



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2022 – 11:07 am BST

PDB ID : 7R3V
Title : Crystal structure of bovine Cytochrome bc1 in complex with inhibitor CK-2-67.
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Deposited on : 2022-02-07
Resolution : 3.20 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

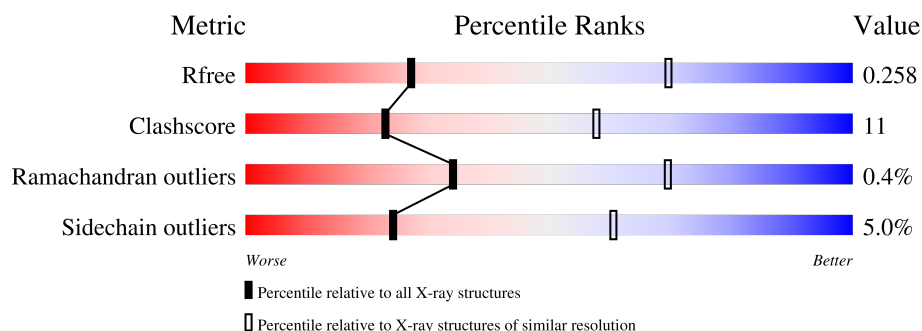
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	445	78% 21% .
2	B	418	73% 25% ..
3	C	379	76% 22% .
4	D	239	79% 20% .
5	E	196	67% 29% .
6	F	99	82% 17% .
7	G	74	74% 26%

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Mol	Chain	Length	Quality of chain
8	H	65	 68% 31%
9	I	46	 57% 28% 15%
10	J	59	 78% 22%

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
16	PEE	C	406	X	-	-	-
16	PEE	E	204	X	-	-	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 16382 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3449	2157	608	664	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLU	ASP	conflict	UNP P31800
A	227	THR	ALA	conflict	UNP P31800

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	0
			3093	1943	546	597	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3004	2012	472	501	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	239	Total	C	N	O	S	0	0	0
			1884	1205	321	343	15			

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

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

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			859	545	156	156	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			620	406	116	97	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	65	Total	C	N	O	S	0	0	0
			525	318	95	107	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			338	209	64	64	1			

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

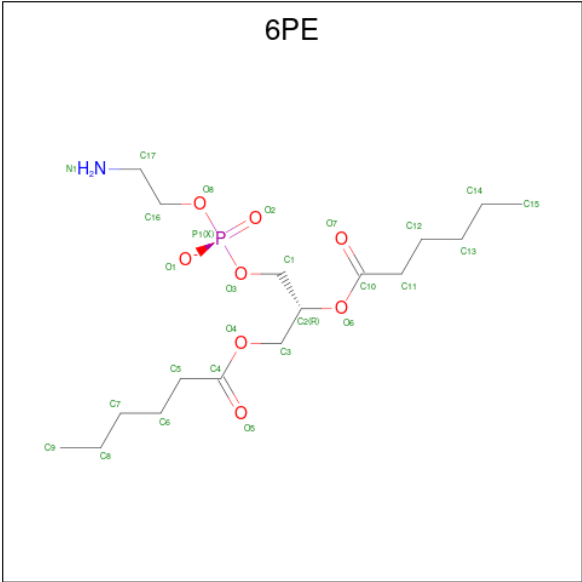
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



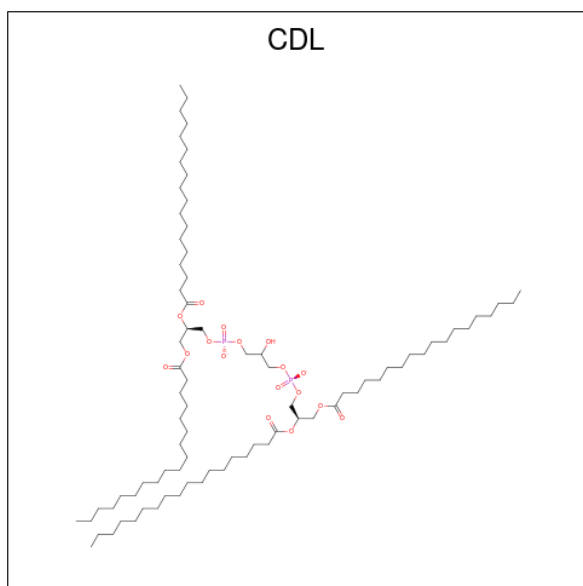
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			13	8	5		
11	C	1	Total	C	O	0	0
			13	8	5		
11	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: C₁₇H₃₃NO₈P).



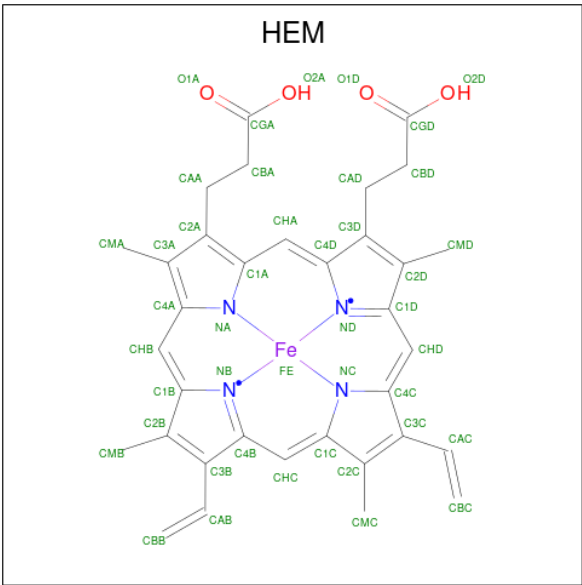
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



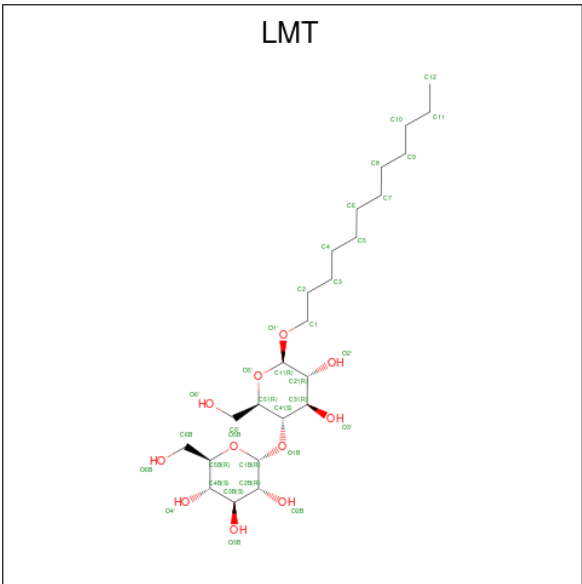
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			34	17	15	2		
13	D	1	Total	C	O	P	0	0
			54	35	17	2		
13	G	1	Total	C	O	P	0	0
			44	25	17	2		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



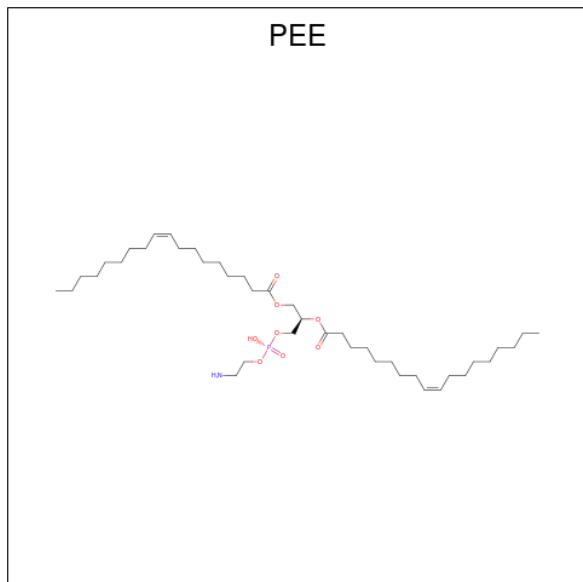
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



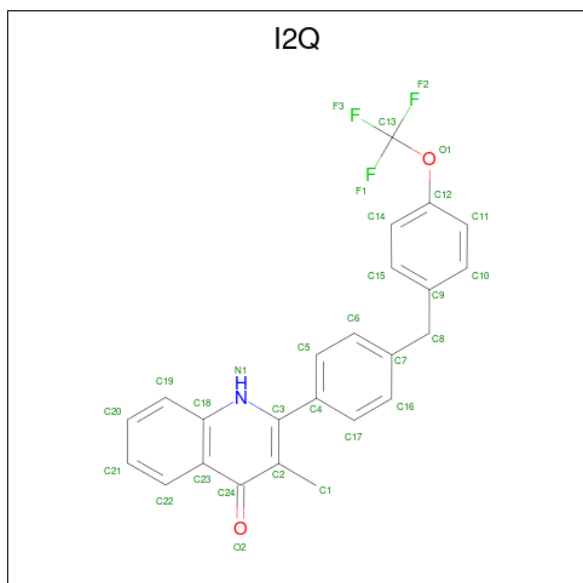
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			35	24	11		

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



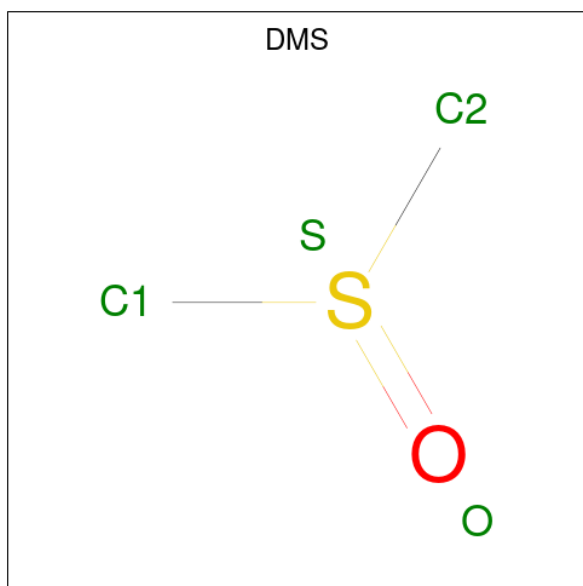
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
16	E	1	Total	C	N	O	P	0	0
			41	31	1	8	1		

- Molecule 17 is 3-methyl-2-[4-[[4-(trifluoromethoxy)phenyl]methyl]phenyl]-1H-quinolin-4-one (three-letter code: I2Q) (formula:) (labeled as "Ligand of Interest" by depositor).



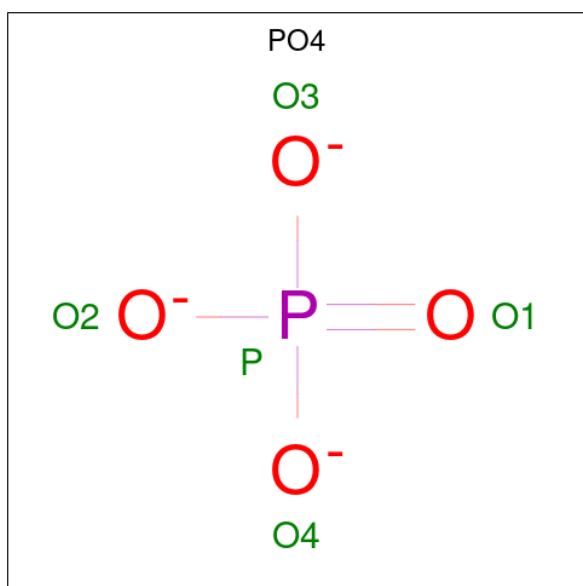
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	F	N	O	0	0
			30	24	3	1	2		

- Molecule 18 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: $\text{C}_2\text{H}_6\text{OS}$).



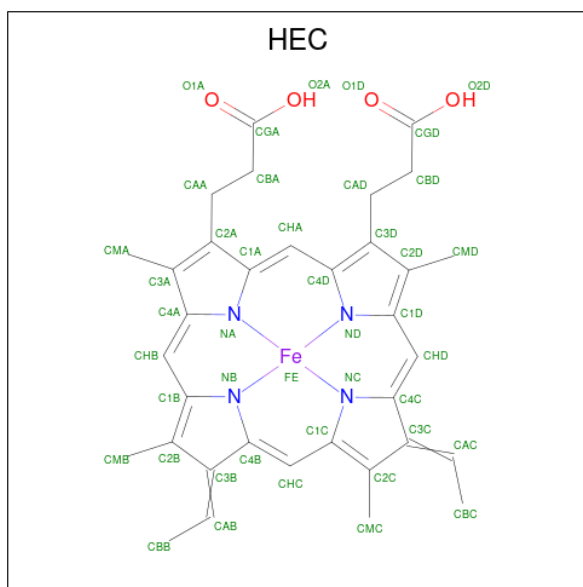
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 19 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



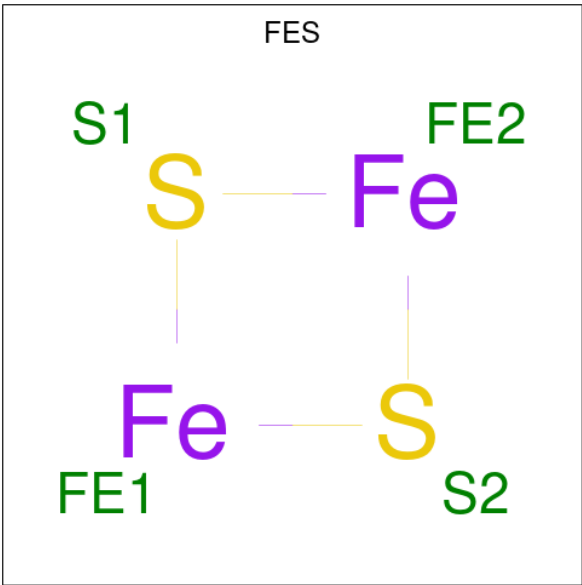
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	C	1	Total O P 5 4 1	0	0
19	C	1	Total O P 5 4 1	0	0
19	D	1	Total O P 5 4 1	0	0
19	E	1	Total O P 5 4 1	0	0
19	F	1	Total O P 5 4 1	0	0
19	F	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0
19	G	1	Total O P 5 4 1	0	0

- Molecule 20 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



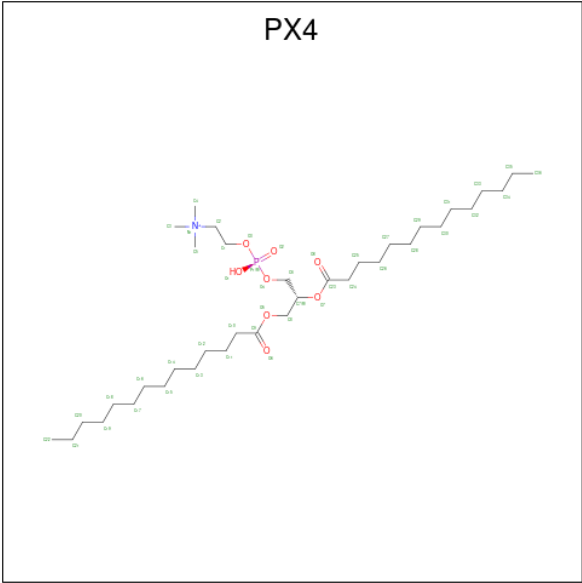
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 22 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	E	1	Total	C	N	O	P	0	0
			37	27	1	8	1		

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	10	Total 10	O 10	0	0
23	B	9	Total 9	O 9	0	0
23	C	10	Total 10	O 10	0	0
23	D	4	Total 4	O 4	0	0
23	E	4	Total 4	O 4	0	0
23	F	5	Total 5	O 5	0	0
23	G	2	Total 2	O 2	0	0
23	J	1	Total 1	O 1	0	0

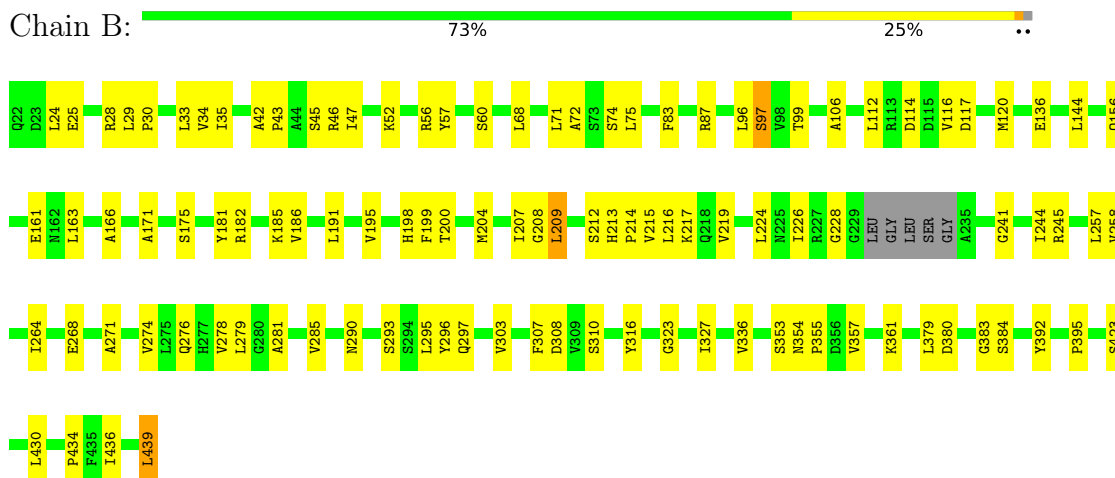
3 Residue-property plots

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. 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. 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.

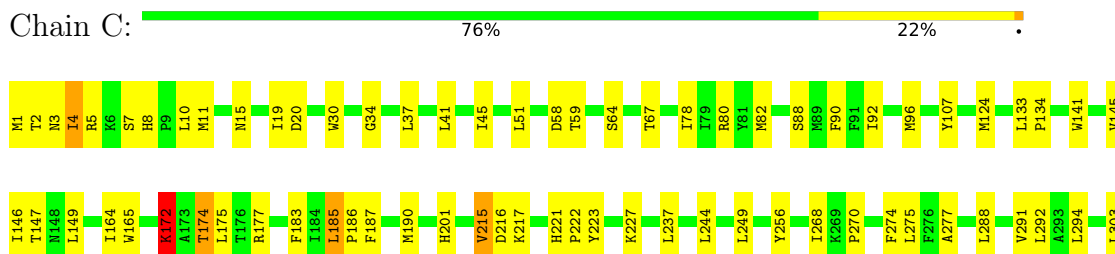
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 3: Cytochrome b





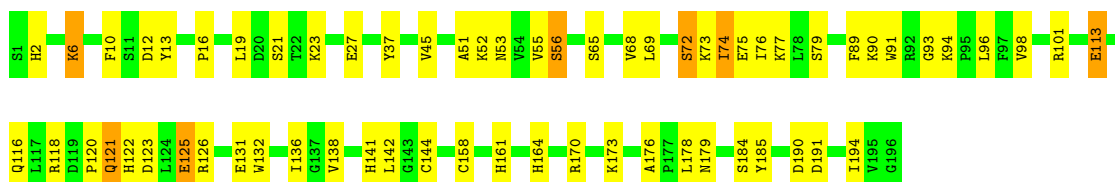
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 79% 20% .



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

Chain E: 67% 29% .



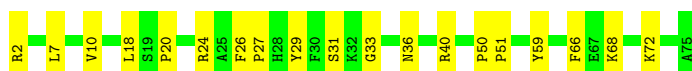
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F: 82% 17% .



- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G: 74% 26% .



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H: 68% 31% .

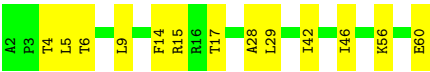
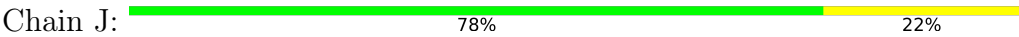


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I: 57% 28% 15% .



- Molecule 10: Cytochrome b-c1 complex subunit 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	209.59Å 209.59Å 342.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.86 – 3.20 49.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.86-3.20) 95.1 (49.81-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.256 0.207 , 0.258	Depositor DCC
R_{free} test set	3441 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	85.7	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16382	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: PX4, PG4, FES, HEM, 6PE, LMT, DMS, I2Q, PEE, CDL, HEC, PO4

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	0.43	0/3522	0.89	0/4781
2	B	0.41	0/3148	0.85	0/4270
3	C	0.39	0/3100	0.78	0/4241
4	D	0.40	0/1943	0.81	0/2642
5	E	0.42	0/1553	0.84	0/2100
6	F	0.42	0/878	0.91	0/1181
7	G	0.43	0/641	0.93	0/868
8	H	0.38	0/530	0.83	0/714
9	I	0.46	0/342	1.11	0/464
10	J	0.39	0/500	0.81	0/675
All	All	0.41	0/16157	0.85	0/21936

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3449	0	3346	81	0
2	B	3093	0	3064	75	0
3	C	3004	0	3070	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1884	0	1814	56	0
5	E	1519	0	1503	45	0
6	F	859	0	836	14	0
7	G	620	0	624	17	0
8	H	525	0	500	23	0
9	I	338	0	356	25	0
10	J	487	0	487	8	0
11	A	13	0	18	0	0
11	C	26	0	36	1	0
12	A	23	0	19	4	0
13	A	34	0	24	3	0
13	D	54	0	52	1	0
13	G	44	0	32	1	0
14	C	86	0	60	12	0
15	C	35	0	46	2	0
16	C	40	0	54	1	0
16	E	41	0	59	3	0
17	C	30	0	0	1	0
18	C	4	0	6	0	0
19	C	10	0	0	0	0
19	D	5	0	0	0	0
19	E	5	0	0	0	0
19	F	10	0	0	0	0
19	G	15	0	0	0	0
20	D	43	0	32	15	0
21	E	4	0	0	0	0
22	E	37	0	51	4	0
23	A	10	0	0	0	0
23	B	9	0	0	0	0
23	C	10	0	0	0	0
23	D	4	0	0	0	0
23	E	4	0	0	1	0
23	F	5	0	0	0	0
23	G	2	0	0	0	0
23	J	1	0	0	0	0
All	All	16382	0	16089	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (369) 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)
14:C:402:HEM:HBC2	14:C:402:HEM:HMC2	1.41	1.00
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.47	0.97
5:E:16:PRO:HA	5:E:19:LEU:HD12	1.51	0.93
1:A:86:LEU:HB3	2:B:285:VAL:HG22	1.54	0.89
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.75	0.87
1:A:8:LEU:O	1:A:11:VAL:HG23	1.75	0.85
14:C:402:HEM:HMB1	14:C:402:HEM:HBB2	1.57	0.85
4:D:40:CYS:SG	20:D:501:HEC:CHD	2.64	0.85
1:A:3:THR:HG22	1:A:6:GLN:HG3	1.58	0.85
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.60	0.83
1:A:305:GLN:NE2	9:I:42:VAL:HG12	1.95	0.81
9:I:42:VAL:O	9:I:43:LEU:HB2	1.81	0.80
8:H:16:PRO:O	8:H:20:VAL:HG23	1.82	0.80
1:A:37:VAL:HG23	1:A:199:ALA:HB2	1.64	0.79
4:D:33:TYR:HA	4:D:37:CYS:SG	2.23	0.79
5:E:37:TYR:CZ	22:E:202:PX4:H9	2.17	0.79
4:D:40:CYS:SG	20:D:501:HEC:CAC	2.72	0.78
1:A:38:GLY:HA2	1:A:113:LEU:HD13	1.67	0.77
14:C:402:HEM:HBB2	14:C:402:HEM:CMB	2.14	0.76
1:A:406:VAL:O	1:A:410:VAL:HG23	1.85	0.76
4:D:40:CYS:SG	20:D:501:HEC:C3C	2.74	0.76
1:A:46:ARG:HH12	1:A:315:ALA:HB3	1.49	0.76
4:D:40:CYS:SG	20:D:501:HEC:C4C	2.75	0.75
2:B:296:TYR:OH	9:I:52:ARG:HD3	1.85	0.75
3:C:141:TRP:O	3:C:145:VAL:HG23	1.86	0.74
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.68	0.74
1:A:158:PHE:O	1:A:164:ALA:HB2	1.87	0.74
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.18	0.73
5:E:74:ILE:HG13	5:E:91:TRP:CD1	2.23	0.73
8:H:19:THR:HG22	8:H:23:GLN:HE21	1.53	0.72
7:G:72:LYS:NZ	8:H:57:GLU:OE1	2.21	0.72
13:D:503:CDL:H511	13:D:503:CDL:H111	1.72	0.71
1:A:75:LEU:O	1:A:79:VAL:HG23	1.91	0.71
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.73	0.70
1:A:86:LEU:HD13	1:A:99:ILE:HD12	1.74	0.70
1:A:444:LEU:HA	10:J:17:THR:HG21	1.73	0.70
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.74	0.69
3:C:319:PRO:HD2	6:F:20:TYR:HE1	1.58	0.68
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.75	0.68
12:A:502:6PE:H28	13:A:503:CDL:HB31	1.76	0.68
12:A:502:6PE:H4	13:A:503:CDL:H512	1.77	0.67
4:D:138:PRO:HG2	4:D:141:VAL:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:167:GLU:HG3	8:H:13:LEU:HD22	1.77	0.66
3:C:15:ASN:HA	3:C:19:ILE:HD12	1.77	0.66
1:A:46:ARG:NH1	1:A:315:ALA:HB3	2.11	0.66
3:C:183:PHE:CE2	14:C:401:HEM:HBC1	2.30	0.66
4:D:40:CYS:SG	20:D:501:HEC:HHH	2.35	0.66
1:A:284:TYR:CZ	9:I:71:ASN:O	2.49	0.65
3:C:349:THR:OG1	15:C:403:LMT:H6E	1.97	0.65
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.37	0.65
2:B:207:ILE:HG22	2:B:379:LEU:HD12	1.78	0.65
2:B:316:TYR:OH	9:I:63:PRO:HB3	1.95	0.65
2:B:56:ARG:HA	2:B:171:ALA:O	1.97	0.64
3:C:41:LEU:O	3:C:45:ILE:HG13	1.97	0.64
2:B:290:ASN:HD21	9:I:56:ARG:HG2	1.62	0.64
1:A:223:TYR:O	1:A:223:TYR:CD1	2.51	0.64
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.80	0.63
9:I:71:ASN:OD1	9:I:71:ASN:N	2.31	0.63
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.27	0.63
2:B:274:VAL:O	2:B:278:VAL:HG23	1.99	0.63
2:B:200:THR:O	2:B:204:MET:HG3	1.99	0.62
5:E:69:LEU:O	5:E:72:SER:HB3	2.00	0.62
1:A:403:ASP:OD1	1:A:406:VAL:HG23	2.00	0.62
5:E:37:TYR:CE1	22:E:202:PX4:H9	2.35	0.61
1:A:106:LEU:O	1:A:109:ALA:HB3	2.01	0.61
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.36	0.61
1:A:152:TYR:HB3	1:A:241:ILE:HG21	1.83	0.61
3:C:319:PRO:HD2	6:F:20:TYR:CE1	2.35	0.61
1:A:286:GLY:HA3	1:A:290:LEU:HD21	1.82	0.61
2:B:308:ASP:OD1	9:I:56:ARG:HD3	2.00	0.60
4:D:83:ARG:HB2	4:D:84:PRO:HD2	1.83	0.60
5:E:121:GLN:HA	5:E:125:GLU:CD	2.22	0.60
5:E:74:ILE:HG13	5:E:91:TRP:HD1	1.66	0.60
9:I:62:ARG:HB2	9:I:78:TYR:HD1	1.67	0.60
4:D:138:PRO:HD3	4:D:149:PHE:CZ	2.37	0.60
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.37	0.60
2:B:380:ASP:O	2:B:384:SER:CB	2.50	0.59
1:A:3:THR:HG22	1:A:6:GLN:CG	2.30	0.59
2:B:268:GLU:O	2:B:271:ALA:HB3	2.02	0.59
1:A:38:GLY:HA2	1:A:113:LEU:CD1	2.33	0.59
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.38	0.58
1:A:70:ARG:HG3	1:A:70:ARG:HH11	1.67	0.58
4:D:166:ASN:HB3	8:H:13:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.33	0.58
2:B:207:ILE:HG13	2:B:383:GLY:CA	2.34	0.58
3:C:107:TYR:HH	3:C:308:HIS:HD1	1.52	0.58
3:C:237:LEU:HD13	4:D:212:MET:HG3	1.85	0.58
2:B:310:SER:HB2	9:I:56:ARG:HH12	1.68	0.58
3:C:145:VAL:HG21	3:C:268:ILE:CD1	2.34	0.57
1:A:267:ASN:O	1:A:271:GLN:HG2	2.05	0.57
3:C:215:VAL:HG11	6:F:59:VAL:HG13	1.87	0.57
2:B:215:VAL:O	2:B:219:VAL:HG23	2.05	0.57
1:A:79:VAL:HG12	1:A:84:ALA:HB3	1.86	0.57
4:D:40:CYS:CB	20:D:501:HEC:C3C	2.83	0.57
1:A:235:ARG:HB2	5:E:23:LYS:O	2.05	0.56
2:B:380:ASP:O	2:B:384:SER:HB2	2.05	0.56
10:J:42:ILE:O	10:J:46:ILE:HD12	2.05	0.56
5:E:52:LYS:O	5:E:56:SER:HB2	2.05	0.56
16:E:204:PEE:H48	16:E:204:PEE:H13	1.88	0.56
1:A:65:LYS:HD2	1:A:126:GLN:NE2	2.21	0.55
3:C:288:LEU:O	3:C:292:LEU:HG	2.05	0.55
4:D:233:ARG:HH21	6:F:67:ASP:HB2	1.71	0.55
7:G:24:ARG:O	7:G:27:PRO:HD3	2.06	0.55
4:D:234:LYS:HZ3	5:E:13:TYR:HE2	1.55	0.55
4:D:166:ASN:HB3	8:H:13:LEU:CD2	2.37	0.55
1:A:412:SER:HB3	10:J:15:ARG:HH22	1.71	0.55
3:C:223:TYR:HB3	4:D:227:TRP:CZ2	2.42	0.55
1:A:436:ARG:NH2	3:C:20:ASP:OD1	2.35	0.55
2:B:25:GLU:HB2	2:B:213:HIS:HD1	1.72	0.55
8:H:50:THR:HG23	8:H:50:THR:O	2.08	0.54
3:C:92:ILE:O	3:C:96:MET:HG2	2.08	0.54
14:C:401:HEM:HBC2	14:C:401:HEM:HMC1	1.89	0.54
4:D:43:MET:CE	4:D:91:PHE:CD2	2.91	0.54
1:A:286:GLY:HA3	1:A:290:LEU:CD2	2.38	0.54
3:C:337:TRP:CH2	7:G:59:TYR:HA	2.43	0.54
1:A:106:LEU:O	1:A:110:VAL:HG23	2.08	0.54
1:A:70:ARG:HG3	1:A:70:ARG:NH1	2.22	0.54
4:D:165:TYR:CE1	4:D:168:VAL:HB	2.43	0.54
2:B:303:VAL:HG21	2:B:336:VAL:HG22	1.90	0.53
14:C:402:HEM:HBC2	14:C:402:HEM:CMC	2.22	0.53
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.90	0.53
1:A:249:PRO:HG3	9:I:45:LEU:HG	1.91	0.53
3:C:149:LEU:HB3	3:C:291:VAL:CG2	2.38	0.53
3:C:5:ARG:HE	3:C:15:ASN:ND2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:O	1:A:245:GLU:HG3	2.09	0.53
3:C:379:TRP:CE3	6:F:33:ARG:NH1	2.77	0.53
8:H:44:VAL:HG23	8:H:50:THR:HG23	1.91	0.53
1:A:222:THR:HG22	1:A:222:THR:O	2.09	0.53
3:C:183:PHE:CZ	14:C:401:HEM:HBC1	2.44	0.52
4:D:164:ILE:CD1	4:D:183:ALA:HB2	2.40	0.52
3:C:256:TYR:CE1	4:D:118:ARG:HD3	2.45	0.52
4:D:116:ILE:HG12	20:D:501:HEC:HMA3	1.91	0.52
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.40	0.52
2:B:24:LEU:HD23	2:B:392:TYR:CD2	2.44	0.52
2:B:209:LEU:N	2:B:209:LEU:HD22	2.25	0.52
3:C:58:ASP:HA	3:C:172:LYS:HE2	1.91	0.52
3:C:346:PRO:HD2	7:G:66:PHE:HB2	1.92	0.52
1:A:223:TYR:HD1	1:A:228:VAL:HG22	1.75	0.52
3:C:324:LEU:O	3:C:327:ALA:HB3	2.09	0.51
2:B:71:LEU:CD2	9:I:68:VAL:HG21	2.40	0.51
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.91	0.51
3:C:133:LEU:HA	3:C:175:LEU:HD11	1.92	0.51
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.30	0.51
1:A:4:TYR:CB	2:B:114:ASP:OD2	2.55	0.51
5:E:96:LEU:HD12	5:E:136:ILE:HD13	1.92	0.51
2:B:96:LEU:HD12	2:B:97:SER:N	2.26	0.50
2:B:156:GLN:NE2	9:I:58:GLN:OE1	2.42	0.50
4:D:40:CYS:SG	20:D:501:HEC:HAC	2.49	0.50
5:E:10:PHE:CG	7:G:18:LEU:HD13	2.46	0.50
2:B:257:LEU:HD22	2:B:439:LEU:HD21	1.93	0.50
3:C:361:LEU:O	3:C:366:MET:HG3	2.10	0.50
4:D:14:HIS:ND1	4:D:21:LEU:HD23	2.26	0.50
4:D:47:ALA:HA	4:D:90:TYR:HA	1.94	0.50
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.92	0.50
3:C:67:THR:HG21	4:D:115:TYR:HE2	1.76	0.50
3:C:78:ILE:O	3:C:82:MET:HB2	2.11	0.50
3:C:124:MET:HG2	3:C:274:PHE:CE1	2.46	0.50
6:F:72:GLN:OE1	6:F:72:GLN:HA	2.11	0.50
1:A:79:VAL:CG1	1:A:84:ALA:HB3	2.41	0.50
14:C:402:HEM:HMB1	14:C:402:HEM:CBB	2.33	0.50
14:C:401:HEM:CMB	14:C:401:HEM:HBB2	2.41	0.50
1:A:92:ARG:NH1	1:A:154:HIS:CE1	2.79	0.50
3:C:4:ILE:HA	3:C:7:SER:HB3	1.93	0.50
3:C:30:TRP:NE1	16:C:406:PEE:H14	2.27	0.50
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:ILE:HD12	11:C:405:PG4:H11	1.93	0.50
22:E:202:PX4:H11	10:J:14:PHE:O	2.12	0.50
2:B:68:LEU:HD13	2:B:144:LEU:HD11	1.94	0.50
4:D:178:THR:HG21	8:H:16:PRO:HD3	1.94	0.50
5:E:94:LYS:HD2	5:E:138:VAL:HG21	1.93	0.50
1:A:15:GLN:O	1:A:26:ALA:HA	2.11	0.49
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.40	0.49
4:D:138:PRO:HG3	8:H:55:THR:HG22	1.94	0.49
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.46	0.49
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.94	0.49
1:A:355:LEU:HD12	1:A:355:LEU:O	2.12	0.49
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.95	0.49
4:D:167:GLU:CG	8:H:13:LEU:HD22	2.39	0.49
2:B:46:ARG:CG	2:B:379:LEU:HD22	2.35	0.49
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.48	0.49
6:F:94:LEU:HD12	6:F:94:LEU:O	2.11	0.49
6:F:13:LEU:HA	6:F:16:ILE:HD12	1.94	0.49
3:C:59:THR:HG23	3:C:172:LYS:HD2	1.95	0.49
4:D:43:MET:CE	4:D:91:PHE:CE2	2.95	0.49
4:D:138:PRO:HG3	8:H:55:THR:HA	1.95	0.49
5:E:136:ILE:HG22	5:E:138:VAL:HG23	1.95	0.49
4:D:165:TYR:CZ	4:D:168:VAL:HG23	2.48	0.48
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.94	0.48
3:C:145:VAL:HG21	3:C:268:ILE:HD12	1.96	0.48
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.95	0.48
4:D:134:TYR:CE2	4:D:162:PRO:HA	2.48	0.48
1:A:355:LEU:HA	1:A:358:LYS:HD3	1.96	0.48
8:H:40:CYS:CB	8:H:43:ARG:NH2	2.76	0.48
1:A:244:ARG:CZ	1:A:429:GLU:HB2	2.44	0.48
1:A:362:ARG:HB3	2:B:112:LEU:HD11	1.94	0.48
5:E:125:GLU:HG3	5:E:125:GLU:O	2.12	0.48
7:G:26:PHE:HB3	7:G:29:TYR:HB2	1.96	0.48
1:A:79:VAL:HG13	1:A:99:ILE:HD11	1.95	0.48
2:B:200:THR:HB	2:B:228:GLY:HA2	1.96	0.48
3:C:51:LEU:HD11	3:C:80:ARG:HA	1.95	0.48
1:A:24:ARG:HD2	1:A:383:LEU:HD12	1.96	0.47
15:C:403:LMT:O6B	15:C:403:LMT:O4'	2.27	0.47
1:A:139:GLN:NE2	9:I:50:LEU:HD22	2.29	0.47
2:B:213:HIS:N	2:B:214:PRO:HD2	2.29	0.47
5:E:51:ALA:O	5:E:55:VAL:HG23	2.14	0.47
5:E:74:ILE:HG22	5:E:76:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:40:ARG:NH2	13:G:101:CDL:OA4	2.42	0.47
2:B:28:ARG:HG3	2:B:34:VAL:HG22	1.96	0.47
2:B:241:GLY:HA2	2:B:423:SER:OG	2.13	0.47
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.96	0.47
2:B:212:SER:OG	2:B:215:VAL:HG22	2.13	0.47
3:C:187:PHE:O	3:C:190:MET:HB3	2.13	0.47
8:H:44:VAL:HG21	8:H:52:GLU:O	2.14	0.47
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.95	0.47
6:F:57:ASP:HB3	6:F:61:ARG:NH1	2.29	0.47
3:C:37:LEU:HD13	14:C:402:HEM:C3B	2.50	0.47
5:E:121:GLN:O	5:E:126:ARG:HD2	2.14	0.47
8:H:48:SER:O	8:H:49:GLN:HB2	2.14	0.47
10:J:56:LYS:HE3	10:J:60:GLU:OE1	2.14	0.47
5:E:121:GLN:HA	5:E:125:GLU:OE1	2.15	0.47
1:A:288:ALA:HB2	1:A:300:THR:CG2	2.45	0.47
3:C:249:LEU:HD12	3:C:249:LEU:O	2.15	0.47
3:C:270:PRO:HD2	3:C:275:LEU:HD23	1.97	0.47
1:A:246:ASP:HB2	7:G:10:VAL:O	2.13	0.47
2:B:353:SER:OG	2:B:355:PRO:HG2	2.15	0.47
6:F:57:ASP:HB3	6:F:61:ARG:HH12	1.80	0.46
2:B:209:LEU:N	2:B:209:LEU:CD2	2.79	0.46
5:E:53:ASN:OD1	16:E:204:PEE:H10	2.15	0.46
1:A:46:ARG:NH1	1:A:315:ALA:CB	2.78	0.46
2:B:57:TYR:HB3	2:B:198:HIS:NE2	2.30	0.46
3:C:133:LEU:N	3:C:134:PRO:CD	2.78	0.46
9:I:49:VAL:HG11	9:I:55:LEU:HD13	1.97	0.46
3:C:244:LEU:HD12	4:D:208:MET:HE2	1.96	0.46
5:E:76:ILE:HG23	5:E:89:PHE:CZ	2.51	0.46
2:B:290:ASN:ND2	9:I:56:ARG:HG2	2.29	0.46
2:B:354:ASN:N	2:B:355:PRO:HD2	2.30	0.46
3:C:8:HIS:CE1	3:C:10:LEU:HB2	2.51	0.46
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.98	0.46
4:D:97:ASN:HB2	4:D:98:PRO:CD	2.46	0.46
5:E:94:LYS:HA	5:E:94:LYS:HD3	1.72	0.46
8:H:44:VAL:HG23	8:H:50:THR:CG2	2.45	0.46
5:E:74:ILE:HD11	5:E:90:LYS:O	2.16	0.45
6:F:51:PRO:HG2	6:F:54:LEU:HB2	1.98	0.45
4:D:216:LEU:N	4:D:217:PRO:HD2	2.31	0.45
20:D:501:HEC:CBB	20:D:501:HEC:HMB1	2.47	0.45
7:G:36:ASN:O	7:G:40:ARG:HG3	2.16	0.45
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:LYS:HD2	3:C:172:LYS:HA	1.44	0.45
2:B:33:LEU:HD11	2:B:224:LEU:HD23	1.99	0.45
2:B:380:ASP:O	2:B:384:SER:HB3	2.16	0.45
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.98	0.45
2:B:207:ILE:HG13	2:B:383:GLY:HA2	1.98	0.45
4:D:40:CYS:HB2	20:D:501:HEC:CAC	2.46	0.45
16:E:204:PEE:O4	16:E:204:PEE:H3	2.17	0.45
1:A:108:LYS:HB2	1:A:108:LYS:HE3	1.75	0.45
4:D:138:PRO:O	4:D:141:VAL:HB	2.17	0.44
2:B:72:ALA:O	2:B:75:LEU:HB2	2.17	0.44
2:B:195:VAL:O	2:B:199:PHE:HB2	2.17	0.44
3:C:8:HIS:HB3	3:C:11:MET:HB2	2.00	0.44
4:D:108:ALA:CB	20:D:501:HEC:HMD1	2.47	0.44
5:E:77:LYS:HG3	5:E:191:ASP:OD1	2.16	0.44
5:E:122:HIS:O	5:E:125:GLU:HG2	2.17	0.44
1:A:331:ILE:HG21	1:A:431:LEU:HB2	2.00	0.44
2:B:161:GLU:OE1	2:B:175:SER:HA	2.17	0.44
2:B:208:GLY:C	2:B:209:LEU:HD22	2.37	0.44
3:C:256:TYR:CZ	4:D:118:ARG:HD3	2.53	0.44
3:C:328:LEU:O	3:C:328:LEU:HD12	2.17	0.44
1:A:3:THR:CG2	1:A:6:GLN:HG3	2.38	0.44
4:D:105:ASN:ND2	20:D:501:HEC:HAC	2.31	0.44
5:E:185:TYR:HE2	23:E:302:HOH:O	2.01	0.44
2:B:357:VAL:O	2:B:361:LYS:HG3	2.17	0.44
2:B:392:TYR:OH	2:B:395:PRO:HD3	2.17	0.44
5:E:94:LYS:HD2	5:E:138:VAL:CG2	2.47	0.44
1:A:301:ASN:O	1:A:302:LYS:C	2.54	0.44
1:A:362:ARG:HG3	1:A:399:ILE:HG21	1.99	0.44
3:C:34:GLY:HA3	14:C:402:HEM:C3A	2.52	0.44
1:A:439:SER:O	12:A:502:6PE:H30	2.18	0.44
2:B:436:ILE:O	2:B:439:LEU:HB2	2.18	0.44
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.53	0.44
7:G:29:TYR:O	7:G:33:GLY:HA3	2.18	0.44
5:E:141:HIS:HB2	5:E:176:ALA:HA	1.99	0.43
2:B:68:LEU:HD22	2:B:186:VAL:HB	1.99	0.43
3:C:373:GLU:HG2	6:F:20:TYR:CE1	2.53	0.43
5:E:113:GLU:OE1	5:E:116:GLN:HG2	2.18	0.43
8:H:29:LYS:HD2	8:H:29:LYS:HA	1.84	0.43
9:I:62:ARG:HB2	9:I:78:TYR:CD1	2.49	0.43
10:J:9:LEU:HD13	10:J:9:LEU:HA	1.92	0.43
2:B:213:HIS:N	2:B:214:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:304:ILE:HB	3:C:305:PRO:HD3	2.00	0.43
20:D:501:HEC:CBC	20:D:501:HEC:HMC1	2.49	0.43
1:A:46:ARG:HH12	1:A:315:ALA:CB	2.27	0.43
9:I:42:VAL:O	9:I:43:LEU:CB	2.55	0.43
2:B:45:SER:CB	2:B:116:VAL:CG1	2.97	0.43
3:C:341:GLN:HB3	3:C:347:TYR:CD2	2.52	0.43
4:D:47:ALA:HB2	4:D:90:TYR:CD1	2.53	0.43
2:B:45:SER:HB2	2:B:116:VAL:CG1	2.49	0.43
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.99	0.43
14:C:401:HEM:HBC2	14:C:401:HEM:CMC	2.49	0.43
7:G:72:LYS:HZ1	8:H:57:GLU:CD	2.19	0.43
1:A:284:TYR:CE1	9:I:71:ASN:O	2.72	0.42
2:B:181:TYR:CE2	2:B:182:ARG:HG2	2.54	0.42
8:H:74:PHE:HA	8:H:77:LEU:HD12	2.01	0.42
1:A:37:VAL:CG2	1:A:199:ALA:HB2	2.42	0.42
5:E:96:LEU:CD1	5:E:136:ILE:HD13	2.49	0.42
3:C:310:SER:OG	3:C:318:ARG:HD2	2.19	0.42
3:C:324:LEU:HD23	3:C:366:MET:HA	2.02	0.42
4:D:138:PRO:HG2	4:D:141:VAL:CG2	2.46	0.42
1:A:196:VAL:HG21	1:A:383:LEU:HB3	2.01	0.42
2:B:75:LEU:HD23	2:B:75:LEU:HA	1.85	0.42
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.51	0.42
6:F:54:LEU:HD23	6:F:54:LEU:HA	1.72	0.42
5:E:10:PHE:CD1	7:G:18:LEU:HD13	2.54	0.42
8:H:40:CYS:HB3	8:H:43:ARG:NH2	2.33	0.42
2:B:307:PHE:CD1	2:B:308:ASP:N	2.88	0.42
5:E:75:GLU:HG2	5:E:194:ILE:HG12	2.02	0.42
1:A:226:GLU:CD	1:A:226:GLU:H	2.22	0.42
2:B:257:LEU:O	2:B:323:GLY:HA3	2.19	0.42
3:C:67:THR:CG2	4:D:115:TYR:HE2	2.33	0.42
3:C:201:HIS:NE2	17:C:407:I2Q:O2	2.46	0.42
1:A:39:VAL:CG1	1:A:195:MET:HE2	2.50	0.42
1:A:286:GLY:HA3	1:A:290:LEU:CG	2.50	0.42
3:C:58:ASP:HA	3:C:172:LYS:CE	2.50	0.42
4:D:105:ASN:O	4:D:106:ASN:HB2	2.20	0.42
1:A:19:LEU:HD22	1:A:213:GLN:HG2	2.01	0.41
2:B:279:LEU:HD22	2:B:295:LEU:HG	2.02	0.41
3:C:174:THR:O	3:C:177:ARG:HG2	2.20	0.41
5:E:101:ARG:HH22	5:E:123:ASP:CG	2.23	0.41
2:B:68:LEU:HD23	2:B:191:LEU:HD11	2.01	0.41
3:C:146:ILE:O	3:C:147:THR:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:LYS:HB3	5:E:6:LYS:HE2	1.84	0.41
2:B:216:LEU:HD23	2:B:216:LEU:HA	1.78	0.41
4:D:37:CYS:O	4:D:39:SER:N	2.53	0.41
2:B:99:THR:O	2:B:106:ALA:N	2.51	0.41
2:B:207:ILE:CG2	2:B:379:LEU:HD12	2.48	0.41
2:B:293:SER:O	2:B:297:GLN:HG2	2.21	0.41
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.56	0.41
13:A:503:CDL:OB3	3:C:5:ARG:NH1	2.54	0.41
2:B:42:ALA:HB1	2:B:43:PRO:CD	2.51	0.41
2:B:163:LEU:HD11	2:B:258:VAL:HG22	2.02	0.41
4:D:40:CYS:CB	20:D:501:HEC:CAC	2.99	0.41
4:D:43:MET:HE1	4:D:91:PHE:CD2	2.56	0.41
1:A:244:ARG:HH11	1:A:244:ARG:HD3	1.72	0.41
1:A:294:LEU:HG	1:A:307:PHE:CE2	2.56	0.41
8:H:50:THR:O	8:H:50:THR:CG2	2.68	0.41
1:A:59:VAL:O	1:A:62:LEU:N	2.53	0.41
1:A:248:LEU:HB3	1:A:249:PRO:HD2	2.03	0.41
1:A:294:LEU:HG	1:A:307:PHE:CZ	2.56	0.41
4:D:105:ASN:HD21	20:D:501:HEC:HAC	1.86	0.41
8:H:53:ASP:OD1	8:H:55:THR:HG23	2.20	0.41
1:A:46:ARG:HG2	1:A:231:LEU:HD22	2.03	0.41
1:A:210:ASP:O	1:A:213:GLN:HB2	2.20	0.41
1:A:284:TYR:CE2	9:I:71:ASN:O	2.73	0.41
3:C:3:ASN:OD1	3:C:5:ARG:NH1	2.54	0.41
3:C:185:LEU:N	3:C:186:PRO:CD	2.84	0.41
4:D:54:VAL:HG11	4:D:192:TRP:CE2	2.56	0.41
5:E:190:ASP:OD1	5:E:190:ASP:N	2.54	0.41
10:J:4:THR:OG1	10:J:5:LEU:N	2.53	0.41
1:A:79:VAL:HG11	1:A:86:LEU:HB2	2.02	0.41
1:A:286:GLY:HA3	1:A:290:LEU:HG	2.02	0.41
3:C:221:HIS:HA	3:C:222:PRO:HA	1.78	0.41
3:C:147:THR:HG21	3:C:165:TRP:NE1	2.36	0.40
9:I:70:LEU:HD22	9:I:70:LEU:HA	1.90	0.40
1:A:223:TYR:CD1	1:A:228:VAL:HG22	2.54	0.40
3:C:145:VAL:HG21	3:C:268:ILE:HD11	2.02	0.40
5:E:76:ILE:HD13	5:E:98:VAL:HG21	2.04	0.40
1:A:152:TYR:HB3	1:A:241:ILE:CG2	2.49	0.40
12:A:502:6PE:H18	22:E:202:PX4:H15	2.02	0.40
5:E:65:SER:OG	5:E:68:VAL:HG23	2.20	0.40
5:E:121:GLN:HB2	5:E:179:ASN:ND2	2.37	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	443/445 (100%)	417 (94%)	25 (6%)	1 (0%)	47	79
2	B	409/418 (98%)	395 (97%)	14 (3%)	0	100	100
3	C	377/379 (100%)	354 (94%)	22 (6%)	1 (0%)	41	74
4	D	237/239 (99%)	224 (94%)	10 (4%)	3 (1%)	12	47
5	E	194/196 (99%)	187 (96%)	5 (3%)	2 (1%)	15	54
6	F	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
7	G	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
8	H	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
9	I	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
10	J	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
All	All	1993/2020 (99%)	1893 (95%)	93 (5%)	7 (0%)	34	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	THR
5	E	120	PRO
3	C	172	LYS
5	E	121	GLN
4	D	162	PRO
4	D	198	HIS
4	D	144	ARG

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	369/370 (100%)	356 (96%)	13 (4%)	36	69
2	B	322/327 (98%)	311 (97%)	11 (3%)	37	70
3	C	326/327 (100%)	311 (95%)	15 (5%)	27	63
4	D	200/204 (98%)	192 (96%)	8 (4%)	31	66
5	E	168/168 (100%)	153 (91%)	15 (9%)	9	35
6	F	88/91 (97%)	82 (93%)	6 (7%)	16	49
7	G	65/66 (98%)	62 (95%)	3 (5%)	27	63
8	H	61/62 (98%)	59 (97%)	2 (3%)	38	71
9	I	38/38 (100%)	28 (74%)	10 (26%)	0	2
10	J	49/49 (100%)	47 (96%)	2 (4%)	30	66
All	All	1686/1702 (99%)	1601 (95%)	85 (5%)	24	60

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	34	THR
1	A	89	TYR
1	A	108	LYS
1	A	181	ASP
1	A	184	GLU
1	A	220	SER
1	A	226	GLU
1	A	232	SER
1	A	245	GLU
1	A	316	ASP
1	A	352	SER
1	A	366	VAL
2	B	52	LYS
2	B	60	SER
2	B	74	SER
2	B	97	SER
2	B	117	ASP
2	B	185	LYS
2	B	209	LEU
2	B	226	ILE
2	B	264	ILE
2	B	434	PRO

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Mol	Chain	Res	Type
2	B	439	LEU
3	C	1	MET
3	C	2	THR
3	C	4	ILE
3	C	64	SER
3	C	88	SER
3	C	90	PHE
3	C	172	LYS
3	C	174	THR
3	C	185	LEU
3	C	215	VAL
3	C	227	LYS
3	C	303	LEU
3	C	349	THR
3	C	356	VAL
3	C	375	LYS
4	D	3	LEU
4	D	17	LEU
4	D	37	CYS
4	D	39	SER
4	D	49	ARG
4	D	88	SER
4	D	109	LEU
4	D	115	TYR
5	E	6	LYS
5	E	12	ASP
5	E	21	SER
5	E	27	GLU
5	E	56	SER
5	E	72	SER
5	E	73	LYS
5	E	74	ILE
5	E	79	SER
5	E	113	GLU
5	E	118	ARG
5	E	125	GLU
5	E	170	ARG
5	E	178	LEU
5	E	184	SER
6	F	11	ARG
6	F	12	TRP
6	F	13	LEU

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Mol	Chain	Res	Type
6	F	17	ARG
6	F	99	ARG
6	F	109	LYS
7	G	2	ARG
7	G	31	SER
7	G	68	LYS
8	H	29	LYS
8	H	37	LEU
9	I	37	THR
9	I	43	LEU
9	I	47	ARG
9	I	49	VAL
9	I	52	ARG
9	I	55	LEU
9	I	70	LEU
9	I	71	ASN
9	I	77	ARG
9	I	78	TYR
10	J	6	THR
10	J	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	18	GLN
1	A	126	GLN
1	A	139	GLN
1	A	165	GLN
1	A	189	HIS
1	A	252	HIS
1	A	305	GLN
1	A	311	ASN
2	B	290	ASN
3	C	15	ASN
3	C	322	GLN
4	D	105	ASN
4	D	225	HIS
5	E	161	HIS
6	F	27	ASN
8	H	23	GLN
8	H	49	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	PG4	A	501	-	12,12,12	0.24	0	11,11,11	0.16	0
13	CDL	A	503	-	33,33,99	0.51	0	37,43,111	0.86	0
17	I2Q	C	407	-	33,33,33	0.78	1 (3%)	46,48,48	0.70	0
16	PEE	E	204	-	40,40,50	0.79	1 (2%)	43,45,55	0.88	1 (2%)
13	CDL	G	101	-	43,43,99	0.66	1 (2%)	49,55,111	1.03	6 (12%)
19	PO4	F	501	-	4,4,4	1.21	1 (25%)	6,6,6	0.49	0
19	PO4	G	103	-	4,4,4	0.93	0	6,6,6	0.45	0
20	HEC	D	501	4	32,50,50	2.38	10 (31%)	24,82,82	2.26	6 (25%)
19	PO4	G	104	-	4,4,4	1.35	1 (25%)	6,6,6	0.52	0
19	PO4	D	502	-	4,4,4	0.69	0	6,6,6	0.54	0
19	PO4	F	502	-	4,4,4	0.65	0	6,6,6	0.46	0
19	PO4	G	102	-	4,4,4	1.11	0	6,6,6	0.38	0
15	LMT	C	403	-	36,36,36	0.88	1 (2%)	47,47,47	1.65	13 (27%)
19	PO4	C	409	-	4,4,4	0.50	0	6,6,6	0.65	0
19	PO4	E	203	-	4,4,4	0.91	0	6,6,6	0.39	0
19	PO4	C	410	-	4,4,4	0.87	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PG4	C	404	-	12,12,12	0.42	0	11,11,11	0.37	0
14	HEM	C	402	3	41,50,50	1.44	5 (12%)	45,82,82	1.88	10 (22%)
13	CDL	D	503	-	53,53,99	0.62	1 (1%)	59,65,111	0.82	1 (1%)
11	PG4	C	405	-	12,12,12	0.30	0	11,11,11	0.30	0
16	PEE	C	406	-	39,39,50	0.80	1 (2%)	42,44,55	0.73	0
18	DMS	C	408	-	3,3,3	0.35	0	3,3,3	0.26	0
22	PX4	E	202	-	36,36,45	0.62	0	42,44,53	0.92	2 (4%)
12	6PE	A	502	-	22,22,26	0.50	0	25,27,31	0.89	1 (4%)
21	FES	E	201	5	0,4,4	-	-	-	-	-
14	HEM	C	401	3	41,50,50	1.53	7 (17%)	45,82,82	2.09	16 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LMT	C	403	-	-	14/21/61/61	0/2/2/2
20	HEC	D	501	4	-	0/10/54/54	-
22	PX4	E	202	-	-	17/40/40/49	-
14	HEM	C	402	3	-	3/12/54/54	-
11	PG4	A	501	-	-	7/10/10/10	-
13	CDL	A	503	-	-	15/41/41/110	-
17	I2Q	C	407	-	-	2/13/13/13	0/4/4/4
12	6PE	A	502	-	-	12/26/26/30	-
16	PEE	E	204	-	1/1/4/8	26/44/44/54	-
11	PG4	C	404	-	-	8/10/10/10	-
13	CDL	G	101	-	-	17/52/52/110	-
13	CDL	D	503	-	-	28/63/63/110	-
21	FES	E	201	5	-	-	0/1/1/1
14	HEM	C	401	3	-	4/12/54/54	-
11	PG4	C	405	-	-	5/10/10/10	-
16	PEE	C	406	-	1/1/4/8	19/43/43/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	501	HEC	C2B-C3B	6.53	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	501	HEC	C3C-C2C	6.32	1.47	1.40
20	D	501	HEC	C3C-C4C	4.47	1.51	1.43
14	C	402	HEM	C1B-NB	-4.24	1.33	1.40
16	C	406	PEE	C18-C19	3.91	1.54	1.31
16	E	204	PEE	C18-C19	3.58	1.52	1.31
20	D	501	HEC	C2A-C3A	3.39	1.47	1.37
20	D	501	HEC	C3D-C2D	3.34	1.47	1.37
20	D	501	HEC	C2A-C1A	3.28	1.50	1.42
14	C	402	HEM	C4B-NB	-3.26	1.32	1.38
15	C	403	LMT	O1'-C1'	3.22	1.45	1.40
14	C	401	HEM	C1B-NB	-3.18	1.34	1.40
14	C	401	HEM	C4D-ND	-3.12	1.34	1.40
14	C	401	HEM	C4B-NB	-3.03	1.32	1.38
20	D	501	HEC	C3A-C4A	2.98	1.49	1.42
14	C	401	HEM	C4D-C3D	2.96	1.50	1.45
20	D	501	HEC	C4B-C3B	2.87	1.48	1.43
14	C	401	HEM	C1D-ND	-2.79	1.33	1.38
14	C	401	HEM	C3B-C4B	2.75	1.50	1.44
19	G	104	PO4	P-O1	2.63	1.57	1.50
20	D	501	HEC	C1C-CHC	2.61	1.48	1.41
14	C	402	HEM	C1D-C2D	2.60	1.49	1.44
14	C	401	HEM	FE-NB	2.46	2.09	1.96
13	G	101	CDL	C11-CA5	2.32	1.57	1.49
14	C	402	HEM	C4D-ND	-2.22	1.36	1.40
14	C	402	HEM	C4D-C3D	2.18	1.48	1.45
17	C	407	I2Q	C3-C2	2.18	1.42	1.37
13	D	503	CDL	C31-CA7	2.16	1.57	1.50
20	D	501	HEC	C4D-CHA	2.08	1.46	1.41
19	F	501	PO4	P-O1	2.05	1.55	1.50

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	501	HEC	C1D-C2D-C3D	-5.95	102.86	107.00
14	C	401	HEM	CBA-CAA-C2A	-5.56	103.13	112.62
14	C	402	HEM	CHC-C4B-NB	5.41	130.31	124.43
20	D	501	HEC	CMB-C2B-C3B	4.82	131.49	125.82
14	C	402	HEM	CMD-C2D-C1D	4.38	131.71	125.04
14	C	401	HEM	CAD-C3D-C4D	4.21	132.02	124.66
15	C	403	LMT	O4'-C4B-C3B	3.67	118.83	110.35
20	D	501	HEC	CBD-CAD-C3D	-3.62	106.44	112.62
15	C	403	LMT	O1B-C4'-C3'	3.57	116.77	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	401	HEM	CHB-C1B-NB	3.53	128.75	124.38
14	C	402	HEM	C1B-NB-C4B	3.49	108.67	105.07
14	C	401	HEM	CMD-C2D-C1D	3.41	130.23	125.04
14	C	401	HEM	CHC-C4B-NB	3.34	128.06	124.43
15	C	403	LMT	C3B-C4B-C5B	-3.34	104.29	110.24
15	C	403	LMT	C3'-C4'-C5'	-3.31	103.34	110.93
14	C	402	HEM	CAD-C3D-C4D	3.26	130.36	124.66
14	C	401	HEM	O2D-CGD-CBD	3.06	123.87	114.03
14	C	401	HEM	C1B-NB-C4B	3.01	108.19	105.07
14	C	402	HEM	CHA-C4D-ND	2.77	127.81	124.38
15	C	403	LMT	O5'-C5'-C6'	2.76	113.31	106.44
14	C	401	HEM	CHD-C1D-C2D	-2.76	120.67	124.98
14	C	401	HEM	CHB-C1B-C2B	-2.71	119.24	126.72
15	C	403	LMT	C4B-C3B-C2B	-2.70	106.11	110.82
13	G	101	CDL	OB6-CB4-CB3	2.70	118.17	108.40
22	E	202	PX4	O7-C7-C6	2.70	118.17	108.40
20	D	501	HEC	CMA-C3A-C2A	2.64	129.92	124.94
22	E	202	PX4	O7-C23-C24	2.61	117.13	111.50
12	A	502	6PE	O6-C10-C11	2.59	117.09	111.50
14	C	401	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
15	C	403	LMT	C1'-O5'-C5'	2.56	118.71	113.69
15	C	403	LMT	C1B-O5B-C5B	2.54	118.67	113.69
13	G	101	CDL	OA6-CA5-OA7	-2.54	117.92	122.96
13	D	503	CDL	OB6-CB5-C51	2.50	116.90	111.50
14	C	402	HEM	CHB-C1B-NB	2.49	127.46	124.38
13	G	101	CDL	OB6-CB5-C51	2.49	117.73	110.80
14	C	401	HEM	CHD-C1D-ND	2.47	127.11	124.43
15	C	403	LMT	O3B-C3B-C4B	2.47	116.05	110.35
20	D	501	HEC	O2D-CGD-CBD	2.42	121.80	114.03
14	C	401	HEM	CHA-C4D-C3D	-2.39	120.84	125.33
15	C	403	LMT	O5B-C1B-C2B	2.38	115.38	110.35
14	C	402	HEM	CAD-C3D-C2D	-2.37	123.47	127.88
13	G	101	CDL	OA2-PA1-OA3	-2.31	100.03	109.07
15	C	403	LMT	O3'-C3'-C2'	2.29	115.65	110.35
14	C	401	HEM	CHA-C4D-ND	2.28	127.20	124.38
14	C	402	HEM	CHA-C4D-C3D	-2.27	121.07	125.33
15	C	403	LMT	O5B-C5B-C6B	2.24	112.00	106.44
16	E	204	PEE	O2-C2-C1	2.19	116.34	108.40
13	G	101	CDL	OA5-PA1-OA3	2.17	117.55	109.07
14	C	401	HEM	O2D-CGD-O1D	-2.17	117.90	123.30
14	C	402	HEM	O2D-CGD-CBD	2.15	120.95	114.03
14	C	401	HEM	C4D-C3D-C2D	-2.15	103.76	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	501	HEC	O2A-CGA-CBA	2.15	120.93	114.03
14	C	401	HEM	C2C-C3C-C4C	-2.07	105.45	106.90
15	C	403	LMT	C2'-C3'-C4'	-2.03	105.04	109.68
13	G	101	CDL	OA6-CA5-C11	2.03	114.82	111.09
14	C	402	HEM	CHB-C1B-C2B	-2.01	121.16	126.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	C	406	PEE	C2
16	E	204	PEE	C2

All (177) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	502	6PE	C1-O3-P1-O1
12	A	502	6PE	C1-O3-P1-O2
12	A	502	6PE	C1-O3-P1-O8
12	A	502	6PE	C11-C10-O6-C2
12	A	502	6PE	O8-C16-C17-N1
13	A	503	CDL	CA3-OA5-PA1-OA2
13	A	503	CDL	CB3-OB5-PB2-OB4
13	D	503	CDL	CA2-C1-CB2-OB2
13	D	503	CDL	CB2-OB2-PB2-OB3
13	D	503	CDL	C51-CB5-OB6-CB4
13	G	101	CDL	CA2-C1-CB2-OB2
13	G	101	CDL	CA3-OA5-PA1-OA4
13	G	101	CDL	CB4-CB3-OB5-PB2
15	C	403	LMT	C2'-C1'-O1'-C1
15	C	403	LMT	C2-C1-O1'-C1'
16	C	406	PEE	C4-O4P-P-O3P
16	C	406	PEE	C4-O4P-P-O2P
16	C	406	PEE	C4-O4P-P-O1P
16	E	204	PEE	O2-C2-C3-O3
16	E	204	PEE	C1-O3P-P-O2P
16	E	204	PEE	C1-O3P-P-O4P
16	E	204	PEE	C4-O4P-P-O1P
16	E	204	PEE	O4P-C4-C5-N
22	E	202	PX4	C6-O4-P1-O1
22	E	202	PX4	C24-C23-O7-C7
13	G	101	CDL	C11-CA5-OA6-CA4
13	D	503	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
22	E	202	PX4	O6-C9-O5-C8
22	E	202	PX4	C10-C9-O5-C8
13	D	503	CDL	OB9-CB7-OB8-CB6
12	A	502	6PE	O7-C10-O6-C2
13	D	503	CDL	OB7-CB5-OB6-CB4
22	E	202	PX4	O8-C23-O7-C7
13	G	101	CDL	OA7-CA5-OA6-CA4
13	D	503	CDL	C31-CA7-OA8-CA6
16	C	406	PEE	C31-C30-O3-C3
16	C	406	PEE	C17-C18-C19-C20
13	D	503	CDL	OA9-CA7-OA8-CA6
16	C	406	PEE	O5-C30-O3-C3
13	A	503	CDL	C51-CB5-OB6-CB4
15	C	403	LMT	C3-C4-C5-C6
13	A	503	CDL	OB7-CB5-OB6-CB4
11	C	404	PG4	O3-C5-C6-O4
11	C	404	PG4	O2-C3-C4-O3
13	D	503	CDL	O1-C1-CB2-OB2
13	G	101	CDL	O1-C1-CB2-OB2
13	D	503	CDL	CA5-C11-C12-C13
11	C	405	PG4	O2-C3-C4-O3
16	E	204	PEE	C30-C31-C32-C33
15	C	403	LMT	O5'-C1'-O1'-C1
13	A	503	CDL	O1-C1-CB2-OB2
13	A	503	CDL	OA5-CA3-CA4-OA6
12	A	502	6PE	C5-C4-O4-C3
12	A	502	6PE	O5-C4-O4-C3
13	G	101	CDL	CA3-OA5-PA1-OA2
16	E	204	PEE	C4-O4P-P-O3P
13	A	503	CDL	CA2-C1-CB2-OB2
13	A	503	CDL	OA5-CA3-CA4-CA6
16	E	204	PEE	C13-C14-C15-C16
16	C	406	PEE	C13-C14-C15-C16
22	E	202	PX4	C13-C14-C15-C16
16	C	406	PEE	C32-C33-C34-C35
13	D	503	CDL	OA5-CA3-CA4-OA6
16	C	406	PEE	C14-C15-C16-C17
15	C	403	LMT	C11-C10-C9-C8
13	D	503	CDL	C53-C54-C55-C56
15	C	403	LMT	C2-C3-C4-C5
15	C	403	LMT	C7-C8-C9-C10
22	E	202	PX4	C1-C2-N1-C5

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Mol	Chain	Res	Type	Atoms
16	C	406	PEE	C11-C12-C13-C14
16	E	204	PEE	C31-C30-O3-C3
13	G	101	CDL	C51-CB5-OB6-CB4
16	C	406	PEE	C31-C32-C33-C34
16	E	204	PEE	O5-C30-O3-C3
13	A	503	CDL	CB2-C1-CA2-OA2
13	G	101	CDL	OB7-CB5-OB6-CB4
15	C	403	LMT	C4-C5-C6-C7
22	E	202	PX4	C9-C10-C11-C12
13	D	503	CDL	C11-C12-C13-C14
15	C	403	LMT	O5B-C1B-O1B-C4'
13	D	503	CDL	O1-C1-CA2-OA2
16	E	204	PEE	C14-C15-C16-C17
22	E	202	PX4	C1-C2-N1-C3
13	G	101	CDL	C71-CB7-OB8-CB6
13	D	503	CDL	CB2-OB2-PB2-OB5
13	D	503	CDL	C51-C52-C53-C54
13	G	101	CDL	OB5-CB3-CB4-CB6
16	E	204	PEE	C15-C16-C17-C18
13	A	503	CDL	O1-C1-CA2-OA2
22	E	202	PX4	C1-C2-N1-C4
11	C	404	PG4	O1-C1-C2-O2
11	C	405	PG4	O4-C7-C8-O5
16	E	204	PEE	C1-C2-C3-O3
16	C	406	PEE	C22-C23-C24-C25
15	C	403	LMT	C6-C7-C8-C9
22	E	202	PX4	C24-C25-C26-C27
15	C	403	LMT	O5B-C5B-C6B-O6B
16	C	406	PEE	C15-C16-C17-C18
11	A	501	PG4	O2-C3-C4-O3
16	E	204	PEE	C24-C25-C26-C27
13	D	503	CDL	CB6-CB4-OB6-CB5
11	A	501	PG4	C3-C4-O3-C5
16	C	406	PEE	O3P-C1-C2-O2
16	E	204	PEE	O3P-C1-C2-O2
16	C	406	PEE	C10-C11-C12-C13
13	G	101	CDL	OB9-CB7-OB8-CB6
16	E	204	PEE	C11-C10-O2-C2
13	D	503	CDL	OA5-CA3-CA4-CA6
13	D	503	CDL	OB5-CB3-CB4-CB6
13	D	503	CDL	CA3-CA4-CA6-OA8
13	A	503	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
16	E	204	PEE	C21-C22-C23-C24
13	D	503	CDL	OB5-CB3-CB4-OB6
13	G	101	CDL	OB5-CB3-CB4-OB6
12	A	502	6PE	C4-C5-C6-C7
13	D	503	CDL	OA6-CA4-CA6-OA8
12	A	502	6PE	C2-C1-O3-P1
13	A	503	CDL	OB5-CB3-CB4-CB6
16	C	406	PEE	O3P-C1-C2-C3
16	C	406	PEE	C16-C17-C18-C19
11	A	501	PG4	C1-C2-O2-C3
11	A	501	PG4	C5-C6-O4-C7
11	C	405	PG4	C6-C5-O3-C4
11	A	501	PG4	C8-C7-O4-C6
11	A	501	PG4	C4-C3-O2-C2
12	A	502	6PE	O6-C2-C3-O4
22	E	202	PX4	O7-C7-C8-O5
11	C	405	PG4	C1-C2-O2-C3
13	A	503	CDL	CA3-OA5-PA1-OA3
13	D	503	CDL	CB2-OB2-PB2-OB4
16	E	204	PEE	C4-O4P-P-O2P
16	E	204	PEE	O3P-C1-C2-C3
12	A	502	6PE	C1-C2-C3-O4
22	E	202	PX4	O3-C1-C2-N1
22	E	202	PX4	C6-C7-C8-O5
16	E	204	PEE	C16-C17-C18-C19
16	E	204	PEE	O4-C10-O2-C2
13	A	503	CDL	OB5-CB3-CB4-OB6
16	E	204	PEE	C10-C11-C12-C13
13	G	101	CDL	CB2-OB2-PB2-OB5
13	D	503	CDL	C32-C33-C34-C35
13	G	101	CDL	C1-CA2-OA2-PA1
14	C	402	HEM	CAA-CBA-CGA-O2A
11	C	405	PG4	C4-C3-O2-C2
14	C	401	HEM	CAA-CBA-CGA-O2A
17	C	407	I2Q	C11-C12-O1-C13
17	C	407	I2Q	C14-C12-O1-C13
15	C	403	LMT	C5-C6-C7-C8
11	C	404	PG4	C6-C5-O3-C4
11	C	404	PG4	C3-C4-O3-C5
14	C	401	HEM	CAA-CBA-CGA-O1A
15	C	403	LMT	C4'-C5'-C6'-O6'
16	E	204	PEE	C1-C2-O2-C10

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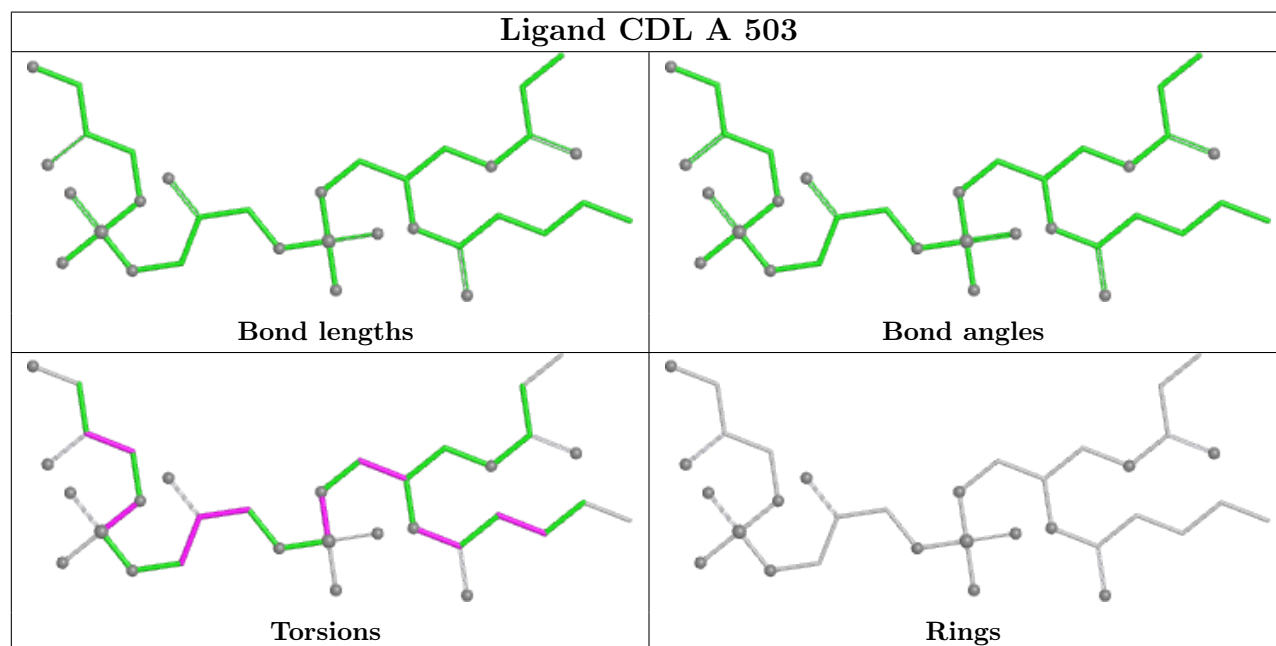
Mol	Chain	Res	Type	Atoms
16	E	204	PEE	C18-C19-C20-C21
13	A	503	CDL	CB3-OB5-PB2-OB2
14	C	402	HEM	CAA-CBA-CGA-O1A
13	D	503	CDL	C52-C53-C54-C55
11	A	501	PG4	O1-C1-C2-O2
16	E	204	PEE	C17-C18-C19-C20
22	E	202	PX4	C18-C19-C20-C21
22	E	202	PX4	C10-C11-C12-C13
11	C	404	PG4	C1-C2-O2-C3
11	C	404	PG4	C4-C3-O2-C2
14	C	401	HEM	CAD-CBD-CGD-O2D
14	C	401	HEM	CAD-CBD-CGD-O1D
15	C	403	LMT	C2B-C1B-O1B-C4'
11	C	404	PG4	C8-C7-O4-C6
13	G	101	CDL	CB3-CB4-CB6-OB8
13	G	101	CDL	CA2-OA2-PA1-OA3
22	E	202	PX4	C6-O4-P1-O2
13	D	503	CDL	OA7-CA5-OA6-CA4
16	C	406	PEE	C21-C22-C23-C24
16	E	204	PEE	C5-C4-O4P-P
14	C	402	HEM	CAD-CBD-CGD-O2D
13	D	503	CDL	C52-C51-CB5-OB7
13	D	503	CDL	C52-C51-CB5-OB6
16	C	406	PEE	O3-C30-C31-C32

There are no ring outliers.

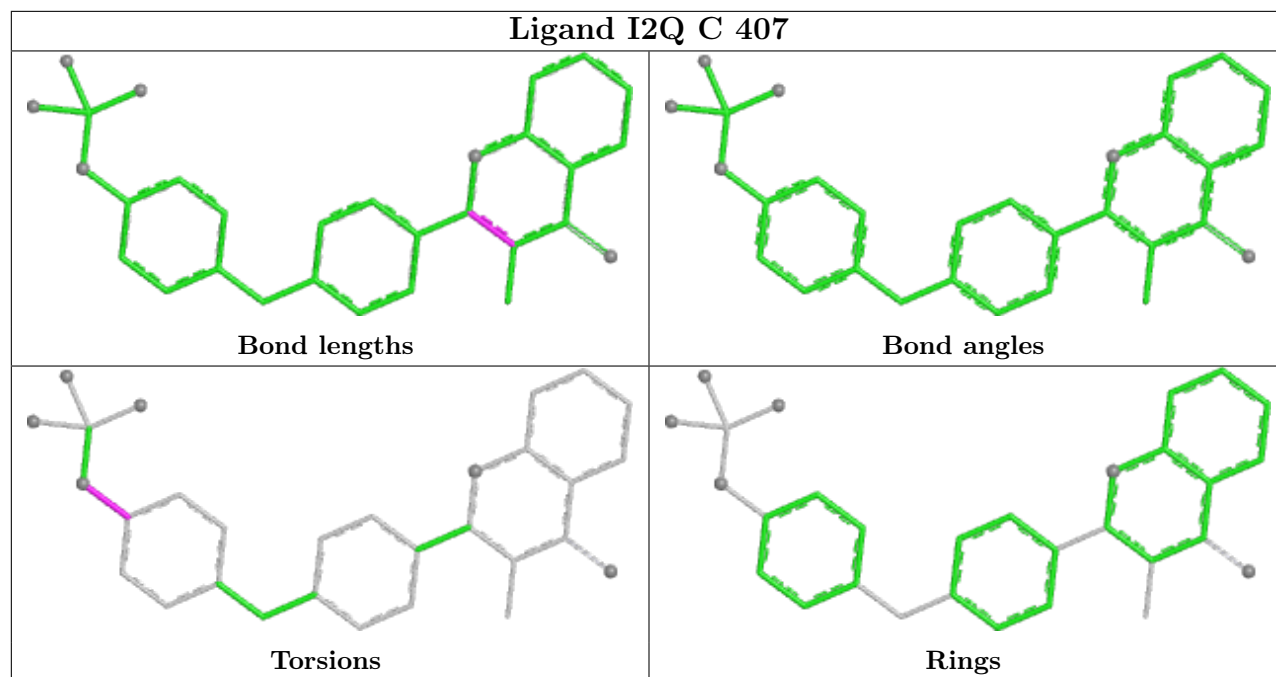
13 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	503	CDL	3	0
17	C	407	I2Q	1	0
16	E	204	PEE	3	0
13	G	101	CDL	1	0
20	D	501	HEC	15	0
15	C	403	LMT	2	0
14	C	402	HEM	7	0
13	D	503	CDL	1	0
11	C	405	PG4	1	0
16	C	406	PEE	1	0
22	E	202	PX4	4	0
12	A	502	6PE	4	0
14	C	401	HEM	5	0

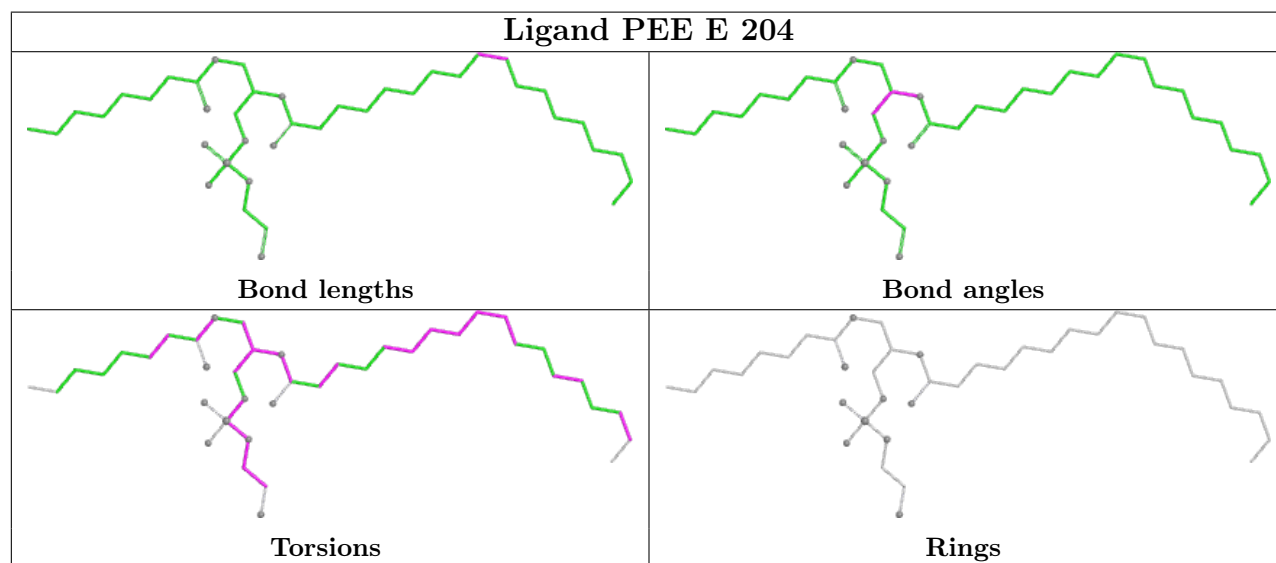
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



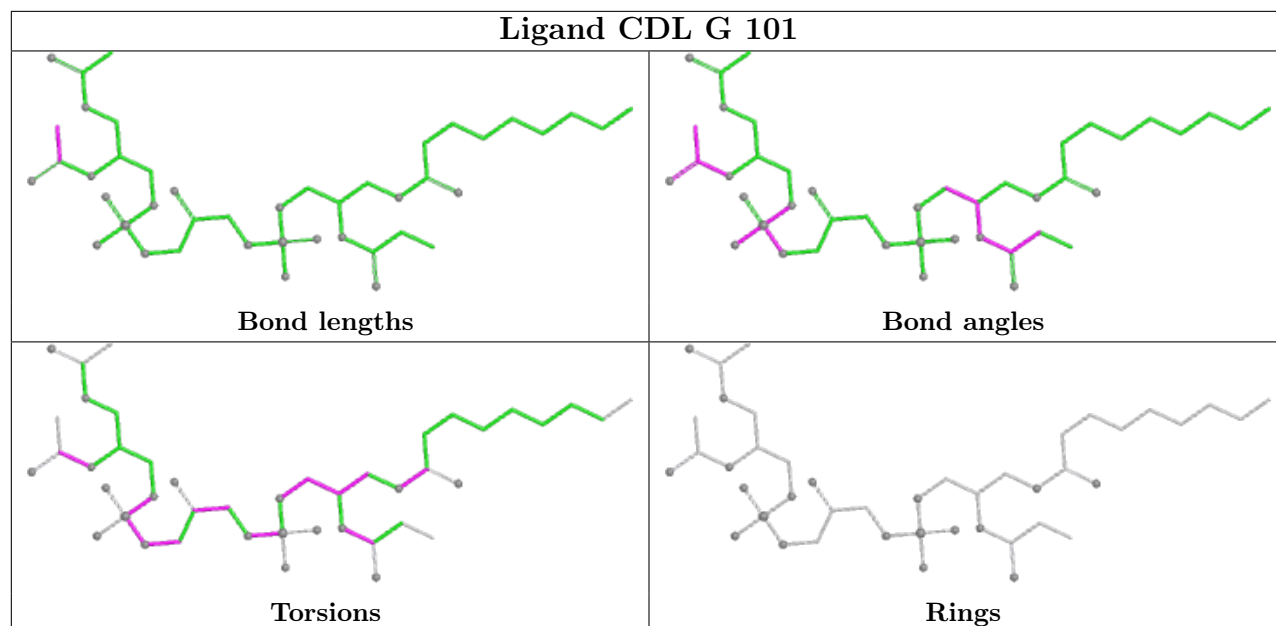
Ligand I2Q C 407



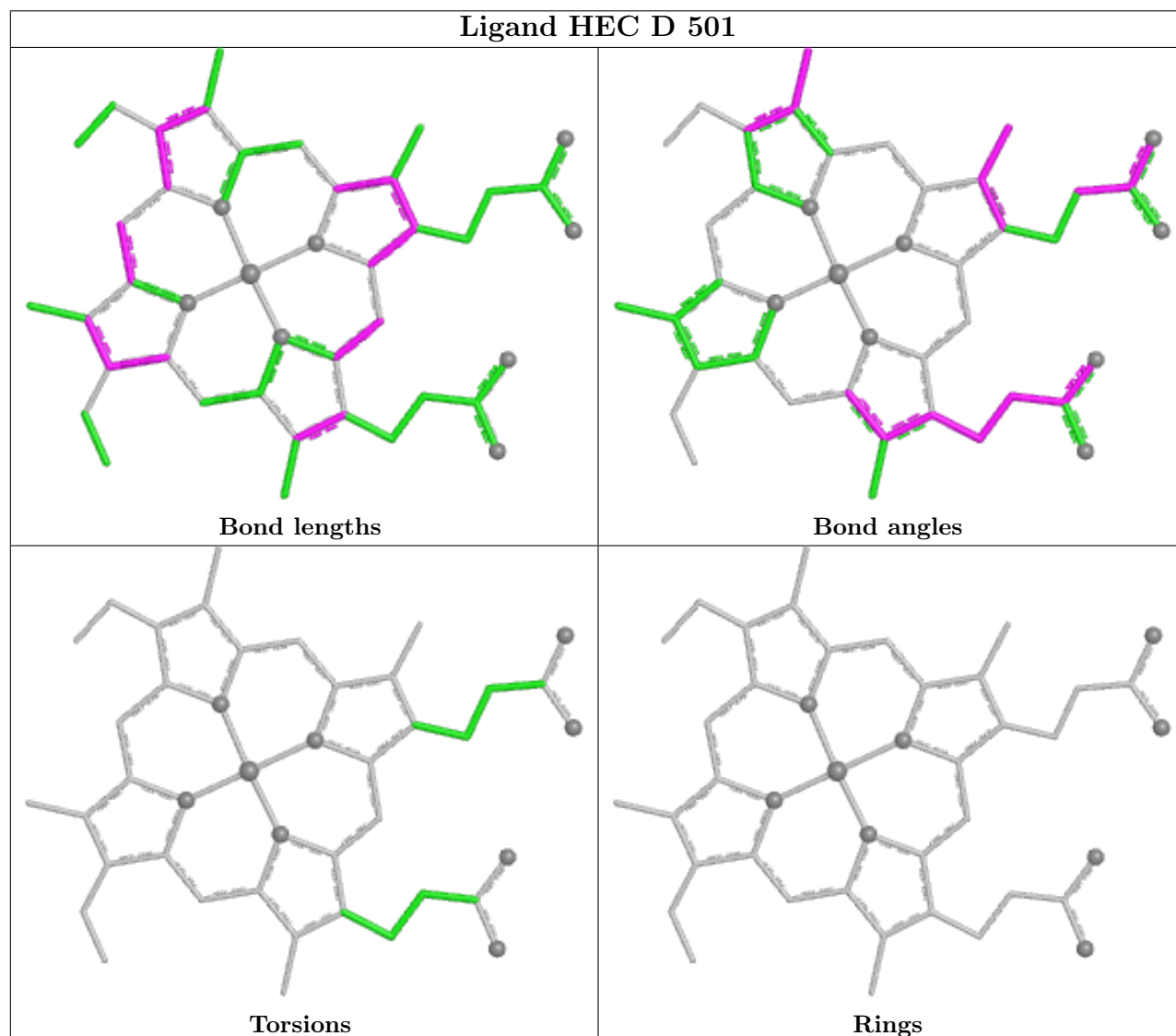
Ligand PEE E 204

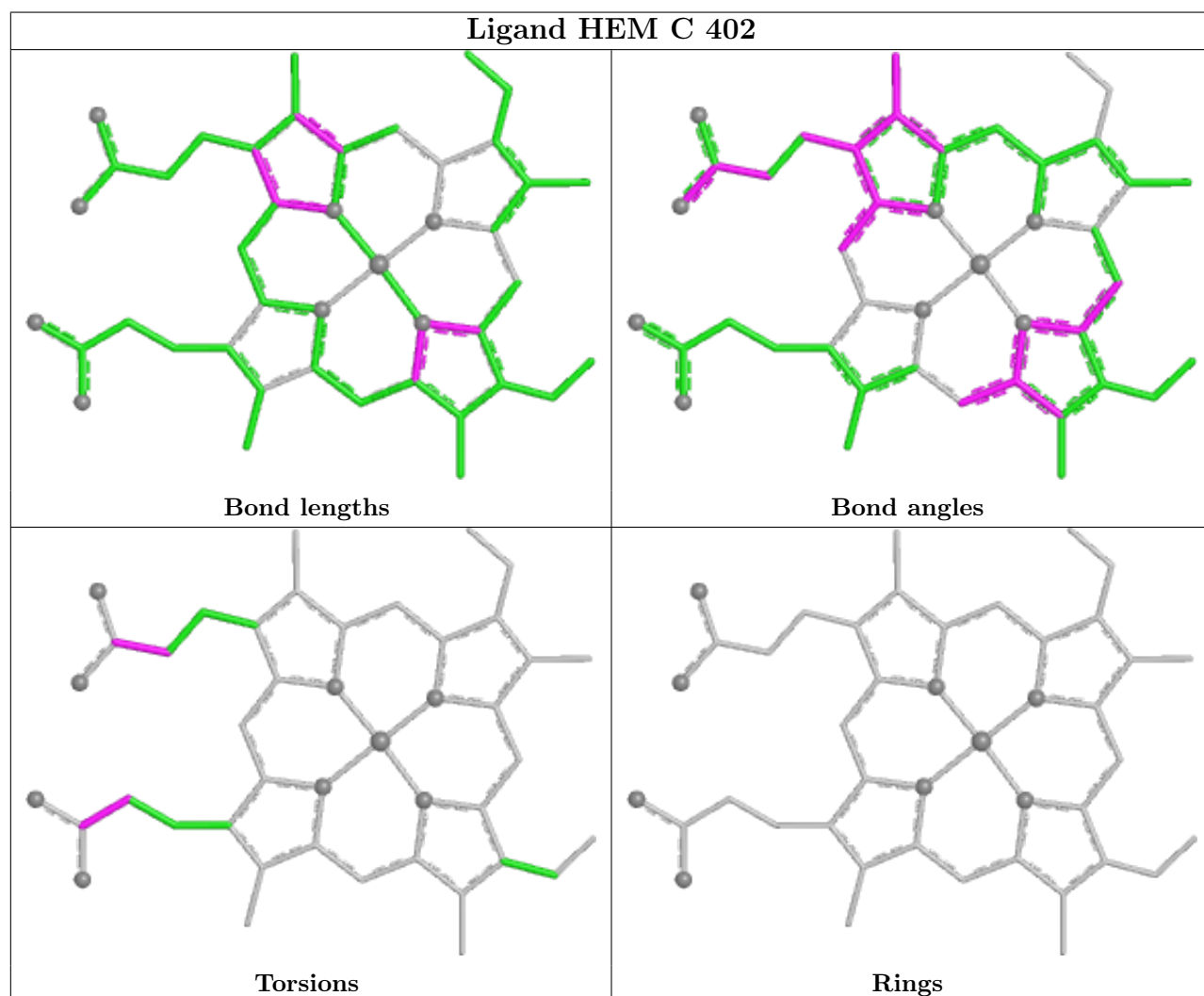
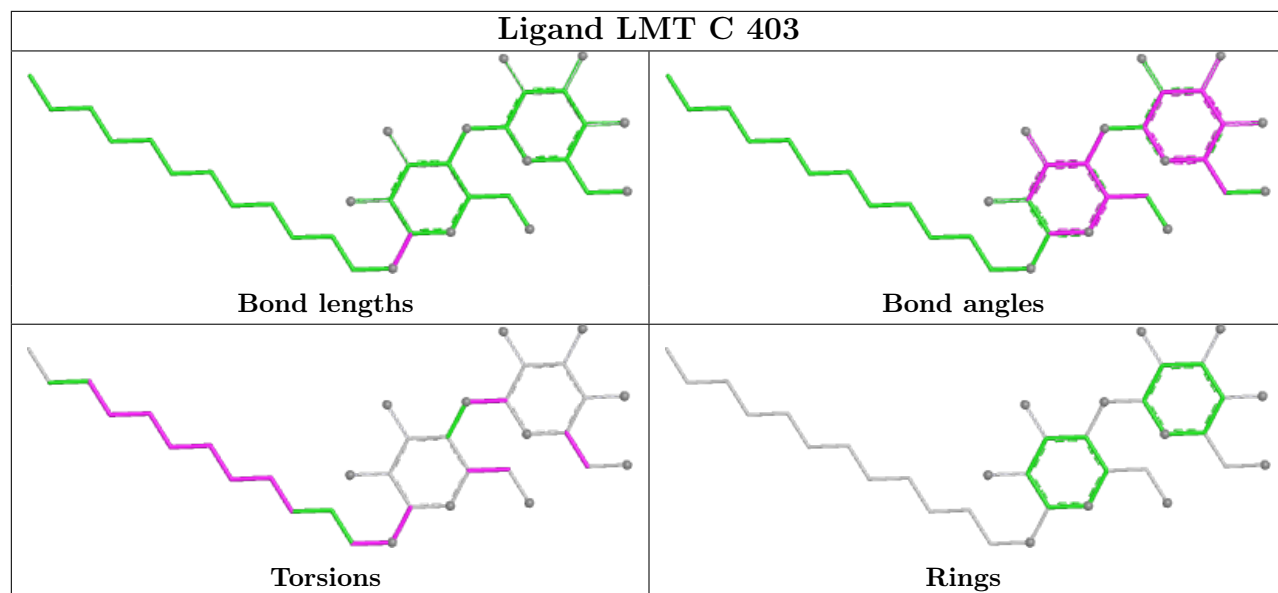


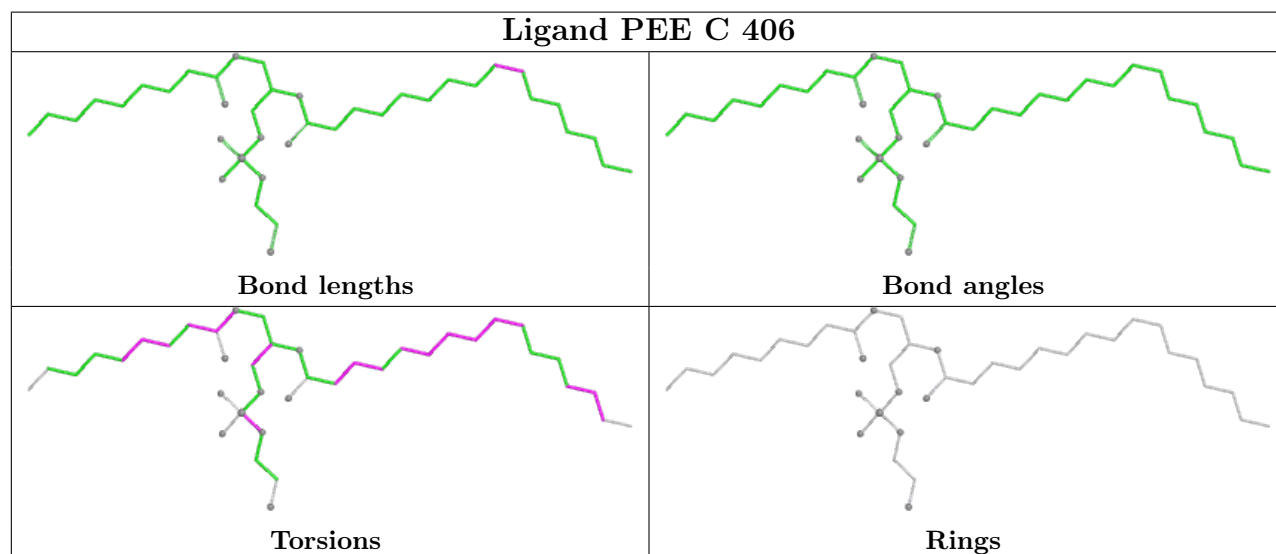
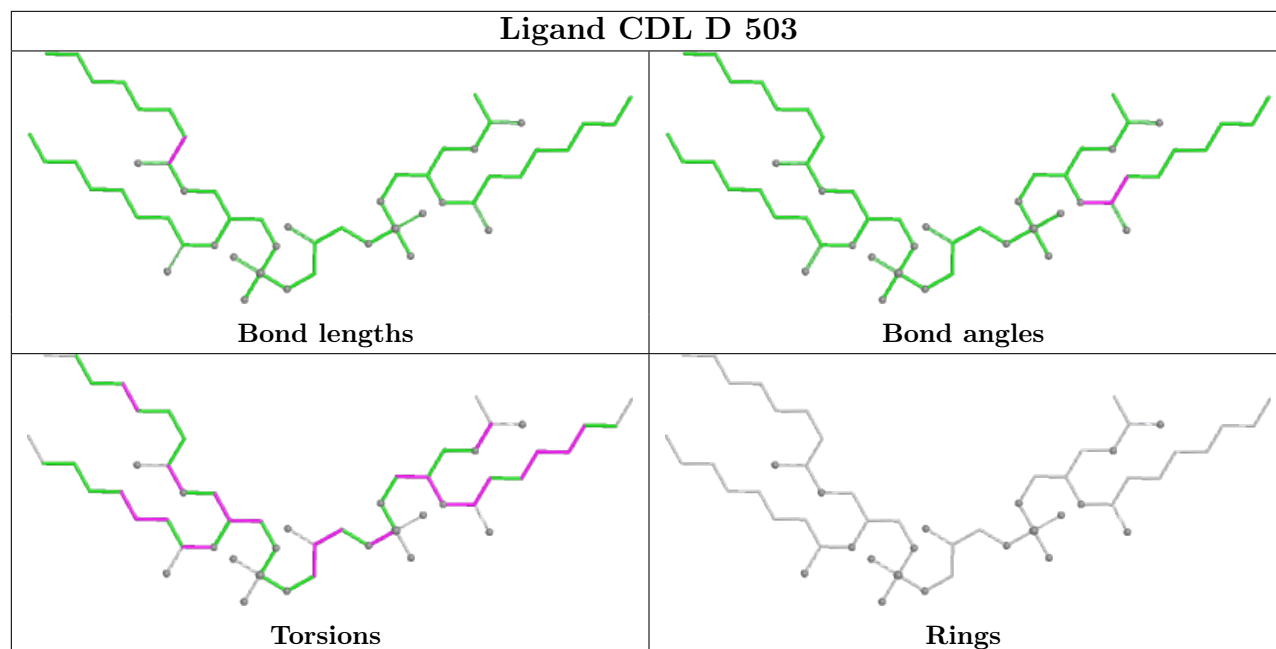
Ligand CDL G 101



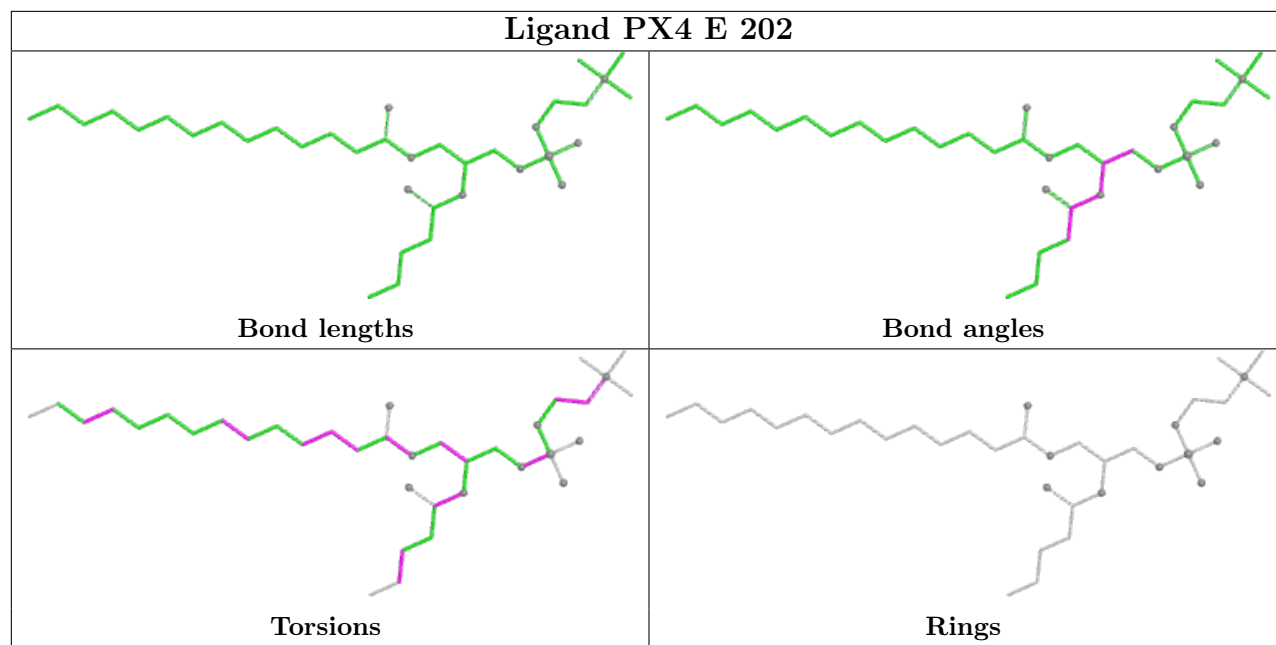
Ligand HEC D 501



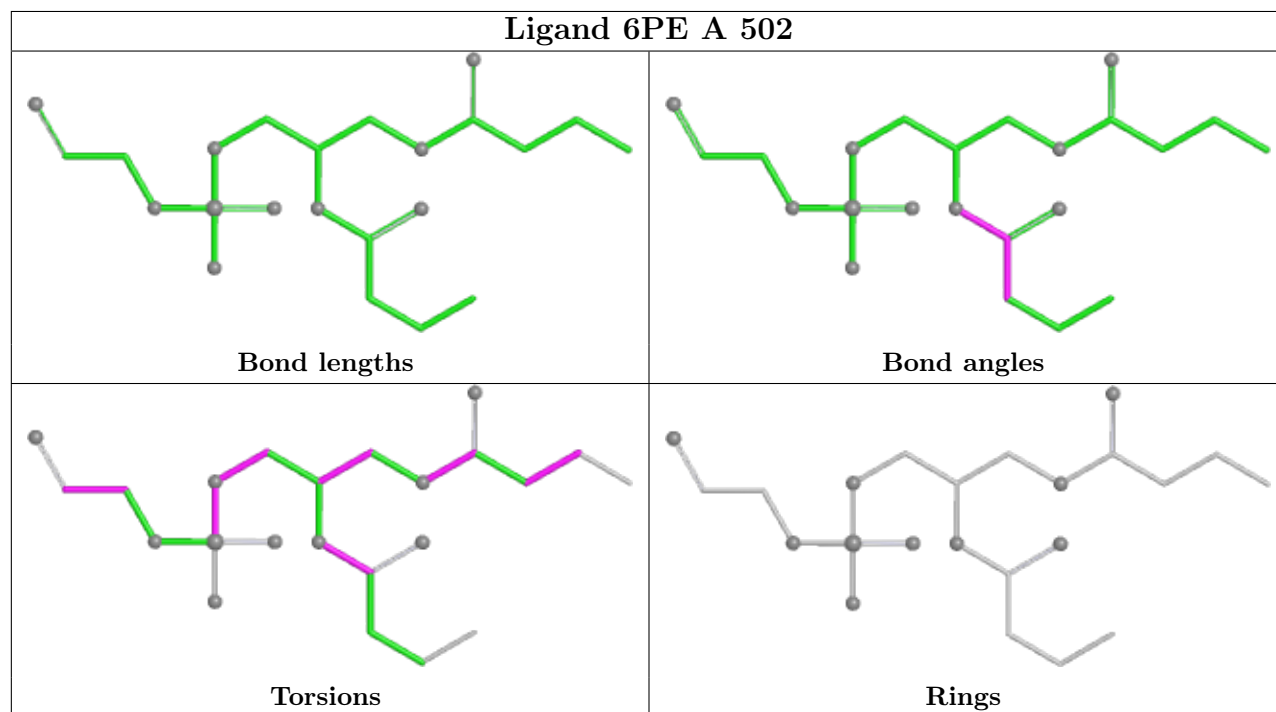


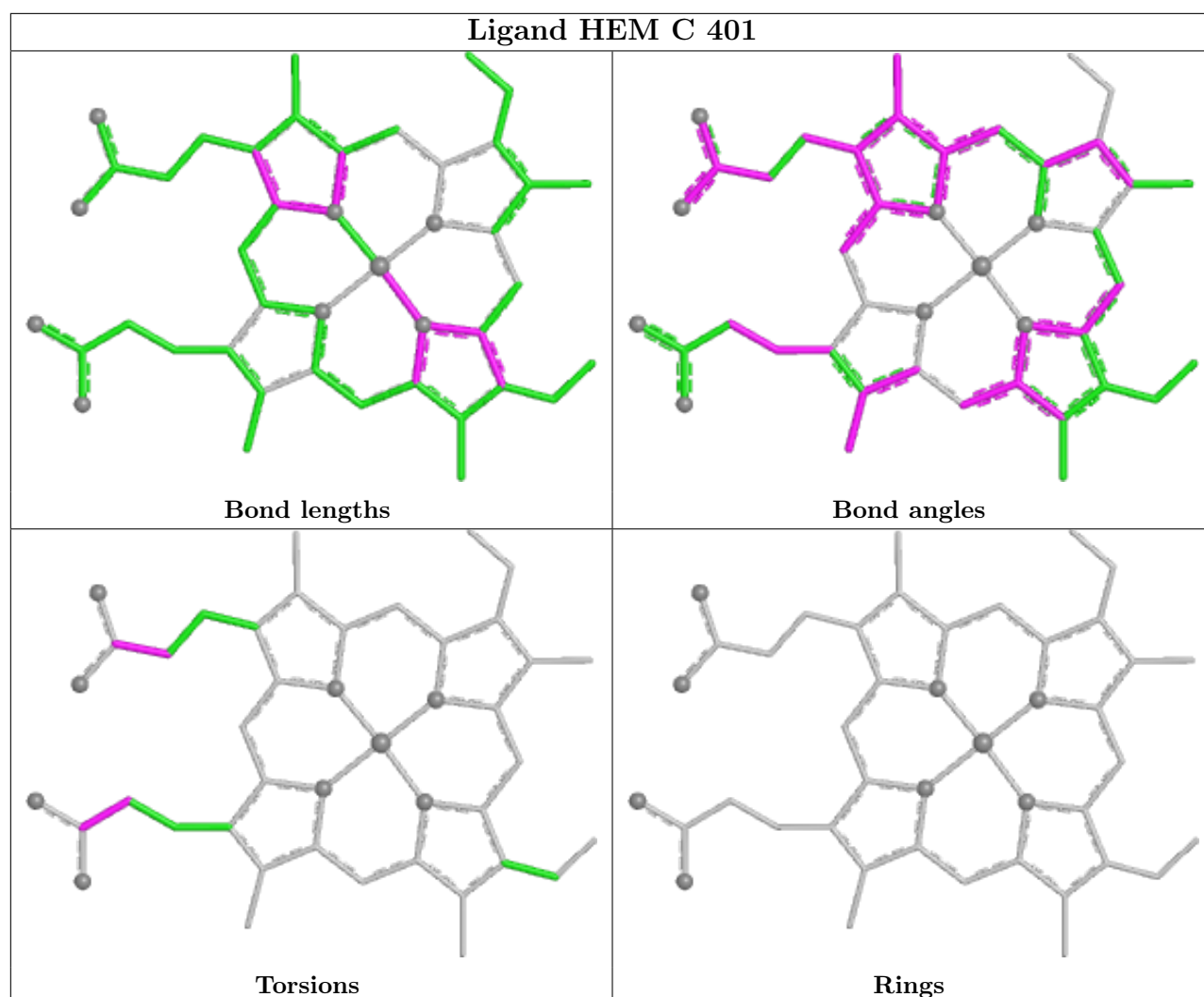


Ligand PX4 E 202



Ligand 6PE A 502





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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

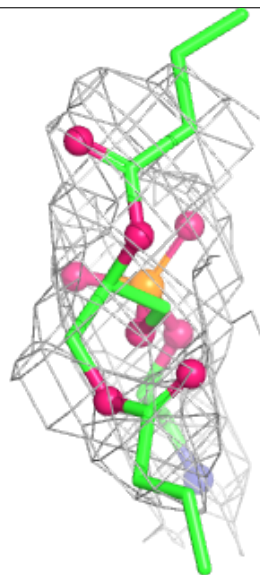
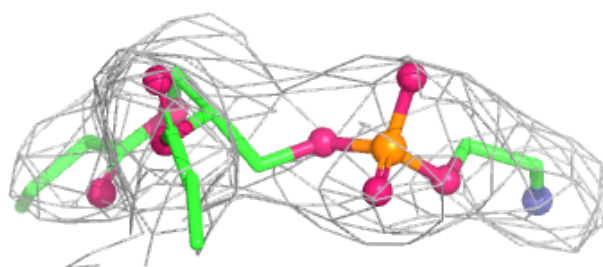
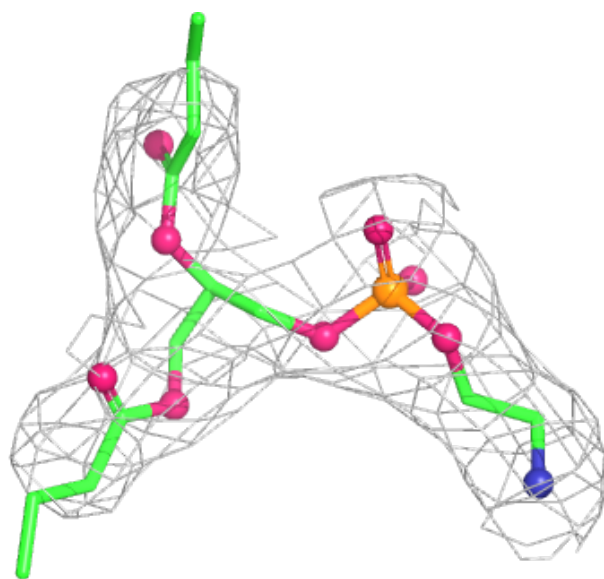
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

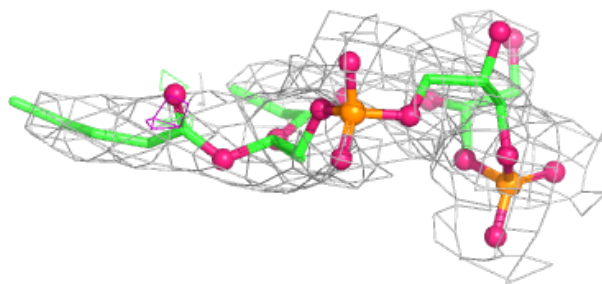
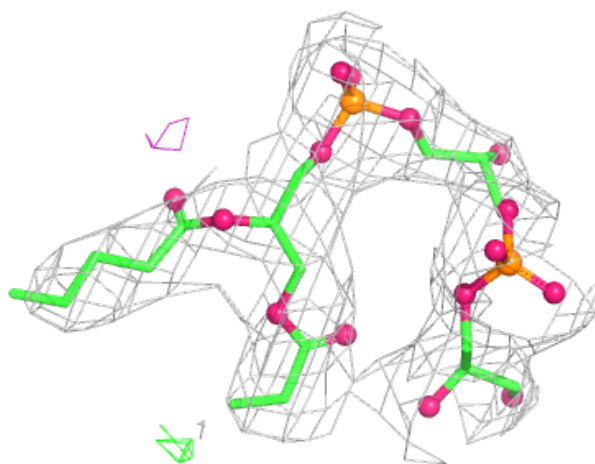
Electron density around 6PE A 502:

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



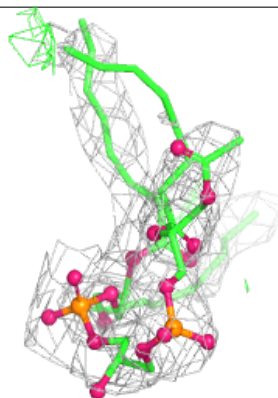
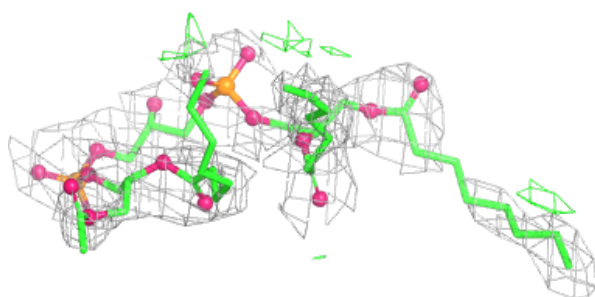
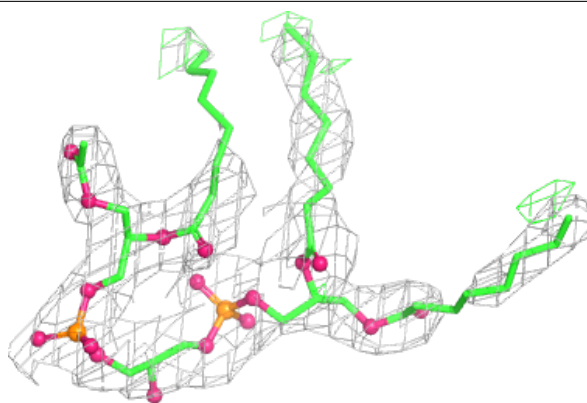
Electron density around CDL A 503:

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



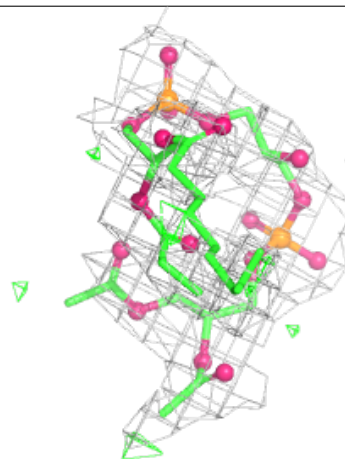
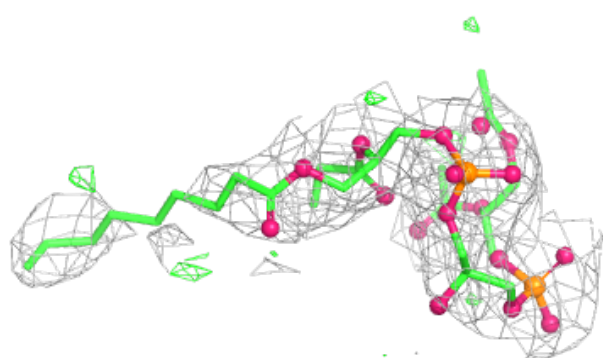
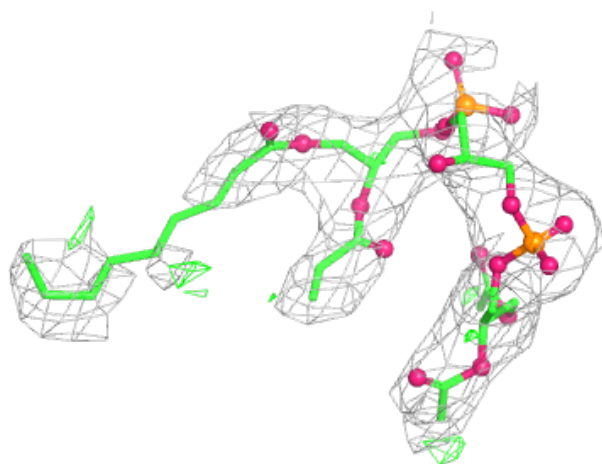
Electron density around CDL D 503:

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



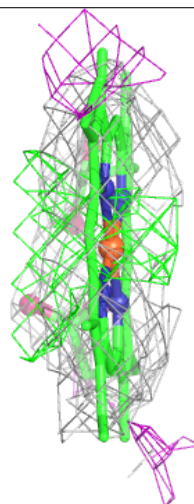
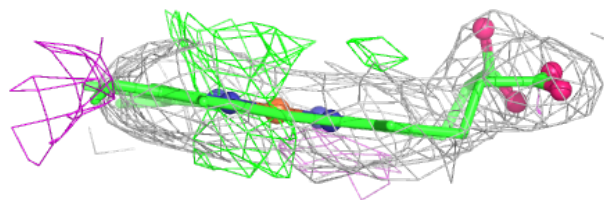
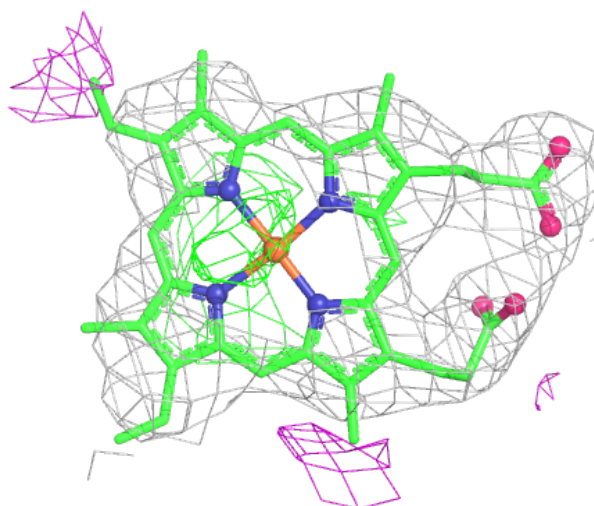
Electron density around CDL G 101:

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



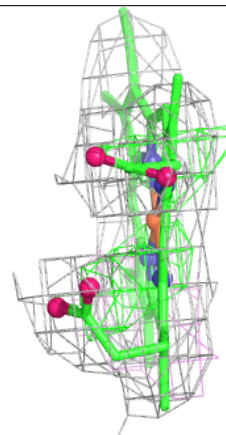
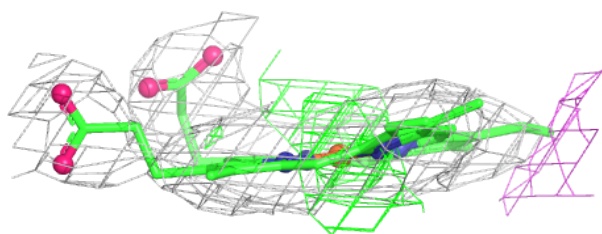
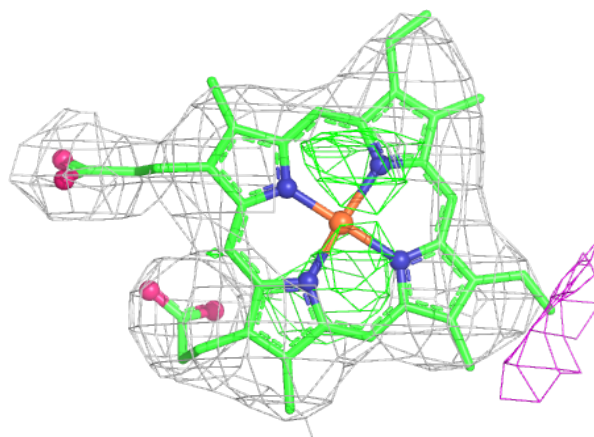
Electron density around HEM C 401:

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

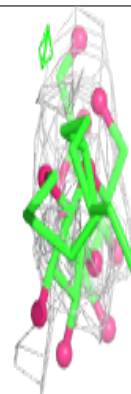
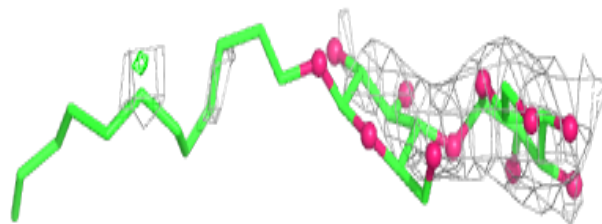
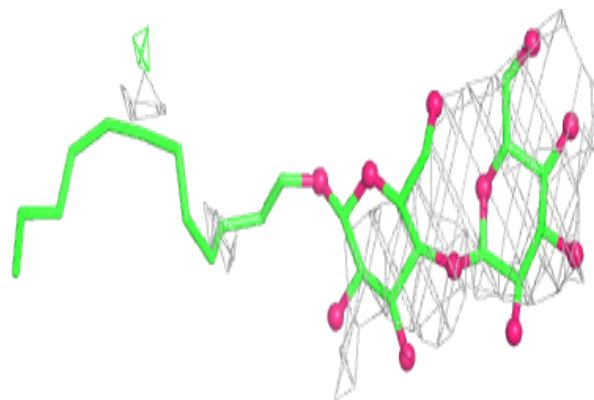


Electron density around HEM C 402:

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

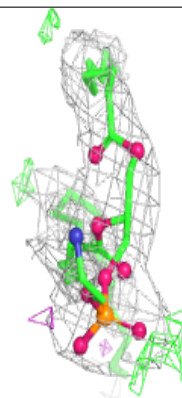
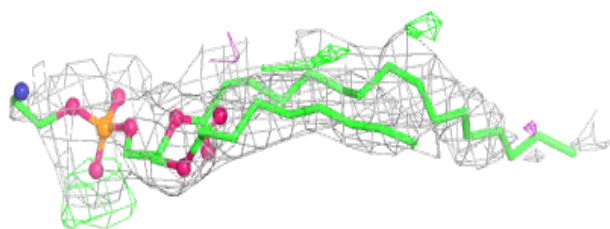
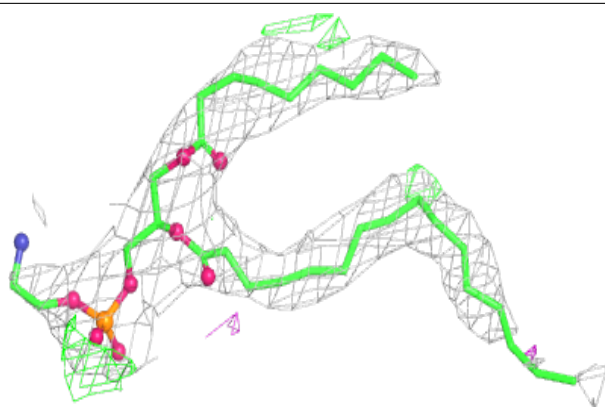
**Electron density around LMT C 403:**

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

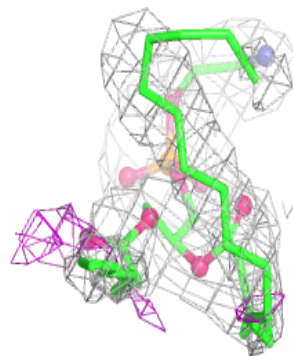
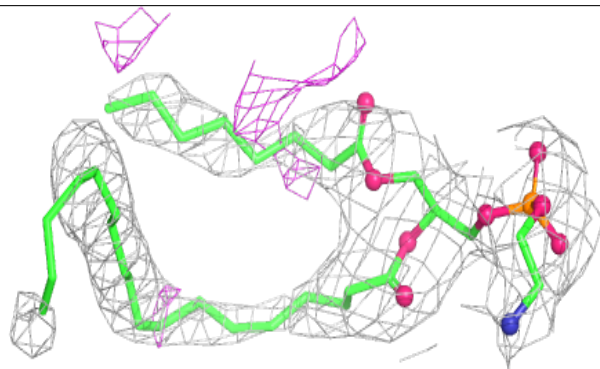
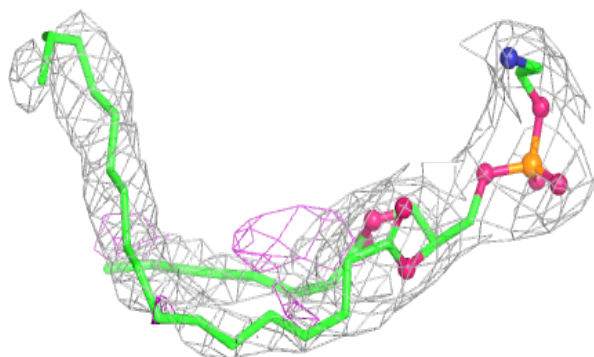


Electron density around PEE C 406:

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

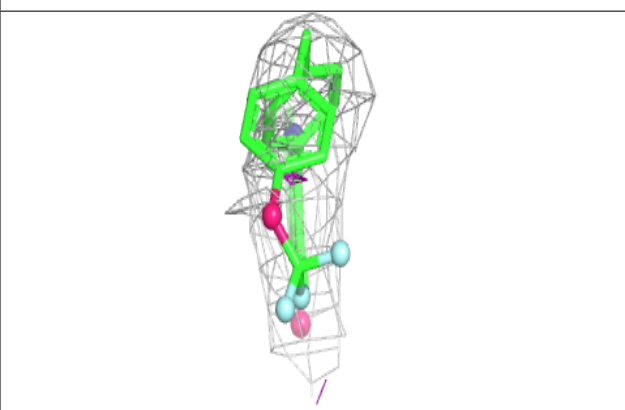
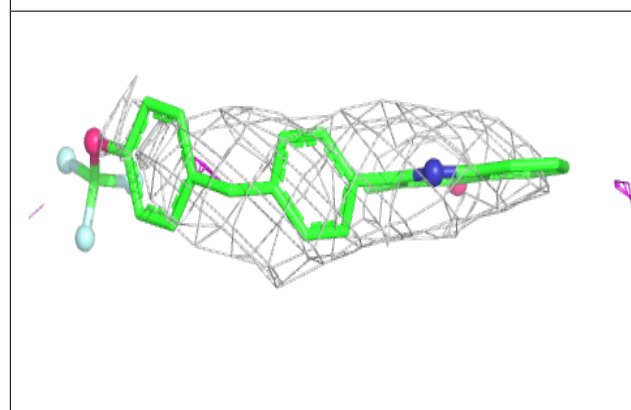
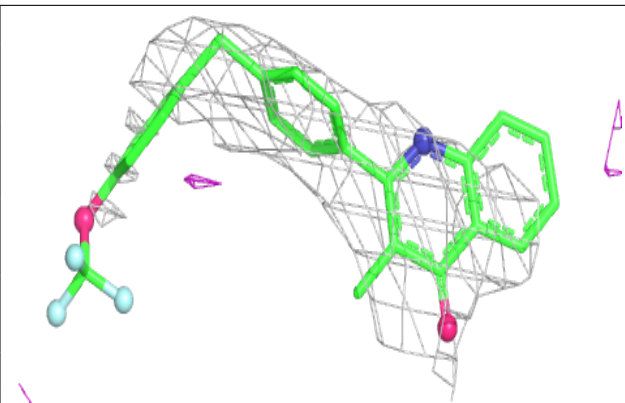
**Electron density around PEE E 204:**

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



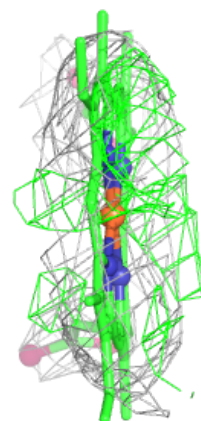
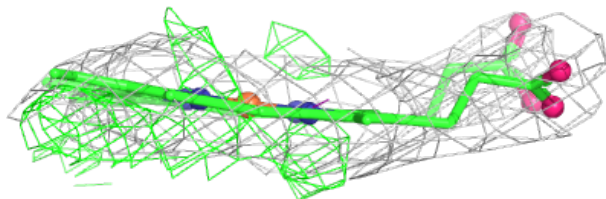
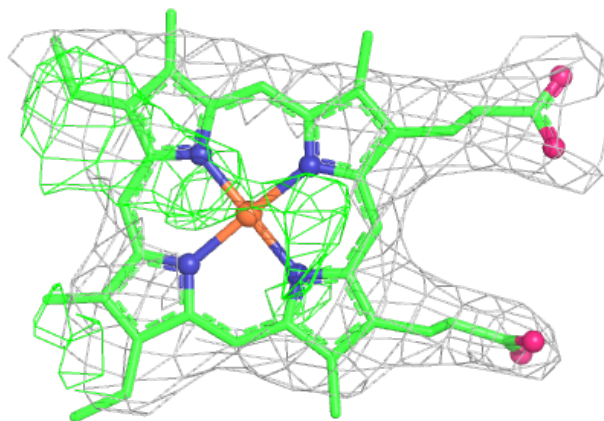
Electron density around I2Q C 407:

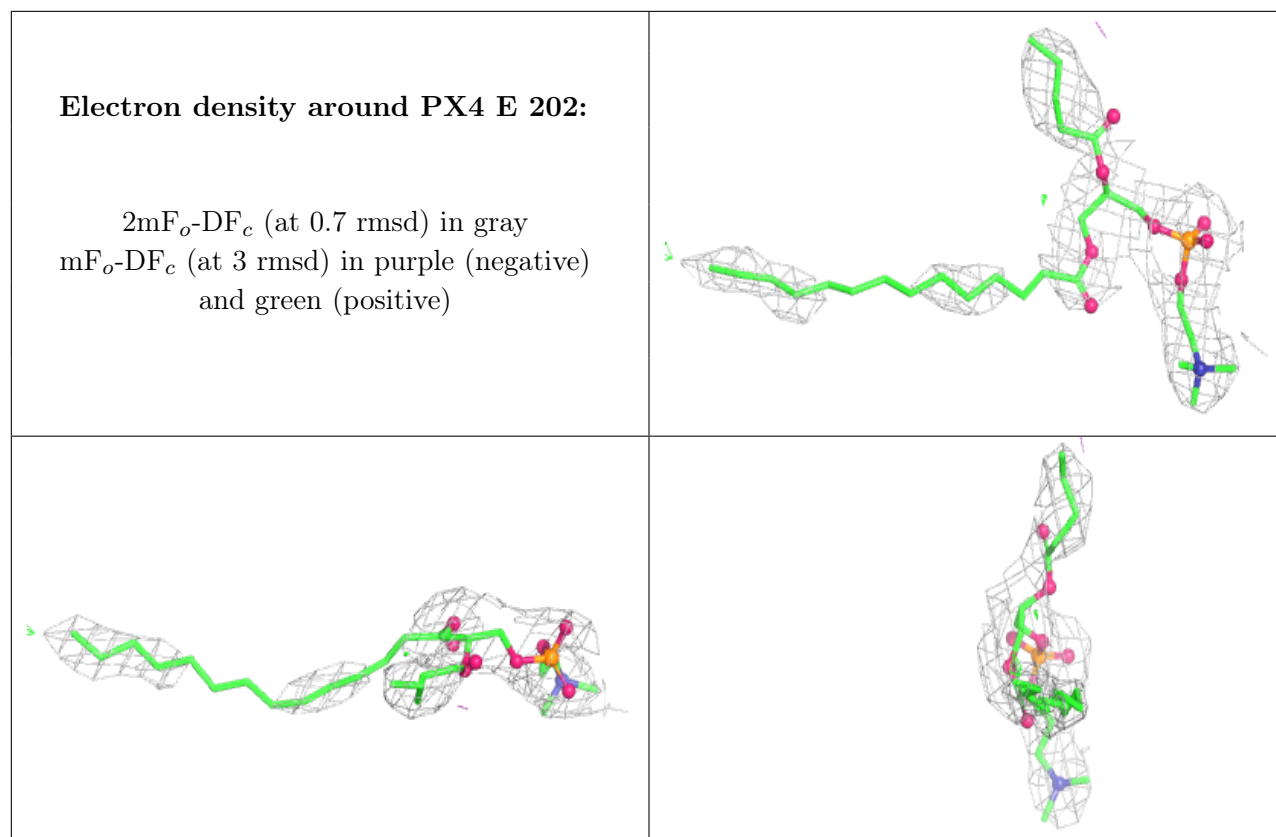
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC D 501:

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.