Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 06:34 AM EDT

PDB ID	:	3L70
Title	:	Cytochrome BC1 complex from chicken with trifloxystrobin bound
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-27
Resolution	:	2.75 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:

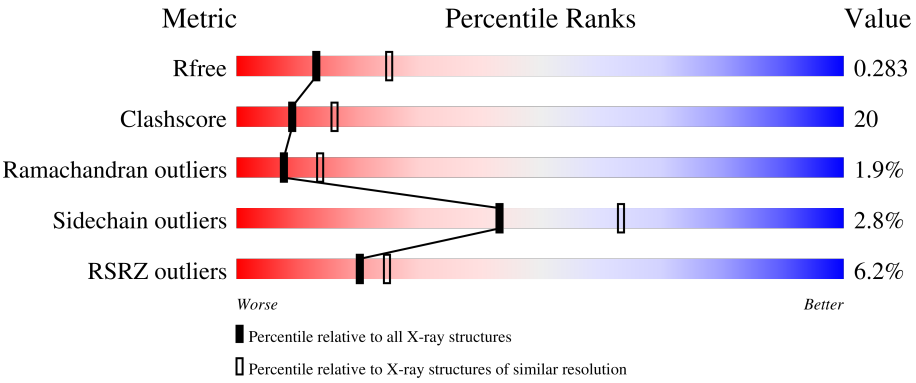
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	446	2% 64% 33% ·
1	N	446	2% 61% 35% · ·
2	B	441	4% 54% 38% · 5%
2	O	441	4% 57% 35% · ·
3	C	380	% 75% 24% ·

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Mol	Chain	Length	Quality of chain
3	P	380	2% 73% 26%
4	D	241	% 74% 25%
4	Q	241	5% 70% 29%
5	E	196	38% 48% 44% 8%
5	R	196	13% 56% 40%
6	F	110	65% 25% 8%
6	S	110	4% 62% 27% 8%
7	G	81	2% 60% 35%
7	T	81	15% 57% 37%
8	H	77	3% 68% 23% 9%
8	U	77	17% 61% 25% 13%
9	I	47	26% 43% 49% 6%
9	V	47	36% 38% 51% 9%
10	J	61	7% 74% 25%
10	W	61	5% 67% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEE	N	3008	-	X	-	-
11	PEE	R	3005	-	-	-	X
18	BOG	D	2091	-	-	-	X
18	BOG	Q	3091	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 32653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3447	2160	607	659	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3133	1968	544	612	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

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

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

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

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein.

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

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

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

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

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

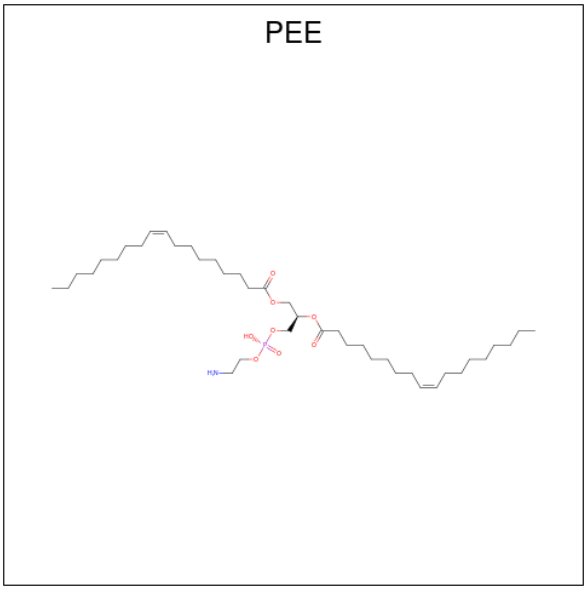
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	43	Total	C	N	O	S	0	0	0
			277	167	55	53	2			

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

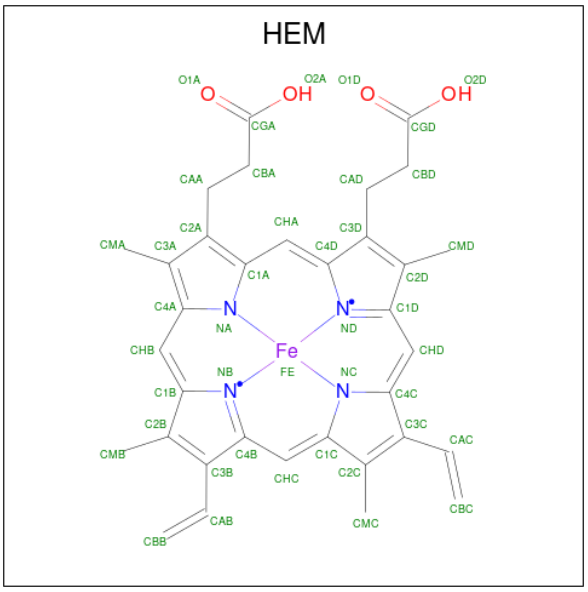
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	61	Total C N O 497 321 87 89	0	0	0
10	W	60	Total C N O 479 311 86 82	0	0	1

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



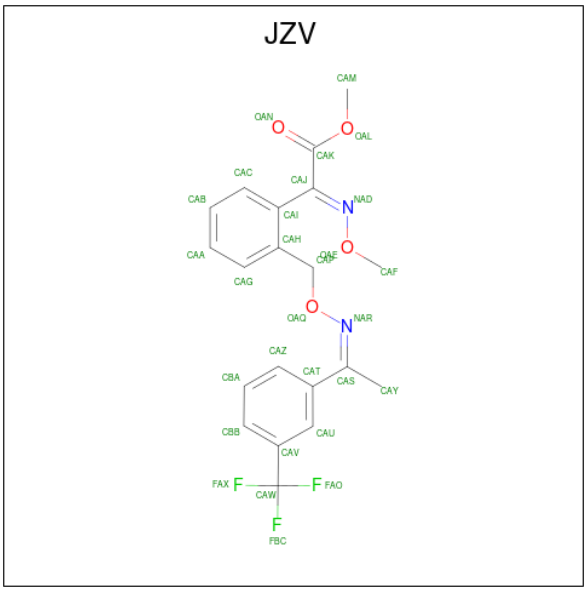
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O P 21 12 8 1	0	0
11	C	1	Total C N O P 49 39 1 8 1	0	0
11	E	1	Total C N O P 50 40 1 8 1	0	0
11	N	1	Total O P 5 4 1	0	0
11	P	1	Total C N O P 49 39 1 8 1	0	0
11	R	1	Total C N O P 50 40 1 8 1	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



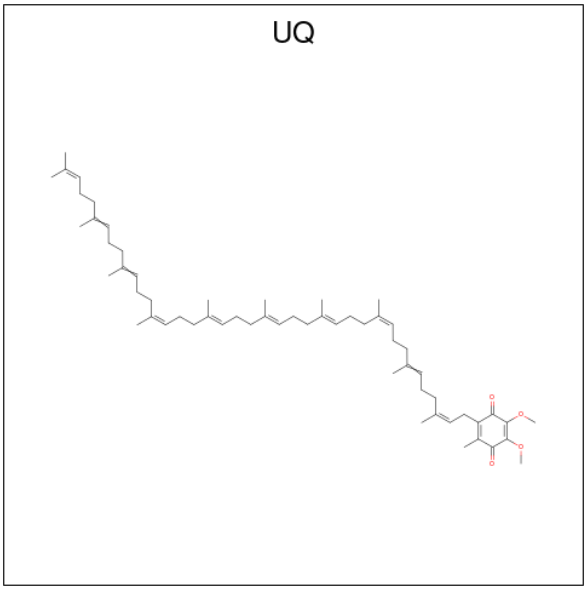
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is methyl (2E)-(methoxyimino)(2-{[({(1Z)-1-[3-(trifluoromethyl)phenyl]ethylidene}amino)oxy]methyl}phenyl)ethanoate (three-letter code: JZV) (formula: $C_{20}H_{19}F_3N_2O_4$).



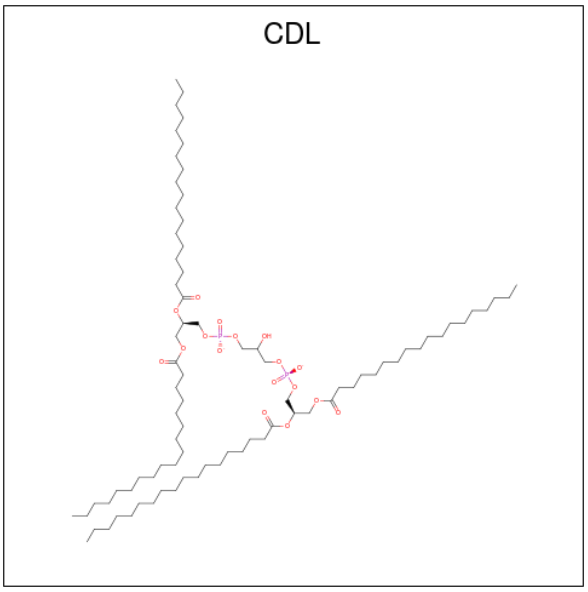
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	0	0
			29	20	3	2	4		
13	P	1	Total	C	F	N	O	0	0
			29	20	3	2	4		

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



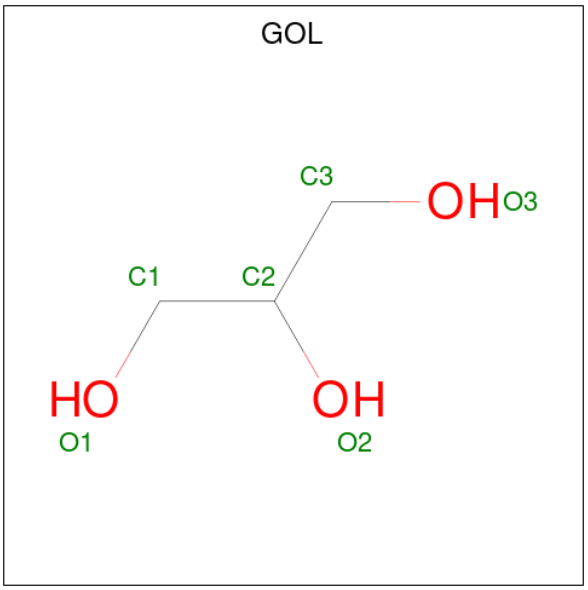
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



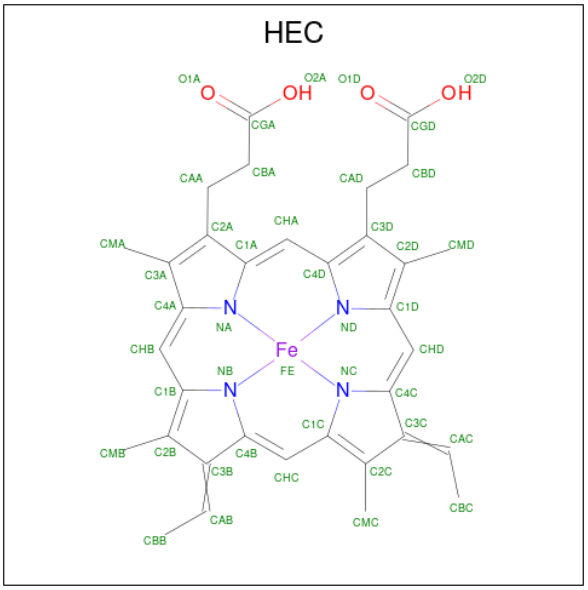
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O	P	0	0
			40	21	17	2		
15	D	1	Total	C	O	P	0	0
			42	23	17	2		
15	P	1	Total	C	O	P	0	0
			40	21	17	2		
15	Q	1	Total	C	O	P	0	0
			42	23	17	2		

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



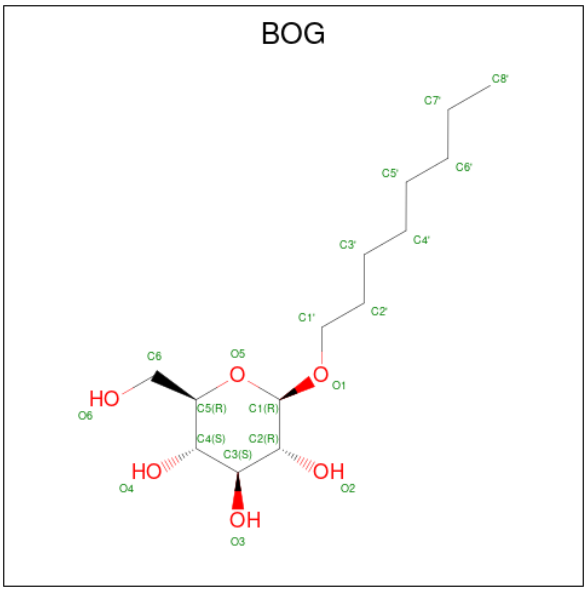
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 6 3 3	0	0
16	P	1	Total C O 6 3 3	0	0

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



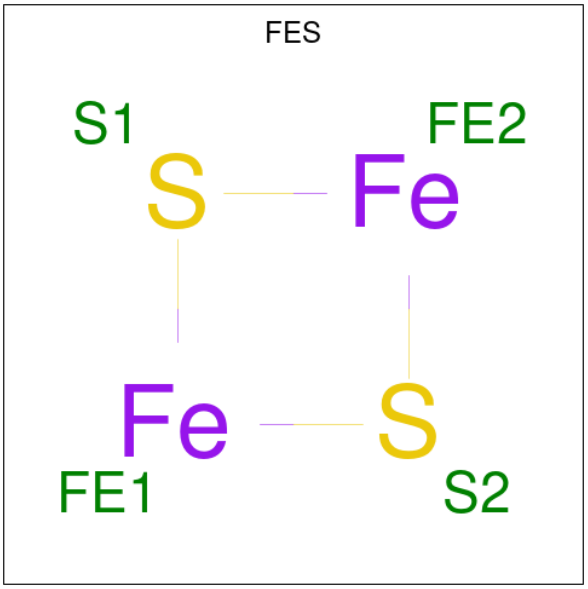
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	D	1	Total C Fe N O 43 34 1 4 4	0	0
17	Q	1	Total C Fe N O 43 34 1 4 4	0	0

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



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

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



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

- Molecule 20 is water.

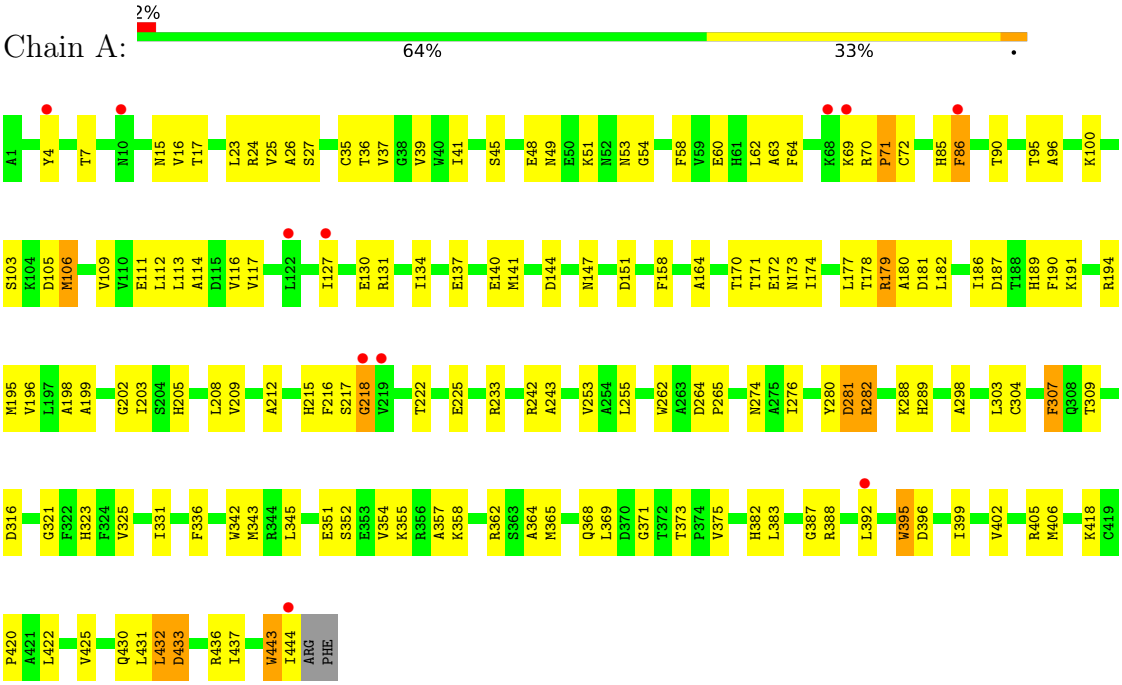
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	8	Total O 8 8	0	0
20	E	1	Total O 1 1	0	0
20	P	9	Total O 9 9	0	0
20	R	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

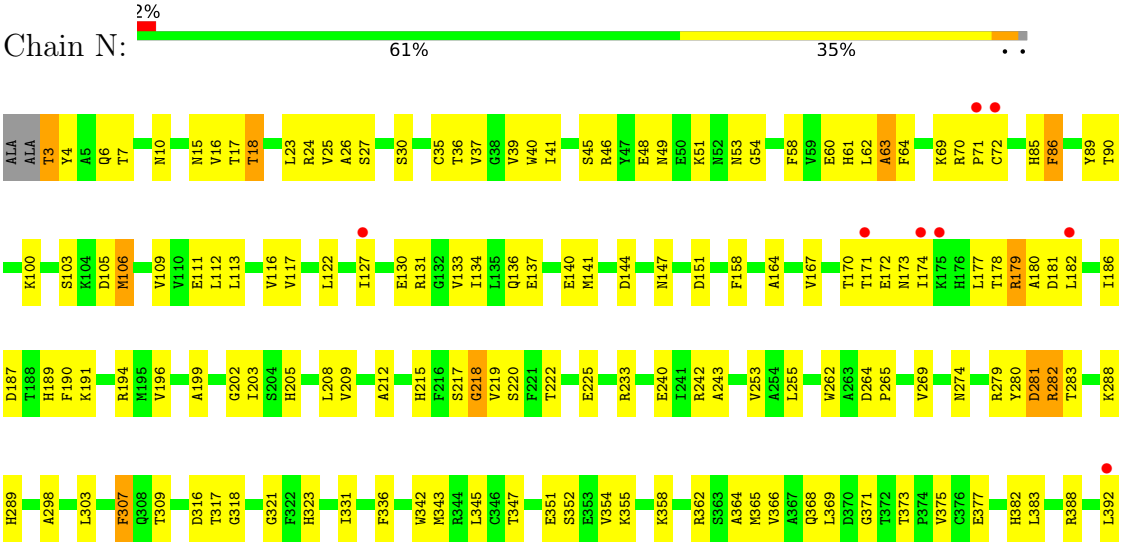
• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

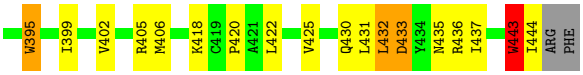
Chain A:



• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

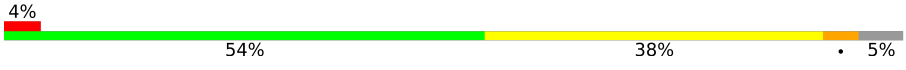
Chain N:

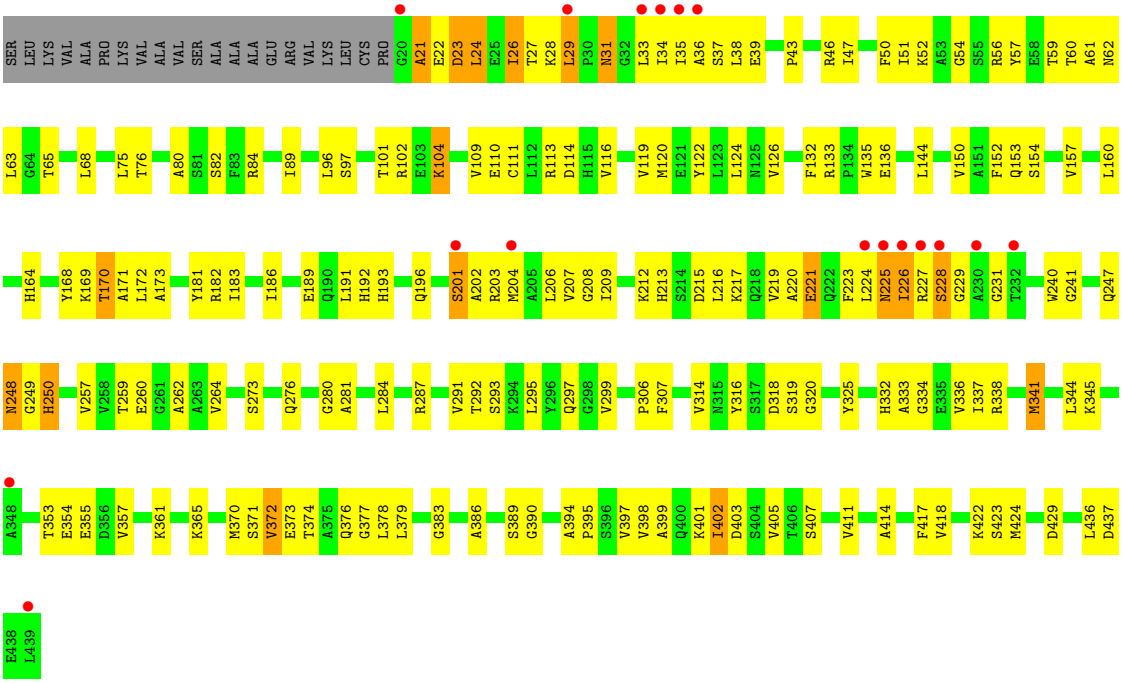




• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

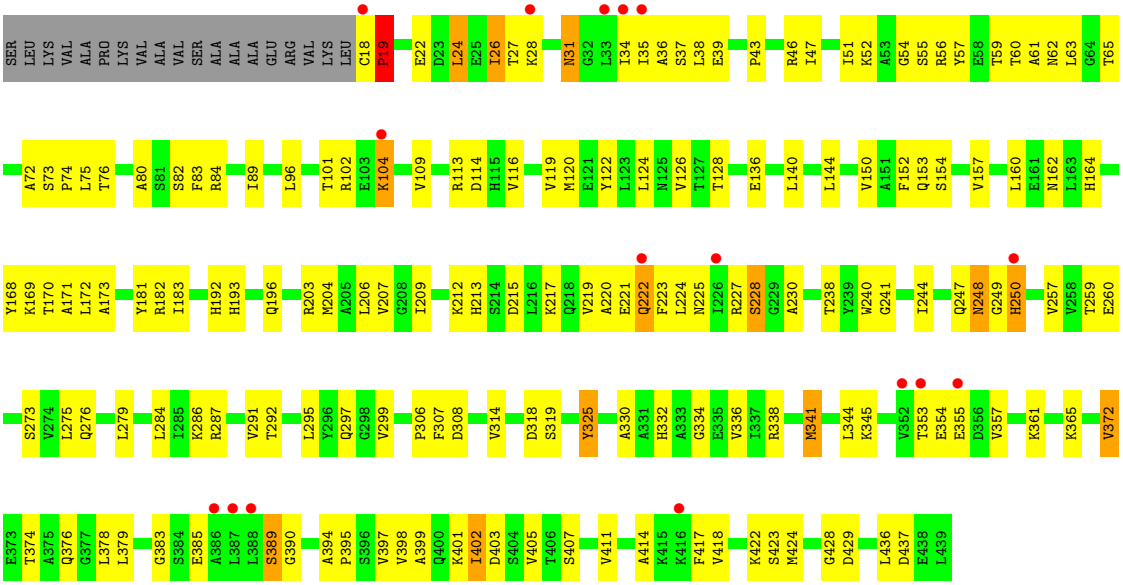
Chain B:



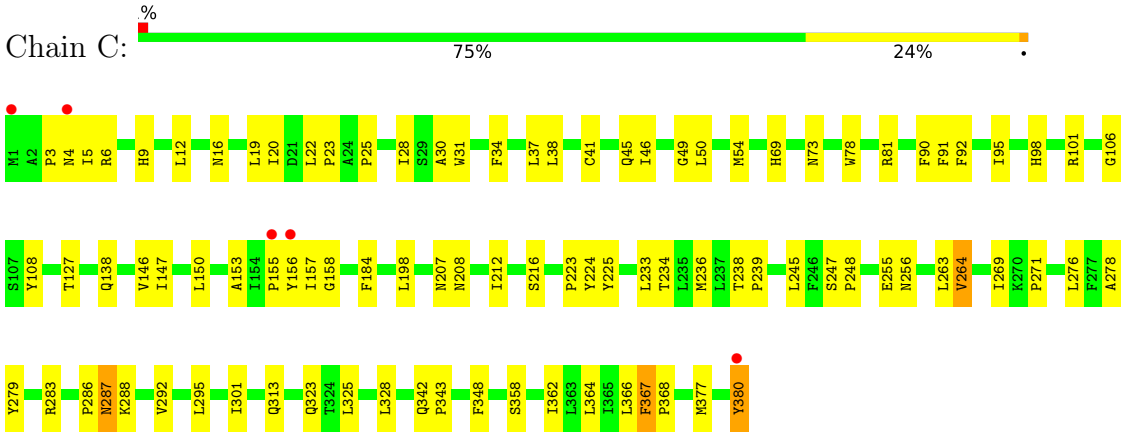


• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

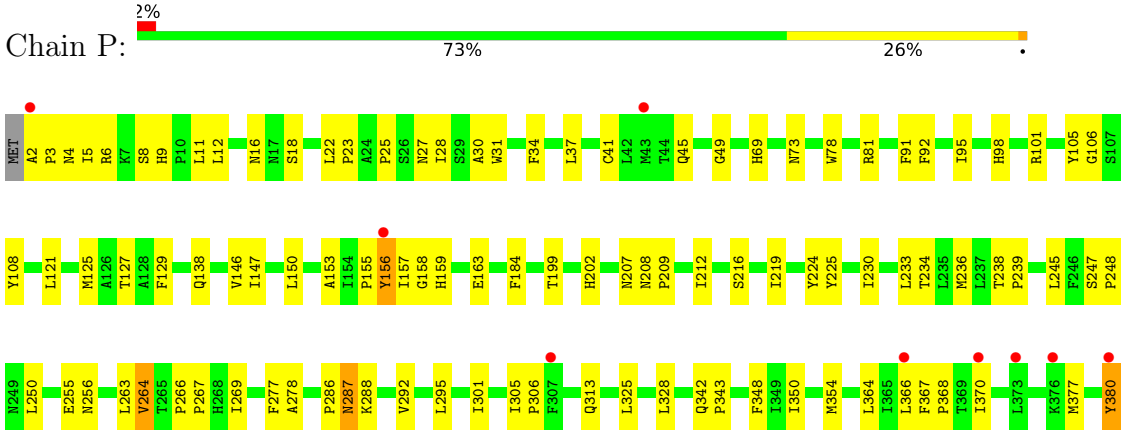
Chain O:



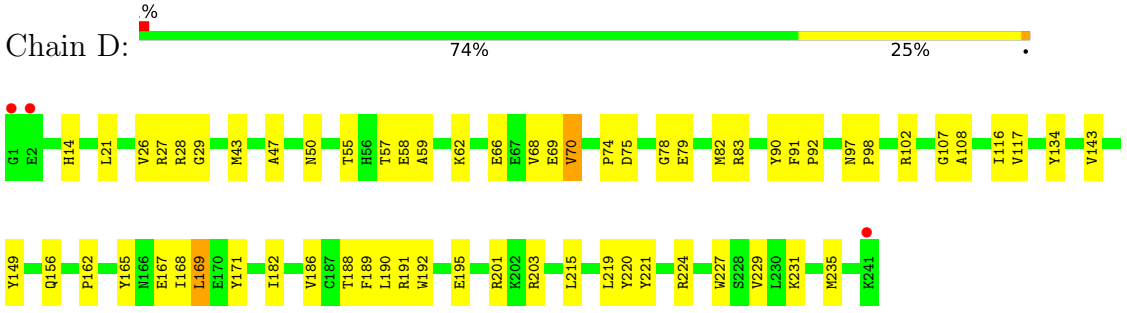
• Molecule 3: Cytochrome b



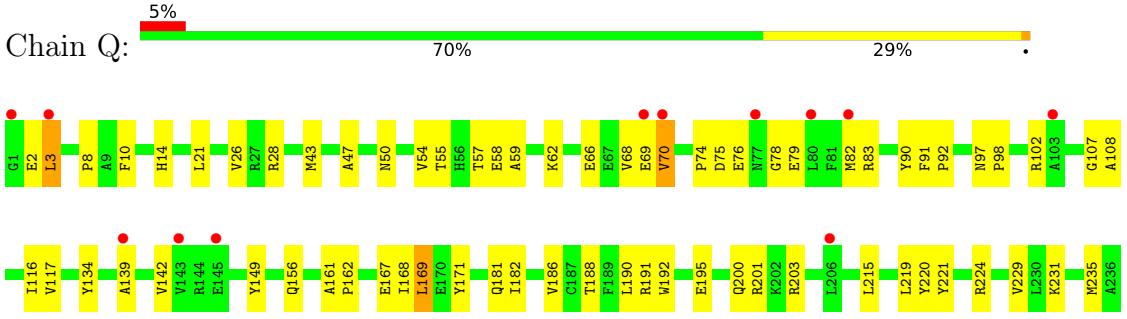
• Molecule 3: Cytochrome b



• Molecule 4: Mitochondrial cytochrome c1, heme protein

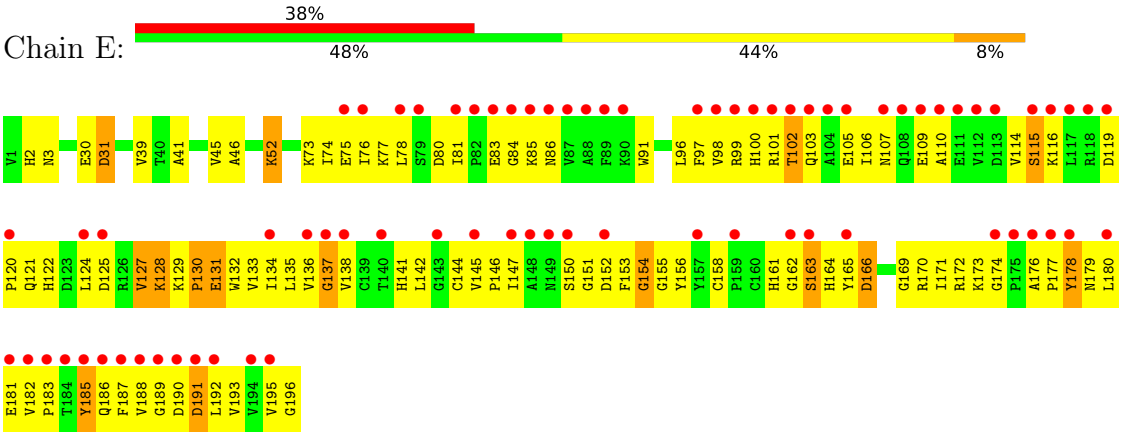


• Molecule 4: Mitochondrial cytochrome c1, heme protein



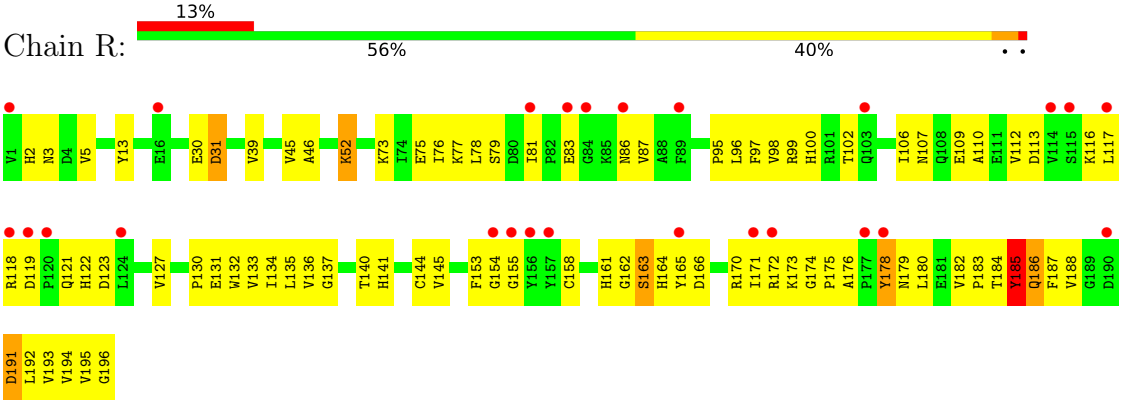
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



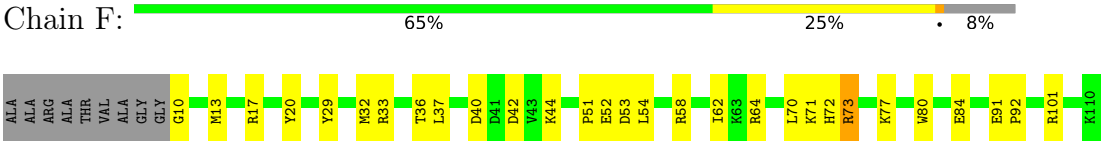
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:



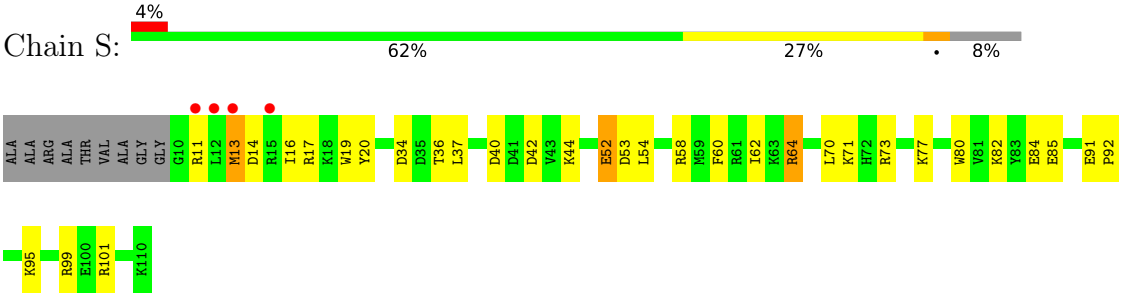
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain F:



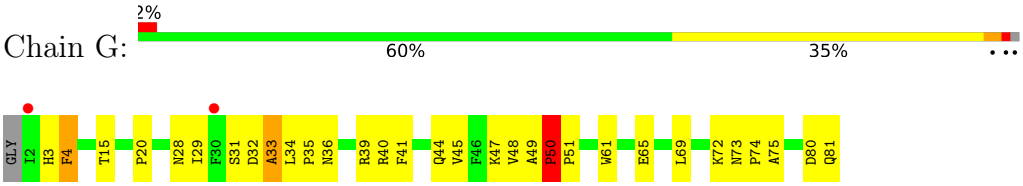
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain S:



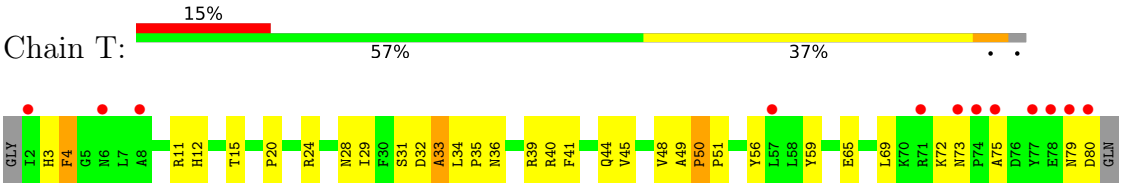
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain G:



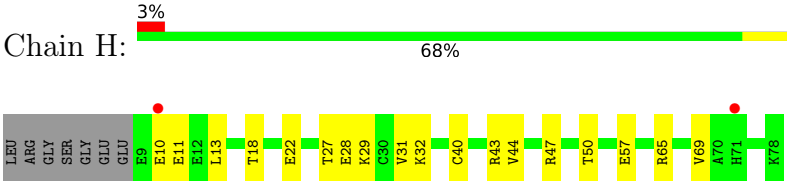
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain T:



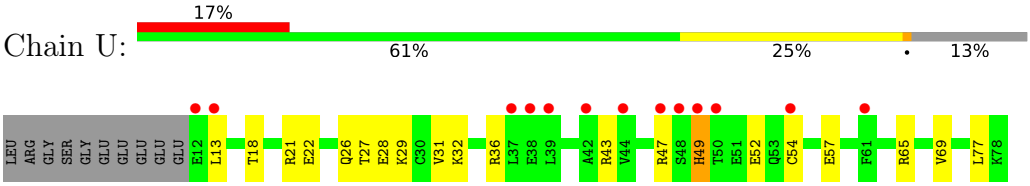
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain H:



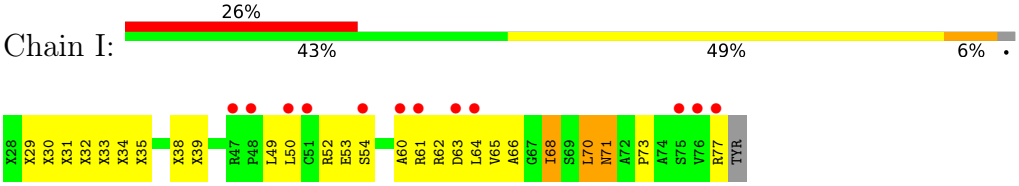
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain U:



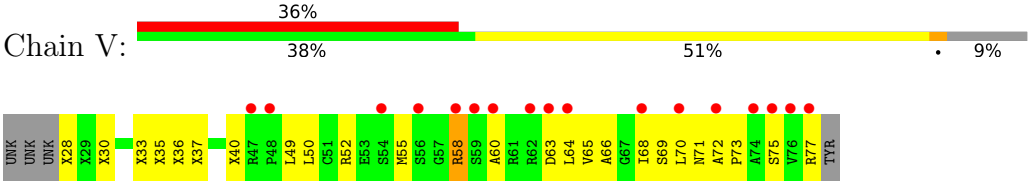
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



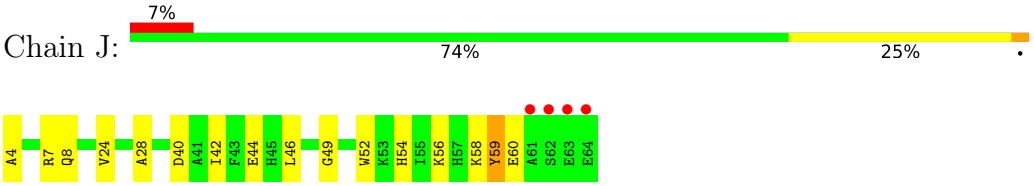
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



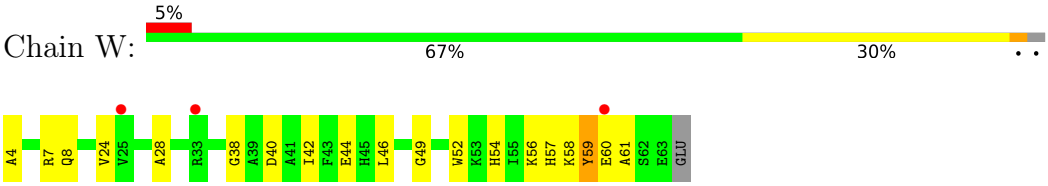
• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain J:



• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	169.61Å 181.99Å 240.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 2.75 58.26 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.99-2.75) 98.8 (58.26-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.267 , 0.297 0.255 , 0.283	Depositor DCC
R_{free} test set	10214 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	32653	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: PEE, GOL, FES, HEC, CDL, JZV, UQ, BOG, HEM

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	0.44	0/3518	0.65	0/4767
1	N	0.42	0/3508	0.64	0/4753
2	B	0.38	0/3187	0.63	0/4321
2	O	0.40	0/3202	0.63	0/4343
3	C	0.50	0/3119	0.66	0/4270
3	P	0.45	0/3114	0.64	0/4263
4	D	0.48	0/1956	0.64	0/2658
4	Q	0.39	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.59	0/2103
5	R	0.37	0/1543	0.60	0/2098
6	F	0.54	1/911 (0.1%)	0.67	0/1219
6	S	0.43	0/911	0.61	0/1219
7	G	0.49	0/694	0.69	0/941
7	T	0.43	0/684	0.64	0/929
8	H	0.44	0/582	0.63	0/779
8	U	0.31	0/561	0.56	0/751
9	I	0.39	0/218	0.60	0/293
9	V	0.36	0/218	0.59	0/293
10	J	0.43	0/508	0.60	0/682
10	W	0.40	0/490	0.60	0/660
All	All	0.43	1/32427 (0.0%)	0.63	0/44000

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	10	GLY	N-CA	5.16	1.53	1.46

There are no bond angle outliers.

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	3447	0	3362	126	0
1	N	3437	0	3349	143	0
2	B	3133	0	3130	187	0
2	O	3147	0	3146	181	0
3	C	3017	0	3063	76	0
3	P	3012	0	3058	95	0
4	D	1898	0	1846	55	0
4	Q	1898	0	1846	67	0
5	E	1513	0	1478	122	0
5	R	1509	0	1474	94	0
6	F	891	0	893	20	0
6	S	891	0	893	33	0
7	G	672	0	653	32	0
7	T	662	0	645	35	0
8	H	574	0	548	16	0
8	U	553	0	535	22	0
9	I	287	0	250	37	0
9	V	277	0	251	32	0
10	J	497	0	490	16	0
10	W	479	0	478	16	0
11	A	21	0	13	0	0
11	C	49	0	72	4	0
11	E	50	0	77	1	0
11	N	5	0	0	0	0
11	P	49	0	72	3	0
11	R	50	0	77	2	0
12	C	86	0	60	9	0
12	P	86	0	60	7	0
13	C	29	0	19	4	0
13	P	29	0	19	4	0
14	C	19	0	17	4	0
14	P	19	0	17	5	0
15	C	40	0	24	4	0
15	D	42	0	28	4	0
15	P	40	0	24	4	0
15	Q	42	0	28	3	0
16	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	6	0	8	0	0
17	D	43	0	30	3	0
17	Q	43	0	30	1	0
18	D	33	0	39	0	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	1	0
20	R	1	0	0	0	0
All	All	32653	0	32160	1298	0

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

All (1298) 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)
9:V:35:UNK:HG3	9:V:36:UNK:H	1.05	1.14
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.15	1.13
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.34	1.07
2:B:76:THR:HG22	2:B:82:SER:H	1.18	1.07
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07
2:O:353:THR:HG22	2:O:355:GLU:H	1.18	1.05
2:B:353:THR:HG22	2:B:355:GLU:H	1.19	1.03
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.27	0.99
3:C:147:ILE:HG13	13:C:2001:JZV:HAP	1.44	0.99
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.28	0.99
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.27	0.99
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.78	0.99
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.42	0.98
1:N:178:THR:HG22	1:N:180:ALA:H	1.25	0.98
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.97
1:A:178:THR:HG22	1:A:180:ALA:H	1.25	0.96
3:P:9:HIS:HD2	3:P:12:LEU:H	1.09	0.95
3:C:9:HIS:HD2	3:C:12:LEU:H	1.11	0.93
4:D:47:ALA:H	4:D:50:ASN:HD22	1.12	0.91
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.50	0.91
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.51	0.90
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.54	0.90
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.36	0.89
3:P:147:ILE:HG13	13:P:3001:JZV:HAP	1.50	0.88
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.54	0.88
9:I:32:UNK:N	9:I:73:PRO:HG2	1.89	0.88
7:T:41:PHE:O	7:T:45:VAL:HG23	1.75	0.87
3:P:238:THR:HB	3:P:239:PRO:HD3	1.56	0.86
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.56	0.86
2:O:27:THR:HG22	2:O:28:LYS:H	1.40	0.86
7:G:41:PHE:O	7:G:45:VAL:HG23	1.76	0.85
1:A:178:THR:HB	1:A:181:ASP:OD1	1.75	0.85
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.57	0.85
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.42	0.85
9:V:35:UNK:HG3	9:V:36:UNK:N	1.89	0.85
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.58	0.85
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.58	0.84
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.60	0.84
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.60	0.84
9:V:64:LEU:HD12	9:V:77:ARG:O	1.78	0.84
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.59	0.83
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.61	0.83
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.04	0.83
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.45	0.82
5:E:127:VAL:HG12	5:E:128:LYS:H	1.43	0.82
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.95	0.81
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.62	0.81
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.45	0.81
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.62	0.81
2:O:192:HIS:O	2:O:196:GLN:HG3	1.81	0.81
12:C:502:HEM:HBC2	12:C:502:HEM:HMC2	1.63	0.81
2:O:248:ASN:HD22	2:O:248:ASN:C	1.83	0.81
9:I:34:UNK:HG3	9:I:35:UNK:N	1.96	0.80
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.45	0.80
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.44	0.80
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.64	0.80
3:C:238:THR:HB	3:C:239:PRO:HD3	1.64	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.65	0.79
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.17	0.79
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.65	0.79
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
2:B:47:ILE:HD13	2:B:120:MET:CE	2.14	0.78
1:A:343:MET:HB3	1:A:444:ILE:HA	1.64	0.78
2:B:248:ASN:C	2:B:248:ASN:HD22	1.87	0.78
1:N:178:THR:HB	1:N:181:ASP:OD1	1.82	0.78
2:O:221:GLU:HG3	2:O:222:GLN:H	1.49	0.77
2:O:154:SER:O	2:O:157:VAL:HG12	1.85	0.77
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.66	0.77
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.49	0.77
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.66	0.77
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.19	0.76
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.86	0.76
4:D:57:THR:HG22	4:D:59:ALA:H	1.49	0.76
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.66	0.76
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.21	0.76
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.34	0.75
2:B:192:HIS:O	2:B:196:GLN:HG3	1.87	0.75
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.68	0.75
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.22	0.75
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.66	0.75
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.51	0.75
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.49	0.75
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.17	0.75
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.68	0.75
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.51	0.74
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.06	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.23	0.74
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.69	0.74
1:N:170:THR:HG22	1:N:171:THR:N	2.03	0.74
2:B:399:ALA:O	2:B:402:ILE:HG22	1.87	0.74
5:R:79:SER:OG	5:R:191:ASP:HB2	1.88	0.74
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.68	0.74
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.70	0.74
2:O:338:ARG:HG3	2:O:338:ARG:NH1	2.00	0.74
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.70	0.73
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.73
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.52	0.73
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.35	0.73
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.24	0.73
2:B:31:ASN:HD22	2:B:31:ASN:N	1.86	0.73
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.52	0.72
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.71	0.72
2:B:27:THR:HG22	2:B:28:LYS:H	1.53	0.72
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.54	0.72
3:P:101:ARG:C	3:P:101:ARG:HD2	2.09	0.72
1:N:10:ASN:HD21	2:O:18:CYS:N	1.88	0.72
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.23	0.72
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.05	0.72
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.70	0.72
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.25	0.72
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.88	0.72
5:E:84:GLY:N	5:E:102:THR:HG23	2.05	0.72
1:N:343:MET:HB3	1:N:444:ILE:HA	1.71	0.72
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.03	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.90	0.72
3:C:9:HIS:CD2	3:C:12:LEU:H	2.03	0.72
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.26	0.71
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.72	0.71
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.07	0.71
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.72	0.71
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.71	0.71
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.01	0.71
2:O:47:ILE:HD13	2:O:120:MET:CE	2.20	0.71
3:C:245:LEU:O	4:D:201:ARG:HD2	1.91	0.71
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.11	0.71
3:P:9:HIS:CD2	3:P:12:LEU:H	2.01	0.71
2:O:399:ALA:O	2:O:402:ILE:HG22	1.90	0.70
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.06	0.70
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.72	0.70
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.71	0.70
2:O:225:ASN:O	2:O:227:ARG:HG3	1.90	0.70
2:B:202:ALA:HB3	2:B:229:GLY:O	1.91	0.70
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.71	0.70
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.22	0.70
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.55	0.70
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.92	0.70
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.56	0.70
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.06	0.70
3:P:245:LEU:O	4:Q:201:ARG:HD2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.74	0.69
4:D:47:ALA:H	4:D:50:ASN:ND2	1.89	0.68
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.93	0.68
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.27	0.68
1:N:15:ASN:O	1:N:26:ALA:HA	1.93	0.68
2:B:76:THR:HG22	2:B:82:SER:N	2.02	0.68
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.26	0.68
2:O:407:SER:O	2:O:411:VAL:HG23	1.94	0.68
2:B:27:THR:HG22	2:B:28:LYS:N	2.07	0.68
2:B:31:ASN:H	2:B:31:ASN:ND2	1.90	0.68
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.94	0.68
1:N:105:ASP:O	1:N:109:VAL:HG23	1.92	0.68
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.76	0.68
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.76	0.68
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.76	0.68
5:E:52:LYS:C	5:E:52:LYS:HD3	2.14	0.68
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.59	0.67
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.75	0.67
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.95	0.67
9:V:35:UNK:CG	9:V:36:UNK:H	1.89	0.67
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.75	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.08	0.67
4:D:57:THR:HG22	4:D:59:ALA:N	2.08	0.67
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.19	0.67
2:O:361:LYS:O	2:O:365:LYS:HG3	1.95	0.67
9:I:31:UNK:C	9:I:73:PRO:HG2	2.25	0.67
1:A:15:ASN:O	1:A:26:ALA:HA	1.95	0.67
2:B:225:ASN:O	2:B:227:ARG:N	2.28	0.67
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.30	0.67
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.10	0.67
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.75	0.66
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.11	0.66
4:D:62:LYS:O	4:D:66:GLU:HG3	1.95	0.66
9:I:70:LEU:HD23	9:I:71:ASN:N	2.10	0.66
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.59	0.66
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.31	0.66
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.78	0.66
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.15	0.66
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.96	0.66
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.26	0.66
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.77	0.66
15:P:3004:CDL:HA32	7:T:40:ARG:HB3	1.77	0.66
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.77	0.66
9:I:64:LEU:HD12	9:I:77:ARG:O	1.95	0.66
2:B:62:ASN:O	2:B:65:THR:HG22	1.96	0.66
1:N:402:VAL:HG22	1:N:406:MET:CE	2.25	0.65
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.28	0.65
5:E:190:ASP:C	5:E:192:LEU:H	1.98	0.65
9:I:70:LEU:HD23	9:I:71:ASN:H	1.61	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.27	0.65
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.61	0.65
5:E:127:VAL:HG12	5:E:128:LYS:N	2.11	0.65
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.78	0.65
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.96	0.65
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.78	0.65
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.77	0.65
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.78	0.65
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.31	0.64
2:O:219:VAL:O	2:O:223:PHE:HB2	1.97	0.64
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.26	0.64
2:O:59:THR:HG22	2:O:61:ALA:H	1.62	0.64
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.78	0.64
12:P:502:HEM:HMC2	12:P:502:HEM:HBC2	1.79	0.64
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.12	0.64
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.12	0.64
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.80	0.64
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.27	0.64
2:O:273:SER:O	2:O:276:GLN:HB3	1.97	0.64
5:R:52:LYS:HD3	5:R:52:LYS:C	2.17	0.64
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.80	0.64
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.79	0.64
3:C:101:ARG:HD2	3:C:101:ARG:C	2.17	0.64
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.33	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.13	0.64
1:N:170:THR:HG22	1:N:172:GLU:H	1.62	0.64
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.13	0.64
9:V:70:LEU:HD23	9:V:71:ASN:N	2.14	0.64
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.12	0.63
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.32	0.63
1:A:178:THR:HG22	1:A:180:ALA:N	2.07	0.63
2:B:31:ASN:N	2:B:31:ASN:ND2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.14	0.63
10:W:7:ARG:CB	10:W:7:ARG:HH11	2.11	0.63
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.79	0.63
5:E:78:LEU:HD12	5:E:190:ASP:O	1.98	0.63
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.79	0.63
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.81	0.63
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.11	0.63
2:B:38:LEU:HD12	2:B:39:GLU:N	2.14	0.63
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.63	0.63
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.99	0.63
3:P:236:MET:O	3:P:239:PRO:HD2	1.99	0.62
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.81	0.62
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.28	0.62
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.80	0.62
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.00	0.62
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.64	0.62
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.82	0.62
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.34	0.62
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.29	0.62
2:O:217:LYS:O	2:O:221:GLU:HG2	1.99	0.62
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.29	0.62
1:A:7:THR:HG21	2:B:113:ARG:CD	2.30	0.62
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.00	0.62
2:O:353:THR:HG22	2:O:355:GLU:N	2.02	0.62
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.82	0.62
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.29	0.62
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.82	0.62
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.80	0.62
8:U:28:GLU:O	8:U:32:LYS:HG3	1.99	0.62
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.00	0.61
7:T:79:ASN:O	7:T:80:ASP:HB2	2.00	0.61
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.10	0.61
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.81	0.61
2:B:407:SER:O	2:B:411:VAL:HG23	2.00	0.61
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.61
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.80	0.61
2:B:353:THR:HG22	2:B:355:GLU:N	2.04	0.61
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.82	0.61
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.30	0.61
2:B:338:ARG:HH11	2:B:338:ARG:CG	2.10	0.61
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.82	0.61
1:N:182:LEU:O	1:N:186:ILE:HG13	2.01	0.61
2:B:292:THR:HG22	2:B:292:THR:O	2.00	0.61
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.61
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.83	0.61
8:H:18:THR:O	8:H:22:GLU:HG3	2.01	0.61
8:H:28:GLU:O	8:H:32:LYS:HG3	2.01	0.61
5:E:130:PRO:HG2	5:E:131:GLU:H	1.66	0.61
2:B:215:ASP:O	2:B:219:VAL:HG23	2.01	0.60
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.16	0.60
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.37	0.60
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.67	0.60
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.01	0.60
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.83	0.60
2:B:96:LEU:H	9:I:70:LEU:HD22	1.66	0.60
1:N:371:GLY:O	1:N:375:VAL:HG23	2.01	0.60
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.81	0.60
1:A:23:LEU:HD23	1:A:24:ARG:N	2.17	0.60
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.83	0.60
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.69	0.60
2:O:27:THR:CG2	2:O:28:LYS:H	2.14	0.60
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.83	0.60
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.60
1:N:219:VAL:HG12	1:N:220:SER:N	2.16	0.60
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.65	0.60
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.83	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.37	0.60
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.37	0.60
5:R:117:LEU:HD11	5:R:172:ARG:NH1	2.16	0.59
1:N:178:THR:HG22	1:N:180:ALA:N	2.08	0.59
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.83	0.59
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.37	0.59
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.85	0.59
6:S:17:ARG:HH11	6:S:17:ARG:HG2	1.68	0.59
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.83	0.59
2:B:59:THR:HG22	2:B:61:ALA:H	1.66	0.59
5:R:109:GLU:OE1	5:R:123:ASP:HB2	2.02	0.59
5:E:116:LYS:HD2	5:E:116:LYS:N	2.17	0.59
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.68	0.59
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.68	0.59
8:H:27:THR:O	8:H:31:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.84	0.59
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.02	0.59
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.84	0.59
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.36	0.59
15:C:2004:CDL:HA32	7:G:40:ARG:HB3	1.85	0.59
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.21	0.59
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.15	0.59
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.84	0.59
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.85	0.59
5:R:171:ILE:HG12	5:R:176:ALA:O	2.02	0.59
8:U:27:THR:O	8:U:31:VAL:HG23	2.02	0.59
2:B:361:LYS:O	2:B:365:LYS:HG3	2.02	0.59
5:E:101:ARG:HA	5:E:105:GLU:OE1	2.03	0.59
5:E:163:SER:HA	5:E:174:GLY:HA3	1.85	0.59
5:R:76:ILE:O	5:R:193:VAL:HG12	2.03	0.59
1:A:170:THR:HG22	1:A:172:GLU:H	1.68	0.58
3:P:34:PHE:HB2	20:P:381:HOH:O	2.03	0.58
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.86	0.58
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.17	0.58
5:E:147:ILE:O	5:E:156:TYR:HA	2.04	0.58
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.33	0.58
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.84	0.58
1:A:430:GLN:HG3	7:G:4:PHE:O	2.03	0.58
2:B:341:MET:CE	2:B:341:MET:HA	2.34	0.58
1:N:63:ALA:O	1:N:116:VAL:HG13	2.03	0.58
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.39	0.58
1:N:282:ARG:NH2	9:V:37:UNK:N	2.51	0.58
1:A:103:SER:HB3	1:A:202:GLY:O	2.04	0.58
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.67	0.58
2:O:422:LYS:O	2:O:436:LEU:HD21	2.02	0.58
8:U:27:THR:HG22	8:U:29:LYS:H	1.67	0.58
1:N:112:LEU:O	1:N:116:VAL:HG23	2.03	0.58
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.51	0.58
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.85	0.58
1:A:371:GLY:O	1:A:375:VAL:HG23	2.04	0.58
5:E:187:PHE:C	5:E:189:GLY:H	2.06	0.58
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.03	0.58
2:O:248:ASN:C	2:O:248:ASN:ND2	2.56	0.58
1:A:402:VAL:HG22	1:A:406:MET:CE	2.34	0.58
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.86	0.58
5:E:106:ILE:C	5:E:110:ALA:HB3	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.84	0.58
2:O:414:ALA:O	2:O:418:VAL:HG23	2.04	0.58
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.86	0.58
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.34	0.58
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.34	0.58
5:E:76:ILE:O	5:E:193:VAL:HG12	2.04	0.58
3:P:313:GLN:HE21	6:S:36:THR:CB	2.17	0.58
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.34	0.57
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.03	0.57
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.86	0.57
2:O:332:HIS:O	2:O:336:VAL:HG23	2.03	0.57
2:O:341:MET:CE	2:O:417:PHE:HE2	2.15	0.57
2:O:215:ASP:O	2:O:219:VAL:HG23	2.04	0.57
3:C:153:ALA:HB2	3:C:288:LYS:HG2	1.85	0.57
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.38	0.57
5:R:102:THR:O	5:R:106:ILE:HG13	2.04	0.57
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.39	0.57
1:A:274:ASN:ND2	1:A:309:THR:HB	2.20	0.57
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.40	0.57
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.04	0.57
3:C:147:ILE:CG1	13:C:2001:JZV:HAP	2.29	0.57
5:E:84:GLY:N	5:E:100:HIS:O	2.33	0.57
2:O:338:ARG:HH11	2:O:338:ARG:CG	2.09	0.57
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.25	0.57
1:A:178:THR:CG2	1:A:179:ARG:N	2.68	0.57
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.57
3:C:30:ALA:HB1	15:D:2003:CDL:H111	1.86	0.57
4:D:231:LYS:O	6:F:71:LYS:HE3	2.05	0.57
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.86	0.57
6:S:95:LYS:O	6:S:99:ARG:HG3	2.03	0.57
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.33	0.57
7:G:65:GLU:O	7:G:69:LEU:HG	2.04	0.57
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.87	0.57
2:O:292:THR:HG22	2:O:292:THR:O	2.02	0.57
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.05	0.57
1:A:364:ALA:O	1:A:368:GLN:HG3	2.05	0.57
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.20	0.57
4:Q:2:GLU:O	4:Q:3:LEU:O	2.22	0.57
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.86	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.05	0.56
1:N:364:ALA:O	1:N:368:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.87	0.56
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.86	0.56
2:O:341:MET:HE2	2:O:341:MET:HA	1.85	0.56
5:R:186:GLN:O	5:R:193:VAL:HG23	2.04	0.56
2:B:31:ASN:HD22	2:B:31:ASN:H	1.48	0.56
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.45	0.56
1:N:36:THR:HG21	1:N:373:THR:HA	1.86	0.56
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.70	0.56
1:N:430:GLN:HG3	7:T:4:PHE:O	2.05	0.56
4:Q:169:LEU:HD22	4:Q:182:ILE:HD11	1.87	0.56
7:G:28:ASN:HB3	7:G:31:SER:OG	2.06	0.56
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.86	0.56
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.87	0.56
2:B:332:HIS:O	2:B:336:VAL:HG23	2.06	0.56
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.35	0.56
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.45	0.56
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.06	0.56
1:N:178:THR:CG2	1:N:179:ARG:N	2.68	0.56
5:R:106:ILE:O	5:R:109:GLU:HB3	2.05	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.41	0.56
3:C:301:ILE:CD1	3:C:364:LEU:HD21	2.34	0.56
1:N:170:THR:CG2	1:N:171:THR:N	2.68	0.56
1:N:382:HIS:HB3	1:N:388:ARG:O	2.06	0.56
9:V:64:LEU:HD12	9:V:77:ARG:C	2.26	0.56
2:B:414:ALA:O	2:B:418:VAL:HG23	2.06	0.56
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.06	0.56
1:N:279:ARG:HH22	9:V:30:UNK:C	2.19	0.56
2:B:28:LYS:O	2:B:29:LEU:O	2.24	0.56
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.88	0.56
1:N:187:ASP:O	1:N:191:LYS:HE3	2.06	0.56
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.70	0.56
6:S:53:ASP:OD1	6:S:54:LEU:N	2.39	0.56
2:O:38:LEU:HD12	2:O:39:GLU:N	2.21	0.55
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.89	0.55
2:O:402:ILE:C	2:O:402:ILE:HD13	2.27	0.55
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.41	0.55
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.20	0.55
2:B:23:ASP:OD1	2:B:24:LEU:N	2.38	0.55
2:B:201:SER:OG	2:B:228:SER:HA	2.07	0.55
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.07	0.55
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:150:VAL:O	2:O:153:GLN:HG3	2.06	0.55
15:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.07	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.40	0.55
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.21	0.55
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.22	0.55
9:I:29:UNK:O	9:I:30:UNK:HB2	2.05	0.55
1:N:170:THR:HG22	1:N:171:THR:H	1.71	0.55
2:O:397:VAL:O	2:O:401:LYS:HG2	2.07	0.55
5:R:118:ARG:NH1	5:R:174:GLY:O	2.40	0.55
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.22	0.55
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.87	0.55
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.06	0.55
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.46	0.55
17:Q:501:HEC:HBB3	17:Q:501:HEC:HMB1	1.89	0.55
1:A:187:ASP:O	1:A:191:LYS:HE3	2.07	0.55
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.71	0.55
5:E:106:ILE:O	5:E:110:ALA:HB3	2.07	0.55
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.41	0.55
3:C:301:ILE:HD11	3:C:364:LEU:CD2	2.34	0.55
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.89	0.55
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.72	0.55
2:B:422:LYS:O	2:B:436:LEU:HD21	2.06	0.55
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.71	0.55
2:O:341:MET:CE	2:O:341:MET:HA	2.37	0.55
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.39	0.55
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.88	0.55
2:B:338:ARG:NH1	2:B:338:ARG:CG	2.69	0.55
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.42	0.55
15:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.22	0.55
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.89	0.55
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.88	0.55
3:C:286:PRO:O	3:C:287:ASN:HB2	2.08	0.54
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.07	0.54
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.70	0.54
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.22	0.54
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.68	0.54
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.37	0.54
2:O:31:ASN:N	2:O:31:ASN:HD22	2.05	0.54
8:U:18:THR:O	8:U:22:GLU:HG3	2.07	0.54
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.88	0.54
1:N:233:ARG:HH21	1:N:316:ASP:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.22	0.54
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.71	0.54
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.88	0.54
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.89	0.54
5:E:188:VAL:HG12	5:E:188:VAL:O	2.08	0.54
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.88	0.54
2:O:357:VAL:O	2:O:361:LYS:HG3	2.07	0.54
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.22	0.54
2:B:76:THR:CG2	2:B:82:SER:H	2.06	0.54
3:P:199:THR:HA	18:P:2010:BOG:O1	2.08	0.54
5:R:184:THR:O	5:R:185:TYR:HB3	2.07	0.54
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.33	0.54
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.89	0.54
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.38	0.54
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.10	0.54
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.90	0.54
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.37	0.54
6:F:53:ASP:OD1	6:F:54:LEU:N	2.39	0.54
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.42	0.54
2:O:374:THR:HG22	2:O:376:GLN:H	1.72	0.54
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.43	0.54
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.70	0.54
3:P:30:ALA:HB1	15:Q:3003:CDL:H111	1.90	0.54
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.43	0.53
5:E:84:GLY:CA	5:E:102:THR:HG23	2.38	0.53
1:N:23:LEU:HD23	1:N:24:ARG:N	2.23	0.53
1:N:209:VAL:O	1:N:212:ALA:HB3	2.07	0.53
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.91	0.53
15:P:3004:CDL:H712	11:P:3007:PEE:H50	1.90	0.53
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.28	0.53
2:B:24:LEU:HD12	2:B:37:SER:O	2.07	0.53
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.53
10:J:56:LYS:O	10:J:60:GLU:HB2	2.08	0.53
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.90	0.53
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.74	0.53
11:R:3005:PEE:H58	10:W:24:VAL:HG11	1.90	0.53
1:A:36:THR:HG21	1:A:373:THR:HA	1.91	0.53
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.73	0.53
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.88	0.53
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.43	0.53
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.23	0.53
8:U:22:GLU:O	8:U:26:GLN:HG2	2.08	0.53
1:A:105:ASP:O	1:A:109:VAL:HG23	2.08	0.53
2:O:372:VAL:HG12	2:O:372:VAL:O	2.08	0.53
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.74	0.53
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.38	0.53
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.90	0.53
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.39	0.53
5:E:165:TYR:HA	5:E:170:ARG:O	2.09	0.53
3:C:45:GLN:CB	12:C:501:HEM:HAB	2.38	0.53
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.91	0.53
1:A:170:THR:CG2	1:A:171:THR:N	2.72	0.53
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.91	0.53
2:B:189:GLU:OE1	2:B:189:GLU:N	2.42	0.53
9:I:65:VAL:HG12	9:I:66:ALA:N	2.24	0.53
1:A:358:LYS:HE3	1:A:399:ILE:O	2.08	0.53
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.91	0.53
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.90	0.53
2:B:374:THR:HG22	2:B:376:GLN:H	1.74	0.53
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.90	0.53
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.90	0.53
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.91	0.53
5:R:131:GLU:OE1	5:R:131:GLU:N	2.40	0.53
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.91	0.52
6:F:84:GLU:H	6:F:84:GLU:CD	2.12	0.52
1:N:7:THR:HG21	2:O:113:ARG:CD	2.38	0.52
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.39	0.52
10:W:52:TRP:O	10:W:56:LYS:HB2	2.09	0.52
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.73	0.52
8:H:27:THR:HG22	8:H:29:LYS:H	1.74	0.52
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.72	0.52
2:B:152:PHE:HA	2:B:157:VAL:CG1	2.40	0.52
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.90	0.52
4:D:169:LEU:C	4:D:169:LEU:HD23	2.30	0.52
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.44	0.52
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.38	0.52
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.92	0.52
4:Q:43:MET:HE1	4:Q:91:PHE:HE2	1.75	0.52
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.39	0.52
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.45	0.52
1:A:280:TYR:CG	1:A:281:ASP:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.09	0.52
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.92	0.52
3:C:313:GLN:HE21	6:F:36:THR:CB	2.22	0.52
4:D:47:ALA:HA	4:D:90:TYR:HA	1.91	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.91	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
2:B:372:VAL:HG12	2:B:372:VAL:O	2.09	0.52
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.90	0.52
3:P:286:PRO:O	3:P:287:ASN:HB2	2.09	0.52
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.40	0.52
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.92	0.52
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.52
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.45	0.52
5:E:102:THR:O	5:E:103:GLN:HG3	2.10	0.52
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.44	0.52
1:N:317:THR:HG23	1:N:318:GLY:N	2.25	0.52
1:N:358:LYS:HE3	1:N:399:ILE:O	2.09	0.52
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.90	0.52
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.24	0.52
14:P:3002:UQ:C8	14:P:3002:UQ:HM51	2.40	0.52
8:U:43:ARG:O	8:U:47:ARG:HG3	2.09	0.52
9:V:65:VAL:HG12	9:V:66:ALA:N	2.25	0.52
1:A:288:LYS:HE3	1:A:289:HIS:CE1	2.45	0.52
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.10	0.52
8:H:10:GLU:O	8:H:11:GLU:HG3	2.10	0.52
1:N:173:ASN:O	1:N:177:LEU:HG	2.10	0.52
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.92	0.52
2:O:222:GLN:O	2:O:222:GLN:HG2	2.10	0.52
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.45	0.52
7:T:48:VAL:O	7:T:51:PRO:HD2	2.10	0.52
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.09	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.92	0.51
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.75	0.51
3:P:301:ILE:HD11	3:P:364:LEU:CD2	2.35	0.51
2:B:264:VAL:HG23	2:B:316:TYR:C	2.30	0.51
2:B:402:ILE:HD13	2:B:402:ILE:C	2.31	0.51
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.43	0.51
3:C:279:TYR:O	3:C:283:ARG:HG3	2.10	0.51
1:N:131:ARG:NH2	1:N:177:LEU:O	2.44	0.51
2:O:203:ARG:HD2	2:O:230:ALA:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.91	0.51
5:R:163:SER:H	5:R:175:PRO:HD2	1.75	0.51
6:S:91:GLU:O	6:S:95:LYS:HG3	2.09	0.51
4:D:169:LEU:HD22	4:D:182:ILE:HD11	1.92	0.51
1:N:45:SER:HA	1:N:48:GLU:HG3	1.92	0.51
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.92	0.51
4:Q:2:GLU:HB3	4:Q:3:LEU:HD12	1.91	0.51
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.93	0.51
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.92	0.51
10:W:40:ASP:O	10:W:44:GLU:HG3	2.09	0.51
1:A:140:GLU:OE2	9:I:49:LEU:HA	2.10	0.51
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.45	0.51
2:O:248:ASN:ND2	2:O:250:HIS:H	2.09	0.51
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.93	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.46	0.51
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.33	0.51
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.46	0.51
2:B:57:TYR:N	2:B:57:TYR:CD1	2.78	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.43	0.51
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.93	0.51
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.51
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.46	0.51
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.45	0.51
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.51
2:O:26:ILE:HG12	2:O:26:ILE:O	2.09	0.51
2:O:57:TYR:CD1	2:O:57:TYR:N	2.78	0.51
2:B:248:ASN:C	2:B:248:ASN:ND2	2.59	0.51
2:B:402:ILE:HG23	2:B:403:ASP:N	2.26	0.51
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.93	0.51
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.40	0.50
9:I:71:ASN:H	9:I:71:ASN:HD22	1.59	0.50
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.46	0.50
2:O:222:GLN:O	2:O:223:PHE:CD2	2.64	0.50
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.72	0.50
9:I:49:LEU:HD22	9:I:54:SER:HB3	1.93	0.50
2:O:43:PRO:O	2:O:113:ARG:HG3	2.11	0.50
6:S:13:MET:HA	6:S:16:ILE:HD12	1.93	0.50
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.40	0.50
1:N:368:GLN:O	1:N:369:LEU:HD23	2.12	0.50
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.41	0.50
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.75	0.50
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.41	0.50
3:C:207:ASN:ND2	3:C:208:ASN:H	2.10	0.50
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.94	0.50
1:N:17:THR:HG23	1:N:205:HIS:NE2	2.27	0.50
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.30	0.50
5:R:165:TYR:HA	5:R:170:ARG:O	2.11	0.50
2:B:402:ILE:HG23	2:B:403:ASP:H	1.77	0.50
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.50
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.46	0.50
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.30	0.50
3:P:147:ILE:CG1	13:P:3001:JZV:HAP	2.32	0.50
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.94	0.50
14:C:2002:UQ:C8	14:C:2002:UQ:HM51	2.41	0.50
5:E:101:ARG:NH2	5:E:130:PRO:O	2.45	0.50
3:P:45:GLN:HB3	12:P:501:HEM:HAB	1.94	0.50
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.41	0.50
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.93	0.50
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.92	0.50
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.94	0.50
1:A:362:ARG:O	1:A:365:MET:HG2	2.11	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
2:B:395:PRO:O	2:B:398:VAL:HG12	2.11	0.50
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.94	0.50
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.41	0.50
17:D:501:HEC:HMB1	17:D:501:HEC:HBB3	1.94	0.50
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.30	0.50
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.42	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.94	0.50
9:I:38:UNK:O	9:I:39:UNK:C	2.59	0.49
9:V:33:UNK:HA	9:V:73:PRO:HB3	1.94	0.49
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.94	0.49
1:N:158:PHE:O	1:N:164:ALA:HB2	2.12	0.49
5:R:178:TYR:N	5:R:178:TYR:CD1	2.80	0.49
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.93	0.49
2:O:76:THR:HG22	2:O:82:SER:N	2.02	0.49
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.94	0.49
2:O:334:GLY:O	2:O:338:ARG:HG2	2.12	0.49
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.37	0.49
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.41	0.49
2:O:52:LYS:O	2:O:203:ARG:NH2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:21:LEU:HD21	4:Q:191:ARG:HG3	1.93	0.49
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.49
2:B:26:ILE:HG12	2:B:26:ILE:O	2.12	0.49
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.94	0.49
3:P:138:GLN:HB2	3:P:255:GLU:O	2.12	0.49
3:P:238:THR:HB	3:P:239:PRO:CD	2.37	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.52	0.49
1:A:307:PHE:CD1	1:A:307:PHE:C	2.85	0.49
2:B:402:ILE:O	2:B:405:VAL:HG23	2.13	0.49
1:N:362:ARG:O	1:N:365:MET:HG2	2.12	0.49
3:P:159:HIS:O	3:P:163:GLU:HG3	2.13	0.49
3:P:301:ILE:CD1	3:P:364:LEU:HD21	2.36	0.49
7:T:28:ASN:HB3	7:T:31:SER:OG	2.13	0.49
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.49
5:E:106:ILE:O	5:E:106:ILE:HG22	2.12	0.49
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.28	0.49
6:S:40:ASP:O	6:S:44:LYS:HG3	2.13	0.49
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.31	0.49
2:B:397:VAL:O	2:B:401:LYS:HG2	2.13	0.49
3:C:34:PHE:HB2	20:C:381:HOH:O	2.12	0.49
3:C:263:LEU:O	3:C:264:VAL:CG2	2.61	0.49
4:D:43:MET:HE1	4:D:91:PHE:HE2	1.78	0.49
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.11	0.49
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.48	0.49
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.94	0.49
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.76	0.49
3:C:138:GLN:HB2	3:C:255:GLU:O	2.13	0.49
4:D:21:LEU:HD21	4:D:191:ARG:HG3	1.94	0.49
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.13	0.49
5:E:127:VAL:O	5:E:128:LYS:HB2	2.13	0.49
1:A:173:ASN:O	1:A:177:LEU:HG	2.13	0.49
1:A:205:HIS:O	1:A:208:LEU:HB3	2.13	0.49
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.95	0.49
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.49
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.94	0.48
2:B:334:GLY:O	2:B:338:ARG:HG2	2.13	0.48
15:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.13	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.31	0.48
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.48	0.48
1:A:95:THR:HG22	1:A:96:ALA:N	2.28	0.48
10:J:52:TRP:O	10:J:56:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:402:VAL:HG22	1:N:406:MET:HE1	1.93	0.48
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.47	0.48
5:E:178:TYR:HD1	5:E:178:TYR:H	1.61	0.48
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.48
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.94	0.48
5:R:73:LYS:HB3	5:R:196:GLY:O	2.14	0.48
6:S:84:GLU:CD	6:S:84:GLU:H	2.15	0.48
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.53	0.48
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.42	0.48
5:E:3:ASN:HD22	5:E:3:ASN:H	1.62	0.48
5:E:131:GLU:H	5:E:131:GLU:CD	2.17	0.48
5:E:187:PHE:C	5:E:189:GLY:N	2.66	0.48
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.36	0.48
1:A:182:LEU:O	1:A:186:ILE:HG13	2.13	0.48
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.76	0.48
3:P:207:ASN:ND2	3:P:208:ASN:H	2.12	0.48
7:T:29:ILE:O	7:T:33:ALA:HB3	2.13	0.48
4:D:167:GLU:HG3	8:H:13:LEU:HD22	1.96	0.48
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.48	0.48
1:N:49:ASN:ND2	1:N:51:LYS:H	2.12	0.48
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.13	0.48
2:O:248:ASN:HD22	2:O:249:GLY:N	2.12	0.48
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.48	0.48
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.96	0.48
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.96	0.48
6:F:40:ASP:O	6:F:44:LYS:HG3	2.14	0.48
6:F:13:MET:O	6:F:17:ARG:HG3	2.12	0.48
6:S:16:ILE:O	6:S:19:TRP:HB3	2.14	0.48
10:W:49:GLY:N	10:W:54:HIS:ND1	2.61	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.14	0.48
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.49	0.48
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.48	0.48
5:E:185:TYR:O	5:E:186:GLN:HB3	2.14	0.48
2:O:164:HIS:O	2:O:173:ALA:HA	2.14	0.48
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.46	0.48
2:B:437:ASP:C	2:B:437:ASP:OD1	2.52	0.48
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.95	0.48
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.95	0.47
5:E:190:ASP:C	5:E:192:LEU:N	2.67	0.47
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.96	0.47
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:433:ASP:OD1	1:N:436:ARG:HG2	2.13	0.47
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.28	0.47
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.49	0.47
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.78	0.47
1:A:37:VAL:HG22	1:A:109:VAL:HG11	1.96	0.47
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.95	0.47
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.42	0.47
1:N:48:GLU:CD	1:N:54:GLY:H	2.18	0.47
1:N:217:SER:O	1:N:218:GLY:C	2.52	0.47
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.14	0.47
1:A:178:THR:HG22	1:A:179:ARG:N	2.29	0.47
4:D:186:VAL:O	4:D:190:LEU:HG	2.14	0.47
4:D:220:TYR:O	4:D:224:ARG:HG2	2.14	0.47
5:E:116:LYS:HD2	5:E:116:LYS:H	1.78	0.47
5:E:141:HIS:HB3	19:E:501:FES:S2	2.54	0.47
1:N:170:THR:CG2	1:N:171:THR:H	2.27	0.47
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.15	0.47
1:A:382:HIS:HB3	1:A:388:ARG:O	2.13	0.47
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.44	0.47
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.44	0.47
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.29	0.47
1:N:137:GLU:O	1:N:141:MET:HG3	2.13	0.47
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.14	0.47
5:E:178:TYR:N	5:E:178:TYR:CD1	2.83	0.47
8:H:43:ARG:O	8:H:47:ARG:HG3	2.15	0.47
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.14	0.47
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.14	0.47
5:E:77:LYS:HG3	5:E:191:ASP:O	2.13	0.47
9:I:34:UNK:CG	9:I:35:UNK:N	2.70	0.47
1:N:178:THR:HG22	1:N:179:ARG:N	2.29	0.47
2:O:73:SER:N	2:O:74:PRO:HD2	2.29	0.47
2:O:89:ILE:HD13	2:O:96:LEU:HB2	1.95	0.47
2:O:295:LEU:O	2:O:299:VAL:HG23	2.14	0.47
2:O:395:PRO:O	2:O:398:VAL:HG12	2.14	0.47
1:A:217:SER:O	1:A:218:GLY:C	2.52	0.47
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.77	0.47
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.96	0.47
5:E:41:ALA:O	5:E:45:VAL:HG23	2.15	0.47
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.44	0.47
5:E:155:GLY:HA3	5:E:166:ASP:O	2.15	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.45	0.47
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.49	0.47
1:N:205:HIS:O	1:N:209:VAL:HG12	2.15	0.47
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.47
1:N:342:TRP:O	1:N:345:LEU:HB2	2.15	0.47
2:O:122:TYR:O	2:O:126:VAL:HG23	2.14	0.47
2:O:221:GLU:C	2:O:223:PHE:H	2.17	0.47
2:O:374:THR:HG22	2:O:376:GLN:N	2.29	0.47
2:O:402:ILE:HG23	2:O:403:ASP:N	2.29	0.47
4:Q:161:ALA:O	4:Q:162:PRO:C	2.53	0.47
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.47	0.47
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.50	0.47
1:A:144:ASP:OD2	1:A:147:ASN:ND2	2.47	0.47
1:A:158:PHE:O	1:A:164:ALA:HB2	2.15	0.47
4:D:102:ARG:HA	4:D:108:ALA:O	2.14	0.47
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.44	0.47
1:N:354:VAL:HG23	1:N:355:LYS:N	2.30	0.47
2:O:31:ASN:N	2:O:31:ASN:ND2	2.63	0.47
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.48	0.47
3:P:350:ILE:O	3:P:354:MET:HG2	2.15	0.47
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.29	0.47
5:E:136:VAL:O	5:E:138:VAL:N	2.44	0.47
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.45	0.47
2:B:122:TYR:O	2:B:126:VAL:HG23	2.15	0.47
3:C:37:LEU:O	3:C:41:CYS:HB2	2.15	0.47
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.45	0.47
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.97	0.47
2:O:59:THR:HG22	2:O:60:THR:N	2.30	0.47
3:P:101:ARG:HD2	3:P:101:ARG:O	2.15	0.47
3:P:155:PRO:O	3:P:156:TYR:HB2	2.15	0.47
4:Q:3:LEU:HD12	4:Q:3:LEU:N	2.29	0.47
7:T:80:ASP:OD1	8:U:47:ARG:HD3	2.14	0.47
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.50	0.46
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.44	0.46
10:J:7:ARG:HH11	10:J:7:ARG:HB2	1.80	0.46
1:N:219:VAL:CG1	1:N:220:SER:N	2.78	0.46
3:P:247:SER:OG	3:P:250:LEU:HB2	2.15	0.46
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.96	0.46
6:F:71:LYS:O	6:F:72:HIS:HB2	2.15	0.46
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.98	0.46
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.97	0.46
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.50	0.46
10:W:4:ALA:O	10:W:8:GLN:HG3	2.15	0.46
2:B:207:VAL:HG12	2:B:208:GLY:N	2.30	0.46
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.30	0.46
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.51	0.46
1:N:130:GLU:O	1:N:134:ILE:HG13	2.16	0.46
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.45	0.46
15:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.48	0.46
5:R:185:TYR:O	5:R:186:GLN:HB3	2.15	0.46
2:B:110:GLU:O	2:B:111:CYS:HB3	2.16	0.46
2:O:259:THR:HG22	2:O:260:GLU:N	2.29	0.46
6:S:17:ARG:HG2	6:S:17:ARG:NH1	2.29	0.46
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.80	0.46
1:A:433:ASP:OD1	1:A:436:ARG:HG2	2.16	0.46
2:B:27:THR:CG2	2:B:28:LYS:H	2.24	0.46
3:C:247:SER:N	3:C:248:PRO:HD3	2.30	0.46
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.51	0.46
5:E:96:LEU:HD12	5:E:135:LEU:O	2.16	0.46
1:N:37:VAL:HG22	1:N:109:VAL:HG11	1.98	0.46
2:O:437:ASP:OD1	2:O:437:ASP:C	2.54	0.46
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.34	0.46
2:B:21:ALA:O	2:B:22:GLU:HB3	2.15	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.16	0.46
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.51	0.46
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.46	0.46
2:O:259:THR:CG2	2:O:260:GLU:N	2.79	0.46
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.43	0.46
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.97	0.46
1:A:49:ASN:ND2	1:A:51:LYS:H	2.14	0.46
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.16	0.46
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.80	0.46
1:N:288:LYS:HE3	1:N:289:HIS:CE1	2.51	0.46
2:O:307:PHE:H	9:V:52:ARG:HG2	1.81	0.46
1:A:48:GLU:CD	1:A:54:GLY:H	2.19	0.46
2:B:50:PHE:N	2:B:50:PHE:CD1	2.83	0.46
2:B:333:ALA:O	2:B:337:ILE:HG13	2.16	0.46
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.51	0.46
5:E:189:GLY:O	5:E:192:LEU:O	2.34	0.46
2:O:24:LEU:HD12	2:O:37:SER:O	2.15	0.46
5:R:109:GLU:HG2	5:R:123:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.64	0.46
1:A:368:GLN:O	1:A:369:LEU:HD23	2.16	0.46
2:B:248:ASN:HD22	2:B:249:GLY:N	2.14	0.46
2:B:259:THR:CG2	2:B:260:GLU:N	2.78	0.46
5:E:133:VAL:O	5:E:133:VAL:HG13	2.16	0.46
10:J:40:ASP:O	10:J:44:GLU:HG3	2.15	0.46
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.80	0.46
2:O:385:GLU:O	2:O:389:SER:HB3	2.15	0.46
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.98	0.46
5:R:141:HIS:HB3	19:R:501:FES:S2	2.56	0.46
9:I:39:UNK:HA	9:V:40:UNK:O	2.16	0.45
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.31	0.45
3:P:153:ALA:CB	3:P:288:LYS:HG2	2.45	0.45
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.46	0.45
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.46	0.45
10:W:42:ILE:HG22	10:W:46:LEU:HD12	1.98	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.16	0.45
1:A:205:HIS:O	1:A:209:VAL:HG12	2.16	0.45
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.81	0.45
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.17	0.45
4:D:169:LEU:HD23	4:D:169:LEU:O	2.16	0.45
4:D:171:TYR:OH	4:D:182:ILE:HA	2.16	0.45
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.45
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.98	0.45
5:R:162:GLY:O	5:R:163:SER:C	2.53	0.45
2:O:31:ASN:ND2	2:O:31:ASN:H	2.13	0.45
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.47	0.45
3:P:380:TYR:CZ	6:S:37:LEU:HD21	2.52	0.45
4:Q:43:MET:HE1	4:Q:91:PHE:CE2	2.52	0.45
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.81	0.45
1:A:418:LYS:O	1:A:420:PRO:HD3	2.16	0.45
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.99	0.45
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.44	0.45
15:C:2004:CDL:H712	11:C:2007:PEE:H50	1.98	0.45
15:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.49	0.45
5:R:163:SER:HA	5:R:174:GLY:HA3	1.99	0.45
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.97	0.45
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.97	0.45
2:B:225:ASN:O	2:B:226:ILE:C	2.54	0.45
2:O:170:THR:O	2:O:172:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.99	0.45
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.17	0.45
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.49	0.45
7:T:36:ASN:O	7:T:40:ARG:HG3	2.17	0.45
1:A:255:LEU:O	1:A:321:GLY:HA3	2.16	0.45
2:B:24:LEU:HD13	2:B:38:LEU:HB2	1.98	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.32	0.45
5:E:144:CYS:CB	5:E:158:CYS:SG	3.05	0.45
5:E:189:GLY:O	5:E:192:LEU:N	2.50	0.45
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.99	0.45
1:A:45:SER:HA	1:A:48:GLU:HG3	1.98	0.45
2:B:28:LYS:O	2:B:28:LYS:HG2	2.17	0.45
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.17	0.45
15:D:2003:CDL:H721	15:D:2003:CDL:HA61	1.98	0.45
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.32	0.45
10:W:38:GLY:O	10:W:42:ILE:HG13	2.16	0.45
2:B:27:THR:CG2	2:B:28:LYS:N	2.77	0.45
2:B:207:VAL:HG12	2:B:208:GLY:H	1.82	0.45
2:B:318:ASP:O	2:B:319:SER:HB2	2.16	0.45
3:C:328:LEU:HD12	3:C:328:LEU:HA	1.83	0.45
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.99	0.45
2:O:75:LEU:HD11	2:O:140:LEU:HD22	1.97	0.45
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.17	0.45
9:V:69:SER:HB2	9:V:72:ALA:H	1.81	0.45
2:B:43:PRO:O	2:B:113:ARG:HG3	2.17	0.45
11:C:2007:PEE:H11	6:F:29:TYR:OH	2.17	0.45
4:D:167:GLU:CG	8:H:13:LEU:HD22	2.46	0.45
5:E:127:VAL:CG1	5:E:128:LYS:H	2.15	0.45
3:P:263:LEU:O	3:P:264:VAL:CG2	2.65	0.45
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.52	0.45
7:T:56:TYR:O	7:T:59:TYR:HB3	2.17	0.45
1:A:27:SER:HA	1:A:199:ALA:O	2.16	0.45
3:C:50:LEU:O	3:C:54:MET:HG3	2.17	0.45
3:P:92:PHE:O	3:P:95:ILE:HG22	2.17	0.45
9:V:55:MET:HA	9:V:58:ARG:HG3	1.99	0.45
10:W:59:TYR:CD1	10:W:59:TYR:N	2.84	0.45
2:B:395:PRO:O	2:B:398:VAL:CG1	2.65	0.44
3:C:19:LEU:C	3:C:20:ILE:HG13	2.36	0.44
7:G:80:ASP:O	7:G:81:GLN:C	2.55	0.44
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.52	0.44
15:P:3004:CDL:HA32	7:T:40:ARG:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:HIS:O	2:B:173:ALA:HA	2.17	0.44
5:E:73:LYS:HB2	5:E:195:VAL:O	2.16	0.44
1:N:255:LEU:O	1:N:321:GLY:HA3	2.17	0.44
3:P:266:PRO:HA	3:P:267:PRO:HD3	1.85	0.44
6:S:82:LYS:HD2	6:S:85:GLU:OE1	2.16	0.44
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.33	0.44
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.52	0.44
4:D:57:THR:CG2	4:D:58:GLU:N	2.79	0.44
6:F:77:LYS:HB3	6:F:77:LYS:HE2	1.81	0.44
3:P:28:ILE:HD11	3:P:225:TYR:CE2	2.52	0.44
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.17	0.44
5:R:178:TYR:N	5:R:178:TYR:HD1	2.15	0.44
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.80	0.44
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.99	0.44
9:I:68:ILE:HD13	9:I:68:ILE:HA	1.84	0.44
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.99	0.44
2:O:221:GLU:O	2:O:223:PHE:N	2.50	0.44
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.99	0.44
8:U:65:ARG:O	8:U:69:VAL:HG23	2.17	0.44
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.47	0.44
1:A:170:THR:HG22	1:A:171:THR:H	1.80	0.44
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.18	0.44
2:B:353:THR:HG22	2:B:354:GLU:N	2.32	0.44
5:E:3:ASN:H	5:E:3:ASN:ND2	2.15	0.44
7:G:48:VAL:O	7:G:51:PRO:HD2	2.17	0.44
14:P:3002:UQ:HM51	14:P:3002:UQ:H8	1.99	0.44
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.52	0.44
4:Q:169:LEU:CD2	4:Q:182:ILE:HD11	2.48	0.44
3:C:358:SER:O	3:C:362:ILE:HG13	2.16	0.44
5:R:75:GLU:O	5:R:75:GLU:HG3	2.17	0.44
3:C:323:GLN:OE1	7:G:47:LYS:HD3	2.18	0.44
3:C:380:TYR:CZ	6:F:37:LEU:HD21	2.53	0.44
12:C:502:HEM:HMC2	12:C:502:HEM:CBC	2.41	0.44
5:E:119:ASP:O	5:E:121:GLN:N	2.49	0.44
5:E:161:HIS:HB2	19:E:501:FES:S1	2.58	0.44
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.47	0.44
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.99	0.44
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.53	0.44
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.99	0.44
5:R:133:VAL:O	5:R:133:VAL:HG13	2.17	0.44
1:A:23:LEU:HD23	1:A:23:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ALA:O	1:A:116:VAL:HG13	2.18	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
3:C:287:ASN:O	3:C:288:LYS:C	2.56	0.44
5:E:171:ILE:O	5:E:171:ILE:HG23	2.17	0.44
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.98	0.44
1:N:243:ALA:O	1:N:425:VAL:HA	2.17	0.44
1:N:365:MET:HG3	1:N:366:VAL:N	2.33	0.44
2:O:361:LYS:HD3	2:O:403:ASP:HA	2.00	0.44
3:P:230:ILE:HG23	11:R:3005:PEE:H25	2.00	0.44
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.32	0.44
2:B:59:THR:CG2	2:B:60:THR:N	2.80	0.44
2:B:104:LYS:HD2	2:B:104:LYS:C	2.38	0.44
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.39	0.44
14:C:2002:UQ:HM51	14:C:2002:UQ:H8	2.00	0.44
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.55	0.43
1:A:281:ASP:OD1	9:I:33:UNK:HB2	2.18	0.43
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.83	0.43
4:D:143:VAL:HG21	4:D:149:TYR:HB2	1.99	0.43
5:E:73:LYS:HB3	5:E:196:GLY:O	2.17	0.43
5:E:97:PHE:O	5:E:134:ILE:HA	2.18	0.43
5:E:136:VAL:HG23	5:E:181:GLU:O	2.17	0.43
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.53	0.43
2:O:227:ARG:HB3	2:O:228:SER:H	1.48	0.43
4:Q:169:LEU:HD22	4:Q:182:ILE:CD1	2.48	0.43
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.99	0.43
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.48	0.43
2:B:341:MET:CE	2:B:417:PHE:HE2	2.14	0.43
3:C:92:PHE:O	3:C:95:ILE:HG22	2.17	0.43
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.85	0.43
4:D:235:MET:HB3	7:G:15:THR:HG22	2.01	0.43
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.51	0.43
2:O:257:VAL:HG22	2:O:424:MET:HG3	2.00	0.43
3:P:121:LEU:O	3:P:125:MET:HG3	2.18	0.43
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.00	0.43
3:P:380:TYR:OH	6:S:34:ASP:OD1	2.32	0.43
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.98	0.43
3:C:46:ILE:HA	12:C:501:HEM:HMC2	2.00	0.43
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.01	0.43
9:I:71:ASN:N	9:I:71:ASN:HD22	2.16	0.43
4:Q:69:GLU:OE1	4:Q:82:MET:HB3	2.18	0.43
4:Q:181:GLN:HA	8:U:77:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.33	0.43
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.82	0.43
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.64	0.43
2:O:345:LYS:HG2	2:O:418:VAL:HG13	2.01	0.43
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.43
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.34	0.43
1:A:130:GLU:O	1:A:134:ILE:HG13	2.18	0.43
2:B:280:GLY:HA3	2:B:293:SER:OG	2.19	0.43
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.43
11:E:2005:PEE:H58	10:J:24:VAL:HG11	2.01	0.43
3:P:156:TYR:C	3:P:158:GLY:H	2.19	0.43
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.48	0.43
2:B:76:THR:HG23	2:B:82:SER:HB2	2.01	0.43
1:N:280:TYR:CG	1:N:281:ASP:N	2.85	0.43
2:O:402:ILE:HG23	2:O:403:ASP:H	1.83	0.43
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.53	0.43
5:R:3:ASN:H	5:R:3:ASN:HD22	1.66	0.43
5:R:170:ARG:HA	5:R:179:ASN:CB	2.45	0.43
1:N:205:HIS:O	1:N:208:LEU:HB3	2.18	0.43
1:N:274:ASN:ND2	1:N:309:THR:HB	2.34	0.43
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.83	0.43
2:B:170:THR:O	2:B:172:LEU:N	2.51	0.43
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.19	0.43
5:E:102:THR:C	5:E:103:GLN:HG3	2.39	0.43
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.01	0.43
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.50	0.43
5:R:96:LEU:HD12	5:R:135:LEU:O	2.19	0.43
3:C:146:VAL:HG21	3:C:269:ILE:HG21	2.00	0.43
4:D:27:ARG:NH1	4:D:55:THR:O	2.52	0.43
5:E:52:LYS:HD3	5:E:52:LYS:O	2.19	0.43
2:O:162:ASN:O	2:O:244:ILE:HD12	2.18	0.43
3:P:129:PHE:CE1	13:P:3001:JZV:HAFB	2.54	0.43
3:P:367:PHE:N	3:P:368:PRO:HD2	2.34	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.54	0.43
8:U:32:LYS:O	8:U:36:ARG:HG3	2.19	0.43
1:A:140:GLU:OE2	9:I:50:LEU:N	2.41	0.43
3:C:155:PRO:O	3:C:157:ILE:N	2.50	0.43
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.54	0.43
5:E:83:GLU:C	5:E:85:LYS:H	2.22	0.43
5:E:127:VAL:CG1	5:E:128:LYS:N	2.78	0.43
10:J:42:ILE:HG22	10:J:46:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:103:SER:HB3	1:N:202:GLY:O	2.19	0.43
2:O:73:SER:N	2:O:74:PRO:CD	2.82	0.43
2:O:221:GLU:HG3	2:O:222:GLN:N	2.26	0.43
3:P:277:PHE:CG	3:P:278:ALA:N	2.86	0.43
1:A:191:LYS:CA	1:A:195:MET:HE2	2.49	0.42
1:A:191:LYS:N	1:A:195:MET:HE2	2.34	0.42
1:A:191:LYS:O	1:A:195:MET:HG3	2.18	0.42
2:B:56:ARG:HB2	2:B:102:ARG:O	2.19	0.42
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.54	0.42
5:E:137:GLY:O	5:E:145:VAL:HG13	2.19	0.42
9:I:31:UNK:O	9:I:32:UNK:O	2.37	0.42
1:N:269:VAL:HG22	1:N:406:MET:CE	2.49	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.42
1:N:436:ARG:HD2	1:N:436:ARG:HA	1.82	0.42
3:P:208:ASN:HB2	3:P:209:PRO:HD2	2.01	0.42
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.53	0.42
5:R:153:PHE:CD1	5:R:153:PHE:N	2.86	0.42
5:R:155:GLY:HA3	5:R:166:ASP:O	2.19	0.42
3:C:286:PRO:O	3:C:287:ASN:CB	2.67	0.42
4:D:69:GLU:OE1	4:D:82:MET:HB3	2.18	0.42
5:E:122:HIS:CE1	5:E:124:LEU:HB2	2.55	0.42
2:B:257:VAL:HG22	2:B:424:MET:HG3	2.01	0.42
2:B:345:LYS:HG2	2:B:418:VAL:HG13	2.02	0.42
3:C:49:GLY:C	12:C:501:HEM:HAC	2.40	0.42
4:D:116:ILE:HG23	4:D:117:VAL:N	2.33	0.42
1:N:90:THR:O	1:N:167:VAL:HG11	2.19	0.42
2:O:96:LEU:H	9:V:70:LEU:HD22	1.84	0.42
3:P:18:SER:CB	3:P:202:HIS:HE1	2.32	0.42
6:S:99:ARG:HH11	6:S:99:ARG:HB3	1.84	0.42
9:V:70:LEU:HD23	9:V:71:ASN:H	1.83	0.42
2:B:52:LYS:O	2:B:203:ARG:NH2	2.46	0.42
2:B:374:THR:HG22	2:B:376:GLN:N	2.33	0.42
5:E:191:ASP:OD2	5:E:191:ASP:N	2.52	0.42
8:H:40:CYS:O	8:H:44:VAL:HG23	2.18	0.42
1:N:27:SER:HA	1:N:199:ALA:O	2.19	0.42
1:A:16:VAL:HA	1:A:25:VAL:O	2.19	0.42
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.35	0.42
1:N:45:SER:HA	1:N:48:GLU:CG	2.49	0.42
1:N:144:ASP:OD2	1:N:147:ASN:ND2	2.52	0.42
1:N:418:LYS:O	1:N:420:PRO:HD3	2.19	0.42
2:O:227:ARG:O	2:O:228:SER:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:353:THR:HG22	2:O:354:GLU:N	2.35	0.42
3:P:5:ILE:O	3:P:5:ILE:HG22	2.20	0.42
3:P:49:GLY:C	12:P:501:HEM:HAC	2.40	0.42
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.48	0.42
5:E:130:PRO:C	5:E:132:TRP:H	2.22	0.42
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.20	0.42
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.84	0.42
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.64	0.42
2:B:22:GLU:O	2:B:23:ASP:OD2	2.38	0.42
9:I:61:ARG:C	9:I:62:ARG:HG3	2.40	0.42
2:O:209:ILE:HD11	2:O:379:LEU:N	2.35	0.42
3:P:101:ARG:C	3:P:101:ARG:CD	2.83	0.42
4:Q:167:GLU:HG2	8:U:13:LEU:HD12	2.01	0.42
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.40	0.42
2:B:144:LEU:HB2	2:B:183:ILE:HD12	2.01	0.42
2:B:287:ARG:NH1	2:B:287:ARG:HG3	2.34	0.42
5:E:122:HIS:O	5:E:125:ASP:HB2	2.19	0.42
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.42
2:O:287:ARG:NH1	2:O:287:ARG:HG3	2.35	0.42
3:P:263:LEU:O	3:P:264:VAL:HG23	2.20	0.42
1:A:17:THR:CG2	1:A:205:HIS:NE2	2.83	0.42
1:A:253:VAL:O	1:A:323:HIS:HA	2.20	0.42
2:B:28:LYS:HG3	2:B:34:ILE:HG12	2.02	0.42
2:B:292:THR:O	2:B:292:THR:CG2	2.66	0.42
2:B:341:MET:HA	2:B:341:MET:HE3	2.00	0.42
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.01	0.42
5:E:75:GLU:HA	5:E:193:VAL:O	2.20	0.42
5:E:162:GLY:O	5:E:163:SER:C	2.58	0.42
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.55	0.42
1:N:4:TYR:CB	2:O:114:ASP:OD2	2.67	0.42
3:P:287:ASN:O	3:P:288:LYS:C	2.58	0.42
1:A:233:ARG:HH21	1:A:316:ASP:HB2	1.83	0.42
2:B:374:THR:HB	2:B:377:GLY:H	1.84	0.42
3:C:150:LEU:HB3	3:C:292:VAL:HG22	2.02	0.42
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.55	0.42
5:E:103:GLN:O	5:E:107:ASN:ND2	2.51	0.42
3:P:150:LEU:HB3	3:P:292:VAL:CG2	2.50	0.42
5:R:77:LYS:HE2	5:R:79:SER:CB	2.49	0.42
6:S:13:MET:O	6:S:17:ARG:HG3	2.19	0.42
10:W:57:HIS:HA	10:W:60:GLU:HB3	2.01	0.42
1:A:304:CYS:HB2	1:A:325:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:81:GLN:OXT	7:G:81:GLN:HG3	2.20	0.41
2:O:403:ASP:C	2:O:405:VAL:H	2.23	0.41
3:P:313:GLN:HE21	6:S:36:THR:HB	1.85	0.41
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.35	0.41
5:R:107:ASN:C	5:R:109:GLU:N	2.73	0.41
5:R:116:LYS:O	5:R:117:LEU:HD23	2.20	0.41
15:C:2004:CDL:HA32	7:G:40:ARG:CB	2.50	0.41
7:G:29:ILE:O	7:G:33:ALA:HB3	2.19	0.41
8:H:50:THR:HG23	8:H:50:THR:O	2.19	0.41
1:N:30:SER:O	1:N:202:GLY:HA2	2.19	0.41
1:N:240:GLU:HA	1:N:422:LEU:O	2.20	0.41
5:E:52:LYS:C	5:E:52:LYS:CD	2.85	0.41
5:E:152:ASP:OD2	5:E:153:PHE:CE1	2.73	0.41
2:O:341:MET:HE2	2:O:341:MET:CA	2.49	0.41
3:P:219:ILE:HD12	3:P:224:TYR:CG	2.55	0.41
5:R:184:THR:HG22	5:R:185:TYR:N	2.35	0.41
1:A:209:VAL:O	1:A:212:ALA:HB3	2.20	0.41
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.02	0.41
1:A:387:GLY:O	1:A:388:ARG:HB3	2.19	0.41
2:B:54:GLY:C	2:B:56:ARG:H	2.22	0.41
3:C:5:ILE:O	3:C:5:ILE:HG22	2.21	0.41
2:O:54:GLY:C	2:O:56:ARG:H	2.23	0.41
2:O:275:LEU:HG	2:O:279:LEU:HD12	2.02	0.41
3:P:9:HIS:CD2	3:P:11:LEU:H	2.38	0.41
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.88	0.41
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.85	0.41
8:U:27:THR:HG22	8:U:29:LYS:N	2.33	0.41
3:C:150:LEU:HB3	3:C:292:VAL:CG2	2.50	0.41
4:D:116:ILE:HG12	17:D:501:HEC:HMA3	2.02	0.41
10:J:56:LYS:HB3	10:J:56:LYS:HE2	1.77	0.41
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.80	0.41
1:N:281:ASP:CB	9:V:33:UNK:HB1	2.50	0.41
4:Q:240:PRO:O	4:Q:241:LYS:C	2.59	0.41
5:R:97:PHE:O	5:R:134:ILE:HA	2.21	0.41
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.35	0.41
6:F:51:PRO:HD2	6:F:54:LEU:HD12	2.01	0.41
8:H:65:ARG:O	8:H:69:VAL:HG23	2.20	0.41
1:N:23:LEU:HD23	1:N:23:LEU:C	2.41	0.41
2:O:169:LYS:HD2	2:O:238:THR:HG21	2.02	0.41
2:O:306:PRO:HA	9:V:52:ARG:CG	2.51	0.41
2:O:307:PHE:CD1	2:O:308:ASP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:395:PRO:O	2:O:398:VAL:CG1	2.69	0.41
5:R:179:ASN:O	5:R:180:LEU:C	2.59	0.41
6:S:91:GLU:HB3	6:S:92:PRO:HD3	2.03	0.41
2:B:399:ALA:O	2:B:402:ILE:CG2	2.65	0.41
8:H:10:GLU:C	8:H:11:GLU:HG3	2.41	0.41
1:N:16:VAL:HA	1:N:25:VAL:O	2.21	0.41
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.39	0.41
1:N:383:LEU:HD23	1:N:388:ARG:HA	2.02	0.41
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.41	0.41
5:R:13:TYR:O	7:T:24:ARG:HG3	2.21	0.41
1:A:26:ALA:O	1:A:198:ALA:HA	2.21	0.41
3:C:367:PHE:N	3:C:368:PRO:HD2	2.36	0.41
3:P:146:VAL:HG21	3:P:269:ILE:HG21	2.03	0.41
13:P:3001:JZV:HAZ	13:P:3001:JZV:HAY	1.81	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.50	0.41
5:R:188:VAL:HG23	5:R:192:LEU:HB2	2.02	0.41
1:A:243:ALA:O	1:A:425:VAL:HA	2.20	0.41
1:A:342:TRP:O	1:A:345:LEU:HB2	2.20	0.41
2:B:262:ALA:O	2:B:320:GLY:HA3	2.20	0.41
2:B:399:ALA:HA	2:B:402:ILE:HG22	2.02	0.41
2:B:403:ASP:C	2:B:405:VAL:H	2.24	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.90	0.41
3:C:271:PRO:HG2	3:C:276:LEU:HD23	2.03	0.41
4:D:21:LEU:HD13	4:D:192:TRP:HB2	2.03	0.41
4:D:165:TYR:CZ	4:D:168:ILE:HG13	2.55	0.41
5:E:151:GLY:O	5:E:154:GLY:N	2.54	0.41
5:E:171:ILE:HG12	5:E:176:ALA:O	2.20	0.41
6:F:32:MET:O	6:F:33:ARG:C	2.58	0.41
1:N:133:VAL:O	1:N:137:GLU:HG3	2.20	0.41
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.51	0.41
2:O:59:THR:CG2	2:O:60:THR:N	2.84	0.41
2:O:169:LYS:CG	2:O:240:TRP:HB2	2.49	0.41
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.21	0.41
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.36	0.41
2:O:318:ASP:O	2:O:319:SER:HB2	2.19	0.41
3:P:45:GLN:CB	12:P:501:HEM:HAB	2.51	0.41
3:P:138:GLN:HA	3:P:138:GLN:OE1	2.21	0.41
3:P:156:TYR:N	3:P:156:TYR:CD2	2.89	0.41
3:P:286:PRO:O	3:P:287:ASN:CB	2.69	0.41
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.56	0.41
4:Q:70:VAL:CG2	4:Q:83:ARG:CZ	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.83	0.41
1:A:45:SER:HA	1:A:48:GLU:CD	2.41	0.41
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.55	0.41
3:C:295:LEU:HD11	13:C:2001:JZV:HAZ	2.02	0.41
2:O:72:ALA:HB1	2:O:75:LEU:HD12	2.03	0.41
3:P:37:LEU:O	3:P:41:CYS:HB2	2.20	0.41
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.83	0.41
5:R:95:PRO:HG2	5:R:145:VAL:CG1	2.51	0.41
1:A:4:TYR:HE2	1:A:396:ASP:OD2	2.04	0.40
1:A:140:GLU:HG2	9:I:50:LEU:HG	2.02	0.40
1:A:276:ILE:HG12	1:A:357:ALA:HB2	2.02	0.40
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.55	0.40
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.56	0.40
2:B:248:ASN:ND2	2:B:250:HIS:H	2.20	0.40
17:D:501:HEC:HAD1	17:D:501:HEC:HMD1	1.92	0.40
5:E:75:GLU:HG3	5:E:75:GLU:O	2.21	0.40
2:O:372:VAL:HG13	2:O:378:LEU:HA	2.03	0.40
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.02	0.40
5:R:134:ILE:HB	5:R:185:TYR:CE1	2.56	0.40
6:S:60:PHE:O	6:S:64:ARG:HB2	2.20	0.40
4:D:70:VAL:CG2	4:D:83:ARG:CZ	2.99	0.40
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.96	0.40
2:O:56:ARG:HB2	2:O:102:ARG:O	2.21	0.40
1:A:170:THR:CG2	1:A:171:THR:H	2.33	0.40
1:A:354:VAL:HG23	1:A:355:LYS:N	2.35	0.40
5:E:109:GLU:OE1	5:E:109:GLU:HA	2.21	0.40
5:E:115:SER:CB	5:E:116:LYS:HD2	2.52	0.40
1:N:62:LEU:O	1:N:64:PHE:N	2.55	0.40
1:N:253:VAL:O	1:N:323:HIS:HA	2.20	0.40
1:N:343:MET:O	1:N:347:THR:HG23	2.21	0.40
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.36	0.40
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.21	0.40
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.52	0.40
5:R:121:GLN:O	5:R:170:ARG:NH1	2.45	0.40
13:C:2001:JZV:HAZ	13:C:2001:JZV:HAY	1.80	0.40
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.51	0.40
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.57	0.40
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.03	0.40
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.36	0.40
3:P:263:LEU:C	3:P:264:VAL:HG23	2.41	0.40
4:Q:79:GLU:OE2	4:Q:79:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:106:ILE:HG21	5:R:130:PRO:HB3	2.02	0.40
5:R:194:VAL:O	5:R:194:VAL:HG12	2.21	0.40
2:B:217:LYS:HE2	2:B:221:GLU:OE2	2.21	0.40
2:B:276:GLN:HG2	2:B:281:ALA:HB2	2.03	0.40
2:B:341:MET:HA	2:B:341:MET:HE2	2.02	0.40
2:B:370:MET:O	2:B:373:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	442/446 (99%)	414 (94%)	22 (5%)	6 (1%)	11 19
1	N	440/446 (99%)	414 (94%)	19 (4%)	7 (2%)	9 16
2	B	418/441 (95%)	358 (86%)	46 (11%)	14 (3%)	4 5
2	O	420/441 (95%)	370 (88%)	40 (10%)	10 (2%)	6 9
3	C	378/380 (100%)	363 (96%)	10 (3%)	5 (1%)	12 21
3	P	377/380 (99%)	358 (95%)	14 (4%)	5 (1%)	12 21
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100 100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	34 53
5	E	194/196 (99%)	152 (78%)	28 (14%)	14 (7%)	1 1
5	R	194/196 (99%)	165 (85%)	22 (11%)	7 (4%)	3 5
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100 100
6	S	99/110 (90%)	91 (92%)	8 (8%)	0	100 100
7	G	78/81 (96%)	69 (88%)	6 (8%)	3 (4%)	3 4
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	5 8
8	H	68/77 (88%)	64 (94%)	4 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	U	65/77 (84%)	60 (92%)	3 (5%)	2 (3%)	4 6
9	I	29/47 (62%)	27 (93%)	2 (7%)	0	100 100
9	V	29/47 (62%)	28 (97%)	1 (3%)	0	100 100
10	J	59/61 (97%)	58 (98%)	1 (2%)	0	100 100
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9 16
All	All	4002/4160 (96%)	3659 (91%)	266 (7%)	77 (2%)	8 14

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY
2	B	21	ALA
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	228	SER
3	C	287	ASN
5	E	127	VAL
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
5	R	163	SER
8	U	52	GLU
10	W	61	ALA
1	A	282	ARG
2	B	231	GLY
5	E	80	ASP
5	E	102	THR
5	E	115	SER
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	282	ARG

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Mol	Chain	Res	Type
2	O	24	LEU
2	O	222	GLN
5	R	185	TYR
5	R	191	ASP
8	U	49	HIS
1	A	72	CYS
2	B	389	SER
5	E	137	GLY
1	N	63	ALA
1	N	72	CYS
1	N	262	TRP
1	N	433	ASP
2	O	372	VAL
2	O	389	SER
3	P	156	TYR
5	R	186	GLN
7	T	33	ALA
1	A	262	TRP
1	A	433	ASP
2	B	372	VAL
2	B	386	ALA
3	C	3	PRO
5	E	154	GLY
2	O	19	PRO
3	P	3	PRO
3	P	157	ILE
5	R	154	GLY
2	B	201	SER
2	B	221	GLU
2	B	371	SER
3	C	156	TYR
5	E	166	ASP
7	G	33	ALA
1	N	443	TRP
5	E	120	PRO
5	E	150	SER
7	G	61	TRP
2	O	55	SER
2	O	330	ALA
3	C	158	GLY
1	A	71	PRO
3	C	264	VAL

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Mol	Chain	Res	Type
5	R	137	GLY
3	P	264	VAL
5	R	127	VAL
7	T	50	PRO
7	G	50	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	354 (97%)	11 (3%)	41	61
1	N	365/368 (99%)	352 (96%)	13 (4%)	35	55
2	B	331/347 (95%)	321 (97%)	10 (3%)	41	61
2	O	333/347 (96%)	324 (97%)	9 (3%)	44	65
3	C	328/329 (100%)	320 (98%)	8 (2%)	49	68
3	P	328/329 (100%)	322 (98%)	6 (2%)	59	75
4	D	200/200 (100%)	197 (98%)	3 (2%)	65	78
4	Q	200/200 (100%)	197 (98%)	3 (2%)	65	78
5	E	166/166 (100%)	161 (97%)	5 (3%)	41	61
5	R	165/166 (99%)	161 (98%)	4 (2%)	49	68
6	F	93/96 (97%)	88 (95%)	5 (5%)	22	38
6	S	93/96 (97%)	88 (95%)	5 (5%)	22	38
7	G	71/71 (100%)	69 (97%)	2 (3%)	43	63
7	T	70/71 (99%)	69 (99%)	1 (1%)	67	79
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	62	77
9	I	23/26 (88%)	20 (87%)	3 (13%)	4	6
9	V	23/26 (88%)	20 (87%)	3 (13%)	4	6
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	72
10	W	47/49 (96%)	46 (98%)	1 (2%)	53	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3378/3446 (98%)	3284 (97%)	94 (3%)	43 63

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	86	PHE
1	A	106	MET
1	A	179	ARG
1	A	281	ASP
1	A	307	PHE
1	A	352	SER
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	104	LYS
2	B	170	THR
2	B	193	HIS
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	341	MET
2	B	402	ILE
3	C	81	ARG
3	C	91	PHE
3	C	184	PHE
3	C	216	SER
3	C	223	PRO
3	C	256	ASN
3	C	367	PHE
3	C	380	TYR
4	D	70	VAL
4	D	169	LEU
4	D	203	ARG
5	E	31	ASP
5	E	52	LYS
5	E	131	GLU
5	E	178	TYR
5	E	185	TYR

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Mol	Chain	Res	Type
6	F	52	GLU
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
6	F	73	ARG
7	G	4	PHE
7	G	50	PRO
9	I	68	ILE
9	I	70	LEU
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	179	ARG
1	N	281	ASP
1	N	307	PHE
1	N	352	SER
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	104	LYS
2	O	193	HIS
2	O	248	ASN
2	O	250	HIS
2	O	325	TYR
2	O	341	MET
2	O	402	ILE
3	P	81	ARG
3	P	91	PHE
3	P	184	PHE
3	P	216	SER
3	P	256	ASN
3	P	380	TYR
4	Q	70	VAL
4	Q	169	LEU
4	Q	203	ARG

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Mol	Chain	Res	Type
5	R	31	ASP
5	R	52	LYS
5	R	178	TYR
5	R	185	TYR
6	S	13	MET
6	S	52	GLU
6	S	58	ARG
6	S	64	ARG
6	S	70	LEU
7	T	4	PHE
8	U	49	HIS
9	V	58	ARG
9	V	68	ILE
9	V	75	SER
10	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	85	HIS
1	A	267	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	311	ASN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	17	ASN
3	C	69	HIS

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Mol	Chain	Res	Type
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	3	ASN
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	32	GLN
1	N	85	HIS
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	267	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	311	ASN
1	N	339	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS

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Mol	Chain	Res	Type
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
5	R	3	ASN
5	R	57	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

29 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	$\#\|Z\|>2$
16	GOL	P	3011	-	5,5,5	1.38	1 (20%)	5,5,5	0.65	0
18	BOG	Q	3009	-	20,20,20	0.98	1 (5%)	25,25,25	0.89	1 (4%)
19	FES	R	501	5	0,4,4	-	-	-		
15	CDL	P	3004	-	39,39,99	1.21	2 (5%)	45,51,111	1.11	4 (8%)
12	HEM	P	501	3	41,50,50	1.59	6 (14%)	45,82,82	1.46	7 (15%)
11	PEE	P	3007	-	48,48,50	1.39	7 (14%)	51,53,55	0.82	2 (3%)
19	FES	E	501	5	0,4,4	-	-	-		
15	CDL	C	2004	-	39,39,99	1.20	2 (5%)	45,51,111	1.09	3 (6%)
17	HEC	D	501	4	32,50,50	1.68	3 (9%)	24,82,82	1.21	2 (8%)
18	BOG	Q	3091	-	13,13,20	1.41	2 (15%)	18,18,25	1.13	2 (11%)
11	PEE	E	2005	-	49,49,50	1.54	10 (20%)	52,54,55	0.88	3 (5%)
14	UQ	C	2002	-	19,19,63	2.71	10 (52%)	23,26,79	1.28	3 (13%)
16	GOL	C	2011	-	5,5,5	1.27	0	5,5,5	0.61	0
14	UQ	P	3002	-	19,19,63	2.69	10 (52%)	23,26,79	1.28	3 (13%)
12	HEM	C	501	3	41,50,50	1.49	4 (9%)	45,82,82	1.60	12 (26%)
12	HEM	P	502	3	41,50,50	1.65	6 (14%)	45,82,82	1.71	9 (20%)
11	PEE	A	2008	-	20,20,50	1.86	6 (30%)	23,25,55	0.67	0
11	PEE	N	3008	-	4,4,50	3.61	4 (100%)	6,6,55	0.65	0
13	JZV	C	2001	-	30,30,30	1.92	5 (16%)	40,41,41	3.73	11 (27%)
11	PEE	C	2007	-	48,48,50	1.42	7 (14%)	51,53,55	0.85	2 (3%)
18	BOG	P	2010	-	12,12,20	1.37	2 (16%)	17,17,25	0.58	0
12	HEM	C	502	3	41,50,50	1.71	7 (17%)	45,82,82	1.91	12 (26%)
18	BOG	D	2009	-	20,20,20	0.95	2 (10%)	25,25,25	0.82	2 (8%)
13	JZV	P	3001	-	30,30,30	1.96	5 (16%)	40,41,41	3.82	11 (27%)
15	CDL	D	2003	-	41,41,99	1.20	4 (9%)	47,53,111	1.03	2 (4%)
18	BOG	D	2091	-	13,13,20	1.31	2 (15%)	18,18,25	1.10	2 (11%)
17	HEC	Q	501	4	32,50,50	2.10	3 (9%)	24,82,82	1.34	2 (8%)
15	CDL	Q	3003	-	41,41,99	1.20	2 (4%)	47,53,111	1.04	2 (4%)
11	PEE	R	3005	-	49,49,50	1.51	10 (20%)	52,54,55	0.87	3 (5%)

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
16	GOL	P	3011	-	-	3/4/4/4	-
18	BOG	Q	3009	-	-	5/11/31/31	0/1/1/1
19	FES	R	501	5	-	-	0/1/1/1
15	CDL	P	3004	-	-	21/49/49/110	-
12	HEM	P	501	3	-	4/12/54/54	-
11	PEE	P	3007	-	-	26/52/52/54	-
19	FES	E	501	5	-	-	0/1/1/1
15	CDL	C	2004	-	-	21/49/49/110	-
17	HEC	D	501	4	-	6/10/54/54	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
11	PEE	E	2005	-	-	27/53/53/54	-
14	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
16	GOL	C	2011	-	-	4/4/4/4	-
14	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
12	HEM	C	501	3	-	6/12/54/54	-
12	HEM	P	502	3	-	6/12/54/54	-
11	PEE	A	2008	-	-	12/24/24/54	-
13	JZV	C	2001	-	-	3/29/29/29	0/2/2/2
11	PEE	C	2007	-	-	23/52/52/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
12	HEM	C	502	3	-	5/12/54/54	-
18	BOG	D	2009	-	-	5/11/31/31	0/1/1/1
13	JZV	P	3001	-	-	3/29/29/29	0/2/2/2
15	CDL	D	2003	-	-	24/51/51/110	-
18	BOG	D	2091	-	-	2/4/24/31	0/1/1/1
17	HEC	Q	501	4	-	6/10/54/54	-
15	CDL	Q	3003	-	-	25/51/51/110	-
11	PEE	R	3005	-	-	27/53/53/54	-

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C2B-C3B	-7.39	1.33	1.40
17	Q	501	HEC	C3C-C2C	-7.29	1.33	1.40
17	D	501	HEC	C3C-C2C	-6.41	1.34	1.40
13	P	3001	JZV	CAT-CAS	-6.21	1.39	1.49
13	C	2001	JZV	CAT-CAS	-6.00	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	UQ	C7-C6	5.80	1.60	1.51
14	C	2002	UQ	C7-C6	5.65	1.60	1.51
14	C	2002	UQ	C6-C5	5.08	1.44	1.35
11	N	3008	PEE	P-O1P	4.90	1.62	1.50
13	C	2001	JZV	CAI-CAJ	-4.75	1.39	1.48
14	P	3002	UQ	C6-C5	4.75	1.43	1.35
13	P	3001	JZV	CAI-CAJ	-4.71	1.39	1.48
17	D	501	HEC	C2B-C3B	-4.62	1.35	1.40
13	P	3001	JZV	CAS-NAR	4.49	1.33	1.28
11	C	2007	PEE	C39-C38	4.32	1.56	1.31
12	P	501	HEM	CBB-CAB	4.23	1.51	1.30
11	P	3007	PEE	C39-C38	4.16	1.55	1.31
13	C	2001	JZV	CAS-NAR	4.15	1.33	1.28
12	C	502	HEM	CBB-CAB	4.11	1.50	1.30
11	E	2005	PEE	C39-C38	4.06	1.55	1.31
12	P	502	HEM	C3C-CAC	-4.06	1.39	1.47
11	R	3005	PEE	C39-C38	3.99	1.54	1.31
14	P	3002	UQ	C6-C1	3.77	1.57	1.46
12	P	502	HEM	CBB-CAB	3.72	1.48	1.30
12	C	501	HEM	CBB-CAB	3.71	1.48	1.30
12	C	501	HEM	CBC-CAC	3.70	1.53	1.29
14	C	2002	UQ	C6-C1	3.70	1.57	1.46
12	C	501	HEM	C3C-CAC	-3.69	1.40	1.47
12	P	501	HEM	C3C-CAC	-3.63	1.40	1.47
11	R	3005	PEE	O2-C10	3.61	1.44	1.34
11	E	2005	PEE	O3-C30	3.54	1.43	1.33
12	P	501	HEM	CBC-CAC	3.51	1.52	1.29
11	N	3008	PEE	P-O4P	3.45	1.65	1.54
11	P	3007	PEE	O3-C30	3.44	1.43	1.33
12	P	501	HEM	CAB-C3B	-3.41	1.38	1.47
11	C	2007	PEE	O3-C30	3.38	1.43	1.33
12	C	501	HEM	CAB-C3B	-3.37	1.38	1.47
11	A	2008	PEE	O2-C10	3.36	1.43	1.34
11	E	2005	PEE	O2-C10	3.34	1.43	1.34
12	C	502	HEM	C3C-CAC	-3.33	1.41	1.47
11	A	2008	PEE	O3-C30	3.27	1.42	1.33
12	C	502	HEM	C3C-C2C	-3.24	1.35	1.40
14	P	3002	UQ	O3-C3	3.24	1.44	1.36
11	R	3005	PEE	O3-C30	3.24	1.42	1.33
11	C	2007	PEE	P-O1P	3.23	1.62	1.50
12	C	502	HEM	C4D-C3D	3.22	1.50	1.45
12	C	502	HEM	CAB-C3B	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2008	PEE	P-O1P	3.17	1.62	1.50
11	N	3008	PEE	P-O3P	3.17	1.64	1.54
14	C	2002	UQ	O3-C3	3.17	1.44	1.36
13	C	2001	JZV	OAQ-NAR	-3.15	1.36	1.42
11	R	3005	PEE	P-O1P	3.15	1.62	1.50
11	E	2005	PEE	P-O1P	3.13	1.62	1.50
12	P	501	HEM	C3C-C2C	-3.11	1.36	1.40
12	P	502	HEM	CAB-C3B	-3.08	1.39	1.47
12	P	502	HEM	CBC-CAC	3.07	1.49	1.29
13	P	3001	JZV	OAQ-NAR	-3.06	1.36	1.42
14	P	3002	UQ	C7-C8	3.05	1.55	1.50
12	C	502	HEM	CBC-CAC	3.01	1.49	1.29
11	C	2007	PEE	C21-C22	-2.99	1.34	1.51
14	C	2002	UQ	C2-C1	2.98	1.57	1.48
11	P	3007	PEE	C21-C22	-2.97	1.34	1.51
11	P	3007	PEE	P-O1P	2.96	1.61	1.50
14	C	2002	UQ	C7-C8	2.90	1.54	1.50
11	R	3005	PEE	C21-C22	-2.88	1.35	1.51
14	C	2002	UQ	CM5-C5	2.87	1.56	1.50
11	E	2005	PEE	C21-C22	-2.83	1.35	1.51
13	P	3001	JZV	CAJ-NAD	2.76	1.33	1.29
14	C	2002	UQ	O2-C2	2.76	1.43	1.36
11	P	3007	PEE	O2-C10	2.73	1.42	1.34
14	P	3002	UQ	C2-C1	2.73	1.56	1.48
11	C	2007	PEE	O2-C10	2.70	1.41	1.34
13	C	2001	JZV	CAJ-NAD	2.62	1.33	1.29
14	P	3002	UQ	CM5-C5	2.61	1.56	1.50
11	E	2005	PEE	C3-C2	2.60	1.58	1.50
14	P	3002	UQ	O2-C2	2.55	1.43	1.36
14	P	3002	UQ	C3-C4	2.55	1.56	1.48
14	P	3002	UQ	C5-C4	2.54	1.56	1.47
11	E	2005	PEE	C31-C30	2.53	1.58	1.50
18	Q	3091	BOG	O5-C1	2.50	1.48	1.41
14	C	2002	UQ	C5-C4	2.49	1.56	1.47
11	N	3008	PEE	P-O2P	2.49	1.62	1.54
11	E	2005	PEE	C1-C2	2.47	1.58	1.50
18	P	2010	BOG	C4-C5	2.46	1.58	1.53
11	A	2008	PEE	C3-C2	2.46	1.58	1.50
11	R	3005	PEE	C11-C10	2.43	1.57	1.50
11	R	3005	PEE	C3-C2	2.42	1.58	1.50
17	D	501	HEC	C2A-C1A	2.39	1.48	1.42
18	D	2091	BOG	C4-C5	2.39	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	2002	UQ	C3-C4	2.38	1.55	1.48
11	R	3005	PEE	C1-C2	2.38	1.58	1.50
12	C	502	HEM	CMB-C2B	2.37	1.55	1.50
11	C	2007	PEE	C31-C30	2.37	1.57	1.50
18	Q	3091	BOG	C4-C5	2.37	1.58	1.53
11	R	3005	PEE	C31-C30	2.33	1.57	1.50
18	D	2091	BOG	O5-C1	2.32	1.47	1.41
11	E	2005	PEE	C11-C10	2.31	1.57	1.50
15	P	3004	CDL	O1-C1	2.31	1.50	1.43
11	A	2008	PEE	C1-C2	2.30	1.57	1.50
15	C	2004	CDL	O1-C1	2.28	1.50	1.43
15	D	2003	CDL	OA6-CA5	2.27	1.40	1.34
18	Q	3009	BOG	O5-C1	2.26	1.47	1.41
15	C	2004	CDL	CB3-CB4	2.25	1.57	1.50
11	P	3007	PEE	C31-C30	2.24	1.57	1.50
11	C	2007	PEE	C3-C2	2.20	1.57	1.50
11	A	2008	PEE	C11-C10	2.20	1.57	1.50
12	P	502	HEM	C4D-C3D	2.19	1.48	1.45
18	P	2010	BOG	C1-C2	2.16	1.57	1.52
15	Q	3003	CDL	O1-C1	2.15	1.49	1.43
11	P	3007	PEE	C3-C2	2.12	1.57	1.50
17	Q	501	HEC	C2A-C1A	2.11	1.47	1.42
12	P	501	HEM	CHD-C1D	-2.10	1.35	1.41
18	D	2009	BOG	O5-C1	2.09	1.47	1.41
15	D	2003	CDL	O1-C1	2.09	1.49	1.43
15	D	2003	CDL	CA3-CA4	2.09	1.57	1.50
15	P	3004	CDL	OB2-CB2	-2.08	1.36	1.44
11	R	3005	PEE	O2-C2	2.08	1.51	1.46
18	D	2009	BOG	C1-C2	2.08	1.58	1.52
11	E	2005	PEE	P-O4P	2.08	1.67	1.59
15	D	2003	CDL	OB8-CB7	2.05	1.39	1.33
15	Q	3003	CDL	OB2-CB2	-2.03	1.37	1.44
16	P	3011	GOL	O2-C2	2.03	1.49	1.43
12	P	502	HEM	CHB-C1B	2.01	1.40	1.35

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	3001	JZV	OAQ-NAR-CAS	14.28	133.72	111.91
13	C	2001	JZV	OAQ-NAR-CAS	12.49	131.00	111.91
13	P	3001	JZV	CAT-CAS-NAR	10.28	133.75	115.28
13	C	2001	JZV	CAT-CAS-NAR	10.15	133.53	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	2001	JZV	CAY-CAS-NAR	-9.97	108.61	123.88
13	P	3001	JZV	CAY-CAS-NAR	-9.42	109.46	123.88
13	P	3001	JZV	OAE-NAD-CAJ	7.88	119.95	111.28
13	C	2001	JZV	OAE-NAD-CAJ	7.50	119.53	111.28
13	C	2001	JZV	OAL-CAK-CAJ	6.49	119.30	111.83
13	P	3001	JZV	OAL-CAK-CAJ	6.41	119.21	111.83
13	C	2001	JZV	CAP-OAQ-NAR	5.58	114.91	107.90
12	C	502	HEM	CAD-C3D-C4D	4.88	133.19	124.66
12	C	502	HEM	C3B-C2B-C1B	-4.82	102.91	106.49
13	C	2001	JZV	OAQ-CAP-CAH	4.69	122.17	109.83
13	P	3001	JZV	CAP-OAQ-NAR	4.43	113.48	107.90
12	P	502	HEM	C2C-C3C-C4C	-4.40	103.82	106.90
17	Q	501	HEC	CBA-CAA-C2A	4.31	119.88	112.60
12	P	502	HEM	CAD-C3D-C4D	4.30	132.17	124.66
12	C	502	HEM	C2C-C3C-C4C	-3.98	104.12	106.90
12	P	502	HEM	C3B-C2B-C1B	-3.89	103.60	106.49
14	P	3002	UQ	C8-C7-C6	3.78	122.23	112.05
12	P	501	HEM	CAD-C3D-C4D	3.74	131.20	124.66
13	P	3001	JZV	OAQ-CAP-CAH	3.74	119.66	109.83
14	C	2002	UQ	C8-C7-C6	3.71	122.06	112.05
18	Q	3091	BOG	C1'-O1-C1	3.60	118.83	113.27
18	D	2091	BOG	C1'-O1-C1	3.34	118.43	113.27
12	C	502	HEM	C2B-C1B-NB	3.32	113.78	109.84
12	C	502	HEM	C2D-C1D-ND	3.32	113.86	109.88
18	Q	3009	BOG	C1'-O1-C1	3.29	119.29	113.84
12	P	501	HEM	CAD-C3D-C2D	-3.25	121.83	127.88
12	C	501	HEM	CAD-C3D-C4D	3.23	130.31	124.66
15	P	3004	CDL	CB4-OB6-CB5	-3.17	109.98	117.79
12	C	501	HEM	C2D-C1D-ND	3.15	113.65	109.88
11	E	2005	PEE	C22-C21-C20	3.13	127.44	113.79
11	R	3005	PEE	C22-C21-C20	3.11	127.34	113.79
17	D	501	HEC	CBA-CAA-C2A	3.10	117.83	112.60
11	C	2007	PEE	C22-C21-C20	3.09	127.27	113.79
12	C	502	HEM	C4D-ND-C1D	-3.08	101.89	105.07
12	C	501	HEM	C3B-C2B-C1B	-3.04	104.23	106.49
11	P	3007	PEE	C22-C21-C20	3.03	126.98	113.79
12	C	502	HEM	C4C-CHD-C1D	3.01	126.53	122.56
12	C	501	HEM	CAD-C3D-C2D	-3.01	122.27	127.88
14	C	2002	UQ	C7-C6-C1	-2.97	114.90	118.48
15	C	2004	CDL	CA4-OA6-CA5	-2.94	110.55	117.79
15	C	2004	CDL	CB4-OB6-CB5	-2.94	110.56	117.79
12	C	502	HEM	CAD-C3D-C2D	-2.93	122.42	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	2001	JZV	OAN-CAK-CAJ	-2.90	119.51	123.46
13	P	3001	JZV	CAP-CAH-CAI	2.87	126.23	121.96
14	P	3002	UQ	C7-C6-C1	-2.80	115.10	118.48
17	Q	501	HEC	CAA-C2A-C3A	-2.77	119.28	127.25
15	P	3004	CDL	CA4-OA6-CA5	-2.76	110.99	117.79
12	C	501	HEM	CBA-CAA-C2A	-2.76	107.91	112.62
12	P	502	HEM	C2B-C1B-NB	2.72	113.07	109.84
12	P	501	HEM	C4B-CHC-C1C	2.70	126.12	122.56
12	P	501	HEM	C2D-C1D-ND	2.68	113.09	109.88
12	P	502	HEM	C4B-CHC-C1C	2.68	126.09	122.56
12	C	501	HEM	C4B-CHC-C1C	2.66	126.07	122.56
11	C	2007	PEE	C21-C22-C23	2.66	127.92	114.42
12	C	502	HEM	C3D-C4D-ND	2.61	113.07	110.17
13	P	3001	JZV	CAP-CAH-CAG	-2.59	113.89	119.52
13	P	3001	JZV	CAM-OAL-CAK	-2.58	110.99	115.86
11	P	3007	PEE	C21-C22-C23	2.54	127.32	114.42
12	P	502	HEM	C2D-C1D-ND	2.51	112.89	109.88
12	C	501	HEM	CBD-CAD-C3D	2.50	119.58	112.63
12	P	502	HEM	CAD-C3D-C2D	-2.49	123.25	127.88
18	D	2009	BOG	C1'-O1-C1	2.47	117.94	113.84
18	D	2091	BOG	O1-C1-C2	2.46	111.04	108.15
12	C	501	HEM	CMD-C2D-C1D	2.46	128.79	125.04
11	E	2005	PEE	C21-C22-C23	2.46	126.90	114.42
18	Q	3091	BOG	O1-C1-C2	2.45	111.02	108.15
13	P	3001	JZV	OAN-CAK-CAJ	-2.43	120.15	123.46
15	D	2003	CDL	CA6-CA4-CA3	-2.42	106.06	111.79
15	D	2003	CDL	CB4-OB6-CB5	-2.40	111.87	117.79
13	C	2001	JZV	CAP-CAH-CAI	2.40	125.53	121.96
11	R	3005	PEE	C21-C22-C23	2.39	126.55	114.42
15	P	3004	CDL	CA6-CA4-CA3	-2.38	106.16	111.79
15	Q	3003	CDL	CB4-OB6-CB5	-2.37	111.95	117.79
12	P	502	HEM	CMC-C2C-C3C	2.37	129.12	124.68
13	C	2001	JZV	CAM-OAL-CAK	-2.34	111.44	115.86
12	P	501	HEM	CMD-C2D-C1D	2.33	128.59	125.04
15	Q	3003	CDL	CA6-CA4-CA3	-2.33	106.28	111.79
12	C	502	HEM	C4D-C3D-C2D	-2.32	103.51	106.90
12	P	502	HEM	C4C-CHD-C1D	2.31	125.61	122.56
11	E	2005	PEE	O3-C3-C2	2.31	115.16	108.43
11	R	3005	PEE	O3-C3-C2	2.29	115.11	108.43
17	D	501	HEC	CAA-C2A-C3A	-2.29	120.68	127.25
12	P	501	HEM	CBD-CAD-C3D	2.26	118.89	112.63
18	D	2009	BOG	O1-C1-C2	2.23	111.78	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	2004	CDL	CA6-CA4-CA3	-2.22	106.53	111.79
13	C	2001	JZV	CAP-CAH-CAG	-2.20	114.73	119.52
12	C	501	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
12	C	501	HEM	C4D-ND-C1D	-2.20	102.81	105.07
14	C	2002	UQ	C10-C9-C8	-2.20	118.05	123.68
14	P	3002	UQ	C10-C9-C8	-2.16	118.14	123.68
12	C	501	HEM	CMB-C2B-C1B	2.13	128.28	125.04
12	P	501	HEM	CMB-C2B-C1B	2.12	128.27	125.04
12	C	501	HEM	C2B-C1B-NB	2.10	112.33	109.84
12	C	502	HEM	CHA-C4D-ND	-2.07	121.83	124.38
15	P	3004	CDL	OB6-CB4-CB3	2.02	115.73	108.40
12	C	502	HEM	C4B-CHC-C1C	2.02	125.22	122.56

There are no chirality outliers.

All (276) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	C	2007	PEE	C4-O4P-P-O1P
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O2P
11	E	2005	PEE	C4-O4P-P-O1P
11	E	2005	PEE	O4P-C4-C5-N
11	P	3007	PEE	C4-O4P-P-O3P
11	P	3007	PEE	C4-O4P-P-O2P
11	P	3007	PEE	C4-O4P-P-O1P
11	R	3005	PEE	C11-C10-O2-C2
11	R	3005	PEE	C4-O4P-P-O2P
11	R	3005	PEE	C4-O4P-P-O1P
12	C	501	HEM	C2B-C3B-CAB-CBB
14	C	2002	UQ	C1-C6-C7-C8
14	C	2002	UQ	C5-C6-C7-C8
14	C	2002	UQ	C12-C11-C9-C8
14	P	3002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C5-C6-C7-C8
14	P	3002	UQ	C12-C11-C9-C8
15	C	2004	CDL	CB2-C1-CA2-OA2
15	C	2004	CDL	CA3-OA5-PA1-OA3
15	C	2004	CDL	CA3-OA5-PA1-OA4
15	C	2004	CDL	CB3-OB5-PB2-OB3
15	C	2004	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
15	D	2003	CDL	CA2-OA2-PA1-OA5
15	D	2003	CDL	OA6-CA4-CA6-OA8
15	P	3004	CDL	CB2-C1-CA2-OA2
15	P	3004	CDL	CA2-C1-CB2-OB2
15	P	3004	CDL	CA3-OA5-PA1-OA3
15	P	3004	CDL	CA3-OA5-PA1-OA4
15	P	3004	CDL	CB3-OB5-PB2-OB3
15	P	3004	CDL	C51-CB5-OB6-CB4
15	Q	3003	CDL	CA2-OA2-PA1-OA5
15	Q	3003	CDL	OA6-CA4-CA6-OA8
16	C	2011	GOL	O1-C1-C2-C3
16	C	2011	GOL	C1-C2-C3-O3
16	P	3011	GOL	C1-C2-C3-O3
17	D	501	HEC	C1A-C2A-CAA-CBA
17	D	501	HEC	C3A-C2A-CAA-CBA
17	Q	501	HEC	C1A-C2A-CAA-CBA
17	Q	501	HEC	C3A-C2A-CAA-CBA
18	Q	3009	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
11	R	3005	PEE	O5-C30-O3-C3
11	E	2005	PEE	O5-C30-O3-C3
15	C	2004	CDL	OB9-CB7-OB8-CB6
15	P	3004	CDL	OB9-CB7-OB8-CB6
15	D	2003	CDL	C31-CA7-OA8-CA6
15	Q	3003	CDL	C31-CA7-OA8-CA6
11	E	2005	PEE	O4-C10-O2-C2
11	R	3005	PEE	O4-C10-O2-C2
15	C	2004	CDL	OB7-CB5-OB6-CB4
15	P	3004	CDL	OB7-CB5-OB6-CB4
11	A	2008	PEE	O5-C30-O3-C3
11	E	2005	PEE	C31-C30-O3-C3
11	R	3005	PEE	C31-C30-O3-C3
15	C	2004	CDL	OA9-CA7-OA8-CA6
15	P	3004	CDL	OA9-CA7-OA8-CA6
11	A	2008	PEE	C31-C30-O3-C3
15	C	2004	CDL	C71-CB7-OB8-CB6
15	P	3004	CDL	C71-CB7-OB8-CB6
15	C	2004	CDL	C31-CA7-OA8-CA6
15	P	3004	CDL	C31-CA7-OA8-CA6
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
15	C	2004	CDL	O1-C1-CA2-OA2
15	P	3004	CDL	O1-C1-CA2-OA2
18	Q	3091	BOG	O5-C5-C6-O6
15	D	2003	CDL	OA9-CA7-OA8-CA6
15	Q	3003	CDL	OA9-CA7-OA8-CA6
15	Q	3003	CDL	C71-CB7-OB8-CB6
15	D	2003	CDL	C71-CB7-OB8-CB6
18	D	2091	BOG	C2-C1-O1-C1'
15	D	2003	CDL	O1-C1-CA2-OA2
15	Q	3003	CDL	O1-C1-CA2-OA2
11	C	2007	PEE	C10-C11-C12-C13
11	P	3007	PEE	C10-C11-C12-C13
18	D	2009	BOG	C2-C1-O1-C1'
18	D	2091	BOG	O5-C1-O1-C1'
15	P	3004	CDL	C11-CA5-OA6-CA4
15	D	2003	CDL	CB7-C71-C72-C73
15	Q	3003	CDL	CB7-C71-C72-C73
15	C	2004	CDL	C11-CA5-OA6-CA4
15	D	2003	CDL	OB9-CB7-OB8-CB6
18	Q	3091	BOG	C4-C5-C6-O6
15	Q	3003	CDL	OB9-CB7-OB8-CB6
18	D	2009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	O1-C1'-C2'-C3'
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
11	E	2005	PEE	C4-O4P-P-O3P
11	R	3005	PEE	C4-O4P-P-O3P
15	C	2004	CDL	CA3-OA5-PA1-OA2
15	D	2003	CDL	CA3-OA5-PA1-OA2
15	D	2003	CDL	CB2-OB2-PB2-OB5
15	D	2003	CDL	CB3-OB5-PB2-OB2
15	P	3004	CDL	CA3-OA5-PA1-OA2
15	Q	3003	CDL	CA3-OA5-PA1-OA2
15	Q	3003	CDL	CB2-OB2-PB2-OB5
15	Q	3003	CDL	CB3-OB5-PB2-OB2
18	D	2009	BOG	O1-C1'-C2'-C3'
15	C	2004	CDL	OA7-CA5-OA6-CA4
15	P	3004	CDL	OA7-CA5-OA6-CA4
11	C	2007	PEE	C35-C36-C37-C38
11	R	3005	PEE	C34-C35-C36-C37
11	E	2005	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C40-C41-C42-C43
12	C	502	HEM	C4D-C3D-CAD-CBD
11	C	2007	PEE	C40-C41-C42-C43
11	R	3005	PEE	O4P-C4-C5-N
11	P	3007	PEE	C21-C22-C23-C24
11	P	3007	PEE	C33-C34-C35-C36
16	C	2011	GOL	O1-C1-C2-O2
11	C	2007	PEE	C33-C34-C35-C36
11	E	2005	PEE	C39-C40-C41-C42
11	P	3007	PEE	C35-C36-C37-C38
15	C	2004	CDL	CA2-C1-CB2-OB2
11	P	3007	PEE	C20-C21-C22-C23
18	D	2009	BOG	C1'-C2'-C3'-C4'
18	Q	3009	BOG	C1'-C2'-C3'-C4'
11	C	2007	PEE	C15-C16-C17-C18
11	P	3007	PEE	C15-C16-C17-C18
11	R	3005	PEE	C39-C40-C41-C42
11	R	3005	PEE	C30-C31-C32-C33
15	D	2003	CDL	C51-CB5-OB6-CB4
15	Q	3003	CDL	C51-CB5-OB6-CB4
15	D	2003	CDL	OB7-CB5-OB6-CB4
11	C	2007	PEE	C20-C21-C22-C23
11	E	2005	PEE	C20-C21-C22-C23
11	P	3007	PEE	C31-C32-C33-C34
12	P	502	HEM	C4D-C3D-CAD-CBD
15	Q	3003	CDL	OB7-CB5-OB6-CB4
15	C	2004	CDL	CB3-OB5-PB2-OB2
15	P	3004	CDL	CB3-OB5-PB2-OB2
11	E	2005	PEE	O3P-C1-C2-C3
11	R	3005	PEE	O3P-C1-C2-C3
11	P	3007	PEE	C11-C12-C13-C14
11	E	2005	PEE	C30-C31-C32-C33
11	E	2005	PEE	C41-C42-C43-C44
11	R	3005	PEE	C20-C21-C22-C23
11	P	3007	PEE	C43-C44-C45-C46
15	D	2003	CDL	CA3-CA4-CA6-OA8
15	Q	3003	CDL	CA3-CA4-CA6-OA8
11	C	2007	PEE	C31-C32-C33-C34
11	C	2007	PEE	C43-C44-C45-C46
16	C	2011	GOL	O2-C2-C3-O3
16	P	3011	GOL	O2-C2-C3-O3
15	D	2003	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C34-C35-C36-C37
15	Q	3003	CDL	C71-C72-C73-C74
11	C	2007	PEE	C11-C12-C13-C14
11	R	3005	PEE	C23-C24-C25-C26
15	C	2004	CDL	OB5-CB3-CB4-OB6
15	P	3004	CDL	OB5-CB3-CB4-OB6
11	E	2005	PEE	C23-C24-C25-C26
15	C	2004	CDL	O1-C1-CB2-OB2
11	C	2007	PEE	C21-C22-C23-C24
13	P	3001	JZV	CAS-NAR-OAQ-CAP
11	C	2007	PEE	C42-C43-C44-C45
11	R	3005	PEE	C41-C42-C43-C44
11	A	2008	PEE	O3P-C1-C2-C3
15	D	2003	CDL	OB5-CB3-CB4-CB6
15	Q	3003	CDL	OB5-CB3-CB4-CB6
15	P	3004	CDL	O1-C1-CB2-OB2
13	C	2001	JZV	CAY-CAS-NAR-OAQ
13	P	3001	JZV	CAY-CAS-NAR-OAQ
13	C	2001	JZV	CAT-CAS-NAR-OAQ
13	P	3001	JZV	CAT-CAS-NAR-OAQ
11	P	3007	PEE	C42-C43-C44-C45
11	E	2005	PEE	C10-C11-C12-C13
11	P	3007	PEE	C34-C35-C36-C37
15	C	2004	CDL	CB5-C51-C52-C53
11	E	2005	PEE	C43-C44-C45-C46
11	A	2008	PEE	O2-C2-C3-O3
11	A	2008	PEE	C11-C10-O2-C2
14	C	2002	UQ	C12-C11-C9-C10
14	P	3002	UQ	C12-C11-C9-C10
11	R	3005	PEE	C43-C44-C45-C46
11	A	2008	PEE	O4-C10-O2-C2
13	C	2001	JZV	CAS-NAR-OAQ-CAP
11	R	3005	PEE	C10-C11-C12-C13
12	P	501	HEM	C2B-C3B-CAB-CBB
11	R	3005	PEE	C31-C32-C33-C34
11	R	3005	PEE	O3P-C1-C2-O2
15	D	2003	CDL	OB5-CB3-CB4-OB6
15	Q	3003	CDL	OB5-CB3-CB4-OB6
12	C	501	HEM	C4B-C3B-CAB-CBB
12	P	502	HEM	C2D-C3D-CAD-CBD
16	P	3011	GOL	O1-C1-C2-O2
11	A	2008	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
15	C	2004	CDL	CB3-OB5-PB2-OB4
15	D	2003	CDL	CA2-OA2-PA1-OA4
15	D	2003	CDL	CA3-OA5-PA1-OA4
15	D	2003	CDL	CB2-OB2-PB2-OB4
15	D	2003	CDL	CB3-OB5-PB2-OB4
15	P	3004	CDL	CB3-OB5-PB2-OB4
15	Q	3003	CDL	CA3-OA5-PA1-OA4
15	Q	3003	CDL	CB2-OB2-PB2-OB4
15	Q	3003	CDL	CB3-OB5-PB2-OB4
11	E	2005	PEE	C31-C32-C33-C34
11	A	2008	PEE	O3P-C1-C2-O2
11	E	2005	PEE	O3P-C1-C2-O2
11	E	2005	PEE	C11-C12-C13-C14
11	E	2005	PEE	C35-C36-C37-C38
11	R	3005	PEE	C11-C12-C13-C14
11	R	3005	PEE	C19-C20-C21-C22
11	P	3007	PEE	C12-C13-C14-C15
15	C	2004	CDL	OB5-CB3-CB4-CB6
15	P	3004	CDL	OB5-CB3-CB4-CB6
11	E	2005	PEE	C14-C15-C16-C17
11	C	2007	PEE	C12-C13-C14-C15
11	R	3005	PEE	C14-C15-C16-C17
11	A	2008	PEE	C10-C11-C12-C13
11	E	2005	PEE	C19-C20-C21-C22
12	P	502	HEM	CAA-CBA-CGA-O2A
11	R	3005	PEE	C35-C36-C37-C38
12	C	502	HEM	CAA-CBA-CGA-O2A
12	P	501	HEM	CAA-CBA-CGA-O2A
12	P	502	HEM	CAA-CBA-CGA-O1A
12	C	502	HEM	CAA-CBA-CGA-O1A
12	C	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	CAD-CBD-CGD-O1D
11	E	2005	PEE	C1-C2-O2-C10
11	R	3005	PEE	C1-C2-O2-C10
12	P	502	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAA-CBA-CGA-O1A
11	E	2005	PEE	C22-C23-C24-C25
11	E	2005	PEE	C37-C38-C39-C40
11	R	3005	PEE	C37-C38-C39-C40
12	C	501	HEM	CAA-CBA-CGA-O2A
17	Q	501	HEC	CAA-CBA-CGA-O2A
12	C	502	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
17	D	501	HEC	CAD-CBD-CGD-O2D
11	P	3007	PEE	C38-C39-C40-C41
11	E	2005	PEE	C40-C41-C42-C43
11	A	2008	PEE	O3-C30-C31-C32
12	C	501	HEM	CAA-CBA-CGA-O1A
11	P	3007	PEE	O2-C10-C11-C12
11	P	3007	PEE	C19-C20-C21-C22
11	C	2007	PEE	C38-C39-C40-C41
11	R	3005	PEE	C22-C23-C24-C25
17	Q	501	HEC	CAD-CBD-CGD-O2D
11	C	2007	PEE	O2-C10-C11-C12
17	D	501	HEC	CAD-CBD-CGD-O1D
17	Q	501	HEC	CAA-CBA-CGA-O1A
11	A	2008	PEE	C1-C2-C3-O3
12	P	501	HEM	C4B-C3B-CAB-CBB
11	A	2008	PEE	O5-C30-C31-C32
11	C	2007	PEE	O2-C2-C3-O3
11	P	3007	PEE	O2-C2-C3-O3
17	Q	501	HEC	CAD-CBD-CGD-O1D
11	P	3007	PEE	C22-C23-C24-C25
17	D	501	HEC	CAA-CBA-CGA-O2A
15	P	3004	CDL	CB5-C51-C52-C53
12	C	501	HEM	CAD-CBD-CGD-O2D
11	P	3007	PEE	O5-C30-O3-C3
11	C	2007	PEE	O4-C10-C11-C12
11	P	3007	PEE	O4-C10-C11-C12
11	P	3007	PEE	C31-C30-O3-C3
15	Q	3003	CDL	C72-C71-CB7-OB8
18	D	2009	BOG	C4'-C5'-C6'-C7'
17	D	501	HEC	CAA-CBA-CGA-O1A
15	D	2003	CDL	CA3-OA5-PA1-OA3
15	Q	3003	CDL	CA2-OA2-PA1-OA4
15	Q	3003	CDL	CA3-OA5-PA1-OA3
15	Q	3003	CDL	CB3-OB5-PB2-OB3
12	C	501	HEM	CAD-CBD-CGD-O1D
11	R	3005	PEE	C40-C41-C42-C43
18	Q	3009	BOG	C4'-C5'-C6'-C7'
15	D	2003	CDL	C72-C71-CB7-OB8
11	C	2007	PEE	C32-C33-C34-C35
15	D	2003	CDL	C72-C71-CB7-OB9
15	Q	3003	CDL	C72-C71-CB7-OB9

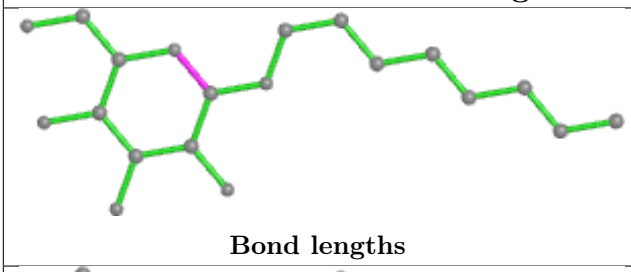
There are no ring outliers.

22 monomers are involved in 66 short contacts:

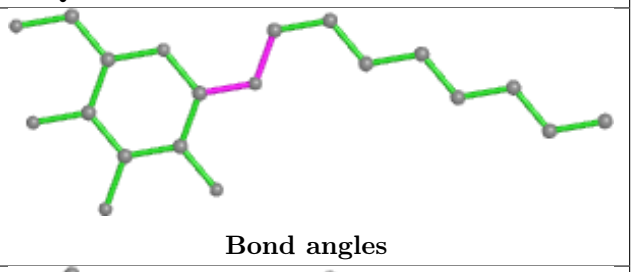
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	R	501	FES	2	0
15	P	3004	CDL	4	0
12	P	501	HEM	4	0
11	P	3007	PEE	3	0
19	E	501	FES	2	0
15	C	2004	CDL	4	0
17	D	501	HEC	3	0
18	Q	3091	BOG	1	0
11	E	2005	PEE	1	0
14	C	2002	UQ	4	0
14	P	3002	UQ	5	0
12	C	501	HEM	5	0
12	P	502	HEM	3	0
13	C	2001	JZV	4	0
11	C	2007	PEE	4	0
18	P	2010	BOG	1	0
12	C	502	HEM	4	0
13	P	3001	JZV	4	0
15	D	2003	CDL	4	0
17	Q	501	HEC	1	0
15	Q	3003	CDL	3	0
11	R	3005	PEE	2	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.

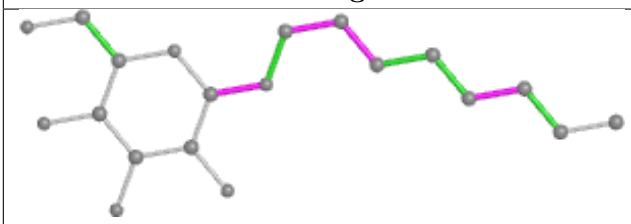
Ligand BOG Q 3009



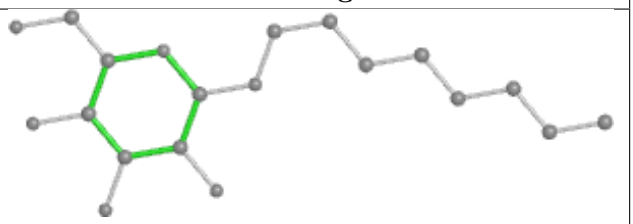
Bond lengths



Bond angles

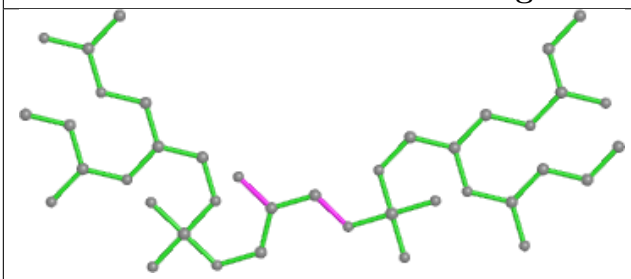


Torsions

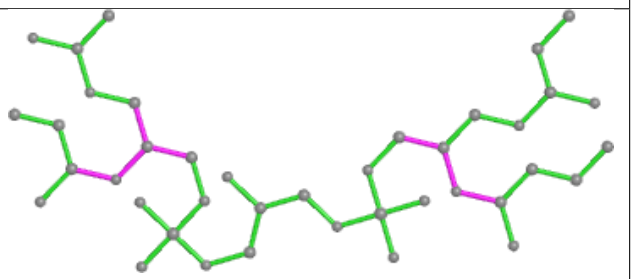


Rings

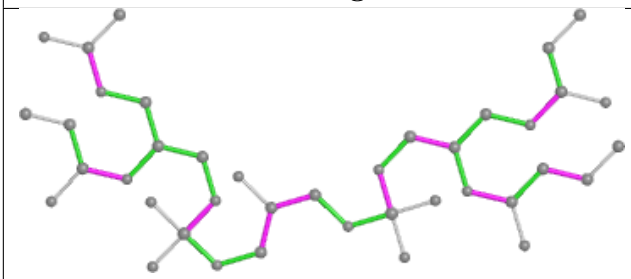
Ligand CDL P 3004



Bond lengths



Bond angles



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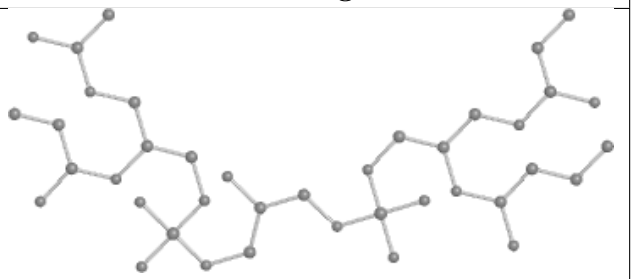
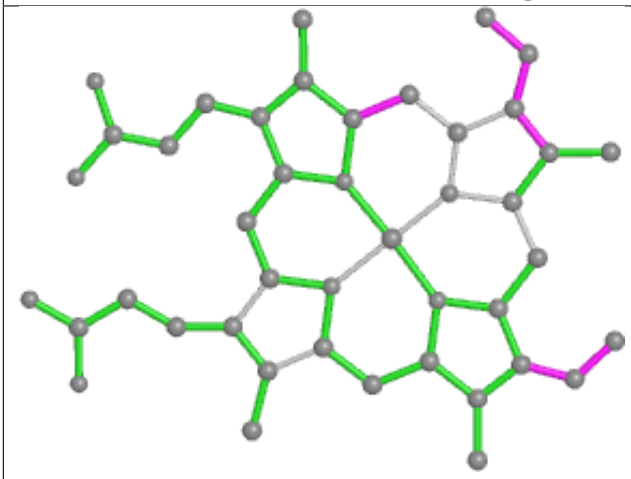


Rings

Ligand HEM P 501



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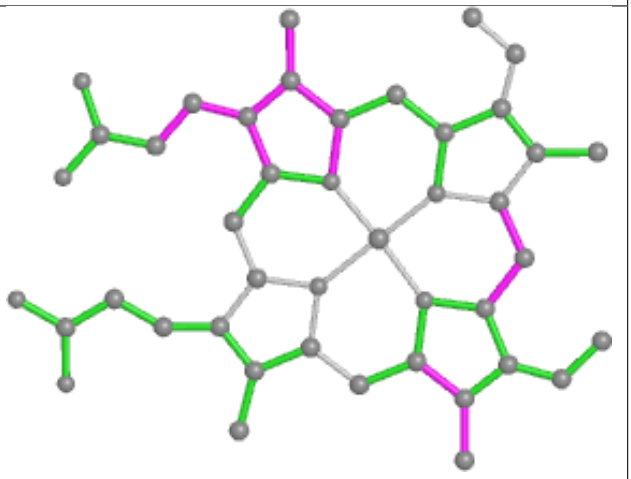
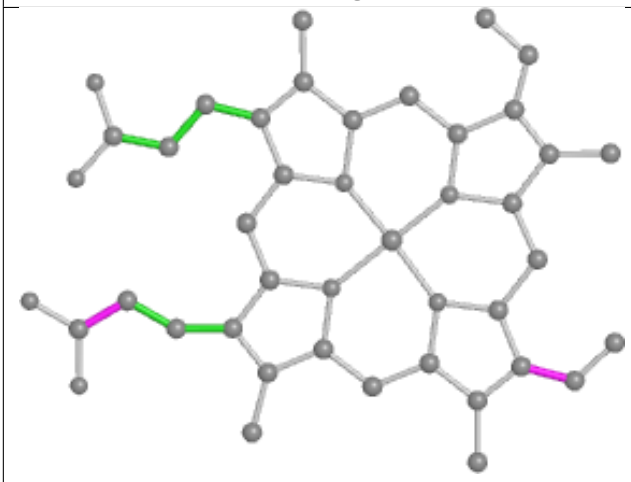
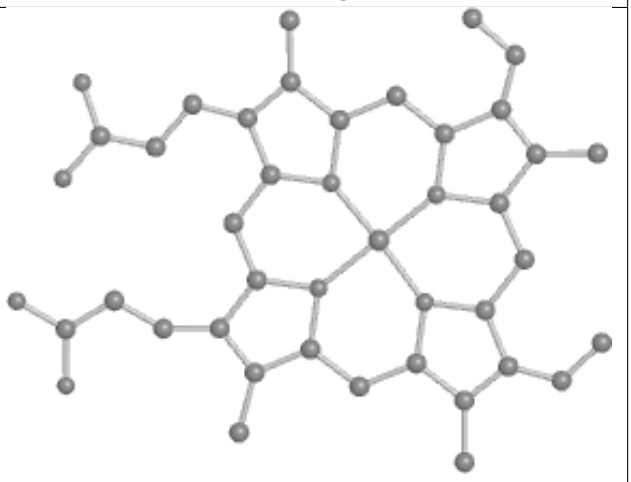


Bond angles

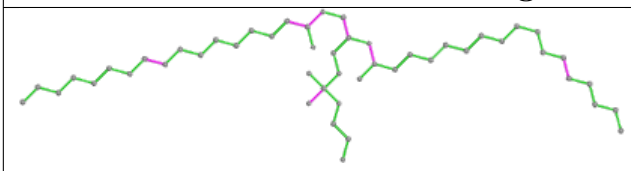


Torsions



Rings

Ligand PEE P 3007



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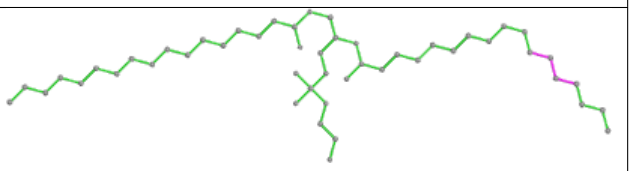
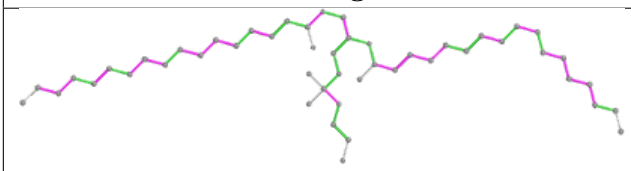


Bond angles



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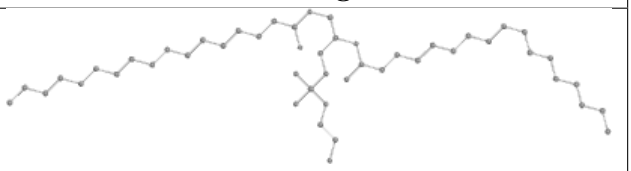
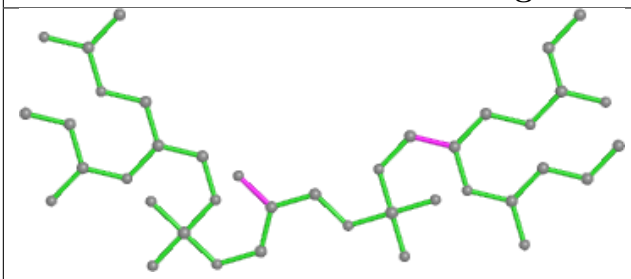


Rings

Ligand CDL C 2004



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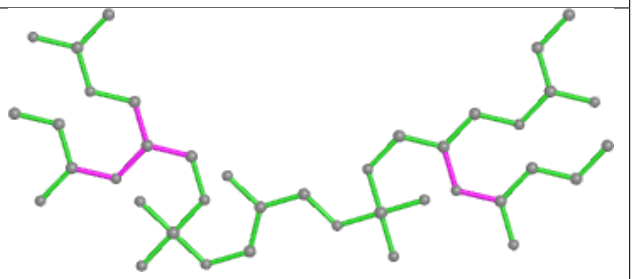

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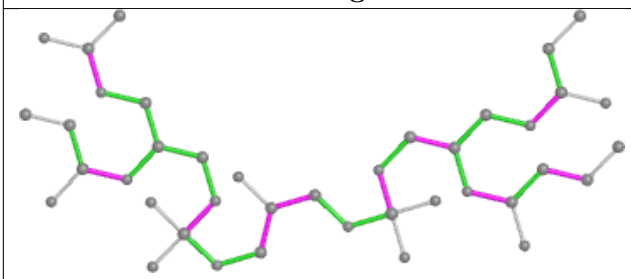

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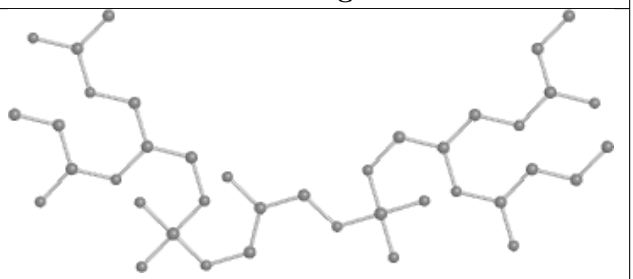
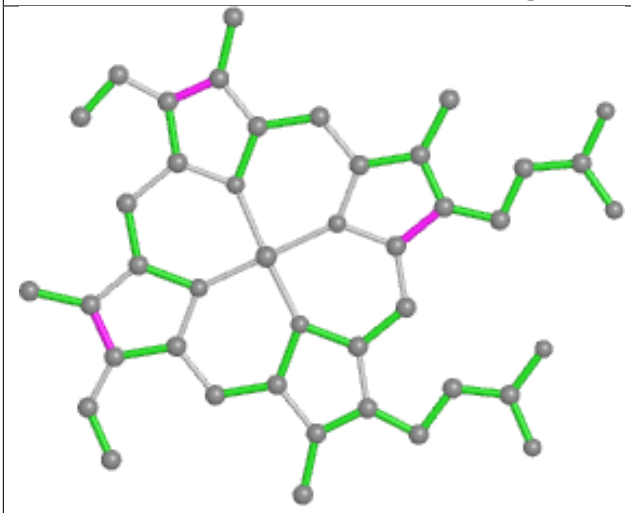


Rings

Ligand HEC D 501



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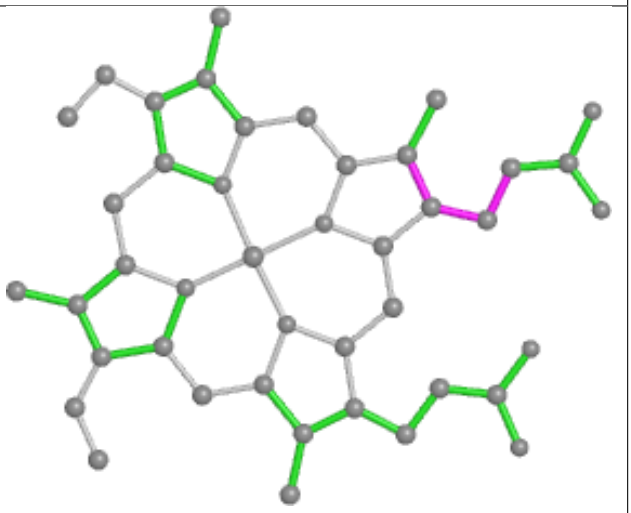

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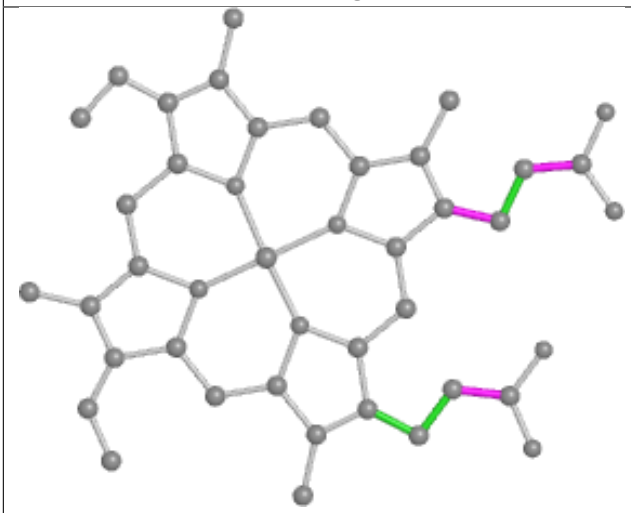

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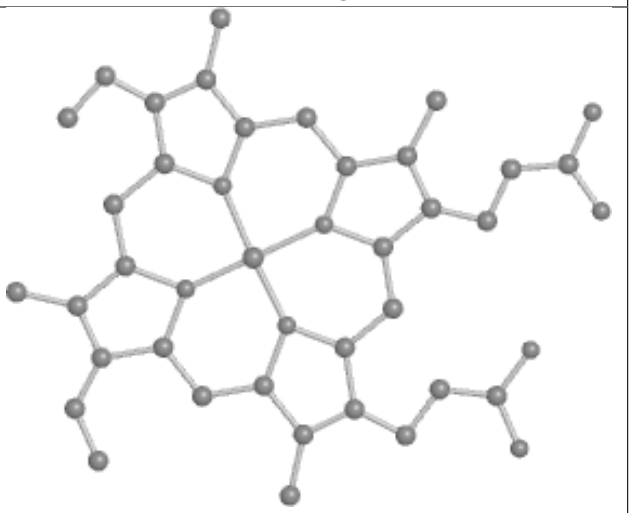
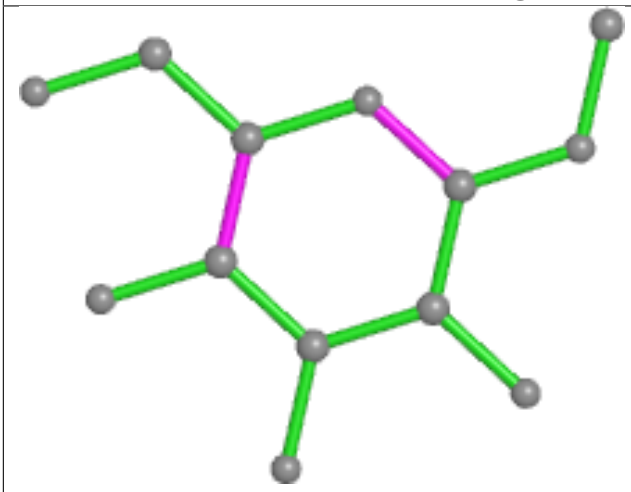


Rings

Ligand BOG Q 3091



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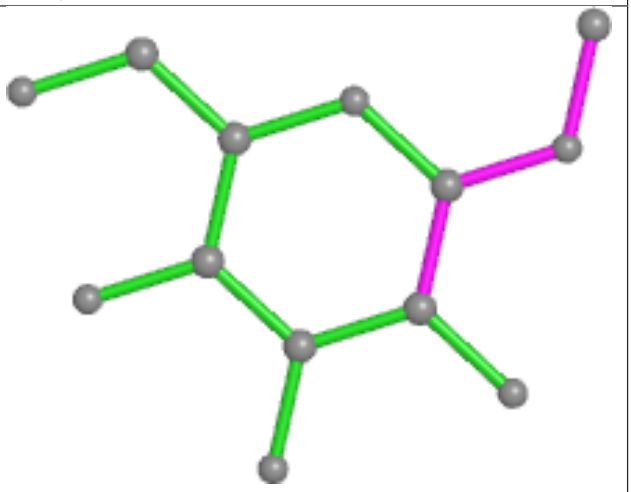

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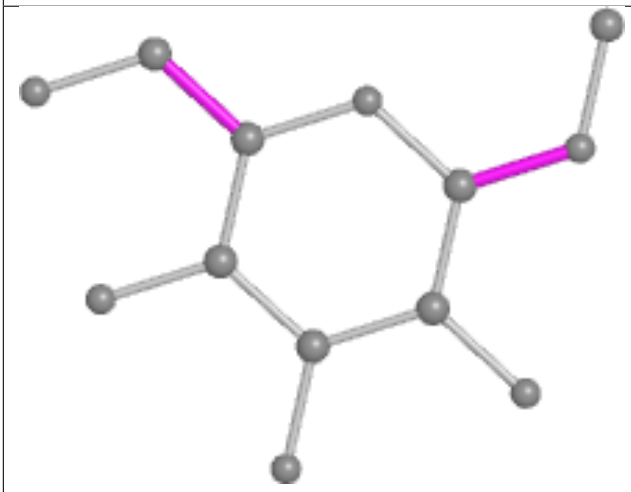

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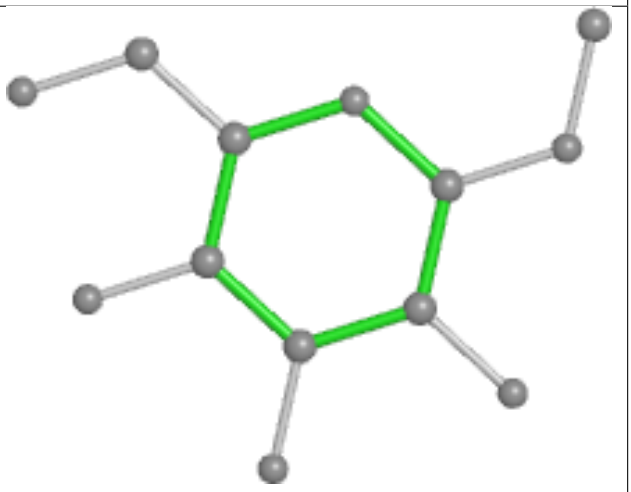
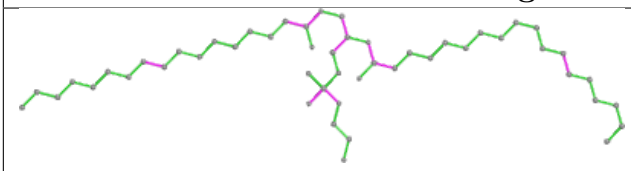


Rings

Ligand PEE E 2005



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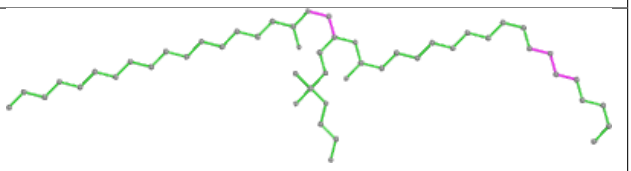
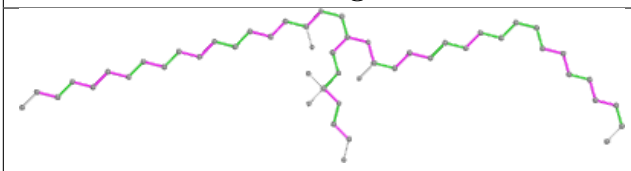
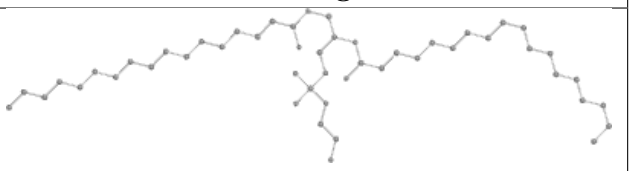


Bond angles

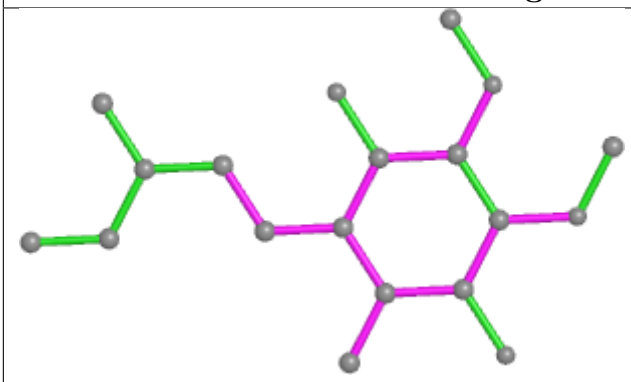


Torsions

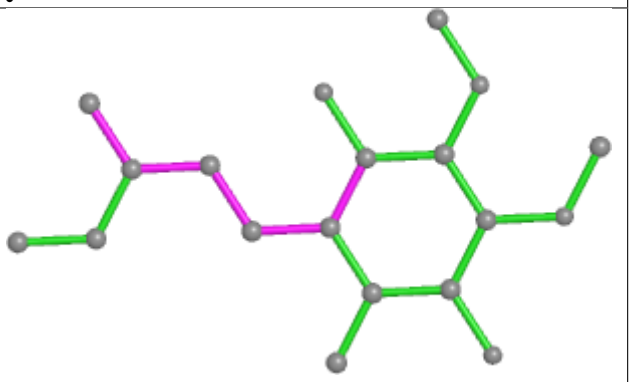


Rings

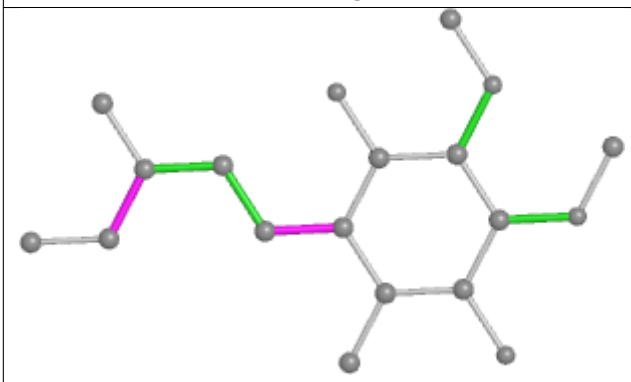
Ligand UQ C 2002



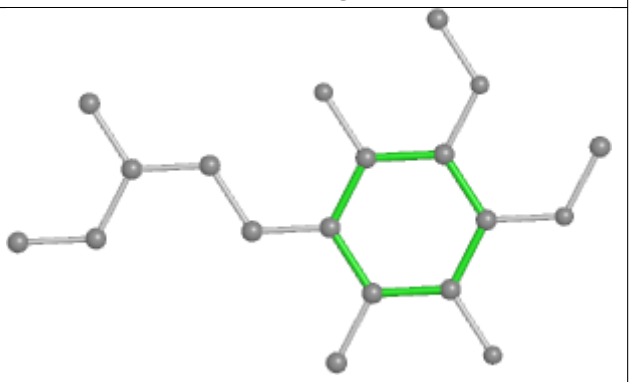
Bond lengths



Bond angles

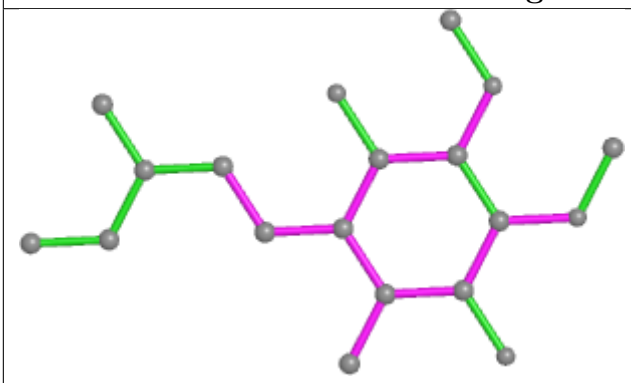


Torsions



Rings

Ligand UQ P 3002



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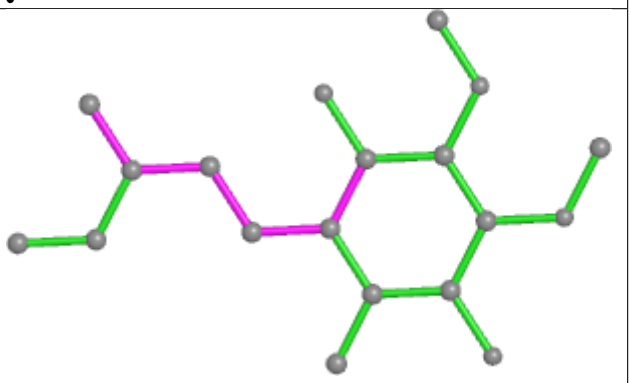
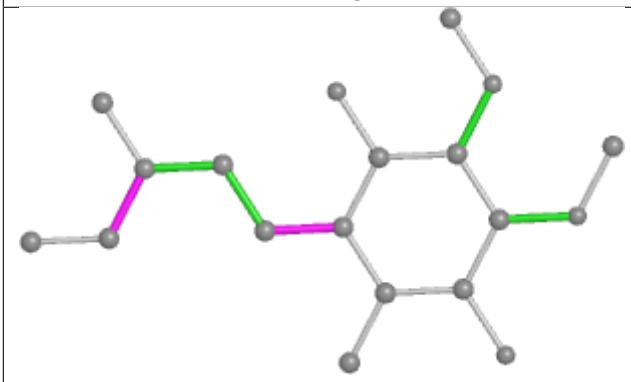
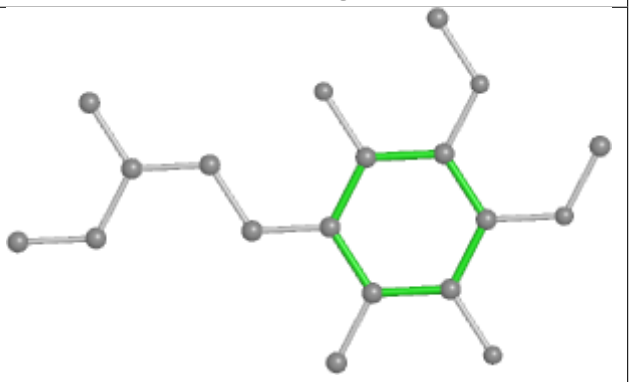


Bond angles

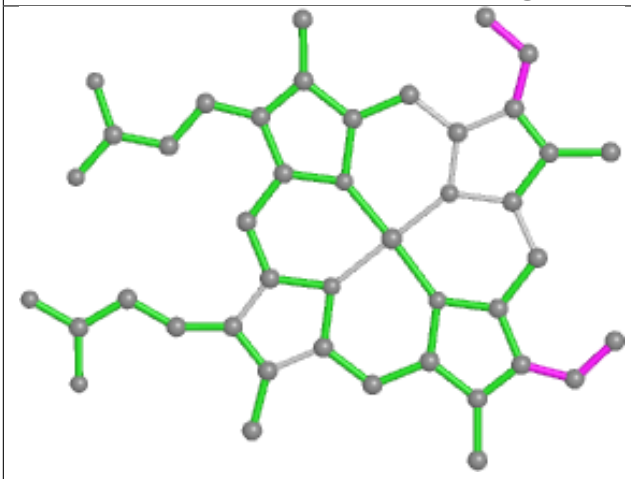


Torsions



Rings

Ligand HEM C 501



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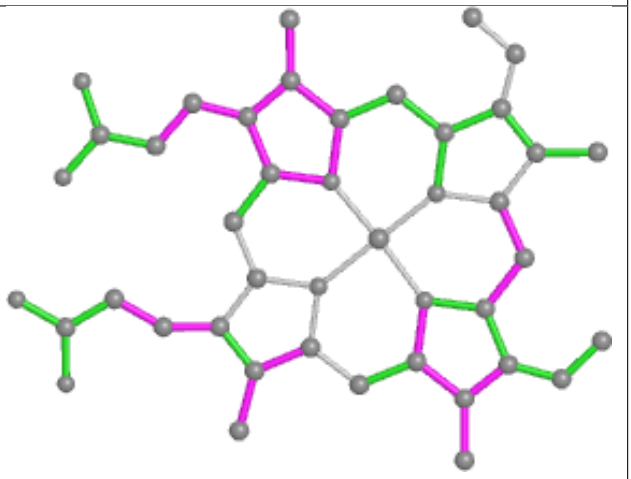
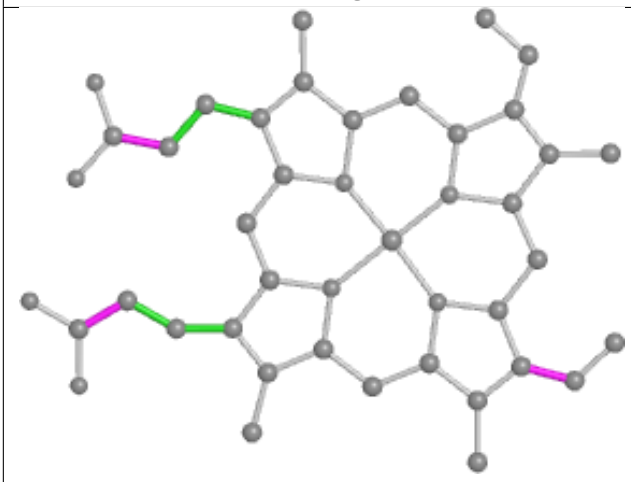


Bond angles



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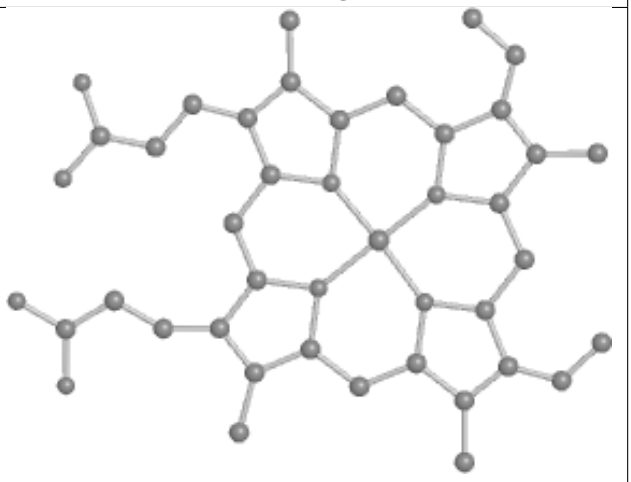
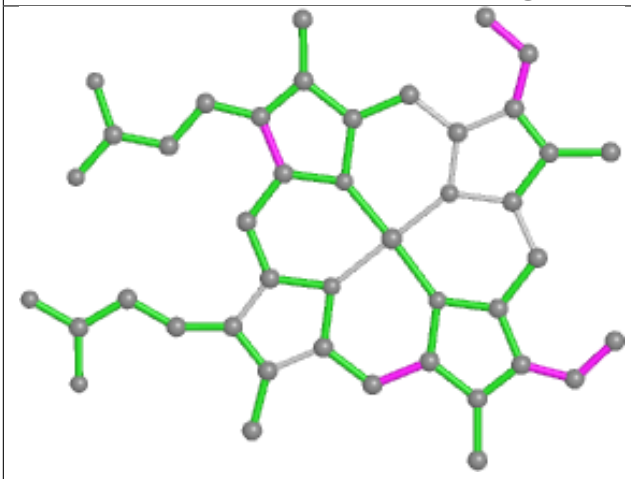
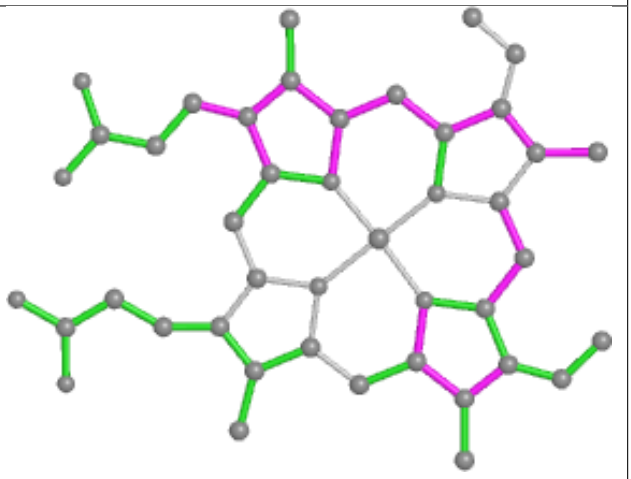


Rings

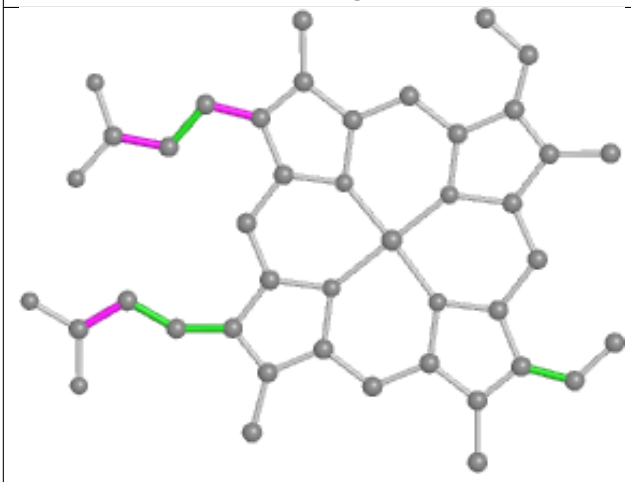
Ligand HEM P 502



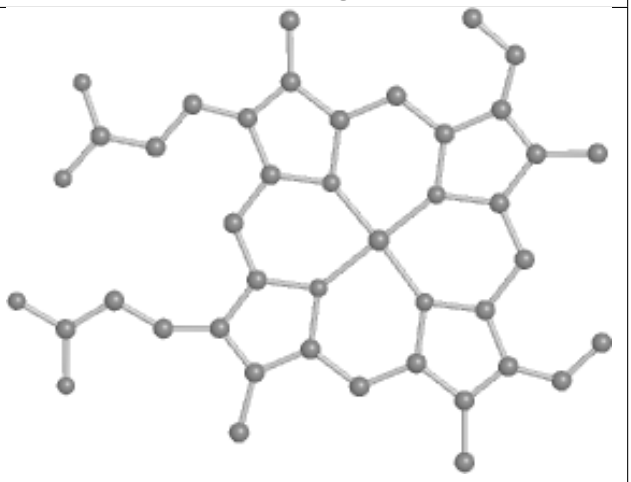
Bond lengths



Bond angles

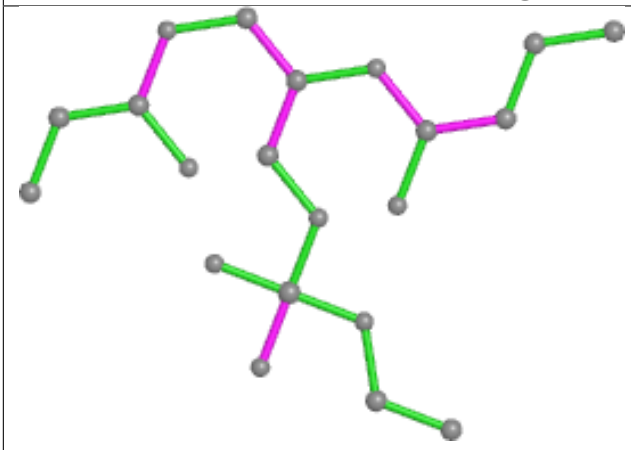


Torsions

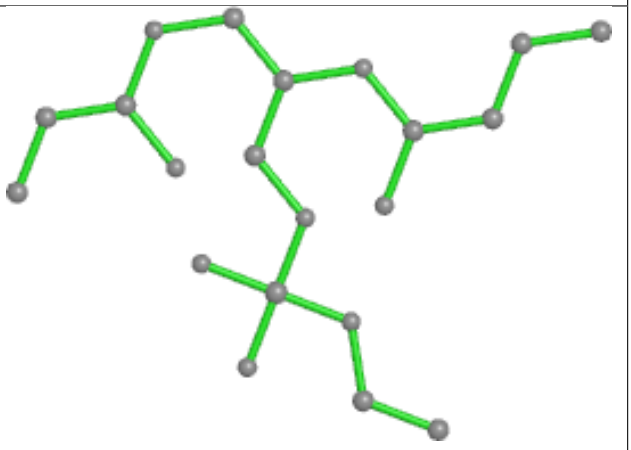


Rings

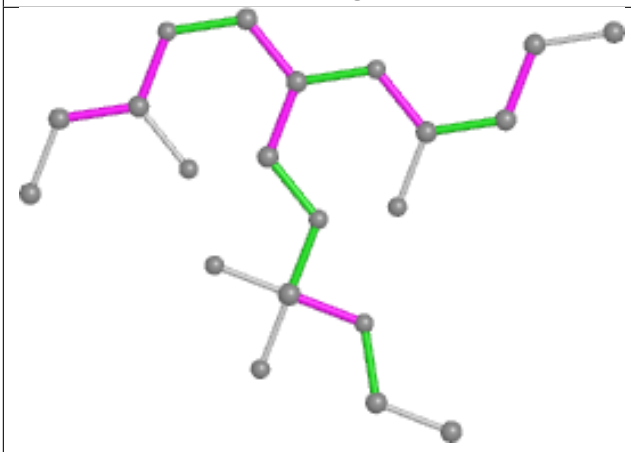
Ligand PEE A 2008



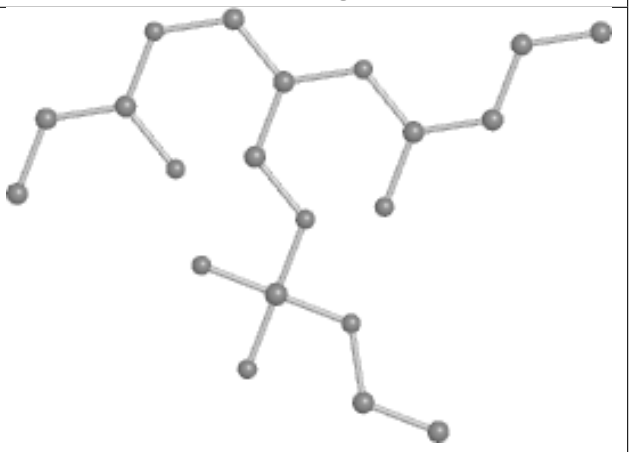
Bond lengths



Bond angles

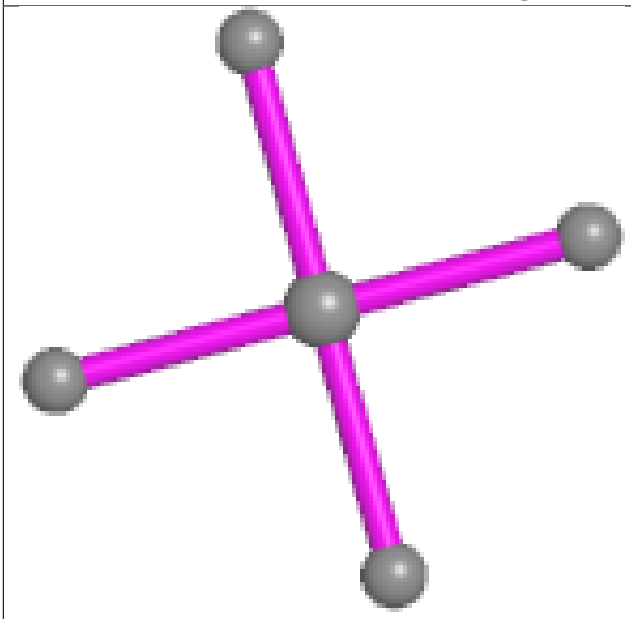


Torsions

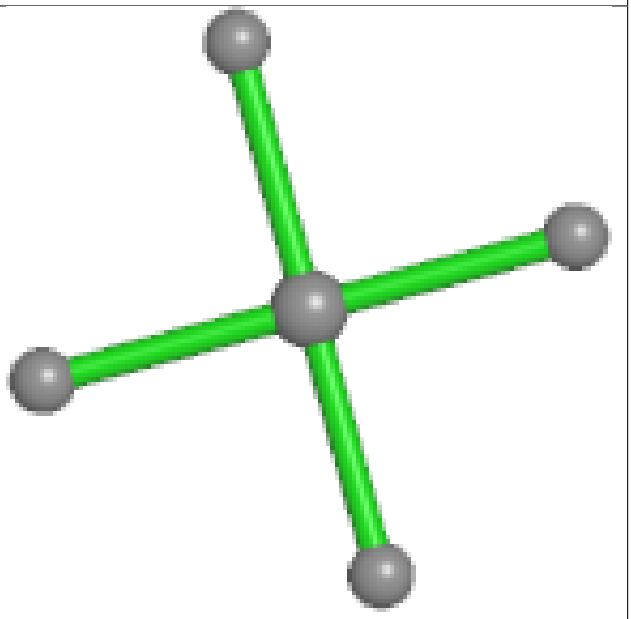


Rings

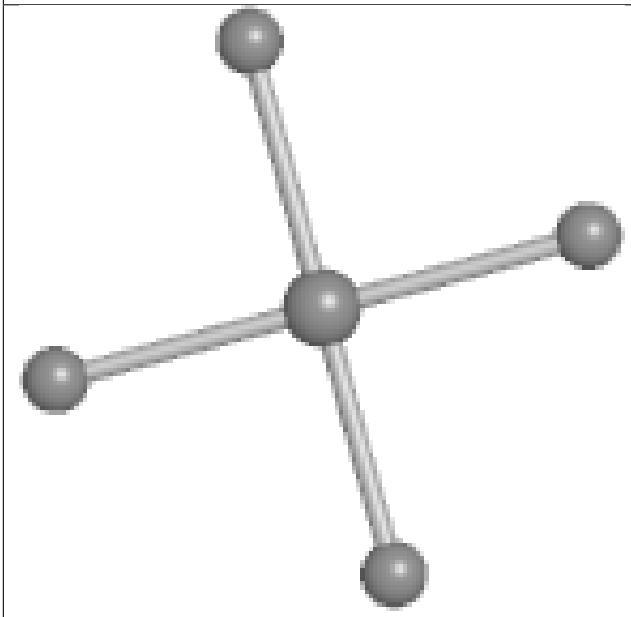
Ligand PEE N 3008



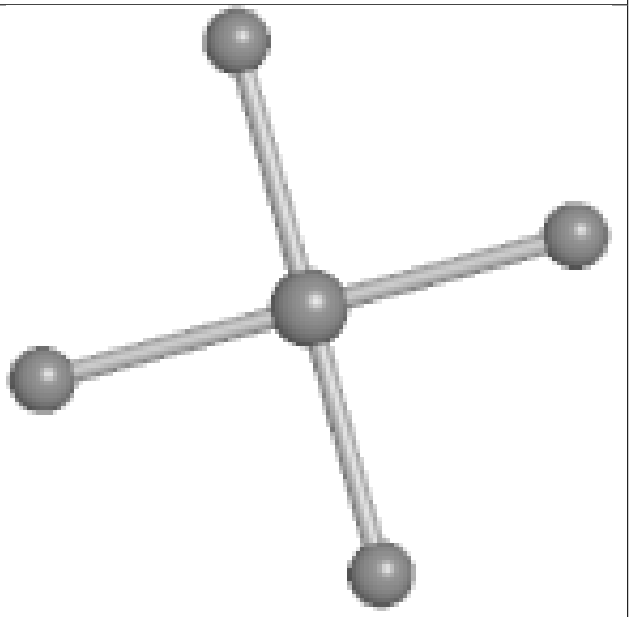
Bond lengths



Bond angles

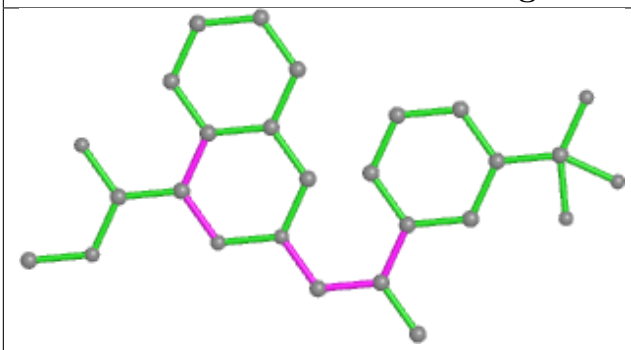


Torsions

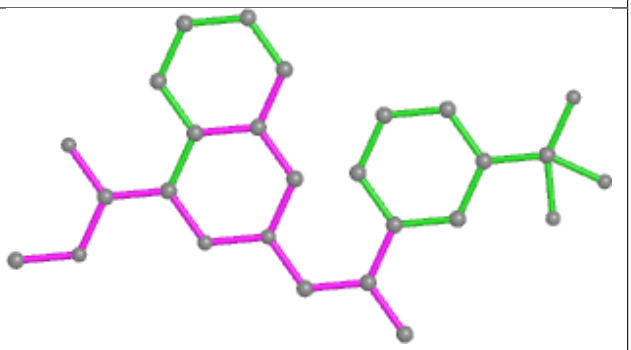


Rings

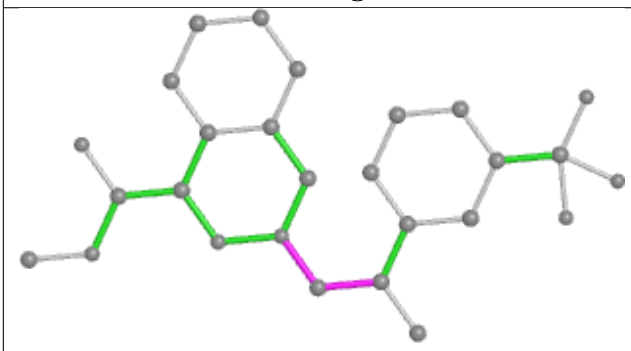
Ligand JZV C 2001



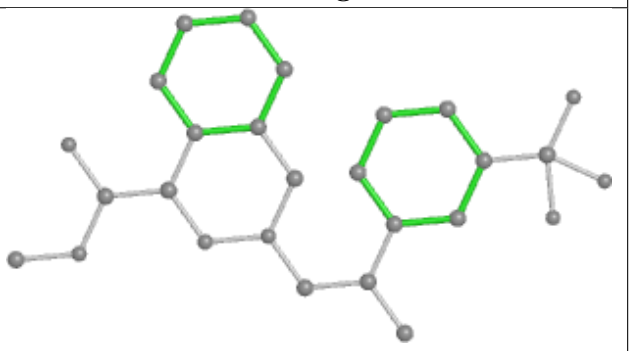
Bond lengths



Bond angles

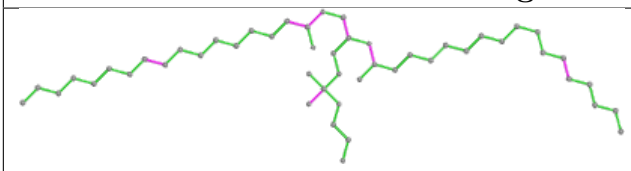


Torsions

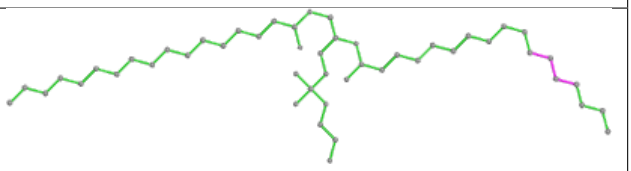


Rings

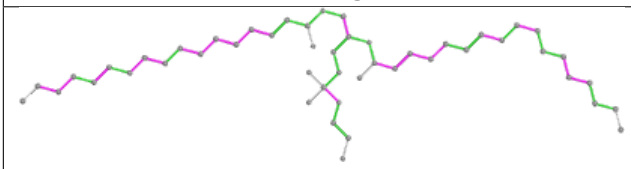
Ligand PEE C 2007



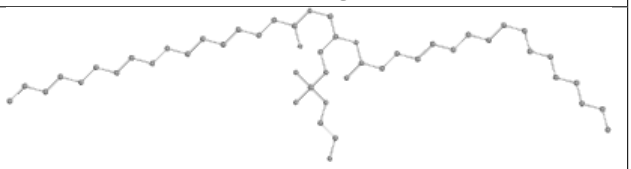
Bond lengths



Bond angles

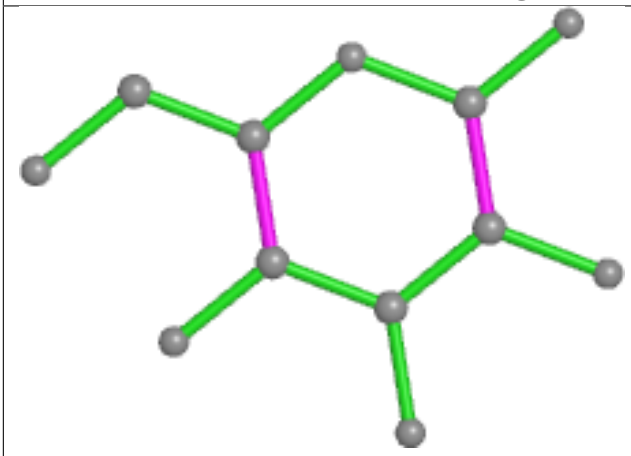


Torsions

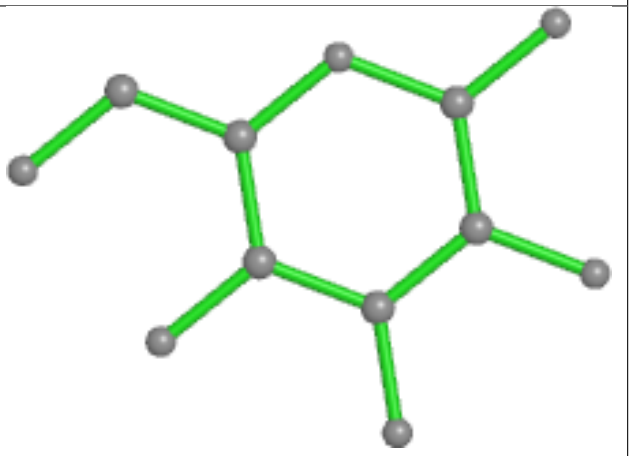


Rings

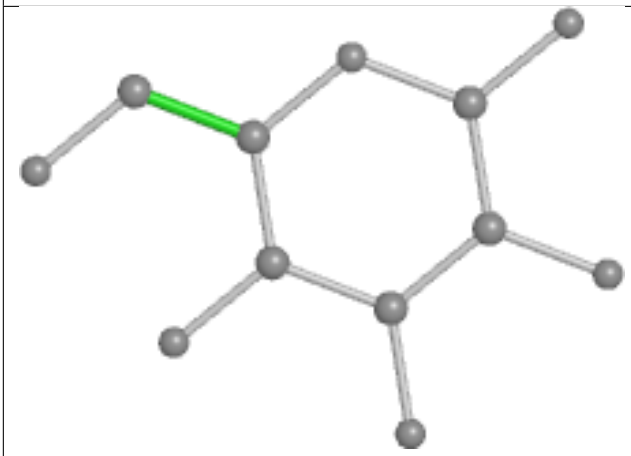
Ligand BOG P 2010



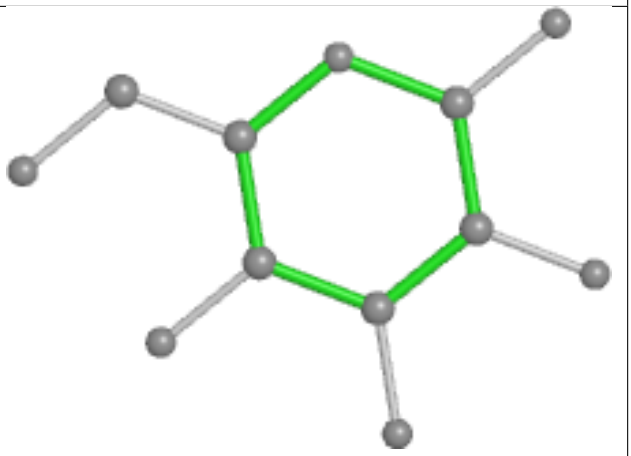
Bond lengths



Bond angles

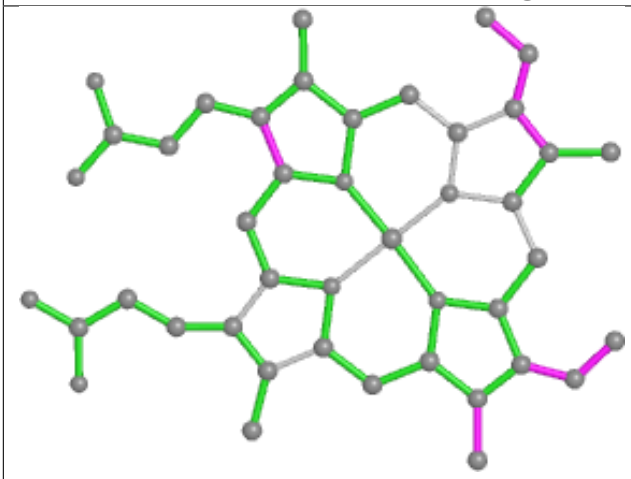


Torsions

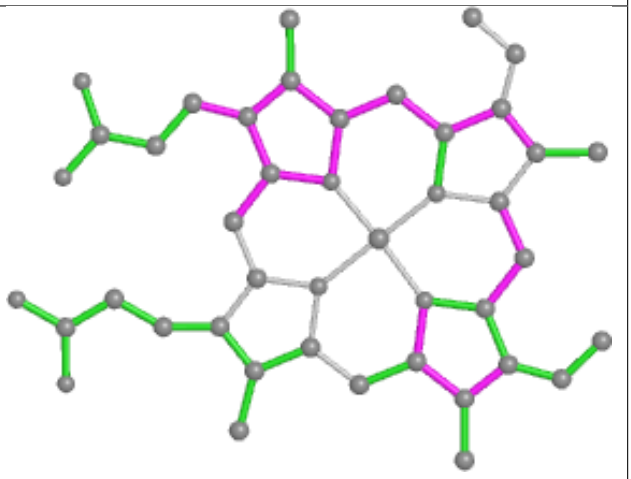


Rings

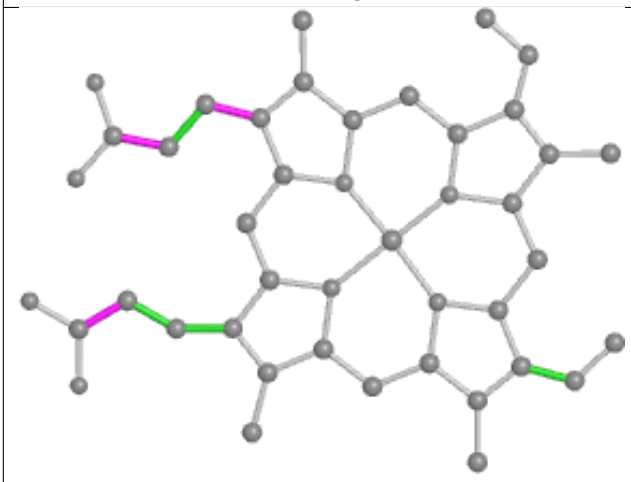
Ligand HEM C 502



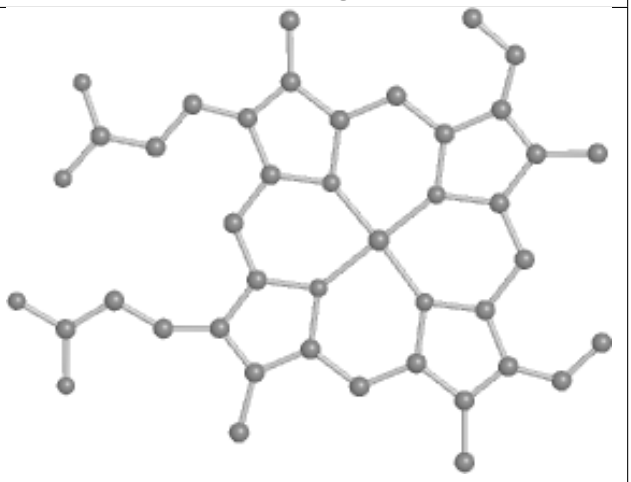
Bond lengths



Bond angles

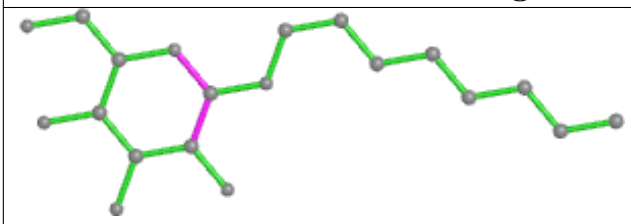


Torsions

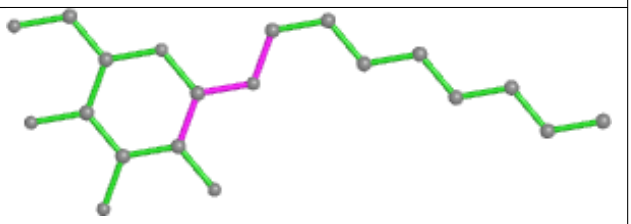


Rings

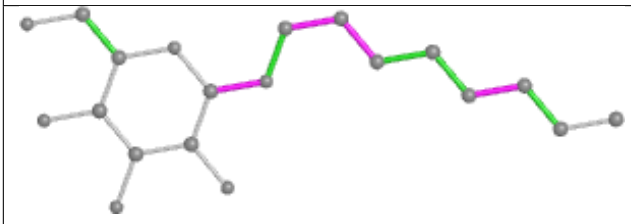
Ligand BOG D 2009



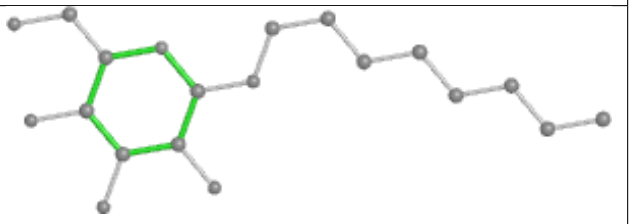
Bond lengths



Bond angles

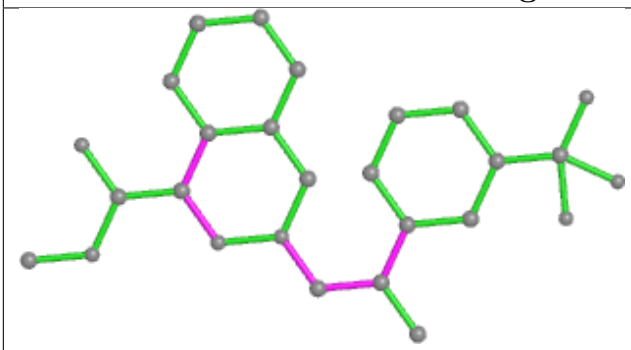


Torsions

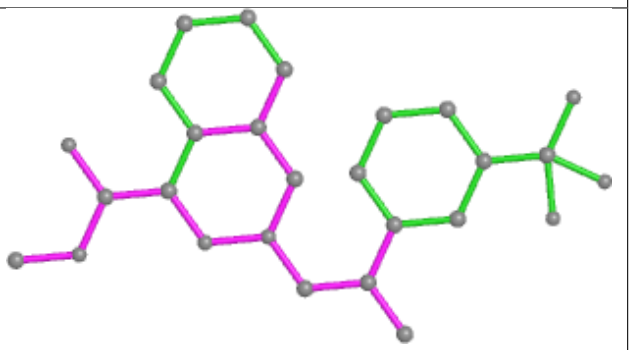


Rings

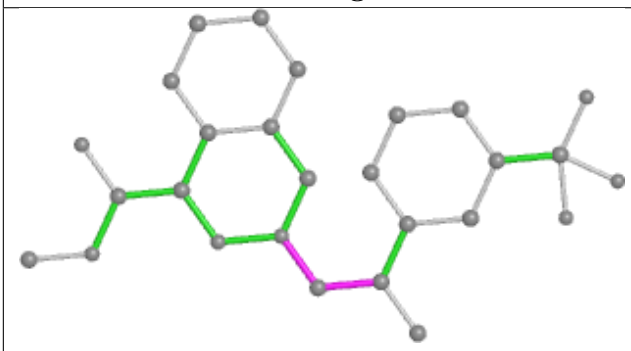
Ligand JZV P 3001



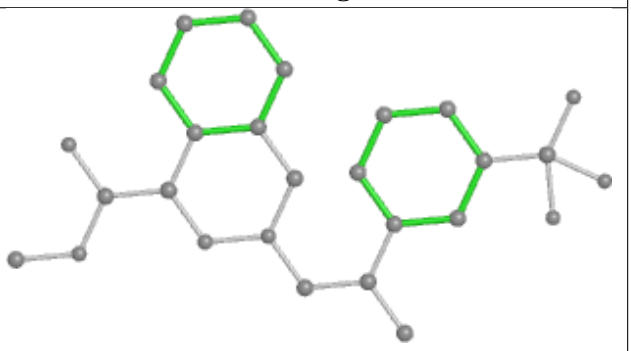
Bond lengths



Bond angles

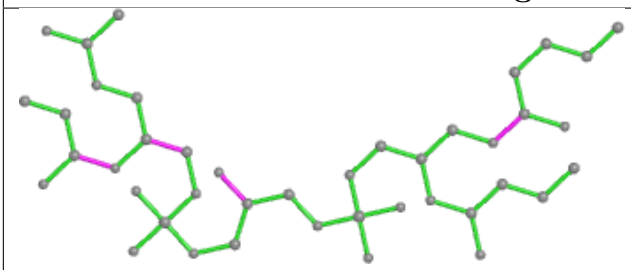


Torsions

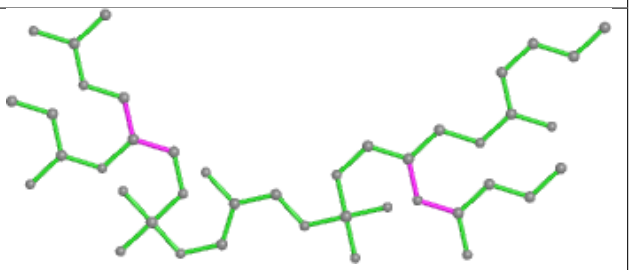


Rings

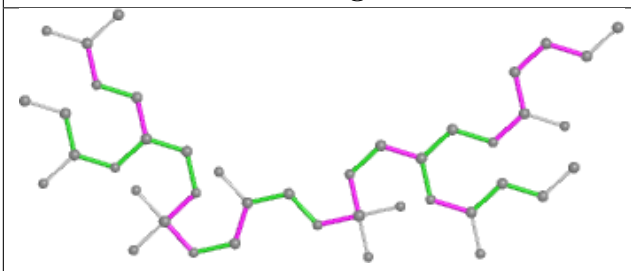
Ligand CDL D 2003



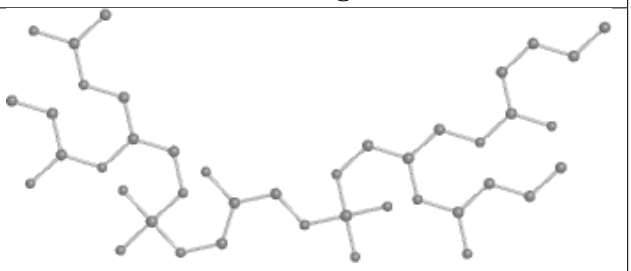
Bond lengths



Bond angles

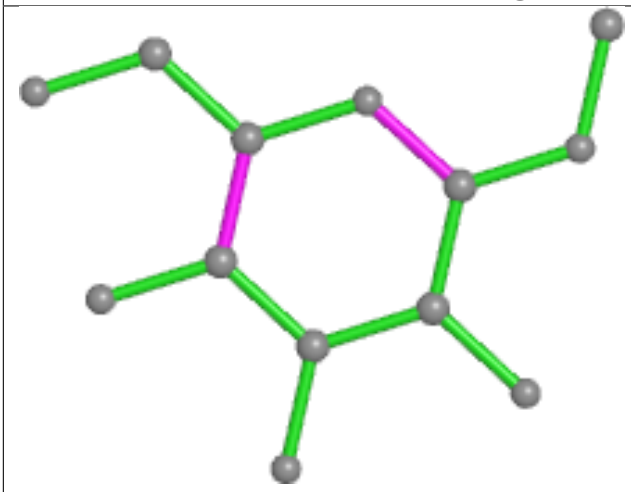


Torsions

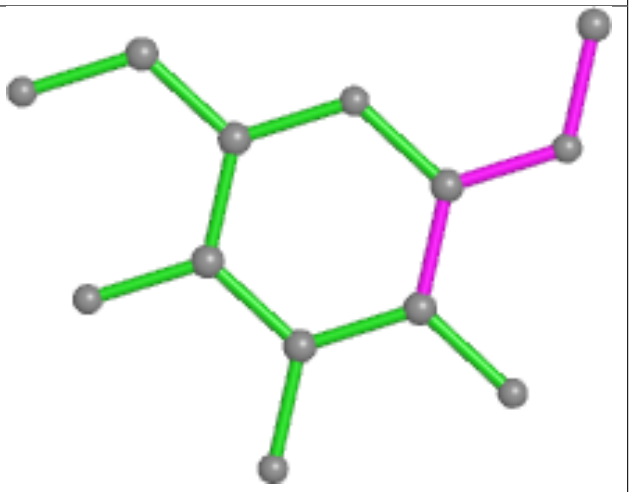


Rings

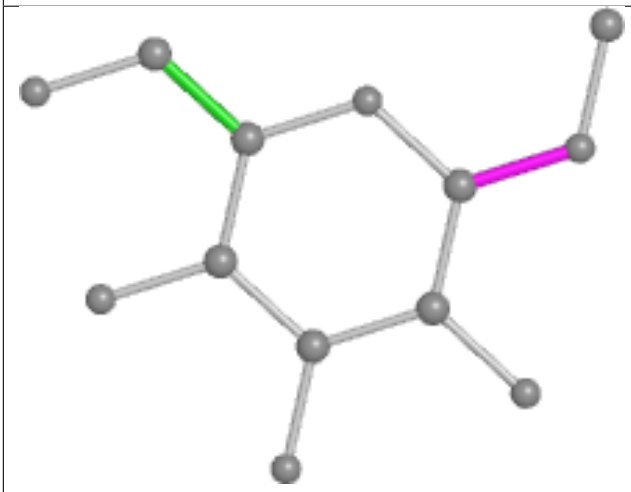
Ligand BOG D 2091



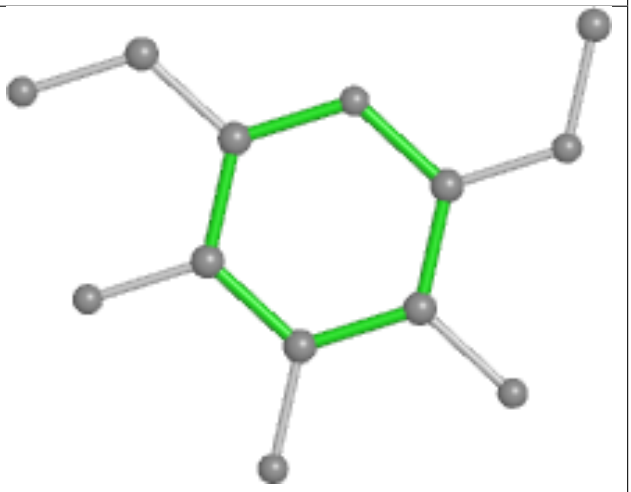
Bond lengths



Bond angles

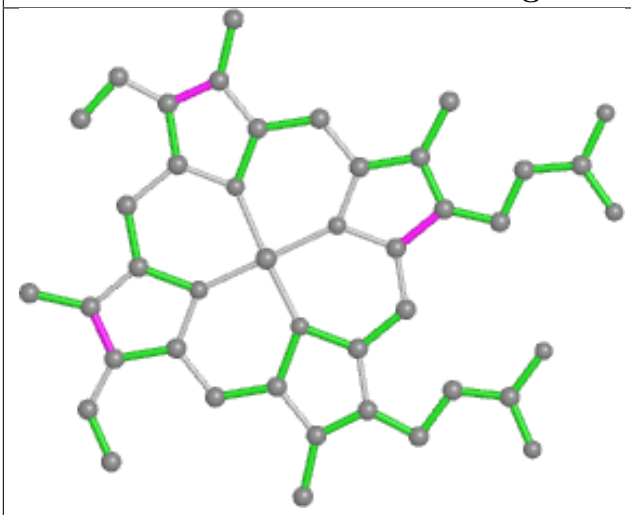


Torsions

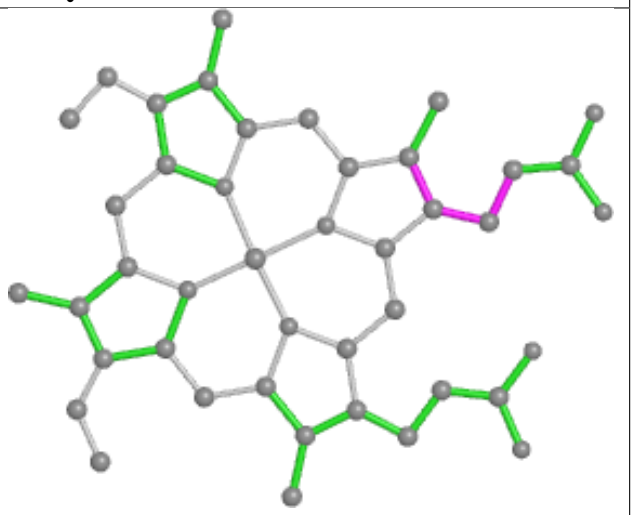


Rings

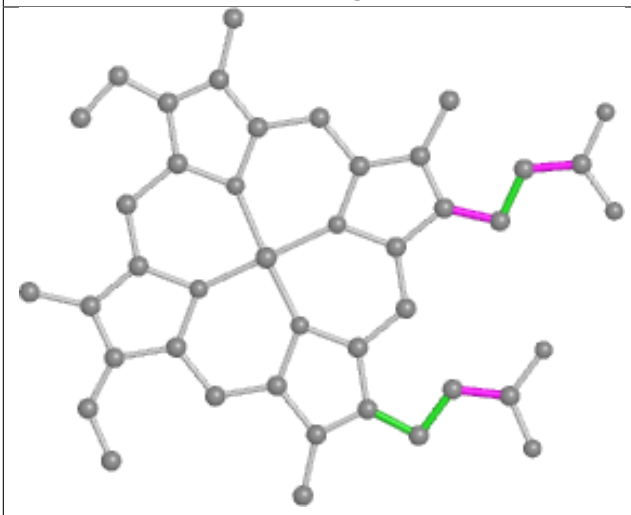
Ligand HEC Q 501



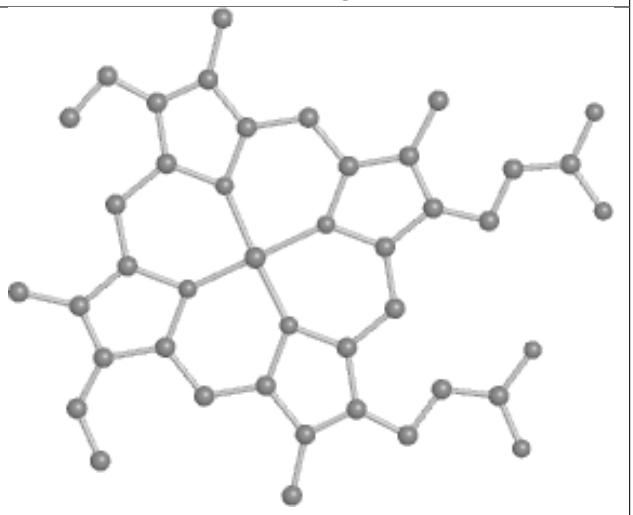
Bond lengths



Bond angles

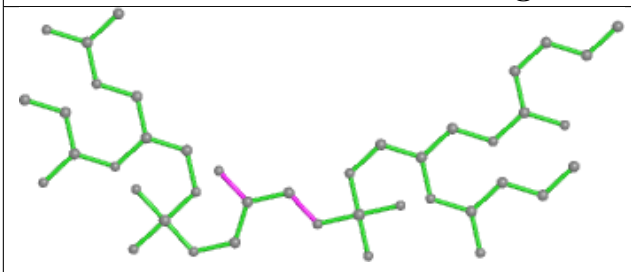


Torsions

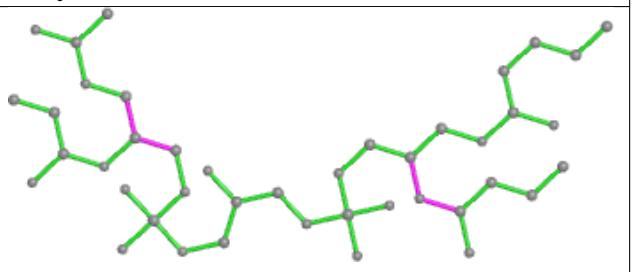


Rings

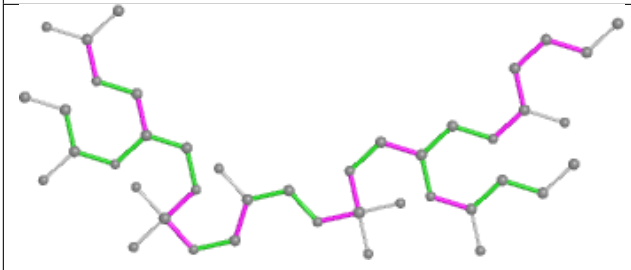
Ligand CDL Q 3003



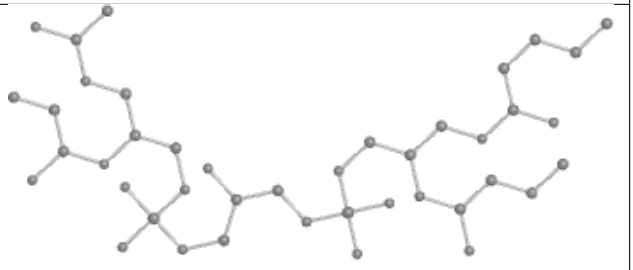
Bond lengths



Bond angles

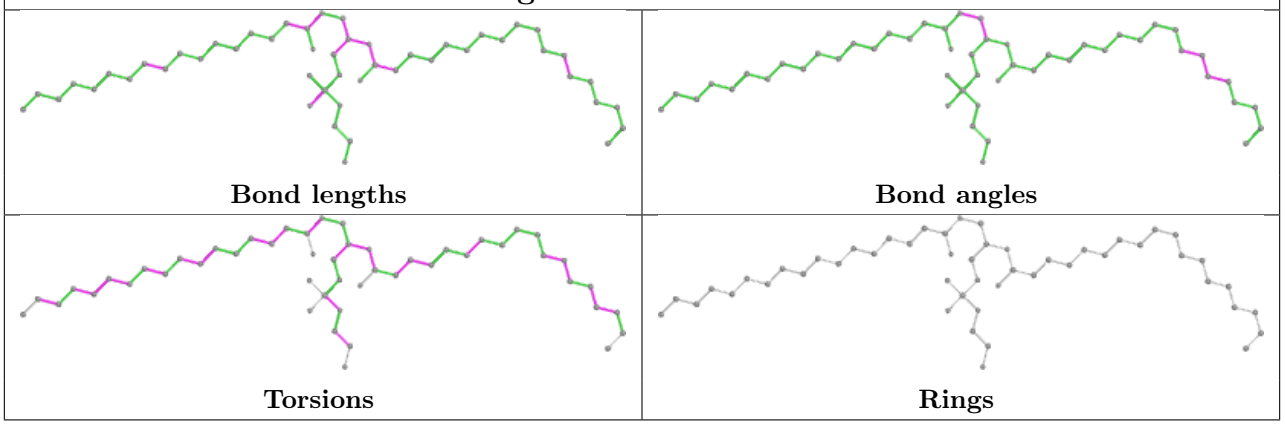


Torsions



Rings

Ligand PEE R 3005



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	444/446 (99%)	0.03	11 (2%) 57 66	32, 58, 86, 100	0
1	N	442/446 (99%)	0.14	8 (1%) 68 76	41, 68, 93, 100	0
2	B	420/441 (95%)	0.25	17 (4%) 38 45	48, 76, 111, 133	0
2	O	422/441 (95%)	0.34	16 (3%) 40 48	39, 74, 103, 122	0
3	C	380/380 (100%)	0.04	5 (1%) 77 84	21, 39, 83, 123	0
3	P	379/380 (99%)	0.19	9 (2%) 59 68	29, 58, 88, 125	0
4	D	241/241 (100%)	-0.09	3 (1%) 79 85	29, 41, 81, 103	0
4	Q	241/241 (100%)	0.17	13 (5%) 25 31	46, 67, 97, 120	0
5	E	196/196 (100%)	1.71	75 (38%) 0 0	34, 135, 167, 175	0
5	R	196/196 (100%)	0.58	25 (12%) 3 4	40, 86, 132, 147	0
6	F	101/110 (91%)	-0.33	0 100 100	26, 43, 61, 94	0
6	S	101/110 (91%)	0.00	4 (3%) 38 45	50, 65, 102, 121	0
7	G	80/81 (98%)	0.10	2 (2%) 57 66	33, 52, 97, 111	0
7	T	79/81 (97%)	0.93	12 (15%) 2 2	46, 78, 139, 149	0
8	H	70/77 (90%)	-0.05	2 (2%) 51 61	34, 58, 80, 119	0
8	U	67/77 (87%)	0.99	13 (19%) 1 1	82, 108, 128, 130	0
9	I	31/47 (65%)	2.17	12 (38%) 0 0	72, 107, 133, 134	0
9	V	31/47 (65%)	2.21	17 (54%) 0 0	66, 107, 132, 136	0
10	J	61/61 (100%)	0.23	4 (6%) 18 21	43, 54, 95, 139	0
10	W	60/61 (98%)	0.53	3 (5%) 28 35	55, 68, 99, 107	0
All	All	4042/4160 (97%)	0.29	251 (6%) 20 25	21, 64, 121, 175	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	11.3
5	E	98	VAL	10.0
5	E	188	VAL	8.7
7	T	2	ILE	7.3
5	E	87	VAL	7.0
5	E	84	GLY	6.9
7	T	77	TYR	6.6
9	I	48	PRO	6.5
5	E	157	TYR	6.5
5	E	102	THR	6.4
7	T	78	GLU	6.1
5	E	83	GLU	6.0
5	E	89	PHE	5.9
5	E	187	PHE	5.8
5	E	79	SER	5.7
5	E	190	ASP	5.7
9	I	77	ARG	5.7
9	I	63	ASP	5.6
5	E	104	ALA	5.5
5	E	148	ALA	5.5
5	R	81	ILE	5.4
5	E	107	ASN	5.4
3	P	2	ALA	5.4
5	E	86	ASN	5.2
5	E	183	PRO	5.2
10	J	63	GLU	5.1
5	E	116	LYS	5.1
9	V	77	ARG	5.1
5	E	85	LYS	5.0
5	R	178	TYR	5.0
7	T	74	PRO	4.9
5	E	76	ILE	4.8
5	E	192	LEU	4.8
2	B	226	ILE	4.8
5	E	81	ILE	4.8
5	E	143	GLY	4.7
2	B	33	LEU	4.6
2	O	386	ALA	4.6
6	S	13	MET	4.4
5	E	163	SER	4.4
9	I	50	LEU	4.4
5	E	82	PRO	4.4
4	Q	145	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
5	E	145	VAL	4.4
10	J	64	GLU	4.3
5	E	100	HIS	4.3
4	Q	241	LYS	4.3
8	U	44	VAL	4.3
5	E	103	GLN	4.2
7	T	6	ASN	4.2
5	E	138	VAL	4.2
5	E	149	ASN	4.2
5	E	88	ALA	4.2
5	E	191	ASP	4.2
5	R	171	ILE	4.2
8	U	49	HIS	4.1
10	J	62	SER	4.1
7	T	80	ASP	4.1
5	E	90	LYS	4.0
8	U	37	LEU	3.9
5	E	108	GLN	3.9
9	V	48	PRO	3.9
5	E	120	PRO	3.8
2	O	355	GLU	3.8
8	U	12	GLU	3.8
9	I	47	ARG	3.7
8	U	50	THR	3.7
3	C	155	PRO	3.7
5	R	155	GLY	3.6
1	A	444	ILE	3.6
5	E	137	GLY	3.6
7	T	73	ASN	3.6
5	E	113	ASP	3.5
10	J	61	ALA	3.5
1	A	10	ASN	3.5
5	E	111	GLU	3.5
5	R	177	PRO	3.5
9	V	47	ARG	3.5
5	E	78	LEU	3.5
5	E	176	ALA	3.5
9	I	61	ARG	3.4
2	O	352	VAL	3.4
2	O	222	GLN	3.3
2	B	232	THR	3.3
2	B	228	SER	3.3

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Mol	Chain	Res	Type	RSRZ
4	D	2	GLU	3.3
9	V	76	VAL	3.3
3	C	4	ASN	3.3
5	R	157	TYR	3.3
8	U	13	LEU	3.3
5	E	115	SER	3.3
5	E	175	PRO	3.3
5	R	117	LEU	3.2
5	E	162	GLY	3.2
1	N	174	ILE	3.2
5	E	180	LEU	3.2
5	E	109	GLU	3.1
4	Q	3	LEU	3.1
3	C	156	TYR	3.1
2	O	226	ILE	3.1
5	E	75	GLU	3.1
5	E	159	PRO	3.1
3	C	1	MET	3.1
5	E	140	THR	3.1
5	E	134	ILE	3.1
1	A	218	GLY	3.1
2	B	224	LEU	3.1
2	B	230	ALA	3.1
5	E	185	TYR	3.1
4	Q	143	VAL	3.1
5	E	117	LEU	3.1
2	B	227	ARG	3.1
4	Q	69	GLU	3.1
10	W	33	ARG	3.1
9	V	60	ALA	3.0
2	B	29	LEU	3.0
5	E	177	PRO	3.0
8	H	71	HIS	3.0
5	E	124	LEU	3.0
5	R	165	TYR	3.0
4	D	1	GLY	3.0
5	E	195	VAL	3.0
6	S	12	LEU	3.0
9	V	59	SER	2.9
2	B	225	ASN	2.9
1	A	86	PHE	2.9
2	O	388	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
9	V	62	ARG	2.9
2	B	34	ILE	2.9
5	E	99	ARG	2.9
2	B	35	ILE	2.9
5	E	150	SER	2.9
3	P	373	LEU	2.9
5	E	178	TYR	2.9
2	O	387	LEU	2.8
7	T	57	LEU	2.8
2	O	18	CYS	2.8
5	R	154	GLY	2.8
5	R	120	PRO	2.7
5	R	115	SER	2.7
2	B	204	MET	2.7
5	R	84	GLY	2.7
9	V	58	ARG	2.7
3	C	380	TYR	2.7
5	R	114	VAL	2.7
1	A	69	LYS	2.7
1	N	71	PRO	2.7
1	N	171	THR	2.7
5	E	181	GLU	2.7
4	Q	80	LEU	2.7
9	I	51	CYS	2.7
7	T	75	ALA	2.6
1	A	127	ILE	2.6
8	U	42	ALA	2.6
2	B	20	GLY	2.6
5	R	156	TYR	2.6
5	E	105	GLU	2.6
5	R	119	ASP	2.6
2	O	34	ILE	2.5
1	A	219	VAL	2.5
1	N	72	CYS	2.5
5	R	190	ASP	2.5
4	Q	206	LEU	2.5
5	E	182	VAL	2.5
9	V	54	SER	2.5
2	B	348	ALA	2.5
5	E	184	THR	2.5
7	T	8	ALA	2.5
8	U	54	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	241	LYS	2.5
7	T	79	ASN	2.5
2	B	201	SER	2.5
5	R	83	GLU	2.4
5	R	172	ARG	2.4
6	S	15	ARG	2.4
5	R	86	ASN	2.4
5	E	189	GLY	2.4
5	E	112	VAL	2.4
2	B	439	LEU	2.4
7	T	71	ARG	2.4
3	P	370	ILE	2.4
1	N	175	LYS	2.4
5	E	118	ARG	2.4
9	I	54	SER	2.4
7	G	2	ILE	2.4
5	E	152	ASP	2.3
9	I	75	SER	2.3
2	O	35	ILE	2.3
1	A	4	TYR	2.3
9	I	60	ALA	2.3
9	V	72	ALA	2.3
5	E	119	ASP	2.3
5	E	97	PHE	2.3
4	Q	1	GLY	2.3
5	E	165	TYR	2.3
5	E	110	ALA	2.3
3	P	376	LYS	2.3
2	B	36	ALA	2.2
4	Q	70	VAL	2.2
5	E	147	ILE	2.2
5	R	1	VAL	2.2
9	I	76	VAL	2.2
9	V	56	SER	2.2
1	A	122	LEU	2.2
1	N	127	ILE	2.2
1	A	68	LYS	2.2
5	R	118	ARG	2.2
2	O	104	LYS	2.2
6	S	11	ARG	2.2
4	Q	103	ALA	2.2
4	Q	77	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	139	ALA	2.2
8	U	47	ARG	2.2
5	E	194	VAL	2.2
1	N	182	LEU	2.2
8	U	39	LEU	2.2
2	O	28	LYS	2.1
5	E	136	VAL	2.1
9	V	68	ILE	2.1
2	O	33	LEU	2.1
3	P	366	LEU	2.1
7	G	30	PHE	2.1
5	R	124	LEU	2.1
5	R	16	GLU	2.1
3	P	156	TYR	2.1
8	H	10	GLU	2.1
9	V	74	ALA	2.1
10	W	60	GLU	2.1
2	O	353	THR	2.1
9	V	75	SER	2.1
2	O	416	LYS	2.1
4	Q	82	MET	2.1
5	E	186	GLN	2.1
5	R	103	GLN	2.1
3	P	43	MET	2.1
2	O	250	HIS	2.1
9	V	70	LEU	2.1
5	E	125	ASP	2.1
5	R	89	PHE	2.1
1	A	392	LEU	2.0
9	I	64	LEU	2.0
5	E	101	ARG	2.0
3	P	380	TYR	2.0
8	U	38	GLU	2.0
8	U	48	SER	2.0
9	V	64	LEU	2.0
5	E	174	GLY	2.0
3	P	307	PHE	2.0
8	U	61	PHE	2.0
1	N	392	LEU	2.0
10	W	25	VAL	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
18	BOG	Q	3091	13/20	0.24	0.61	183,186,187,187	0
18	BOG	D	2091	13/20	0.26	0.62	200,201,201,201	0
18	BOG	P	2010	12/20	0.46	0.35	135,137,138,138	0
11	PEE	A	2008	21/51	0.54	0.39	129,133,134,135	0
11	PEE	R	3005	50/51	0.71	0.42	80,98,108,110	0
15	CDL	Q	3003	42/100	0.73	0.29	109,121,139,139	0
14	UQ	P	3002	19/63	0.76	0.38	119,124,125,126	0
16	GOL	P	3011	6/6	0.80	0.40	73,75,76,77	0
15	CDL	D	2003	42/100	0.81	0.29	82,92,106,108	0
11	PEE	E	2005	50/51	0.82	0.35	68,89,95,97	0
11	PEE	N	3008	5/51	0.83	0.20	110,111,112,112	0
11	PEE	P	3007	49/51	0.83	0.33	53,79,93,94	0
14	UQ	C	2002	19/63	0.84	0.30	88,90,90,91	0
16	GOL	C	2011	6/6	0.85	0.34	67,70,72,72	0
11	PEE	C	2007	49/51	0.86	0.30	43,58,70,73	0
15	CDL	P	3004	40/100	0.86	0.21	96,102,111,111	0
18	BOG	Q	3009	20/20	0.89	0.23	62,75,77,78	0
13	JZV	P	3001	29/29	0.89	0.24	59,66,104,106	0
15	CDL	C	2004	40/100	0.91	0.22	66,80,91,93	0
13	JZV	C	2001	29/29	0.93	0.23	38,46,86,87	0
18	BOG	D	2009	20/20	0.93	0.17	53,59,62,64	0
19	FES	E	501	4/4	0.93	0.11	144,144,145,145	0
17	HEC	Q	501	43/43	0.96	0.18	52,56,64,65	0
12	HEM	P	501	43/43	0.97	0.22	33,40,48,54	0
17	HEC	D	501	43/43	0.98	0.17	21,29,34,35	0
12	HEM	C	501	43/43	0.98	0.21	23,30,37,42	0
12	HEM	P	502	43/43	0.98	0.17	29,41,54,59	0

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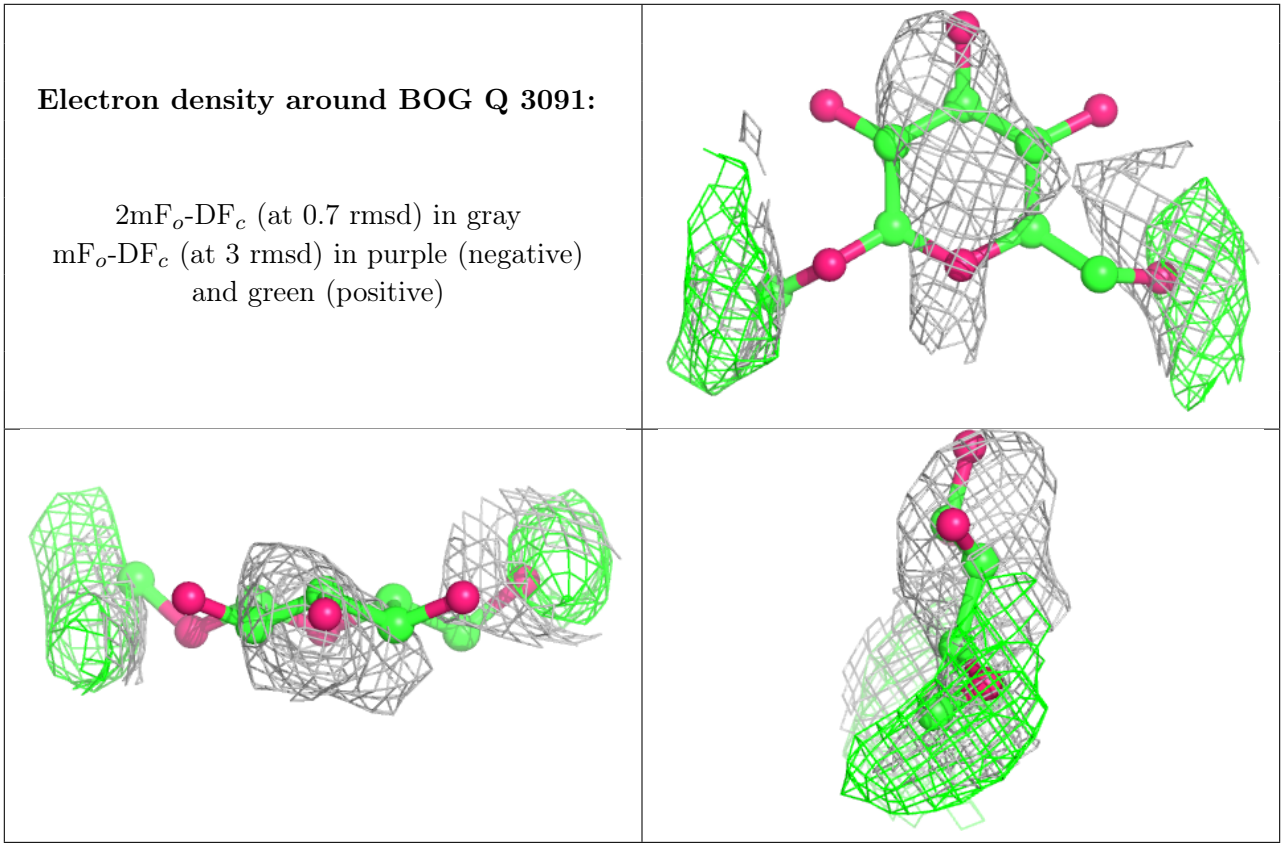
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	HEM	C	502	43/43	0.98	0.17	24,27,35,41	0
19	FES	R	501	4/4	0.98	0.06	74,76,77,78	0

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

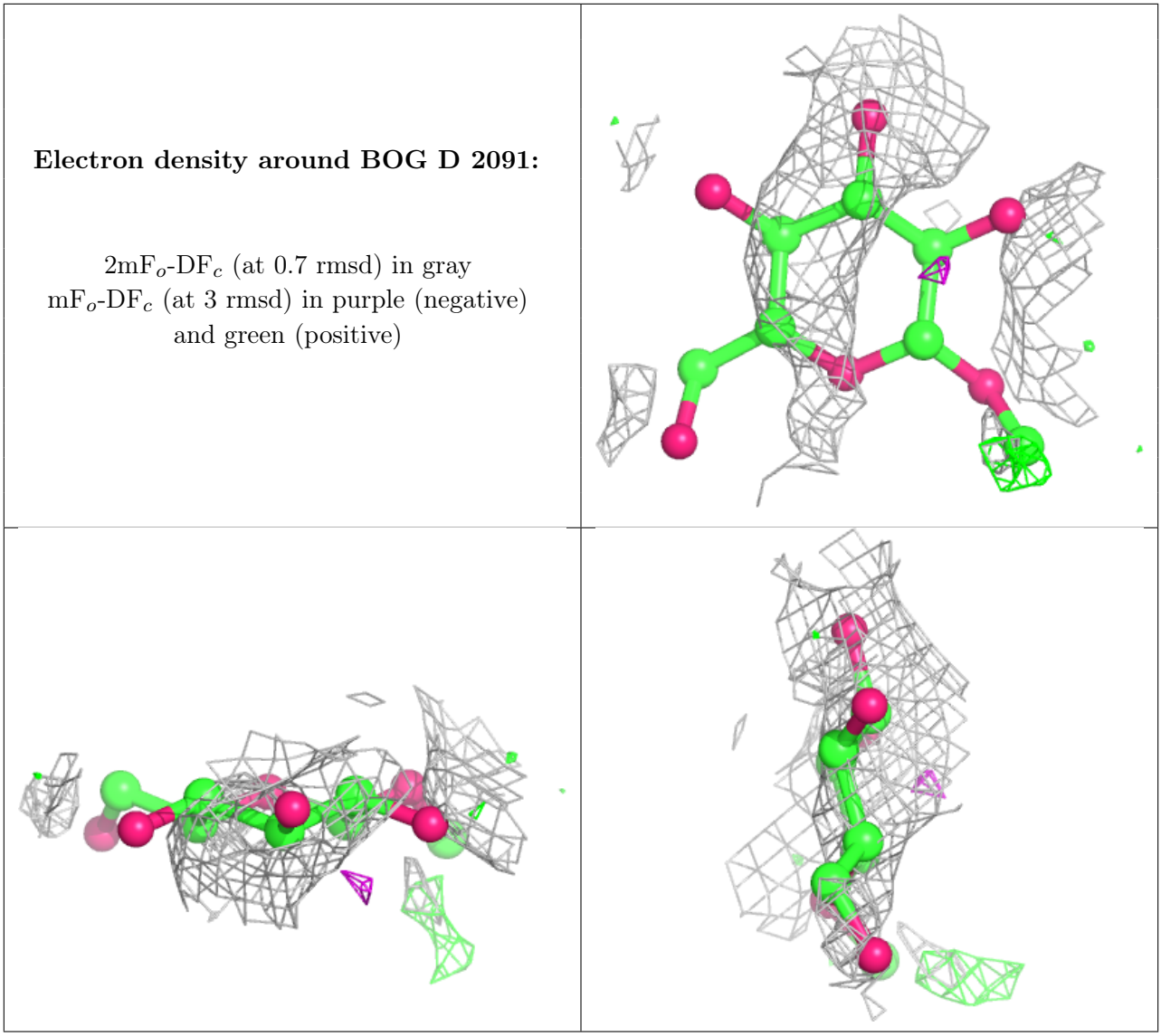
Electron density around BOG Q 3091:

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



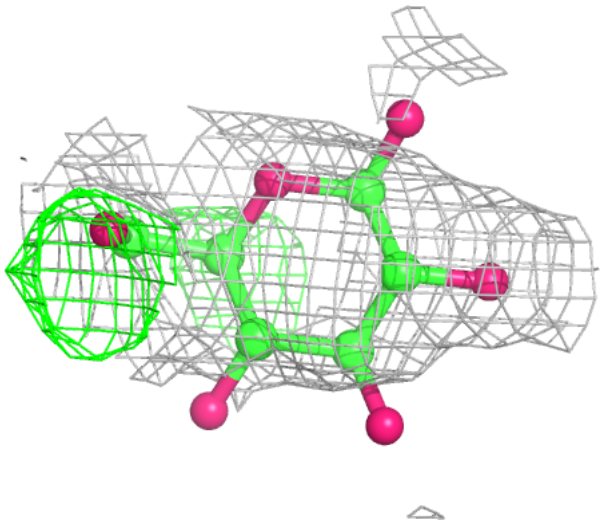
Electron density around BOG D 2091:

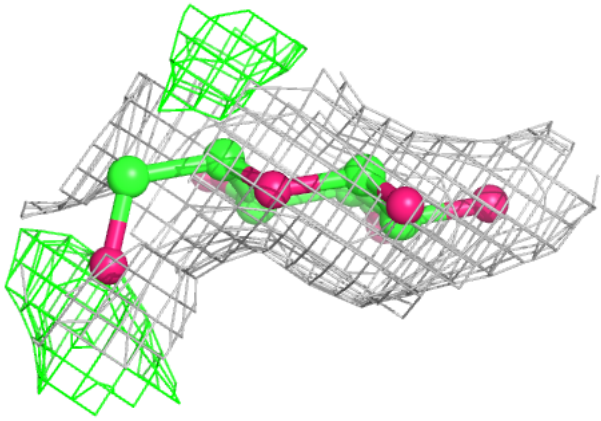
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

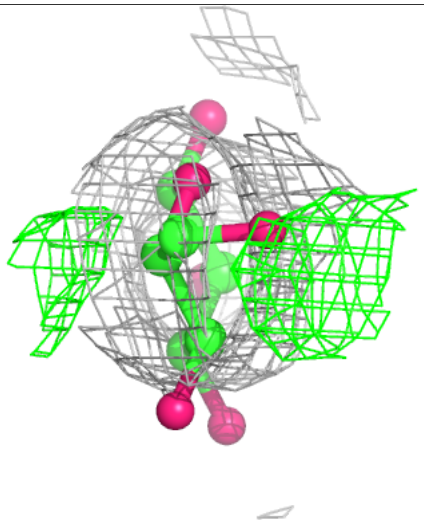


Electron density around BOG P 2010:

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

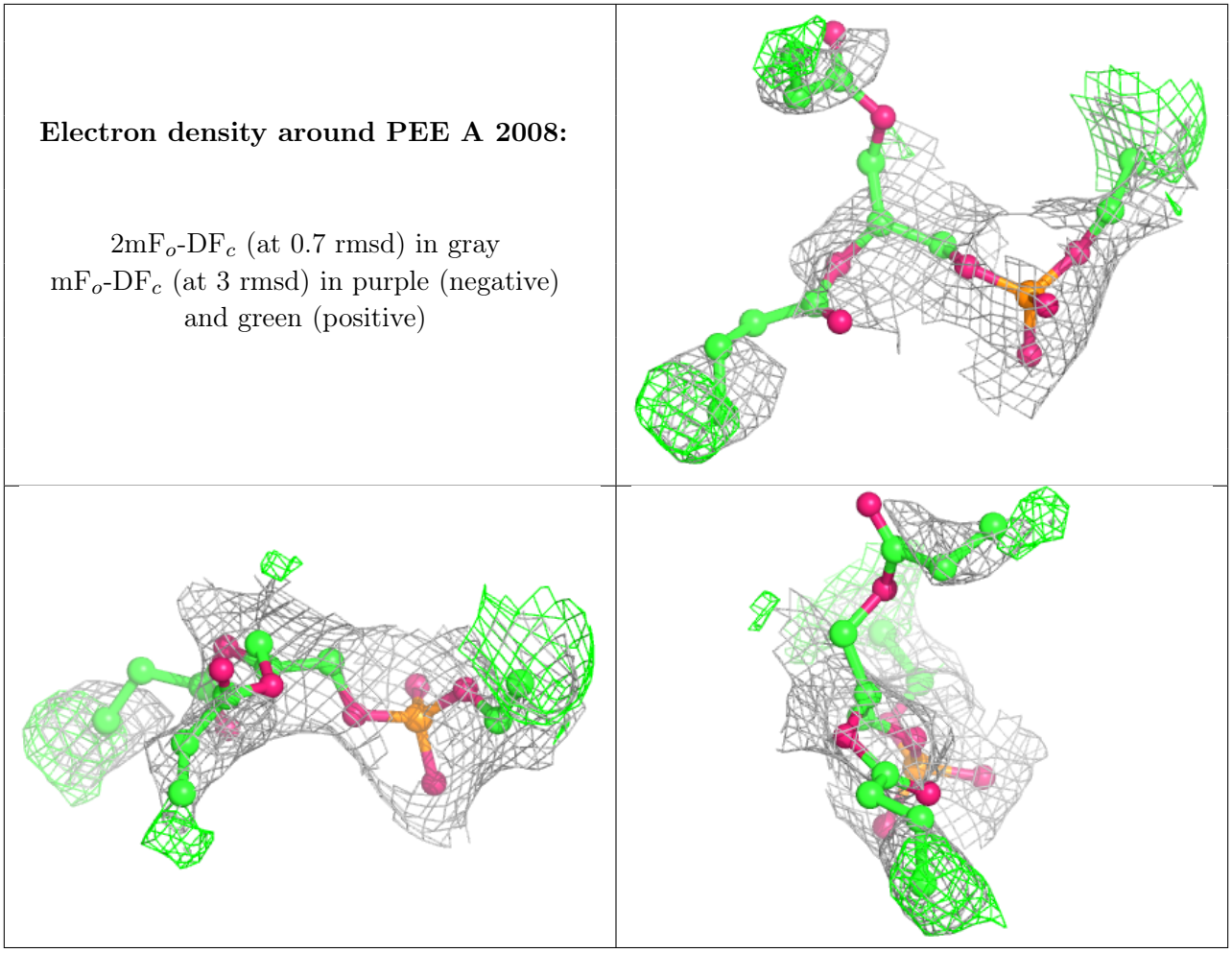






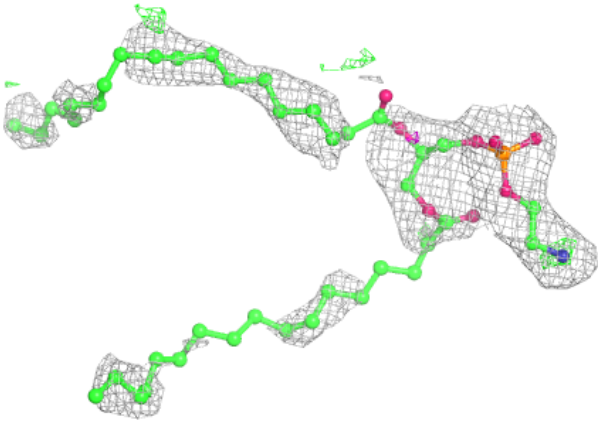
Electron density around PEE A 2008:

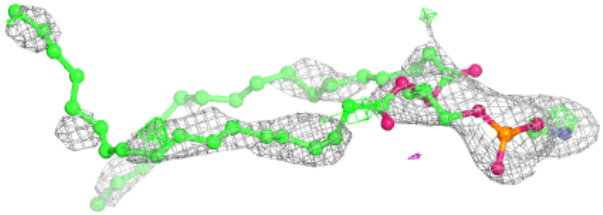
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

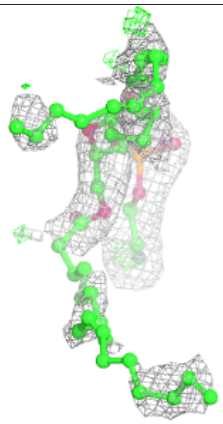


Electron density around PEE R 3005:

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

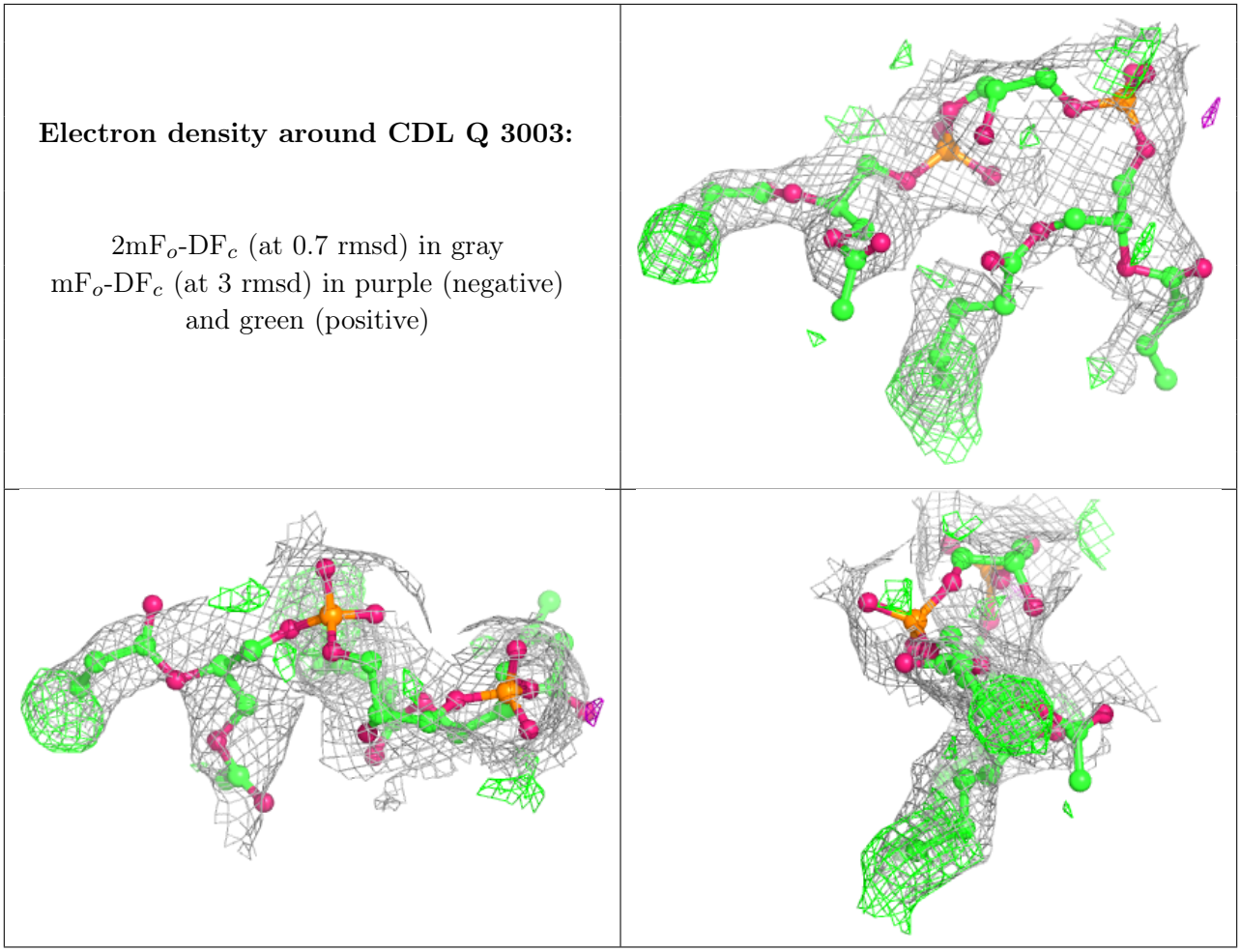






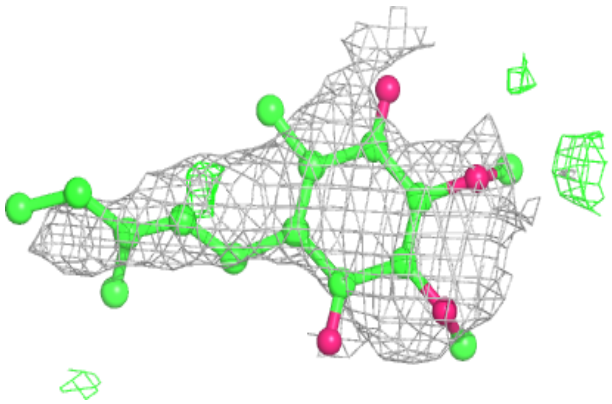
Electron density around CDL Q 3003:

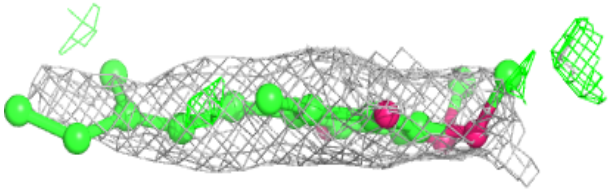
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

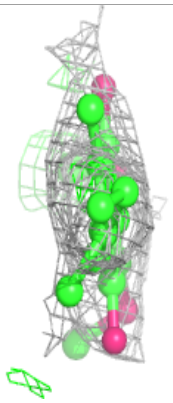


Electron density around UQ P 3002:

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

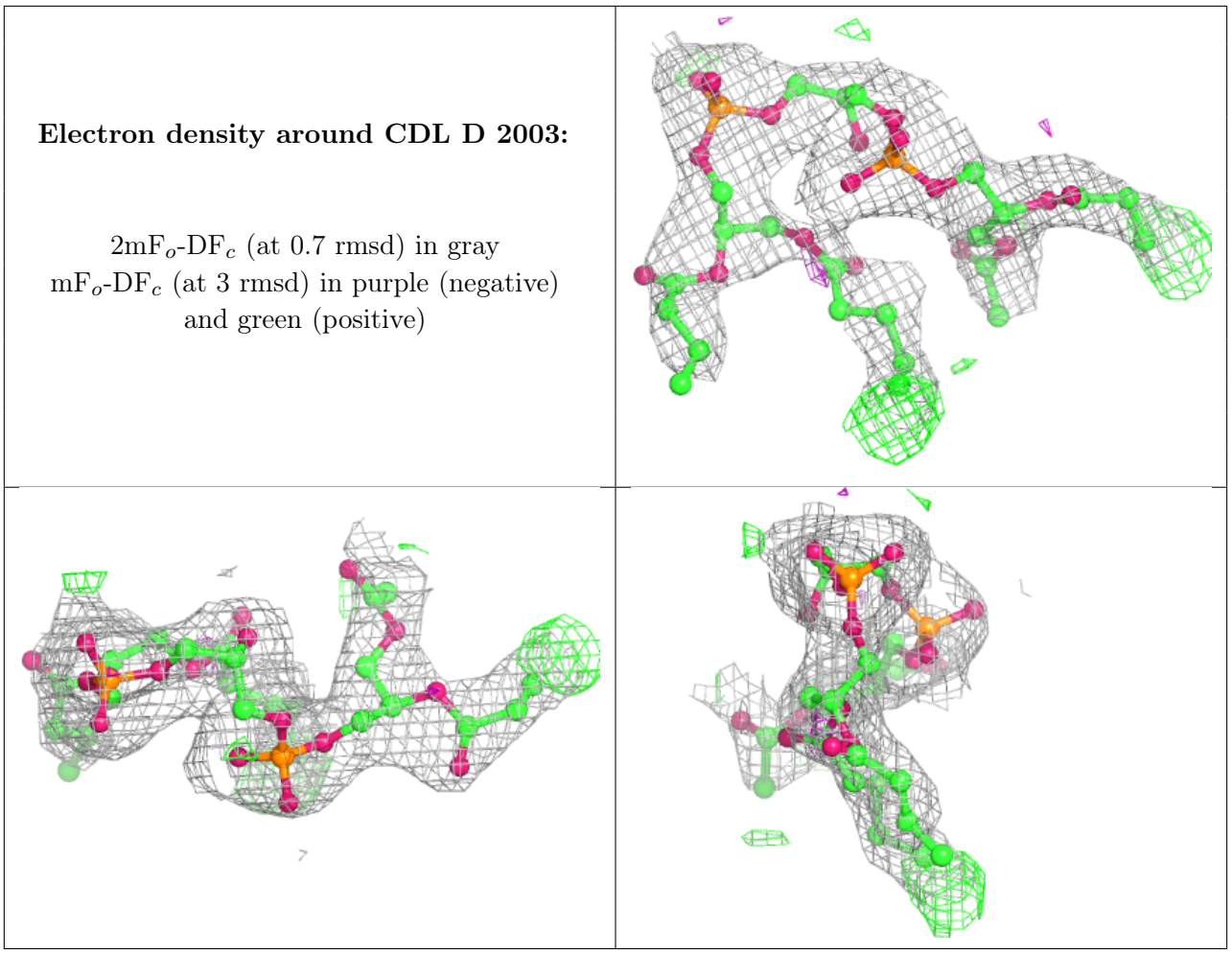






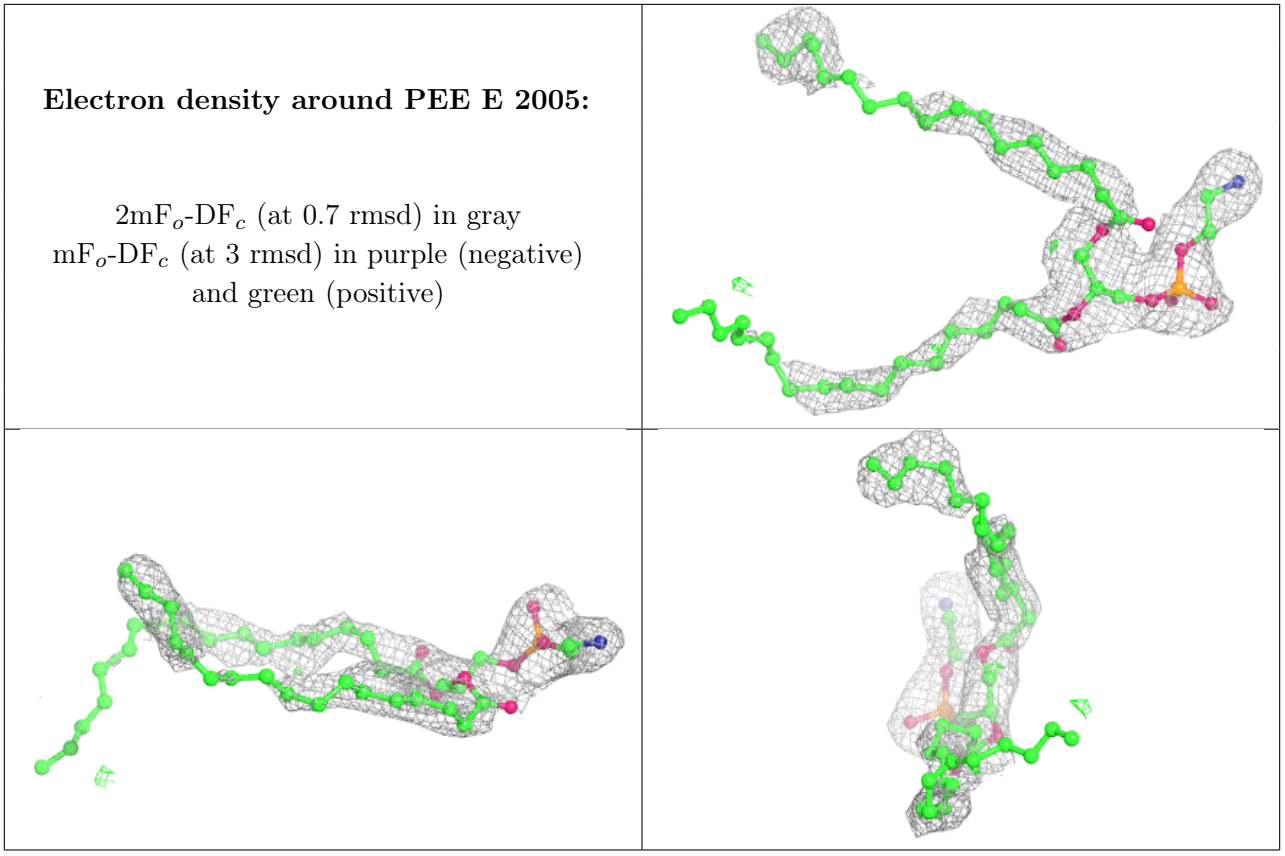
Electron density around CDL D 2003:

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



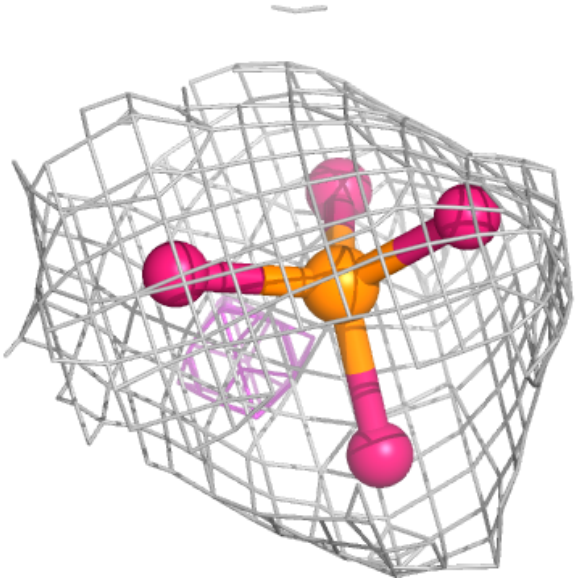
Electron density around PEE E 2005:

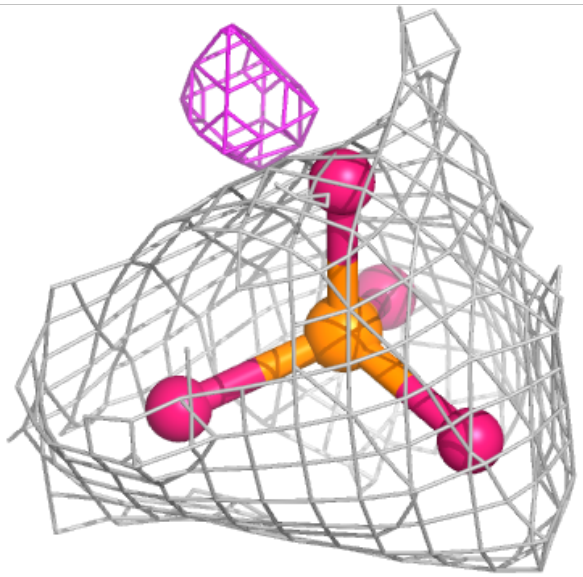
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

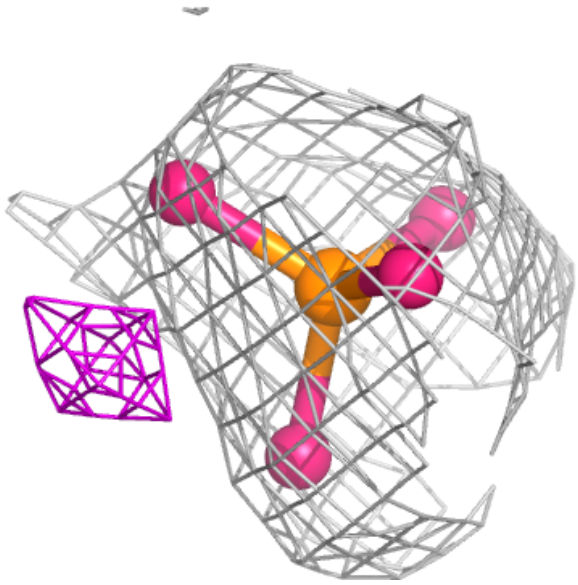


Electron density around PEE N 3008:

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

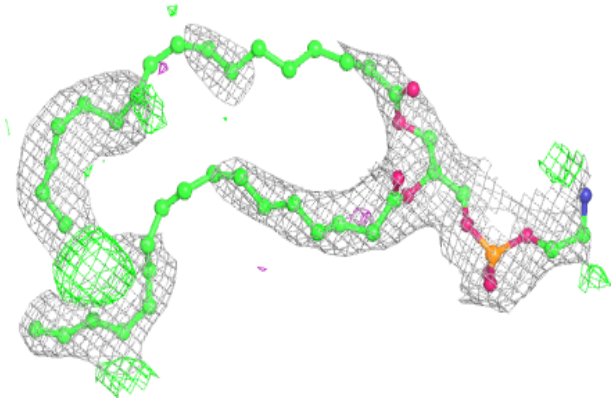


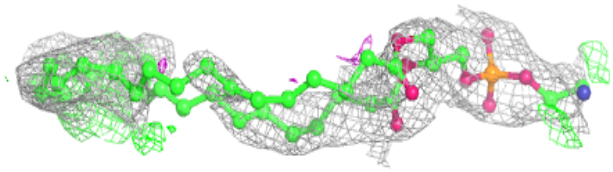


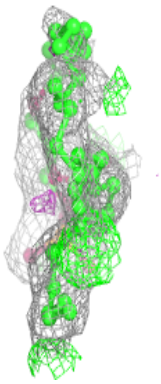


Electron density around PEE P 3007:

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

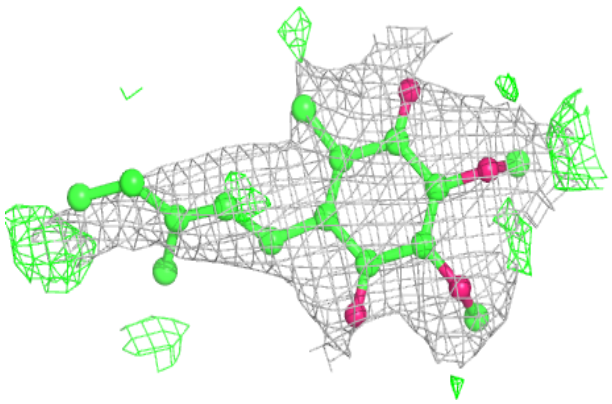


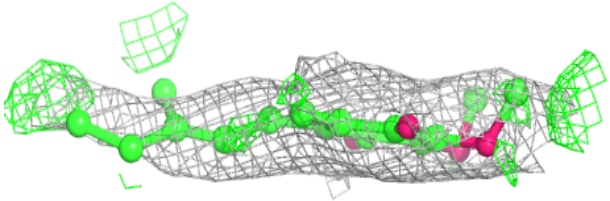


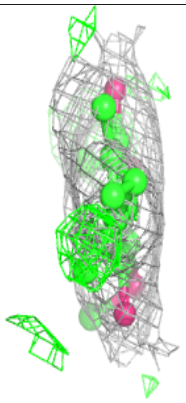


Electron density around UQ C 2002:

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

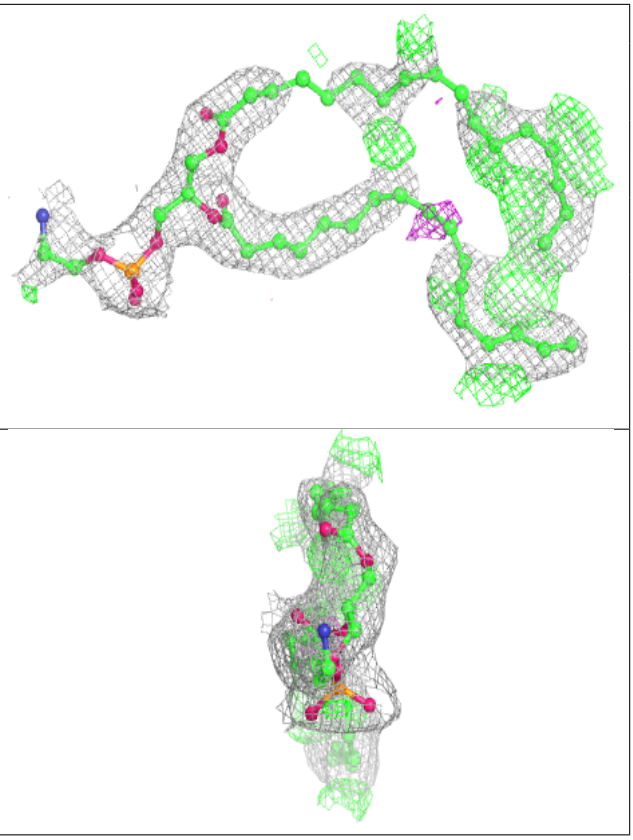


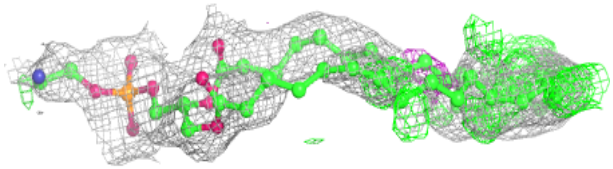




Electron density around PEE C 2007:

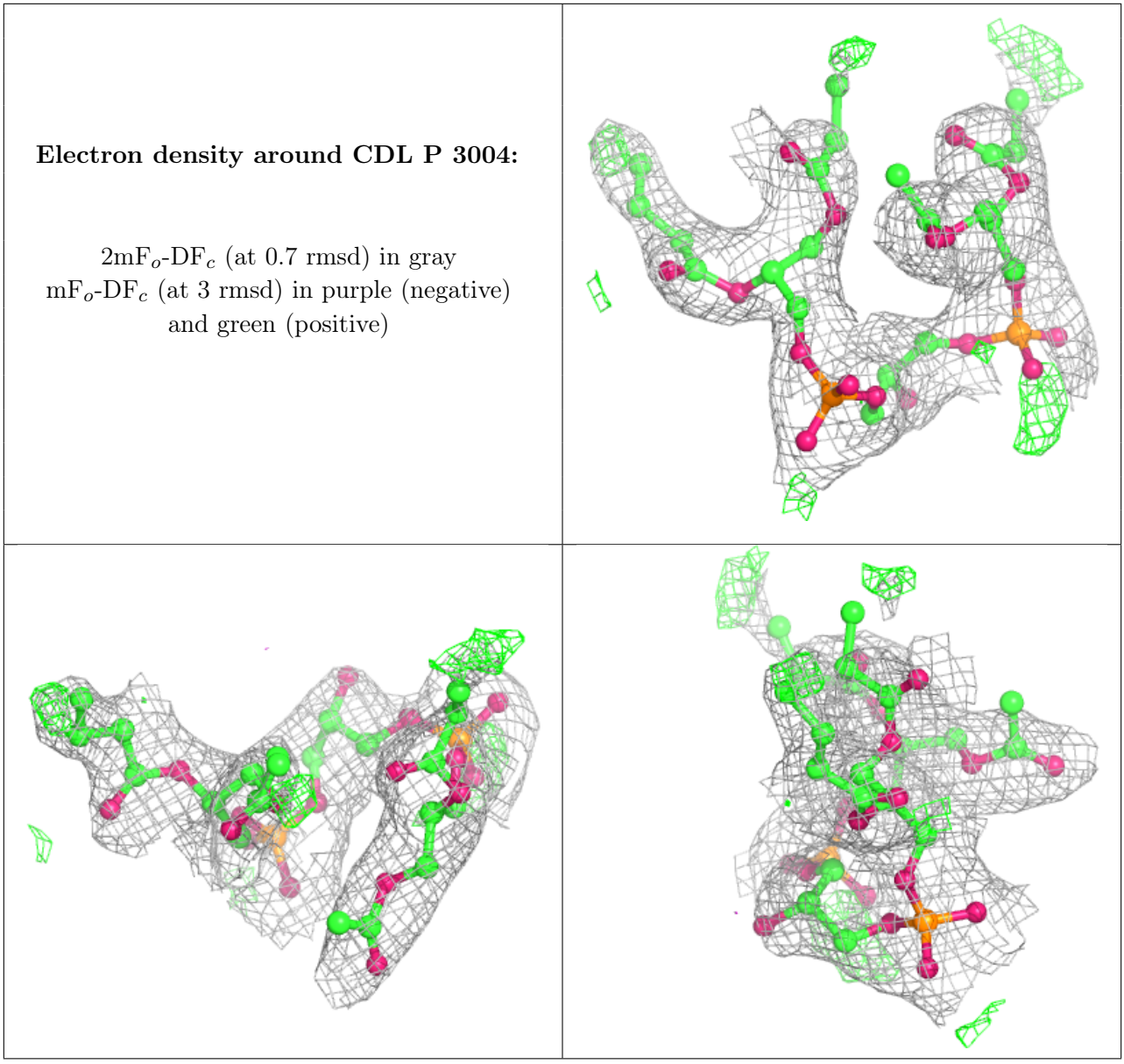
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





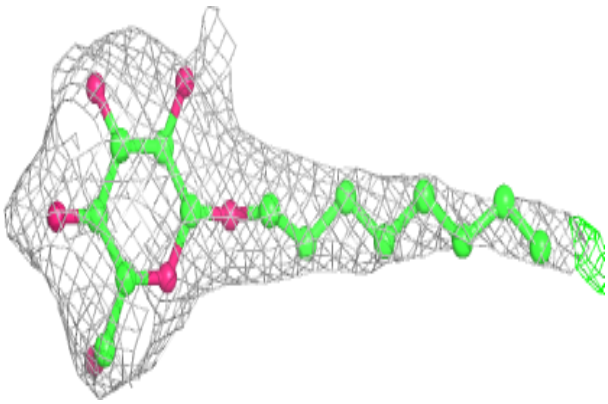
Electron density around CDL P 3004:

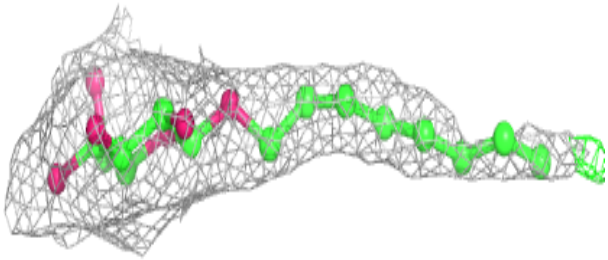
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

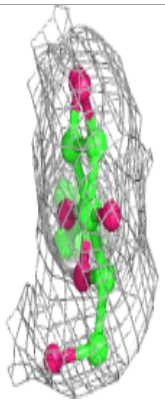


Electron density around BOG Q 3009:

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

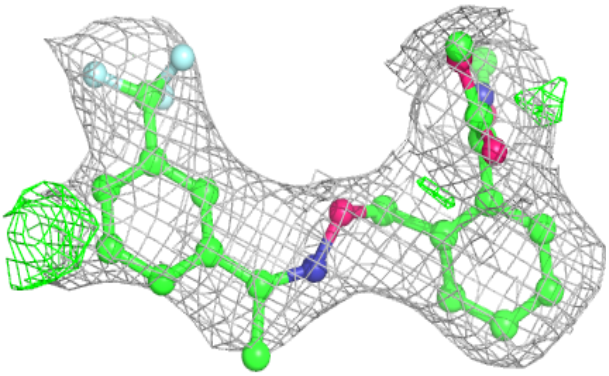


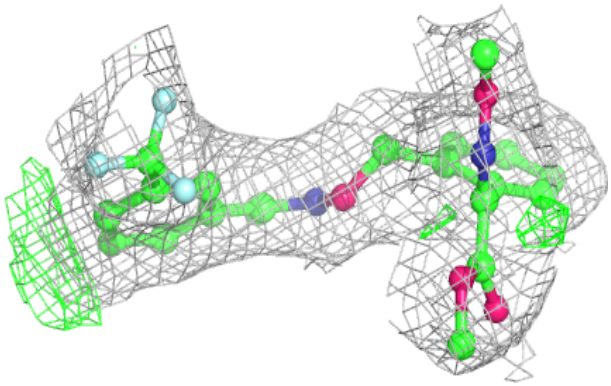


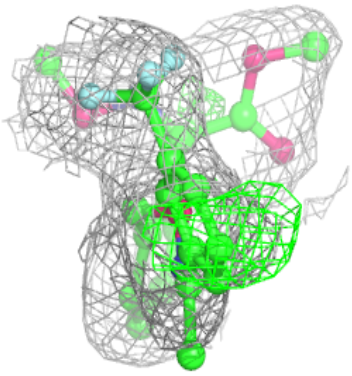


Electron density around JZV P 3001:

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

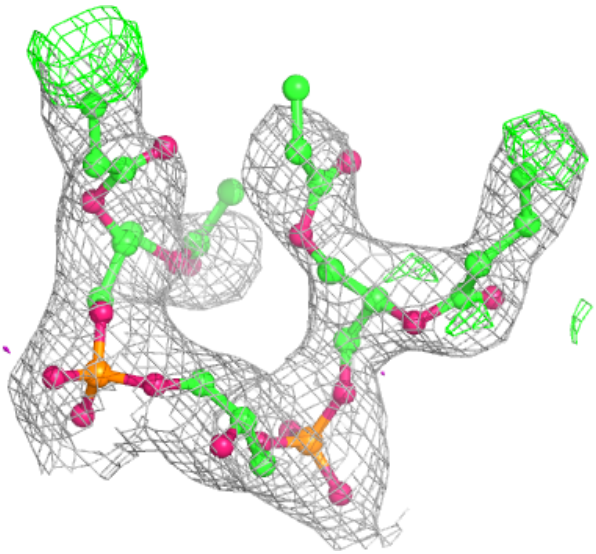


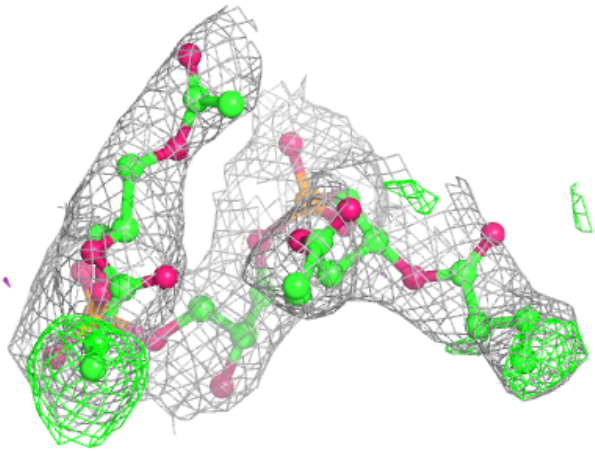


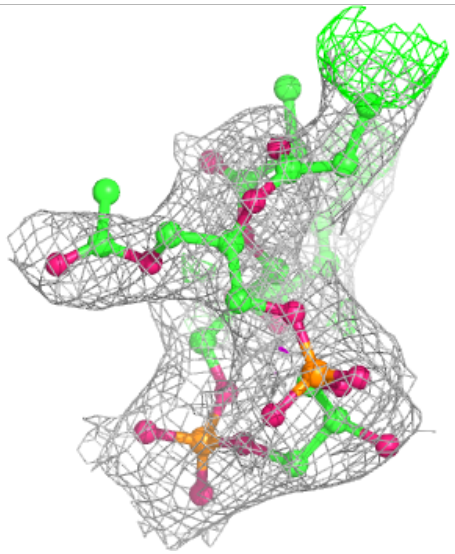


Electron density around CDL C 2004:

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

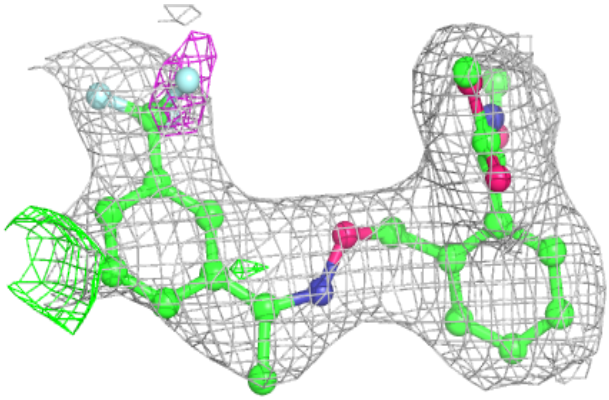


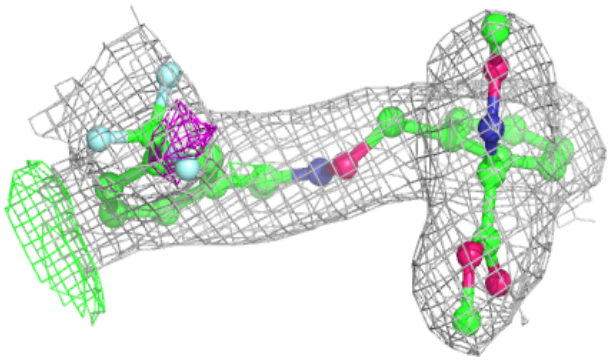


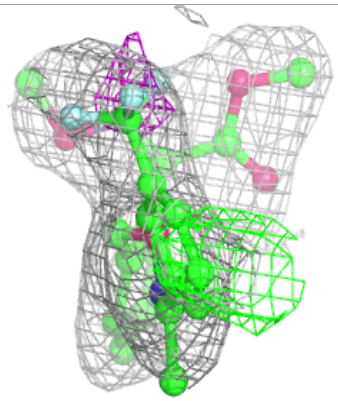


Electron density around JZV C 2001:

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

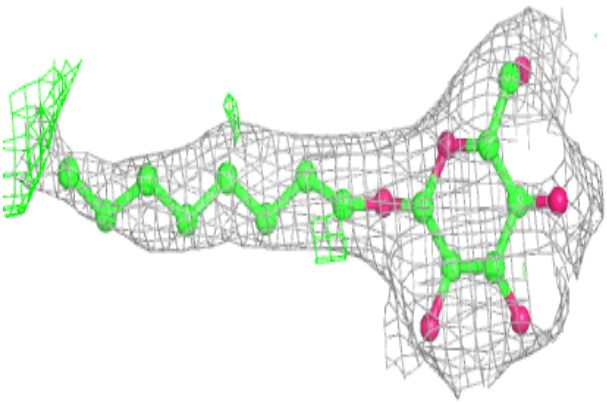


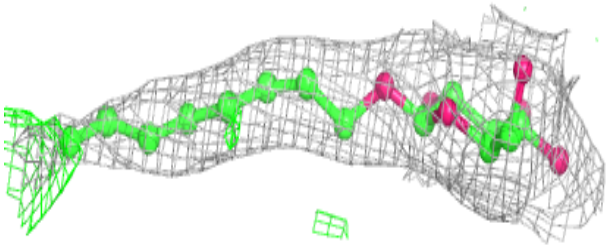


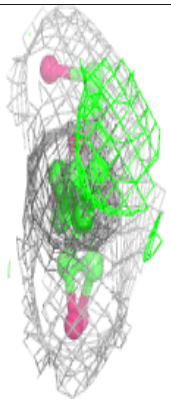


Electron density around BOG D 2009:

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

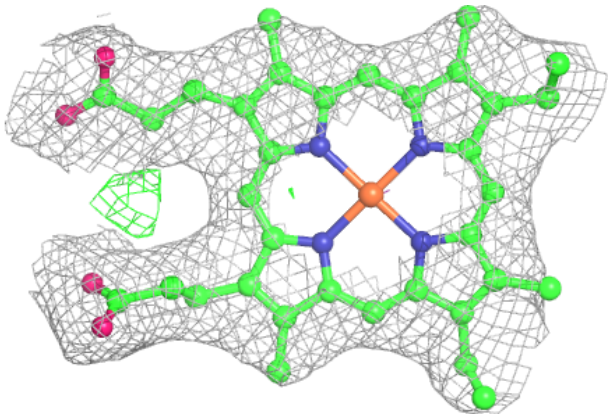


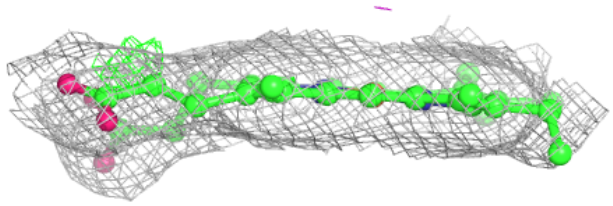


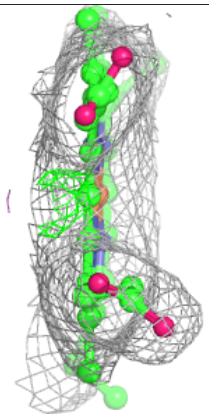


Electron density around HEC Q 501:

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

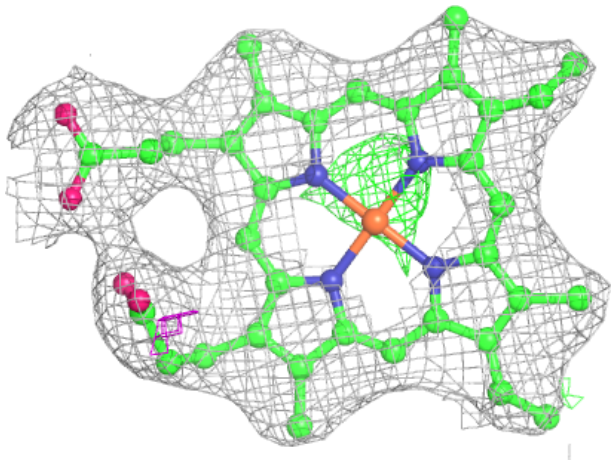


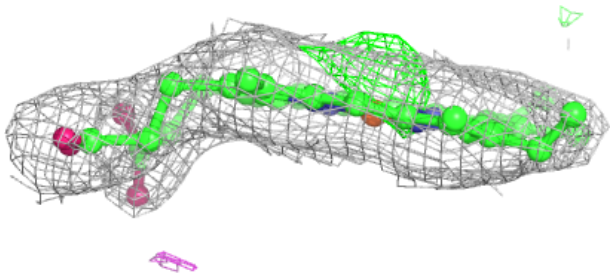


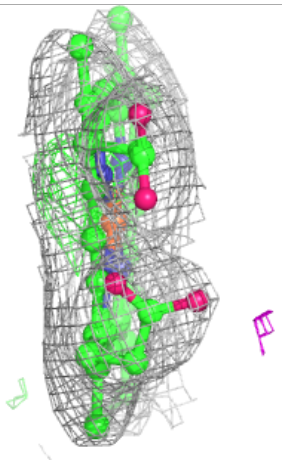


Electron density around HEM P 501:

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

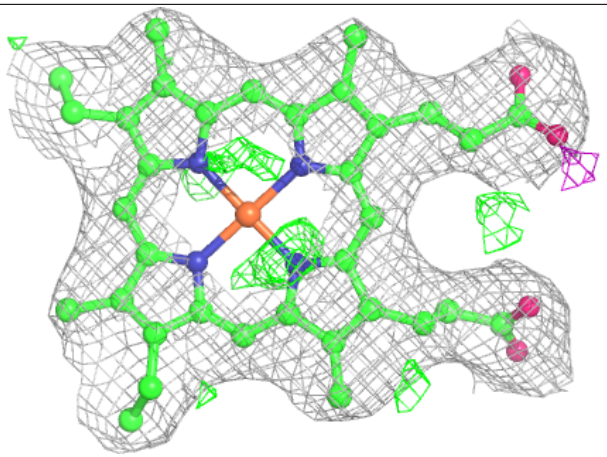


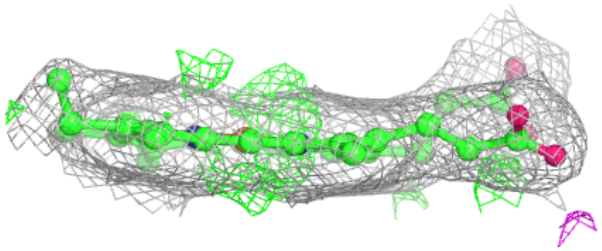


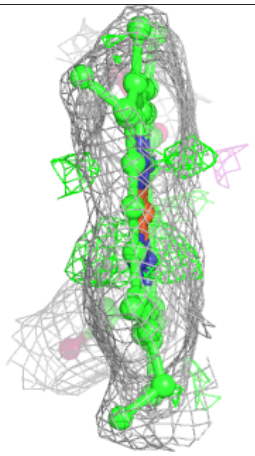


Electron density around HEC D 501:

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

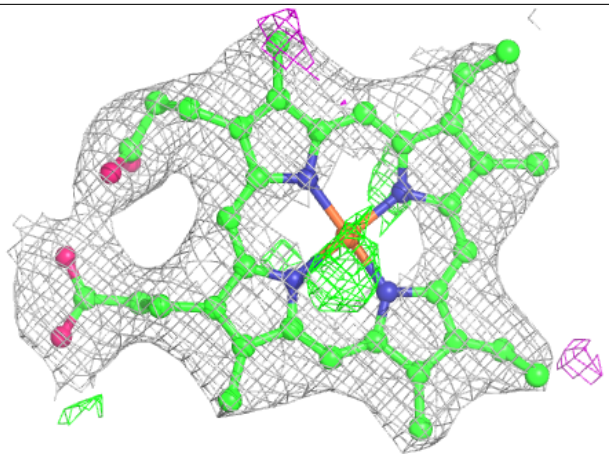


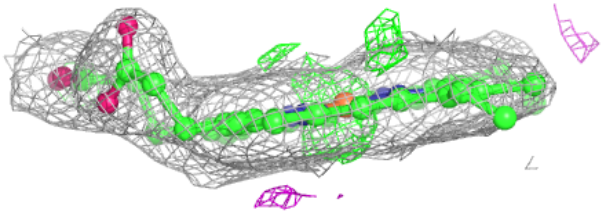


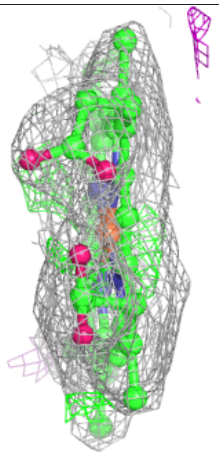


Electron density around HEM C 501:

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

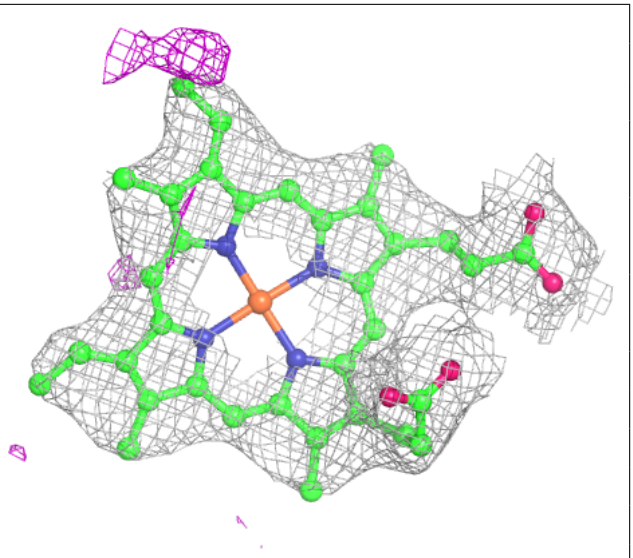


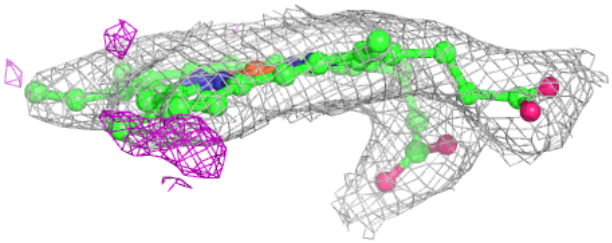


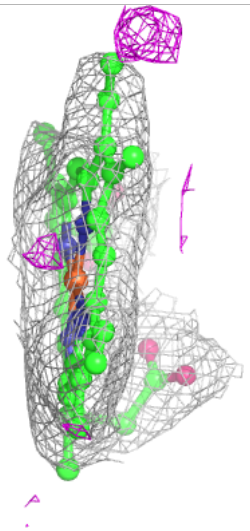


Electron density around HEM P 502:

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

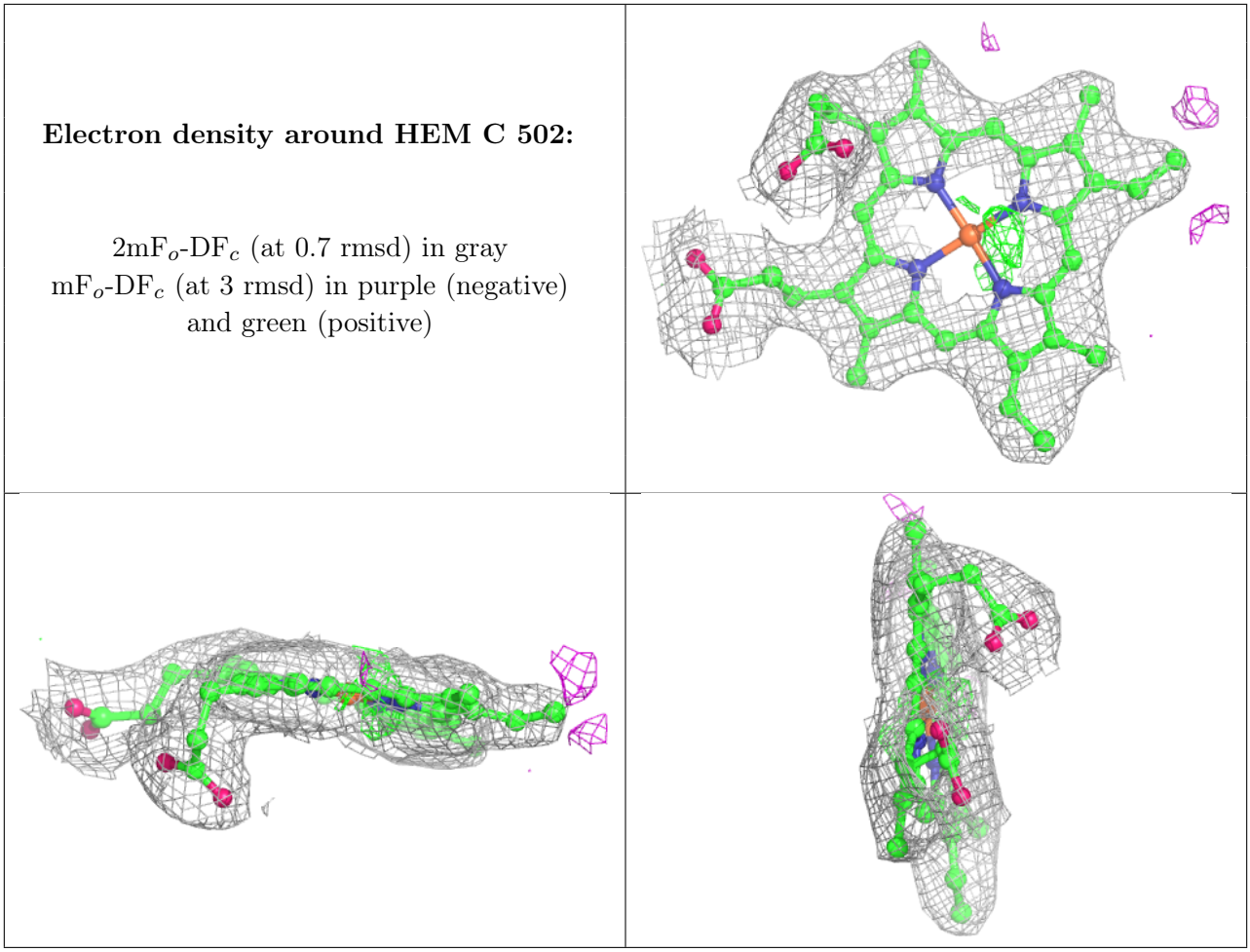






Electron density around HEM C 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.