Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 12:57 AM EDT

PDB ID	:	1PP9
Title	:	Bovine cytochrome bc1 complex with stigmatellin bound
Authors	:	Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on	:	2003-06-16
Resolution	:	2.10 Å(reported)

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

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

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

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

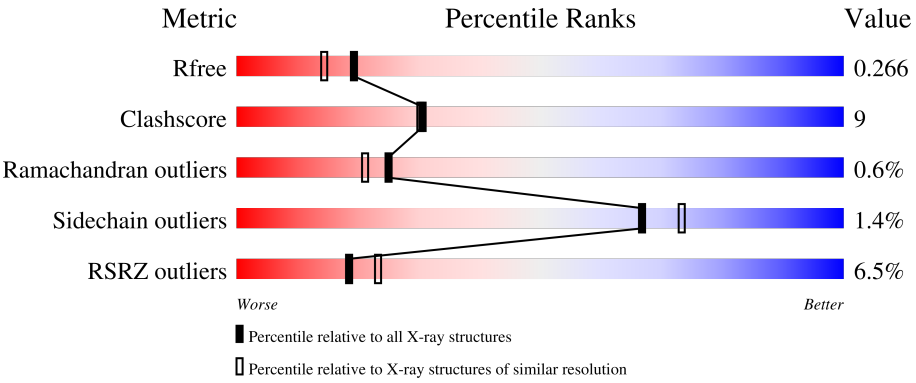
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	4% 82% 17%
1	N	446	3% 83% 15%
2	B	439	3% 82% 15%
2	O	439	6% 83% 13%
3	C	379	2% 84% 12%

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Mol	Chain	Length	Quality of chain
3	P	379	6% 84% 12%
4	D	241	2% 88% 11%
4	Q	241	6% 87% 12%
5	E	196	16% 81% 17%
5	R	196	2% 84% 15%
6	F	110	4% 75% 15% 10%
6	S	110	9% 75% 15% 10%
7	G	81	6% 68% 23% 7%
7	T	81	10% 70% 21% 6%
8	H	78	12% 64% 18% 15%
8	U	78	13% 68% 17% 15%
9	I	78	29% 28% 26% 46%
9	V	78	19% 32% 21% 46%
10	J	62	19% 76% 21%
10	W	62	15% 74% 21% 5%

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	JZR	A	4002	-	-	-	X
11	JZR	C	2008	-	-	-	X
11	JZR	F	3011	-	-	-	X
11	JZR	F	4001	-	-	-	X
11	JZR	S	2011	-	-	-	X
12	AZI	P	3014	-	-	-	X
13	PEE	C	2012	-	X	-	-
13	PEE	G	2005	-	-	-	X
13	PEE	N	3012	-	X	-	-
13	PEE	T	3005	-	-	-	X
14	PO4	B	3010	-	X	-	-
14	PO4	O	2010	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	GOL	B	2013	-	-	-	X
15	GOL	O	3013	-	-	-	X

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 33959 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	10	0	1
			3403	2121	602	660	20			
1	N	443	Total	C	N	O	S	10	0	1
			3403	2121	602	660	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3177	1996	562	612	7			
2	O	424	Total	C	N	O	S	0	0	0
			3180	1998	562	613	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2892	1940	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2931	1968	455	490	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	R	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

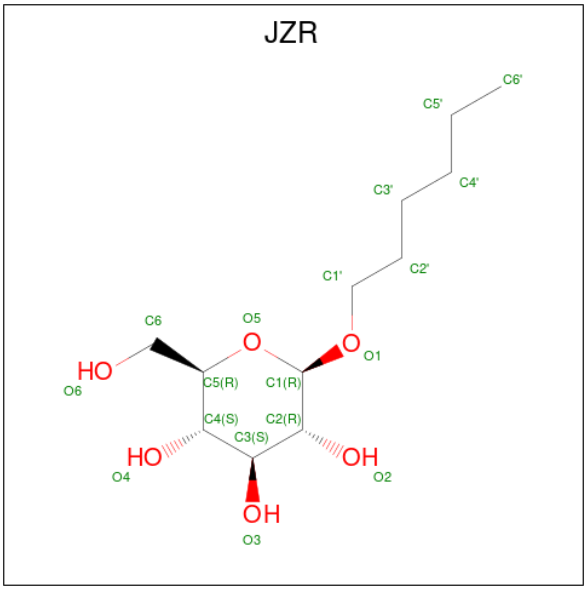
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			
9	V	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

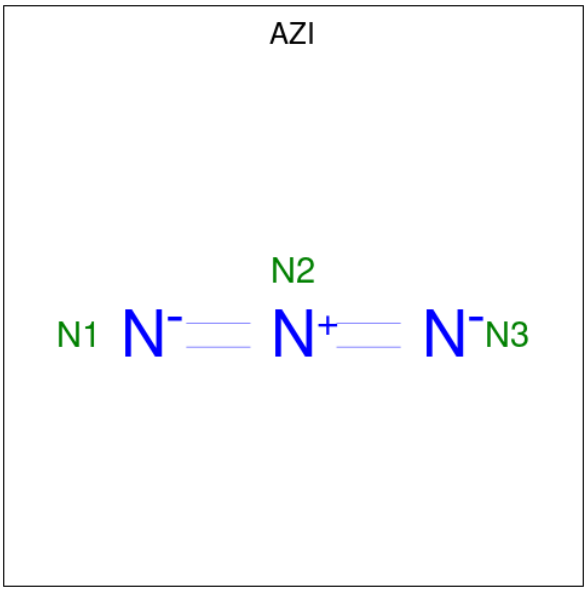
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	62	Total C N O 507 333 88 86	0	0	0
10	W	62	Total C N O 507 333 88 86	0	0	0

- Molecule 11 is hexyl beta-D-glucopyranoside (three-letter code: JZR) (formula: $C_{12}H_{24}O_6$).



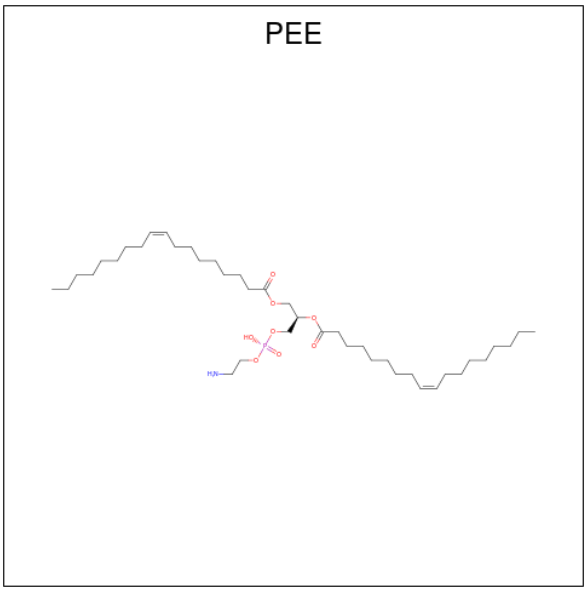
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 18 12 6	0	0
11	C	1	Total C O 18 12 6	0	0
11	F	1	Total C O 18 12 6	0	0
11	F	1	Total C O 18 12 6	0	0
11	P	1	Total C O 18 12 6	0	0
11	S	1	Total C O 18 12 6	0	0

- Molecule 12 is AZIDE ION (three-letter code: AZI) (formula: N_3).



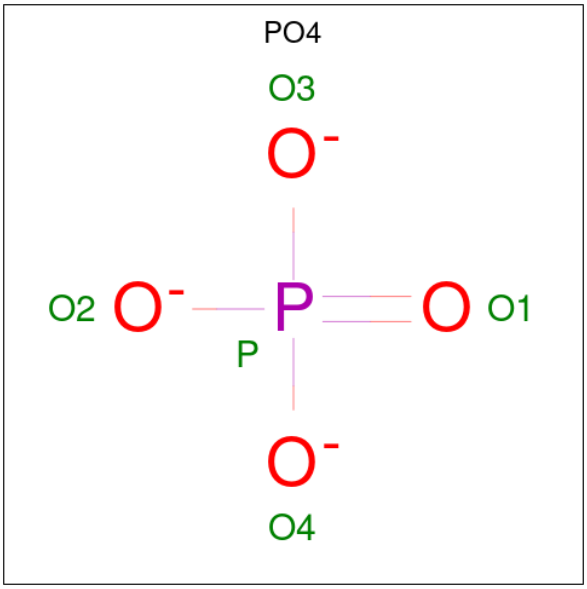
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total N 3 3	0	0
12	C	1	Total N 3 3	0	0
12	D	1	Total N 3 3	0	0
12	P	1	Total N 3 3	0	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



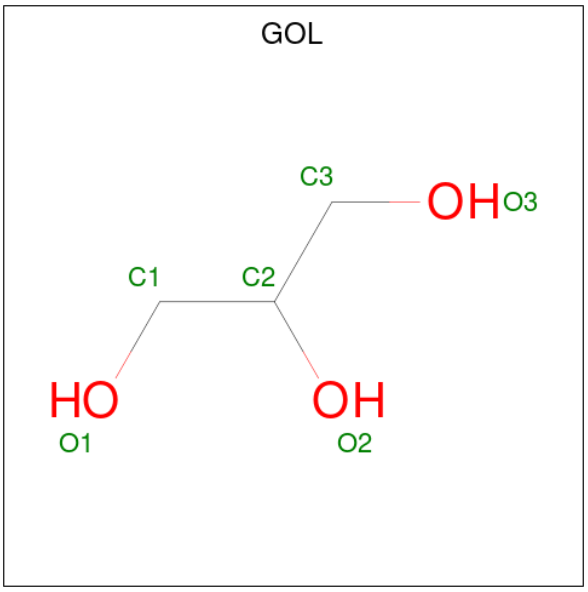
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 6 3 3	0	0
13	C	1	Total C N O P 49 39 1 8 1	0	0
13	C	1	Total O P 5 4 1	0	0
13	D	1	Total C N O P 51 41 1 8 1	0	0
13	G	1	Total C N O P 49 39 1 8 1	0	0
13	N	1	Total O P 5 4 1	0	0
13	P	1	Total C N O P 49 39 1 8 1	0	0
13	Q	1	Total C N O P 51 41 1 8 1	0	0
13	T	1	Total C N O P 49 39 1 8 1	0	0

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



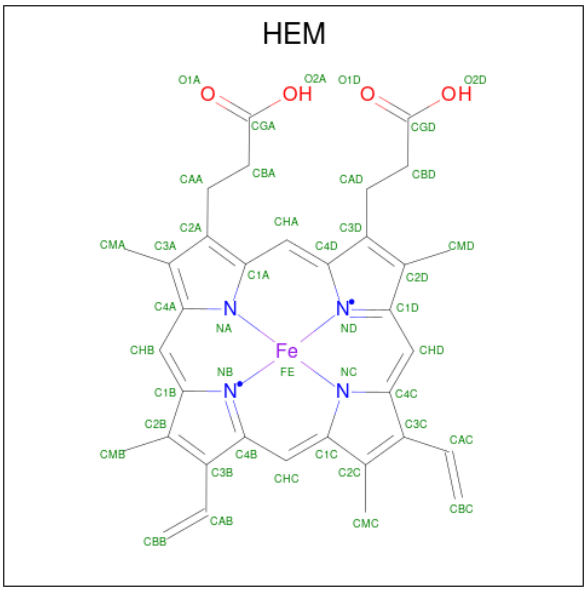
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total O P 5 4 1	0	0
14	O	1	Total O P 5 4 1	0	0

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



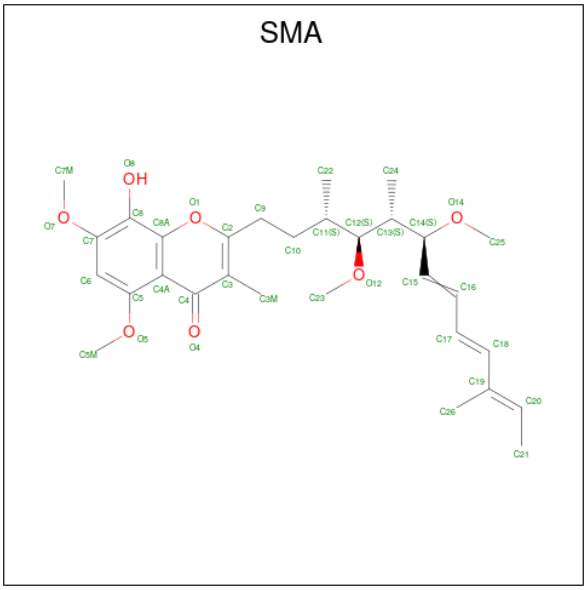
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C O 6 3 3	0	0
15	C	1	Total C O 6 3 3	0	0
15	O	1	Total C O 6 3 3	0	0
15	P	1	Total C O 6 3 3	0	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



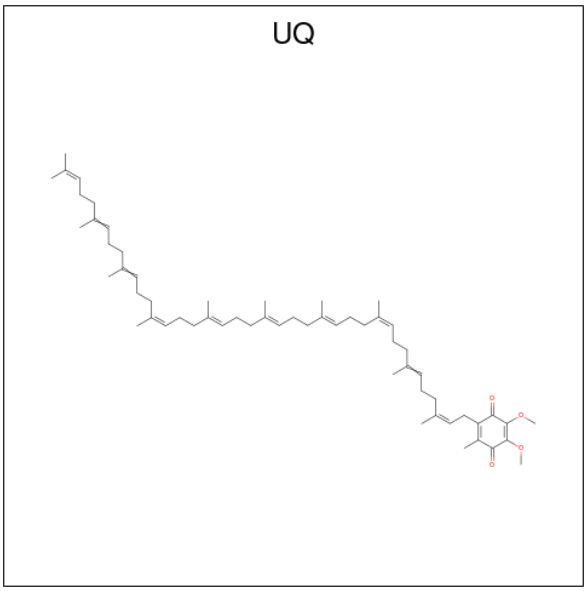
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



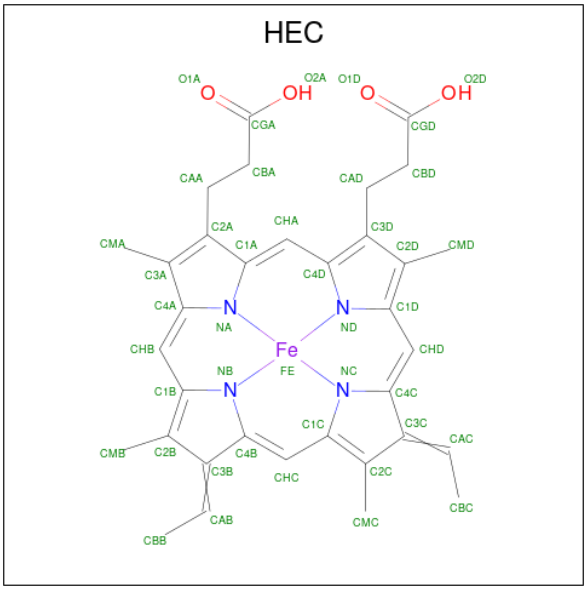
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	P	1	Total	C	O	0	0
			37	30	7		

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



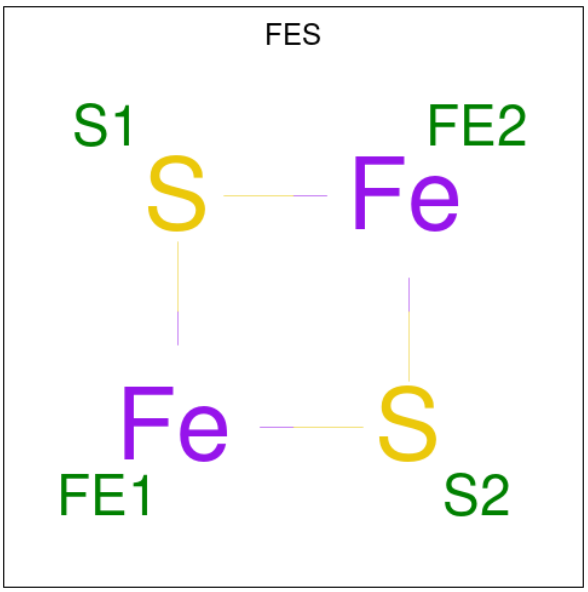
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	C	1	Total C O 14 10 4	0	0
18	P	1	Total C O 14 10 4	0	0

- Molecule 19 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



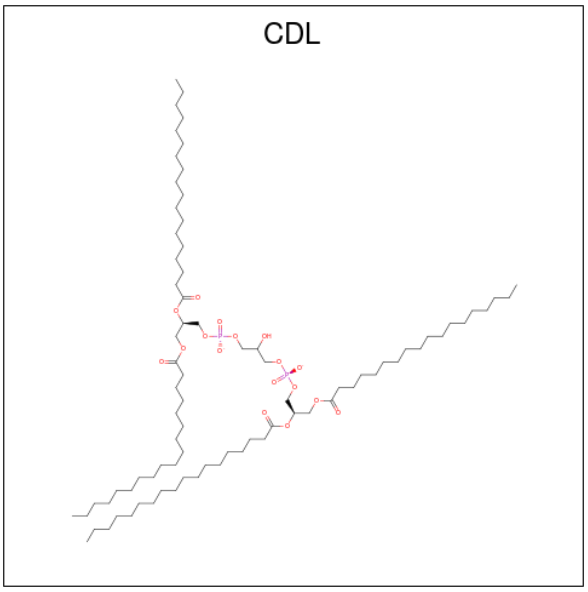
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	D	1	Total C Fe N O 43 34 1 4 4	0	0
19	Q	1	Total C Fe N O 43 34 1 4 4	0	0

- 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	0	0
			4	2	2		
20	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 21 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	G	1	Total	C	O	P	0	0
			50	31	17	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	G	1	Total C O P 44 25 17 2	0	0
21	Q	1	Total C O P 50 31 17 2	0	0
21	T	1	Total C O P 49 30 17 2	0	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	187	Total O 187 187	0	0
22	B	149	Total O 149 149	0	0
22	C	125	Total O 125 125	0	0
22	D	118	Total O 118 118	0	0
22	E	54	Total O 54 54	0	0
22	F	57	Total O 57 57	0	0
22	G	24	Total O 24 24	0	0
22	H	14	Total O 14 14	0	0
22	I	16	Total O 16 16	0	0
22	J	5	Total O 5 5	0	0
22	N	134	Total O 134 134	0	0
22	O	130	Total O 130 130	0	0
22	P	122	Total O 122 122	0	0
22	Q	109	Total O 109 109	0	0
22	R	64	Total O 64 64	0	0
22	S	73	Total O 73 73	0	0

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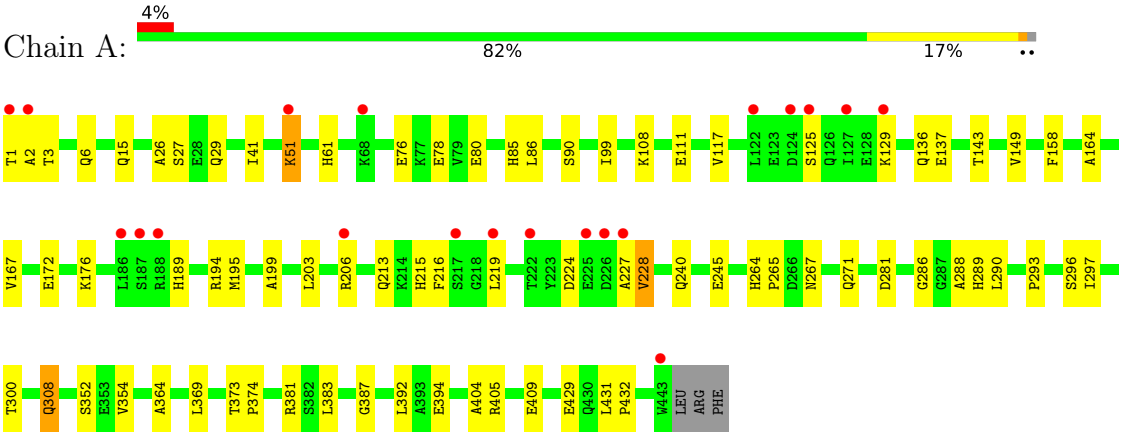
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	T	21	Total O 21 21	0	0
22	U	16	Total O 16 16	0	0
22	V	10	Total O 10 10	0	0
22	W	9	Total O 9 9	0	0

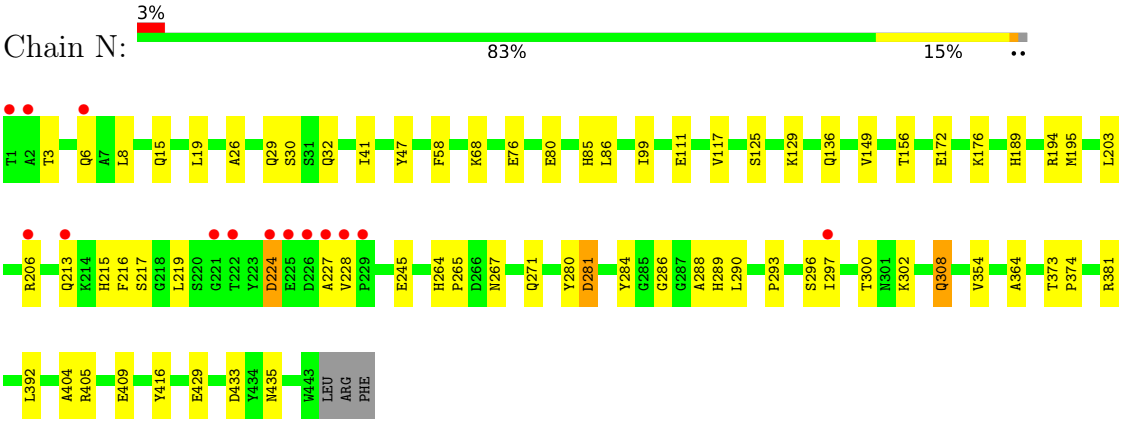
3 Residue-property plots (i)

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

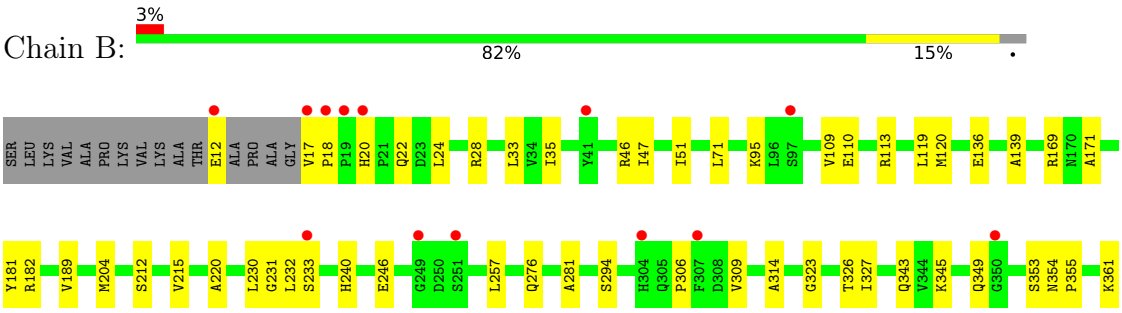
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial



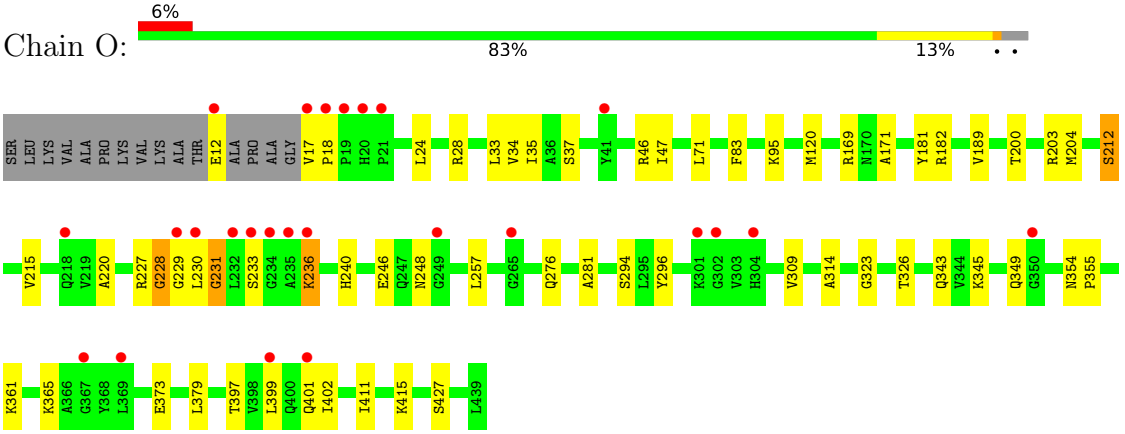
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial



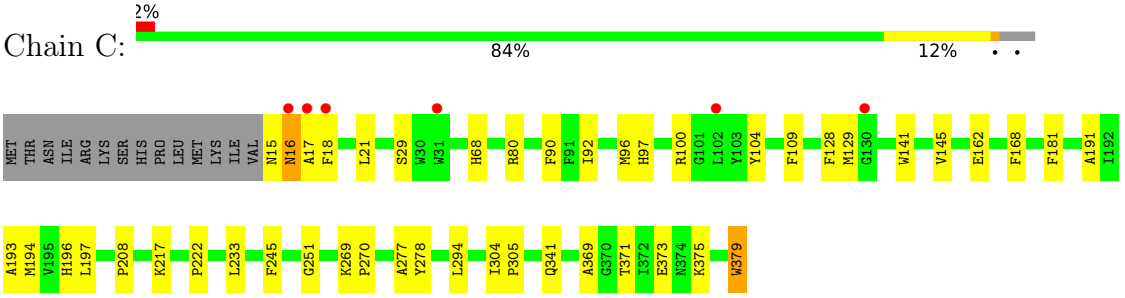
• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial



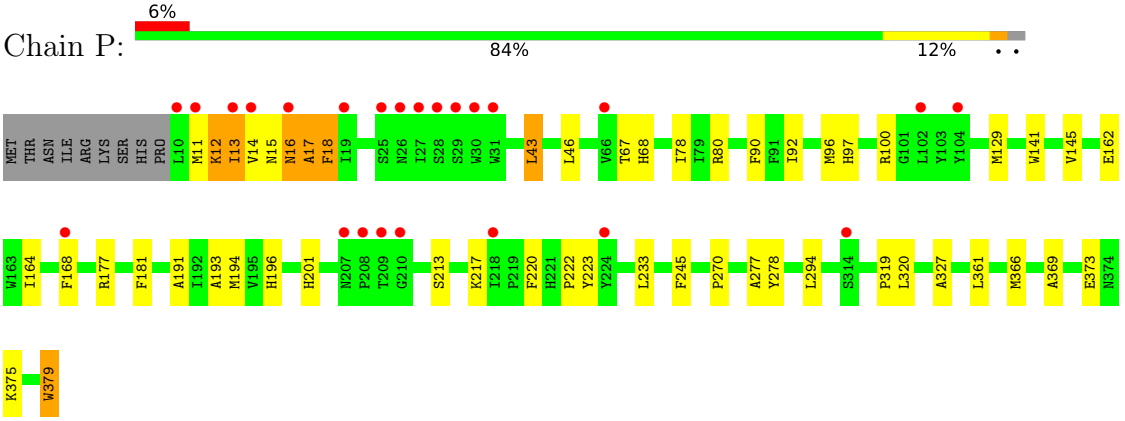
• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial



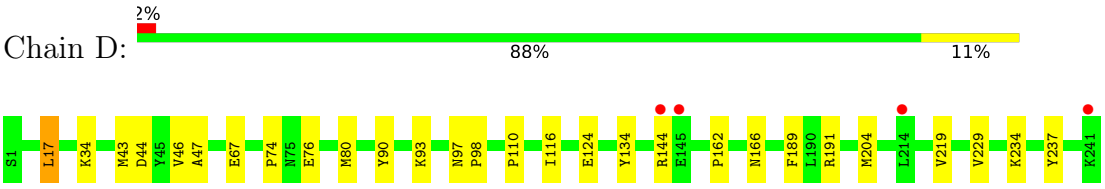
• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b

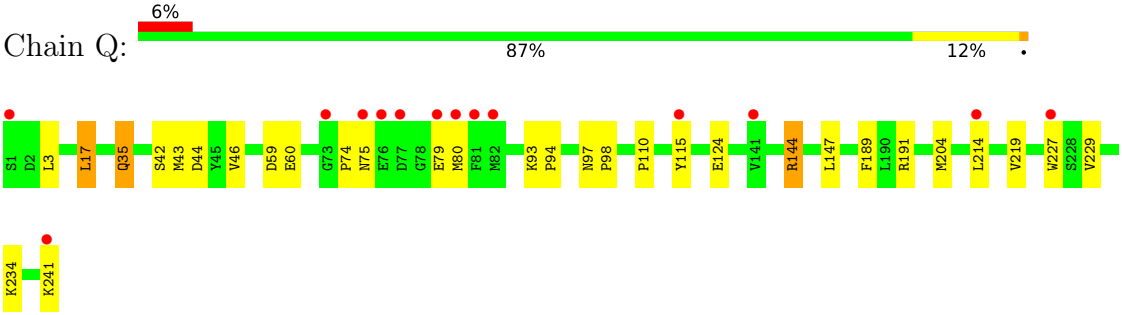


• Molecule 4: Cytochrome c1, heme protein, mitochondrial



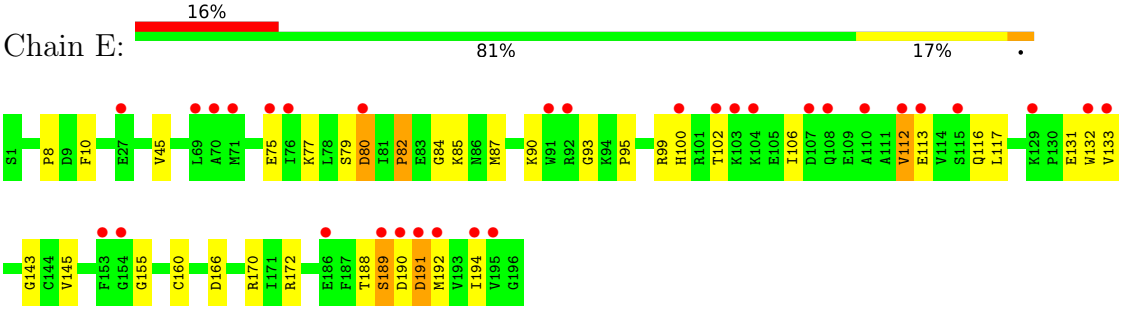
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:



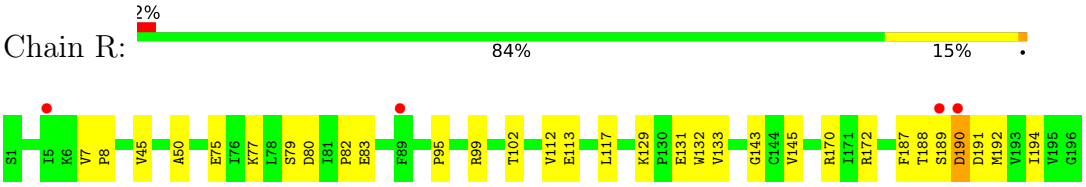
• Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain E:



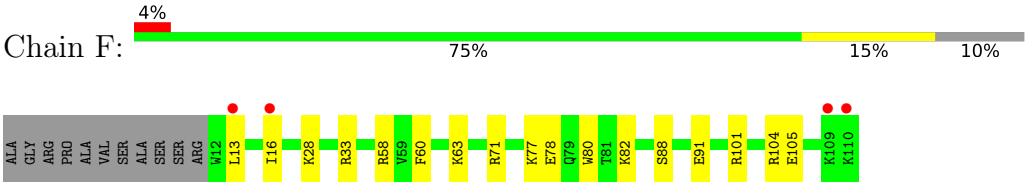
• Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain R:



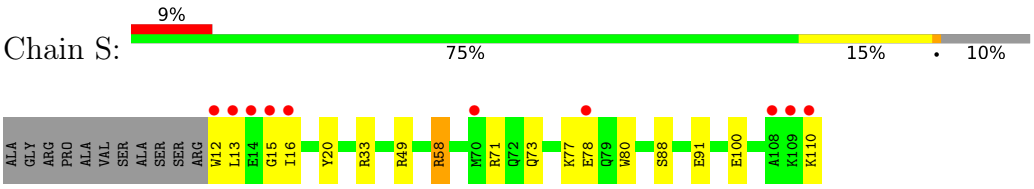
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



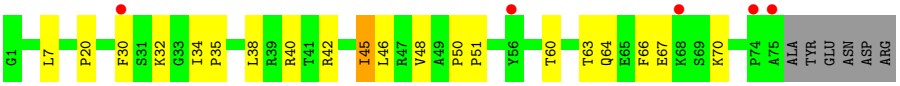
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain S:

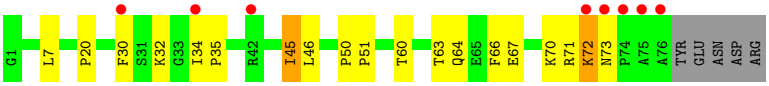


• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

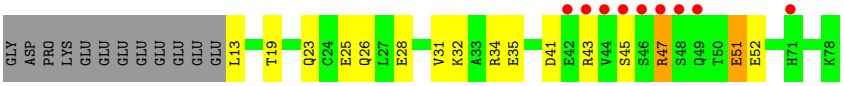
Chain G:



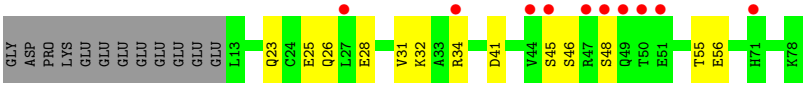
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



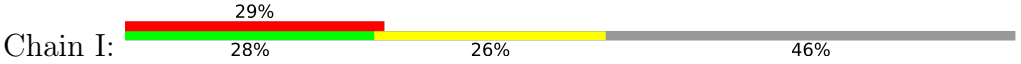
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

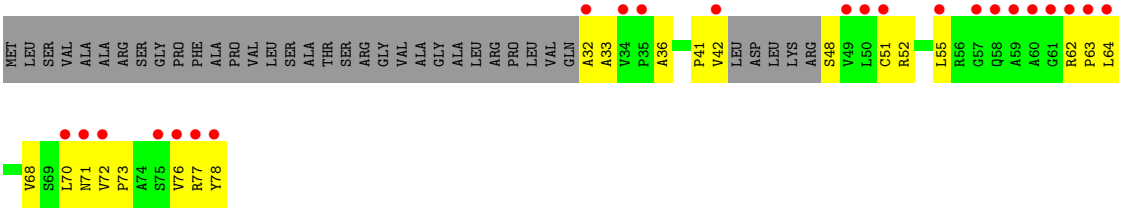


• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

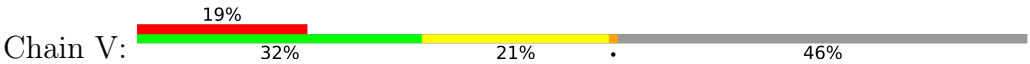


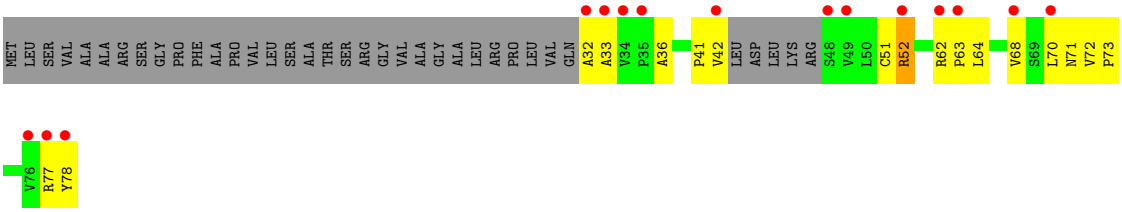
• Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial





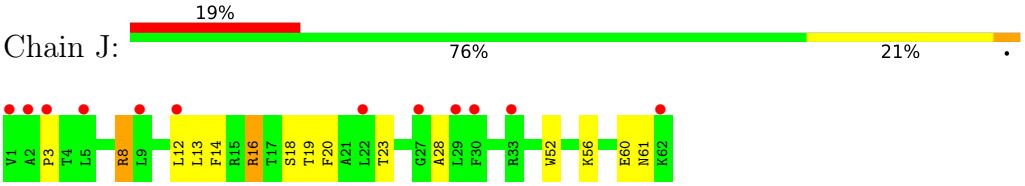
• Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial





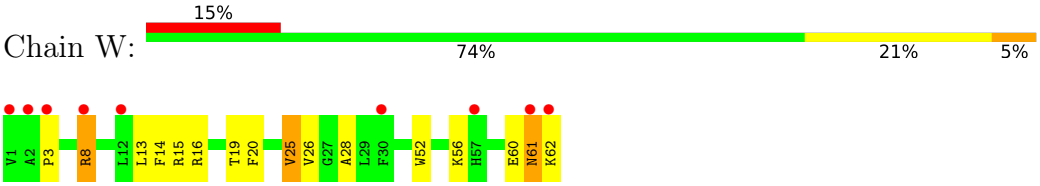
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.12Å 171.06Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.10 40.02 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.98-2.10) 96.1 (40.02-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.287 0.246 , 0.266	Depositor DCC
R_{free} test set	15323 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33959	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: CDL, PO4, PEE, UQ, HEC, SMA, FES, HEM, AZI, JZR, GOL

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	0.32	0/3472	0.66	0/4714
1	N	0.33	0/3472	0.67	0/4714
2	B	0.32	0/3235	0.65	0/4387
2	O	0.31	0/3239	0.65	1/4393 (0.0%)
3	C	0.36	0/2986	0.65	1/4089 (0.0%)
3	P	0.35	0/3024	0.64	0/4137
4	D	0.34	0/1978	0.65	0/2684
4	Q	0.34	0/1978	0.65	0/2684
5	E	0.31	0/1553	0.67	1/2100 (0.0%)
5	R	0.35	0/1553	0.69	1/2100 (0.0%)
6	F	0.32	0/878	0.64	0/1175
6	S	0.32	0/878	0.65	0/1175
7	G	0.32	0/642	0.65	0/869
7	T	0.34	0/647	0.68	0/876
8	H	0.30	0/544	0.60	0/729
8	U	0.31	0/544	0.56	0/729
9	I	0.32	0/285	0.66	0/384
9	V	0.32	0/285	0.69	0/384
10	J	0.36	0/520	0.65	0/699
10	W	0.36	0/520	0.65	0/699
All	All	0.33	0/32233	0.65	4/43721 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	228	GLY	N-CA-C	-6.96	95.71	113.10
5	R	143	GLY	N-CA-C	5.70	127.36	113.10
5	E	143	GLY	N-CA-C	5.38	126.54	113.10
3	C	109	PHE	N-CA-C	-5.22	96.91	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	3403	0	3302	63	0
1	N	3403	0	3302	53	0
2	B	3177	0	3152	64	0
2	O	3180	0	3156	56	0
3	C	2892	0	2938	39	0
3	P	2931	0	2989	59	0
4	D	1919	0	1868	25	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	30	0
5	R	1519	0	1503	25	0
6	F	861	0	854	14	0
6	S	861	0	854	20	0
7	G	621	0	626	17	0
7	T	626	0	631	23	0
8	H	539	0	524	14	0
8	U	539	0	524	10	0
9	I	285	0	288	37	0
9	V	285	0	288	31	0
10	J	507	0	513	24	0
10	W	507	0	513	27	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	3	0
11	P	18	0	24	0	0
11	S	18	0	24	8	0
12	A	3	0	0	0	0
12	C	3	0	0	0	0
12	D	3	0	0	0	0
12	P	3	0	0	0	0
13	A	6	0	5	0	0
13	C	54	0	72	2	0
13	D	51	0	82	1	0
13	G	49	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	5	0	0	0	0
13	P	49	0	72	2	0
13	Q	51	0	82	9	0
13	T	49	0	72	1	0
14	B	5	0	0	0	0
14	O	5	0	0	0	0
15	B	6	0	8	0	0
15	C	6	0	8	0	0
15	O	6	0	8	0	0
15	P	6	0	8	0	0
16	C	86	0	60	5	0
16	P	86	0	60	3	0
17	C	37	0	42	1	0
17	P	37	0	42	2	0
18	C	14	0	9	3	0
18	P	14	0	9	5	0
19	D	43	0	30	3	0
19	Q	43	0	30	2	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	G	94	0	76	5	0
21	Q	50	0	44	0	0
21	T	49	0	42	0	0
22	A	187	0	0	8	0
22	B	149	0	0	2	0
22	C	125	0	0	4	0
22	D	118	0	0	2	0
22	E	54	0	0	2	0
22	F	57	0	0	3	0
22	G	24	0	0	1	0
22	H	14	0	0	0	0
22	I	16	0	0	1	0
22	J	5	0	0	0	0
22	N	134	0	0	1	0
22	O	130	0	0	1	0
22	P	122	0	0	6	0
22	Q	109	0	0	1	0
22	R	64	0	0	0	0
22	S	73	0	0	2	0
22	T	21	0	0	1	0
22	U	16	0	0	0	0
22	V	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	9	0	0	0	0
All	All	33959	0	32273	593	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 9.

All (593) 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:95:LYS:HB2	9:V:32:ALA:HB2	1.20	1.12
2:B:12:GLU:HG2	2:B:17:VAL:H	1.15	1.09
7:T:45:ILE:HG22	7:T:46:LEU:HD22	1.31	1.04
2:O:200:THR:HB	2:O:229:GLY:HA2	1.36	1.04
3:P:43:LEU:HD21	13:Q:3006:PEE:H30	1.40	1.01
5:E:166:ASP:HA	22:E:541:HOH:O	1.59	1.01
1:A:136:GLN:HE21	9:I:51:CYS:HB3	1.34	0.91
4:Q:59:ASP:OD2	10:W:62:LYS:HB3	1.71	0.91
6:S:13:LEU:HD12	6:S:16:ILE:HD11	1.52	0.91
6:F:104:ARG:HH11	11:F:3011:JZR:H6	1.36	0.91
1:A:293:PRO:O	1:A:297:ILE:HG12	1.71	0.90
1:N:136:GLN:HE21	9:V:51:CYS:HB3	1.37	0.89
2:O:229:GLY:C	2:O:231:GLY:H	1.76	0.89
9:V:64:LEU:HD12	9:V:77:ARG:O	1.73	0.88
9:I:32:ALA:N	9:I:72:VAL:HG23	1.88	0.88
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.56	0.87
1:A:1:THR:HG21	2:B:212:SER:HB3	1.55	0.86
9:V:52:ARG:HH11	9:V:52:ARG:HB3	1.40	0.86
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.41	0.85
2:B:12:GLU:HG2	2:B:17:VAL:N	1.90	0.85
2:O:236:LYS:H	2:O:236:LYS:HD2	1.42	0.84
2:O:95:LYS:CB	9:V:32:ALA:HB2	2.06	0.84
1:N:293:PRO:O	1:N:297:ILE:HG12	1.78	0.83
4:D:74:PRO:HG3	4:D:80:MET:HE1	1.59	0.83
2:B:95:LYS:HB2	9:I:32:ALA:HB2	1.57	0.83
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.61	0.83
3:P:12:LYS:HE2	3:P:16:ASN:H	1.42	0.82
9:V:52:ARG:HB3	9:V:52:ARG:NH1	1.94	0.82
10:J:16:ARG:HB2	10:J:19:THR:HG22	1.58	0.82
9:I:64:LEU:HD12	9:I:77:ARG:O	1.78	0.81
1:N:29:GLN:HB3	2:O:12:GLU:O	1.80	0.80
7:T:72:LYS:HG3	8:U:56:GLU:OE2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:12:LYS:HA	3:P:12:LYS:HE3	1.62	0.80
2:O:200:THR:CB	2:O:229:GLY:HA2	2.11	0.79
1:A:1:THR:HG21	2:B:212:SER:CB	2.13	0.78
10:J:16:ARG:NH1	10:J:19:THR:HG21	1.99	0.78
9:I:32:ALA:N	9:I:71:ASN:HB3	1.99	0.77
4:Q:110:PRO:HG3	19:Q:501:HEC:HMD3	1.66	0.77
10:W:13:LEU:O	10:W:19:THR:HG23	1.84	0.76
1:A:2:ALA:HB1	1:A:6:GLN:HB2	1.65	0.76
10:W:3:PRO:HB2	10:W:8:ARG:NH1	2.01	0.76
3:P:43:LEU:HD21	13:Q:3006:PEE:C19	2.17	0.75
4:Q:74:PRO:HG3	4:Q:80:MET:HE1	1.69	0.74
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.22	0.74
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.52	0.74
9:I:32:ALA:N	9:I:71:ASN:CB	2.51	0.74
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.69	0.74
10:W:16:ARG:HH11	10:W:19:THR:HG21	1.54	0.73
1:A:3:THR:OG1	1:A:6:GLN:HG3	1.88	0.73
8:U:28:GLU:O	8:U:31:VAL:HG22	1.89	0.73
1:A:352:SER:HB3	6:S:110:LYS:HD2	1.71	0.72
8:H:43:ARG:O	8:H:47:ARG:HD2	1.89	0.72
6:F:13:LEU:O	6:F:16:ILE:HG12	1.89	0.72
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.70	0.72
10:J:16:ARG:HB2	10:J:16:ARG:HH11	1.55	0.72
3:C:129:MET:CE	3:C:181:PHE:HD2	2.02	0.71
5:E:113:GLU:HB3	5:E:116:GLN:HE21	1.55	0.71
5:E:113:GLU:HB3	5:E:116:GLN:NE2	2.05	0.71
10:J:13:LEU:O	10:J:19:THR:HG23	1.90	0.71
4:Q:35:GLN:HG3	22:Q:3086:HOH:O	1.91	0.71
1:A:51:LYS:HZ1	1:A:51:LYS:H	1.39	0.70
4:Q:74:PRO:HG3	4:Q:80:MET:CE	2.22	0.70
3:P:96:MET:HE2	13:P:3007:PEE:H27	1.74	0.70
3:C:129:MET:HE1	3:C:181:PHE:CD2	2.26	0.70
2:B:47:ILE:HG21	2:B:120:MET:HE3	1.73	0.69
8:H:28:GLU:O	8:H:31:VAL:HG22	1.92	0.69
1:A:352:SER:HB3	6:S:110:LYS:CD	2.23	0.69
2:B:231:GLY:N	2:B:233:SER:H	1.90	0.69
3:P:68:HIS:HD2	22:P:3131:HOH:O	1.75	0.69
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.28	0.69
4:Q:75:ASN:HD21	4:Q:79:GLU:HG2	1.58	0.69
1:A:136:GLN:HE21	9:I:51:CYS:CB	2.04	0.68
22:A:4185:HOH:O	9:I:73:PRO:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:GLN:HG3	1:N:203:LEU:O	1.94	0.68
2:B:353:SER:HB3	2:B:355:PRO:HD2	1.76	0.68
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.23	0.68
5:R:79:SER:HB3	5:R:191:ASP:OD1	1.93	0.68
2:B:95:LYS:HD3	2:B:110:GLU:OE2	1.94	0.68
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.76	0.67
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.76	0.67
6:S:100:GLU:HB3	11:S:2011:JZR:H6A	1.76	0.67
10:W:16:ARG:NH1	10:W:19:THR:HG21	2.10	0.67
1:N:32:GLN:OE1	2:O:373:GLU:HB2	1.94	0.67
3:P:129:MET:CE	3:P:181:PHE:HD2	2.08	0.66
1:A:2:ALA:O	2:B:113:ARG:NE	2.28	0.66
10:W:8:ARG:HG2	10:W:8:ARG:HH11	1.60	0.65
5:R:190:ASP:HB2	5:R:192:MET:HG2	1.79	0.65
7:G:60:THR:O	7:G:64:GLN:HG3	1.95	0.65
10:J:16:ARG:HB2	10:J:19:THR:CG2	2.26	0.65
2:O:365:LYS:HG2	2:O:399:LEU:HD22	1.78	0.65
6:S:13:LEU:HA	6:S:16:ILE:HG12	1.78	0.65
4:D:74:PRO:HG3	4:D:80:MET:CE	2.27	0.64
3:P:96:MET:CE	13:P:3007:PEE:H27	2.27	0.64
2:B:95:LYS:HD2	9:I:32:ALA:HB2	1.79	0.64
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.32	0.64
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.78	0.64
1:N:136:GLN:NE2	9:V:51:CYS:HB3	2.11	0.64
2:B:231:GLY:N	2:B:232:LEU:N	2.46	0.64
7:T:60:THR:O	7:T:64:GLN:HG3	1.98	0.64
10:J:16:ARG:HH11	10:J:16:ARG:CB	2.10	0.64
8:H:25:GLU:HG2	8:H:34:ARG:HH22	1.62	0.64
2:O:95:LYS:HB2	9:V:32:ALA:CB	2.12	0.63
2:O:236:LYS:H	2:O:236:LYS:CD	2.07	0.63
2:B:95:LYS:CB	9:I:32:ALA:HB2	2.26	0.63
2:O:47:ILE:HG21	2:O:120:MET:HE3	1.81	0.63
6:F:28:LYS:HE3	22:F:4052:HOH:O	1.98	0.63
4:Q:75:ASN:ND2	4:Q:79:GLU:HG2	2.13	0.63
7:T:71:ARG:HH11	7:T:72:LYS:HZ2	1.45	0.63
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.80	0.62
5:E:113:GLU:CB	5:E:116:GLN:HE21	2.12	0.62
10:J:14:PHE:HA	10:J:20:PHE:HD2	1.64	0.62
10:J:16:ARG:HH11	10:J:16:ARG:CG	2.12	0.62
9:V:32:ALA:N	9:V:71:ASN:CB	2.63	0.62
2:B:397:THR:O	2:B:401:GLN:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:296:TYR:OH	9:V:52:ARG:NE	2.33	0.62
3:C:29:SER:HB2	21:G:2004:CDL:HA31	1.82	0.62
2:B:47:ILE:HG21	2:B:120:MET:CE	2.30	0.61
3:C:96:MET:HE2	13:C:2007:PEE:H27	1.80	0.61
2:B:412:ASN:HA	2:B:415:LYS:HD2	1.80	0.61
10:J:3:PRO:HD2	10:J:8:ARG:CZ	2.30	0.61
1:N:41:ILE:HG12	1:N:195:MET:HG2	1.83	0.61
2:O:397:THR:O	2:O:401:GLN:HG3	2.01	0.61
2:O:227:ARG:C	2:O:229:GLY:N	2.50	0.61
4:Q:60:GLU:HG3	10:W:62:LYS:NZ	2.15	0.61
1:A:29:GLN:HG3	1:A:203:LEU:O	2.00	0.61
9:V:32:ALA:N	9:V:71:ASN:HB2	2.15	0.61
2:O:35:ILE:N	2:O:35:ILE:HD12	2.16	0.60
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.01	0.60
2:O:203:ARG:HH12	2:O:233:SER:HA	1.65	0.60
4:D:116:ILE:HG12	19:D:501:HEC:HMA3	1.83	0.60
3:P:145:VAL:HG21	17:P:3001:SMA:H6	1.84	0.60
4:Q:43:MET:HE2	4:Q:46:VAL:HG21	1.84	0.60
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.31	0.60
1:N:308:GLN:HG2	22:N:3026:HOH:O	2.01	0.60
3:P:14:VAL:O	3:P:18:PHE:HB3	2.01	0.60
7:T:71:ARG:HH11	7:T:72:LYS:NZ	1.99	0.60
2:O:47:ILE:HG21	2:O:120:MET:CE	2.32	0.60
1:N:86:LEU:HD13	1:N:99:ILE:HG12	1.82	0.60
5:E:85:LYS:NZ	5:E:87:MET:SD	2.75	0.60
1:N:216:PHE:HD2	1:N:219:LEU:HD22	1.67	0.59
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.33	0.59
2:B:412:ASN:HD22	2:B:415:LYS:HD2	1.67	0.59
3:P:43:LEU:HD21	13:Q:3006:PEE:C20	2.33	0.59
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.84	0.59
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.37	0.59
2:O:227:ARG:C	2:O:229:GLY:H	2.02	0.59
1:A:296:SER:O	1:A:300:THR:HG23	2.02	0.59
7:G:40:ARG:HB3	21:G:2004:CDL:HB32	1.85	0.59
7:G:45:ILE:HG22	7:G:46:LEU:HD12	1.85	0.59
10:J:3:PRO:HD2	10:J:8:ARG:NH2	2.18	0.59
2:B:354:ASN:N	2:B:355:PRO:CD	2.66	0.59
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.84	0.59
7:T:66:PHE:CZ	7:T:70:LYS:HD2	2.38	0.58
3:C:96:MET:CE	13:C:2007:PEE:H27	2.34	0.58
2:B:189:VAL:HG23	22:B:3089:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:77:LYS:HE3	5:E:79:SER:OG	2.03	0.58
2:B:309:VAL:HG23	2:B:326:THR:HG22	1.85	0.58
1:N:8:LEU:HD22	1:N:392:LEU:HB3	1.84	0.58
1:A:289:HIS:HE1	11:S:2011:JZR:H1'A	1.69	0.58
2:B:20:HIS:HB2	2:B:22:GLN:HG3	1.84	0.58
10:J:12:LEU:O	10:J:13:LEU:HD23	2.04	0.58
9:V:32:ALA:N	9:V:72:VAL:HG23	2.18	0.58
2:B:365:LYS:HG2	2:B:399:LEU:HD22	1.86	0.58
1:N:30:SER:HA	2:O:18:PRO:HG3	1.85	0.58
1:N:286:GLY:HA3	1:N:290:LEU:HD21	1.85	0.58
2:O:229:GLY:C	2:O:231:GLY:N	2.47	0.57
2:B:139:ALA:HB3	11:S:2011:JZR:H5'	1.86	0.57
10:W:8:ARG:HH11	10:W:8:ARG:CG	2.18	0.57
1:A:136:GLN:NE2	9:I:51:CYS:CB	2.67	0.57
7:T:71:ARG:HD3	7:T:72:LYS:HZ3	1.70	0.57
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.84	0.57
6:F:82:LYS:HE3	22:F:4032:HOH:O	2.04	0.57
1:N:373:THR:HB	1:N:374:PRO:HD3	1.86	0.57
9:V:62:ARG:O	9:V:78:TYR:HB3	2.05	0.57
3:P:129:MET:HE2	3:P:181:PHE:HB2	1.87	0.56
10:J:3:PRO:HB2	10:J:8:ARG:HD3	1.86	0.56
10:W:25:VAL:HG12	10:W:26:VAL:N	2.20	0.56
2:B:95:LYS:CG	9:I:32:ALA:HB2	2.35	0.56
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.36	0.56
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.69	0.56
9:I:32:ALA:N	9:I:71:ASN:HB2	2.19	0.56
8:H:25:GLU:CG	8:H:34:ARG:HH22	2.19	0.56
5:E:190:ASP:O	5:E:192:MET:HG2	2.05	0.56
7:T:30:PHE:O	7:T:34:ILE:HG12	2.06	0.56
8:U:25:GLU:HG2	8:U:34:ARG:HH22	1.71	0.56
3:P:319:PRO:HD2	22:P:3113:HOH:O	2.05	0.55
7:G:63:THR:O	7:G:67:GLU:HG2	2.06	0.55
5:E:90:LYS:HE2	5:E:93:GLY:HA2	1.87	0.55
7:G:30:PHE:O	7:G:34:ILE:HG12	2.06	0.55
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.89	0.55
11:F:3011:JZR:H6A	2:O:83:PHE:HB2	1.89	0.55
3:P:201:HIS:NE2	18:P:3002:UQ:O4	2.28	0.55
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.89	0.55
4:Q:241:LYS:OXT	4:Q:241:LYS:HD3	2.06	0.55
1:A:51:LYS:H	1:A:51:LYS:NZ	2.03	0.55
9:I:62:ARG:O	9:I:78:TYR:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:GLU:CG	2:B:17:VAL:H	2.04	0.55
1:N:136:GLN:HE21	9:V:51:CYS:CB	2.15	0.55
2:B:95:LYS:HD2	9:I:32:ALA:CB	2.37	0.55
1:N:364:ALA:HB2	9:V:33:ALA:HB1	1.89	0.55
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.41	0.54
3:C:341:GLN:NE2	22:C:2099:HOH:O	2.39	0.54
5:R:77:LYS:HE3	5:R:79:SER:OG	2.07	0.54
6:F:63:LYS:HE2	22:G:1280:HOH:O	2.06	0.54
7:T:63:THR:O	7:T:67:GLU:HG2	2.07	0.54
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.89	0.54
3:P:12:LYS:HA	3:P:12:LYS:CE	2.37	0.54
1:A:216:PHE:HD2	1:A:219:LEU:HD22	1.71	0.54
1:A:172:GLU:OE2	1:A:176:LYS:HE3	2.06	0.54
7:T:45:ILE:HG22	7:T:46:LEU:CD2	2.22	0.54
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.07	0.54
2:B:12:GLU:O	2:B:18:PRO:HD3	2.08	0.54
2:O:411:ILE:O	2:O:415:LYS:HG3	2.08	0.54
5:R:191:ASP:OD2	5:R:191:ASP:N	2.40	0.54
10:W:56:LYS:HG2	10:W:60:GLU:CD	2.28	0.54
1:A:41:ILE:HG12	1:A:195:MET:HG2	1.89	0.53
3:P:100:ARG:HD2	3:P:100:ARG:C	2.28	0.53
2:B:306:PRO:HA	9:I:52:ARG:HE	1.74	0.53
3:P:43:LEU:HD21	13:Q:3006:PEE:H31	1.89	0.53
4:Q:59:ASP:OD2	10:W:62:LYS:CB	2.52	0.53
5:R:188:THR:HG21	5:R:194:ILE:CD1	2.37	0.53
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.74	0.53
2:B:294:SER:OG	2:B:343:GLN:NE2	2.42	0.53
4:D:166:ASN:HB3	8:H:13:LEU:HD23	1.91	0.53
2:O:229:GLY:O	2:O:230:LEU:HB2	2.07	0.53
3:P:220:PHE:HE1	18:P:3002:UQ:CM2	2.22	0.53
10:W:56:LYS:O	10:W:60:GLU:HG3	2.09	0.53
9:V:32:ALA:N	9:V:71:ASN:HB3	2.24	0.53
2:B:353:SER:CB	2:B:355:PRO:HD2	2.38	0.52
4:D:34:LYS:NZ	4:D:67:GLU:OE1	2.31	0.52
5:E:90:LYS:CE	5:E:93:GLY:HA2	2.40	0.52
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.91	0.52
9:I:72:VAL:HG13	9:I:73:PRO:HD2	1.92	0.52
2:O:95:LYS:HG3	9:V:32:ALA:N	2.24	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HD3	2.40	0.52
8:H:41:ASP:O	8:H:45:SER:HB2	2.09	0.52
2:B:314:ALA:HA	9:I:63:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:234:LYS:HD3	5:E:8:PRO:HB2	1.91	0.52
10:J:13:LEU:HB3	10:J:23:THR:OG1	2.10	0.52
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.09	0.52
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.91	0.52
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.92	0.52
2:O:189:VAL:HG23	22:O:3052:HOH:O	2.10	0.52
1:A:289:HIS:HE1	11:S:2011:JZR:C1'	2.23	0.52
1:N:30:SER:CA	2:O:18:PRO:HG3	2.39	0.52
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.44	0.52
4:D:34:LYS:HE3	22:D:4097:HOH:O	2.09	0.52
9:V:72:VAL:HG13	9:V:73:PRO:HD2	1.91	0.52
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.91	0.52
5:E:102:THR:O	5:E:106:ILE:HG13	2.09	0.52
3:P:12:LYS:CE	3:P:15:ASN:HB3	2.39	0.52
3:P:220:PHE:HE1	18:P:3002:UQ:HM22	1.74	0.52
3:C:129:MET:HE2	3:C:181:PHE:HB2	1.91	0.51
3:P:162:GLU:OE2	3:P:168:PHE:HD1	1.93	0.51
6:S:88:SER:OG	6:S:91:GLU:HB2	2.09	0.51
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.44	0.51
6:S:71:ARG:O	6:S:73:GLN:HG3	2.10	0.51
3:P:12:LYS:HE3	3:P:12:LYS:CA	2.36	0.51
10:W:52:TRP:O	10:W:56:LYS:HB2	2.11	0.51
1:N:206:ARG:HG3	1:N:206:ARG:HH11	1.75	0.51
5:R:77:LYS:HD3	5:R:80:ASP:OD2	2.10	0.51
1:A:227:ALA:O	1:A:228:VAL:C	2.49	0.51
2:B:33:LEU:CD2	2:B:220:ALA:HB1	2.41	0.51
16:C:502:HEM:HBA1	18:C:2002:UQ:O2	2.11	0.51
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.46	0.51
2:O:294:SER:OG	2:O:343:GLN:NE2	2.44	0.51
2:O:309:VAL:HG23	2:O:326:THR:HG22	1.93	0.51
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.59	0.51
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.76	0.51
7:G:40:ARG:CB	21:G:2004:CDL:HB32	2.41	0.51
1:N:68:LYS:HE3	1:N:68:LYS:HA	1.93	0.51
6:S:12:TRP:O	6:S:16:ILE:N	2.36	0.51
10:W:16:ARG:HB2	10:W:19:THR:CG2	2.33	0.51
1:N:381:ARG:HH11	1:N:381:ARG:HG2	1.75	0.51
8:U:25:GLU:CG	8:U:34:ARG:HH22	2.24	0.51
3:C:369:ALA:O	3:C:373:GLU:HG3	2.11	0.50
5:E:189:SER:C	5:E:190:ASP:OD1	2.49	0.50
5:R:188:THR:HG21	5:R:194:ILE:HD12	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:HG2	22:A:4140:HOH:O	2.10	0.50
7:T:71:ARG:HB2	7:T:72:LYS:HD3	1.93	0.50
3:C:68:HIS:HD2	22:C:2126:HOH:O	1.95	0.50
1:N:136:GLN:NE2	9:V:51:CYS:CB	2.72	0.50
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.42	0.50
2:B:35:ILE:N	2:B:35:ILE:HD12	2.27	0.50
3:P:245:PHE:CG	4:Q:17:LEU:HD13	2.47	0.50
5:R:129:LYS:HG3	5:R:187:PHE:CE1	2.47	0.50
6:F:88:SER:OG	6:F:91:GLU:HB2	2.12	0.50
11:F:3011:JZR:H4	1:N:289:HIS:CE1	2.47	0.50
1:A:373:THR:HB	1:A:374:PRO:HD3	1.92	0.50
2:O:229:GLY:O	2:O:231:GLY:N	2.44	0.50
3:P:15:ASN:O	3:P:17:ALA:N	2.44	0.50
4:Q:124:GLU:OE2	4:Q:191:ARG:CD	2.60	0.50
1:A:90:SER:HB3	22:A:4116:HOH:O	2.11	0.50
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.42	0.50
2:O:200:THR:O	2:O:204:MET:HG3	2.12	0.50
5:R:80:ASP:O	5:R:82:PRO:HD3	2.12	0.50
1:A:289:HIS:CE1	11:S:2011:JZR:H1'A	2.47	0.50
3:C:191:ALA:HA	3:C:194:MET:HE2	1.94	0.50
7:G:66:PHE:CZ	7:G:70:LYS:HD2	2.47	0.50
1:N:125:SER:O	1:N:129:LYS:HG3	2.11	0.50
1:A:125:SER:O	1:A:129:LYS:HG3	2.12	0.49
2:O:354:ASN:N	2:O:355:PRO:CD	2.75	0.49
3:P:164:ILE:O	3:P:177:ARG:HD2	2.12	0.49
13:Q:3006:PEE:H56	5:R:50:ALA:CB	2.42	0.49
9:V:32:ALA:HA	9:V:71:ASN:HD22	1.77	0.49
3:C:96:MET:HE2	3:C:96:MET:HA	1.93	0.49
19:D:501:HEC:HMC1	19:D:501:HEC:HBC3	1.94	0.49
10:W:3:PRO:HB2	10:W:8:ARG:HH11	1.74	0.49
5:E:82:PRO:O	5:E:100:HIS:HB3	2.12	0.49
1:A:364:ALA:HB2	9:I:33:ALA:HB1	1.95	0.49
5:R:99:ARG:HB3	5:R:133:VAL:HG12	1.94	0.49
1:N:405:ARG:O	1:N:409:GLU:HG3	2.13	0.49
1:A:172:GLU:HG3	1:A:176:LYS:HE3	1.95	0.49
8:H:28:GLU:O	8:H:32:LYS:HG2	2.13	0.49
1:N:227:ALA:O	1:N:228:VAL:HB	2.13	0.49
3:C:15:ASN:O	3:C:16:ASN:C	2.50	0.49
1:N:264:HIS:ND1	1:N:265:PRO:HD2	2.28	0.49
6:S:78:GLU:CD	6:S:78:GLU:H	2.16	0.48
3:C:191:ALA:HA	3:C:194:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:191:ALA:HA	3:P:194:MET:CE	2.43	0.48
6:S:100:GLU:OE1	11:S:2011:JZR:H4	2.13	0.48
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.94	0.48
3:C:21:LEU:HD21	18:C:2002:UQ:HM32	1.95	0.48
3:C:251:GLY:HA3	22:C:2091:HOH:O	2.13	0.48
3:C:371:THR:O	3:C:375:LYS:HG2	2.13	0.48
10:J:16:ARG:NH1	10:J:16:ARG:CG	2.75	0.48
5:R:79:SER:CB	5:R:191:ASP:OD1	2.61	0.48
6:S:13:LEU:HB3	22:S:2070:HOH:O	2.13	0.48
1:A:143:THR:OG1	9:I:48:SER:HB3	2.13	0.48
3:C:97:HIS:CD2	16:C:502:HEM:NC	2.81	0.48
4:D:110:PRO:HG3	19:D:501:HEC:HMD3	1.95	0.48
3:P:245:PHE:CD1	4:Q:17:LEU:HD13	2.48	0.48
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.29	0.48
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.49	0.48
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.96	0.48
3:C:379:TRP:CE3	6:F:33:ARG:HD3	2.47	0.48
2:O:365:LYS:HG2	2:O:399:LEU:CD2	2.42	0.48
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.96	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.49	0.48
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.14	0.48
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.49	0.48
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.49	0.48
4:Q:3:LEU:HD12	8:U:55:THR:HG22	1.96	0.48
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.79	0.48
10:W:61:ASN:C	10:W:62:LYS:HG3	2.35	0.48
5:E:155:GLY:N	22:E:541:HOH:O	2.46	0.47
6:F:78:GLU:H	6:F:78:GLU:CD	2.16	0.47
2:O:354:ASN:HB3	2:O:355:PRO:HD3	1.96	0.47
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.95	0.47
10:J:16:ARG:CB	10:J:19:THR:HG22	2.38	0.47
10:J:16:ARG:O	10:J:19:THR:HG22	2.14	0.47
10:W:8:ARG:NH1	10:W:8:ARG:CG	2.75	0.47
1:A:213:GLN:HG2	22:A:4055:HOH:O	2.15	0.47
2:B:212:SER:OG	2:B:215:VAL:HG23	2.15	0.47
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.44	0.47
3:P:14:VAL:O	3:P:15:ASN:O	2.32	0.47
1:A:429:GLU:OE2	7:G:7:LEU:HB2	2.14	0.47
10:J:52:TRP:O	10:J:56:LYS:HB2	2.13	0.47
1:N:296:SER:O	1:N:300:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.96	0.47
3:C:100:ARG:HD2	3:C:100:ARG:C	2.35	0.47
2:O:361:LYS:HE2	2:O:402:ILE:O	2.14	0.47
3:P:14:VAL:C	3:P:15:ASN:CA	2.83	0.47
1:A:167:VAL:HG13	22:A:4111:HOH:O	2.15	0.47
2:B:246:GLU:O	2:B:427:SER:HA	2.15	0.47
2:B:345:LYS:O	2:B:349:GLN:HG3	2.14	0.47
3:P:193:ALA:O	3:P:196:HIS:HB3	2.15	0.47
2:B:396:SER:HB3	22:B:3031:HOH:O	2.14	0.47
1:N:111:GLU:HG3	1:N:215:HIS:CE1	2.50	0.47
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.50	0.47
7:T:46:LEU:HD23	22:T:3018:HOH:O	2.13	0.47
8:U:28:GLU:O	8:U:32:LYS:HG2	2.15	0.47
1:A:394:GLU:HA	11:A:4002:JZR:H2	1.96	0.47
3:C:162:GLU:OE2	3:C:168:PHE:HD1	1.98	0.47
2:O:17:VAL:HG13	2:O:18:PRO:HD2	1.96	0.47
4:Q:234:LYS:HD3	5:R:8:PRO:HB2	1.95	0.47
2:B:95:LYS:HE3	9:I:72:VAL:HG21	1.97	0.47
2:B:257:LEU:O	2:B:323:GLY:HA3	2.15	0.47
5:E:79:SER:HB3	5:E:191:ASP:OD2	2.15	0.47
1:N:172:GLU:HG3	1:N:176:LYS:HE3	1.96	0.47
3:P:97:HIS:CD2	16:P:502:HEM:NC	2.83	0.47
7:T:46:LEU:HD22	7:T:46:LEU:N	2.30	0.47
1:A:286:GLY:HA3	1:A:290:LEU:HD21	1.95	0.47
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.97	0.47
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.63	0.46
3:P:361:LEU:O	3:P:366:MET:HG3	2.15	0.46
16:P:502:HEM:HBA1	18:P:3002:UQ:O2	2.15	0.46
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.51	0.46
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.15	0.46
5:E:85:LYS:HZ3	5:E:87:MET:HA	1.80	0.46
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.45	0.46
3:P:375:LYS:HD2	3:P:375:LYS:N	2.29	0.46
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.81	0.46
2:B:46:ARG:HD2	2:B:375:SER:OG	2.14	0.46
3:C:245:PHE:CG	4:D:17:LEU:HD13	2.50	0.46
3:P:92:ILE:O	3:P:96:MET:HG2	2.16	0.46
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.95	0.46
8:H:31:VAL:HG23	8:H:32:LYS:N	2.30	0.46
10:J:16:ARG:HH12	10:J:19:THR:HG21	1.76	0.46
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:47:TYR:HB3	1:N:189:HIS:CE1	2.51	0.46
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.45	0.46
22:P:3113:HOH:O	6:S:20:TYR:HE1	1.99	0.46
22:A:4072:HOH:O	6:S:110:LYS:HD2	2.15	0.46
2:O:24:LEU:HD12	2:O:37:SER:O	2.15	0.46
19:Q:501:HEC:HBC3	19:Q:501:HEC:HMC1	1.98	0.46
3:C:233:LEU:HD11	4:D:219:VAL:HG21	1.98	0.46
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.96	0.46
3:P:129:MET:CE	3:P:181:PHE:CD2	2.94	0.46
13:Q:3006:PEE:H56	5:R:50:ALA:HB1	1.98	0.46
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.46	0.46
1:A:29:GLN:HB3	2:B:12:GLU:O	2.16	0.46
9:I:70:LEU:HB3	22:I:1016:HOH:O	2.16	0.46
4:Q:124:GLU:OE2	4:Q:191:ARG:HD2	2.16	0.46
1:A:15:GLN:O	1:A:26:ALA:HA	2.16	0.46
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.51	0.46
9:I:36:ALA:CB	9:I:73:PRO:HB2	2.46	0.46
2:B:365:LYS:HG2	2:B:399:LEU:CD2	2.45	0.45
3:C:193:ALA:O	3:C:196:HIS:HB3	2.16	0.45
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.98	0.45
8:U:31:VAL:HG23	8:U:32:LYS:N	2.30	0.45
9:V:36:ALA:CB	9:V:73:PRO:HB2	2.46	0.45
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.82	0.45
7:G:40:ARG:NH2	21:G:2004:CDL:HB31	2.32	0.45
3:P:43:LEU:CD2	13:Q:3006:PEE:H30	2.29	0.45
8:U:41:ASP:O	8:U:45:SER:HB2	2.15	0.45
2:O:71:LEU:CD2	9:V:68:VAL:HG21	2.43	0.45
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.98	0.45
9:V:62:ARG:HB3	9:V:63:PRO:HD2	1.99	0.45
10:W:16:ARG:O	10:W:19:THR:HG22	2.17	0.45
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.52	0.45
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.99	0.45
3:P:96:MET:HE2	3:P:96:MET:HA	1.99	0.45
1:A:85:HIS:O	1:A:99:ILE:HA	2.16	0.45
1:N:195:MET:HE1	1:N:219:LEU:HD21	1.99	0.45
3:P:217:LYS:HG3	7:T:7:LEU:HD13	1.99	0.45
10:J:16:ARG:NH1	10:J:16:ARG:HG3	2.32	0.45
9:V:36:ALA:HB3	9:V:73:PRO:CG	2.46	0.45
3:C:92:ILE:O	3:C:96:MET:HG2	2.17	0.44
1:N:19:LEU:HD22	1:N:213:GLN:HG3	1.99	0.44
3:P:12:LYS:HE2	3:P:16:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:13:ILE:HG22	3:P:13:ILE:O	2.17	0.44
3:P:213:SER:OG	3:P:217:LYS:NZ	2.42	0.44
5:R:112:VAL:CG2	5:R:172:ARG:NH2	2.80	0.44
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.98	0.44
2:B:28:ARG:HH21	2:B:390:GLY:HA3	1.81	0.44
3:C:304:ILE:HB	3:C:305:PRO:HD3	1.99	0.44
7:G:38:LEU:HB3	7:G:42:ARG:NH1	2.32	0.44
8:H:51:GLU:HG3	8:H:52:GLU:N	2.32	0.44
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.47	0.44
8:H:31:VAL:O	8:H:35:GLU:HG3	2.17	0.44
9:I:76:VAL:HG13	9:I:76:VAL:O	2.16	0.44
1:N:213:GLN:O	1:N:217:SER:OG	2.25	0.44
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	2.18	0.44
4:Q:144:ARG:HG3	4:Q:147:LEU:HD12	1.98	0.44
7:T:71:ARG:NH1	7:T:72:LYS:HD2	2.31	0.44
6:S:110:LYS:O	6:S:110:LYS:HG3	2.17	0.44
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.98	0.44
3:P:270:PRO:HG2	3:P:278:TYR:CG	2.53	0.44
7:G:40:ARG:CZ	21:G:2004:CDL:HB31	2.47	0.44
5:R:75:GLU:HG2	5:R:194:ILE:HG12	2.00	0.44
2:B:230:LEU:HB3	2:B:233:SER:OG	2.18	0.44
3:C:197:LEU:HD21	16:C:502:HEM:HMA1	2.00	0.44
18:P:3002:UQ:HM31	22:P:3116:HOH:O	2.17	0.44
6:S:58:ARG:HD3	22:S:2031:HOH:O	2.18	0.44
16:C:501:HEM:HMC1	16:C:501:HEM:HBC2	2.00	0.43
4:Q:42:SER:HB3	4:Q:94:PRO:HD2	2.00	0.43
5:R:117:LEU:HD13	5:R:170:ARG:HD2	2.00	0.43
6:S:49:ARG:HH22	11:S:2011:JZR:H4	1.83	0.43
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.45	0.43
2:B:361:LYS:HE2	2:B:402:ILE:O	2.18	0.43
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.39	0.43
2:O:314:ALA:HA	9:V:63:PRO:HD3	2.00	0.43
5:R:112:VAL:HG22	5:R:172:ARG:NH2	2.33	0.43
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.54	0.43
3:C:129:MET:CE	3:C:181:PHE:CD2	2.90	0.43
4:D:204:MET:HE3	13:D:2006:PEE:O4	2.18	0.43
8:H:19:THR:O	8:H:23:GLN:HG3	2.19	0.43
1:N:288:ALA:HB2	1:N:300:THR:HG22	2.01	0.43
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.17	0.43
1:A:27:SER:HA	1:A:199:ALA:O	2.18	0.43
1:N:15:GLN:O	1:N:26:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:78:ILE:HD12	4:Q:204:MET:CE	2.49	0.43
3:P:369:ALA:O	3:P:373:GLU:HG3	2.19	0.43
3:C:68:HIS:HE1	22:C:2049:HOH:O	2.01	0.43
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.01	0.43
2:B:136:GLU:HG2	11:S:2011:JZR:H2'	2.00	0.43
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.54	0.43
22:D:4077:HOH:O	6:F:71:ARG:HD3	2.18	0.43
5:E:112:VAL:HG22	5:E:172:ARG:NH2	2.34	0.43
2:O:228:GLY:O	2:O:231:GLY:HA2	2.18	0.43
16:C:501:HEM:O2D	16:C:501:HEM:O2A	2.37	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.43
9:I:36:ALA:HB2	9:I:73:PRO:CD	2.40	0.43
7:T:72:LYS:CG	8:U:56:GLU:OE2	2.62	0.43
1:A:61:HIS:CE1	1:A:137:GLU:OE1	2.72	0.43
1:A:383:LEU:O	1:A:387:GLY:HA2	2.18	0.43
1:N:224:ASP:OD1	1:N:227:ALA:HB2	2.18	0.43
2:O:345:LYS:O	2:O:349:GLN:HG3	2.19	0.43
4:Q:74:PRO:HG3	4:Q:80:MET:HE2	1.99	0.43
4:Q:204:MET:HE3	4:Q:204:MET:HB3	1.83	0.43
5:E:75:GLU:HG2	5:E:194:ILE:HG12	2.00	0.43
7:G:32:LYS:C	7:G:35:PRO:HD2	2.39	0.43
1:N:416:TYR:HB3	10:W:15:ARG:NH2	2.33	0.43
1:A:381:ARG:HG2	22:A:4120:HOH:O	2.19	0.42
2:B:181:TYR:CE1	2:B:182:ARG:HG2	2.54	0.42
7:G:48:VAL:O	7:G:51:PRO:HD2	2.19	0.42
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.19	0.42
1:A:111:GLU:HG3	1:A:215:HIS:CE1	2.54	0.42
3:C:269:LYS:HA	3:C:270:PRO:HD3	1.81	0.42
9:I:77:ARG:O	9:I:78:TYR:HB2	2.19	0.42
1:N:280:TYR:HA	1:N:284:TYR:CE2	2.54	0.42
1:A:117:VAL:HG11	1:A:195:MET:CE	2.49	0.42
1:A:240:GLN:NE2	22:A:4184:HOH:O	2.51	0.42
3:P:67:THR:HB	4:Q:115:TYR:OH	2.20	0.42
3:P:68:HIS:HE1	22:P:3053:HOH:O	2.03	0.42
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.84	0.42
2:O:28:ARG:HB2	2:O:28:ARG:NH1	2.35	0.42
8:U:23:GLN:O	8:U:26:GLN:HG2	2.20	0.42
1:A:78:GLU:OE2	1:A:108:LYS:HD2	2.20	0.42
1:A:158:PHE:O	1:A:164:ALA:HB2	2.20	0.42
3:C:270:PRO:HG2	3:C:278:TYR:CG	2.54	0.42
4:D:43:MET:CE	4:D:46:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:286:GLY:HA3	1:N:290:LEU:CD2	2.47	0.42
4:D:97:ASN:HB2	4:D:98:PRO:HD2	2.01	0.42
1:A:267:ASN:O	1:A:271:GLN:HG2	2.20	0.42
3:P:320:LEU:HG	22:P:3113:HOH:O	2.19	0.42
7:T:71:ARG:HB2	7:T:72:LYS:H	1.66	0.42
3:P:46:LEU:HD11	13:Q:3006:PEE:H81	2.01	0.42
4:Q:43:MET:HE2	4:Q:46:VAL:CG2	2.48	0.42
4:Q:75:ASN:HD21	4:Q:79:GLU:CG	2.30	0.42
5:R:95:PRO:HG2	5:R:145:VAL:HG22	2.02	0.42
1:N:267:ASN:O	1:N:271:GLN:HG2	2.19	0.42
1:N:281:ASP:C	1:N:281:ASP:OD1	2.58	0.42
2:O:17:VAL:HA	2:O:18:PRO:HD3	1.85	0.42
2:O:257:LEU:O	2:O:323:GLY:HA3	2.19	0.42
7:T:32:LYS:C	7:T:35:PRO:HD2	2.40	0.42
10:W:14:PHE:HA	10:W:20:PHE:HD2	1.85	0.41
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.49	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.56	0.41
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.41
2:O:203:ARG:HH12	2:O:233:SER:CA	2.32	0.41
2:O:212:SER:OG	2:O:215:VAL:HG23	2.20	0.41
5:E:117:LEU:HD13	5:E:170:ARG:HD2	2.03	0.41
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.55	0.41
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.68	0.41
2:O:246:GLU:O	2:O:427:SER:HA	2.19	0.41
2:B:46:ARG:O	2:B:47:ILE:HD13	2.21	0.41
9:I:36:ALA:HB3	9:I:73:PRO:HB2	2.02	0.41
1:N:302:LYS:HA	1:N:302:LYS:HD3	1.93	0.41
2:B:412:ASN:HA	2:B:412:ASN:HD22	1.67	0.41
8:H:31:VAL:CG2	8:H:32:LYS:N	2.83	0.41
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.21	0.41
5:E:84:GLY:N	5:E:100:HIS:O	2.54	0.41
5:E:160:CYS:HB3	17:P:3001:SMA:H4	2.03	0.41
7:T:50:PRO:HB2	7:T:51:PRO:HD3	2.03	0.41
1:A:264:HIS:ND1	1:A:265:PRO:HD2	2.36	0.41
6:F:63:LYS:HG3	22:F:4045:HOH:O	2.20	0.41
8:H:51:GLU:HG3	8:H:52:GLU:H	1.86	0.41
4:Q:124:GLU:OE2	4:Q:191:ARG:HD3	2.21	0.41
6:S:12:TRP:O	6:S:15:GLY:N	2.53	0.41
10:W:16:ARG:NH1	10:W:16:ARG:HG3	2.36	0.41
6:F:101:ARG:O	6:F:105:GLU:HG3	2.21	0.41
8:H:23:GLN:O	8:H:26:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:85:HIS:O	1:N:99:ILE:HA	2.20	0.41
2:B:71:LEU:CD2	9:I:68:VAL:HG21	2.44	0.41
10:J:14:PHE:N	10:J:14:PHE:CD1	2.87	0.41
2:O:34:VAL:C	2:O:35:ILE:HD12	2.41	0.41
2:O:47:ILE:HG13	2:O:120:MET:CE	2.51	0.41
1:A:288:ALA:HB2	1:A:300:THR:HG22	2.02	0.41
1:A:405:ARG:O	1:A:409:GLU:HG3	2.20	0.41
9:I:62:ARG:HB3	9:I:63:PRO:HD2	2.02	0.41
3:P:162:GLU:OE2	3:P:168:PHE:CD1	2.73	0.41
2:B:95:LYS:HB2	9:I:32:ALA:CB	2.41	0.40
5:E:80:ASP:O	5:E:82:PRO:HD3	2.21	0.40
1:N:19:LEU:CD2	1:N:213:GLN:HG3	2.51	0.40
4:D:43:MET:HE2	4:D:46:VAL:HG21	2.01	0.40
10:J:56:LYS:HB3	10:J:56:LYS:HE2	1.76	0.40
4:Q:204:MET:HE3	13:Q:3006:PEE:O4	2.21	0.40
10:J:18:SER:OG	10:J:19:THR:N	2.55	0.40
3:P:223:TYR:HB3	4:Q:227:TRP:CZ2	2.56	0.40
4:Q:214:LEU:HA	13:T:3005:PEE:H58	2.03	0.40
9:V:62:ARG:HB2	9:V:78:TYR:CG	2.56	0.40
2:B:47:ILE:HG13	2:B:120:MET:CE	2.52	0.40
3:P:191:ALA:HA	3:P:194:MET:HE2	2.03	0.40
3:P:233:LEU:HD11	4:Q:219:VAL:HG21	2.03	0.40
9:V:70:LEU:HB3	22:V:1017:HOH:O	2.22	0.40
10:W:56:LYS:HE2	10:W:56:LYS:HB3	1.75	0.40
3:C:21:LEU:HD21	18:C:2002:UQ:CM3	2.52	0.40
5:E:188:THR:C	5:E:189:SER:O	2.60	0.40
16:P:501:HEM:HMC1	16:P:501:HEM:HBC2	2.02	0.40
10:W:14:PHE:CD1	10:W:14:PHE:N	2.89	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%)	425 (96%)	14 (3%)	2 (0%)	29 26
1	N	441/446 (99%)	425 (96%)	15 (3%)	1 (0%)	47 49
2	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	47 49
2	O	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	29 26
3	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	19 15
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	11 6
4	D	239/241 (99%)	234 (98%)	5 (2%)	0	100 100
4	Q	239/241 (99%)	235 (98%)	4 (2%)	0	100 100
5	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	7 3
5	R	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	29 26
6	F	97/110 (88%)	96 (99%)	1 (1%)	0	100 100
6	S	97/110 (88%)	96 (99%)	1 (1%)	0	100 100
7	G	73/81 (90%)	72 (99%)	1 (1%)	0	100 100
7	T	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	11 6
8	H	64/78 (82%)	61 (95%)	3 (5%)	0	100 100
8	U	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	9 5
9	I	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	5 2
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	5 2
10	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9 4
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9 4
All	All	3980/4220 (94%)	3851 (97%)	104 (3%)	25 (1%)	25 21

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP
3	C	16	ASN
3	C	17	ALA
9	I	41	PRO
10	J	61	ASN
1	N	224	ASP
3	P	17	ALA
7	T	72	LYS
9	V	41	PRO
10	W	61	ASN
2	B	171	ALA

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Mol	Chain	Res	Type
5	E	112	VAL
2	O	171	ALA
2	O	231	GLY
3	P	16	ASN
8	U	48	SER
5	R	189	SER
1	A	228	VAL
3	C	18	PHE
5	E	189	SER
5	E	191	ASP
3	P	11	MET
3	P	18	PHE
5	E	82	PRO
3	P	13	ILE

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	364/370 (98%)	359 (99%)	5 (1%)	67	73
1	N	364/370 (98%)	359 (99%)	5 (1%)	67	73
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	332/343 (97%)	330 (99%)	2 (1%)	86	90
3	C	312/327 (95%)	307 (98%)	5 (2%)	62	69
3	P	316/327 (97%)	310 (98%)	6 (2%)	57	63
4	D	206/206 (100%)	203 (98%)	3 (2%)	65	71
4	Q	206/206 (100%)	203 (98%)	3 (2%)	65	71
5	E	168/168 (100%)	167 (99%)	1 (1%)	86	90
5	R	168/168 (100%)	166 (99%)	2 (1%)	71	77
6	F	90/98 (92%)	89 (99%)	1 (1%)	73	79
6	S	90/98 (92%)	89 (99%)	1 (1%)	73	79
7	G	66/71 (93%)	65 (98%)	1 (2%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	66/71 (93%)	64 (97%)	2 (3%)	41	44
8	H	63/74 (85%)	61 (97%)	2 (3%)	39	41
8	U	63/74 (85%)	62 (98%)	1 (2%)	62	69
9	I	28/60 (47%)	27 (96%)	1 (4%)	35	36
9	V	28/60 (47%)	26 (93%)	2 (7%)	14	11
10	J	51/52 (98%)	49 (96%)	2 (4%)	32	33
10	W	51/52 (98%)	49 (96%)	2 (4%)	32	33
All	All	3364/3538 (95%)	3317 (99%)	47 (1%)	67	73

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	149	VAL
1	A	245	GLU
1	A	281	ASP
1	A	308	GLN
3	C	80	ARG
3	C	90	PHE
3	C	128	PHE
3	C	222	PRO
3	C	379	TRP
4	D	17	LEU
4	D	76	GLU
4	D	144	ARG
5	E	80	ASP
6	F	58	ARG
7	G	45	ILE
8	H	47	ARG
8	H	51	GLU
9	I	42	VAL
10	J	8	ARG
10	J	16	ARG
1	N	58	PHE
1	N	149	VAL
1	N	245	GLU
1	N	281	ASP
1	N	308	GLN
2	O	212	SER
2	O	236	LYS

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Mol	Chain	Res	Type
3	P	12	LYS
3	P	43	LEU
3	P	80	ARG
3	P	90	PHE
3	P	222	PRO
3	P	379	TRP
4	Q	17	LEU
4	Q	35	GLN
4	Q	144	ARG
5	R	113	GLU
5	R	190	ASP
6	S	58	ARG
7	T	45	ILE
7	T	73	ASN
8	U	46	SER
9	V	42	VAL
9	V	52	ARG
10	W	8	ARG
10	W	25	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	61	HIS
1	A	136	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS
2	B	22	GLN
2	B	104	ASN
2	B	343	GLN
2	B	412	ASN
3	C	68	HIS
3	C	159	ASN
4	D	106	ASN
5	E	57	GLN
5	E	116	GLN
7	G	73	ASN
1	N	15	GLN
1	N	61	HIS
1	N	136	GLN

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Mol	Chain	Res	Type
1	N	165	GLN
1	N	213	GLN
1	N	271	GLN
2	O	104	ASN
2	O	240	HIS
2	O	343	GLN
2	O	412	ASN
3	P	68	HIS
3	P	159	ASN
4	Q	106	ASN
4	Q	121	HIS
5	R	57	GLN
6	S	73	GLN
7	T	28	HIS
9	V	71	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

41 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	PO4	B	3010	-	4,4,4	1.30	0	6,6,6	5.82	5 (83%)
20	FES	R	501	5	0,4,4	-	-	-		
11	JZR	S	2011	-	18,18,18	1.83	3 (16%)	23,23,23	0.77	0
11	JZR	F	3011	-	18,18,18	1.90	5 (27%)	23,23,23	0.71	0
19	HEC	D	501	4	32,50,50	1.91	6 (18%)	24,82,82	1.40	4 (16%)
19	HEC	Q	501	4	32,50,50	1.88	5 (15%)	24,82,82	1.23	3 (12%)
21	CDL	Q	3003	-	49,49,99	1.08	4 (8%)	55,61,111	1.14	4 (7%)
21	CDL	G	2004	-	43,43,99	1.12	2 (4%)	49,55,111	1.20	4 (8%)
16	HEM	P	501	3	41,50,50	1.83	7 (17%)	45,82,82	1.49	7 (15%)
13	PEE	C	2007	-	48,48,50	1.27	5 (10%)	51,53,55	0.76	2 (3%)
13	PEE	Q	3006	-	50,50,50	1.31	6 (12%)	53,55,55	0.78	2 (3%)
12	AZI	C	2014	-	0,2,2	-	-	0,1,1	-	-
15	GOL	O	3013	-	5,5,5	1.29	0	5,5,5	0.69	0
11	JZR	P	3008	-	18,18,18	1.83	6 (33%)	23,23,23	0.68	0
11	JZR	C	2008	-	18,18,18	1.82	6 (33%)	23,23,23	0.69	0
13	PEE	T	3005	-	48,48,50	1.37	7 (14%)	51,53,55	0.76	3 (5%)
16	HEM	C	502	3	41,50,50	1.75	7 (17%)	45,82,82	1.97	16 (35%)
13	PEE	N	3012	-	4,4,50	3.06	4 (100%)	6,6,55	0.58	0
11	JZR	A	4002	-	18,18,18	1.90	5 (27%)	23,23,23	0.77	1 (4%)
16	HEM	P	502	3	41,50,50	1.87	10 (24%)	45,82,82	1.68	7 (15%)
13	PEE	D	2006	-	50,50,50	1.33	7 (14%)	53,55,55	0.80	2 (3%)
12	AZI	D	4004	-	0,2,2	-	-	0,1,1	-	-
15	GOL	B	2013	-	5,5,5	1.29	0	5,5,5	0.64	0
13	PEE	P	3007	-	48,48,50	1.32	5 (10%)	51,53,55	0.74	2 (3%)
13	PEE	G	2005	-	48,48,50	1.33	7 (14%)	51,53,55	0.77	2 (3%)
18	UQ	C	2002	-	14,14,63	2.25	8 (57%)	18,20,79	0.53	0
15	GOL	P	3009	-	5,5,5	1.35	0	5,5,5	0.61	0
20	FES	E	501	5	0,4,4	-	-	-		
14	PO4	O	2010	-	4,4,4	1.32	0	6,6,6	5.81	5 (83%)
16	HEM	C	501	3	41,50,50	1.92	7 (17%)	45,82,82	1.99	12 (26%)
17	SMA	C	2001	-	38,38,38	1.40	7 (18%)	48,52,52	1.09	4 (8%)
17	SMA	P	3001	-	38,38,38	1.55	9 (23%)	48,52,52	1.12	4 (8%)
18	UQ	P	3002	-	14,14,63	2.05	8 (57%)	18,20,79	0.40	0
21	CDL	T	3004	-	48,48,99	1.14	4 (8%)	54,60,111	1.10	2 (3%)
13	PEE	C	2012	-	4,4,50	3.24	4 (100%)	6,6,55	0.58	0
13	PEE	A	4003	-	5,5,50	1.30	0	5,5,55	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	AZI	P	3014	-	0,2,2	-	-	0,1,1	-	-
12	AZI	A	4005	-	0,2,2	-	-	0,1,1	-	-
11	JZR	F	4001	-	18,18,18	1.80	5 (27%)	23,23,23	0.66	0
21	CDL	G	2003	-	49,49,99	1.09	2 (4%)	55,61,111	1.07	4 (7%)
15	GOL	C	2009	-	5,5,5	1.32	0	5,5,5	0.63	0

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
20	FES	R	501	5	-	-	0/1/1/1
11	JZR	S	2011	-	-	6/9/29/29	0/1/1/1
11	JZR	F	3011	-	-	4/9/29/29	0/1/1/1
19	HEC	D	501	4	-	4/10/54/54	-
19	HEC	Q	501	4	-	4/10/54/54	-
21	CDL	Q	3003	-	-	37/58/58/110	-
21	CDL	G	2004	-	-	34/52/52/110	-
16	HEM	P	501	3	-	4/12/54/54	-
13	PEE	C	2007	-	-	16/52/52/54	-
13	PEE	Q	3006	-	-	18/54/54/54	-
15	GOL	O	3013	-	-	2/4/4/4	-
11	JZR	P	3008	-	-	3/9/29/29	0/1/1/1
11	JZR	C	2008	-	-	4/9/29/29	0/1/1/1
13	PEE	T	3005	-	-	28/52/52/54	-
16	HEM	C	502	3	-	4/12/54/54	-
11	JZR	A	4002	-	-	5/9/29/29	0/1/1/1
16	HEM	P	502	3	-	4/12/54/54	-
13	PEE	D	2006	-	-	17/54/54/54	-
15	GOL	B	2013	-	-	4/4/4/4	-
13	PEE	P	3007	-	-	16/52/52/54	-
13	PEE	G	2005	-	-	26/52/52/54	-
18	UQ	C	2002	-	-	0/4/28/87	0/1/1/1
15	GOL	P	3009	-	-	2/4/4/4	-
20	FES	E	501	5	-	-	0/1/1/1
16	HEM	C	501	3	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SMA	C	2001	-	-	2/34/34/34	0/2/2/2
17	SMA	P	3001	-	-	2/34/34/34	0/2/2/2
18	UQ	P	3002	-	-	2/4/28/87	0/1/1/1
21	CDL	T	3004	-	-	22/57/57/110	-
13	PEE	A	4003	-	-	4/4/4/54	-
11	JZR	F	4001	-	-	5/9/29/29	0/1/1/1
21	CDL	G	2003	-	-	26/58/58/110	-
15	GOL	C	2009	-	-	0/4/4/4	-

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	501	HEC	C3C-C2C	-6.07	1.34	1.40
19	D	501	HEC	C2B-C3B	-5.97	1.34	1.40
16	C	501	HEM	C3C-CAC	-5.60	1.36	1.47
16	P	502	HEM	CBB-CAB	5.38	1.57	1.30
16	P	501	HEM	CBB-CAB	5.31	1.56	1.30
16	P	501	HEM	C3C-CAC	-5.10	1.37	1.47
16	C	502	HEM	C3C-CAC	-5.08	1.37	1.47
11	F	3011	JZR	O1-C1	5.03	1.48	1.40
16	P	502	HEM	C3C-CAC	-4.99	1.37	1.47
11	S	2011	JZR	O1-C1	4.92	1.48	1.40
11	A	4002	JZR	O1-C1	4.91	1.48	1.40
16	C	501	HEM	CBB-CAB	4.88	1.54	1.30
19	D	501	HEC	C3C-C2C	-4.88	1.35	1.40
16	C	502	HEM	CBB-CAB	4.75	1.53	1.30
11	P	3008	JZR	O1-C1	4.62	1.48	1.40
11	C	2008	JZR	O1-C1	4.60	1.48	1.40
19	Q	501	HEC	C4B-C3B	4.57	1.51	1.43
11	F	4001	JZR	O1-C1	4.55	1.48	1.40
13	C	2012	PEE	P-O1P	4.46	1.61	1.50
13	N	3012	PEE	P-O1P	4.15	1.60	1.50
13	P	3007	PEE	C39-C38	4.13	1.55	1.31
13	C	2007	PEE	C39-C38	4.11	1.55	1.31
13	Q	3006	PEE	C39-C38	4.08	1.55	1.31
16	P	501	HEM	CAB-C3B	-4.08	1.36	1.47
13	D	2006	PEE	C39-C38	4.08	1.55	1.31
13	T	3005	PEE	C39-C38	4.05	1.55	1.31
13	G	2005	PEE	C39-C38	3.92	1.54	1.31
16	C	501	HEM	CBC-CAC	3.72	1.54	1.29
11	S	2011	JZR	O5-C1	3.67	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	502	HEM	CBC-CAC	3.63	1.53	1.29
16	P	502	HEM	CAB-C3B	-3.62	1.37	1.47
17	P	3001	SMA	C6-C5	3.55	1.45	1.38
11	F	3011	JZR	O5-C1	3.51	1.50	1.41
16	P	502	HEM	CBC-CAC	3.49	1.52	1.29
19	Q	501	HEC	C2B-C3B	-3.46	1.37	1.40
16	P	501	HEM	CBC-CAC	3.42	1.52	1.29
16	C	501	HEM	CAB-C3B	-3.42	1.38	1.47
13	D	2006	PEE	O3-C30	3.35	1.43	1.33
16	C	501	HEM	C4D-C3D	3.34	1.50	1.45
11	A	4002	JZR	O5-C1	3.33	1.50	1.41
19	D	501	HEC	C3C-C4C	3.27	1.49	1.43
17	C	2001	SMA	C4A-C5	3.25	1.46	1.40
16	P	502	HEM	C1A-NA	3.23	1.42	1.36
18	C	2002	UQ	O3-C3	3.22	1.44	1.36
13	P	3007	PEE	P-O1P	3.21	1.62	1.50
17	P	3001	SMA	O1-C2	3.21	1.40	1.36
11	F	4001	JZR	O5-C1	3.21	1.50	1.41
13	P	3007	PEE	O3-C30	3.19	1.42	1.33
11	C	2008	JZR	O5-C1	3.17	1.49	1.41
17	P	3001	SMA	C6-C7	3.17	1.44	1.38
11	P	3008	JZR	O5-C1	3.17	1.49	1.41
13	C	2007	PEE	O3-C30	3.07	1.42	1.33
13	Q	3006	PEE	P-O1P	3.07	1.61	1.50
13	G	2005	PEE	C21-C22	-3.07	1.34	1.51
16	C	501	HEM	C2C-C1C	3.06	1.49	1.42
13	T	3005	PEE	C21-C22	-3.05	1.34	1.51
13	D	2006	PEE	P-O1P	3.05	1.61	1.50
13	Q	3006	PEE	C21-C22	-3.05	1.34	1.51
13	T	3005	PEE	P-O1P	3.05	1.61	1.50
13	C	2012	PEE	P-O4P	3.05	1.63	1.54
18	C	2002	UQ	C3-C4	3.04	1.57	1.48
13	Q	3006	PEE	O3-C30	3.02	1.42	1.33
18	C	2002	UQ	C2-C1	3.02	1.57	1.48
17	C	2001	SMA	C6-C7	3.01	1.44	1.38
18	P	3002	UQ	C7-C6	3.01	1.57	1.50
18	C	2002	UQ	C7-C6	3.00	1.57	1.50
13	D	2006	PEE	C21-C22	-2.98	1.34	1.51
13	P	3007	PEE	C21-C22	-2.97	1.34	1.51
13	G	2005	PEE	P-O1P	2.96	1.61	1.50
17	C	2001	SMA	C6-C5	2.94	1.44	1.38
17	C	2001	SMA	C7-C8	2.93	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	3001	SMA	C4A-C5	2.93	1.45	1.40
13	T	3005	PEE	O3-C30	2.93	1.41	1.33
13	N	3012	PEE	P-O4P	2.91	1.63	1.54
18	C	2002	UQ	O2-C2	2.90	1.44	1.36
13	C	2007	PEE	C21-C22	-2.90	1.35	1.51
13	C	2007	PEE	P-O1P	2.88	1.61	1.50
19	Q	501	HEC	C3C-C4C	2.85	1.48	1.43
13	C	2012	PEE	P-O3P	2.85	1.63	1.54
18	C	2002	UQ	CM5-C5	2.83	1.56	1.50
13	G	2005	PEE	O2-C10	2.81	1.42	1.34
13	N	3012	PEE	P-O3P	2.79	1.63	1.54
13	D	2006	PEE	O2-C10	2.79	1.42	1.34
13	Q	3006	PEE	O2-C10	2.78	1.42	1.34
19	D	501	HEC	C2A-C1A	2.78	1.48	1.42
18	P	3002	UQ	CM5-C5	2.77	1.56	1.50
13	T	3005	PEE	O2-C10	2.77	1.42	1.34
13	G	2005	PEE	O3-C30	2.74	1.41	1.33
17	P	3001	SMA	C7-C8	2.73	1.44	1.40
13	P	3007	PEE	O2-C10	2.71	1.42	1.34
13	C	2007	PEE	O2-C10	2.69	1.41	1.34
17	P	3001	SMA	C20-C19	2.69	1.35	1.33
16	P	501	HEM	C4A-NA	2.68	1.41	1.36
16	P	501	HEM	C4D-C3D	2.66	1.49	1.45
11	P	3008	JZR	C4-C5	2.66	1.58	1.53
18	P	3002	UQ	C2-C1	2.61	1.56	1.48
21	G	2004	CDL	O1-C1	2.59	1.51	1.43
11	A	4002	JZR	C4-C5	2.58	1.58	1.53
18	P	3002	UQ	O2-C2	2.57	1.43	1.36
16	C	502	HEM	C2C-C1C	2.56	1.48	1.42
18	P	3002	UQ	O3-C3	2.55	1.43	1.36
16	P	502	HEM	C1B-C2B	2.55	1.49	1.44
19	D	501	HEC	C4B-C3B	2.54	1.47	1.43
11	C	2008	JZR	C4-C5	2.52	1.58	1.53
11	S	2011	JZR	O5-C5	2.52	1.50	1.44
18	P	3002	UQ	C6-C1	2.50	1.56	1.47
16	C	502	HEM	C1D-C2D	2.48	1.49	1.44
16	C	502	HEM	C3B-C4B	2.48	1.49	1.44
17	P	3001	SMA	C3-C2	2.48	1.39	1.34
21	T	3004	CDL	O1-C1	2.45	1.50	1.43
21	T	3004	CDL	OB8-CB6	-2.43	1.39	1.45
19	Q	501	HEC	C4D-ND	2.42	1.41	1.36
11	F	4001	JZR	C4-C5	2.41	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	2002	UQ	C6-C1	2.38	1.55	1.47
18	P	3002	UQ	C3-C4	2.37	1.55	1.48
11	A	4002	JZR	O5-C5	2.37	1.50	1.44
21	T	3004	CDL	OA8-CA6	-2.35	1.39	1.45
18	P	3002	UQ	C5-C4	2.35	1.55	1.47
11	F	3011	JZR	C4-C5	2.34	1.58	1.53
21	T	3004	CDL	CB3-CB4	2.33	1.57	1.50
11	F	3011	JZR	O5-C5	2.31	1.50	1.44
17	C	2001	SMA	C3-C2	2.31	1.39	1.34
18	C	2002	UQ	C5-C4	2.31	1.55	1.47
21	Q	3003	CDL	O1-C1	2.31	1.50	1.43
16	P	502	HEM	C1D-C2D	2.29	1.49	1.44
16	C	502	HEM	C4D-C3D	2.28	1.49	1.45
21	G	2003	CDL	O1-C1	2.23	1.50	1.43
13	C	2012	PEE	P-O2P	2.20	1.61	1.54
17	C	2001	SMA	C20-C19	2.20	1.35	1.33
19	D	501	HEC	C4D-ND	2.20	1.40	1.36
16	P	502	HEM	CMC-C2C	2.19	1.56	1.51
17	C	2001	SMA	O1-C2	2.19	1.39	1.36
17	P	3001	SMA	C8-C8A	2.15	1.43	1.39
17	P	3001	SMA	C4A-C4	2.14	1.52	1.46
11	C	2008	JZR	O5-C5	2.14	1.49	1.44
16	C	501	HEM	CHD-C1D	-2.13	1.34	1.41
16	P	501	HEM	C2C-C1C	2.12	1.47	1.42
11	P	3008	JZR	O5-C5	2.12	1.49	1.44
11	F	4001	JZR	O5-C5	2.11	1.49	1.44
11	F	4001	JZR	C1-C2	2.11	1.58	1.52
13	G	2005	PEE	C3-C2	2.11	1.57	1.50
13	D	2006	PEE	C31-C30	2.09	1.56	1.50
11	P	3008	JZR	C1-C2	2.08	1.58	1.52
11	C	2008	JZR	C1-C2	2.08	1.58	1.52
13	T	3005	PEE	C3-C2	2.08	1.57	1.50
13	G	2005	PEE	C1-C2	2.08	1.57	1.50
21	G	2003	CDL	CA3-CA4	2.07	1.57	1.50
21	Q	3003	CDL	OA8-CA6	-2.06	1.40	1.45
11	A	4002	JZR	C1-C2	2.06	1.58	1.52
11	C	2008	JZR	C4-C3	2.06	1.57	1.52
11	P	3008	JZR	C4-C3	2.05	1.57	1.52
21	G	2004	CDL	OA8-CA6	-2.05	1.40	1.45
13	Q	3006	PEE	C3-C2	2.04	1.57	1.50
21	Q	3003	CDL	OB8-CB6	-2.04	1.40	1.45
13	T	3005	PEE	C31-C30	2.04	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	502	HEM	CHB-C1B	2.02	1.40	1.35
13	N	3012	PEE	P-O2P	2.01	1.60	1.54
21	Q	3003	CDL	CA3-CA4	2.01	1.56	1.50
13	D	2006	PEE	C3-C2	2.01	1.56	1.50
16	P	502	HEM	CHA-C4D	2.01	1.40	1.35
11	F	3011	JZR	C1-C2	2.00	1.58	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	3010	PO4	O4-P-O1	-8.10	81.24	110.89
14	O	2010	PO4	O4-P-O1	-8.04	81.46	110.89
14	O	2010	PO4	O4-P-O2	-7.75	83.09	107.97
14	B	3010	PO4	O4-P-O2	-7.67	83.37	107.97
14	O	2010	PO4	O4-P-O3	-7.08	85.24	107.97
14	B	3010	PO4	O4-P-O3	-7.06	85.29	107.97
16	C	501	HEM	C4A-C3A-C2A	-5.84	102.93	107.00
16	P	502	HEM	C4C-CHD-C1D	5.57	129.91	122.56
16	C	501	HEM	C4C-CHD-C1D	4.93	129.07	122.56
14	B	3010	PO4	O2-P-O1	4.74	128.24	110.89
16	C	502	HEM	C4B-C3B-C2B	-4.71	103.38	107.11
17	P	3001	SMA	C9-C10-C11	-4.70	105.94	114.52
16	P	502	HEM	CMA-C3A-C4A	-4.55	121.48	128.46
14	O	2010	PO4	O2-P-O1	4.52	127.43	110.89
21	G	2004	CDL	CB4-OB6-CB5	-4.33	109.83	117.90
16	C	501	HEM	C2D-C1D-ND	4.28	115.01	109.88
17	C	2001	SMA	C9-C10-C11	-4.26	106.74	114.52
16	P	501	HEM	C4C-CHD-C1D	3.91	127.71	122.56
16	C	502	HEM	CHD-C1D-ND	-3.88	120.21	124.43
21	Q	3003	CDL	CA4-OA6-CA5	-3.79	110.83	117.90
21	T	3004	CDL	CB4-OB6-CB5	-3.79	110.84	117.90
16	P	502	HEM	CMC-C2C-C3C	3.68	131.57	124.68
16	C	502	HEM	C4C-CHD-C1D	3.68	127.41	122.56
16	C	502	HEM	CHC-C4B-NB	-3.62	120.50	124.43
16	P	501	HEM	C4A-C3A-C2A	-3.61	104.48	107.00
16	C	501	HEM	CHD-C1D-ND	-3.59	120.53	124.43
21	G	2003	CDL	CA4-OA6-CA5	-3.55	111.28	117.90
19	D	501	HEC	CMD-C2D-C1D	-3.37	123.28	128.46
16	P	501	HEM	C4B-CHC-C1C	3.35	126.98	122.56
16	C	502	HEM	C1B-NB-C4B	-3.34	101.62	105.07
16	C	501	HEM	C4B-CHC-C1C	3.29	126.90	122.56
16	C	501	HEM	CBA-CAA-C2A	-3.22	107.13	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	501	HEM	C4D-ND-C1D	-3.13	101.84	105.07
16	C	502	HEM	C4B-CHC-C1C	3.13	126.68	122.56
16	C	502	HEM	CMC-C2C-C3C	3.11	130.50	124.68
13	D	2006	PEE	C22-C21-C20	3.06	127.13	113.79
13	P	3007	PEE	C22-C21-C20	3.03	126.99	113.79
13	C	2007	PEE	C22-C21-C20	3.02	126.95	113.79
16	C	502	HEM	CBD-CAD-C3D	-3.01	104.27	112.63
21	T	3004	CDL	CA4-OA6-CA5	-3.00	110.42	117.79
13	G	2005	PEE	C22-C21-C20	2.98	126.78	113.79
16	P	502	HEM	CMA-C3A-C2A	2.98	130.56	124.94
13	T	3005	PEE	C22-C21-C20	2.98	126.77	113.79
16	P	501	HEM	CMC-C2C-C3C	2.98	130.25	124.68
21	Q	3003	CDL	CB6-CB4-CB3	-2.93	104.86	111.79
16	C	501	HEM	C4B-C3B-C2B	-2.88	104.83	107.11
13	Q	3006	PEE	C22-C21-C20	2.88	126.36	113.79
16	C	501	HEM	C1D-C2D-C3D	-2.88	103.93	106.96
17	P	3001	SMA	C4A-C4-C3	-2.83	114.62	118.79
16	C	502	HEM	CMA-C3A-C2A	2.73	130.09	124.94
21	G	2004	CDL	CA6-CA4-CA3	-2.71	105.37	111.79
21	G	2003	CDL	CB4-OB6-CB5	-2.69	111.16	117.79
16	C	502	HEM	CMA-C3A-C4A	-2.67	124.35	128.46
17	C	2001	SMA	C4A-C4-C3	-2.66	114.88	118.79
16	C	502	HEM	C4D-ND-C1D	-2.65	102.34	105.07
14	O	2010	PO4	O3-P-O2	2.62	116.38	107.97
16	P	502	HEM	C4B-CHC-C1C	2.61	126.00	122.56
21	Q	3003	CDL	CB4-OB6-CB5	-2.59	111.41	117.79
19	D	501	HEC	CMA-C3A-C2A	2.59	129.83	124.94
16	P	502	HEM	CMD-C2D-C1D	2.57	128.96	125.04
16	C	502	HEM	C2D-C1D-ND	2.57	112.96	109.88
16	C	502	HEM	CHB-C1B-NB	-2.56	121.22	124.38
14	B	3010	PO4	O3-P-O2	2.55	116.17	107.97
13	C	2007	PEE	C21-C22-C23	2.45	126.88	114.42
13	P	3007	PEE	C21-C22-C23	2.44	126.80	114.42
16	C	502	HEM	C2B-C1B-NB	2.41	112.69	109.84
19	Q	501	HEC	CMC-C2C-C1C	-2.40	124.77	128.46
16	P	501	HEM	CMA-C3A-C2A	2.38	129.43	124.94
21	G	2003	CDL	CB6-CB4-CB3	-2.35	106.23	111.79
19	D	501	HEC	C2B-C3B-C4B	2.34	108.88	106.35
13	G	2005	PEE	C21-C22-C23	2.31	126.14	114.42
19	D	501	HEC	CMD-C2D-C3D	2.29	129.26	124.94
13	T	3005	PEE	C21-C22-C23	2.28	126.00	114.42
16	C	501	HEM	CHA-C4D-ND	-2.26	121.58	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	501	HEM	CAD-C3D-C4D	2.25	128.59	124.66
17	P	3001	SMA	O1-C2-C9	-2.24	105.83	110.58
16	P	501	HEM	CMD-C2D-C1D	2.22	128.41	125.04
11	A	4002	JZR	C1'-O1-C1	2.21	117.51	113.84
13	D	2006	PEE	C21-C22-C23	2.21	125.63	114.42
16	C	502	HEM	CHA-C4D-ND	-2.20	121.66	124.38
13	Q	3006	PEE	C21-C22-C23	2.20	125.58	114.42
21	Q	3003	CDL	CA6-OA8-CA7	-2.20	111.59	117.10
21	G	2004	CDL	CA4-OA6-CA5	-2.18	112.42	117.79
16	C	501	HEM	C3B-C2B-C1B	2.13	108.07	106.49
19	Q	501	HEC	C1D-C2D-C3D	2.12	108.47	107.00
21	G	2003	CDL	CA6-OA8-CA7	-2.09	111.85	117.10
16	P	502	HEM	CAD-C3D-C4D	2.08	128.30	124.66
13	T	3005	PEE	O3-C3-C2	2.08	114.49	108.43
16	C	502	HEM	C4A-C3A-C2A	-2.08	105.55	107.00
21	G	2004	CDL	CB6-CB4-CB3	-2.08	106.88	111.79
17	P	3001	SMA	C9-C2-C3	2.07	130.10	127.07
19	Q	501	HEC	CBA-CAA-C2A	-2.07	109.12	112.60
16	C	501	HEM	CHC-C4B-NB	-2.06	122.19	124.43
17	C	2001	SMA	C9-C2-C3	2.06	130.09	127.07
17	C	2001	SMA	O1-C2-C9	-2.06	106.22	110.58

There are no chirality outliers.

All (309) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	4003	PEE	O3P-C1-C2-C3
13	G	2005	PEE	C1-O3P-P-O1P
13	T	3005	PEE	C11-C10-O2-C2
13	T	3005	PEE	O4-C10-O2-C2
13	T	3005	PEE	C4-O4P-P-O3P
13	T	3005	PEE	C4-O4P-P-O2P
13	T	3005	PEE	C4-O4P-P-O1P
13	T	3005	PEE	O4P-C4-C5-N
15	B	2013	GOL	O1-C1-C2-C3
15	B	2013	GOL	C1-C2-C3-O3
15	P	3009	GOL	O1-C1-C2-C3
17	C	2001	SMA	C3-C2-C9-C10
17	C	2001	SMA	O1-C2-C9-C10
17	P	3001	SMA	C3-C2-C9-C10
17	P	3001	SMA	O1-C2-C9-C10
21	G	2003	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
21	G	2003	CDL	C11-CA5-OA6-CA4
21	G	2003	CDL	CB2-OB2-PB2-OB3
21	G	2003	CDL	OB5-CB3-CB4-OB6
21	G	2004	CDL	CA2-C1-CB2-OB2
21	G	2004	CDL	CA2-OA2-PA1-OA3
21	G	2004	CDL	CA2-OA2-PA1-OA4
21	G	2004	CDL	CA3-OA5-PA1-OA3
21	G	2004	CDL	CA3-OA5-PA1-OA4
21	G	2004	CDL	OA7-CA5-OA6-CA4
21	G	2004	CDL	CB3-OB5-PB2-OB3
21	G	2004	CDL	CB3-OB5-PB2-OB4
21	G	2004	CDL	C51-CB5-OB6-CB4
21	Q	3003	CDL	CA2-OA2-PA1-OA3
21	Q	3003	CDL	CA2-OA2-PA1-OA4
21	Q	3003	CDL	CA2-OA2-PA1-OA5
21	Q	3003	CDL	CA3-OA5-PA1-OA3
21	Q	3003	CDL	CB2-OB2-PB2-OB3
21	Q	3003	CDL	CB2-OB2-PB2-OB4
21	Q	3003	CDL	CB2-OB2-PB2-OB5
21	Q	3003	CDL	CB3-OB5-PB2-OB2
21	Q	3003	CDL	CB3-OB5-PB2-OB3
21	Q	3003	CDL	CB3-OB5-PB2-OB4
21	Q	3003	CDL	OB6-CB4-CB6-OB8
21	T	3004	CDL	CA2-C1-CB2-OB2
21	T	3004	CDL	CB2-OB2-PB2-OB4
21	T	3004	CDL	CB3-OB5-PB2-OB3
21	Q	3003	CDL	C11-CA5-OA6-CA4
21	T	3004	CDL	C51-CB5-OB6-CB4
21	G	2003	CDL	C31-CA7-OA8-CA6
21	Q	3003	CDL	C31-CA7-OA8-CA6
21	Q	3003	CDL	OA7-CA5-OA6-CA4
21	T	3004	CDL	OB7-CB5-OB6-CB4
21	G	2004	CDL	OB7-CB5-OB6-CB4
21	T	3004	CDL	C31-CA7-OA8-CA6
21	G	2004	CDL	C11-CA5-OA6-CA4
21	G	2003	CDL	OA9-CA7-OA8-CA6
21	G	2003	CDL	C71-CB7-OB8-CB6
21	Q	3003	CDL	OA9-CA7-OA8-CA6
21	T	3004	CDL	OA9-CA7-OA8-CA6
11	C	2008	JZR	O5-C5-C6-O6
21	G	2004	CDL	O1-C1-CB2-OB2
21	T	3004	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
13	G	2005	PEE	C31-C30-O3-C3
21	G	2003	CDL	OB9-CB7-OB8-CB6
11	F	3011	JZR	O5-C5-C6-O6
13	G	2005	PEE	O5-C30-O3-C3
21	Q	3003	CDL	CB2-C1-CA2-OA2
11	C	2008	JZR	C4-C5-C6-O6
11	S	2011	JZR	C4-C5-C6-O6
21	Q	3003	CDL	O1-C1-CA2-OA2
21	T	3004	CDL	C11-CA5-OA6-CA4
13	T	3005	PEE	C31-C30-O3-C3
13	P	3007	PEE	C10-C11-C12-C13
13	C	2007	PEE	C10-C11-C12-C13
13	G	2005	PEE	C30-C31-C32-C33
21	Q	3003	CDL	CB7-C71-C72-C73
11	P	3008	JZR	O1-C1'-C2'-C3'
11	F	4001	JZR	O1-C1'-C2'-C3'
13	T	3005	PEE	C10-C11-C12-C13
21	Q	3003	CDL	CB5-C51-C52-C53
11	F	3011	JZR	C4-C5-C6-O6
21	G	2003	CDL	O1-C1-CA2-OA2
13	T	3005	PEE	C37-C38-C39-C40
13	T	3005	PEE	O5-C30-O3-C3
21	G	2003	CDL	CB2-OB2-PB2-OB5
21	G	2004	CDL	CA2-OA2-PA1-OA5
21	G	2004	CDL	CA3-OA5-PA1-OA2
21	G	2004	CDL	CB2-OB2-PB2-OB5
21	G	2004	CDL	CB3-OB5-PB2-OB2
21	T	3004	CDL	CB2-OB2-PB2-OB5
21	G	2003	CDL	CB2-C1-CA2-OA2
21	T	3004	CDL	OA7-CA5-OA6-CA4
11	C	2008	JZR	C2'-C3'-C4'-C5'
13	C	2007	PEE	C34-C35-C36-C37
13	G	2005	PEE	C21-C22-C23-C24
21	T	3004	CDL	C31-C32-C33-C34
21	T	3004	CDL	CA7-C31-C32-C33
13	D	2006	PEE	C17-C18-C19-C20
13	Q	3006	PEE	C37-C38-C39-C40
13	D	2006	PEE	C13-C14-C15-C16
13	P	3007	PEE	C34-C35-C36-C37
11	S	2011	JZR	O5-C5-C6-O6
11	A	4002	JZR	C2'-C3'-C4'-C5'
13	Q	3006	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
13	P	3007	PEE	C12-C13-C14-C15
13	P	3007	PEE	C42-C43-C44-C45
21	Q	3003	CDL	C77-C78-C79-C80
13	C	2007	PEE	C42-C43-C44-C45
15	O	3013	GOL	C1-C2-C3-O3
21	G	2003	CDL	C51-CB5-OB6-CB4
13	P	3007	PEE	C41-C42-C43-C44
13	T	3005	PEE	C11-C12-C13-C14
13	G	2005	PEE	C35-C36-C37-C38
13	C	2007	PEE	C41-C42-C43-C44
13	G	2005	PEE	C40-C41-C42-C43
13	C	2007	PEE	C21-C22-C23-C24
21	G	2004	CDL	C33-C34-C35-C36
13	G	2005	PEE	C22-C23-C24-C25
21	Q	3003	CDL	C71-C72-C73-C74
13	G	2005	PEE	C12-C13-C14-C15
13	Q	3006	PEE	C42-C43-C44-C45
21	Q	3003	CDL	C78-C79-C80-C81
13	D	2006	PEE	C42-C43-C44-C45
13	T	3005	PEE	C41-C42-C43-C44
13	D	2006	PEE	C37-C38-C39-C40
13	G	2005	PEE	C37-C38-C39-C40
13	Q	3006	PEE	C17-C18-C19-C20
13	C	2007	PEE	C12-C13-C14-C15
13	G	2005	PEE	C11-C10-O2-C2
13	A	4003	PEE	O3P-C1-C2-O2
15	B	2013	GOL	O1-C1-C2-O2
15	B	2013	GOL	O2-C2-C3-O3
15	O	3013	GOL	O2-C2-C3-O3
13	G	2005	PEE	C33-C34-C35-C36
13	P	3007	PEE	C21-C22-C23-C24
21	G	2004	CDL	O1-C1-CA2-OA2
11	C	2008	JZR	C1'-C2'-C3'-C4'
13	G	2005	PEE	O4-C10-O2-C2
13	D	2006	PEE	C22-C23-C24-C25
13	T	3005	PEE	C21-C22-C23-C24
21	Q	3003	CDL	C76-C77-C78-C79
13	C	2007	PEE	C17-C18-C19-C20
13	P	3007	PEE	C17-C18-C19-C20
21	Q	3003	CDL	C73-C74-C75-C76
13	D	2006	PEE	C35-C36-C37-C38
13	T	3005	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	G	2003	CDL	OB7-CB5-OB6-CB4
13	G	2005	PEE	C42-C43-C44-C45
13	C	2007	PEE	C22-C23-C24-C25
21	T	3004	CDL	C13-C14-C15-C16
11	A	4002	JZR	O1-C1'-C2'-C3'
13	Q	3006	PEE	C22-C23-C24-C25
13	P	3007	PEE	C31-C32-C33-C34
21	G	2004	CDL	C31-C32-C33-C34
13	G	2005	PEE	C39-C40-C41-C42
13	P	3007	PEE	C15-C16-C17-C18
13	Q	3006	PEE	C35-C36-C37-C38
13	T	3005	PEE	C39-C40-C41-C42
21	Q	3003	CDL	CA3-OA5-PA1-OA2
21	G	2004	CDL	OA5-CA3-CA4-CA6
13	P	3007	PEE	C32-C33-C34-C35
13	D	2006	PEE	C15-C16-C17-C18
13	Q	3006	PEE	C15-C16-C17-C18
21	G	2004	CDL	C31-CA7-OA8-CA6
13	C	2007	PEE	C31-C32-C33-C34
13	C	2007	PEE	C32-C33-C34-C35
13	G	2005	PEE	C1-C2-C3-O3
13	T	3005	PEE	C1-C2-C3-O3
21	G	2003	CDL	CB3-CB4-CB6-OB8
21	Q	3003	CDL	CB3-CB4-CB6-OB8
21	T	3004	CDL	CA3-CA4-CA6-OA8
21	G	2003	CDL	C73-C74-C75-C76
11	S	2011	JZR	C2'-C3'-C4'-C5'
21	Q	3003	CDL	C72-C73-C74-C75
15	P	3009	GOL	O1-C1-C2-O2
13	P	3007	PEE	C22-C23-C24-C25
13	P	3007	PEE	C20-C21-C22-C23
13	C	2007	PEE	C39-C40-C41-C42
13	P	3007	PEE	C39-C40-C41-C42
11	S	2011	JZR	O1-C1'-C2'-C3'
13	T	3005	PEE	C33-C34-C35-C36
11	A	4002	JZR	C3'-C4'-C5'-C6'
13	G	2005	PEE	C15-C16-C17-C18
21	G	2004	CDL	OA6-CA4-CA6-OA8
21	G	2004	CDL	OA9-CA7-OA8-CA6
21	T	3004	CDL	C14-C15-C16-C17
21	Q	3003	CDL	C79-C80-C81-C82
13	A	4003	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
13	D	2006	PEE	C43-C44-C45-C46
13	Q	3006	PEE	C43-C44-C45-C46
21	G	2003	CDL	OB5-CB3-CB4-CB6
21	Q	3003	CDL	OB5-CB3-CB4-CB6
21	Q	3003	CDL	C75-C76-C77-C78
11	F	4001	JZR	C4-C5-C6-O6
21	G	2004	CDL	CA3-CA4-CA6-OA8
13	T	3005	PEE	C17-C18-C19-C20
11	F	4001	JZR	C1'-C2'-C3'-C4'
11	A	4002	JZR	C4-C5-C6-O6
13	T	3005	PEE	O3P-C1-C2-O2
21	T	3004	CDL	OB5-CB3-CB4-OB6
11	P	3008	JZR	C1'-C2'-C3'-C4'
13	G	2005	PEE	C34-C35-C36-C37
13	C	2007	PEE	C15-C16-C17-C18
21	G	2004	CDL	CB2-C1-CA2-OA2
13	Q	3006	PEE	C34-C35-C36-C37
21	T	3004	CDL	OB5-CB3-CB4-CB6
13	P	3007	PEE	C18-C19-C20-C21
13	G	2005	PEE	C43-C44-C45-C46
21	G	2004	CDL	C71-CB7-OB8-CB6
11	A	4002	JZR	O5-C5-C6-O6
13	D	2006	PEE	C40-C41-C42-C43
13	D	2006	PEE	C34-C35-C36-C37
13	C	2007	PEE	C20-C21-C22-C23
21	G	2004	CDL	CB3-CB4-CB6-OB8
21	G	2004	CDL	OA5-CA3-CA4-OA6
21	Q	3003	CDL	OB5-CB3-CB4-OB6
21	G	2003	CDL	C72-C73-C74-C75
13	T	3005	PEE	O2-C2-C3-O3
21	G	2003	CDL	OB6-CB4-CB6-OB8
11	S	2011	JZR	C1'-C2'-C3'-C4'
13	D	2006	PEE	C23-C24-C25-C26
13	P	3007	PEE	C43-C44-C45-C46
21	Q	3003	CDL	C74-C75-C76-C77
13	T	3005	PEE	C1-O3P-P-O4P
13	T	3005	PEE	C12-C13-C14-C15
13	Q	3006	PEE	C23-C24-C25-C26
21	G	2003	CDL	CB2-OB2-PB2-OB4
21	G	2004	CDL	CB2-OB2-PB2-OB3
21	T	3004	CDL	CB2-OB2-PB2-OB3
13	C	2007	PEE	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
13	Q	3006	PEE	C40-C41-C42-C43
13	T	3005	PEE	O3P-C1-C2-C3
21	G	2003	CDL	C71-C72-C73-C74
13	G	2005	PEE	C5-C4-O4P-P
13	C	2007	PEE	C18-C19-C20-C21
21	G	2003	CDL	CB7-C71-C72-C73
13	G	2005	PEE	O2-C2-C3-O3
21	T	3004	CDL	OA6-CA4-CA6-OA8
13	D	2006	PEE	C31-C32-C33-C34
11	F	4001	JZR	O5-C5-C6-O6
21	G	2004	CDL	OB5-CB3-CB4-CB6
13	G	2005	PEE	C14-C15-C16-C17
13	D	2006	PEE	C11-C12-C13-C14
16	C	501	HEM	CAD-CBD-CGD-O1D
16	P	502	HEM	CAA-CBA-CGA-O1A
16	P	501	HEM	CAD-CBD-CGD-O1D
13	D	2006	PEE	C16-C17-C18-C19
13	T	3005	PEE	C18-C19-C20-C21
16	C	502	HEM	CAA-CBA-CGA-O2A
16	C	502	HEM	CAA-CBA-CGA-O1A
16	P	502	HEM	CAA-CBA-CGA-O2A
21	T	3004	CDL	C12-C13-C14-C15
21	Q	3003	CDL	C51-C52-C53-C54
16	P	501	HEM	CAD-CBD-CGD-O2D
21	G	2003	CDL	OA5-CA3-CA4-OA6
16	C	501	HEM	CAA-CBA-CGA-O1A
16	C	501	HEM	CAD-CBD-CGD-O2D
18	P	3002	UQ	C4-C3-O3-CM3
21	G	2003	CDL	C78-C79-C80-C81
16	C	501	HEM	CAA-CBA-CGA-O2A
21	G	2004	CDL	OB9-CB7-OB8-CB6
13	G	2005	PEE	C11-C12-C13-C14
11	F	4001	JZR	C2'-C3'-C4'-C5'
13	G	2005	PEE	C17-C18-C19-C20
13	D	2006	PEE	C36-C37-C38-C39
21	G	2003	CDL	C76-C77-C78-C79
13	D	2006	PEE	C20-C21-C22-C23
13	Q	3006	PEE	C32-C33-C34-C35
21	G	2004	CDL	C12-C11-CA5-OA6
13	Q	3006	PEE	C31-C32-C33-C34
19	D	501	HEC	CAD-CBD-CGD-O1D
13	Q	3006	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
13	T	3005	PEE	C36-C37-C38-C39
13	G	2005	PEE	C1-O3P-P-O4P
13	T	3005	PEE	O2-C10-C11-C12
13	Q	3006	PEE	C16-C17-C18-C19
16	P	502	HEM	CAD-CBD-CGD-O2D
19	D	501	HEC	CAA-CBA-CGA-O2A
11	F	3011	JZR	C2'-C3'-C4'-C5'
21	Q	3003	CDL	C72-C71-CB7-OB8
13	D	2006	PEE	C39-C40-C41-C42
13	P	3007	PEE	C19-C20-C21-C22
16	P	501	HEM	CAA-CBA-CGA-O2A
19	Q	501	HEC	CAD-CBD-CGD-O1D
16	P	501	HEM	CAA-CBA-CGA-O1A
16	P	502	HEM	CAD-CBD-CGD-O1D
11	P	3008	JZR	C2'-C3'-C4'-C5'
19	D	501	HEC	CAA-CBA-CGA-O1A
19	Q	501	HEC	CAA-CBA-CGA-O2A
11	S	2011	JZR	C3'-C4'-C5'-C6'
21	G	2003	CDL	OA5-CA3-CA4-CA6
21	G	2003	CDL	C51-C52-C53-C54
19	Q	501	HEC	CAD-CBD-CGD-O2D
13	A	4003	PEE	O2-C2-C3-O3
21	G	2004	CDL	C32-C31-CA7-OA8
18	P	3002	UQ	C2-C3-O3-CM3
16	C	502	HEM	CAD-CBD-CGD-O2D
13	G	2005	PEE	C10-C11-C12-C13
11	F	3011	JZR	O1-C1'-C2'-C3'
19	D	501	HEC	CAD-CBD-CGD-O2D
13	Q	3006	PEE	C11-C12-C13-C14
19	Q	501	HEC	CAA-CBA-CGA-O1A
13	C	2007	PEE	C4-O4P-P-O1P
21	T	3004	CDL	CA2-OA2-PA1-OA3
13	T	3005	PEE	O4-C10-C11-C12
21	Q	3003	CDL	C52-C51-CB5-OB6
21	G	2004	CDL	C32-C31-CA7-OA9
21	Q	3003	CDL	C72-C71-CB7-OB9
16	C	502	HEM	CAD-CBD-CGD-O1D
13	T	3005	PEE	C5-C4-O4P-P
21	Q	3003	CDL	OB9-CB7-OB8-CB6
13	Q	3006	PEE	O2-C10-C11-C12
13	Q	3006	PEE	C41-C42-C43-C44

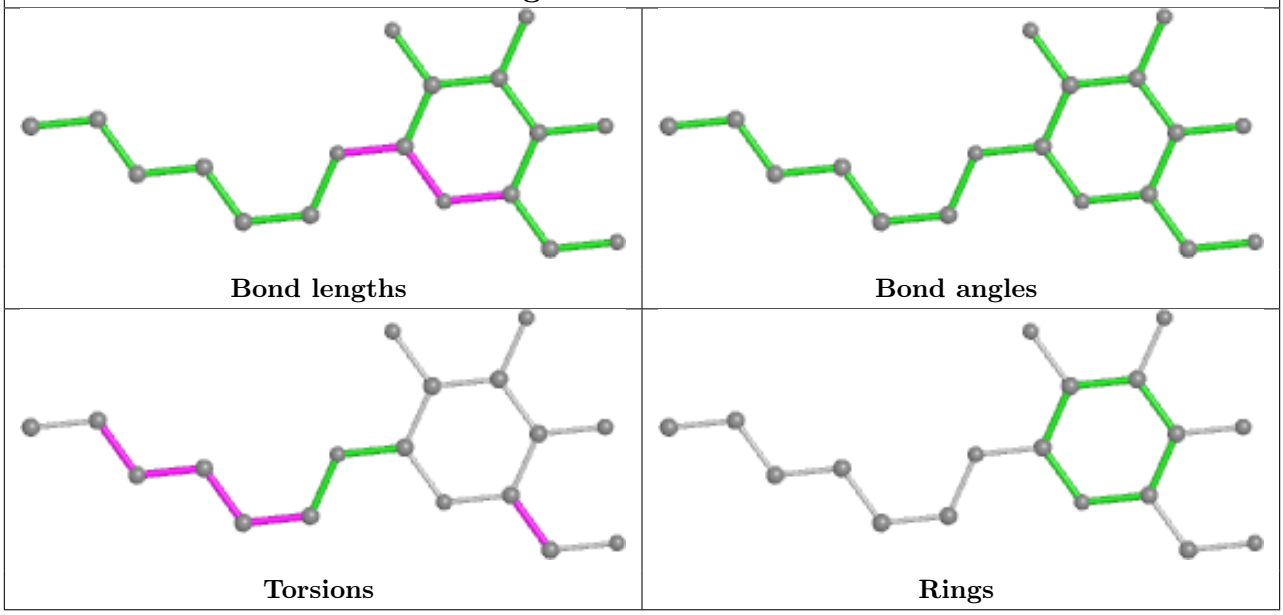
There are no ring outliers.

19 monomers are involved in 54 short contacts:

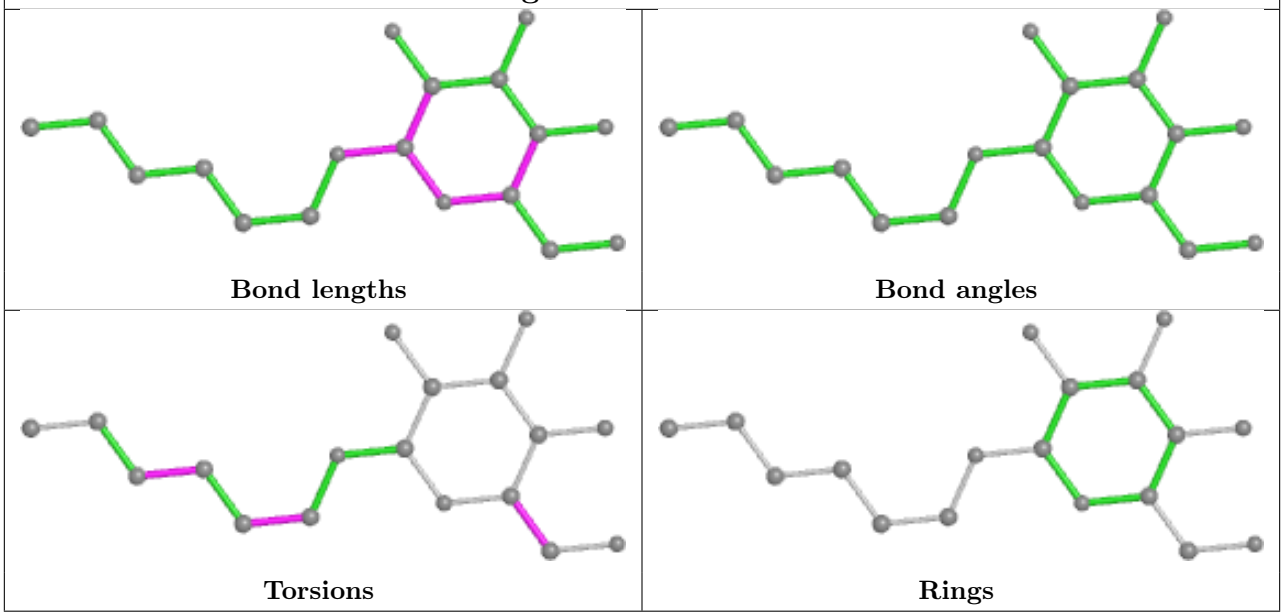
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	S	2011	JZR	8	0
11	F	3011	JZR	3	0
19	D	501	HEC	3	0
19	Q	501	HEC	2	0
21	G	2004	CDL	5	0
16	P	501	HEM	1	0
13	C	2007	PEE	2	0
13	Q	3006	PEE	9	0
13	T	3005	PEE	1	0
16	C	502	HEM	3	0
11	A	4002	JZR	1	0
16	P	502	HEM	2	0
13	D	2006	PEE	1	0
13	P	3007	PEE	2	0
18	C	2002	UQ	3	0
16	C	501	HEM	2	0
17	C	2001	SMA	1	0
17	P	3001	SMA	2	0
18	P	3002	UQ	5	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.

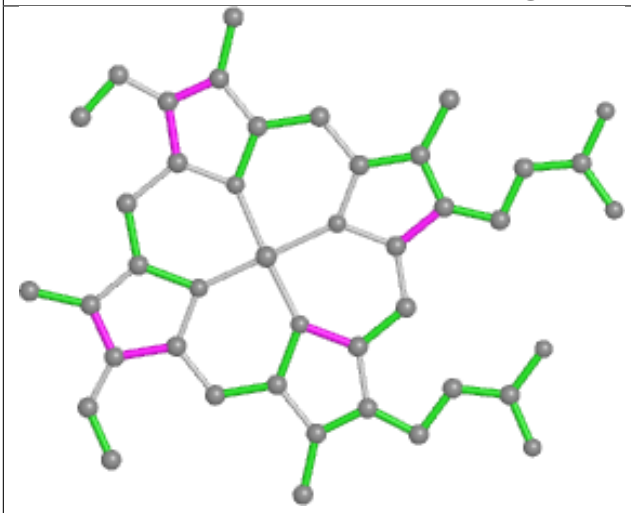
Ligand JZR S 2011



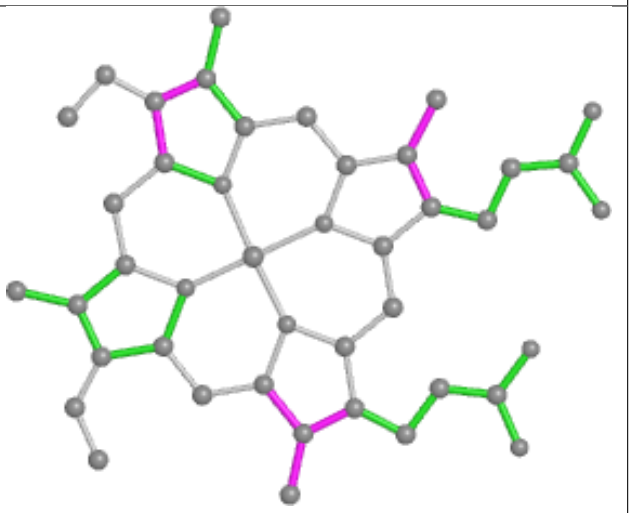
Ligand JZR F 3011



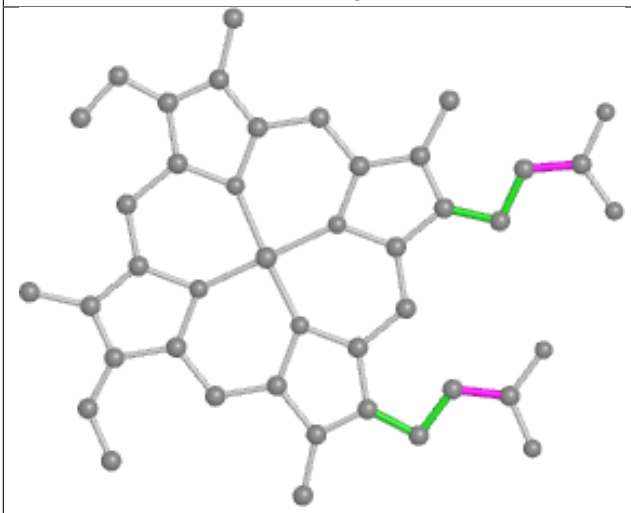
Ligand HEC D 501



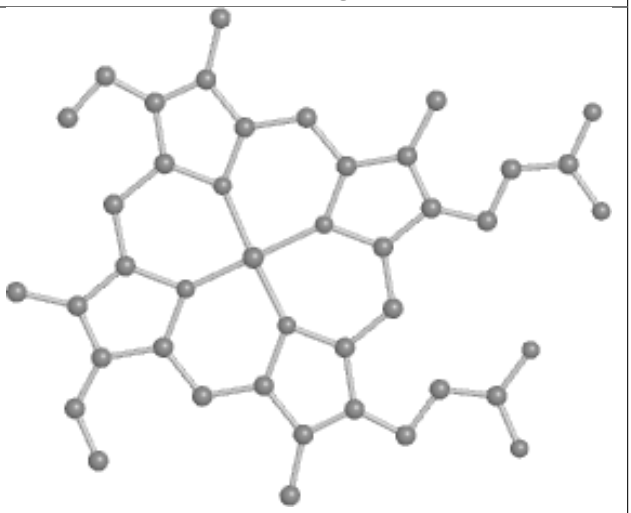
Bond lengths



Bond angles

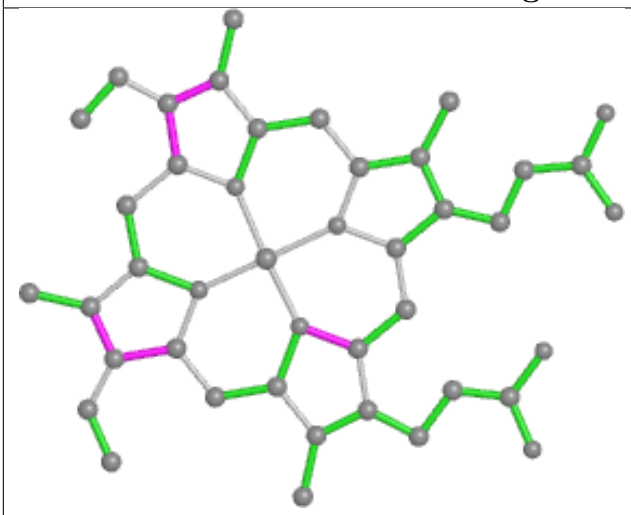


Torsions

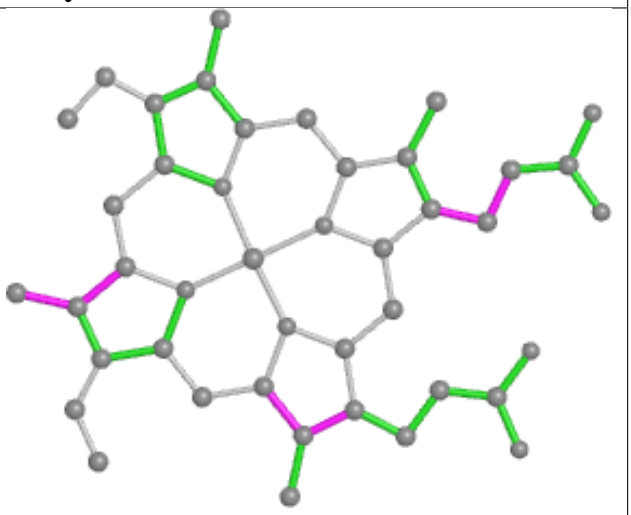


Rings

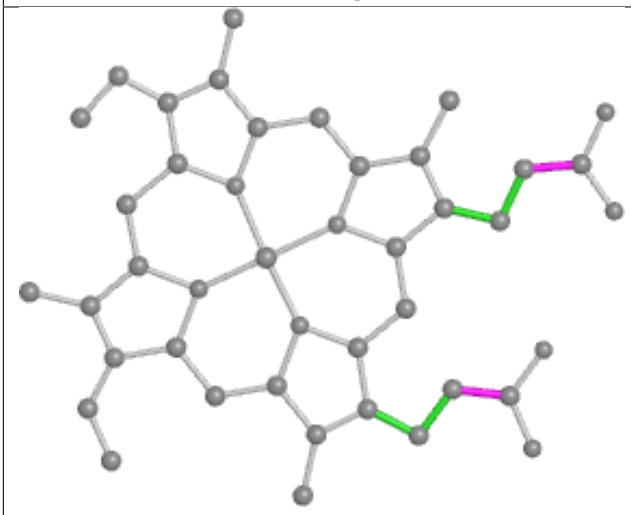
Ligand HEC Q 501



Bond lengths



Bond angles



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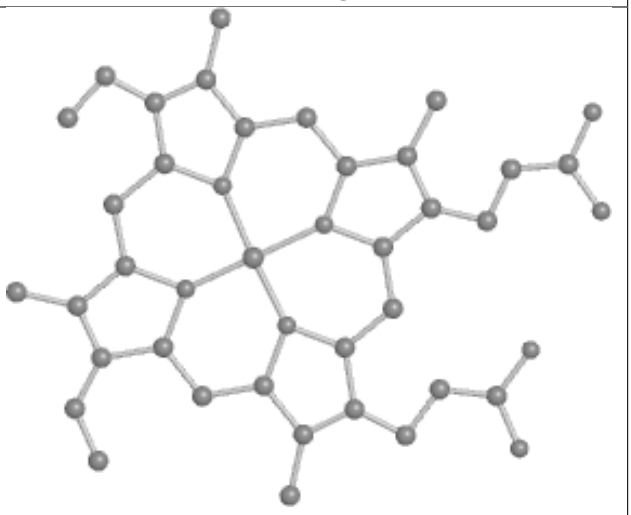
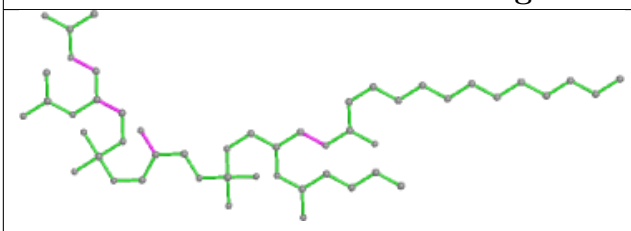
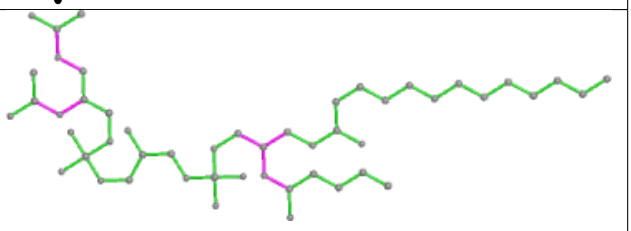


Rings

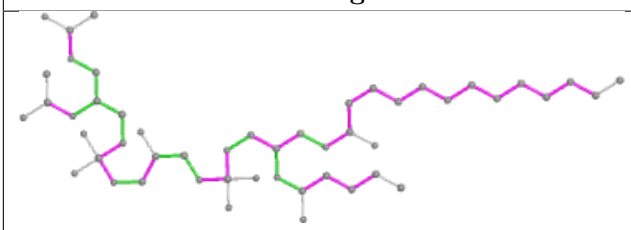
Ligand CDL Q 3003



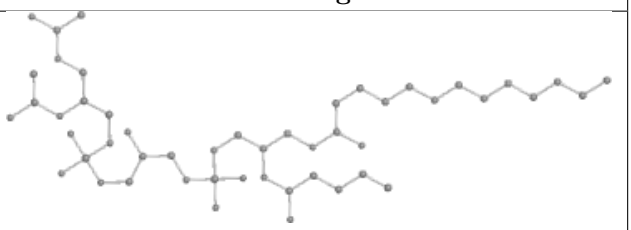
Bond lengths



Bond angles

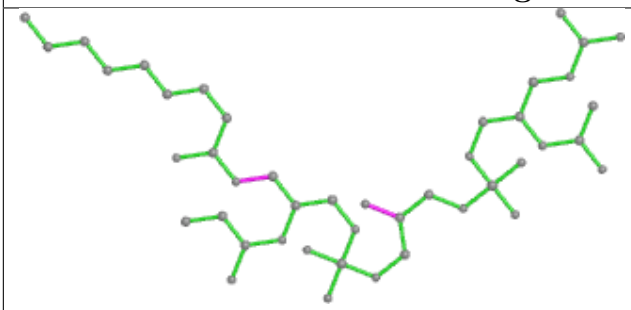


Torsions

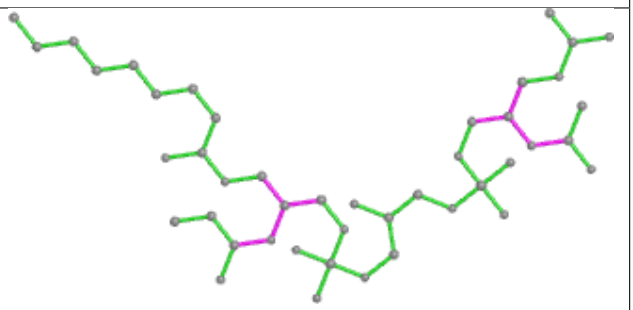


Rings

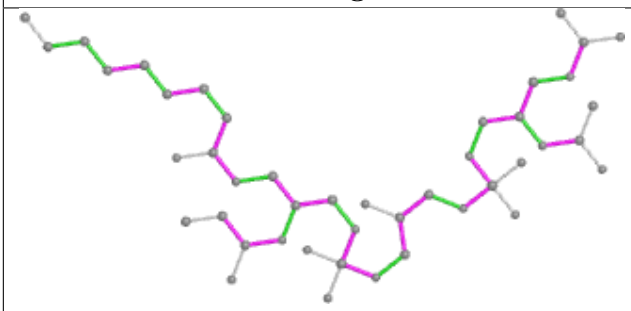
Ligand CDL G 2004



Bond lengths



Bond angles



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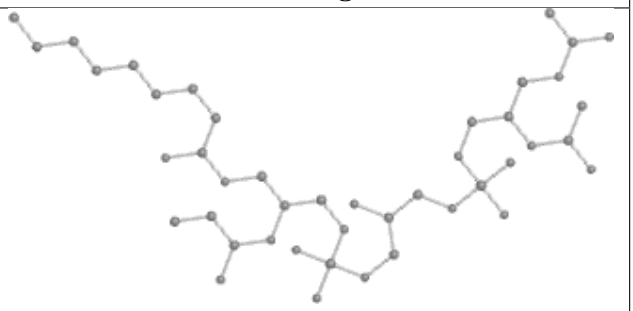
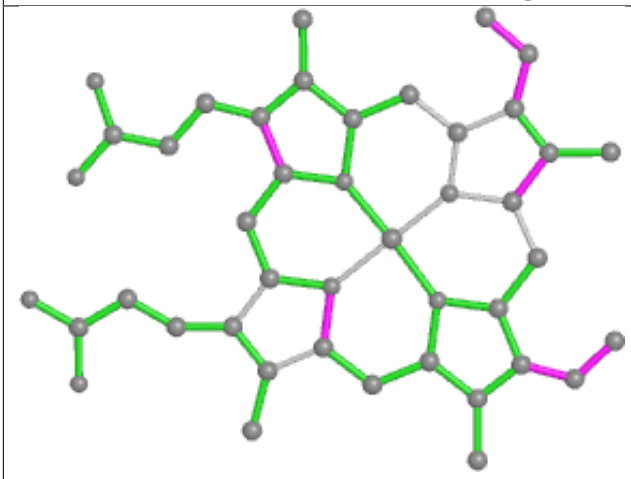
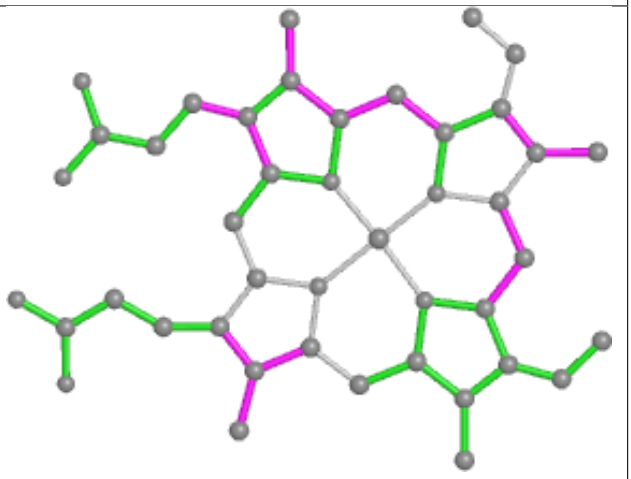


Rings

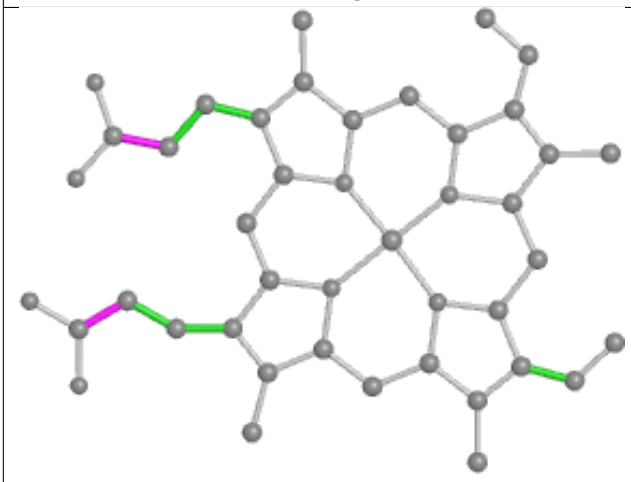
Ligand HEM P 501



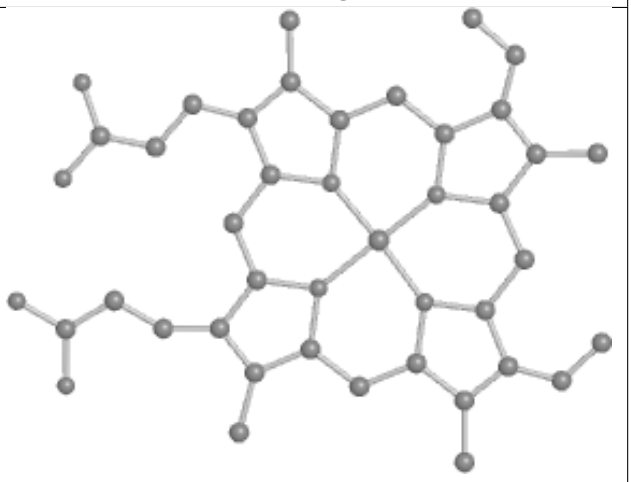
Bond lengths



Bond angles

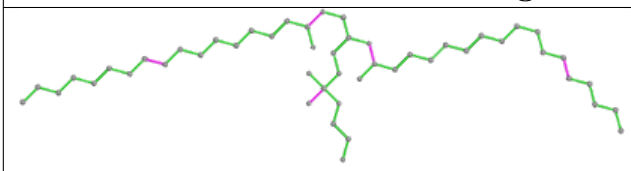


Torsions

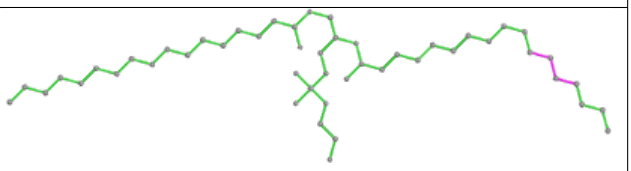


Rings

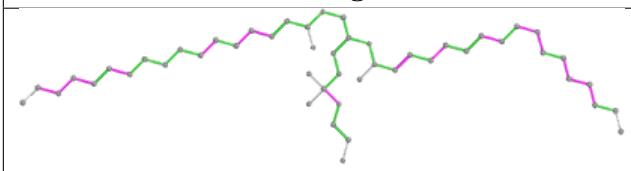
Ligand PEE C 2007



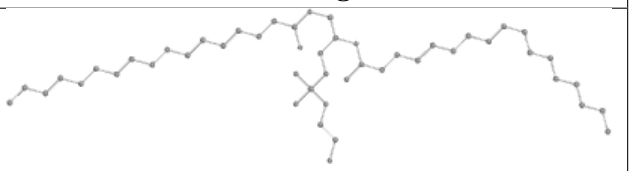
Bond lengths



Bond angles

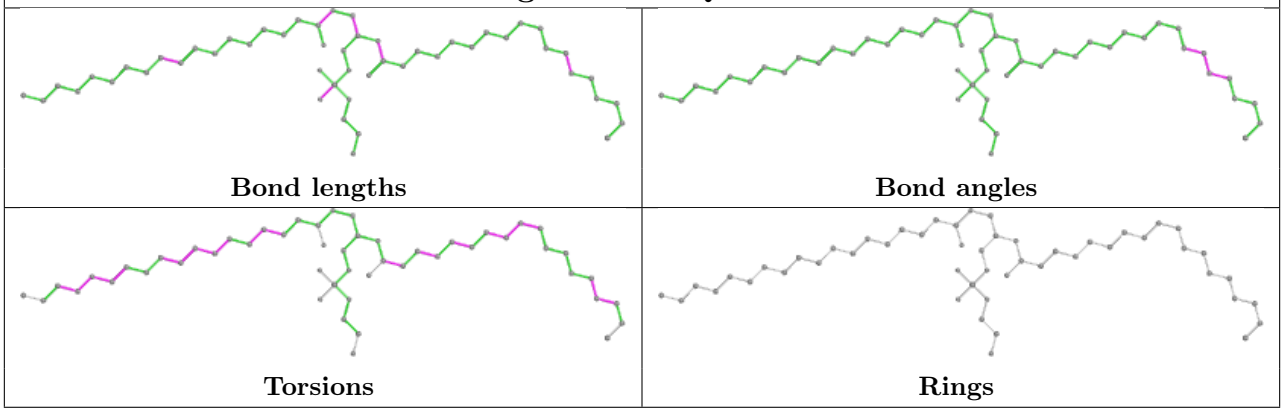


Torsions

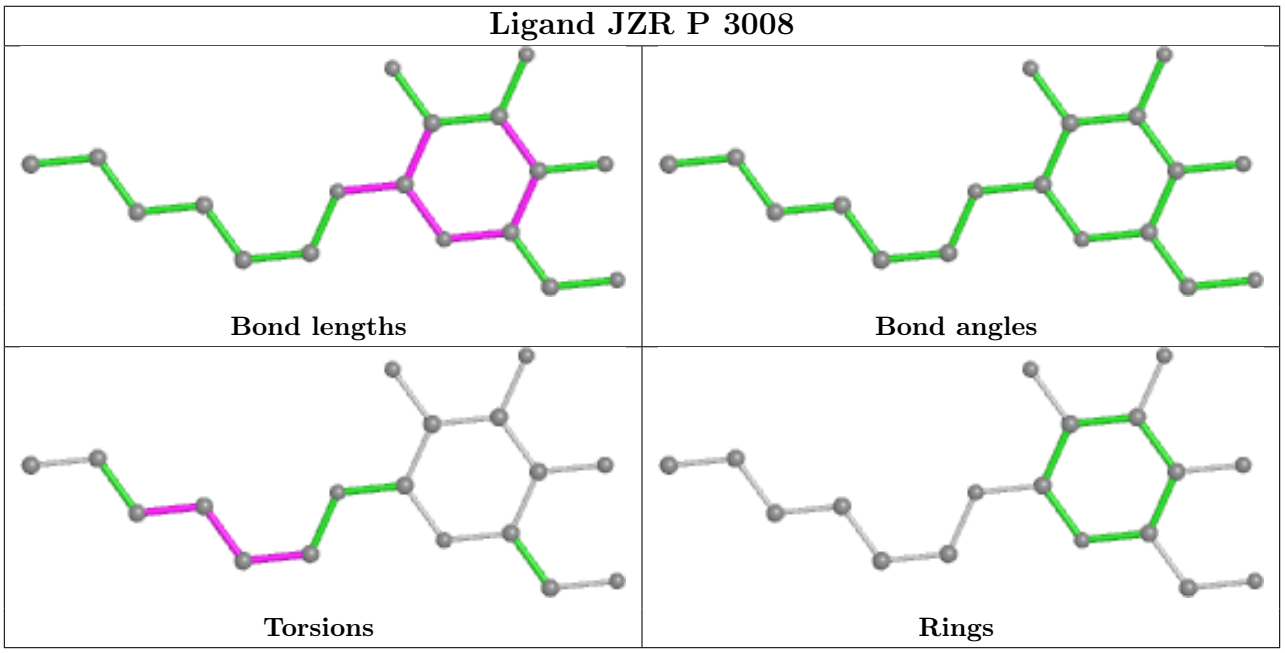


Rings

Ligand PEE Q 3006



Ligand JZR P 3008



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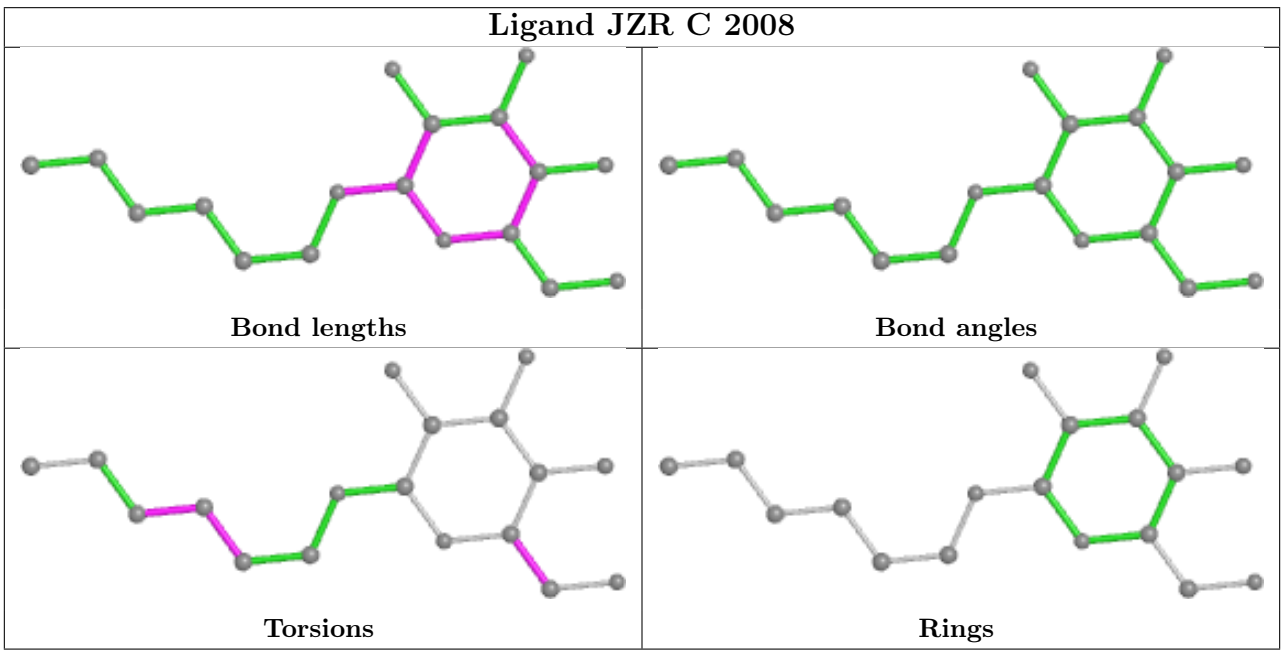
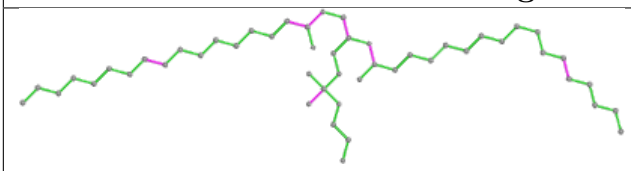
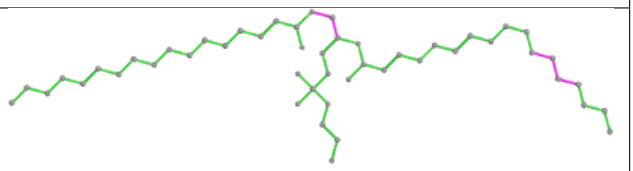


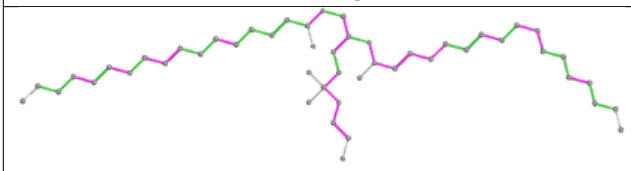
Ligand PEE T 3005



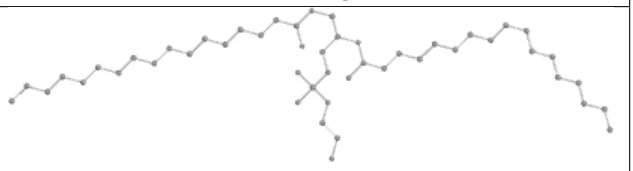
Bond lengths



Bond angles

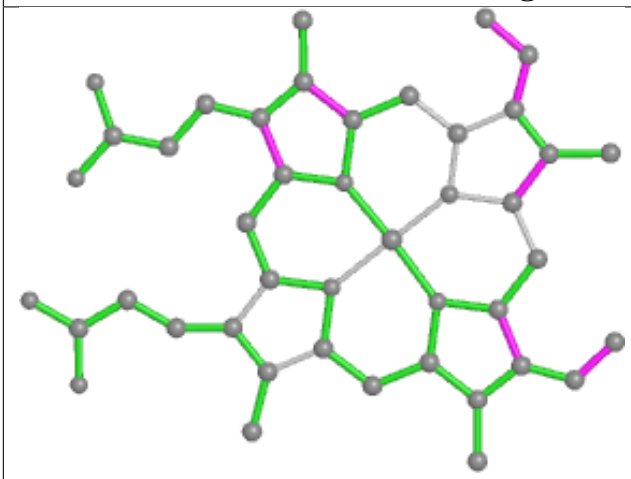


Torsions



Rings

Ligand HEM C 502



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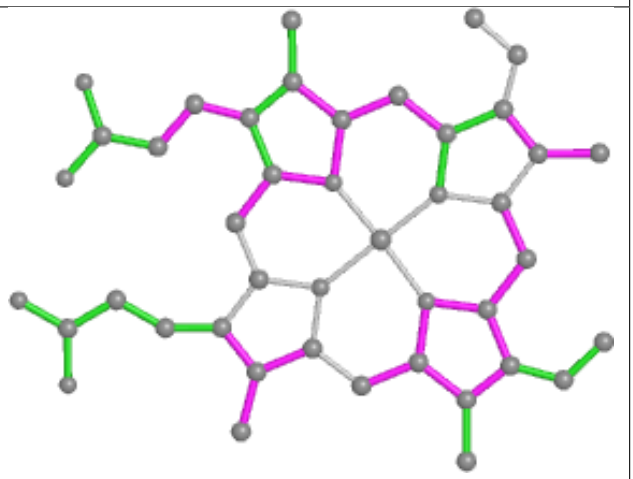
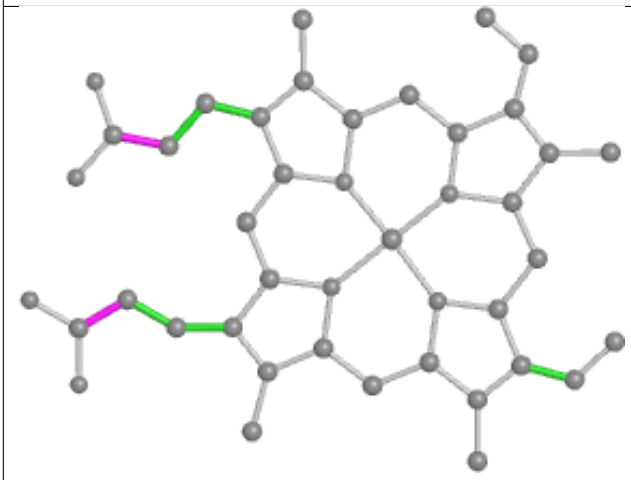
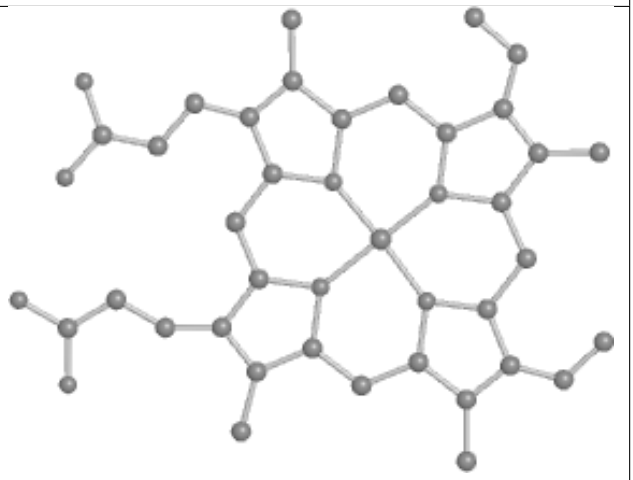


Bond angles

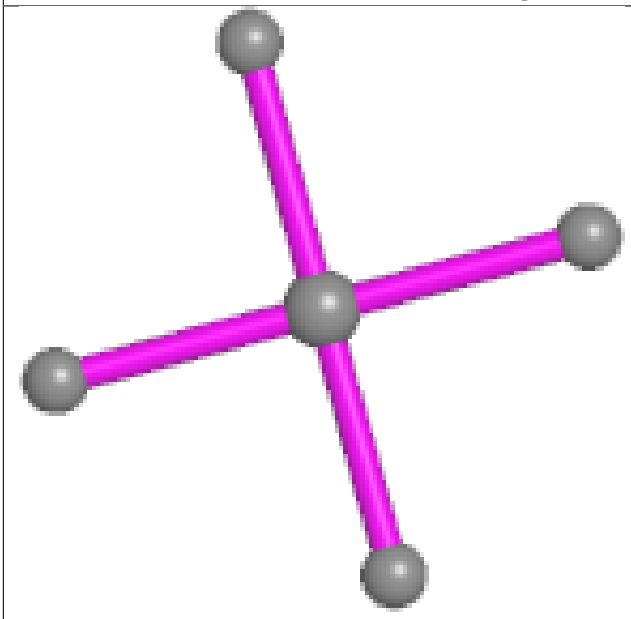


Torsions



Rings

Ligand PEE N 3012



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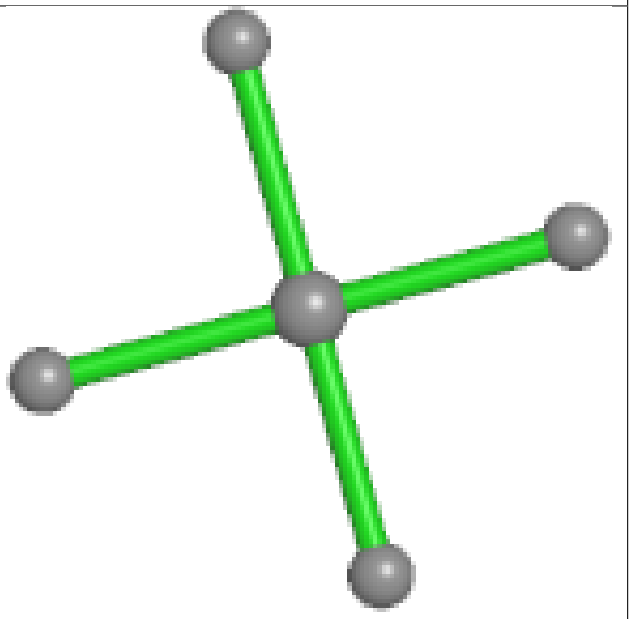
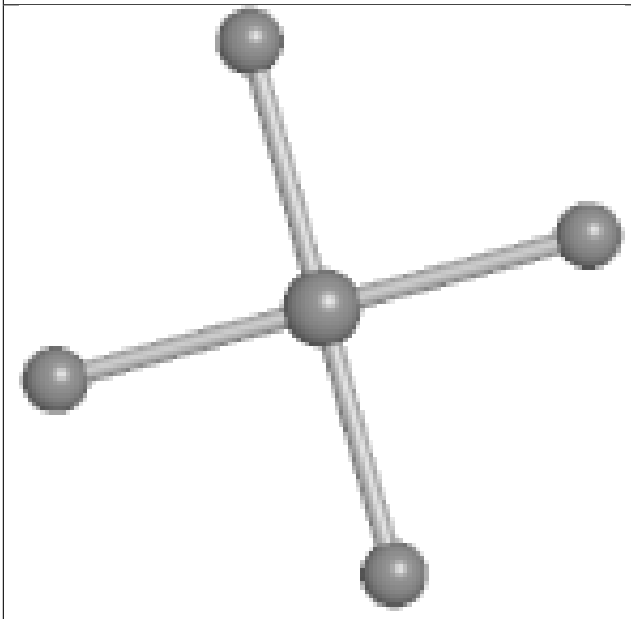


Bond angles



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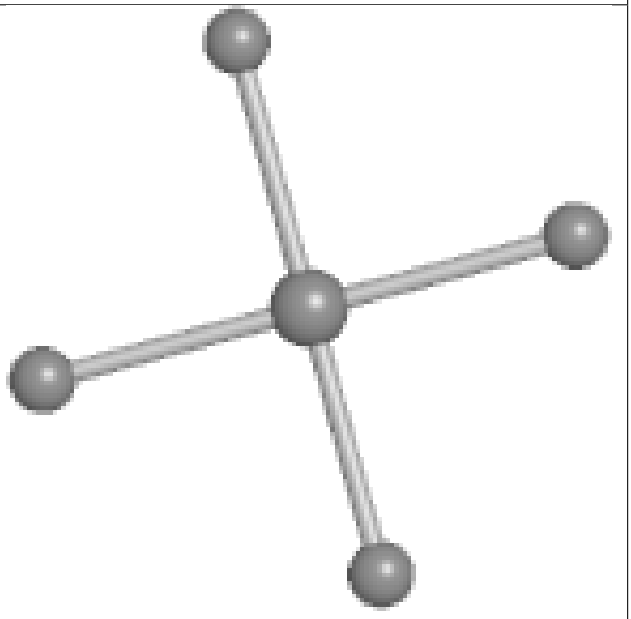
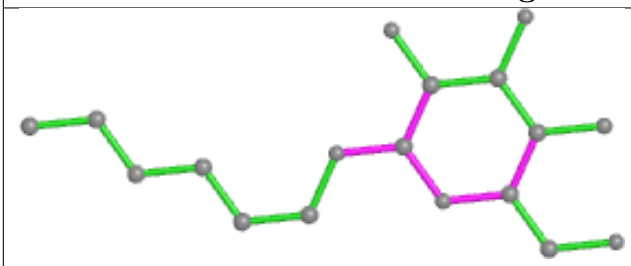


Rings

Ligand JZR A 4002



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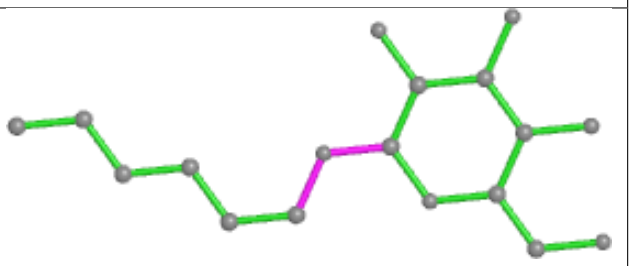
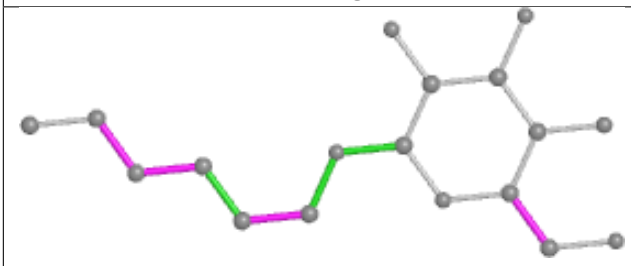


Bond angles



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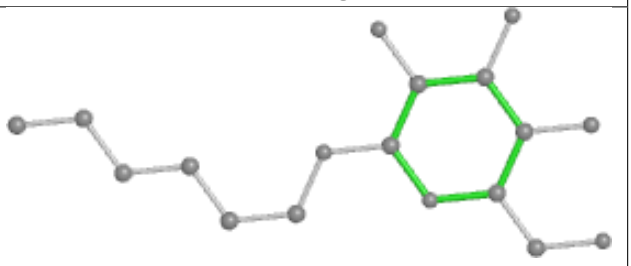
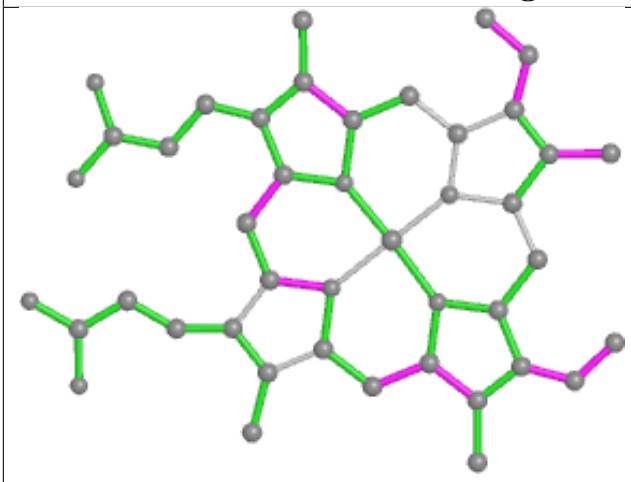


Rings

Ligand HEM P 502



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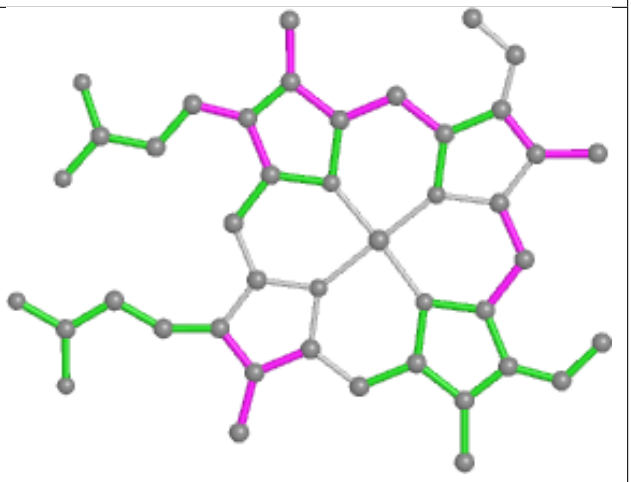
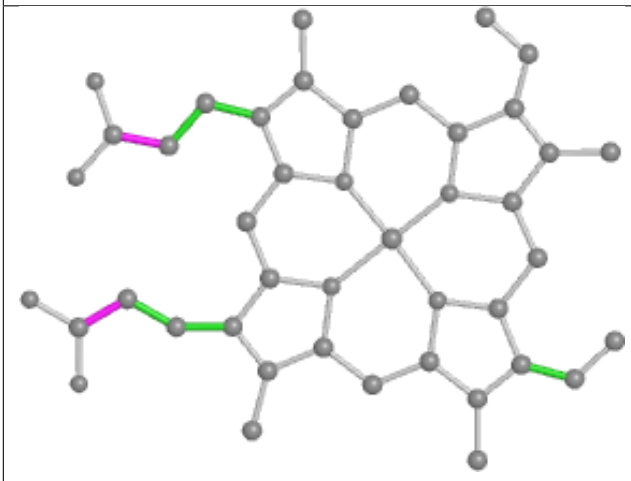


Bond angles



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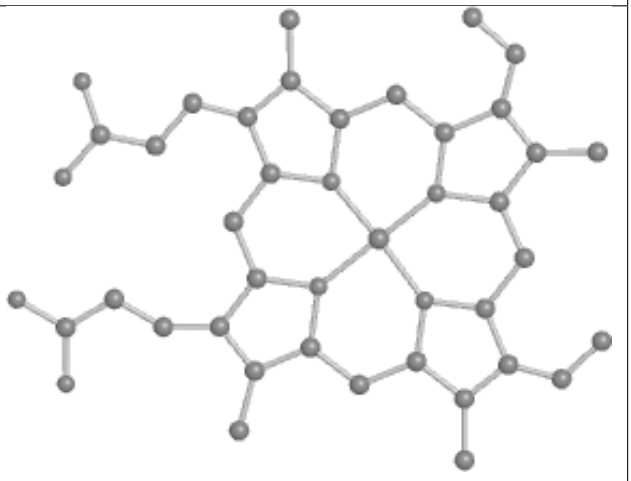
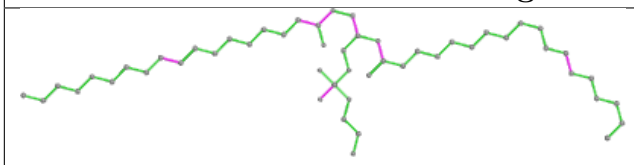


Rings

Ligand PEE D 2006



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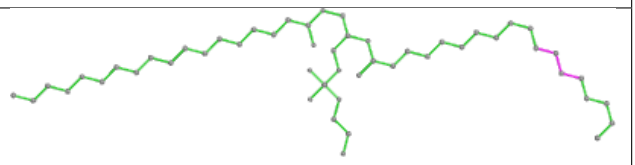
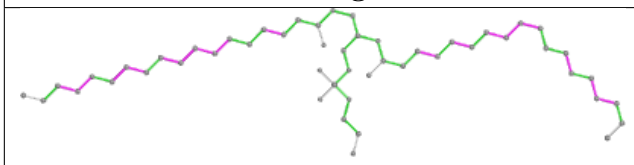
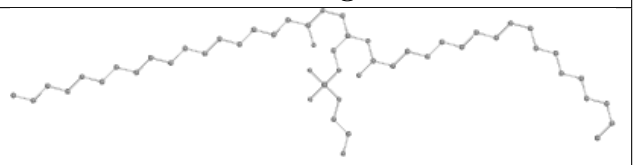


Bond angles

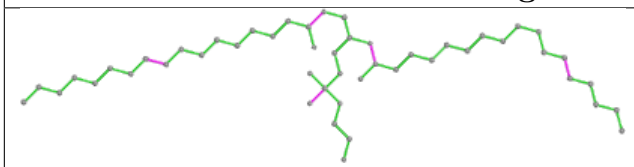


Torsions

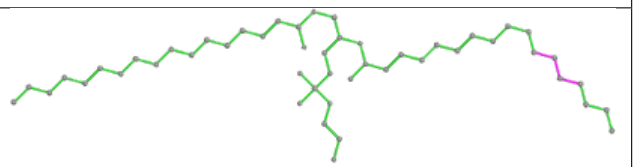


Rings

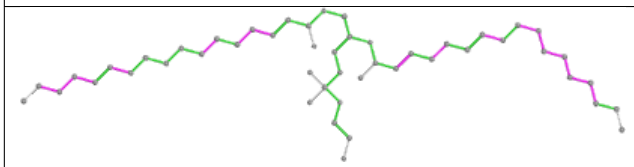
Ligand PEE P 3007



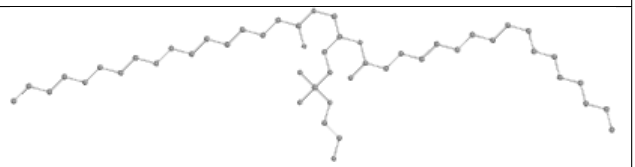
Bond lengths



Bond angles

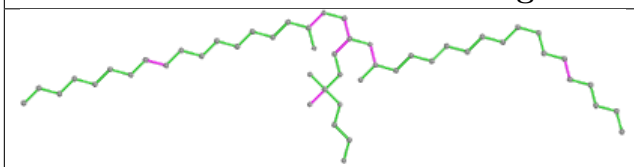


Torsions



Rings

Ligand PEE G 2005



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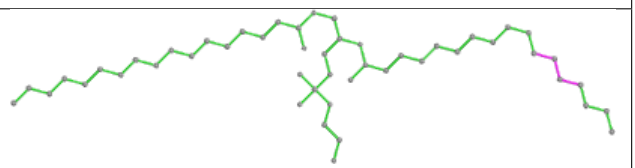
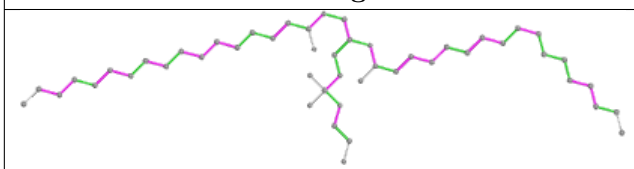
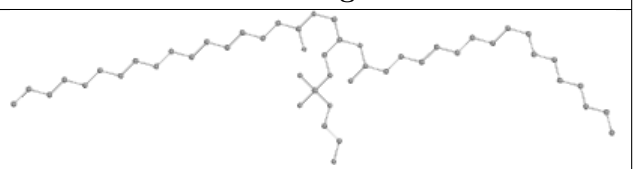


Bond angles

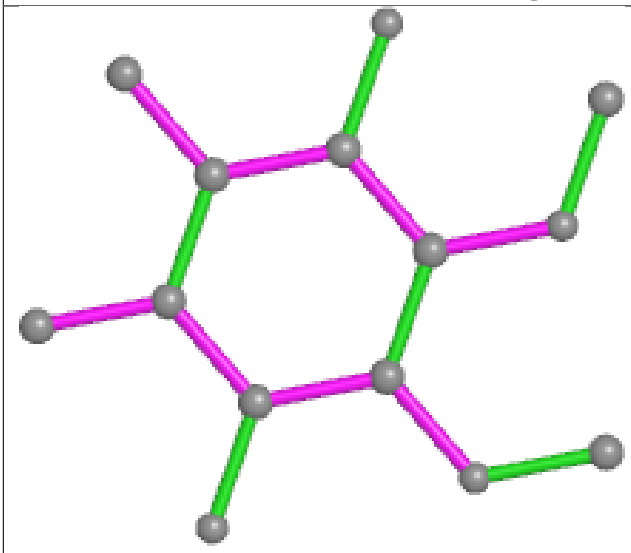


Torsions



Rings

Ligand UQ C 2002



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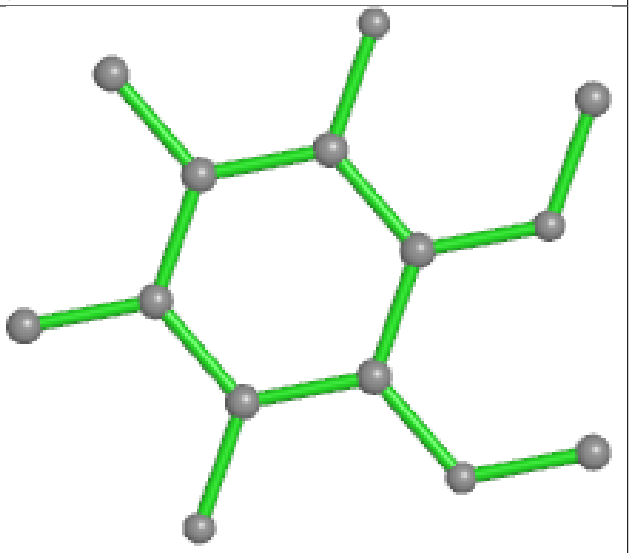
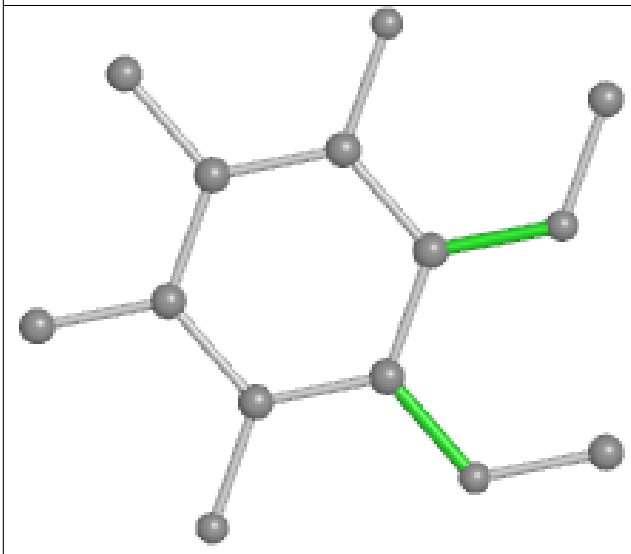
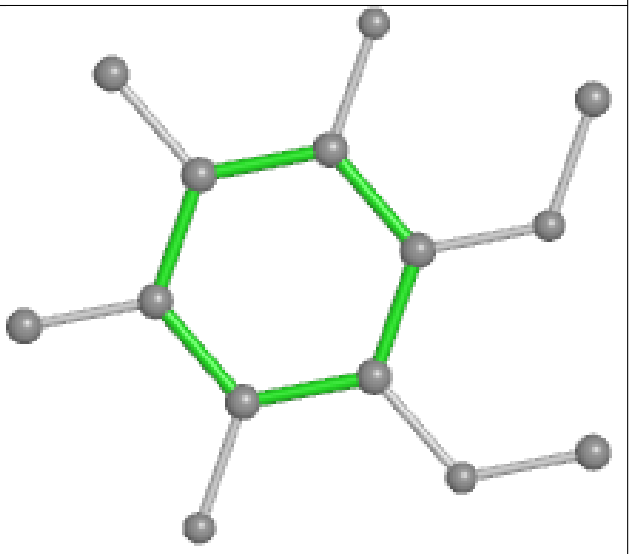


Bond angles

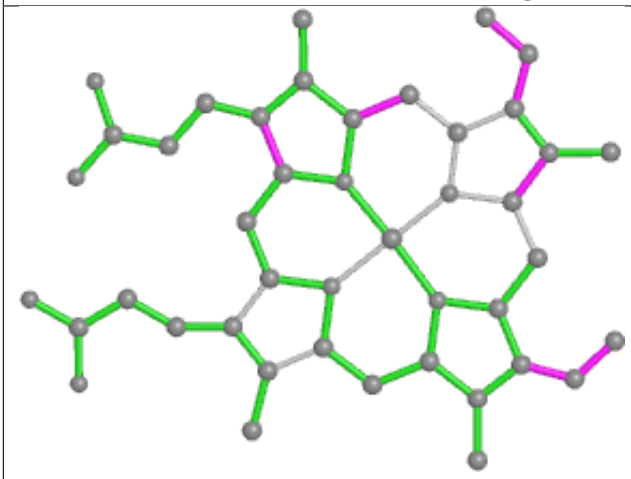


Torsions



Rings

Ligand HEM C 501



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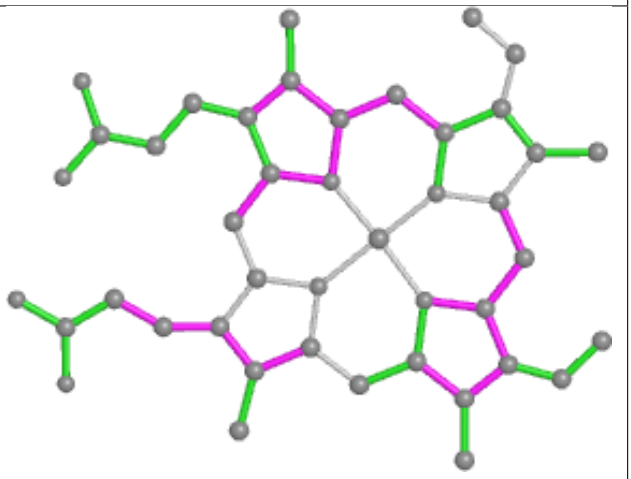
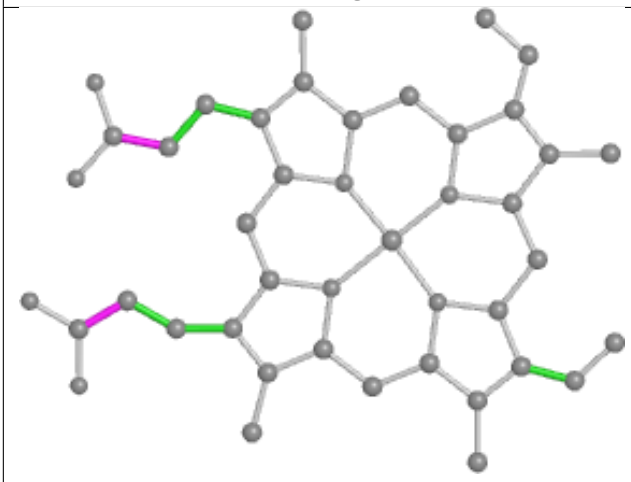
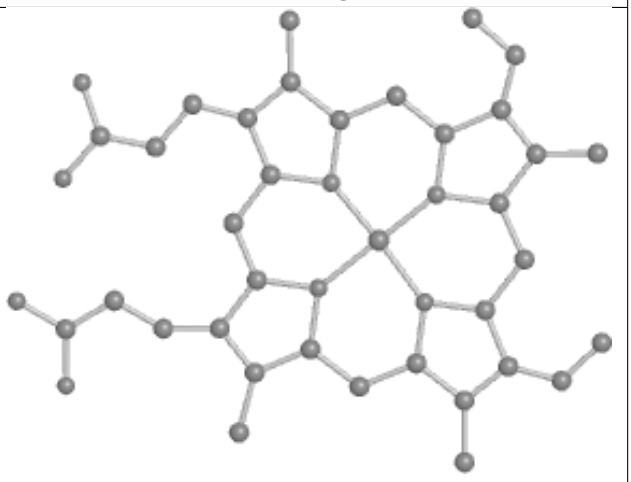


Bond angles

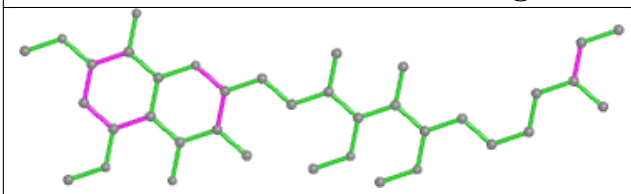


Torsions



Rings

Ligand SMA C 2001



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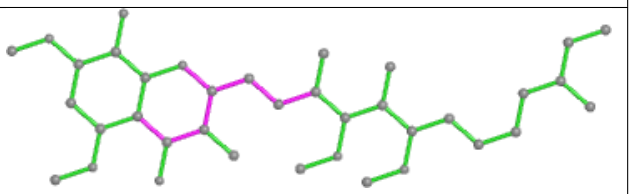
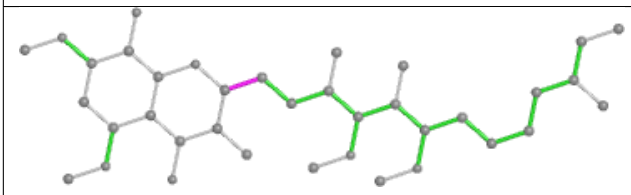
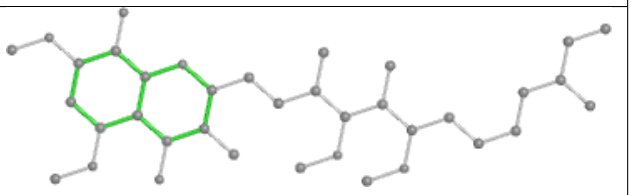


Bond angles

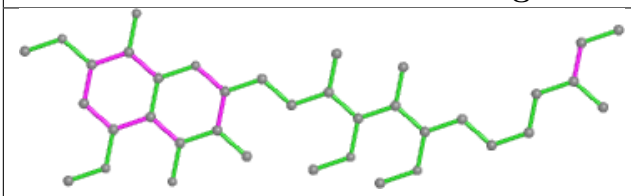


Torsions



Rings

Ligand SMA P 3001



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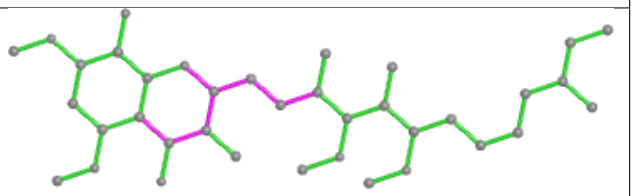
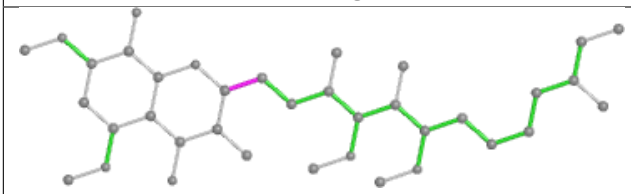
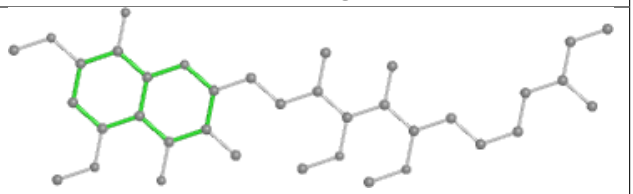


Bond angles

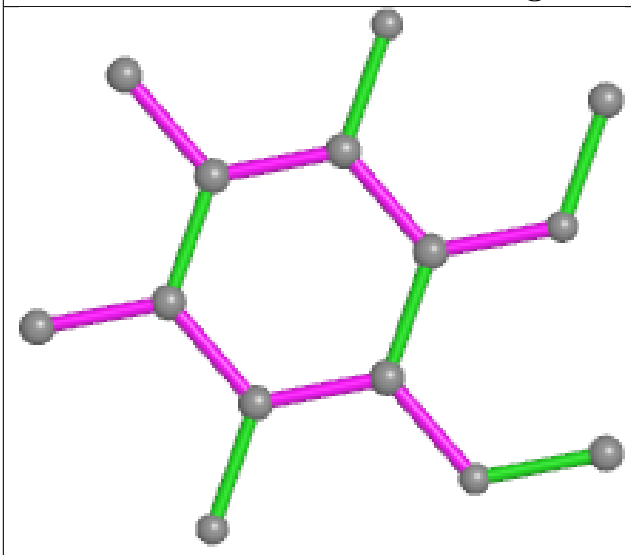


Torsions

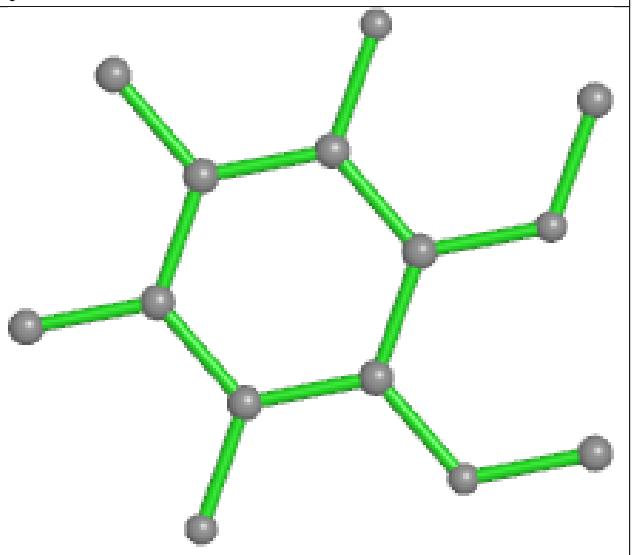


Rings

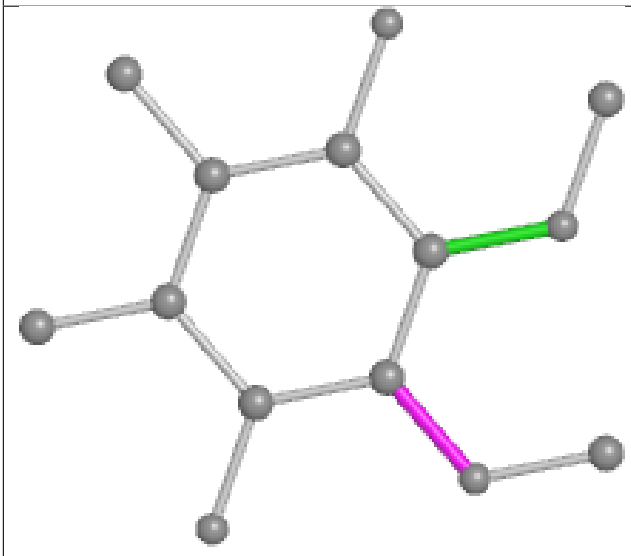
Ligand UQ P 3002



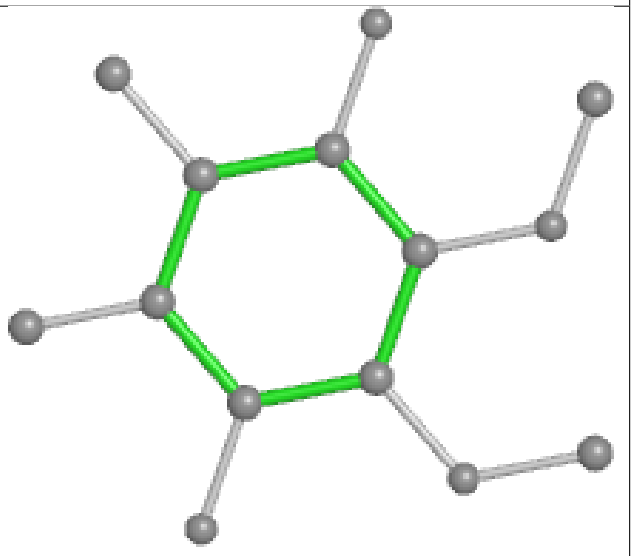
Bond lengths



Bond angles

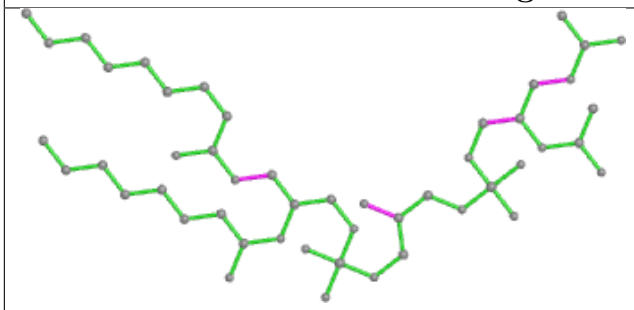


Torsions

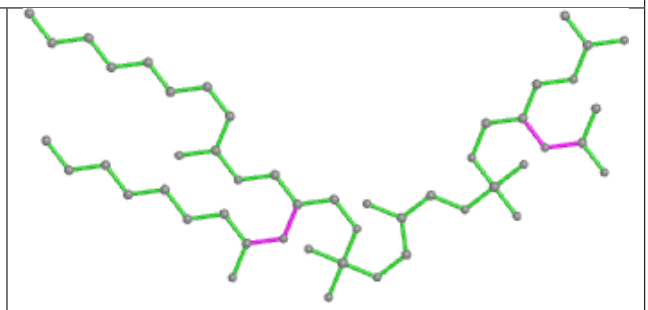


Rings

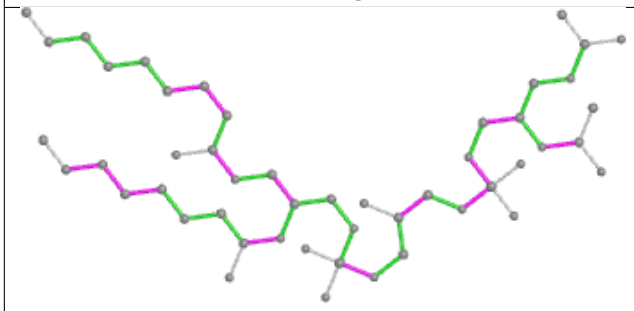
Ligand CDL T 3004



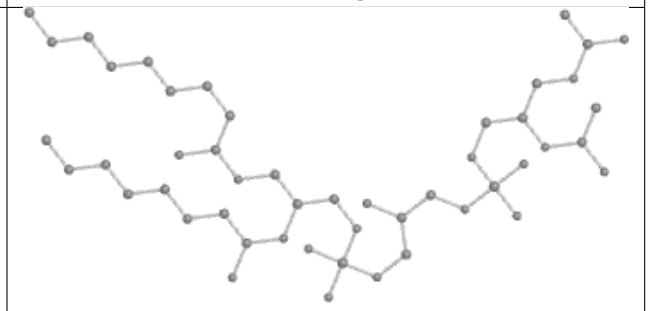
Bond lengths



Bond angles

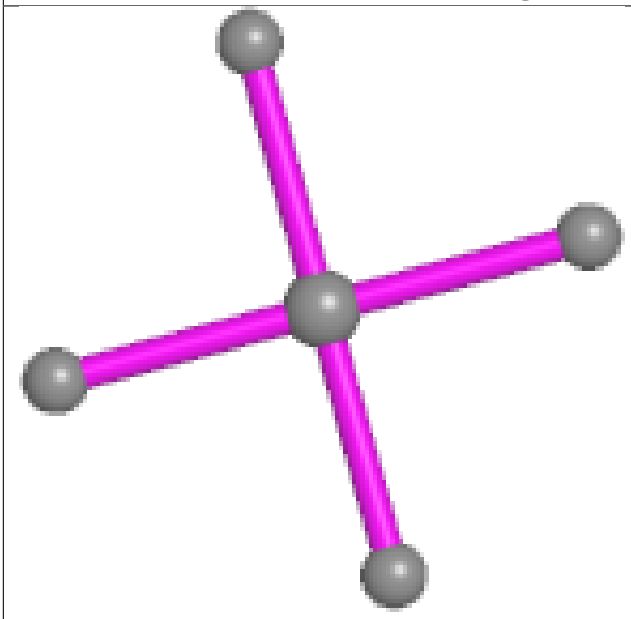


Torsions

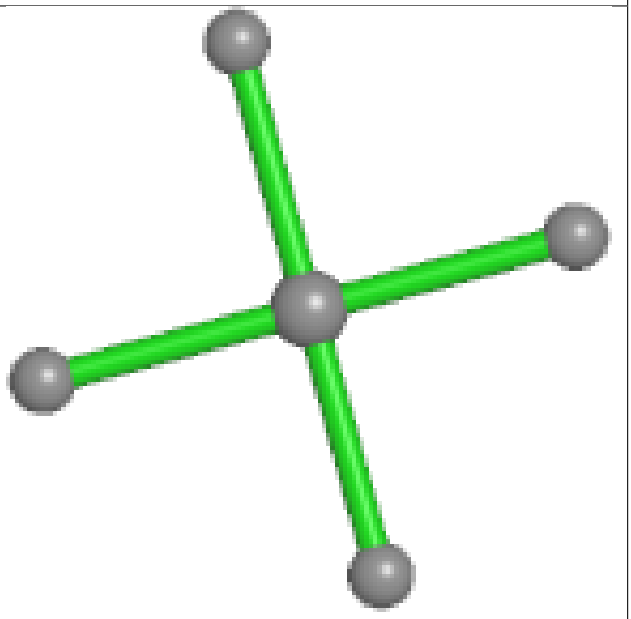


Rings

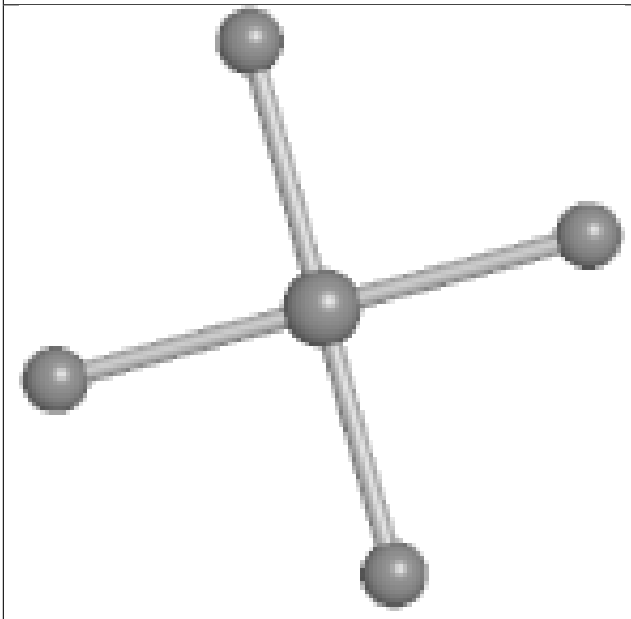
Ligand PEE C 2012



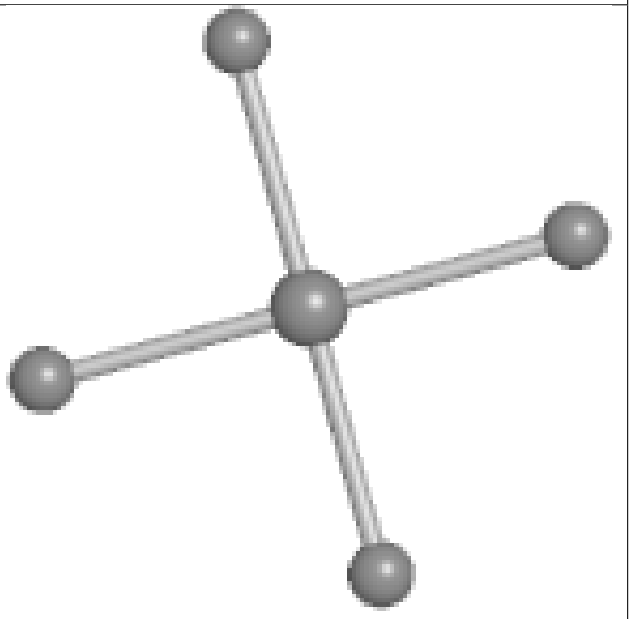
Bond lengths



Bond angles

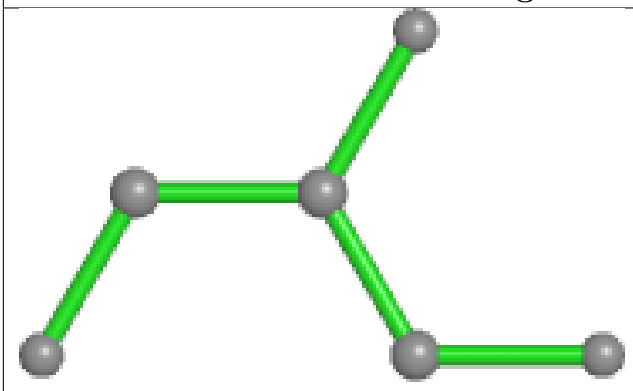


Torsions

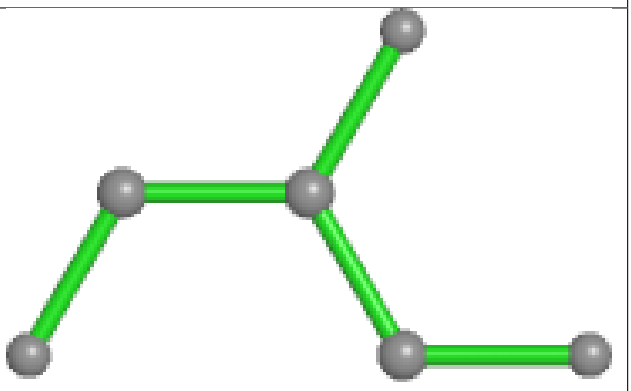


Rings

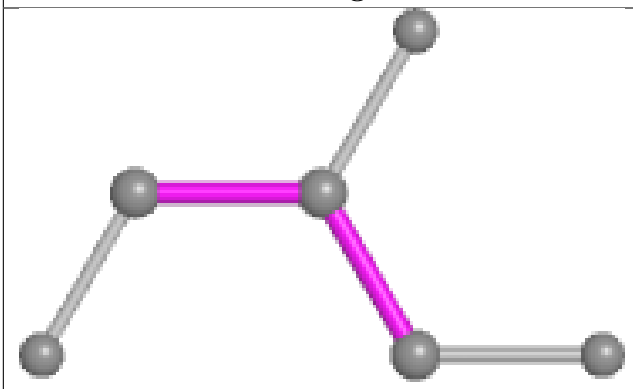
Ligand PEE A 4003



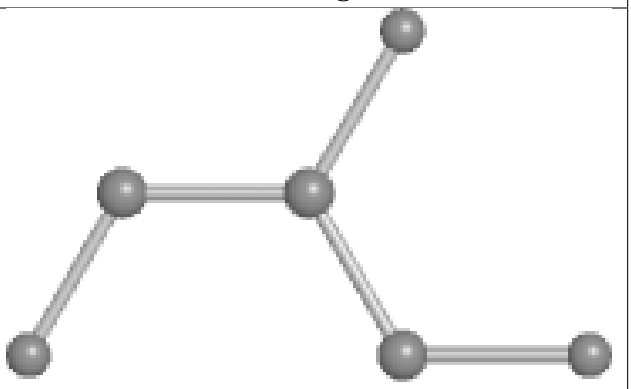
Bond lengths



Bond angles

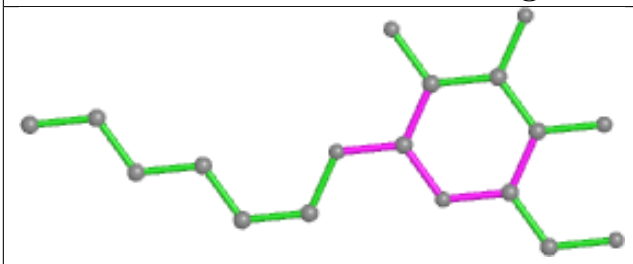


Torsions

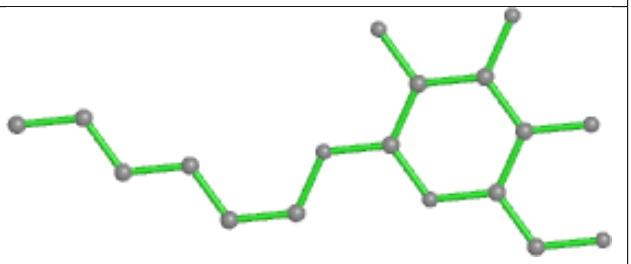


Rings

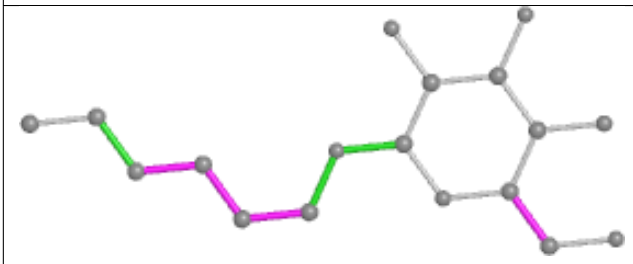
Ligand JZR F 4001



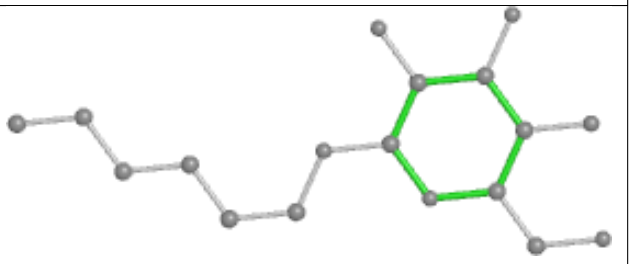
Bond lengths



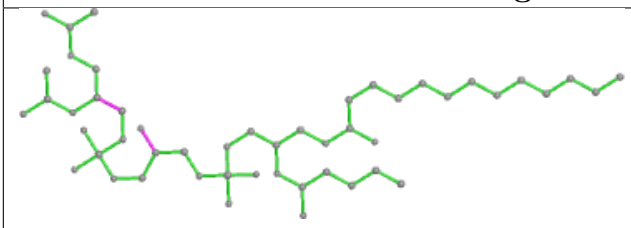
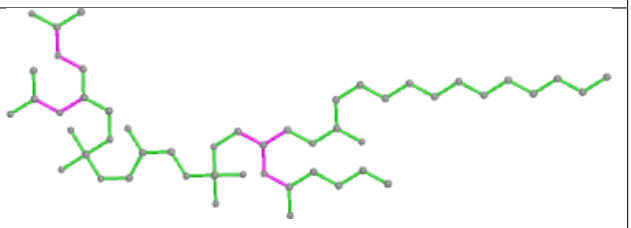
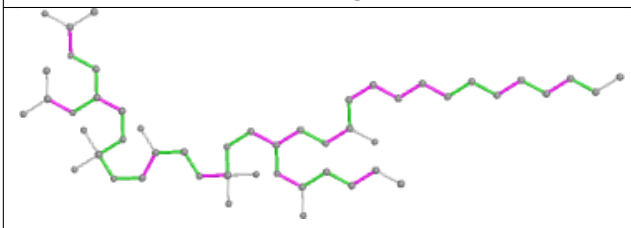
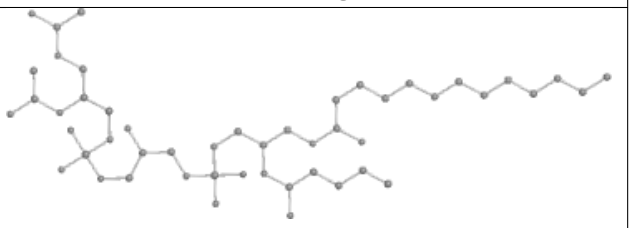
Bond angles



Torsions



Rings

Ligand CDL G 2003	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	442/446 (99%)	0.09	20 (4%) 33 38	27, 43, 65, 115	1 (0%)
1	N	442/446 (99%)	0.15	14 (3%) 47 54	28, 43, 63, 128	1 (0%)
2	B	424/439 (96%)	0.14	15 (3%) 44 50	29, 45, 67, 132	0
2	O	424/439 (96%)	0.25	25 (5%) 22 27	33, 47, 73, 162	0
3	C	365/379 (96%)	0.21	6 (1%) 72 75	25, 34, 47, 106	0
3	P	370/379 (97%)	0.28	24 (6%) 18 23	26, 34, 52, 165	0
4	D	241/241 (100%)	-0.00	4 (1%) 70 74	28, 39, 59, 80	0
4	Q	241/241 (100%)	0.06	14 (5%) 23 28	28, 38, 59, 81	0
5	E	196/196 (100%)	0.73	31 (15%) 2 2	29, 54, 96, 117	0
5	R	196/196 (100%)	0.01	4 (2%) 65 69	29, 43, 61, 85	0
6	F	99/110 (90%)	0.23	4 (4%) 38 44	29, 44, 70, 80	0
6	S	99/110 (90%)	0.35	10 (10%) 7 9	28, 39, 79, 109	0
7	G	75/81 (92%)	0.45	5 (6%) 17 22	31, 50, 72, 80	0
7	T	76/81 (93%)	0.92	8 (10%) 6 8	30, 50, 97, 117	0
8	H	66/78 (84%)	0.84	9 (13%) 3 4	40, 55, 87, 101	0
8	U	66/78 (84%)	0.69	10 (15%) 2 3	40, 54, 79, 89	0
9	I	42/78 (53%)	2.49	23 (54%) 0 0	40, 75, 88, 93	0
9	V	42/78 (53%)	1.94	15 (35%) 0 0	45, 72, 92, 97	0
10	J	62/62 (100%)	1.08	12 (19%) 1 1	35, 60, 85, 116	0
10	W	62/62 (100%)	0.91	9 (14%) 2 3	34, 51, 80, 111	0
All	All	4030/4220 (95%)	0.29	262 (6%) 18 23	25, 42, 76, 165	2 (0%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	76	ALA	32.7
10	J	1	VAL	16.1
1	N	1	THR	11.4
2	O	19	PRO	9.9
3	P	13	ILE	9.5
10	W	2	ALA	9.3
1	A	222	THR	8.8
2	O	233	SER	8.5
6	S	12	TRP	8.3
2	O	232	LEU	8.1
7	T	73	ASN	7.7
10	W	62	LYS	7.6
3	C	17	ALA	7.5
1	A	1	THR	7.0
5	E	71	MET	6.9
2	O	18	PRO	6.8
2	O	229	GLY	6.6
10	W	61	ASN	6.6
2	B	41	TYR	6.5
2	O	230	LEU	6.5
9	I	78	TYR	6.4
2	O	17	VAL	6.4
2	O	234	GLY	6.2
10	W	1	VAL	6.2
7	T	75	ALA	6.2
1	N	2	ALA	6.1
5	E	191	ASP	5.9
4	Q	241	LYS	5.9
5	E	103	LYS	5.9
1	N	229	PRO	5.8
2	B	233	SER	5.7
6	S	110	LYS	5.6
9	I	63	PRO	5.5
5	E	194	ILE	5.5
9	V	32	ALA	5.4
9	V	78	TYR	5.4
2	B	19	PRO	5.3
1	A	2	ALA	5.2
9	I	49	VAL	5.1
1	N	227	ALA	5.0
3	P	16	ASN	5.0
6	F	13	LEU	5.0
5	E	190	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	4.9
9	V	63	PRO	4.9
10	J	2	ALA	4.9
1	N	222	THR	4.7
9	I	62	ARG	4.7
10	J	62	LYS	4.7
5	E	70	ALA	4.7
2	B	304	HIS	4.6
7	T	74	PRO	4.5
2	O	12	GLU	4.5
5	E	108	GLN	4.5
7	G	30	PHE	4.4
10	J	30	PHE	4.4
9	I	59	ALA	4.3
9	I	77	ARG	4.3
3	P	168	PHE	4.3
8	H	46	SER	4.2
5	E	112	VAL	4.2
1	N	226	ASP	4.2
2	B	18	PRO	4.1
8	H	47	ARG	4.1
6	S	13	LEU	4.1
5	E	76	ILE	4.0
2	B	12	GLU	4.0
8	U	47	ARG	4.0
3	P	11	MET	4.0
8	U	45	SER	3.9
8	U	48	SER	3.9
3	P	10	LEU	3.9
5	E	110	ALA	3.9
5	E	132	TRP	3.8
5	E	92	ARG	3.7
1	A	443	TRP	3.7
1	A	227	ALA	3.7
5	E	80	ASP	3.7
9	I	76	VAL	3.7
2	B	249	GLY	3.7
10	J	33	ARG	3.7
1	A	51	LYS	3.6
10	J	29	LEU	3.6
7	T	72	LYS	3.6
10	J	27	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
7	G	56	TYR	3.6
9	I	51	CYS	3.6
9	V	42	VAL	3.6
9	V	33	ALA	3.5
9	I	50	LEU	3.5
2	B	20	HIS	3.5
7	G	74	PRO	3.5
9	V	62	ARG	3.5
9	I	61	GLY	3.5
9	V	70	LEU	3.5
10	J	3	PRO	3.5
9	I	35	PRO	3.4
9	I	32	ALA	3.4
2	O	41	TYR	3.4
10	W	12	LEU	3.4
8	H	49	GLN	3.4
9	I	70	LEU	3.3
9	I	57	GLY	3.3
5	E	189	SER	3.2
3	P	14	VAL	3.2
2	O	20	HIS	3.2
2	O	21	PRO	3.1
5	E	107	ASP	3.1
1	N	206	ARG	3.1
4	Q	73	GLY	3.1
6	S	108	ALA	3.1
9	I	55	LEU	3.0
5	R	189	SER	3.0
9	I	60	ALA	3.0
9	V	34	VAL	3.0
6	S	14	GLU	3.0
8	U	27	LEU	3.0
3	C	16	ASN	3.0
6	S	16	ILE	3.0
4	D	241	LYS	3.0
5	E	133	VAL	2.9
2	O	235	ALA	2.9
5	E	104	LYS	2.9
3	P	218	ILE	2.9
5	E	154	GLY	2.9
1	N	225	GLU	2.9
8	U	44	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	N	224	ASP	2.9
1	A	219	LEU	2.9
1	A	122	LEU	2.9
5	E	69	LEU	2.9
4	Q	141	VAL	2.8
9	V	48	SER	2.8
3	P	31	TRP	2.8
8	H	44	VAL	2.8
9	I	72	VAL	2.8
9	V	49	VAL	2.8
5	E	129	LYS	2.8
8	H	42	GLU	2.8
3	P	208	PRO	2.8
4	Q	81	PHE	2.8
2	O	369	LEU	2.8
1	A	68	LYS	2.7
6	F	109	LYS	2.7
2	O	218	GLN	2.7
2	O	265	GLY	2.7
4	D	145	GLU	2.7
1	N	297	ILE	2.7
1	A	217	SER	2.7
1	N	228	VAL	2.7
1	A	206	ARG	2.7
6	S	109	LYS	2.7
2	B	17	VAL	2.6
8	U	71	HIS	2.6
9	V	35	PRO	2.6
5	E	195	VAL	2.6
2	B	350	GLY	2.6
5	E	75	GLU	2.6
8	U	50	THR	2.6
10	W	57	HIS	2.6
1	A	125	SER	2.6
3	P	25	SER	2.6
5	R	190	ASP	2.5
4	Q	76	GLU	2.5
7	T	42	ARG	2.5
2	O	367	GLY	2.5
3	P	26	ASN	2.5
6	S	78	GLU	2.5
4	D	144	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
8	H	43	ARG	2.5
5	R	89	PHE	2.5
4	Q	1	SER	2.5
9	I	71	ASN	2.5
10	J	5	LEU	2.5
3	P	19	ILE	2.5
5	E	186	GLU	2.5
5	E	192	MET	2.4
4	Q	75	ASN	2.4
2	B	251	SER	2.4
4	Q	79	GLU	2.4
3	P	29	SER	2.4
7	G	68	LYS	2.4
2	O	304	HIS	2.4
1	A	187	SER	2.4
3	P	314	SER	2.4
1	N	213	GLN	2.4
4	Q	77	ASP	2.4
9	I	75	SER	2.4
10	W	30	PHE	2.4
7	G	75	ALA	2.4
10	J	12	LEU	2.4
2	O	301	LYS	2.4
5	E	102	THR	2.4
10	W	8	ARG	2.3
8	U	51	GLU	2.3
3	P	27	ILE	2.3
3	P	104	TYR	2.3
3	C	18	PHE	2.3
2	O	350	GLY	2.3
8	H	48	SER	2.3
9	I	64	LEU	2.3
7	T	30	PHE	2.3
1	A	225	GLU	2.3
3	P	209	THR	2.3
3	P	30	TRP	2.3
2	O	399	LEU	2.2
4	Q	115	TYR	2.2
6	F	110	LYS	2.2
4	Q	82	MET	2.2
8	H	71	HIS	2.2
8	U	34	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
9	V	68	VAL	2.2
4	Q	227	TRP	2.2
6	S	70	MET	2.2
1	A	186	LEU	2.2
5	E	153	PHE	2.2
3	P	207	ASN	2.2
1	N	221	GLY	2.2
2	B	97	SER	2.2
1	A	124	ASP	2.2
3	P	66	VAL	2.2
9	I	58	GLN	2.2
1	A	127	ILE	2.2
5	E	91	TRP	2.2
7	T	34	ILE	2.2
3	P	102	LEU	2.2
10	W	3	PRO	2.2
5	R	5	ILE	2.1
5	E	27	GLU	2.1
9	I	42	VAL	2.1
4	Q	80	MET	2.1
6	S	15	GLY	2.1
1	A	129	LYS	2.1
4	Q	214	LEU	2.1
9	V	77	ARG	2.1
2	O	249	GLY	2.1
9	V	76	VAL	2.1
8	U	49	GLN	2.1
2	B	411	ILE	2.1
2	O	302	GLY	2.1
3	P	210	GLY	2.1
4	D	214	LEU	2.1
10	J	9	LEU	2.1
10	J	22	LEU	2.1
3	P	224	TYR	2.1
1	N	6	GLN	2.1
2	B	439	LEU	2.1
3	C	102	LEU	2.1
3	P	28	SER	2.1
5	E	115	SER	2.1
9	I	34	VAL	2.1
8	H	45	SER	2.0
1	A	188	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	401	GLN	2.0
5	E	113	GLU	2.0
9	V	52	ARG	2.0
6	F	16	ILE	2.0
2	B	307	PHE	2.0
3	C	31	TRP	2.0
5	E	100	HIS	2.0
2	O	236	LYS	2.0
3	C	130	GLY	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
15	GOL	B	2013	6/6	0.09	0.93	145,148,148,149	0
11	JZR	A	4002	18/18	0.28	0.63	130,143,145,145	0
11	JZR	F	4001	18/18	0.30	0.52	168,171,173,173	0
11	JZR	S	2011	18/18	0.31	0.42	73,86,91,91	0
15	GOL	O	3013	6/6	0.35	0.66	112,115,116,116	0
12	AZI	P	3014	3/3	0.41	0.42	54,54,55,61	0
11	JZR	C	2008	18/18	0.46	0.42	109,112,116,116	0
11	JZR	F	3011	18/18	0.49	0.59	114,118,122,122	0
12	AZI	C	2014	3/3	0.52	0.38	53,53,57,59	0
12	AZI	D	4004	3/3	0.53	0.30	69,69,72,73	0
11	JZR	P	3008	18/18	0.57	0.40	100,102,107,109	0
13	PEE	G	2005	49/51	0.62	0.43	105,123,129,129	0
13	PEE	A	4003	6/51	0.68	0.31	110,111,112,113	0
13	PEE	T	3005	49/51	0.71	0.53	96,121,136,136	0

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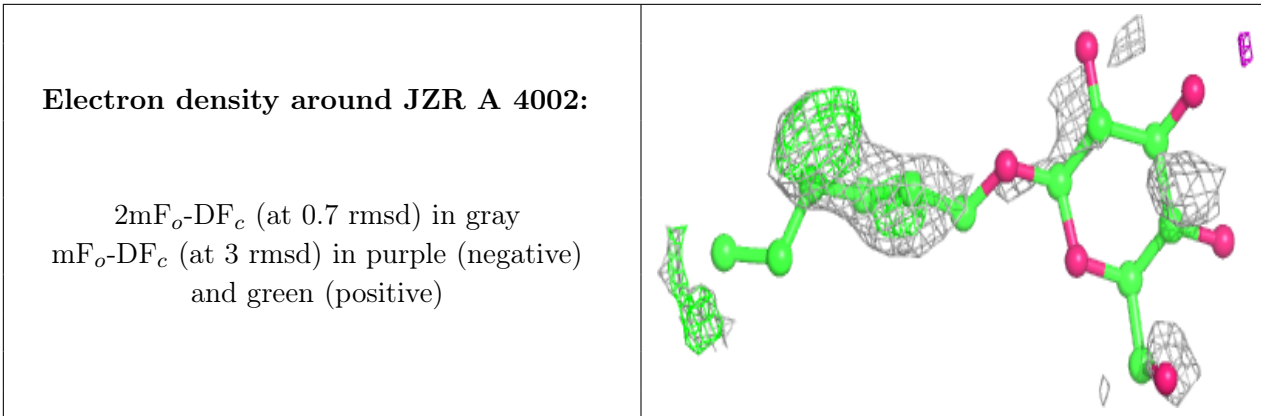
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	UQ	P	3002	14/63	0.71	0.37	90,93,97,97	0
13	PEE	C	2012	5/51	0.73	0.26	116,116,116,116	0
21	CDL	G	2003	50/100	0.74	0.27	62,96,113,113	0
13	PEE	N	3012	5/51	0.77	0.20	94,94,94,96	0
18	UQ	C	2002	14/63	0.77	0.28	74,78,80,82	0
12	AZI	A	4005	3/3	0.79	0.32	72,72,73,74	0
15	GOL	P	3009	6/6	0.80	0.35	59,65,67,68	0
15	GOL	C	2009	6/6	0.85	0.40	56,59,63,67	0
21	CDL	Q	3003	50/100	0.85	0.21	55,78,90,92	0
14	PO4	B	3010	5/5	0.86	0.16	99,100,100,100	0
21	CDL	T	3004	49/100	0.87	0.26	54,69,98,101	0
13	PEE	C	2007	49/51	0.88	0.25	39,53,68,69	0
21	CDL	G	2004	44/100	0.88	0.25	62,79,105,107	0
13	PEE	D	2006	51/51	0.90	0.21	52,66,94,95	0
13	PEE	Q	3006	51/51	0.91	0.18	45,59,83,83	0
14	PO4	O	2010	5/5	0.92	0.11	106,106,107,108	0
17	SMA	P	3001	37/37	0.92	0.15	24,32,37,37	0
13	PEE	P	3007	49/51	0.93	0.22	35,54,62,63	0
17	SMA	C	2001	37/37	0.94	0.13	25,30,32,38	0
16	HEM	P	502	43/43	0.97	0.14	24,27,32,37	0
19	HEC	D	501	43/43	0.97	0.12	29,33,36,38	0
20	FES	E	501	4/4	0.98	0.10	34,35,37,37	0
16	HEM	C	501	43/43	0.98	0.14	21,26,33,37	0
16	HEM	C	502	43/43	0.98	0.13	22,26,31,33	0
16	HEM	P	501	43/43	0.98	0.14	25,29,37,42	0
19	HEC	Q	501	43/43	0.98	0.10	32,35,36,37	0
20	FES	R	501	4/4	0.99	0.09	31,31,33,33	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.

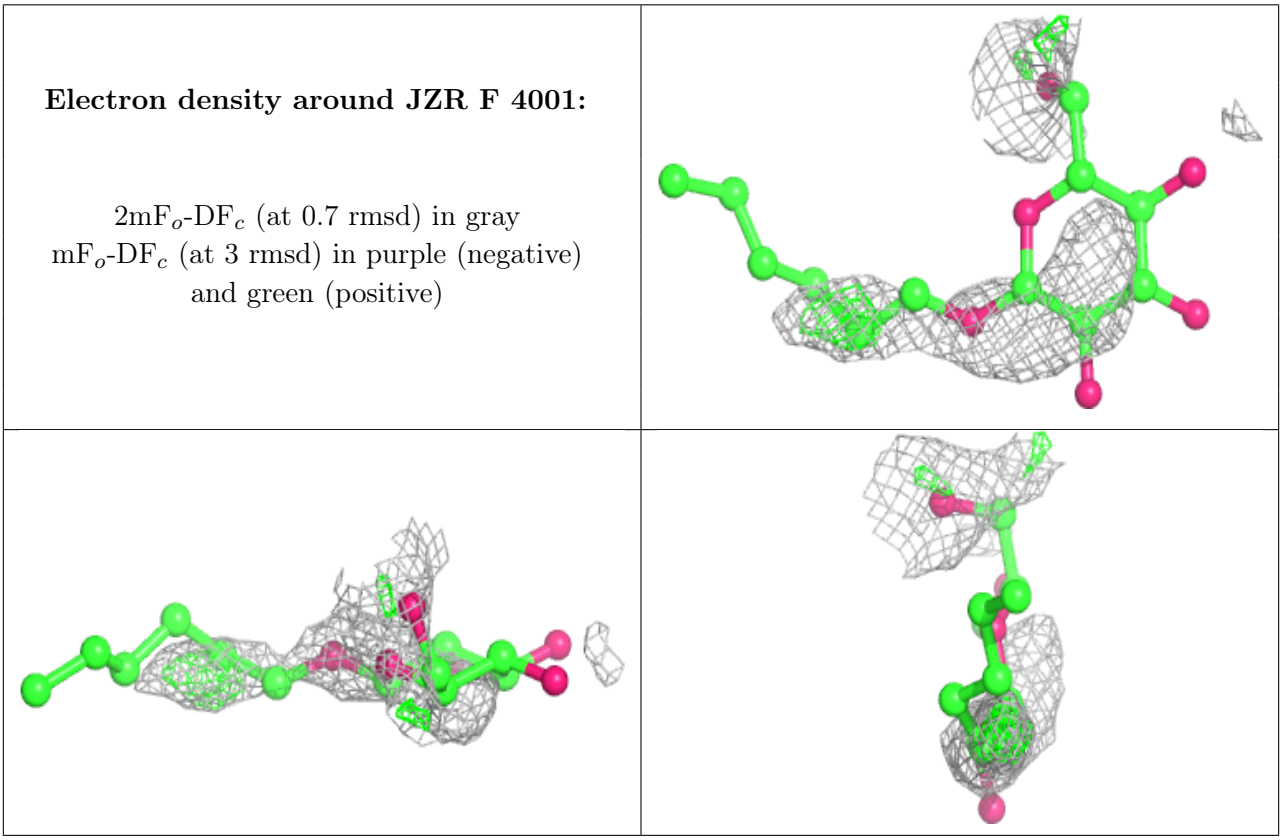
Electron density around JZR A 4002:

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



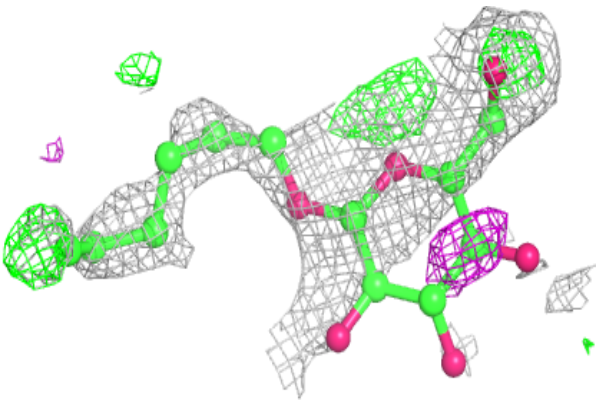
Electron density around JZR F 4001:

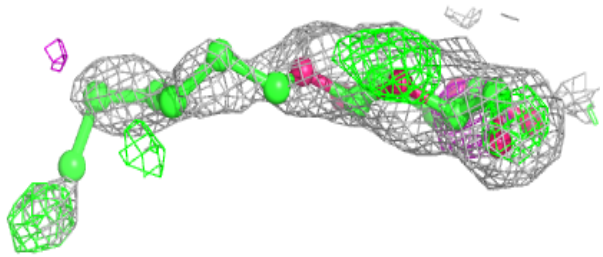
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

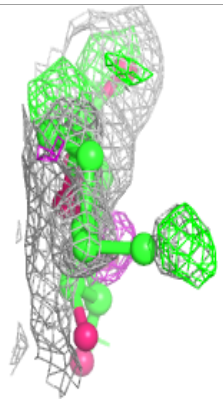


Electron density around JZR S 2011:

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

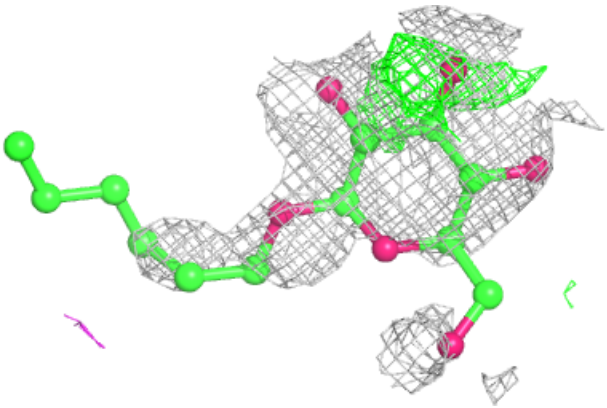


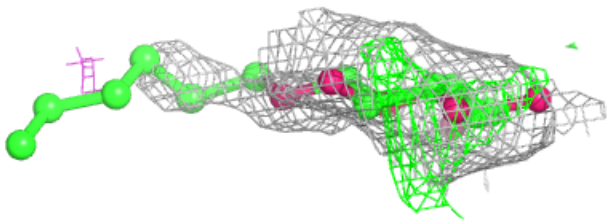


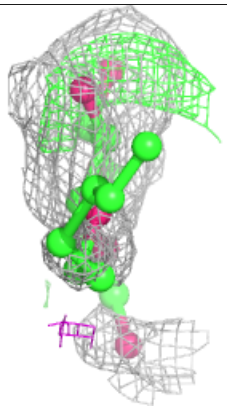


Electron density around JZR C 2008:

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

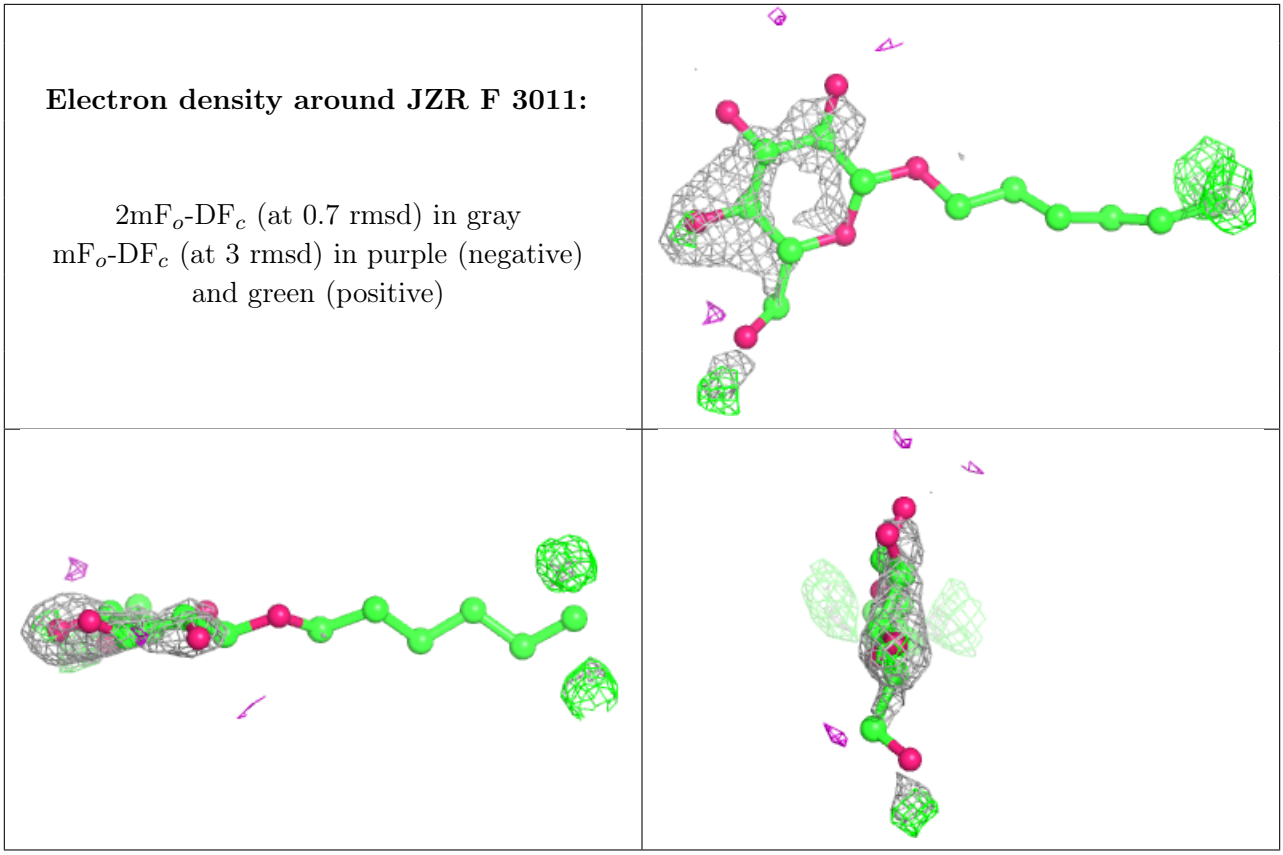






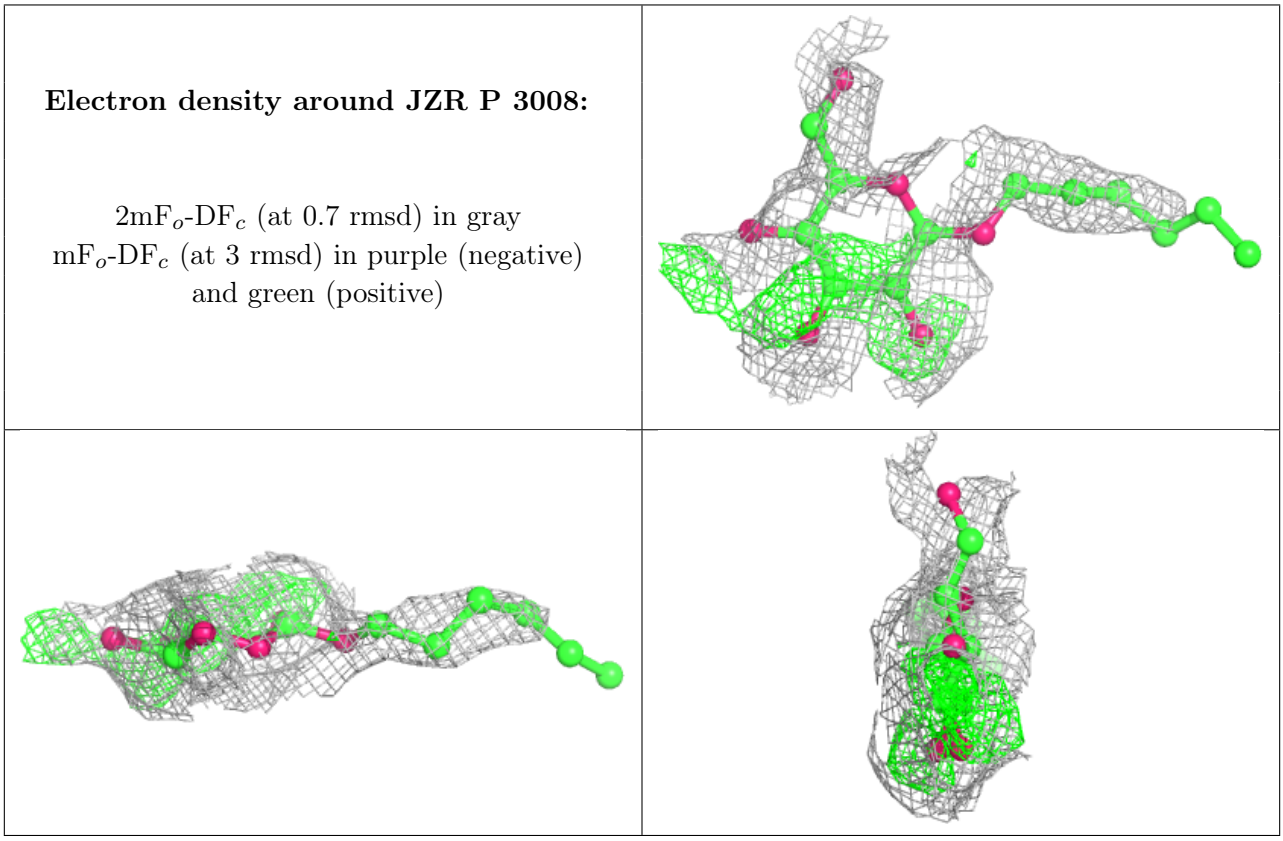
Electron density around JZR F 3011:

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



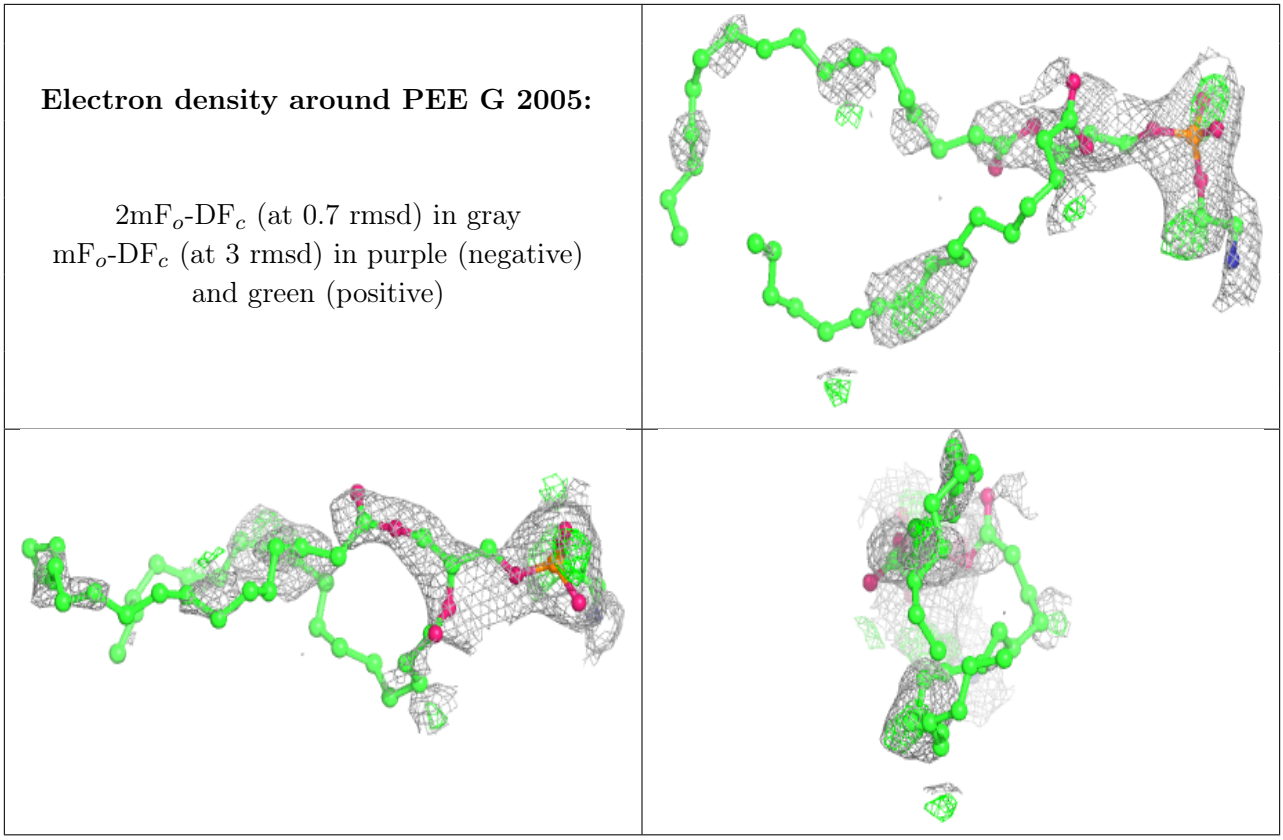
Electron density around JZR P 3008:

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



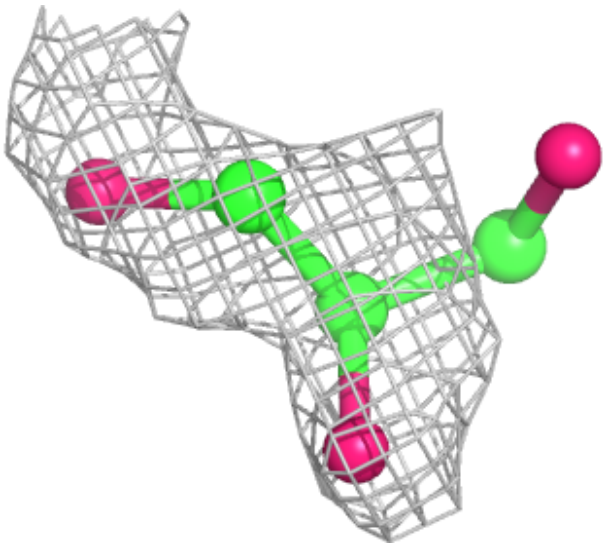
Electron density around PEE G 2005:

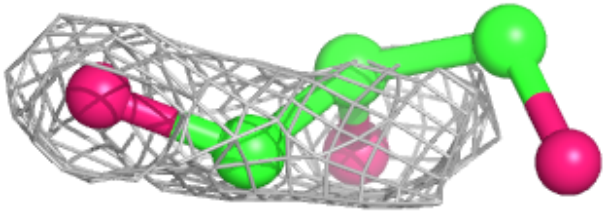
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

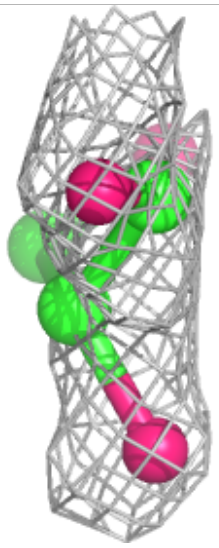


Electron density around PEE A 4003:

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

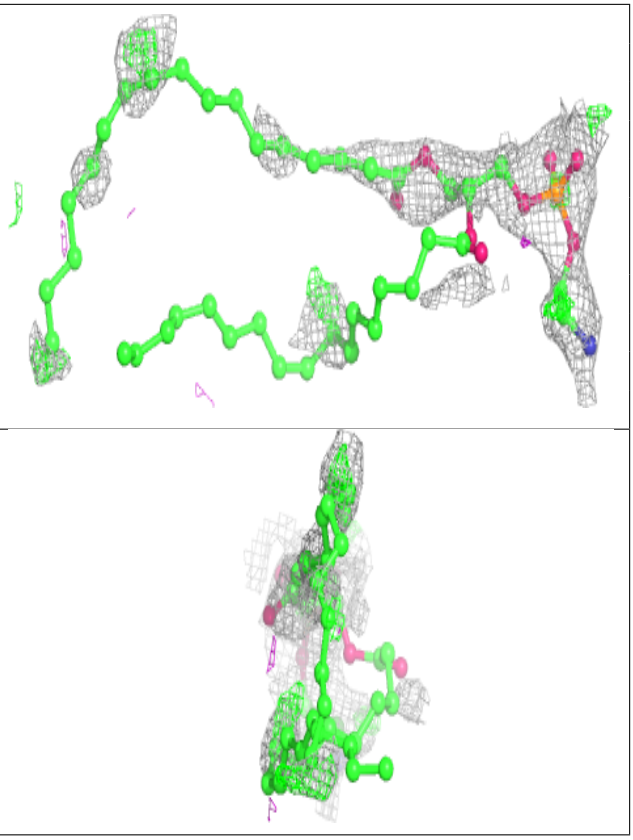


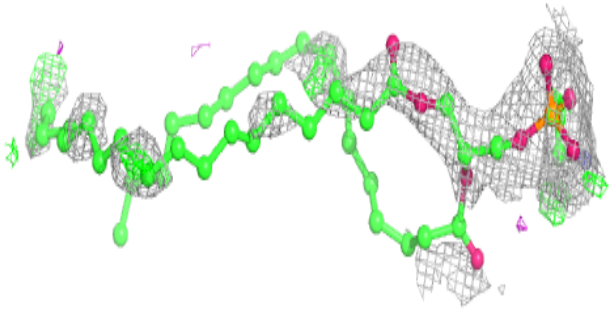




Electron density around PEE T 3005:

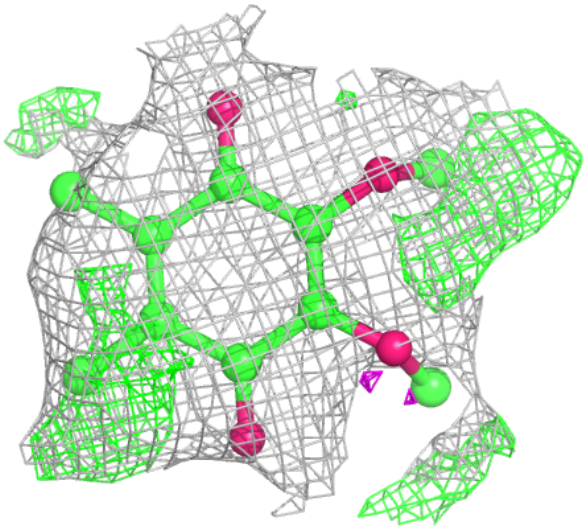
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

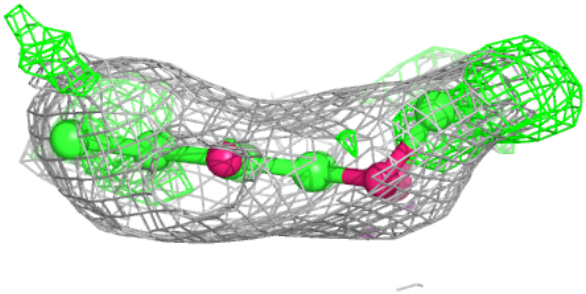


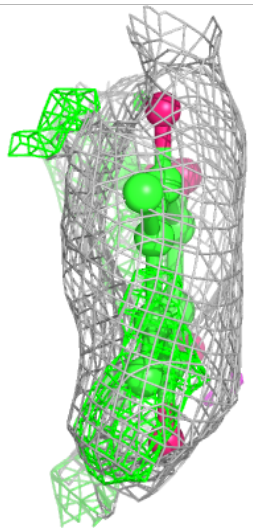


Electron density around UQ P 3002:

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

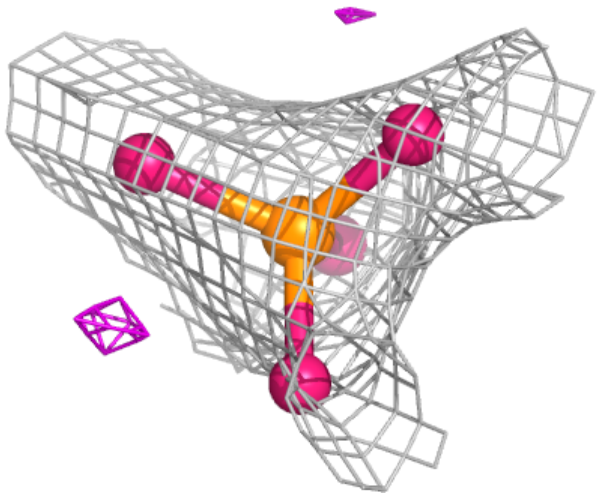


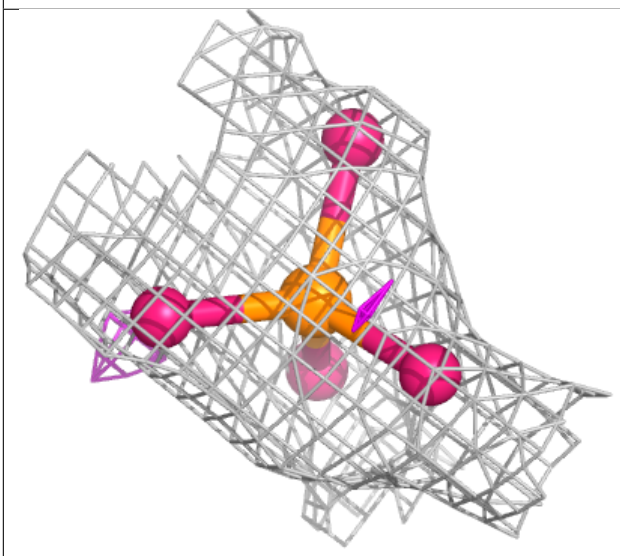


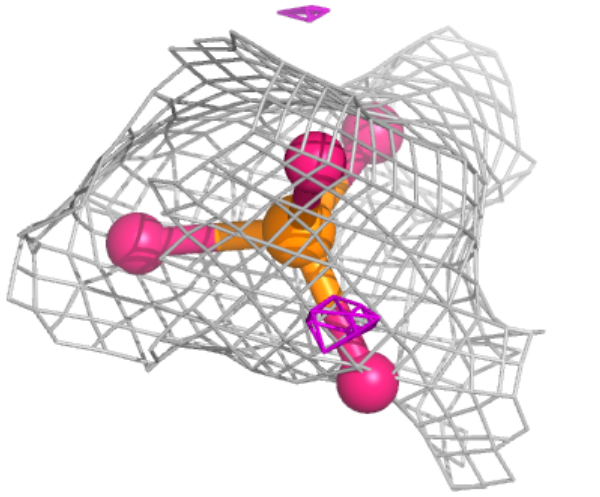


Electron density around PEE C 2012:

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

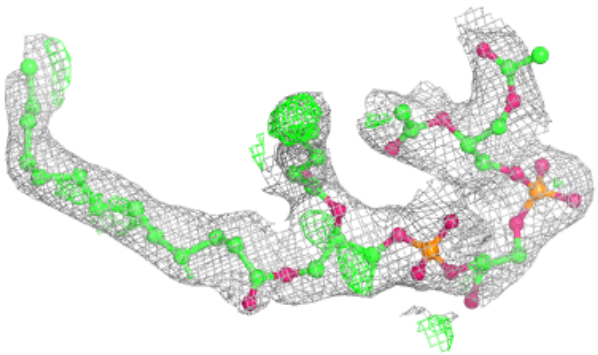


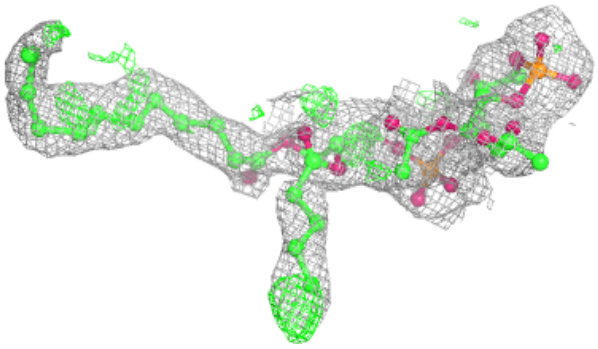


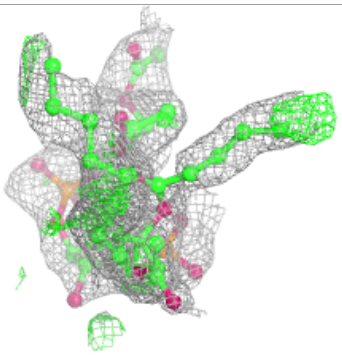


Electron density around CDL G 2003:

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

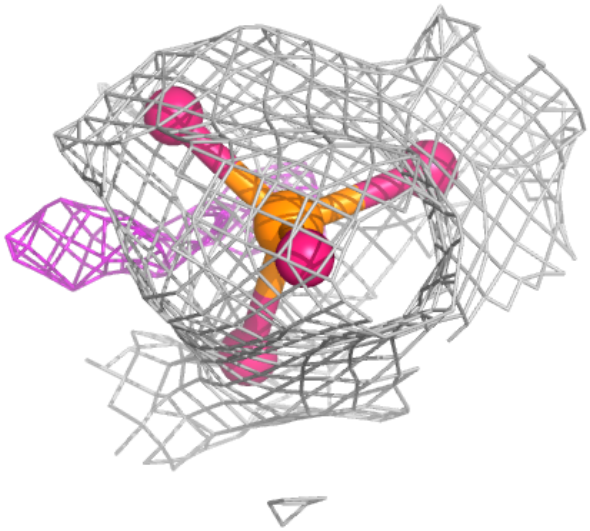


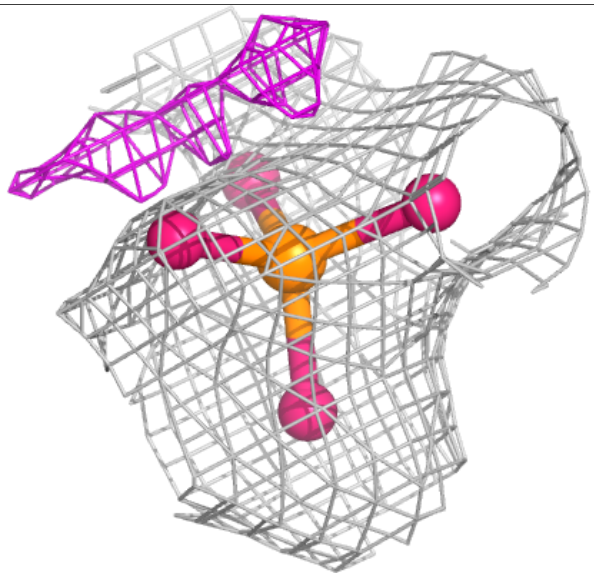


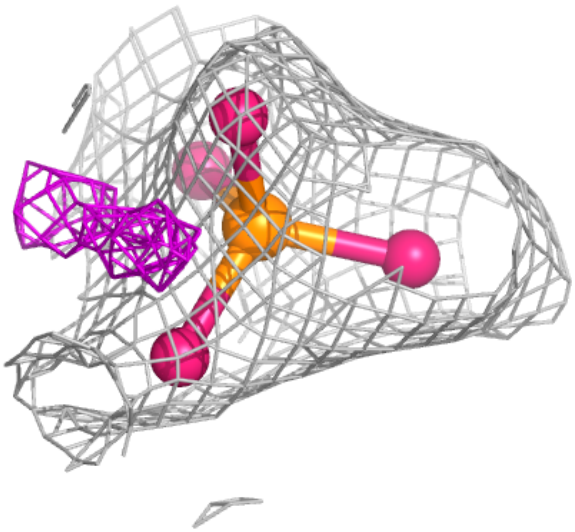


Electron density around PEE N 3012:

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

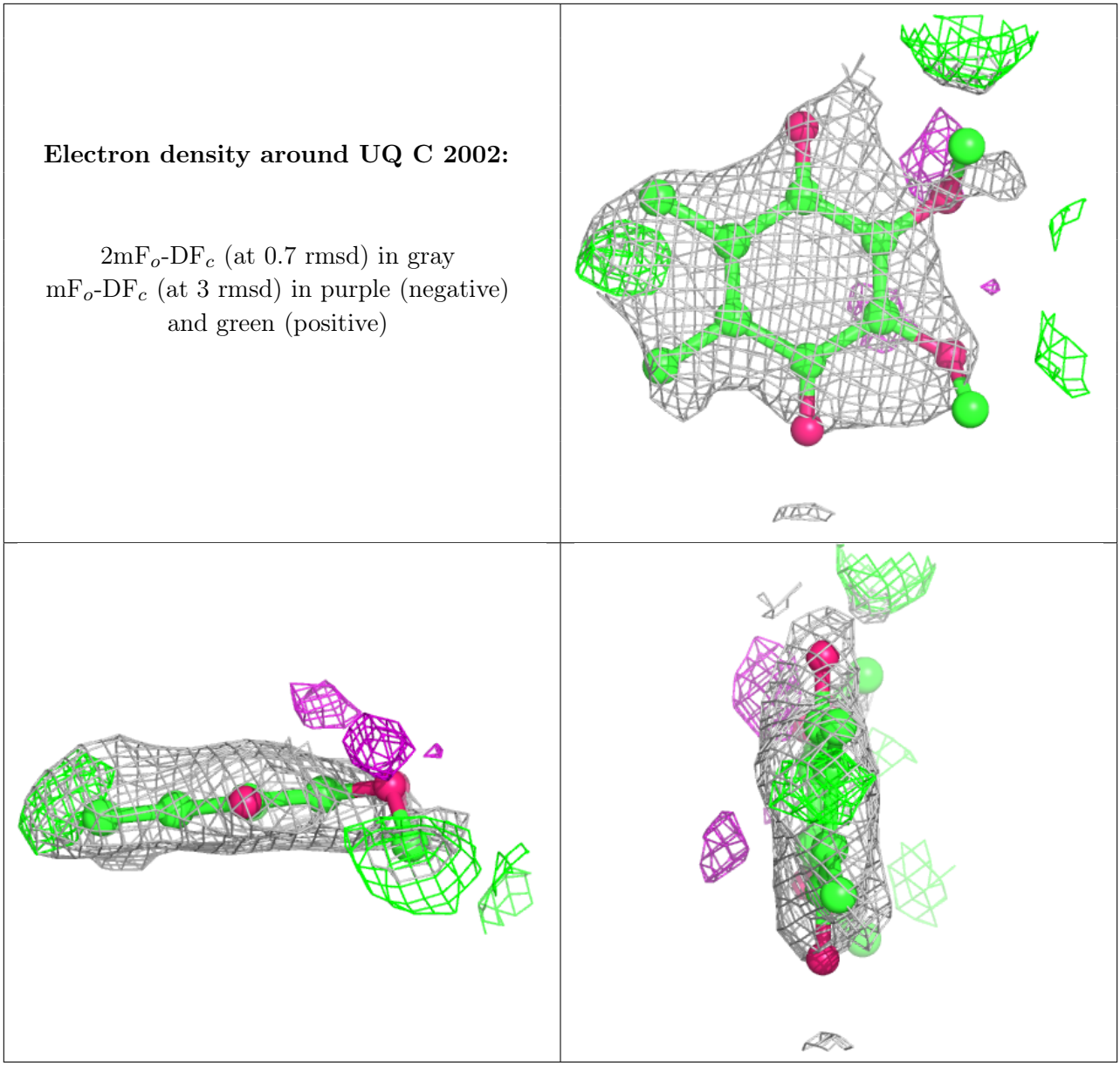






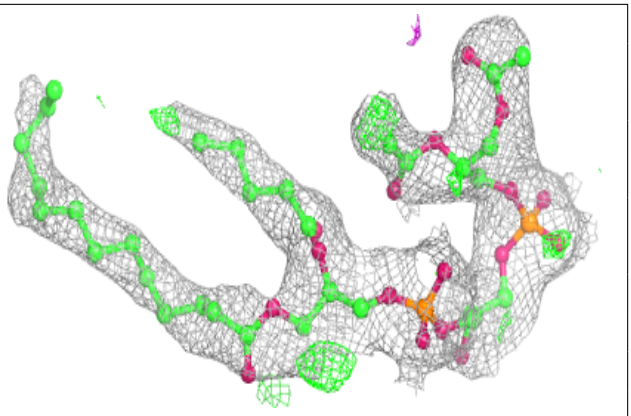
Electron density around UQ C 2002:

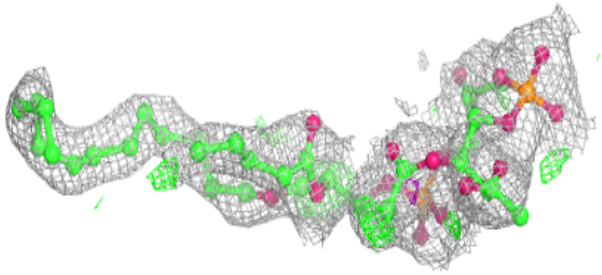
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

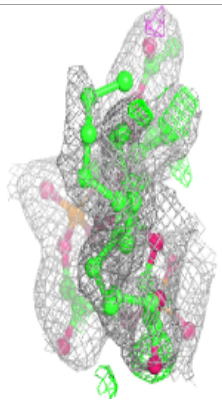


Electron density around CDL Q 3003:

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

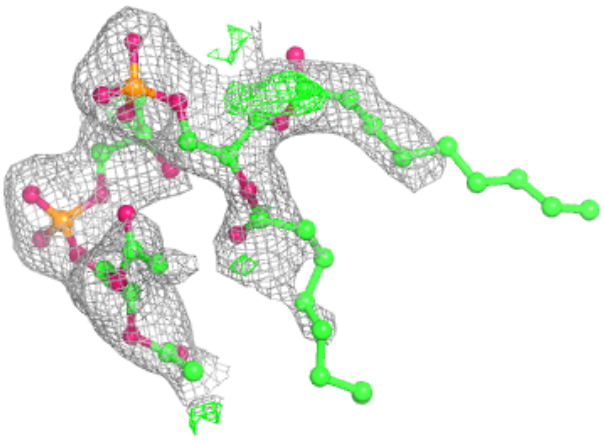


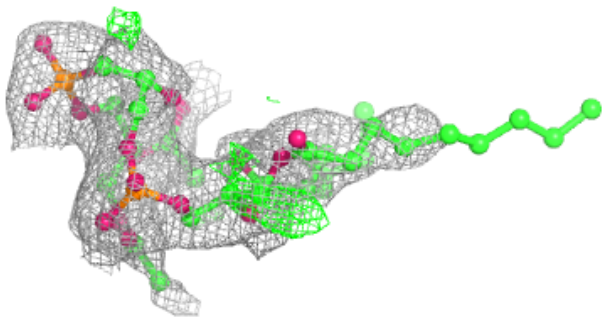


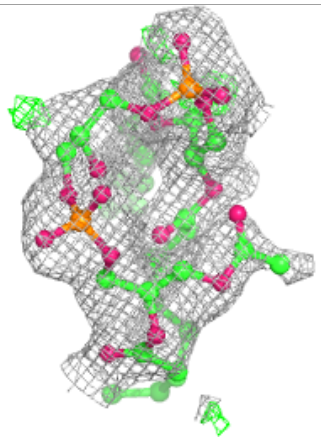


Electron density around CDL T 3004:

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

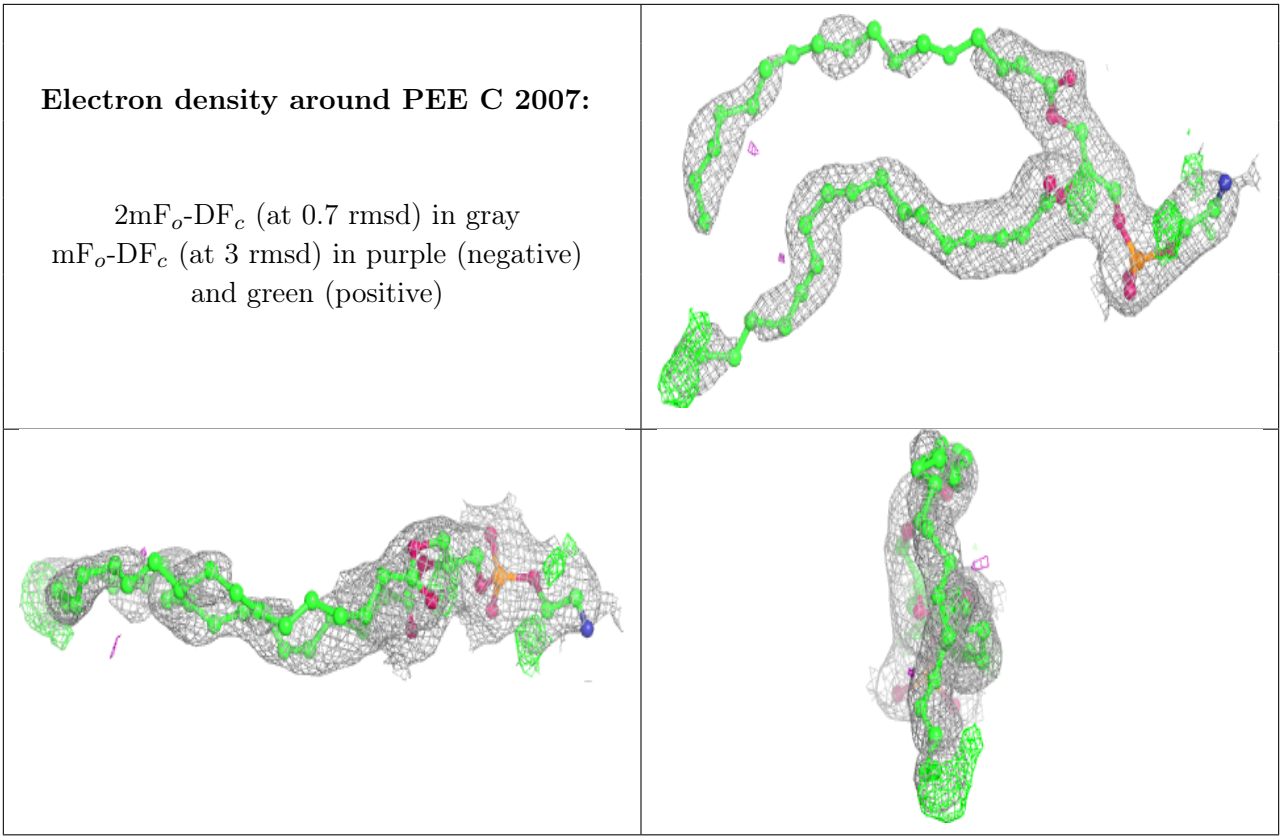






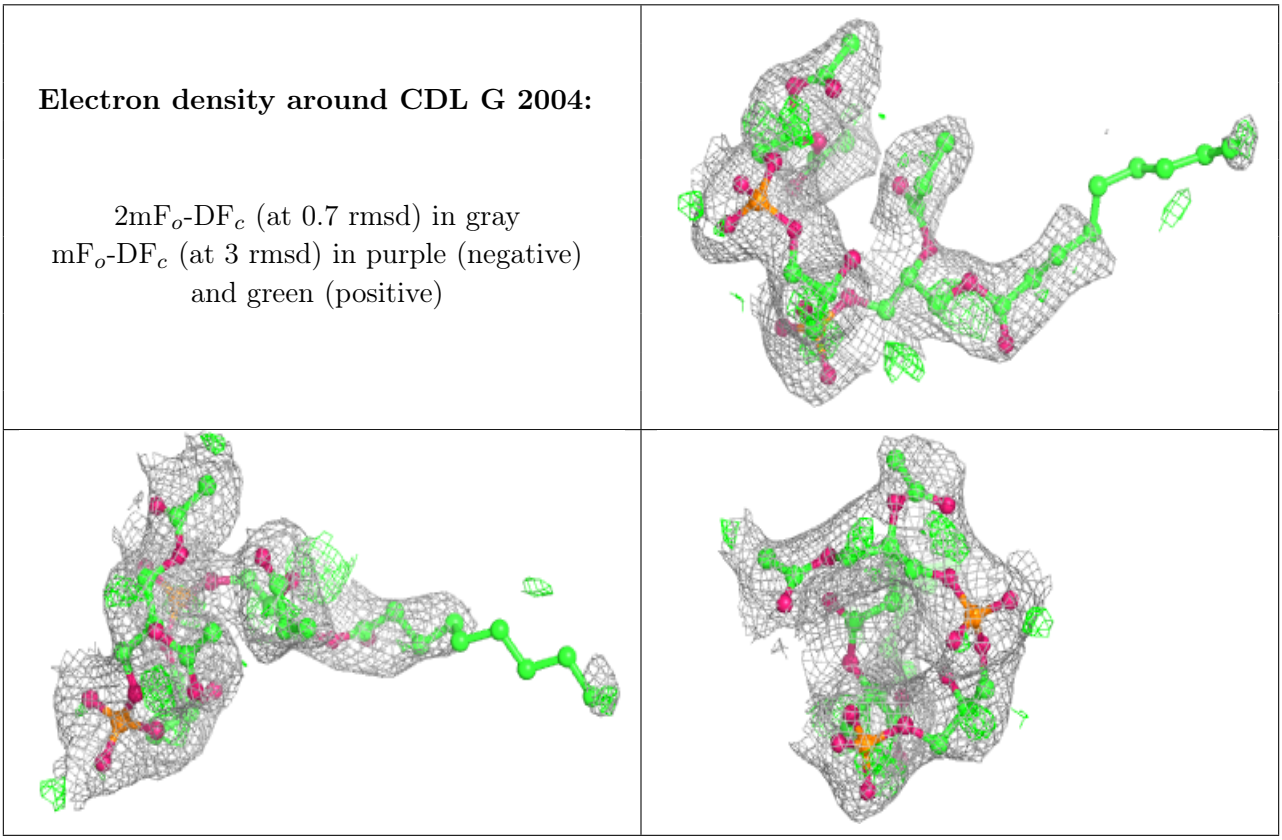
Electron density around PEE C 2007:

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



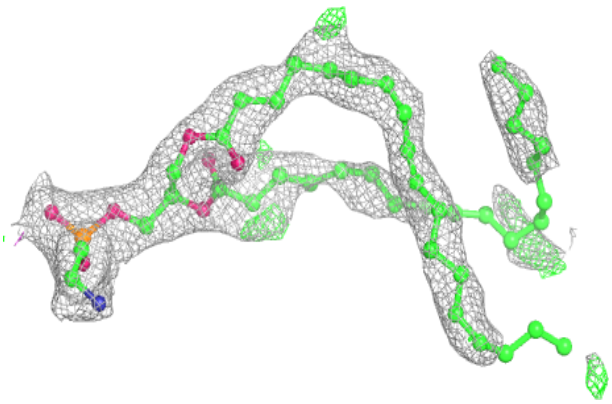
Electron density around CDL G 2004:

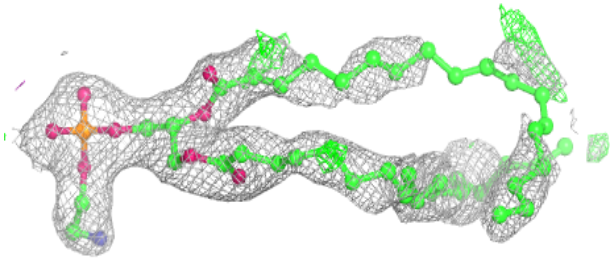
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

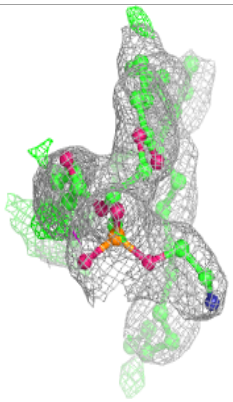


Electron density around PEE D 2006:

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

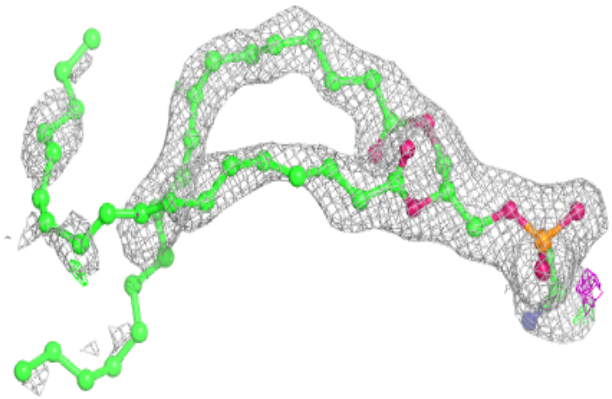


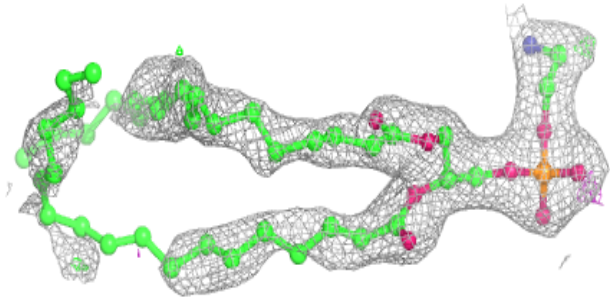


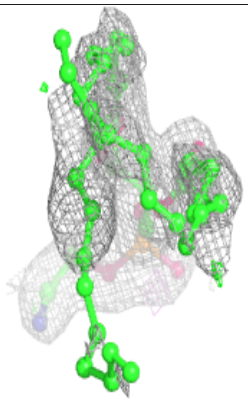


Electron density around PEE Q 3006:

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

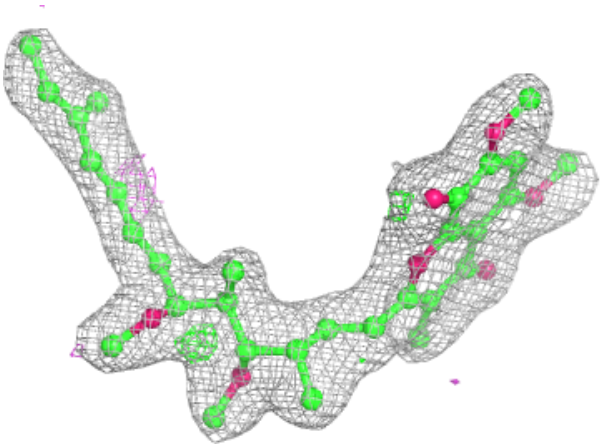


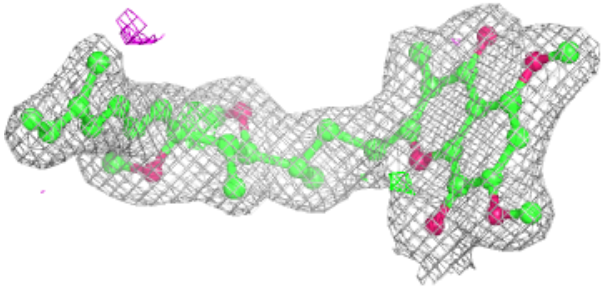


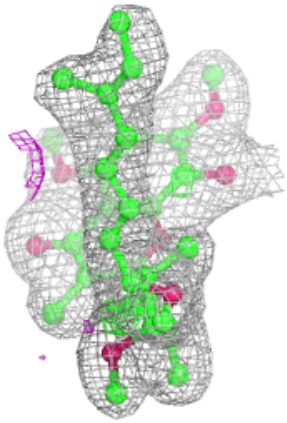


Electron density around SMA P 3001:

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

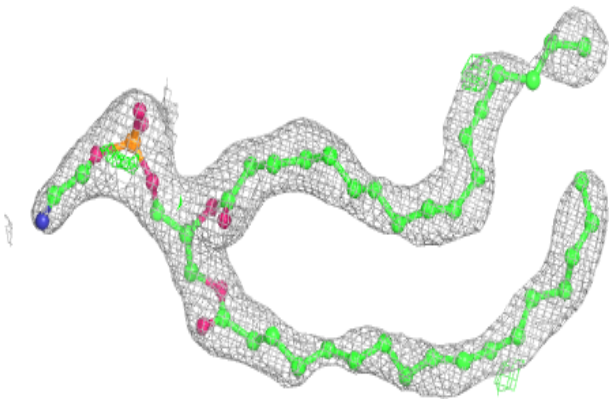


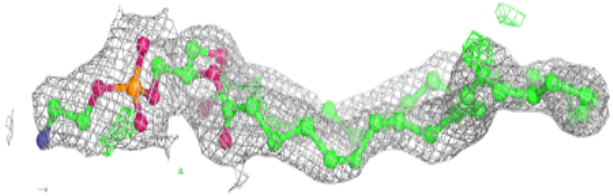


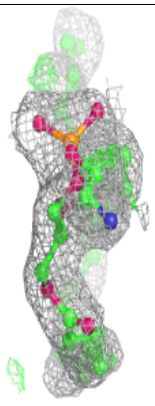


Electron density around PEE P 3007:

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

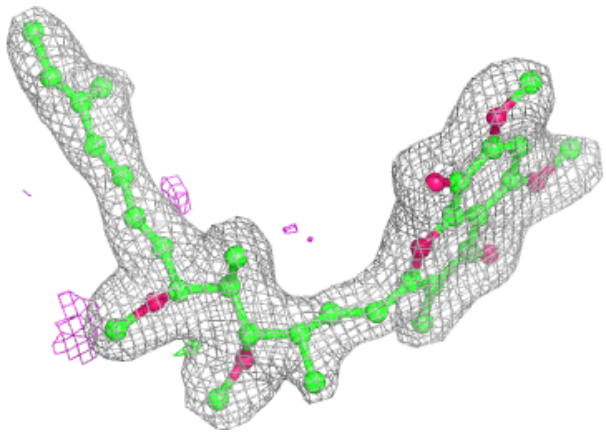


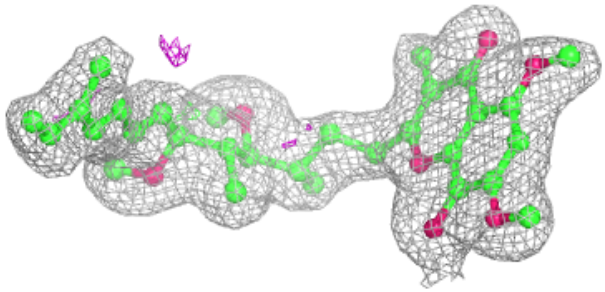




Electron density around SMA C 2001:

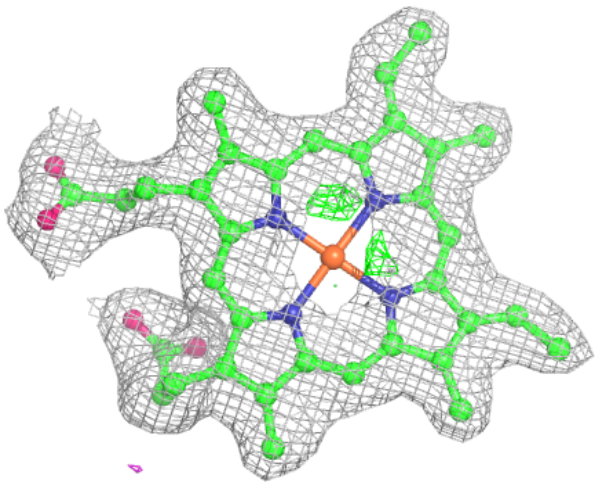
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

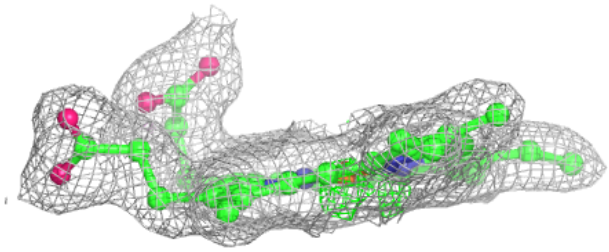


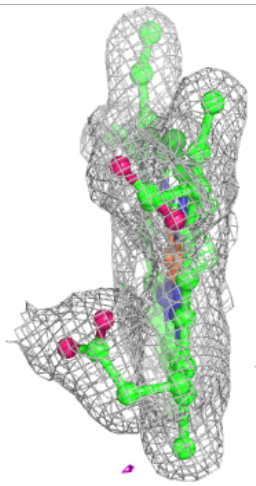


Electron density around HEM P 502:

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

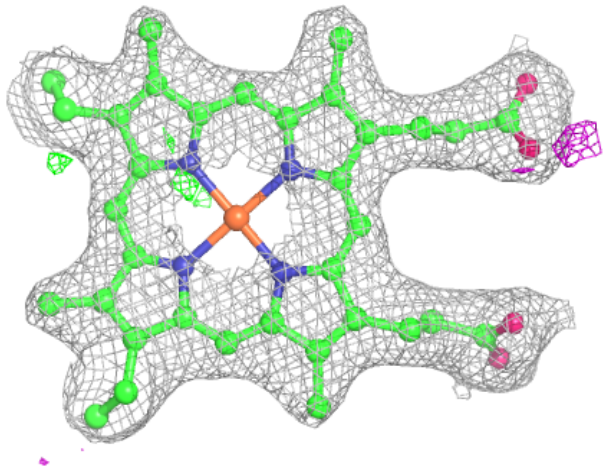


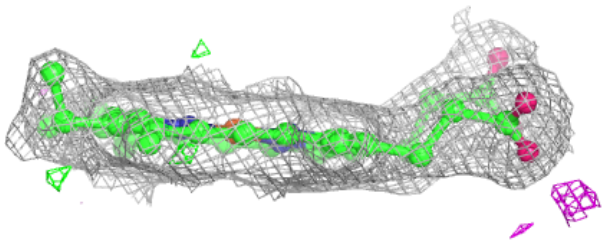


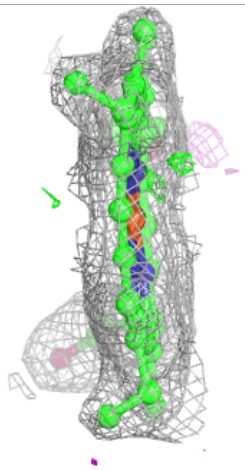


Electron density around HEC D 501:

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

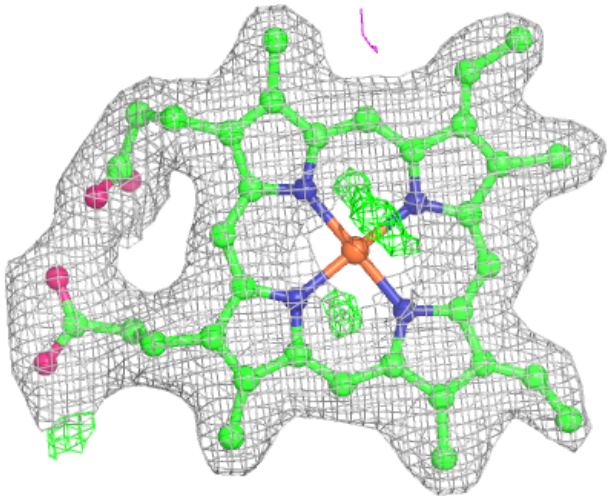


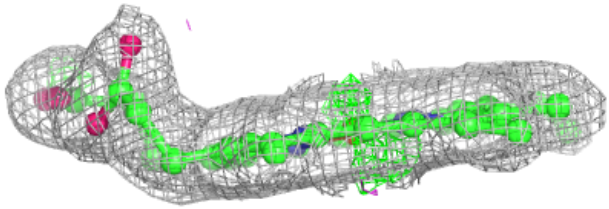


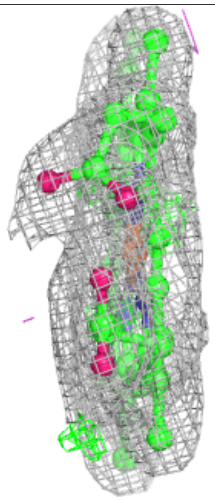


Electron density around HEM C 501:

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

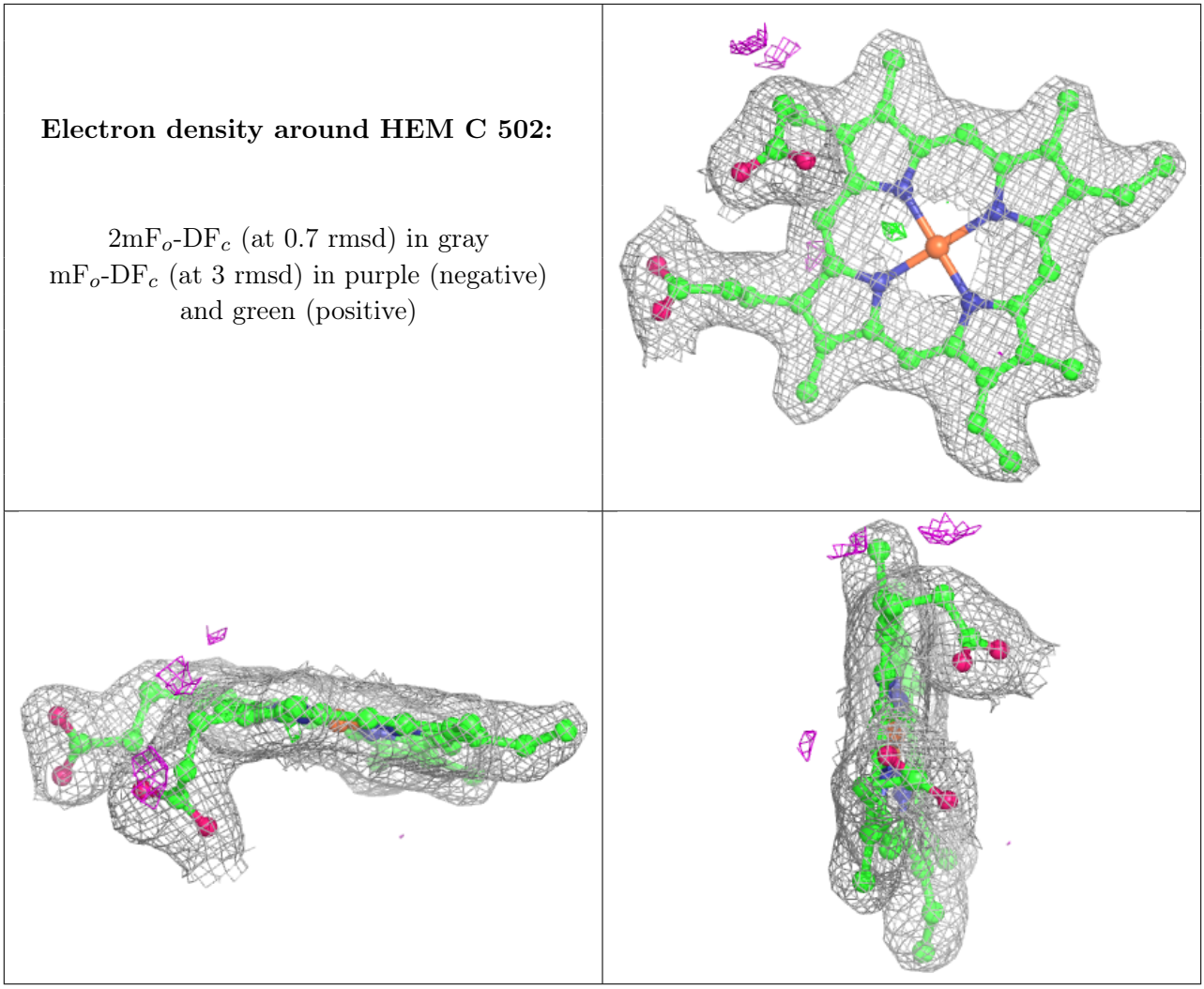






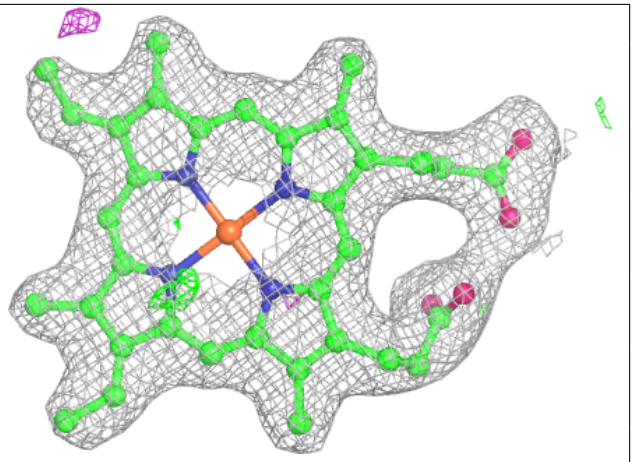
Electron density around HEM C 502:

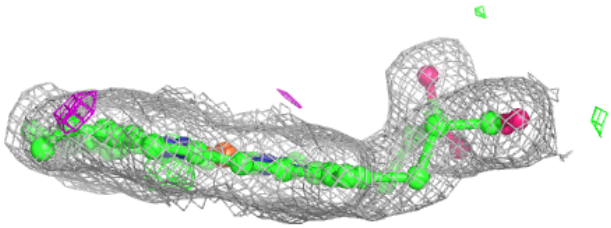
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

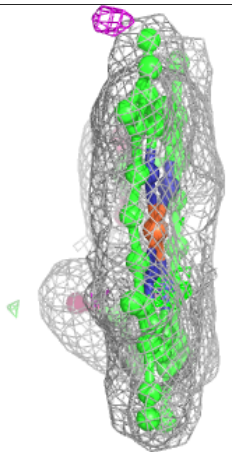


Electron density around HEM P 501:

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

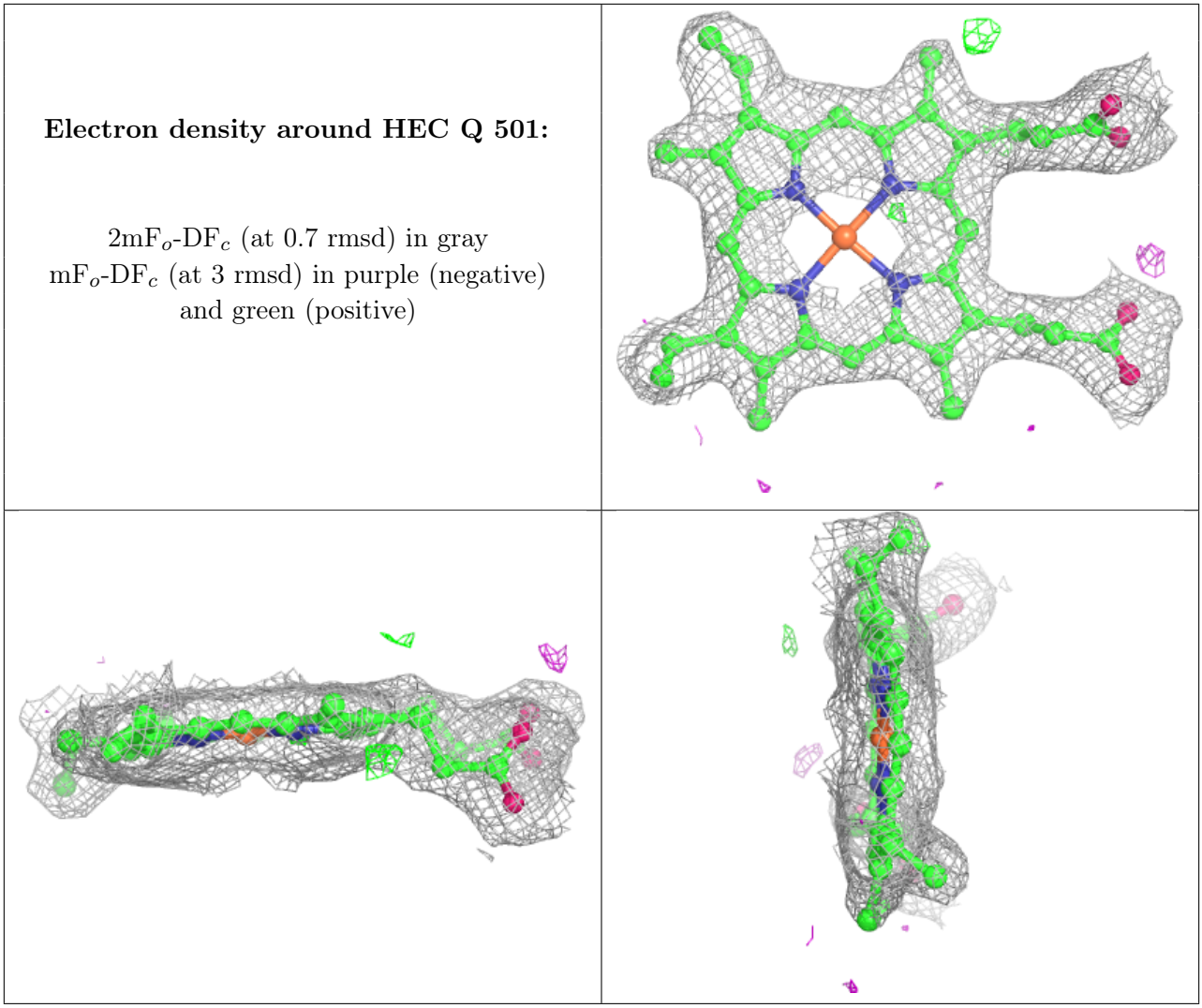






Electron density around HEC Q 501:

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



6.5 Other polymers

There are no such residues in this entry.