



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:20 AM BST

PDB ID : 2A06
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2005-06-16
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

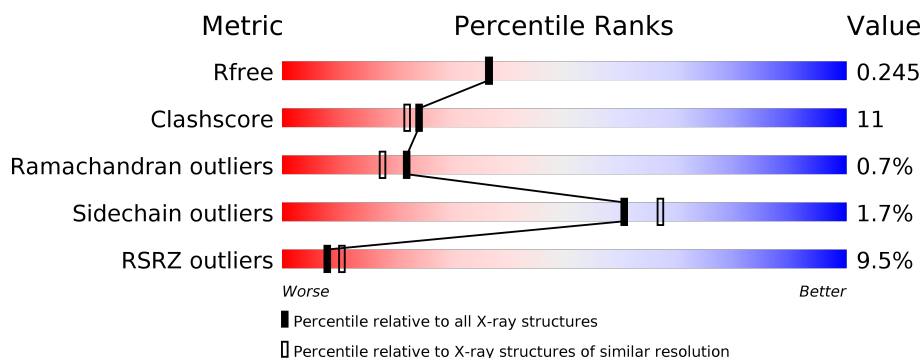
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$. 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	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	N	446	<div> <div>7%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
2	B	439	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
2	O	439	<div> <div>9%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
3	C	379	<div> <div>5%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
3	P	379	<div> <div>6%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
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	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	JZR	C	2011	-	-	-	X
11	JZR	F	3012	-	-	-	X
11	JZR	F	4003	-	-	-	X
11	JZR	P	3011	-	-	-	X
11	JZR	S	2012	-	-	-	X
12	PO4	A	2010	-	X	-	-
12	PO4	B	3009	-	X	-	-
12	PO4	D	4010	-	X	-	-
12	PO4	D	4011	-	X	-	-
12	PO4	I	4015	-	X	-	-
12	PO4	O	2009	-	X	-	-
12	PO4	P	3010	-	X	-	-
12	PO4	Q	4012	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	PO4	R	4013	-	X	-	-
12	PO4	R	4014	-	X	-	X
12	PO4	T	4016	-	X	-	-
13	AZI	A	4002	-	-	-	X
14	UNL	A	4035	-	-	-	X
14	UNL	A	4038	-	-	-	X
14	UNL	A	4076	-	-	-	X
14	UNL	A	4081	-	-	-	X
14	UNL	A	4091	-	-	-	X
14	UNL	B	4025	-	-	-	X
14	UNL	B	4026	-	-	-	X
14	UNL	B	4034	-	-	-	X
14	UNL	B	4057	-	-	-	X
14	UNL	B	4080	-	-	-	X
14	UNL	C	4045	-	-	-	X
14	UNL	C	4068	-	-	-	X
14	UNL	D	4059	-	-	-	X
14	UNL	D	4083	-	-	-	X
14	UNL	I	4072	-	-	-	X
14	UNL	N	4022	-	-	-	X
14	UNL	N	4029	-	-	-	X
14	UNL	O	4037	-	-	-	X
14	UNL	O	4043	-	-	X	-
14	UNL	O	4071	-	-	-	X
14	UNL	Q	4044	-	-	-	X
14	UNL	U	4049	-	-	-	X
14	UNL	U	4056	-	-	-	X
14	UNL	V	4024	-	-	-	X
14	UNL	V	4088	-	-	-	X
15	PEE	B	4017	-	-	-	X
20	GOL	E	4007	-	-	-	X
20	GOL	O	4005	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 33890 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			
1	N	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			

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

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

- Molecule 3 is a protein called Cytochrome b, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2897	1945	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2936	1973	455	490	18			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	R	196	Total	C	N	O	S	0	0	0
			1517	955	263	291	8			

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

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

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

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

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

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

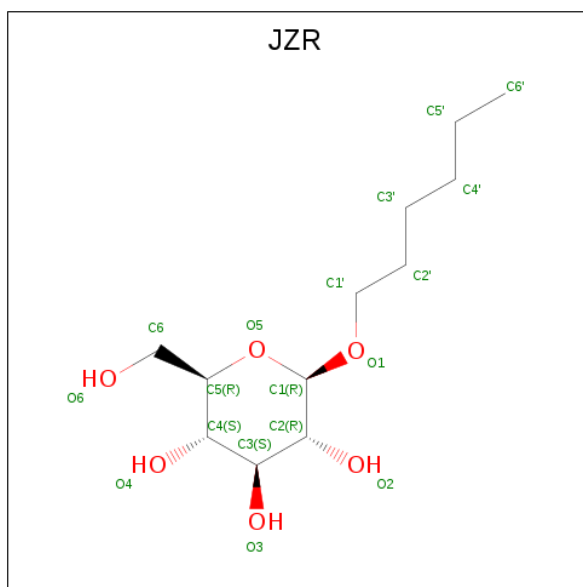
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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

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

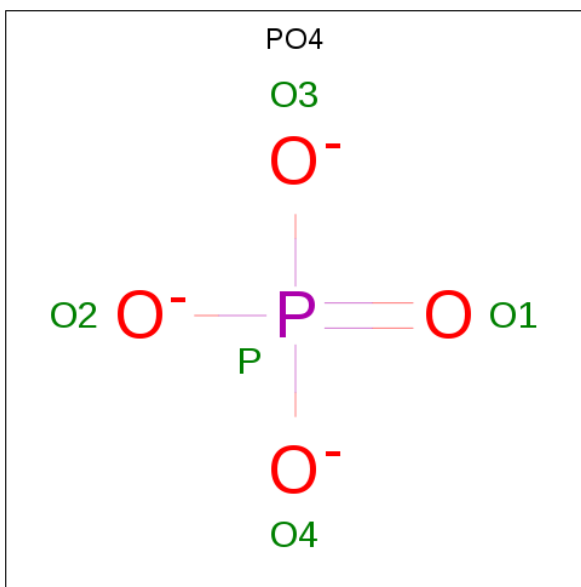
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (three-letter code: JZR) (formula: C₁₂H₂₄O₆).



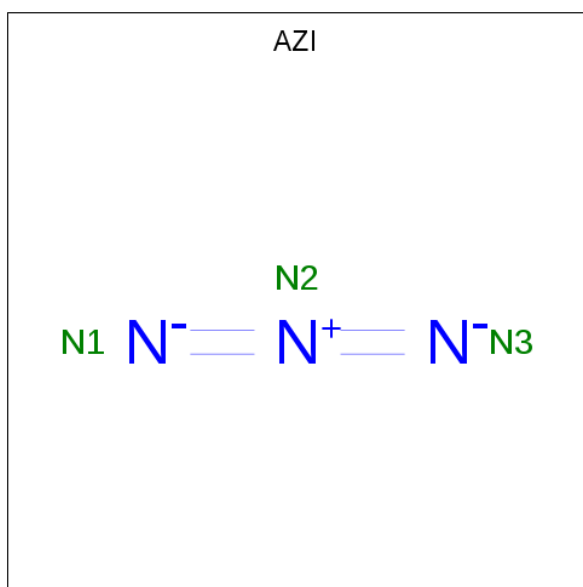
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			5	4	1		
12	B	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	I	1	Total	O	P	0	0
			5	4	1		
12	O	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		
12	Q	1	Total	O	P	0	0
			5	4	1		
12	R	1	Total	O	P	0	0
			5	4	1		
12	R	1	Total	O	P	0	0
			5	4	1		
12	T	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total N 3 3	0	0
13	C	1	Total N 3 3	0	0
13	G	1	Total N 3 3	0	0
13	P	1	Total N 3 3	0	0

- Molecule 14 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

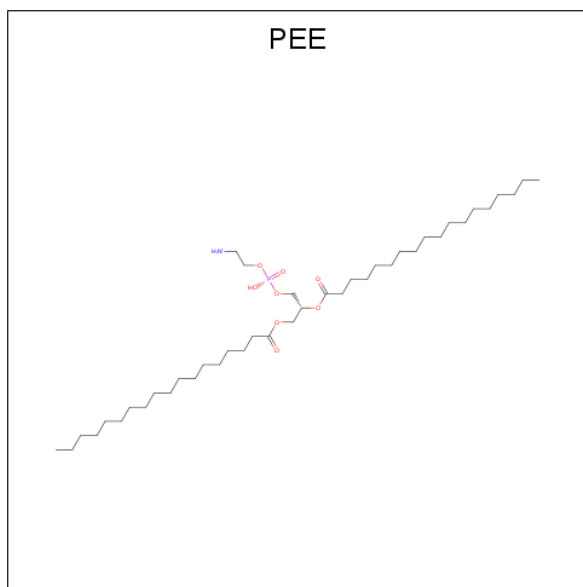
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	P	7	Total O 8 8	0	0
14	G	3	Total O 3 3	0	0
14	Q	1	Total O 1 1	0	0
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	B	11	Total O 11 11	0	0
14	I	2	Total O 2 2	0	0
14	C	6	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	V	4	Total	O	0	0
			4	4		
14	W	1	Total	O	0	0
			1	1		
14	A	10	Total	O	0	0
			10	10		
14	T	2	Total	O	0	0
			2	2		
14	N	4	Total	O	0	0
			5	5		
14	U	2	Total	O	0	0
			2	2		
14	O	8	Total	O	0	0
			9	9		
14	R	2	Total	O	0	0
			2	2		
14	S	1	Total	O	0	0
			1	1		
14	F	1	Total	O	0	0
			1	1		

- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



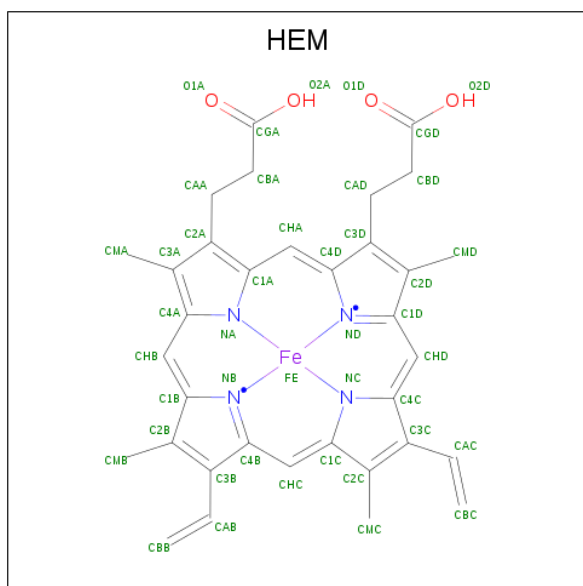
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			8	6	2		

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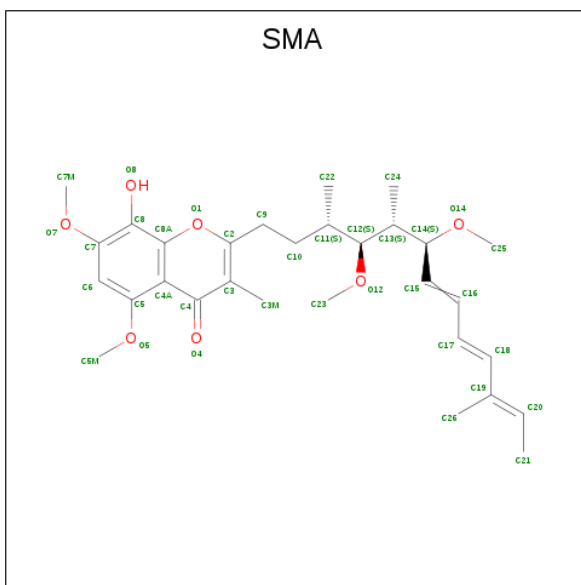
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

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



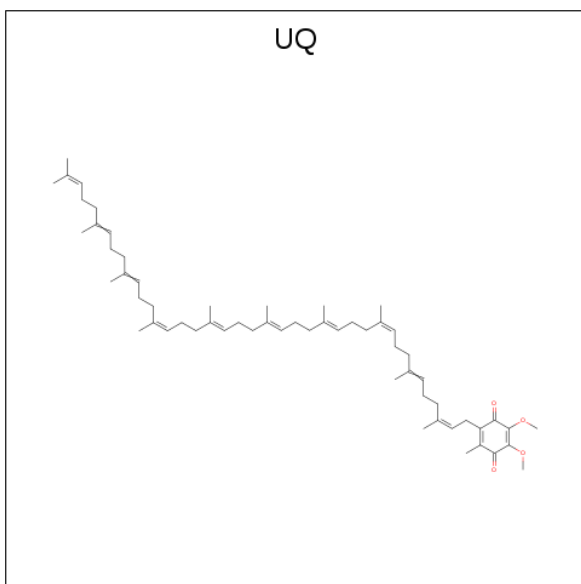
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 18 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



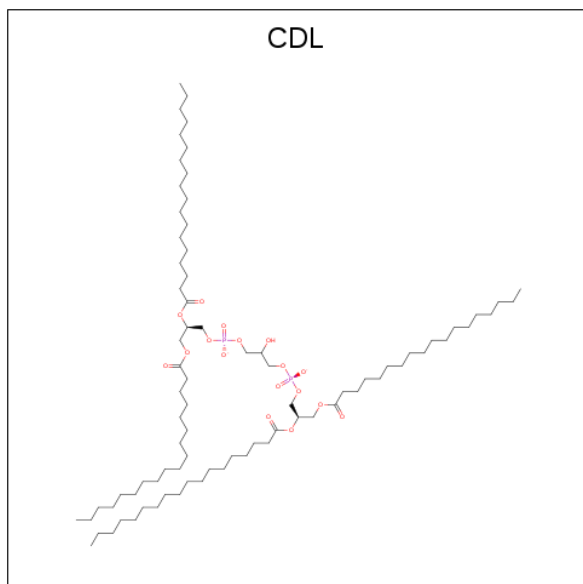
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			18	14	4		

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

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



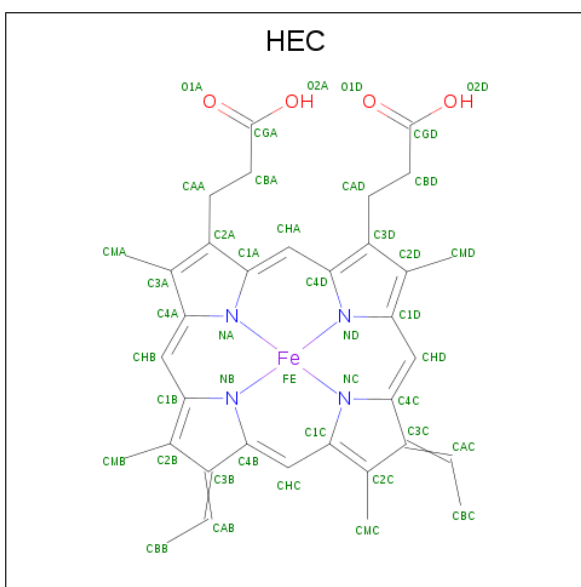
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	C	1	Total	C	O	P	0	0
			44	25	17	2		
19	D	1	Total	C	O	P	0	0
			39	24	13	2		
19	P	1	Total	C	O	P	0	0
			49	30	17	2		
19	Q	1	Total	C	O	P	0	0
			39	24	13	2		

- Molecule 20 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



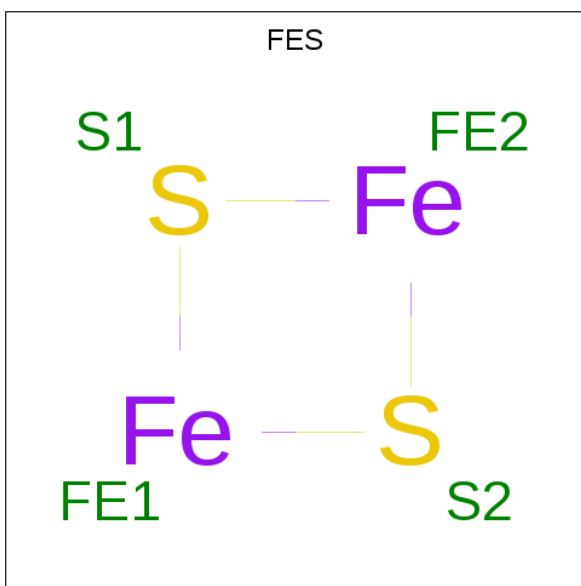
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	C	1	Total	C	O	0	0
			6	3	3		
20	C	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			5	3	2		
20	O	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 21 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

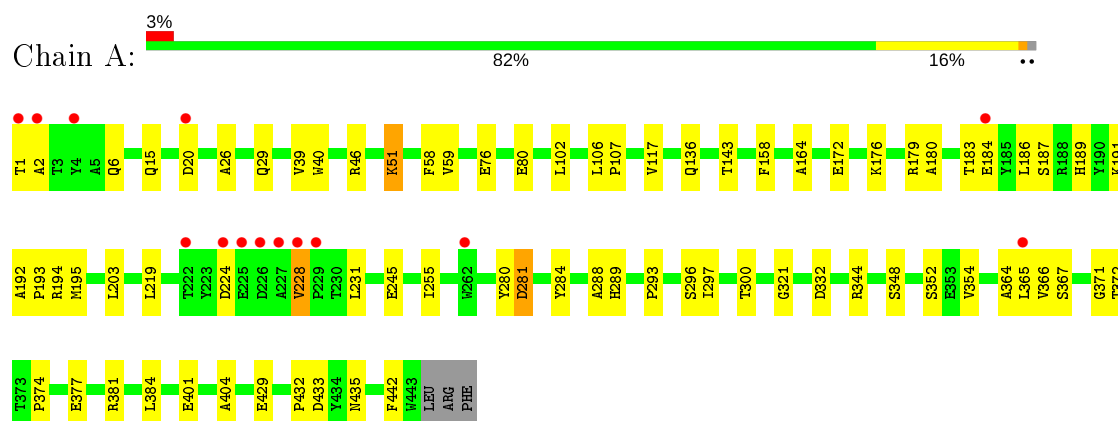
- Molecule 23 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	209	Total O 209 209	0	0
23	B	170	Total O 170 170	0	0
23	C	137	Total O 137 137	0	0
23	D	133	Total O 133 133	0	0
23	E	63	Total O 63 63	0	0
23	F	68	Total O 68 68	0	0
23	G	31	Total O 31 31	0	0
23	H	15	Total O 15 15	0	0
23	I	18	Total O 18 18	0	0
23	J	7	Total O 7 7	0	0
23	N	145	Total O 145 145	0	0
23	O	136	Total O 136 136	0	0
23	P	135	Total O 135 135	0	0
23	Q	126	Total O 126 126	0	0
23	R	77	Total O 77 77	0	0
23	S	81	Total O 81 81	0	0
23	T	17	Total O 17 17	0	0
23	U	16	Total O 16 16	0	0
23	V	16	Total O 16 16	0	0
23	W	12	Total O 12 12	0	0

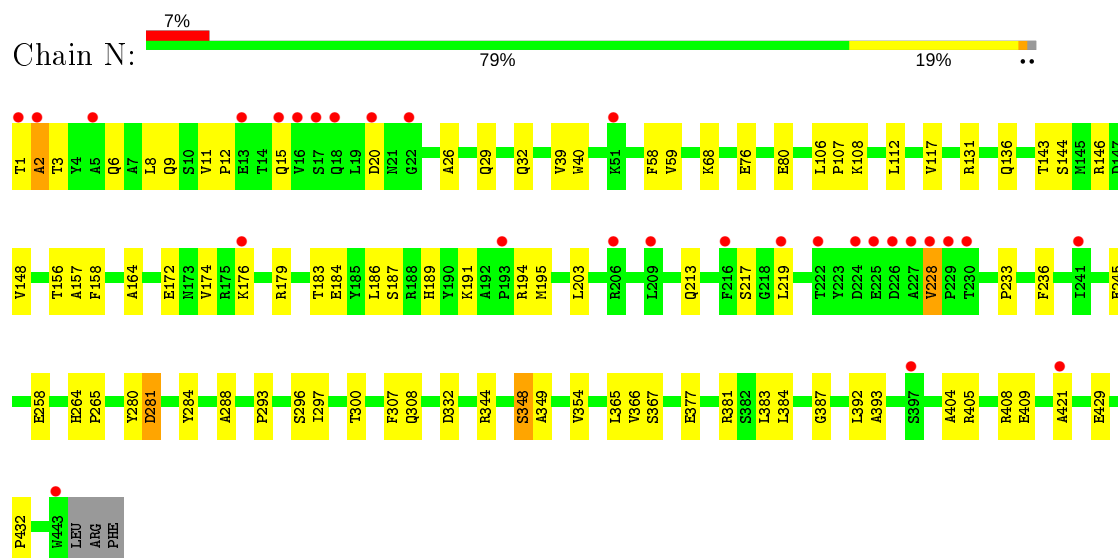
3 Residue-property plots [i](#)

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

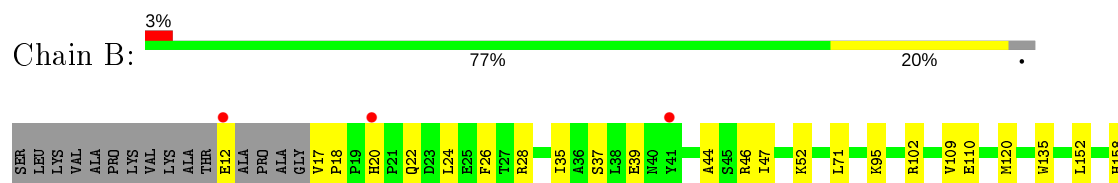
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

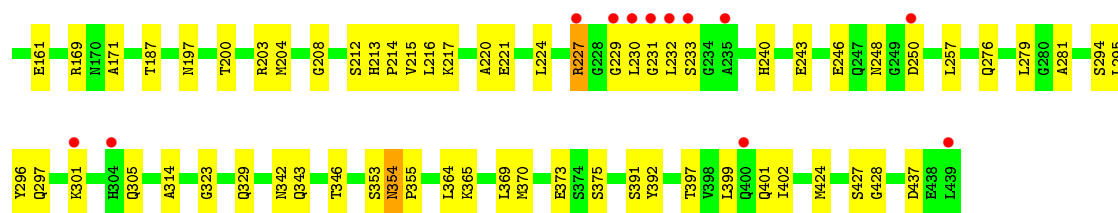


- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

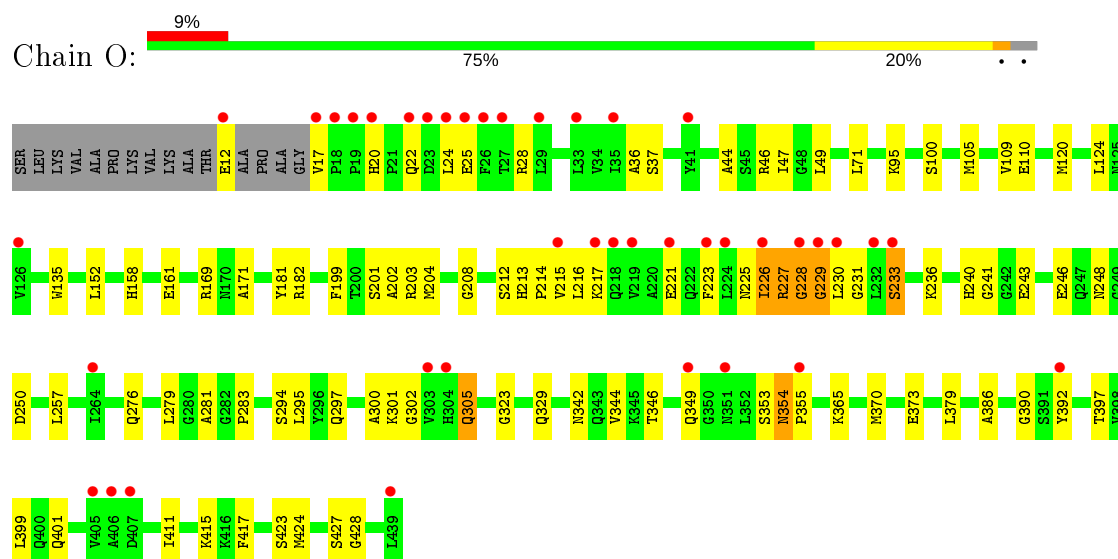


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

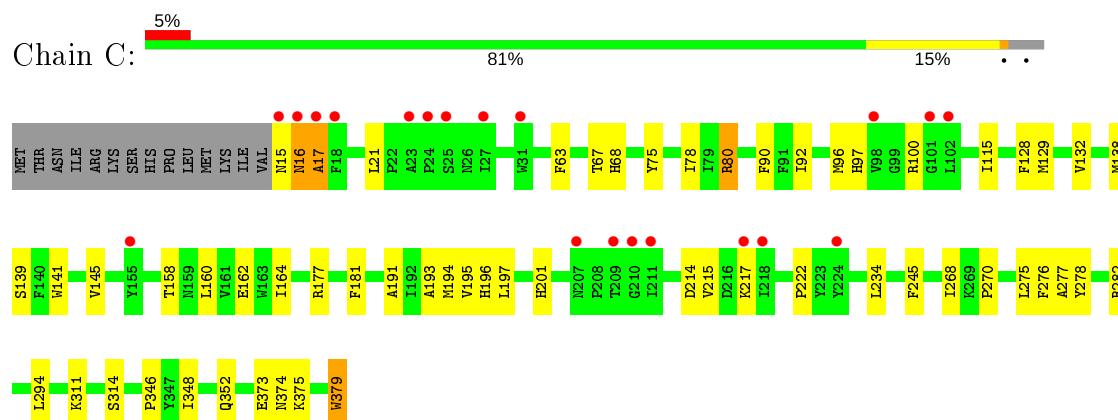




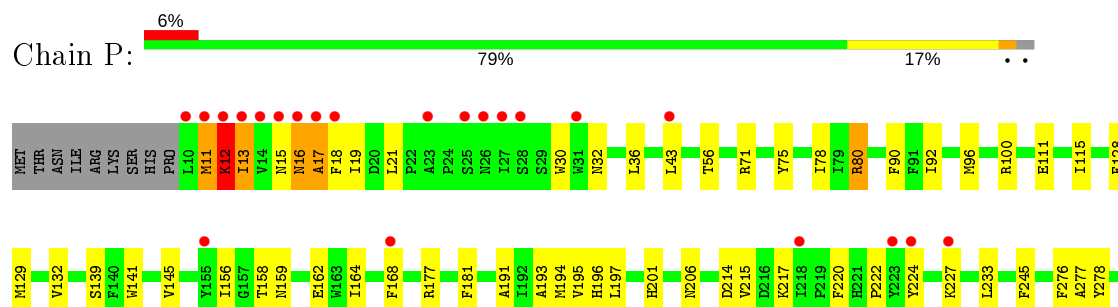
- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

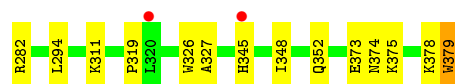


- Molecule 3: Cytochrome b, heme protein, mitochondrial

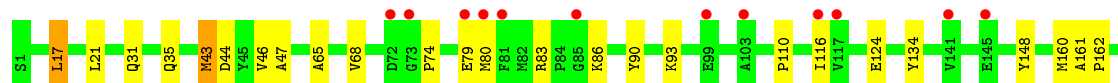
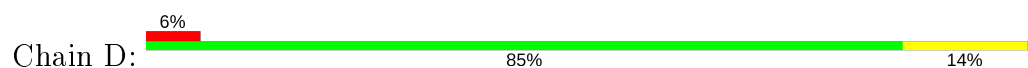


- Molecule 3: Cytochrome b, heme protein, mitochondrial

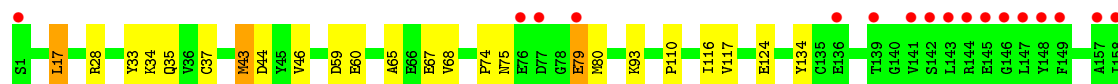
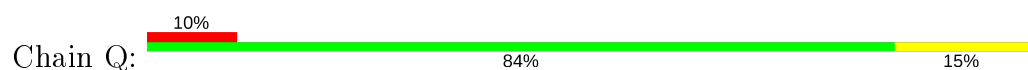




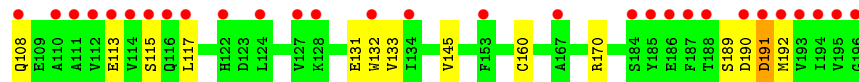
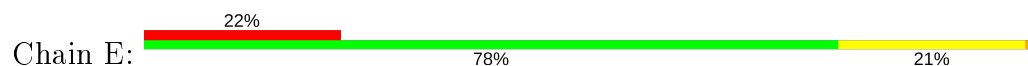
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



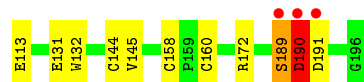
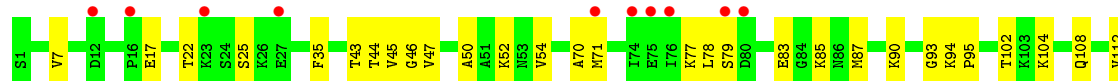
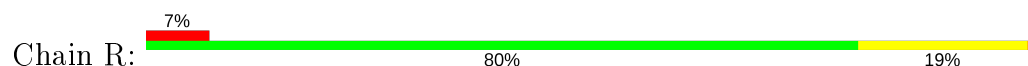
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



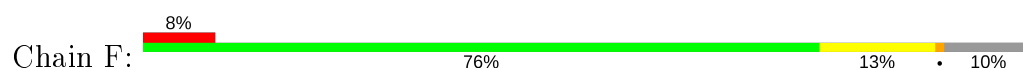
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



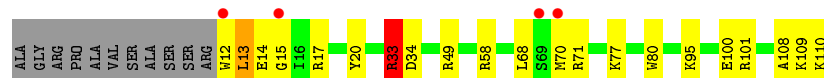
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



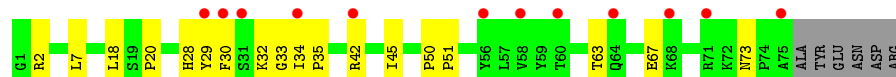
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



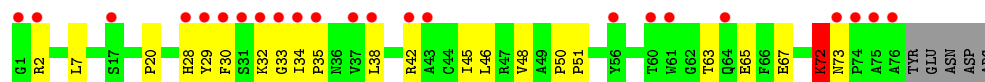
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



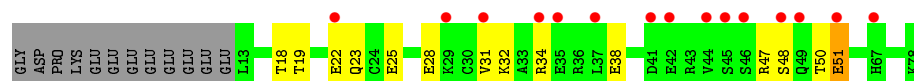
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



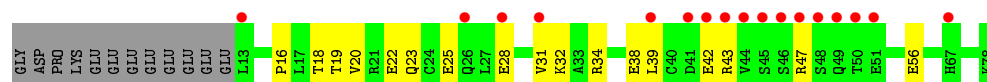
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



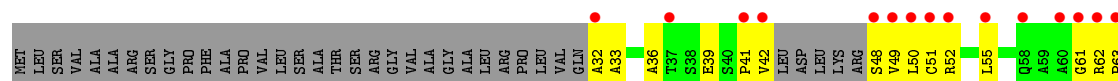
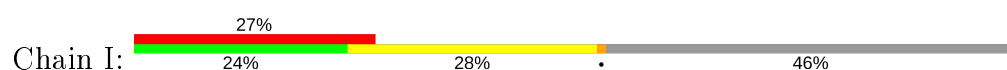
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

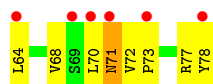


- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

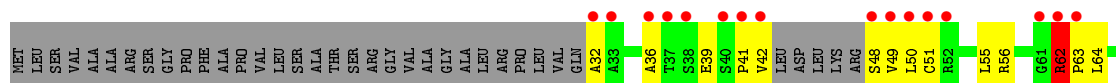
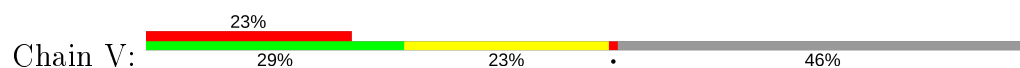


- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

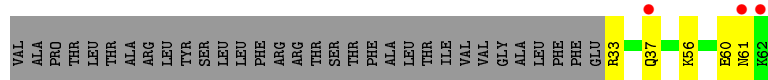
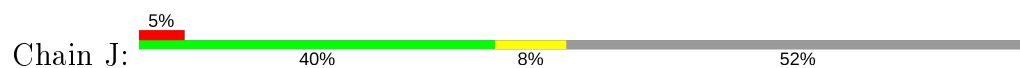




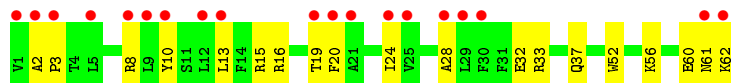
- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



- Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.25Å 168.80Å 230.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.87 – 2.10 37.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (37.87-2.10) 91.8 (37.87-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.258 0.212 , 0.245	Depositor DCC
R_{free} test set	15254 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, UNL, PO4, UQ, FES, HEC, HEM, PEE, JZR, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3467	0.67	0/4706
1	N	0.38	0/3467	0.64	0/4706
2	B	0.42	0/3235	0.65	0/4387
2	O	0.39	0/3239	0.65	1/4393 (0.0%)
3	C	0.48	0/2992	0.66	0/4097
3	P	0.44	0/3030	0.64	0/4145
4	D	0.44	0/1978	0.64	0/2684
4	Q	0.41	0/1978	0.62	0/2684
5	E	0.35	0/1553	0.70	3/2100 (0.1%)
5	R	0.41	0/1550	0.69	0/2094
6	F	0.45	0/878	0.66	0/1175
6	S	0.44	0/878	0.68	1/1175 (0.1%)
7	G	0.42	0/642	0.63	0/869
7	T	0.39	0/647	0.65	0/876
8	H	0.34	0/544	0.61	0/729
8	U	0.34	0/544	0.56	0/729
9	I	0.60	0/285	0.96	0/384
9	V	0.50	0/285	0.94	1/384 (0.3%)
10	J	0.38	0/252	0.56	0/333
10	W	0.36	0/520	0.59	0/699
All	All	0.42	0/31964	0.66	6/43349 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	70	ALA	C-N-CA	-6.85	104.57	121.70
2	O	228	GLY	N-CA-C	-6.31	97.33	113.10
5	E	71	MET	C-N-CA	-6.26	106.05	121.70
6	S	33	ARG	NE-CZ-NH2	-6.11	117.24	120.30
9	V	62	ARG	NE-CZ-NH2	5.70	123.15	120.30
5	E	69	LEU	C-N-CA	-5.27	108.53	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	70	ALA	Peptide

5.2 Too-close contacts ⓘ

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	3398	0	3295	68	0
1	N	3398	0	3295	64	0
2	B	3177	0	3152	88	0
2	O	3180	0	3156	87	0
3	C	2897	0	2943	47	0
3	P	2936	0	2994	74	0
4	D	1919	0	1868	38	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	34	0
5	R	1517	0	1498	38	0
6	F	861	0	854	20	0
6	S	861	0	854	26	0
7	G	621	0	626	14	0
7	T	626	0	631	18	0
8	H	539	0	524	17	0
8	U	539	0	524	18	0
9	I	285	0	288	41	0
9	V	285	0	288	32	0
10	J	245	0	229	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	507	0	513	22	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	4	0
11	P	18	0	24	0	0
11	S	18	0	24	6	0
12	A	5	0	0	0	0
12	B	5	0	0	0	0
12	D	10	0	0	0	0
12	I	5	0	0	1	0
12	O	5	0	0	0	0
12	P	5	0	0	0	0
12	Q	5	0	0	1	0
12	R	10	0	0	0	0
12	T	5	0	0	0	0
13	A	3	0	0	0	0
13	C	3	0	0	0	0
13	G	3	0	0	1	0
13	P	3	0	0	0	0
14	A	10	0	0	0	0
14	B	11	0	0	0	0
14	C	7	0	0	0	0
14	D	7	0	0	1	0
14	E	2	0	0	0	0
14	F	1	0	0	0	0
14	G	3	0	0	0	0
14	I	2	0	0	0	0
14	N	5	0	0	0	0
14	O	9	0	0	2	0
14	P	8	0	0	0	0
14	Q	1	0	0	0	0
14	R	2	0	0	0	0
14	S	1	0	0	0	0
14	T	2	0	0	0	0
14	U	2	0	0	0	0
14	V	4	0	0	0	0
14	W	1	0	0	0	0
15	B	8	0	8	1	0
15	C	49	0	72	0	0
15	D	51	0	82	2	0
15	P	49	0	72	3	0
15	Q	51	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C	86	0	60	5	0
16	P	86	0	60	3	0
17	C	37	0	42	3	0
17	P	37	0	42	3	0
18	C	18	0	14	4	0
18	P	18	0	14	5	0
19	C	44	0	32	0	0
19	D	39	0	39	1	0
19	P	49	0	42	0	0
19	Q	39	0	39	0	0
20	C	12	0	16	0	0
20	E	11	0	13	0	0
20	O	6	0	8	0	0
20	P	12	0	16	2	0
21	D	43	0	30	4	0
21	Q	43	0	30	5	0
22	E	4	0	0	0	0
22	R	4	0	0	0	0
23	A	209	0	0	4	0
23	B	170	0	0	2	0
23	C	137	0	0	6	0
23	D	133	0	0	0	0
23	E	63	0	0	0	0
23	F	68	0	0	4	0
23	G	31	0	0	2	0
23	H	15	0	0	0	0
23	I	18	0	0	4	0
23	J	7	0	0	0	0
23	N	145	0	0	3	0
23	O	136	0	0	6	0
23	P	135	0	0	8	0
23	Q	126	0	0	0	0
23	R	77	0	0	1	0
23	S	81	0	0	2	0
23	T	17	0	0	0	0
23	U	16	0	0	0	0
23	V	16	0	0	0	0
23	W	12	0	0	0	0
All	All	33890	0	31860	708	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 11.

All (708) 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:226:ILE:HG13	14:O:4043:UNL:O1	1.38	1.23
9:I:32:ALA:N	9:I:71:ASN:HB2	1.70	1.05
2:B:12:GLU:HG2	2:B:17:VAL:H	1.16	1.04
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.34	1.04
5:R:90:LYS:HE2	5:R:93:GLY:HA2	1.39	1.03
2:B:95:LYS:HD2	9:I:32:ALA:HB2	1.42	1.00
1:A:1:THR:HG21	2:B:212:SER:HB3	1.46	0.97
8:H:25:GLU:HB3	8:H:34:ARG:NH2	1.79	0.97
3:P:12:LYS:HE2	3:P:16:ASN:H	1.28	0.96
9:I:32:ALA:N	9:I:71:ASN:CB	2.31	0.92
2:B:12:GLU:HG2	2:B:17:VAL:N	1.86	0.90
8:U:25:GLU:HB3	8:U:34:ARG:NH2	1.87	0.89
2:B:95:LYS:HB2	9:I:32:ALA:HB2	1.55	0.86
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.55	0.85
2:O:202:ALA:HB3	2:O:229:GLY:C	1.96	0.85
4:D:241:LYS:HA	4:D:241:LYS:NZ	1.92	0.85
2:B:397:THR:HG22	2:B:401:GLN:HE21	1.41	0.83
1:A:187:SER:O	1:A:191:LYS:HE2	1.79	0.82
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.63	0.81
9:V:49:VAL:HG11	9:V:55:LEU:HD13	1.63	0.80
2:O:397:THR:HG22	2:O:401:GLN:HE21	1.46	0.80
3:P:21:LEU:HD21	18:P:3002:UQ:HM32	1.64	0.80
23:C:4219:HOH:O	3:P:56:THR:HG22	1.82	0.80
1:A:51:LYS:H	1:A:51:LYS:HE3	1.47	0.80
3:C:21:LEU:HD21	18:C:2002:UQ:HM32	1.64	0.80
1:A:29:GLN:HB3	2:B:12:GLU:O	1.81	0.79
23:A:4261:HOH:O	9:I:73:PRO:HG3	1.83	0.78
1:A:352:SER:HB3	6:S:110:LYS:HD2	1.65	0.78
2:B:95:LYS:HD2	9:I:32:ALA:CB	2.13	0.78
2:O:20:HIS:HB2	2:O:22:GLN:HG2	1.66	0.77
10:W:3:PRO:HB2	10:W:8:ARG:HD3	1.65	0.77
1:N:179:ARG:O	1:N:183:THR:HG23	1.85	0.77
4:D:116:ILE:HG12	21:D:501:HEC:HMA3	1.66	0.77
1:A:401:GLU:HG3	11:A:4004:JZR:H6'	1.67	0.77
2:B:397:THR:HG22	2:B:401:GLN:NE2	1.99	0.77
15:B:4017:PEE:C15	9:I:77:ARG:HH22	1.98	0.76
2:B:20:HIS:HB2	2:B:22:GLN:HG2	1.66	0.75
9:I:49:VAL:HG11	9:I:55:LEU:HD13	1.68	0.75
6:F:58:ARG:HD3	23:F:4062:HOH:O	1.86	0.75
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:59:ASP:OD2	10:W:62:LYS:HB3	1.87	0.74
8:H:31:VAL:HA	8:H:34:ARG:NH1	2.02	0.74
9:I:62:ARG:O	9:I:78:TYR:HB3	1.87	0.74
2:O:161:GLU:OE1	9:V:64:LEU:HD12	1.88	0.74
2:O:95:LYS:HD2	2:O:110:GLU:OE2	1.88	0.74
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.51	0.74
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.69	0.73
8:U:31:VAL:HA	8:U:34:ARG:NH1	2.03	0.73
4:D:241:LYS:HZ3	4:D:241:LYS:HA	1.50	0.73
3:P:43:LEU:HD21	15:Q:3006:PEE:H30	1.71	0.72
5:E:90:LYS:HE2	5:E:93:GLY:HA2	1.70	0.72
8:H:25:GLU:HB3	8:H:34:ARG:HH21	1.51	0.72
1:A:2:ALA:HB1	1:A:6:GLN:HB2	1.71	0.72
9:V:62:ARG:O	9:V:78:TYR:HB3	1.88	0.72
7:T:72:LYS:HG3	8:U:56:GLU:OE2	1.90	0.71
10:W:13:LEU:O	10:W:19:THR:HG23	1.91	0.71
8:U:25:GLU:HB3	8:U:34:ARG:HH21	1.55	0.71
10:W:33:ARG:O	10:W:37:GLN:HG3	1.91	0.70
7:G:63:THR:O	7:G:67:GLU:HG2	1.91	0.70
4:D:74:PRO:HD3	4:D:80:MET:HE1	1.73	0.70
2:O:397:THR:HG22	2:O:401:GLN:NE2	2.07	0.70
3:C:68:HIS:HD2	23:C:4195:HOH:O	1.74	0.69
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.75	0.69
5:R:44:THR:HG21	10:W:24:ILE:HD13	1.73	0.69
2:O:95:LYS:HE2	9:V:32:ALA:CB	2.22	0.69
2:B:197:ASN:HB3	2:B:230:LEU:HG	1.74	0.69
5:R:70:ALA:N	5:R:71:MET:HE2	2.07	0.69
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.21	0.68
4:D:110:PRO:HG3	21:D:501:HEC:HMD3	1.75	0.68
1:N:187:SER:O	1:N:191:LYS:HE2	1.93	0.68
4:Q:231:LYS:HD3	6:S:70:MET:HE3	1.75	0.68
7:T:63:THR:O	7:T:67:GLU:HG2	1.94	0.68
2:O:203:ARG:HH12	2:O:233:SER:HB3	1.58	0.68
2:O:49:LEU:HD11	2:O:204:MET:HE3	1.73	0.68
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.28	0.67
10:J:33:ARG:O	10:J:37:GLN:HG3	1.94	0.67
8:U:28:GLU:HA	8:U:31:VAL:HG22	1.76	0.67
8:H:18:THR:O	8:H:22:GLU:HG3	1.94	0.67
4:Q:110:PRO:HG3	21:Q:501:HEC:HMD3	1.77	0.67
9:V:32:ALA:N	9:V:71:ASN:HB3	2.08	0.67
5:R:90:LYS:HE2	5:R:93:GLY:CA	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:12:LYS:HA	3:P:12:LYS:HE3	1.77	0.66
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.60	0.66
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.76	0.66
2:B:95:LYS:CB	9:I:32:ALA:HB2	2.25	0.66
9:I:32:ALA:N	9:I:71:ASN:HB3	2.11	0.66
5:E:87:MET:CE	5:E:88:ALA:H	2.09	0.65
1:A:293:PRO:O	1:A:297:ILE:HG12	1.97	0.65
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.61	0.65
9:V:32:ALA:N	9:V:71:ASN:CB	2.59	0.65
3:P:12:LYS:HE2	3:P:16:ASN:N	2.06	0.65
2:O:95:LYS:HE2	9:V:32:ALA:HB3	1.78	0.65
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.27	0.65
2:O:203:ARG:HH12	2:O:233:SER:CA	2.09	0.65
2:B:200:THR:HG21	2:B:229:GLY:CA	2.26	0.65
16:P:501:HEM:HMC1	16:P:501:HEM:HBC2	1.79	0.65
1:A:179:ARG:O	1:A:183:THR:HG23	1.97	0.65
4:D:231:LYS:HD3	6:F:70:MET:HE3	1.78	0.64
1:A:372:THR:HA	23:A:4296:HOH:O	1.96	0.64
3:C:92:ILE:O	3:C:96:MET:HG2	1.96	0.64
5:E:83:GLU:HG2	5:E:100:HIS:CE1	2.33	0.64
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	1.97	0.64
5:E:85:LYS:NZ	5:E:87:MET:SD	2.69	0.64
5:E:79:SER:HB3	5:E:191:ASP:OD2	1.98	0.64
2:B:203:ARG:HH11	2:B:232:LEU:HA	1.63	0.64
8:U:18:THR:O	8:U:22:GLU:HG3	1.97	0.64
8:H:28:GLU:HA	8:H:31:VAL:HG22	1.80	0.63
2:B:35:ILE:HD11	2:B:220:ALA:CB	2.28	0.63
3:P:12:LYS:NZ	3:P:16:ASN:HD22	1.95	0.63
4:Q:74:PRO:HD3	4:Q:80:MET:HE1	1.80	0.63
2:B:35:ILE:HD11	2:B:220:ALA:HB3	1.80	0.63
1:N:59:VAL:HG11	1:N:186:LEU:HD21	1.80	0.63
1:N:293:PRO:O	1:N:297:ILE:HG12	1.99	0.63
2:O:250:ASP:HB3	23:O:4203:HOH:O	1.99	0.63
3:P:129:MET:CE	3:P:181:PHE:HD2	2.12	0.63
2:B:12:GLU:CG	2:B:17:VAL:H	2.03	0.62
6:S:108:ALA:C	6:S:110:LYS:H	2.00	0.62
2:O:158:HIS:HB3	23:O:4207:HOH:O	1.98	0.62
2:O:202:ALA:HB3	2:O:229:GLY:O	1.99	0.62
6:S:14:GLU:HG2	23:S:4108:HOH:O	1.98	0.62
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.64	0.62
1:N:344:ARG:HG2	1:N:344:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:4237:HOH:O	5:E:26:LYS:HE2	1.99	0.62
2:O:95:LYS:CE	9:V:32:ALA:HB3	2.29	0.62
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.82	0.62
2:B:296:TYR:OH	9:I:52:ARG:HD3	2.00	0.62
8:H:25:GLU:HB3	8:H:34:ARG:HH22	1.63	0.62
1:A:136:GLN:NE2	9:I:51:CYS:HB2	2.15	0.62
2:B:24:LEU:HD13	2:B:392:TYR:CE2	2.35	0.61
2:B:354:ASN:N	2:B:355:PRO:HD2	2.15	0.61
1:A:143:THR:OG1	9:I:48:SER:HB3	2.00	0.61
5:E:160:CYS:HB3	17:P:3001:SMA:H4	1.82	0.61
2:B:200:THR:HG21	2:B:229:GLY:HA3	1.80	0.61
2:B:95:LYS:HB2	9:I:32:ALA:CB	2.29	0.61
2:B:95:LYS:HD3	2:B:110:GLU:OE2	2.01	0.61
1:A:117:VAL:HG11	1:A:195:MET:CE	2.30	0.61
1:A:366:VAL:HG21	2:B:44:ALA:HB2	1.82	0.61
1:N:366:VAL:HG21	2:O:44:ALA:HB2	1.82	0.61
5:R:17:GLU:OE2	5:R:17:GLU:N	2.28	0.61
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.83	0.61
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.01	0.61
5:E:77:LYS:HD3	5:E:80:ASP:OD2	2.01	0.61
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.36	0.61
2:O:28:ARG:HB2	2:O:28:ARG:NH1	2.16	0.61
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.82	0.60
3:P:92:ILE:O	3:P:96:MET:HG2	2.01	0.60
8:U:34:ARG:O	8:U:38:GLU:HG3	2.01	0.60
2:O:226:ILE:CG1	14:O:4043:UNL:O1	2.32	0.60
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.83	0.60
2:B:212:SER:OG	2:B:215:VAL:HG13	2.02	0.60
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.50	0.60
2:O:203:ARG:HH12	2:O:233:SER:CB	2.13	0.60
3:P:21:LEU:HD11	23:P:4171:HOH:O	2.01	0.60
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.01	0.60
2:O:24:LEU:HD23	2:O:392:TYR:CD2	2.37	0.60
10:W:10:TYR:OH	10:W:15:ARG:NH1	2.35	0.60
1:N:68:LYS:HA	1:N:68:LYS:HE3	1.83	0.60
2:O:226:ILE:HD11	23:O:4141:HOH:O	2.00	0.60
23:P:4186:HOH:O	6:S:20:TYR:HE1	1.84	0.60
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.31	0.60
8:H:34:ARG:O	8:H:38:GLU:HG3	2.01	0.59
5:R:112:VAL:HG22	5:R:172:ARG:NH2	2.16	0.59
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:SER:O	1:A:300:THR:HG23	2.01	0.59
9:I:32:ALA:N	9:I:72:VAL:HG23	2.17	0.59
2:O:20:HIS:HB2	2:O:22:GLN:CG	2.32	0.59
2:O:279:LEU:HA	2:O:294:SER:HB3	1.84	0.59
2:B:161:GLU:OE1	9:I:64:LEU:HD12	2.02	0.59
1:N:195:MET:SD	1:N:219:LEU:HD21	2.43	0.59
9:V:32:ALA:N	9:V:72:VAL:HG23	2.18	0.59
5:R:112:VAL:CG2	5:R:172:ARG:NH2	2.66	0.59
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.83	0.59
2:O:28:ARG:HB2	2:O:28:ARG:HH11	1.67	0.59
8:U:28:GLU:O	8:U:31:VAL:HG22	2.03	0.59
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.84	0.59
2:B:250:ASP:HB3	23:B:4230:HOH:O	2.02	0.59
5:E:71:MET:HE2	5:E:92:ARG:HD3	1.85	0.59
4:Q:60:GLU:HG3	10:W:62:LYS:NZ	2.18	0.58
4:Q:124:GLU:OE2	4:Q:191:ARG:HD2	2.03	0.58
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.38	0.58
8:H:28:GLU:O	8:H:31:VAL:HG22	2.03	0.58
5:R:79:SER:HB3	5:R:191:ASP:CG	2.23	0.58
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.49	0.58
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.39	0.58
5:E:17:GLU:N	5:E:17:GLU:OE2	2.28	0.58
1:N:1:THR:O	1:N:2:ALA:HB2	2.03	0.58
2:B:203:ARG:HH12	2:B:233:SER:H	1.50	0.58
2:O:365:LYS:HG2	2:O:399:LEU:HD22	1.85	0.58
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.85	0.58
3:P:100:ARG:C	3:P:100:ARG:HD2	2.24	0.58
3:C:129:MET:CE	3:C:181:PHE:HD2	2.16	0.57
1:N:29:GLN:HG3	1:N:203:LEU:O	2.05	0.57
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.86	0.57
8:U:31:VAL:HA	8:U:34:ARG:HH12	1.68	0.57
5:E:191:ASP:O	5:E:192:MET:HG2	2.04	0.57
9:I:70:LEU:O	9:I:71:ASN:HB2	2.02	0.57
2:B:208:GLY:HA3	2:B:216:LEU:HD11	1.84	0.57
3:P:43:LEU:HD21	15:Q:3006:PEE:C19	2.34	0.57
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.85	0.57
2:O:365:LYS:HG2	2:O:399:LEU:CD2	2.35	0.57
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.19	0.57
2:B:365:LYS:HG2	2:B:399:LEU:CD2	2.35	0.57
2:O:297:GLN:O	2:O:301:LYS:HG3	2.05	0.57
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:GLU:HG2	5:E:100:HIS:NE2	2.19	0.57
2:B:297:GLN:O	2:B:301:LYS:HG3	2.03	0.57
4:Q:75:ASN:HD21	4:Q:79:GLU:HG3	1.69	0.57
5:R:79:SER:HB3	5:R:191:ASP:OD2	2.05	0.57
1:A:117:VAL:HG11	1:A:195:MET:HE3	1.87	0.57
2:B:305:GLN:HB3	2:B:329:GLN:OE1	2.04	0.57
2:O:354:ASN:N	2:O:355:PRO:CD	2.68	0.57
2:O:427:SER:HB3	23:O:4207:HOH:O	2.04	0.57
1:A:172:GLU:OE2	1:A:176:LYS:HE3	2.05	0.56
2:O:236:LYS:H	2:O:236:LYS:HD2	1.70	0.56
6:S:49:ARG:HH22	11:S:2012:JZR:H4	1.70	0.56
1:N:189:HIS:HB3	1:N:194:ARG:HH21	1.71	0.56
2:B:365:LYS:HG2	2:B:399:LEU:HD22	1.87	0.56
2:O:212:SER:OG	2:O:215:VAL:HG13	2.05	0.56
5:E:94:LYS:HE3	3:P:168:PHE:O	2.05	0.56
6:S:100:GLU:HB3	11:S:2012:JZR:H6A	1.88	0.56
17:C:2001:SMA:H4	5:R:160:CYS:HB3	1.87	0.56
9:I:70:LEU:HB2	23:I:1826:HOH:O	2.04	0.56
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.05	0.56
2:O:227:ARG:HA	23:O:4150:HOH:O	2.06	0.56
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.35	0.56
7:G:42:ARG:HG3	7:G:42:ARG:HH11	1.71	0.56
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.88	0.56
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.87	0.56
16:C:501:HEM:HBC2	16:C:501:HEM:HMC1	1.88	0.56
3:C:373:GLU:HB2	23:C:4111:HOH:O	2.06	0.55
9:I:62:ARG:HD3	12:I:4015:PO4:O3	2.07	0.55
4:Q:116:ILE:HG12	21:Q:501:HEC:HMA3	1.89	0.55
6:F:95:LYS:HB2	6:F:95:LYS:NZ	2.20	0.55
1:A:289:HIS:HE1	11:S:2012:JZR:H1'A	1.71	0.55
1:N:189:HIS:CB	1:N:194:ARG:HH21	2.19	0.55
6:S:49:ARG:NH2	11:S:2012:JZR:H4	2.21	0.55
10:W:16:ARG:HB2	10:W:19:THR:CG2	2.36	0.55
6:F:101:ARG:HG2	6:F:101:ARG:HH11	1.71	0.55
8:H:47:ARG:HD3	8:H:50:THR:HB	1.89	0.55
6:S:13:LEU:O	6:S:17:ARG:N	2.40	0.55
3:P:96:MET:HE2	3:P:96:MET:HA	1.89	0.55
4:D:241:LYS:HZ2	4:D:241:LYS:HA	1.70	0.55
5:E:104:LYS:O	5:E:108:GLN:HG3	2.07	0.55
5:E:82:PRO:O	5:E:100:HIS:HB3	2.07	0.55
3:C:15:ASN:O	3:C:16:ASN:C	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.89	0.55
9:I:62:ARG:HB3	9:I:63:PRO:HD2	1.89	0.54
2:O:353:SER:HB3	2:O:355:PRO:HD2	1.89	0.54
5:R:25:SER:HA	23:R:4077:HOH:O	2.06	0.54
8:H:31:VAL:HA	8:H:34:ARG:HH12	1.69	0.54
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.08	0.54
2:B:46:ARG:HD2	2:B:375:SER:OG	2.07	0.54
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.38	0.54
1:A:189:HIS:CB	1:A:194:ARG:HH21	2.19	0.54
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.42	0.54
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.72	0.54
2:O:12:GLU:HG3	2:O:17:VAL:H	1.72	0.54
8:U:16:PRO:O	8:U:20:VAL:HG23	2.08	0.54
2:B:231:GLY:N	2:B:233:SER:OG	2.40	0.54
8:H:51:GLU:H	8:H:51:GLU:CD	2.10	0.54
4:Q:34:LYS:HE3	4:Q:67:GLU:OE1	2.07	0.54
1:A:189:HIS:HB3	1:A:194:ARG:HH21	1.72	0.54
1:N:296:SER:O	1:N:300:THR:HG23	2.07	0.54
3:P:156:ILE:HA	3:P:159:ASN:HD22	1.73	0.54
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.90	0.54
5:E:87:MET:HE3	5:E:88:ALA:H	1.71	0.54
2:O:228:GLY:O	2:O:231:GLY:N	2.40	0.54
3:P:197:LEU:HD13	18:P:3002:UQ:HM53	1.89	0.54
5:E:50:ALA:O	5:E:54:VAL:HG23	2.08	0.54
1:N:381:ARG:HH11	1:N:381:ARG:HG2	1.73	0.53
2:O:225:ASN:HD21	2:O:227:ARG:NH2	2.06	0.53
1:A:39:VAL:HG11	1:A:195:MET:CE	2.37	0.53
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.89	0.53
3:P:12:LYS:CA	3:P:12:LYS:HE3	2.39	0.53
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.90	0.53
8:U:19:THR:O	8:U:23:GLN:HG3	2.07	0.53
1:A:51:LYS:N	1:A:51:LYS:HE3	2.21	0.53
2:B:203:ARG:NH1	2:B:233:SER:H	2.07	0.53
6:F:63:LYS:HE2	23:G:4088:HOH:O	2.08	0.53
2:O:225:ASN:HD21	2:O:227:ARG:CZ	2.22	0.53
5:R:104:LYS:O	5:R:108:GLN:HG3	2.09	0.53
6:S:12:TRP:O	6:S:15:GLY:N	2.41	0.53
3:P:145:VAL:HG21	17:P:3001:SMA:H6	1.91	0.53
3:C:375:LYS:O	6:F:17:ARG:NH1	2.42	0.53
2:B:279:LEU:HA	2:B:294:SER:HB3	1.91	0.53
3:P:201:HIS:NE2	18:P:3002:UQ:O4	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:TYR:O	7:T:33:GLY:HA3	2.09	0.53
1:A:429:GLU:OE2	7:G:7:LEU:HB2	2.09	0.52
1:N:106:LEU:HB3	1:N:107:PRO:HD3	1.92	0.52
2:O:279:LEU:HB3	2:O:295:LEU:HG	1.89	0.52
1:A:29:GLN:HG3	1:A:203:LEU:O	2.09	0.52
3:C:201:HIS:NE2	18:C:2002:UQ:O4	2.37	0.52
16:C:502:HEM:HMC2	16:C:502:HEM:HBC2	1.92	0.52
2:O:225:ASN:ND2	2:O:227:ARG:CZ	2.72	0.52
1:N:117:VAL:HG11	1:N:195:MET:CE	2.40	0.52
21:Q:501:HEC:HBC3	21:Q:501:HEC:HMC1	1.91	0.52
3:C:138:MET:SD	3:C:268:ILE:HG13	2.49	0.52
1:N:2:ALA:HA	1:N:6:GLN:OE1	2.10	0.52
2:O:217:LYS:O	2:O:221:GLU:HG3	2.10	0.52
4:Q:75:ASN:OD1	4:Q:79:GLU:HG2	2.10	0.52
1:A:136:GLN:HB3	9:I:51:CYS:HB3	1.91	0.52
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.37	0.52
3:P:311:LYS:HG2	3:P:374:ASN:CG	2.30	0.52
6:S:95:LYS:HB2	6:S:95:LYS:NZ	2.25	0.52
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.92	0.52
3:C:100:ARG:C	3:C:100:ARG:HD2	2.29	0.52
1:N:228:VAL:O	1:N:228:VAL:HG13	2.11	0.52
9:V:36:ALA:HB3	9:V:73:PRO:CG	2.40	0.52
5:E:87:MET:HE2	5:E:88:ALA:H	1.75	0.51
1:N:146:ARG:HH21	1:N:308:GLN:HE22	1.57	0.51
1:A:281:ASP:OD2	9:I:73:PRO:HB3	2.10	0.51
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.09	0.51
1:N:408:ARG:HD2	23:N:4206:HOH:O	2.09	0.51
1:N:405:ARG:O	1:N:409:GLU:HG3	2.10	0.51
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.75	0.51
4:Q:231:LYS:HD3	6:S:70:MET:CE	2.40	0.51
7:T:32:LYS:C	7:T:35:PRO:HD2	2.31	0.51
9:V:32:ALA:N	9:V:71:ASN:HB2	2.25	0.51
1:N:39:VAL:HG11	1:N:195:MET:CE	2.40	0.51
3:P:158:THR:HB	23:P:4121:HOH:O	2.11	0.51
2:O:236:LYS:N	2:O:236:LYS:HD2	2.26	0.51
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.45	0.50
21:D:501:HEC:HMC1	21:D:501:HEC:HBC3	1.92	0.50
7:G:29:TYR:O	7:G:33:GLY:HA3	2.09	0.50
2:B:227:ARG:HD3	2:B:227:ARG:N	2.26	0.50
5:E:102:THR:OG1	5:E:105:GLU:HG3	2.11	0.50
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:LEU:HD21	4:D:191:ARG:HG2	1.94	0.50
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.47	0.50
2:B:248:ASN:OD1	2:B:428:GLY:HA2	2.11	0.50
1:A:180:ALA:O	1:A:184:GLU:HG3	2.11	0.50
5:R:50:ALA:O	5:R:54:VAL:HG23	2.11	0.50
5:E:190:ASP:O	5:E:192:MET:HG2	2.12	0.50
9:I:64:LEU:HD23	9:I:77:ARG:O	2.12	0.50
4:Q:195:GLU:HG2	4:Q:198:HIS:HB2	1.94	0.50
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.12	0.50
1:N:136:GLN:NE2	9:V:51:CYS:HB2	2.27	0.50
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.47	0.50
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.32	0.50
2:O:305:GLN:NE2	2:O:329:GLN:OE1	2.45	0.49
3:C:160:LEU:O	3:C:164:ILE:HG12	2.11	0.49
1:N:344:ARG:HG2	1:N:344:ARG:NH1	2.27	0.49
4:Q:208:MET:HA	15:Q:3006:PEE:H49	1.94	0.49
2:O:95:LYS:CE	9:V:32:ALA:CB	2.90	0.49
2:O:283:PRO:HB3	9:V:56:ARG:HG3	1.93	0.49
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.94	0.49
10:W:15:ARG:HG3	10:W:15:ARG:HH11	1.76	0.49
6:F:104:ARG:HH11	11:F:3012:JZR:H6	1.77	0.49
3:P:217:LYS:HG3	7:T:7:LEU:HD13	1.94	0.49
8:U:25:GLU:HB3	8:U:34:ARG:HH22	1.72	0.49
2:B:203:ARG:NH1	2:B:232:LEU:HA	2.28	0.49
3:C:197:LEU:HD13	18:C:2002:UQ:HM53	1.94	0.49
4:D:17:LEU:HD21	14:D:4083:UNL:O1	2.13	0.49
1:N:280:TYR:HA	1:N:284:TYR:CE2	2.47	0.49
1:N:383:LEU:O	1:N:387:GLY:HA2	2.12	0.49
2:O:203:ARG:HH12	2:O:233:SER:HA	1.78	0.49
2:O:95:LYS:O	2:O:109:VAL:HA	2.12	0.49
3:P:11:MET:HG2	3:P:12:LYS:N	2.27	0.49
7:G:32:LYS:C	7:G:35:PRO:HD2	2.33	0.49
3:P:164:ILE:O	3:P:177:ARG:HD2	2.13	0.49
2:O:47:ILE:HG21	2:O:120:MET:HE3	1.95	0.49
7:T:46:LEU:N	7:T:46:LEU:HD22	2.27	0.49
1:A:344:ARG:HG2	1:A:344:ARG:NH1	2.25	0.48
3:P:13:ILE:O	3:P:13:ILE:HG22	2.13	0.48
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.95	0.48
1:A:39:VAL:HG11	1:A:195:MET:HE2	1.93	0.48
2:B:246:GLU:O	2:B:427:SER:HA	2.13	0.48
2:B:243:GLU:HA	2:B:424:MET:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:208:MET:HA	15:D:2006:PEE:H49	1.94	0.48
1:N:15:GLN:O	1:N:26:ALA:HA	2.13	0.48
8:U:39:LEU:O	8:U:42:GLU:HB3	2.13	0.48
2:O:95:LYS:HB2	9:V:32:ALA:CB	2.25	0.48
2:B:52:LYS:NZ	2:B:232:LEU:HD11	2.28	0.48
3:C:158:THR:O	3:C:162:GLU:HG3	2.13	0.48
3:C:68:HIS:CD2	23:C:4195:HOH:O	2.59	0.48
1:N:233:PRO:O	5:R:22:THR:HA	2.13	0.48
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.40	0.48
3:P:311:LYS:HG2	3:P:374:ASN:OD1	2.14	0.48
5:R:77:LYS:HE3	5:R:79:SER:OG	2.13	0.48
23:A:4251:HOH:O	9:I:39:GLU:CG	2.62	0.48
1:N:308:GLN:HB3	23:N:4088:HOH:O	2.13	0.48
2:O:199:PHE:O	2:O:226:ILE:HD13	2.14	0.48
2:B:217:LYS:HE2	2:B:221:GLU:OE2	2.14	0.48
2:B:354:ASN:N	2:B:355:PRO:CD	2.76	0.48
2:B:47:ILE:HG13	2:B:120:MET:HE1	1.96	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.47	0.48
2:O:201:SER:H	2:O:226:ILE:HG23	1.78	0.48
2:O:246:GLU:O	2:O:427:SER:HA	2.14	0.48
4:D:160:MET:HB2	21:D:501:HEC:C1D	2.44	0.48
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
2:O:202:ALA:HB3	2:O:230:LEU:N	2.28	0.48
4:Q:43:MET:HE2	4:Q:189:PHE:CZ	2.49	0.48
2:B:232:LEU:O	2:B:233:SER:HB3	2.13	0.48
6:F:49:ARG:NH2	11:F:3012:JZR:H1	2.28	0.48
2:B:437:ASP:OD2	2:O:240:HIS:CD2	2.67	0.48
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.42	0.47
10:W:56:LYS:O	10:W:60:GLU:HG3	2.13	0.47
2:B:397:THR:CG2	2:B:401:GLN:HE21	2.18	0.47
1:N:158:PHE:O	1:N:164:ALA:HB2	2.14	0.47
2:O:124:LEU:HD13	2:O:223:PHE:CB	2.44	0.47
3:P:115:ILE:HD13	3:P:195:VAL:HG12	1.95	0.47
3:P:319:PRO:HD2	23:P:4186:HOH:O	2.13	0.47
4:Q:43:MET:HE2	4:Q:189:PHE:HZ	1.80	0.47
4:D:74:PRO:CD	4:D:80:MET:HE1	2.41	0.47
2:O:397:THR:CG2	2:O:401:GLN:HE21	2.23	0.47
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.54	0.47
1:A:15:GLN:O	1:A:26:ALA:HA	2.14	0.47
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.50	0.47
5:E:77:LYS:HE3	5:E:79:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:ASP:O	6:F:58:ARG:NH2	2.47	0.47
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.97	0.47
6:F:104:ARG:HH11	11:F:3012:JZR:C6	2.27	0.47
4:D:231:LYS:HD3	6:F:70:MET:CE	2.44	0.47
9:I:71:ASN:ND2	23:I:1406:HOH:O	2.47	0.47
9:I:78:TYR:HA	23:I:1201:HOH:O	2.14	0.47
3:P:214:ASP:CG	7:T:2:ARG:HH22	2.18	0.47
3:C:191:ALA:HA	3:C:194:MET:CE	2.45	0.47
3:C:96:MET:HA	3:C:96:MET:HE2	1.97	0.47
6:S:68:LEU:HD23	6:S:71:ARG:HH22	1.80	0.47
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.95	0.47
1:N:348:SER:O	1:N:349:ALA:C	2.54	0.47
10:W:2:ALA:HA	10:W:3:PRO:HD3	1.77	0.47
1:A:40:TRP:HB3	1:A:384:LEU:HD11	1.96	0.46
2:B:12:GLU:O	2:B:18:PRO:HD3	2.14	0.46
2:O:370:MET:O	2:O:373:GLU:HG2	2.15	0.46
5:R:189:SER:O	5:R:190:ASP:C	2.53	0.46
2:B:135:TRP:CE2	6:S:49:ARG:HD3	2.50	0.46
9:I:72:VAL:CG1	9:I:73:PRO:HD2	2.45	0.46
4:D:211:MET:HG3	15:D:2006:PEE:H48	1.97	0.46
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.50	0.46
10:W:20:PHE:CE1	10:W:24:ILE:HD11	2.49	0.46
4:D:47:ALA:HA	4:D:90:TYR:HA	1.96	0.46
8:H:19:THR:O	8:H:23:GLN:HG3	2.15	0.46
1:N:264:HIS:HA	1:N:265:PRO:HD3	1.83	0.46
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.15	0.46
6:S:101:ARG:HG2	6:S:101:ARG:HH11	1.80	0.46
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.46	0.46
3:P:12:LYS:HA	3:P:12:LYS:CE	2.43	0.46
5:R:93:GLY:O	5:R:94:LYS:HG3	2.14	0.46
2:O:213:HIS:N	2:O:214:PRO:CD	2.79	0.46
2:O:344:VAL:HG11	2:O:417:PHE:CD2	2.50	0.46
4:Q:74:PRO:HB3	4:Q:80:MET:CE	2.45	0.46
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.98	0.46
2:B:102:ARG:HH22	2:B:161:GLU:CD	2.19	0.46
2:B:370:MET:O	2:B:373:GLU:HG2	2.16	0.46
3:C:215:VAL:HG13	23:C:4154:HOH:O	2.15	0.46
3:C:75:TYR:O	3:C:78:ILE:HG22	2.15	0.46
4:D:83:ARG:CZ	4:D:86:LYS:HE2	2.45	0.46
1:N:281:ASP:OD2	9:V:73:PRO:HB3	2.15	0.46
3:P:373:GLU:HB2	23:P:4170:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:13:LEU:HD22	23:S:4129:HOH:O	2.15	0.46
3:P:375:LYS:O	6:S:17:ARG:NH1	2.49	0.46
2:B:342:ASN:O	2:B:346:THR:HG23	2.15	0.46
2:B:354:ASN:H	2:B:355:PRO:HD2	1.81	0.46
6:S:108:ALA:C	6:S:110:LYS:N	2.68	0.46
10:W:3:PRO:CB	10:W:8:ARG:HD3	2.41	0.46
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.51	0.46
2:O:25:GLU:O	2:O:36:ALA:HA	2.15	0.46
8:U:28:GLU:CA	8:U:31:VAL:HG22	2.44	0.46
6:F:71:ARG:HD3	23:F:4076:HOH:O	2.15	0.46
3:C:214:ASP:CG	7:G:2:ARG:HH22	2.19	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.98	0.46
3:P:278:TYR:CZ	3:P:282:ARG:HD3	2.50	0.46
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.51	0.46
4:Q:74:PRO:CD	4:Q:80:MET:HE1	2.46	0.46
23:O:4201:HOH:O	9:V:32:ALA:HB1	2.16	0.46
9:V:50:LEU:O	9:V:51:CYS:HB3	2.16	0.46
3:C:115:ILE:HD13	3:C:195:VAL:HG12	1.98	0.45
16:C:502:HEM:HBA1	18:C:2002:UQ:O2	2.16	0.45
1:N:29:GLN:HB3	2:O:12:GLU:O	2.16	0.45
1:A:228:VAL:O	1:A:228:VAL:HG13	2.16	0.45
7:G:2:ARG:HA	23:G:4101:HOH:O	2.16	0.45
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.51	0.45
3:P:15:ASN:O	3:P:17:ALA:N	2.49	0.45
8:U:28:GLU:HA	8:U:31:VAL:CG2	2.44	0.45
10:W:3:PRO:HB2	10:W:8:ARG:CD	2.43	0.45
7:T:28:HIS:ND1	7:T:32:LYS:HD2	2.31	0.45
3:C:276:PHE:CG	3:C:277:ALA:N	2.84	0.45
6:S:109:LYS:O	6:S:110:LYS:HG2	2.16	0.45
4:D:148:TYR:CZ	4:D:161:ALA:HB2	2.52	0.45
2:O:386:ALA:O	2:O:390:GLY:HA2	2.17	0.45
5:R:190:ASP:HB2	5:R:191:ASP:H	1.42	0.45
3:P:158:THR:O	3:P:162:GLU:HG3	2.16	0.45
2:B:217:LYS:O	2:B:221:GLU:HG3	2.17	0.45
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.45
2:B:95:LYS:O	2:B:109:VAL:HA	2.17	0.45
3:C:80:ARG:C	3:C:80:ARG:HD3	2.37	0.45
3:C:164:ILE:O	3:C:177:ARG:HD2	2.16	0.45
1:A:39:VAL:CG1	1:A:195:MET:HE2	2.47	0.45
6:F:101:ARG:HG2	6:F:101:ARG:NH1	2.32	0.45
9:I:61:GLY:C	9:I:62:ARG:HG3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:213:GLN:O	1:N:217:SER:OG	2.27	0.45
2:O:342:ASN:O	2:O:346:THR:HG23	2.16	0.45
5:R:44:THR:HG22	10:W:24:ILE:HG21	1.97	0.45
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.99	0.44
2:O:100:SER:OG	2:O:105:MET:HG2	2.17	0.44
3:P:13:ILE:HA	3:P:17:ALA:HB2	1.99	0.44
1:A:288:ALA:CB	1:A:300:THR:HG22	2.46	0.44
2:O:227:ARG:HD2	2:O:227:ARG:N	2.32	0.44
3:P:348:ILE:O	3:P:352:GLN:HG3	2.17	0.44
3:P:75:TYR:O	3:P:78:ILE:HG22	2.17	0.44
8:U:42:GLU:HG2	8:U:43:ARG:N	2.32	0.44
4:D:74:PRO:HB3	4:D:80:MET:CE	2.47	0.44
3:P:220:PHE:HE1	18:P:3002:UQ:HM23	1.82	0.44
3:P:129:MET:HE1	17:P:3001:SMA:H26	1.98	0.44
4:Q:160:MET:HB2	21:Q:501:HEC:C1D	2.47	0.44
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.81	0.44
5:R:112:VAL:HG22	5:R:172:ARG:HH22	1.82	0.44
3:C:270:PRO:HG2	3:C:278:TYR:CG	2.52	0.44
1:A:102:LEU:CD2	2:B:369:LEU:HD12	2.47	0.44
3:C:348:ILE:O	3:C:352:GLN:HG3	2.17	0.44
4:D:195:GLU:HG2	4:D:198:HIS:HB2	2.00	0.44
10:J:56:LYS:O	10:J:60:GLU:HG3	2.17	0.44
2:O:248:ASN:OD1	2:O:428:GLY:HA2	2.17	0.44
3:P:11:MET:HE3	3:P:12:LYS:HB2	1.99	0.44
5:R:102:THR:OG1	5:R:104:LYS:HG2	2.18	0.44
10:W:52:TRP:O	10:W:56:LYS:HB2	2.17	0.44
4:D:74:PRO:HA	4:D:79:GLU:O	2.18	0.44
6:F:95:LYS:NZ	6:F:95:LYS:CB	2.80	0.44
1:N:39:VAL:HG11	1:N:195:MET:HE2	1.98	0.44
16:P:502:HEM:HBA1	18:P:3002:UQ:O2	2.18	0.44
1:A:371:GLY:O	1:A:374:PRO:HD2	2.18	0.44
3:C:191:ALA:HA	3:C:194:MET:HE3	2.00	0.44
4:D:214:LEU:O	4:D:217:PRO:HG2	2.17	0.44
9:V:32:ALA:N	9:V:72:VAL:CG2	2.80	0.44
2:B:46:ARG:O	2:B:47:ILE:HD13	2.17	0.44
3:C:132:VAL:HA	3:C:139:SER:HB3	1.98	0.44
2:O:217:LYS:HE2	2:O:221:GLU:OE2	2.18	0.44
5:R:112:VAL:HG21	5:R:172:ARG:NH2	2.32	0.44
5:R:43:THR:O	5:R:47:VAL:HG23	2.17	0.44
9:V:72:VAL:HG13	9:V:73:PRO:HD2	2.00	0.44
9:V:72:VAL:CG1	9:V:73:PRO:HD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:GLU:HG2	5:E:100:HIS:CD2	2.53	0.43
4:D:43:MET:CE	4:D:189:PHE:CZ	3.01	0.43
9:I:50:LEU:O	9:I:51:CYS:HB3	2.18	0.43
2:O:215:VAL:CG2	2:O:216:LEU:N	2.80	0.43
6:S:34:ASP:O	6:S:58:ARG:NH2	2.50	0.43
1:A:195:MET:SD	1:A:219:LEU:HD21	2.58	0.43
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.01	0.43
1:N:1:THR:O	1:N:2:ALA:CB	2.66	0.43
3:P:100:ARG:O	3:P:100:ARG:HD2	2.18	0.43
3:P:282:ARG:NH2	23:P:4173:HOH:O	2.51	0.43
3:P:43:LEU:HD21	15:Q:3006:PEE:H27	2.00	0.43
9:V:64:LEU:HD23	9:V:78:TYR:C	2.38	0.43
1:A:289:HIS:HE1	11:S:2012:JZR:C1'	2.32	0.43
2:B:28:ARG:CG	2:B:28:ARG:HH11	2.32	0.43
2:O:46:ARG:HG2	2:O:379:LEU:HD22	2.00	0.43
4:Q:195:GLU:O	4:Q:195:GLU:HG2	2.19	0.43
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.19	0.43
2:B:52:LYS:HZ3	2:B:232:LEU:HD11	1.82	0.43
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.66	0.43
8:H:25:GLU:CB	8:H:34:ARG:NH2	2.67	0.43
4:Q:211:MET:HG3	15:Q:3006:PEE:H48	2.00	0.43
1:A:352:SER:OG	6:S:110:LYS:HB2	2.18	0.43
3:P:378:LYS:HE3	6:S:17:ARG:NE	2.34	0.43
2:B:46:ARG:HG2	2:B:110:GLU:HG2	2.00	0.43
1:A:364:ALA:HB2	9:I:33:ALA:HB1	2.01	0.43
2:O:46:ARG:O	2:O:47:ILE:HD13	2.19	0.43
3:P:227:LYS:HE3	20:P:4009:GOL:O1	2.18	0.43
3:P:80:ARG:C	3:P:80:ARG:HD3	2.39	0.43
2:B:187:THR:HB	23:B:4154:HOH:O	2.18	0.43
1:N:236:PHE:CG	1:N:258:GLU:HB2	2.54	0.43
7:T:30:PHE:O	7:T:34:ILE:HG12	2.18	0.43
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.67	0.43
4:D:195:GLU:HG2	4:D:195:GLU:O	2.19	0.43
5:E:191:ASP:CG	5:E:191:ASP:O	2.56	0.43
3:P:191:ALA:HA	3:P:194:MET:CE	2.48	0.43
9:V:62:ARG:HB3	9:V:63:PRO:HD2	2.01	0.43
2:O:203:ARG:HD2	2:O:230:LEU:O	2.19	0.43
4:Q:229:VAL:CG2	7:T:20:PRO:HD3	2.48	0.43
3:C:100:ARG:CZ	16:C:502:HEM:HBD1	2.49	0.43
4:D:239:PRO:O	4:D:241:LYS:HE2	2.19	0.43
9:I:64:LEU:HD23	9:I:78:TYR:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:43:ARG:HD2	8:U:47:ARG:HH21	1.83	0.43
2:B:213:HIS:N	2:B:214:PRO:CD	2.81	0.42
5:E:113:GLU:HG3	5:E:115:SER:OG	2.19	0.42
5:R:17:GLU:H	5:R:17:GLU:CD	2.17	0.42
1:A:192:ALA:HB3	1:A:193:PRO:HD3	1.99	0.42
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.00	0.42
3:C:97:HIS:CD2	16:C:502:HEM:NC	2.86	0.42
7:G:30:PHE:O	7:G:34:ILE:HG12	2.19	0.42
4:Q:65:ALA:O	4:Q:68:VAL:HG22	2.18	0.42
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42
3:C:270:PRO:HD2	3:C:275:LEU:HD23	2.01	0.42
4:D:31:GLN:O	4:D:35:GLN:HG2	2.19	0.42
6:F:39:GLU:HG3	23:F:4047:HOH:O	2.19	0.42
1:N:157:ALA:HB2	1:N:421:ALA:CB	2.49	0.42
1:N:8:LEU:HD22	1:N:392:LEU:HB3	2.01	0.42
1:N:40:TRP:HB3	1:N:384:LEU:HD11	2.00	0.42
3:P:193:ALA:O	3:P:196:HIS:HB3	2.19	0.42
1:A:352:SER:CB	6:S:110:LYS:HB2	2.50	0.42
3:P:378:LYS:HE3	6:S:17:ARG:CD	2.49	0.42
1:N:8:LEU:O	1:N:11:VAL:HG23	2.19	0.42
1:A:195:MET:HE2	1:A:195:MET:HB3	1.91	0.42
5:E:43:THR:O	5:E:47:VAL:HG23	2.20	0.42
5:E:10:PHE:HB3	7:G:18:LEU:HD11	2.02	0.42
3:P:276:PHE:CG	3:P:277:ALA:N	2.87	0.42
4:Q:43:MET:CE	4:Q:189:PHE:CZ	3.02	0.42
1:A:289:HIS:CE1	11:S:2012:JZR:H1'A	2.52	0.42
2:O:95:LYS:HE2	9:V:32:ALA:N	2.35	0.42
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.02	0.42
7:G:28:HIS:ND1	7:G:32:LYS:HD2	2.34	0.42
2:B:314:ALA:HA	9:I:63:PRO:HD3	2.02	0.42
5:R:112:VAL:HG21	5:R:172:ARG:HH21	1.84	0.42
5:E:15:ARG:NH2	13:G:4001:AZI:N1	2.68	0.42
5:E:117:LEU:HD13	5:E:170:ARG:HD2	2.01	0.42
5:R:85:LYS:NZ	5:R:87:MET:SD	2.72	0.42
1:N:284:TYR:HE1	9:V:73:PRO:HG3	1.84	0.42
10:W:16:ARG:O	10:W:19:THR:HG22	2.20	0.42
2:B:294:SER:OG	2:B:343:GLN:NE2	2.53	0.42
3:C:314:SER:O	23:C:4170:HOH:O	2.21	0.42
4:D:231:LYS:HA	4:D:231:LYS:HD3	1.89	0.42
1:N:131:ARG:NH1	1:N:174:VAL:O	2.51	0.42
2:O:241:GLY:HA2	2:O:423:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:SER:HB3	2:B:355:PRO:HG2	2.01	0.42
4:D:116:ILE:HA	4:D:116:ILE:HD12	1.86	0.42
2:O:152:LEU:HD13	2:O:158:HIS:CE1	2.55	0.42
3:P:12:LYS:HE2	3:P:16:ASN:HB2	2.02	0.42
3:P:345:HIS:HE1	7:T:65:GLU:OE2	2.02	0.42
5:R:78:LEU:HB2	5:R:191:ASP:HB2	2.02	0.42
1:A:281:ASP:C	1:A:281:ASP:OD1	2.59	0.42
2:B:204:MET:HE1	2:B:224:LEU:HD22	2.01	0.42
3:C:311:LYS:HG2	3:C:374:ASN:CG	2.41	0.42
3:C:234:LEU:HD12	19:D:2003:CDL:H712	2.01	0.42
6:F:102:LYS:HD3	6:F:102:LYS:HA	1.83	0.42
8:H:28:GLU:CA	8:H:31:VAL:HG22	2.47	0.42
3:P:18:PHE:CD2	3:P:19:ILE:HD13	2.55	0.42
3:P:215:VAL:HG13	23:P:4193:HOH:O	2.18	0.42
3:P:233:LEU:HD11	4:Q:219:VAL:HG21	2.01	0.42
1:A:1:THR:CG2	2:B:212:SER:HB3	2.34	0.41
2:B:364:LEU:HG	2:B:402:ILE:HD13	2.00	0.41
1:N:143:THR:OG1	9:V:48:SER:HB3	2.20	0.41
3:P:326:TRP:NE1	7:T:48:VAL:HG22	2.35	0.41
3:P:224:TYR:HB3	20:P:4009:GOL:H31	2.02	0.41
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.55	0.41
1:A:117:VAL:HG11	1:A:195:MET:HE1	2.01	0.41
3:C:15:ASN:O	3:C:17:ALA:N	2.53	0.41
9:I:52:ARG:NH1	23:I:859:HOH:O	2.54	0.41
1:N:11:VAL:HA	1:N:12:PRO:HD3	1.92	0.41
1:N:146:ARG:NH2	1:N:308:GLN:HE22	2.17	0.41
2:O:257:LEU:O	2:O:323:GLY:HA3	2.21	0.41
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.55	0.41
3:C:277:ALA:HB1	3:C:294:LEU:HD12	2.02	0.41
3:C:278:TYR:CZ	3:C:282:ARG:HD3	2.56	0.41
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.50	0.41
5:E:189:SER:C	5:E:190:ASP:OD1	2.59	0.41
6:F:99:ARG:NH2	23:F:4055:HOH:O	2.53	0.41
8:H:31:VAL:HA	8:H:34:ARG:HH11	1.84	0.41
1:N:39:VAL:CG1	1:N:195:MET:HE2	2.51	0.41
3:P:30:TRP:CZ3	15:P:3007:PEE:H21	2.55	0.41
3:P:96:MET:HE2	15:P:3007:PEE:H27	2.03	0.41
4:Q:215:LEU:HD21	5:R:46:GLY:HA3	2.02	0.41
5:R:70:ALA:C	5:R:71:MET:HE2	2.40	0.41
23:N:4088:HOH:O	9:V:39:GLU:CG	2.69	0.41
2:B:28:ARG:HG2	2:B:28:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:19:TRP:CD2	11:F:4003:JZR:H1'A	2.56	0.41
1:N:108:LYS:O	1:N:112:LEU:HG	2.21	0.41
2:O:411:ILE:O	2:O:415:LYS:HG3	2.20	0.41
5:R:44:THR:CG2	10:W:24:ILE:HG21	2.51	0.41
5:R:95:PRO:HG2	5:R:145:VAL:HG22	2.02	0.41
1:A:1:THR:HG22	2:B:39:GLU:OE1	2.20	0.41
2:B:46:ARG:HD2	2:B:375:SER:CB	2.50	0.41
3:C:129:MET:HE1	17:C:2001:SMA:H26	2.02	0.41
4:Q:28:ARG:HB3	4:Q:171:PHE:CE1	2.55	0.41
21:Q:501:HEC:HMB1	21:Q:501:HEC:HBB3	2.02	0.41
8:U:31:VAL:HG23	8:U:32:LYS:N	2.35	0.41
1:A:46:ARG:HG2	1:A:231:LEU:HD22	2.03	0.41
2:B:152:LEU:HD13	2:B:158:HIS:CE1	2.55	0.41
2:O:236:LYS:CD	2:O:236:LYS:H	2.32	0.41
5:R:52:LYS:NZ	10:W:32:GLU:OE2	2.48	0.41
2:B:257:LEU:O	2:B:323:GLY:HA3	2.21	0.41
2:B:26:PHE:CZ	2:B:391:SER:HA	2.56	0.41
1:N:332:ASP:OD1	1:N:432:PRO:HG3	2.21	0.41
4:Q:117:VAL:O	12:Q:4012:PO4:O2	2.38	0.41
1:A:332:ASP:OD1	1:A:432:PRO:HG3	2.21	0.41
3:P:206:ASN:HB3	16:P:502:HEM:O2D	2.20	0.41
1:A:366:VAL:HG23	1:A:367:SER:N	2.35	0.40
2:O:37:SER:HA	2:O:208:GLY:O	2.21	0.40
2:O:243:GLU:HA	2:O:424:MET:O	2.22	0.40
3:P:245:PHE:CD1	4:Q:17:LEU:HD13	2.56	0.40
4:D:74:PRO:CA	4:D:80:MET:HE2	2.51	0.40
3:P:326:TRP:CH2	15:P:3007:PEE:H51	2.57	0.40
3:P:32:ASN:O	3:P:36:LEU:HG	2.22	0.40
1:A:255:ILE:O	1:A:321:GLY:HA3	2.22	0.40
1:A:442:PHE:C	1:A:442:PHE:CD1	2.95	0.40
3:C:63:PHE:O	3:C:67:THR:HG23	2.22	0.40
4:D:65:ALA:O	4:D:68:VAL:HG22	2.21	0.40
9:I:72:VAL:HG13	9:I:73:PRO:HD2	2.03	0.40
1:N:9:GLN:HE22	1:N:393:ALA:HB1	1.87	0.40
3:P:197:LEU:HA	3:P:197:LEU:HD23	1.73	0.40
3:P:71:ARG:HD3	23:P:4196:HOH:O	2.22	0.40
7:T:50:PRO:HB2	7:T:51:PRO:HD3	2.02	0.40
7:T:72:LYS:HE2	7:T:72:LYS:HB2	1.97	0.40
1:A:2:ALA:HB1	1:A:6:GLN:CB	2.48	0.40
1:N:144:SER:O	1:N:148:VAL:HG23	2.20	0.40
1:N:307:PHE:CD1	1:N:307:PHE:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:366:VAL:HG23	1:N:367:SER:N	2.37	0.40
2:O:120:MET:HE2	2:O:120:MET:HB2	1.92	0.40
2:O:300:ALA:C	2:O:302:GLY:H	2.25	0.40
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.56	0.40
4:Q:79:GLU:HG2	4:Q:79:GLU:H	1.62	0.40
8:H:28:GLU:HA	8:H:31:VAL:CG2	2.48	0.40
8:H:31:VAL:HG23	8:H:32:LYS:N	2.36	0.40
3:P:111:GLU:CD	3:P:111:GLU:H	2.25	0.40
3:P:132:VAL:HA	3:P:139:SER:HB3	2.03	0.40
4:Q:116:ILE:HD12	4:Q:116:ILE:HA	1.90	0.40
4:Q:161:ALA:O	4:Q:162:PRO:C	2.60	0.40
7:T:38:LEU:O	7:T:42:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	427 (97%)	12 (3%)	2 (0%)	29	26
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	29	26
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	47	49
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	13	8
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	25	21
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	11	6
4	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
4	Q	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	179 (92%)	14 (7%)	1 (0%)	29	26
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	15	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	97/110 (88%)	97 (100%)	0	0	100	100
6	S	97/110 (88%)	95 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	71 (96%)	2 (3%)	1 (1%)	11	6
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
9	I	38/78 (49%)	35 (92%)	1 (3%)	2 (5%)	2	0
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	5	2
10	J	28/62 (45%)	26 (93%)	1 (4%)	1 (4%)	3	1
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
All	All	3947/4220 (94%)	3811 (97%)	110 (3%)	26 (1%)	22	18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	41	PRO
10	J	61	ASN
1	N	2	ALA
2	O	226	ILE
2	O	233	SER
3	P	11	MET
3	P	16	ASN
3	P	17	ALA
9	V	41	PRO
10	W	61	ASN
1	A	224	ASP
2	B	171	ALA
3	C	17	ALA
5	E	191	ASP
2	O	171	ALA
3	P	12	LYS
5	R	190	ASP
7	T	72	LYS
3	C	16	ASN
9	I	71	ASN
2	O	227	ARG
5	R	189	SER
2	O	229	GLY

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Mol	Chain	Res	Type
1	A	228	VAL
3	P	13	ILE
1	N	228	VAL

5.3.2 Protein sidechains ⓘ

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	363/370 (98%)	356 (98%)	7 (2%)	57	63
1	N	363/370 (98%)	355 (98%)	8 (2%)	52	57
2	B	332/343 (97%)	330 (99%)	2 (1%)	86	90
2	O	332/343 (97%)	329 (99%)	3 (1%)	78	84
3	C	313/327 (96%)	307 (98%)	6 (2%)	57	63
3	P	317/327 (97%)	311 (98%)	6 (2%)	57	63
4	D	206/206 (100%)	203 (98%)	3 (2%)	65	71
4	Q	206/206 (100%)	202 (98%)	4 (2%)	57	63
5	E	168/168 (100%)	167 (99%)	1 (1%)	86	90
5	R	168/168 (100%)	165 (98%)	3 (2%)	59	65
6	F	90/98 (92%)	89 (99%)	1 (1%)	73	79
6	S	90/98 (92%)	88 (98%)	2 (2%)	52	57
7	G	66/71 (93%)	64 (97%)	2 (3%)	41	44
7	T	66/71 (93%)	63 (96%)	3 (4%)	27	27
8	H	63/74 (85%)	61 (97%)	2 (3%)	39	41
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	27 (96%)	1 (4%)	35	36
9	V	28/60 (47%)	26 (93%)	2 (7%)	14	11
10	J	23/52 (44%)	23 (100%)	0	100	100
10	W	51/52 (98%)	51 (100%)	0	100	100
All	All	3336/3538 (94%)	3280 (98%)	56 (2%)	60	67

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	51	LYS
1	A	58	PHE
1	A	245	GLU
1	A	281	ASP
1	A	348	SER
1	A	365	LEU
2	B	227	ARG
2	B	354	ASN
3	C	80	ARG
3	C	90	PHE
3	C	128	PHE
3	C	222	PRO
3	C	346	PRO
3	C	379	TRP
4	D	17	LEU
4	D	43	MET
4	D	241	LYS
5	E	35	PHE
6	F	33	ARG
7	G	45	ILE
7	G	73	ASN
8	H	48	SER
8	H	51	GLU
9	I	42	VAL
1	N	20	ASP
1	N	32	GLN
1	N	58	PHE
1	N	184	GLU
1	N	245	GLU
1	N	281	ASP
1	N	348	SER
1	N	365	LEU
2	O	305	GLN
2	O	349	GLN
2	O	354	ASN
3	P	12	LYS
3	P	80	ARG
3	P	90	PHE
3	P	128	PHE
3	P	222	PRO
3	P	379	TRP

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Mol	Chain	Res	Type
4	Q	17	LEU
4	Q	35	GLN
4	Q	43	MET
4	Q	79	GLU
5	R	35	PHE
5	R	113	GLU
5	R	190	ASP
6	S	13	LEU
6	S	33	ARG
7	T	45	ILE
7	T	72	LYS
7	T	73	ASN
9	V	42	VAL
9	V	62	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	119	ASN
1	A	136	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS
1	A	308	GLN
2	B	104	ASN
2	B	240	HIS
2	B	305	GLN
2	B	343	GLN
2	B	401	GLN
2	B	412	ASN
2	B	432	HIS
3	C	54	HIS
3	C	159	ASN
3	C	345	HIS
5	E	57	GLN
7	G	73	ASN
1	N	9	GLN
1	N	32	GLN
1	N	119	ASN
1	N	136	GLN
1	N	213	GLN

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Mol	Chain	Res	Type
1	N	271	GLN
1	N	301	ASN
1	N	308	GLN
2	O	104	ASN
2	O	154	ASN
2	O	240	HIS
2	O	305	GLN
2	O	401	GLN
2	O	412	ASN
2	O	432	HIS
3	P	16	ASN
3	P	159	ASN
3	P	345	HIS
4	Q	35	GLN
5	R	57	GLN
5	R	116	GLN
8	U	49	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 123 ligands modelled in this entry, 74 are unknown - leaving 49 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
12	PO4	T	4016	-	4,4,4	1.39	1 (25%)	6,6,6	5.79	5 (83%)
12	PO4	A	2010	-	4,4,4	1.42	1 (25%)	6,6,6	5.79	5 (83%)
11	JZR	F	3012	-	18,18,18	1.89	5 (27%)	23,23,23	0.73	0
20	GOL	P	4009	-	5,5,5	1.08	0	5,5,5	0.53	0
15	PEE	C	2007	-	48,48,50	1.08	5 (10%)	51,53,55	0.85	4 (7%)
12	PO4	P	3010	-	4,4,4	1.33	1 (25%)	6,6,6	5.79	5 (83%)
22	FES	R	501	5	0,4,4	0.00	-	-	-	-
12	PO4	D	4011	-	4,4,4	1.33	1 (25%)	6,6,6	5.82	5 (83%)
20	GOL	E	4007	-	3,4,5	1.10	0	1,4,5	0.42	0
15	PEE	D	2006	-	50,50,50	1.24	5 (10%)	53,55,55	0.85	4 (7%)
15	PEE	P	3007	-	48,48,50	1.11	4 (8%)	51,53,55	0.85	4 (7%)
16	HEM	C	501	3	27,50,50	1.84	7 (25%)	17,82,82	1.73	5 (29%)
22	FES	E	501	5	0,4,4	0.00	-	-	-	-
20	GOL	C	4008	-	5,5,5	1.23	0	5,5,5	0.56	0
20	GOL	C	2008	-	5,5,5	1.28	0	5,5,5	0.67	0
15	PEE	B	4017	-	4,7,50	0.50	0	3,7,55	0.41	0
12	PO4	O	2009	-	4,4,4	1.37	0	6,6,6	5.78	5 (83%)
13	AZI	C	2005	-	0,2,2	0.00	-	0,1,1	0.00	-
11	JZR	A	4004	-	18,18,18	1.36	4 (22%)	23,23,23	0.58	0
20	GOL	P	3008	-	5,5,5	1.23	0	5,5,5	0.53	0
19	CDL	C	2004	-	43,43,99	1.14	3 (6%)	49,55,111	1.23	4 (8%)
20	GOL	O	4005	-	5,5,5	1.29	0	5,5,5	0.63	0
11	JZR	C	2011	-	18,18,18	1.84	5 (27%)	23,23,23	0.70	0
12	PO4	I	4015	-	4,4,4	1.37	1 (25%)	6,6,6	5.82	5 (83%)
18	UQ	C	2002	-	18,18,63	2.45	9 (50%)	19,24,79	0.84	1 (5%)
11	JZR	S	2012	-	18,18,18	1.88	6 (33%)	23,23,23	0.70	0
17	SMA	C	2001	-	35,38,38	1.35	5 (14%)	46,52,52	1.82	8 (17%)
17	SMA	P	3001	-	35,38,38	1.41	5 (14%)	46,52,52	1.70	6 (13%)
12	PO4	B	3009	-	4,4,4	1.37	1 (25%)	6,6,6	5.80	5 (83%)
20	GOL	E	4006	-	5,5,5	1.31	0	5,5,5	0.64	0
15	PEE	Q	3006	-	50,50,50	1.22	6 (12%)	53,55,55	0.84	4 (7%)
16	HEM	P	502	3	27,50,50	1.69	6 (22%)	17,82,82	1.75	6 (35%)
19	CDL	P	3004	-	48,48,99	1.12	2 (4%)	54,60,111	1.11	3 (5%)
13	AZI	A	4002	-	0,2,2	0.00	-	0,1,1	0.00	-
16	HEM	P	501	3	27,50,50	1.74	6 (22%)	17,82,82	1.65	4 (23%)
12	PO4	D	4010	-	4,4,4	1.38	1 (25%)	6,6,6	5.80	5 (83%)
16	HEM	C	502	3	27,50,50	1.55	5 (18%)	17,82,82	1.78	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CDL	Q	3003	-	38,38,99	1.08	3 (7%)	43,47,111	1.04	3 (6%)
18	UQ	P	3002	-	18,18,63	2.26	9 (50%)	19,24,79	0.76	1 (5%)
19	CDL	D	2003	-	38,38,99	1.04	1 (2%)	43,47,111	1.08	3 (6%)
11	JZR	P	3011	-	18,18,18	1.84	5 (27%)	23,23,23	0.70	0
21	HEC	Q	501	4	26,50,50	1.80	6 (23%)	18,82,82	1.02	1 (5%)
21	HEC	D	501	4	26,50,50	1.98	5 (19%)	18,82,82	0.99	1 (5%)
12	PO4	R	4014	-	4,4,4	1.40	1 (25%)	6,6,6	5.80	5 (83%)
11	JZR	F	4003	-	18,18,18	1.85	5 (27%)	23,23,23	0.67	0
13	AZI	G	4001	-	0,2,2	0.00	-	0,1,1	0.00	-
13	AZI	P	3005	-	0,2,2	0.00	-	0,1,1	0.00	-
12	PO4	R	4013	-	4,4,4	1.41	1 (25%)	6,6,6	5.80	5 (83%)
12	PO4	Q	4012	-	4,4,4	1.50	1 (25%)	6,6,6	5.80	5 (83%)

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
19	CDL	D	2003	-	-	21/43/43/110	-
20	GOL	P	4009	-	-	2/4/4/4	-
15	PEE	C	2007	-	-	21/52/52/54	-
22	FES	R	501	5	-	-	0/1/1/1
15	PEE	D	2006	-	-	23/54/54/54	-
15	PEE	P	3007	-	-	22/52/52/54	-
16	HEM	C	501	3	-	0/6/54/54	-
22	FES	E	501	5	-	-	0/1/1/1
20	GOL	C	4008	-	-	0/4/4/4	-
20	GOL	C	2008	-	-	2/4/4/4	-
15	PEE	B	4017	-	-	1/3/5/54	-
11	JZR	A	4004	-	-	1/9/29/29	0/1/1/1
20	GOL	P	3008	-	-	0/4/4/4	-
19	CDL	C	2004	-	-	30/52/52/110	-
20	GOL	O	4005	-	-	3/4/4/4	-
11	JZR	C	2011	-	-	4/9/29/29	0/1/1/1
20	GOL	E	4007	-	-	2/2/2/4	-
18	UQ	C	2002	-	-	1/9/33/87	0/1/1/1
11	JZR	S	2012	-	-	5/9/29/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SMA	C	2001	-	-	1/33/34/34	0/2/2/2
17	SMA	P	3001	-	-	3/33/34/34	0/2/2/2
15	PEE	Q	3006	-	-	23/54/54/54	-
16	HEM	P	502	3	-	0/6/54/54	-
19	CDL	P	3004	-	-	27/57/57/110	-
16	HEM	P	501	3	-	0/6/54/54	-
16	HEM	C	502	3	-	0/6/54/54	-
19	CDL	Q	3003	-	-	22/43/43/110	-
18	UQ	P	3002	-	-	3/9/33/87	0/1/1/1
11	JZR	F	3012	-	-	2/9/29/29	0/1/1/1
11	JZR	P	3011	-	-	3/9/29/29	0/1/1/1
21	HEC	Q	501	4	-	0/6/54/54	-
21	HEC	D	501	4	-	0/6/54/54	-
11	JZR	F	4003	-	-	4/9/29/29	0/1/1/1
20	GOL	E	4006	-	-	4/4/4/4	-

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	C3B-C2B	-6.39	1.34	1.40
21	Q	501	HEC	C3B-C2B	-5.19	1.35	1.40
21	D	501	HEC	C3C-C2C	-4.98	1.35	1.40
11	S	2012	JZR	O1-C1	4.81	1.48	1.40
11	F	3012	JZR	O1-C1	4.79	1.48	1.40
11	P	3011	JZR	O1-C1	4.78	1.48	1.40
11	C	2011	JZR	O1-C1	4.72	1.48	1.40
11	F	4003	JZR	O1-C1	4.69	1.48	1.40
18	C	2002	UQ	C7-C6	4.65	1.59	1.51
18	P	3002	UQ	C7-C6	3.93	1.57	1.51
16	P	501	HEM	C3C-CAC	-3.85	1.39	1.47
16	C	501	HEM	C3C-CAC	-3.83	1.40	1.47
18	C	2002	UQ	C6-C5	3.67	1.41	1.35
17	C	2001	SMA	C4-C3	3.65	1.51	1.41
21	Q	501	HEC	C3C-C2C	-3.64	1.36	1.40
17	P	3001	SMA	O1-C2	3.57	1.40	1.35
18	C	2002	UQ	C6-C1	3.55	1.56	1.46
18	P	3002	UQ	C6-C1	3.54	1.56	1.46
11	F	3012	JZR	O5-C1	3.52	1.50	1.41
16	P	501	HEM	CBC-CAC	3.50	1.52	1.29
11	S	2012	JZR	O5-C1	3.50	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	2002	UQ	O2-C2	3.46	1.45	1.36
16	C	501	HEM	C3C-C2C	-3.43	1.35	1.40
16	C	501	HEM	CBB-CAB	3.41	1.51	1.29
11	F	4003	JZR	O5-C1	3.38	1.50	1.41
16	P	502	HEM	CBC-CAC	3.34	1.51	1.29
16	C	501	HEM	CMA-C3A	3.34	1.58	1.51
18	P	3002	UQ	C6-C5	3.30	1.41	1.35
17	C	2001	SMA	C20-C19	3.30	1.36	1.33
18	P	3002	UQ	O2-C2	3.26	1.44	1.36
16	P	502	HEM	C3C-CAC	-3.24	1.41	1.47
18	C	2002	UQ	C2-C1	3.21	1.58	1.48
11	C	2011	JZR	O5-C1	3.21	1.50	1.41
16	P	501	HEM	C3C-C2C	-3.14	1.36	1.40
17	C	2001	SMA	O1-C2	3.13	1.39	1.35
16	C	502	HEM	C3C-CAC	-3.13	1.41	1.47
15	P	3007	PEE	C22-C21	-3.12	1.34	1.51
17	P	3001	SMA	C4-C3	3.11	1.50	1.41
16	P	501	HEM	C4B-NB	3.10	1.42	1.36
16	P	502	HEM	CBB-CAB	3.10	1.49	1.29
18	C	2002	UQ	O3-C3	3.06	1.44	1.36
15	D	2006	PEE	P-O1P	3.05	1.61	1.50
15	P	3007	PEE	O3-C30	3.05	1.42	1.33
15	C	2007	PEE	C22-C21	-3.04	1.34	1.51
11	P	3011	JZR	O5-C1	3.03	1.49	1.41
16	P	502	HEM	C3C-C2C	-3.03	1.36	1.40
15	Q	3006	PEE	C19-C18	-3.03	1.34	1.51
17	P	3001	SMA	C20-C19	3.01	1.36	1.33
15	C	2007	PEE	C19-C18	-3.01	1.34	1.51
15	D	2006	PEE	C19-C18	-3.00	1.34	1.51
15	Q	3006	PEE	O3-C30	2.99	1.42	1.33
15	D	2006	PEE	C22-C21	-2.97	1.34	1.51
15	P	3007	PEE	C19-C18	-2.96	1.34	1.51
15	Q	3006	PEE	C22-C21	-2.93	1.35	1.51
16	C	502	HEM	CBB-CAB	2.93	1.48	1.29
11	A	4004	JZR	O1-C1	2.93	1.45	1.40
17	P	3001	SMA	C7-C8	2.92	1.44	1.40
16	P	501	HEM	C3B-CAB	-2.90	1.42	1.47
18	P	3002	UQ	O3-C3	2.88	1.43	1.36
11	A	4004	JZR	C4-C5	2.85	1.59	1.53
15	D	2006	PEE	O3-C30	2.84	1.41	1.33
16	P	501	HEM	CBB-CAB	2.84	1.48	1.29
18	P	3002	UQ	C2-C1	2.84	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	C3C-C4C	2.84	1.48	1.43
18	P	3002	UQ	CM5-C5	2.83	1.56	1.50
16	C	501	HEM	CBC-CAC	2.82	1.48	1.29
15	D	2006	PEE	O2-C10	2.81	1.42	1.34
16	C	502	HEM	CBC-CAC	2.77	1.47	1.29
15	Q	3006	PEE	P-O1P	2.76	1.60	1.50
18	C	2002	UQ	CM5-C5	2.75	1.56	1.50
15	Q	3006	PEE	O2-C10	2.72	1.42	1.34
16	P	502	HEM	C3B-CAB	-2.70	1.42	1.47
21	D	501	HEC	C3B-C4B	2.66	1.47	1.43
21	Q	501	HEC	C1C-NC	2.66	1.41	1.36
16	P	502	HEM	C1D-ND	2.64	1.41	1.36
15	C	2007	PEE	P-O1P	2.63	1.60	1.50
11	C	2011	JZR	C4-C5	2.62	1.58	1.53
18	C	2002	UQ	C5-C4	2.50	1.56	1.47
11	P	3011	JZR	C4-C5	2.48	1.58	1.53
11	F	4003	JZR	C4-C5	2.46	1.58	1.53
15	P	3007	PEE	P-O1P	2.46	1.59	1.50
11	S	2012	JZR	C4-C5	2.44	1.58	1.53
11	A	4004	JZR	O5-C1	2.44	1.48	1.41
16	C	502	HEM	C3B-CAB	-2.42	1.43	1.47
11	F	3012	JZR	O5-C5	2.42	1.50	1.44
16	C	502	HEM	C1D-ND	2.38	1.41	1.36
15	C	2007	PEE	O3-C30	2.38	1.40	1.33
18	P	3002	UQ	C3-C4	2.36	1.55	1.48
16	C	501	HEM	C4D-C3D	2.35	1.47	1.42
21	Q	501	HEC	C3B-C4B	2.33	1.47	1.43
11	S	2012	JZR	O5-C5	2.31	1.49	1.44
18	P	3002	UQ	C5-C4	2.31	1.55	1.47
19	Q	3003	CDL	O1-C1	2.30	1.50	1.43
19	D	2003	CDL	O1-C1	2.29	1.50	1.43
17	P	3001	SMA	C6-C7	2.29	1.42	1.38
19	C	2004	CDL	OA8-CA6	-2.27	1.40	1.45
19	P	3004	CDL	O1-C1	2.27	1.50	1.43
11	F	3012	JZR	C4-C5	2.26	1.57	1.53
21	Q	501	HEC	C3C-C4C	2.24	1.47	1.43
19	P	3004	CDL	OA8-CA6	-2.22	1.40	1.45
12	T	4016	PO4	P-O1	2.22	1.56	1.50
11	F	3012	JZR	C1-C2	2.22	1.58	1.52
18	C	2002	UQ	C3-C4	2.21	1.55	1.48
11	P	3011	JZR	C1-C2	2.20	1.58	1.52
12	A	2010	PO4	P-O1	2.19	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	4003	JZR	O5-C5	2.17	1.49	1.44
16	C	501	HEM	C3B-CAB	-2.17	1.43	1.47
11	C	2011	JZR	C1-C2	2.16	1.58	1.52
21	Q	501	HEC	C1B-NB	2.15	1.40	1.36
19	Q	3003	CDL	OB8-CB6	-2.15	1.40	1.45
11	C	2011	JZR	O5-C5	2.13	1.49	1.44
15	Q	3006	PEE	C3-C2	2.12	1.57	1.50
12	R	4014	PO4	P-O1	2.12	1.55	1.50
12	Q	4012	PO4	P-O1	2.11	1.55	1.50
15	C	2007	PEE	O2-C10	2.10	1.40	1.34
12	B	3009	PO4	P-O1	2.10	1.55	1.50
12	R	4013	PO4	P-O1	2.10	1.55	1.50
17	C	2001	SMA	C6-C7	2.08	1.42	1.38
12	P	3010	PO4	P-O1	2.08	1.55	1.50
11	F	4003	JZR	C1-C2	2.07	1.58	1.52
12	D	4010	PO4	P-O1	2.06	1.55	1.50
12	D	4011	PO4	P-O1	2.06	1.55	1.50
11	A	4004	JZR	C4-C3	2.05	1.57	1.52
11	P	3011	JZR	O5-C5	2.04	1.49	1.44
11	S	2012	JZR	C1-C2	2.03	1.58	1.52
17	C	2001	SMA	C7-C8	2.03	1.43	1.40
12	I	4015	PO4	P-O1	2.03	1.55	1.50
11	S	2012	JZR	C4-C3	2.02	1.57	1.52
19	Q	3003	CDL	OB5-CB3	-2.01	1.37	1.44
19	C	2004	CDL	OA5-CA3	-2.01	1.37	1.44
19	C	2004	CDL	O1-C1	2.00	1.49	1.43
21	D	501	HEC	C1C-NC	2.00	1.40	1.36

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	2009	PO4	O4-P-O1	-8.18	80.98	110.89
12	R	4013	PO4	O4-P-O1	-8.15	81.06	110.89
12	I	4015	PO4	O4-P-O1	-8.12	81.16	110.89
12	D	4010	PO4	O4-P-O1	-8.12	81.18	110.89
12	T	4016	PO4	O4-P-O1	-8.10	81.25	110.89
12	A	2010	PO4	O4-P-O1	-8.10	81.27	110.89
12	Q	4012	PO4	O4-P-O1	-8.09	81.30	110.89
12	B	3009	PO4	O4-P-O1	-8.08	81.32	110.89
12	R	4014	PO4	O4-P-O1	-8.08	81.33	110.89
12	P	3010	PO4	O4-P-O1	-8.07	81.38	110.89
12	D	4011	PO4	O4-P-O1	-8.02	81.55	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	4015	PO4	O4-P-O2	-7.92	82.56	107.97
12	D	4011	PO4	O4-P-O2	-7.77	83.02	107.97
12	Q	4012	PO4	O4-P-O2	-7.74	83.11	107.97
12	R	4014	PO4	O4-P-O2	-7.73	83.15	107.97
12	P	3010	PO4	O4-P-O2	-7.73	83.16	107.97
12	D	4010	PO4	O4-P-O2	-7.70	83.25	107.97
12	A	2010	PO4	O4-P-O2	-7.69	83.28	107.97
12	B	3009	PO4	O4-P-O2	-7.68	83.33	107.97
12	R	4013	PO4	O4-P-O2	-7.63	83.47	107.97
12	T	4016	PO4	O4-P-O2	-7.61	83.54	107.97
12	O	2009	PO4	O4-P-O2	-7.50	83.89	107.97
12	D	4011	PO4	O4-P-O3	-7.11	85.16	107.97
12	T	4016	PO4	O4-P-O3	-7.09	85.22	107.97
12	B	3009	PO4	O4-P-O3	-7.04	85.37	107.97
12	O	2009	PO4	O4-P-O3	-7.04	85.38	107.97
12	Q	4012	PO4	O4-P-O3	-7.03	85.40	107.97
12	R	4013	PO4	O4-P-O3	-7.02	85.43	107.97
12	R	4014	PO4	O4-P-O3	-7.02	85.45	107.97
12	D	4010	PO4	O4-P-O3	-7.00	85.52	107.97
12	A	2010	PO4	O4-P-O3	-6.98	85.58	107.97
12	P	3010	PO4	O4-P-O3	-6.97	85.60	107.97
12	I	4015	PO4	O4-P-O3	-6.78	86.21	107.97
17	C	2001	SMA	C9-C2-C3	6.52	129.63	120.39
17	C	2001	SMA	C3-C4-C4A	-5.70	114.85	120.58
17	P	3001	SMA	C3-C4-C4A	-5.54	115.01	120.58
17	P	3001	SMA	C9-C2-C3	5.45	128.12	120.39
12	I	4015	PO4	O2-P-O1	4.69	128.06	110.89
12	B	3009	PO4	O2-P-O1	4.65	127.91	110.89
12	P	3010	PO4	O2-P-O1	4.63	127.82	110.89
12	R	4014	PO4	O2-P-O1	4.61	127.78	110.89
12	O	2009	PO4	O2-P-O1	4.61	127.75	110.89
12	A	2010	PO4	O2-P-O1	4.60	127.73	110.89
12	T	4016	PO4	O2-P-O1	4.60	127.71	110.89
12	D	4011	PO4	O2-P-O1	4.58	127.67	110.89
12	D	4010	PO4	O2-P-O1	4.57	127.63	110.89
12	R	4013	PO4	O2-P-O1	4.56	127.58	110.89
12	Q	4012	PO4	O2-P-O1	4.47	127.26	110.89
16	P	501	HEM	C4A-C3A-C2A	-4.26	104.03	107.00
19	C	2004	CDL	CA4-OA6-CA5	-4.25	109.98	117.90
17	P	3001	SMA	C9-C10-C11	-4.20	109.07	114.72
17	C	2001	SMA	O1-C2-C9	-4.03	107.13	111.91
17	C	2001	SMA	C9-C10-C11	-3.99	109.35	114.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	501	HEM	C4A-C3A-C2A	-3.65	104.46	107.00
19	P	3004	CDL	CA4-OA6-CA5	-3.63	111.14	117.90
16	C	501	HEM	C1D-C2D-C3D	-3.62	104.48	107.00
17	P	3001	SMA	C4-C3-C2	3.58	120.56	116.63
16	C	502	HEM	CBD-CAD-C3D	-3.49	106.04	112.48
16	P	502	HEM	CBD-CAD-C3D	-3.30	106.39	112.48
19	C	2004	CDL	CB4-OB6-CB5	-3.28	109.72	117.79
17	C	2001	SMA	C4-C3-C2	3.15	120.08	116.63
16	P	501	HEM	CMA-C3A-C2A	3.01	130.62	124.94
15	P	3007	PEE	C20-C19-C18	2.92	129.27	114.42
15	C	2007	PEE	C20-C19-C18	2.89	129.07	114.42
21	Q	501	HEC	CBD-CAD-C3D	-2.85	107.23	112.49
19	P	3004	CDL	CA6-OA8-CA7	-2.83	109.98	117.10
15	Q	3006	PEE	C20-C19-C18	2.82	128.72	114.42
15	D	2006	PEE	C20-C19-C18	2.79	128.60	114.42
19	P	3004	CDL	CB4-OB6-CB5	-2.79	110.93	117.79
19	D	2003	CDL	CB6-CB4-CB3	-2.78	105.20	111.79
17	P	3001	SMA	O1-C2-C9	-2.78	108.62	111.91
19	Q	3003	CDL	CB4-OB6-CB5	-2.71	111.12	117.79
16	C	502	HEM	CMB-C2B-C3B	2.67	129.67	124.68
12	D	4011	PO4	O3-P-O2	2.65	116.46	107.97
16	C	502	HEM	CBA-CAA-C2A	-2.62	107.66	112.49
17	C	2001	SMA	C10-C9-C2	2.61	119.21	113.59
12	R	4013	PO4	O3-P-O2	2.60	116.32	107.97
12	D	4010	PO4	O3-P-O2	2.59	116.28	107.97
19	D	2003	CDL	CB4-OB6-CB5	-2.58	111.43	117.79
19	Q	3003	CDL	CB6-CB4-CB3	-2.58	105.69	111.79
15	D	2006	PEE	C19-C18-C17	2.57	127.48	114.42
12	Q	4012	PO4	O3-P-O2	2.57	116.22	107.97
12	I	4015	PO4	O3-P-O2	2.57	116.21	107.97
15	C	2007	PEE	C19-C18-C17	2.56	127.41	114.42
12	R	4014	PO4	O3-P-O2	2.55	116.15	107.97
16	C	501	HEM	C3B-C4B-NB	2.54	112.50	109.21
12	P	3010	PO4	O3-P-O2	2.54	116.13	107.97
15	P	3007	PEE	C19-C18-C17	2.54	127.32	114.42
12	T	4016	PO4	O3-P-O2	2.54	116.11	107.97
12	B	3009	PO4	O3-P-O2	2.52	116.07	107.97
12	O	2009	PO4	O3-P-O2	2.52	116.05	107.97
12	A	2010	PO4	O3-P-O2	2.52	116.05	107.97
15	Q	3006	PEE	C22-C21-C20	2.50	127.14	114.42
15	D	2006	PEE	C22-C21-C20	2.50	127.12	114.42
16	C	501	HEM	CBA-CAA-C2A	-2.49	107.90	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	3006	PEE	C19-C18-C17	2.49	127.05	114.42
16	P	502	HEM	CMC-C2C-C3C	2.48	129.32	124.68
16	C	502	HEM	CMC-C2C-C3C	2.47	129.29	124.68
19	C	2004	CDL	CA6-CA4-CA3	-2.44	106.01	111.79
17	P	3001	SMA	C10-C9-C2	2.43	118.81	113.59
15	C	2007	PEE	C22-C21-C20	2.43	126.74	114.42
15	P	3007	PEE	C22-C21-C20	2.42	126.72	114.42
19	C	2004	CDL	CA6-OA8-CA7	-2.42	111.03	117.10
15	C	2007	PEE	C23-C22-C21	2.41	126.68	114.42
16	P	502	HEM	C3B-C4B-NB	2.41	112.32	109.21
15	P	3007	PEE	C23-C22-C21	2.37	126.47	114.42
18	C	2002	UQ	C6-C5-C4	2.36	121.05	119.18
16	C	501	HEM	CMB-C2B-C3B	2.30	128.98	124.68
15	D	2006	PEE	C23-C22-C21	2.29	126.06	114.42
15	Q	3006	PEE	C23-C22-C21	2.28	126.02	114.42
16	P	502	HEM	C4C-C3C-C2C	2.25	108.47	106.90
16	P	502	HEM	CBA-CAA-C2A	2.24	116.61	112.49
16	C	502	HEM	C3B-C4B-NB	2.19	112.04	109.21
16	C	502	HEM	CMD-C2D-C1D	-2.18	125.12	128.46
21	D	501	HEC	CBD-CAD-C3D	-2.13	108.56	112.49
17	C	2001	SMA	O8-C8-C8A	2.12	123.52	119.62
17	C	2001	SMA	C8-C8A-C4A	2.12	123.86	119.44
19	D	2003	CDL	OA4-PA1-OA2	2.10	112.33	106.73
18	P	3002	UQ	C6-C5-C4	2.06	120.81	119.18
16	P	501	HEM	C4C-C3C-C2C	-2.06	105.46	106.90
16	P	502	HEM	CMB-C2B-C3B	2.05	128.52	124.68
16	P	501	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
19	Q	3003	CDL	OA4-PA1-OA2	2.01	112.07	106.73

There are no chirality outliers.

All (230) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	2006	PEE	O4P-C4-C5-N
15	D	2006	PEE	C1-O3P-P-O2P
15	D	2006	PEE	C4-O4P-P-O2P
19	C	2004	CDL	CA3-OA5-PA1-OA3
19	C	2004	CDL	CA3-OA5-PA1-OA4
19	C	2004	CDL	C11-CA5-OA6-CA4
19	C	2004	CDL	CB2-OB2-PB2-OB4
19	C	2004	CDL	C51-CB5-OB6-CB4
19	Q	3003	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
19	Q	3003	CDL	CB2-OB2-PB2-OB5
19	Q	3003	CDL	CB3-OB5-PB2-OB4
19	Q	3003	CDL	OB6-CB4-CB6-OB8
19	D	2003	CDL	CB2-OB2-PB2-OB3
19	D	2003	CDL	CB2-OB2-PB2-OB4
19	D	2003	CDL	CB2-OB2-PB2-OB5
15	Q	3006	PEE	O4P-C4-C5-N
15	Q	3006	PEE	C1-O3P-P-O2P
15	Q	3006	PEE	C4-O4P-P-O2P
19	P	3004	CDL	C11-CA5-OA6-CA4
20	E	4007	GOL	O1-C1-C2-O2
20	E	4007	GOL	O1-C1-C2-C3
18	P	3002	UQ	C12-C11-C9-C8
20	E	4006	GOL	C1-C2-C3-O3
20	P	4009	GOL	O1-C1-C2-C3
19	P	3004	CDL	C31-CA7-OA8-CA6
19	C	2004	CDL	OA9-CA7-OA8-CA6
19	C	2004	CDL	OB9-CB7-OB8-CB6
19	P	3004	CDL	OB9-CB7-OB8-CB6
19	C	2004	CDL	C31-CA7-OA8-CA6
19	C	2004	CDL	OB7-CB5-OB6-CB4
19	C	2004	CDL	OA7-CA5-OA6-CA4
19	P	3004	CDL	OA7-CA5-OA6-CA4
19	P	3004	CDL	OA9-CA7-OA8-CA6
19	C	2004	CDL	C71-CB7-OB8-CB6
19	Q	3003	CDL	C71-CB7-OB8-CB6
19	P	3004	CDL	C71-CB7-OB8-CB6
11	F	3012	JZR	O5-C5-C6-O6
19	Q	3003	CDL	OB9-CB7-OB8-CB6
19	P	3004	CDL	C51-CB5-OB6-CB4
15	P	3007	PEE	C18-C19-C20-C21
15	C	2007	PEE	C18-C19-C20-C21
11	C	2011	JZR	O5-C5-C6-O6
11	S	2012	JZR	C4-C5-C6-O6
11	F	3012	JZR	C4-C5-C6-O6
11	C	2011	JZR	C4-C5-C6-O6
11	S	2012	JZR	O5-C5-C6-O6
15	D	2006	PEE	C30-C31-C32-C33
20	E	4006	GOL	O2-C2-C3-O3
15	Q	3006	PEE	C30-C31-C32-C33
19	P	3004	CDL	OB7-CB5-OB6-CB4
15	P	3007	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
11	F	4003	JZR	O1-C1'-C2'-C3'
19	Q	3003	CDL	O1-C1-CB2-OB2
15	C	2007	PEE	C10-C11-C12-C13
15	D	2006	PEE	C4-O4P-P-O3P
19	C	2004	CDL	CA3-OA5-PA1-OA2
19	C	2004	CDL	CB2-OB2-PB2-OB5
19	Q	3003	CDL	CB3-OB5-PB2-OB2
15	Q	3006	PEE	C4-O4P-P-O3P
19	Q	3003	CDL	CA2-C1-CB2-OB2
19	Q	3003	CDL	C75-C76-C77-C78
15	P	3007	PEE	C31-C32-C33-C34
15	Q	3006	PEE	C13-C14-C15-C16
15	C	2007	PEE	C20-C21-C22-C23
15	C	2007	PEE	C31-C32-C33-C34
19	P	3004	CDL	C72-C73-C74-C75
15	D	2006	PEE	C13-C14-C15-C16
19	P	3004	CDL	C71-C72-C73-C74
15	P	3007	PEE	C20-C21-C22-C23
15	Q	3006	PEE	C38-C39-C40-C41
19	D	2003	CDL	O1-C1-CA2-OA2
15	D	2006	PEE	C34-C35-C36-C37
15	Q	3006	PEE	C14-C15-C16-C17
15	Q	3006	PEE	C37-C38-C39-C40
15	Q	3006	PEE	C22-C23-C24-C25
15	Q	3006	PEE	C43-C44-C45-C46
15	D	2006	PEE	C14-C15-C16-C17
15	D	2006	PEE	C22-C23-C24-C25
15	D	2006	PEE	C37-C38-C39-C40
15	D	2006	PEE	C38-C39-C40-C41
15	D	2006	PEE	C43-C44-C45-C46
19	Q	3003	CDL	C77-C78-C79-C80
15	Q	3006	PEE	C23-C24-C25-C26
15	Q	3006	PEE	C34-C35-C36-C37
15	D	2006	PEE	C23-C24-C25-C26
15	P	3007	PEE	C41-C42-C43-C44
15	C	2007	PEE	C41-C42-C43-C44
11	P	3011	JZR	C2'-C3'-C4'-C5'
15	C	2007	PEE	C16-C17-C18-C19
20	O	4005	GOL	C1-C2-C3-O3
20	C	2008	GOL	O1-C1-C2-C3
20	E	4006	GOL	O1-C1-C2-C3
19	C	2004	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
19	P	3004	CDL	C74-C75-C76-C77
19	Q	3003	CDL	C73-C74-C75-C76
19	D	2003	CDL	C72-C73-C74-C75
15	P	3007	PEE	C16-C17-C18-C19
15	C	2007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C35-C36-C37-C38
19	D	2003	CDL	C76-C77-C78-C79
19	D	2003	CDL	C75-C76-C77-C78
19	C	2004	CDL	C71-C72-C73-C74
11	C	2011	JZR	C1'-C2'-C3'-C4'
19	D	2003	CDL	C71-C72-C73-C74
15	P	3007	PEE	C34-C35-C36-C37
15	C	2007	PEE	C34-C35-C36-C37
19	P	3004	CDL	CB7-C71-C72-C73
19	C	2004	CDL	O1-C1-CA2-OA2
11	F	4003	JZR	C4-C5-C6-O6
11	P	3011	JZR	C1'-C2'-C3'-C4'
19	Q	3003	CDL	C76-C77-C78-C79
15	P	3007	PEE	C42-C43-C44-C45
15	P	3007	PEE	C15-C16-C17-C18
19	Q	3003	CDL	C78-C79-C80-C81
19	Q	3003	CDL	CB5-C51-C52-C53
15	P	3007	PEE	C32-C33-C34-C35
15	P	3007	PEE	C12-C13-C14-C15
15	C	2007	PEE	C15-C16-C17-C18
15	C	2007	PEE	C32-C33-C34-C35
15	C	2007	PEE	C42-C43-C44-C45
19	D	2003	CDL	C51-CB5-OB6-CB4
19	P	3004	CDL	OA6-CA4-CA6-OA8
19	D	2003	CDL	OB7-CB5-OB6-CB4
19	Q	3003	CDL	C51-CB5-OB6-CB4
15	D	2006	PEE	C1-O3P-P-O4P
15	Q	3006	PEE	C1-O3P-P-O4P
19	C	2004	CDL	OA5-CA3-CA4-CA6
15	C	2007	PEE	C12-C13-C14-C15
11	F	4003	JZR	C1'-C2'-C3'-C4'
19	C	2004	CDL	CB3-CB4-CB6-OB8
19	P	3004	CDL	CB3-CB4-CB6-OB8
15	P	3007	PEE	C37-C38-C39-C40
20	O	4005	GOL	O2-C2-C3-O3
20	C	2008	GOL	O1-C1-C2-O2
20	P	4009	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
15	D	2006	PEE	C41-C42-C43-C44
19	C	2004	CDL	CB7-C71-C72-C73
15	Q	3006	PEE	C41-C42-C43-C44
15	C	2007	PEE	C37-C38-C39-C40
15	D	2006	PEE	C35-C36-C37-C38
19	D	2003	CDL	C79-C80-C81-C82
15	C	2007	PEE	C19-C20-C21-C22
19	Q	3003	CDL	OB7-CB5-OB6-CB4
19	C	2004	CDL	C75-C76-C77-C78
15	Q	3006	PEE	C35-C36-C37-C38
15	P	3007	PEE	C43-C44-C45-C46
11	S	2012	JZR	C1'-C2'-C3'-C4'
11	F	4003	JZR	O5-C5-C6-O6
19	P	3004	CDL	C53-C54-C55-C56
19	P	3004	CDL	CA3-CA4-CA6-OA8
19	P	3004	CDL	CB2-OB2-PB2-OB5
20	E	4006	GOL	O1-C1-C2-O2
19	C	2004	CDL	OA5-CA3-CA4-OA6
15	P	3007	PEE	C19-C20-C21-C22
19	Q	3003	CDL	C51-C52-C53-C54
15	C	2007	PEE	C43-C44-C45-C46
11	C	2011	JZR	C2'-C3'-C4'-C5'
15	P	3007	PEE	C23-C24-C25-C26
19	P	3004	CDL	OA5-CA3-CA4-CA6
15	P	3007	PEE	C22-C23-C24-C25
19	D	2003	CDL	C78-C79-C80-C81
15	C	2007	PEE	C22-C23-C24-C25
18	P	3002	UQ	C1-C2-O2-CM2
19	Q	3003	CDL	CB3-CB4-CB6-OB8
15	C	2007	PEE	C23-C24-C25-C26
19	D	2003	CDL	CB2-C1-CA2-OA2
19	P	3004	CDL	OB6-CB4-CB6-OB8
19	D	2003	CDL	C73-C74-C75-C76
15	C	2007	PEE	C36-C37-C38-C39
19	P	3004	CDL	O1-C1-CA2-OA2
15	D	2006	PEE	C1-O3P-P-O1P
15	D	2006	PEE	C4-O4P-P-O1P
19	C	2004	CDL	CB2-OB2-PB2-OB3
19	C	2004	CDL	CB3-OB5-PB2-OB4
19	Q	3003	CDL	CB2-OB2-PB2-OB3
19	Q	3003	CDL	CB3-OB5-PB2-OB3
15	Q	3006	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
15	Q	3006	PEE	C4-O4P-P-O1P
19	P	3004	CDL	CB3-OB5-PB2-OB4
15	Q	3006	PEE	C20-C21-C22-C23
15	D	2006	PEE	C20-C21-C22-C23
19	C	2004	CDL	OB6-CB4-CB6-OB8
15	P	3007	PEE	C36-C37-C38-C39
19	P	3004	CDL	C51-C52-C53-C54
19	C	2004	CDL	C73-C74-C75-C76
15	C	2007	PEE	C11-C12-C13-C14
19	D	2003	CDL	OB9-CB7-OB8-CB6
19	P	3004	CDL	CB5-C51-C52-C53
19	D	2003	CDL	OB5-CB3-CB4-OB6
19	P	3004	CDL	OA5-CA3-CA4-OA6
19	D	2003	CDL	C71-CB7-OB8-CB6
15	D	2006	PEE	C1-C2-C3-O3
15	Q	3006	PEE	C1-C2-C3-O3
18	C	2002	UQ	C1-C2-O2-CM2
11	S	2012	JZR	C2'-C3'-C4'-C5'
15	Q	3006	PEE	C39-C40-C41-C42
15	P	3007	PEE	O4P-C4-C5-N
19	C	2004	CDL	C72-C73-C74-C75
15	D	2006	PEE	C39-C40-C41-C42
15	D	2006	PEE	C40-C41-C42-C43
17	P	3001	SMA	O14-C14-C15-C16
17	P	3001	SMA	C17-C18-C19-C26
19	Q	3003	CDL	OB5-CB3-CB4-CB6
11	A	4004	JZR	O1-C1'-C2'-C3'
19	C	2004	CDL	OA6-CA4-CA6-OA8
11	S	2012	JZR	O1-C1'-C2'-C3'
11	P	3011	JZR	O5-C5-C6-O6
19	D	2003	CDL	OB5-CB3-CB4-CB6
19	D	2003	CDL	C72-C71-CB7-OB8
19	P	3004	CDL	C72-C71-CB7-OB8
19	C	2004	CDL	C72-C71-CB7-OB8
15	Q	3006	PEE	C40-C41-C42-C43
17	P	3001	SMA	C17-C18-C19-C20
15	P	3007	PEE	C11-C12-C13-C14
15	C	2007	PEE	O3-C30-C31-C32
20	O	4005	GOL	O1-C1-C2-O2
15	B	4017	PEE	C12-C13-C14-C15
15	P	3007	PEE	O3-C30-C31-C32
17	C	2001	SMA	O14-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
15	P	3007	PEE	O5-C30-C31-C32
19	P	3004	CDL	C72-C71-CB7-OB9
19	C	2004	CDL	CA3-CA4-CA6-OA8
19	D	2003	CDL	C72-C71-CB7-OB9
19	P	3004	CDL	CB2-OB2-PB2-OB4
19	C	2004	CDL	C72-C71-CB7-OB9
19	D	2003	CDL	C74-C75-C76-C77
15	D	2006	PEE	C16-C17-C18-C19
15	Q	3006	PEE	C11-C12-C13-C14
18	P	3002	UQ	C3-C2-O2-CM2
15	C	2007	PEE	O5-C30-C31-C32

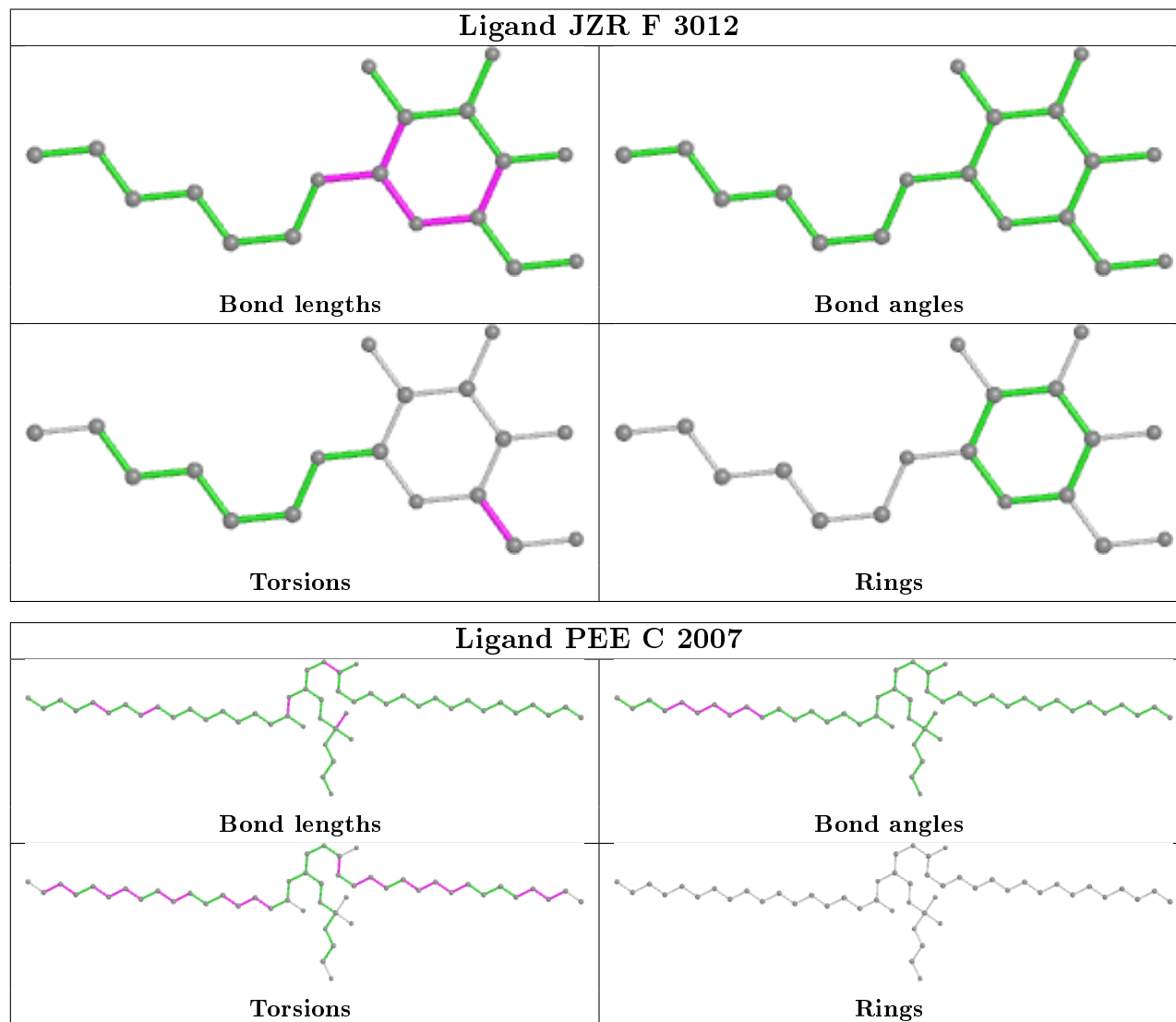
There are no ring outliers.

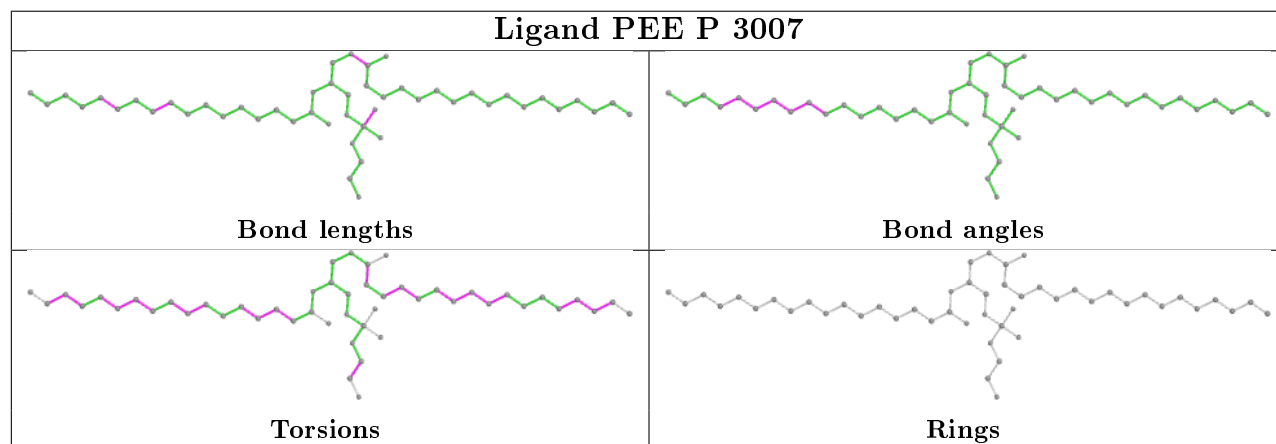
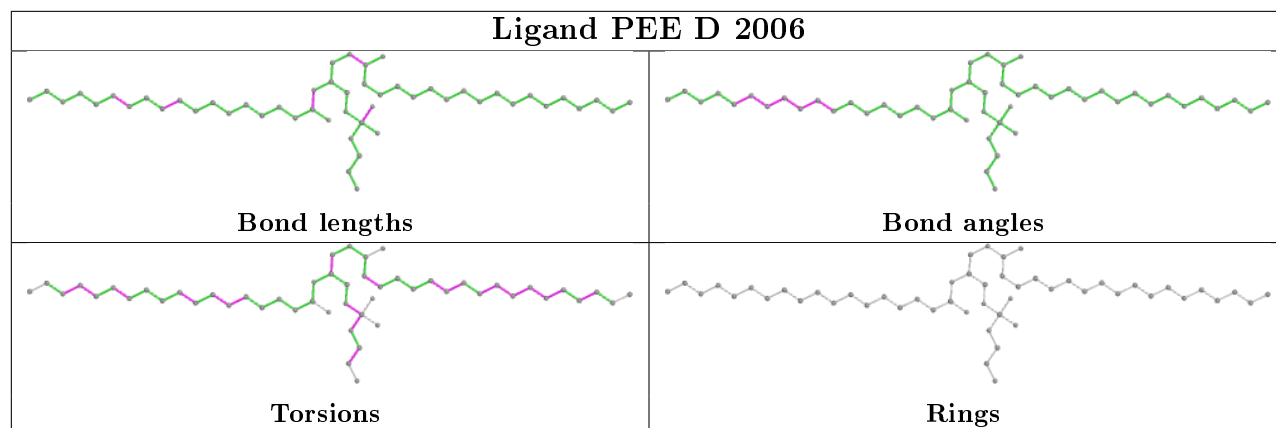
23 monomers are involved in 58 short contacts:

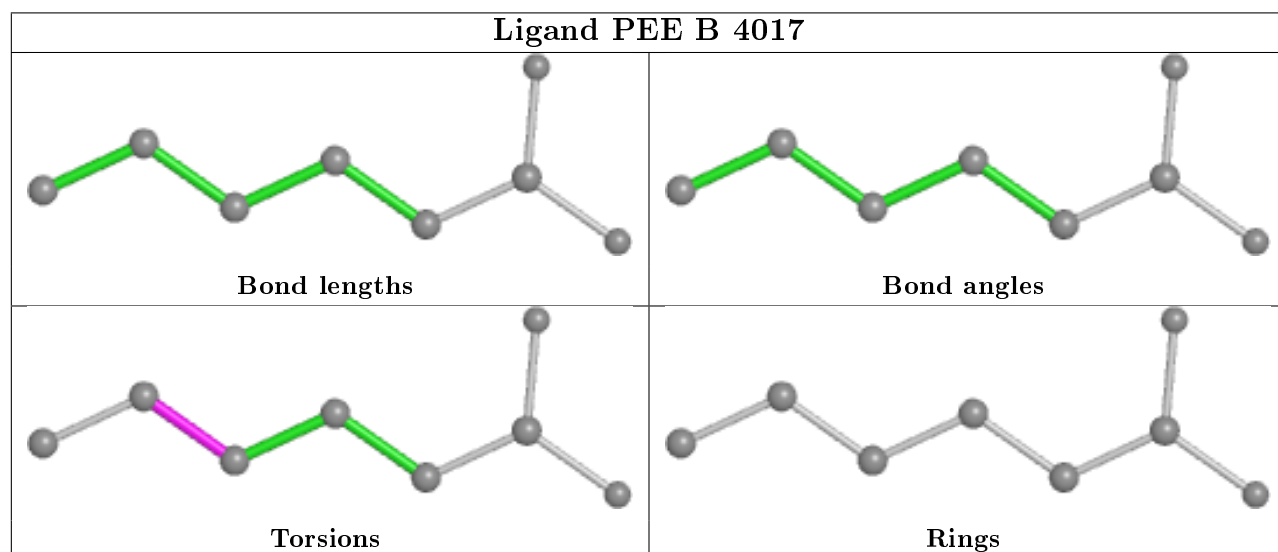
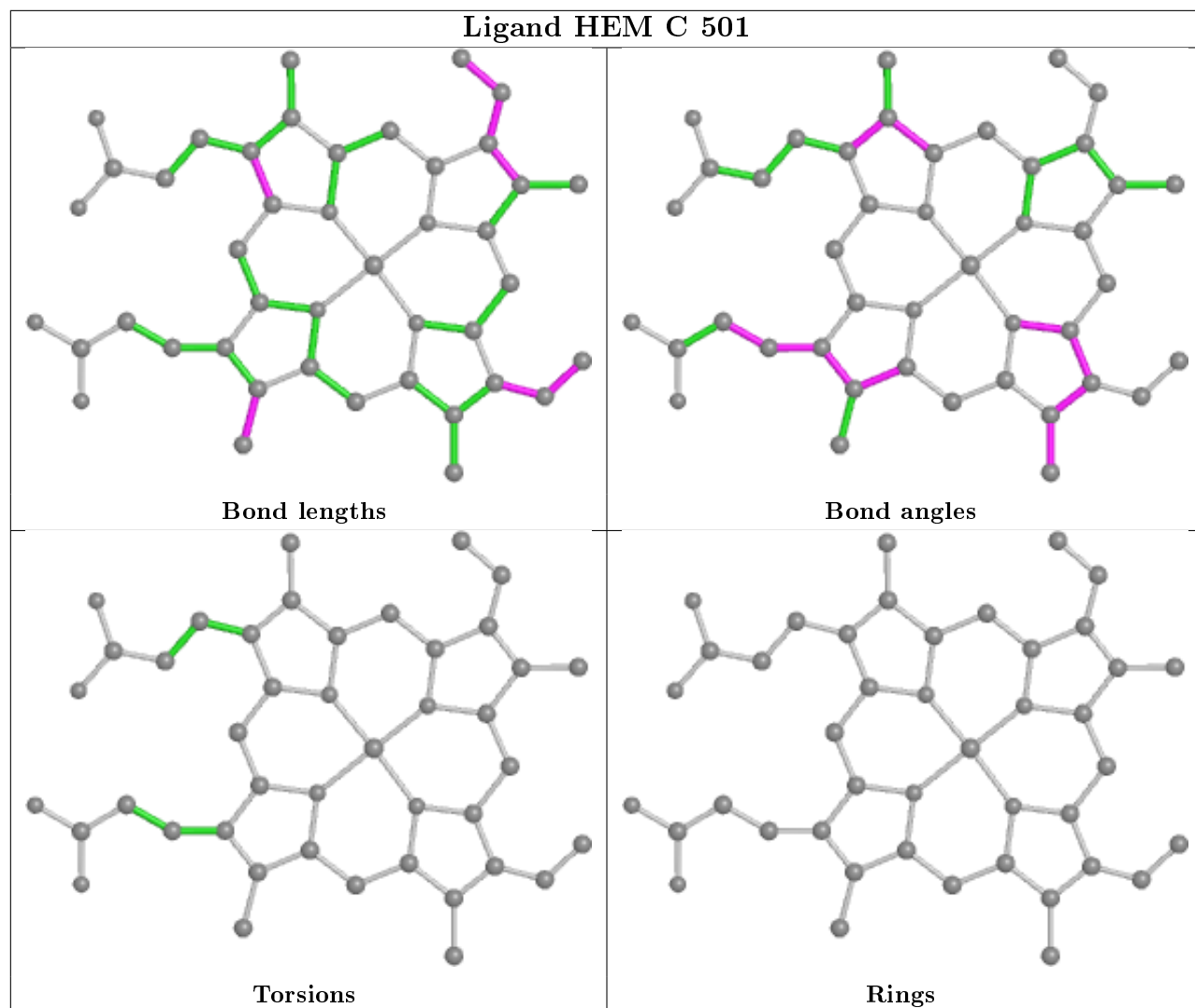
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	3012	JZR	3	0
20	P	4009	GOL	2	0
15	D	2006	PEE	2	0
15	P	3007	PEE	3	0
16	C	501	HEM	1	0
15	B	4017	PEE	1	0
11	A	4004	JZR	1	0
12	I	4015	PO4	1	0
18	C	2002	UQ	4	0
11	S	2012	JZR	6	0
17	C	2001	SMA	3	0
17	P	3001	SMA	3	0
15	Q	3006	PEE	5	0
16	P	502	HEM	2	0
16	P	501	HEM	1	0
16	C	502	HEM	4	0
18	P	3002	UQ	5	0
19	D	2003	CDL	1	0
21	Q	501	HEC	5	0
21	D	501	HEC	4	0
11	F	4003	JZR	1	0
13	G	4001	AZI	1	0
12	Q	4012	PO4	1	0

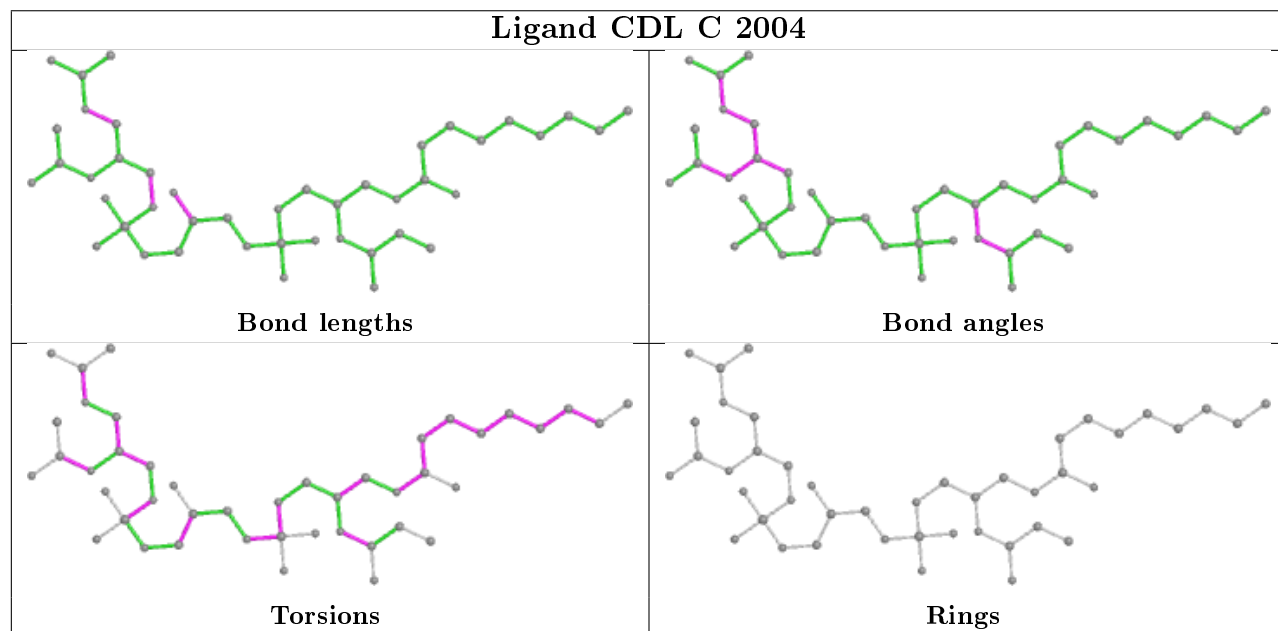
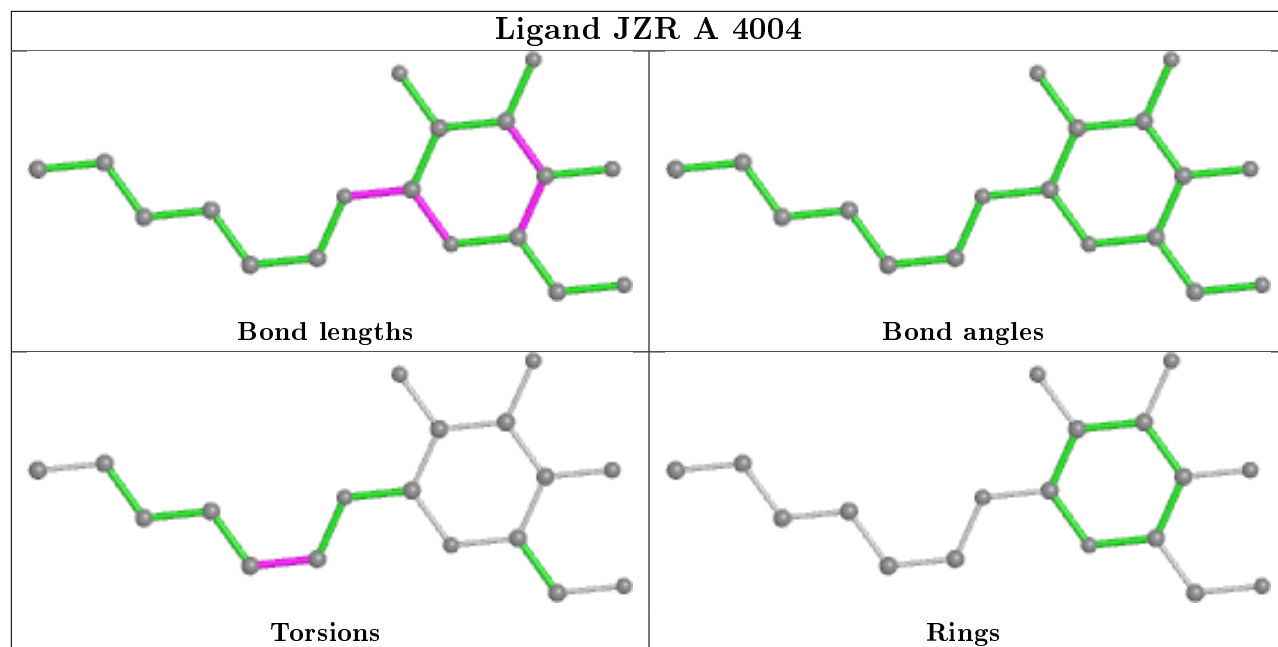
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

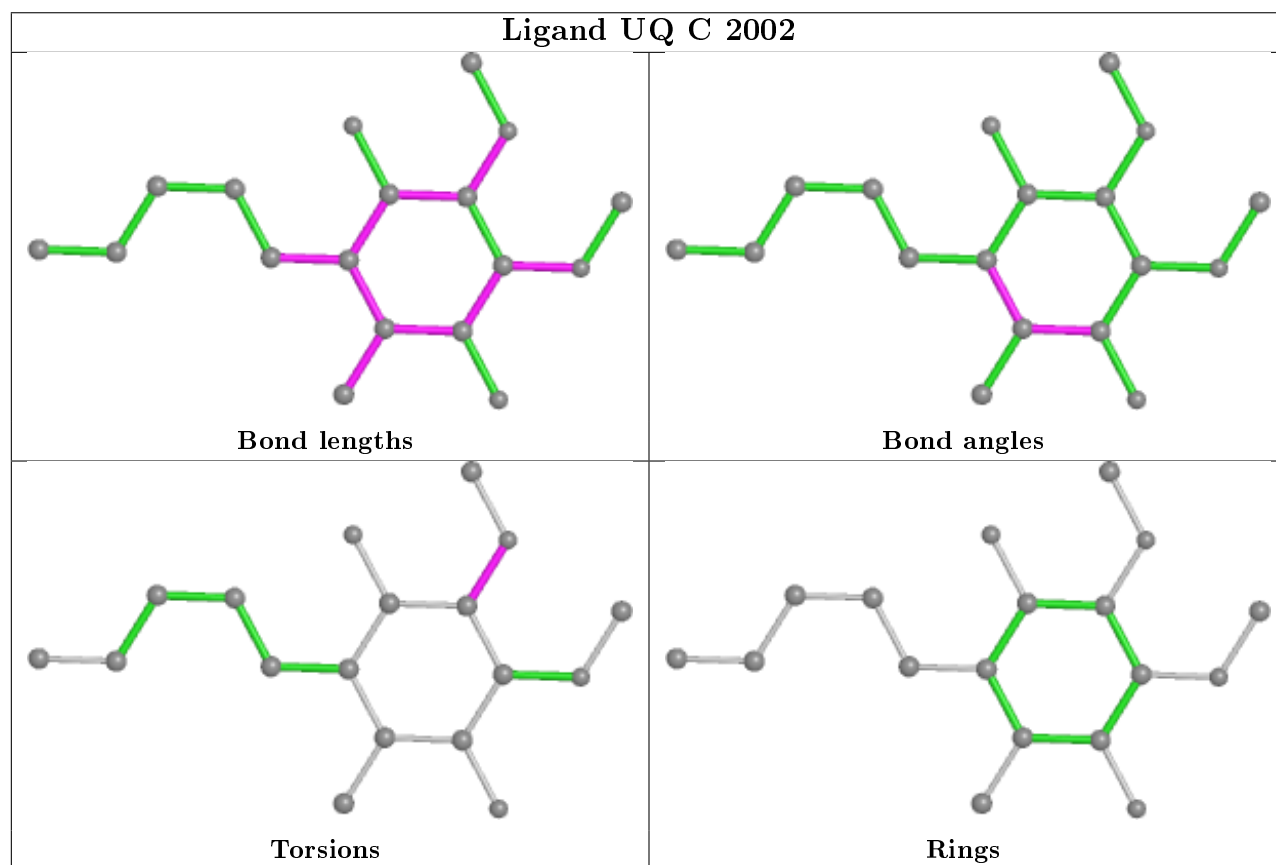
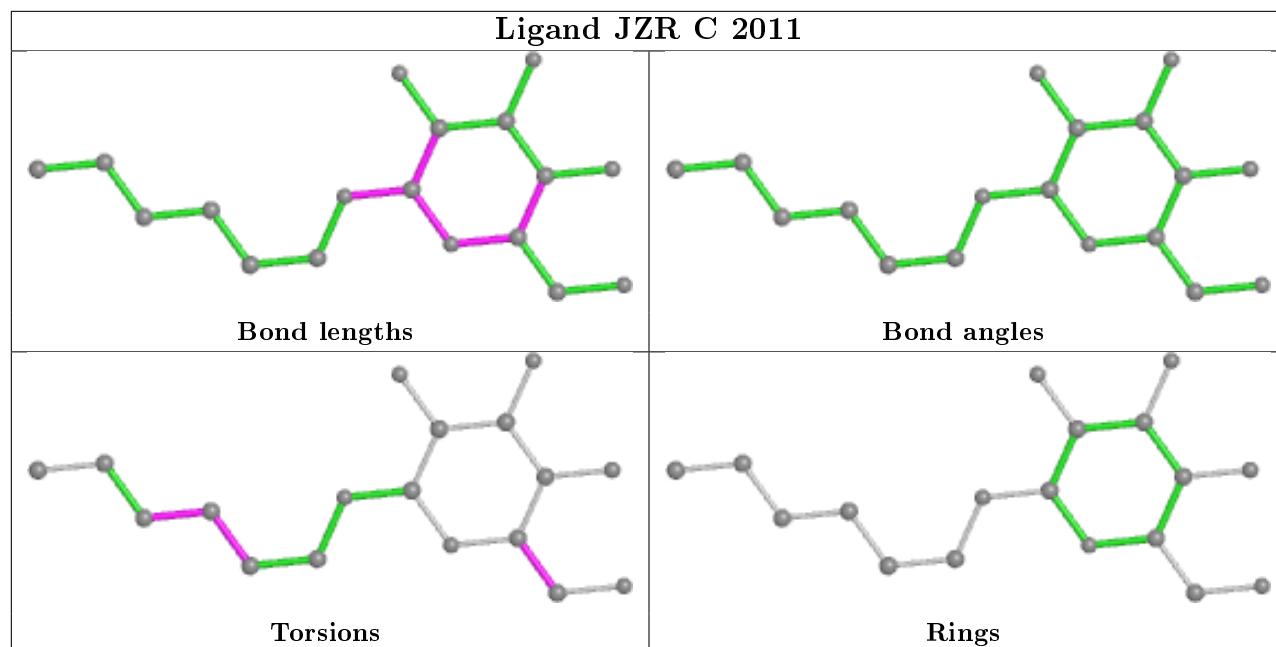
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

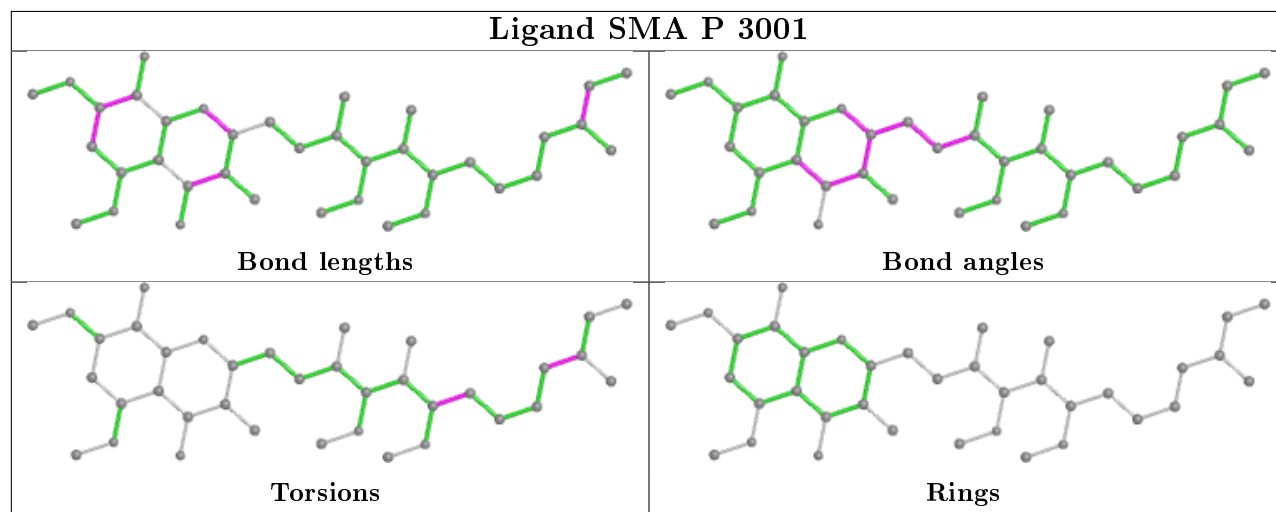
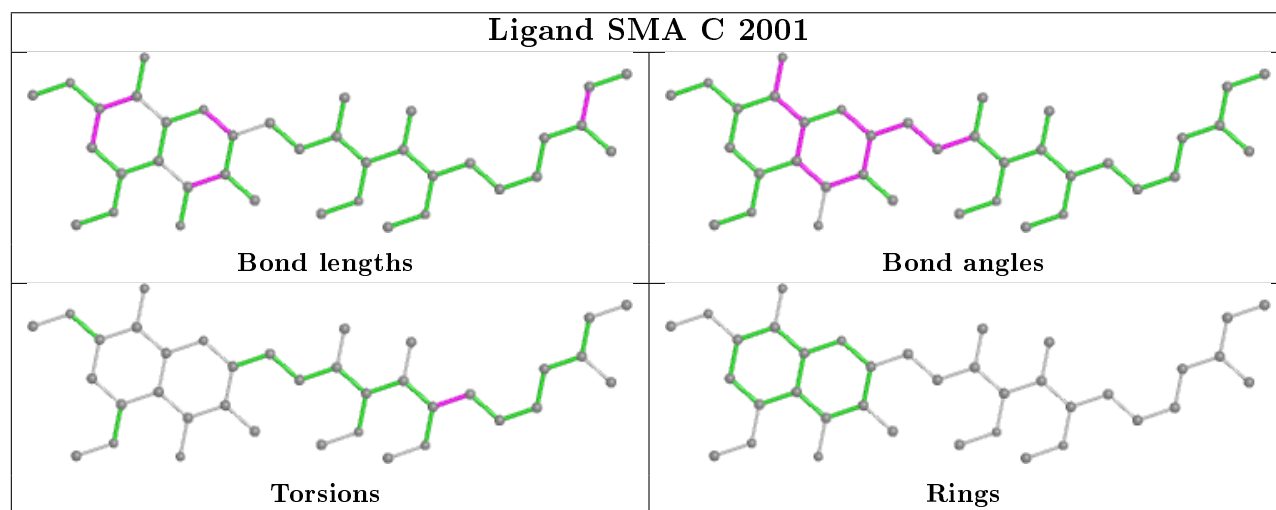
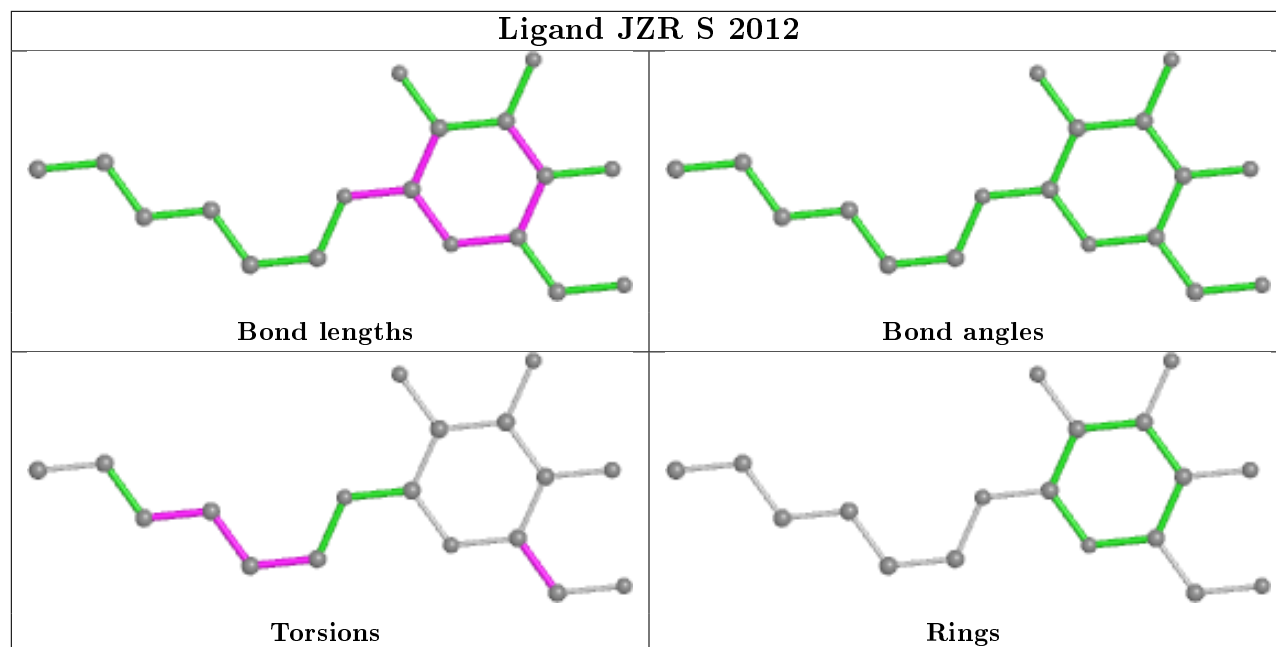


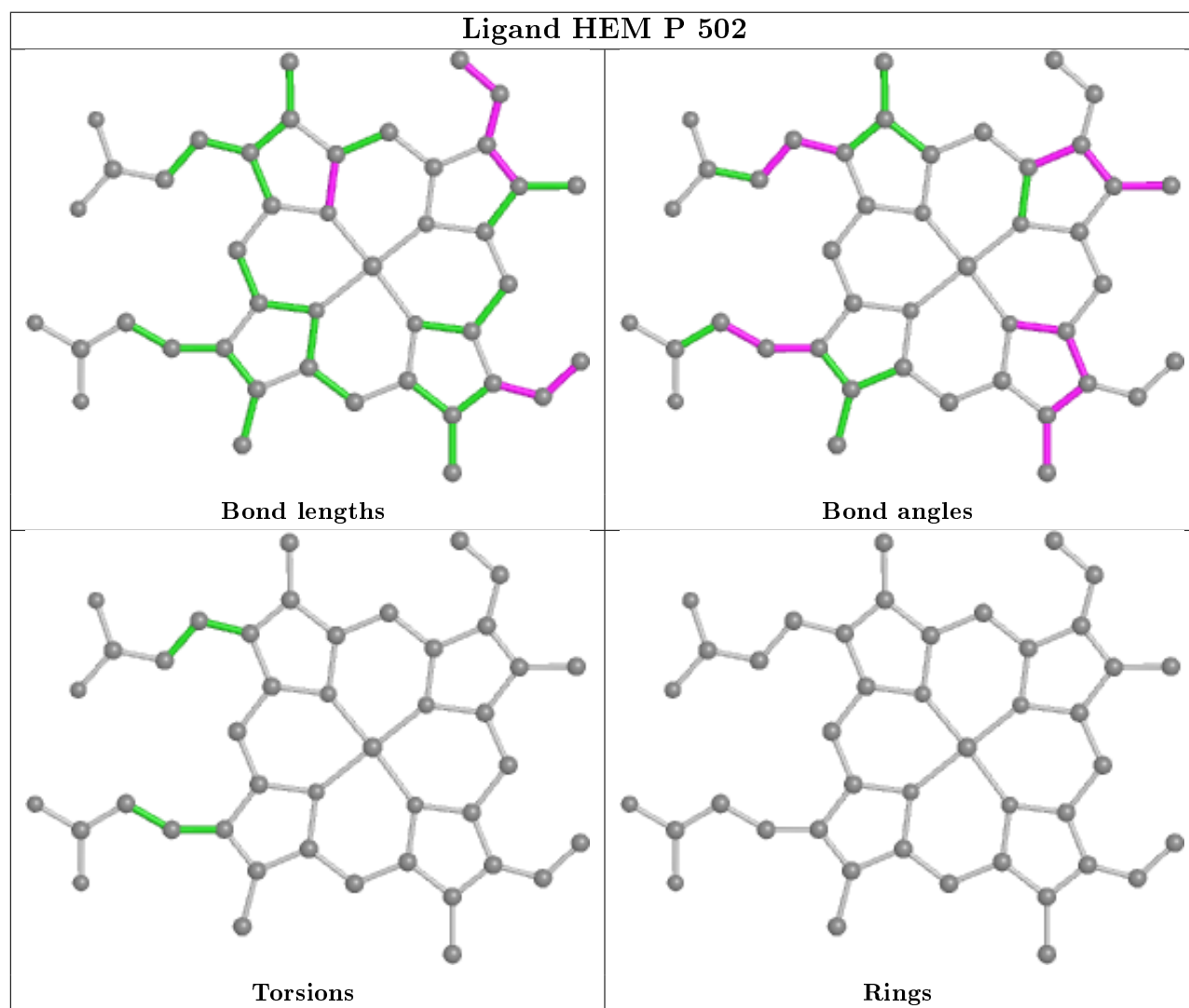
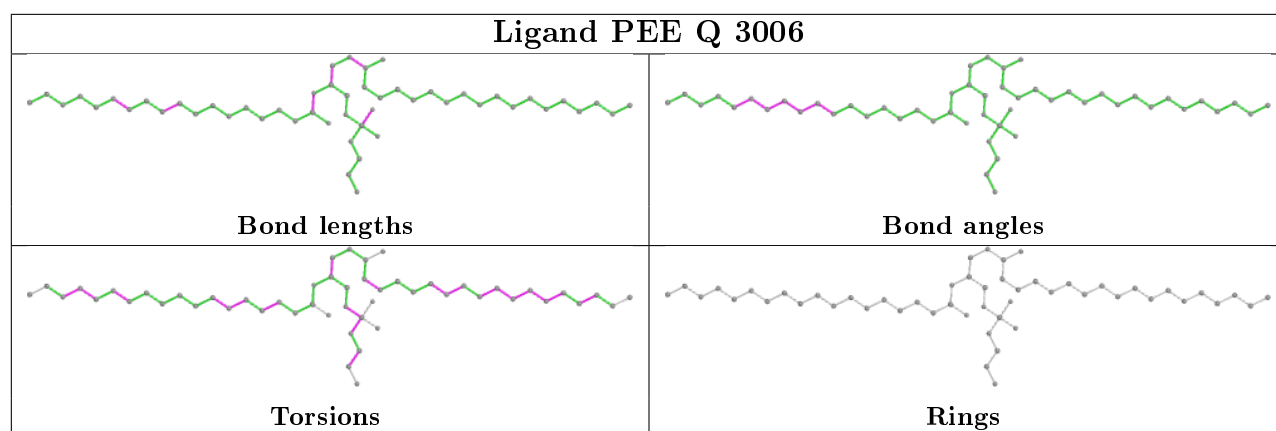




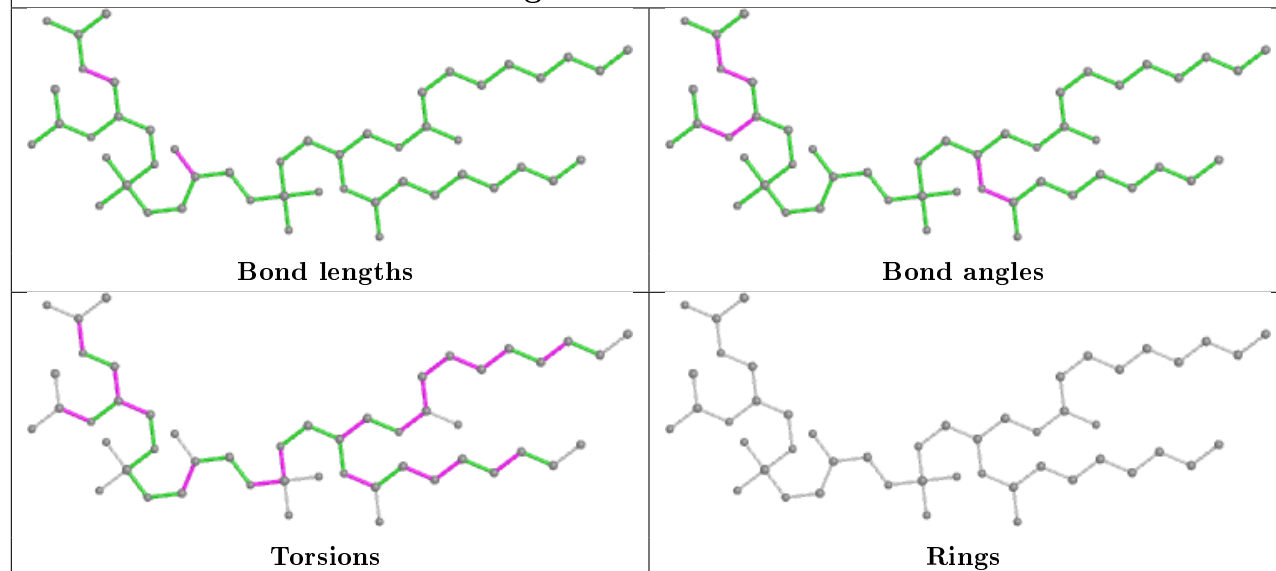




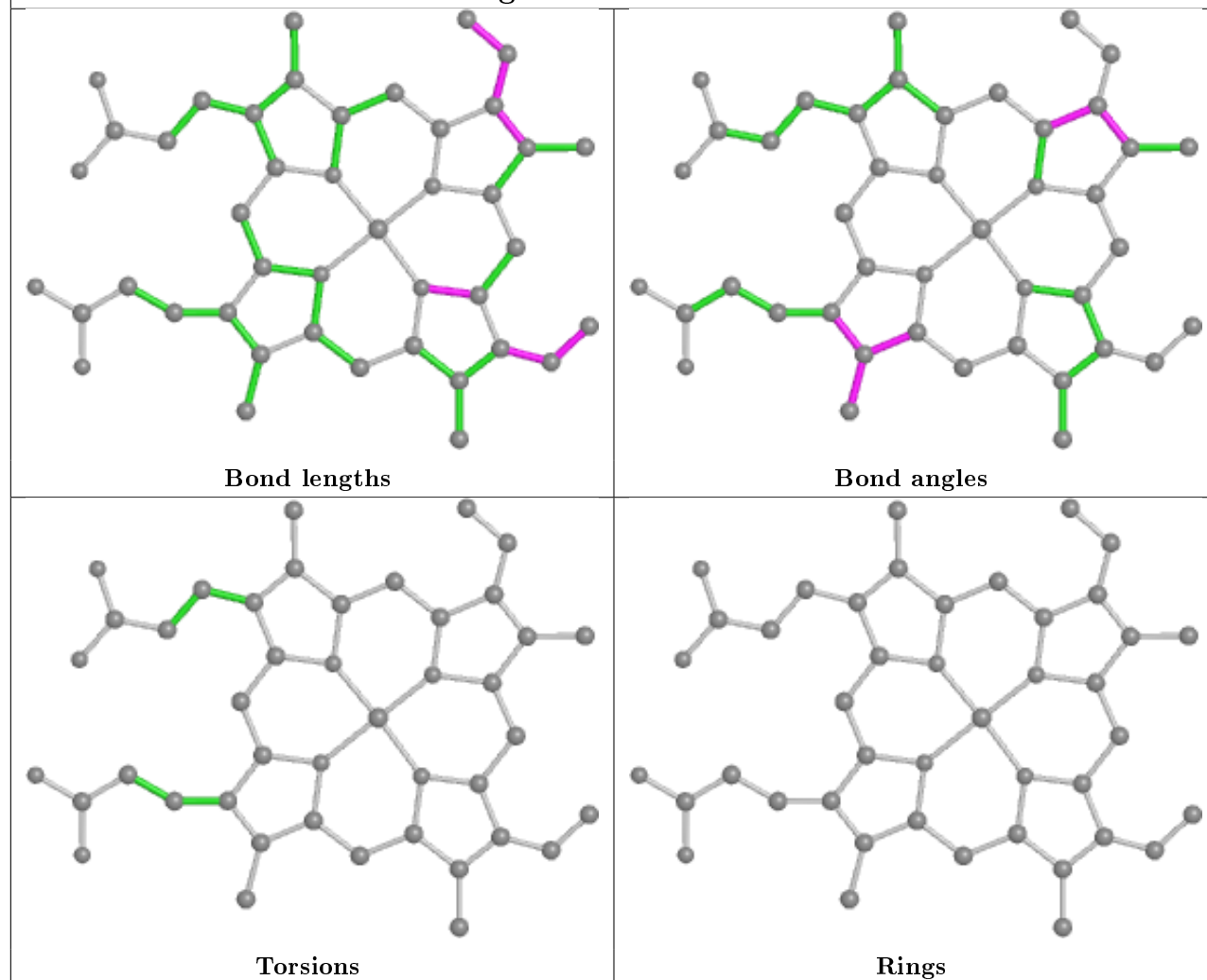


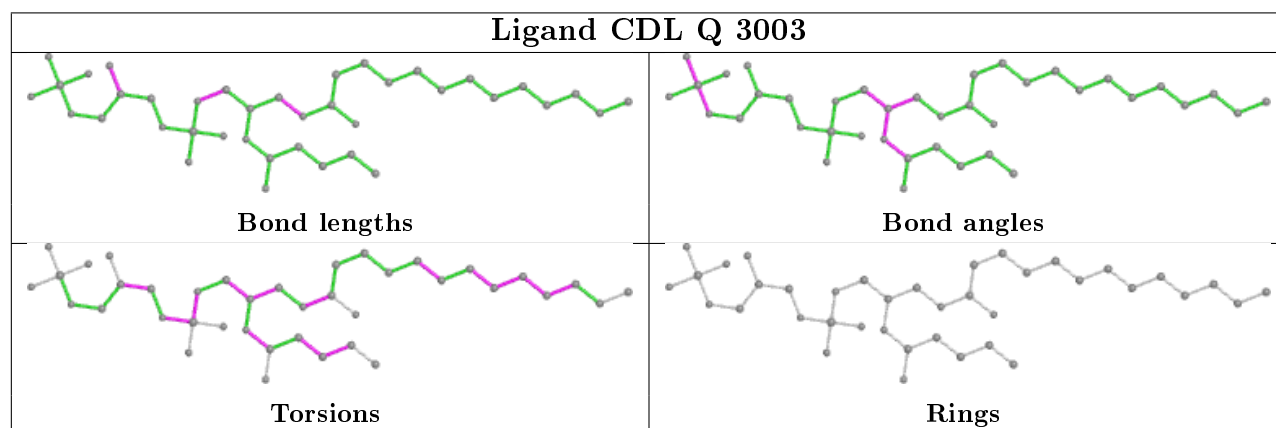
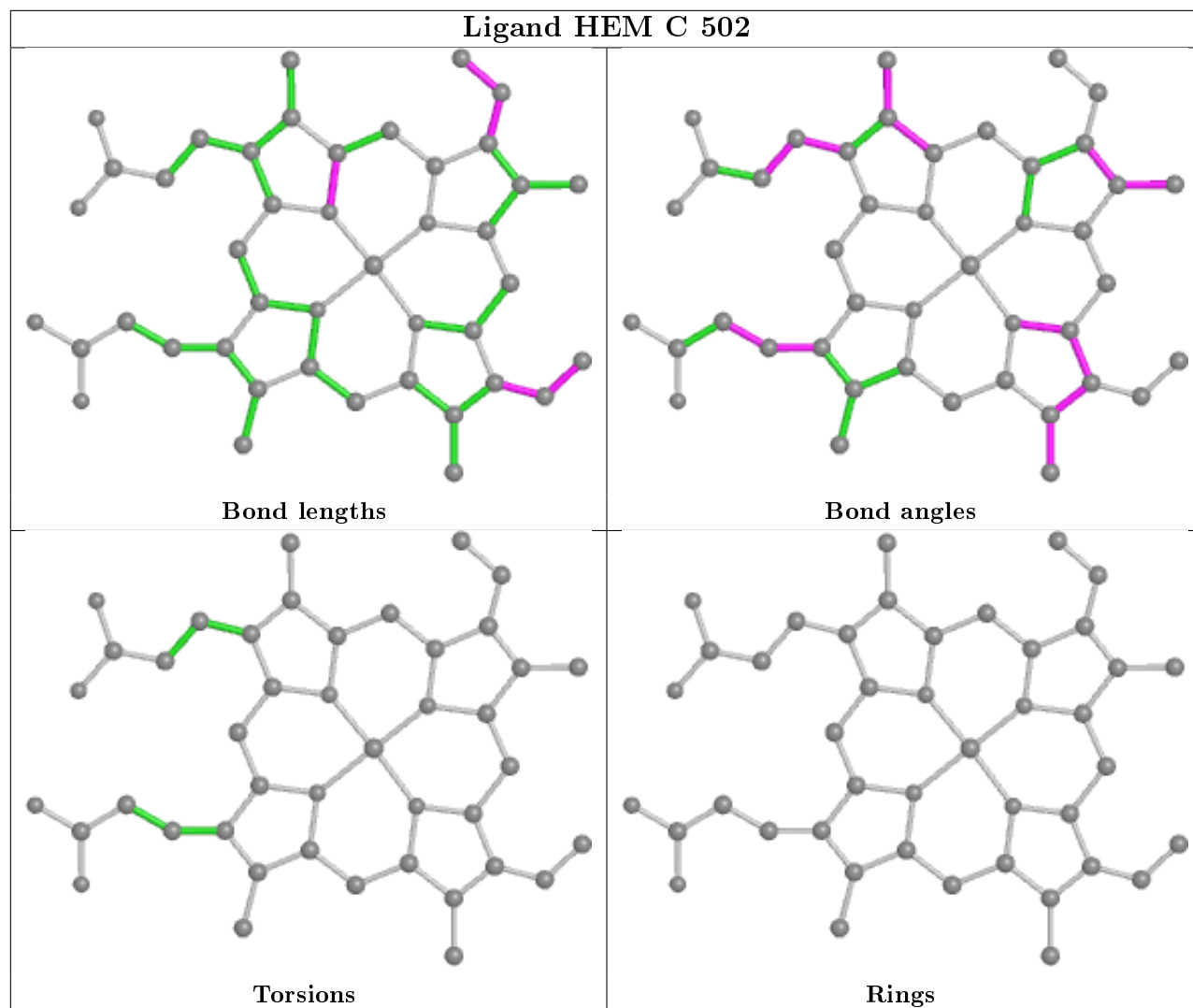


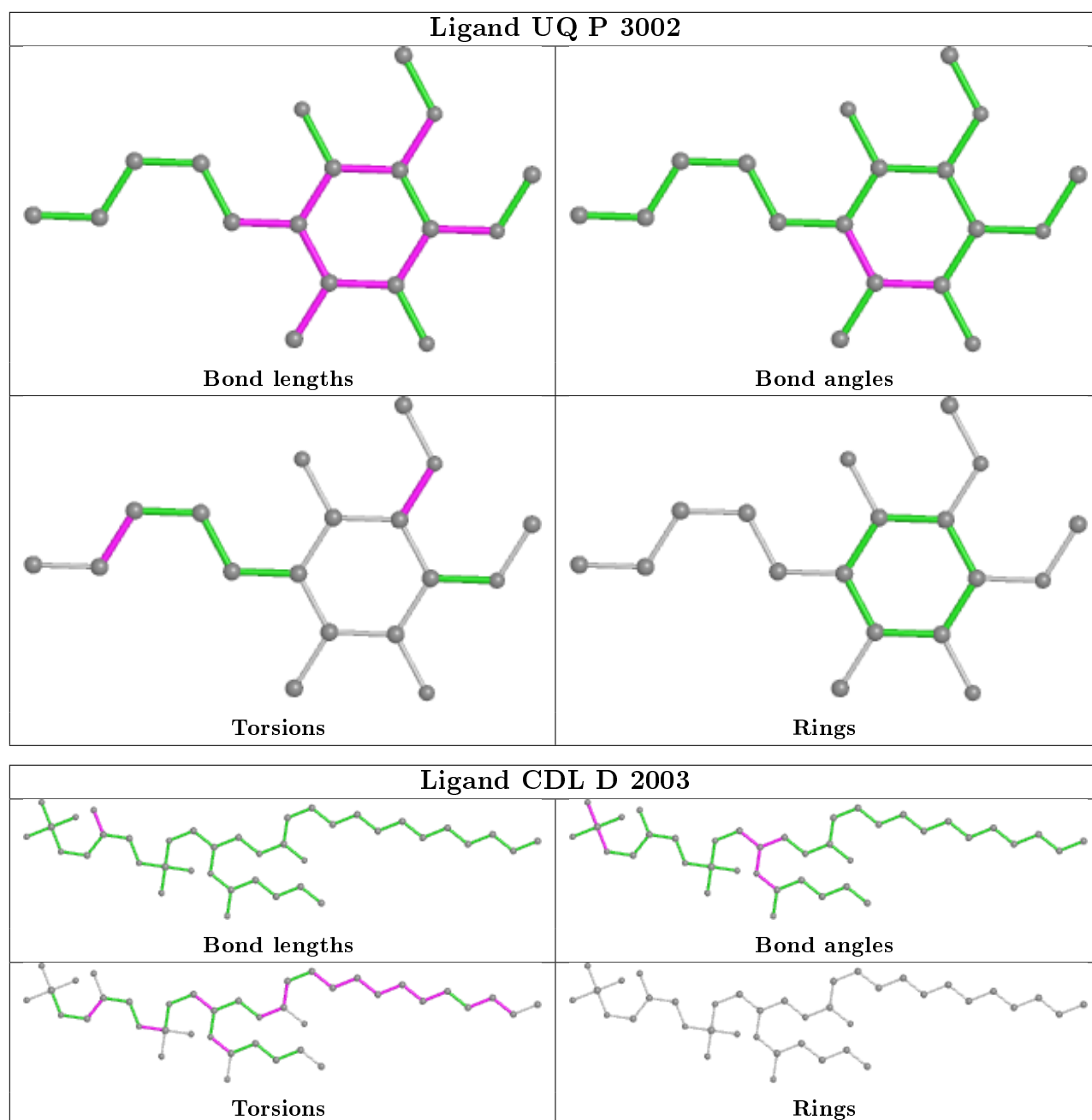
Ligand CDL P 3004

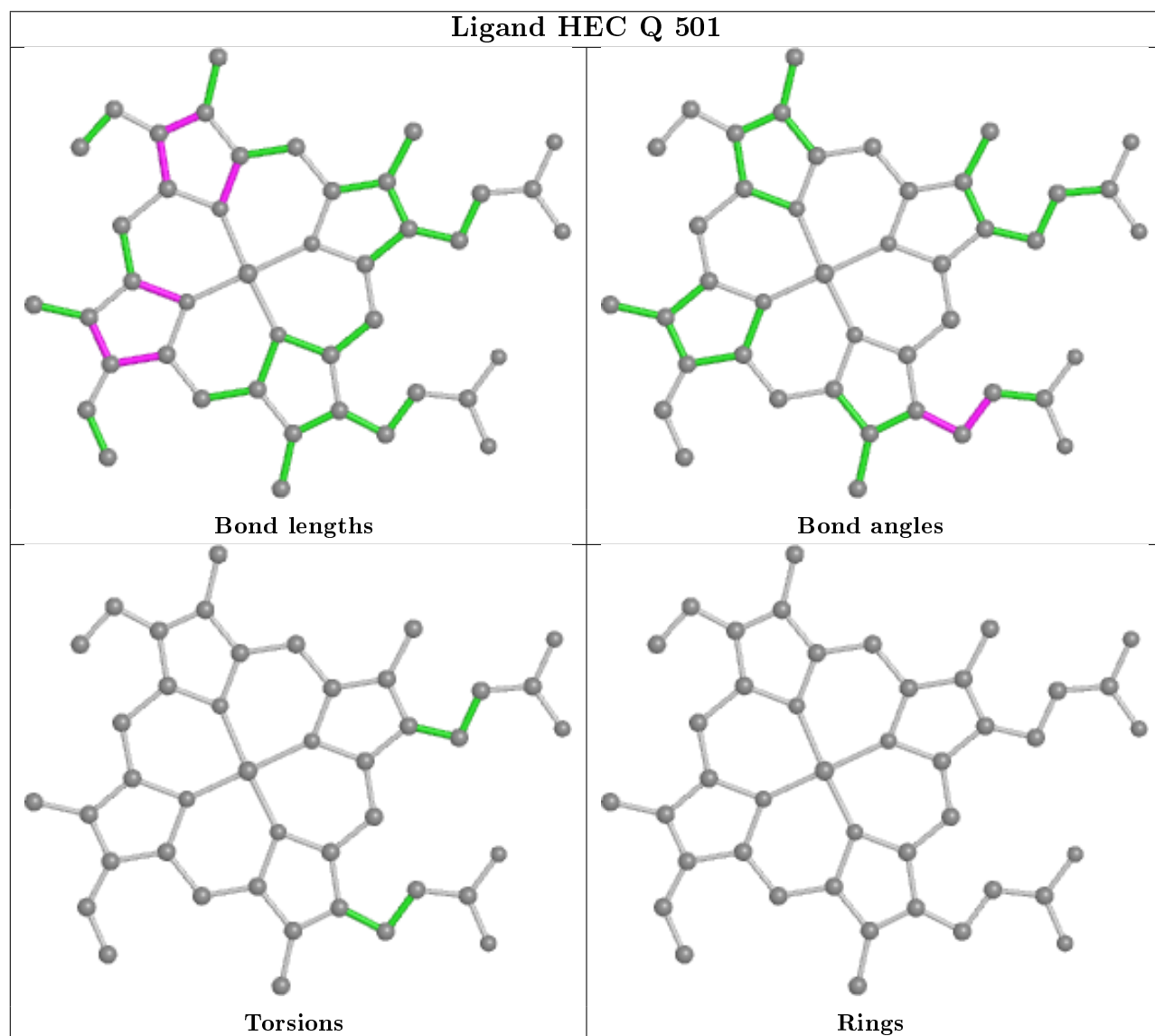
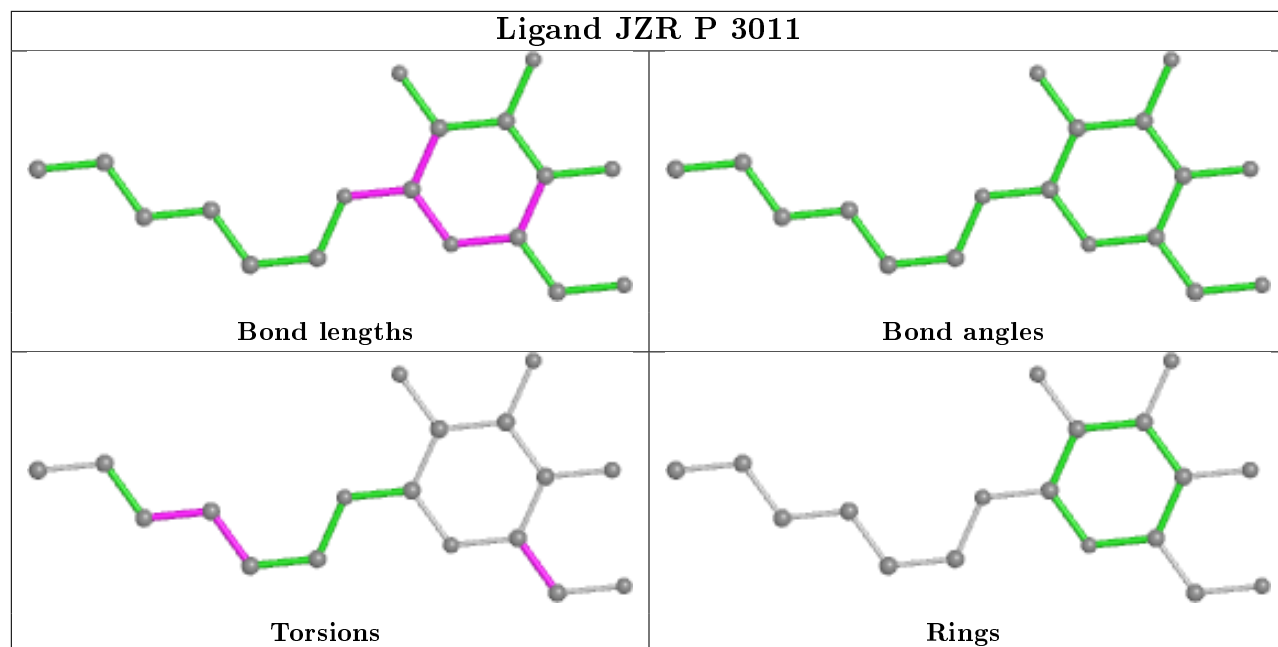


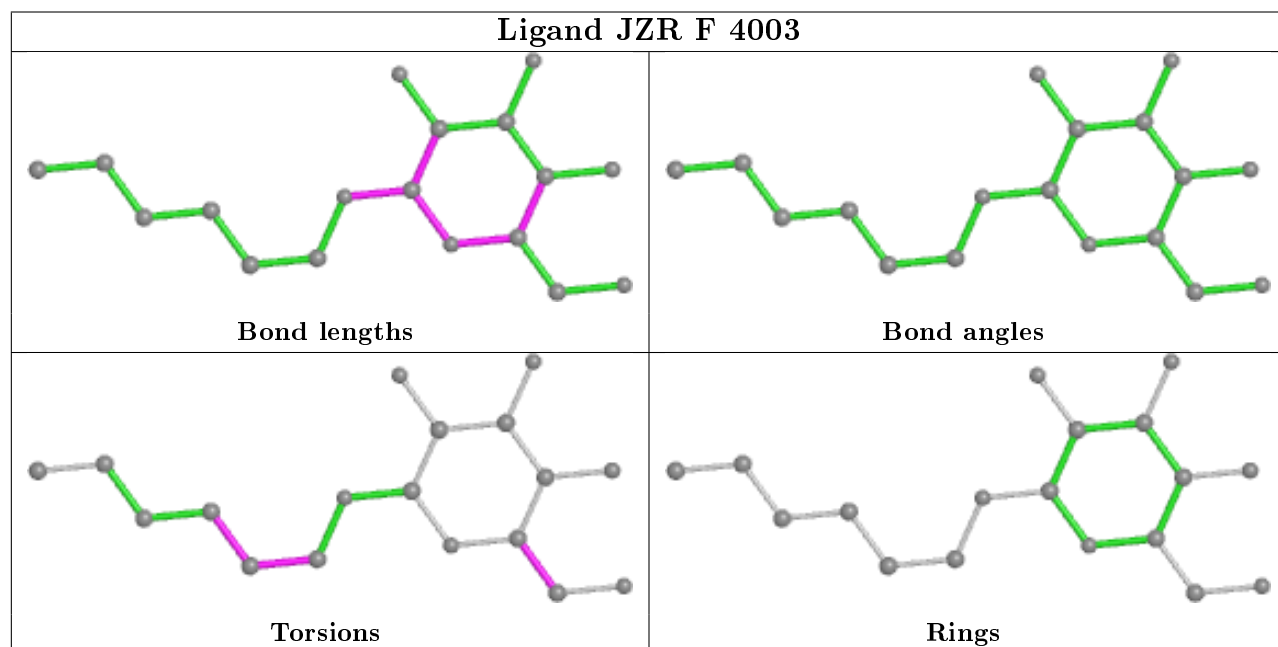
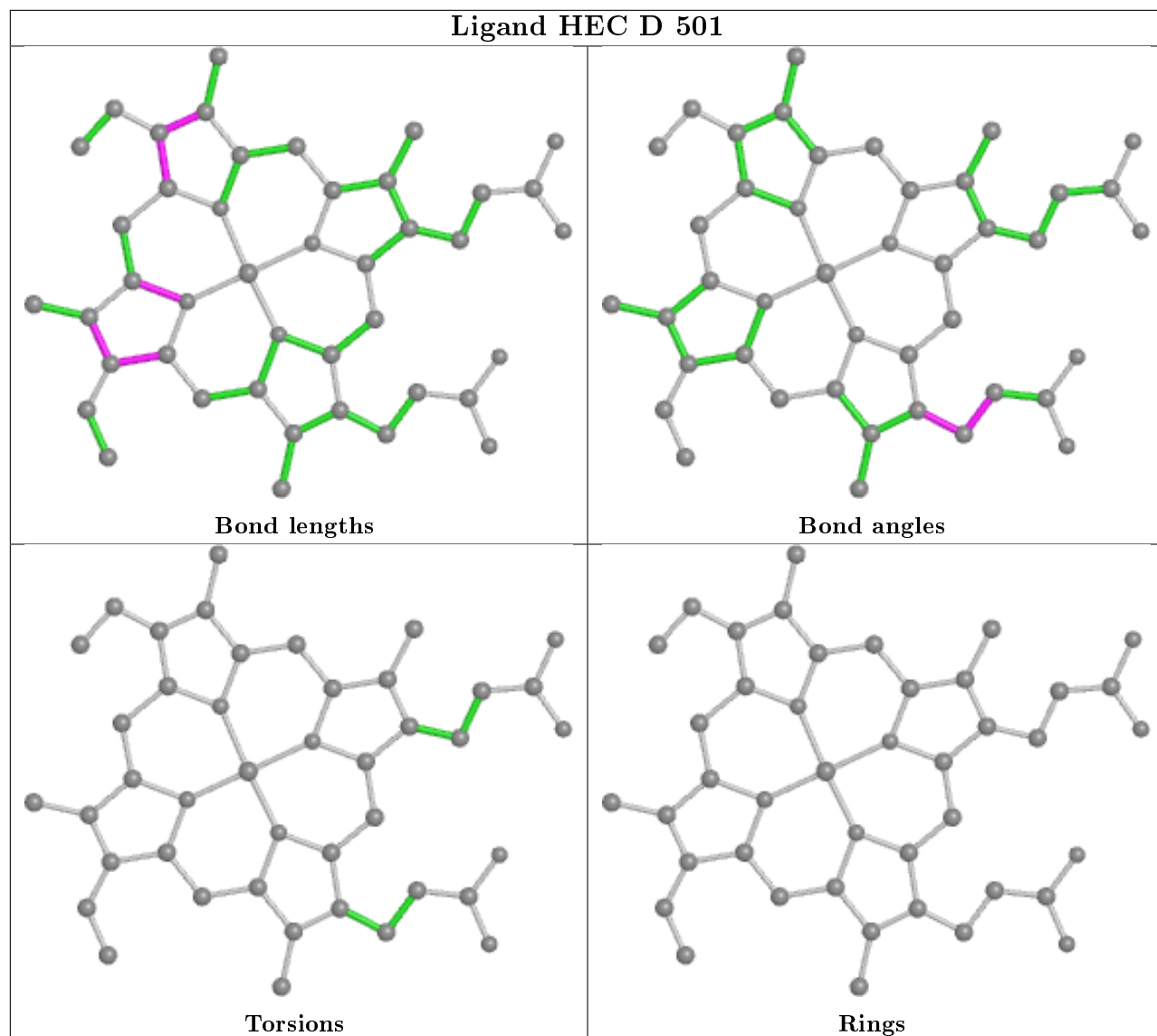
Ligand HEM P 501











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/446 (99%)	0.08	14 (3%) 47 54	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.48	29 (6%) 18 23	31, 50, 77, 132	1 (0%)
2	B	424/439 (96%)	0.19	15 (3%) 44 50	28, 41, 66, 102	0
2	O	424/439 (96%)	0.48	40 (9%) 8 11	31, 48, 87, 185	0
3	C	365/379 (96%)	0.35	20 (5%) 25 31	24, 34, 48, 108	0
3	P	370/379 (97%)	0.46	24 (6%) 18 23	28, 37, 52, 218	0
4	D	241/241 (100%)	0.42	15 (6%) 20 25	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.58	24 (9%) 7 9	31, 45, 67, 87	0
5	E	196/196 (100%)	1.09	43 (21%) 0 0	32, 57, 105, 117	0
5	R	196/196 (100%)	0.30	13 (6%) 18 23	27, 46, 71, 99	0
6	F	99/110 (90%)	0.38	9 (9%) 9 12	24, 39, 71, 83	0
6	S	99/110 (90%)	0.27	4 (4%) 38 44	28, 40, 67, 88	0
7	G	75/81 (92%)	0.91	12 (16%) 1 2	26, 49, 77, 86	0
7	T	76/81 (93%)	1.51	23 (30%) 0 0	32, 55, 98, 114	0
8	H	66/78 (84%)	1.08	15 (22%) 0 0	40, 56, 73, 78	0
8	U	66/78 (84%)	1.16	17 (25%) 0 0	44, 63, 94, 104	0
9	I	42/78 (53%)	2.19	21 (50%) 0 0	33, 62, 90, 93	0
9	V	42/78 (53%)	2.05	18 (42%) 0 0	36, 78, 94, 100	0
10	J	30/62 (48%)	0.81	3 (10%) 7 9	40, 52, 80, 109	0
10	W	62/62 (100%)	2.06	19 (30%) 0 0	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.52	378 (9%) 8 10	24, 43, 80, 218	2 (0%)

All (378) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	13	ILE	22.1
10	W	1	VAL	21.3
10	W	62	LYS	12.6
2	O	12	GLU	10.6
10	W	2	ALA	10.6
7	T	76	ALA	10.3
9	I	50	LEU	10.3
7	T	1	GLY	9.5
3	P	18	PHE	9.4
3	P	11	MET	9.3
2	O	19	PRO	8.9
5	E	112	VAL	8.5
4	Q	241	LYS	8.5
1	A	2	ALA	8.2
9	I	49	VAL	8.2
1	N	222	THR	8.1
10	W	12	LEU	8.0
2	B	233	SER	8.0
9	V	50	LEU	7.9
3	C	17	ALA	7.7
1	N	1	THR	7.4
2	B	230	LEU	7.3
1	N	227	ALA	7.2
10	J	62	LYS	7.0
5	E	115	SER	6.9
3	P	12	LYS	6.8
2	B	231	GLY	6.8
2	O	228	GLY	6.7
8	U	50	THR	6.6
1	A	222	THR	6.5
1	A	225	GLU	6.5
2	B	232	LEU	6.2
2	B	20	HIS	6.0
1	A	1	THR	5.9
3	P	16	ASN	5.9
4	Q	1	SER	5.8
1	A	227	ALA	5.8
1	N	2	ALA	5.8
7	G	30	PHE	5.7
5	R	189	SER	5.5
9	V	38	SER	5.4
1	A	226	ASP	5.4
8	U	47	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
2	O	218	GLN	5.4
7	T	34	ILE	5.3
7	T	30	PHE	5.3
3	P	14	VAL	5.3
5	E	114	VAL	5.3
9	I	78	TYR	5.3
7	T	32	LYS	5.3
3	P	17	ALA	5.1
5	E	196	GLY	5.1
1	N	229	PRO	5.1
10	W	5	LEU	5.1
3	P	10	LEU	5.0
1	N	206	ARG	4.9
6	S	12	TRP	4.9
5	E	124	LEU	4.9
5	E	194	ILE	4.8
3	C	18	PHE	4.8
1	N	228	VAL	4.8
10	W	3	PRO	4.8
4	Q	76	GLU	4.8
4	D	241	LYS	4.7
5	E	117	LEU	4.7
8	H	34	ARG	4.7
3	C	16	ASN	4.7
7	T	73	ASN	4.7
7	T	31	SER	4.6
8	U	48	SER	4.6
5	R	191	ASP	4.6
4	D	81	PHE	4.6
9	I	51	CYS	4.5
2	O	232	LEU	4.5
9	V	49	VAL	4.5
5	E	116	GLN	4.4
2	B	12	GLU	4.4
9	V	52	ARG	4.4
10	J	61	ASN	4.3
1	N	230	THR	4.3
2	O	20	HIS	4.3
7	T	61	TRP	4.3
5	E	108	GLN	4.3
8	U	49	GLN	4.2
1	N	225	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	304	HIS	4.2
8	U	44	VAL	4.2
10	W	8	ARG	4.2
5	E	188	THR	4.2
5	E	111	ALA	4.1
5	E	80	ASP	4.1
5	E	186	GLU	4.1
2	O	17	VAL	4.1
2	O	41	TYR	4.1
7	T	29	TYR	4.1
10	W	13	LEU	4.1
4	Q	158	ILE	4.0
5	E	35	PHE	4.0
5	E	191	ASP	4.0
5	E	113	GLU	4.0
3	C	27	ILE	4.0
10	W	9	LEU	3.9
3	C	218	ILE	3.9
5	E	5	ILE	3.9
1	A	4	TYR	3.9
2	B	229	GLY	3.9
2	O	230	LEU	3.8
9	V	61	GLY	3.8
9	V	42	VAL	3.8
10	W	30	PHE	3.8
2	O	229	GLY	3.8
5	E	185	TYR	3.8
9	V	78	TYR	3.8
7	G	29	TYR	3.7
5	R	71	MET	3.7
10	W	61	ASN	3.7
1	N	15	GLN	3.7
5	E	107	ASP	3.7
8	U	45	SER	3.7
4	Q	146	GLY	3.7
4	Q	139	THR	3.7
8	H	46	SER	3.7
4	D	73	GLY	3.7
5	R	74	ILE	3.6
2	O	221	GLU	3.6
5	E	27	GLU	3.6
6	F	13	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	N	193	PRO	3.6
2	B	41	TYR	3.6
4	D	79	GLU	3.5
8	U	51	GLU	3.5
5	E	128	LYS	3.5
9	I	42	VAL	3.5
4	Q	227	TRP	3.5
6	S	70	MET	3.5
1	N	226	ASP	3.5
5	E	127	VAL	3.5
1	A	224	ASP	3.5
5	E	187	PHE	3.5
9	I	62	ARG	3.5
2	O	215	VAL	3.4
4	Q	77	ASP	3.4
4	Q	157	ALA	3.4
3	P	27	ILE	3.4
7	G	42	ARG	3.4
5	E	190	ASP	3.4
5	R	76	ILE	3.3
3	P	218	ILE	3.3
9	I	52	ARG	3.3
8	H	44	VAL	3.3
5	R	190	ASP	3.3
10	W	25	VAL	3.3
6	F	110	LYS	3.3
4	Q	145	GLU	3.3
2	O	18	PRO	3.3
2	O	233	SER	3.3
4	D	230	LEU	3.3
3	C	23	ALA	3.3
3	P	223	TYR	3.2
1	N	209	LEU	3.2
8	U	39	LEU	3.2
8	H	42	GLU	3.2
5	R	23	LYS	3.2
2	O	439	LEU	3.2
7	G	34	ILE	3.2
5	E	184	SER	3.2
3	C	15	ASN	3.2
4	Q	141	VAL	3.2
9	I	48	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	TRP	3.1
5	E	122	HIS	3.1
8	H	31	VAL	3.1
4	D	80	MET	3.1
9	I	73	PRO	3.1
8	H	41	ASP	3.1
4	D	141	VAL	3.1
1	N	22	GLY	3.1
1	A	228	VAL	3.1
7	T	28	HIS	3.1
2	O	25	GLU	3.1
7	T	75	ALA	3.1
1	N	443	TRP	3.1
3	C	31	TRP	3.0
9	I	55	LEU	3.0
3	C	211	ILE	3.0
9	V	51	CYS	3.0
8	H	45	SER	3.0
2	O	217	LYS	3.0
6	S	15	GLY	3.0
3	C	25	SER	3.0
4	D	145	GLU	3.0
5	E	49	TYR	3.0
4	D	72	ASP	3.0
2	O	355	PRO	3.0
9	I	63	PRO	3.0
4	D	85	GLY	2.9
1	N	224	ASP	2.9
4	Q	79	GLU	2.9
5	R	75	GLU	2.9
6	F	108	ALA	2.9
9	V	32	ALA	2.8
4	Q	148	TYR	2.8
3	C	209	THR	2.8
5	E	103	LYS	2.8
5	E	110	ALA	2.8
2	O	224	LEU	2.8
4	Q	230	LEU	2.8
1	N	51	LYS	2.8
3	P	26	ASN	2.8
1	N	16	VAL	2.8
4	Q	229	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
9	I	37	THR	2.8
9	V	37	THR	2.8
5	E	84	GLY	2.8
5	E	79	SER	2.8
8	U	42	GLU	2.8
10	W	19	THR	2.8
9	I	58	GLN	2.8
10	W	29	LEU	2.8
3	P	224	TYR	2.8
5	E	53	ASN	2.7
3	C	155	TYR	2.7
9	I	70	LEU	2.7
4	D	229	VAL	2.7
7	T	42	ARG	2.7
4	Q	167	GLU	2.7
1	N	13	GLU	2.7
2	O	26	PHE	2.7
5	E	89	PHE	2.7
9	I	71	ASN	2.7
8	U	13	LEU	2.7
4	Q	144	ARG	2.7
4	Q	147	LEU	2.7
8	H	51	GLU	2.7
9	V	40	SER	2.6
2	B	250	ASP	2.6
1	N	219	LEU	2.6
4	Q	143	LEU	2.6
3	C	224	TYR	2.6
8	U	43	ARG	2.6
1	N	176	LYS	2.6
10	W	20	PHE	2.6
9	V	41	PRO	2.6
4	D	116	ILE	2.6
5	R	12	ASP	2.6
2	O	405	VAL	2.6
2	O	22	GLN	2.6
7	T	2	ARG	2.6
9	I	60	ALA	2.6
9	V	48	SER	2.6
2	O	304	HIS	2.6
4	Q	149	PHE	2.6
2	B	235	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
7	T	17	SER	2.5
2	O	392	TYR	2.5
3	P	320	LEU	2.5
7	G	31	SER	2.5
7	G	75	ALA	2.5
3	P	31	TRP	2.5
10	W	21	ALA	2.5
2	O	27	THR	2.5
7	G	56	TYR	2.5
7	T	74	PRO	2.5
8	H	49	GLN	2.5
5	R	80	ASP	2.5
2	O	303	VAL	2.5
3	P	227	LYS	2.5
3	P	15	ASN	2.5
8	U	46	SER	2.5
1	N	5	ALA	2.5
7	G	60	THR	2.5
1	A	20	ASP	2.5
9	V	33	ALA	2.5
7	T	35	PRO	2.4
2	O	226	ILE	2.4
4	D	103	ALA	2.4
9	I	32	ALA	2.4
7	G	58	VAL	2.4
2	B	227	ARG	2.4
5	E	134	ILE	2.4
3	P	25	SER	2.4
3	P	345	HIS	2.4
4	Q	142	SER	2.4
7	G	64	GLN	2.4
7	T	64	GLN	2.4
3	P	155	TYR	2.4
8	H	22	GLU	2.3
6	S	69	SER	2.3
8	H	29	LYS	2.3
2	O	223	PHE	2.3
9	V	77	ARG	2.3
4	D	117	VAL	2.3
2	O	29	LEU	2.3
2	O	33	LEU	2.3
10	J	37	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	17	SER	2.3
5	E	38	LEU	2.3
6	F	106	GLU	2.3
8	U	67	HIS	2.3
5	R	79	SER	2.3
1	A	365	LEU	2.3
6	F	66	LEU	2.3
8	H	37	LEU	2.3
1	A	184	GLU	2.3
3	P	168	PHE	2.3
7	T	43	ALA	2.3
1	N	241	ILE	2.3
3	C	207	ASN	2.2
6	F	107	TRP	2.2
8	H	48	SER	2.2
9	V	63	PRO	2.2
10	W	24	ILE	2.2
5	E	71	MET	2.2
3	P	43	LEU	2.2
7	T	38	LEU	2.2
9	I	64	LEU	2.2
4	Q	171	PHE	2.2
2	O	126	VAL	2.2
2	O	351	ASN	2.2
1	N	397	SER	2.2
1	N	20	ASP	2.2
8	U	26	GLN	2.2
8	H	67	HIS	2.2
2	O	406	ALA	2.2
9	I	61	GLY	2.2
10	W	28	ALA	2.2
5	R	27	GLU	2.2
2	B	439	LEU	2.2
5	R	16	PRO	2.2
2	O	349	GLN	2.2
5	E	193	VAL	2.2
8	U	31	VAL	2.2
7	T	33	GLY	2.2
2	O	264	ILE	2.1
2	O	23	ASP	2.1
1	N	18	GLN	2.1
1	A	229	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	78	LEU	2.1
6	F	22	ASN	2.1
5	E	195	VAL	2.1
8	U	41	ASP	2.1
4	Q	233	ARG	2.1
3	P	23	ALA	2.1
4	D	99	GLU	2.1
5	E	192	MET	2.1
6	F	70	MET	2.1
9	I	69	SER	2.1
2	O	24	LEU	2.1
3	C	210	GLY	2.1
3	P	28	SER	2.1
7	G	68	LYS	2.1
1	N	421	ALA	2.1
4	Q	136	GLU	2.1
3	C	101	GLY	2.1
2	O	219	VAL	2.1
3	C	98	VAL	2.1
7	T	60	THR	2.1
1	N	216	PHE	2.1
7	T	56	TYR	2.1
8	U	28	GLU	2.0
5	E	167	ALA	2.0
5	E	153	PHE	2.0
10	W	10	TYR	2.0
9	V	62	ARG	2.0
2	B	400	GLN	2.0
2	O	35	ILE	2.0
3	C	102	LEU	2.0
9	V	36	ALA	2.0
7	G	71	ARG	2.0
3	C	217	LYS	2.0
3	C	24	PRO	2.0
9	I	41	PRO	2.0
5	E	132	TRP	2.0
6	F	19	TRP	2.0
8	H	35	GLU	2.0
2	B	301	LYS	2.0
2	O	407	ASP	2.0
7	T	37	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	JZR	F	3012	18/18	0.17	0.72	159,162,164,164	0
14	UNL	U	4056	1/-	0.24	1.01	101,101,101,101	0
20	GOL	O	4005	6/6	0.25	0.74	166,167,167,168	0
14	UNL	P	4060	1/-	0.32	0.34	88,88,88,88	0
11	JZR	S	2012	18/18	0.38	0.46	89,103,106,107	0
11	JZR	F	4003	18/18	0.39	0.66	176,180,181,181	0
14	UNL	I	4072	1/-	0.39	2.21	93,93,93,93	0
14	UNL	D	4036	1/-	0.44	0.35	83,83,83,83	0
14	UNL	B	4034	1/-	0.47	0.70	87,87,87,87	0
14	UNL	S	4047	1/-	0.52	0.38	71,71,71,71	0
14	UNL	C	4068	1/-	0.55	0.58	72,72,72,72	0
11	JZR	P	3011	18/18	0.56	0.40	99,107,109,109	0
20	GOL	E	4007	5/6	0.58	0.50	97,100,101,102	0
14	UNL	P	4040	1/-	0.58	0.30	73,73,73,73	0
14	UNL	V	4024	1/-	0.59	1.07	96,96,96,96	0
14	UNL	E	4061	1/-	0.60	0.19	79,79,79,79	0
11	JZR	C	2011	18/18	0.60	0.47	106,118,123,125	0
14	UNL	B	4080	1/-	0.60	0.68	67,67,67,67	0
14	UNL	O	4020	2/-	0.61	0.23	96,96,96,97	0
12	PO4	A	2010	5/5	0.61	0.23	133,133,134,134	0
14	UNL	G	4070	1/-	0.63	0.26	67,67,67,67	0
14	UNL	Q	4044	1/-	0.63	1.63	88,88,88,88	0
14	UNL	U	4049	1/-	0.64	0.69	77,77,77,77	0
14	UNL	B	4025	1/-	0.64	1.82	93,93,93,93	0
14	UNL	N	4022	1/-	0.64	0.51	81,81,81,81	0
18	UQ	C	2002	18/63	0.65	0.30	61,73,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	PO4	D	4010	5/5	0.65	0.30	169,169,170,170	0
14	UNL	O	4071	1/-	0.67	0.86	70,70,70,70	0
15	PEE	B	4017	8/51	0.67	0.42	85,88,91,92	0
14	UNL	V	4088	1/-	0.68	0.92	80,80,80,80	0
14	UNL	A	4076	1/-	0.69	0.44	68,68,68,68	0
14	UNL	A	4081	1/-	0.71	0.47	71,71,71,71	0
13	AZI	A	4002	3/3	0.71	0.49	48,48,58,65	0
14	UNL	D	4054	1/-	0.72	0.27	76,76,76,76	0
14	UNL	N	4029	1/-	0.72	1.40	94,94,94,94	0
14	UNL	O	4037	1/-	0.73	0.82	62,62,62,62	0
14	UNL	A	4038	1/-	0.73	0.60	85,85,85,85	0
14	UNL	B	4026	1/-	0.73	1.33	92,92,92,92	0
14	UNL	D	4027	1/-	0.74	0.29	87,87,87,87	0
14	UNL	R	4055	1/-	0.74	0.13	73,73,73,73	0
12	PO4	R	4014	5/5	0.75	0.43	173,174,174,174	0
14	UNL	D	4059	1/-	0.75	0.90	57,57,57,57	0
14	UNL	A	4091	1/-	0.75	0.75	72,72,72,72	0
14	UNL	A	4048	1/-	0.75	0.38	72,72,72,72	0
14	UNL	D	4083	1/-	0.76	0.55	82,82,82,82	0
14	UNL	B	4057	1/-	0.77	0.85	57,57,57,57	0
14	UNL	N	4019	2/-	0.77	0.31	76,76,76,76	0
15	PEE	D	2006	51/51	0.77	0.32	85,98,115,118	0
18	UQ	P	3002	18/63	0.78	0.24	60,82,85,86	0
13	AZI	P	3005	3/3	0.78	0.35	54,54,59,63	0
12	PO4	R	4013	5/5	0.78	0.25	114,114,116,116	0
14	UNL	G	4053	1/-	0.79	0.23	77,77,77,77	0
14	UNL	P	4074	1/-	0.79	0.17	59,59,59,59	0
14	UNL	C	4045	1/-	0.79	0.41	71,71,71,71	0
12	PO4	D	4011	5/5	0.79	0.31	130,130,130,131	0
14	UNL	N	4073	1/-	0.79	0.17	69,69,69,69	0
14	UNL	B	4042	1/-	0.80	0.42	81,81,81,81	0
13	AZI	C	2005	3/3	0.80	0.35	41,41,55,60	0
14	UNL	A	4035	1/-	0.80	0.99	69,69,69,69	0
14	UNL	B	4079	1/-	0.80	0.44	66,66,66,66	0
14	UNL	P	4021	2/-	0.80	0.18	71,71,71,73	0
14	UNL	O	4031	1/-	0.81	0.46	86,86,86,86	0
14	UNL	O	4082	1/-	0.81	0.14	73,73,73,73	0
14	UNL	B	4030	1/-	0.82	0.44	70,70,70,70	0
12	PO4	P	3010	5/5	0.83	0.18	115,115,115,116	0
14	UNL	C	4023	1/-	0.83	0.52	55,55,55,55	0
20	GOL	E	4006	6/6	0.83	0.25	67,71,72,75	0
14	UNL	F	4028	1/-	0.84	0.58	82,82,82,82	0

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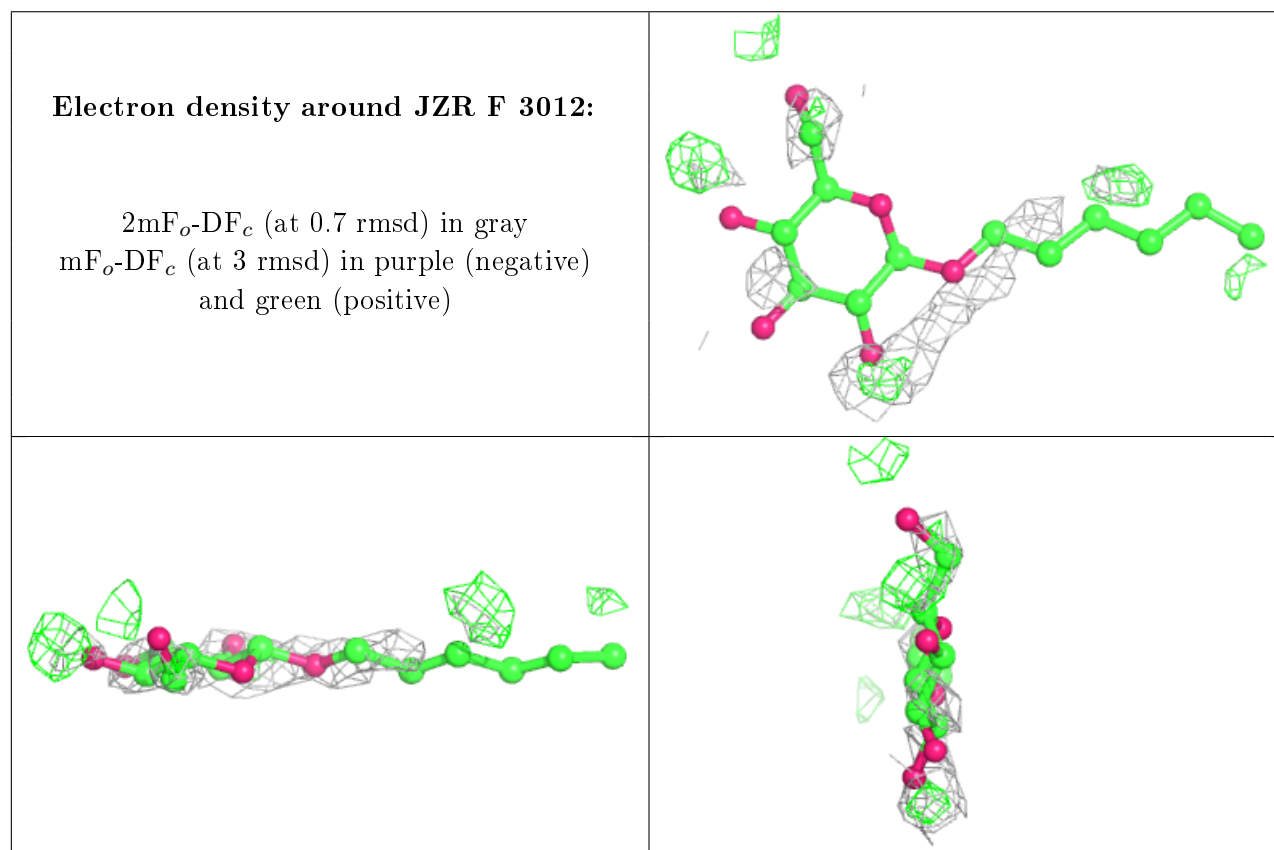
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	PO4	I	4015	5/5	0.84	0.31	122,122,123,123	0
14	UNL	B	4051	1/-	0.84	0.22	78,78,78,78	0
14	UNL	O	4043	1/-	0.84	0.29	80,80,80,80	0
14	UNL	P	4058	1/-	0.84	0.34	61,61,61,61	0
14	UNL	A	4032	1/-	0.84	0.71	65,65,65,65	0
14	UNL	O	4084	1/-	0.84	0.68	67,67,67,67	0
14	UNL	D	4067	1/-	0.84	0.58	58,58,58,58	0
14	UNL	T	4065	1/-	0.84	0.73	66,66,66,66	0
14	UNL	V	4078	1/-	0.85	1.63	94,94,94,94	0
14	UNL	D	4062	1/-	0.85	0.27	90,90,90,90	0
14	UNL	B	4052	1/-	0.85	0.17	60,60,60,60	0
14	UNL	W	4077	1/-	0.86	0.14	60,60,60,60	0
19	CDL	D	2003	39/100	0.86	0.20	64,84,106,107	0
14	UNL	A	4087	1/-	0.86	0.33	60,60,60,60	0
14	UNL	O	4041	1/-	0.87	0.36	71,71,71,71	0
14	UNL	B	4039	1/-	0.87	0.31	73,73,73,73	0
14	UNL	I	4033	1/-	0.87	0.87	69,69,69,69	0
12	PO4	Q	4012	5/5	0.87	0.18	108,109,110,110	0
14	UNL	A	4085	1/-	0.88	0.18	56,56,56,56	0
14	UNL	T	4066	1/-	0.88	0.07	70,70,70,70	0
14	UNL	G	4064	1/-	0.88	0.52	56,56,56,56	0
19	CDL	Q	3003	39/100	0.88	0.23	54,90,96,96	0
20	GOL	C	2008	6/6	0.88	0.31	60,63,63,70	0
12	PO4	B	3009	5/5	0.89	0.17	97,99,100,101	0
14	UNL	E	4050	1/-	0.89	0.38	65,65,65,65	0
20	GOL	P	3008	6/6	0.89	0.50	83,84,85,88	0
14	UNL	C	4018	2/-	0.90	0.35	74,74,74,76	0
19	CDL	P	3004	49/100	0.90	0.26	54,81,117,120	0
15	PEE	Q	3006	51/51	0.91	0.20	53,65,110,110	0
14	UNL	P	4089	1/-	0.91	0.47	63,63,63,63	0
19	CDL	C	2004	44/100	0.91	0.21	54,83,104,106	0
14	UNL	P	4046	1/-	0.91	0.48	65,65,65,65	0
15	PEE	P	3007	49/51	0.92	0.23	35,58,75,76	0
13	AZI	G	4001	3/3	0.92	0.15	47,47,57,59	0
14	UNL	V	4090	1/-	0.92	0.98	74,74,74,74	0
15	PEE	C	2007	49/51	0.93	0.23	33,58,74,74	0
12	PO4	T	4016	5/5	0.93	0.09	107,108,108,108	0
14	UNL	R	4069	1/-	0.93	0.41	62,62,62,62	0
14	UNL	C	4086	1/-	0.93	0.24	50,50,50,50	0
14	UNL	A	4075	1/-	0.94	0.90	64,64,64,64	0
17	SMA	P	3001	37/37	0.95	0.16	30,39,47,52	0
20	GOL	P	4009	6/6	0.95	0.23	67,70,71,72	0

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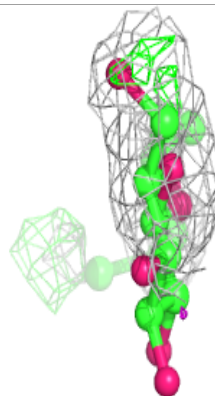
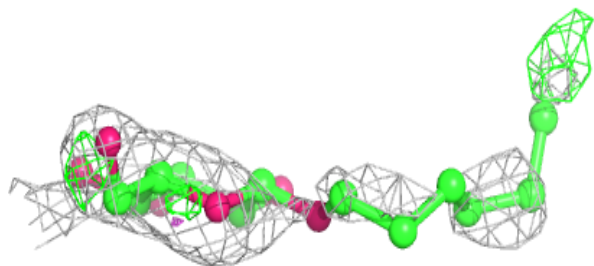
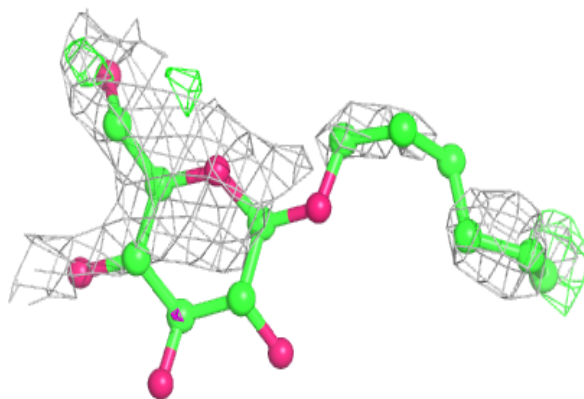
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	GOL	C	4008	6/6	0.95	0.20	53,55,60,60	0
17	SMA	C	2001	37/37	0.96	0.16	25,33,44,46	0
11	JZR	A	4004	18/18	0.96	0.13	29,36,42,44	0
14	UNL	C	4063	1/-	0.96	1.03	74,74,74,74	0
21	HEC	D	501	43/43	0.97	0.13	26,33,37,38	0
12	PO4	O	2009	5/5	0.97	0.09	76,79,81,81	0
21	HEC	Q	501	43/43	0.98	0.11	29,36,41,45	0
16	HEM	C	502	43/43	0.98	0.16	23,26,33,36	0
16	HEM	C	501	43/43	0.98	0.12	21,27,34,38	0
16	HEM	P	501	43/43	0.98	0.14	22,26,33,40	0
22	FES	R	501	4/4	0.99	0.12	27,29,30,30	0
22	FES	E	501	4/4	0.99	0.13	38,39,40,40	0
16	HEM	P	502	43/43	0.99	0.11	23,27,37,39	0

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

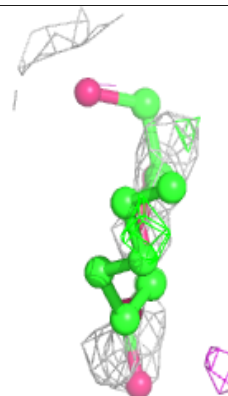
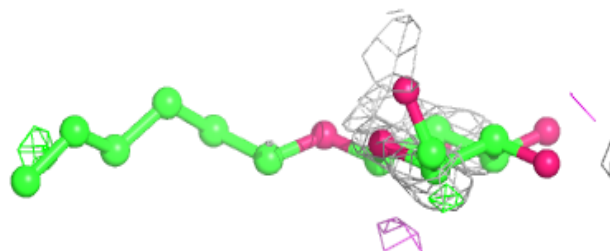
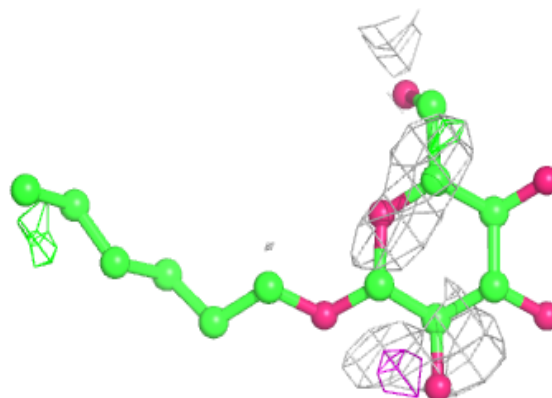


Electron density around JZR S 2012:

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

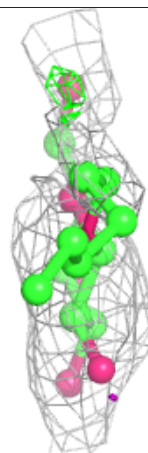
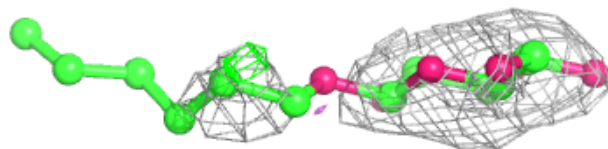
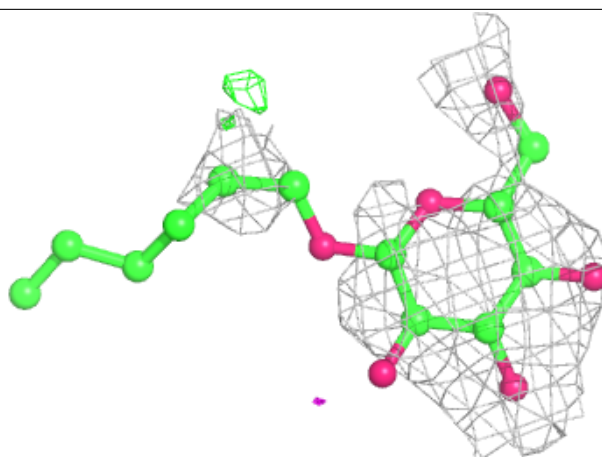
**Electron density around JZR F 4003:**

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



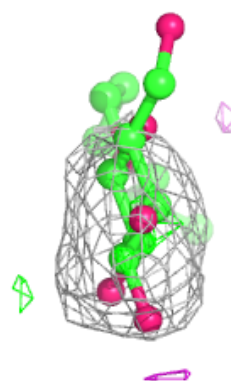
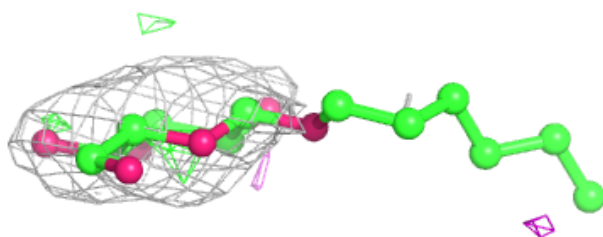
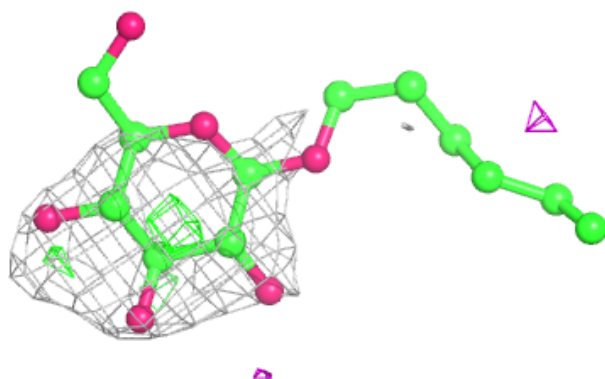
Electron density around JZR P 3011:

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

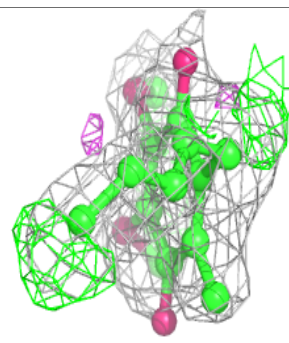
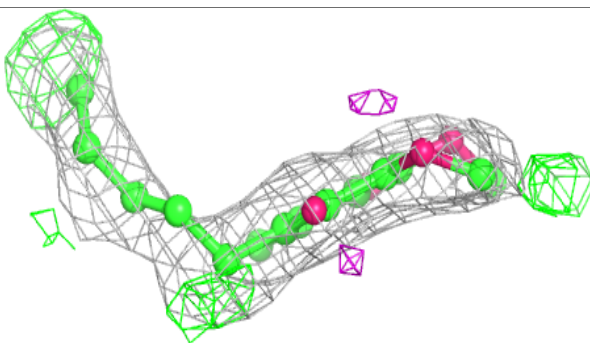
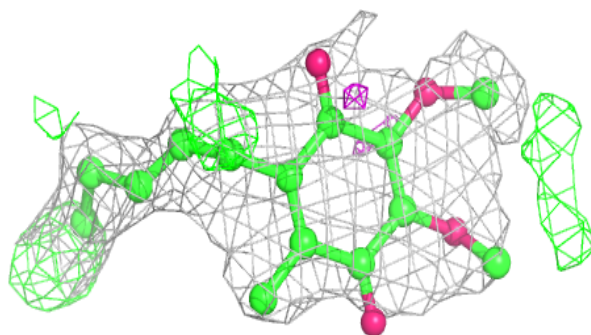


Electron density around JZR C 2011:

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

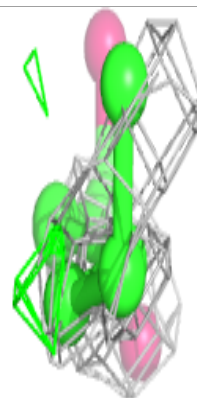
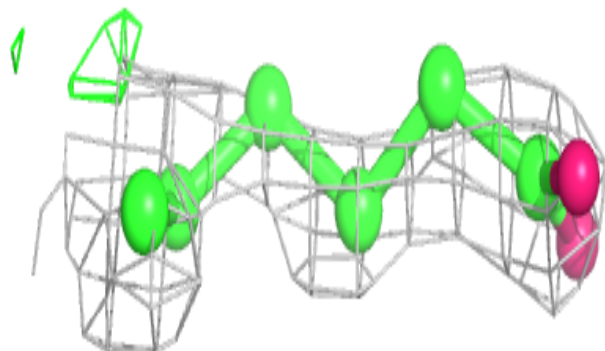
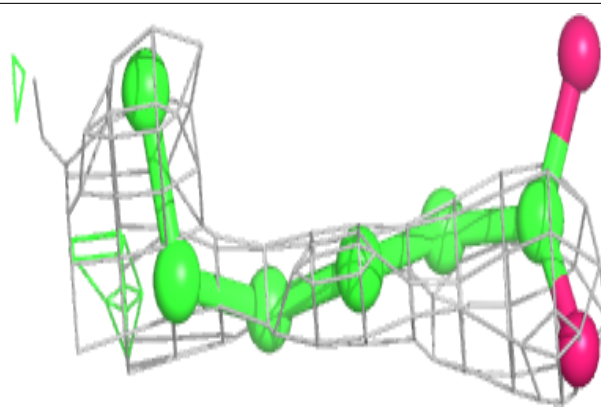
**Electron density around UQ C 2002:**

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

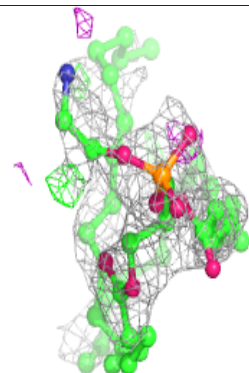
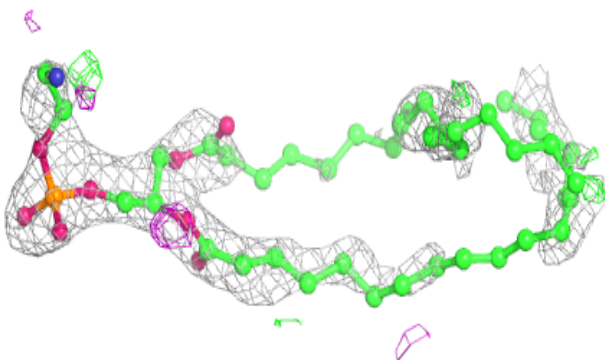
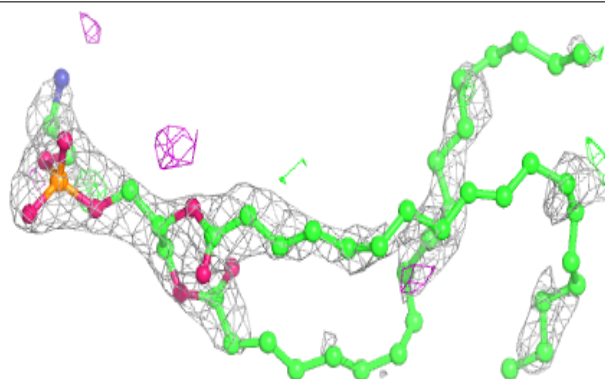


Electron density around PEE B 4017:

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

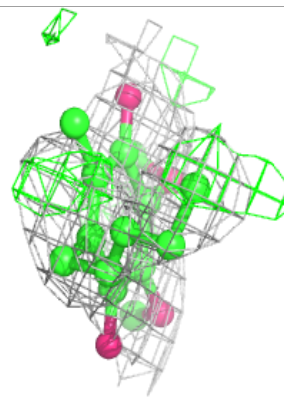
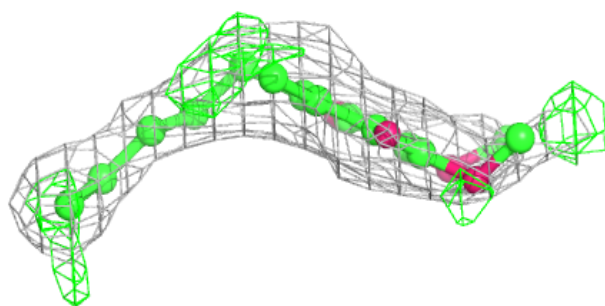
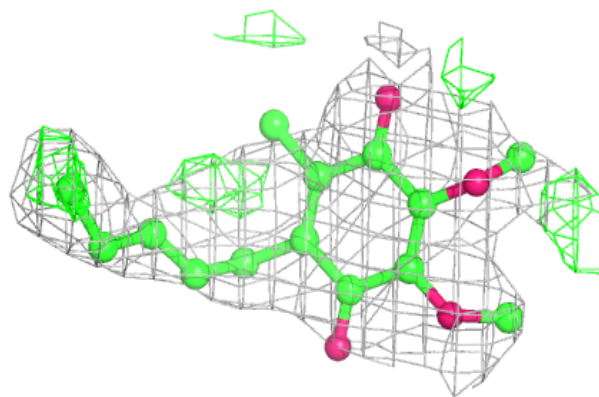
**Electron density around PEE D 2006:**

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

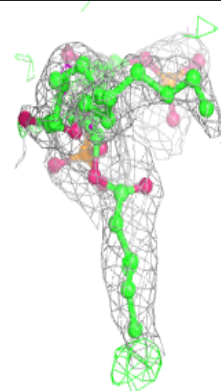
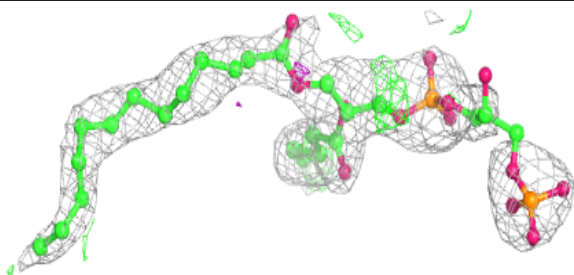
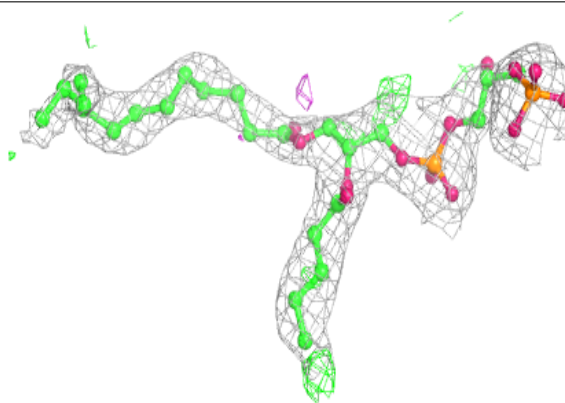


Electron density around UQ P 3002:

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

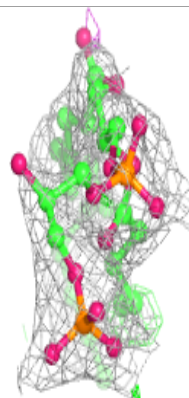
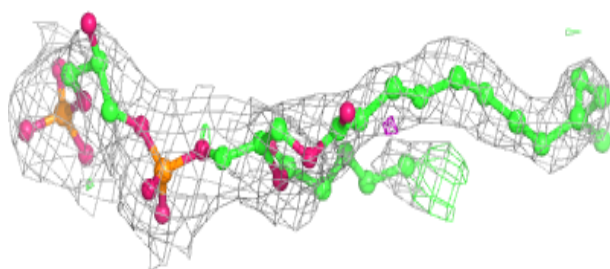
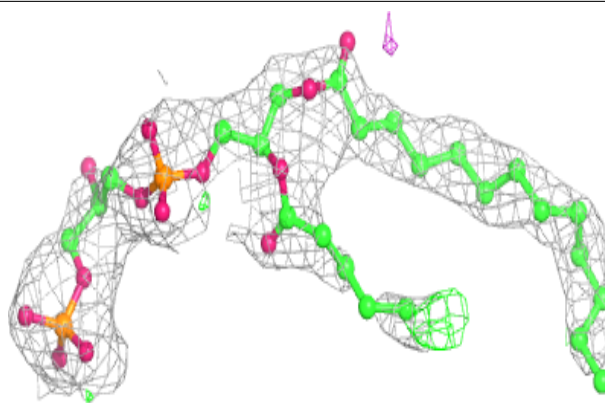
**Electron density around CDL D 2003:**

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

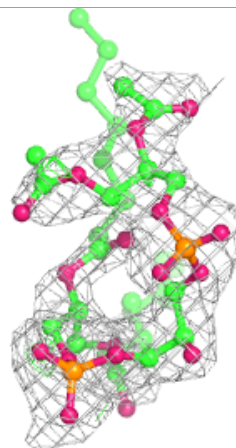
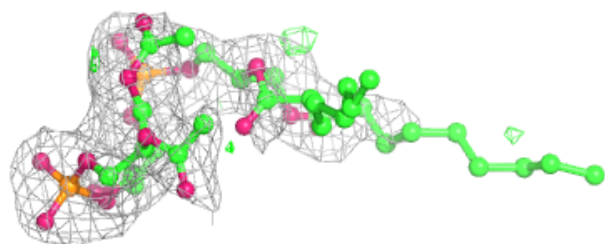
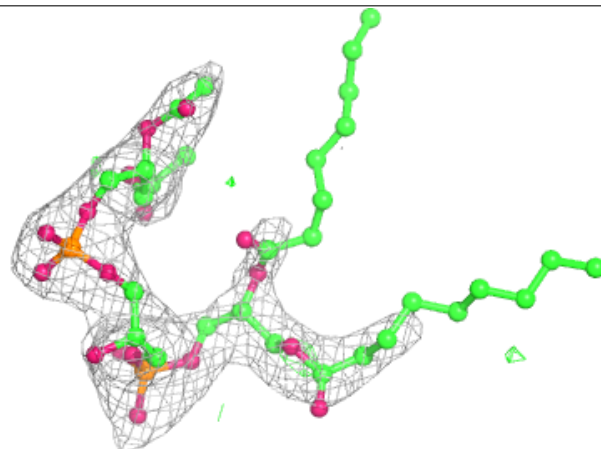


Electron density around CDL Q 3003:

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

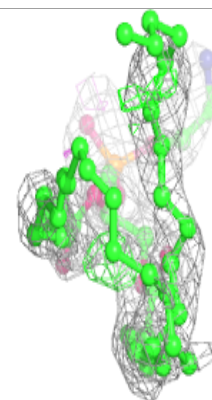
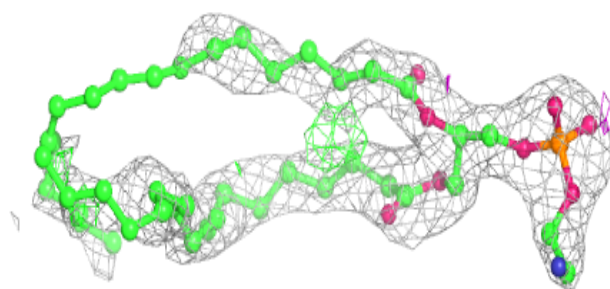
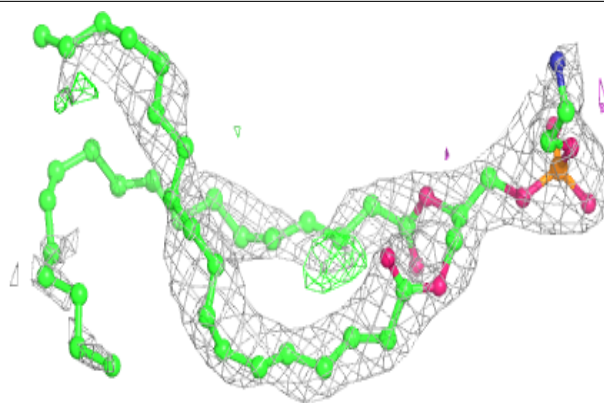
**Electron density around CDL P 3004:**

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

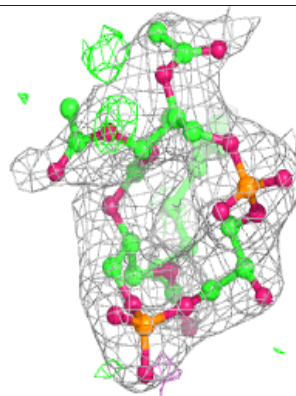
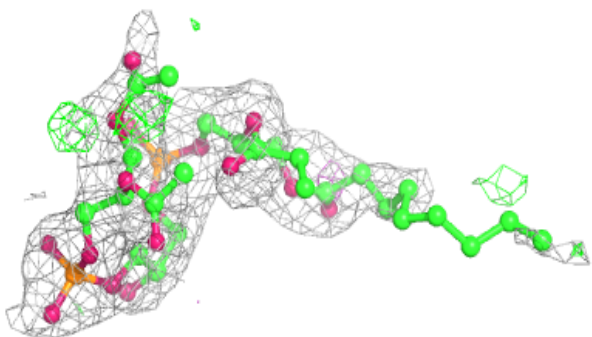
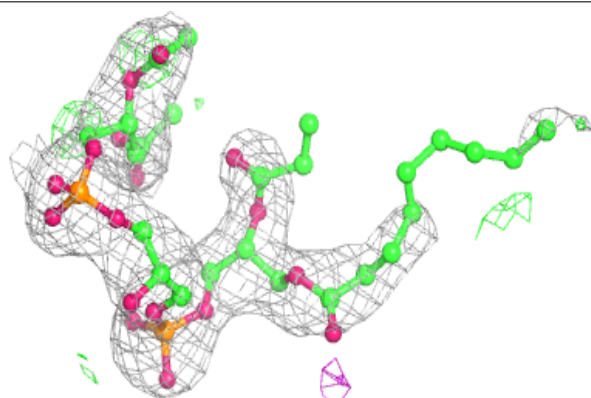


Electron density around PEE Q 3006:

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

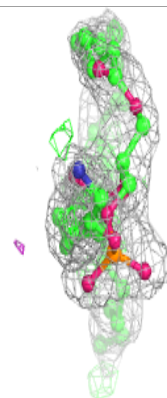
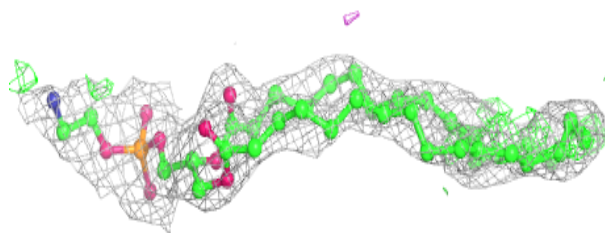
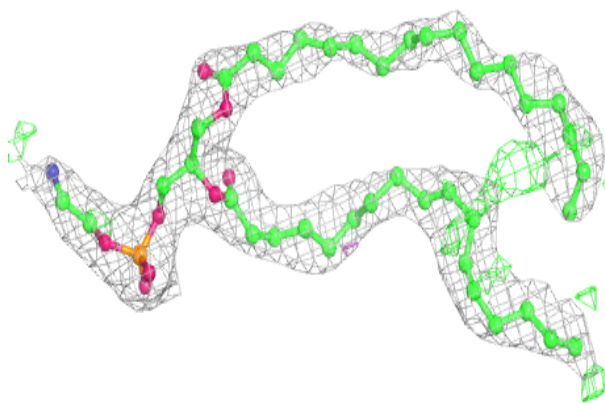
**Electron density around CDL C 2004:**

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

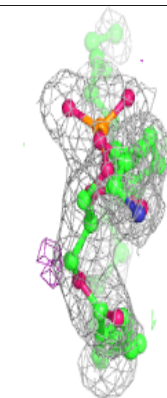
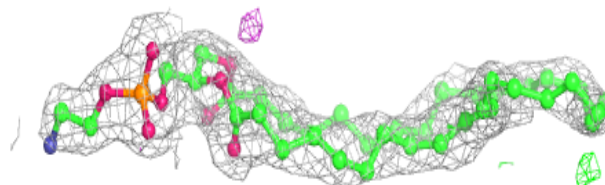
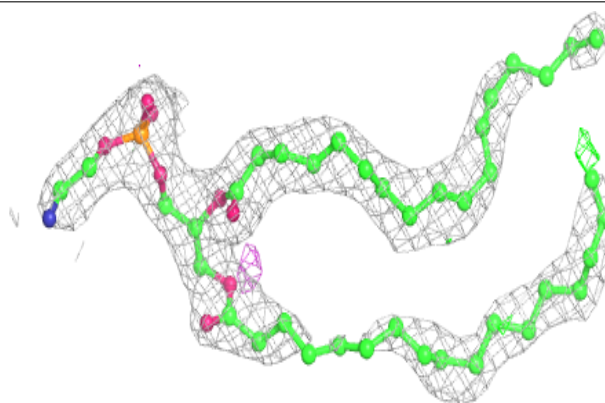


Electron density around PEE P 3007:

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

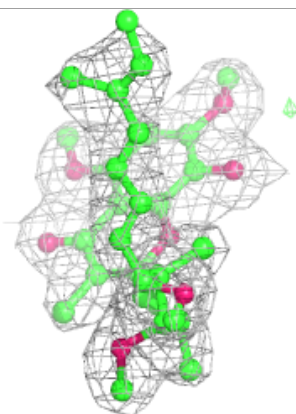
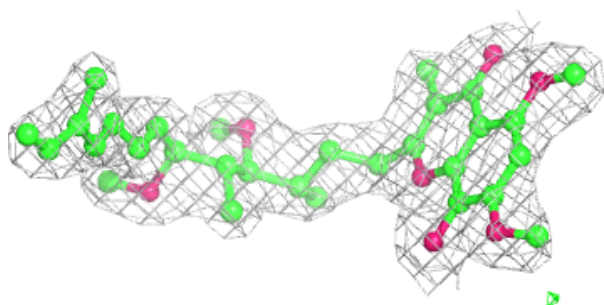
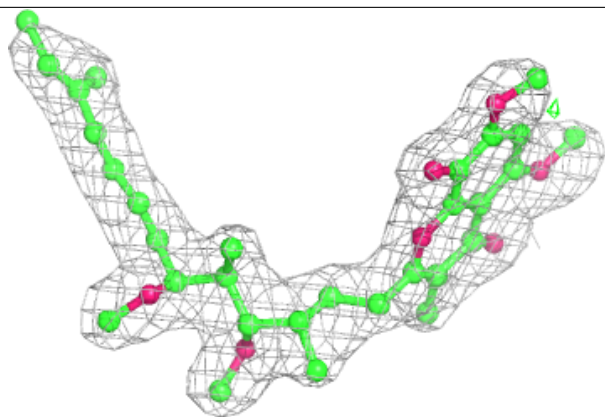
**Electron density around PEE C 2007:**

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

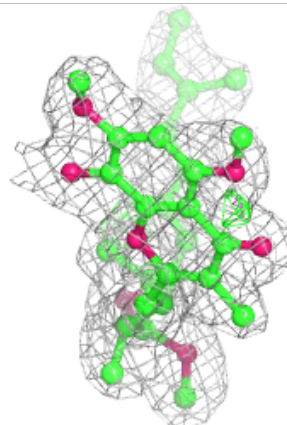
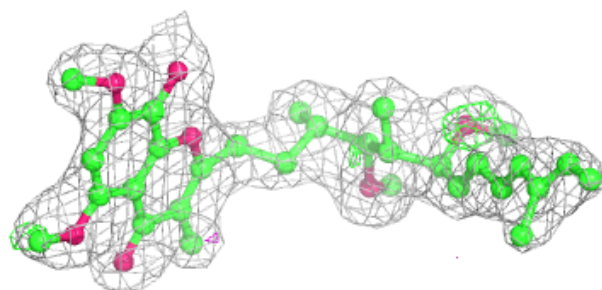
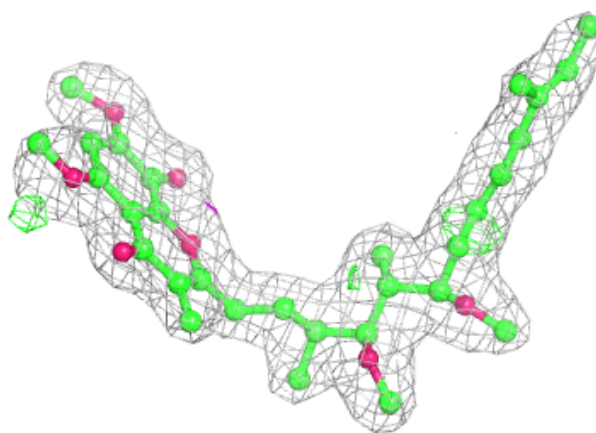


Electron density around SMA P 3001:

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

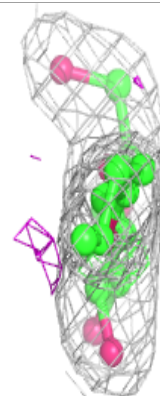
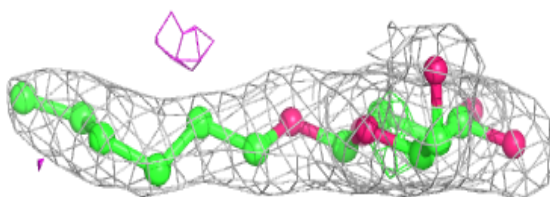
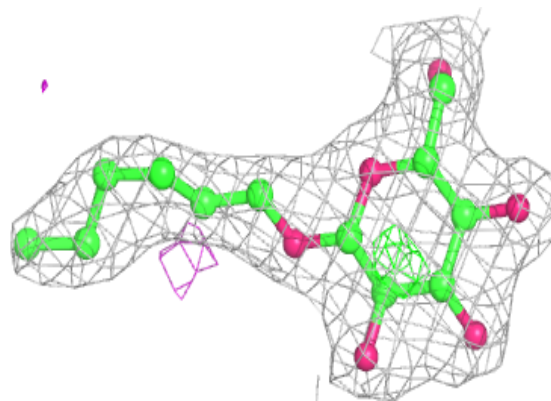
**Electron density around SMA C 2001:**

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



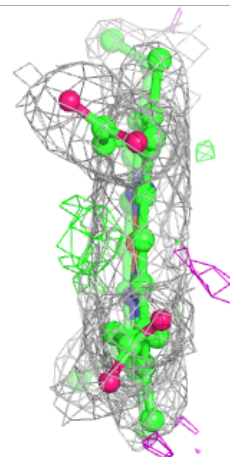
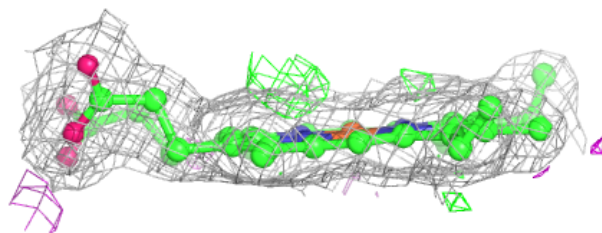
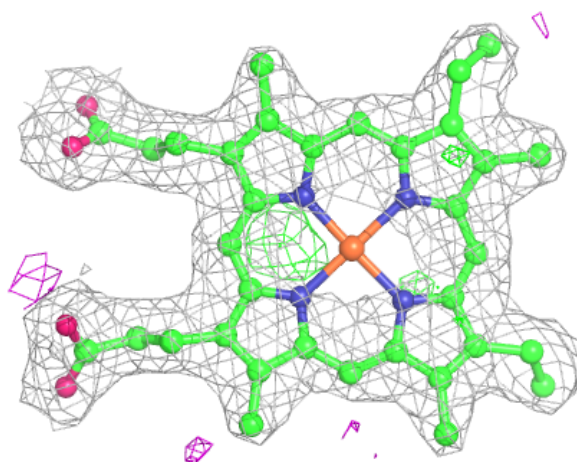
Electron density around JZR A 4004:

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



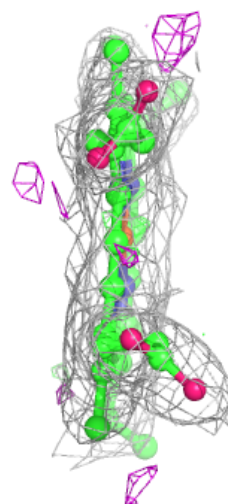
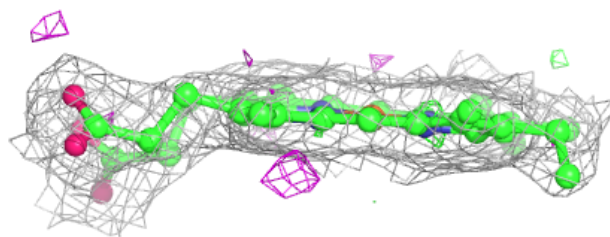
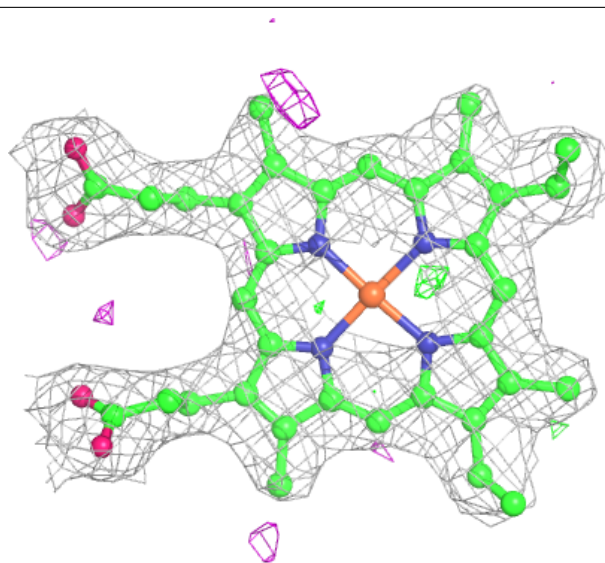
Electron density around HEC D 501:

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



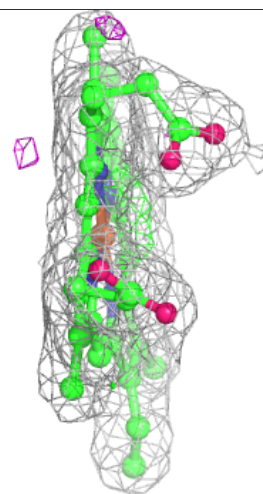
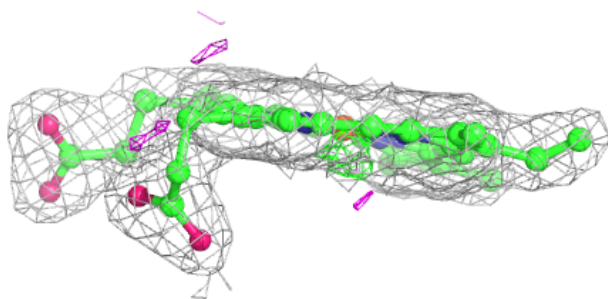
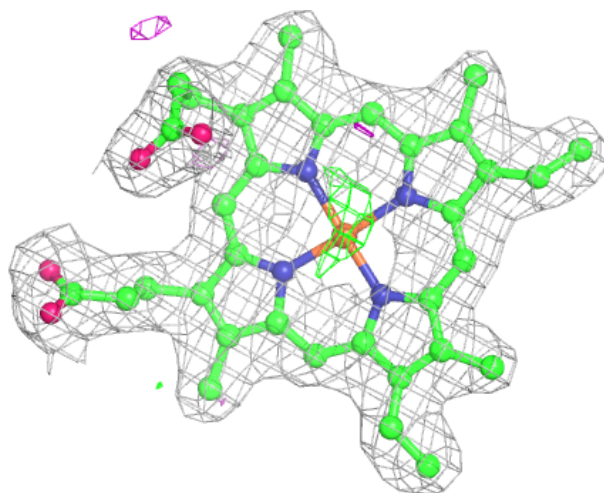
Electron density around HEC Q 501:

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



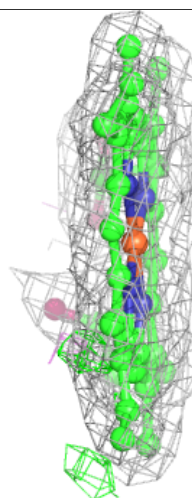
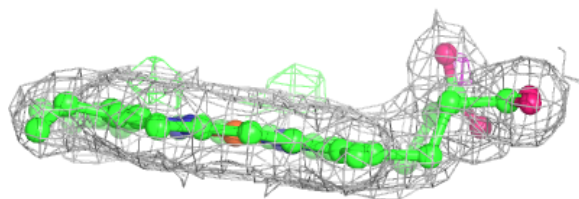
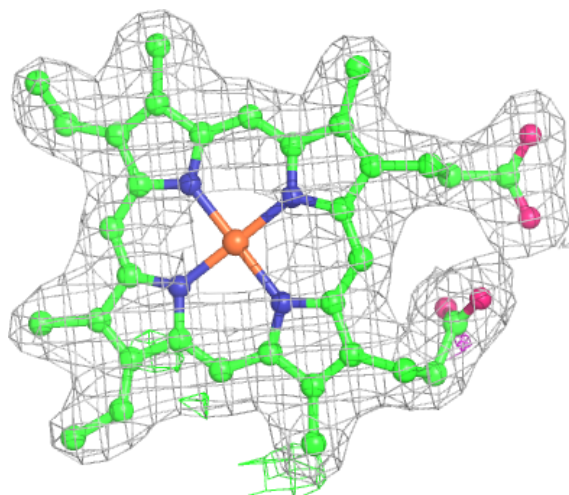
Electron density around HEM C 502:

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



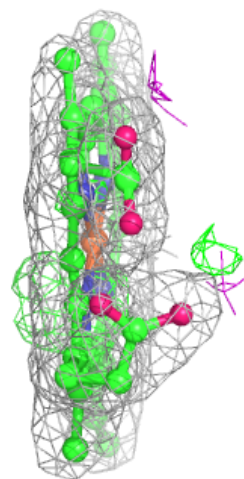
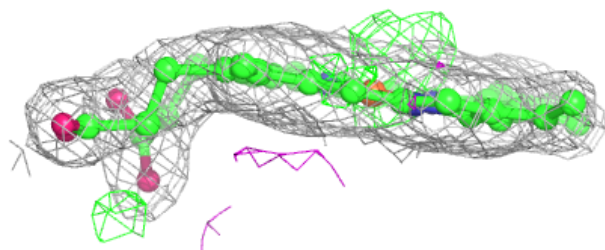
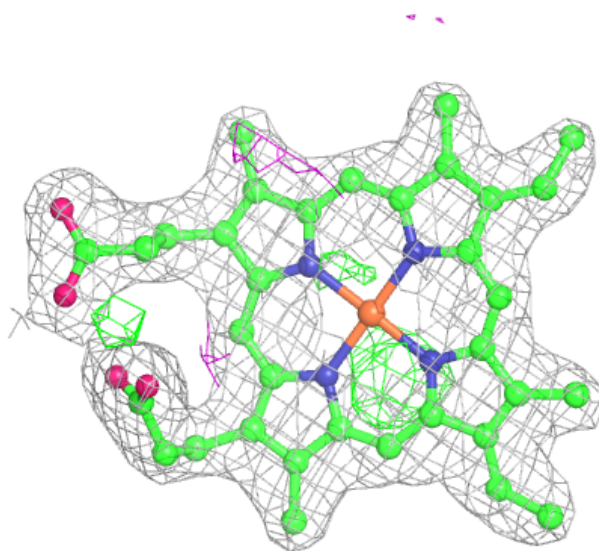
Electron density around HEM C 501:

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



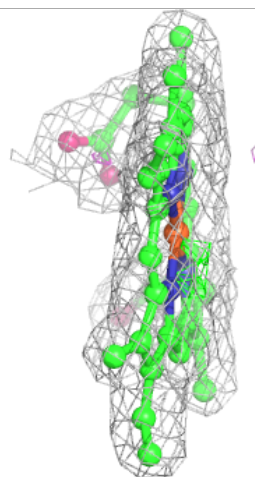
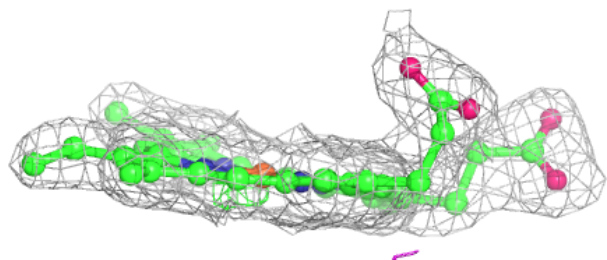
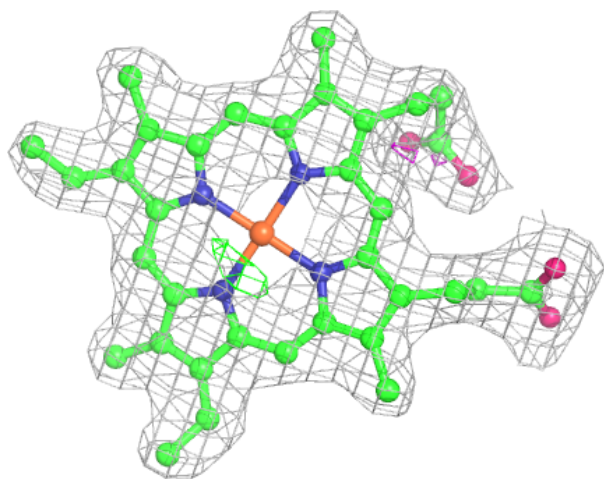
Electron density around HEM P 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.