



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:33 AM EDT

PDB ID : 2A06 / pdb_00002a06
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

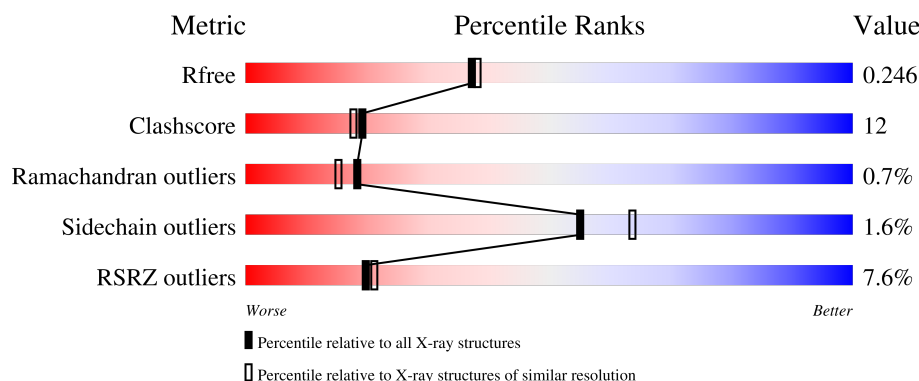
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

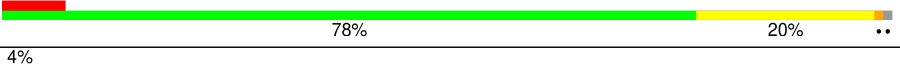
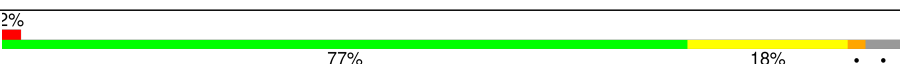
The reported resolution of this entry is 2.10 Å.

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	N	446	
2	B	439	
2	O	439	
3	C	379	

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Mol	Chain	Length	Quality of chain
3	P	379	
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	F	3012	-	-	-	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	-	-
12	PO4	R	4013	-	X	-	-
12	PO4	R	4014	-	X	-	-
12	PO4	T	4016	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	AZI	A	4002	-	X	-	-
13	AZI	C	2005	-	X	-	-
13	AZI	G	4001	-	X	-	-
13	AZI	P	3005	-	X	-	-
14	UNL	O	4043	-	-	X	-
21	HEC	D	501	X	-	-	-
21	HEC	Q	501	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			

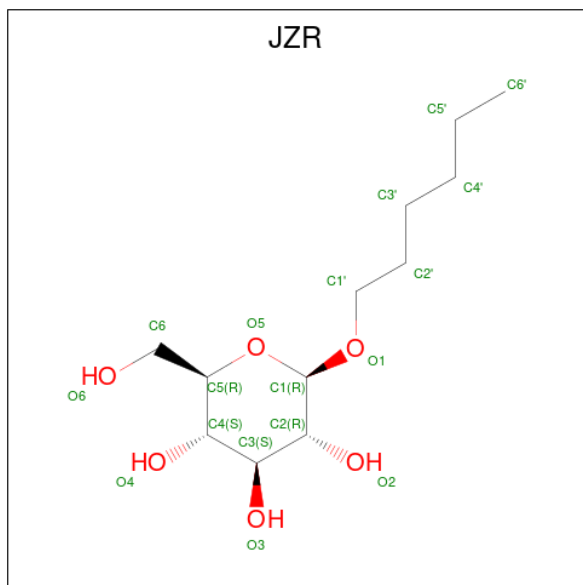
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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.

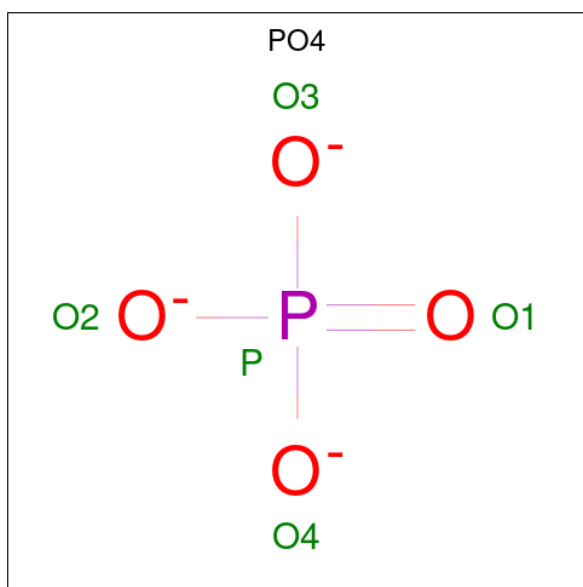
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: C₁₂H₂₄O₆).



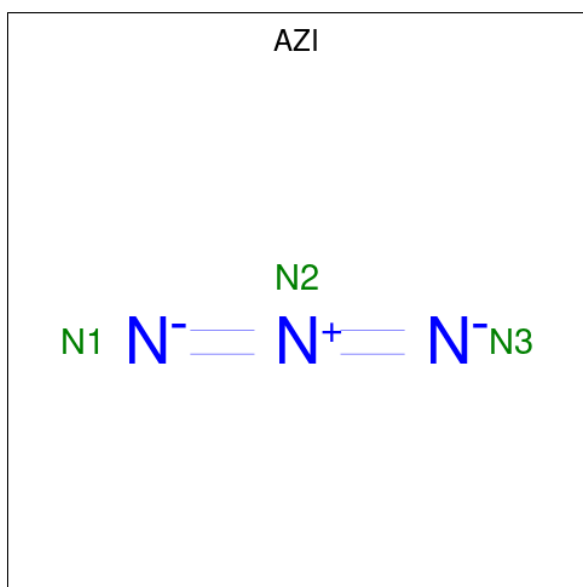
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is PHOSPHATE ION (CCD ID: 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 (CCD ID: 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 (CCD ID: UNL) (formula:).

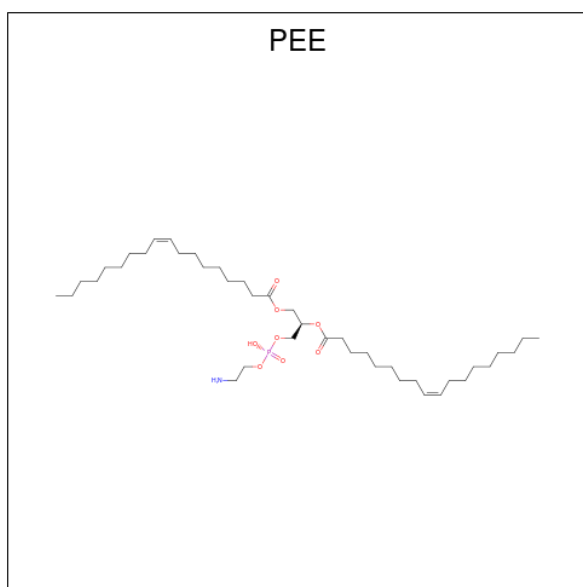
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	10	Total O 10 10	0	0
14	B	11	Total O 11 11	0	0
14	C	6	Total O 7 7	0	0
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	F	1	Total O 1 1	0	0
14	G	3	Total O 3 3	0	0
14	I	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	N	4	Total	O	0	0
			5	5		
14	O	8	Total	O	0	0
			9	9		
14	P	7	Total	O	0	0
			8	8		
14	Q	1	Total	O	0	0
			1	1		
14	R	2	Total	O	0	0
			2	2		
14	S	1	Total	O	0	0
			1	1		
14	T	2	Total	O	0	0
			2	2		
14	U	2	Total	O	0	0
			2	2		
14	V	4	Total	O	0	0
			4	4		
14	W	1	Total	O	0	0
			1	1		

- Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



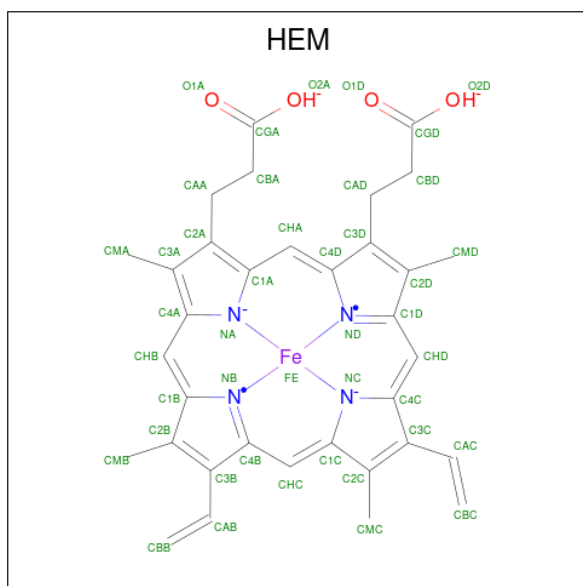
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			8	6	2		

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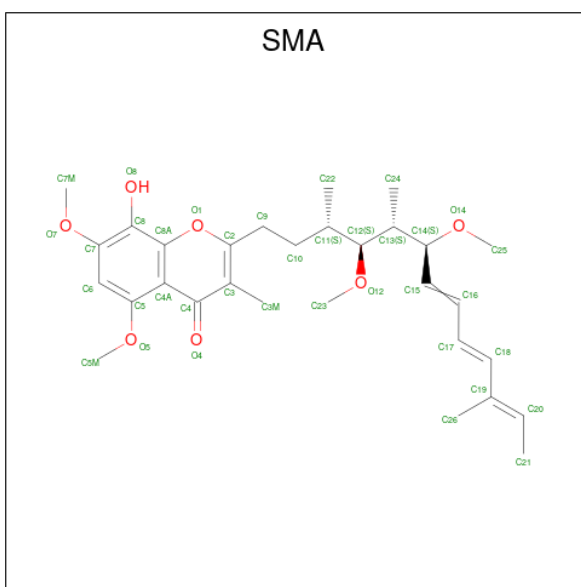
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	D	1	Total 51	C 41	N 1	O 8	P 1	0	0
15	P	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0

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



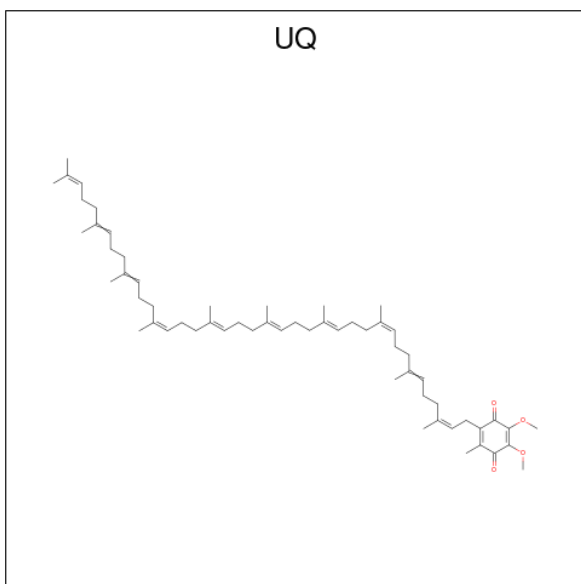
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 17 is STIGMATELLIN A (CCD ID: 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 (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



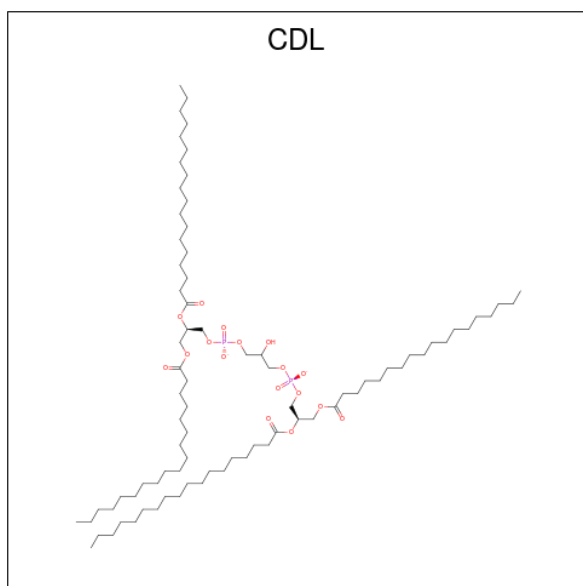
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			18	14	4		

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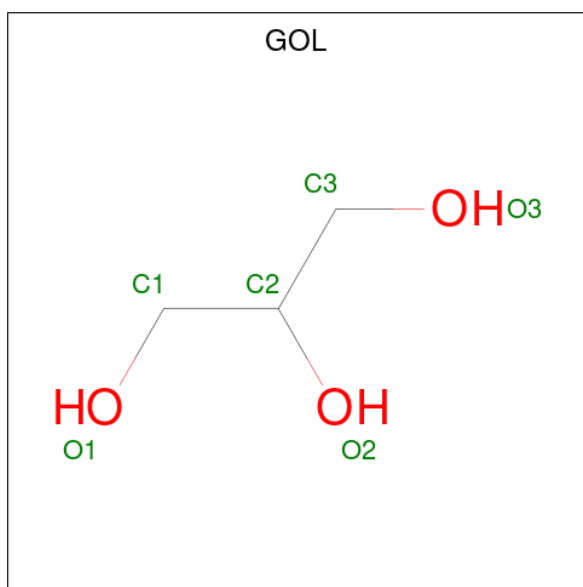
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	P	1	Total	C	O	0	0
			18	14	4		

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



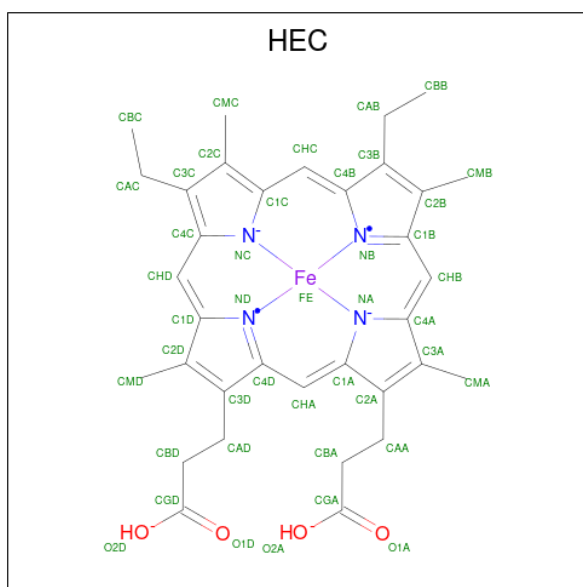
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	C	1	Total	C	O	P	0	0
			44	25	17	2		
19	D	1	Total	C	O	P	0	0
			39	24	13	2		
19	P	1	Total	C	O	P	0	0
			49	30	17	2		
19	Q	1	Total	C	O	P	0	0
			39	24	13	2		

- Molecule 20 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



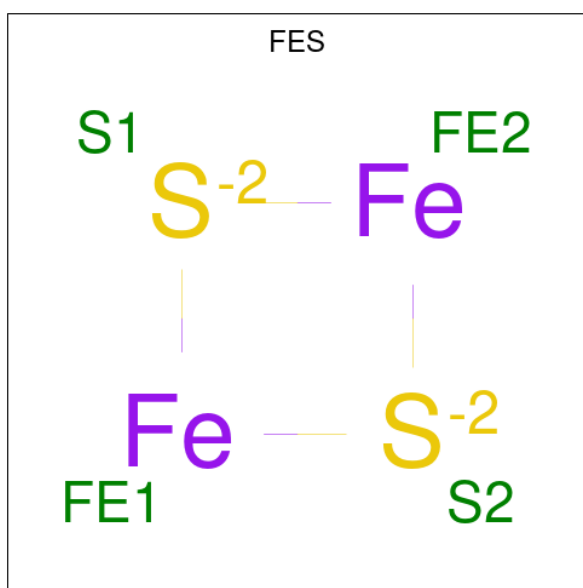
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	C	1	Total	C	O	0	0
			6	3	3		
20	C	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			5	3	2		
20	O	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 21 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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 (CCD ID: 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

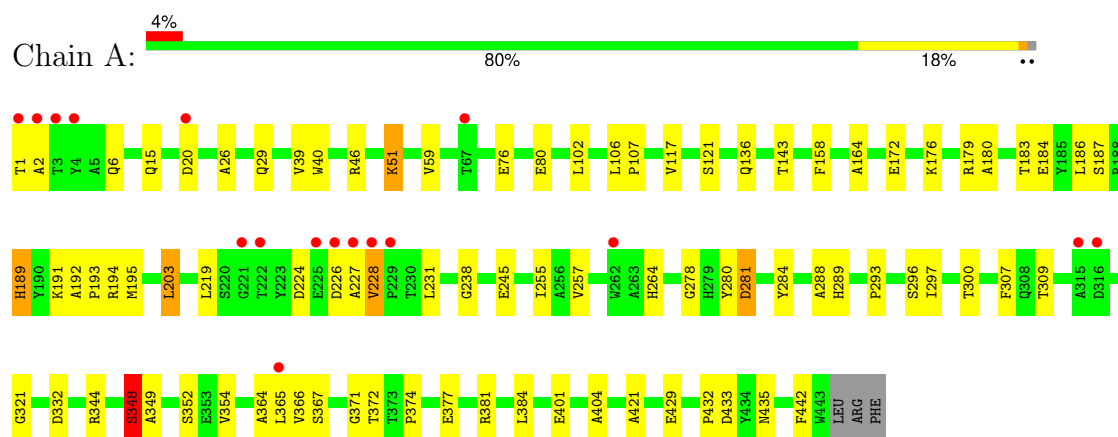
- Molecule 23 is water.

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

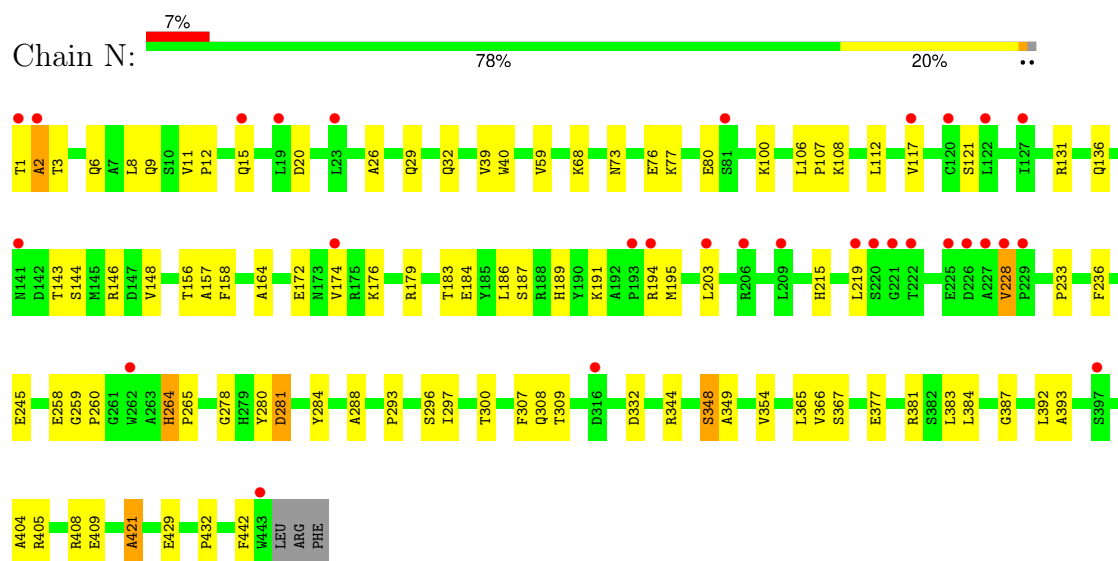
3 Residue-property plots

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

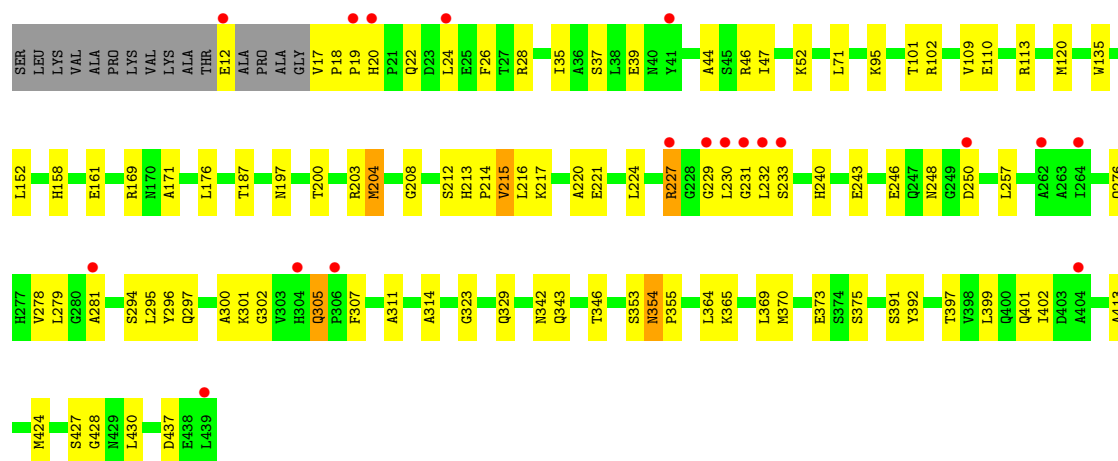


- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

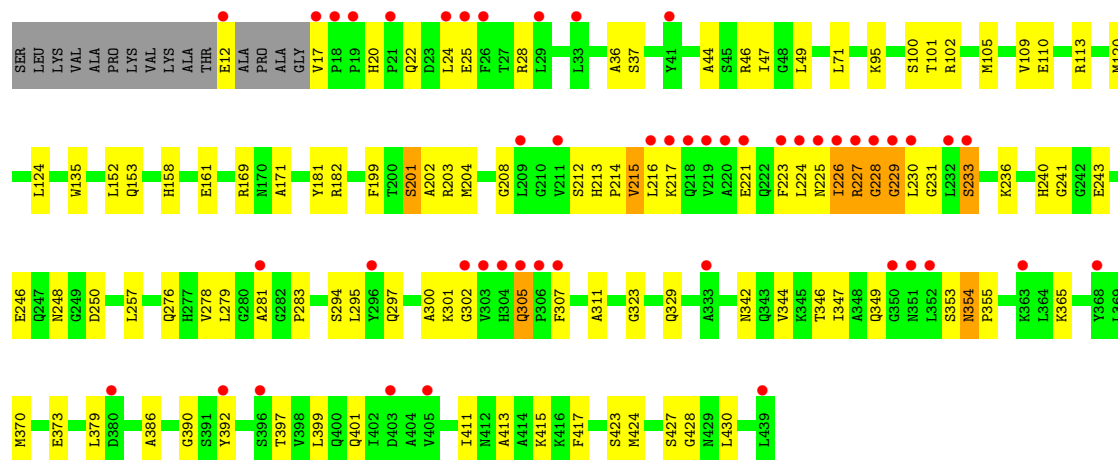
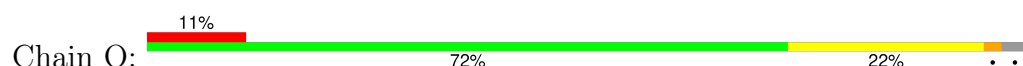


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

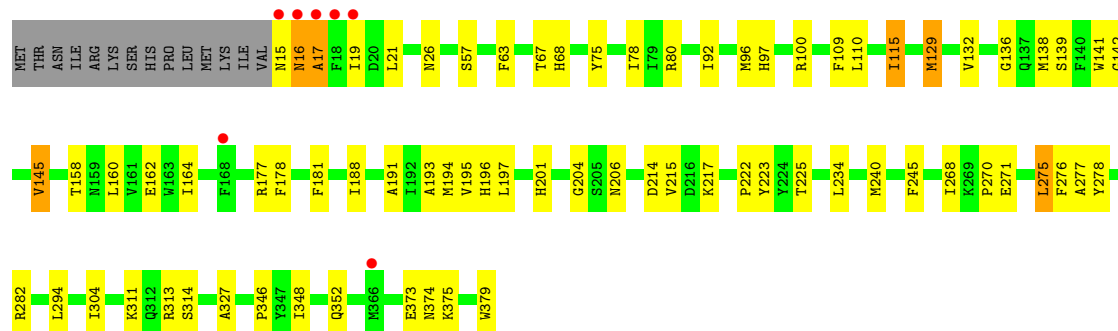




- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

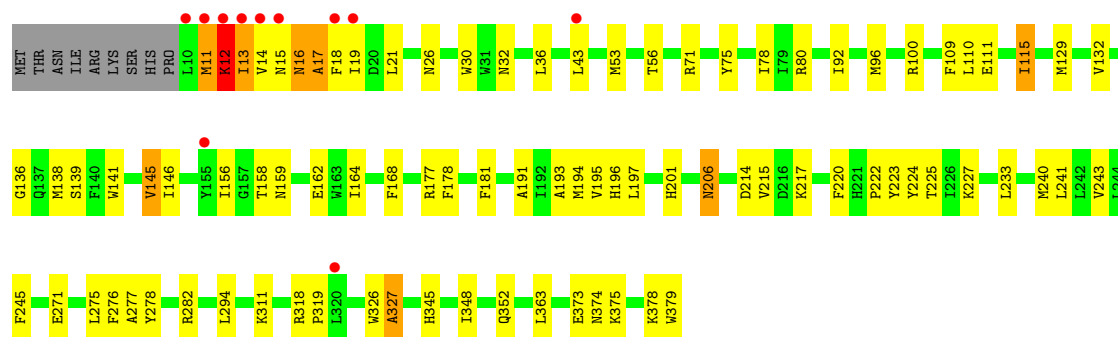


- Molecule 3: Cytochrome b, heme protein, mitochondrial

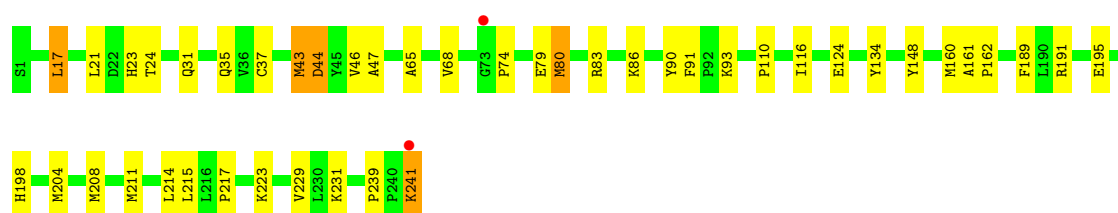
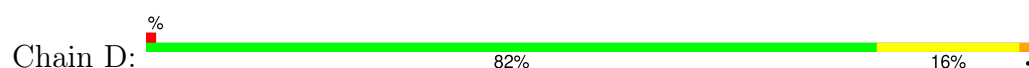


- Molecule 3: Cytochrome b, heme protein, mitochondrial

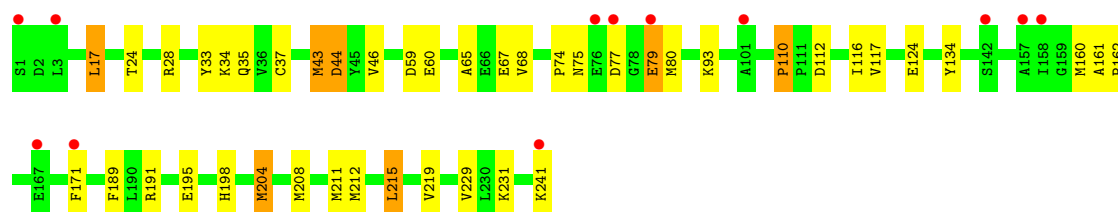
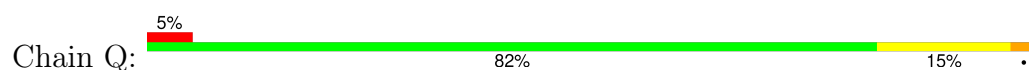




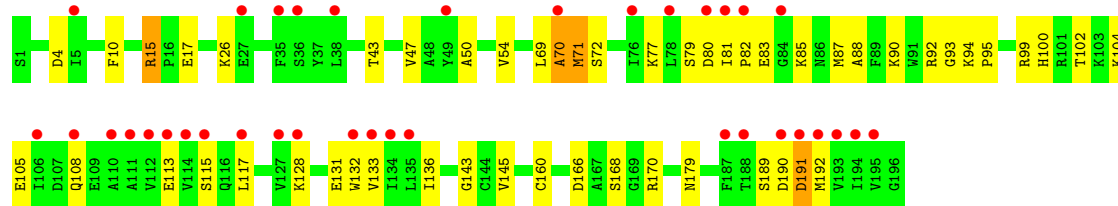
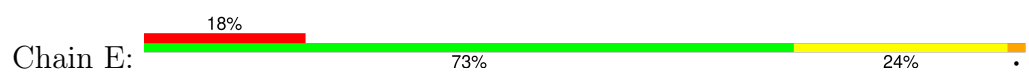
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



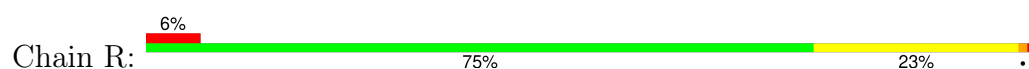
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

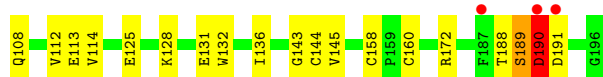


- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



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

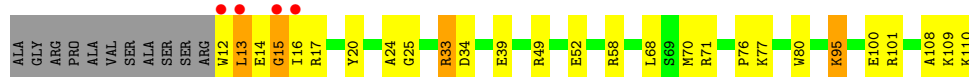




- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



- 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



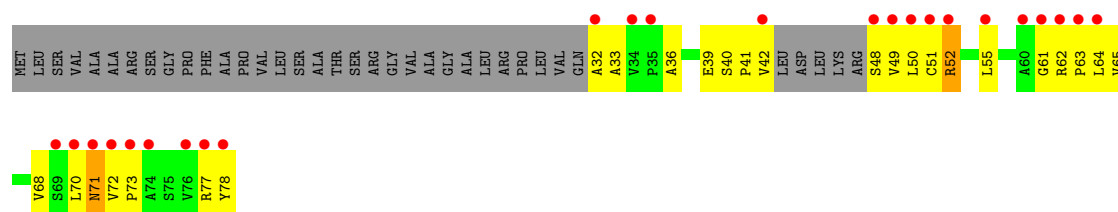
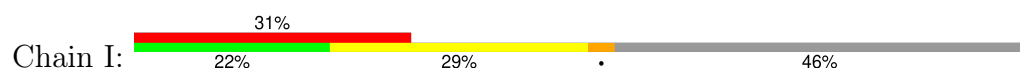
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



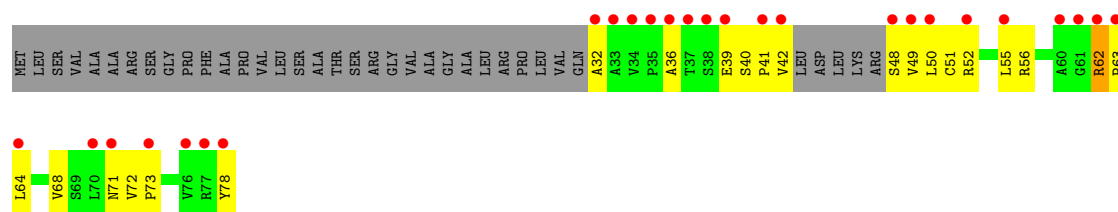
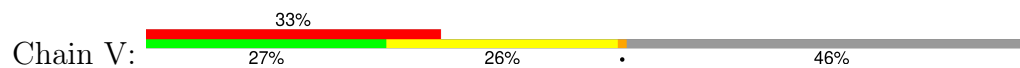
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



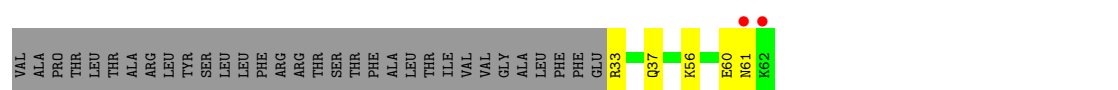
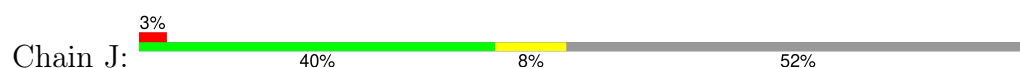
- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



- 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 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.3 (37.87-2.10) 95.3 (37.87-2.10)	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 , 0.246	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)	0.37 , 57.0	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: UQ, GOL, HEM, CDL, UNL, FES, JZR, PO4, AZI, HEC, SMA, PEE

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	0.54	0/3467	0.96	10/4706 (0.2%)
1	N	0.46	0/3467	0.94	10/4706 (0.2%)
2	B	0.54	1/3235 (0.0%)	0.97	8/4387 (0.2%)
2	O	0.49	0/3239	0.99	11/4393 (0.3%)
3	C	0.60	1/2992 (0.0%)	0.99	18/4097 (0.4%)
3	P	0.56	0/3030	0.97	18/4145 (0.4%)
4	D	0.55	0/1978	0.96	6/2684 (0.2%)
4	Q	0.52	1/1978 (0.1%)	0.97	6/2684 (0.2%)
5	E	0.45	0/1553	1.12	14/2100 (0.7%)
5	R	0.51	0/1550	1.01	12/2094 (0.6%)
6	F	0.57	0/878	0.93	4/1175 (0.3%)
6	S	0.54	0/878	0.91	5/1175 (0.4%)
7	G	0.49	0/642	1.01	5/869 (0.6%)
7	T	0.44	0/647	1.02	7/876 (0.8%)
8	H	0.40	0/544	0.95	3/729 (0.4%)
8	U	0.38	0/544	0.88	0/729
9	I	0.72	0/285	1.33	3/384 (0.8%)
9	V	0.62	0/285	1.28	3/384 (0.8%)
10	J	0.44	0/252	0.83	0/333
10	W	0.41	0/520	0.91	1/699 (0.1%)
All	All	0.52	3/31964 (0.0%)	0.98	144/43349 (0.3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	129	MET	SD-CE	-5.69	1.65	1.79
2	B	204	MET	SD-CE	-5.68	1.65	1.79
4	Q	204	MET	SD-CE	-5.64	1.65	1.79

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	228	GLY	N-CA-C	-11.53	97.33	115.08
5	E	70	ALA	CA-C-N	-10.57	104.57	122.33
5	E	70	ALA	C-N-CA	-10.57	104.57	122.33
5	E	69	LEU	CA-C-N	-9.66	108.53	123.13
5	E	69	LEU	C-N-CA	-9.66	108.53	123.13
5	E	71	MET	CA-C-N	-8.69	106.05	122.73
5	E	71	MET	C-N-CA	-8.69	106.05	122.73
8	H	48	SER	N-CA-C	-7.82	104.34	114.04
4	Q	44	ASP	N-CA-C	7.77	121.69	111.75
4	D	44	ASP	N-CA-C	7.75	121.66	111.75
2	O	101	THR	N-CA-C	-7.63	98.09	108.86
9	V	40	SER	CA-C-N	7.63	129.38	119.84
9	V	40	SER	C-N-CA	7.63	129.38	119.84
5	R	114	VAL	N-CA-C	7.46	119.12	110.62
3	C	110	LEU	N-CA-C	7.24	119.79	111.11
9	I	40	SER	CA-C-N	7.22	128.86	119.84
9	I	40	SER	C-N-CA	7.22	128.86	119.84
2	B	278	VAL	N-CA-C	-7.08	103.88	110.53
5	E	143	GLY	N-CA-C	7.04	125.04	115.32
1	A	309	THR	N-CA-C	-6.90	100.31	110.52
3	P	110	LEU	N-CA-C	6.85	119.33	111.11
3	C	223	TYR	N-CA-C	6.75	119.25	111.02
3	P	206	ASN	N-CA-C	-6.64	100.07	110.36
3	P	223	TYR	N-CA-C	6.53	118.06	111.07
3	C	275	LEU	N-CA-C	6.53	118.39	111.28
2	B	430	LEU	N-CA-C	6.50	120.21	112.93
2	O	278	VAL	N-CA-C	-6.46	104.56	110.82
4	D	24	THR	N-CA-C	-6.45	103.76	111.69
3	P	26	ASN	N-CA-C	6.44	120.44	112.59
3	C	206	ASN	N-CA-C	-6.42	100.41	110.36
5	E	136	ILE	N-CA-C	-6.41	99.06	108.54
3	C	26	ASN	N-CA-C	6.36	120.34	112.59
7	T	49	ALA	N-CA-C	6.29	120.78	112.35
3	C	115	ILE	N-CA-C	-6.28	104.38	110.72
4	Q	24	THR	N-CA-C	-6.26	104.54	111.36
4	D	215	LEU	N-CA-C	6.26	118.90	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	15	ARG	N-CA-C	-6.24	101.47	110.08
6	F	25	GLY	N-CA-C	6.17	124.19	115.30
5	R	136	ILE	N-CA-C	-6.11	99.49	108.54
5	R	143	GLY	N-CA-C	6.09	123.73	115.32
9	I	65	VAL	N-CA-C	-6.06	99.48	108.45
3	P	275	LEU	N-CA-C	6.04	117.87	111.28
7	G	53	VAL	N-CA-C	-6.04	104.42	111.00
3	C	327	ALA	N-CA-C	-6.02	104.79	111.36
3	C	109	PHE	N-CA-C	-5.99	98.09	108.52
4	Q	110	PRO	CA-C-N	-5.99	114.11	120.03
4	Q	110	PRO	C-N-CA	-5.99	114.11	120.03
2	O	430	LEU	N-CA-C	5.96	120.07	113.21
1	A	238	GLY	N-CA-C	-5.94	101.71	110.97
4	Q	215	LEU	N-CA-C	5.92	118.52	111.71
3	C	225	THR	N-CA-C	-5.89	104.94	111.36
5	E	15	ARG	N-CA-C	-5.87	101.69	109.84
6	F	15	GLY	N-CA-C	-5.86	105.40	112.49
6	F	76	PRO	N-CA-C	-5.85	102.01	111.14
3	P	109	PHE	N-CA-C	-5.85	98.37	108.56
3	C	142	GLY	N-CA-C	-5.84	105.42	112.49
5	E	81	ILE	N-CA-C	5.83	113.32	107.55
1	N	421	ALA	N-CA-C	-5.83	99.69	109.07
1	N	100	LYS	N-CA-C	-5.81	99.72	109.07
5	R	81	ILE	CA-C-N	5.75	125.70	119.78
5	R	81	ILE	C-N-CA	5.75	125.70	119.78
1	A	264	HIS	N-CA-C	5.73	117.93	109.50
1	N	259	GLY	CA-C-N	5.73	125.27	119.19
1	N	259	GLY	C-N-CA	5.73	125.27	119.19
2	O	201	SER	N-CA-C	5.73	118.27	111.33
1	A	421	ALA	N-CA-C	-5.72	99.92	109.24
3	P	115	ILE	N-CA-C	-5.72	103.94	111.09
7	T	71	ARG	N-CA-C	5.70	118.89	109.94
3	P	243	VAL	N-CA-C	5.70	116.44	110.62
8	H	73	LEU	N-CA-C	5.70	120.78	111.37
6	S	39	GLU	N-CA-C	5.70	118.71	108.17
2	O	113	ARG	N-CA-C	5.69	118.25	111.71
10	W	14	PHE	N-CA-C	5.68	120.34	112.90
6	F	39	GLU	N-CA-C	5.67	118.66	108.17
2	B	176	LEU	N-CA-C	-5.64	106.35	113.18
1	N	264	HIS	N-CA-C	5.64	117.79	109.50
3	C	136	GLY	N-CA-C	-5.63	103.96	112.41
3	P	318	ARG	CA-C-N	5.62	125.08	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	318	ARG	C-N-CA	5.62	125.08	119.24
2	B	413	ALA	N-CA-C	-5.61	105.17	111.28
2	B	101	THR	N-CA-C	-5.58	98.91	110.80
2	B	311	ALA	N-CA-C	-5.57	102.23	110.48
7	G	50	PRO	N-CA-C	5.57	117.49	110.70
1	A	257	VAL	N-CA-C	-5.57	101.39	109.29
7	G	23	GLN	N-CA-C	5.55	118.13	109.52
5	R	38	LEU	N-CA-C	-5.52	104.67	111.40
2	O	153	GLN	N-CA-C	-5.51	106.51	113.18
6	S	24	ALA	N-CA-C	-5.50	105.29	111.28
4	D	37	CYS	N-CA-C	5.49	117.26	111.28
3	P	136	GLY	N-CA-C	-5.49	104.18	112.41
2	O	413	ALA	N-CA-C	-5.48	105.39	111.36
7	G	49	ALA	N-CA-C	5.45	119.65	112.35
1	A	278	GLY	N-CA-C	5.44	122.15	112.02
5	R	128	LYS	N-CA-C	-5.43	106.33	113.12
4	D	23	HIS	N-CA-C	5.42	119.16	112.54
1	N	260	PRO	N-CA-C	5.42	120.67	113.57
8	H	67	HIS	N-CA-C	-5.41	105.46	111.36
3	C	188	ILE	N-CA-C	-5.40	105.27	110.72
5	E	72	SER	N-CA-C	5.39	118.40	109.94
3	P	241	LEU	N-CA-C	-5.38	105.49	111.36
9	V	52	ARG	CB-CG-CD	-5.38	98.94	111.30
3	P	225	THR	N-CA-C	-5.36	105.33	111.07
7	T	53	VAL	N-CA-C	-5.35	105.31	110.72
5	R	125	GLU	N-CA-C	-5.34	106.76	113.28
5	E	179	ASN	N-CA-C	-5.34	103.48	110.53
6	S	76	PRO	N-CA-C	-5.33	102.82	111.14
6	S	15	GLY	N-CA-C	-5.33	106.05	112.49
1	A	348	SER	N-CA-C	5.31	118.83	111.71
1	A	226	ASP	N-CA-C	-5.31	106.58	113.16
4	Q	112	ASP	N-CA-C	-5.29	103.03	110.50
7	T	48	VAL	N-CA-C	5.29	117.19	111.58
3	P	327	ALA	N-CA-C	-5.29	105.60	111.36
1	A	121	SER	N-CA-C	5.28	116.72	111.07
2	B	113	ARG	N-CA-C	5.26	117.76	111.71
3	C	19	ILE	N-CA-C	5.25	115.69	110.23
3	C	313	ARG	N-CA-C	5.25	116.81	111.14
7	G	34	ILE	CB-CA-C	-5.25	108.72	113.70
4	D	80	MET	N-CA-C	-5.24	102.72	110.48
2	O	224	LEU	N-CA-C	5.24	121.95	110.80
5	E	128	LYS	N-CA-C	-5.23	106.58	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	309	THR	N-CA-C	-5.23	102.78	110.52
1	A	189	HIS	N-CA-C	5.20	119.75	113.41
2	B	305	GLN	N-CA-C	-5.19	103.61	110.40
3	P	146	ILE	N-CA-C	5.18	115.91	110.62
3	C	145	VAL	N-CA-C	5.17	115.39	110.42
3	C	304	ILE	CB-CA-C	-5.17	108.79	113.70
2	O	311	ALA	N-CA-C	-5.17	102.83	110.48
3	P	145	VAL	N-CA-C	5.17	115.38	110.42
3	P	271	GLU	N-CA-C	-5.17	103.32	110.35
1	N	215	HIS	N-CA-C	5.17	119.85	113.50
1	N	278	GLY	N-CA-C	5.16	121.62	112.02
7	T	34	ILE	CB-CA-C	-5.15	108.80	113.70
6	S	25	GLY	N-CA-C	5.15	122.46	115.30
7	T	45	ILE	N-CA-C	5.14	118.27	111.17
1	N	121	SER	N-CA-C	5.08	116.51	111.07
3	C	271	GLU	N-CA-C	-5.08	103.45	110.35
5	R	188	THR	CB-CA-C	-5.07	108.06	114.40
2	O	347	ILE	N-CA-C	-5.07	105.60	110.72
3	P	363	LEU	N-CA-C	5.06	118.60	112.23
7	T	50	PRO	N-CA-C	5.05	116.86	110.70
5	R	90	LYS	N-CA-C	-5.03	101.11	109.46
3	C	204	GLY	N-CA-C	-5.03	105.37	112.81
5	R	4	ASP	N-CA-C	-5.02	107.15	113.28
5	E	4	ASP	N-CA-C	-5.02	107.16	113.28

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3177	0	3152	91	0
2	O	3180	0	3156	90	0
3	C	2897	0	2943	53	0
3	P	2936	0	2994	80	0
4	D	1919	0	1868	44	0
4	Q	1919	0	1868	45	0
5	E	1519	0	1503	38	0
5	R	1517	0	1498	40	0
6	F	861	0	854	24	0
6	S	861	0	854	31	0
7	G	621	0	626	14	0
7	T	626	0	631	18	0
8	H	539	0	524	19	0
8	U	539	0	524	20	0
9	I	285	0	288	41	0
9	V	285	0	288	32	0
10	J	245	0	229	3	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
15	D	51	0	82	3	0
15	P	49	0	72	3	0
15	Q	51	0	82	7	0
16	C	86	0	60	5	0
16	P	86	0	60	3	0
17	C	37	0	42	2	0
17	P	37	0	42	2	0
18	C	18	0	14	3	0
18	P	18	0	14	4	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	3	0
21	Q	43	0	30	3	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	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	751	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 12.

All (751) 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
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.17	1.08
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
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.42	1.01
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.22	1.01
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
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.51	0.93
9:I:32:ALA:N	9:I:71:ASN:CB	2.31	0.92
2:O:202:ALA:HB3	2:O:229:GLY:C	1.96	0.90
5:R:70:ALA:C	5:R:71:MET:HE2	1.96	0.90
8:U:25:GLU:HB3	8:U:34:ARG:NH2	1.87	0.89
2:B:12:GLU:HG2	2:B:17:VAL:N	1.86	0.89
5:E:87:MET:HE3	5:E:88:ALA:H	1.38	0.88
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LYS:HB2	9:I:32:ALA:HB2	1.55	0.86
4:D:241:LYS:HA	4:D:241:LYS:NZ	1.92	0.85
3:C:129:MET:HE1	3:C:181:PHE:CD2	2.13	0.83
2:B:397:THR:HG22	2:B:401:GLN:HE21	1.41	0.83
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.14	0.82
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:HE3	1:A:51:LYS:H	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
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.17	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:43:MET:HE3	4:D:46:VAL:HG21	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
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.67	0.75
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.69	0.75
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
4:Q:231:LYS:HD3	6:S:70:MET:HE3	1.69	0.74
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.68	0.74
2:O:95:LYS:HD2	2:O:110:GLU:OE2	1.88	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:HA	4:D:241:LYS:HZ3	1.50	0.73
3:P:43:LEU:HD21	15:Q:3006:PEE:H30	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:O:95:LYS:HE2	9:V:32:ALA:CB	2.22	0.69
5:R:44:THR:HG21	10:W:24:ILE:HD13	1.73	0.69
2:B:197:ASN:HB3	2:B:230:LEU:HG	1.74	0.69
3:C:191:ALA:HA	3:C:194:MET:HE3	1.75	0.69
6:S:108:ALA:C	6:S:110:LYS:H	2.00	0.68
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.21	0.68
1:N:187:SER:O	1:N:191:LYS:HE2	1.93	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
4:D:231:LYS:HD3	6:F:70:MET:HE3	1.76	0.67
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
6:F:70:MET:HE2	6:F:71:ARG:HG3	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
3:P:12:LYS:HA	3:P:12:LYS:HE3	1.77	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
4:D:74:PRO:CD	4:D:80:MET:HE1	2.26	0.66
9:I:32:ALA:N	9:I:71:ASN:HB3	2.11	0.66
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.78	0.65
1:A:39:VAL:HG11	1:A:195:MET:HE3	1.78	0.65
1:A:293:PRO:O	1:A:297:ILE:HG12	1.97	0.65
1:A:344:ARG:HH11	1:A:344:ARG:HG2	1.61	0.65
9:V:32:ALA:N	9:V:71:ASN:CB	2.59	0.65
2:O:95:LYS:HE2	9:V:32:ALA:HB3	1.78	0.65
3:P:12:LYS:HE2	3:P:16:ASN:N	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:O:49:LEU:HD11	2:O:204:MET:HE3	1.80	0.64
8:U:18:THR:O	8:U:22:GLU:HG3	1.97	0.64
4:Q:74:PRO:HD3	4:Q:80:MET:HE1	1.80	0.64
6:S:70:MET:HE2	6:S:71:ARG:HG3	1.79	0.64
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.79	0.63
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
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
5:E:87:MET:CE	5:E:88:ALA:H	2.09	0.63
2:B:12:GLU:CG	2:B:17:VAL:H	2.03	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
3:P:100:ARG:HD2	3:P:100:ARG:C	2.24	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
23:A:4237:HOH:O	5:E:26:LYS:HE2	1.99	0.62
5:R:79:SER:HB3	5:R:191:ASP:CG	2.23	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
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:LYS:HB2	9:I:32:ALA:CB	2.29	0.61
2:B:200:THR:HG21	2:B:229:GLY:HA3	1.80	0.61
2:B:95:LYS:HD3	2:B:110:GLU:OE2	2.01	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
3:P:191:ALA:HA	3:P:194:MET:HE3	1.83	0.60
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.83	0.60
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.65	0.60
1:N:39:VAL:HG11	1:N:195:MET:HE3	1.82	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:HE3	1:N:68:LYS:HA	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
1:A:296:SER:O	1:A:300:THR:HG23	2.01	0.59
3:C:15:ASN:O	3:C:16:ASN:C	2.46	0.59
8:H:51:GLU:H	8:H:51:GLU:CD	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:Q:74:PRO:CD	4:Q:80:MET:HE1	2.32	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
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
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:OE2	5:E:17:GLU:N	2.28	0.58
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.39	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
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
4:D:116:ILE:HG12	21:D:501:HEC:HMA3	1.87	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:427:SER:HB3	23:O:4207:HOH:O	2.04	0.57
1:N:1:THR:O	1:N:2:ALA:HB2	2.03	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
3:P:311:LYS:HG2	3:P:374:ASN:CG	2.30	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
3:C:100:ARG:HD2	3:C:100:ARG:C	2.29	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:HMC1	16:C:501:HEM:HBC2	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
1:A:289:HIS:HE1	11:S:2012:JZR:H1'A	1.71	0.55
6:F:95:LYS:HB2	6:F:95:LYS:NZ	2.20	0.55
5:E:87:MET:HE3	5:E:88:ALA:N	2.16	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:HH11	6:F:101:ARG:HG2	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
7:T:32:LYS:C	7:T:35:PRO:HD2	2.31	0.55
4:D:241:LYS:HA	4:D:241:LYS:HZ2	1.70	0.55
5:E:82:PRO:O	5:E:100:HIS:HB3	2.07	0.55
5:E:104:LYS:O	5:E:108:GLN:HG3	2.07	0.55
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
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:P:96:MET:HE2	3:P:96:MET:HA	1.89	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
2:O:228:GLY:O	2:O:231:GLY:N	2.40	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:32:LYS:C	7:G:35:PRO:HD2	2.33	0.53
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.89	0.53
3:P:12:LYS:HE3	3:P:12:LYS:CA	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:HE3	1:A:51:LYS:N	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
4:Q:231:LYS:CD	6:S:70:MET:HE3	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:HIS:NE2	18:C:2002:UQ:O4	2.37	0.52
16:C:502:HEM:HBC2	16:C:502:HEM:HMC2	1.92	0.52
2:O:225:ASN:ND2	2:O:227:ARG:CZ	2.72	0.52
3:P:11:MET:HE3	3:P:12:LYS:CE	2.40	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:214:ASP:CG	7:T:2:ARG:HH22	2.18	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
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
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
2:B:47:ILE:HG13	2:B:120:MET:HE1	1.90	0.51
3:C:181:PHE:HE1	3:P:53:MET:HE2	1.75	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:348:SER:O	1:N:349:ALA:C	2.54	0.51
1:N:405:ARG:O	1:N:409:GLU:HG3	2.10	0.51
5:R:189:SER:O	5:R:190:ASP:C	2.53	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
9:V:32:ALA:N	9:V:71:ASN:HB2	2.25	0.51
4:D:110:PRO:HG3	21:D:501:HEC:HMD2	1.92	0.51
3:P:158:THR:HB	23:P:4121:HOH:O	2.11	0.51
1:N:39:VAL:HG11	1:N:195:MET:CE	2.40	0.51
2:O:236:LYS:HD2	2:O:236:LYS:N	2.26	0.51
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.45	0.50
2:B:102:ARG:HH22	2:B:161:GLU:CD	2.19	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
6:S:108:ALA:C	6:S:110:LYS:N	2.68	0.50
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.91	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:ASP:CG	7:G:2:ARG:HH22	2.19	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
6:F:70:MET:HE2	6:F:71:ARG:CG	2.42	0.50
9:I:64:LEU:HD23	9:I:77:ARG:O	2.12	0.50
1:N:136:GLN:NE2	9:V:51:CYS:HB2	2.27	0.50
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.12	0.50
4:Q:195:GLU:HG2	4:Q:198:HIS:HB2	1.94	0.50
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.47	0.50
2:O:305:GLN:NE2	2:O:329:GLN:OE1	2.45	0.49
3:C:80:ARG:C	3:C:80:ARG:HD3	2.37	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
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
4:Q:208:MET:HA	15:Q:3006:PEE:H49	1.94	0.49
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.94	0.49
10:W:15:ARG:HH11	10:W:15:ARG:HG3	1.76	0.49
6:F:104:ARG:HH11	11:F:3012:JZR:H6	1.77	0.49
6:F:95:LYS:HB2	6:F:95:LYS:HZ2	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
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:95:LYS:O	2:O:109:VAL:HA	2.12	0.49
2:O:203:ARG:HH12	2:O:233:SER:HA	1.78	0.49
3:P:11:MET:HG2	3:P:12:LYS:N	2.27	0.49
3:P:164:ILE:O	3:P:177:ARG:HD2	2.13	0.49
2:O:47:ILE:HG13	2:O:120:MET:HE1	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:HG22	3:P:13:ILE:O	2.13	0.48
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.95	0.48
2:B:243:GLU:HA	2:B:424:MET:O	2.13	0.48
2:B:246:GLU:O	2:B:427:SER:HA	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:61:GLY:C	9:I:62:ARG:HG3	2.37	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:68:HIS:CD2	23:C:4195:HOH:O	2.59	0.48
3:C:158:THR:O	3:C:162:GLU:HG3	2.13	0.48
1:N:233:PRO:O	5:R:22:THR:HA	2.13	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
9:V:64:LEU:HD23	9:V:78:TYR:C	2.38	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
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:B:232:LEU:O	2:B:233:SER:HB3	2.13	0.48
2:B:437:ASP:OD2	2:O:240:HIS:CD2	2.67	0.48
6:F:49:ARG:NH2	11:F:3012:JZR:H1	2.28	0.48
3:P:80:ARG:HD3	3:P:80:ARG:C	2.39	0.48
5:E:191:ASP:O	5:E:191:ASP:CG	2.56	0.47
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
9:I:64:LEU:HD23	9:I:78:TYR:C	2.39	0.47
2:O:397:THR:CG2	2:O:401:GLN:HE21	2.23	0.47
5:R:17:GLU:H	5:R:17:GLU:CD	2.17	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
6:F:34:ASP:O	6:F:58:ARG:NH2	2.47	0.47
4:D:231:LYS:HD3	6:F:70:MET:CE	2.44	0.47
6:F:104:ARG:HH11	11:F:3012:JZR:C6	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:R:70:ALA:N	5:R:71:MET:HE3	2.29	0.47
3:C:96:MET:HE2	3:C:96:MET:HA	1.96	0.47
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.95	0.47
6:S:68:LEU:HD23	6:S:71:ARG:HH22	1.80	0.47
3:P:78:ILE:CD1	4:Q:204:MET:HE1	2.45	0.47
5:R:71:MET:HE2	5:R:71:MET:N	2.30	0.47
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.78	0.47
2:O:202:ALA:HB3	2:O:230:LEU:N	2.28	0.47
4:Q:74:PRO:HB3	4:Q:80:MET:HE1	1.96	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
1:A:281:ASP:OD1	1:A:281:ASP:C	2.59	0.46
2:B:135:TRP:CE2	6:S:49:ARG:HD3	2.50	0.46
3:C:311:LYS:HG2	3:C:374:ASN:CG	2.41	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:3:THR:OG1	1:N:6:GLN:HG3	2.15	0.46
1:N:264:HIS:HA	1:N:265:PRO:HD3	1.83	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:370:MET:O	2:B:373:GLU:HG2	2.16	0.46
3:C:75:TYR:O	3:C:78:ILE:HG22	2.15	0.46
3:C:78:ILE:CD1	4:D:204:MET:HE1	2.46	0.46
3:C:215:VAL:HG13	23:C:4154:HOH:O	2.15	0.46
4:D:83:ARG:CZ	4:D:86:LYS:HE2	2.45	0.46
5:E:189:SER:C	5:E:190:ASP:OD1	2.59	0.46
1:N:281:ASP:OD2	9:V:73:PRO:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:373:GLU:HB2	23:P:4170:HOH:O	2.16	0.46
3:P:375:LYS:O	6:S:17:ARG:NH1	2.49	0.46
6:S:13:LEU:HD22	23:S:4129:HOH:O	2.15	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
3:C:129:MET:HE2	3:C:178:PHE:CD1	2.50	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
1:N:156:THR:HA	5:R:7:VAL:HG21	1.98	0.46
23:O:4201:HOH:O	9:V:32:ALA:HB1	2.16	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
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:191:ALA:HA	3:C:194:MET:CE	2.45	0.45
3:C:276:PHE:CG	3:C:277:ALA:N	2.84	0.45
4:Q:231:LYS:CE	6:S:70:MET:HE3	2.46	0.45
6:S:109:LYS:O	6:S:110:LYS:HG2	2.16	0.45
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.52	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
1:A:442:PHE:CD1	1:A:442:PHE:C	2.95	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
4:D:74:PRO:N	4:D:80:MET:HE1	2.32	0.45
1:N:307:PHE:CD1	1:N:307:PHE:C	2.94	0.45
2:O:300:ALA:C	2:O:302:GLY:H	2.25	0.45
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LYS:O	2:B:109:VAL:HA	2.17	0.45
3:P:111:GLU:H	3:P:111:GLU:CD	2.25	0.45
4:Q:161:ALA:O	4:Q:162:PRO:C	2.60	0.45
3:C:164:ILE:O	3:C:177:ARG:HD2	2.16	0.45
6:F:101:ARG:HG2	6:F:101:ARG:NH1	2.32	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
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
3:P:96:MET:HE2	15:P:3007:PEE:H27	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:75:TYR:O	3:P:78:ILE:HG22	2.17	0.44
3:P:348:ILE:O	3:P:352:GLN:HG3	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
4:Q:74:PRO:CB	4:Q:80:MET:HE1	2.47	0.44
4:Q:160:MET:HB2	21:Q:501:HEC:C1D	2.47	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
3:P:100:ARG:C	3:P:100:ARG:CD	2.90	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
4:D:231:LYS:CD	6:F:70:MET:HE3	2.46	0.44
5:E:87:MET:HE3	5:E:87:MET:HA	1.99	0.44
10:J:56:LYS:O	10:J:60:GLU:HG3	2.17	0.44
2:O:307:PHE:CD1	2:O:307:PHE:C	2.95	0.44
6:S:70:MET:HE2	6:S:71:ARG:CG	2.47	0.44
2:O:248:ASN:OD1	2:O:428:GLY:HA2	2.17	0.44
3:P:240:MET:HE2	15:Q:3006:PEE:H17	2.00	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
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
4:D:74:PRO:HB3	4:D:80:MET:HE1	2.00	0.44
4:D:214:LEU:O	4:D:217:PRO:HG2	2.17	0.44
4:D:223:LYS:HD3	4:D:223:LYS:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:32:ALA:N	9:V:72:VAL:CG2	2.80	0.44
2:B:19:PRO:C	2:B:20:HIS:O	2.60	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:43:THR:O	5:R:47:VAL:HG23	2.17	0.44
5:R:112:VAL:HG21	5:R:172:ARG:NH2	2.32	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
5:E:83:GLU:HG2	5:E:100:HIS:CD2	2.53	0.43
5:E:191:ASP:C	5:E:192:MET:HG2	2.43	0.43
2:B:307:PHE:CD1	2:B:307:PHE:C	2.95	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
3:C:96:MET:HE2	15:C:2007:PEE:H27	2.01	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:43:LEU:HD21	15:Q:3006:PEE:H27	2.00	0.43
3:P:100:ARG:HD2	3:P:100:ARG:O	2.18	0.43
3:P:282:ARG:NH2	23:P:4173:HOH:O	2.51	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:HG2	4:Q:195:GLU:O	2.19	0.43
1:A:352:SER:OG	6:S:110:LYS:HB2	2.18	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
3:P:378:LYS:HE3	6:S:17:ARG:NE	2.34	0.43
4:Q:211:MET:HG3	15:Q:3006:PEE:H48	2.00	0.43
5:R:77:LYS:HE3	5:R:79:SER:HG	1.83	0.43
1:A:364:ALA:HB2	9:I:33:ALA:HB1	2.01	0.43
2:B:46:ARG:HG2	2:B:110:GLU:HG2	2.00	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
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
1:N:442:PHE:CD1	1:N:442:PHE:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:225:ASN:CG	2:O:227:ARG:NH1	2.77	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
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
4:Q:37:CYS:SG	21:Q:501:HEC:HMB1	2.59	0.43
8:U:43:ARG:HD2	8:U:47:ARG:HH21	1.83	0.43
1:A:227:ALA:O	1:A:228:VAL:C	2.61	0.42
1:A:307:PHE:CD1	1:A:307:PHE:C	2.96	0.42
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
1:N:73:ASN:CG	1:N:77:LYS:HE3	2.44	0.42
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.00	0.42
1:A:192:ALA:HB3	1:A:193:PRO:HD3	1.99	0.42
2:B:300:ALA:C	2:B:302:GLY:H	2.27	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
1:A:352:SER:CB	6:S:110:LYS:HB2	2.50	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: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
1:N:157:ALA:HB2	1:N:421:ALA:CB	2.49	0.42
3:P:193:ALA:O	3:P:196:HIS:HB3	2.19	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:289:HIS:CE1	11:S:2012:JZR:H1'A	2.52	0.42
5:E:10:PHE:HB3	7:G:18:LEU:HD11	2.02	0.42
5:E:43:THR:O	5:E:47:VAL:HG23	2.20	0.42
5:E:71:MET:HE2	5:E:92:ARG:HD3	2.01	0.42
2:O:95:LYS:HE2	9:V:32:ALA:N	2.35	0.42
3:P:276:PHE:CG	3:P:277:ALA:N	2.87	0.42
8:U:28:GLU:C	8:U:31:VAL:HG22	2.44	0.42
2:B:314:ALA:HA	9:I:63:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.02	0.42
3:C:240:MET:HE2	15:D:2006:PEE:H17	2.02	0.42
7:G:28:HIS:ND1	7:G:32:LYS:HD2	2.34	0.42
5:R:112:VAL:HG21	5:R:172:ARG:HH21	1.84	0.42
3:C:129:MET:HE2	3:C:178:PHE:CG	2.54	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
1:N:281:ASP:C	1:N:281:ASP:OD1	2.62	0.42
1:N:284:TYR:HE1	9:V:73:PRO:HG3	1.84	0.42
5:R:85:LYS:NZ	5:R:87:MET:SD	2.72	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:HD3	4:D:231:LYS:HA	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
2:B:353:SER:HB3	2:B:355:PRO:HG2	2.01	0.42
4:D:116:ILE:HD12	4:D:116:ILE:HA	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
4:Q:110:PRO:HG3	21:Q:501:HEC:HMD3	2.01	0.42
5:R:78:LEU:HB2	5:R:191:ASP:HB2	2.02	0.42
3:C:234:LEU:HD12	19:D:2003:CDL:H712	2.01	0.42
6:F:102:LYS:HA	6:F:102:LYS:HD3	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
4:D:74:PRO:CB	4:D:80:MET:HE1	2.49	0.41
1:N:143:THR:OG1	9:V:48:SER:HB3	2.20	0.41
3:P:224:TYR:HB3	20:P:4009:GOL:H31	2.02	0.41
3:P:326:TRP:NE1	7:T:48:VAL:HG22	2.35	0.41
1:A:348:SER:O	1:A:349:ALA:C	2.61	0.41
8:H:28:GLU:C	8:H:31:VAL:HG22	2.45	0.41
3:C:57:SER:C	23:C:4219:HOH:O	2.63	0.41
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:138:MET:HA	3:P:138:MET:HE2	2.02	0.41
3:P:191:ALA:HA	3:P:194:MET:CE	2.48	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
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
23:N:4088:HOH:O	9:V:39:GLU:CG	2.69	0.41
3:P:30:TRP:CZ3	15:P:3007:PEE:H21	2.55	0.41
3:P:129:MET:HE2	3:P:178:PHE:CG	2.56	0.41
4:Q:215:LEU:HD21	5:R:46:GLY:HA3	2.02	0.41
2:B:28:ARG:HH11	2:B:28:ARG:HG2	1.86	0.41
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
3:P:12:LYS:C	3:P:14:VAL:N	2.77	0.41
4:Q:74:PRO:N	4:Q:80:MET:HE1	2.35	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
5:E:190:ASP:O	5:E:191:ASP:C	2.63	0.41
4:Q:28:ARG:HB3	4:Q:171:PHE:CE1	2.55	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
1:A:117:VAL:HG11	1:A:195:MET:CE	2.30	0.41
2:B:26:PHE:CZ	2:B:391:SER:HA	2.56	0.41
2:B:152:LEU:HD13	2:B:158:HIS:CE1	2.55	0.41
2:B:257:LEU:O	2:B:323:GLY:HA3	2.21	0.41
8:H:53:ASP:OD1	8:H:53:ASP:C	2.63	0.41
1:N:332:ASP:OD1	1:N:432:PRO:HG3	2.21	0.41
2:O:236:LYS:H	2:O:236:LYS:CD	2.32	0.41
4:Q:77:ASP:HB2	4:Q:79:GLU:CD	2.46	0.41
4:Q:117:VAL:O	12:Q:4012:PO4:O2	2.38	0.41
4:Q:208:MET:HE3	4:Q:208:MET:HB3	2.00	0.41
5:R:52:LYS:NZ	10:W:32:GLU:OE2	2.48	0.41
6:S:12:TRP:O	6:S:13:LEU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:53:ASP:OD1	8:U:53:ASP:C	2.63	0.41
1:A:332:ASP:OD1	1:A:432:PRO:HG3	2.21	0.41
2:O:102:ARG:HH22	2:O:161:GLU:CD	2.29	0.41
3:P:12:LYS:C	3:P:14:VAL:H	2.29	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
3:C:100:ARG:C	3:C:100:ARG:CD	2.95	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
3:P:32:ASN:O	3:P:36:LEU:HG	2.22	0.40
3:P:326:TRP:CH2	15:P:3007:PEE:H51	2.57	0.40
1:A:255:ILE:O	1:A:321:GLY:HA3	2.22	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:71:ARG:HD3	23:P:4196:HOH:O	2.22	0.40
3:P:197:LEU:HD23	3:P:197:LEU:HA	1.73	0.40
4:Q:241:LYS:HD3	4:Q:241:LYS:C	2.46	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:366:VAL:HG23	1:N:367:SER:N	2.37	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
5:E:166:ASP:C	5:E:168:SER:H	2.30	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: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:212:MET:HE2	15:Q:3006:PEE:H54	2.03	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

5.3.1 Protein backbone

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%)	24	22
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	24	22
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	43	44
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	10	7
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	21	18
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	9	5
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%)	24	22
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	12	9
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%)	9	5
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%)	1	0
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	4	1
10	J	28/62 (45%)	26 (93%)	1 (4%)	1 (4%)	2	1
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
All	All	3947/4220 (94%)	3811 (97%)	110 (3%)	26 (1%)	18	15

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	41	PRO

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Mol	Chain	Res	Type
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
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%)	50	58
1	N	363/370 (98%)	356 (98%)	7 (2%)	50	58
2	B	332/343 (97%)	329 (99%)	3 (1%)	70	78
2	O	332/343 (97%)	328 (99%)	4 (1%)	63	72
3	C	313/327 (96%)	311 (99%)	2 (1%)	78	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	317/327 (97%)	315 (99%)	2 (1%)	78	86
4	D	206/206 (100%)	203 (98%)	3 (2%)	57	65
4	Q	206/206 (100%)	202 (98%)	4 (2%)	50	58
5	E	168/168 (100%)	168 (100%)	0	100	100
5	R	168/168 (100%)	166 (99%)	2 (1%)	63	72
6	F	90/98 (92%)	86 (96%)	4 (4%)	25	26
6	S	90/98 (92%)	85 (94%)	5 (6%)	19	18
7	G	66/71 (93%)	64 (97%)	2 (3%)	36	41
7	T	66/71 (93%)	63 (96%)	3 (4%)	24	25
8	H	63/74 (85%)	61 (97%)	2 (3%)	34	38
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	26 (93%)	2 (7%)	13	11
9	V	28/60 (47%)	26 (93%)	2 (7%)	13	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%)	3282 (98%)	54 (2%)	55	64

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	51	LYS
1	A	203	LEU
1	A	245	GLU
1	A	281	ASP
1	A	348	SER
1	A	365	LEU
2	B	215	VAL
2	B	227	ARG
2	B	354	ASN
3	C	222	PRO
3	C	346	PRO
4	D	17	LEU
4	D	43	MET
4	D	241	LYS
6	F	16	ILE
6	F	33	ARG

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Mol	Chain	Res	Type
6	F	52	GLU
6	F	95	LYS
7	G	45	ILE
7	G	67	GLU
8	H	48	SER
8	H	51	GLU
9	I	42	VAL
9	I	52	ARG
1	N	20	ASP
1	N	32	GLN
1	N	184	GLU
1	N	245	GLU
1	N	281	ASP
1	N	348	SER
1	N	365	LEU
2	O	215	VAL
2	O	305	GLN
2	O	349	GLN
2	O	354	ASN
3	P	12	LYS
3	P	222	PRO
4	Q	17	LEU
4	Q	35	GLN
4	Q	43	MET
4	Q	79	GLU
5	R	113	GLU
5	R	190	ASP
6	S	13	LEU
6	S	16	ILE
6	S	33	ARG
6	S	52	GLU
6	S	95	LYS
7	T	45	ILE
7	T	72	LYS
7	T	73	ASN
9	V	42	VAL
9	V	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN

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Mol	Chain	Res	Type
1	A	119	ASN
1	A	136	GLN
1	A	165	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS
1	A	339	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	15	ASN
3	C	159	ASN
3	C	312	GLN
3	C	345	HIS
5	E	57	GLN
6	F	79	GLN
7	G	73	ASN
8	H	71	HIS
1	N	9	GLN
1	N	32	GLN
1	N	119	ASN
1	N	136	GLN
1	N	139	GLN
1	N	165	GLN
1	N	213	GLN
1	N	215	HIS
1	N	267	ASN
1	N	271	GLN
1	N	311	ASN
1	N	435	ASN
2	O	104	ASN
2	O	240	HIS
2	O	305	GLN
2	O	343	GLN
2	O	401	GLN
2	O	412	ASN
2	O	432	HIS
3	P	16	ASN

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Mol	Chain	Res	Type
3	P	159	ASN
3	P	267	HIS
3	P	312	GLN
3	P	345	HIS
4	Q	35	GLN
4	Q	225	HIS
5	R	57	GLN
5	R	116	GLN
6	S	79	GLN
8	U	49	GLN
8	U	67	HIS
8	U	71	HIS

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 oligosaccharides 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	$\# Z > 2$
20	GOL	P	4009	-	5,5,5	1.11	0	5,5,5	0.54	0
12	PO4	R	4013	-	4,4,4	1.48	1 (25%)	6,6,6	5.98	5 (83%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CDL	P	3004	-	48,48,99	1.14	3 (6%)	54,60,111	1.15	5 (9%)
13	AZI	C	2005	-	2,2,2	2.43	2 (100%)	0,1,1	-	-
12	PO4	R	4014	-	4,4,4	1.46	1 (25%)	6,6,6	5.99	5 (83%)
20	GOL	P	3008	-	5,5,5	1.27	0	5,5,5	0.54	0
11	JZR	F	4003	-	18,18,18	1.86	5 (27%)	23,23,23	0.68	0
12	PO4	B	3009	-	4,4,4	1.43	1 (25%)	6,6,6	5.99	5 (83%)
17	SMA	P	3001	-	38,38,38	1.38	7 (18%)	47,52,52	0.90	2 (4%)
20	GOL	E	4007	-	4,4,5	1.38	0	4,4,5	0.55	0
13	AZI	A	4002	-	2,2,2	2.82	2 (100%)	0,1,1	-	-
11	JZR	P	3011	-	18,18,18	1.84	5 (27%)	23,23,23	0.72	0
12	PO4	O	2009	-	4,4,4	1.44	1 (25%)	6,6,6	5.96	5 (83%)
12	PO4	T	4016	-	4,4,4	1.45	1 (25%)	6,6,6	5.98	5 (83%)
19	CDL	D	2003	-	38,38,99	1.06	1 (2%)	42,47,111	1.07	3 (7%)
13	AZI	G	4001	-	2,2,2	3.30	2 (100%)	0,1,1	-	-
16	HEM	P	502	3	50,50,50	1.42	6 (12%)	67,82,82	1.17	4 (5%)
19	CDL	Q	3003	-	38,38,99	1.10	2 (5%)	42,47,111	1.04	3 (7%)
20	GOL	O	4005	-	5,5,5	1.33	0	5,5,5	0.64	0
15	PEE	P	3007	-	48,48,50	1.22	4 (8%)	51,53,55	0.73	2 (3%)
17	SMA	C	2001	-	38,38,38	1.35	5 (13%)	47,52,52	0.92	2 (4%)
11	JZR	C	2011	-	18,18,18	1.85	5 (27%)	23,23,23	0.71	0
15	PEE	D	2006	-	50,50,50	1.34	5 (10%)	53,55,55	0.74	2 (3%)
11	JZR	F	3012	-	18,18,18	1.89	5 (27%)	23,23,23	0.74	0
12	PO4	Q	4012	-	4,4,4	1.57	2 (50%)	6,6,6	5.98	5 (83%)
16	HEM	C	502	3	50,50,50	1.42	6 (12%)	67,82,82	1.07	4 (5%)
12	PO4	P	3010	-	4,4,4	1.40	1 (25%)	6,6,6	5.98	5 (83%)
12	PO4	D	4010	-	4,4,4	1.44	1 (25%)	6,6,6	5.99	5 (83%)
20	GOL	E	4006	-	5,5,5	1.35	1 (20%)	5,5,5	0.66	0
21	HEC	Q	501	4	50,50,50	0.93	1 (2%)	68,82,82	1.37	8 (11%)
21	HEC	D	501	4	50,50,50	1.10	3 (6%)	68,82,82	1.08	6 (8%)
15	PEE	Q	3006	-	50,50,50	1.31	7 (14%)	53,55,55	0.74	2 (3%)
12	PO4	I	4015	-	4,4,4	1.43	1 (25%)	6,6,6	6.01	5 (83%)
18	UQ	P	3002	-	18,18,63	2.26	9 (50%)	23,24,79	0.83	1 (4%)
19	CDL	C	2004	-	43,43,99	1.16	3 (6%)	49,55,111	1.27	4 (8%)
22	FES	R	501	5	0,4,4	-	-	-	-	-
13	AZI	P	3005	-	2,2,2	2.97	2 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	JZR	A	4004	-	18,18,18	1.36	4 (22%)	23,23,23	0.58	0
22	FES	E	501	5	0,4,4	-	-	-	-	-
16	HEM	P	501	3	50,50,50	1.42	7 (14%)	67,82,82	1.15	6 (8%)
12	PO4	A	2010	-	4,4,4	1.49	1 (25%)	6,6,6	5.97	5 (83%)
18	UQ	C	2002	-	18,18,63	2.44	9 (50%)	23,24,79	0.90	1 (4%)
20	GOL	C	4008	-	5,5,5	1.27	0	5,5,5	0.57	0
15	PEE	B	4017	-	7,7,50	1.51	2 (28%)	7,7,55	0.33	0
12	PO4	D	4011	-	4,4,4	1.39	1 (25%)	6,6,6	6.01	5 (83%)
16	HEM	C	501	3	50,50,50	1.56	8 (16%)	67,82,82	1.28	7 (10%)
11	JZR	S	2012	-	18,18,18	1.89	4 (22%)	23,23,23	0.71	0
20	GOL	C	2008	-	5,5,5	1.32	0	5,5,5	0.69	0
15	PEE	C	2007	-	48,48,50	1.20	5 (10%)	51,53,55	0.73	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GOL	P	4009	-	-	2/4/4/4	-
19	CDL	P	3004	-	-	26/57/57/110	-
20	GOL	P	3008	-	-	0/4/4/4	-
11	JZR	F	4003	-	-	4/9/29/29	0/1/1/1
17	SMA	P	3001	-	-	4/34/34/34	0/2/2/2
20	GOL	E	4007	-	-	2/2/2/4	-
11	JZR	P	3011	-	-	3/9/29/29	0/1/1/1
19	CDL	D	2003	-	-	21/43/43/110	-
16	HEM	P	502	3	-	2/14/54/54	-
19	CDL	Q	3003	-	-	22/43/43/110	-
20	GOL	O	4005	-	-	3/4/4/4	-
15	PEE	P	3007	-	-	22/52/52/54	-
17	SMA	C	2001	-	-	4/34/34/34	0/2/2/2
11	JZR	C	2011	-	-	4/9/29/29	0/1/1/1
15	PEE	D	2006	-	-	23/54/54/54	-
11	JZR	F	3012	-	-	2/9/29/29	0/1/1/1
16	HEM	C	502	3	-	2/14/54/54	-
20	GOL	E	4006	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	HEC	D	501	4	1/1/3/7	8/14/54/54	-
15	PEE	Q	3006	-	-	25/54/54/54	-
18	UQ	P	3002	-	-	3/9/33/87	0/1/1/1
19	CDL	C	2004	-	-	30/52/52/110	-
22	FES	R	501	5	-	-	0/1/1/1
11	JZR	A	4004	-	-	1/9/29/29	0/1/1/1
22	FES	E	501	5	-	-	0/1/1/1
15	PEE	C	2007	-	-	19/52/52/54	-
16	HEM	P	501	3	-	4/14/54/54	-
18	UQ	C	2002	-	-	1/9/33/87	0/1/1/1
20	GOL	C	4008	-	-	0/4/4/4	-
15	PEE	B	4017	-	-	3/5/5/54	-
20	GOL	C	2008	-	-	2/4/4/4	-
11	JZR	S	2012	-	-	5/9/29/29	0/1/1/1
21	HEC	Q	501	4	1/1/3/7	8/14/54/54	-
16	HEM	C	501	3	-	4/14/54/54	-

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	S	2012	JZR	O1-C1	4.93	1.48	1.40
11	F	3012	JZR	O1-C1	4.91	1.48	1.40
11	P	3011	JZR	O1-C1	4.89	1.48	1.40
11	C	2011	JZR	O1-C1	4.84	1.48	1.40
11	F	4003	JZR	O1-C1	4.81	1.48	1.40
16	P	501	HEM	CBC-CAC	4.60	1.52	1.30
16	C	501	HEM	CBB-CAB	4.48	1.51	1.30
16	P	502	HEM	CBC-CAC	4.39	1.51	1.30
18	C	2002	UQ	C7-C6	4.12	1.59	1.51
15	P	3007	PEE	C39-C38	4.11	1.55	1.31
15	C	2007	PEE	C39-C38	4.09	1.54	1.31
16	P	502	HEM	CBB-CAB	4.05	1.49	1.30
15	D	2006	PEE	C39-C38	4.01	1.54	1.31
15	Q	3006	PEE	C39-C38	4.00	1.54	1.31
16	C	502	HEM	CBB-CAB	3.82	1.48	1.30
16	C	501	HEM	CMA-C3A	3.81	1.58	1.50
18	C	2002	UQ	C6-C5	3.74	1.41	1.35
17	C	2001	SMA	C20-C19	3.74	1.36	1.33
16	P	501	HEM	CBB-CAB	3.68	1.48	1.30
16	C	501	HEM	CBC-CAC	3.66	1.48	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	502	HEM	CBC-CAC	3.59	1.47	1.30
18	C	2002	UQ	C6-C1	3.59	1.56	1.46
18	P	3002	UQ	C6-C1	3.58	1.56	1.46
15	P	3007	PEE	C21-C22	-3.56	1.34	1.51
18	C	2002	UQ	O2-C2	3.55	1.45	1.36
13	G	4001	AZI	N1-N2	-3.52	1.15	1.23
11	F	3012	JZR	O5-C1	3.49	1.50	1.41
18	P	3002	UQ	C7-C6	3.47	1.57	1.51
15	C	2007	PEE	C21-C22	-3.47	1.34	1.51
11	S	2012	JZR	O5-C1	3.46	1.50	1.41
17	P	3001	SMA	C20-C19	3.42	1.36	1.33
15	D	2006	PEE	C21-C22	-3.39	1.34	1.51
18	P	3002	UQ	C6-C5	3.36	1.41	1.35
15	Q	3006	PEE	C21-C22	-3.35	1.35	1.51
11	F	4003	JZR	O5-C1	3.34	1.50	1.41
13	P	3005	AZI	N1-N2	-3.34	1.16	1.23
18	P	3002	UQ	O2-C2	3.34	1.44	1.36
18	C	2002	UQ	C2-C1	3.22	1.58	1.48
15	B	4017	PEE	O2-C10	3.19	1.41	1.30
11	C	2011	JZR	O5-C1	3.18	1.50	1.41
16	C	501	HEM	FE-ND	3.15	2.04	1.94
18	C	2002	UQ	O3-C3	3.15	1.44	1.36
15	D	2006	PEE	P-O1P	3.15	1.61	1.50
17	P	3001	SMA	O1-C2	3.13	1.40	1.36
13	A	4002	AZI	N1-N2	-3.12	1.16	1.23
16	C	502	HEM	FE-NA	3.12	2.05	1.95
13	G	4001	AZI	N3-N2	-3.06	1.16	1.23
15	P	3007	PEE	O3-C30	3.05	1.42	1.33
11	P	3011	JZR	O5-C1	3.00	1.49	1.41
15	Q	3006	PEE	O3-C30	2.99	1.42	1.33
11	A	4004	JZR	O1-C1	2.99	1.45	1.40
18	P	3002	UQ	O3-C3	2.96	1.43	1.36
18	P	3002	UQ	CM5-C5	2.93	1.56	1.50
15	Q	3006	PEE	P-O1P	2.85	1.60	1.50
18	C	2002	UQ	CM5-C5	2.85	1.56	1.50
18	P	3002	UQ	C2-C1	2.85	1.57	1.48
15	D	2006	PEE	O3-C30	2.84	1.41	1.33
11	A	4004	JZR	C4-C5	2.82	1.59	1.53
15	D	2006	PEE	O2-C10	2.81	1.42	1.34
16	P	501	HEM	CAC-C3C	-2.80	1.39	1.47
17	C	2001	SMA	C6-C5	2.80	1.43	1.38
21	D	501	HEC	C4B-NB	-2.79	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	501	HEM	CAC-C3C	-2.78	1.40	1.47
17	P	3001	SMA	C7-C8	2.76	1.44	1.40
15	Q	3006	PEE	O2-C10	2.73	1.42	1.34
16	C	502	HEM	C4A-NA	-2.72	1.34	1.39
15	C	2007	PEE	P-O1P	2.72	1.60	1.50
16	C	502	HEM	FE-NB	2.72	2.03	1.94
16	C	501	HEM	C3C-C4C	-2.69	1.41	1.46
13	C	2005	AZI	N1-N2	-2.66	1.17	1.23
18	C	2002	UQ	C5-C4	2.60	1.56	1.47
11	C	2011	JZR	C4-C5	2.59	1.58	1.53
17	C	2001	SMA	O1-C2	2.57	1.39	1.36
13	P	3005	AZI	N3-N2	-2.55	1.17	1.23
15	P	3007	PEE	P-O1P	2.54	1.59	1.50
17	P	3001	SMA	C6-C5	2.51	1.43	1.38
16	P	502	HEM	CMB-C2B	2.50	1.55	1.50
13	A	4002	AZI	N3-N2	-2.49	1.18	1.23
16	P	502	HEM	C3D-C2D	2.48	1.42	1.36
21	D	501	HEC	FE-NB	2.46	2.02	1.94
11	P	3011	JZR	C4-C5	2.46	1.58	1.53
21	Q	501	HEC	CMA-C3A	2.44	1.55	1.50
11	F	4003	JZR	C4-C5	2.44	1.58	1.53
17	P	3001	SMA	C4A-C5	2.42	1.45	1.40
16	P	501	HEM	C4C-NC	-2.42	1.35	1.39
11	A	4004	JZR	O5-C1	2.42	1.48	1.41
11	S	2012	JZR	C4-C5	2.41	1.58	1.53
17	P	3001	SMA	C6-C7	2.41	1.42	1.38
11	F	3012	JZR	O5-C5	2.39	1.50	1.44
18	P	3002	UQ	C5-C4	2.39	1.55	1.47
15	C	2007	PEE	O3-C30	2.38	1.40	1.33
19	Q	3003	CDL	O1-C1	2.37	1.50	1.43
18	P	3002	UQ	C3-C4	2.37	1.55	1.48
19	D	2003	CDL	O1-C1	2.36	1.50	1.43
21	D	501	HEC	FE-NC	2.35	2.02	1.95
19	P	3004	CDL	O1-C1	2.34	1.50	1.43
12	T	4016	PO4	P-O1	2.33	1.56	1.50
16	P	502	HEM	CAC-C3C	-2.33	1.41	1.47
16	P	501	HEM	C4A-C3A	2.33	1.48	1.43
19	C	2004	CDL	OA8-CA6	-2.33	1.40	1.45
12	A	2010	PO4	P-O1	2.30	1.56	1.50
17	C	2001	SMA	C4A-C5	2.29	1.44	1.40
11	S	2012	JZR	O5-C5	2.28	1.49	1.44
19	P	3004	CDL	OA8-CA6	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	502	HEM	CHC-C1C	-2.26	1.33	1.38
16	C	502	HEM	CAC-C3C	-2.25	1.41	1.47
11	F	3012	JZR	C4-C5	2.24	1.57	1.53
12	R	4014	PO4	P-O1	2.24	1.55	1.50
12	Q	4012	PO4	P-O1	2.23	1.55	1.50
18	C	2002	UQ	C3-C4	2.22	1.55	1.48
12	B	3009	PO4	P-O1	2.21	1.55	1.50
12	R	4013	PO4	P-O1	2.21	1.55	1.50
19	Q	3003	CDL	OB8-CB6	-2.20	1.40	1.45
17	C	2001	SMA	C6-C7	2.19	1.42	1.38
12	P	3010	PO4	P-O1	2.19	1.55	1.50
12	D	4010	PO4	P-O1	2.17	1.55	1.50
12	D	4011	PO4	P-O1	2.17	1.55	1.50
11	F	3012	JZR	C1-C2	2.17	1.58	1.52
13	C	2005	AZI	N3-N2	-2.17	1.18	1.23
11	P	3011	JZR	C1-C2	2.15	1.58	1.52
11	F	4003	JZR	O5-C5	2.14	1.49	1.44
12	I	4015	PO4	P-O1	2.14	1.55	1.50
16	C	501	HEM	CMC-C2C	2.12	1.55	1.50
11	C	2011	JZR	C1-C2	2.12	1.58	1.52
15	C	2007	PEE	O2-C10	2.11	1.40	1.34
11	C	2011	JZR	O5-C5	2.10	1.49	1.44
12	O	2009	PO4	P-O1	2.10	1.55	1.50
16	P	501	HEM	CMC-C2C	2.10	1.55	1.50
17	P	3001	SMA	C3-C2	2.09	1.38	1.34
16	C	501	HEM	C1B-NB	-2.07	1.36	1.40
19	C	2004	CDL	O1-C1	2.07	1.49	1.43
15	Q	3006	PEE	C3-C2	2.05	1.57	1.50
15	B	4017	PEE	C11-C10	2.04	1.55	1.50
19	P	3004	CDL	OB8-CB6	-2.04	1.40	1.45
11	F	4003	JZR	C1-C2	2.03	1.58	1.52
19	C	2004	CDL	OB8-CB6	-2.03	1.40	1.45
20	E	4006	GOL	O2-C2	2.02	1.49	1.43
11	P	3011	JZR	O5-C5	2.01	1.49	1.44
16	P	501	HEM	CAB-C3B	-2.01	1.42	1.47
12	Q	4012	PO4	P-O2	-2.01	1.48	1.54
11	A	4004	JZR	C4-C3	2.01	1.57	1.52
15	Q	3006	PEE	C31-C30	2.00	1.56	1.50

All (119) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	2009	PO4	O4-P-O1	-8.48	80.98	110.95
12	R	4013	PO4	O4-P-O1	-8.45	81.06	110.95
12	I	4015	PO4	O4-P-O1	-8.42	81.16	110.95
12	D	4010	PO4	O4-P-O1	-8.42	81.18	110.95
12	T	4016	PO4	O4-P-O1	-8.40	81.25	110.95
12	A	2010	PO4	O4-P-O1	-8.39	81.27	110.95
12	Q	4012	PO4	O4-P-O1	-8.39	81.30	110.95
12	B	3009	PO4	O4-P-O1	-8.38	81.32	110.95
12	R	4014	PO4	O4-P-O1	-8.38	81.33	110.95
12	P	3010	PO4	O4-P-O1	-8.36	81.38	110.95
12	D	4011	PO4	O4-P-O1	-8.31	81.55	110.95
12	I	4015	PO4	O4-P-O2	-8.15	82.56	107.91
12	D	4011	PO4	O4-P-O2	-8.00	83.02	107.91
12	Q	4012	PO4	O4-P-O2	-7.97	83.11	107.91
12	R	4014	PO4	O4-P-O2	-7.96	83.15	107.91
12	P	3010	PO4	O4-P-O2	-7.95	83.16	107.91
12	D	4010	PO4	O4-P-O2	-7.93	83.25	107.91
12	A	2010	PO4	O4-P-O2	-7.92	83.28	107.91
12	B	3009	PO4	O4-P-O2	-7.90	83.33	107.91
12	R	4013	PO4	O4-P-O2	-7.86	83.47	107.91
12	T	4016	PO4	O4-P-O2	-7.83	83.54	107.91
12	O	2009	PO4	O4-P-O2	-7.72	83.89	107.91
12	D	4011	PO4	O4-P-O3	-7.31	85.16	107.91
12	T	4016	PO4	O4-P-O3	-7.29	85.22	107.91
12	B	3009	PO4	O4-P-O3	-7.24	85.37	107.91
12	O	2009	PO4	O4-P-O3	-7.24	85.38	107.91
12	Q	4012	PO4	O4-P-O3	-7.24	85.40	107.91
12	R	4013	PO4	O4-P-O3	-7.23	85.43	107.91
12	R	4014	PO4	O4-P-O3	-7.22	85.45	107.91
12	D	4010	PO4	O4-P-O3	-7.20	85.52	107.91
12	A	2010	PO4	O4-P-O3	-7.18	85.58	107.91
12	P	3010	PO4	O4-P-O3	-7.17	85.60	107.91
12	I	4015	PO4	O4-P-O3	-6.98	86.21	107.91
12	I	4015	PO4	O2-P-O1	4.84	128.06	110.95
12	B	3009	PO4	O2-P-O1	4.80	127.91	110.95
12	P	3010	PO4	O2-P-O1	4.77	127.82	110.95
12	R	4014	PO4	O2-P-O1	4.76	127.78	110.95
12	O	2009	PO4	O2-P-O1	4.75	127.75	110.95
12	A	2010	PO4	O2-P-O1	4.75	127.73	110.95
12	T	4016	PO4	O2-P-O1	4.74	127.71	110.95
12	D	4011	PO4	O2-P-O1	4.73	127.67	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	4010	PO4	O2-P-O1	4.72	127.63	110.95
12	R	4013	PO4	O2-P-O1	4.70	127.58	110.95
12	Q	4012	PO4	O2-P-O1	4.61	127.26	110.95
19	C	2004	CDL	CA4-OA6-CA5	-4.45	109.98	117.85
16	C	501	HEM	C3B-C4B-NB	4.22	112.50	109.47
16	P	502	HEM	C3B-C4B-NB	3.98	112.32	109.47
19	P	3004	CDL	CA4-OA6-CA5	-3.80	111.14	117.85
16	C	502	HEM	C3B-C4B-NB	3.59	112.04	109.47
21	Q	501	HEC	CMA-C3A-C4A	3.45	130.80	124.73
19	C	2004	CDL	CB4-OB6-CB5	-3.37	109.72	117.80
21	Q	501	HEC	CAC-C3C-C4C	-3.18	120.54	124.91
16	P	501	HEM	C3B-C4B-NB	2.97	111.60	109.47
16	P	502	HEM	C3C-C2C-C1C	-2.96	104.24	107.05
16	C	502	HEM	C4B-C3B-C2B	-2.90	104.62	107.28
17	P	3001	SMA	C9-C10-C11	-2.89	109.07	114.46
19	P	3004	CDL	CA6-OA8-CA7	-2.88	109.98	117.08
19	P	3004	CDL	CB4-OB6-CB5	-2.87	110.93	117.80
16	C	501	HEM	C4B-C3B-C2B	-2.84	104.67	107.28
21	Q	501	HEC	CAC-C3C-C2C	2.83	131.36	126.89
19	D	2003	CDL	CB6-CB4-CB3	-2.82	105.20	111.78
19	Q	3003	CDL	CB4-OB6-CB5	-2.79	111.12	117.80
15	Q	3006	PEE	C22-C21-C20	2.76	127.14	113.86
15	D	2006	PEE	C22-C21-C20	2.76	127.12	113.86
12	D	4011	PO4	O3-P-O2	2.75	116.46	107.91
17	C	2001	SMA	C9-C10-C11	-2.74	109.35	114.46
12	R	4013	PO4	O3-P-O2	2.70	116.32	107.91
12	D	4010	PO4	O3-P-O2	2.69	116.28	107.91
15	C	2007	PEE	C22-C21-C20	2.68	126.74	113.86
15	P	3007	PEE	C22-C21-C20	2.67	126.72	113.86
12	Q	4012	PO4	O3-P-O2	2.67	116.22	107.91
17	C	2001	SMA	C4A-C4-C3	-2.67	114.85	118.78
12	I	4015	PO4	O3-P-O2	2.67	116.21	107.91
19	D	2003	CDL	CB4-OB6-CB5	-2.66	111.43	117.80
12	R	4014	PO4	O3-P-O2	2.65	116.15	107.91
12	P	3010	PO4	O3-P-O2	2.64	116.13	107.91
16	C	501	HEM	C2D-C1D-ND	2.64	112.95	109.90
12	T	4016	PO4	O3-P-O2	2.64	116.11	107.91
21	D	501	HEC	CAB-C3B-C4B	-2.63	121.37	124.79
12	B	3009	PO4	O3-P-O2	2.62	116.07	107.91
12	O	2009	PO4	O3-P-O2	2.62	116.05	107.91
12	A	2010	PO4	O3-P-O2	2.62	116.05	107.91
19	Q	3003	CDL	CB6-CB4-CB3	-2.61	105.69	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	501	HEC	C3D-C4D-ND	2.59	112.85	110.35
17	P	3001	SMA	C4A-C4-C3	-2.56	115.01	118.78
16	P	501	HEM	CMD-C2D-C1D	2.55	129.02	125.03
21	D	501	HEC	C2B-C1B-NB	2.55	112.85	109.90
21	D	501	HEC	CAC-C3C-C4C	-2.54	121.41	124.91
21	Q	501	HEC	CMB-C2B-C1B	2.51	128.95	125.03
19	C	2004	CDL	CA6-CA4-CA3	-2.48	106.01	111.78
19	C	2004	CDL	CA6-OA8-CA7	-2.45	111.03	117.08
16	C	501	HEM	CMA-C3A-C4A	2.45	129.15	125.42
15	C	2007	PEE	C21-C22-C23	2.44	126.68	114.37
16	P	501	HEM	C4A-C3A-C2A	-2.43	104.03	106.82
21	D	501	HEC	CAC-C3C-C2C	2.42	130.71	126.89
15	P	3007	PEE	C21-C22-C23	2.39	126.47	114.37
16	C	501	HEM	C1D-C2D-C3D	-2.38	104.48	106.98
18	C	2002	UQ	C6-C5-C4	2.38	121.05	119.17
16	P	501	HEM	CMA-C3A-C2A	2.36	130.62	125.62
16	C	502	HEM	CBD-CAD-C3D	-2.35	106.04	112.53
15	D	2006	PEE	C21-C22-C23	2.31	126.06	114.37
15	Q	3006	PEE	C21-C22-C23	2.31	126.02	114.37
16	C	502	HEM	C2B-C1B-NB	2.29	112.47	109.84
21	Q	501	HEC	C2B-C1B-NB	2.27	112.53	109.90
21	D	501	HEC	CMC-C2C-C1C	2.23	128.82	125.42
16	P	502	HEM	CBD-CAD-C3D	-2.22	106.39	112.53
16	P	501	HEM	C2D-C1D-ND	2.20	112.45	109.90
16	P	502	HEM	C2D-C1D-ND	2.19	112.43	109.90
21	Q	501	HEC	CHB-C1B-C2B	-2.18	121.59	125.03
19	D	2003	CDL	OA4-PA1-OA2	2.17	112.33	106.67
21	D	501	HEC	CAB-C3B-C2B	2.15	131.51	127.56
16	P	501	HEM	CAD-C3D-C4D	2.10	128.36	124.70
18	P	3002	UQ	C6-C5-C4	2.08	120.81	119.17
19	Q	3003	CDL	OA4-PA1-OA2	2.07	112.07	106.67
16	C	501	HEM	C4A-C3A-C2A	-2.06	104.46	106.82
16	C	501	HEM	C4C-NC-C1C	-2.06	102.47	105.82
21	Q	501	HEC	C4A-C3A-C2A	-2.04	103.95	106.97
19	P	3004	CDL	CB6-CB4-CB3	-2.01	107.09	111.78
19	P	3004	CDL	OA6-CA5-OA7	2.00	126.86	122.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	D	501	HEC	NA
21	Q	501	HEC	NA

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	2006	PEE	C1-O3P-P-O2P
15	D	2006	PEE	C1-O3P-P-O4P
15	D	2006	PEE	C4-O4P-P-O2P
15	D	2006	PEE	O4P-C4-C5-N
15	Q	3006	PEE	C1-O3P-P-O2P
15	Q	3006	PEE	C1-O3P-P-O4P
15	Q	3006	PEE	C4-O4P-P-O2P
15	Q	3006	PEE	O4P-C4-C5-N
17	C	2001	SMA	C3-C2-C9-C10
17	C	2001	SMA	O1-C2-C9-C10
19	C	2004	CDL	CA3-OA5-PA1-OA2
19	C	2004	CDL	CA3-OA5-PA1-OA3
19	C	2004	CDL	CA3-OA5-PA1-OA4
19	C	2004	CDL	CB2-OB2-PB2-OB4
19	C	2004	CDL	C51-CB5-OB6-CB4
19	D	2003	CDL	CB2-OB2-PB2-OB3
19	D	2003	CDL	CB2-OB2-PB2-OB4
19	D	2003	CDL	CB2-OB2-PB2-OB5
19	Q	3003	CDL	CB2-OB2-PB2-OB4
19	Q	3003	CDL	CB2-OB2-PB2-OB5
19	Q	3003	CDL	CB3-OB5-PB2-OB2
19	Q	3003	CDL	CB3-OB5-PB2-OB4
19	Q	3003	CDL	OB6-CB4-CB6-OB8
20	E	4006	GOL	C1-C2-C3-O3
20	P	4009	GOL	O1-C1-C2-C3
19	C	2004	CDL	C11-CA5-OA6-CA4
19	P	3004	CDL	C11-CA5-OA6-CA4
19	P	3004	CDL	C31-CA7-OA8-CA6
19	C	2004	CDL	OB9-CB7-OB8-CB6
19	P	3004	CDL	OB9-CB7-OB8-CB6
19	C	2004	CDL	OA9-CA7-OA8-CA6
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	OA9-CA7-OA8-CA6
19	P	3004	CDL	OA7-CA5-OA6-CA4
19	C	2004	CDL	C71-CB7-OB8-CB6
19	P	3004	CDL	C71-CB7-OB8-CB6
19	Q	3003	CDL	C71-CB7-OB8-CB6
15	P	3007	PEE	C37-C38-C39-C40
15	Q	3006	PEE	C37-C38-C39-C40
19	Q	3003	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
11	F	3012	JZR	O5-C5-C6-O6
19	P	3004	CDL	C51-CB5-OB6-CB4
11	C	2011	JZR	O5-C5-C6-O6
11	S	2012	JZR	C4-C5-C6-O6
15	C	2007	PEE	C37-C38-C39-C40
15	D	2006	PEE	C37-C38-C39-C40
11	F	3012	JZR	C4-C5-C6-O6
21	Q	501	HEC	C2B-C3B-CAB-CBB
21	Q	501	HEC	C4C-C3C-CAC-CBC
11	S	2012	JZR	O5-C5-C6-O6
20	E	4006	GOL	O2-C2-C3-O3
15	D	2006	PEE	C30-C31-C32-C33
19	P	3004	CDL	OB7-CB5-OB6-CB4
11	C	2011	JZR	C4-C5-C6-O6
15	Q	3006	PEE	C30-C31-C32-C33
19	Q	3003	CDL	O1-C1-CB2-OB2
15	P	3007	PEE	C10-C11-C12-C13
11	F	4003	JZR	O1-C1'-C2'-C3'
15	C	2007	PEE	C10-C11-C12-C13
21	D	501	HEC	C4C-C3C-CAC-CBC
19	Q	3003	CDL	CA2-C1-CB2-OB2
19	D	2003	CDL	O1-C1-CA2-OA2
21	D	501	HEC	C2B-C3B-CAB-CBB
20	C	2008	GOL	O1-C1-C2-C3
20	E	4006	GOL	O1-C1-C2-C3
20	O	4005	GOL	C1-C2-C3-O3
15	C	2007	PEE	C20-C21-C22-C23
15	C	2007	PEE	C31-C32-C33-C34
19	Q	3003	CDL	C75-C76-C77-C78
15	P	3007	PEE	C20-C21-C22-C23
15	P	3007	PEE	C31-C32-C33-C34
15	Q	3006	PEE	C13-C14-C15-C16
19	P	3004	CDL	C72-C73-C74-C75
11	C	2011	JZR	C1'-C2'-C3'-C4'
19	P	3004	CDL	C71-C72-C73-C74
15	D	2006	PEE	C13-C14-C15-C16
15	Q	3006	PEE	C14-C15-C16-C17
15	Q	3006	PEE	C22-C23-C24-C25
11	P	3011	JZR	C2'-C3'-C4'-C5'
15	D	2006	PEE	C14-C15-C16-C17
19	Q	3003	CDL	C77-C78-C79-C80
15	D	2006	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
15	D	2006	PEE	C34-C35-C36-C37
11	P	3011	JZR	C1'-C2'-C3'-C4'
15	Q	3006	PEE	C23-C24-C25-C26
15	Q	3006	PEE	C43-C44-C45-C46
15	D	2006	PEE	C43-C44-C45-C46
19	D	2003	CDL	C72-C73-C74-C75
21	Q	501	HEC	C2C-C3C-CAC-CBC
11	F	4003	JZR	C4-C5-C6-O6
15	P	3007	PEE	C41-C42-C43-C44
15	Q	3006	PEE	C34-C35-C36-C37
19	D	2003	CDL	C76-C77-C78-C79
15	C	2007	PEE	C41-C42-C43-C44
15	D	2006	PEE	C23-C24-C25-C26
19	P	3004	CDL	C74-C75-C76-C77
19	C	2004	CDL	C74-C75-C76-C77
19	P	3004	CDL	CB7-C71-C72-C73
19	C	2004	CDL	O1-C1-CA2-OA2
19	Q	3003	CDL	C73-C74-C75-C76
19	D	2003	CDL	C51-CB5-OB6-CB4
19	Q	3003	CDL	C76-C77-C78-C79
15	C	2007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C35-C36-C37-C38
15	P	3007	PEE	C42-C43-C44-C45
19	D	2003	CDL	C75-C76-C77-C78
19	Q	3003	CDL	CB5-C51-C52-C53
19	Q	3003	CDL	C78-C79-C80-C81
19	Q	3003	CDL	C51-CB5-OB6-CB4
19	P	3004	CDL	OA6-CA4-CA6-OA8
19	C	2004	CDL	C71-C72-C73-C74
15	P	3007	PEE	C34-C35-C36-C37
19	D	2003	CDL	C71-C72-C73-C74
15	C	2007	PEE	C34-C35-C36-C37
15	C	2007	PEE	C42-C43-C44-C45
19	D	2003	CDL	OB7-CB5-OB6-CB4
20	C	2008	GOL	O1-C1-C2-O2
20	O	4005	GOL	O2-C2-C3-O3
20	P	4009	GOL	O1-C1-C2-O2
15	C	2007	PEE	C19-C20-C21-C22
19	C	2004	CDL	OA5-CA3-CA4-CA6
20	E	4007	GOL	O1-C1-C2-O2
15	P	3007	PEE	C32-C33-C34-C35
15	P	3007	PEE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
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	C15-C16-C17-C18
15	C	2007	PEE	C32-C33-C34-C35
15	C	2007	PEE	C12-C13-C14-C15
19	C	2004	CDL	CB7-C71-C72-C73
15	C	2007	PEE	C15-C16-C17-C18
15	D	2006	PEE	C41-C42-C43-C44
15	Q	3006	PEE	C41-C42-C43-C44
19	Q	3003	CDL	OB7-CB5-OB6-CB4
20	E	4006	GOL	O1-C1-C2-O2
19	D	2003	CDL	C79-C80-C81-C82
19	C	2004	CDL	C75-C76-C77-C78
11	F	4003	JZR	O5-C5-C6-O6
15	P	3007	PEE	C43-C44-C45-C46
21	D	501	HEC	C4B-C3B-CAB-CBB
11	S	2012	JZR	C1'-C2'-C3'-C4'
19	P	3004	CDL	CA3-CA4-CA6-OA8
19	C	2004	CDL	OA5-CA3-CA4-OA6
19	P	3004	CDL	C53-C54-C55-C56
15	P	3007	PEE	C19-C20-C21-C22
18	P	3002	UQ	C12-C11-C9-C8
19	Q	3003	CDL	C51-C52-C53-C54
19	P	3004	CDL	OA5-CA3-CA4-CA6
21	Q	501	HEC	C4B-C3B-CAB-CBB
11	C	2011	JZR	C2'-C3'-C4'-C5'
15	C	2007	PEE	C43-C44-C45-C46
18	P	3002	UQ	C1-C2-O2-CM2
15	P	3007	PEE	C22-C23-C24-C25
19	Q	3003	CDL	CB3-CB4-CB6-OB8
15	P	3007	PEE	C23-C24-C25-C26
19	D	2003	CDL	C78-C79-C80-C81
19	P	3004	CDL	OB6-CB4-CB6-OB8
15	C	2007	PEE	C22-C23-C24-C25
19	D	2003	CDL	CB2-C1-CA2-OA2
19	D	2003	CDL	C73-C74-C75-C76
15	C	2007	PEE	C23-C24-C25-C26
19	C	2004	CDL	OB6-CB4-CB6-OB8
15	Q	3006	PEE	C20-C21-C22-C23
17	P	3001	SMA	O14-C14-C15-C16
15	D	2006	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
15	D	2006	PEE	C1-O3P-P-O1P
15	D	2006	PEE	C4-O4P-P-O3P
15	D	2006	PEE	C4-O4P-P-O1P
15	P	3007	PEE	O4P-C4-C5-N
15	Q	3006	PEE	C1-O3P-P-O1P
15	Q	3006	PEE	C4-O4P-P-O3P
15	Q	3006	PEE	C4-O4P-P-O1P
19	C	2004	CDL	CB2-OB2-PB2-OB3
19	C	2004	CDL	CB2-OB2-PB2-OB5
19	C	2004	CDL	CB3-OB5-PB2-OB4
19	P	3004	CDL	CB2-OB2-PB2-OB5
19	P	3004	CDL	CB3-OB5-PB2-OB4
19	Q	3003	CDL	CB2-OB2-PB2-OB3
19	Q	3003	CDL	CB3-OB5-PB2-OB3
15	C	2007	PEE	C18-C19-C20-C21
19	C	2004	CDL	C73-C74-C75-C76
19	P	3004	CDL	C51-C52-C53-C54
19	D	2003	CDL	OB9-CB7-OB8-CB6
19	D	2003	CDL	OB5-CB3-CB4-OB6
19	P	3004	CDL	OA5-CA3-CA4-OA6
15	C	2007	PEE	C11-C12-C13-C14
19	P	3004	CDL	O1-C1-CA2-OA2
19	D	2003	CDL	C71-CB7-OB8-CB6
19	P	3004	CDL	CB5-C51-C52-C53
15	D	2006	PEE	C35-C36-C37-C38
18	C	2002	UQ	C1-C2-O2-CM2
11	S	2012	JZR	C2'-C3'-C4'-C5'
15	Q	3006	PEE	C35-C36-C37-C38
16	C	501	HEM	CAA-CBA-CGA-O1A
16	P	501	HEM	CAA-CBA-CGA-O1A
15	D	2006	PEE	C1-C2-C3-O3
15	Q	3006	PEE	C1-C2-C3-O3
19	C	2004	CDL	C72-C73-C74-C75
17	C	2001	SMA	O14-C14-C15-C16
16	C	502	HEM	CAA-CBA-CGA-O1A
20	E	4007	GOL	O1-C1-C2-C3
16	C	501	HEM	CAA-CBA-CGA-O2A
16	P	501	HEM	CAA-CBA-CGA-O2A
16	P	501	HEM	CAD-CBD-CGD-O1D
15	D	2006	PEE	C40-C41-C42-C43
15	B	4017	PEE	O2-C10-C11-C12
11	A	4004	JZR	O1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
16	C	501	HEM	CAD-CBD-CGD-O1D
21	Q	501	HEC	CAD-CBD-CGD-O1D
19	C	2004	CDL	OA6-CA4-CA6-OA8
16	P	502	HEM	CAA-CBA-CGA-O1A
16	P	502	HEM	CAA-CBA-CGA-O2A
17	P	3001	SMA	C17-C18-C19-C26
15	B	4017	PEE	O4-C10-C11-C12
21	Q	501	HEC	CAD-CBD-CGD-O2D
16	P	501	HEM	CAD-CBD-CGD-O2D
21	D	501	HEC	CAD-CBD-CGD-O1D
15	P	3007	PEE	C18-C19-C20-C21
15	Q	3006	PEE	C39-C40-C41-C42
16	C	501	HEM	CAD-CBD-CGD-O2D
20	O	4005	GOL	O1-C1-C2-O2
11	S	2012	JZR	O1-C1'-C2'-C3'
11	P	3011	JZR	O5-C5-C6-O6
19	Q	3003	CDL	OB5-CB3-CB4-CB6
21	D	501	HEC	C2C-C3C-CAC-CBC
21	D	501	HEC	CAA-CBA-CGA-O2A
16	C	502	HEM	CAA-CBA-CGA-O2A
15	P	3007	PEE	C38-C39-C40-C41
15	Q	3006	PEE	C18-C19-C20-C21
15	D	2006	PEE	C39-C40-C41-C42
21	Q	501	HEC	CAA-CBA-CGA-O2A
21	D	501	HEC	CAA-CBA-CGA-O1A
21	Q	501	HEC	CAA-CBA-CGA-O1A
15	D	2006	PEE	C18-C19-C20-C21
15	C	2007	PEE	C38-C39-C40-C41
15	Q	3006	PEE	C40-C41-C42-C43
15	P	3007	PEE	C11-C12-C13-C14
15	D	2006	PEE	C36-C37-C38-C39
15	Q	3006	PEE	C36-C37-C38-C39
19	D	2003	CDL	C72-C71-CB7-OB8
19	D	2003	CDL	OB5-CB3-CB4-CB6
19	P	3004	CDL	C72-C71-CB7-OB8
21	D	501	HEC	CAD-CBD-CGD-O2D
15	Q	3006	PEE	C16-C17-C18-C19
17	C	2001	SMA	C13-C14-C15-C16
17	P	3001	SMA	C13-C14-C15-C16
19	C	2004	CDL	C72-C71-CB7-OB8
15	B	4017	PEE	C12-C13-C14-C15
15	C	2007	PEE	O3-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
19	C	2004	CDL	CA3-CA4-CA6-OA8
17	P	3001	SMA	C17-C18-C19-C20
15	P	3007	PEE	O3-C30-C31-C32
18	P	3002	UQ	C3-C2-O2-CM2
19	D	2003	CDL	C74-C75-C76-C77
15	P	3007	PEE	O5-C30-C31-C32
19	P	3004	CDL	C72-C71-CB7-OB9
19	C	2004	CDL	C72-C71-CB7-OB9
19	D	2003	CDL	C72-C71-CB7-OB9
15	P	3007	PEE	C17-C18-C19-C20
15	Q	3006	PEE	C11-C12-C13-C14

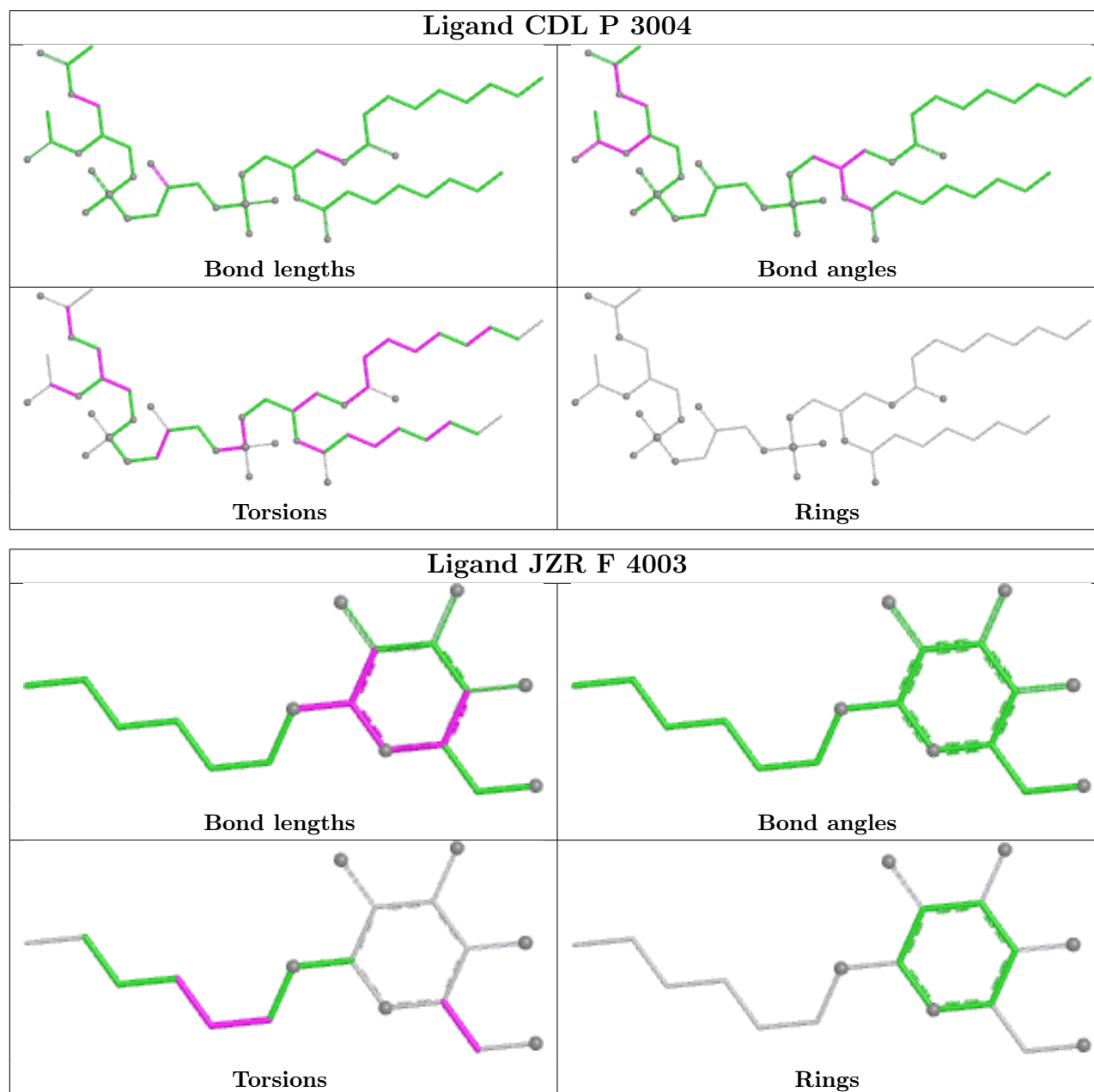
There are no ring outliers.

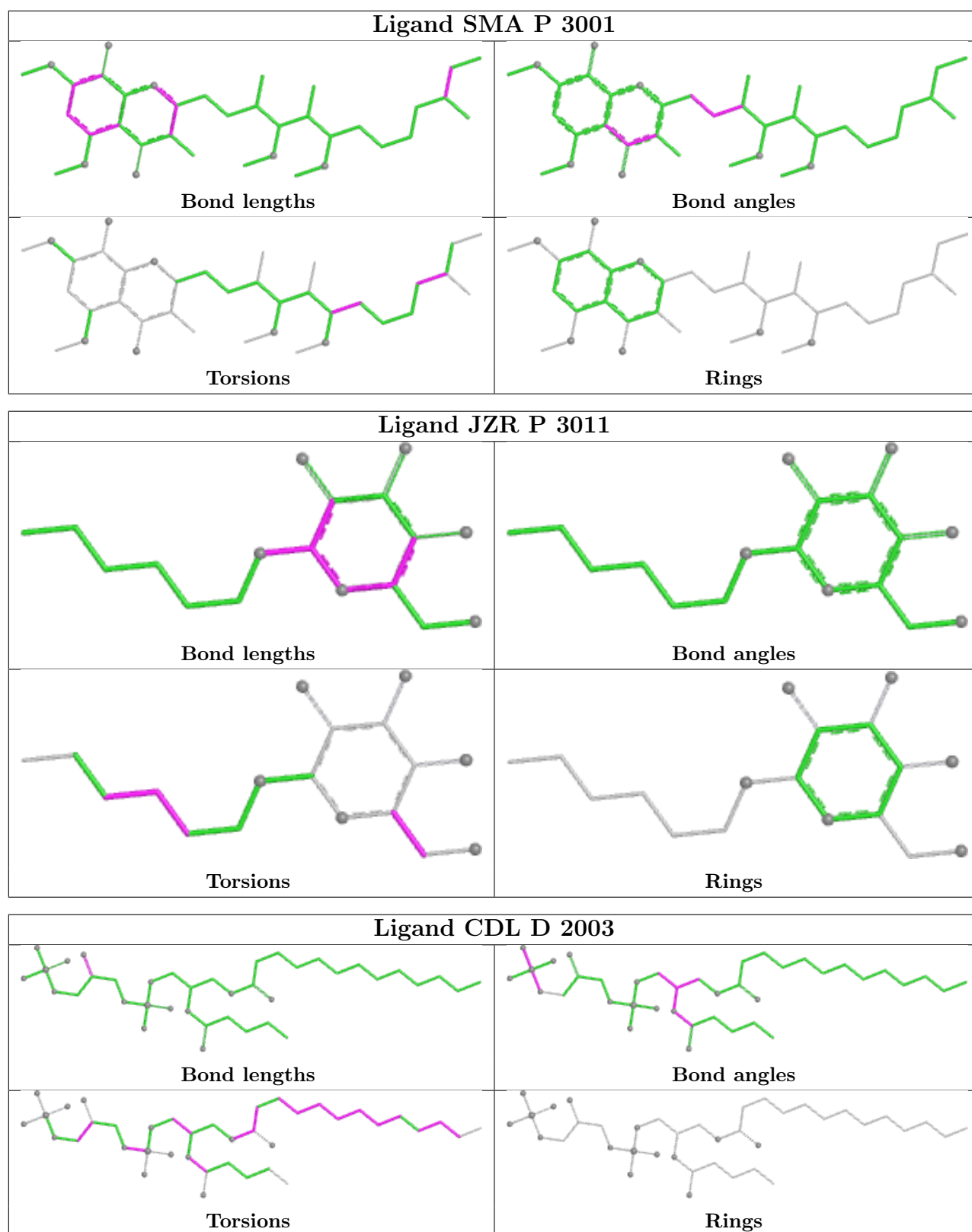
24 monomers are involved in 55 short contacts:

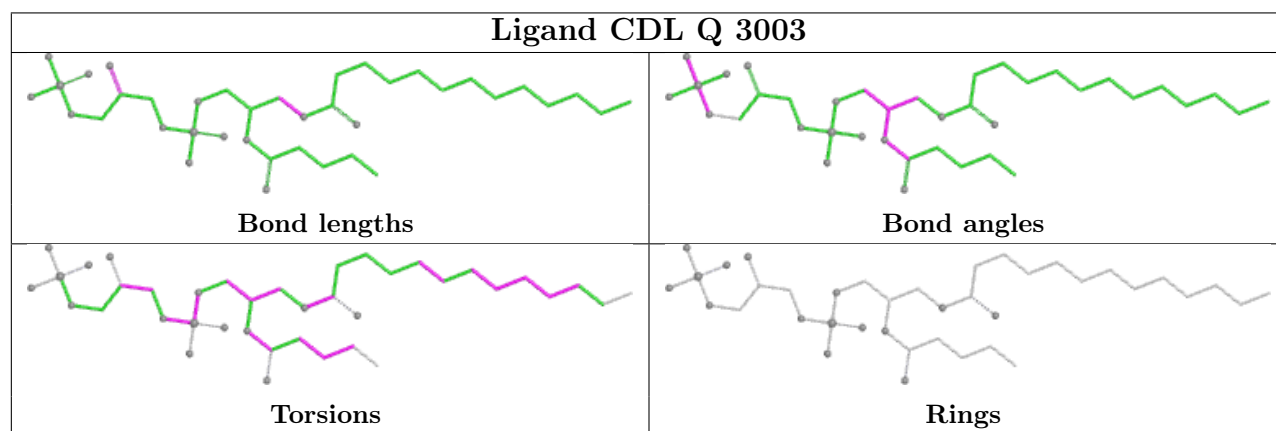
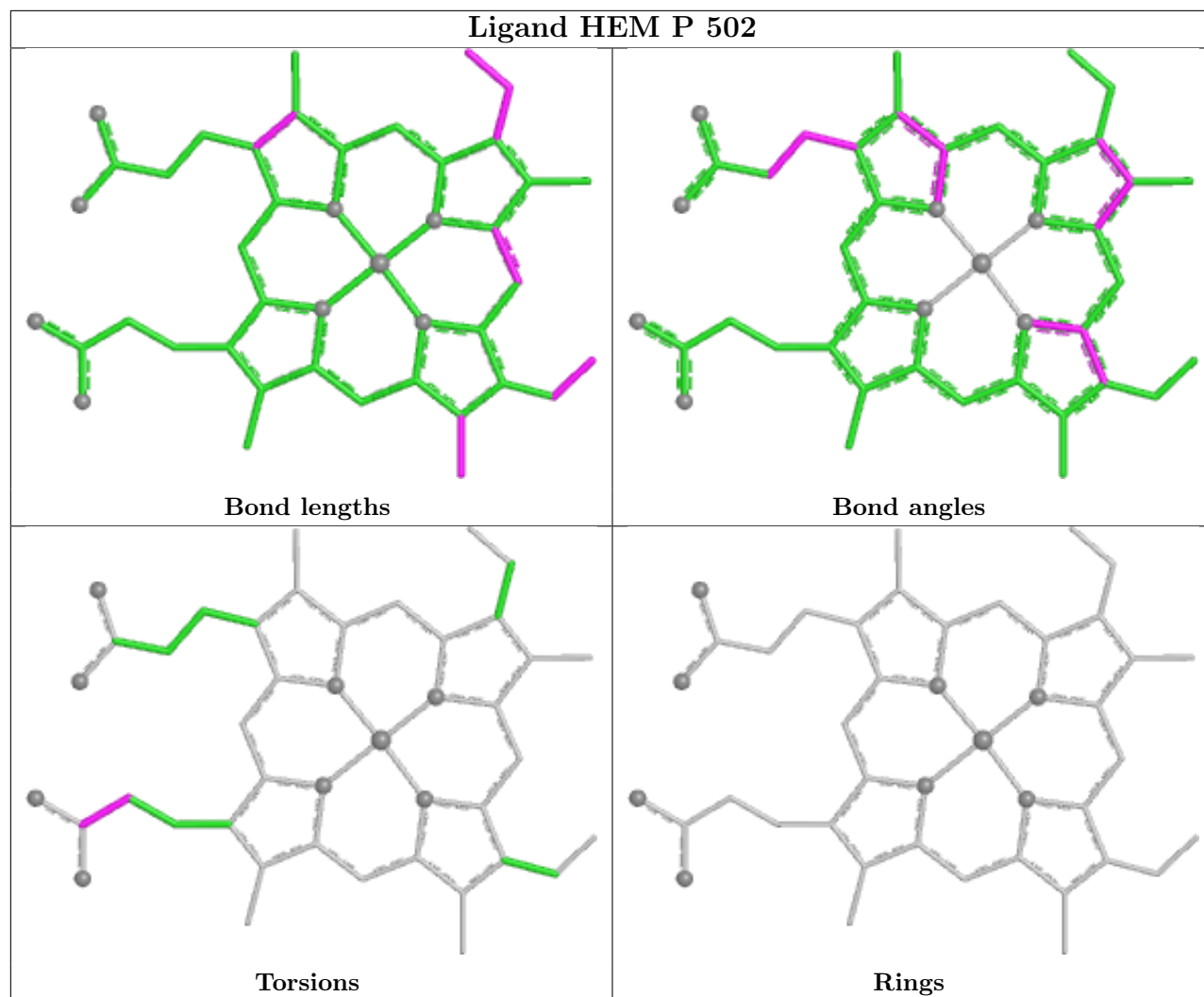
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	4009	GOL	2	0
11	F	4003	JZR	1	0
17	P	3001	SMA	2	0
19	D	2003	CDL	1	0
13	G	4001	AZI	1	0
16	P	502	HEM	2	0
15	P	3007	PEE	3	0
17	C	2001	SMA	2	0
15	D	2006	PEE	3	0
11	F	3012	JZR	3	0
12	Q	4012	PO4	1	0
16	C	502	HEM	4	0
21	Q	501	HEC	3	0
21	D	501	HEC	3	0
15	Q	3006	PEE	7	0
12	I	4015	PO4	1	0
18	P	3002	UQ	4	0
11	A	4004	JZR	1	0
16	P	501	HEM	1	0
18	C	2002	UQ	3	0
15	B	4017	PEE	1	0
16	C	501	HEM	1	0
11	S	2012	JZR	6	0
15	C	2007	PEE	1	0

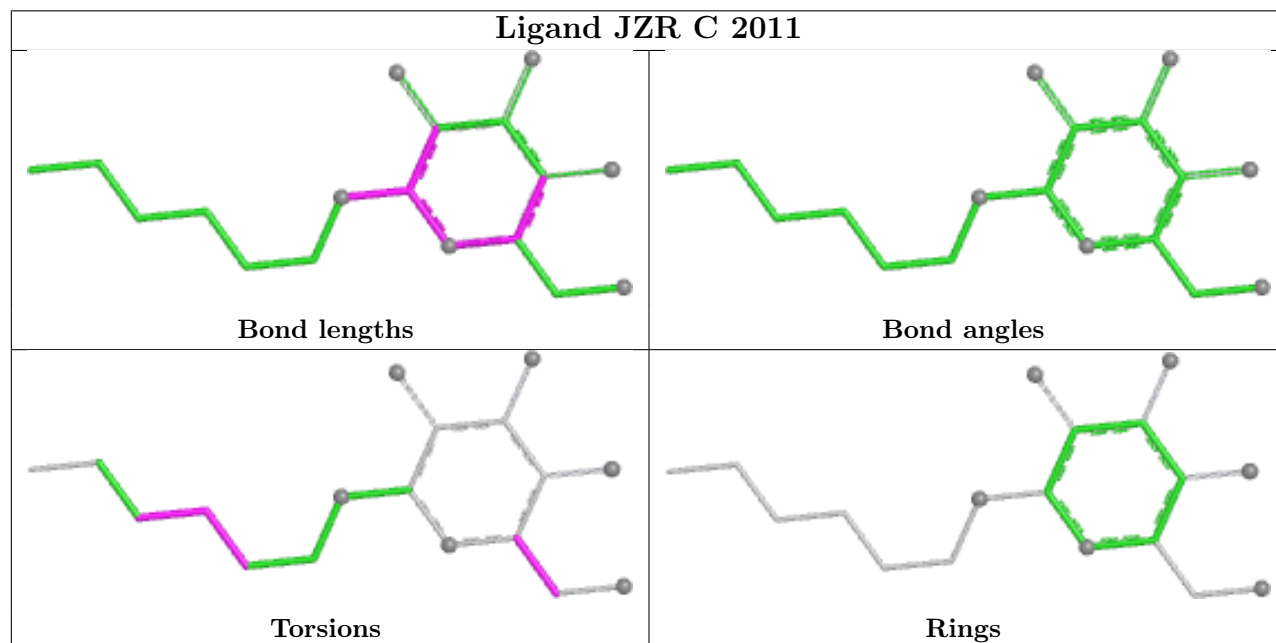
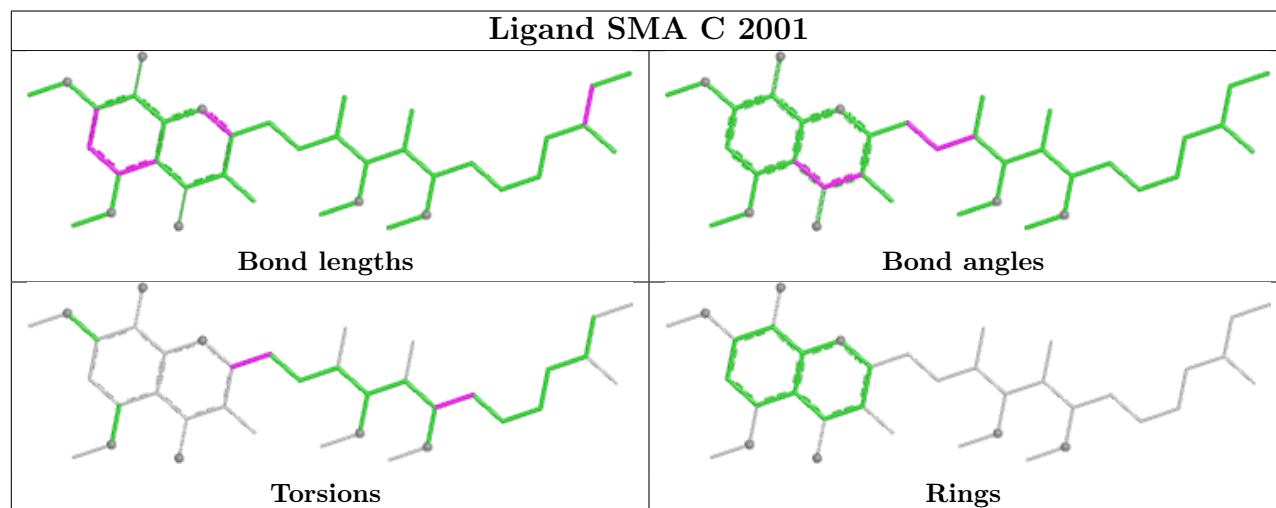
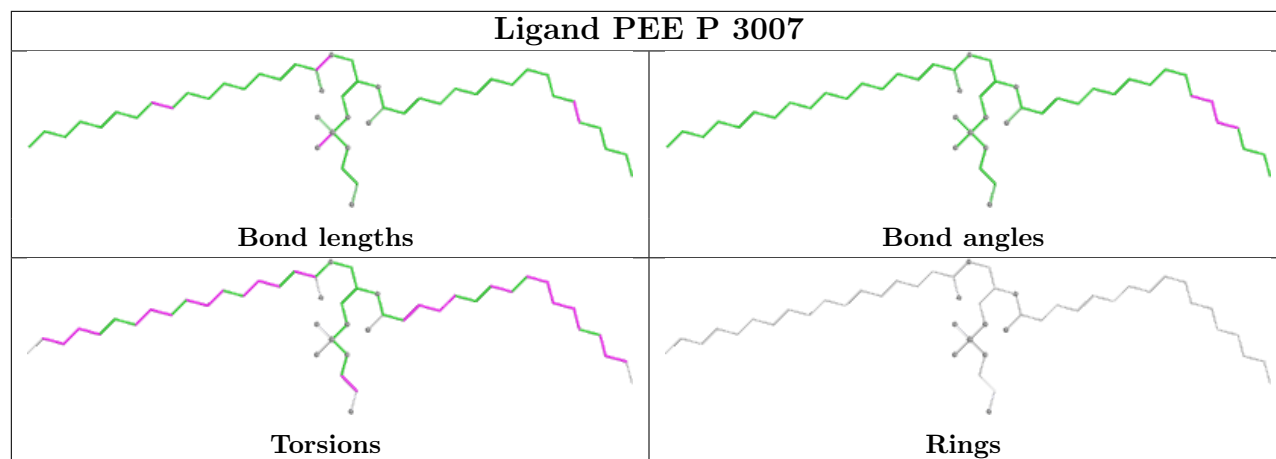
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

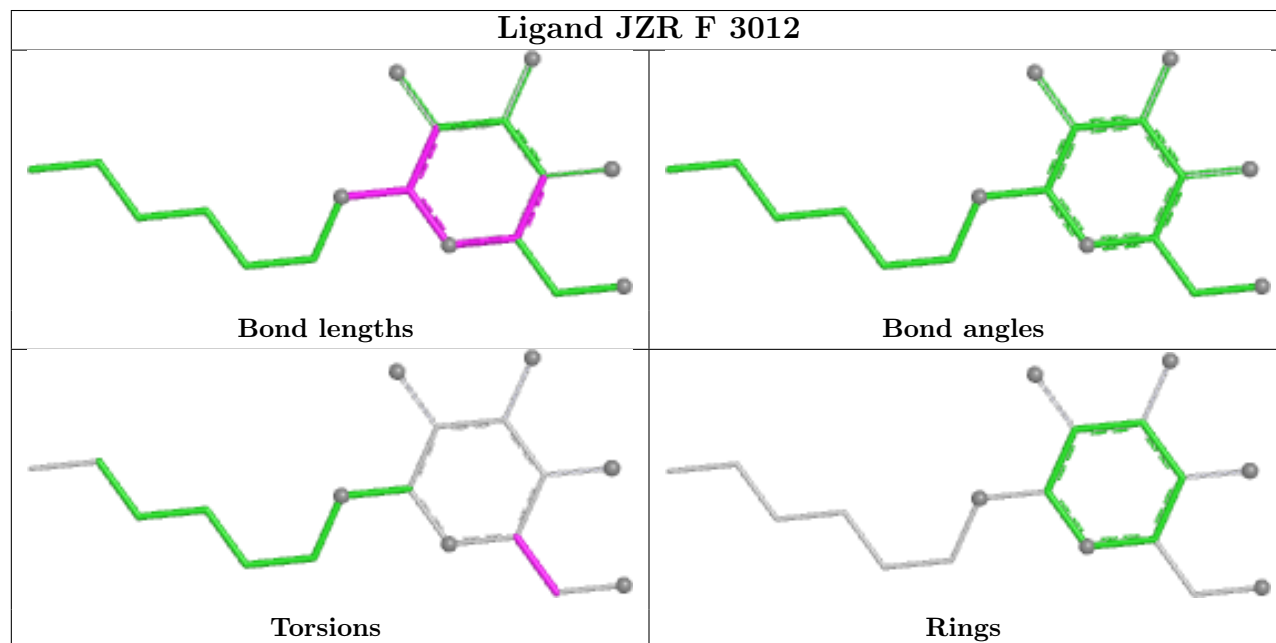
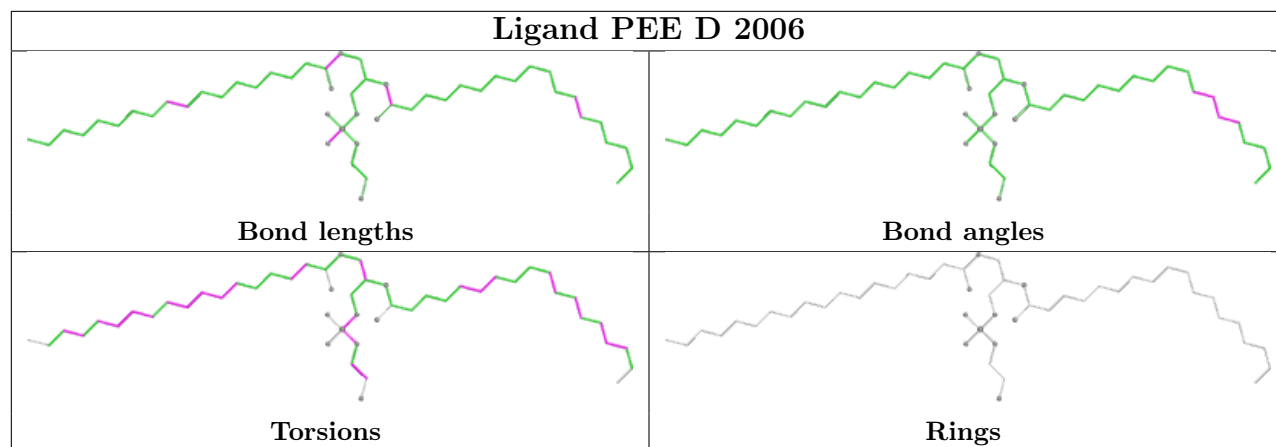
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

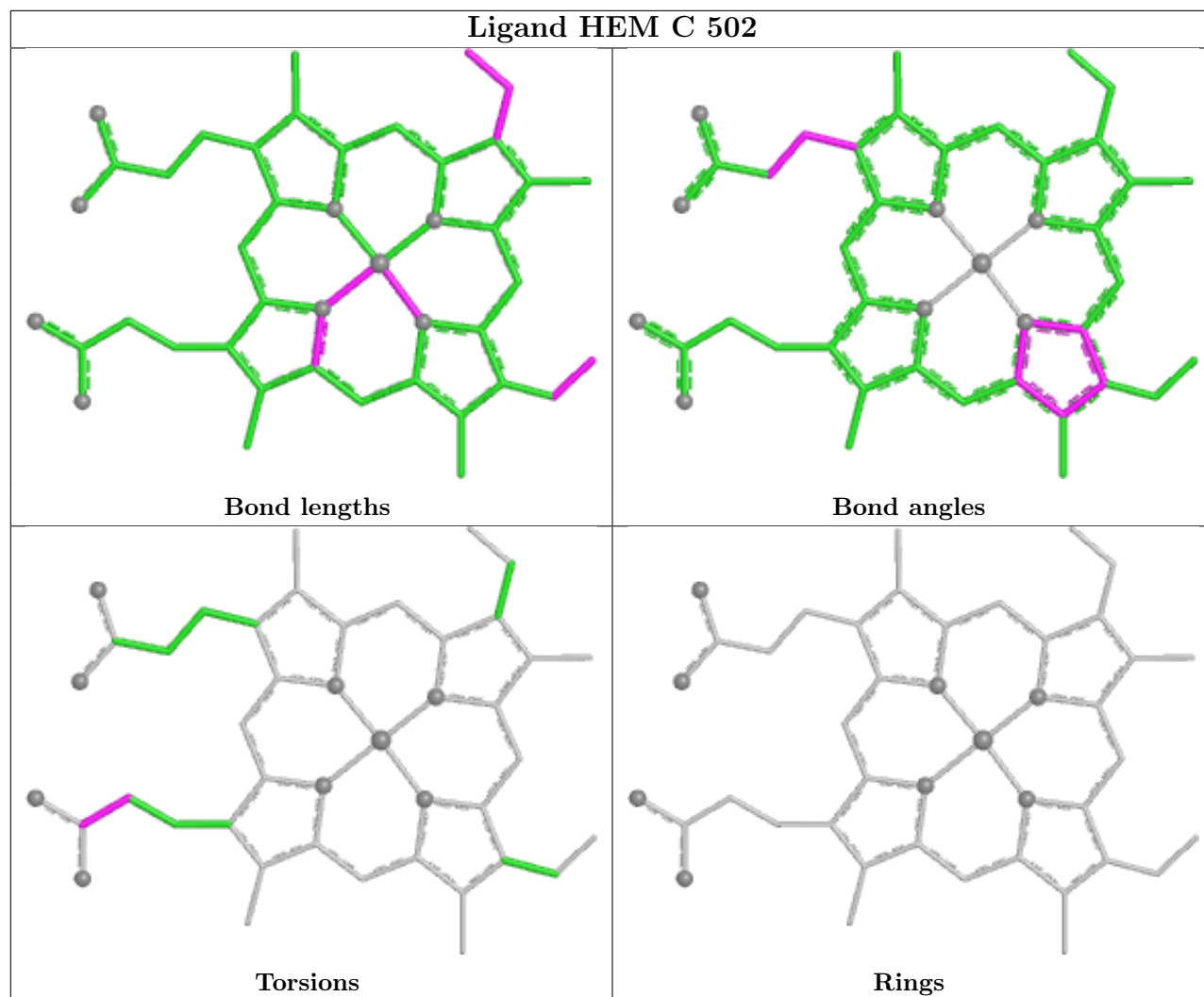


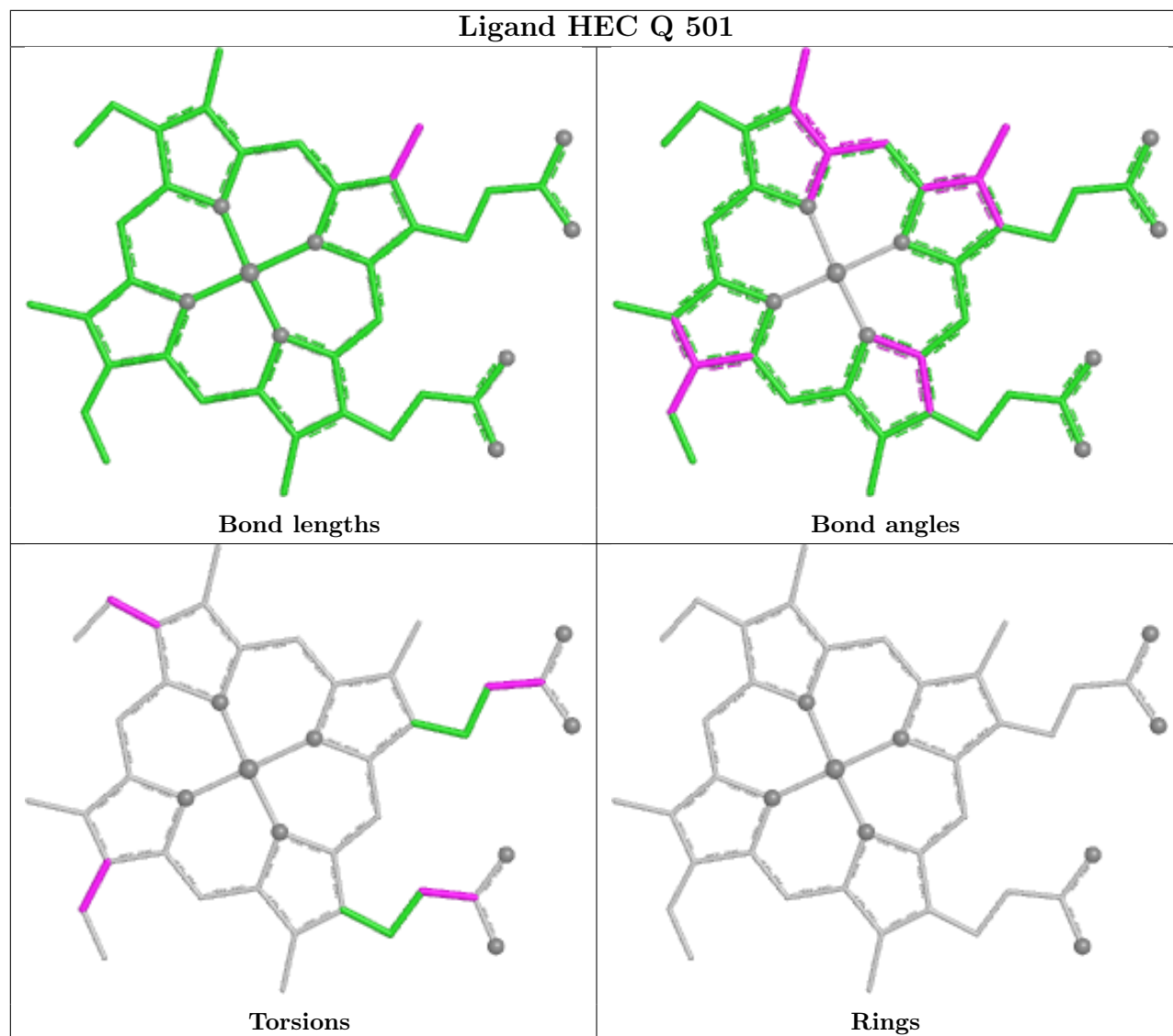




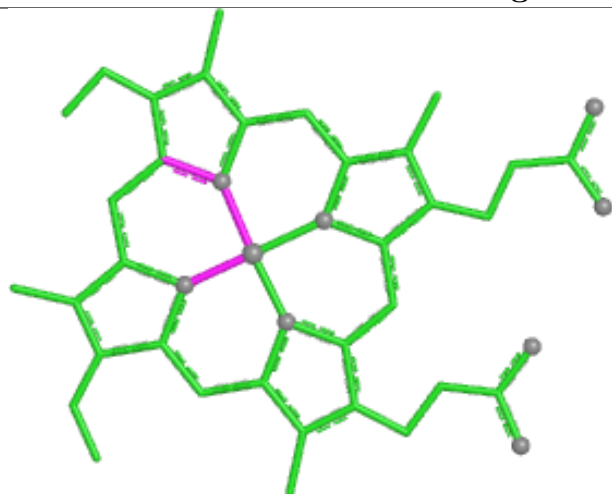




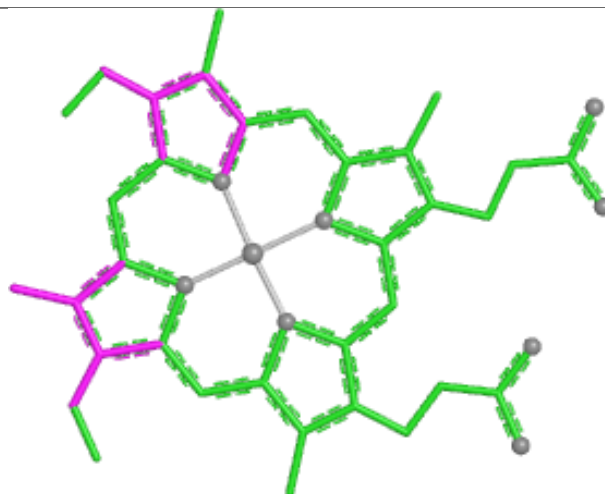




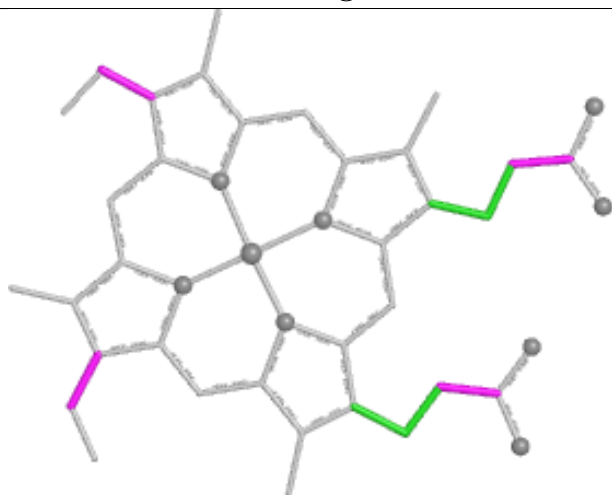
Ligand HEC D 501



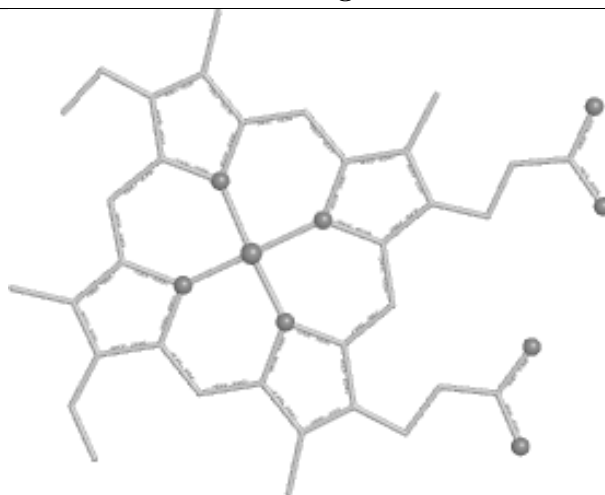
Bond lengths



Bond angles

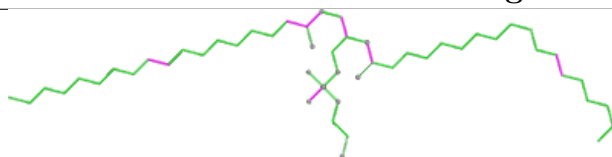


Torsions

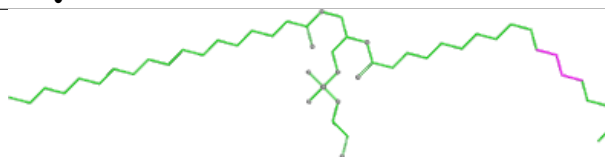


Rings

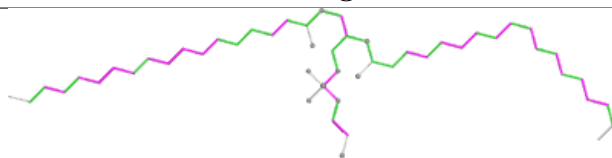
Ligand PEE Q 3006



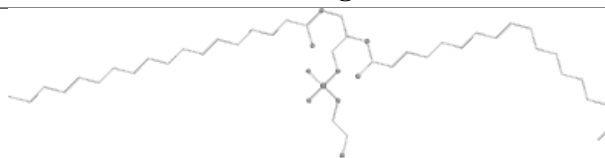
Bond lengths



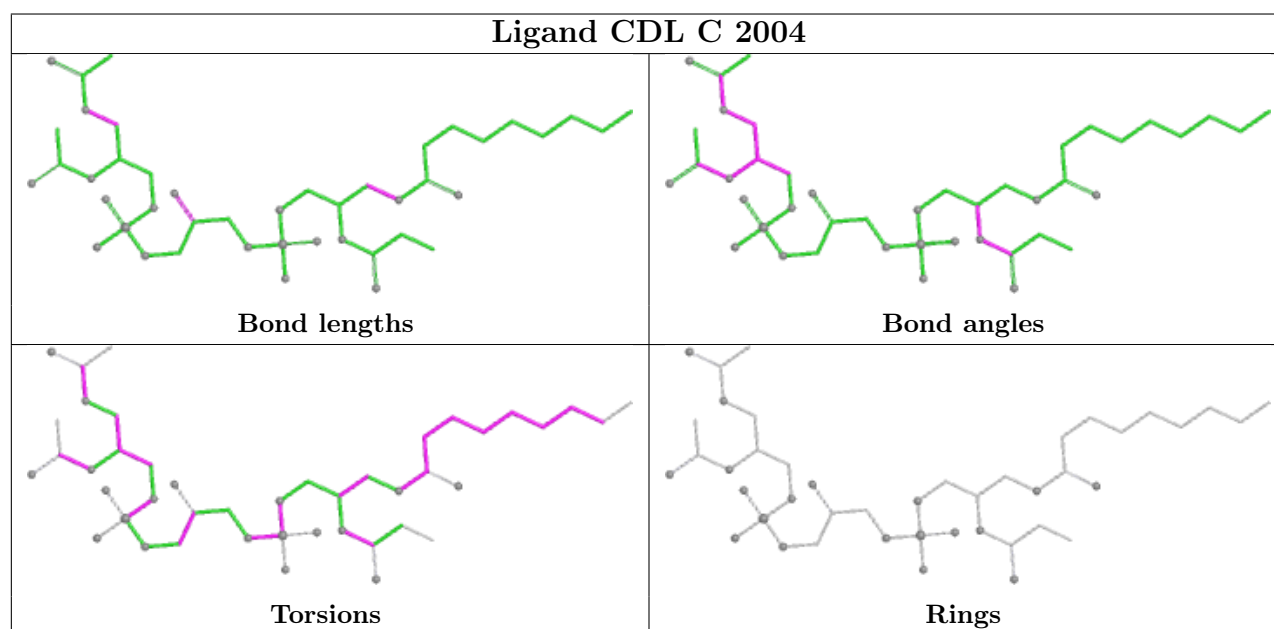
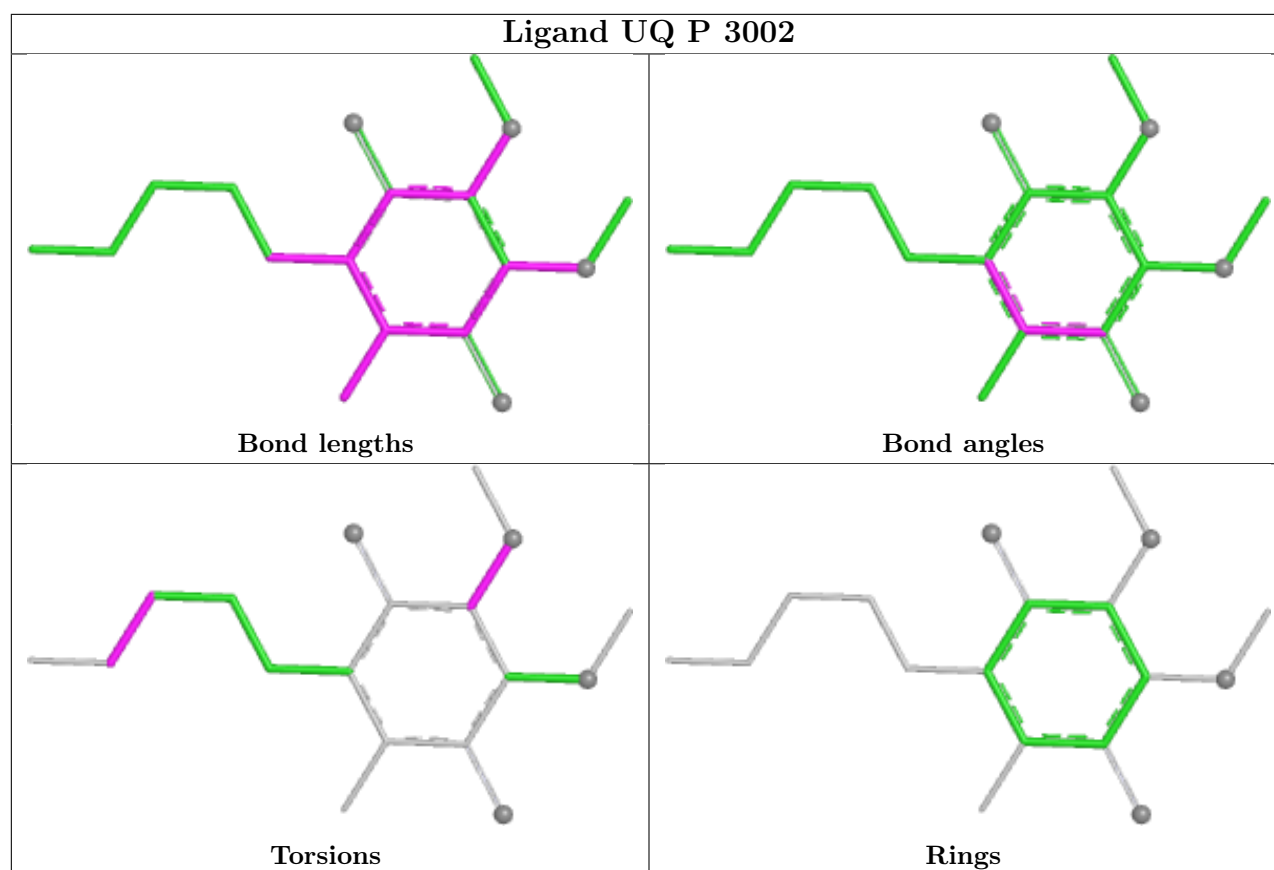
Bond angles

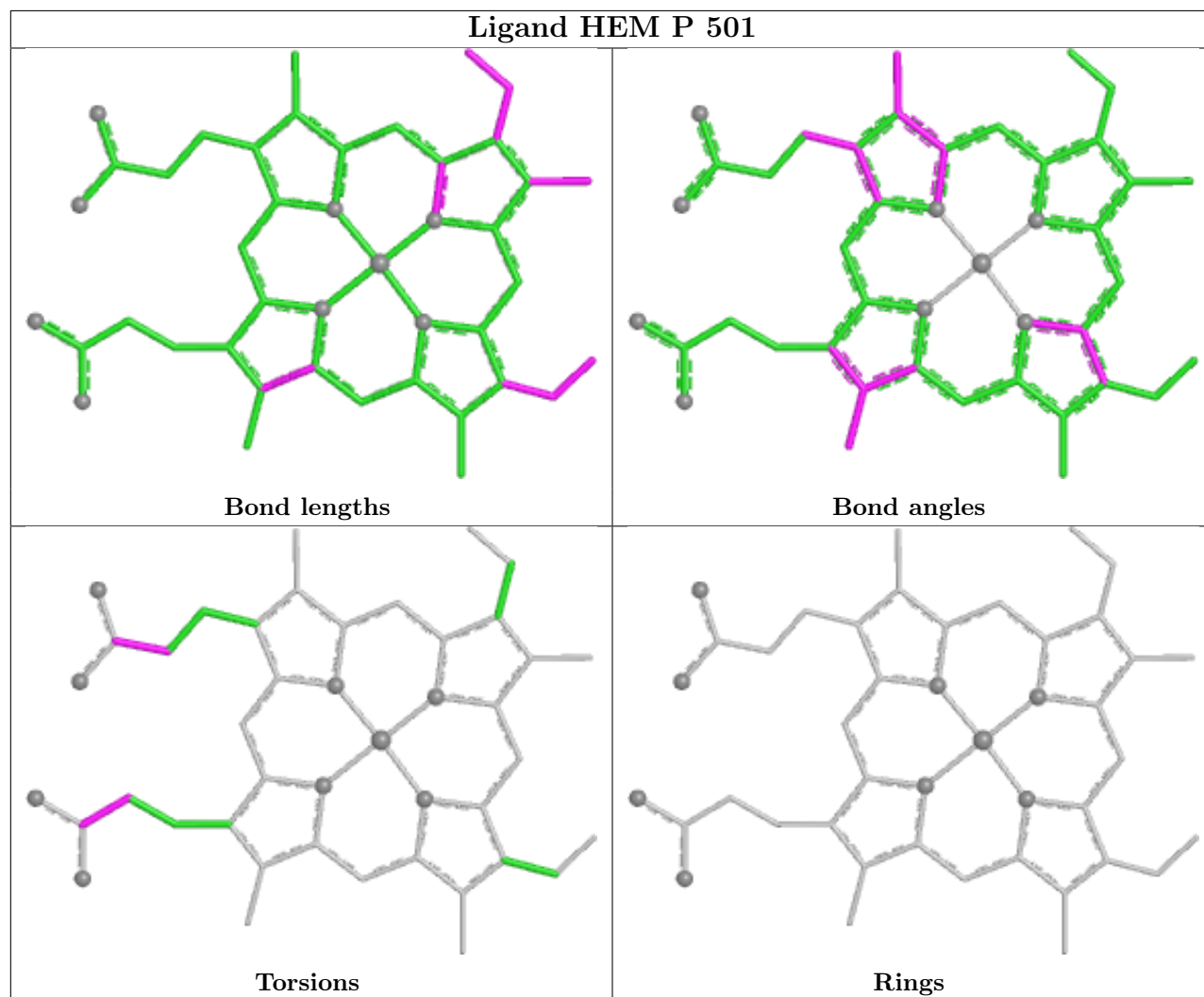
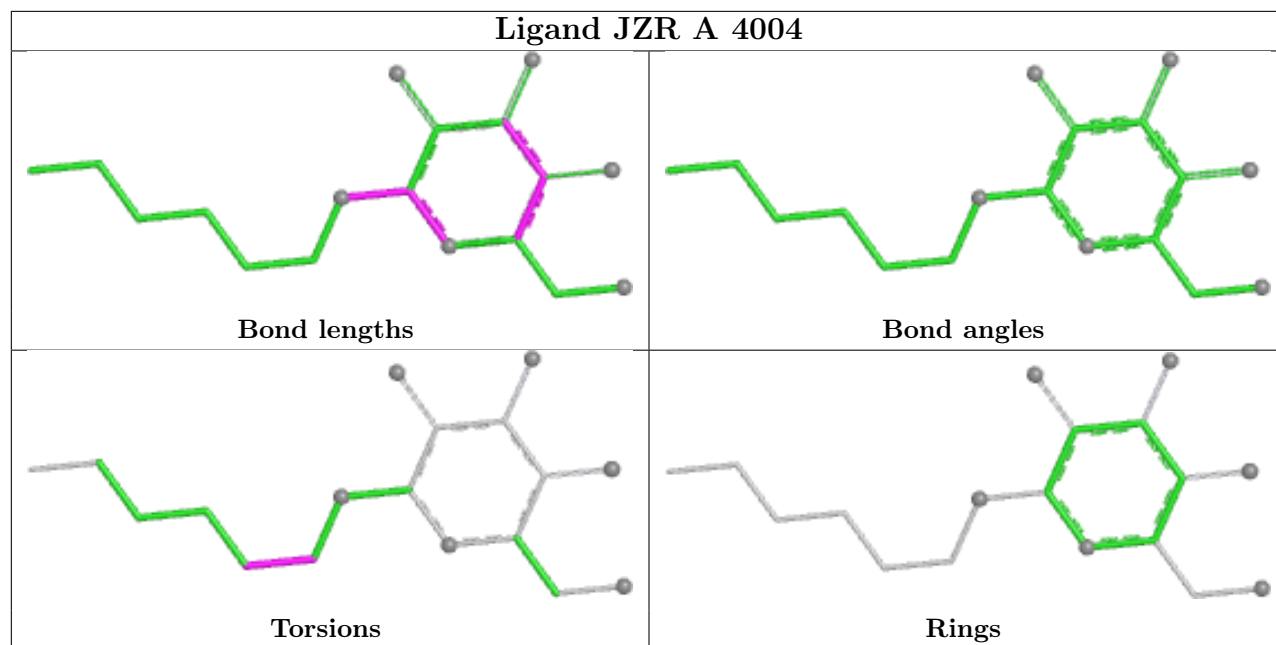


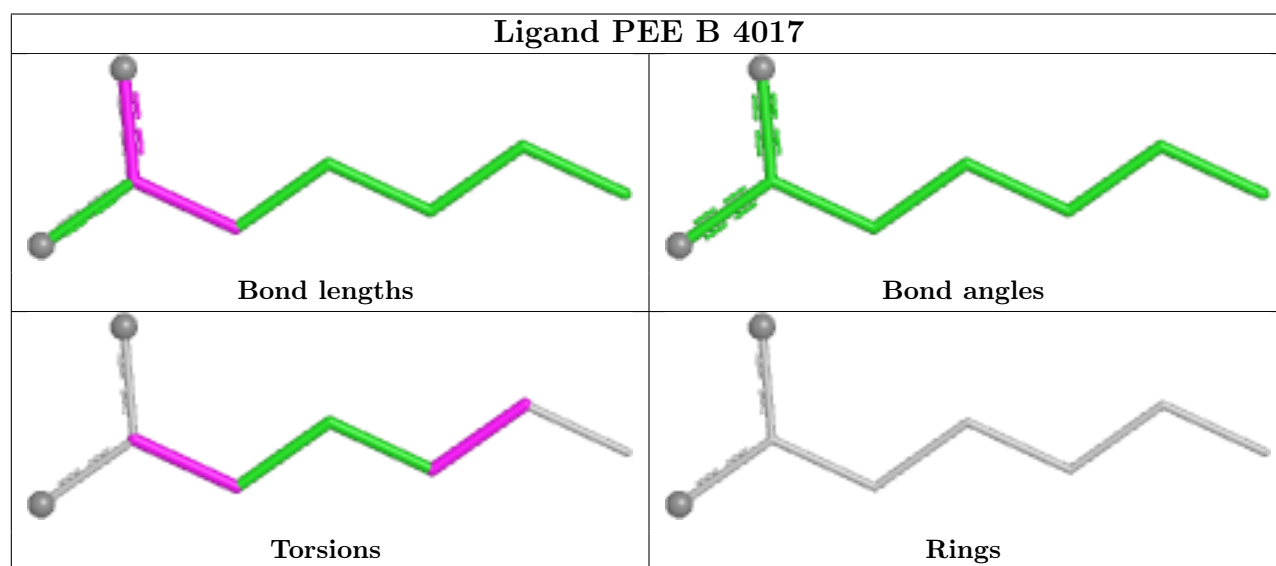
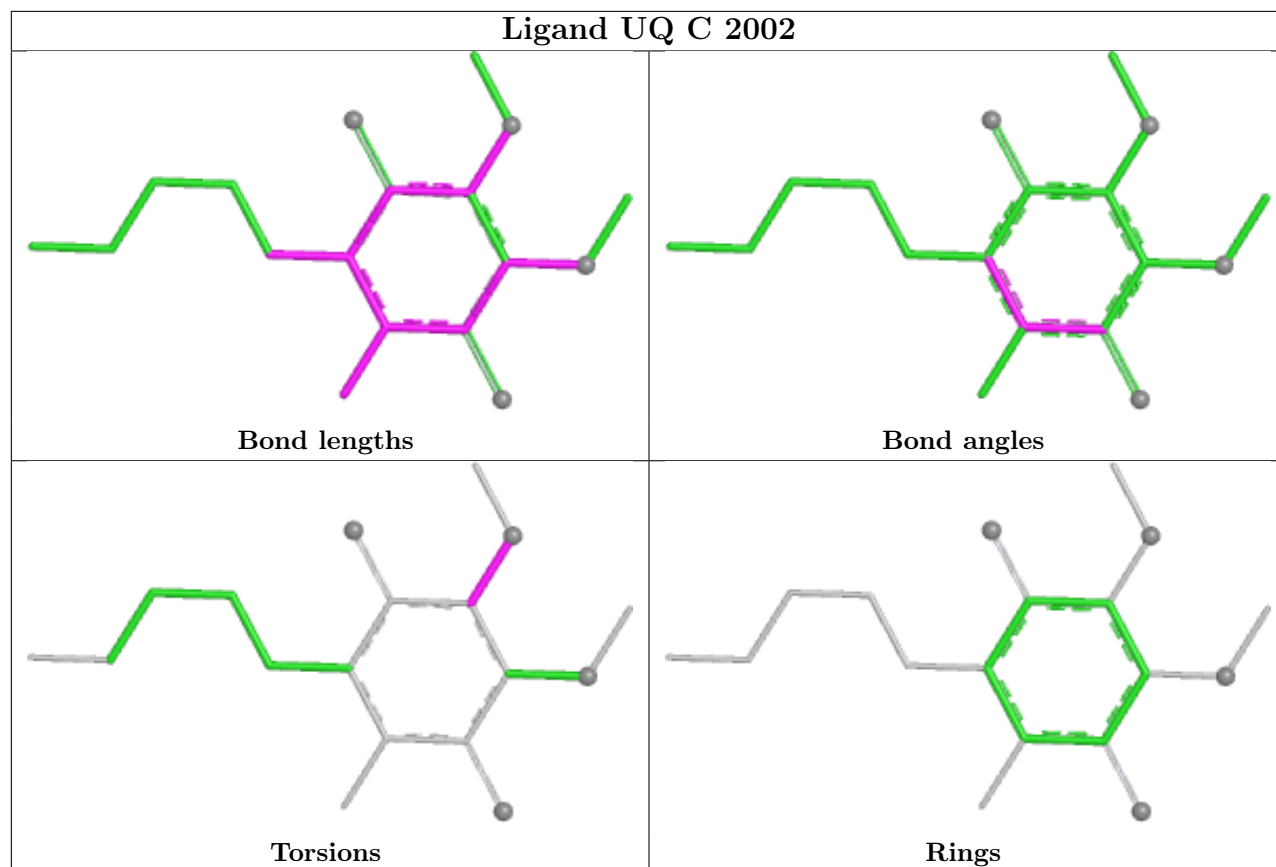
Torsions

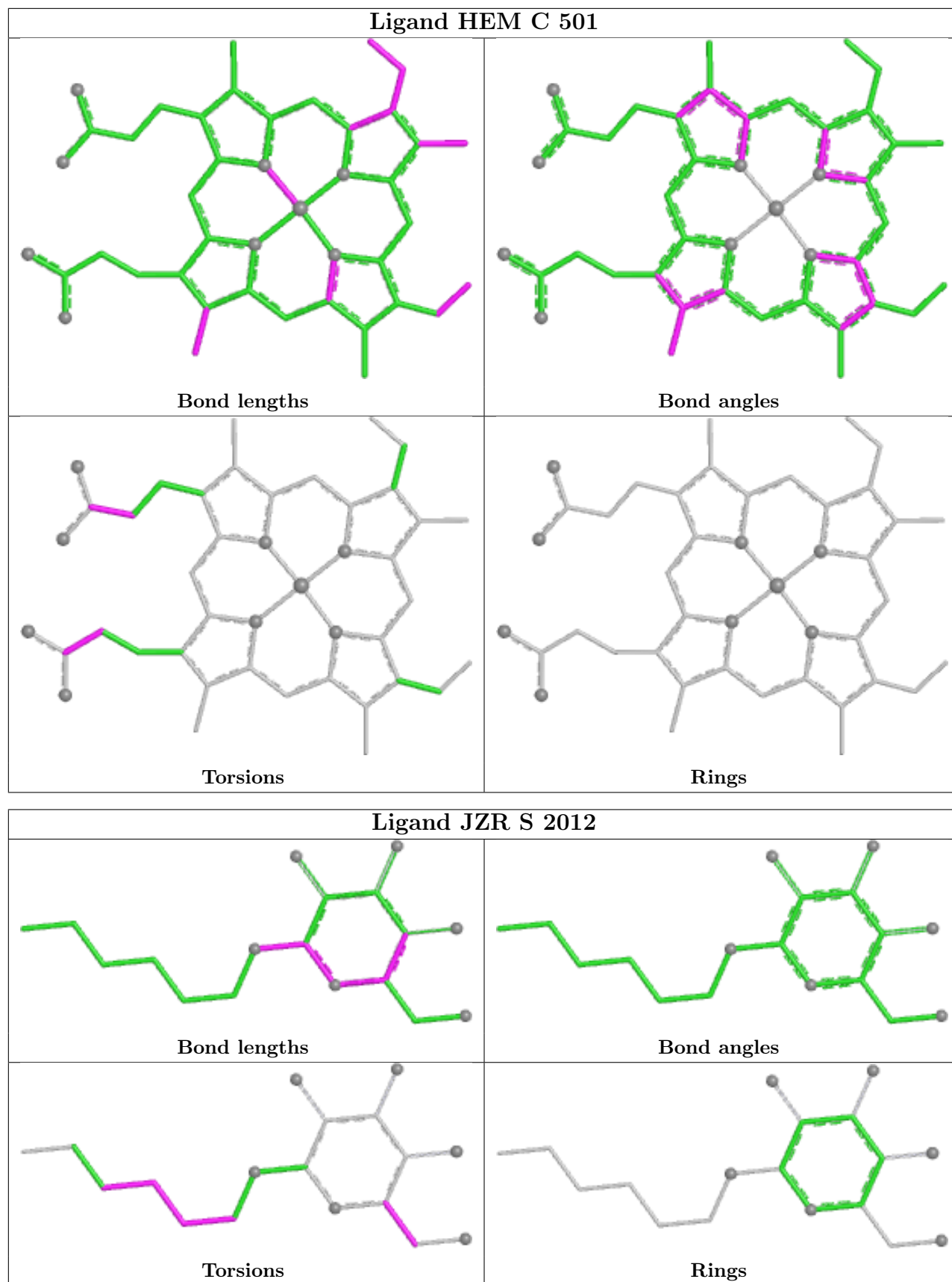


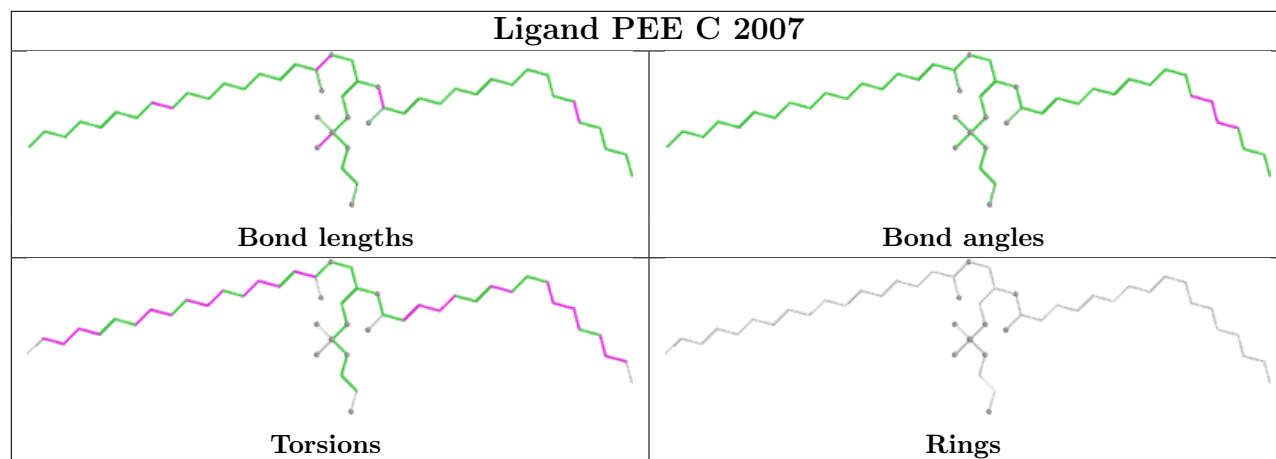
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.18	17 (3%) 44 46	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.63	30 (6%) 23 25	31, 49, 76, 132	1 (0%)
2	B	424/439 (96%)	0.30	19 (4%) 38 40	28, 41, 66, 102	0
2	O	424/439 (96%)	0.71	49 (11%) 9 10	31, 48, 87, 185	0
3	C	365/379 (96%)	0.03	7 (1%) 66 69	24, 34, 48, 108	0
3	P	370/379 (97%)	0.12	11 (2%) 52 55	28, 37, 52, 218	0
4	D	241/241 (100%)	0.13	2 (0%) 82 84	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.45	12 (4%) 34 36	31, 45, 67, 87	0
5	E	196/196 (100%)	1.02	36 (18%) 3 3	32, 57, 105, 117	0
5	R	196/196 (100%)	0.49	11 (5%) 30 32	27, 46, 71, 99	0
6	F	99/110 (90%)	0.24	7 (7%) 22 23	24, 39, 70, 83	0
6	S	99/110 (90%)	0.35	4 (4%) 42 44	28, 40, 67, 88	0
7	G	75/81 (92%)	0.77	5 (6%) 24 25	26, 49, 77, 86	0
7	T	76/81 (93%)	0.94	17 (22%) 2 2	32, 55, 98, 114	0
8	H	66/78 (84%)	0.72	2 (3%) 52 55	40, 56, 73, 78	0
8	U	66/78 (84%)	1.11	9 (13%) 7 7	44, 63, 94, 104	0
9	I	42/78 (53%)	2.49	24 (57%) 0 0	33, 62, 90, 93	0
9	V	42/78 (53%)	2.47	26 (61%) 0 0	36, 78, 94, 100	0
10	J	30/62 (48%)	0.95	2 (6%) 24 25	40, 52, 80, 109	0
10	W	62/62 (100%)	1.30	12 (19%) 3 3	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.48	302 (7%) 20 21	24, 43, 80, 218	2 (0%)

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	THR	10.5
1	N	222	THR	9.6
3	P	18	PHE	7.8
6	S	12	TRP	7.4
3	P	13	ILE	7.2
6	S	13	LEU	6.8
2	O	232	LEU	6.6
2	B	232	LEU	6.5
1	A	2	ALA	6.0
2	O	228	GLY	5.9
3	P	10	LEU	5.8
3	P	14	VAL	5.8
7	G	1	GLY	5.6
1	N	221	GLY	5.5
9	V	78	TYR	5.5
9	I	78	TYR	5.5
2	O	230	LEU	5.3
2	O	17	VAL	5.3
9	I	48	SER	5.2
2	B	230	LEU	5.1
2	O	19	PRO	5.1
9	V	48	SER	5.1
10	W	1	VAL	5.0
2	O	224	LEU	5.0
10	J	61	ASN	4.7
9	I	61	GLY	4.6
1	A	228	VAL	4.6
1	A	1	THR	4.5
9	I	42	VAL	4.5
7	T	1	GLY	4.5
9	V	41	PRO	4.5
2	O	12	GLU	4.5
9	I	71	ASN	4.4
9	I	63	PRO	4.4
10	W	61	ASN	4.3
9	V	61	GLY	4.3
9	I	60	ALA	4.2
1	A	262	TRP	4.2
9	I	73	PRO	4.2
9	I	50	LEU	4.1
1	N	1	THR	4.1
2	O	233	SER	4.1
4	Q	241	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
9	V	42	VAL	4.0
6	F	12	TRP	4.0
9	V	32	ALA	4.0
1	A	225	GLU	4.0
9	I	76	VAL	3.9
3	C	18	PHE	3.8
10	W	5	LEU	3.7
9	I	35	PRO	3.7
2	B	233	SER	3.7
2	O	26	PHE	3.7
5	E	35	PHE	3.7
2	B	229	GLY	3.7
5	E	194	ILE	3.7
9	I	70	LEU	3.6
6	S	15	GLY	3.6
2	O	226	ILE	3.6
8	U	39	LEU	3.6
2	O	229	GLY	3.6
2	O	225	ASN	3.6
9	V	70	LEU	3.6
5	E	193	VAL	3.5
9	I	72	VAL	3.5
1	A	4	TYR	3.5
9	V	39	GLU	3.5
3	P	12	LYS	3.5
5	E	187	PHE	3.5
4	Q	1	SER	3.5
5	E	106	ILE	3.4
5	E	112	VAL	3.4
4	Q	76	GLU	3.4
1	N	228	VAL	3.4
8	U	44	VAL	3.4
9	V	49	VAL	3.4
7	T	75	ALA	3.4
4	Q	3	LEU	3.4
3	C	17	ALA	3.4
9	V	37	THR	3.3
9	V	63	PRO	3.3
2	O	209	LEU	3.3
5	E	191	ASP	3.3
1	A	221	GLY	3.3
10	W	2	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	365	LEU	3.3
1	A	229	PRO	3.2
2	O	304	HIS	3.2
1	N	2	ALA	3.2
9	V	35	PRO	3.2
4	Q	167	GLU	3.1
2	O	303	VAL	3.1
9	I	62	ARG	3.1
9	V	34	VAL	3.1
5	R	93	GLY	3.1
2	O	18	PRO	3.1
3	C	16	ASN	3.1
1	N	225	GLU	3.1
9	I	64	LEU	3.1
5	E	27	GLU	3.0
9	I	49	VAL	3.0
2	B	12	GLU	3.0
5	R	191	ASP	3.0
7	T	43	ALA	3.0
1	N	397	SER	3.0
10	J	62	LYS	3.0
6	S	16	ILE	3.0
5	R	12	ASP	3.0
2	O	219	VAL	2.9
10	W	24	ILE	2.9
2	B	41	TYR	2.9
2	O	25	GLU	2.9
9	V	62	ARG	2.9
2	O	41	TYR	2.9
1	N	443	TRP	2.9
7	T	73	ASN	2.9
2	O	439	LEU	2.9
5	E	195	VAL	2.9
9	I	32	ALA	2.9
5	E	133	VAL	2.8
9	V	73	PRO	2.8
7	G	75	ALA	2.8
9	V	60	ALA	2.8
5	E	82	PRO	2.8
3	C	15	ASN	2.8
3	P	11	MET	2.8
10	W	12	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
9	V	38	SER	2.8
5	E	84	GLY	2.8
2	O	216	LEU	2.7
9	V	55	LEU	2.7
5	R	70	ALA	2.7
2	O	29	LEU	2.7
9	V	50	LEU	2.7
1	N	117	VAL	2.7
5	E	36	SER	2.7
10	W	62	LYS	2.7
1	A	227	ALA	2.7
9	V	36	ALA	2.7
10	W	3	PRO	2.7
2	O	405	VAL	2.7
1	A	316	ASP	2.7
9	I	55	LEU	2.6
1	A	20	ASP	2.6
1	N	81	SER	2.6
7	T	45	ILE	2.6
1	N	120	CYS	2.6
2	B	227	ARG	2.6
5	E	188	THR	2.6
5	E	78	LEU	2.6
5	R	190	ASP	2.6
5	E	192	MET	2.6
1	N	193	PRO	2.6
1	N	209	LEU	2.6
2	O	24	LEU	2.6
4	Q	171	PHE	2.6
7	G	26	PHE	2.6
8	H	34	ARG	2.6
3	P	19	ILE	2.6
5	E	5	ILE	2.6
1	A	3	THR	2.6
4	Q	157	ALA	2.6
5	E	38	LEU	2.6
6	F	107	TRP	2.6
5	E	128	LYS	2.5
5	E	190	ASP	2.5
5	R	11	SER	2.5
3	P	15	ASN	2.5
8	U	50	THR	2.5

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Mol	Chain	Res	Type	RSRZ
7	G	30	PHE	2.5
2	B	231	GLY	2.5
5	E	81	ILE	2.5
10	W	4	THR	2.5
2	O	21	PRO	2.5
7	T	74	PRO	2.5
5	R	71	MET	2.5
10	W	19	THR	2.4
8	U	16	PRO	2.4
9	V	33	ALA	2.4
2	B	24	LEU	2.4
5	E	135	LEU	2.4
2	O	227	ARG	2.4
2	O	350	GLY	2.4
1	A	226	ASP	2.4
9	I	34	VAL	2.4
9	V	76	VAL	2.4
1	N	227	ALA	2.4
5	E	110	ALA	2.4
2	O	351	ASN	2.4
6	F	22	ASN	2.4
5	E	108	GLN	2.4
2	O	380	ASP	2.4
2	O	211	VAL	2.4
5	E	132	TRP	2.4
7	T	70	LYS	2.4
9	I	51	CYS	2.4
7	T	29	TYR	2.4
1	N	219	LEU	2.4
3	P	320	LEU	2.4
3	C	168	PHE	2.4
2	B	264	ILE	2.4
5	E	134	ILE	2.4
1	N	220	SER	2.4
5	E	70	ALA	2.3
2	O	218	GLN	2.3
2	B	250	ASP	2.3
7	T	2	ARG	2.3
1	N	127	ILE	2.3
4	Q	79	GLU	2.3
4	Q	101	ALA	2.3
5	E	117	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
6	F	71	ARG	2.3
9	V	77	ARG	2.3
3	C	19	ILE	2.3
4	Q	158	ILE	2.3
1	N	15	GLN	2.3
1	N	262	TRP	2.3
2	O	33	LEU	2.3
2	O	392	TYR	2.3
3	P	43	LEU	2.3
3	P	155	TYR	2.3
8	U	37	LEU	2.3
7	T	72	LYS	2.3
9	I	69	SER	2.3
2	O	223	PHE	2.3
5	R	35	PHE	2.3
5	E	114	VAL	2.3
2	B	306	PRO	2.3
2	B	439	LEU	2.3
2	O	368	TYR	2.3
7	T	30	PHE	2.2
5	E	76	ILE	2.2
7	G	45	ILE	2.2
1	A	67	THR	2.2
9	V	71	ASN	2.2
5	E	80	ASP	2.2
2	O	220	ALA	2.2
2	O	307	PHE	2.2
9	V	52	ARG	2.2
2	O	306	PRO	2.2
7	T	32	LYS	2.2
1	N	316	ASP	2.2
1	A	315	ALA	2.2
1	N	23	LEU	2.2
1	N	122	LEU	2.2
1	N	203	LEU	2.2
2	O	352	LEU	2.2
5	R	187	PHE	2.2
2	O	403	ASP	2.2
5	E	113	GLU	2.2
5	E	115	SER	2.2
2	O	217	LYS	2.2
4	D	241	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	19	TRP	2.2
7	T	61	TRP	2.2
2	B	19	PRO	2.1
1	N	174	VAL	2.1
5	E	127	VAL	2.1
10	W	26	VAL	2.1
9	I	77	ARG	2.1
8	U	68	CYS	2.1
8	U	78	LYS	2.1
4	Q	77	ASP	2.1
2	B	304	HIS	2.1
2	B	262	ALA	2.1
9	I	74	ALA	2.1
5	R	19	LEU	2.1
8	H	48	SER	2.1
8	U	45	SER	2.1
9	V	64	LEU	2.1
1	N	229	PRO	2.1
9	I	52	ARG	2.1
10	W	14	PHE	2.1
2	B	404	ALA	2.1
2	O	281	ALA	2.1
4	Q	142	SER	2.1
2	O	221	GLU	2.1
3	C	366	MET	2.1
1	N	226	ASP	2.1
7	T	64	GLN	2.1
5	E	111	ALA	2.1
7	T	67	GLU	2.0
1	N	19	LEU	2.0
1	N	141	ASN	2.0
2	O	305	GLN	2.0
1	N	206	ARG	2.0
8	U	67	HIS	2.0
2	O	296	TYR	2.0
6	F	110	LYS	2.0
4	D	73	GLY	2.0
7	T	34	ILE	2.0
2	O	396	SER	2.0
5	R	25	SER	2.0
2	B	281	ALA	2.0
2	O	333	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
6	F	108	ALA	2.0
1	N	194	ARG	2.0
2	B	20	HIS	2.0
2	O	363	LYS	2.0
7	T	60	THR	2.0
2	O	302	GLY	2.0
5	E	49	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
11	JZR	F	4003	18/18	0.53	0.25	176,180,181,181	0
12	PO4	D	4010	5/5	0.53	0.10	169,169,170,170	0
14	UNL	I	4072	1/-	0.55	0.11	93,93,93,93	0
12	PO4	A	2010	5/5	0.57	0.15	133,133,134,134	0
14	UNL	V	4078	1/-	0.59	0.13	94,94,94,94	0
14	UNL	D	4062	1/-	0.61	0.13	90,90,90,90	0
18	UQ	C	2002	18/63	0.64	0.28	61,73,76,76	0
14	UNL	V	4024	1/-	0.65	0.17	96,96,96,96	0
14	UNL	R	4055	1/-	0.66	0.12	73,73,73,73	0
20	GOL	E	4007	5/6	0.66	0.27	97,100,101,102	0
12	PO4	P	3010	5/5	0.67	0.15	115,115,115,116	0
11	JZR	F	3012	18/18	0.67	0.44	159,162,164,164	0
12	PO4	I	4015	5/5	0.68	0.18	122,122,123,123	0
13	AZI	P	3005	3/3	0.69	0.25	54,54,59,63	0
12	PO4	D	4011	5/5	0.69	0.18	130,130,130,131	0
14	UNL	D	4083	1/-	0.69	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	UNL	I	4033	1/-	0.69	0.18	69,69,69,69	0
12	PO4	R	4014	5/5	0.69	0.11	173,174,174,174	0
14	UNL	N	4029	1/-	0.71	0.19	94,94,94,94	0
14	UNL	U	4056	1/-	0.71	0.21	101,101,101,101	0
13	AZI	C	2005	3/3	0.72	0.20	41,41,55,60	0
11	JZR	S	2012	18/18	0.73	0.26	89,103,106,107	0
18	UQ	P	3002	18/63	0.74	0.23	60,82,85,86	0
14	UNL	V	4090	1/-	0.74	0.09	74,74,74,74	0
20	GOL	O	4005	6/6	0.74	0.29	166,167,167,168	0
14	UNL	A	4091	1/-	0.75	0.20	72,72,72,72	0
14	UNL	C	4045	1/-	0.75	0.17	71,71,71,71	0
14	UNL	V	4088	1/-	0.75	0.20	80,80,80,80	0
14	UNL	N	4022	1/-	0.75	0.13	81,81,81,81	0
14	UNL	O	4020	2/-	0.76	0.11	96,96,96,97	0
13	AZI	A	4002	3/3	0.76	0.27	48,48,58,65	0
15	PEE	B	4017	8/51	0.76	0.32	85,88,91,92	0
14	UNL	U	4049	1/-	0.76	0.21	77,77,77,77	0
14	UNL	A	4081	1/-	0.76	0.18	71,71,71,71	0
12	PO4	T	4016	5/5	0.76	0.11	107,108,108,108	0
14	UNL	F	4028	1/-	0.76	0.13	82,82,82,82	0
11	JZR	C	2011	18/18	0.77	0.26	106,118,123,125	0
14	UNL	G	4053	1/-	0.78	0.17	77,77,77,77	0
14	UNL	A	4085	1/-	0.78	0.10	56,56,56,56	0
14	UNL	N	4073	1/-	0.78	0.28	69,69,69,69	0
14	UNL	B	4042	1/-	0.78	0.14	81,81,81,81	0
11	JZR	P	3011	18/18	0.79	0.22	99,107,109,109	0
14	UNL	R	4069	1/-	0.80	0.19	62,62,62,62	0
14	UNL	D	4036	1/-	0.80	0.18	83,83,83,83	0
14	UNL	E	4061	1/-	0.81	0.06	79,79,79,79	0
14	UNL	O	4037	1/-	0.81	0.44	62,62,62,62	0
12	PO4	Q	4012	5/5	0.81	0.13	108,109,110,110	0
19	CDL	D	2003	39/100	0.81	0.20	64,84,106,107	0
14	UNL	B	4051	1/-	0.81	0.10	78,78,78,78	0
12	PO4	R	4013	5/5	0.81	0.20	114,114,116,116	0
14	UNL	A	4032	1/-	0.82	0.25	65,65,65,65	0
14	UNL	A	4035	1/-	0.82	0.19	69,69,69,69	0
14	UNL	C	4063	1/-	0.82	0.35	74,74,74,74	0
12	PO4	B	3009	5/5	0.83	0.10	97,99,100,101	0
14	UNL	O	4084	1/-	0.83	0.19	67,67,67,67	0
15	PEE	D	2006	51/51	0.83	0.24	85,98,115,118	0
14	UNL	B	4025	1/-	0.83	0.11	93,93,93,93	0
14	UNL	G	4064	1/-	0.84	0.31	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	UNL	S	4047	1/-	0.84	0.18	71,71,71,71	0
14	UNL	P	4040	1/-	0.84	0.19	73,73,73,73	0
14	UNL	Q	4044	1/-	0.84	0.36	88,88,88,88	0
14	UNL	B	4034	1/-	0.84	0.28	87,87,87,87	0
14	UNL	D	4054	1/-	0.85	0.13	76,76,76,76	0
14	UNL	B	4030	1/-	0.86	0.13	70,70,70,70	0
14	UNL	A	4075	1/-	0.86	0.08	64,64,64,64	0
19	CDL	Q	3003	39/100	0.86	0.16	54,90,96,96	0
14	UNL	G	4070	1/-	0.86	0.11	67,67,67,67	0
14	UNL	O	4031	1/-	0.86	0.10	86,86,86,86	0
14	UNL	D	4059	1/-	0.87	0.14	57,57,57,57	0
19	CDL	C	2004	44/100	0.87	0.17	54,83,104,106	0
13	AZI	G	4001	3/3	0.87	0.19	47,47,57,59	0
14	UNL	C	4018	2/-	0.87	0.14	74,74,74,76	0
12	PO4	O	2009	5/5	0.87	0.09	76,79,81,81	0
14	UNL	O	4071	1/-	0.87	0.17	70,70,70,70	0
14	UNL	C	4068	1/-	0.88	0.20	72,72,72,72	0
14	UNL	O	4043	1/-	0.88	0.10	80,80,80,80	0
14	UNL	A	4048	1/-	0.88	0.15	72,72,72,72	0
14	UNL	E	4050	1/-	0.88	0.19	65,65,65,65	0
14	UNL	P	4021	2/-	0.88	0.14	71,71,71,73	0
14	UNL	B	4026	1/-	0.88	0.20	92,92,92,92	0
14	UNL	P	4058	1/-	0.88	0.09	61,61,61,61	0
20	GOL	E	4006	6/6	0.88	0.14	67,71,72,75	0
14	UNL	P	4060	1/-	0.88	0.14	88,88,88,88	0
14	UNL	B	4079	1/-	0.88	0.19	66,66,66,66	0
14	UNL	B	4052	1/-	0.89	0.09	60,60,60,60	0
20	GOL	C	2008	6/6	0.89	0.14	60,63,63,70	0
14	UNL	A	4076	1/-	0.89	0.20	68,68,68,68	0
14	UNL	P	4089	1/-	0.89	0.13	63,63,63,63	0
15	PEE	Q	3006	51/51	0.89	0.18	53,65,110,110	0
20	GOL	P	3008	6/6	0.89	0.25	83,84,85,88	0
14	UNL	C	4023	1/-	0.90	0.11	55,55,55,55	0
14	UNL	A	4038	1/-	0.90	0.23	85,85,85,85	0
14	UNL	D	4067	1/-	0.90	0.14	58,58,58,58	0
19	CDL	P	3004	49/100	0.90	0.17	54,81,117,120	0
14	UNL	N	4019	2/-	0.90	0.11	76,76,76,76	0
14	UNL	T	4065	1/-	0.91	0.27	66,66,66,66	0
14	UNL	T	4066	1/-	0.91	0.11	70,70,70,70	0
14	UNL	B	4080	1/-	0.91	0.30	67,67,67,67	0
14	UNL	W	4077	1/-	0.91	0.13	60,60,60,60	0
14	UNL	C	4086	1/-	0.91	0.10	50,50,50,50	0

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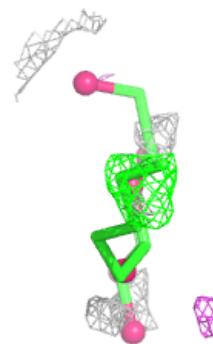
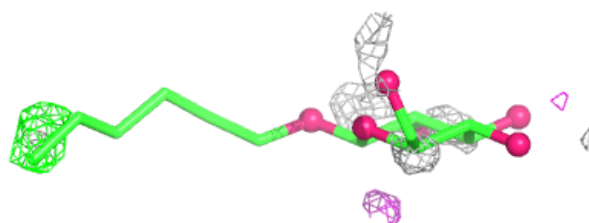
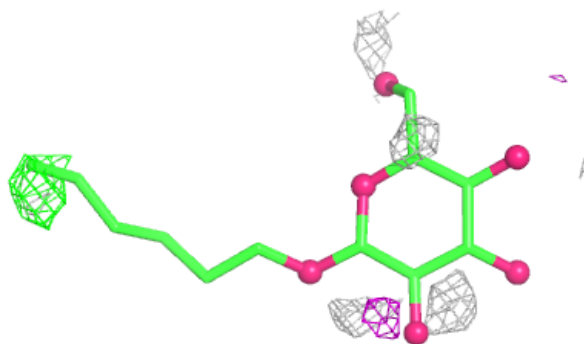
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	UNL	D	4027	1/-	0.91	0.20	87,87,87,87	0
20	GOL	P	4009	6/6	0.91	0.14	67,70,71,72	0
14	UNL	P	4074	1/-	0.92	0.09	59,59,59,59	0
15	PEE	P	3007	49/51	0.92	0.15	35,58,75,76	0
14	UNL	O	4082	1/-	0.92	0.12	73,73,73,73	0
14	UNL	B	4039	1/-	0.92	0.10	73,73,73,73	0
14	UNL	B	4057	1/-	0.92	0.17	57,57,57,57	0
20	GOL	C	4008	6/6	0.93	0.10	53,55,60,60	0
14	UNL	A	4087	1/-	0.93	0.21	60,60,60,60	0
14	UNL	O	4041	1/-	0.94	0.10	71,71,71,71	0
15	PEE	C	2007	49/51	0.94	0.13	33,58,74,74	0
11	JZR	A	4004	18/18	0.94	0.09	29,36,42,44	0
17	SMA	C	2001	37/37	0.95	0.07	25,33,44,46	0
14	UNL	P	4046	1/-	0.95	0.20	65,65,65,65	0
17	SMA	P	3001	37/37	0.96	0.08	30,39,47,52	0
16	HEM	C	501	43/43	0.98	0.06	21,27,34,38	0
16	HEM	C	502	43/43	0.98	0.06	23,26,33,36	0
16	HEM	P	501	43/43	0.98	0.07	22,26,33,40	0
21	HEC	D	501	43/43	0.98	0.07	26,33,37,38	0
21	HEC	Q	501	43/43	0.98	0.06	29,36,41,45	0
22	FES	E	501	4/4	0.98	0.04	38,39,40,40	0
16	HEM	P	502	43/43	0.99	0.05	23,27,37,39	0
22	FES	R	501	4/4	0.99	0.03	27,29,30,30	0

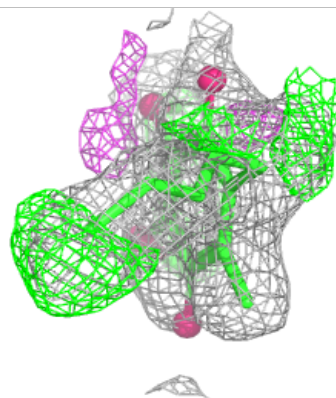
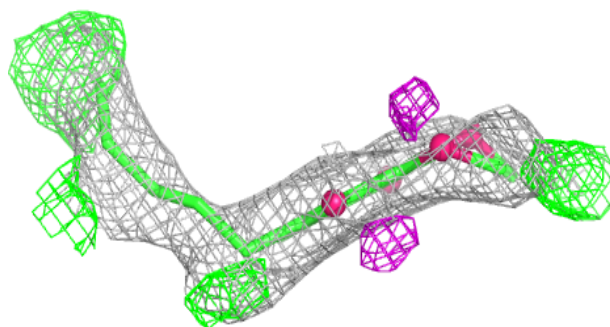
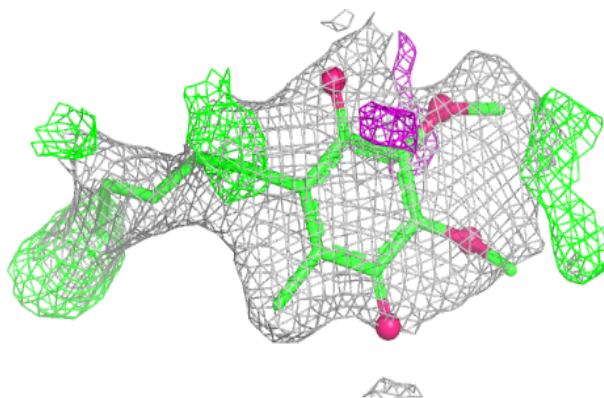
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JZR 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)

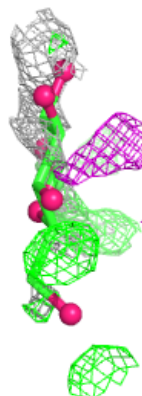
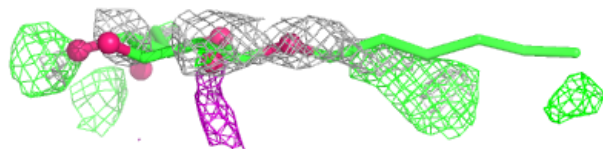
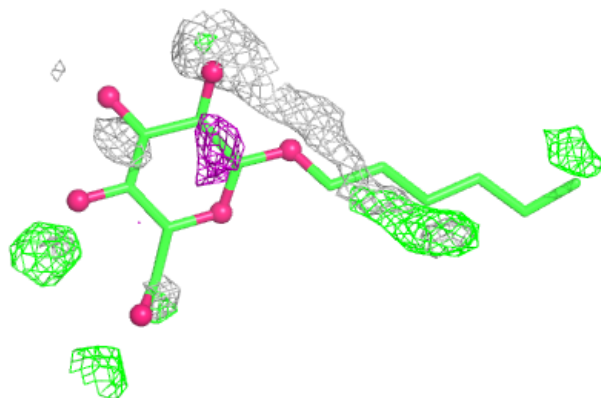
**Electron density around UQ C 2002:**

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

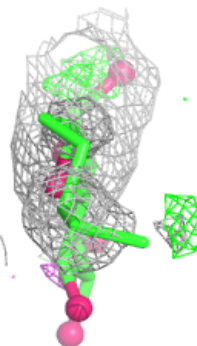
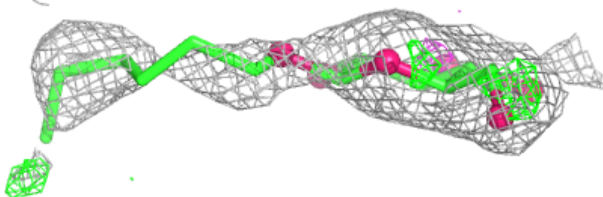
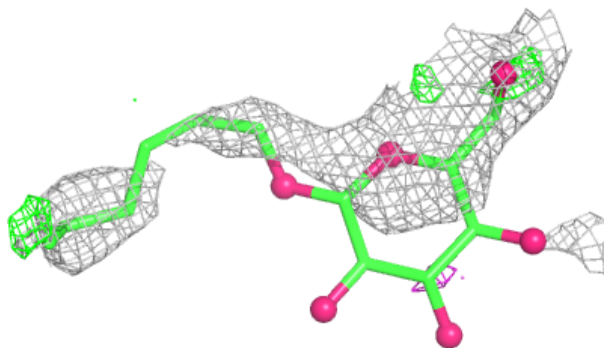


Electron density around JZR F 3012:

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

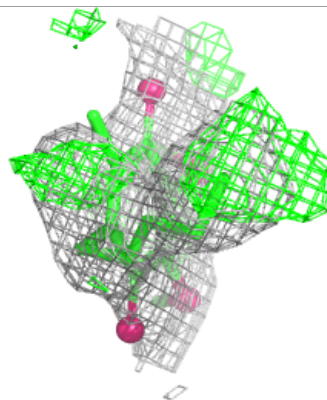
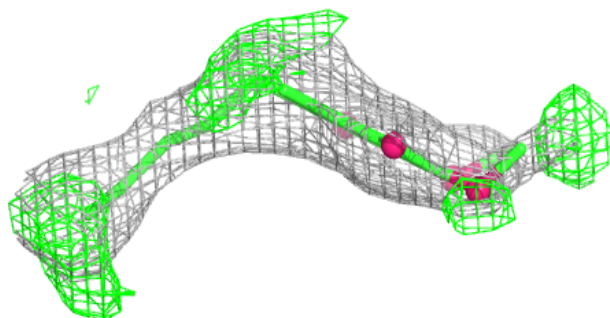
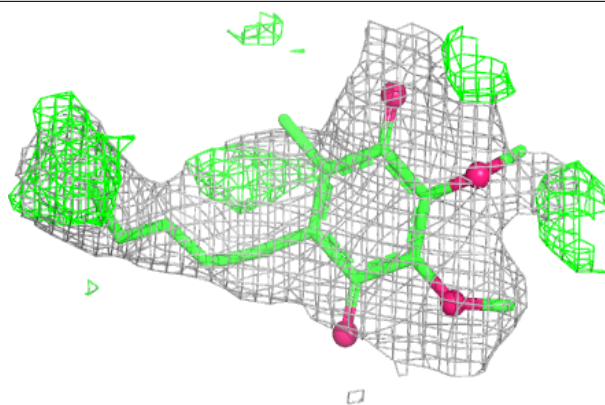
**Electron density around JZR S 2012:**

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

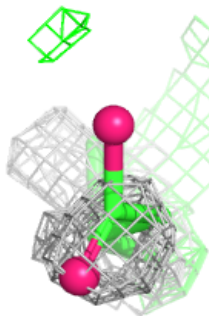
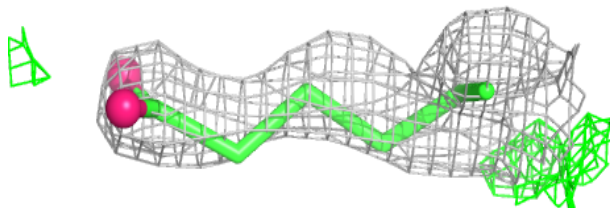
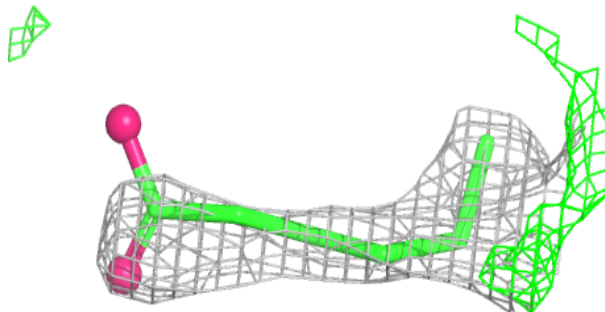


Electron density around UQ P 3002:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

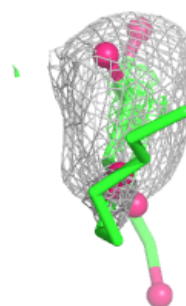
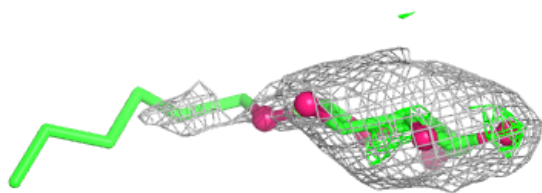
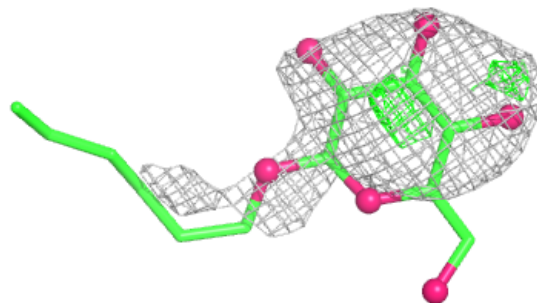
**Electron density around PEE B 4017:**

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

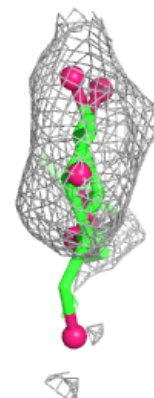
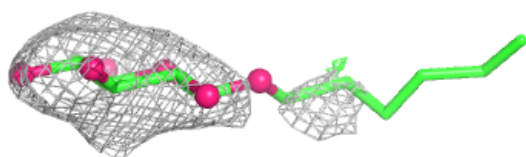
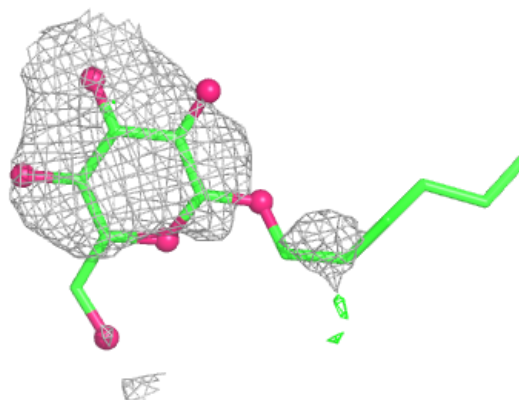


Electron density around JZR C 2011:

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

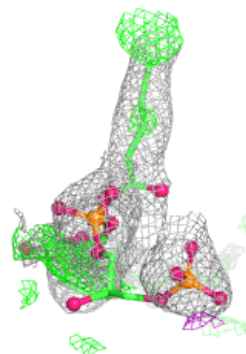
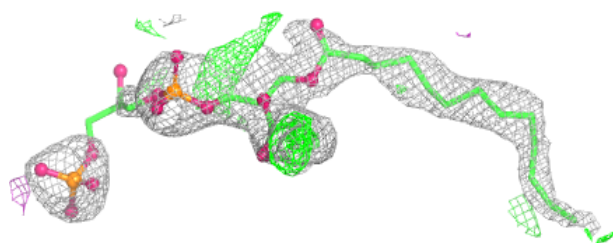
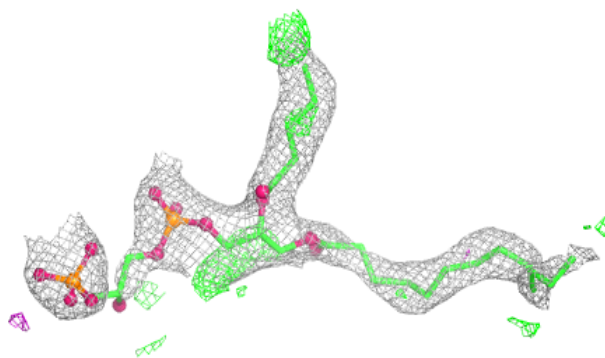
**Electron density around JZR P 3011:**

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

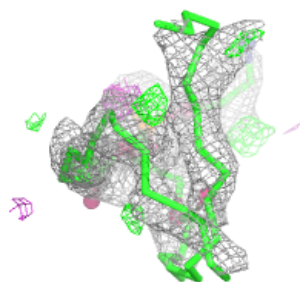
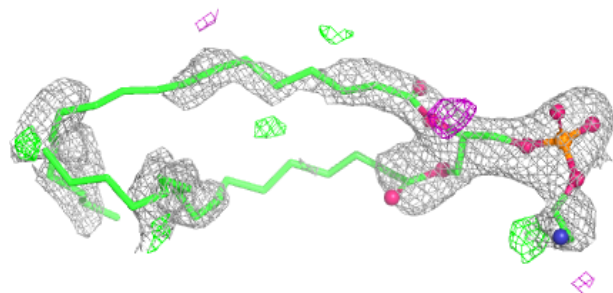
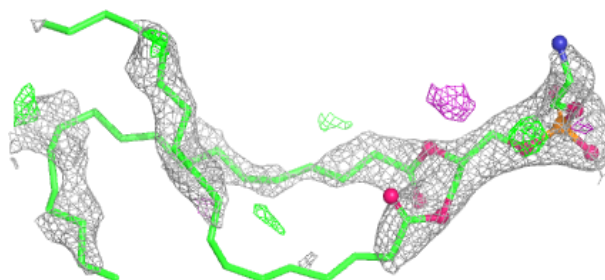


Electron density around CDL D 2003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

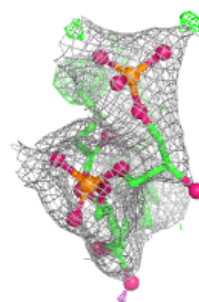
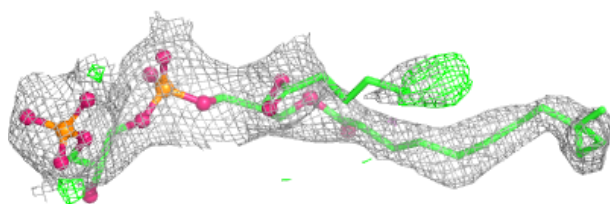
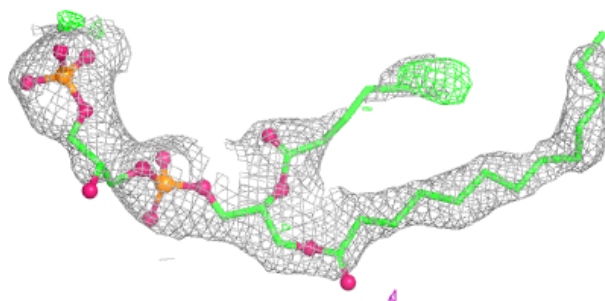
**Electron density around PEE D 2006:**

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and green (positive)

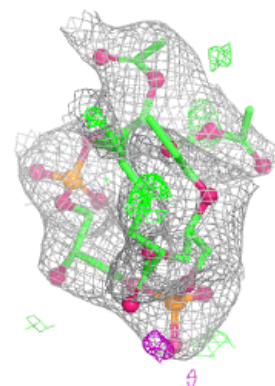
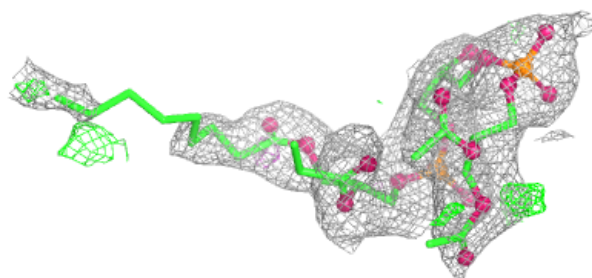
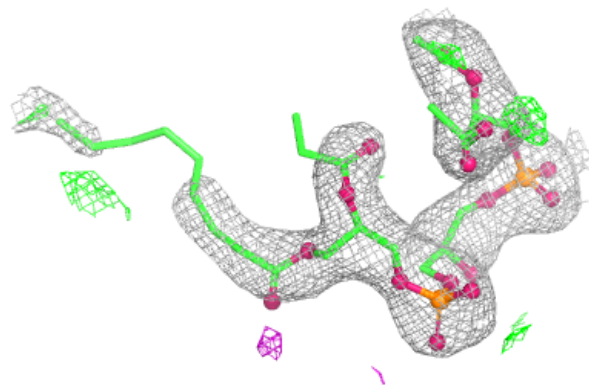


Electron density around CDL Q 3003:

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and green (positive)

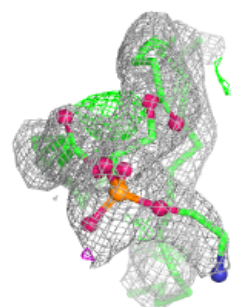
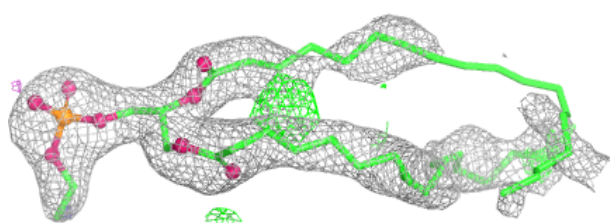
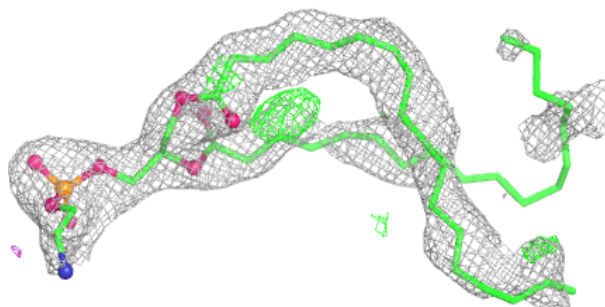
**Electron density around CDL C 2004:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

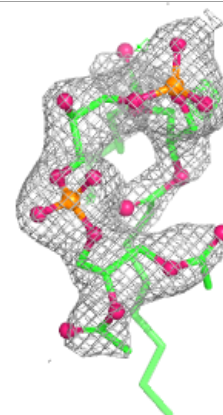
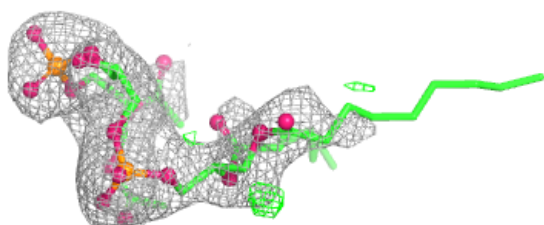
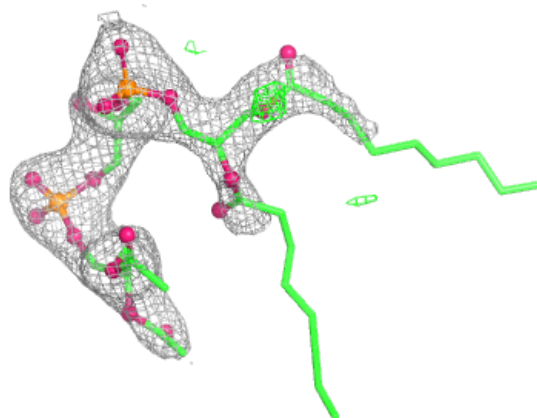


Electron density around PEE Q 3006:

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and green (positive)

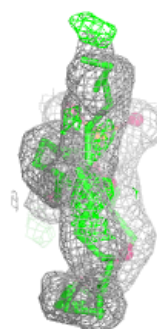
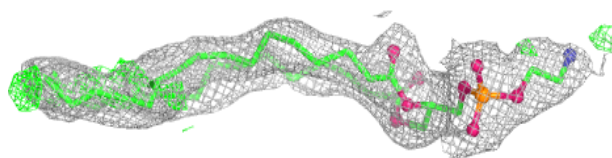
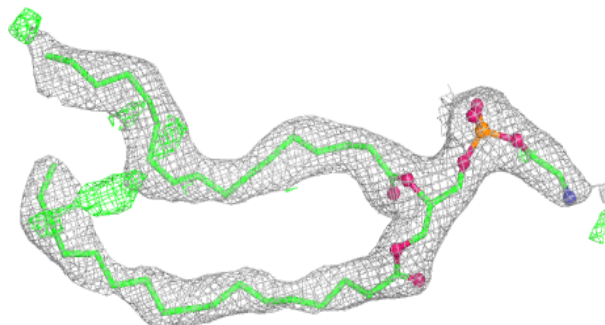
**Electron density around CDL P 3004:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

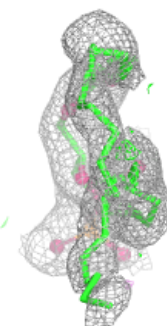
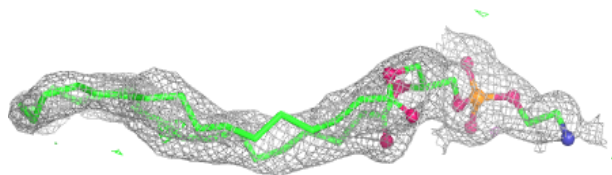
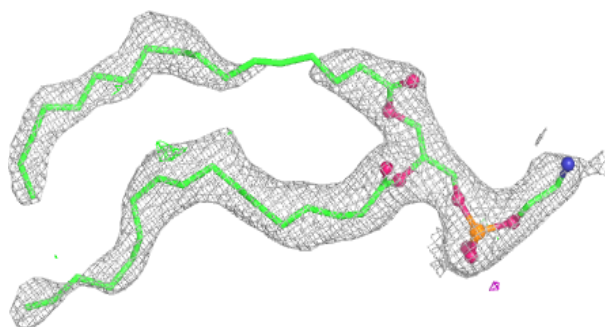


Electron density around PEE P 3007:

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and green (positive)

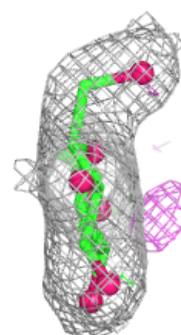
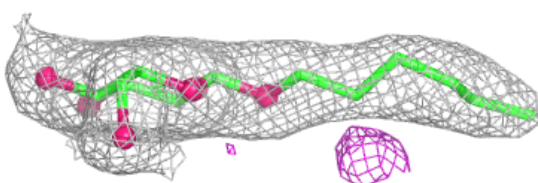
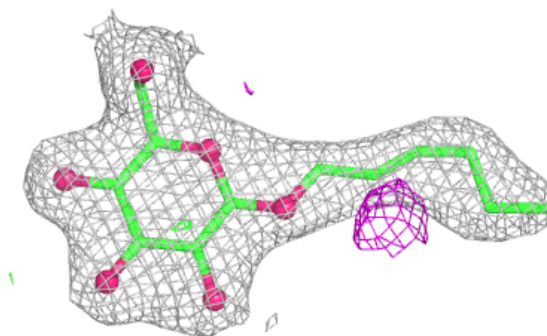
**Electron density around PEE C 2007:**

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

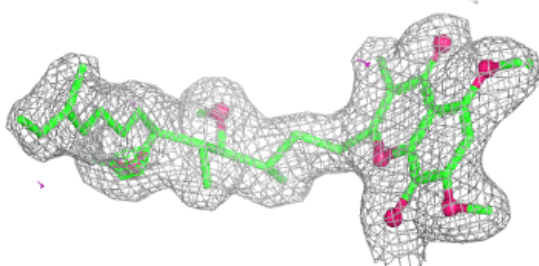
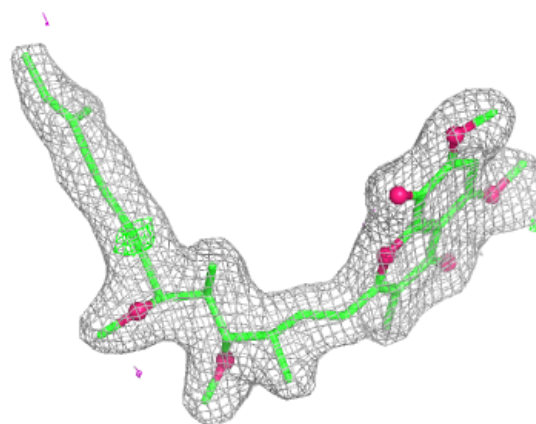


Electron density around JZR A 4004:

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

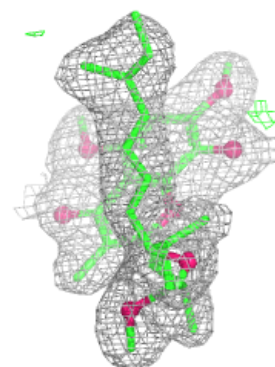
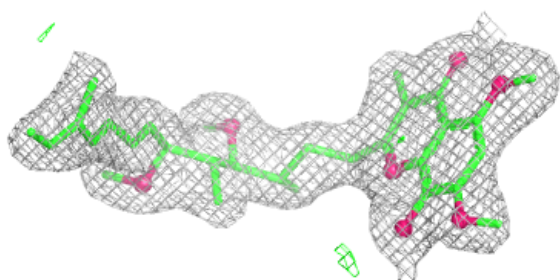
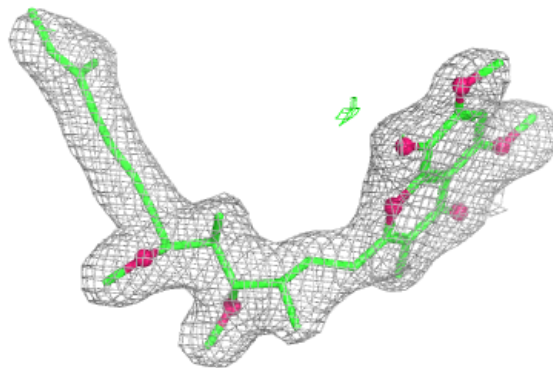
**Electron density around SMA C 2001:**

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



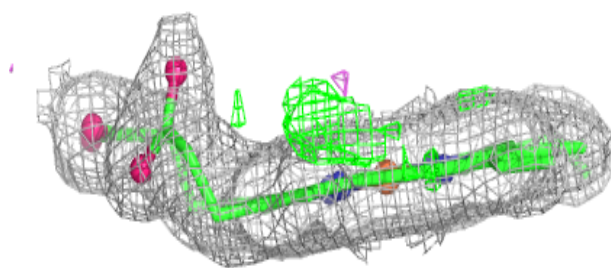
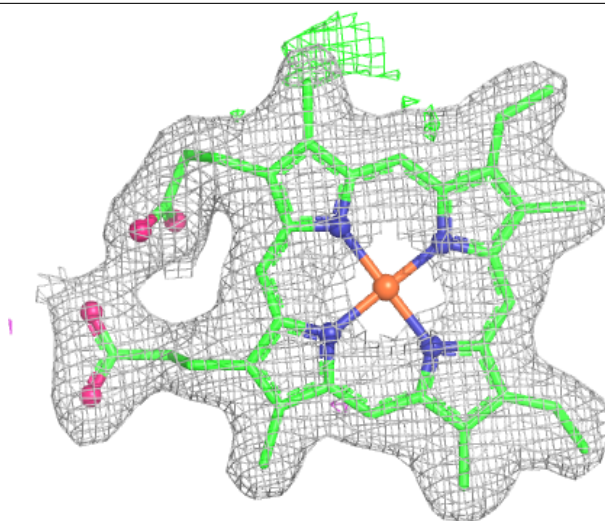
Electron density around SMA P 3001:

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



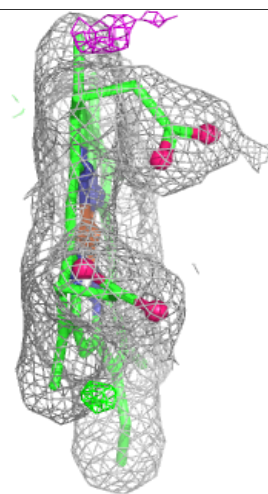
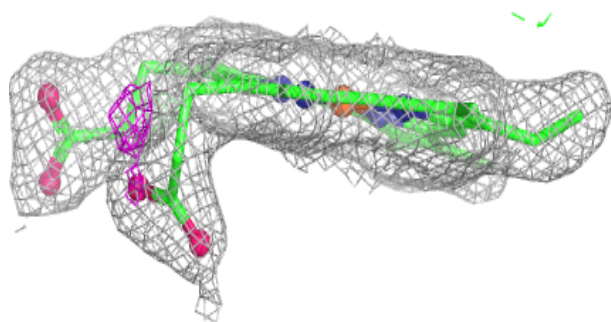
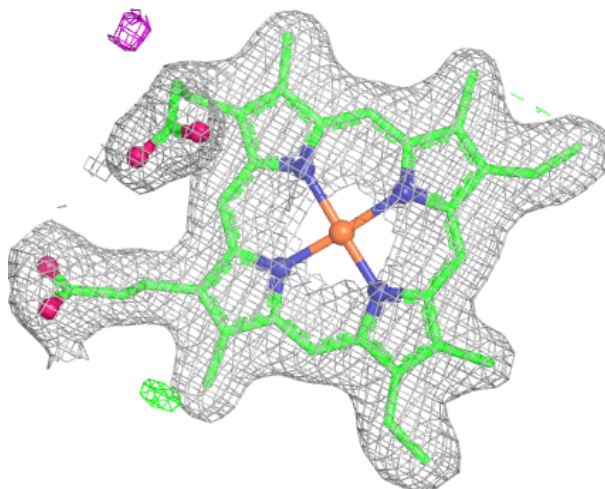
Electron density around HEM C 501:

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



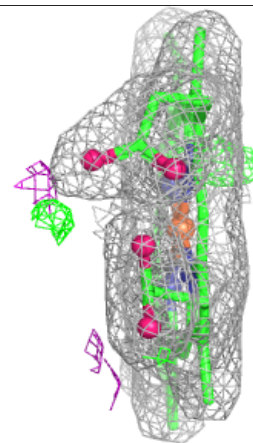
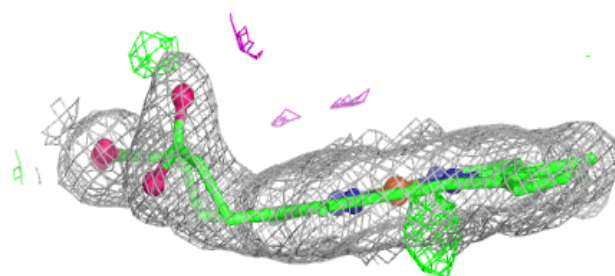
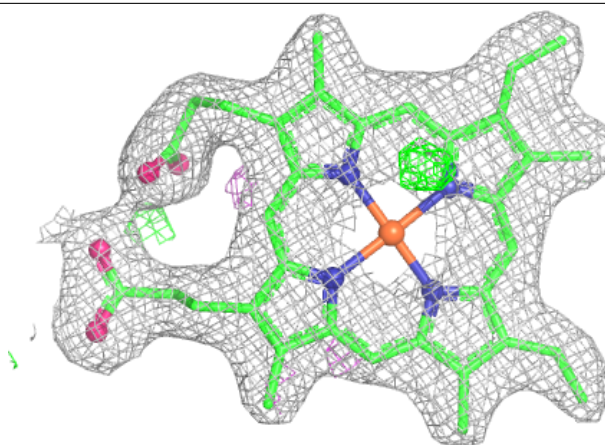
Electron density around HEM C 502:

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



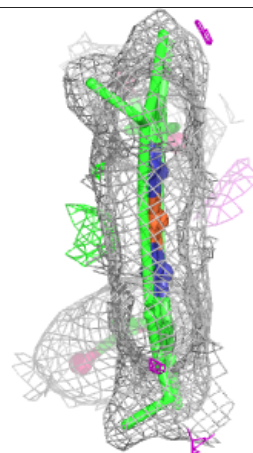
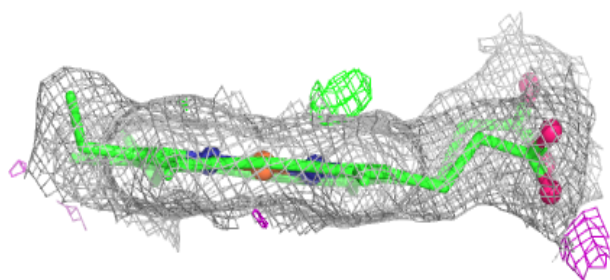
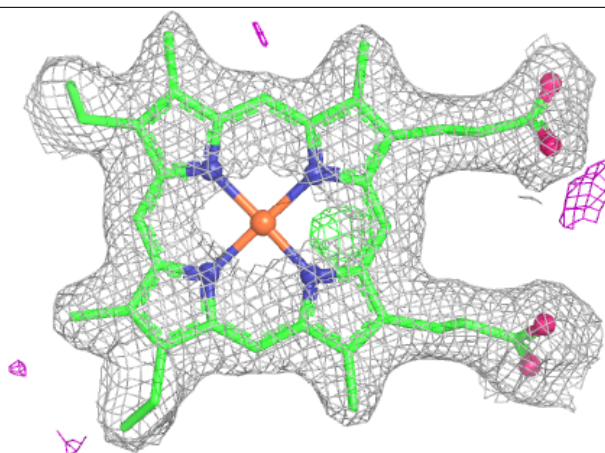
Electron density around HEM P 501:

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



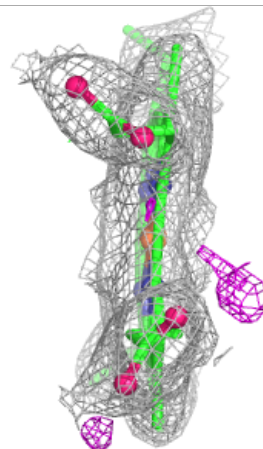
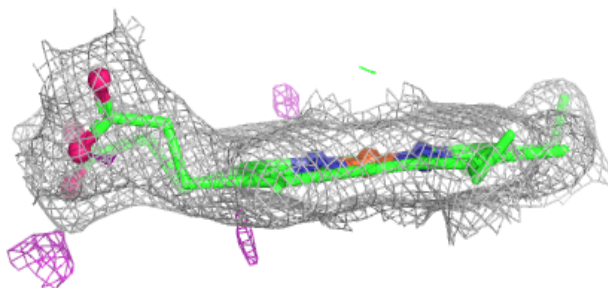
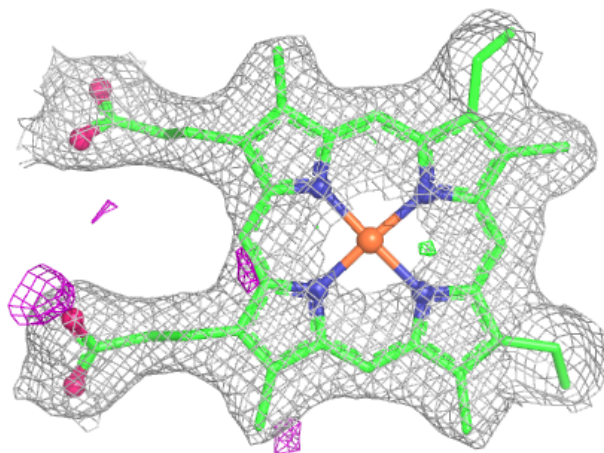
Electron density around HEC D 501:

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



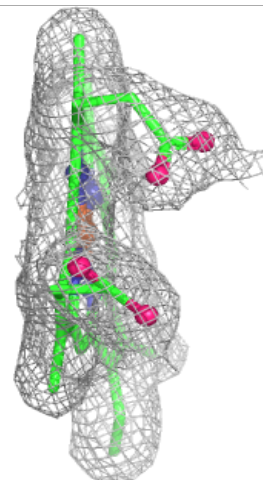
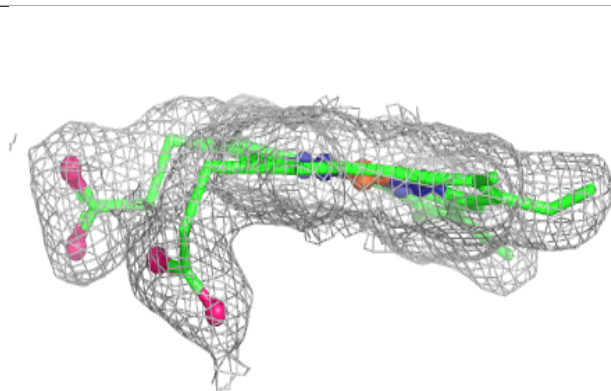
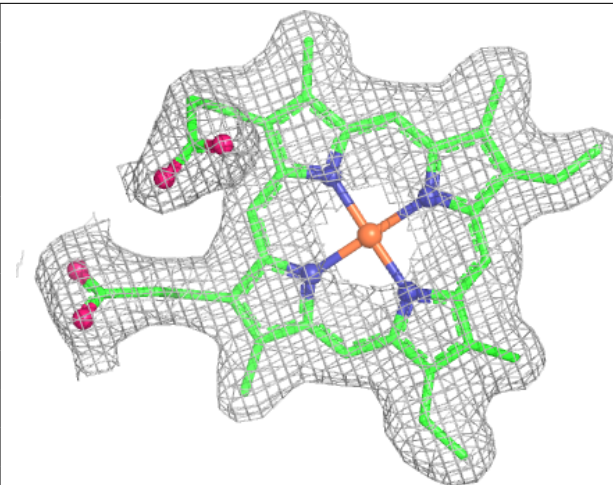
Electron density around HEC Q 501:

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



Electron density around HEM P 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.