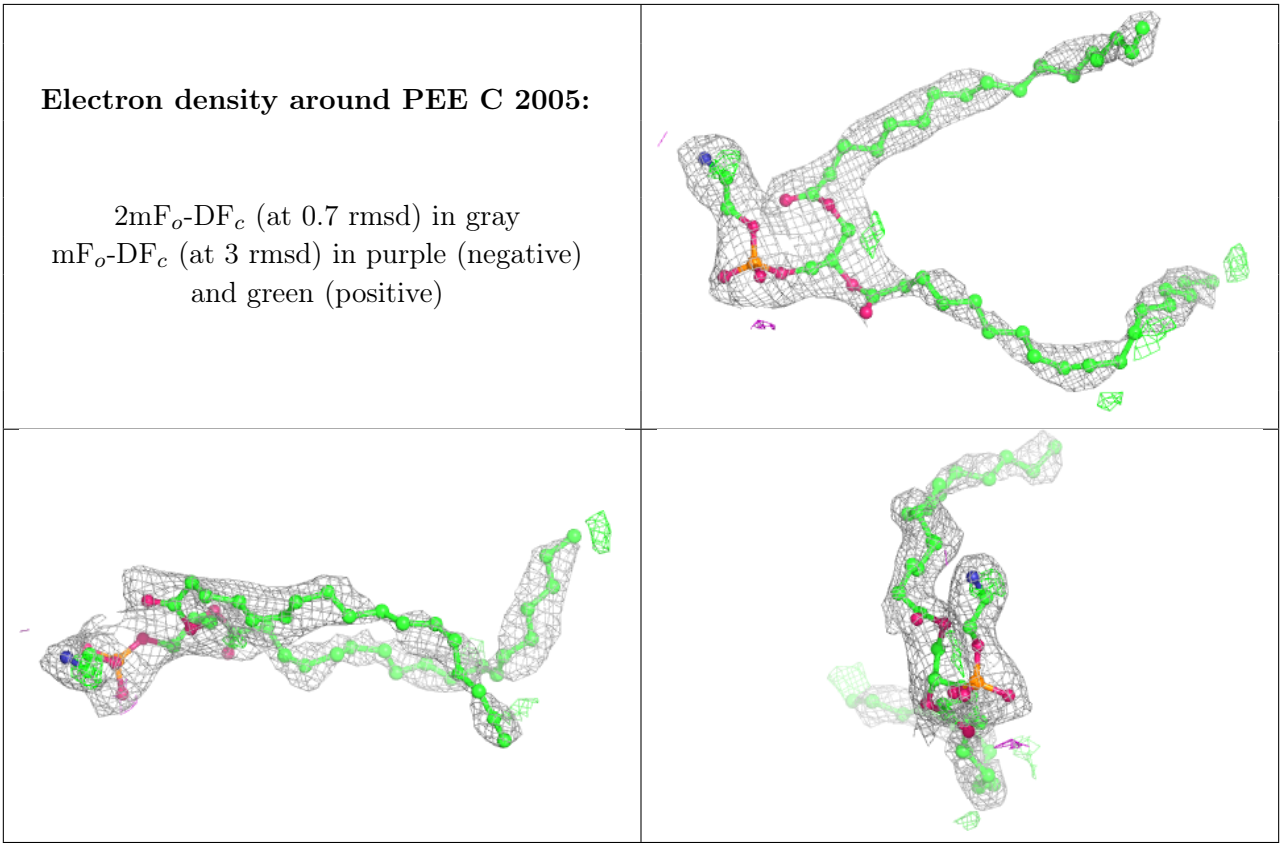
Electron density around PEE P 3005:

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



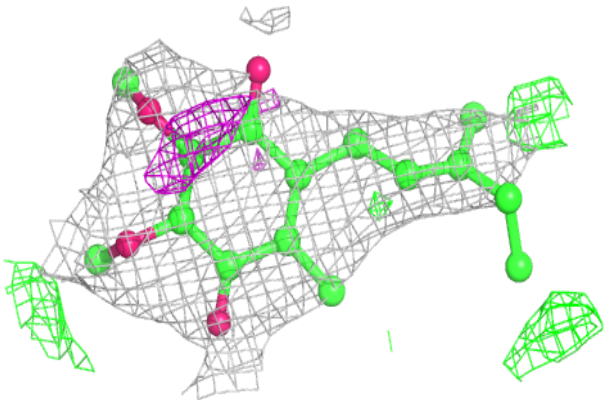
Electron density around PEE C 2005:

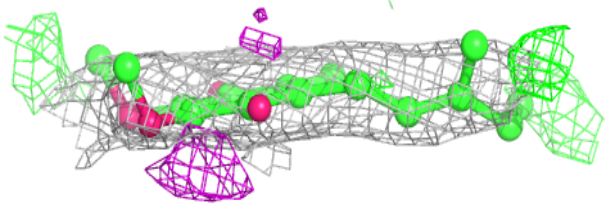
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

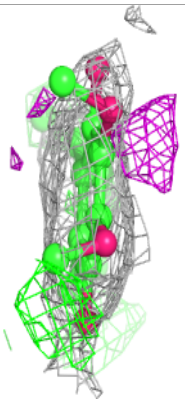


Electron density around UQ C 2002:

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

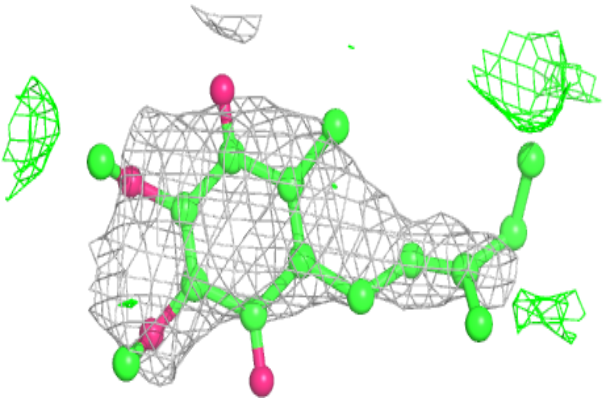


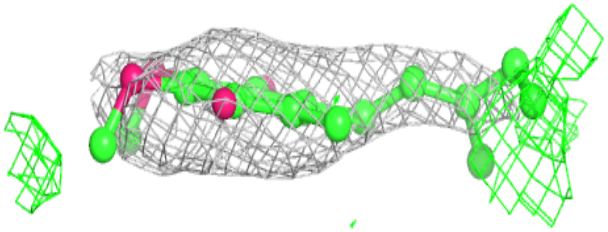


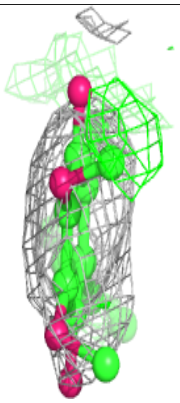


Electron density around UQ P 3002:

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

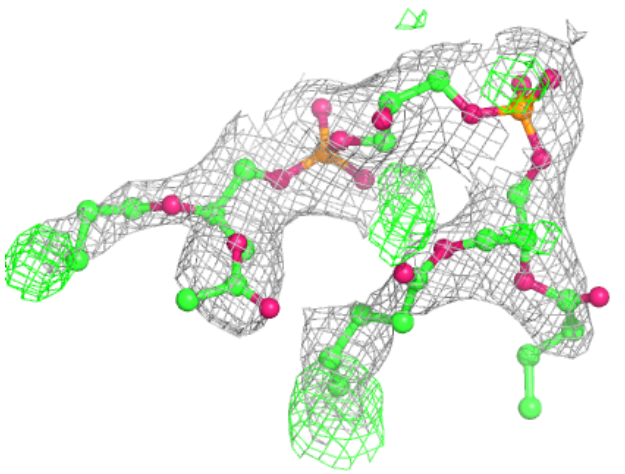


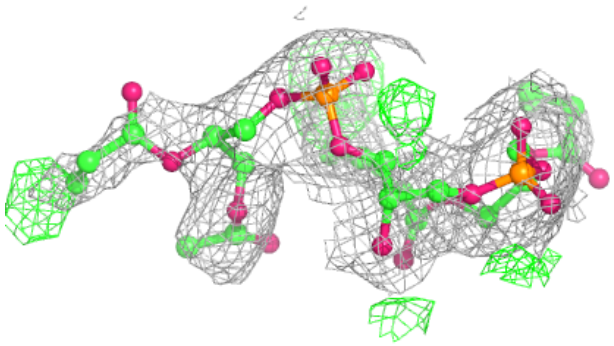


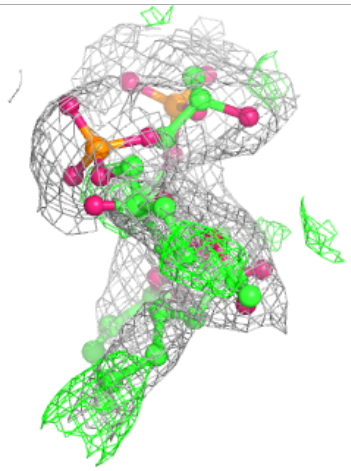


Electron density around CDL Q 3003:

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

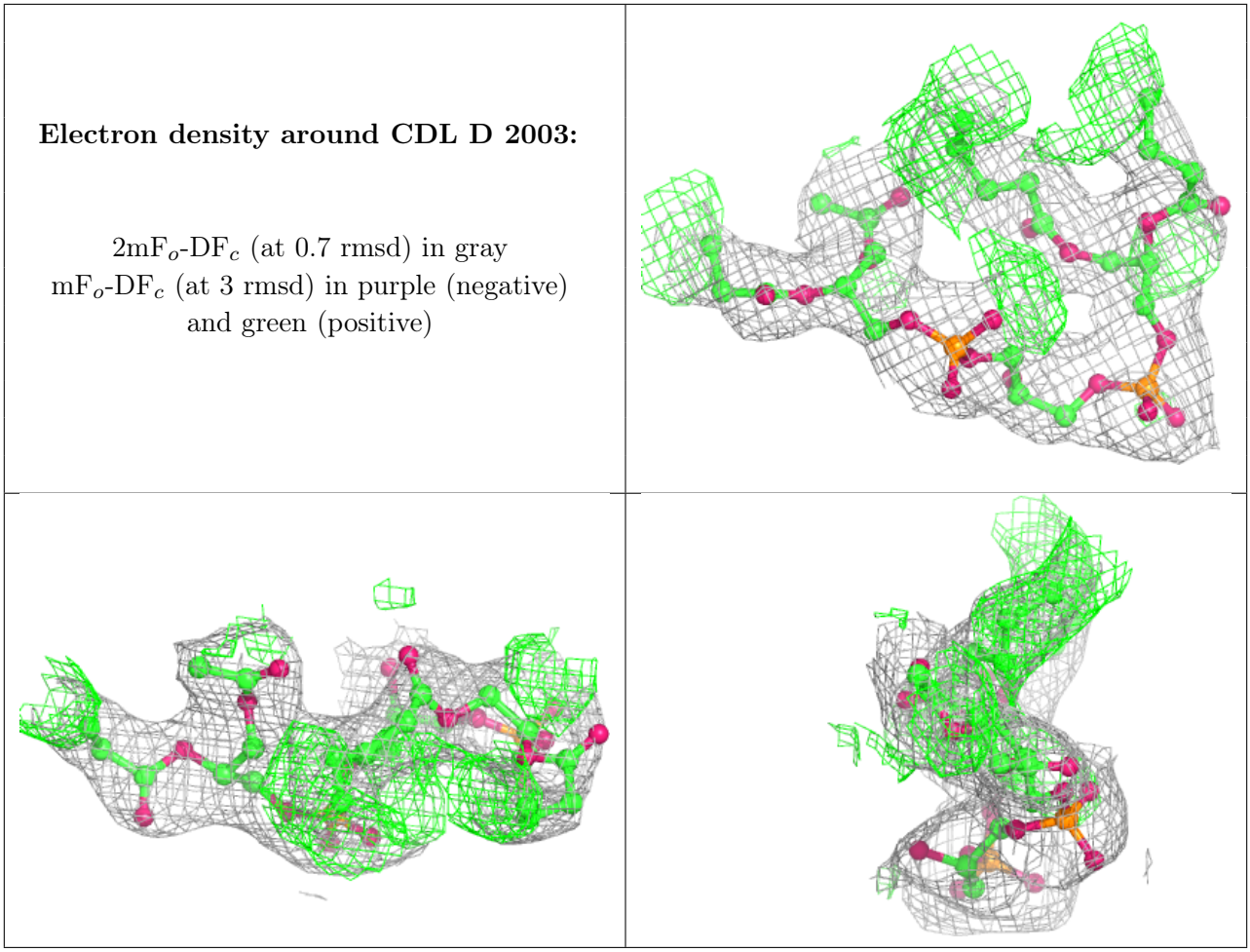






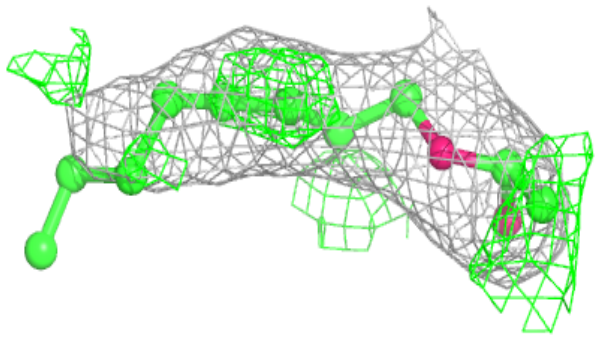
Electron density around CDL D 2003:

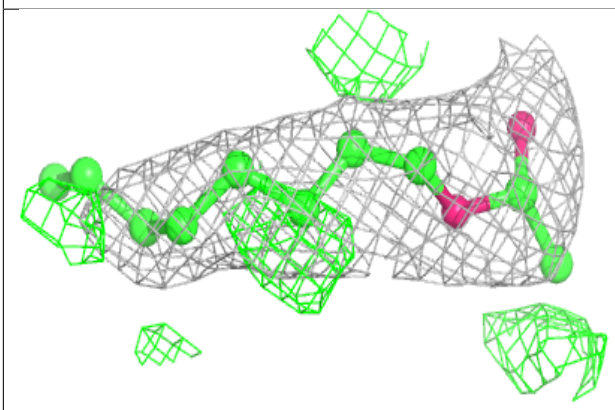
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

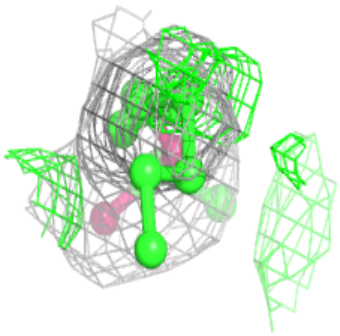


Electron density around BOG C 3010:

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

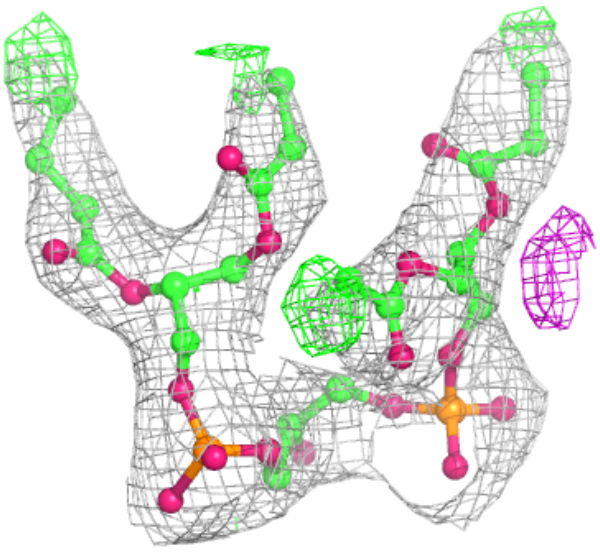


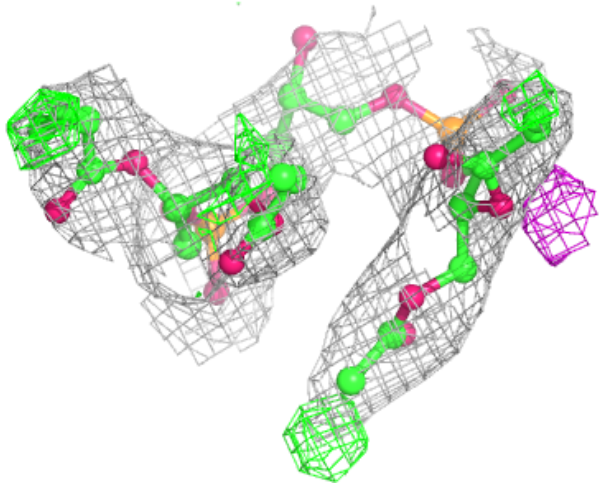


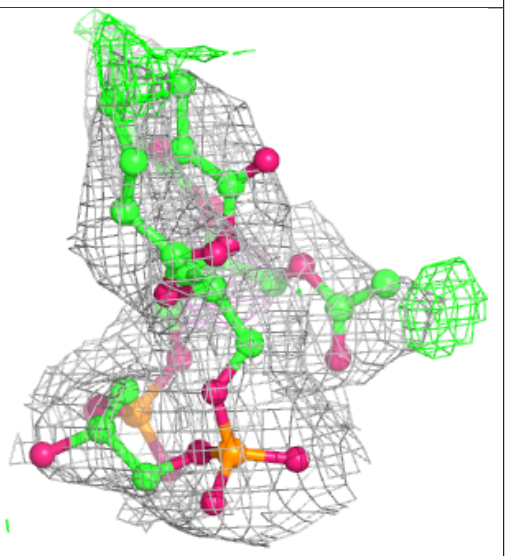


Electron density around CDL T 3004:

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

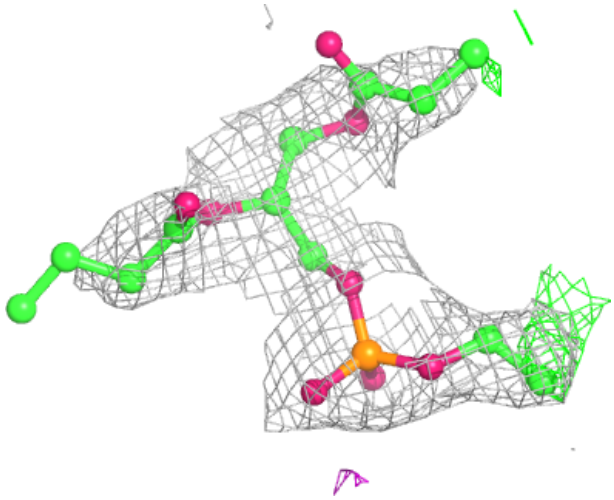


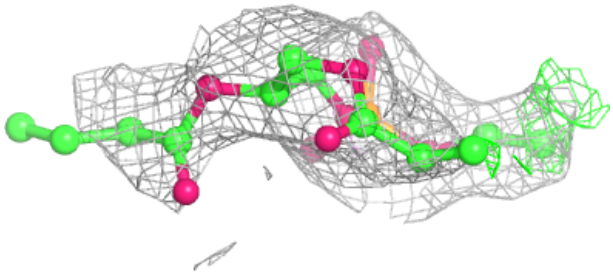


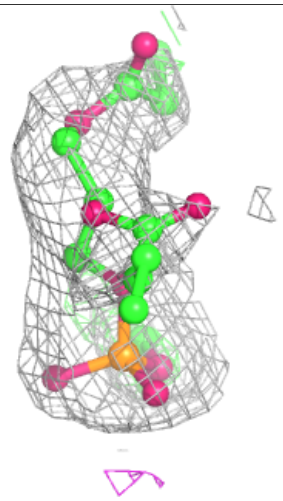


Electron density around PEE A 2008:

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

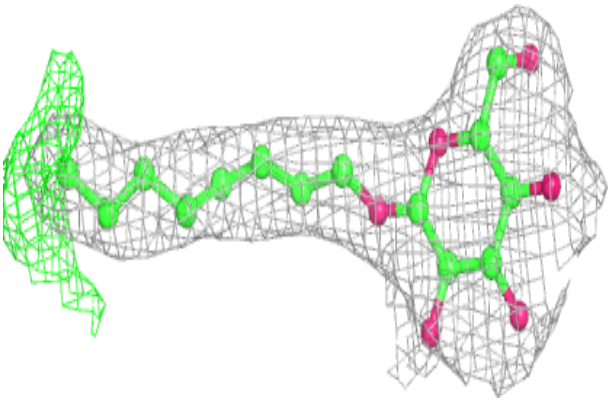


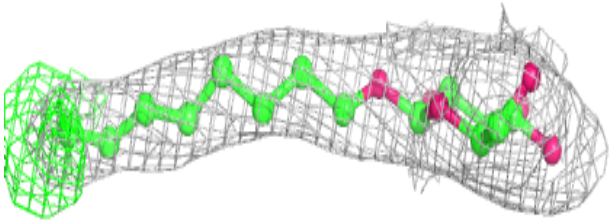


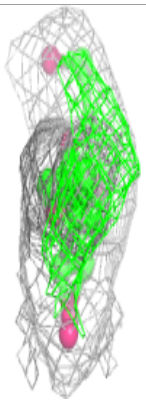


Electron density around BOG D 2009:

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

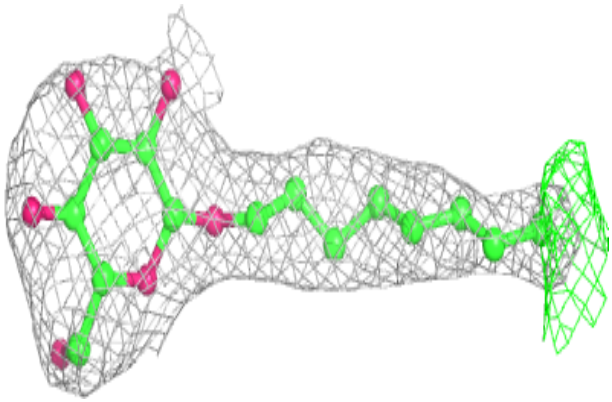


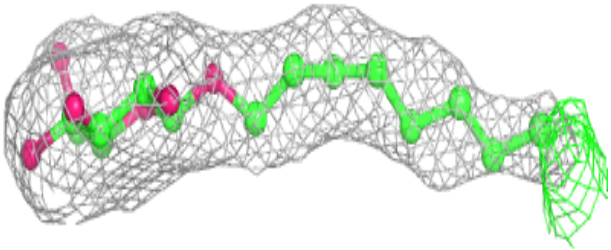


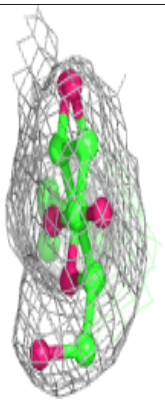


Electron density around BOG Q 3009:

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

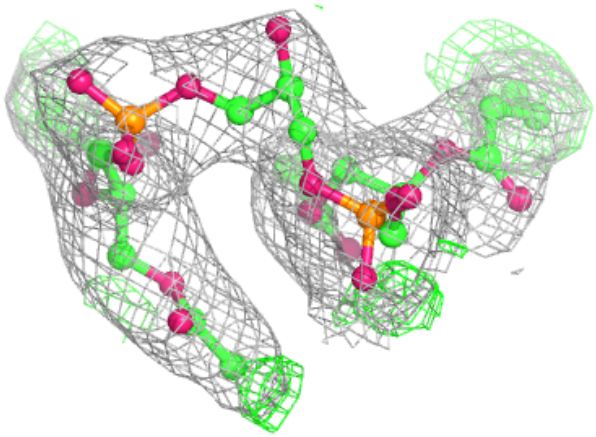


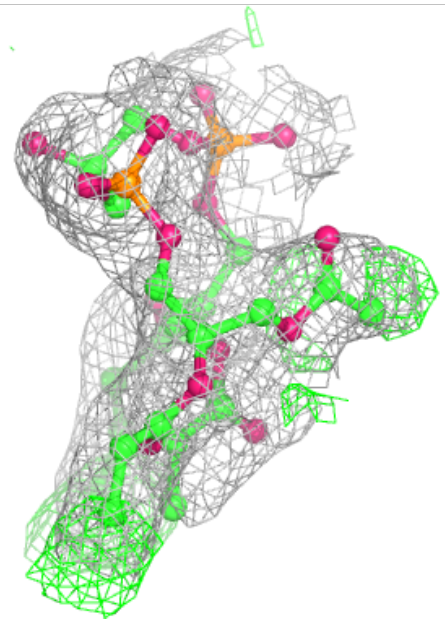




Electron density around CDL G 2004:

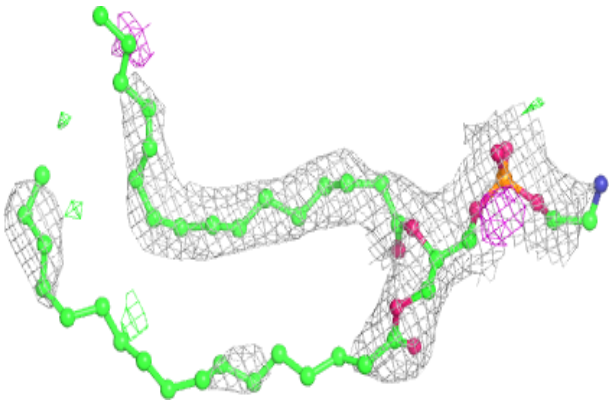
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

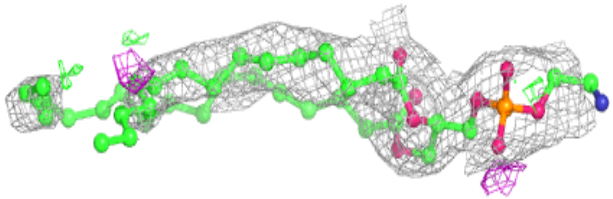


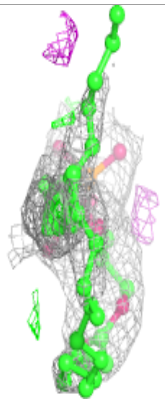


Electron density around PEE P 3007:

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

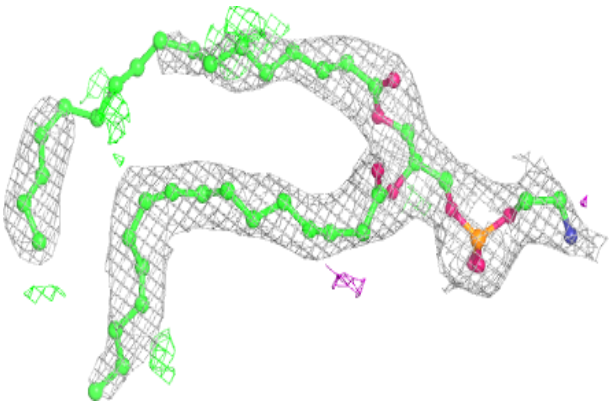


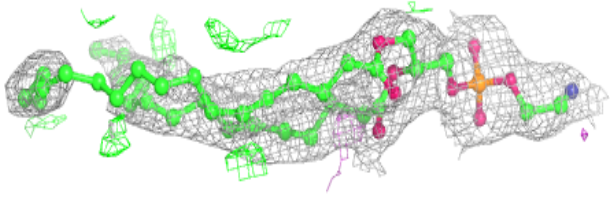


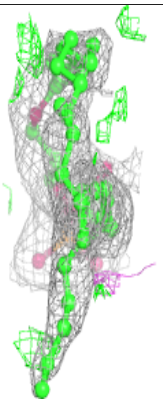


Electron density around PEE C 2007:

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

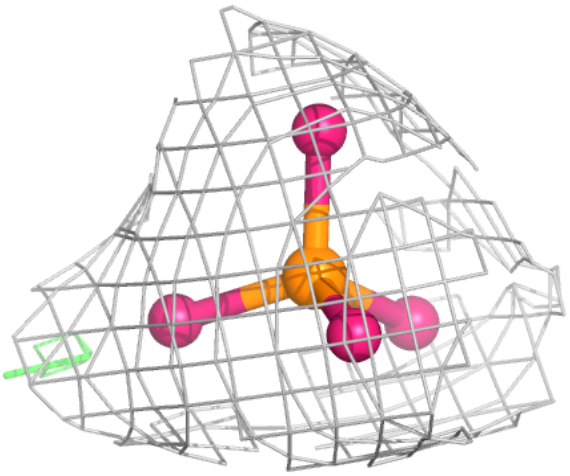


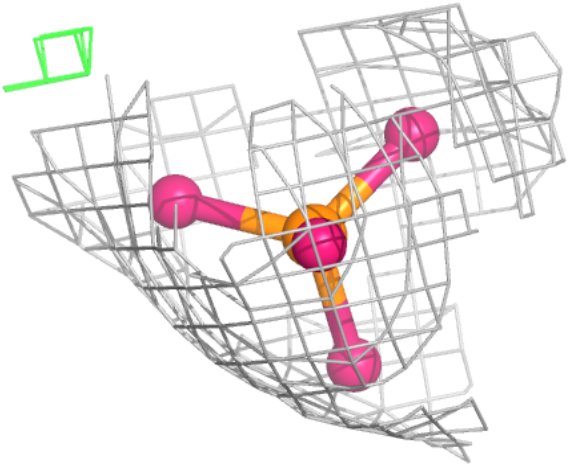


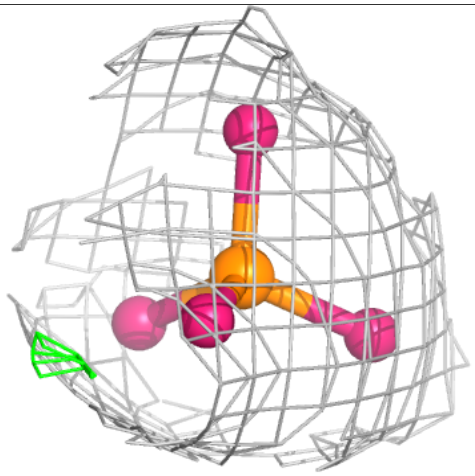


Electron density around PEE N 3008:

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

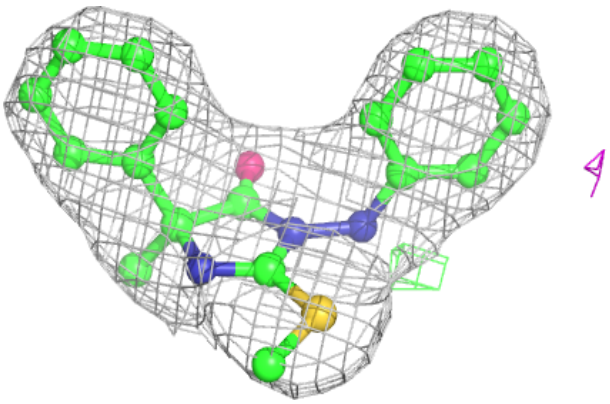


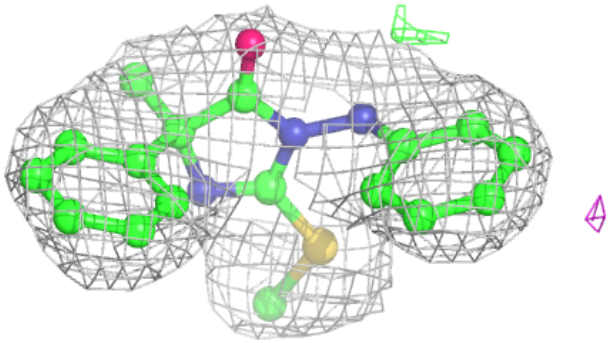


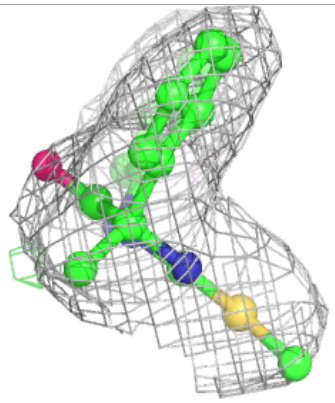


Electron density around FNM P 3001:

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

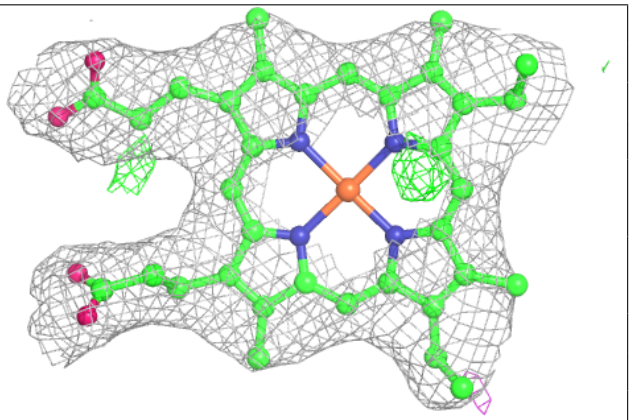


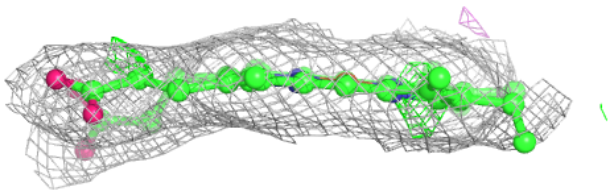


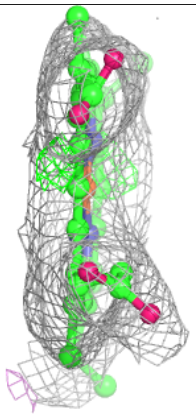


Electron density around HEC Q 501:

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

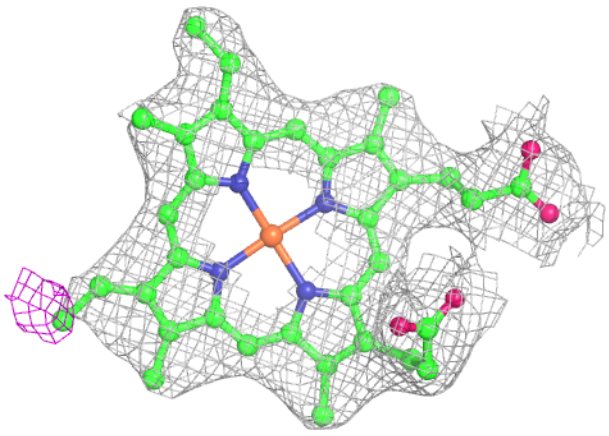


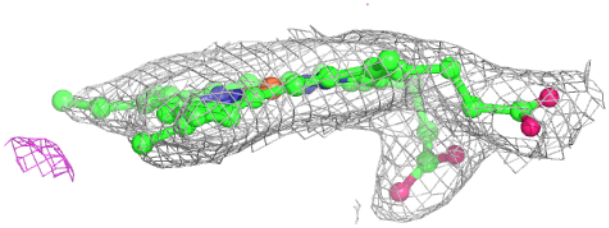


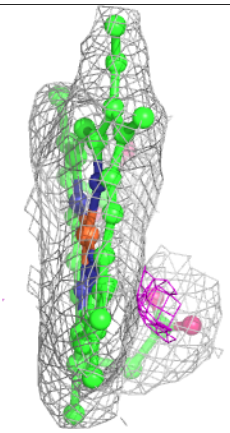


Electron density around HEM P 502:

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

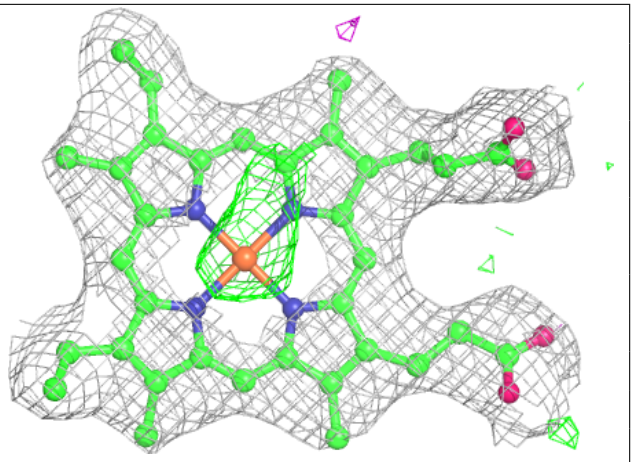


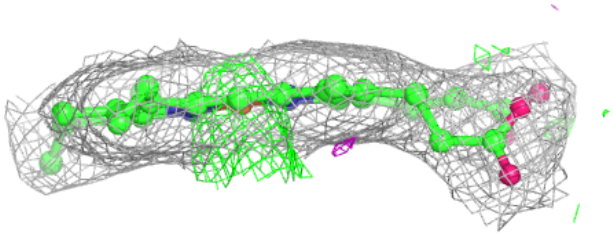


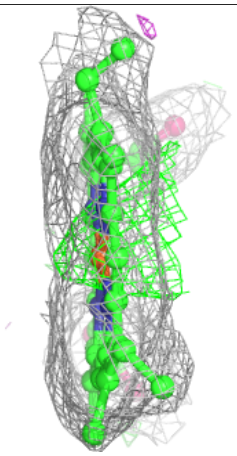


Electron density around HEC D 501:

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

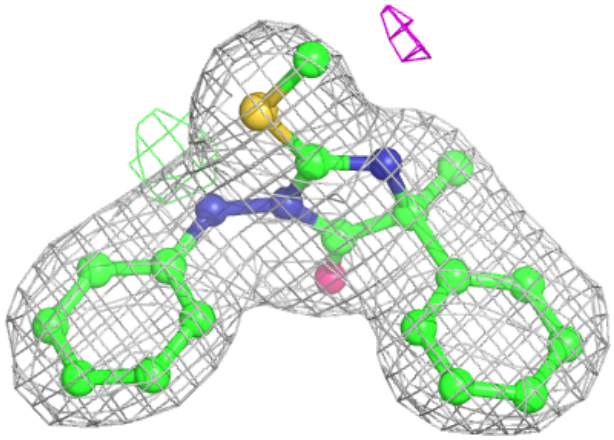


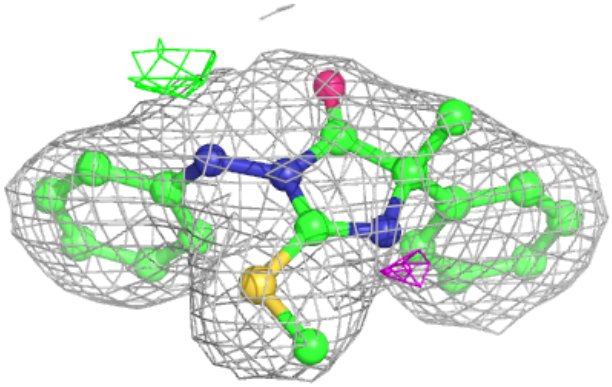


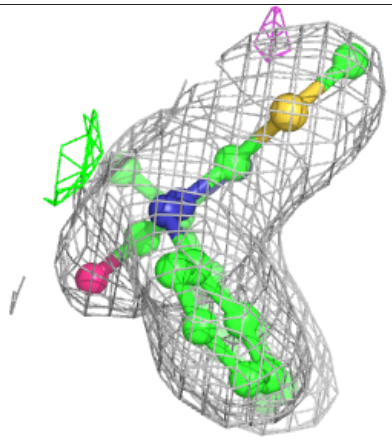


Electron density around FNM C 2001:

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

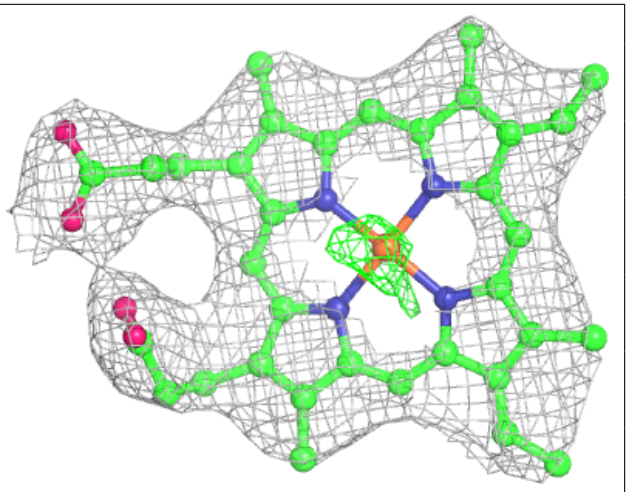


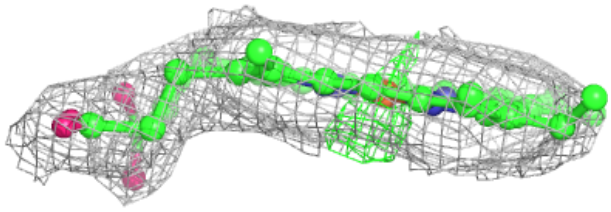


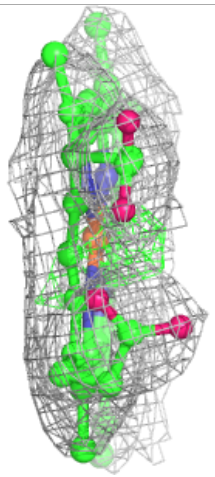


Electron density around HEM P 501:

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

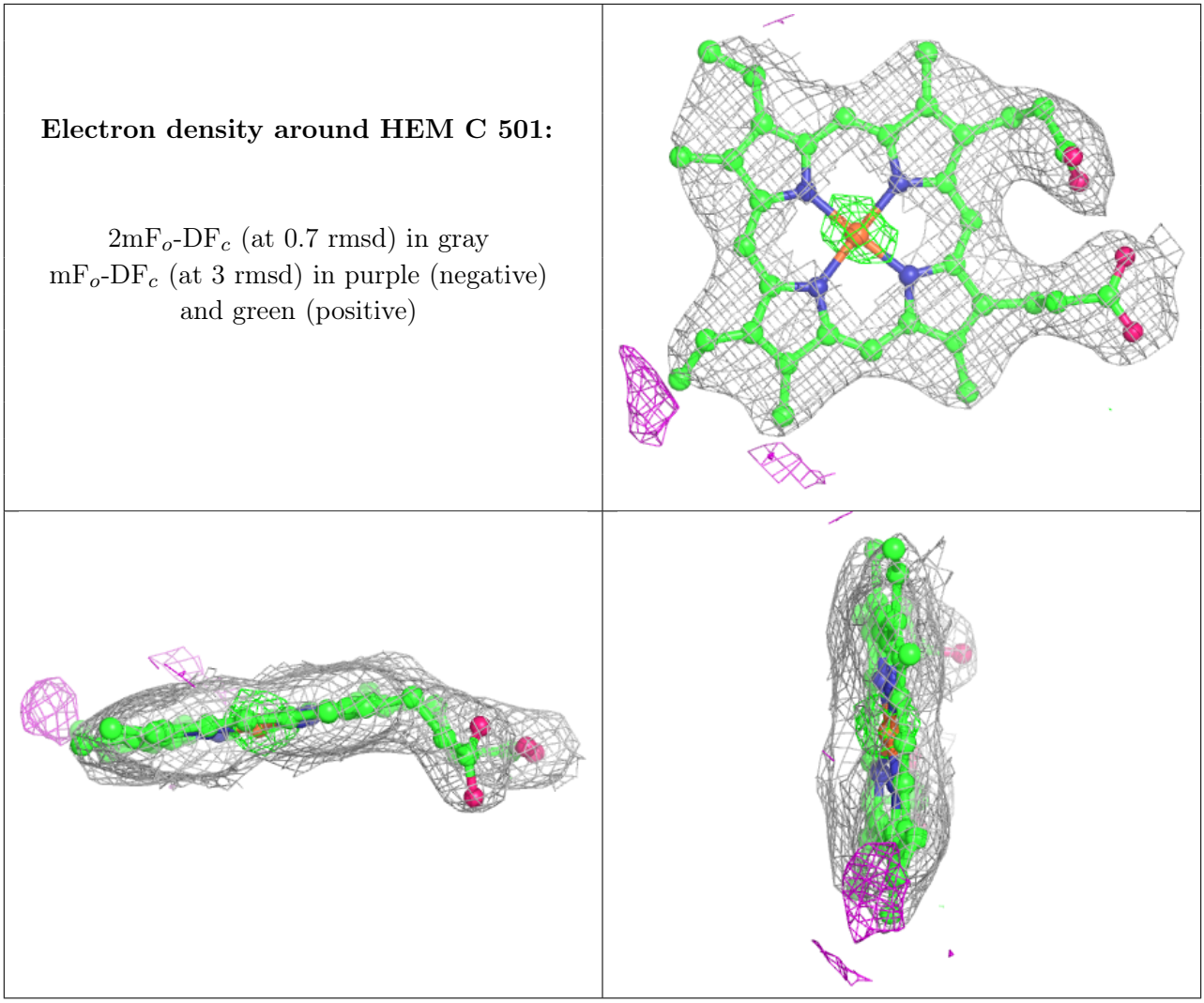






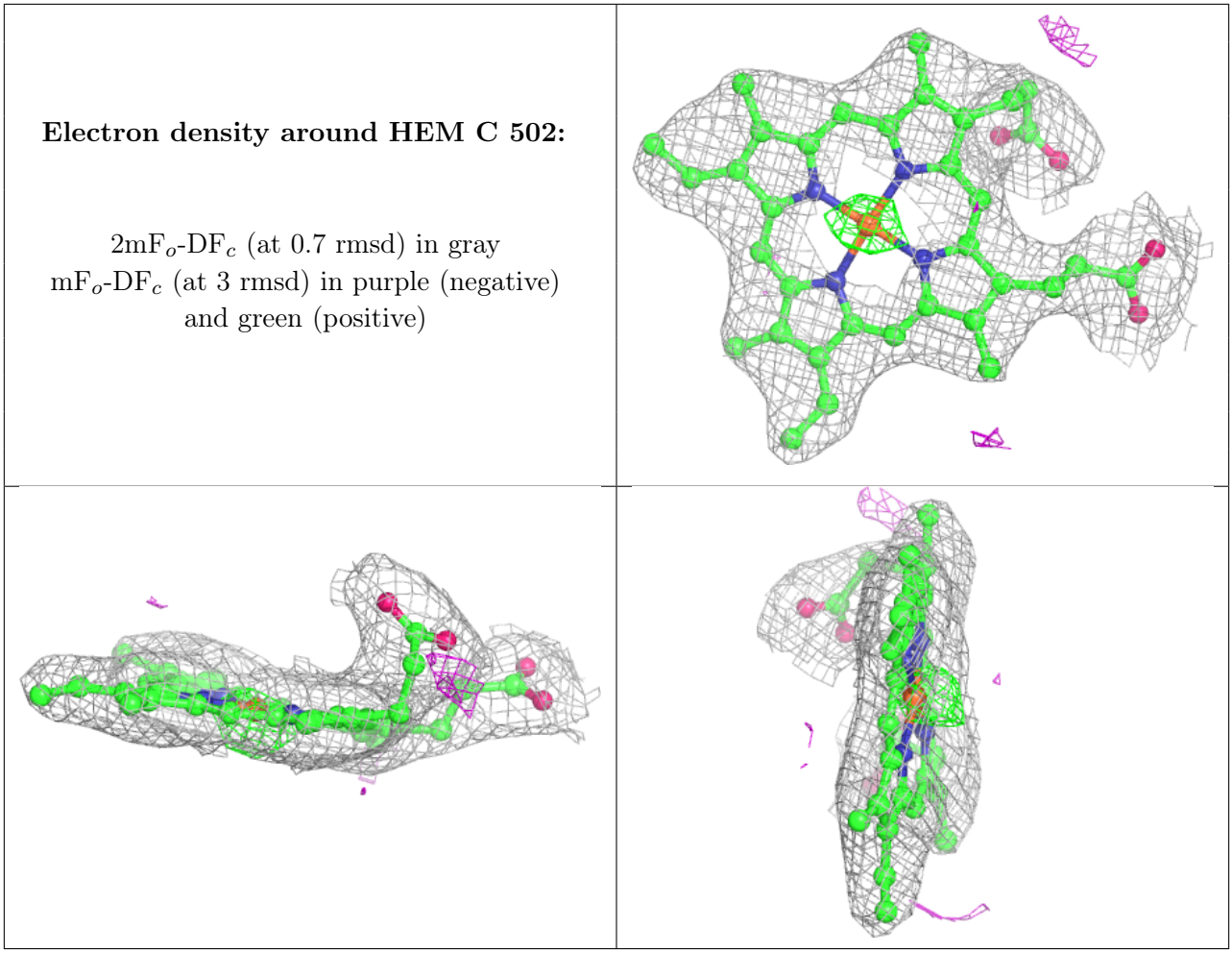
Electron density around HEM C 501:

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



Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.