Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 05:05 PM EDT

PDB ID	:	3TGU
Title	:	Cytochrome bc1 complex from chicken with pfvs-designed moa inhibitor bound
Authors	:	Huang, L.-S.; Yang, G.-F.; Berry, E.A.
Deposited on	:	2011-08-17
Resolution	:	2.70 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:

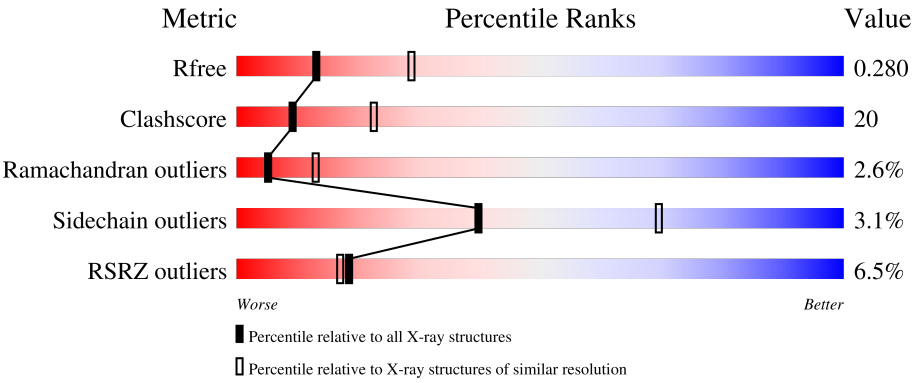
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	67% 29%
1	N	446	64% 33%
2	B	441	52% 39% 5%
2	O	441	5% 52% 39%
3	C	380	3% 73% 26%

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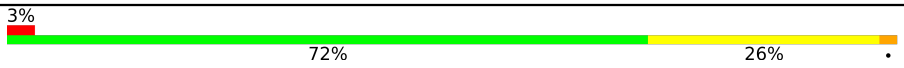
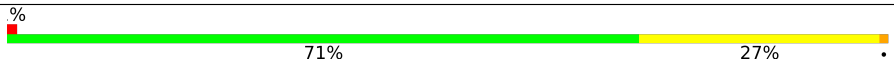
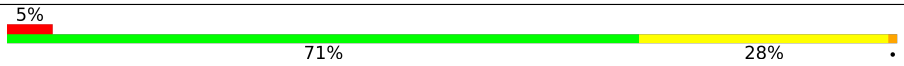
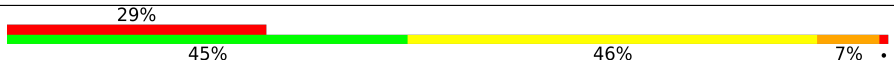
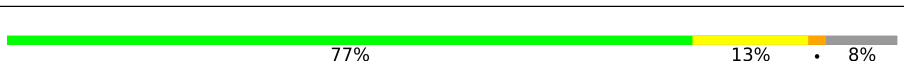
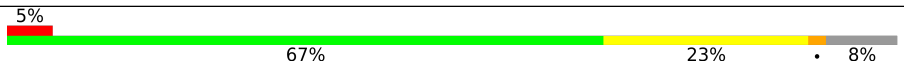
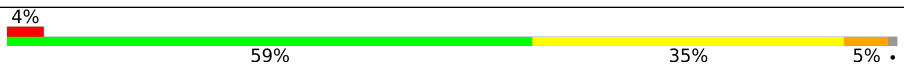
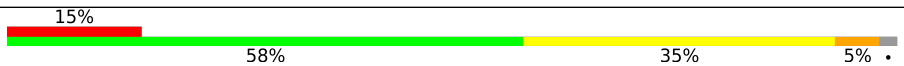
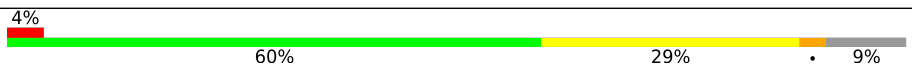
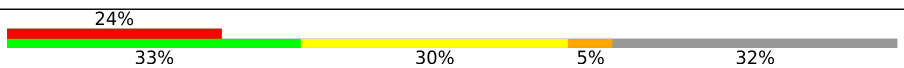
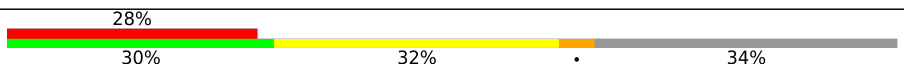
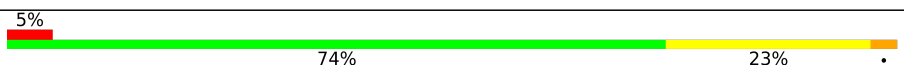
Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	76	
9	V	76	
10	J	61	
10	W	61	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	UQ	P	505	-	-	-	X
15	CDL	Q	502	-	-	-	X
16	PEE	N	502	-	X	-	-
19	BOG	D	503	-	-	-	X
19	BOG	Q	504	-	-	-	X
3	FME	C	1	-	-	-	X

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 32733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3021	2025	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	-	initiating methionine	UNP P18946
P	1	FME	-	initiating methionine	UNP P18946

- 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	52	Total	C	N	O	S	0	0	2
			319	190	65	61	3			
9	V	50	Total	C	N	O	S	0	0	2
			311	186	63	59	3			

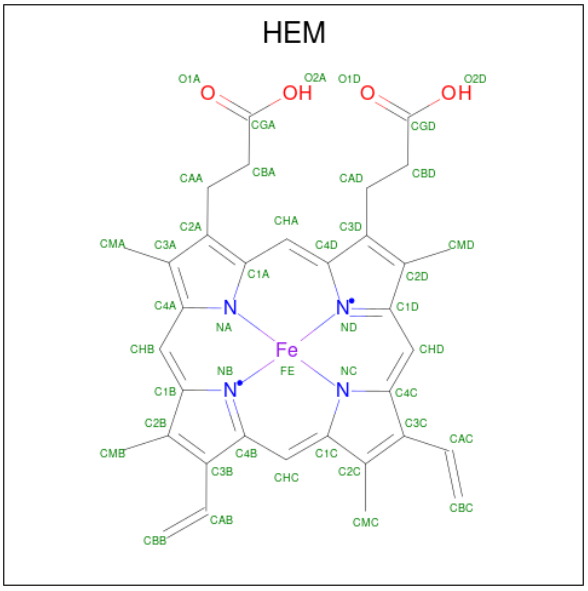
- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

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

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

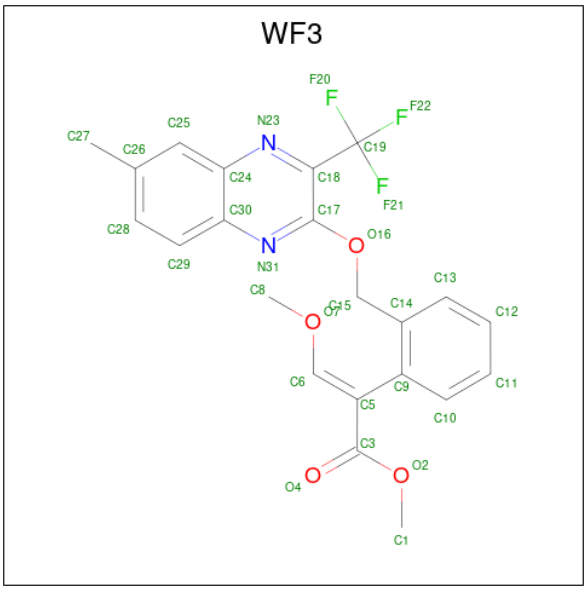
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	O	0	0
			1	1		
11	N	1	Total	O	0	0
			1	1		

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



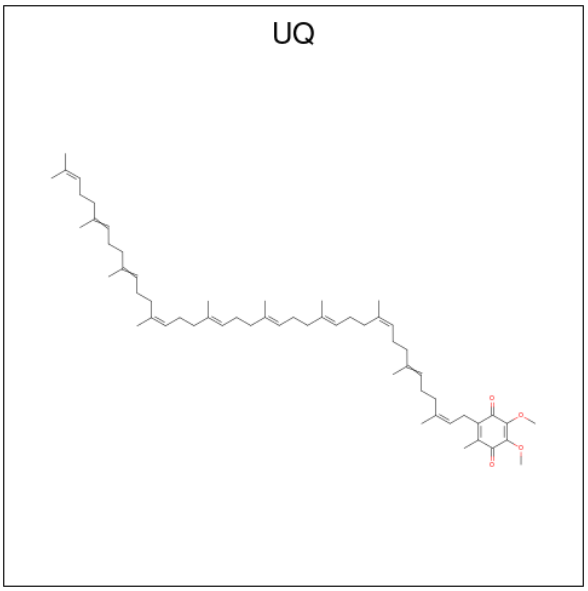
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is methyl (2E)-3-methoxy-2-[2-({[6-methyl-3-(trifluoromethyl)quinoxalin-2-yl]oxy}methyl)phenyl]prop-2-enoate (three-letter code: WF3) (formula: $C_{22}H_{19}F_3N_2O_4$).



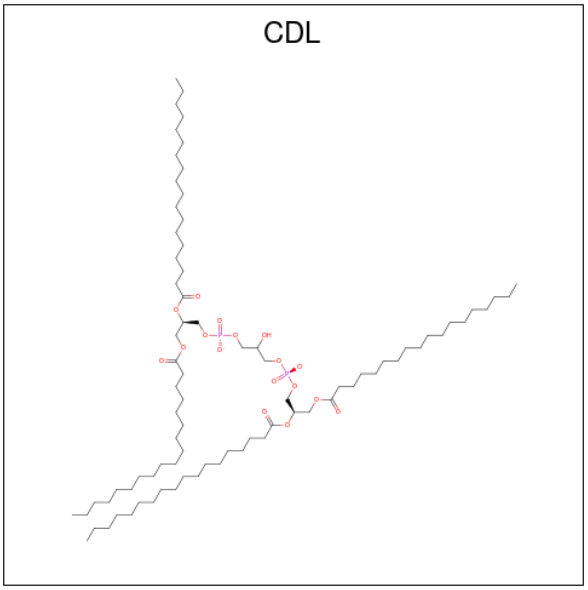
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	0	0
			31	22	3	2	4		
13	P	1	Total	C	F	N	O	0	0
			31	22	3	2	4		

- 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 19 15 4	0	0
14	P	1	Total C O 19 15 4	0	0

- 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 42 23 17 2	0	0
15	G	1	Total C O P 40 21 17 2	0	0

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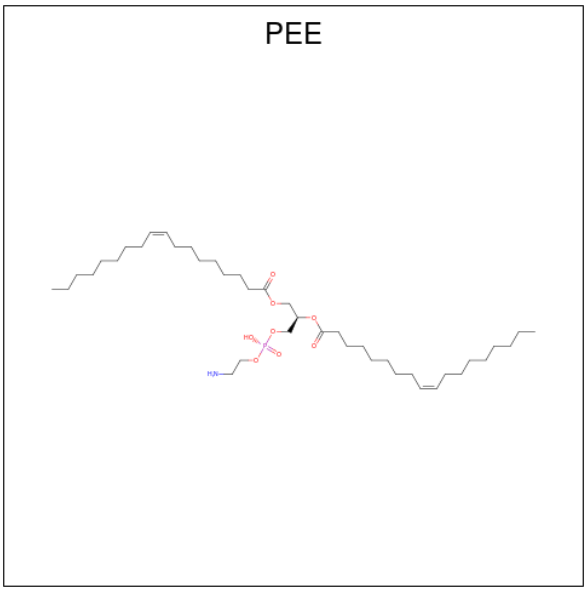
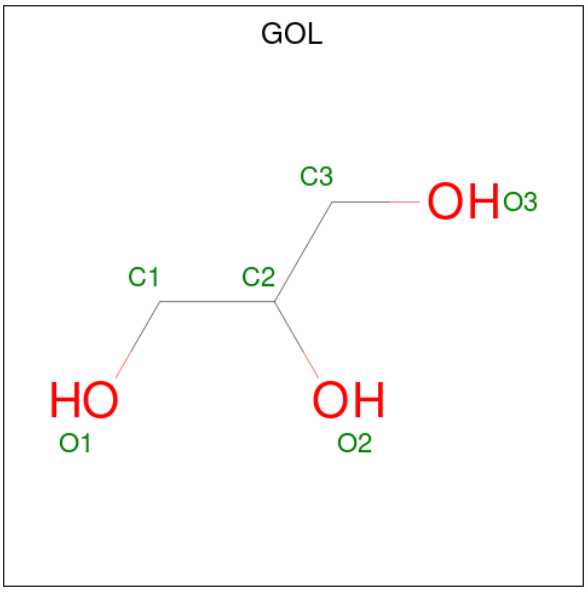
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	P	1	Total C O P 40 21 17 2	0	0
15	Q	1	Total C O P 42 23 17 2	0	0

- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



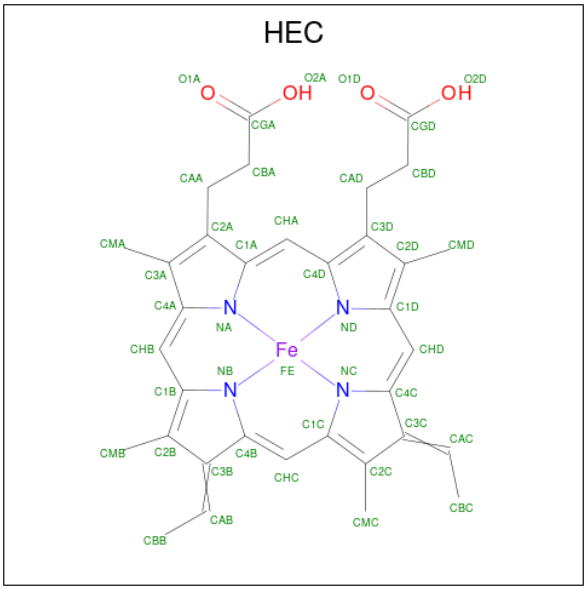
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C N O P 49 39 1 8 1	0	0
16	C	1	Total C O P 21 12 8 1	0	0
16	E	1	Total C N O P 50 40 1 8 1	0	0
16	N	1	Total O P 5 4 1	0	0
16	P	1	Total C N O P 49 39 1 8 1	0	0
16	R	1	Total C N O P 49 39 1 8 1	0	0

- Molecule 17 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



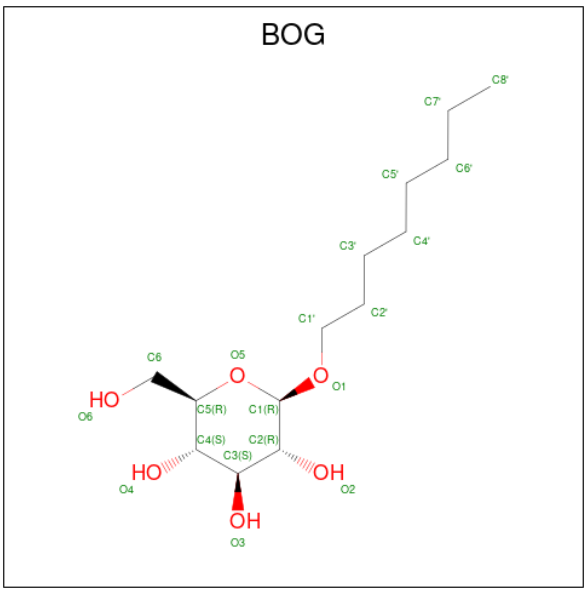
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total C O 6 3 3	0	0
17	P	1	Total C O 6 3 3	0	0

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



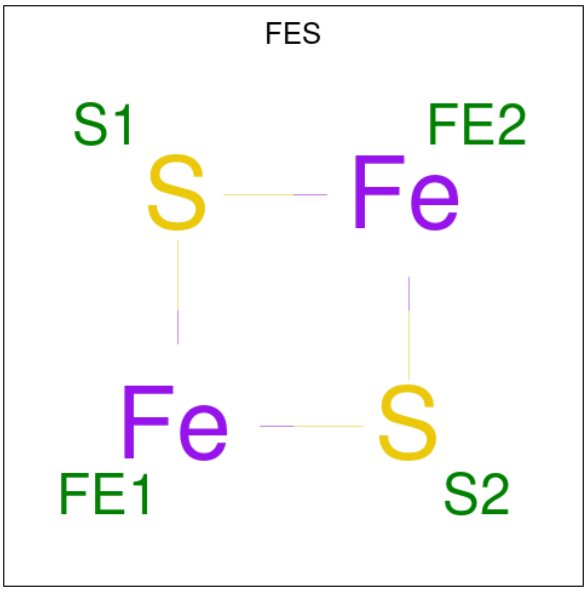
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	D	1	Total C Fe N O 43 34 1 4 4	0	0
18	Q	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 19 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

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



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

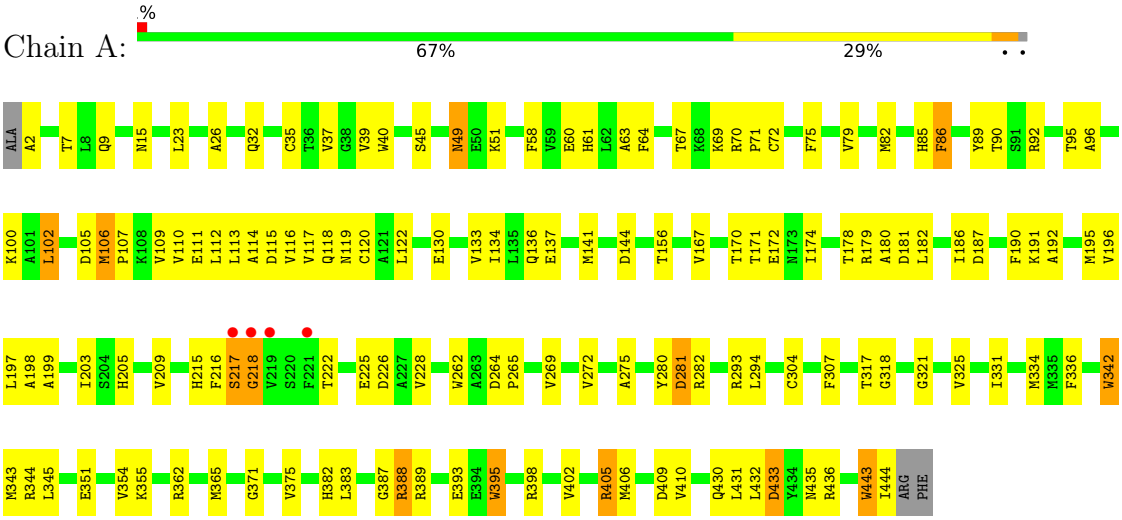
- Molecule 21 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	C	9	Total O 9 9	0	0
21	E	1	Total O 1 1	0	0
21	P	10	Total O 10 10	0	0
21	R	1	Total O 1 1	0	0

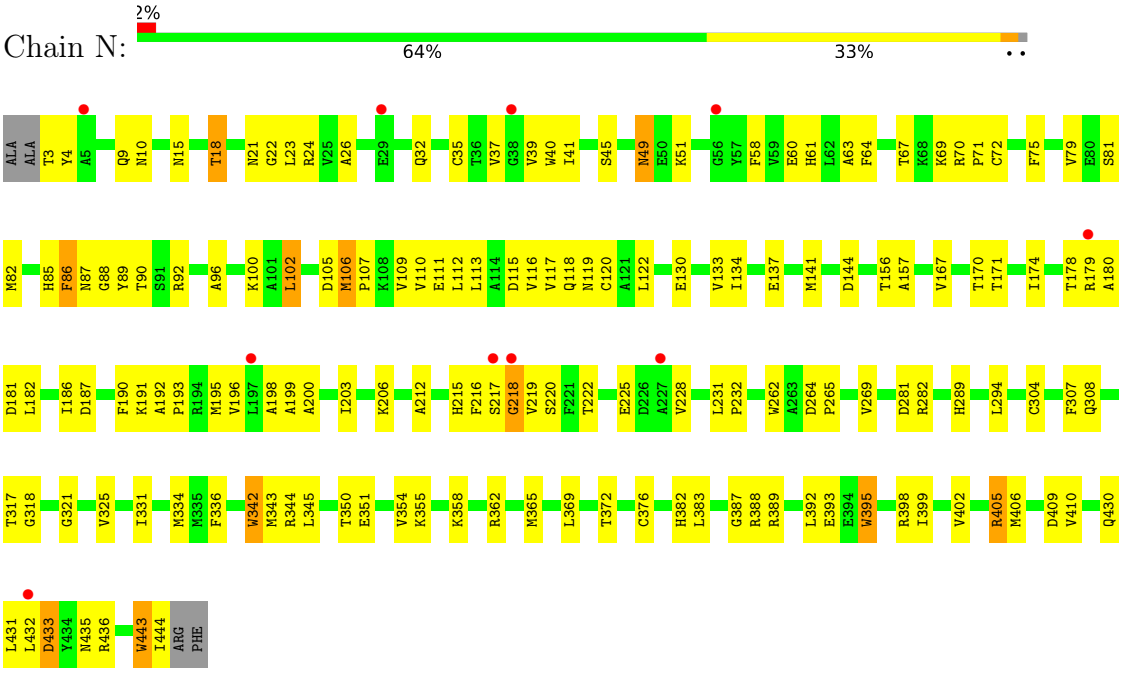
3 Residue-property plots (i)

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

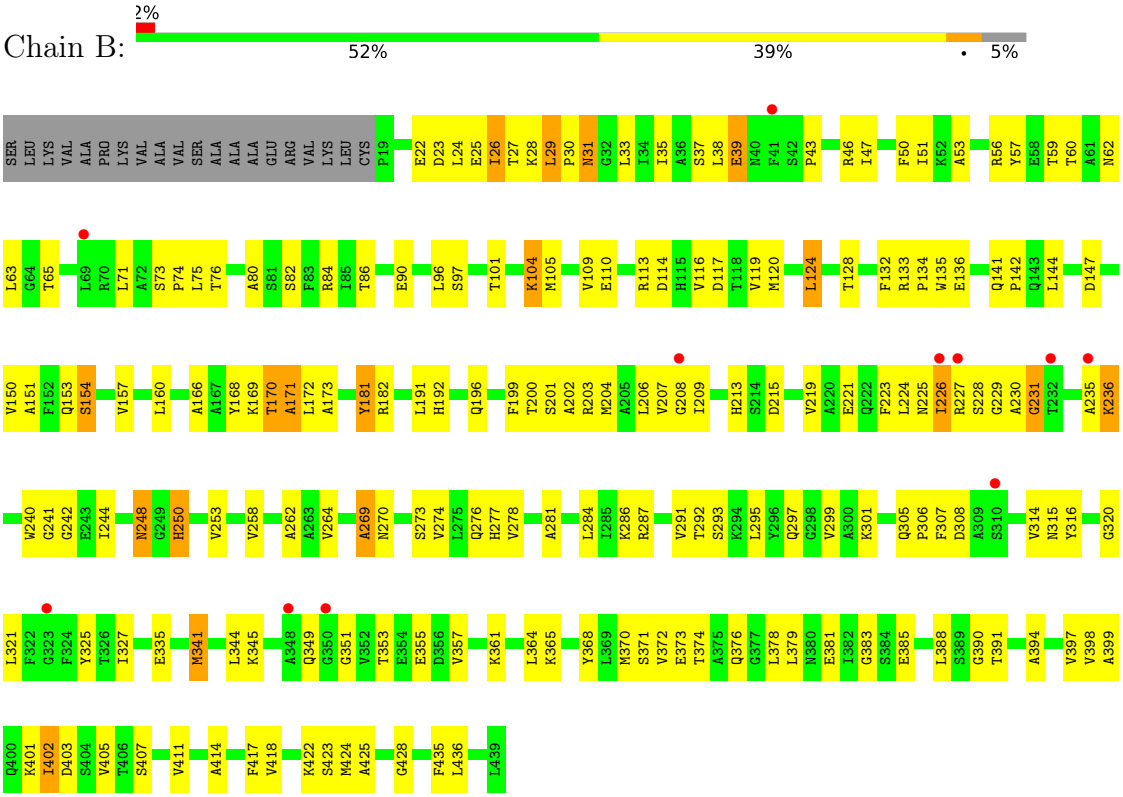


• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



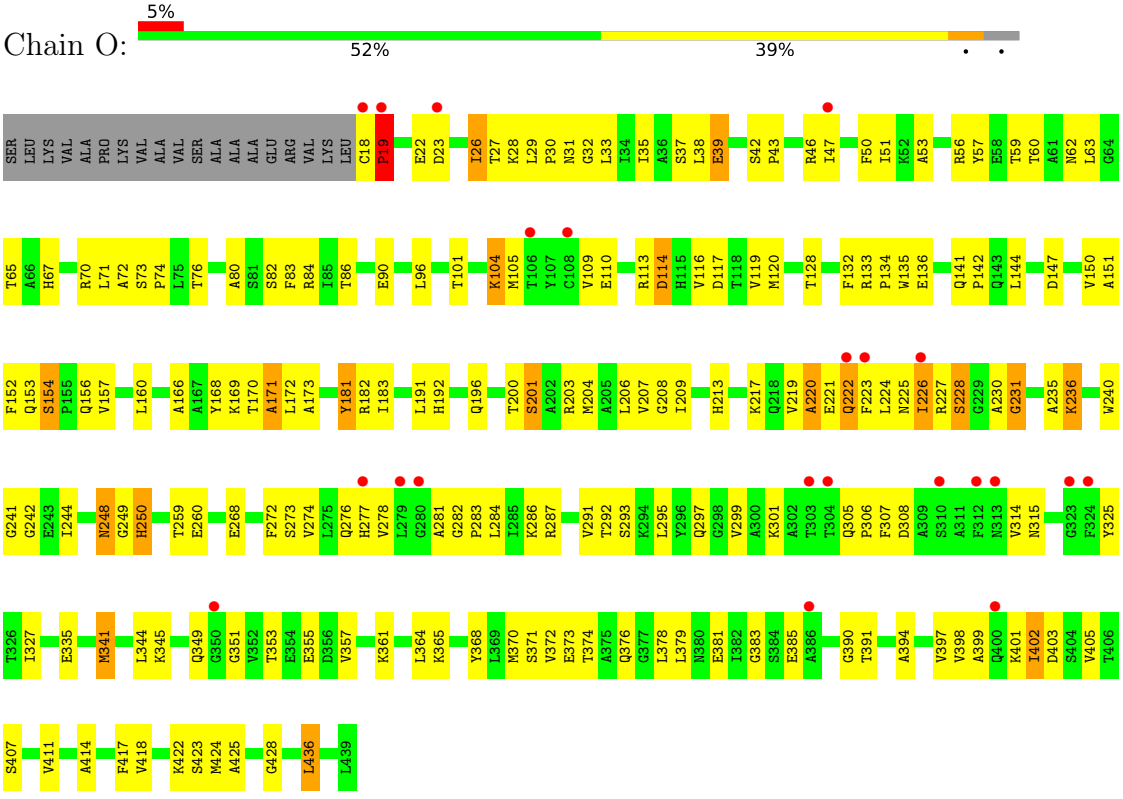
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain B:

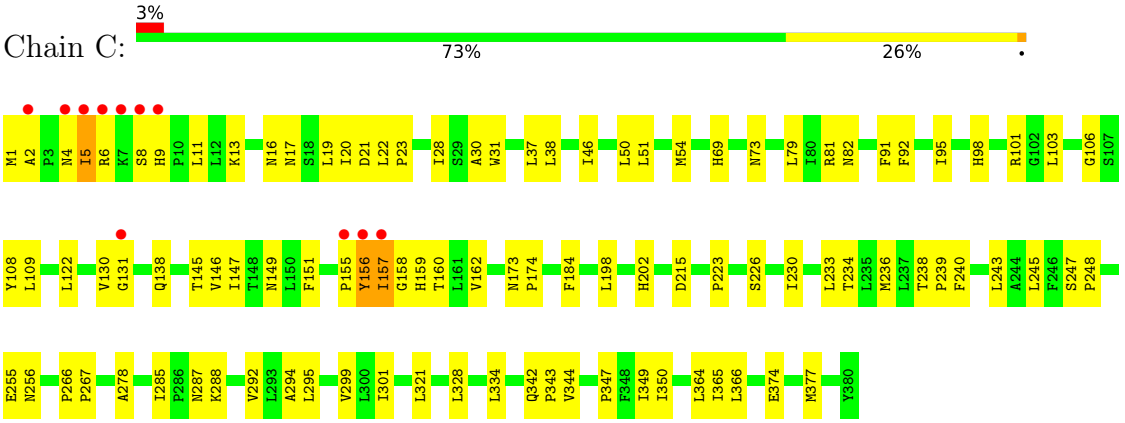


• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

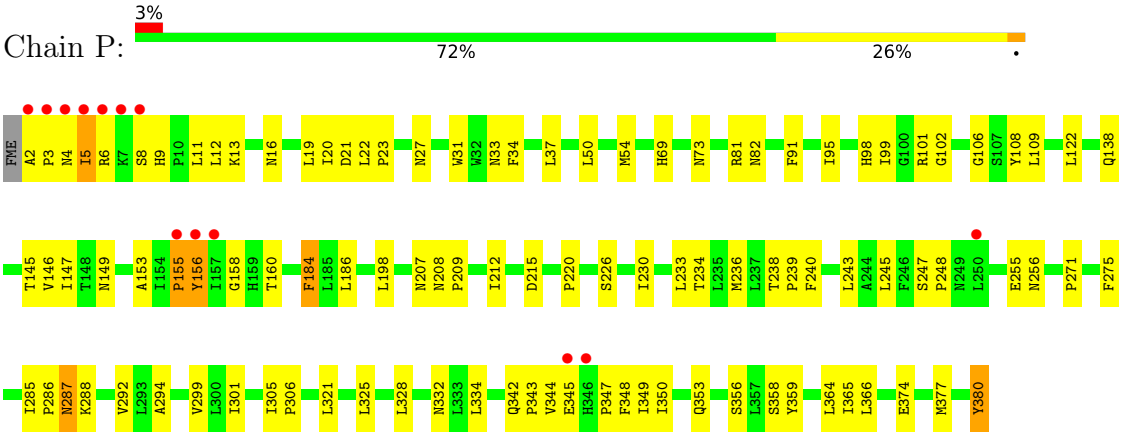
Chain O:



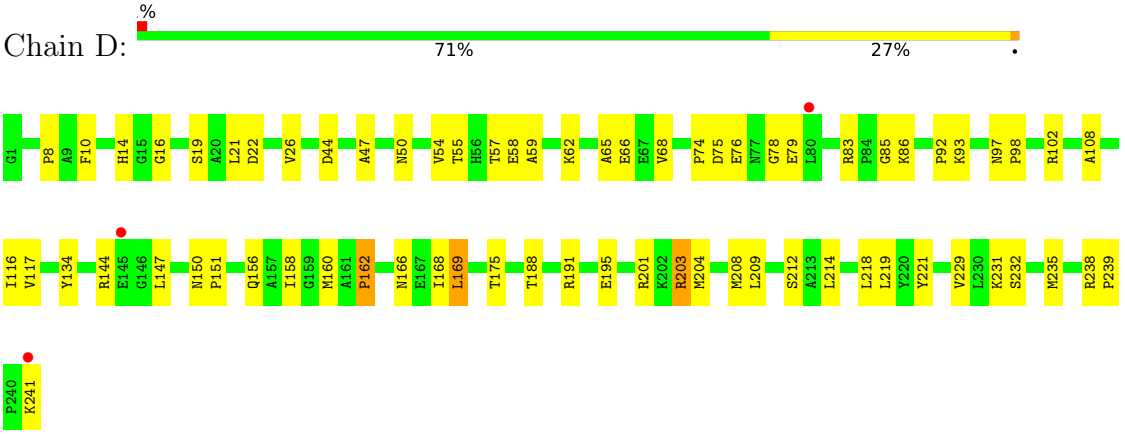
• Molecule 3: Cytochrome b



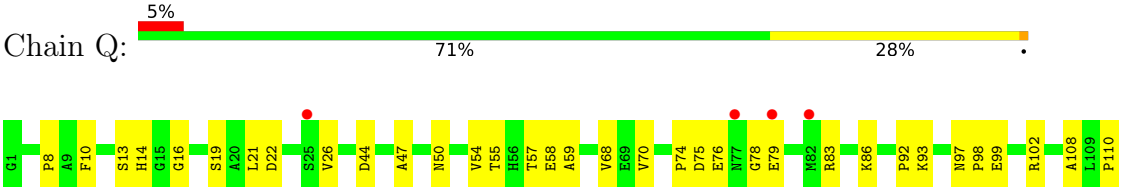
• Molecule 3: Cytochrome b

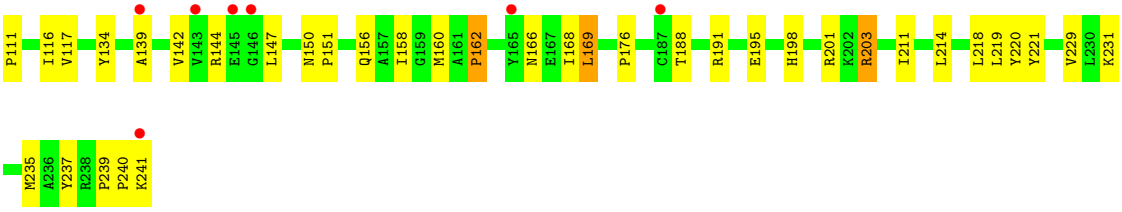


• Molecule 4: Mitochondrial cytochrome c1, heme protein

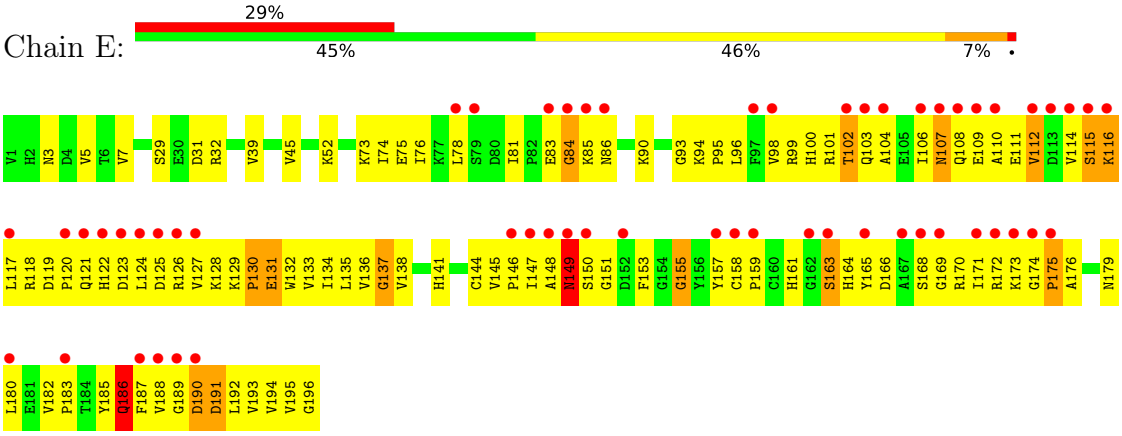


• Molecule 4: Mitochondrial cytochrome c1, heme protein

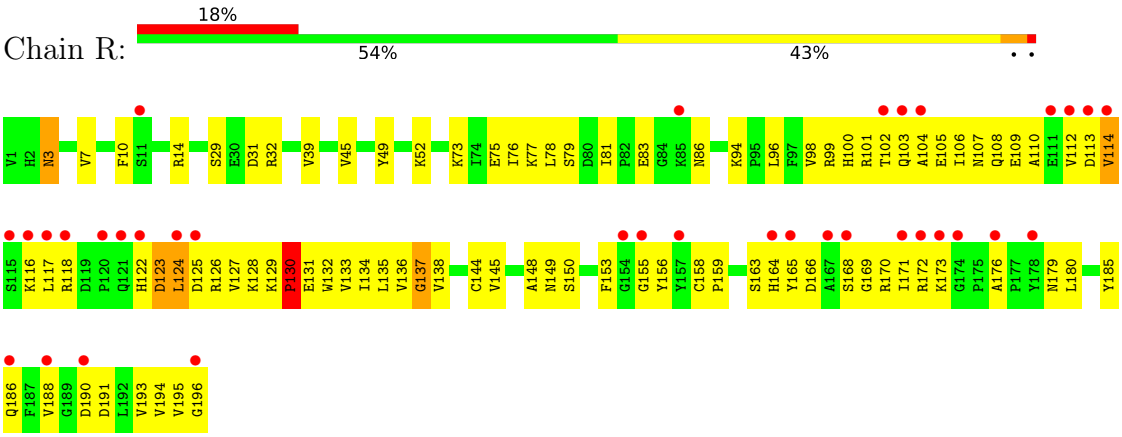




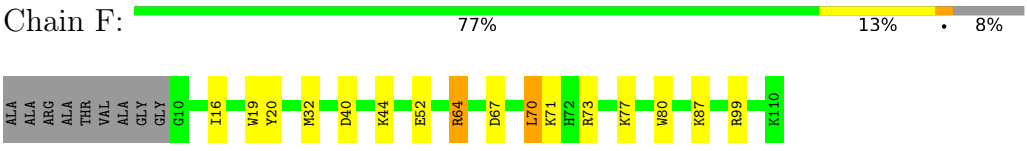
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



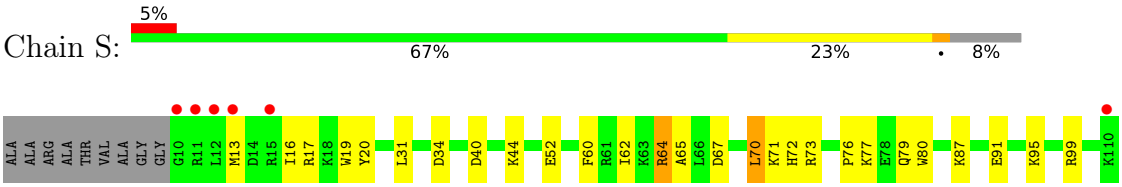
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

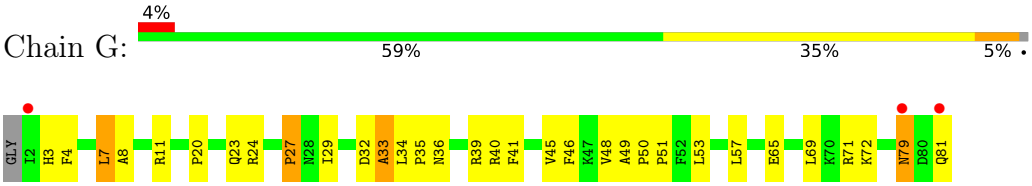


• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



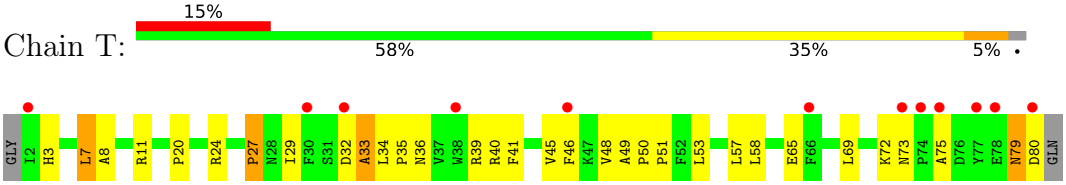
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain G:



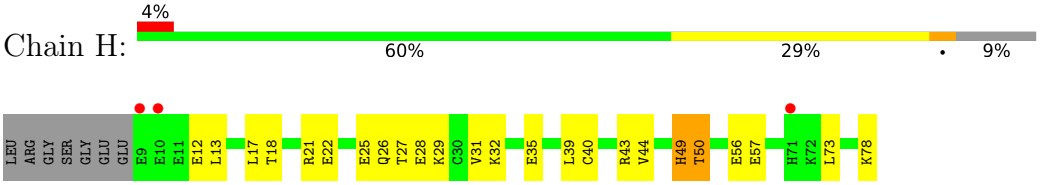
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain T:



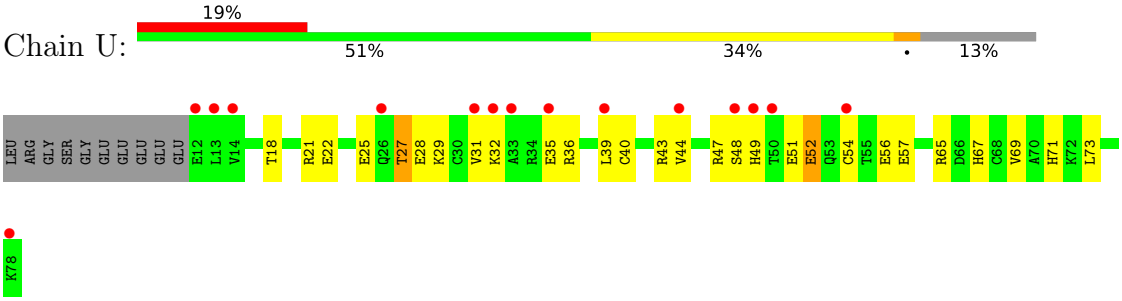
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain H:



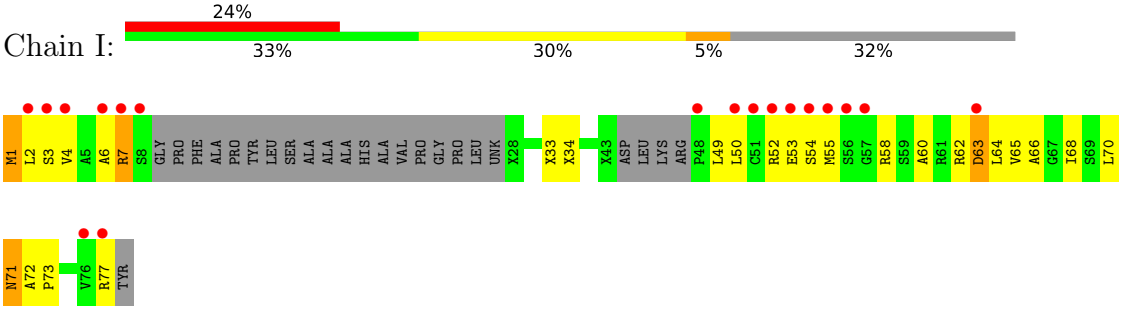
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain U:



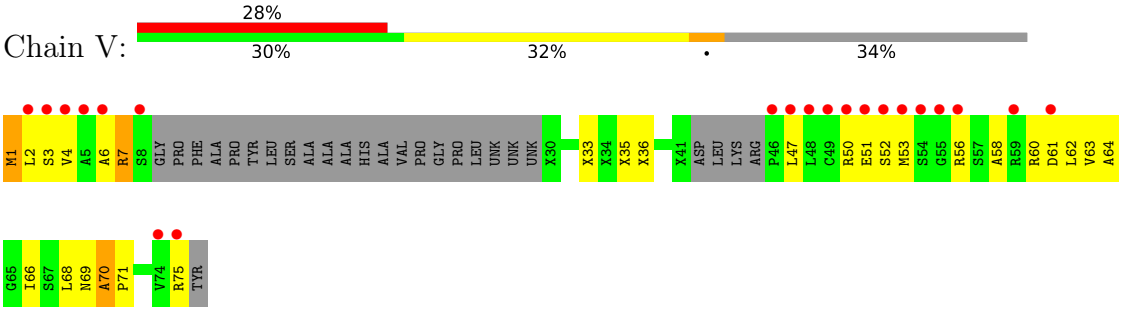
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



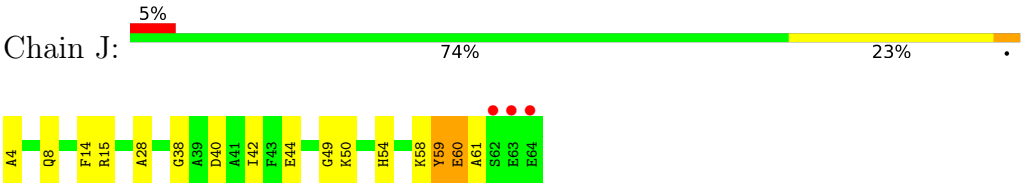
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



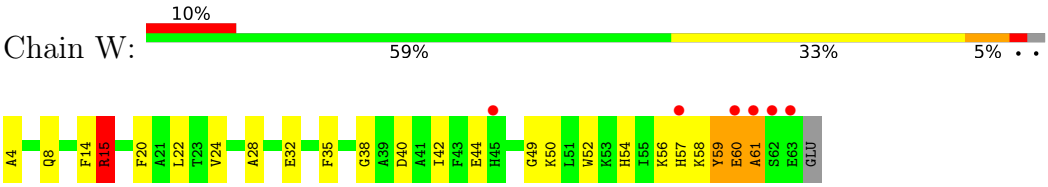
• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain J:



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

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	172.68Å 183.31Å 241.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.70 24.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.1 (24.98-2.70) 91.2 (24.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.289 0.247 , 0.280	Depositor DCC
R_{free} test set	3737 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.1	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	0.93	EDS
Total number of atoms	32733	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, UNL, HEM, FME, HEC, UQ, AME, WF3, FES, GOL, PEE, BOG

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	0.39	0/3513	0.64	0/4760
1	N	0.40	0/3508	0.63	0/4753
2	B	0.35	0/3196	0.62	0/4334
2	O	0.37	0/3202	0.63	0/4343
3	C	0.45	0/3114	0.65	0/4263
3	P	0.42	0/3114	0.63	0/4263
4	D	0.41	0/1956	0.62	0/2658
4	Q	0.37	0/1956	0.60	0/2658
5	E	0.35	0/1547	0.59	0/2103
5	R	0.35	0/1543	0.60	0/2098
6	F	0.47	0/911	0.65	0/1219
6	S	0.38	0/911	0.60	0/1219
7	G	0.44	0/694	0.65	0/941
7	T	0.41	0/684	0.64	0/929
8	H	0.39	0/582	0.60	0/779
8	U	0.32	0/561	0.58	0/751
9	I	0.36	0/251	0.62	0/336
9	V	0.34	0/251	0.60	0/336
10	J	0.39	0/508	0.59	0/682
10	W	0.41	0/490	0.58	0/660
All	All	0.39	0/32492	0.62	0/44085

There are no bond length outliers.

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	3442	0	3354	119	0
1	N	3437	0	3349	134	0
2	B	3141	0	3142	195	0
2	O	3147	0	3146	213	0
3	C	3021	0	3068	74	0
3	P	3012	0	3058	79	0
4	D	1898	0	1846	58	0
4	Q	1898	0	1846	59	0
5	E	1513	0	1478	108	0
5	R	1509	0	1474	92	0
6	F	891	0	893	16	0
6	S	891	0	893	29	0
7	G	672	0	653	29	0
7	T	662	0	645	33	0
8	H	574	0	548	18	0
8	U	553	0	535	29	0
9	I	319	0	281	43	0
9	V	311	0	283	48	0
10	J	497	0	490	13	0
10	W	479	0	478	22	0
11	A	1	0	0	0	0
11	N	1	0	0	0	0
12	C	86	0	60	5	0
12	P	86	0	60	4	0
13	C	31	0	19	1	0
13	P	31	0	19	1	0
14	C	19	0	17	3	0
14	P	19	0	17	2	0
15	C	42	0	28	1	0
15	G	40	0	24	1	0
15	P	40	0	24	3	0
15	Q	42	0	28	1	0
16	C	70	0	85	2	0
16	E	50	0	77	0	0
16	N	5	0	0	0	0
16	P	49	0	72	2	0
16	R	49	0	71	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	6	0	8	0	0
17	P	6	0	8	0	0
18	D	43	0	30	2	0
18	Q	43	0	30	1	0
19	D	33	0	39	0	0
19	P	12	0	11	0	0
19	Q	33	0	39	0	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	C	9	0	0	0	0
21	E	1	0	0	0	0
21	P	10	0	0	2	0
21	R	1	0	0	0	0
All	All	32733	0	32226	1293	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 (1293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:76:THR:HG22	2:O:82:SER:H	1.05	1.19
1:N:178:THR:HG22	1:N:180:ALA:H	1.10	1.14
1:A:178:THR:HG22	1:A:180:ALA:H	1.11	1.13
2:B:76:THR:HG22	2:B:82:SER:H	1.12	1.12
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.12	1.10
8:U:36:ARG:HH11	8:U:36:ARG:HB3	1.18	1.08
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.17	1.07
1:N:102:LEU:HD12	1:N:102:LEU:H	1.18	1.06
9:V:35:UNK:HG3	9:V:36:UNK:H	1.15	1.05
2:B:22:GLU:HG3	2:B:23:ASP:H	1.20	1.05
9:I:33:UNK:HG3	9:I:34:UNK:H	1.19	1.02
1:A:102:LEU:HD12	1:A:102:LEU:H	1.23	1.02
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.39	1.01
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.44	0.98
4:D:47:ALA:H	4:D:50:ASN:HD22	1.02	0.98
8:U:36:ARG:HB3	8:U:36:ARG:NH1	1.80	0.96
2:O:341:MET:HE2	2:O:341:MET:HA	1.46	0.96
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.80	0.96
2:B:341:MET:HE2	2:B:341:MET:HA	1.49	0.95
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.51	0.93
2:O:101:THR:HG21	9:V:4:VAL:HG11	1.48	0.93
5:E:116:LYS:H	5:E:116:LYS:HD2	1.33	0.93
2:B:353:THR:HG22	2:B:355:GLU:H	1.33	0.92
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.52	0.91
2:O:353:THR:HG22	2:O:355:GLU:H	1.33	0.90
2:O:157:VAL:HG23	9:V:62:LEU:HD21	1.53	0.90
1:N:206:LYS:H	1:N:206:LYS:HD2	1.37	0.89
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.71	0.88
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.54	0.88
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.09	0.87
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.55	0.87
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.53	0.87
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.57	0.86
2:O:76:THR:HG22	2:O:82:SER:N	1.89	0.86
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.91	0.86
5:R:117:LEU:HD21	5:R:172:ARG:NH1	1.91	0.86
2:O:385:GLU:HG2	9:V:2:LEU:HD13	1.58	0.85
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.41	0.84
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.75	0.84
1:A:178:THR:HG22	1:A:180:ALA:N	1.94	0.83
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.44	0.83
2:B:315:ASN:HD22	9:I:7:ARG:HD3	1.43	0.82
6:S:13:MET:HA	6:S:16:ILE:HD12	1.62	0.82
5:E:107:ASN:N	5:E:107:ASN:HD22	1.78	0.82
2:O:27:THR:HG22	2:O:28:LYS:H	1.42	0.82
4:D:57:THR:HG22	4:D:59:ALA:H	1.43	0.82
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.60	0.82
1:A:178:THR:HB	1:A:181:ASP:OD1	1.78	0.82
1:N:178:THR:HG22	1:N:180:ALA:N	1.92	0.82
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.63	0.81
2:O:96:LEU:HB3	9:V:68:LEU:HD22	1.62	0.81
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.62	0.81
2:O:221:GLU:HG3	2:O:222:GLN:H	1.45	0.81
8:H:27:THR:HG22	8:H:29:LYS:H	1.45	0.80
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.44	0.80
8:U:27:THR:HG22	8:U:29:LYS:H	1.44	0.80
2:B:76:THR:HG22	2:B:82:SER:N	1.94	0.80
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.64	0.80
1:A:69:LYS:HD2	1:A:70:ARG:NH2	1.95	0.80
2:O:38:LEU:HG	2:O:39:GLU:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:ALA:H	4:D:50:ASN:ND2	1.77	0.80
2:O:291:VAL:HA	2:O:297:GLN:NE2	1.96	0.79
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.65	0.79
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.65	0.79
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.62	0.79
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.46	0.79
10:W:60:GLU:O	10:W:60:GLU:HG2	1.80	0.78
2:O:381:GLU:OE1	9:V:3:SER:HB2	1.83	0.78
2:B:38:LEU:HG	2:B:39:GLU:H	1.49	0.78
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.48	0.78
2:B:27:THR:HG22	2:B:28:LYS:H	1.48	0.78
3:P:238:THR:HB	3:P:239:PRO:HD3	1.66	0.78
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.66	0.77
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.63	0.77
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.00	0.77
4:D:57:THR:HG22	4:D:59:ALA:N	2.00	0.77
1:N:69:LYS:HD2	1:N:70:ARG:NH2	1.98	0.77
5:R:112:VAL:HG21	5:R:170:ARG:HH22	1.49	0.76
2:B:291:VAL:HA	2:B:297:GLN:NE2	1.99	0.76
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.67	0.76
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.01	0.76
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.21	0.75
1:N:182:LEU:O	1:N:186:ILE:HG13	1.86	0.75
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.22	0.75
2:O:62:ASN:O	2:O:65:THR:HG22	1.86	0.75
9:V:3:SER:HB3	9:V:6:ALA:HB3	1.69	0.75
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.68	0.75
2:O:154:SER:O	2:O:157:VAL:HG12	1.87	0.75
1:A:2:ALA:HB3	2:B:113:ARG:HH21	1.52	0.74
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.67	0.74
9:I:49:LEU:HD22	9:I:54:SER:O	1.87	0.74
1:N:102:LEU:HD12	1:N:102:LEU:N	2.00	0.74
9:V:47:LEU:HD22	9:V:52:SER:O	1.86	0.74
1:N:178:THR:HB	1:N:181:ASP:OD1	1.85	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.22	0.74
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.68	0.74
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.23	0.74
1:N:187:ASP:O	1:N:191:LYS:HE3	1.88	0.73
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.69	0.73
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.22	0.73
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:315:ASN:HD22	9:V:7:ARG:HD3	1.53	0.73
1:N:206:LYS:HD2	1:N:206:LYS:N	2.04	0.73
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.69	0.73
2:O:327:ILE:HD11	9:V:56:ARG:O	1.89	0.73
2:O:361:LYS:O	2:O:365:LYS:HG3	1.89	0.73
2:O:248:ASN:HD22	2:O:248:ASN:C	1.89	0.73
9:I:3:SER:HB3	9:I:6:ALA:HB3	1.71	0.73
2:B:22:GLU:HG3	2:B:23:ASP:N	2.01	0.72
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.70	0.72
9:V:63:VAL:HB	9:V:75:ARG:HD3	1.70	0.72
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.03	0.72
1:A:187:ASP:O	1:A:191:LYS:HE3	1.88	0.72
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.71	0.72
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.90	0.72
9:I:64:LEU:HD12	9:I:77:ARG:C	2.10	0.72
6:F:32:MET:HE1	6:F:87:LYS:HG2	1.71	0.72
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.24	0.72
1:N:102:LEU:H	1:N:102:LEU:CD1	1.97	0.72
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.72	0.72
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.04	0.72
3:C:238:THR:HB	3:C:239:PRO:HD3	1.71	0.72
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.72
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.54	0.72
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.71	0.72
2:B:62:ASN:O	2:B:65:THR:HG22	1.90	0.72
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.72	0.72
3:P:101:ARG:C	3:P:101:ARG:HD2	2.11	0.71
10:W:40:ASP:O	10:W:44:GLU:HG3	1.89	0.71
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.55	0.71
9:I:70:LEU:HD23	9:I:71:ASN:HD22	1.55	0.71
5:R:94:LYS:HD3	5:R:138:VAL:HG21	1.72	0.71
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.70	0.71
1:A:182:LEU:O	1:A:186:ILE:HG13	1.89	0.71
4:D:231:LYS:O	6:F:71:LYS:HE3	1.90	0.71
2:O:221:GLU:HG3	2:O:222:GLN:N	2.05	0.71
2:O:295:LEU:O	2:O:299:VAL:HG23	1.91	0.71
2:O:314:VAL:HG13	9:V:61:ASP:HB3	1.73	0.71
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.71	0.71
2:B:38:LEU:CG	2:B:39:GLU:H	2.04	0.70
2:B:27:THR:HG22	2:B:28:LYS:N	2.06	0.70
2:O:38:LEU:CG	2:O:39:GLU:H	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:O	2:B:299:VAL:HG23	1.91	0.70
2:B:202:ALA:HB3	2:B:229:GLY:O	1.92	0.70
1:A:102:LEU:HD12	1:A:102:LEU:N	2.02	0.70
5:E:78:LEU:HD12	5:E:190:ASP:O	1.92	0.70
2:O:22:GLU:HG3	2:O:23:ASP:H	1.56	0.70
2:B:150:VAL:O	2:B:153:GLN:HG3	1.91	0.70
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.73	0.70
2:B:399:ALA:O	2:B:402:ILE:HG22	1.92	0.69
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.27	0.69
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.57	0.69
9:V:35:UNK:HG3	9:V:36:UNK:N	1.95	0.69
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.72	0.69
15:P:506:CDL:OA4	7:T:40:ARG:HD2	1.92	0.69
2:O:150:VAL:O	2:O:153:GLN:HG3	1.92	0.69
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.76	0.68
5:R:169:GLY:O	5:R:179:ASN:HB3	1.92	0.68
2:B:31:ASN:HD22	2:B:31:ASN:N	1.91	0.68
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.09	0.68
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.93	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.59	0.68
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.27	0.68
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.76	0.68
2:O:399:ALA:O	2:O:402:ILE:HG22	1.93	0.68
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.76	0.67
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.29	0.67
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.28	0.67
2:O:26:ILE:HD13	2:O:391:THR:HA	1.76	0.67
2:B:361:LYS:O	2:B:365:LYS:HG3	1.94	0.67
10:J:40:ASP:O	10:J:44:GLU:HG3	1.95	0.67
3:P:22:LEU:HD21	14:P:505:UQ:HM32	1.77	0.67
2:B:248:ASN:C	2:B:248:ASN:HD22	1.98	0.67
1:A:69:LYS:CD	1:A:70:ARG:HH21	1.99	0.67
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.77	0.67
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.67
3:C:236:MET:O	3:C:239:PRO:HD2	1.94	0.67
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.77	0.67
18:Q:501:HEC:HBB3	18:Q:501:HEC:HMB1	1.77	0.67
9:V:62:LEU:HD12	9:V:75:ARG:C	2.15	0.67
2:B:101:THR:HG21	9:I:4:VAL:HG11	1.77	0.66
4:D:102:ARG:HA	4:D:108:ALA:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:501:HEC:HMB1	18:D:501:HEC:HBB3	1.76	0.66
7:G:40:ARG:HD2	15:G:101:CDL:OA4	1.95	0.66
10:J:15:ARG:HG2	10:J:15:ARG:HH11	1.59	0.66
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.77	0.66
1:A:102:LEU:H	1:A:102:LEU:CD1	2.01	0.66
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.31	0.66
2:B:307:PHE:H	9:I:52:ARG:HG2	1.58	0.66
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.78	0.66
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.10	0.66
5:E:84:GLY:N	5:E:102:THR:HG23	2.10	0.66
1:N:170:THR:HG22	1:N:171:THR:N	2.11	0.66
7:T:29:ILE:O	7:T:33:ALA:HB3	1.95	0.66
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.77	0.66
8:H:40:CYS:O	8:H:44:VAL:HG23	1.96	0.66
9:V:35:UNK:CG	9:V:36:UNK:H	2.00	0.66
2:B:169:LYS:O	2:B:170:THR:HG23	1.95	0.66
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.78	0.65
5:E:96:LEU:HD12	5:E:135:LEU:O	1.96	0.65
10:W:15:ARG:HG2	10:W:15:ARG:HH11	1.61	0.65
3:P:9:HIS:O	3:P:13:LYS:HB3	1.95	0.65
1:N:105:ASP:O	1:N:109:VAL:HG23	1.96	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.26	0.65
2:O:414:ALA:O	2:O:418:VAL:HG23	1.96	0.65
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.61	0.65
5:E:117:LEU:HD21	5:E:170:ARG:HD2	1.78	0.65
5:E:163:SER:HA	5:E:174:GLY:HA3	1.79	0.65
1:N:69:LYS:CD	1:N:70:ARG:HH21	2.03	0.65
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.26	0.65
1:N:32:GLN:OE1	2:O:373:GLU:HG2	1.97	0.65
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.62	0.65
2:B:26:ILE:HD13	2:B:391:THR:HA	1.79	0.65
5:R:73:LYS:HB3	5:R:196:GLY:O	1.97	0.65
5:R:96:LEU:HD12	5:R:135:LEU:O	1.97	0.65
5:R:128:LYS:O	5:R:130:PRO:HD3	1.97	0.64
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.78	0.64
5:E:186:GLN:HG3	5:E:188:VAL:HG23	1.78	0.64
3:P:155:PRO:O	3:P:156:TYR:HB2	1.97	0.64
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.98	0.64
3:C:9:HIS:O	3:C:13:LYS:HB3	1.96	0.64
5:R:101:ARG:HA	5:R:105:GLU:OE1	1.97	0.64
2:B:327:ILE:HD11	9:I:58:ARG:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.78	0.64
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.80	0.64
2:O:407:SER:O	2:O:411:VAL:HG23	1.98	0.64
2:B:96:LEU:HB3	9:I:70:LEU:HD22	1.80	0.63
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.33	0.63
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.63	0.63
1:N:206:LYS:H	1:N:206:LYS:CD	2.10	0.63
4:D:175:THR:HG23	8:H:78:LYS:HD2	1.79	0.63
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.80	0.63
2:O:225:ASN:O	2:O:226:ILE:C	2.35	0.63
9:V:47:LEU:HD13	9:V:53:MET:HG2	1.80	0.63
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.81	0.63
4:Q:102:ARG:HA	4:Q:108:ALA:O	1.99	0.63
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.99	0.63
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.98	0.63
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.14	0.63
1:N:112:LEU:O	1:N:116:VAL:HG23	1.99	0.62
2:O:47:ILE:HD13	2:O:120:MET:CE	2.29	0.62
9:V:1:AME:C	9:V:3:SER:H	2.12	0.62
3:P:236:MET:O	3:P:239:PRO:HD2	1.99	0.62
10:W:57:HIS:HA	10:W:60:GLU:OE2	1.99	0.62
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.38	0.62
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.80	0.62
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.64	0.62
2:O:306:PRO:HA	9:V:50:ARG:HG3	1.81	0.62
2:B:264:VAL:HG23	2:B:316:TYR:C	2.19	0.62
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.00	0.62
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.62
5:E:115:SER:HB2	5:E:116:LYS:HD2	1.81	0.62
5:E:119:ASP:HB3	5:E:179:ASN:CG	2.20	0.62
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.35	0.62
2:B:47:ILE:HD13	2:B:120:MET:CE	2.30	0.61
7:T:46:PHE:O	7:T:50:PRO:HG2	2.00	0.61
5:R:102:THR:O	5:R:106:ILE:HG13	2.01	0.61
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.82	0.61
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.02	0.61
1:A:170:THR:HG22	1:A:171:THR:N	2.15	0.61
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.29	0.61
8:U:21:ARG:O	8:U:25:GLU:HG3	2.01	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.97	0.61
2:O:341:MET:CE	2:O:417:PHE:HE2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.16	0.61
1:A:32:GLN:OE1	2:B:373:GLU:HG2	2.01	0.61
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.35	0.61
2:O:225:ASN:O	2:O:227:ARG:HB3	2.01	0.61
1:A:106:MET:HE2	1:A:107:PRO:HA	1.83	0.61
5:E:144:CYS:O	5:E:146:PRO:HD3	2.01	0.61
9:I:33:UNK:HG3	9:I:34:UNK:N	1.99	0.61
9:V:68:LEU:HD21	9:V:69:ASN:ND2	2.15	0.61
10:W:49:GLY:N	10:W:54:HIS:ND1	2.48	0.61
2:B:397:VAL:O	2:B:401:LYS:HG2	2.01	0.61
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.30	0.61
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.36	0.61
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.83	0.60
5:E:163:SER:H	5:E:175:PRO:HD2	1.66	0.60
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.83	0.60
2:O:248:ASN:ND2	2:O:250:HIS:H	1.99	0.60
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.01	0.60
2:B:76:THR:CG2	2:B:82:SER:H	2.01	0.60
5:E:73:LYS:HB3	5:E:196:GLY:O	2.01	0.60
5:R:112:VAL:HG11	5:R:170:ARG:NH1	2.16	0.60
2:O:397:VAL:O	2:O:401:LYS:HG2	2.01	0.60
5:E:94:LYS:HD3	5:E:138:VAL:HG21	1.84	0.60
6:F:99:ARG:HH11	6:F:99:ARG:HG3	1.66	0.60
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.83	0.60
2:O:169:LYS:O	2:O:170:THR:HG23	2.01	0.60
2:B:385:GLU:HG2	9:I:2:LEU:HD13	1.81	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.35	0.60
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.84	0.60
4:D:47:ALA:N	4:D:50:ASN:HD22	1.87	0.60
1:A:102:LEU:HD13	1:A:105:ASP:OD2	2.02	0.60
2:B:43:PRO:O	2:B:113:ARG:HG3	2.00	0.60
2:B:341:MET:CE	2:B:417:PHE:HE2	2.15	0.60
5:E:190:ASP:C	5:E:192:LEU:H	2.04	0.60
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.82	0.60
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.67	0.60
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.67	0.60
7:T:79:ASN:N	7:T:79:ASN:HD22	1.99	0.60
8:U:40:CYS:O	8:U:44:VAL:HG23	2.02	0.59
9:V:6:ALA:O	9:V:7:ARG:HG3	2.01	0.59
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.83	0.59
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:29:LEU:HD11	2:O:221:GLU:HB3	1.83	0.59
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.37	0.59
2:O:341:MET:HE2	2:O:341:MET:CA	2.27	0.59
5:E:106:ILE:C	5:E:107:ASN:HD22	2.06	0.59
8:H:27:THR:HG22	8:H:29:LYS:N	2.16	0.59
9:I:70:LEU:HD23	9:I:71:ASN:N	2.17	0.59
2:O:374:THR:HG22	2:O:376:GLN:H	1.68	0.59
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.02	0.59
2:O:357:VAL:O	2:O:361:LYS:HG3	2.02	0.59
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.83	0.59
2:B:407:SER:O	2:B:411:VAL:HG23	2.01	0.59
8:H:21:ARG:O	8:H:25:GLU:HG3	2.02	0.59
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.85	0.59
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.38	0.59
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.85	0.59
3:C:46:ILE:HA	12:C:501:HEM:HMC3	1.85	0.59
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.03	0.59
2:O:53:ALA:O	2:O:105:MET:HG3	2.03	0.59
2:O:101:THR:CG2	2:O:104:LYS:HE3	2.29	0.59
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.67	0.59
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.03	0.58
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.18	0.58
2:B:357:VAL:O	2:B:361:LYS:HG3	2.02	0.58
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.18	0.58
5:R:118:ARG:NH1	5:R:118:ARG:HB2	2.18	0.58
2:B:22:GLU:CG	2:B:23:ASP:H	1.99	0.58
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.68	0.58
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.84	0.58
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.39	0.58
9:V:69:ASN:O	9:V:70:ALA:HB2	2.03	0.58
3:C:288:LYS:O	3:C:292:VAL:HG23	2.03	0.58
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.32	0.58
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.17	0.58
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.35	0.58
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.19	0.58
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.85	0.58
2:B:315:ASN:ND2	9:I:7:ARG:HD3	2.17	0.58
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.86	0.58
1:N:106:MET:HE2	1:N:107:PRO:HA	1.86	0.58
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.86	0.58
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.85	0.58
3:P:145:THR:O	3:P:149:ASN:HB2	2.04	0.58
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.33	0.58
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.04	0.58
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.84	0.58
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.39	0.57
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.34	0.57
9:I:6:ALA:O	9:I:7:ARG:HG3	2.03	0.57
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.85	0.57
3:C:101:ARG:HD2	3:C:101:ARG:C	2.24	0.57
1:N:102:LEU:HD13	1:N:105:ASP:OD2	2.04	0.57
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.51	0.57
2:B:374:THR:HG22	2:B:376:GLN:H	1.69	0.57
2:O:59:THR:HG22	2:O:60:THR:N	2.19	0.57
2:O:422:LYS:O	2:O:436:LEU:HD21	2.03	0.57
1:A:133:VAL:O	1:A:137:GLU:HG3	2.04	0.57
7:T:41:PHE:O	7:T:45:VAL:HG23	2.04	0.57
7:G:29:ILE:O	7:G:33:ALA:HB3	2.04	0.57
9:I:33:UNK:CG	9:I:34:UNK:H	2.03	0.57
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.86	0.57
1:N:402:VAL:HG22	1:N:406:MET:CE	2.35	0.57
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.40	0.57
3:P:5:ILE:O	3:P:5:ILE:HG22	2.05	0.57
2:B:381:GLU:OE1	9:I:3:SER:HB2	2.05	0.57
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.23	0.57
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.87	0.57
4:D:22:ASP:HA	10:J:50:LYS:HB3	1.87	0.57
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.04	0.57
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.85	0.57
1:A:362:ARG:O	1:A:365:MET:HG2	2.05	0.56
3:P:138:GLN:HB2	3:P:255:GLU:O	2.05	0.56
2:B:341:MET:HE2	2:B:341:MET:CA	2.28	0.56
2:B:368:TYR:HB2	9:I:1:AME:HE3	1.87	0.56
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.41	0.56
1:N:4:TYR:HB2	2:O:114:ASP:OD1	2.05	0.56
1:N:21:ASN:HB3	1:N:219:VAL:HG22	1.86	0.56
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.87	0.56
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.35	0.56
1:A:137:GLU:O	1:A:141:MET:HG3	2.05	0.56
3:C:22:LEU:HD21	14:C:504:UQ:HM32	1.88	0.56
10:W:60:GLU:O	10:W:61:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.87	0.56
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.86	0.56
2:O:192:HIS:O	2:O:196:GLN:HG3	2.04	0.56
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.23	0.56
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.87	0.56
3:C:5:ILE:O	3:C:5:ILE:HG22	2.06	0.56
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.35	0.56
5:R:117:LEU:HD21	5:R:172:ARG:HH11	1.70	0.56
2:B:53:ALA:O	2:B:105:MET:HG3	2.06	0.56
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.88	0.56
2:O:182:ARG:HG2	2:O:182:ARG:HH11	1.70	0.56
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.40	0.56
1:A:2:ALA:HB3	2:B:113:ARG:NH2	2.20	0.56
2:B:297:GLN:O	2:B:301:LYS:HG3	2.05	0.56
7:G:65:GLU:O	7:G:69:LEU:HG	2.06	0.56
1:N:90:THR:O	1:N:167:VAL:HG11	2.05	0.56
10:W:38:GLY:O	10:W:42:ILE:HG13	2.05	0.56
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.88	0.56
4:D:203:ARG:HB2	4:D:203:ARG:HH11	1.70	0.56
2:O:273:SER:O	2:O:276:GLN:HB3	2.06	0.56
3:P:153:ALA:O	3:P:155:PRO:HD3	2.06	0.56
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.70	0.55
2:B:31:ASN:N	2:B:31:ASN:ND2	2.52	0.55
2:B:101:THR:CG2	2:B:104:LYS:HE3	2.33	0.55
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.71	0.55
6:S:13:MET:O	6:S:16:ILE:HB	2.05	0.55
1:A:67:THR:HG21	1:A:115:ASP:CG	2.26	0.55
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.21	0.55
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.41	0.55
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.21	0.55
2:O:297:GLN:O	2:O:301:LYS:HG3	2.06	0.55
7:G:46:PHE:O	7:G:50:PRO:HG2	2.06	0.55
3:P:230:ILE:HG23	16:R:502:PEE:H25	1.89	0.55
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.05	0.55
5:R:134:ILE:HD11	5:R:193:VAL:HG21	1.88	0.55
7:G:41:PHE:O	7:G:45:VAL:HG23	2.07	0.55
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.42	0.55
2:B:414:ALA:O	2:B:418:VAL:HG23	2.07	0.55
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.41	0.55
3:P:365:ILE:HG22	3:P:366:LEU:N	2.22	0.55
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.88	0.55
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.89	0.55
6:F:40:ASP:O	6:F:44:LYS:HG2	2.07	0.55
1:A:112:LEU:O	1:A:116:VAL:HG23	2.07	0.55
2:O:292:THR:HG22	2:O:292:THR:O	2.07	0.55
1:A:387:GLY:O	1:A:388:ARG:HB3	2.07	0.54
2:B:38:LEU:HG	2:B:39:GLU:N	2.21	0.54
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.42	0.54
8:U:43:ARG:HD2	8:U:47:ARG:HH22	1.72	0.54
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.88	0.54
5:E:189:GLY:O	5:E:192:LEU:N	2.39	0.54
1:N:134:ILE:HG22	1:N:174:ILE:HD13	1.89	0.54
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.72	0.54
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.07	0.54
9:V:47:LEU:HD11	9:V:56:ARG:HH11	1.72	0.54
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.42	0.54
2:O:248:ASN:C	2:O:248:ASN:ND2	2.60	0.54
5:R:3:ASN:ND2	5:R:3:ASN:H	2.06	0.54
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.89	0.54
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.23	0.54
2:B:417:PHE:O	2:B:422:LYS:HE3	2.08	0.54
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.38	0.54
1:N:294:LEU:HD11	1:N:334:MET:HE3	1.89	0.54
1:N:362:ARG:O	1:N:365:MET:HG2	2.08	0.54
5:R:3:ASN:H	5:R:3:ASN:HD22	1.55	0.54
1:N:67:THR:HG21	1:N:115:ASP:CG	2.27	0.54
4:Q:203:ARG:HH11	4:Q:203:ARG:HB2	1.73	0.54
2:B:166:ALA:O	2:B:242:GLY:N	2.35	0.54
3:C:145:THR:O	3:C:149:ASN:HB2	2.08	0.54
4:D:150:ASN:O	4:D:156:GLN:HA	2.06	0.54
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.38	0.54
8:U:32:LYS:O	8:U:36:ARG:HG3	2.06	0.54
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.23	0.54
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.43	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.90	0.54
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.90	0.54
5:R:126:ARG:NH2	5:R:169:GLY:O	2.41	0.54
6:S:40:ASP:O	6:S:44:LYS:HG2	2.06	0.54
5:E:169:GLY:O	5:E:179:ASN:HB3	2.07	0.54
5:E:194:VAL:HG12	5:E:194:VAL:O	2.07	0.54
2:O:160:LEU:HD12	9:V:62:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.89	0.54
2:O:227:ARG:HG3	2:O:228:SER:N	2.22	0.54
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.89	0.54
1:A:402:VAL:HG22	1:A:406:MET:CE	2.38	0.54
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.38	0.54
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.71	0.54
2:O:307:PHE:H	9:V:50:ARG:HG2	1.72	0.54
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.43	0.54
5:R:102:THR:OG1	5:R:105:GLU:HG3	2.07	0.54
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.89	0.54
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.54
2:B:292:THR:HG22	2:B:292:THR:O	2.07	0.53
3:C:28:ILE:CD1	14:C:504:UQ:HM21	2.38	0.53
5:R:10:PHE:O	5:R:14:ARG:HG3	2.08	0.53
5:R:83:GLU:HB3	5:R:102:THR:CG2	2.27	0.53
5:E:3:ASN:HD22	5:E:3:ASN:H	1.56	0.53
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.26	0.53
4:Q:83:ARG:HH12	4:Q:86:LYS:HG3	1.73	0.53
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.08	0.53
3:C:245:LEU:O	4:D:201:ARG:HD2	2.08	0.53
5:E:109:GLU:OE2	5:E:166:ASP:HB2	2.08	0.53
2:O:27:THR:CG2	2:O:28:LYS:H	2.16	0.53
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.38	0.53
5:E:191:ASP:OD2	5:E:191:ASP:N	2.42	0.53
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.91	0.53
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.48	0.53
7:G:79:ASN:N	7:G:79:ASN:ND2	2.56	0.53
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.90	0.53
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.23	0.53
2:B:124:LEU:HD11	2:B:223:PHE:CD2	2.43	0.53
5:E:95:PRO:HG2	5:E:145:VAL:HG11	1.89	0.53
2:O:402:ILE:C	2:O:402:ILE:HD13	2.28	0.53
2:O:417:PHE:O	2:O:422:LYS:HE3	2.09	0.53
3:P:243:LEU:O	3:P:243:LEU:HD12	2.08	0.53
5:R:78:LEU:HB3	5:R:132:TRP:HZ2	1.69	0.53
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.90	0.53
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.38	0.53
10:J:38:GLY:O	10:J:42:ILE:HG13	2.09	0.53
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.24	0.53
2:O:402:ILE:HD13	2:O:402:ILE:O	2.09	0.53
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:148:ALA:O	5:R:155:GLY:O	2.26	0.53
7:T:79:ASN:N	7:T:79:ASN:ND2	2.54	0.53
2:B:35:ILE:O	2:B:213:HIS:HE1	1.92	0.53
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.90	0.53
2:B:199:PHE:O	2:B:226:ILE:HG21	2.08	0.53
5:R:166:ASP:OD1	5:R:168:SER:HB3	2.09	0.53
3:C:122:LEU:HD21	3:C:299:VAL:HG11	1.90	0.53
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.53
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.90	0.53
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.74	0.52
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.90	0.52
2:O:46:ARG:HH22	2:O:376:GLN:HG3	1.73	0.52
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.91	0.52
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.24	0.52
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.91	0.52
5:E:96:LEU:HD21	5:E:195:VAL:HG21	1.91	0.52
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.08	0.52
2:O:219:VAL:O	2:O:223:PHE:HB2	2.09	0.52
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.73	0.52
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.90	0.52
1:A:178:THR:CG2	1:A:179:ARG:N	2.73	0.52
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.91	0.52
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.43	0.52
5:E:134:ILE:HD11	5:E:193:VAL:HG21	1.91	0.52
7:G:79:ASN:N	7:G:79:ASN:HD22	2.07	0.52
5:R:155:GLY:HA3	5:R:166:ASP:C	2.30	0.52
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.92	0.52
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.45	0.52
2:B:207:VAL:HG12	2:B:208:GLY:N	2.25	0.52
9:I:49:LEU:HB3	9:I:55:MET:HG3	1.92	0.52
2:O:76:THR:CG2	2:O:82:SER:H	1.98	0.52
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.25	0.52
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.39	0.52
2:O:147:ASP:OD1	9:V:66:ILE:HD11	2.09	0.52
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.91	0.52
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.10	0.52
1:A:49:ASN:ND2	1:A:51:LYS:H	2.06	0.52
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.52
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.52
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.75	0.52
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:95:LYS:O	6:S:99:ARG:HG3	2.10	0.52
9:V:1:AME:C	9:V:3:SER:N	2.73	0.52
2:B:38:LEU:CG	2:B:39:GLU:N	2.72	0.52
2:B:402:ILE:HD13	2:B:402:ILE:C	2.30	0.52
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.23	0.52
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.45	0.52
4:D:238:ARG:CZ	5:E:5:VAL:HG22	2.40	0.52
1:N:49:ASN:HD21	1:N:51:LYS:H	1.58	0.52
2:O:314:VAL:CG1	9:V:61:ASP:HB3	2.38	0.52
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.45	0.51
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.51
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.40	0.51
1:N:178:THR:CG2	1:N:179:ARG:N	2.72	0.51
1:N:294:LEU:HD11	1:N:334:MET:CE	2.40	0.51
2:O:29:LEU:CD1	2:O:221:GLU:HB3	2.39	0.51
1:A:191:LYS:O	1:A:195:MET:HG3	2.10	0.51
3:C:202:HIS:NE2	14:C:504:UQ:O4	2.43	0.51
5:E:95:PRO:HG2	5:E:145:VAL:CG1	2.40	0.51
2:O:38:LEU:CG	2:O:39:GLU:N	2.73	0.51
3:P:347:PRO:O	3:P:350:ILE:HG22	2.10	0.51
3:P:380:TYR:OH	6:S:34:ASP:OD1	2.27	0.51
1:A:105:ASP:O	1:A:109:VAL:HG23	2.10	0.51
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.51
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.51
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.09	0.51
6:S:13:MET:HA	6:S:16:ILE:CD1	2.37	0.51
5:E:107:ASN:N	5:E:107:ASN:ND2	2.51	0.51
8:U:27:THR:HG22	8:U:29:LYS:N	2.20	0.51
3:C:365:ILE:HG22	3:C:366:LEU:N	2.26	0.51
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.45	0.51
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.76	0.51
3:P:95:ILE:O	3:P:99:ILE:HG13	2.10	0.51
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.40	0.51
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.93	0.51
1:N:133:VAL:O	1:N:137:GLU:HG3	2.10	0.51
1:N:137:GLU:O	1:N:141:MET:HG3	2.11	0.51
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.74	0.51
7:T:3:HIS:O	7:T:7:LEU:HG	2.11	0.51
2:O:273:SER:OG	9:V:7:ARG:NH1	2.44	0.51
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.11	0.51
7:G:53:LEU:O	7:G:57:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:63:ALA:O	1:N:116:VAL:HG13	2.11	0.51
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.91	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.46	0.51
1:A:343:MET:HB3	1:A:444:ILE:HA	1.92	0.51
5:E:165:TYR:HA	5:E:170:ARG:O	2.11	0.51
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.92	0.51
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.93	0.51
2:B:273:SER:OG	9:I:7:ARG:NH1	2.44	0.51
8:H:12:GLU:HG2	8:H:13:LEU:N	2.25	0.51
2:B:287:ARG:HD3	9:I:53:GLU:HG2	1.92	0.50
1:N:75:PHE:O	1:N:79:VAL:HG23	2.11	0.50
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.41	0.50
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.74	0.50
2:B:150:VAL:HG23	2:B:151:ALA:N	2.26	0.50
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.92	0.50
7:T:80:ASP:C	8:U:47:ARG:HD3	2.30	0.50
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.92	0.50
2:B:50:PHE:N	2:B:50:PHE:CD1	2.79	0.50
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.76	0.50
5:E:3:ASN:H	5:E:3:ASN:ND2	2.09	0.50
5:E:147:ILE:HG22	5:E:149:ASN:H	1.76	0.50
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.93	0.50
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.27	0.50
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.45	0.50
2:O:38:LEU:HG	2:O:39:GLU:N	2.21	0.50
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.42	0.50
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.94	0.50
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.41	0.50
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.77	0.50
9:I:49:LEU:HD11	9:I:58:ARG:HH11	1.74	0.50
3:P:50:LEU:O	3:P:54:MET:HG3	2.11	0.50
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.52	0.50
1:A:405:ARG:HD3	1:A:409:ASP:OD2	2.11	0.50
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.93	0.50
5:E:52:LYS:C	5:E:52:LYS:HD3	2.31	0.50
1:N:343:MET:HB3	1:N:444:ILE:HA	1.93	0.50
2:O:307:PHE:CD1	2:O:308:ASP:N	2.80	0.50
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.41	0.50
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.94	0.50
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.42	0.50
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.93	0.50
1:N:405:ARG:HG2	1:N:405:ARG:HH11	1.77	0.50
10:W:14:PHE:N	10:W:14:PHE:CD2	2.79	0.50
3:C:147:ILE:HG13	13:C:503:WF3:H15	1.94	0.50
2:B:206:LEU:HG	2:B:206:LEU:O	2.12	0.50
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.76	0.50
9:I:49:LEU:HB3	9:I:55:MET:CG	2.42	0.50
10:W:22:LEU:O	10:W:22:LEU:HD23	2.12	0.50
1:A:40:TRP:CZ3	1:A:198:ALA:HB3	2.47	0.49
9:I:65:VAL:HG12	9:I:66:ALA:N	2.26	0.49
6:S:91:GLU:O	6:S:95:LYS:HG3	2.11	0.49
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.12	0.49
7:G:81:GLN:OXT	7:G:81:GLN:HG3	2.11	0.49
2:O:315:ASN:HD21	9:V:7:ARG:HH11	1.60	0.49
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.12	0.49
4:Q:16:GLY:CA	4:Q:19:SER:OG	2.60	0.49
2:B:368:TYR:HB2	9:I:1:AME:CE	2.42	0.49
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.31	0.49
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.44	0.49
2:O:287:ARG:HD3	9:V:51:GLU:HG2	1.93	0.49
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.94	0.49
5:R:118:ARG:CB	5:R:118:ARG:HH11	2.26	0.49
5:R:165:TYR:HA	5:R:170:ARG:O	2.12	0.49
7:T:48:VAL:O	7:T:51:PRO:HD2	2.11	0.49
1:A:95:THR:HG22	1:A:96:ALA:N	2.27	0.49
2:B:27:THR:CG2	2:B:28:LYS:H	2.21	0.49
2:O:71:LEU:HD23	9:V:66:ILE:HG13	1.94	0.49
2:O:73:SER:N	2:O:74:PRO:HD2	2.28	0.49
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.94	0.49
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.12	0.49
2:B:307:PHE:CD1	2:B:308:ASP:N	2.81	0.49
12:C:502:HEM:HBC2	12:C:502:HEM:HMC2	1.93	0.49
3:P:288:LYS:O	3:P:292:VAL:HG23	2.12	0.49
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.76	0.49
2:B:262:ALA:CB	2:B:269:ALA:HA	2.43	0.49
3:C:173:ASN:N	3:C:174:PRO:HD2	2.27	0.49
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.26	0.49
5:E:107:ASN:O	5:E:111:GLU:HG3	2.13	0.49
8:H:18:THR:O	8:H:22:GLU:HG3	2.13	0.49
2:O:268:GLU:HG2	2:O:272:PHE:CE1	2.47	0.49
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:133:VAL:O	5:R:133:VAL:HG13	2.12	0.49
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.47	0.49
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.42	0.49
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.42	0.49
1:A:293:ARG:HD3	1:A:344:ARG:NH1	2.27	0.49
2:B:315:ASN:HD21	9:I:7:ARG:HH11	1.61	0.49
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.47	0.49
2:O:341:MET:HE3	2:O:417:PHE:CE2	2.48	0.49
2:B:398:VAL:HG13	2:B:399:ALA:N	2.28	0.49
4:D:166:ASN:H	4:D:166:ASN:ND2	2.10	0.49
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.94	0.49
1:N:219:VAL:HG12	1:N:220:SER:N	2.27	0.49
2:B:248:ASN:ND2	2:B:250:HIS:H	2.11	0.49
2:O:306:PRO:HA	9:V:50:ARG:CG	2.43	0.49
2:O:345:LYS:O	2:O:349:GLN:HG3	2.13	0.49
3:P:334:LEU:HD21	16:P:507:PEE:H65	1.95	0.49
5:R:114:VAL:HG12	5:R:114:VAL:O	2.13	0.49
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.42	0.48
1:N:35:CYS:HB2	1:N:200:ALA:O	2.13	0.48
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.48	0.48
3:P:33:ASN:HB3	21:P:608:HOH:O	2.13	0.48
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.95	0.48
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.95	0.48
5:R:186:GLN:HE21	5:R:188:VAL:CG1	2.25	0.48
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.95	0.48
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.78	0.48
5:E:137:GLY:O	5:E:145:VAL:HG13	2.13	0.48
5:E:155:GLY:HA3	5:E:166:ASP:C	2.34	0.48
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.42	0.48
1:A:134:ILE:HG22	1:A:174:ILE:HD13	1.94	0.48
5:R:118:ARG:NH1	5:R:118:ARG:CB	2.77	0.48
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.46	0.48
8:U:28:GLU:O	8:U:32:LYS:HG3	2.14	0.48
2:B:27:THR:CG2	2:B:28:LYS:N	2.76	0.48
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.48
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.95	0.48
5:E:84:GLY:CA	5:E:102:THR:HG23	2.42	0.48
7:G:3:HIS:O	7:G:7:LEU:HG	2.14	0.48
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.48	0.48
5:R:29:SER:HA	5:R:32:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:67:ASP:CG	6:S:71:LYS:HZ3	2.16	0.48
9:V:33:UNK:C	9:V:71:PRO:HG2	2.43	0.48
2:B:402:ILE:HD13	2:B:402:ILE:O	2.14	0.48
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.48	0.48
5:E:130:PRO:HG2	5:E:131:GLU:H	1.79	0.48
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.95	0.48
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.49	0.48
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.96	0.48
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	1.94	0.48
5:R:107:ASN:O	5:R:110:ALA:N	2.43	0.48
9:V:47:LEU:HB3	9:V:53:MET:CG	2.44	0.48
2:B:38:LEU:O	2:B:39:GLU:HB2	2.14	0.48
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.96	0.48
2:B:370:MET:O	2:B:373:GLU:HG3	2.14	0.48
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.79	0.48
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.48
2:B:248:ASN:C	2:B:248:ASN:ND2	2.67	0.48
2:B:274:VAL:O	2:B:278:VAL:HG23	2.14	0.48
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.41	0.48
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.43	0.48
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.79	0.48
8:U:73:LEU:HD12	8:U:73:LEU:O	2.13	0.48
1:A:170:THR:HG22	1:A:172:GLU:H	1.79	0.48
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.43	0.48
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.14	0.48
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.95	0.48
5:E:119:ASP:O	5:E:121:GLN:N	2.46	0.48
1:N:342:TRP:O	1:N:345:LEU:HB2	2.12	0.48
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.43	0.48
5:R:194:VAL:O	5:R:194:VAL:HG12	2.14	0.48
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.13	0.48
2:O:268:GLU:HG2	2:O:272:PHE:HE1	1.78	0.48
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.95	0.48
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.08	0.48
1:A:178:THR:HG22	1:A:179:ARG:N	2.29	0.47
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.29	0.47
9:I:1:AME:C	9:I:3:SER:H	2.27	0.47
2:O:38:LEU:O	2:O:39:GLU:HB2	2.14	0.47
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.85	0.47
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.96	0.47
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.21	0.47
4:D:57:THR:CG2	4:D:58:GLU:N	2.76	0.47
8:H:35:GLU:O	8:H:39:LEU:HG	2.14	0.47
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.96	0.47
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.96	0.47
2:B:225:ASN:O	2:B:226:ILE:C	2.52	0.47
2:B:307:PHE:N	9:I:52:ARG:HG2	2.27	0.47
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.14	0.47
2:O:156:GLN:NE2	9:V:75:ARG:C	2.68	0.47
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.78	0.47
2:O:403:ASP:C	2:O:405:VAL:H	2.16	0.47
3:P:332:ASN:ND2	3:P:358:SER:OG	2.47	0.47
5:R:166:ASP:OD2	5:R:172:ARG:HD3	2.13	0.47
1:A:170:THR:CG2	1:A:171:THR:N	2.78	0.47
2:B:402:ILE:O	2:B:405:VAL:HG23	2.13	0.47
3:C:103:LEU:HD12	3:C:103:LEU:O	2.13	0.47
3:C:344:VAL:HG12	3:C:349:ILE:HD11	1.97	0.47
1:N:387:GLY:O	1:N:388:ARG:HB3	2.13	0.47
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.47
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.49	0.47
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.96	0.47
2:B:207:VAL:HG12	2:B:208:GLY:H	1.79	0.47
1:N:228:VAL:O	1:N:228:VAL:HG13	2.13	0.47
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.45	0.47
5:E:161:HIS:HB2	5:E:175:PRO:HG3	1.96	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.96	0.47
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.47
5:R:129:LYS:HG2	5:R:131:GLU:OE1	2.14	0.47
6:S:16:ILE:O	6:S:19:TRP:HB3	2.15	0.47
1:A:228:VAL:O	1:A:228:VAL:HG13	2.14	0.47
2:B:403:ASP:C	2:B:405:VAL:H	2.18	0.47
3:C:138:GLN:HB2	3:C:255:GLU:O	2.15	0.47
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.14	0.47
8:H:26:GLN:HA	8:H:26:GLN:OE1	2.14	0.47
1:N:18:THR:HG23	1:N:24:ARG:CG	2.40	0.47
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.97	0.47
1:N:317:THR:HG23	1:N:318:GLY:N	2.30	0.47
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.50	0.47
2:O:166:ALA:O	2:O:242:GLY:N	2.45	0.47
2:O:207:VAL:HG12	2:O:208:GLY:N	2.30	0.47
3:P:34:PHE:HB2	21:P:601:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:13:MET:HE3	6:S:17:ARG:HH12	1.80	0.47
6:S:13:MET:CE	6:S:17:ARG:HH12	2.27	0.47
6:S:70:LEU:HD12	6:S:70:LEU:C	2.35	0.47
5:E:116:LYS:HD2	5:E:116:LYS:N	2.13	0.47
5:E:127:VAL:HG12	5:E:128:LYS:N	2.30	0.47
1:A:75:PHE:O	1:A:79:VAL:HG23	2.15	0.47
3:C:156:TYR:N	3:C:156:TYR:CD2	2.81	0.47
3:C:243:LEU:HD12	3:C:243:LEU:O	2.14	0.47
2:O:150:VAL:HG23	2:O:151:ALA:N	2.29	0.47
2:O:235:ALA:O	2:O:236:LYS:C	2.53	0.47
5:R:100:HIS:HA	5:R:131:GLU:O	2.14	0.47
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.50	0.47
5:E:133:VAL:O	5:E:133:VAL:HG13	2.15	0.47
2:O:398:VAL:HG13	2:O:399:ALA:N	2.30	0.47
4:Q:235:MET:HE1	6:S:64:ARG:N	2.30	0.47
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.78	0.47
5:R:156:TYR:N	5:R:165:TYR:O	2.37	0.47
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.50	0.47
5:E:151:GLY:HA2	5:E:157:TYR:HB2	1.96	0.46
1:N:23:LEU:HA	1:N:192:ALA:O	2.16	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.46
2:O:28:LYS:CE	2:O:32:GLY:HA2	2.45	0.46
9:V:47:LEU:HB3	9:V:53:MET:HG3	1.95	0.46
2:B:46:ARG:HH22	2:B:376:GLN:HG3	1.80	0.46
2:B:235:ALA:O	2:B:236:LYS:C	2.53	0.46
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.50	0.46
2:O:73:SER:N	2:O:74:PRO:CD	2.78	0.46
3:P:146:VAL:HG12	3:P:147:ILE:N	2.31	0.46
3:P:147:ILE:HG13	13:P:504:WF3:H15	1.97	0.46
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.15	0.46
5:R:52:LYS:HD3	5:R:52:LYS:C	2.35	0.46
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.48	0.46
3:C:19:LEU:C	3:C:20:ILE:HG13	2.36	0.46
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.79	0.46
4:D:16:GLY:N	4:D:19:SER:OG	2.49	0.46
4:D:158:ILE:HG12	4:D:160:MET:H	1.80	0.46
4:D:168:ILE:HG12	4:D:168:ILE:O	2.15	0.46
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.44	0.46
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.74	0.46
5:R:83:GLU:OE1	5:R:103:GLN:NE2	2.49	0.46
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TRP:O	1:A:345:LEU:HB2	2.16	0.46
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.45	0.46
3:C:146:VAL:HG12	3:C:147:ILE:N	2.30	0.46
5:E:29:SER:HA	5:E:32:ARG:NH2	2.30	0.46
5:E:102:THR:HB	5:E:103:GLN:OE1	2.15	0.46
5:E:104:ALA:O	5:E:108:GLN:HB3	2.15	0.46
5:E:134:ILE:O	5:E:182:VAL:HG13	2.15	0.46
2:O:67:HIS:O	2:O:70:ARG:HB3	2.15	0.46
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.83	0.46
4:Q:13:SER:O	10:W:50:LYS:NZ	2.46	0.46
9:V:2:LEU:HD12	9:V:2:LEU:H	1.78	0.46
2:B:230:ALA:O	2:B:231:GLY:C	2.54	0.46
4:D:57:THR:CG2	4:D:59:ALA:H	2.23	0.46
3:P:101:ARG:HD2	3:P:102:GLY:N	2.31	0.46
1:A:15:ASN:O	1:A:26:ALA:HA	2.16	0.46
1:A:294:LEU:HD11	1:A:334:MET:CE	2.46	0.46
1:A:294:LEU:HD11	1:A:334:MET:HE3	1.98	0.46
2:B:86:THR:O	2:B:90:GLU:HG3	2.15	0.46
2:B:141:GLN:N	2:B:142:PRO:HD2	2.31	0.46
5:E:186:GLN:O	5:E:193:VAL:HA	2.16	0.46
9:I:49:LEU:CD1	9:I:55:MET:HG2	2.44	0.46
1:N:178:THR:HG22	1:N:179:ARG:N	2.30	0.46
4:Q:22:ASP:HA	10:W:50:LYS:HB3	1.98	0.46
3:C:157:ILE:O	3:C:157:ILE:HG12	2.15	0.46
4:D:239:PRO:C	4:D:241:LYS:H	2.18	0.46
7:T:53:LEU:O	7:T:57:LEU:HG	2.15	0.46
1:A:405:ARG:HG2	1:A:405:ARG:NH1	2.30	0.46
3:C:334:LEU:HD21	16:C:506:PEE:H65	1.97	0.46
2:O:35:ILE:O	2:O:213:HIS:HE1	1.98	0.46
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.51	0.46
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.97	0.46
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.42	0.46
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.96	0.46
6:F:16:ILE:O	6:F:19:TRP:HB3	2.16	0.46
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.98	0.46
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.31	0.46
2:B:76:THR:HG23	2:B:82:SER:HB2	1.98	0.46
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.46	0.46
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.49	0.46
1:A:307:PHE:CD1	1:A:307:PHE:C	2.89	0.45
4:D:208:MET:O	4:D:212:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:398:ARG:NH1	1:N:398:ARG:HG2	2.30	0.45
2:O:201:SER:H	2:O:227:ARG:HA	1.81	0.45
2:O:201:SER:HB3	2:O:227:ARG:HB2	1.98	0.45
9:V:63:VAL:HG12	9:V:64:ALA:N	2.31	0.45
6:F:77:LYS:HB3	6:F:77:LYS:HE2	1.71	0.45
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.98	0.45
5:R:109:GLU:HA	5:R:109:GLU:OE2	2.17	0.45
6:S:76:PRO:HD2	6:S:79:GLN:OE1	2.16	0.45
1:A:354:VAL:HG23	1:A:355:LYS:N	2.32	0.45
2:B:262:ALA:O	2:B:320:GLY:HA3	2.16	0.45
3:C:156:TYR:C	3:C:158:GLY:H	2.19	0.45
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.76	0.45
1:N:307:PHE:CD1	1:N:307:PHE:C	2.88	0.45
8:U:27:THR:O	8:U:31:VAL:HG23	2.17	0.45
1:A:272:VAL:O	1:A:275:ALA:HB3	2.17	0.45
2:B:345:LYS:O	2:B:349:GLN:HG3	2.16	0.45
3:C:158:GLY:O	3:C:160:THR:N	2.49	0.45
4:D:65:ALA:O	4:D:85:GLY:HA3	2.16	0.45
4:D:235:MET:HE1	6:F:64:ARG:HA	1.99	0.45
5:E:185:TYR:O	5:E:186:GLN:HB3	2.16	0.45
10:J:4:ALA:O	10:J:8:GLN:HG3	2.17	0.45
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.46	0.45
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.80	0.45
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.65	0.45
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.74	0.45
3:C:122:LEU:HD21	3:C:299:VAL:CG1	2.47	0.45
10:J:14:PHE:CD2	10:J:14:PHE:N	2.82	0.45
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.52	0.45
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.98	0.45
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.98	0.45
2:O:305:GLN:HB3	2:O:306:PRO:HD2	1.99	0.45
5:R:136:VAL:O	5:R:138:VAL:N	2.46	0.45
2:B:341:MET:HE3	2:B:417:PHE:HE2	1.82	0.45
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.38	0.45
1:A:130:GLU:O	1:A:134:ILE:HG13	2.17	0.45
1:A:136:GLN:NE2	9:I:50:LEU:HB3	2.32	0.45
2:B:368:TYR:O	2:B:372:VAL:HG23	2.17	0.45
3:C:31:TRP:CZ3	16:C:506:PEE:H20	2.52	0.45
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.47	0.45
1:N:395:TRP:CE3	1:N:398:ARG:HD2	2.52	0.45
2:O:166:ALA:HB1	2:O:242:GLY:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.47	0.45
2:O:286:LYS:O	2:O:287:ARG:HB2	2.17	0.45
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.80	0.45
4:Q:214:LEU:O	4:Q:218:LEU:HG	2.17	0.45
1:A:122:LEU:HD11	1:A:186:ILE:HD12	1.99	0.45
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.32	0.45
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.20	0.45
6:F:70:LEU:C	6:F:70:LEU:HD12	2.36	0.45
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.50	0.45
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.32	0.45
5:R:130:PRO:C	5:R:132:TRP:H	2.20	0.45
1:A:90:THR:O	1:A:167:VAL:HG11	2.17	0.45
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.52	0.45
3:C:155:PRO:O	3:C:157:ILE:HG22	2.16	0.45
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.99	0.45
6:F:32:MET:HE3	6:F:87:LYS:HE3	1.99	0.45
7:G:71:ARG:NH1	8:H:56:GLU:HG3	2.32	0.45
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.38	0.45
3:P:122:LEU:HD21	3:P:299:VAL:HG11	1.98	0.45
4:Q:16:GLY:N	4:Q:19:SER:OG	2.50	0.45
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.52	0.45
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.38	0.44
3:C:122:LEU:CD2	3:C:299:VAL:HG11	2.46	0.44
12:C:502:HEM:HMC2	12:C:502:HEM:CBC	2.47	0.44
5:E:100:HIS:HA	5:E:131:GLU:O	2.17	0.44
1:N:10:ASN:OD1	2:O:18:CYS:HB3	2.16	0.44
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.99	0.44
3:P:31:TRP:CZ3	16:P:507:PEE:H20	2.51	0.44
3:P:287:ASN:O	3:P:288:LYS:C	2.56	0.44
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.82	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
4:D:169:LEU:C	4:D:169:LEU:HD23	2.38	0.44
1:N:405:ARG:HD3	1:N:409:ASP:OD2	2.18	0.44
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.52	0.44
9:V:47:LEU:CD1	9:V:53:MET:HG2	2.46	0.44
10:W:20:PHE:CD1	10:W:20:PHE:C	2.90	0.44
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.44
1:A:269:VAL:HG21	1:A:410:VAL:HG21	2.00	0.44
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.17	0.44
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.98	0.44
5:E:171:ILE:HG12	5:E:176:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.99	0.44
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.48	0.44
9:V:69:ASN:O	9:V:70:ALA:CB	2.65	0.44
1:A:82:MET:HE3	1:A:105:ASP:HB3	1.99	0.44
3:C:215:ASP:HB3	7:G:8:ALA:HB2	2.00	0.44
5:E:74:ILE:CG2	5:E:195:VAL:HB	2.47	0.44
1:N:15:ASN:O	1:N:26:ALA:HA	2.18	0.44
2:O:50:PHE:CD1	2:O:50:PHE:N	2.85	0.44
2:O:221:GLU:CG	2:O:222:GLN:H	2.25	0.44
2:O:248:ASN:HD22	2:O:250:HIS:H	1.63	0.44
5:R:122:HIS:O	5:R:124:LEU:N	2.51	0.44
2:O:26:ILE:HG23	2:O:26:ILE:O	2.18	0.44
2:O:150:VAL:CG2	2:O:151:ALA:N	2.81	0.44
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.44
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.82	0.44
8:U:35:GLU:O	8:U:39:LEU:HG	2.17	0.44
3:C:247:SER:N	3:C:248:PRO:HD3	2.33	0.44
5:E:191:ASP:O	5:E:192:LEU:HD23	2.18	0.44
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.47	0.44
2:O:182:ARG:HG2	2:O:182:ARG:NH1	2.32	0.44
2:O:402:ILE:O	2:O:405:VAL:HG23	2.18	0.44
8:U:18:THR:O	8:U:22:GLU:HG3	2.17	0.44
1:A:106:MET:HE3	1:A:110:VAL:HG23	1.99	0.44
2:B:150:VAL:CG2	2:B:151:ALA:N	2.80	0.44
4:D:83:ARG:HH12	4:D:86:LYS:HG3	1.81	0.44
4:D:151:PRO:HA	4:D:156:GLN:HG3	1.98	0.44
2:O:42:SER:O	2:O:113:ARG:HD2	2.17	0.44
2:O:156:GLN:HE22	9:V:75:ARG:C	2.21	0.44
3:P:50:LEU:HD23	12:P:501:HEM:HBC1	1.99	0.44
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.99	0.44
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.57	0.44
5:E:166:ASP:OD2	5:E:172:ARG:HD3	2.17	0.44
1:N:106:MET:CG	1:N:203:ILE:HD13	2.40	0.44
2:O:62:ASN:O	2:O:65:THR:CG2	2.62	0.44
2:B:424:MET:HG2	2:B:425:ALA:N	2.33	0.44
1:N:22:GLY:O	1:N:193:PRO:HA	2.18	0.44
2:O:76:THR:HG23	2:O:82:SER:HB2	2.00	0.44
2:O:370:MET:C	2:O:372:VAL:H	2.21	0.44
1:A:106:MET:HE2	1:A:107:PRO:CA	2.48	0.43
2:B:182:ARG:HH11	2:B:182:ARG:HG2	1.83	0.43
3:C:92:PHE:O	3:C:95:ILE:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:190:ASP:C	5:E:192:LEU:N	2.71	0.43
2:O:206:LEU:O	2:O:206:LEU:HG	2.17	0.43
5:R:118:ARG:NH1	5:R:171:ILE:HG13	2.33	0.43
2:B:422:LYS:O	2:B:436:LEU:HD21	2.18	0.43
4:D:209:LEU:HD23	4:D:209:LEU:HA	1.89	0.43
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.53	0.43
2:B:26:ILE:HG12	2:B:26:ILE:O	2.18	0.43
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.99	0.43
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.48	0.43
5:E:185:TYR:HB3	5:E:195:VAL:HA	1.99	0.43
8:H:28:GLU:O	8:H:32:LYS:HG3	2.18	0.43
1:N:354:VAL:HG23	1:N:355:LYS:N	2.33	0.43
4:Q:166:ASN:ND2	4:Q:166:ASN:H	2.14	0.43
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.89	0.43
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.43
2:B:258:VAL:HG21	2:B:321:LEU:HD22	2.00	0.43
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.83	0.43
2:O:315:ASN:ND2	9:V:7:ARG:HD3	2.27	0.43
3:P:285:ILE:HD12	3:P:294:ALA:HB2	2.00	0.43
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.99	0.43
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.54	0.43
1:A:23:LEU:HA	1:A:192:ALA:O	2.19	0.43
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.18	0.43
2:B:291:VAL:C	2:B:293:SER:H	2.22	0.43
2:O:315:ASN:HD21	9:V:7:ARG:NH1	2.16	0.43
1:A:7:THR:HG21	2:B:113:ARG:CD	2.48	0.43
1:A:331:ILE:HG21	1:A:431:LEU:HB2	2.01	0.43
8:H:49:HIS:O	8:H:50:THR:HB	2.18	0.43
1:N:398:ARG:HG2	1:N:398:ARG:HH11	1.84	0.43
1:N:430:GLN:O	1:N:430:GLN:HG2	2.19	0.43
3:P:247:SER:N	3:P:248:PRO:HD3	2.33	0.43
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.99	0.43
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.54	0.43
1:A:205:HIS:O	1:A:209:VAL:HG12	2.19	0.43
2:B:59:THR:HG22	2:B:60:THR:HG22	2.01	0.43
3:C:9:HIS:CD2	3:C:11:LEU:H	2.36	0.43
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.84	0.43
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.43
1:N:304:CYS:HB2	1:N:325:VAL:O	2.19	0.43
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.01	0.43
2:O:424:MET:HG2	2:O:425:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.54	0.43
8:U:65:ARG:O	8:U:69:VAL:HG23	2.19	0.43
10:W:52:TRP:O	10:W:56:LYS:HB2	2.18	0.43
1:A:317:THR:HG23	1:A:318:GLY:N	2.34	0.43
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.01	0.43
1:A:395:TRP:CE3	1:A:398:ARG:HD2	2.54	0.43
2:B:38:LEU:CD1	2:B:39:GLU:H	2.32	0.43
5:E:83:GLU:O	5:E:85:LYS:N	2.43	0.43
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.38	0.43
3:P:365:ILE:HG22	3:P:366:LEU:HD23	2.01	0.43
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.19	0.43
5:R:186:GLN:O	5:R:193:VAL:HG23	2.19	0.43
3:C:6:ARG:O	3:C:13:LYS:HA	2.19	0.43
3:C:50:LEU:O	3:C:54:MET:HG3	2.19	0.43
2:O:47:ILE:HD11	2:O:116:VAL:HG13	2.01	0.43
2:O:59:THR:HG22	2:O:60:THR:HG22	1.99	0.43
2:O:230:ALA:O	2:O:231:GLY:C	2.56	0.43
2:O:341:MET:HE3	2:O:417:PHE:HE2	1.79	0.43
3:P:344:VAL:O	3:P:345:GLU:HG3	2.18	0.43
5:R:104:ALA:HA	5:R:107:ASN:HD22	1.83	0.43
1:A:63:ALA:O	1:A:116:VAL:HG13	2.19	0.43
2:B:128:THR:HG21	2:B:224:LEU:CD2	2.49	0.43
3:C:198:LEU:HD21	12:C:502:HEM:HMA3	2.00	0.43
3:P:9:HIS:ND1	3:P:12:LEU:HD12	2.34	0.43
3:P:345:GLU:O	3:P:348:PHE:HB2	2.18	0.43
10:W:15:ARG:HH11	10:W:15:ARG:CG	2.31	0.43
2:B:31:ASN:ND2	2:B:31:ASN:H	2.16	0.42
2:B:372:VAL:HG12	2:B:372:VAL:O	2.19	0.42
3:C:347:PRO:O	3:C:350:ILE:HG22	2.18	0.42
5:E:101:ARG:HB2	5:E:131:GLU:HA	2.00	0.42
8:H:27:THR:O	8:H:31:VAL:HG23	2.19	0.42
2:O:33:LEU:HD22	2:O:224:LEU:HD12	2.01	0.42
2:O:72:ALA:C	2:O:74:PRO:HD2	2.39	0.42
2:O:152:PHE:HA	2:O:157:VAL:HG11	2.01	0.42
2:O:268:GLU:HG2	2:O:268:GLU:O	2.18	0.42
9:V:47:LEU:HD11	9:V:56:ARG:NH1	2.34	0.42
5:E:125:ASP:C	5:E:126:ARG:HG3	2.39	0.42
1:N:106:MET:HE3	1:N:110:VAL:CG2	2.49	0.42
1:N:191:LYS:O	1:N:195:MET:HG3	2.19	0.42
2:O:28:LYS:HE3	2:O:32:GLY:HA2	2.01	0.42
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:374:THR:HG22	2:O:376:GLN:N	2.33	0.42
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.54	0.42
8:U:48:SER:O	8:U:49:HIS:HB2	2.18	0.42
2:B:253:VAL:O	2:B:327:ILE:HA	2.20	0.42
2:B:305:GLN:HB3	2:B:306:PRO:HD2	2.00	0.42
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.42
3:C:79:LEU:HD22	4:D:204:MET:HE3	2.01	0.42
6:F:32:MET:CE	6:F:87:LYS:HG2	2.42	0.42
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.19	0.42
1:N:119:ASN:O	1:N:120:CYS:C	2.57	0.42
1:N:219:VAL:CG1	1:N:220:SER:N	2.82	0.42
1:N:358:LYS:HE3	1:N:399:ILE:O	2.19	0.42
3:P:215:ASP:HB3	7:T:8:ALA:HB2	2.01	0.42
5:R:153:PHE:C	5:R:155:GLY:H	2.22	0.42
2:B:28:LYS:O	2:B:28:LYS:HG2	2.18	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.49	0.42
2:O:291:VAL:C	2:O:293:SER:H	2.22	0.42
2:O:368:TYR:O	2:O:372:VAL:HG23	2.20	0.42
3:P:2:ALA:CB	3:P:8:SER:HB3	2.41	0.42
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	2.02	0.42
6:S:17:ARG:HH11	6:S:17:ARG:HG2	1.82	0.42
1:A:443:TRP:CE3	1:A:443:TRP:CA	3.00	0.42
2:B:341:MET:HE3	2:B:417:PHE:CE2	2.55	0.42
5:E:114:VAL:HG11	5:E:117:LEU:HD12	2.01	0.42
5:E:153:PHE:C	5:E:155:GLY:H	2.23	0.42
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.37	0.42
1:N:436:ARG:NH1	3:P:220:PRO:HB2	2.34	0.42
2:O:86:THR:O	2:O:90:GLU:HG3	2.20	0.42
3:P:9:HIS:CD2	3:P:11:LEU:H	2.37	0.42
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.50	0.42
9:V:75:ARG:N	9:V:75:ARG:HD2	2.34	0.42
10:W:20:PHE:O	10:W:24:VAL:HG23	2.20	0.42
3:C:151:PHE:HB2	3:C:162:VAL:HG22	2.00	0.42
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.20	0.42
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.60	0.42
2:O:399:ALA:C	2:O:402:ILE:HG22	2.39	0.42
3:P:349:ILE:O	3:P:353:GLN:HG3	2.19	0.42
4:Q:235:MET:CE	6:S:64:ARG:HA	2.49	0.42
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.69	0.42
1:A:49:ASN:HD21	1:A:51:LYS:H	1.68	0.42
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:LYS:O	4:D:66:GLU:HG3	2.19	0.42
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.84	0.42
3:P:23:PRO:HG2	7:T:3:HIS:HB2	2.00	0.42
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.42
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.54	0.42
1:A:37:VAL:HG12	1:A:199:ALA:HB1	2.01	0.42
3:C:130:VAL:HG23	3:C:131:GLY:N	2.34	0.42
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.20	0.42
4:D:76:GLU:OE1	4:D:76:GLU:N	2.43	0.42
4:D:232:SER:CB	7:G:23:GLN:HE22	2.32	0.42
1:N:269:VAL:HG21	1:N:410:VAL:HG21	2.02	0.42
2:O:259:THR:CG2	2:O:260:GLU:N	2.82	0.42
3:P:31:TRP:CH2	15:P:506:CDL:H512	2.55	0.42
8:U:51:GLU:O	8:U:52:GLU:O	2.38	0.42
1:A:119:ASN:O	1:A:120:CYS:C	2.58	0.42
2:B:73:SER:N	2:B:74:PRO:HD2	2.34	0.42
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.93	0.42
3:C:156:TYR:C	3:C:158:GLY:N	2.73	0.42
3:C:158:GLY:C	3:C:160:THR:N	2.73	0.42
2:O:315:ASN:ND2	9:V:7:ARG:HH11	2.18	0.42
2:O:372:VAL:HG12	2:O:372:VAL:O	2.20	0.42
2:O:374:THR:HG22	2:O:376:GLN:HB3	2.01	0.42
3:P:184:PHE:HD2	3:P:184:PHE:O	2.03	0.42
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.55	0.42
9:V:4:VAL:HG12	9:V:61:ASP:OD2	2.19	0.42
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.55	0.42
2:B:215:ASP:O	2:B:219:VAL:HG23	2.20	0.42
4:D:169:LEU:HD23	4:D:169:LEU:O	2.20	0.42
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.50	0.42
5:E:116:LYS:H	5:E:116:LYS:CD	2.14	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.55	0.42
1:N:382:HIS:HB3	1:N:388:ARG:O	2.20	0.42
5:R:79:SER:C	5:R:81:ILE:H	2.22	0.42
2:B:128:THR:HG21	2:B:224:LEU:HD22	2.01	0.41
4:D:57:THR:HG22	4:D:58:GLU:N	2.34	0.41
9:I:49:LEU:HD11	9:I:58:ARG:NH1	2.35	0.41
10:J:15:ARG:HG2	10:J:15:ARG:NH1	2.30	0.41
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.20	0.41
1:N:217:SER:O	1:N:218:GLY:C	2.59	0.41
1:N:405:ARG:HG2	1:N:405:ARG:NH1	2.35	0.41
2:O:151:ALA:O	2:O:157:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:227:ARG:O	2:O:228:SER:O	2.38	0.41
2:O:274:VAL:O	2:O:278:VAL:HG23	2.20	0.41
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.63	0.41
3:P:286:PRO:O	3:P:287:ASN:HB2	2.20	0.41
2:B:62:ASN:O	2:B:65:THR:CG2	2.63	0.41
2:B:370:MET:C	2:B:372:VAL:H	2.23	0.41
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.87	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.54	0.41
5:E:126:ARG:O	5:E:127:VAL:HG23	2.19	0.41
5:E:146:PRO:HG2	5:E:180:LEU:HD21	2.01	0.41
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.93	0.41
5:R:148:ALA:O	5:R:150:SER:N	2.53	0.41
1:A:304:CYS:HB2	1:A:325:VAL:O	2.20	0.41
2:B:57:TYR:N	2:B:57:TYR:CD1	2.87	0.41
3:C:13:LYS:HG3	3:C:17:ASN:ND2	2.36	0.41
18:D:501:HEC:HMD1	18:D:501:HEC:HAD1	1.94	0.41
1:N:35:CYS:HA	1:N:372:THR:HG21	2.02	0.41
2:O:207:VAL:HG12	2:O:208:GLY:H	1.86	0.41
12:P:501:HEM:HMC1	12:P:501:HEM:HBC2	2.02	0.41
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.19	0.41
5:R:134:ILE:HB	5:R:185:TYR:CE2	2.54	0.41
1:A:430:GLN:O	1:A:430:GLN:HG2	2.19	0.41
3:C:30:ALA:HB1	15:C:505:CDL:H111	2.02	0.41
1:N:45:SER:OG	1:N:92:ARG:HG2	2.20	0.41
2:O:59:THR:HG22	2:O:60:THR:H	1.83	0.41
2:O:96:LEU:HB3	9:V:68:LEU:CD2	2.41	0.41
4:Q:211:ILE:HG12	10:W:35:PHE:CZ	2.55	0.41
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.35	0.41
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.55	0.41
1:A:106:MET:HE3	1:A:110:VAL:CG2	2.50	0.41
2:B:166:ALA:HB1	2:B:242:GLY:C	2.40	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.83	0.41
4:D:16:GLY:CA	4:D:19:SER:OG	2.68	0.41
5:E:106:ILE:O	5:E:106:ILE:HG22	2.21	0.41
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.56	0.41
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.55	0.41
1:N:87:ASN:CG	1:N:88:GLY:N	2.73	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.25	0.41
3:P:2:ALA:HA	3:P:3:PRO:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:506:CDL:HA32	7:T:40:ARG:HB3	2.03	0.41
5:R:83:GLU:HA	5:R:100:HIS:O	2.20	0.41
5:R:137:GLY:O	5:R:145:VAL:HG13	2.21	0.41
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.49	0.41
3:C:51:LEU:HD23	3:C:51:LEU:HA	1.92	0.41
5:R:170:ARG:HG2	5:R:179:ASN:ND2	2.36	0.41
1:A:280:TYR:CG	1:A:281:ASP:N	2.88	0.41
3:C:285:ILE:HD12	3:C:294:ALA:HB2	2.03	0.41
4:D:68:VAL:HG11	4:D:92:PRO:CG	2.50	0.41
1:N:156:THR:CG2	1:N:157:ALA:N	2.83	0.41
1:N:350:THR:HG22	1:N:351:GLU:N	2.35	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:22:GLU:HG3	2:O:23:ASP:N	2.30	0.41
4:Q:220:TYR:CE2	15:Q:502:CDL:H722	2.55	0.41
5:R:77:LYS:HG3	5:R:191:ASP:OD2	2.20	0.41
5:R:193:VAL:HG13	5:R:193:VAL:O	2.21	0.41
1:A:106:MET:HG3	1:A:203:ILE:HG21	2.02	0.41
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.02	0.41
1:N:106:MET:HE2	1:N:107:PRO:CA	2.50	0.41
2:O:144:LEU:HB2	2:O:183:ILE:HD12	2.03	0.41
2:O:248:ASN:HD22	2:O:249:GLY:N	2.18	0.41
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.61	0.41
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.56	0.41
8:U:67:HIS:CE1	8:U:71:HIS:HE1	2.38	0.41
10:W:4:ALA:O	10:W:8:GLN:HG3	2.21	0.41
1:A:388:ARG:HH21	1:A:388:ARG:HG3	1.86	0.41
2:B:75:LEU:HD22	2:B:136:GLU:HB3	2.02	0.41
2:B:374:THR:HG22	2:B:376:GLN:N	2.35	0.41
3:C:285:ILE:O	3:C:285:ILE:HG22	2.19	0.41
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.56	0.41
4:D:117:VAL:HG21	4:D:191:ARG:HA	2.03	0.41
5:E:128:LYS:O	5:E:129:LYS:C	2.58	0.41
5:E:134:ILE:CD1	5:E:193:VAL:HG21	2.50	0.41
8:H:17:LEU:HD13	8:H:73:LEU:HD22	2.01	0.41
1:N:45:SER:OG	1:N:92:ARG:HA	2.21	0.41
1:N:212:ALA:O	1:N:216:PHE:HB2	2.21	0.41
1:N:331:ILE:HG21	1:N:431:LEU:HB2	2.03	0.41
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.20	0.41
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.55	0.41
3:P:19:LEU:C	3:P:20:ILE:HG13	2.41	0.41
3:P:101:ARG:C	3:P:101:ARG:CD	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:186:LEU:HD23	3:P:186:LEU:HA	1.89	0.41
4:Q:240:PRO:O	4:Q:241:LYS:C	2.58	0.41
5:R:112:VAL:HG11	5:R:170:ARG:HH12	1.83	0.41
8:U:51:GLU:O	8:U:52:GLU:C	2.58	0.41
1:A:156:THR:HA	5:E:7:VAL:HG21	2.02	0.41
2:B:26:ILE:CD1	2:B:391:THR:HA	2.48	0.41
1:N:144:ASP:C	1:N:144:ASP:OD1	2.59	0.41
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.92	0.41
1:A:109:VAL:HA	1:A:112:LEU:HD12	2.03	0.40
3:C:23:PRO:HG3	7:G:4:PHE:CD1	2.55	0.40
4:D:116:ILE:HG23	4:D:117:VAL:N	2.36	0.40
2:O:141:GLN:N	2:O:142:PRO:HD2	2.36	0.40
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.20	0.40
2:O:230:ALA:O	2:O:231:GLY:O	2.39	0.40
3:P:109:LEU:HD23	3:P:109:LEU:HA	1.81	0.40
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.52	0.40
6:S:87:LYS:HA	6:S:87:LYS:HD3	1.93	0.40
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.57	0.40
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.56	0.40
5:E:131:GLU:H	5:E:131:GLU:CD	2.23	0.40
7:T:57:LEU:O	7:T:58:LEU:C	2.59	0.40
1:A:45:SER:OG	1:A:92:ARG:HA	2.22	0.40
1:A:144:ASP:C	1:A:144:ASP:OD1	2.60	0.40
1:A:217:SER:O	1:A:218:GLY:C	2.60	0.40
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.56	0.40
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.02	0.40
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.36	0.40
1:A:371:GLY:O	1:A:375:VAL:HG23	2.21	0.40
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.21	0.40
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.33	0.40
10:J:15:ARG:HH11	10:J:15:ARG:CG	2.30	0.40
1:N:156:THR:HG23	1:N:157:ALA:N	2.37	0.40
3:P:271:PRO:HB2	3:P:275:PHE:HB2	2.03	0.40
3:P:356:SER:O	3:P:359:TYR:HB3	2.21	0.40
14:P:505:UQ:HM51	14:P:505:UQ:C8	2.51	0.40
5:R:78:LEU:N	5:R:191:ASP:O	2.48	0.40
6:S:71:LYS:O	6:S:72:HIS:HB2	2.22	0.40
4:D:214:LEU:O	4:D:218:LEU:HG	2.21	0.40
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.57	0.40
9:I:65:VAL:HG12	9:I:66:ALA:H	1.85	0.40
1:N:82:MET:CE	1:N:105:ASP:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:239:PRO:C	4:Q:241:LYS:H	2.25	0.40
7:T:24:ARG:O	7:T:27:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	441/446 (99%)	408 (92%)	25 (6%)	8 (2%)	8 21
1	N	440/446 (99%)	409 (93%)	24 (6%)	7 (2%)	9 24
2	B	419/441 (95%)	351 (84%)	52 (12%)	16 (4%)	3 7
2	O	420/441 (95%)	359 (86%)	46 (11%)	15 (4%)	3 7
3	C	378/380 (100%)	350 (93%)	24 (6%)	4 (1%)	14 34
3	P	377/380 (99%)	348 (92%)	23 (6%)	6 (2%)	9 24
4	D	239/241 (99%)	222 (93%)	16 (7%)	1 (0%)	34 60
4	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	12 30
5	E	194/196 (99%)	147 (76%)	31 (16%)	16 (8%)	1 1
5	R	194/196 (99%)	151 (78%)	32 (16%)	11 (6%)	1 2
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100 100
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100 100
7	G	78/81 (96%)	65 (83%)	11 (14%)	2 (3%)	5 13
7	T	77/81 (95%)	66 (86%)	9 (12%)	2 (3%)	5 13
8	H	68/77 (88%)	63 (93%)	4 (6%)	1 (2%)	10 26
8	U	65/77 (84%)	55 (85%)	8 (12%)	2 (3%)	4 9
9	I	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0 0
9	V	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	59/61 (97%)	54 (92%)	5 (8%)	0	100 100
10	W	58/61 (95%)	52 (90%)	4 (7%)	2 (3%)	3 8
All	All	4012/4218 (95%)	3556 (89%)	352 (9%)	104 (3%)	5 13

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY
1	A	433	ASP
2	B	26	ILE
2	B	39	GLU
2	B	226	ILE
3	C	287	ASN
5	E	102	THR
5	E	149	ASN
5	E	150	SER
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	39	GLU
2	O	228	SER
3	P	287	ASN
5	R	124	LEU
5	R	125	ASP
8	U	52	GLU
10	W	61	ALA
1	A	262	TRP
2	B	171	ALA
2	B	201	SER
2	B	227	ARG
2	B	228	SER
2	B	231	GLY
2	B	236	LYS
2	B	371	SER
5	E	118	ARG
5	E	163	SER
5	E	190	ASP
9	I	7	ARG
9	I	60	ALA
9	I	63	ASP
1	N	218	GLY

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Mol	Chain	Res	Type
1	N	262	TRP
1	N	282	ARG
2	O	171	ALA
2	O	201	SER
2	O	220	ALA
2	O	231	GLY
2	O	371	SER
5	R	127	VAL
5	R	163	SER
9	V	58	ALA
9	V	70	ALA
1	A	217	SER
1	A	282	ARG
2	B	29	LEU
3	C	159	HIS
5	E	84	GLY
5	E	115	SER
5	E	120	PRO
5	E	137	GLY
2	O	236	LYS
3	P	155	PRO
3	P	160	THR
5	R	149	ASN
7	T	33	ALA
9	V	7	ARG
9	V	60	ARG
1	A	71	PRO
1	A	72	CYS
2	B	221	GLU
3	C	5	ILE
5	E	112	VAL
7	G	33	ALA
1	N	81	SER
2	O	222	GLN
3	P	5	ILE
3	P	156	TYR
5	R	123	ASP
5	R	137	GLY
1	A	388	ARG
2	B	269	ALA
2	B	270	ASN
2	B	390	GLY

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Mol	Chain	Res	Type
3	C	156	TYR
5	E	186	GLN
7	G	7	LEU
8	H	50	THR
9	I	62	ARG
1	N	71	PRO
1	N	72	CYS
2	O	390	GLY
4	Q	162	PRO
5	R	108	GLN
7	T	7	LEU
8	U	27	THR
10	W	15	ARG
4	D	162	PRO
5	E	130	PRO
2	O	226	ILE
2	O	436	LEU
3	P	158	GLY
4	Q	198	HIS
5	R	130	PRO
5	R	159	PRO
4	Q	176	PRO
5	R	114	VAL
5	E	159	PRO
2	O	351	GLY
2	B	351	GLY
5	E	155	GLY
5	E	175	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%)	353 (97%)	12 (3%)	38	67
1	N	365/368 (99%)	351 (96%)	14 (4%)	33	62
2	B	332/347 (96%)	317 (96%)	15 (4%)	27	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	333/347 (96%)	320 (96%)	13 (4%)	32	61
3	C	328/328 (100%)	318 (97%)	10 (3%)	41	70
3	P	328/328 (100%)	318 (97%)	10 (3%)	41	70
4	D	200/200 (100%)	198 (99%)	2 (1%)	76	91
4	Q	200/200 (100%)	198 (99%)	2 (1%)	76	91
5	E	166/166 (100%)	158 (95%)	8 (5%)	25	53
5	R	165/166 (99%)	161 (98%)	4 (2%)	49	77
6	F	93/96 (97%)	91 (98%)	2 (2%)	52	79
6	S	93/96 (97%)	91 (98%)	2 (2%)	52	79
7	G	71/71 (100%)	69 (97%)	2 (3%)	43	73
7	T	70/71 (99%)	68 (97%)	2 (3%)	42	71
8	H	65/71 (92%)	64 (98%)	1 (2%)	65	86
8	U	63/71 (89%)	63 (100%)	0	100	100
9	I	26/45 (58%)	25 (96%)	1 (4%)	33	62
9	V	26/45 (58%)	26 (100%)	0	100	100
10	J	49/49 (100%)	47 (96%)	2 (4%)	30	59
10	W	47/49 (96%)	44 (94%)	3 (6%)	17	39
All	All	3385/3482 (97%)	3280 (97%)	105 (3%)	40	69

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	102	LEU
1	A	106	MET
1	A	226	ASP
1	A	281	ASP
1	A	342	TRP
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	97	SER

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Mol	Chain	Res	Type
2	B	104	LYS
2	B	114	ASP
2	B	117	ASP
2	B	124	LEU
2	B	154	SER
2	B	170	THR
2	B	181	TYR
2	B	248	ASN
2	B	250	HIS
2	B	325	TYR
2	B	335	GLU
2	B	341	MET
2	B	402	ILE
3	C	21	ASP
3	C	81	ARG
3	C	82	ASN
3	C	91	PHE
3	C	157	ILE
3	C	184	PHE
3	C	223	PRO
3	C	226	SER
3	C	240	PHE
3	C	256	ASN
4	D	169	LEU
4	D	203	ARG
5	E	31	ASP
5	E	107	ASN
5	E	116	LYS
5	E	123	ASP
5	E	131	GLU
5	E	149	ASN
5	E	186	GLN
5	E	191	ASP
6	F	64	ARG
6	F	70	LEU
7	G	27	PRO
7	G	79	ASN
8	H	49	HIS
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	3	THR

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Mol	Chain	Res	Type
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	102	LEU
1	N	106	MET
1	N	281	ASP
1	N	308	GLN
1	N	342	TRP
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	114	ASP
2	O	117	ASP
2	O	154	SER
2	O	181	TYR
2	O	248	ASN
2	O	250	HIS
2	O	325	TYR
2	O	335	GLU
2	O	341	MET
2	O	402	ILE
3	P	21	ASP
3	P	81	ARG
3	P	82	ASN
3	P	91	PHE
3	P	184	PHE
3	P	207	ASN
3	P	226	SER
3	P	240	PHE
3	P	256	ASN
3	P	380	TYR
4	Q	169	LEU
4	Q	203	ARG
5	R	3	ASN
5	R	31	ASP
5	R	130	PRO
5	R	190	ASP

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Mol	Chain	Res	Type
6	S	64	ARG
6	S	70	LEU
7	T	27	PRO
7	T	79	ASN
10	W	15	ARG
10	W	59	TYR
10	W	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	156	GLN
2	B	225	ASN
2	B	248	ASN
2	B	276	GLN
2	B	315	ASN
2	B	343	GLN
2	B	362	ASN
2	B	380	ASN
3	C	9	HIS
3	C	17	ASN
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
4	D	166	ASN
5	E	3	ASN
5	E	57	GLN
5	E	107	ASN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS

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Mol	Chain	Res	Type
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
9	I	71	ASN
1	N	118	GLN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	156	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	315	ASN
2	O	332	HIS
2	O	343	GLN
2	O	362	ASN
2	O	380	ASN
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
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	122	HIS
5	R	164	HIS
5	R	186	GLN
6	S	72	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	71	HIS

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Mol	Chain	Res	Type
9	V	69	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
9	AME	I	1	9	7,8,11	1.96	1 (14%)	5,8,13	1.45	1 (20%)
3	FME	C	1	3	7,8,10	2.00	1 (14%)	5,8,11	1.43	1 (20%)
9	AME	V	1	9	7,8,11	1.97	1 (14%)	5,8,13	1.54	1 (20%)

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
9	AME	I	1	9	-	0/5/8/12	-
3	FME	C	1	3	-	1/5/8/11	-
9	AME	V	1	9	-	0/5/8/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	AME	CT1-N	-5.07	1.33	1.46
9	I	1	AME	CT1-N	-5.06	1.33	1.46
3	C	1	FME	CN-N	-5.02	1.33	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	AME	CT1-N-CA	2.63	121.83	113.64
3	C	1	FME	CN-N-CA	2.62	121.79	113.64
9	I	1	AME	CT1-N-CA	2.58	121.66	113.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1	AME	3	0
9	V	1	AME	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 2 are unknown - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	CDL	Q	502	-	41,41,99	1.19	1 (2%)	47,53,111	1.06	4 (8%)
19	BOG	Q	504	-	13,13,20	1.32	2 (15%)	18,18,25	1.09	2 (11%)
12	HEM	C	501	3	41,50,50	1.58	5 (12%)	45,82,82	1.51	9 (20%)
20	FES	R	501	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CDL	G	101	-	39,39,99	1.21	1 (2%)	45,51,111	1.10	4 (8%)
13	WF3	C	503	-	32,33,33	2.80	12 (37%)	44,47,47	2.35	15 (34%)
14	UQ	C	504	-	19,19,63	2.64	9 (47%)	23,26,79	1.09	1 (4%)
17	GOL	C	508	-	5,5,5	1.39	0	5,5,5	0.67	0
15	CDL	P	506	-	39,39,99	1.23	2 (5%)	45,51,111	1.11	4 (8%)
12	HEM	P	501	3	41,50,50	1.56	5 (12%)	45,82,82	1.39	7 (15%)
20	FES	E	501	5	0,4,4	-	-	-		
18	HEC	D	501	4	32,50,50	1.90	4 (12%)	24,82,82	1.39	3 (12%)
16	PEE	N	502	-	4,4,50	3.51	4 (100%)	6,6,55	0.56	0
16	PEE	C	506	-	48,48,50	1.36	6 (12%)	51,53,55	0.79	2 (3%)
12	HEM	P	502	3	41,50,50	1.55	6 (14%)	45,82,82	1.53	7 (15%)
16	PEE	P	507	-	48,48,50	1.33	6 (12%)	51,53,55	0.77	2 (3%)
13	WF3	P	504	-	32,33,33	2.94	14 (43%)	44,47,47	2.34	15 (34%)
19	BOG	D	503	-	13,13,20	1.41	3 (23%)	18,18,25	1.18	2 (11%)
19	BOG	D	502	-	20,20,20	0.87	0	25,25,25	0.88	1 (4%)
19	BOG	Q	503	-	20,20,20	0.95	2 (10%)	25,25,25	0.89	1 (4%)
16	PEE	R	502	-	47,47,50	1.47	8 (17%)	49,51,55	0.71	1 (2%)
17	GOL	P	508	-	5,5,5	1.41	1 (20%)	5,5,5	0.67	0
12	HEM	C	502	3	41,50,50	1.56	6 (14%)	45,82,82	1.79	10 (22%)
16	PEE	C	507	-	20,20,50	1.78	7 (35%)	23,25,55	0.61	0
15	CDL	C	505	-	41,41,99	1.19	2 (4%)	47,53,111	1.05	3 (6%)
16	PEE	E	502	-	49,49,50	1.52	10 (20%)	52,54,55	0.92	3 (5%)
19	BOG	P	503	-	12,12,20	1.39	3 (25%)	17,17,25	0.53	0
14	UQ	P	505	-	19,19,63	2.62	10 (52%)	23,26,79	1.08	2 (8%)
18	HEC	Q	501	4	32,50,50	1.80	3 (9%)	24,82,82	1.46	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	Q	502	-	-	20/51/51/110	-
19	BOG	Q	504	-	-	4/4/24/31	0/1/1/1
12	HEM	C	501	3	-	4/12/54/54	-
20	FES	R	501	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	G	101	-	-	17/49/49/110	-
13	WF3	C	503	-	-	0/24/24/24	0/3/3/3
14	UQ	C	504	-	-	3/11/35/87	0/1/1/1
17	GOL	C	508	-	-	4/4/4/4	-
15	CDL	P	506	-	-	19/49/49/110	-
12	HEM	P	501	3	-	4/12/54/54	-
20	FES	E	501	5	-	-	0/1/1/1
18	HEC	D	501	4	-	8/10/54/54	-
16	PEE	C	506	-	-	20/52/52/54	-
12	HEM	P	502	3	-	6/12/54/54	-
16	PEE	P	507	-	-	20/52/52/54	-
13	WF3	P	504	-	-	6/24/24/24	0/3/3/3
19	BOG	D	503	-	-	0/4/24/31	0/1/1/1
19	BOG	D	502	-	-	4/11/31/31	0/1/1/1
19	BOG	Q	503	-	-	4/11/31/31	0/1/1/1
16	PEE	R	502	-	-	25/49/49/54	-
17	GOL	P	508	-	-	3/4/4/4	-
12	HEM	C	502	3	-	5/12/54/54	-
16	PEE	C	507	-	-	7/24/24/54	-
15	CDL	C	505	-	-	19/51/51/110	-
16	PEE	E	502	-	-	27/53/53/54	-
19	BOG	P	503	-	-	0/2/22/31	0/1/1/1
14	UQ	P	505	-	-	3/11/35/87	0/1/1/1
18	HEC	Q	501	4	-	7/10/54/54	-

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	504	WF3	C6-C5	9.16	1.54	1.34
13	C	503	WF3	C6-C5	8.78	1.53	1.34
18	Q	501	HEC	C2B-C3B	-6.50	1.34	1.40
18	D	501	HEC	C3C-C2C	-6.19	1.34	1.40
13	P	504	WF3	C18-N23	5.95	1.38	1.30
14	P	505	UQ	C7-C6	5.59	1.60	1.51
14	C	504	UQ	C7-C6	5.57	1.60	1.51
13	P	504	WF3	C9-C14	5.54	1.47	1.40
18	D	501	HEC	C2B-C3B	-5.48	1.35	1.40
18	Q	501	HEC	C3C-C2C	-5.44	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	503	WF3	C18-N23	5.42	1.37	1.30
13	P	504	WF3	C9-C5	-5.35	1.42	1.49
13	C	503	WF3	C9-C14	5.19	1.47	1.40
14	C	504	UQ	C6-C5	4.87	1.44	1.35
13	C	503	WF3	C9-C5	-4.81	1.42	1.49
16	N	502	PEE	P-O1P	4.77	1.62	1.50
14	P	505	UQ	C6-C5	4.74	1.43	1.35
12	P	501	HEM	CBB-CAB	4.49	1.52	1.30
12	C	501	HEM	CBB-CAB	4.33	1.51	1.30
12	C	502	HEM	CBB-CAB	4.30	1.51	1.30
12	C	501	HEM	C3C-CAC	-4.20	1.39	1.47
12	P	501	HEM	C3C-CAC	-4.17	1.39	1.47
16	R	502	PEE	C39-C38	4.11	1.55	1.31
14	C	504	UQ	C6-C1	4.07	1.58	1.46
16	C	506	PEE	C39-C38	4.00	1.54	1.31
16	P	507	PEE	C39-C38	3.95	1.54	1.31
13	P	504	WF3	C15-C14	-3.94	1.40	1.50
16	E	502	PEE	C39-C38	3.92	1.54	1.31
13	C	503	WF3	C15-C14	-3.81	1.40	1.50
12	P	502	HEM	CBB-CAB	3.80	1.49	1.30
14	P	505	UQ	C6-C1	3.76	1.57	1.46
12	P	501	HEM	CBC-CAC	3.73	1.54	1.29
12	C	501	HEM	CBC-CAC	3.73	1.54	1.29
12	P	502	HEM	CBC-CAC	3.72	1.54	1.29
16	E	502	PEE	O2-C10	3.57	1.44	1.34
12	C	502	HEM	CBC-CAC	3.56	1.52	1.29
12	P	502	HEM	C3C-CAC	-3.54	1.40	1.47
13	C	503	WF3	C25-C26	3.36	1.44	1.37
16	C	506	PEE	O3-C30	3.35	1.43	1.33
16	N	502	PEE	P-O4P	3.35	1.64	1.54
16	R	502	PEE	O2-C10	3.31	1.43	1.34
13	P	504	WF3	C29-C28	3.31	1.43	1.36
12	C	502	HEM	C3C-C2C	-3.30	1.35	1.40
16	E	502	PEE	P-O1P	3.23	1.62	1.50
13	P	504	WF3	C17-N31	3.23	1.38	1.30
13	C	503	WF3	C29-C28	3.21	1.43	1.36
16	E	502	PEE	O3-C30	3.20	1.42	1.33
16	R	502	PEE	O3-C30	3.20	1.42	1.33
14	P	505	UQ	O3-C3	3.18	1.44	1.36
13	C	503	WF3	C10-C9	3.18	1.45	1.39
12	C	501	HEM	CAB-C3B	-3.17	1.38	1.47
13	P	504	WF3	C13-C14	3.17	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	504	UQ	O3-C3	3.16	1.44	1.36
16	N	502	PEE	P-O3P	3.12	1.64	1.54
16	P	507	PEE	O3-C30	3.10	1.42	1.33
16	C	507	PEE	P-O1P	3.07	1.61	1.50
16	P	507	PEE	C21-C22	-3.06	1.34	1.51
12	P	502	HEM	CAB-C3B	-3.06	1.39	1.47
16	R	502	PEE	P-O1P	3.06	1.61	1.50
12	C	502	HEM	CAB-C3B	-3.05	1.39	1.47
13	C	503	WF3	C17-N31	3.04	1.37	1.30
16	C	507	PEE	O2-C10	3.03	1.42	1.34
12	P	501	HEM	CAB-C3B	-2.99	1.39	1.47
14	C	504	UQ	C2-C1	2.96	1.57	1.48
13	P	504	WF3	C25-C26	2.90	1.43	1.37
16	C	506	PEE	C21-C22	-2.89	1.35	1.51
16	C	506	PEE	P-O1P	2.86	1.61	1.50
16	P	507	PEE	O2-C10	2.84	1.42	1.34
16	C	507	PEE	O3-C30	2.83	1.41	1.33
14	P	505	UQ	C2-C1	2.81	1.57	1.48
16	E	502	PEE	C21-C22	-2.80	1.35	1.51
16	P	507	PEE	P-O1P	2.80	1.60	1.50
13	P	504	WF3	C10-C9	2.78	1.44	1.39
14	P	505	UQ	CM5-C5	2.78	1.56	1.50
14	C	504	UQ	CM5-C5	2.77	1.56	1.50
16	C	506	PEE	O2-C10	2.72	1.42	1.34
12	C	501	HEM	C3C-C2C	-2.67	1.36	1.40
19	D	503	BOG	C4-C5	2.66	1.58	1.53
14	C	504	UQ	C3-C4	2.64	1.56	1.48
14	P	505	UQ	O2-C2	2.62	1.43	1.36
13	C	503	WF3	C13-C14	2.61	1.44	1.39
14	C	504	UQ	C5-C4	2.57	1.56	1.47
14	P	505	UQ	C5-C4	2.57	1.56	1.47
13	P	504	WF3	C19-C18	2.56	1.55	1.51
14	P	505	UQ	C7-C8	2.55	1.54	1.50
15	C	505	CDL	O1-C1	2.55	1.51	1.43
18	D	501	HEC	C4B-C3B	2.53	1.47	1.43
16	R	502	PEE	C11-C10	2.53	1.58	1.50
16	E	502	PEE	C3-C2	2.51	1.58	1.50
16	E	502	PEE	C1-C2	2.51	1.58	1.50
16	C	507	PEE	C1-C2	2.49	1.58	1.50
14	P	505	UQ	C3-C4	2.49	1.56	1.48
18	D	501	HEC	C1D-CHD	-2.46	1.34	1.41
16	E	502	PEE	C11-C10	2.46	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	504	UQ	O2-C2	2.45	1.42	1.36
15	Q	502	CDL	O1-C1	2.44	1.50	1.43
13	C	503	WF3	C19-C18	2.41	1.55	1.51
19	P	503	BOG	C4-C5	2.37	1.58	1.53
16	N	502	PEE	P-O2P	2.36	1.61	1.54
19	Q	504	BOG	C4-C5	2.36	1.58	1.53
19	Q	504	BOG	O5-C1	2.35	1.47	1.41
12	P	501	HEM	C3C-C2C	-2.32	1.37	1.40
15	P	506	CDL	O1-C1	2.29	1.50	1.43
19	D	503	BOG	O5-C1	2.28	1.47	1.41
13	C	503	WF3	C28-C26	2.27	1.45	1.38
12	C	502	HEM	C3C-CAC	-2.27	1.43	1.47
16	R	502	PEE	C3-C2	2.25	1.57	1.50
16	R	502	PEE	C1-C2	2.23	1.57	1.50
19	Q	503	BOG	C4-C5	2.20	1.57	1.53
16	C	507	PEE	C11-C10	2.20	1.57	1.50
13	P	504	WF3	C11-C10	2.19	1.43	1.38
16	E	502	PEE	C31-C30	2.18	1.57	1.50
16	R	502	PEE	C31-C30	2.18	1.57	1.50
15	C	505	CDL	OA6-CA5	2.18	1.40	1.34
15	P	506	CDL	CB3-CB4	2.15	1.57	1.50
19	P	503	BOG	O5-C1	2.14	1.48	1.42
16	C	507	PEE	P-O4P	2.13	1.67	1.59
13	P	504	WF3	C28-C26	2.12	1.44	1.38
16	C	506	PEE	C3-C2	2.11	1.57	1.50
13	P	504	WF3	C12-C11	2.11	1.43	1.38
19	P	503	BOG	C1-C2	2.11	1.57	1.52
16	E	502	PEE	O2-C2	2.09	1.51	1.46
12	C	502	HEM	C3B-C4B	2.08	1.49	1.44
19	Q	503	BOG	O5-C1	2.07	1.47	1.41
18	Q	501	HEC	C1D-CHD	-2.06	1.35	1.41
12	P	502	HEM	C2C-C1C	2.05	1.47	1.42
19	D	503	BOG	C1-C2	2.04	1.58	1.52
16	P	507	PEE	C3-C2	2.04	1.57	1.50
15	G	101	CDL	O1-C1	2.04	1.49	1.43
12	P	502	HEM	C1A-NA	2.03	1.40	1.36
17	P	508	GOL	O2-C2	2.03	1.49	1.43
16	C	507	PEE	C3-C2	2.03	1.56	1.50

All (102) bond angle outliers are listed below:

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	504	WF3	O2-C3-C5	9.26	125.61	112.01
13	C	503	WF3	O2-C3-C5	9.00	125.22	112.01
12	C	502	HEM	C2C-C3C-C4C	-5.00	103.41	106.90
12	P	502	HEM	CBA-CAA-C2A	4.32	119.99	112.62
13	C	503	WF3	C26-C25-C24	-4.21	118.09	121.19
12	C	502	HEM	CAD-C3D-C4D	4.19	131.99	124.66
18	Q	501	HEC	CBA-CAA-C2A	4.09	119.50	112.60
13	P	504	WF3	C8-O7-C6	-4.04	108.57	115.61
13	P	504	WF3	C26-C25-C24	-3.90	118.32	121.19
13	C	503	WF3	C1-O2-C3	3.76	122.97	115.86
13	P	504	WF3	C18-N23-C24	3.75	122.81	115.00
13	C	503	WF3	C18-N23-C24	3.72	122.75	115.00
13	C	503	WF3	C19-C18-N23	3.72	119.97	113.57
13	C	503	WF3	O2-C3-O4	-3.69	116.42	123.53
13	C	503	WF3	C8-O7-C6	-3.68	109.20	115.61
12	C	502	HEM	C4C-CHD-C1D	3.67	127.41	122.56
19	D	503	BOG	C1'-O1-C1	3.66	118.93	113.27
12	P	502	HEM	CAD-C3D-C4D	3.66	131.04	124.66
12	C	502	HEM	CBA-CAA-C2A	3.63	118.81	112.62
13	P	504	WF3	C1-O2-C3	3.61	122.70	115.86
13	P	504	WF3	O2-C3-O4	-3.55	116.69	123.53
13	P	504	WF3	C19-C18-N23	3.52	119.63	113.57
12	C	501	HEM	CAD-C3D-C4D	3.47	130.72	124.66
19	Q	504	BOG	C1'-O1-C1	3.40	118.53	113.27
12	P	502	HEM	C2C-C3C-C4C	-3.37	104.54	106.90
19	Q	503	BOG	C1'-O1-C1	3.33	119.36	113.84
12	C	501	HEM	C4B-CHC-C1C	3.29	126.90	122.56
15	P	506	CDL	CB4-OB6-CB5	-3.27	109.75	117.79
18	D	501	HEC	CBA-CAA-C2A	3.17	117.95	112.60
14	C	504	UQ	C8-C7-C6	3.17	120.58	112.05
12	C	502	HEM	CAD-C3D-C2D	-3.12	122.06	127.88
15	G	101	CDL	CB4-OB6-CB5	-3.12	110.12	117.79
16	E	502	PEE	C22-C21-C20	3.10	127.31	113.79
19	D	502	BOG	C1'-O1-C1	3.06	118.92	113.84
12	P	502	HEM	C4C-CHD-C1D	3.00	126.52	122.56
14	P	505	UQ	C8-C7-C6	2.99	120.10	112.05
13	C	503	WF3	C17-N31-C30	2.98	123.01	116.41
18	D	501	HEC	CBD-CAD-C3D	2.95	117.66	112.62
12	P	501	HEM	C4B-CHC-C1C	2.91	126.39	122.56
13	P	504	WF3	O4-C3-C5	-2.87	117.70	124.34
13	P	504	WF3	C17-N31-C30	2.86	122.76	116.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	501	HEC	CBD-CAD-C3D	2.83	117.44	112.62
16	P	507	PEE	C22-C21-C20	2.80	125.97	113.79
16	C	506	PEE	C22-C21-C20	2.79	125.93	113.79
12	C	502	HEM	C2B-C1B-NB	2.75	113.10	109.84
12	P	501	HEM	CAD-C3D-C4D	2.72	129.41	124.66
12	C	501	HEM	C2B-C1B-NB	2.70	113.03	109.84
12	C	502	HEM	C2D-C1D-ND	2.70	113.11	109.88
12	P	502	HEM	CAD-C3D-C2D	-2.69	122.86	127.88
13	P	504	WF3	C10-C9-C5	-2.69	115.53	119.79
19	D	503	BOG	O1-C1-C2	2.68	111.29	108.15
13	C	503	WF3	C28-C26-C25	2.65	121.67	118.40
12	C	501	HEM	C3B-C2B-C1B	-2.64	104.53	106.49
15	P	506	CDL	CA6-CA4-CA3	-2.61	105.61	111.79
13	C	503	WF3	C10-C9-C5	-2.60	115.68	119.79
13	C	503	WF3	O4-C3-C5	-2.59	118.35	124.34
12	P	501	HEM	C4A-C3A-C2A	-2.55	105.22	107.00
15	G	101	CDL	CA6-CA4-CA3	-2.52	105.82	111.79
18	D	501	HEC	CAA-C2A-C3A	-2.49	120.09	127.25
13	C	503	WF3	C24-C30-N31	-2.48	117.95	121.18
12	P	501	HEM	C2B-C1B-NB	2.48	112.78	109.84
12	C	502	HEM	C4A-C3A-C2A	-2.48	105.27	107.00
12	P	502	HEM	C2D-C1D-ND	2.48	112.85	109.88
16	E	502	PEE	C21-C22-C23	2.46	126.94	114.42
16	C	506	PEE	C21-C22-C23	2.46	126.90	114.42
12	C	501	HEM	CBD-CAD-C3D	2.45	119.45	112.63
19	Q	504	BOG	O1-C1-C2	2.42	110.98	108.15
12	C	501	HEM	C3D-C4D-ND	2.40	112.84	110.17
18	Q	501	HEC	CAA-C2A-C3A	-2.39	120.36	127.25
16	P	507	PEE	C21-C22-C23	2.37	126.46	114.42
12	C	501	HEM	C4A-C3A-C2A	-2.35	105.36	107.00
13	P	504	WF3	C28-C26-C25	2.33	121.27	118.40
15	C	505	CDL	CA6-CA4-CA3	-2.31	106.31	111.79
15	G	101	CDL	CA4-OA6-CA5	-2.31	112.11	117.79
12	C	502	HEM	C4D-ND-C1D	-2.29	102.71	105.07
12	P	501	HEM	CBD-CAD-C3D	2.24	118.86	112.63
12	P	501	HEM	C2D-C1D-ND	2.23	112.55	109.88
15	Q	502	CDL	CA6-CA4-CA3	-2.22	106.53	111.79
16	E	502	PEE	O3-C3-C2	2.22	114.90	108.43
15	Q	502	CDL	CA6-OA8-CA7	-2.18	111.63	117.10
15	C	505	CDL	CA6-OA8-CA7	-2.17	111.64	117.10
16	R	502	PEE	O3-C3-C2	2.17	114.74	108.43
15	C	505	CDL	CB4-OB6-CB5	-2.16	112.47	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Q	502	CDL	CA4-OA6-CA5	-2.16	112.48	117.79
15	P	506	CDL	OB6-CB4-CB3	2.15	116.19	108.40
12	C	501	HEM	CAD-C3D-C2D	-2.15	123.88	127.88
12	P	501	HEM	CMC-C2C-C3C	2.15	128.69	124.68
13	P	504	WF3	C24-C30-N31	-2.14	118.39	121.18
12	C	502	HEM	C3B-C2B-C1B	-2.14	104.90	106.49
18	Q	501	HEC	CMD-C2D-C1D	-2.12	125.21	128.46
13	P	504	WF3	C14-C9-C5	2.11	125.06	122.24
15	P	506	CDL	CA4-OA6-CA5	-2.11	112.60	117.79
15	Q	502	CDL	CB4-OB6-CB5	-2.09	112.66	117.79
13	C	503	WF3	C14-C9-C5	2.08	125.02	122.24
14	P	505	UQ	C7-C6-C1	-2.07	115.98	118.48
13	P	504	WF3	C28-C29-C30	-2.07	118.23	120.84
13	C	503	WF3	C28-C29-C30	-2.06	118.24	120.84
12	C	501	HEM	CBA-CAA-C2A	-2.06	109.10	112.62
13	C	503	WF3	O16-C15-C14	2.05	115.45	109.38
15	G	101	CDL	OB6-CB4-CB3	2.04	115.79	108.40
12	P	502	HEM	C2B-C1B-NB	2.01	112.22	109.84
13	P	504	WF3	O16-C15-C14	2.00	115.30	109.38

There are no chirality outliers.

All (239) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	505	CDL	O1-C1-CB2-OB2
15	C	505	CDL	CB2-OB2-PB2-OB3
15	C	505	CDL	CB2-OB2-PB2-OB4
15	C	505	CDL	CB2-OB2-PB2-OB5
15	G	101	CDL	O1-C1-CA2-OA2
15	G	101	CDL	CA3-OA5-PA1-OA2
15	G	101	CDL	CA3-OA5-PA1-OA3
15	G	101	CDL	CA3-OA5-PA1-OA4
15	G	101	CDL	CB3-OB5-PB2-OB3
15	G	101	CDL	CB3-OB5-PB2-OB4
15	G	101	CDL	C51-CB5-OB6-CB4
15	P	506	CDL	O1-C1-CA2-OA2
15	P	506	CDL	CA3-OA5-PA1-OA2
15	P	506	CDL	CA3-OA5-PA1-OA3
15	P	506	CDL	CA3-OA5-PA1-OA4
15	P	506	CDL	CB3-OB5-PB2-OB3
15	P	506	CDL	C51-CB5-OB6-CB4
15	Q	502	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
15	Q	502	CDL	CB2-OB2-PB2-OB3
15	Q	502	CDL	CB2-OB2-PB2-OB4
15	Q	502	CDL	CB2-OB2-PB2-OB5
16	C	506	PEE	O4P-C4-C5-N
16	C	507	PEE	C1-O3P-P-O1P
16	C	507	PEE	C1-O3P-P-O4P
16	E	502	PEE	C11-C10-O2-C2
16	E	502	PEE	O4-C10-O2-C2
16	E	502	PEE	C4-O4P-P-O3P
16	E	502	PEE	C4-O4P-P-O2P
16	E	502	PEE	C4-O4P-P-O1P
16	P	507	PEE	O4P-C4-C5-N
16	R	502	PEE	C17-C18-C19-C20
16	R	502	PEE	C11-C10-O2-C2
16	R	502	PEE	C1-O3P-P-O2P
16	R	502	PEE	C1-O3P-P-O4P
16	R	502	PEE	O4P-C4-C5-N
17	C	508	GOL	O1-C1-C2-C3
17	C	508	GOL	C1-C2-C3-O3
17	P	508	GOL	C1-C2-C3-O3
18	D	501	HEC	C1A-C2A-CAA-CBA
18	D	501	HEC	C3A-C2A-CAA-CBA
18	D	501	HEC	C2D-C3D-CAD-CBD
18	Q	501	HEC	C1A-C2A-CAA-CBA
18	Q	501	HEC	C3A-C2A-CAA-CBA
15	C	505	CDL	C31-CA7-OA8-CA6
15	Q	502	CDL	C31-CA7-OA8-CA6
15	G	101	CDL	OB9-CB7-OB8-CB6
15	P	506	CDL	OB9-CB7-OB8-CB6
16	R	502	PEE	O5-C30-O3-C3
16	E	502	PEE	O5-C30-O3-C3
16	R	502	PEE	C31-C30-O3-C3
19	Q	504	BOG	O5-C5-C6-O6
15	G	101	CDL	C31-CA7-OA8-CA6
15	P	506	CDL	C31-CA7-OA8-CA6
19	Q	504	BOG	O5-C1-O1-C1'
15	G	101	CDL	C71-CB7-OB8-CB6
15	P	506	CDL	C71-CB7-OB8-CB6
16	E	502	PEE	C31-C30-O3-C3
15	C	505	CDL	OA9-CA7-OA8-CA6
15	Q	502	CDL	OA9-CA7-OA8-CA6
15	G	101	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
15	P	506	CDL	OB7-CB5-OB6-CB4
16	R	502	PEE	O4-C10-O2-C2
19	Q	504	BOG	C2-C1-O1-C1'
15	C	505	CDL	C71-CB7-OB8-CB6
15	Q	502	CDL	C71-CB7-OB8-CB6
19	Q	504	BOG	C4-C5-C6-O6
15	C	505	CDL	OB9-CB7-OB8-CB6
15	Q	502	CDL	OB9-CB7-OB8-CB6
15	G	101	CDL	OA9-CA7-OA8-CA6
15	P	506	CDL	OA9-CA7-OA8-CA6
16	E	502	PEE	C30-C31-C32-C33
16	C	506	PEE	C17-C18-C19-C20
19	D	502	BOG	O1-C1'-C2'-C3'
19	Q	503	BOG	O1-C1'-C2'-C3'
16	R	502	PEE	C30-C31-C32-C33
16	C	506	PEE	C10-C11-C12-C13
16	E	502	PEE	C10-C11-C12-C13
16	P	507	PEE	C17-C18-C19-C20
15	G	101	CDL	CB3-OB5-PB2-OB2
15	P	506	CDL	CB3-OB5-PB2-OB2
15	C	505	CDL	CA2-C1-CB2-OB2
15	G	101	CDL	CB2-C1-CA2-OA2
15	P	506	CDL	CB2-C1-CA2-OA2
15	Q	502	CDL	CA2-C1-CB2-OB2
16	E	502	PEE	C34-C35-C36-C37
16	C	506	PEE	C37-C38-C39-C40
16	P	507	PEE	C37-C38-C39-C40
19	D	502	BOG	C2-C1-O1-C1'
19	Q	503	BOG	C2-C1-O1-C1'
16	R	502	PEE	C11-C12-C13-C14
16	P	507	PEE	C10-C11-C12-C13
16	E	502	PEE	C22-C23-C24-C25
16	R	502	PEE	C39-C40-C41-C42
16	E	502	PEE	C32-C33-C34-C35
16	E	502	PEE	C20-C21-C22-C23
17	C	508	GOL	O1-C1-C2-O2
17	C	508	GOL	O2-C2-C3-O3
16	C	506	PEE	C35-C36-C37-C38
16	P	507	PEE	C35-C36-C37-C38
19	D	502	BOG	C1'-C2'-C3'-C4'
19	Q	503	BOG	C1'-C2'-C3'-C4'
16	C	507	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
16	R	502	PEE	C34-C35-C36-C37
16	E	502	PEE	C35-C36-C37-C38
16	R	502	PEE	C41-C42-C43-C44
16	C	507	PEE	O5-C30-O3-C3
19	D	502	BOG	O5-C1-O1-C1'
19	Q	503	BOG	O5-C1-O1-C1'
16	C	506	PEE	C21-C22-C23-C24
16	R	502	PEE	C42-C43-C44-C45
16	P	507	PEE	C21-C22-C23-C24
16	C	506	PEE	C15-C16-C17-C18
16	P	507	PEE	C15-C16-C17-C18
16	R	502	PEE	C35-C36-C37-C38
16	P	507	PEE	C20-C21-C22-C23
16	C	506	PEE	C11-C12-C13-C14
16	E	502	PEE	O3P-C1-C2-C3
16	P	507	PEE	C11-C12-C13-C14
16	E	502	PEE	C14-C15-C16-C17
15	Q	502	CDL	C71-C72-C73-C74
16	P	507	PEE	C33-C34-C35-C36
12	C	502	HEM	C4D-C3D-CAD-CBD
14	C	504	UQ	C5-C6-C7-C8
14	P	505	UQ	C5-C6-C7-C8
16	R	502	PEE	C24-C25-C26-C27
15	C	505	CDL	C71-C72-C73-C74
17	P	508	GOL	O2-C2-C3-O3
16	E	502	PEE	C19-C20-C21-C22
16	C	506	PEE	C20-C21-C22-C23
14	C	504	UQ	C1-C6-C7-C8
14	P	505	UQ	C1-C6-C7-C8
13	P	504	WF3	C5-C3-O2-C1
16	R	502	PEE	C14-C15-C16-C17
16	R	502	PEE	C43-C44-C45-C46
15	C	505	CDL	OA5-CA3-CA4-OA6
15	G	101	CDL	OA6-CA4-CA6-OA8
15	P	506	CDL	OA6-CA4-CA6-OA8
16	C	506	PEE	C33-C34-C35-C36
16	R	502	PEE	C22-C23-C24-C25
16	C	506	PEE	C12-C13-C14-C15
16	E	502	PEE	C41-C42-C43-C44
15	Q	502	CDL	OA5-CA3-CA4-OA6
14	P	505	UQ	C12-C11-C9-C10
16	E	502	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
16	P	507	PEE	C12-C13-C14-C15
12	P	502	HEM	C4D-C3D-CAD-CBD
13	P	504	WF3	O2-C3-C5-C9
16	E	502	PEE	C1-C2-O2-C10
17	P	508	GOL	O1-C1-C2-O2
16	P	507	PEE	C43-C44-C45-C46
13	P	504	WF3	O4-C3-O2-C1
15	C	505	CDL	CA2-OA2-PA1-OA5
15	Q	502	CDL	CA2-OA2-PA1-OA5
13	P	504	WF3	O2-C3-C5-C6
13	P	504	WF3	O4-C3-C5-C6
15	P	506	CDL	CB3-OB5-PB2-OB4
16	R	502	PEE	C1-O3P-P-O1P
15	Q	502	CDL	OA5-CA3-CA4-CA6
16	C	506	PEE	C43-C44-C45-C46
16	R	502	PEE	C12-C13-C14-C15
16	E	502	PEE	C13-C14-C15-C16
16	E	502	PEE	O3P-C1-C2-O2
18	D	501	HEC	C4D-C3D-CAD-CBD
18	Q	501	HEC	C2D-C3D-CAD-CBD
16	P	507	PEE	C42-C43-C44-C45
15	C	505	CDL	OA5-CA3-CA4-CA6
15	G	101	CDL	C1-CB2-OB2-PB2
15	G	101	CDL	CA3-CA4-CA6-OA8
15	P	506	CDL	CA3-CA4-CA6-OA8
15	C	505	CDL	C1-CA2-OA2-PA1
15	Q	502	CDL	C1-CA2-OA2-PA1
16	C	507	PEE	C10-C11-C12-C13
12	C	502	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAA-CBA-CGA-O1A
16	E	502	PEE	C38-C39-C40-C41
16	C	506	PEE	C42-C43-C44-C45
15	P	506	CDL	C1-CB2-OB2-PB2
16	E	502	PEE	C23-C24-C25-C26
16	P	507	PEE	C14-C15-C16-C17
16	E	502	PEE	C18-C19-C20-C21
12	P	502	HEM	CAA-CBA-CGA-O2A
12	C	502	HEM	CAA-CBA-CGA-O2A
16	C	507	PEE	O3-C30-C31-C32
18	D	501	HEC	CAA-CBA-CGA-O2A
15	P	506	CDL	OA7-CA5-OA6-CA4
13	P	504	WF3	O4-C3-C5-C9

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Mol	Chain	Res	Type	Atoms
12	P	501	HEM	CAA-CBA-CGA-O2A
16	C	506	PEE	C14-C15-C16-C17
18	Q	501	HEC	CAA-CBA-CGA-O2A
14	C	504	UQ	C12-C11-C9-C10
12	C	501	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAD-CBD-CGD-O2D
18	D	501	HEC	CAD-CBD-CGD-O2D
18	D	501	HEC	CAA-CBA-CGA-O1A
16	E	502	PEE	C43-C44-C45-C46
12	P	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	CAD-CBD-CGD-O2D
16	C	506	PEE	O3-C30-C31-C32
12	P	501	HEM	CAA-CBA-CGA-O1A
16	R	502	PEE	C36-C37-C38-C39
16	R	502	PEE	C10-C11-C12-C13
16	P	507	PEE	O3-C30-C31-C32
18	Q	501	HEC	CAD-CBD-CGD-O2D
15	C	505	CDL	C72-C71-CB7-OB8
16	C	506	PEE	O2-C10-C11-C12
16	P	507	PEE	O2-C10-C11-C12
12	C	501	HEM	CAD-CBD-CGD-O1D
12	C	501	HEM	CAA-CBA-CGA-O1A
12	C	501	HEM	CAA-CBA-CGA-O2A
12	C	502	HEM	CAD-CBD-CGD-O1D
12	P	501	HEM	CAD-CBD-CGD-O1D
18	D	501	HEC	CAD-CBD-CGD-O1D
18	Q	501	HEC	CAA-CBA-CGA-O1A
12	C	502	HEM	CAD-CBD-CGD-O2D
16	P	507	PEE	C38-C39-C40-C41
16	R	502	PEE	C23-C24-C25-C26
18	Q	501	HEC	CAD-CBD-CGD-O1D
15	Q	502	CDL	C72-C71-CB7-OB8
15	Q	502	CDL	C52-C51-CB5-OB6
16	C	507	PEE	O5-C30-C31-C32
16	C	506	PEE	C38-C39-C40-C41
16	P	507	PEE	C16-C17-C18-C19
15	C	505	CDL	C52-C51-CB5-OB6
15	C	505	CDL	C12-C11-CA5-OA6
15	Q	502	CDL	C12-C11-CA5-OA6
15	P	506	CDL	C11-CA5-OA6-CA4
12	P	502	HEM	C2A-CAA-CBA-CGA
16	P	507	PEE	O5-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
15	Q	502	CDL	C72-C71-CB7-OB9
16	C	506	PEE	O5-C30-C31-C32
16	C	506	PEE	O4-C10-C11-C12
15	C	505	CDL	C72-C71-CB7-OB9
16	P	507	PEE	O4-C10-C11-C12
16	C	506	PEE	C16-C17-C18-C19
16	R	502	PEE	O3P-C1-C2-O2
16	E	502	PEE	C16-C17-C18-C19
15	Q	502	CDL	CB7-C71-C72-C73
15	C	505	CDL	C52-C51-CB5-OB7
15	Q	502	CDL	C52-C51-CB5-OB7

There are no ring outliers.

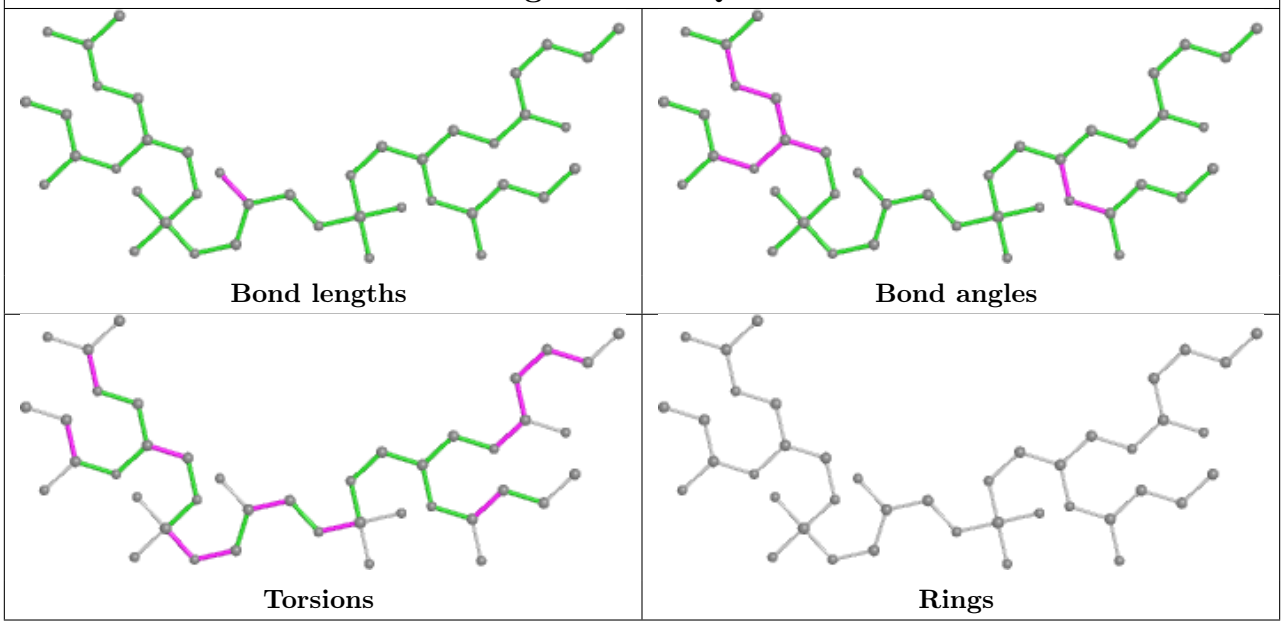
17 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Q	502	CDL	1	0
12	C	501	HEM	1	0
15	G	101	CDL	1	0
13	C	503	WF3	1	0
14	C	504	UQ	3	0
15	P	506	CDL	3	0
12	P	501	HEM	2	0
18	D	501	HEC	2	0
16	C	506	PEE	2	0
12	P	502	HEM	2	0
16	P	507	PEE	2	0
13	P	504	WF3	1	0
16	R	502	PEE	1	0
12	C	502	HEM	4	0
15	C	505	CDL	1	0
14	P	505	UQ	2	0
18	Q	501	HEC	1	0

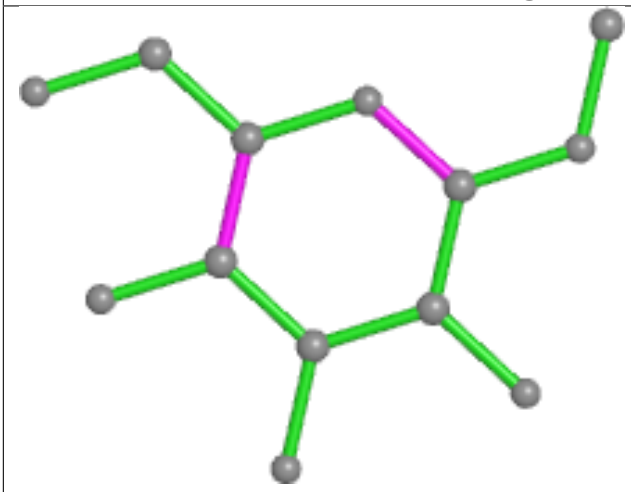
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

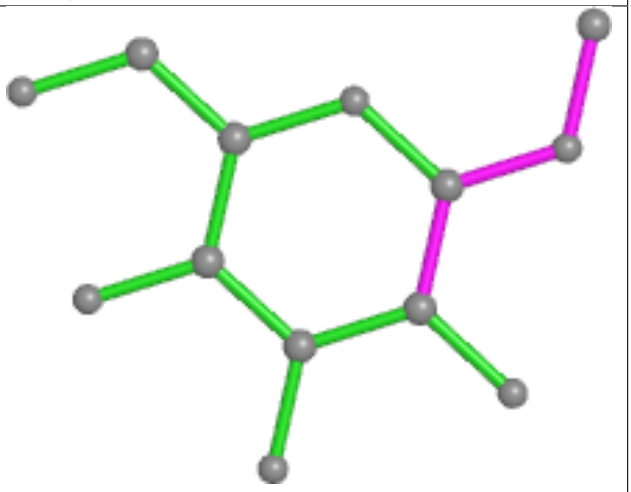
Ligand CDL Q 502



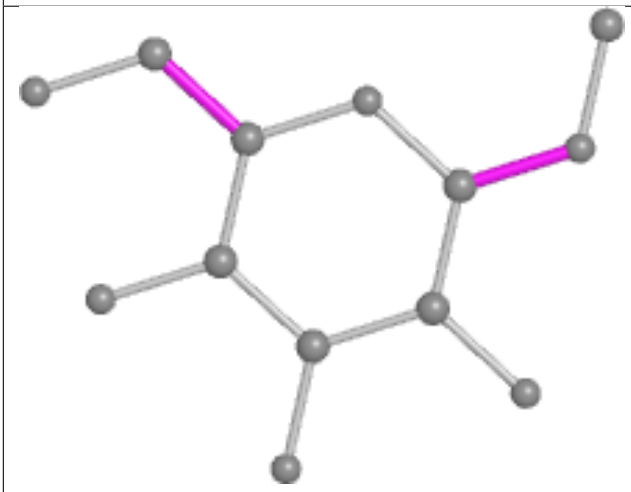
Ligand BOG Q 504



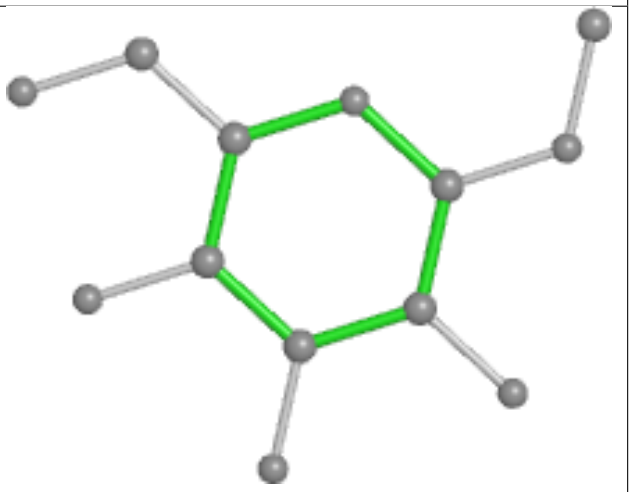
Bond lengths



Bond angles

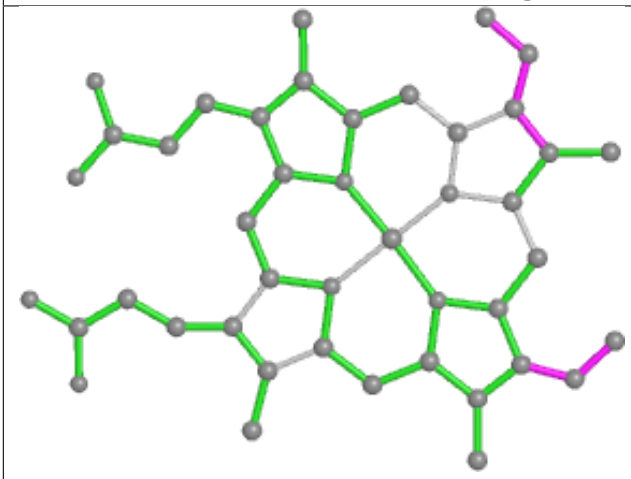


Torsions

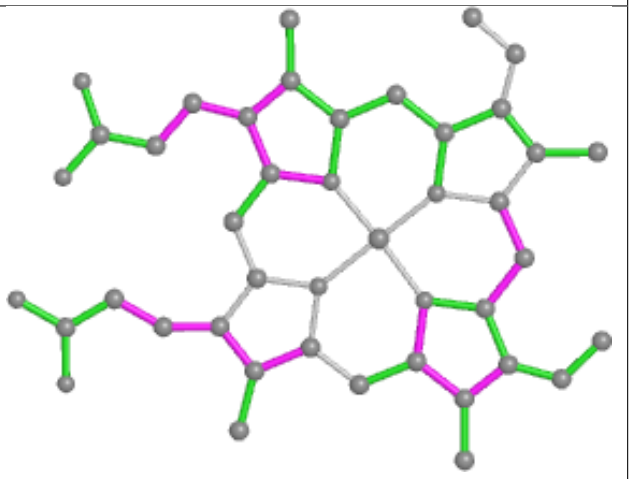


Rings

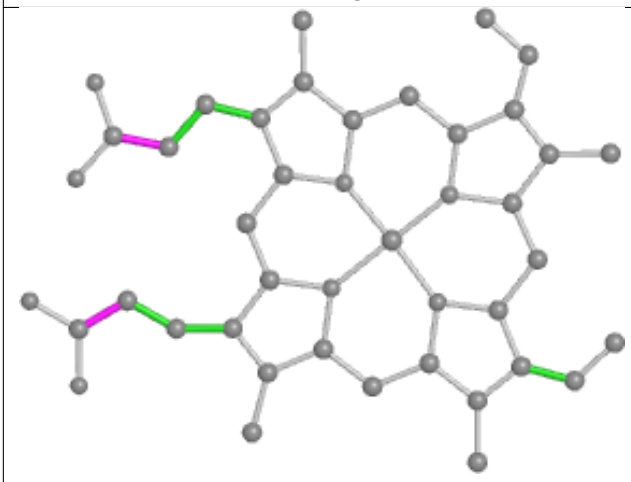
Ligand HEM C 501



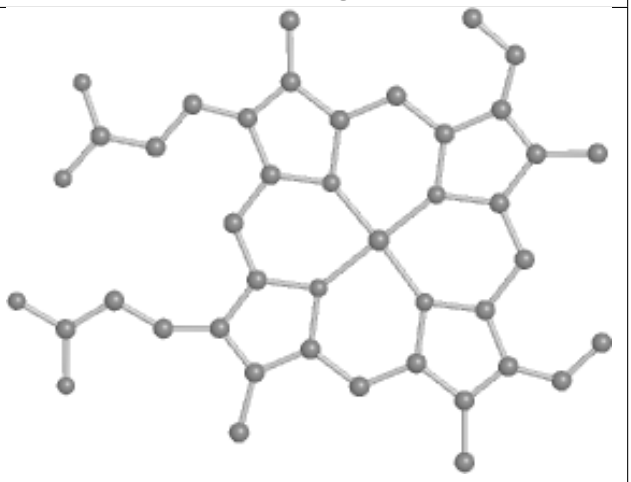
Bond lengths



Bond angles

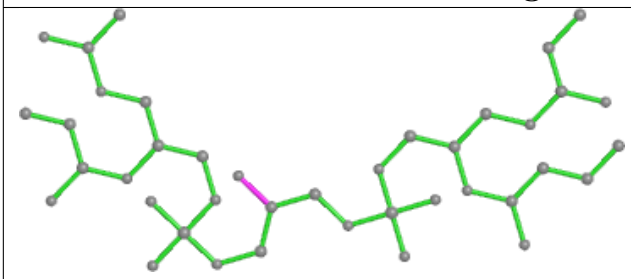


Torsions

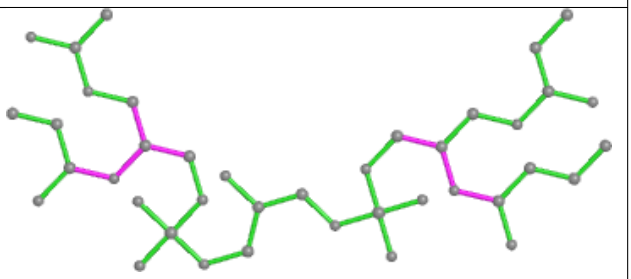


Rings

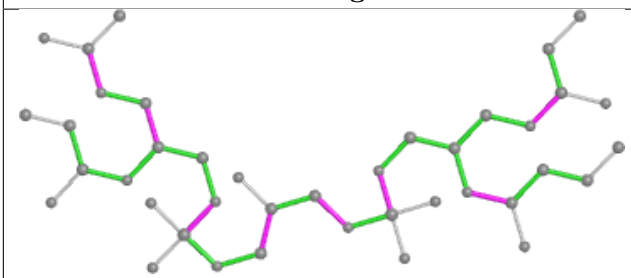
Ligand CDL G 101



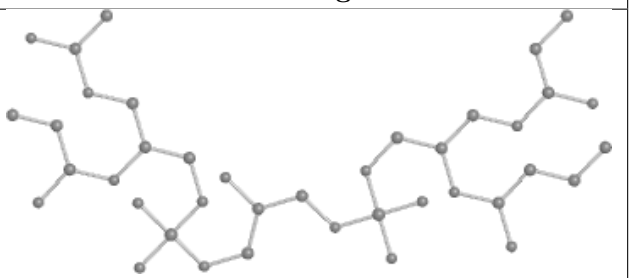
Bond lengths



Bond angles

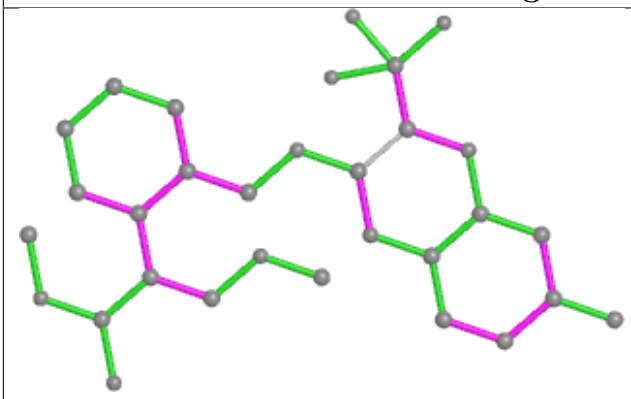


Torsions

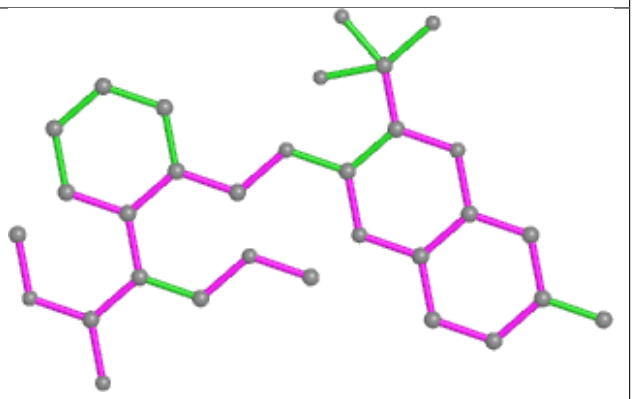


Rings

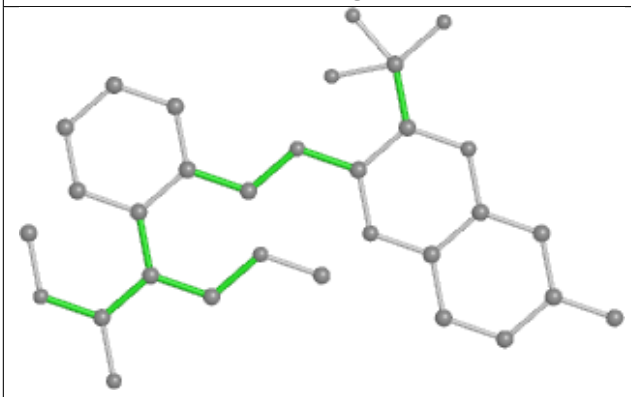
Ligand WF3 C 503



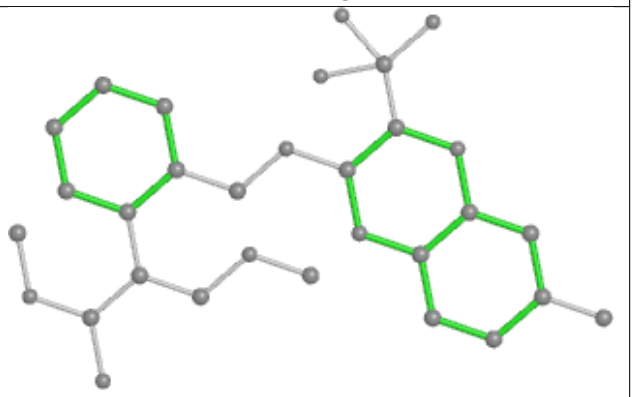
Bond lengths



Bond angles

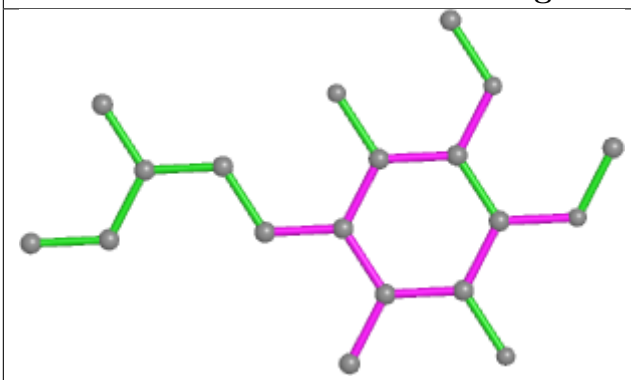


Torsions

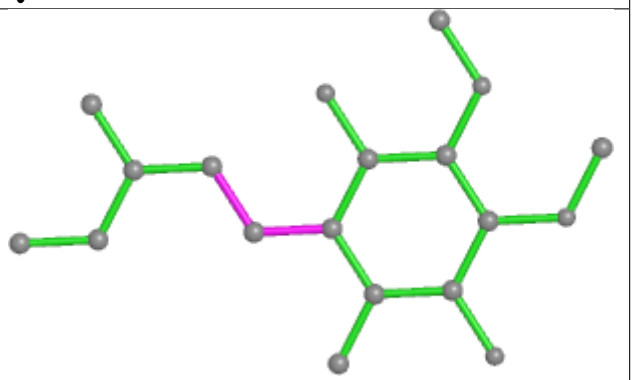


Rings

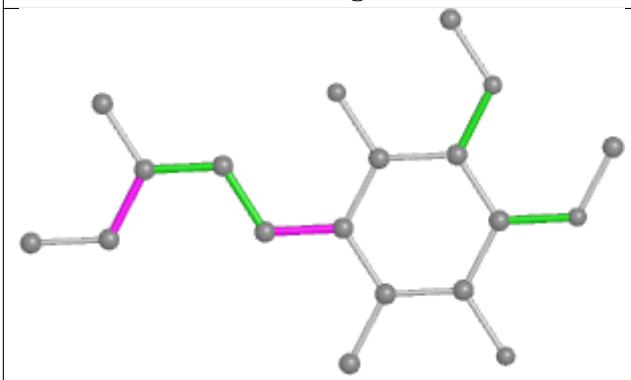
Ligand UQ C 504



Bond lengths



Bond angles



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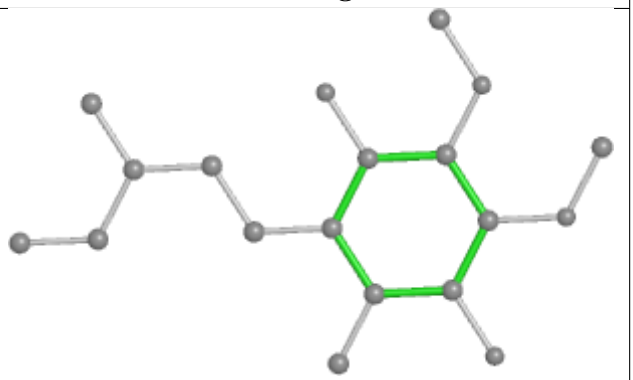
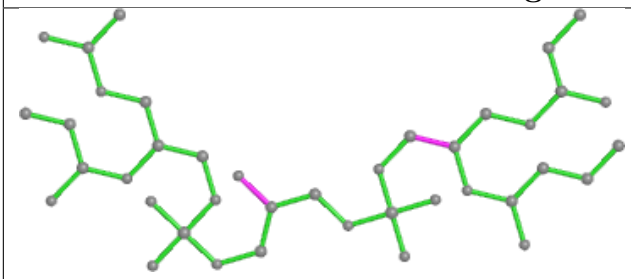


Rings

Ligand CDL P 506



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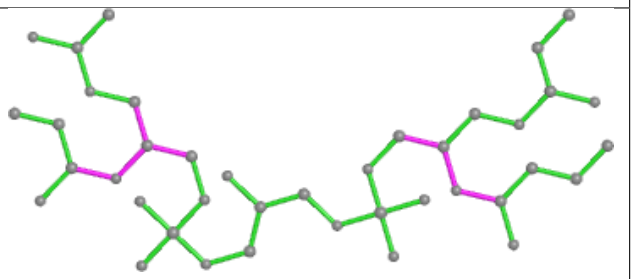
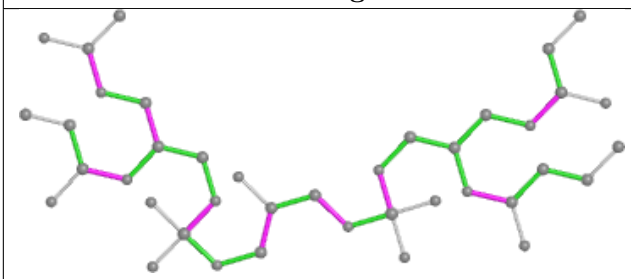


Bond angles



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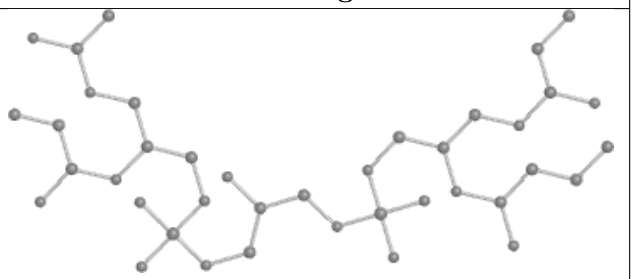
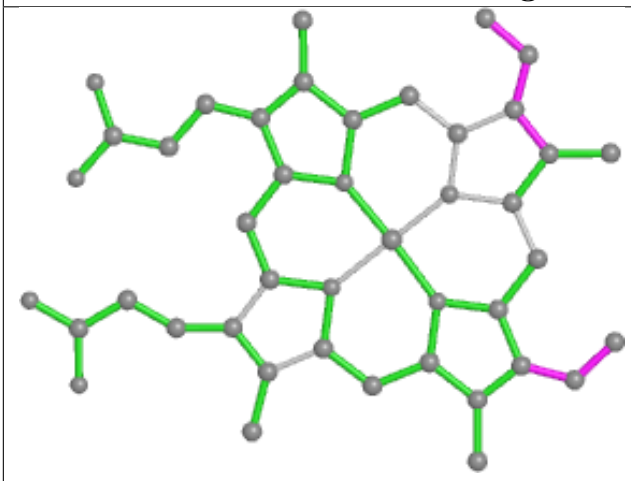


Rings

Ligand HEM P 501



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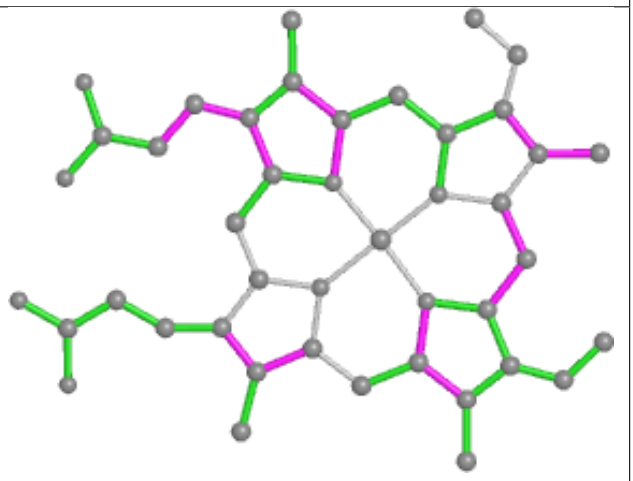

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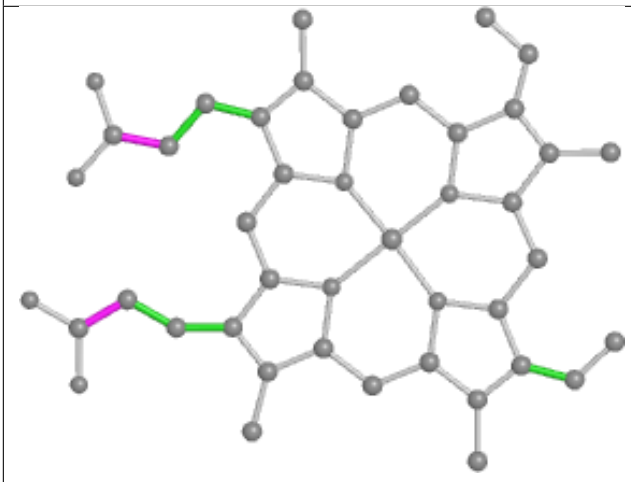

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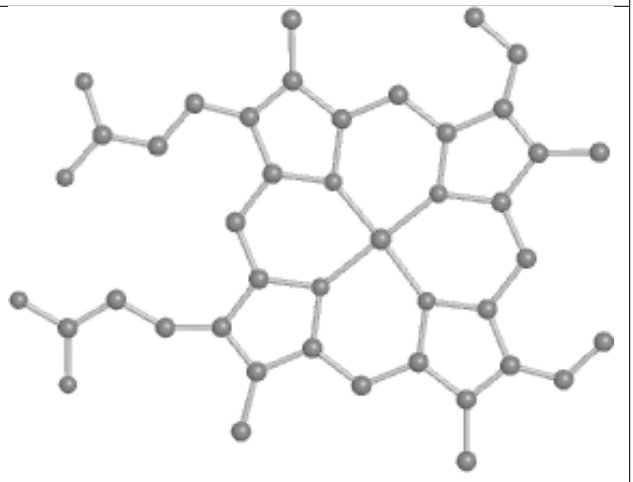
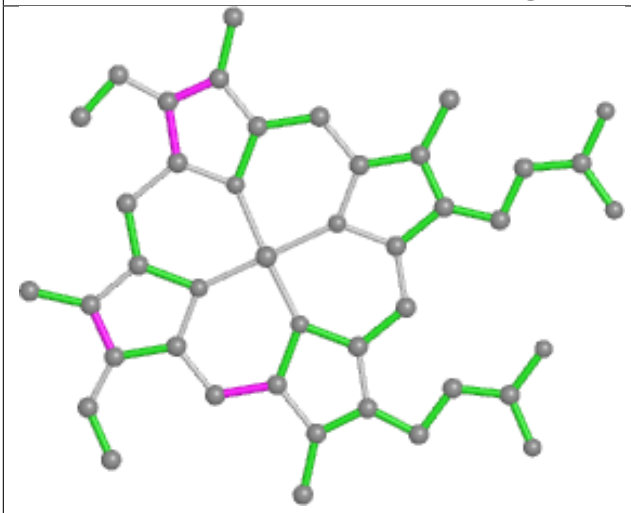


Rings

Ligand HEC D 501



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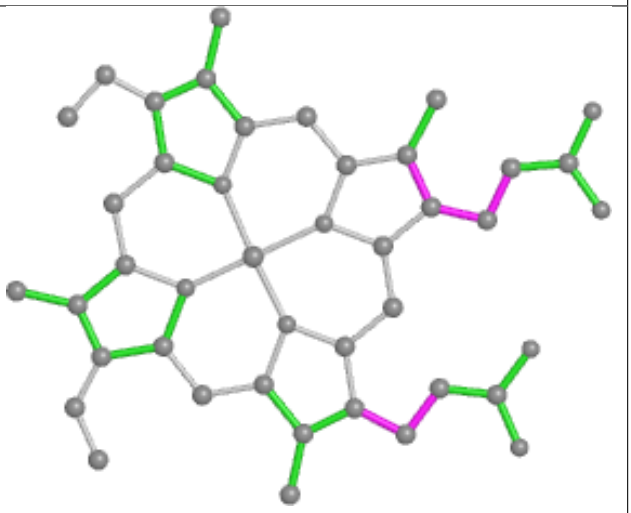
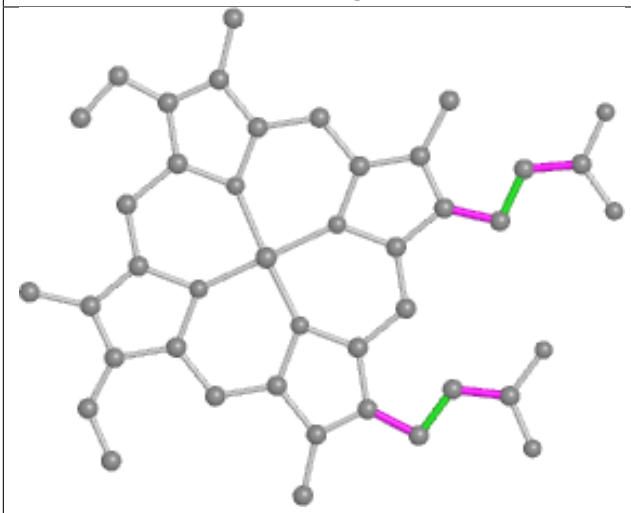


Bond angles



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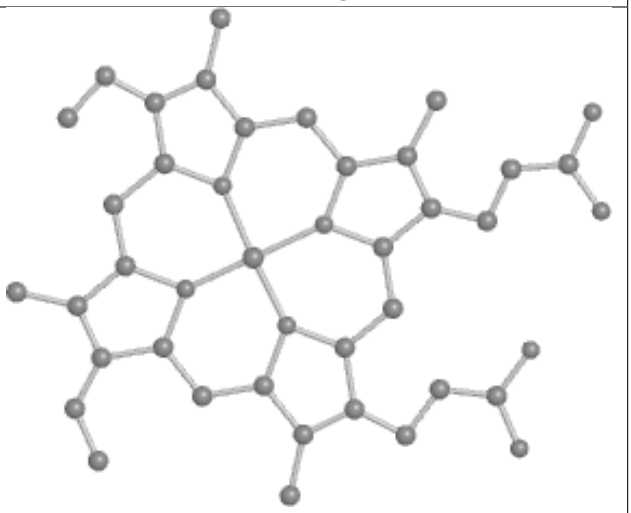
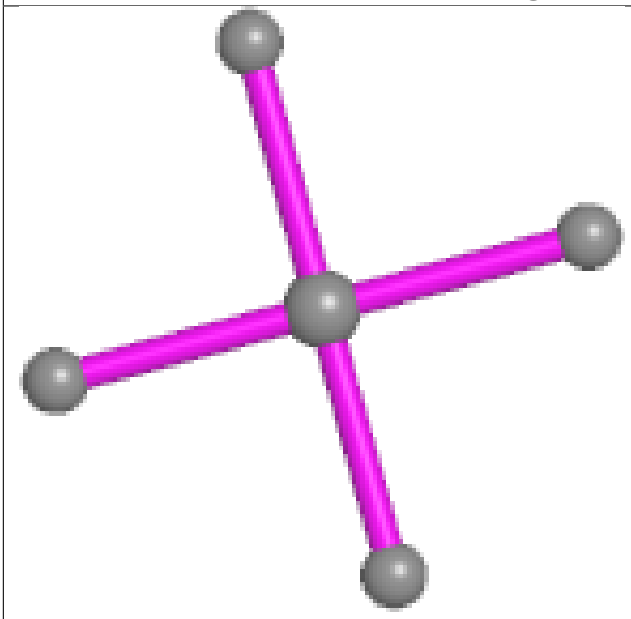
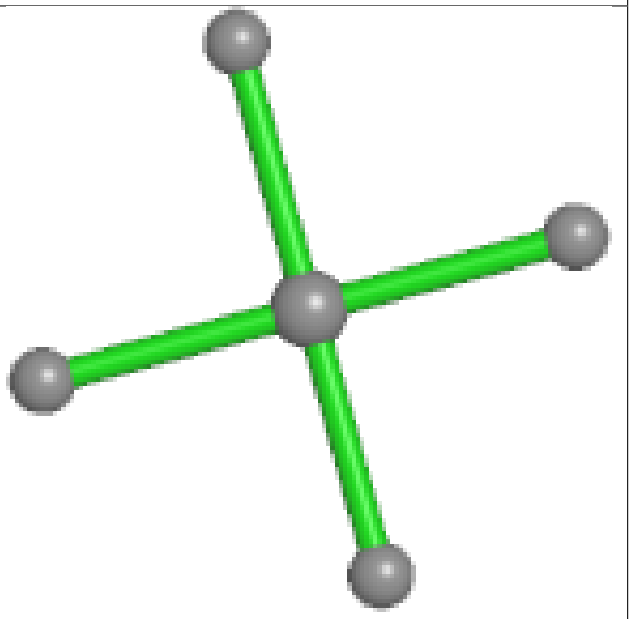


Rings

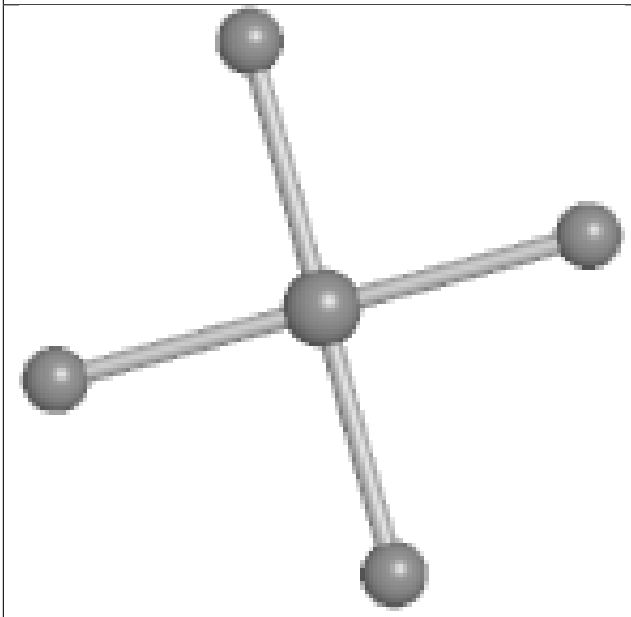
Ligand PEE N 502



Bond lengths



Bond angles



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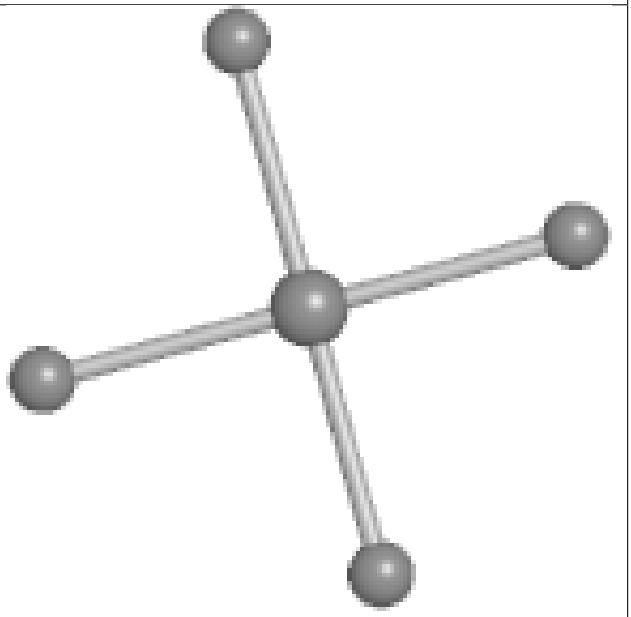
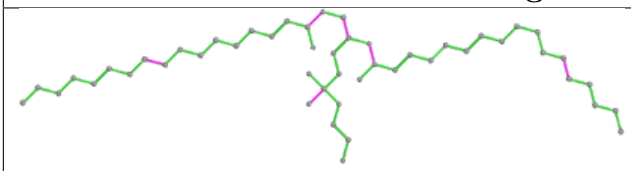
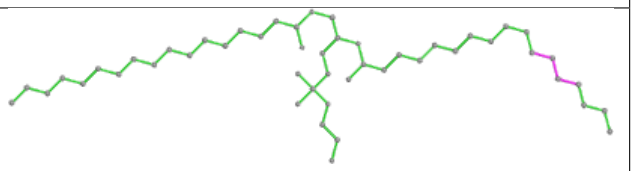


Rings

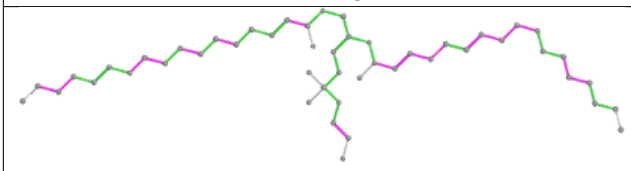
Ligand PEE C 506



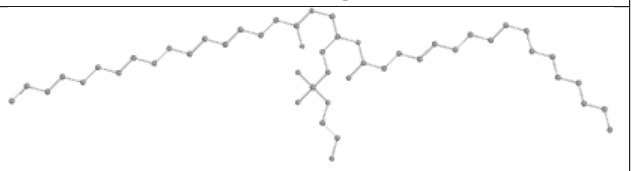
Bond lengths



Bond angles

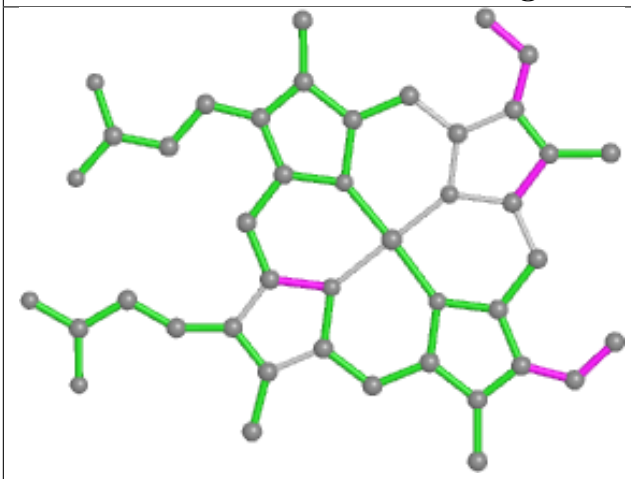


Torsions



Rings

Ligand HEM P 502



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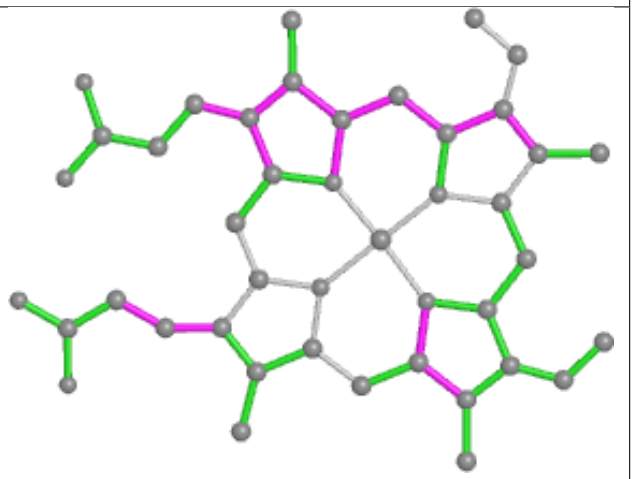
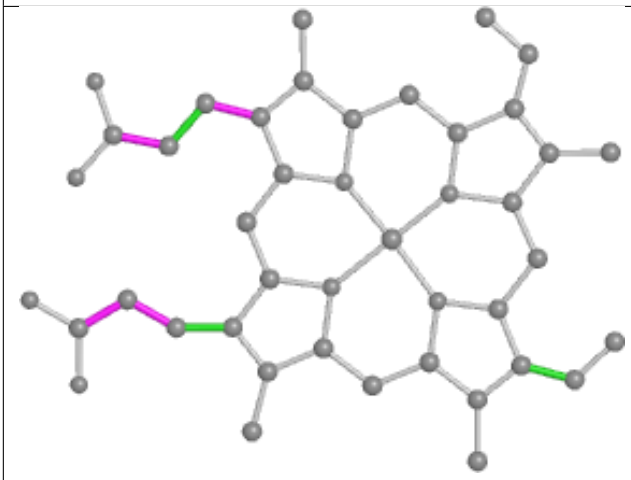


Bond angles



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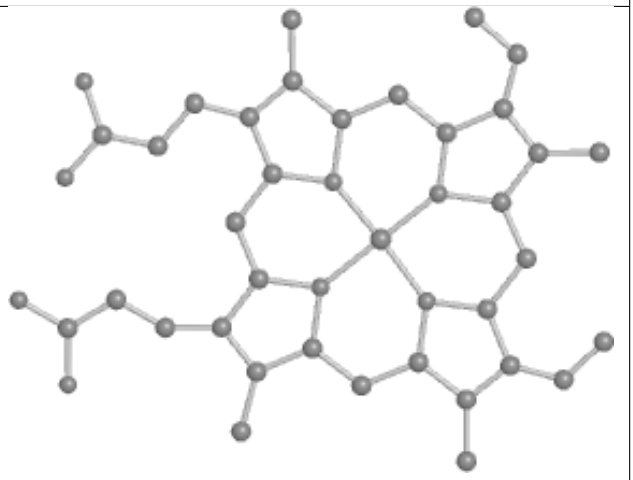
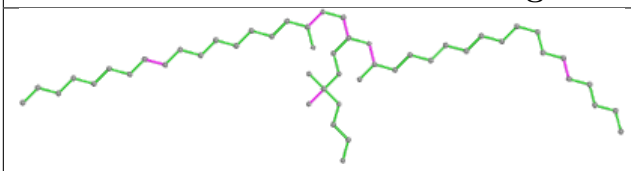


Rings

Ligand PEE P 507



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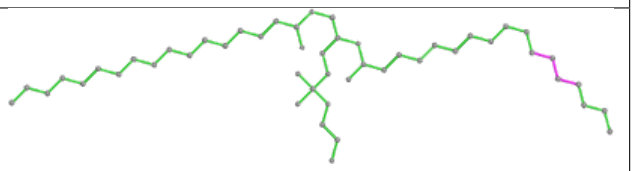
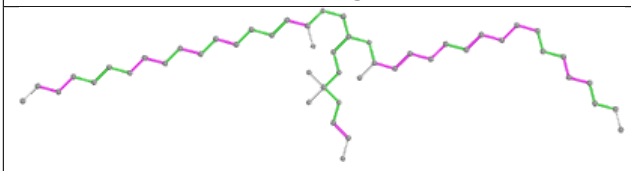


Bond angles



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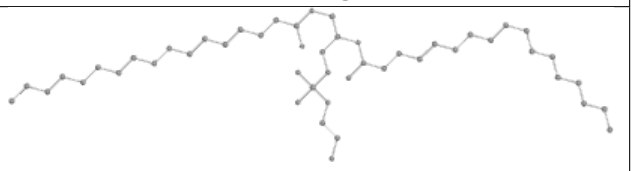
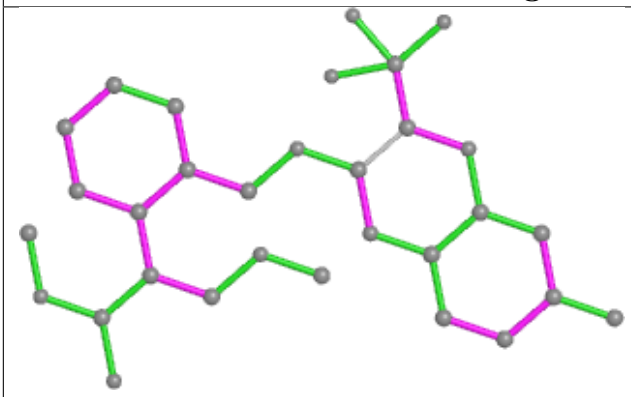


Rings

Ligand WF3 P 504



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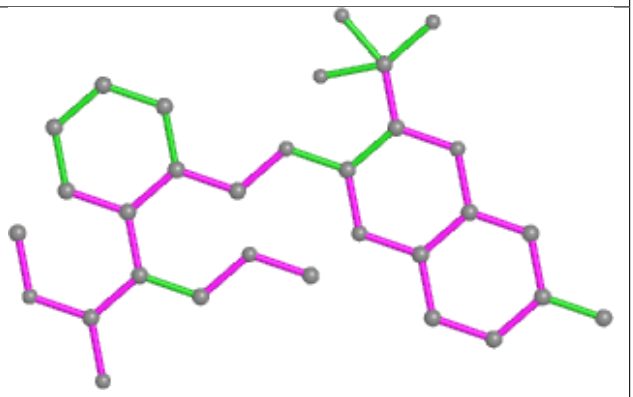
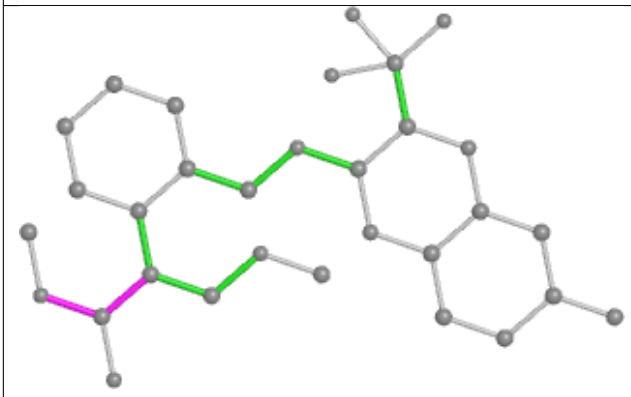


Bond angles



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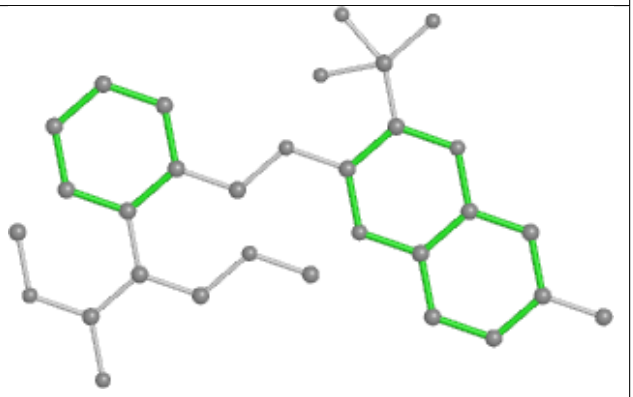
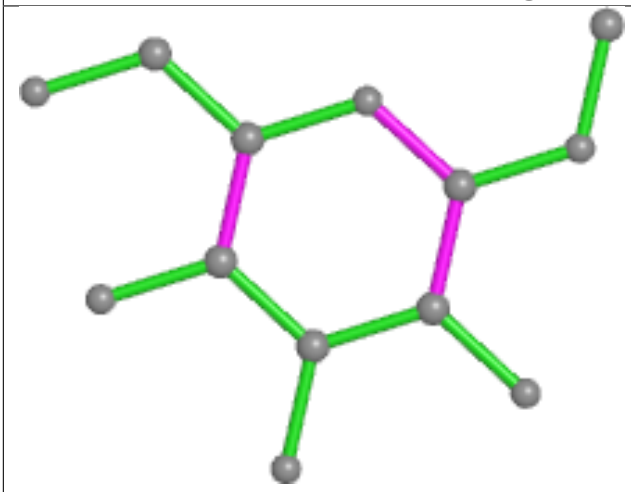


Rings

Ligand BOG D 503



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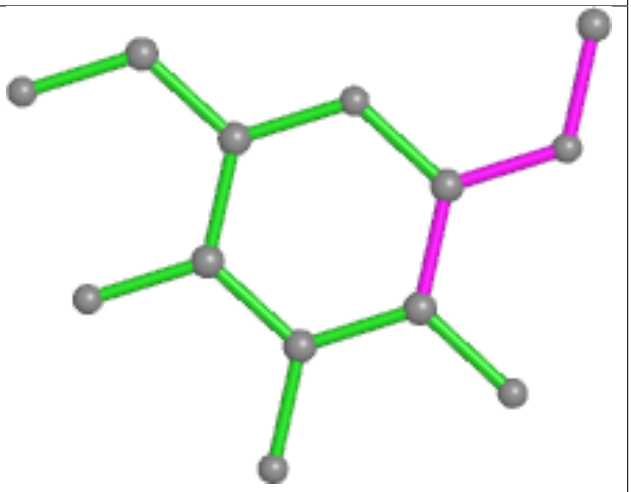
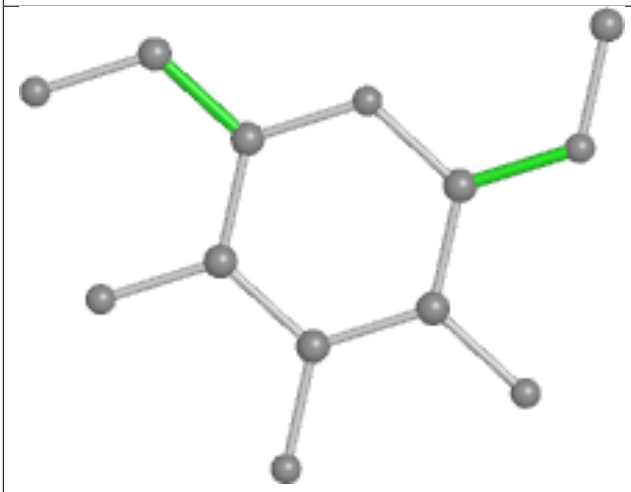


Bond angles



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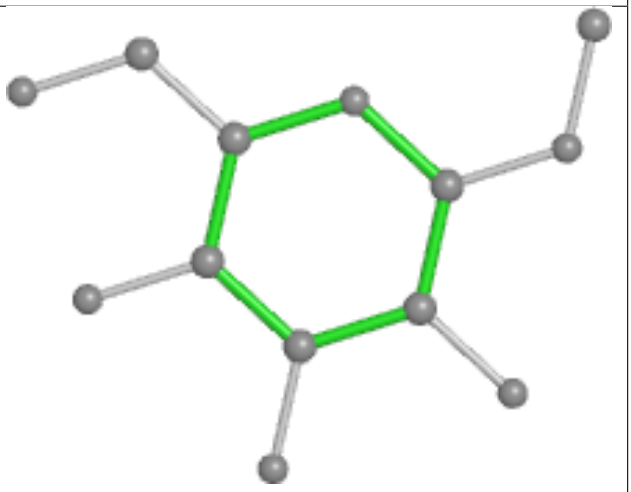

Rings

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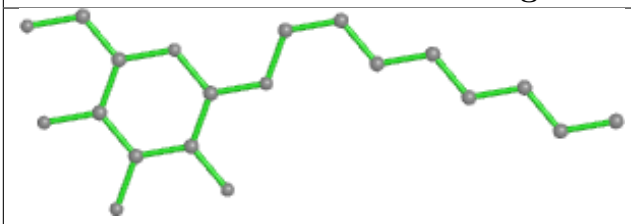

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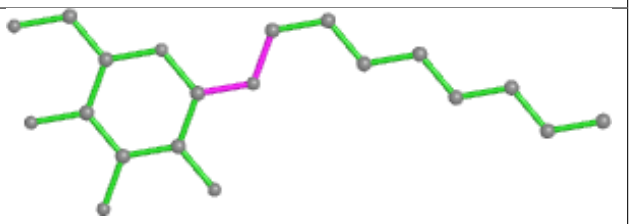
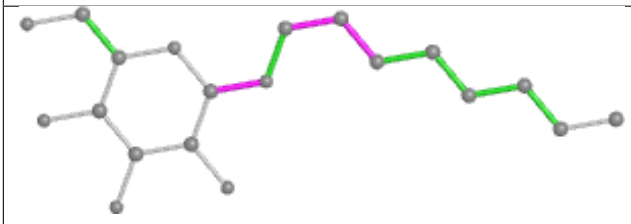


Bond angles



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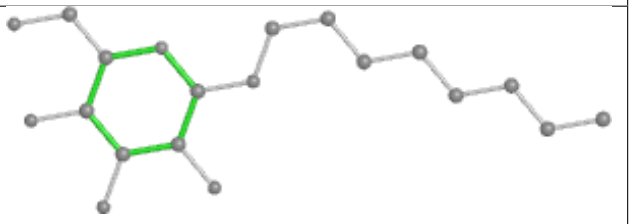
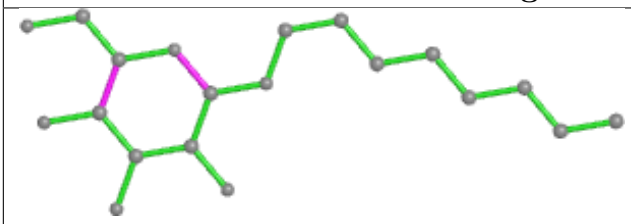


Rings

Ligand BOG Q 503



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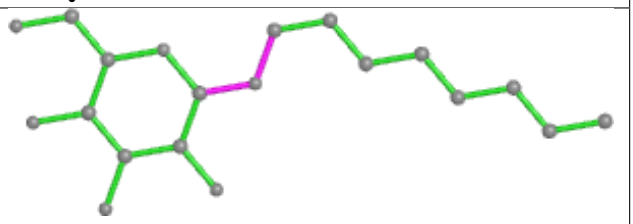

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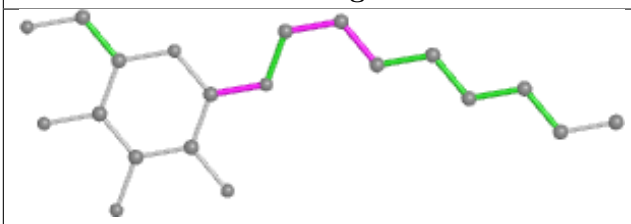

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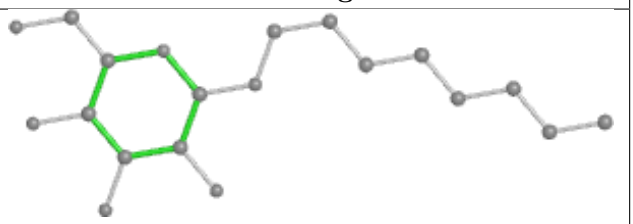
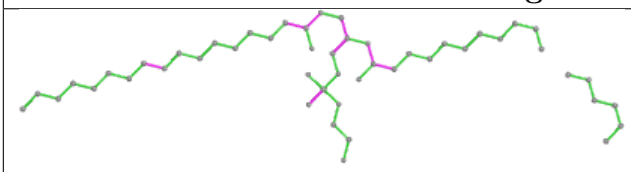


Rings

Ligand PEE R 502



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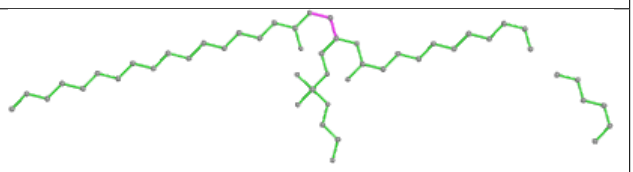
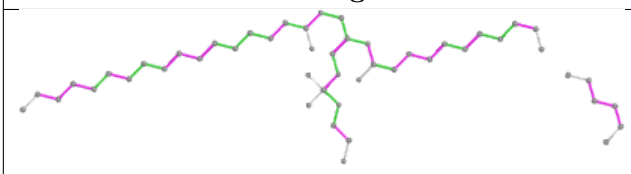


Bond angles



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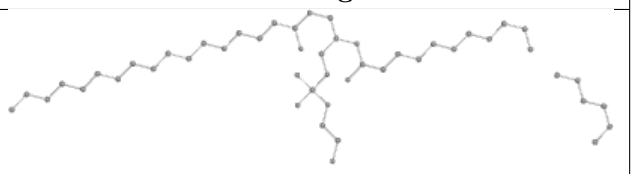
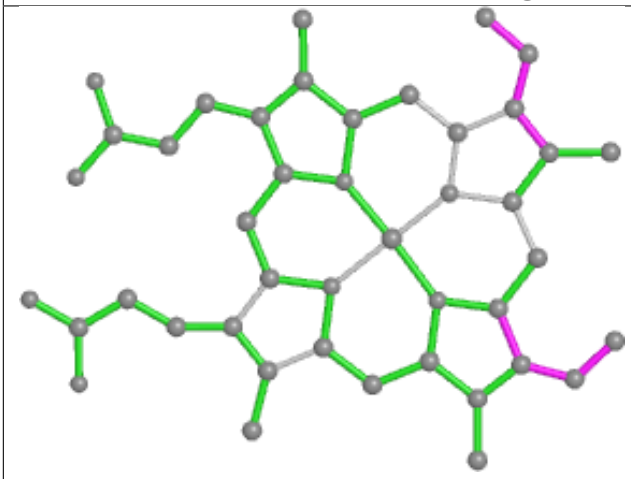


Rings

Ligand HEM C 502



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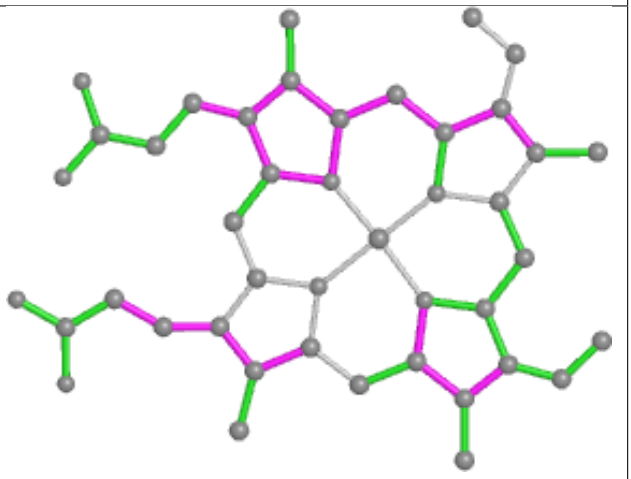
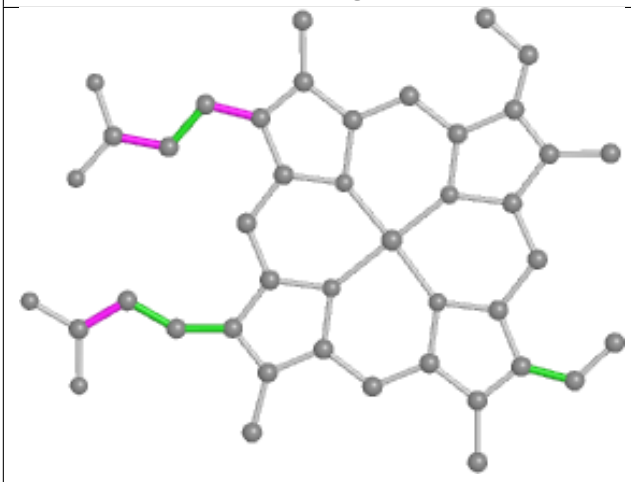


Bond angles



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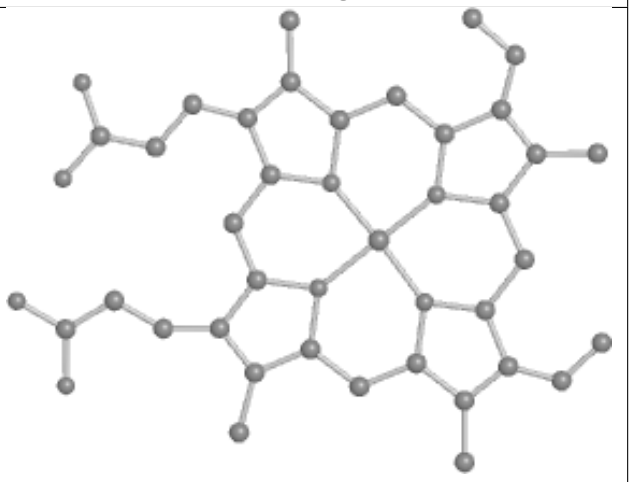
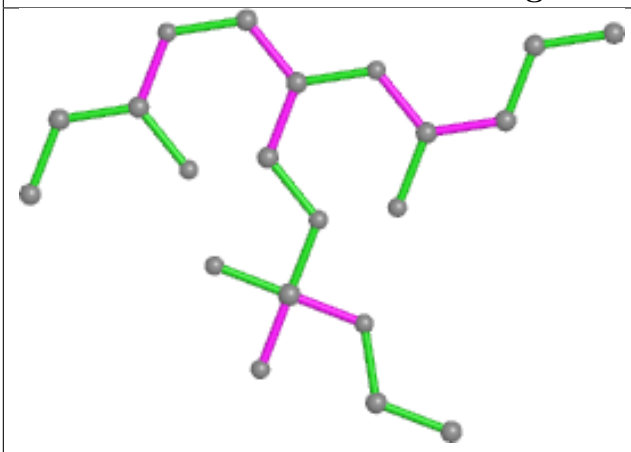


Rings

Ligand PEE C 507



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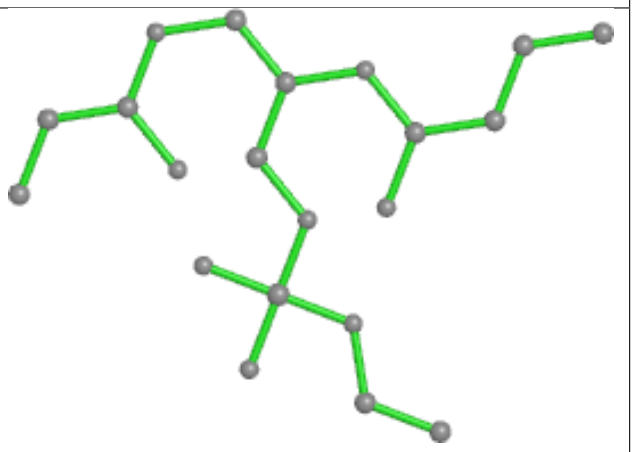
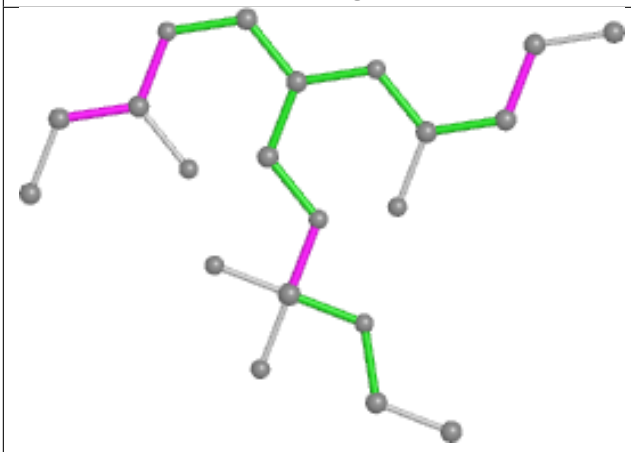


Bond angles



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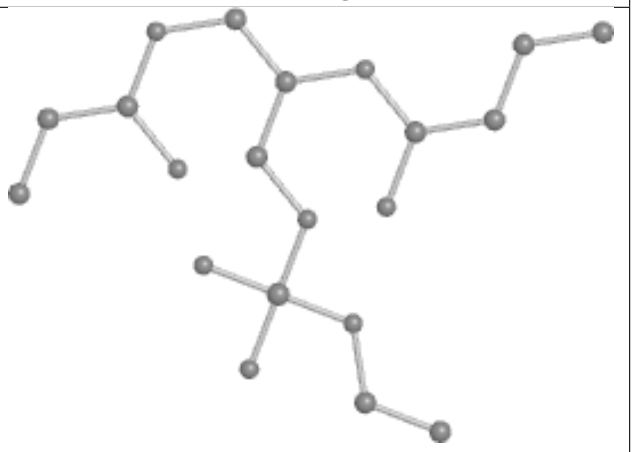
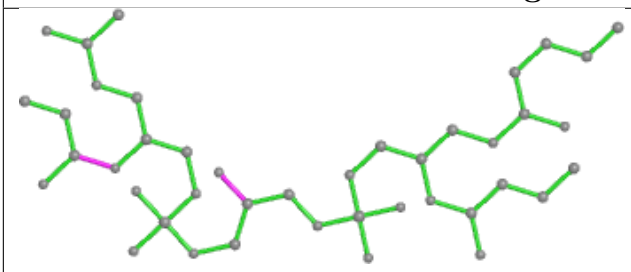


Rings

Ligand CDL C 505



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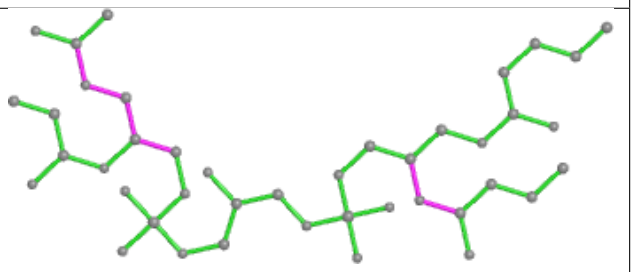

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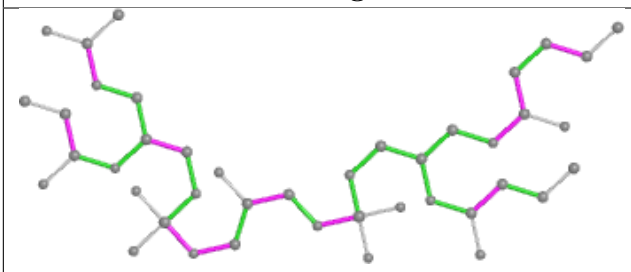

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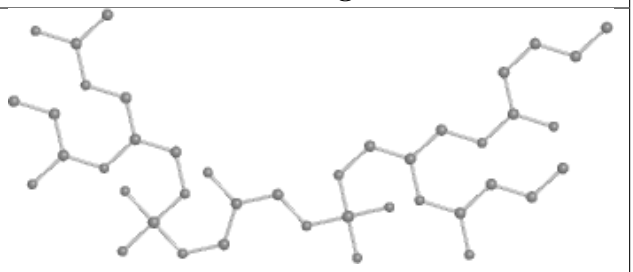
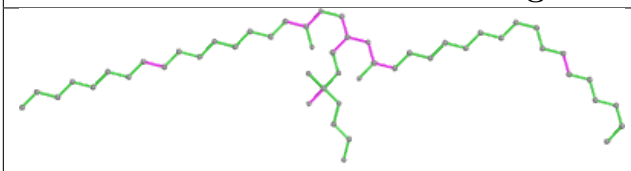


Rings

Ligand PEE E 502



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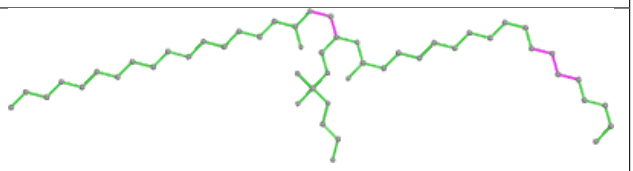
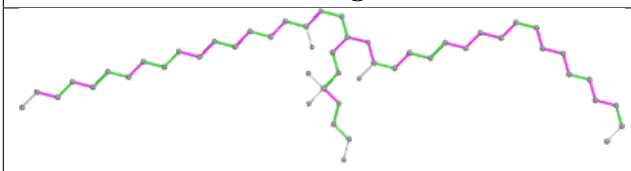


Bond angles



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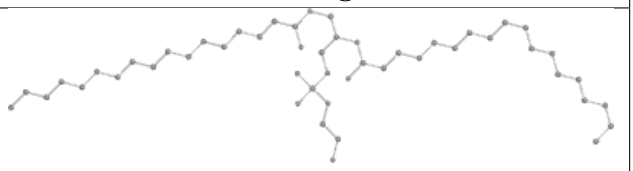
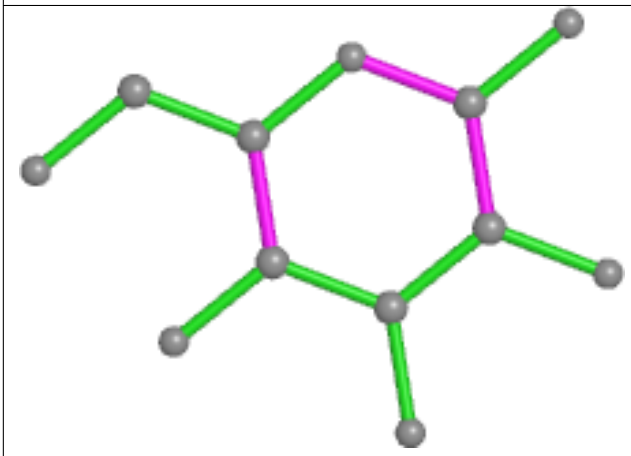


Rings

Ligand BOG P 503



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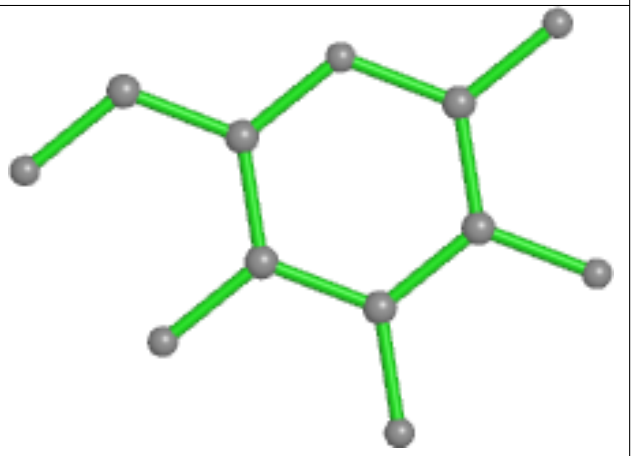
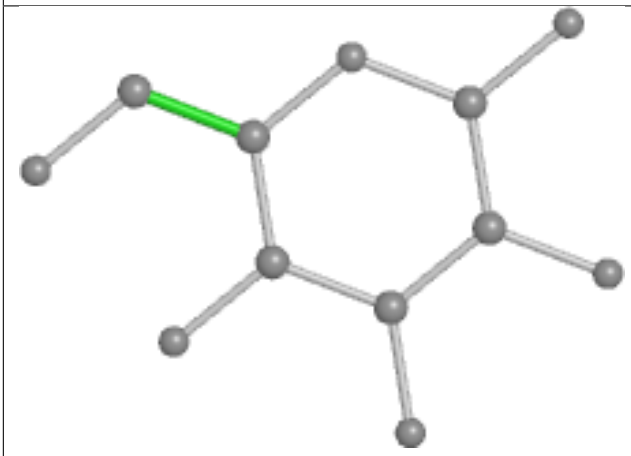


Bond angles



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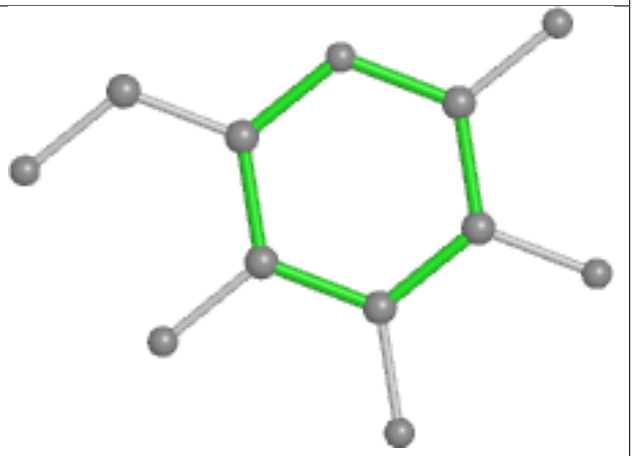
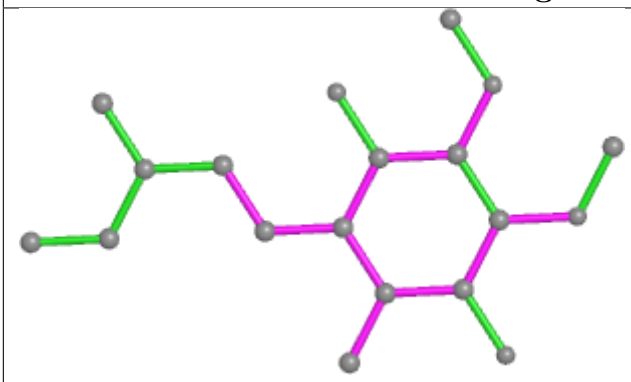


Rings

Ligand UQ P 505



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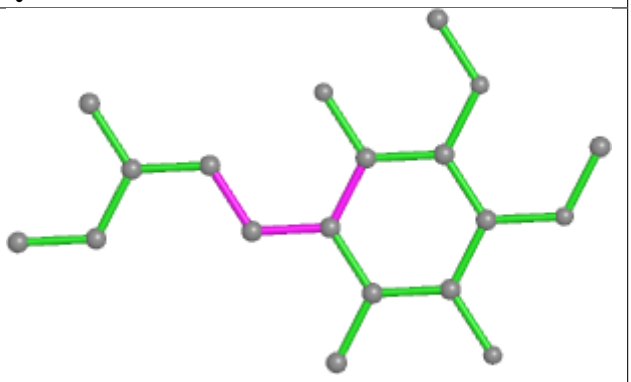
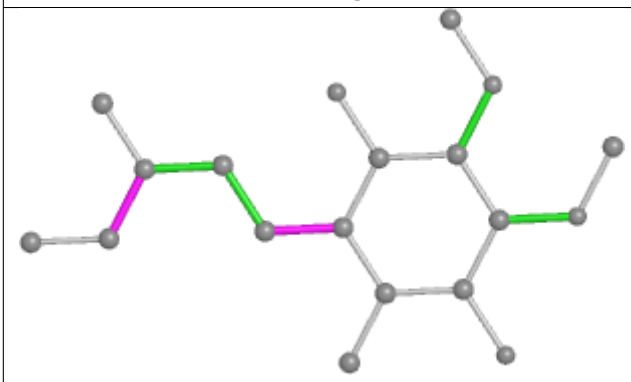


Bond angles



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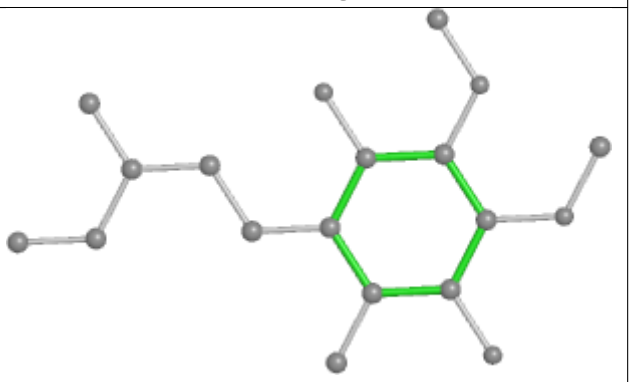
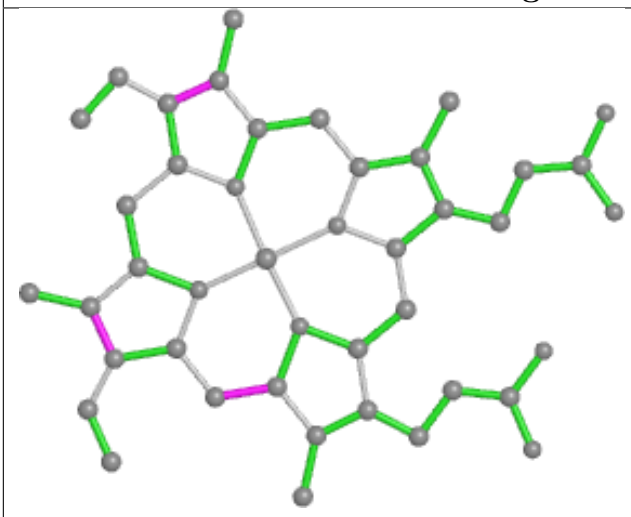
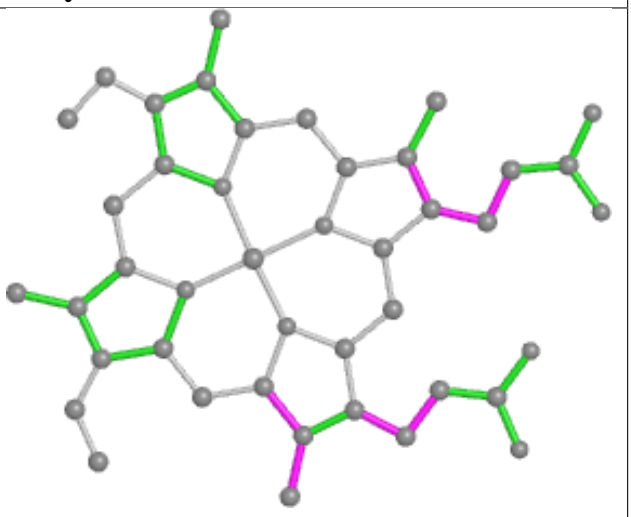


Rings

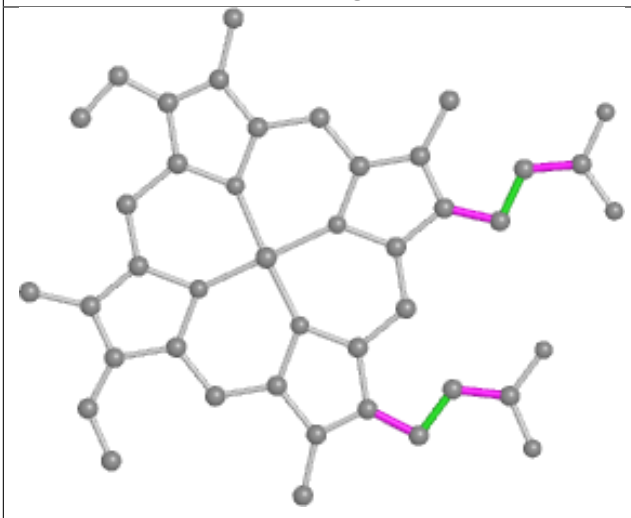
Ligand HEC Q 501



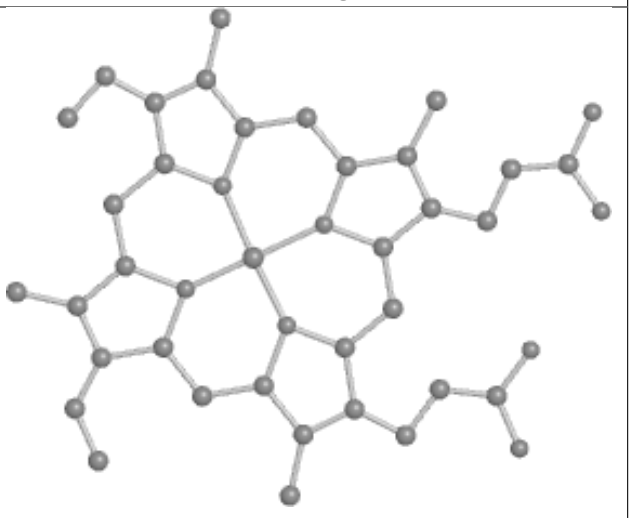
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	443/446 (99%)	-0.13	4 (0%) 84 85	40, 70, 101, 123	0
1	N	442/446 (99%)	0.06	10 (2%) 60 62	44, 76, 104, 117	0
2	B	421/441 (95%)	0.15	11 (2%) 56 57	55, 88, 120, 147	0
2	O	422/441 (95%)	0.17	22 (5%) 27 25	49, 81, 114, 133	0
3	C	379/380 (99%)	-0.20	11 (2%) 51 52	29, 47, 92, 135	0
3	P	379/380 (99%)	-0.05	13 (3%) 45 45	37, 68, 106, 127	0
4	D	241/241 (100%)	-0.24	3 (1%) 79 80	37, 49, 89, 118	0
4	Q	241/241 (100%)	0.39	11 (4%) 32 31	51, 82, 115, 128	0
5	E	196/196 (100%)	1.34	56 (28%) 0 0	41, 118, 173, 190	0
5	R	196/196 (100%)	0.71	35 (17%) 1 1	49, 99, 152, 173	0
6	F	101/110 (91%)	-0.45	0 100 100	31, 51, 71, 100	0
6	S	101/110 (91%)	0.20	6 (5%) 22 21	60, 79, 123, 146	0
7	G	80/81 (98%)	0.07	3 (3%) 40 39	37, 62, 116, 128	0
7	T	79/81 (97%)	0.75	12 (15%) 2 1	55, 91, 150, 165	0
8	H	70/77 (90%)	-0.02	3 (4%) 35 33	45, 69, 101, 145	0
8	U	67/77 (87%)	1.18	15 (22%) 0 0	96, 129, 149, 155	0
9	I	37/76 (48%)	2.36	18 (48%) 0 0	80, 124, 163, 166	0
9	V	37/76 (48%)	2.39	21 (56%) 0 0	61, 126, 162, 163	0
10	J	61/61 (100%)	-0.11	3 (4%) 29 28	46, 65, 107, 170	0
10	W	60/61 (98%)	0.24	6 (10%) 7 5	62, 81, 128, 138	0
All	All	4053/4218 (96%)	0.18	263 (6%) 18 17	29, 74, 134, 190	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	113	ASP	12.5
8	H	9	GLU	9.4
5	E	104	ALA	7.7
5	E	108	GLN	7.6
5	E	126	ARG	7.4
5	E	110	ALA	7.3
8	U	13	LEU	7.2
9	I	3	SER	7.2
9	V	54	SER	7.2
9	I	57	GLY	7.2
5	E	109	GLU	7.0
5	E	114	VAL	7.0
5	E	157	TYR	7.0
5	E	112	VAL	7.0
5	E	124	LEU	6.7
5	E	102	THR	6.7
5	E	115	SER	6.4
5	E	173	LYS	6.1
7	T	77	TYR	6.1
9	V	55	GLY	6.0
5	E	107	ASN	6.0
7	T	74	PRO	6.0
9	V	2	LEU	6.0
5	E	103	GLN	6.0
5	E	188	VAL	5.9
7	T	78	GLU	5.9
5	E	120	PRO	5.7
9	I	51	CYS	5.6
10	J	64	GLU	5.6
2	O	19	PRO	5.6
9	V	61	ASP	5.6
9	I	50	LEU	5.5
5	E	174	GLY	5.3
8	H	10	GLU	5.2
7	T	2	ILE	5.1
9	I	6	ALA	5.1
5	E	116	LYS	5.0
5	E	127	VAL	4.9
6	S	11	ARG	4.9
9	I	48	PRO	4.8
5	R	186	GLN	4.8
2	O	222	GLN	4.8
3	C	5	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	4	ASN	4.8
6	S	12	LEU	4.8
5	E	125	ASP	4.8
9	V	46	PRO	4.7
4	D	241	LYS	4.7
5	E	149	ASN	4.6
9	I	2	LEU	4.6
5	R	112	VAL	4.6
3	P	8	SER	4.6
3	C	8	SER	4.6
5	E	147	ILE	4.4
9	V	51	GLU	4.4
5	R	120	PRO	4.4
9	V	50	ARG	4.3
5	E	122	HIS	4.3
5	E	190	ASP	4.3
9	I	55	MET	4.2
10	J	62	SER	4.2
9	V	48	LEU	4.2
8	U	12	GLU	4.1
3	C	7	LYS	4.1
9	I	63	ASP	4.1
9	I	56	SER	4.1
10	J	63	GLU	4.1
5	R	111	GLU	4.1
5	R	114	VAL	4.1
9	I	53	GLU	4.1
5	E	117	LEU	4.0
2	B	350	GLY	4.0
7	T	75	ALA	3.9
9	V	3	SER	3.9
5	R	171	ILE	3.9
3	P	156	TYR	3.8
2	O	18	CYS	3.8
4	Q	241	LYS	3.8
8	U	49	HIS	3.7
5	E	86	ASN	3.7
7	G	81	GLN	3.7
9	I	52	ARG	3.7
3	C	6	ARG	3.7
5	E	169	GLY	3.7
9	V	53	MET	3.6

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Mol	Chain	Res	Type	RSRZ
5	R	102	THR	3.6
3	C	156	TYR	3.6
7	T	73	ASN	3.6
3	P	2	ALA	3.6
7	G	2	ILE	3.6
5	R	157	TYR	3.6
3	C	2	ALA	3.6
2	B	226	ILE	3.6
9	V	8	SER	3.5
3	P	5	ILE	3.5
8	U	50	THR	3.5
5	E	165	TYR	3.5
5	R	122	HIS	3.5
5	R	167	ALA	3.5
5	R	188	VAL	3.5
1	N	29	GLU	3.4
7	T	80	ASP	3.4
5	E	172	ARG	3.4
5	R	196	GLY	3.4
9	V	59	ARG	3.4
9	V	52	SER	3.4
6	S	13	MET	3.4
5	E	159	PRO	3.4
5	E	121	GLN	3.4
5	R	124	LEU	3.4
2	O	323	GLY	3.3
5	R	118	ARG	3.3
5	R	104	ALA	3.3
9	I	76	VAL	3.3
1	A	219	VAL	3.3
3	P	4	ASN	3.3
7	T	38	TRP	3.2
7	T	30	PHE	3.2
5	E	146	PRO	3.2
2	O	310	SER	3.2
5	R	173	LYS	3.1
9	I	54	SER	3.1
2	O	23	ASP	3.1
5	R	164	HIS	3.1
5	R	125	ASP	3.1
2	B	227	ARG	3.1
5	R	168	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	N	56	GLY	3.1
5	E	150	SER	3.1
5	R	113	ASP	3.1
1	A	218	GLY	3.1
3	P	7	LYS	3.1
5	E	162	GLY	3.0
5	R	172	ARG	3.0
2	O	223	PHE	3.0
5	E	79	SER	3.0
10	W	45	HIS	3.0
10	W	62	SER	3.0
3	P	6	ARG	3.0
8	U	44	VAL	2.9
2	O	350	GLY	2.9
3	C	155	PRO	2.9
1	N	179	ARG	2.9
9	I	8	SER	2.9
2	O	280	GLY	2.9
1	N	227	ALA	2.9
6	S	10	GLY	2.9
5	R	178	TYR	2.9
8	U	35	GLU	2.9
5	E	148	ALA	2.8
4	Q	77	ASN	2.8
9	V	5	ALA	2.8
9	I	7	ARG	2.8
9	V	49	CYS	2.8
5	R	121	GLN	2.8
5	E	167	ALA	2.8
5	R	85	LYS	2.8
8	U	78	LYS	2.7
10	W	63	GLU	2.7
5	R	103	GLN	2.7
6	S	110	LYS	2.7
2	B	323	GLY	2.7
1	N	217	SER	2.7
5	E	78	LEU	2.7
2	B	232	THR	2.7
9	V	4	VAL	2.7
9	V	47	LEU	2.6
2	O	279	LEU	2.6
2	O	304	THR	2.6

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Mol	Chain	Res	Type	RSRZ
8	U	54	CYS	2.6
5	E	175	PRO	2.6
4	Q	143	VAL	2.6
7	T	66	PHE	2.6
5	E	163	SER	2.6
5	E	83	GLU	2.6
5	R	165	TYR	2.6
8	U	26	GLN	2.6
5	R	176	ALA	2.5
5	R	116	LYS	2.5
5	R	11	SER	2.5
10	W	60	GLU	2.5
7	T	32	ASP	2.5
4	Q	139	ALA	2.5
5	R	155	GLY	2.5
10	W	61	ALA	2.5
5	E	98	VAL	2.5
4	Q	82	MET	2.5
9	V	6	ALA	2.5
4	Q	187	CYS	2.4
3	P	3	PRO	2.4
5	E	85	LYS	2.4
5	E	168	SER	2.4
8	U	31	VAL	2.4
4	Q	25	SER	2.4
6	S	15	ARG	2.4
2	B	348	ALA	2.4
9	V	74	VAL	2.4
7	T	46	PHE	2.3
5	R	117	LEU	2.3
5	R	115	SER	2.3
9	I	77	ARG	2.3
1	A	221	PHE	2.3
9	V	56	ARG	2.3
5	E	171	ILE	2.3
4	Q	79	GLU	2.3
5	E	180	LEU	2.3
5	E	152	ASP	2.3
2	B	208	GLY	2.3
4	Q	146	GLY	2.3
3	C	9	HIS	2.3
8	H	71	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	158	CYS	2.3
2	B	310	SER	2.2
1	N	432	LEU	2.2
3	P	157	ILE	2.2
8	U	14	VAL	2.2
3	P	250	LEU	2.2
8	U	39	LEU	2.2
4	D	145	GLU	2.2
8	U	32	LYS	2.2
9	I	4	VAL	2.2
5	E	183	PRO	2.2
4	Q	145	GLU	2.2
5	E	84	GLY	2.2
5	R	154	GLY	2.2
5	R	174	GLY	2.2
2	O	106	THR	2.2
2	O	303	THR	2.2
2	B	41	PHE	2.2
3	C	157	ILE	2.2
5	E	106	ILE	2.2
3	P	346	HIS	2.2
1	N	5	ALA	2.2
1	N	38	GLY	2.2
3	C	131	GLY	2.2
5	R	190	ASP	2.2
8	U	33	ALA	2.2
5	E	97	PHE	2.2
5	E	187	PHE	2.2
3	P	345	GLU	2.1
2	O	277	HIS	2.1
2	O	400	GLN	2.1
2	O	47	ILE	2.1
4	D	80	LEU	2.1
9	V	75	ARG	2.1
4	Q	165	TYR	2.1
2	O	108	CYS	2.1
2	B	69	LEU	2.1
7	G	79	ASN	2.1
1	A	217	SER	2.1
2	O	386	ALA	2.1
2	O	324	PHE	2.1
5	E	123	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
10	W	57	HIS	2.1
2	O	313	ASN	2.0
1	N	218	GLY	2.0
8	U	48	SER	2.0
1	N	197	LEU	2.0
2	O	226	ILE	2.0
3	P	155	PRO	2.0
2	B	235	ALA	2.0
2	O	312	PHE	2.0
5	E	189	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	FME	C	1	9/11	0.64	0.62	139,141,148,153	0
9	AME	I	1	9/12	0.75	0.39	150,155,160,160	0
9	AME	V	1	9/12	0.78	0.31	136,148,153,154	0

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
19	BOG	D	503	13/20	0.49	0.58	140,156,162,164	0
19	BOG	Q	504	13/20	0.53	0.50	179,186,190,192	0
15	CDL	Q	502	42/100	0.56	0.46	79,169,202,203	0
19	BOG	P	503	12/20	0.58	0.39	126,144,149,158	0
15	CDL	C	505	42/100	0.70	0.35	65,134,159,163	0

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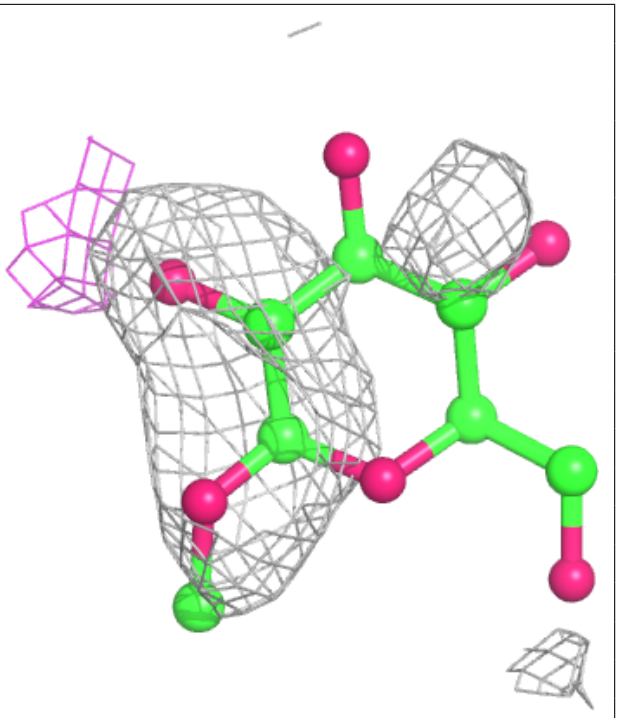
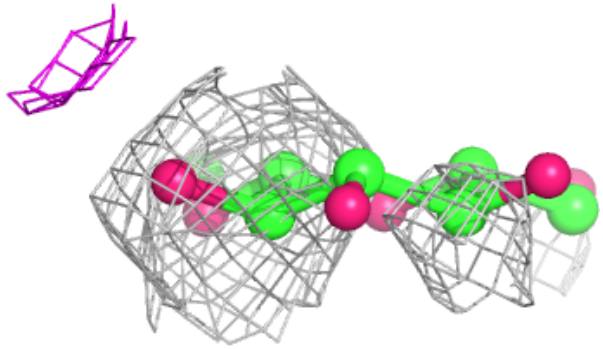
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	PEE	C	507	21/51	0.73	0.31	64,135,154,156	0
14	UQ	P	505	19/63	0.76	0.41	80,127,140,146	0
16	PEE	R	502	49/51	0.77	0.31	51,98,121,125	0
14	UQ	C	504	19/63	0.82	0.32	73,96,104,108	0
16	PEE	E	502	50/51	0.82	0.33	59,86,114,117	0
15	CDL	P	506	40/100	0.83	0.27	110,125,138,141	0
16	PEE	N	502	5/51	0.84	0.20	132,134,139,140	0
16	PEE	P	507	49/51	0.87	0.31	72,91,119,123	0
17	GOL	C	508	6/6	0.90	0.26	64,72,75,76	0
11	UNL	A	501	1/-	0.90	0.47	48,48,48,48	0
19	BOG	Q	503	20/20	0.91	0.27	72,100,105,113	0
16	PEE	C	506	49/51	0.92	0.23	33,60,91,103	0
17	GOL	P	508	6/6	0.92	0.26	67,76,82,84	0
15	CDL	G	101	40/100	0.92	0.21	46,83,125,131	0
11	UNL	N	501	1/-	0.95	0.66	47,47,47,47	0
19	BOG	D	502	20/20	0.95	0.14	44,64,72,76	0
13	WF3	P	504	31/31	0.96	0.18	51,64,73,78	0
20	FES	E	501	4/4	0.96	0.08	125,129,129,130	0
13	WF3	C	503	31/31	0.97	0.17	30,40,53,60	0
18	HEC	Q	501	43/43	0.97	0.15	48,60,77,85	0
12	HEM	P	502	43/43	0.98	0.17	36,50,69,74	0
12	HEM	C	501	43/43	0.98	0.21	23,41,51,66	0
12	HEM	C	502	43/43	0.98	0.21	21,39,48,59	0
12	HEM	P	501	43/43	0.98	0.22	39,58,68,81	0
18	HEC	D	501	43/43	0.99	0.12	7,31,49,55	0
20	FES	R	501	4/4	0.99	0.08	78,88,91,94	0

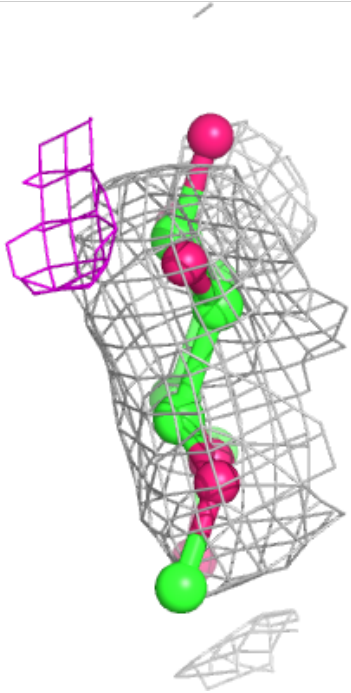
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG D 503:

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

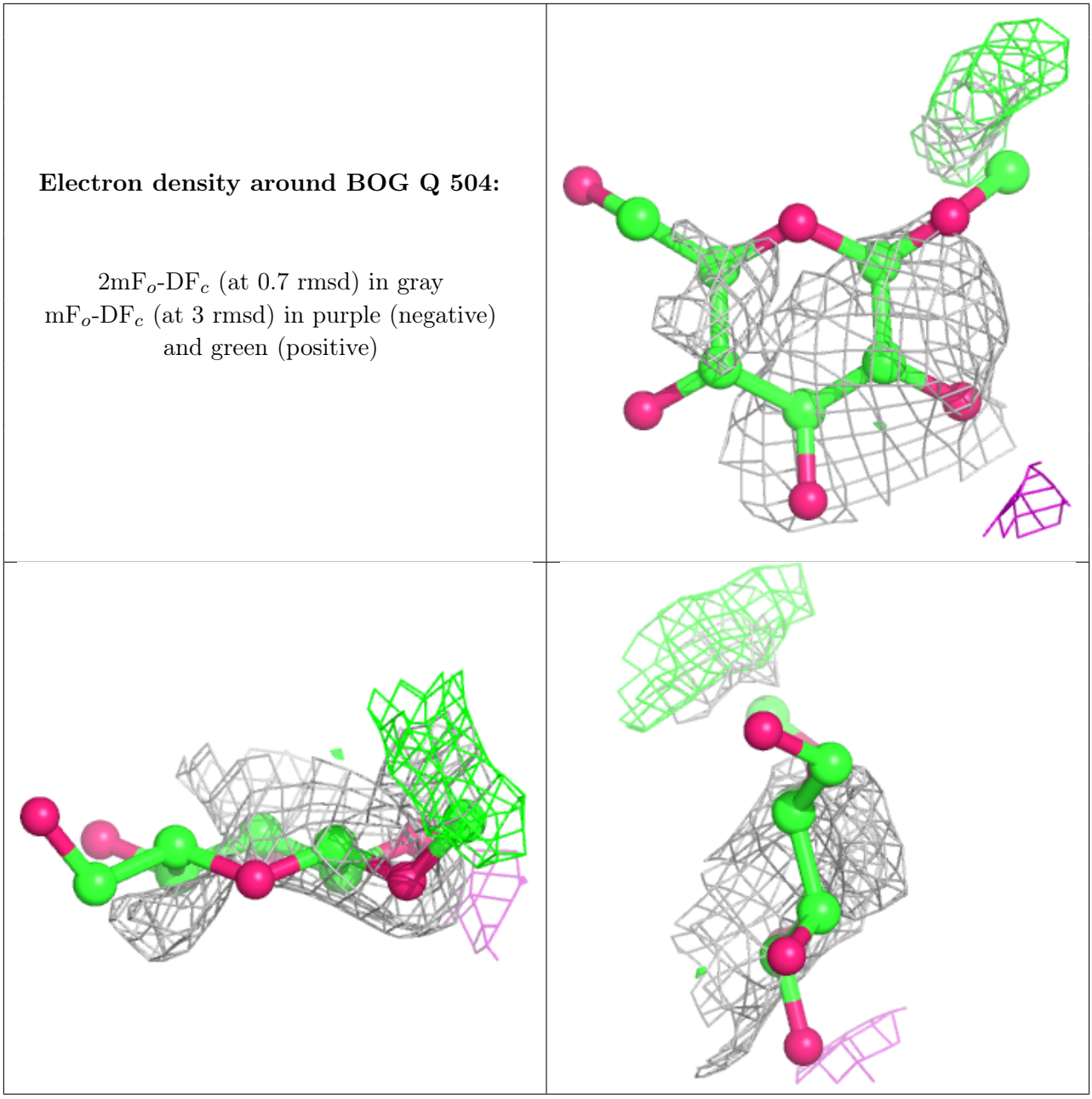






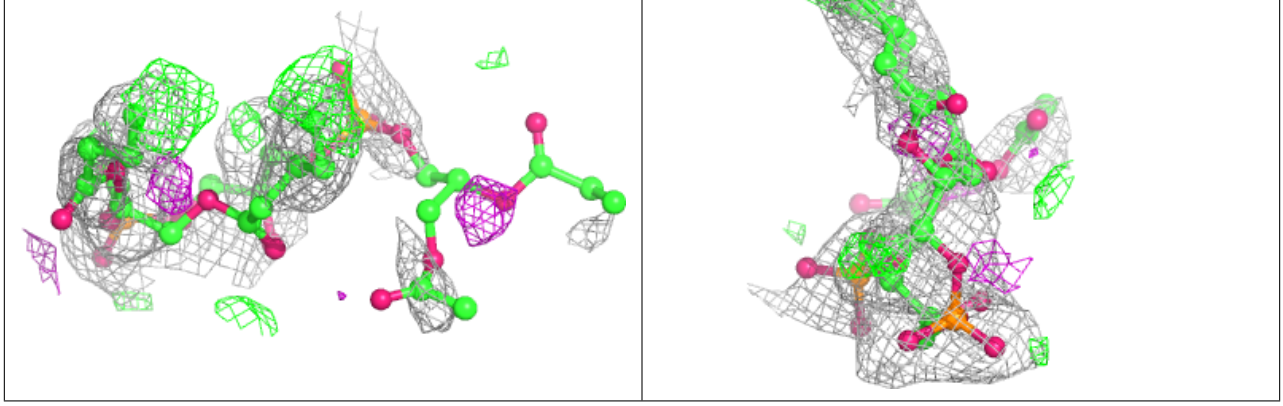
Electron density around BOG Q 504:

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



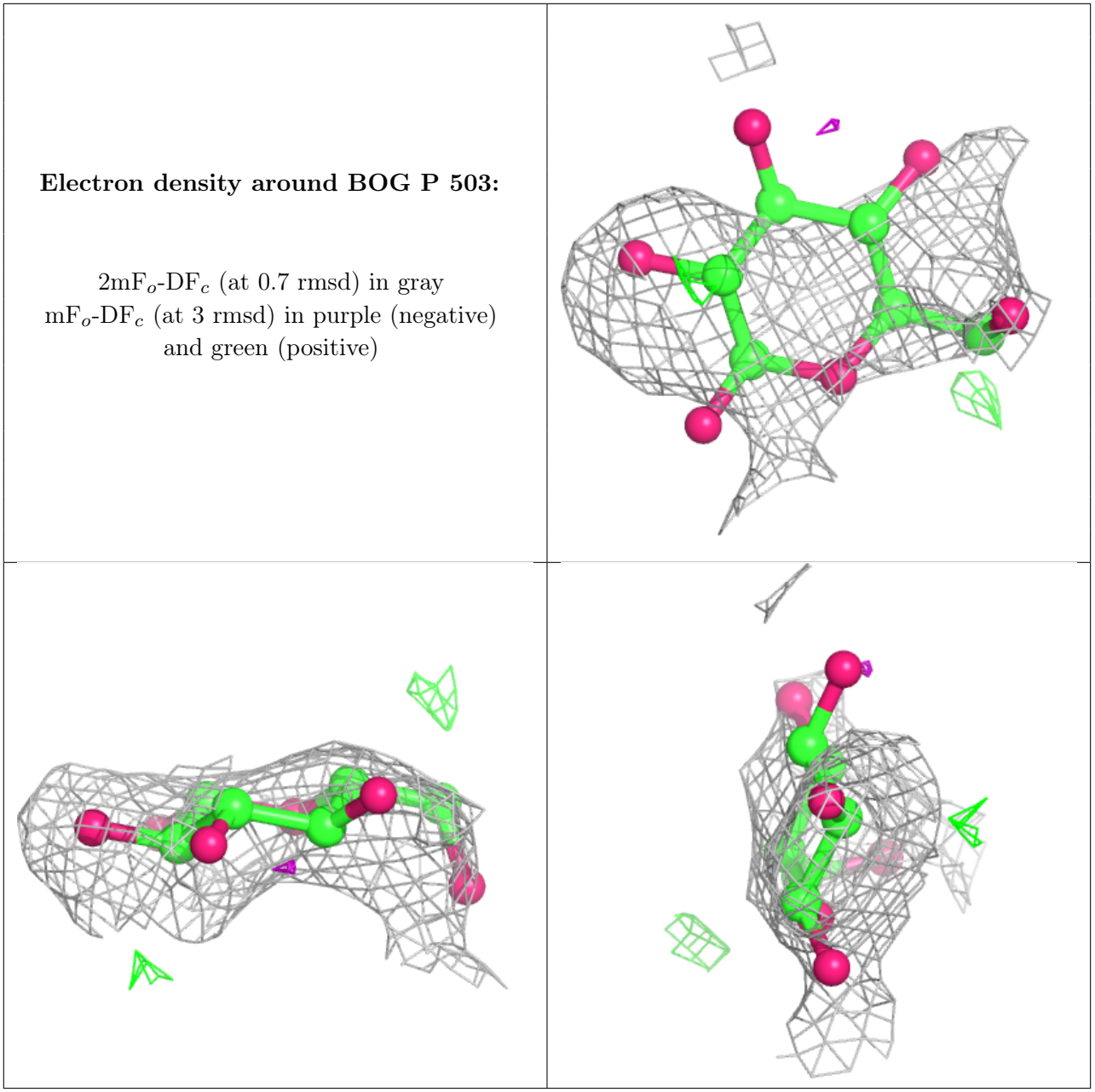
Electron density around CDL Q 502:

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



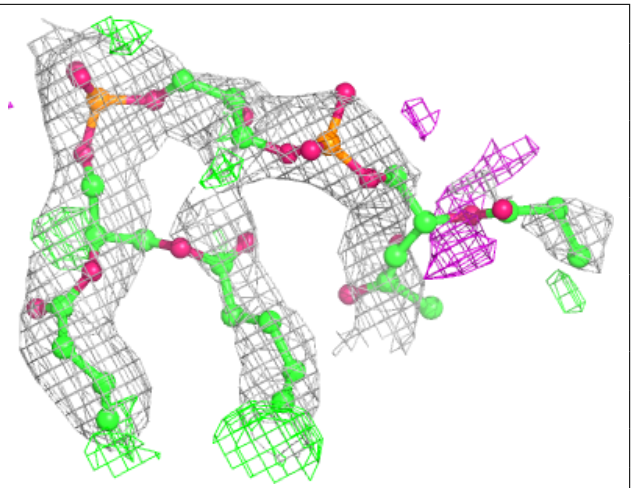
Electron density around BOG P 503:

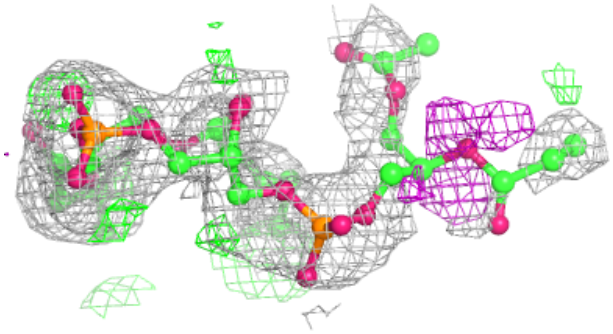
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

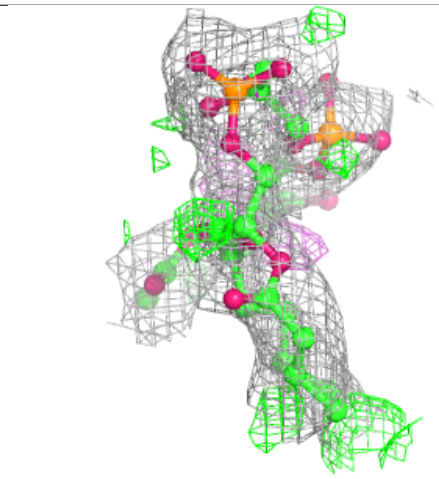


Electron density around CDL C 505:

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

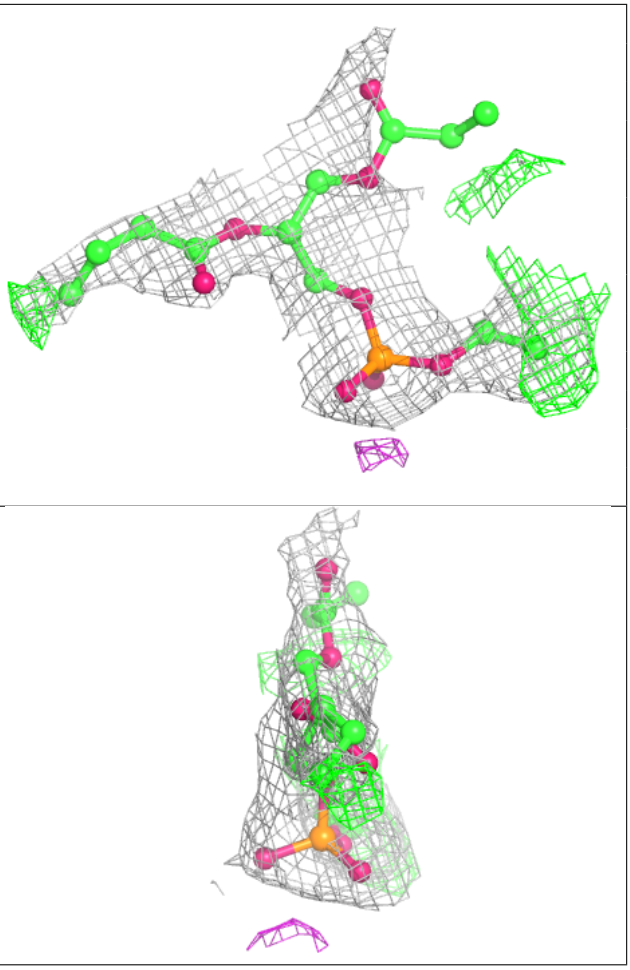






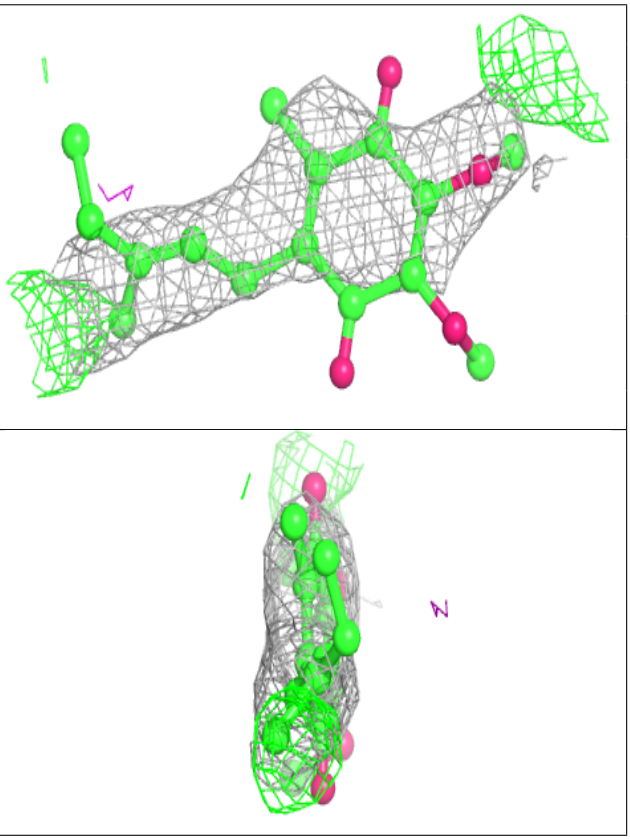
Electron density around PEE C 507:

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



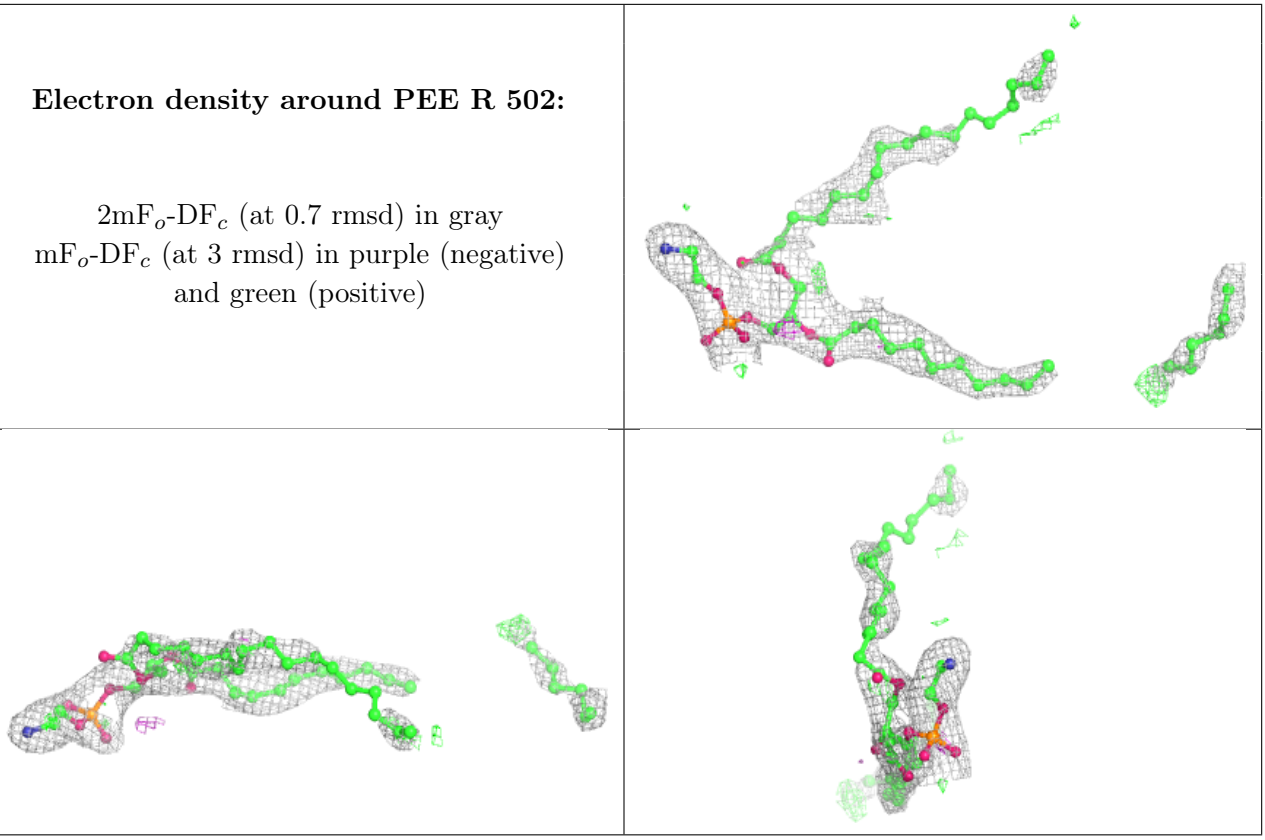
Electron density around UQ P 505:

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



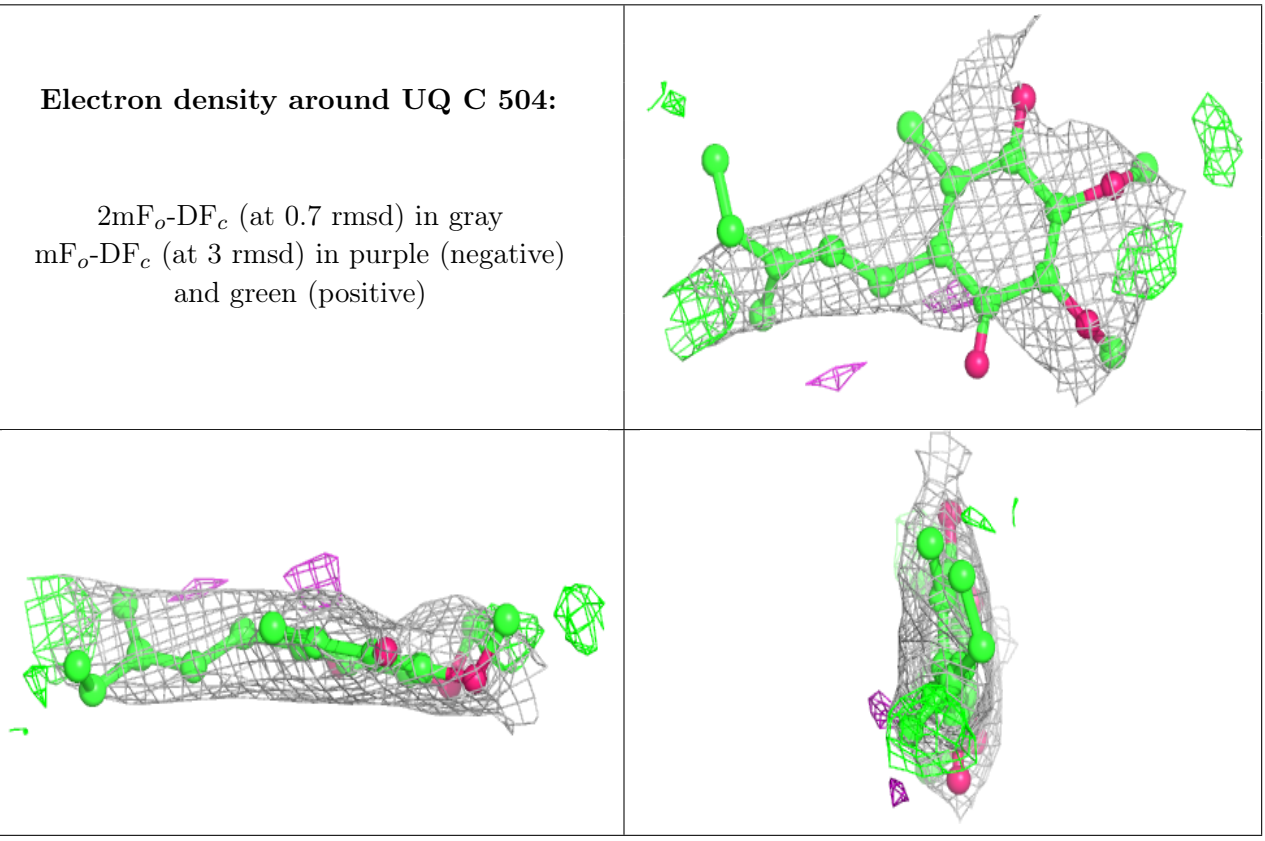
Electron density around PEE R 502:

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



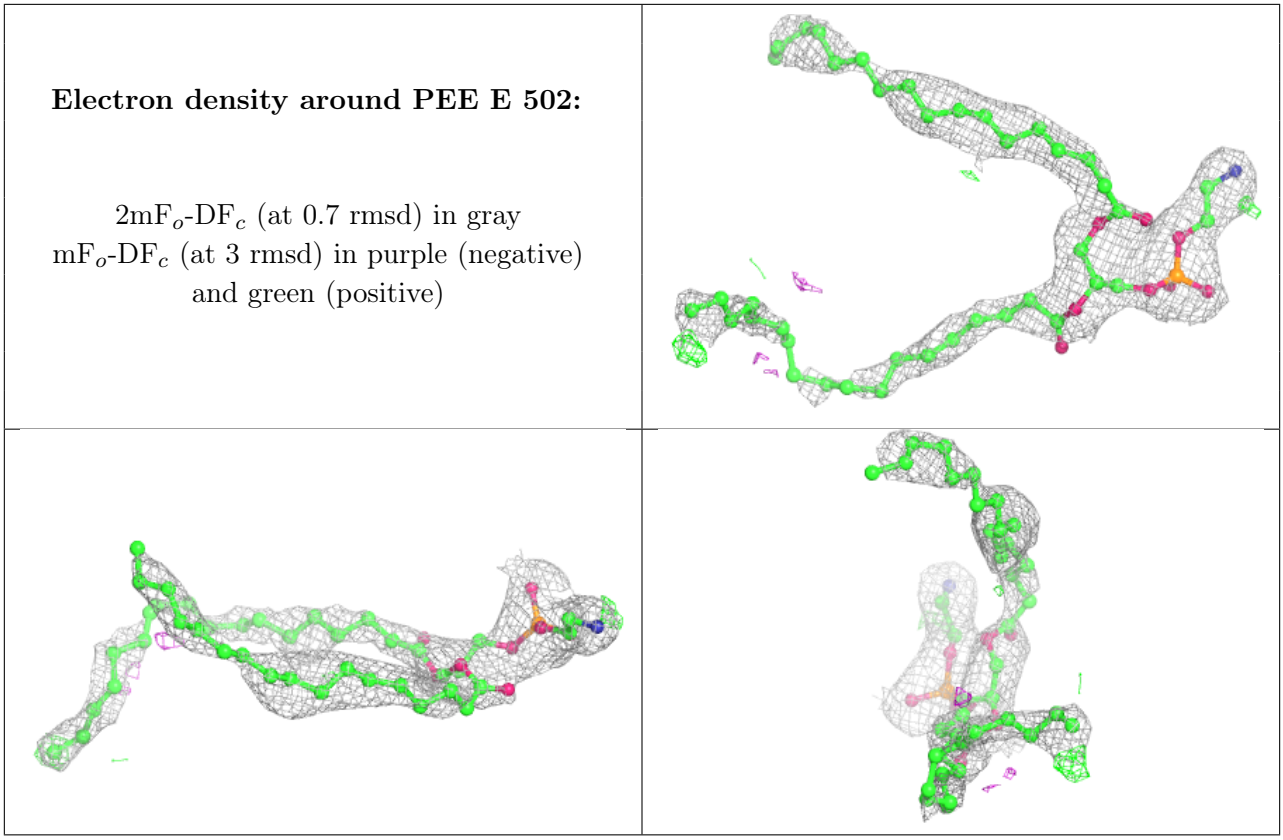
Electron density around UQ C 504:

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



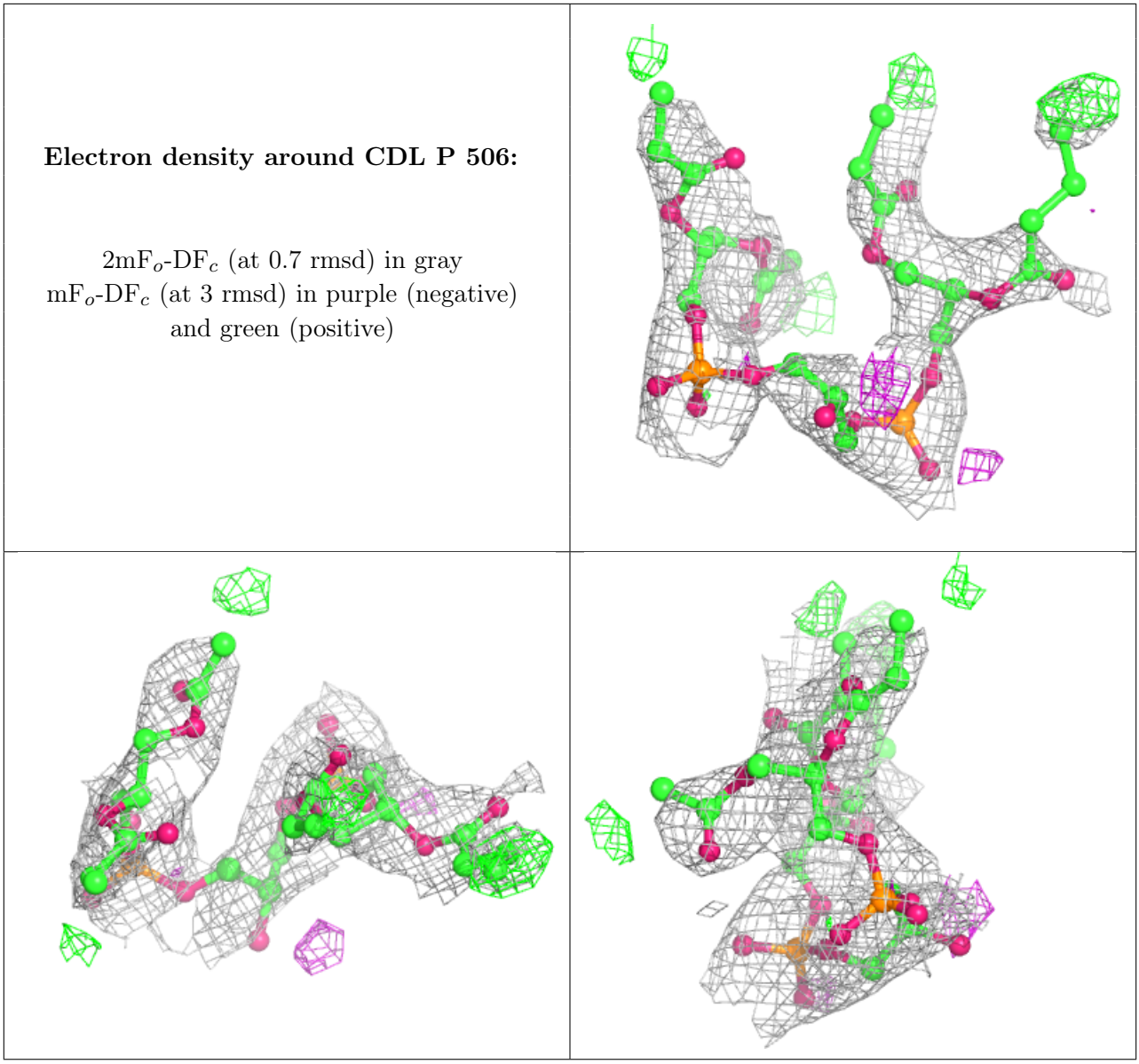
Electron density around PEE E 502:

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



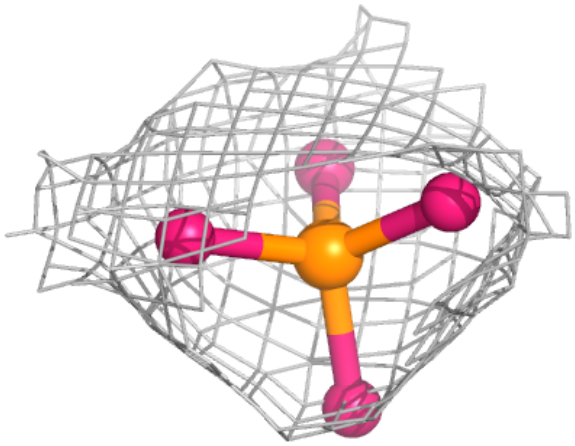
Electron density around CDL P 506:

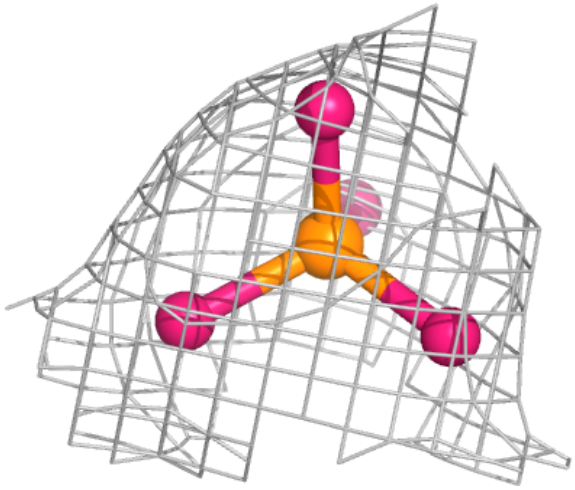
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

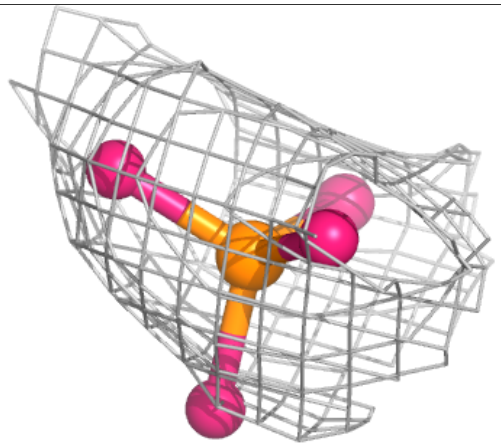


Electron density around PEE N 502:

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

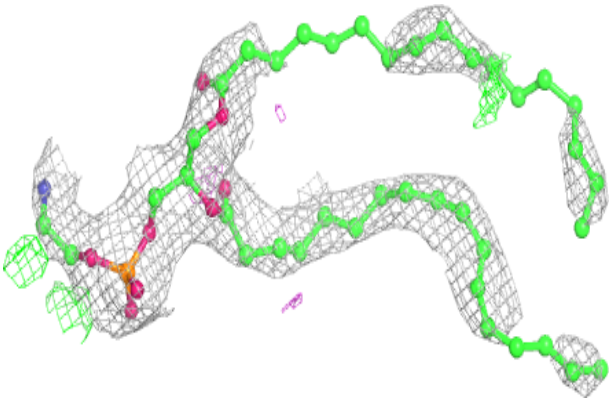


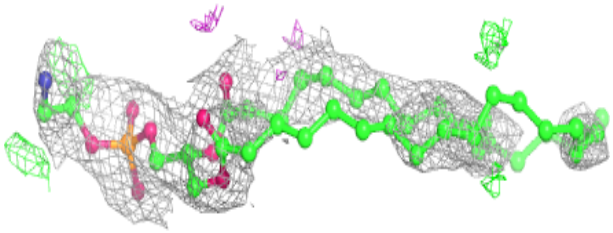


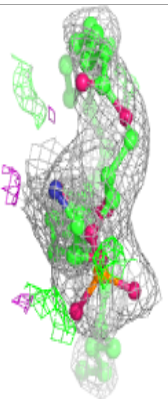


Electron density around PEE P 507:

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

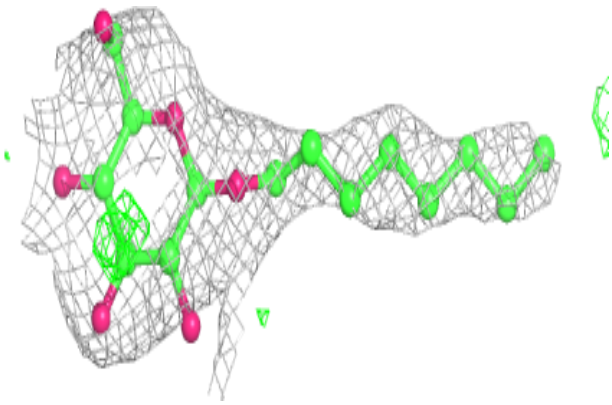


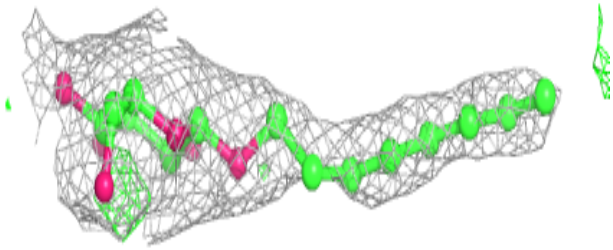


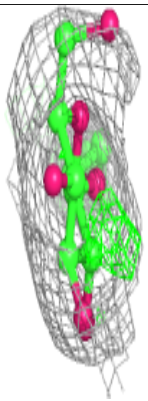


Electron density around BOG Q 503:

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

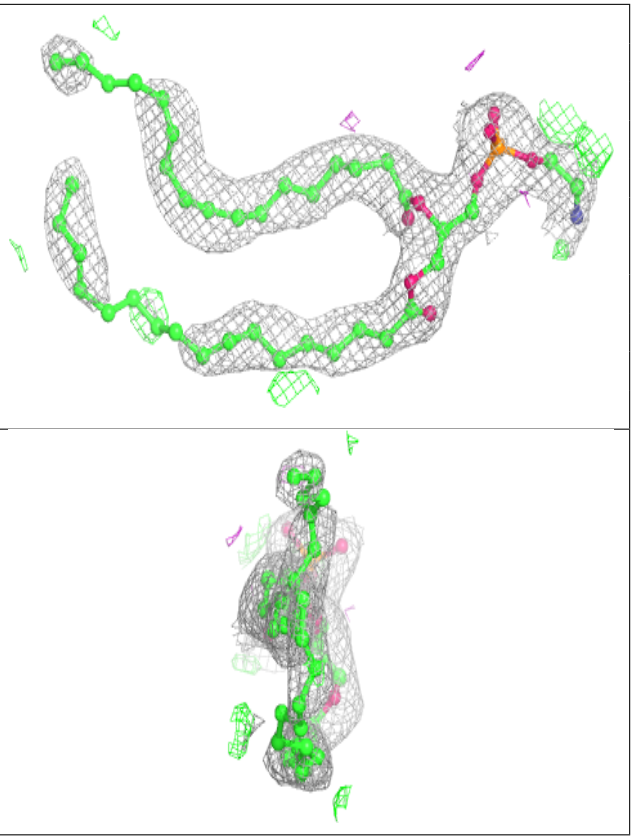






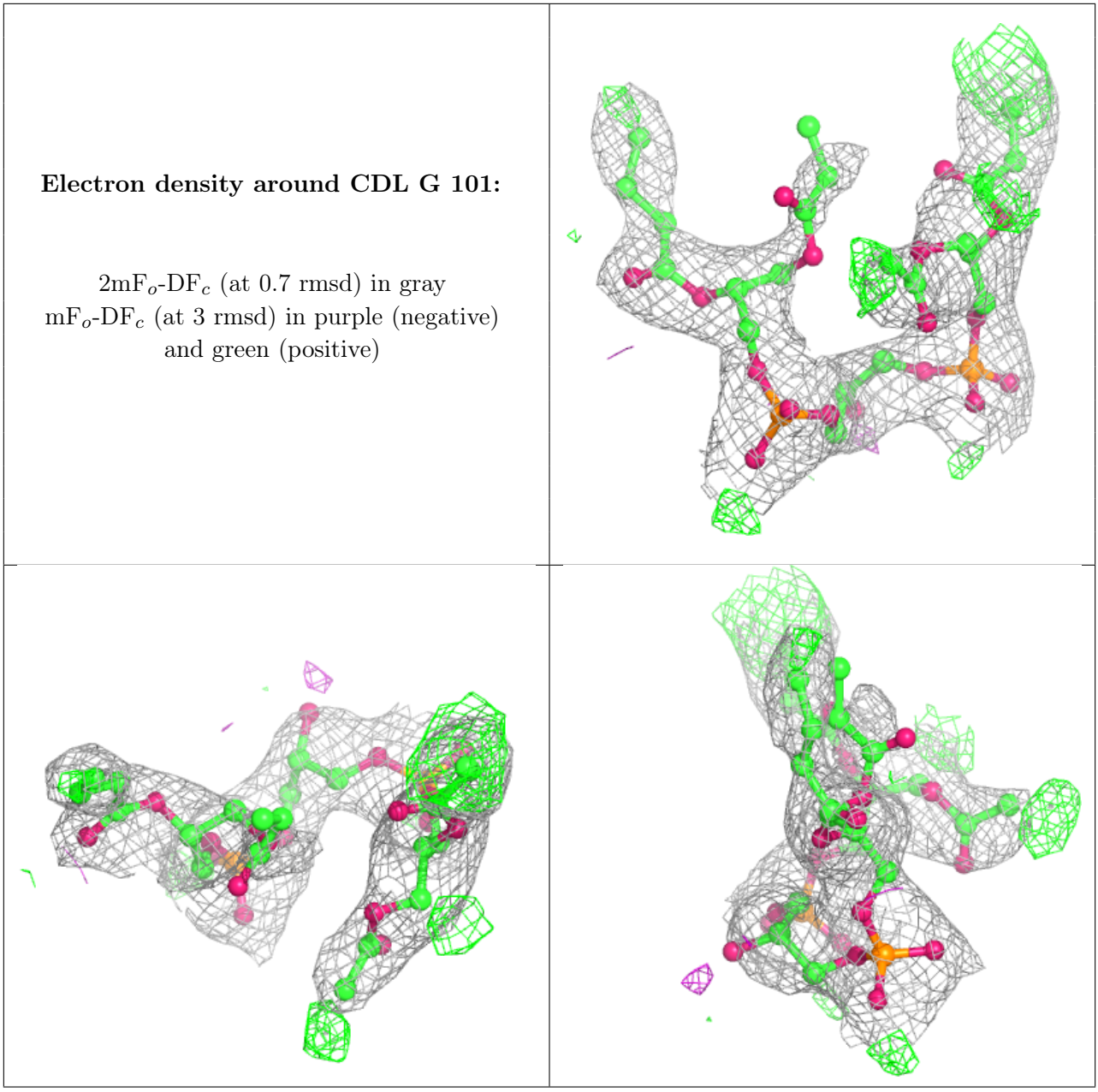
Electron density around PEE C 506:

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



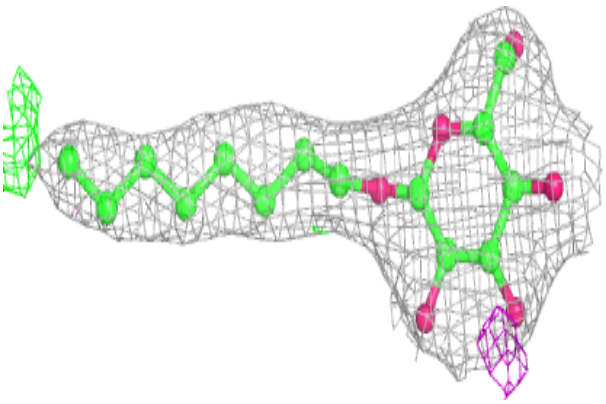
Electron density around CDL G 101:

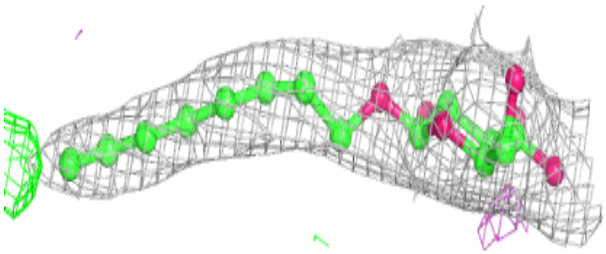
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

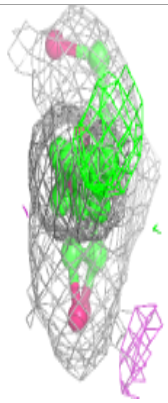


Electron density around BOG D 502:

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

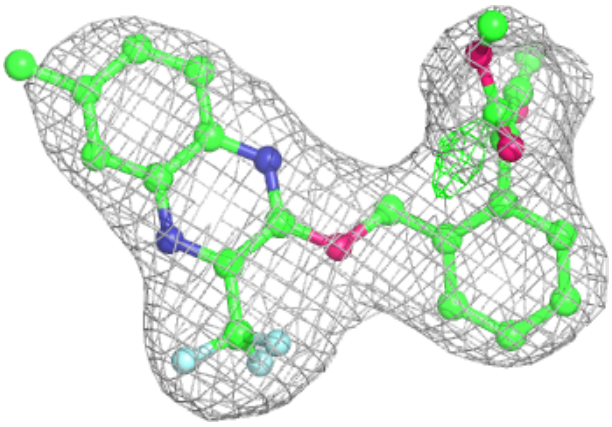


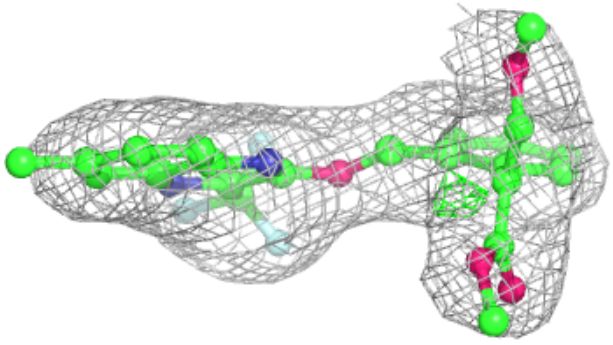


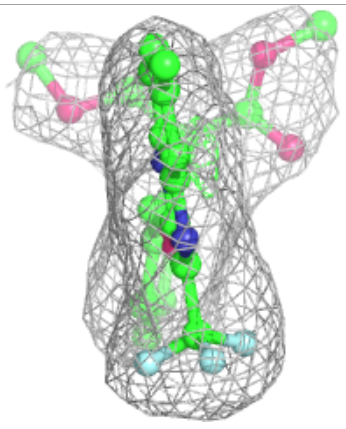


Electron density around WF3 P 504:

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

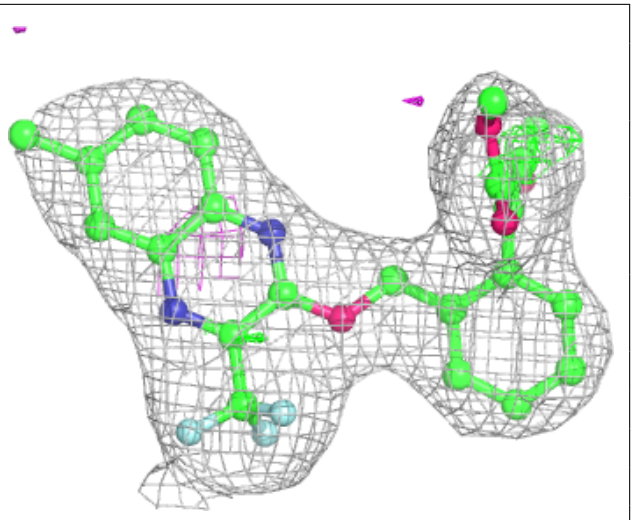


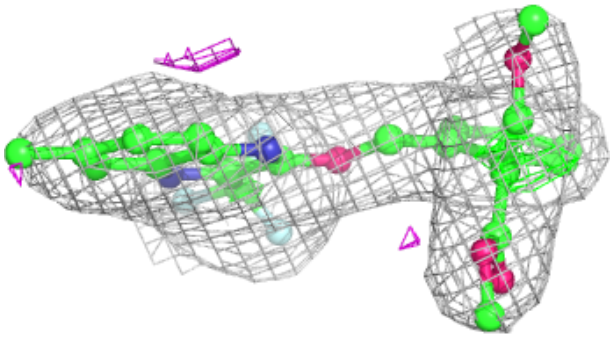


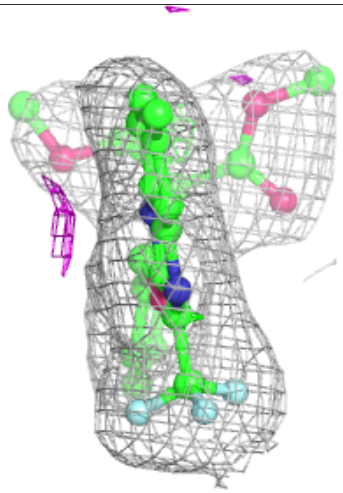


Electron density around WF3 C 503:

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

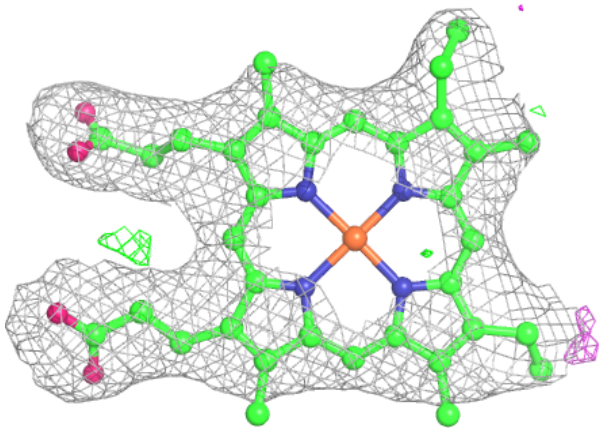


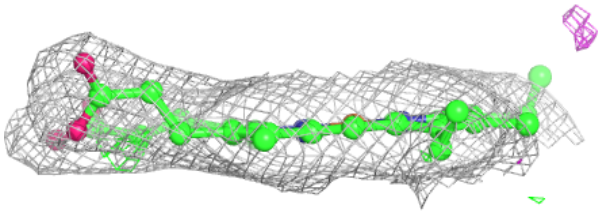


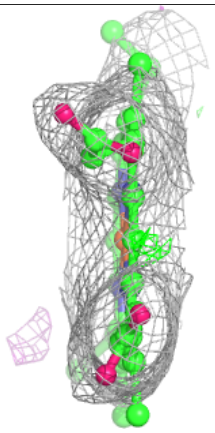


Electron density around HEC Q 501:

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

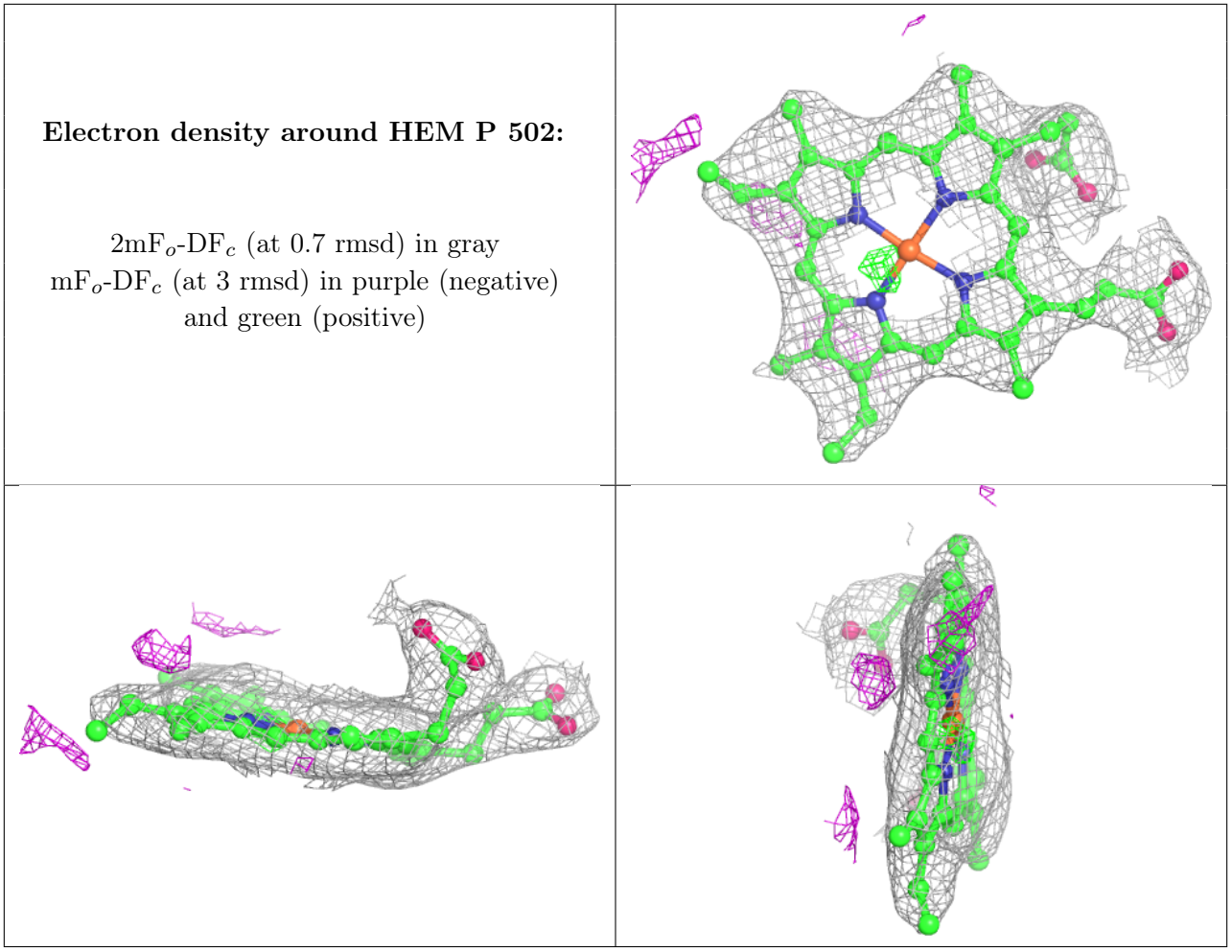






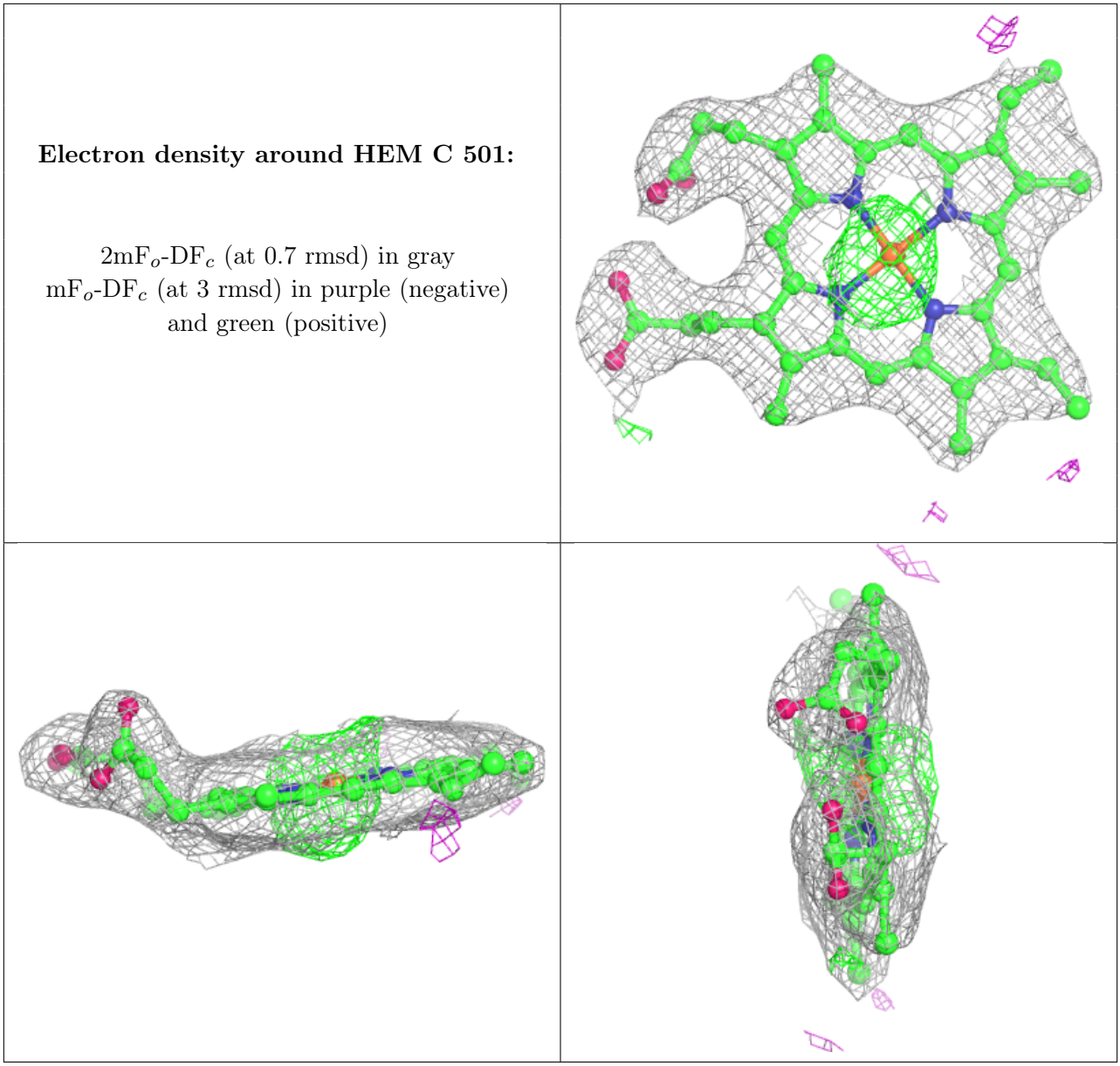
Electron density around HEM P 502:

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



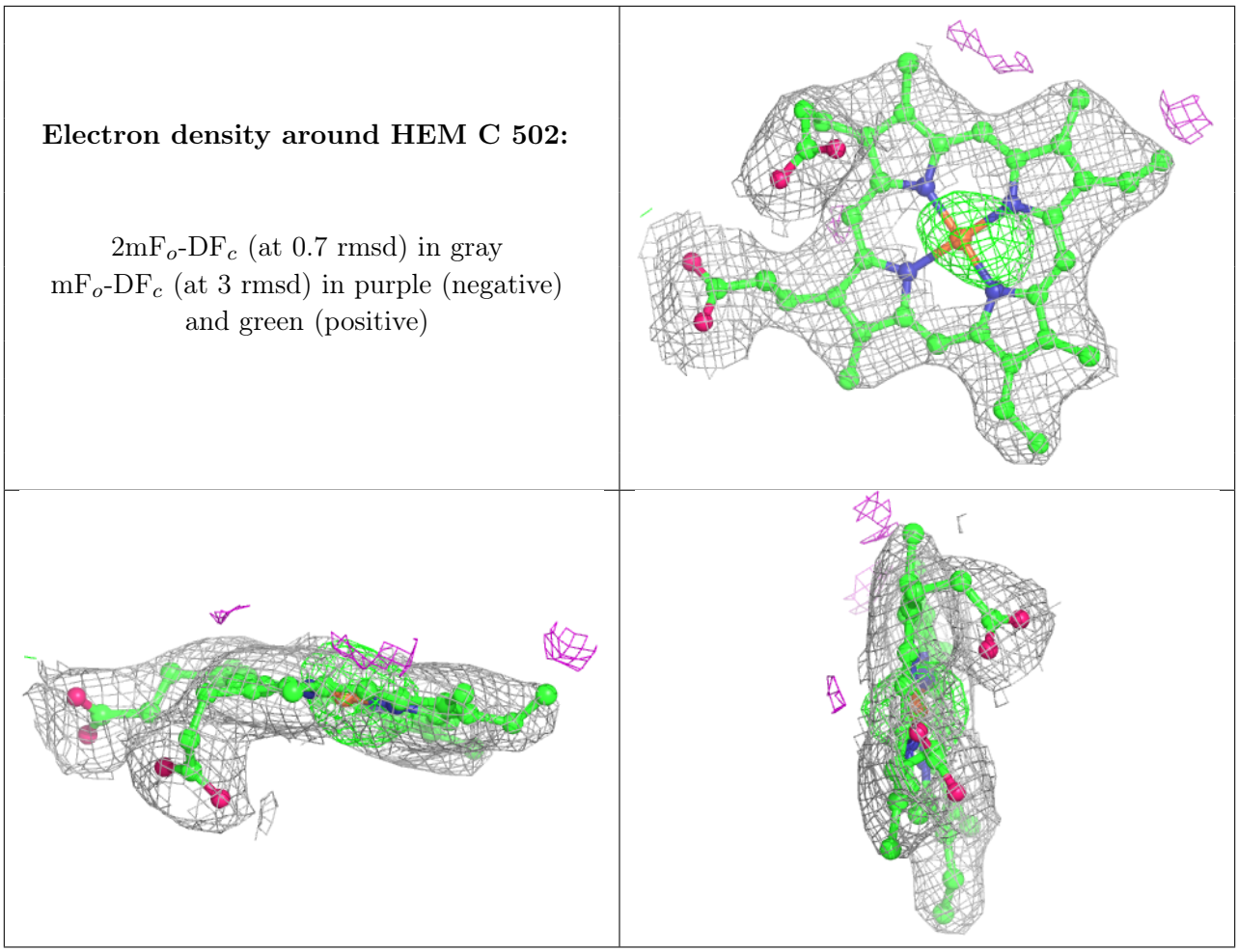
Electron density around HEM C 501:

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



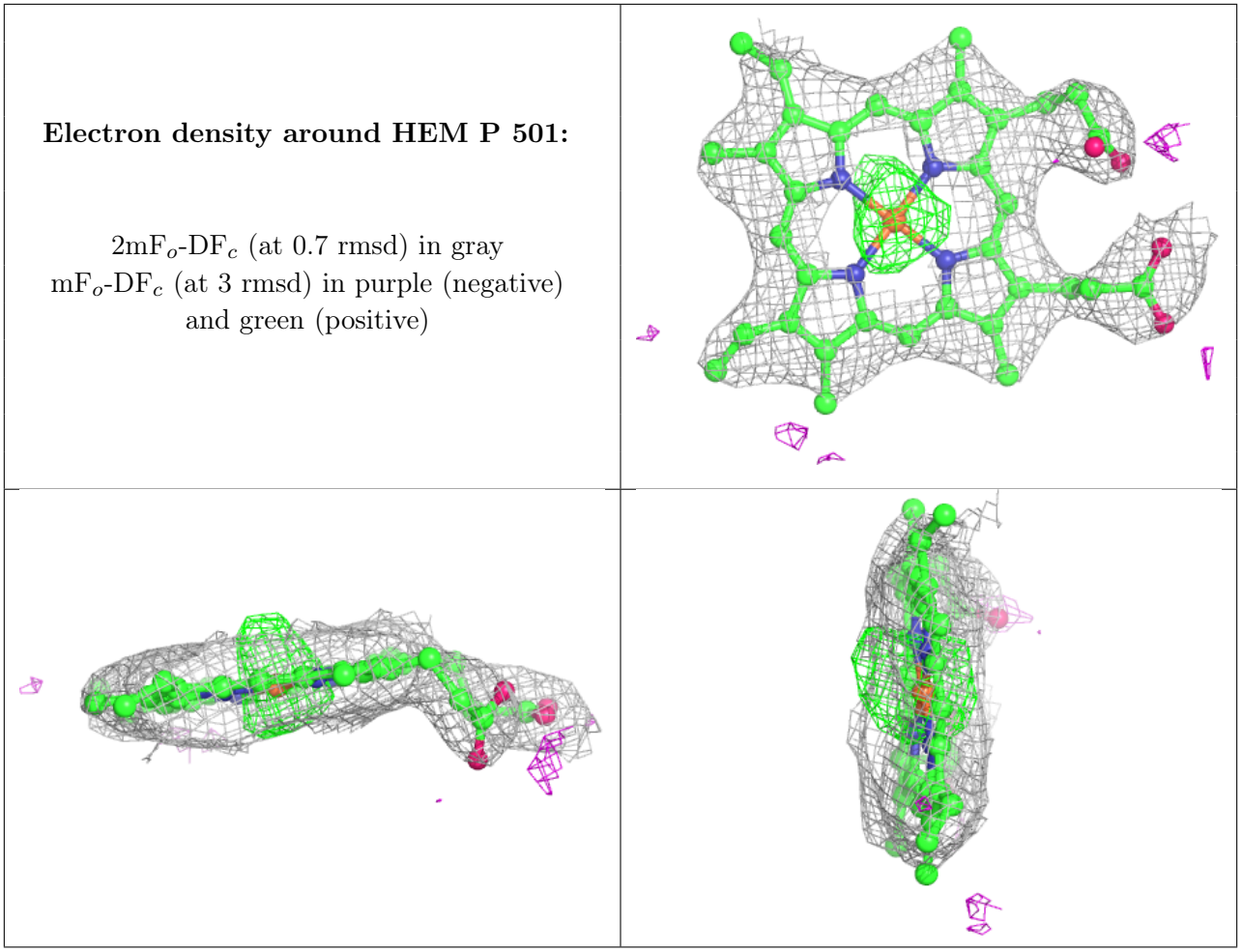
Electron density around HEM C 502:

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



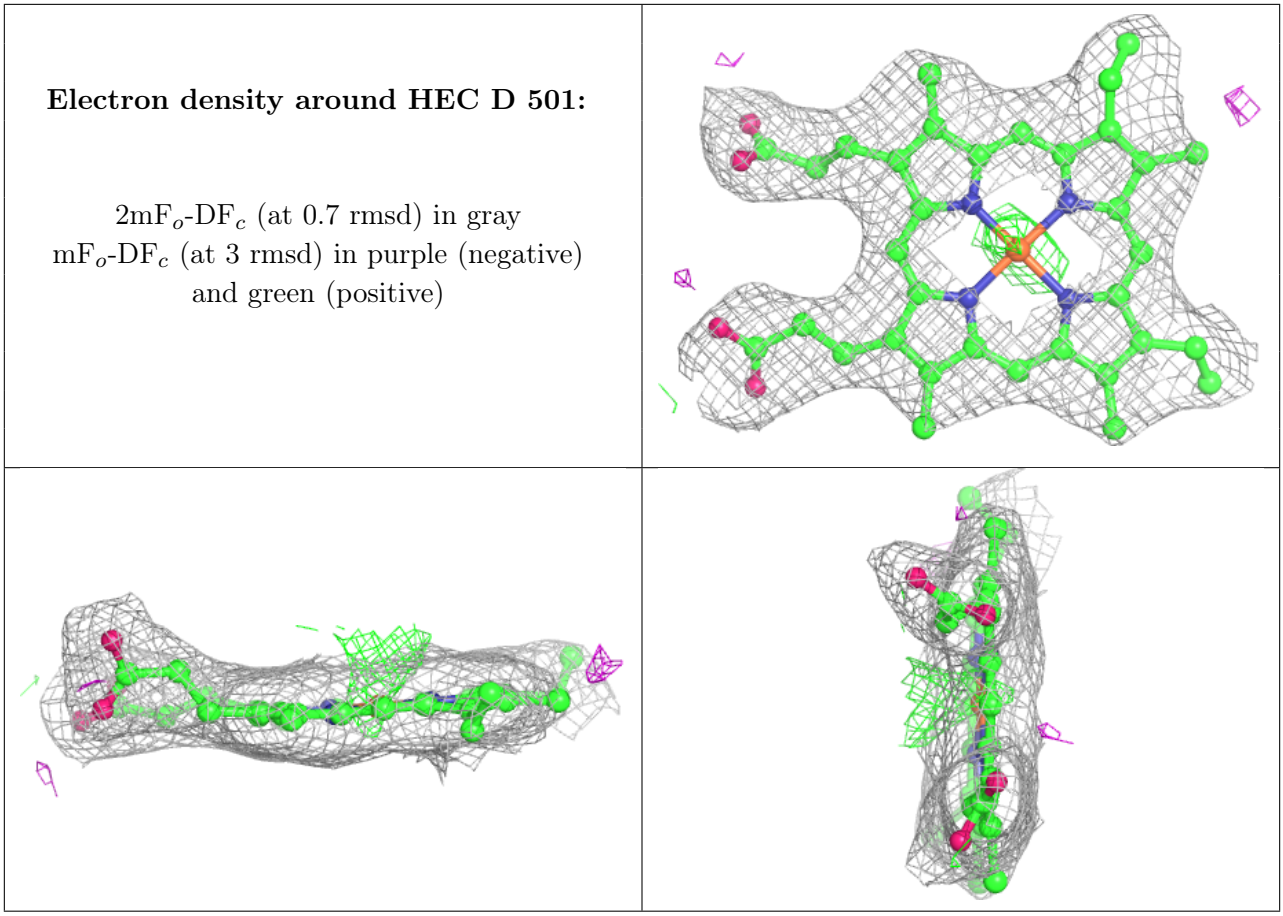
Electron density around HEM P 501:

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



Electron density around HEC D 501:

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



6.5 Other polymers

There are no such residues in this entry.