



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:24 am BST

PDB ID : 2BS2
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINO-
GENES
Authors : Lancaster, C.R.D.
Deposited on : 2005-05-14
Resolution : 1.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

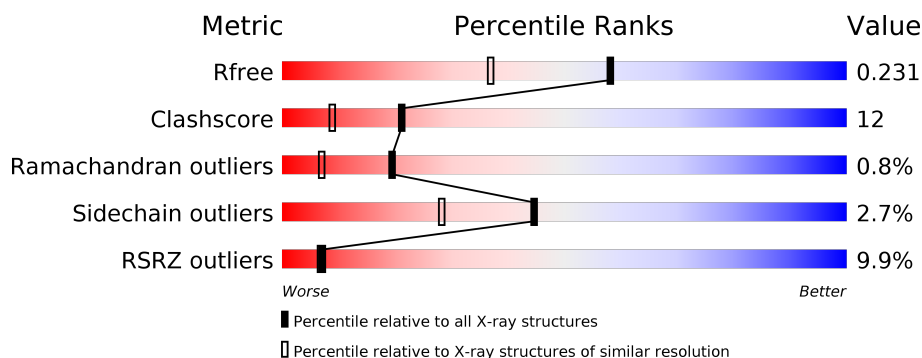
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	660	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	660	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
2	B	241	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>.</div> </div> </div>
2	E	241	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>.</div> </div> </div>
3	C	256	<div> <div>18%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>
3	F	256	<div> <div>14%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>.</div> </div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19666 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 QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	27	5	1
			5145	3219	927	967	32			
1	D	656	Total	C	N	O	S	32	3	1
			5125	3207	921	965	32			

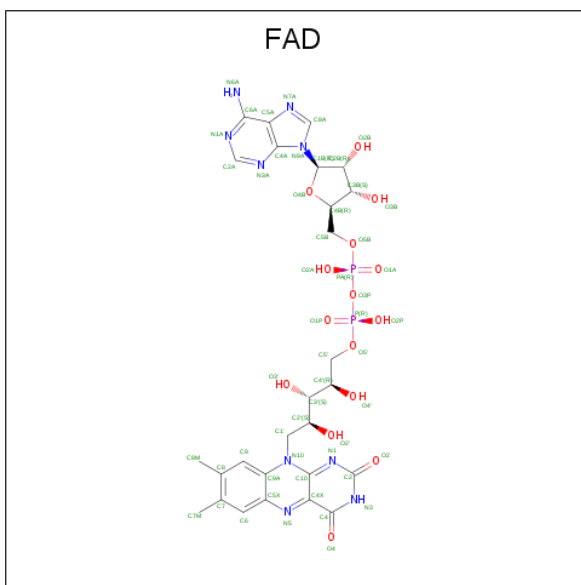
- Molecule 2 is a protein called QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			
2	E	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			

- Molecule 3 is a protein called QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C.

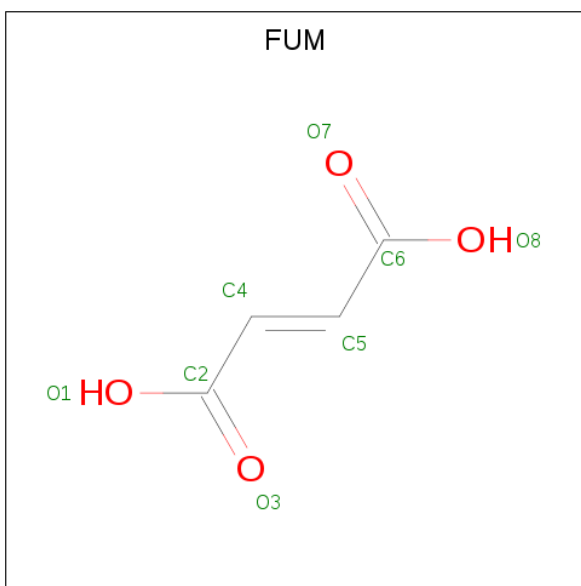
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	255	Total	C	N	O	S	16	2	1
			2099	1398	336	351	14			
3	F	255	Total	C	N	O	S	12	2	1
			2099	1398	336	351	14			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).

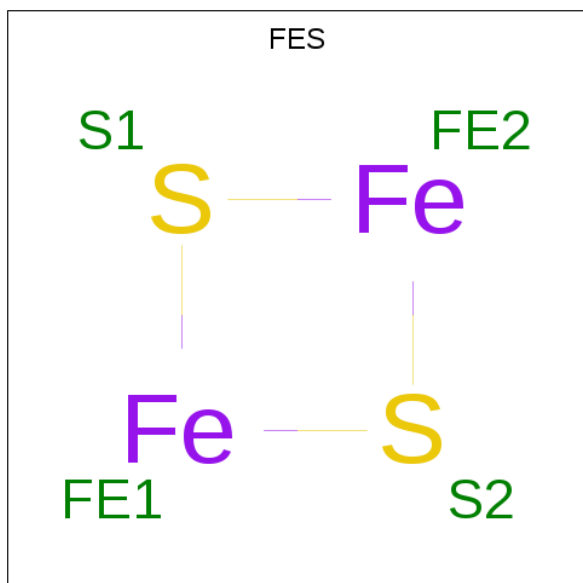


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	C 4	O 4	0	0
5	D	1	Total 8	C 4	O 4	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

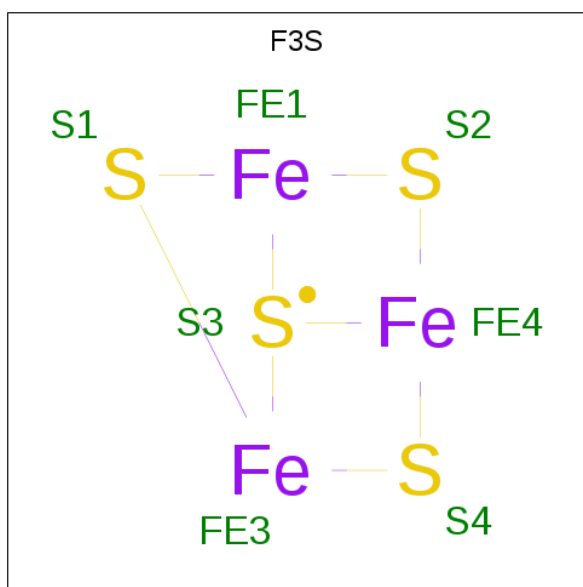
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



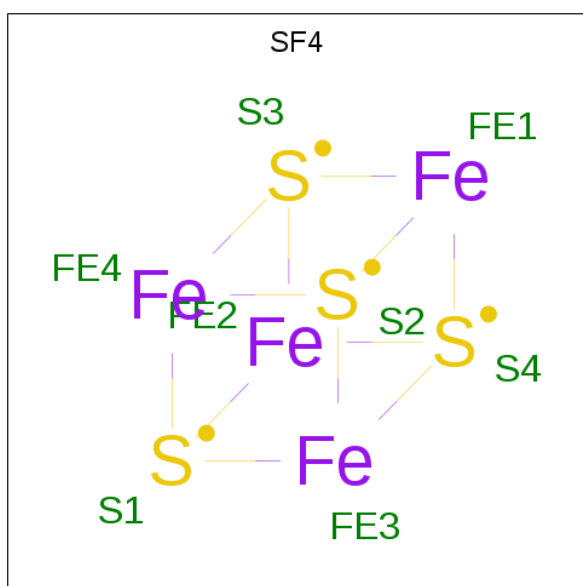
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

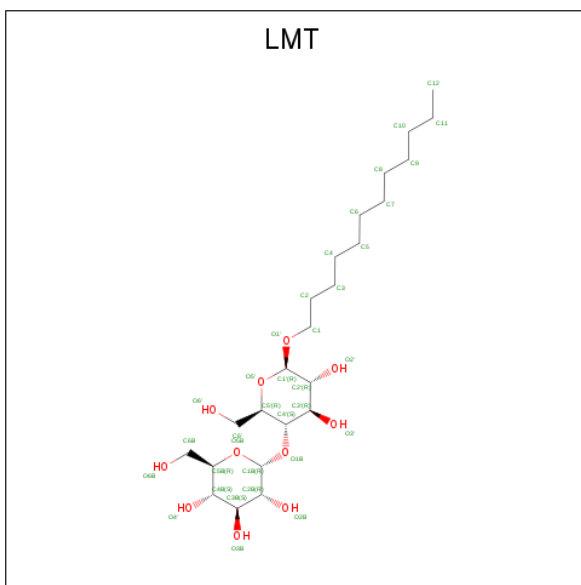


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		

- # HEM

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total 35	C 24	O 11	16	0
11	F	1	Total 35	C 24	O 11	16	0

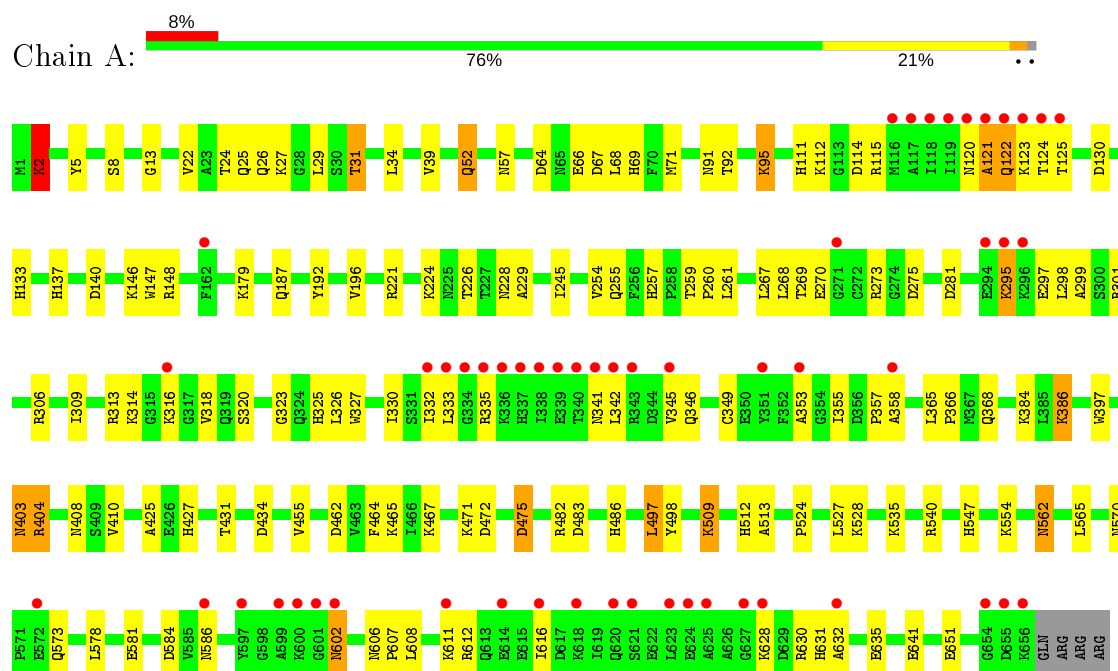
- Molecule 12 is water.

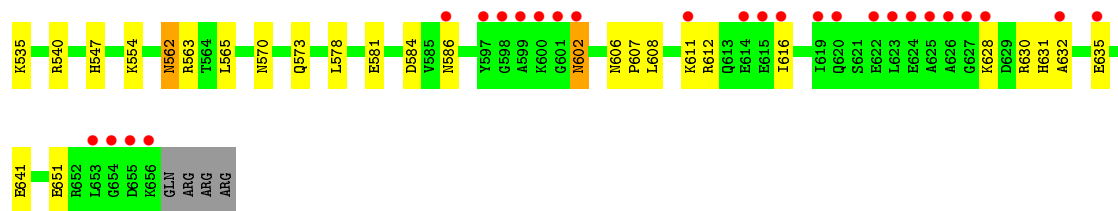
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	273	Total O 273 273	1	0
12	B	155	Total O 155 155	0	0
12	C	55	Total O 55 55	0	0
12	D	287	Total O 287 287	4	0
12	E	164	Total O 164 164	0	0
12	F	56	Total O 56 56	0	0

3 Residue-property plots

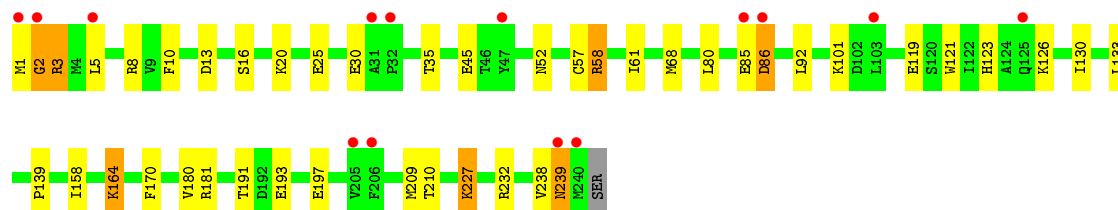
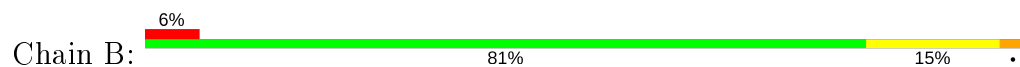
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

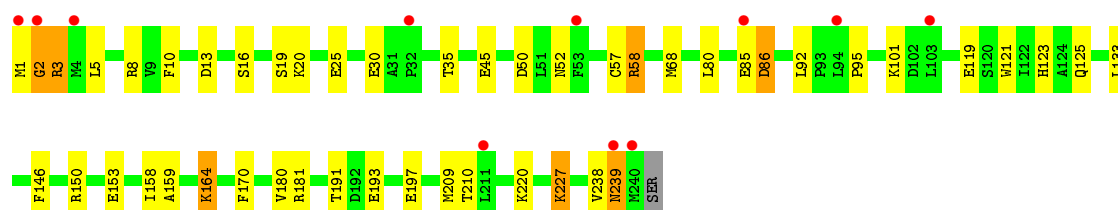
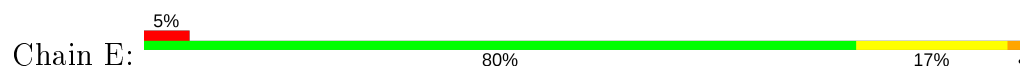




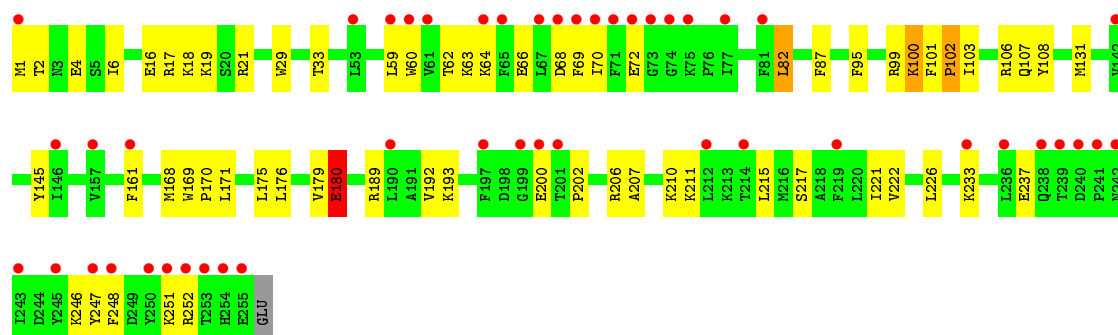
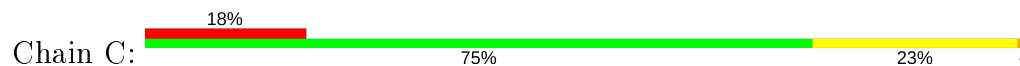
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B



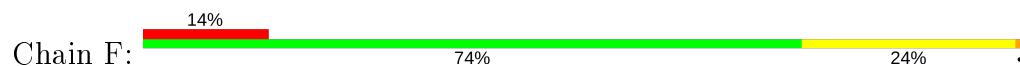
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

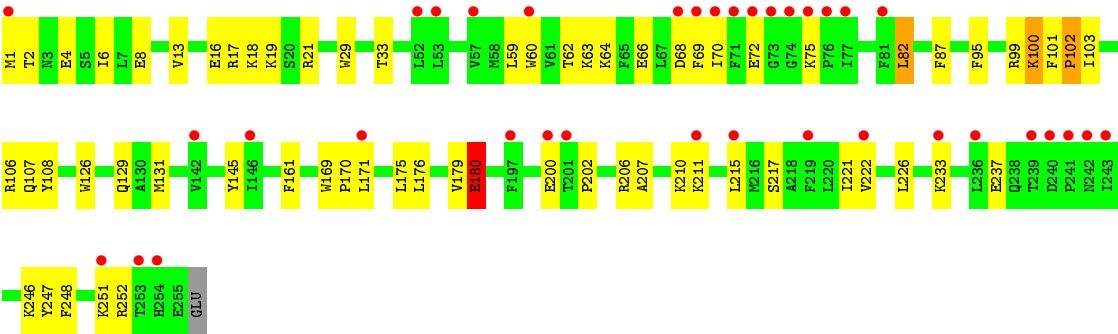


• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C



• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.10Å 188.77Å 117.82Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	28.70 – 1.78 28.70 – 1.78	Depositor EDS
% Data completeness (in resolution range)	92.5 (28.70-1.78) 92.3 (28.70-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.237 0.224 , 0.231	Depositor DCC
R_{free} test set	4488 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19666	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.55% 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: NA, SF4, LMT, F3S, FES, HEM, FUM, FAD

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	2.00	2/5241 (0.0%)	0.61	3/7063 (0.0%)
1	D	0.32	0/5221	0.59	1/7038 (0.0%)
2	B	0.34	0/1939	0.59	0/2616
2	E	0.35	0/1939	0.59	0/2616
3	C	2.35	2/2165 (0.1%)	2.34	3/2930 (0.1%)
3	F	7.27	6/2165 (0.3%)	2.64	9/2930 (0.3%)
All	All	2.82	10/18670 (0.1%)	1.31	16/25193 (0.1%)

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
3	C	0	1
3	F	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	180[A]	GLU	CD-OE2	220.23	3.67	1.25
3	F	180[B]	GLU	CD-OE2	220.23	3.67	1.25
1	A	2[A]	LYS	CE-NZ	101.15	4.01	1.49
1	A	2[B]	LYS	CE-NZ	101.15	4.01	1.49
3	F	180[A]	GLU	CG-CD	83.46	2.77	1.51
3	F	180[B]	GLU	CG-CD	83.46	2.77	1.51
3	C	180[A]	GLU	CD-OE2	76.70	2.10	1.25
3	C	180[B]	GLU	CD-OE2	76.70	2.10	1.25
3	F	180[A]	GLU	CD-OE1	40.43	1.70	1.25
3	F	180[B]	GLU	CD-OE1	40.43	1.70	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	180[A]	GLU	OE1-CD-OE2	-87.28	18.56	123.30
3	C	180[B]	GLU	OE1-CD-OE2	-87.28	18.56	123.30
3	F	180[A]	GLU	OE1-CD-OE2	-84.43	21.99	123.30
3	F	180[B]	GLU	OE1-CD-OE2	-84.43	21.99	123.30
3	F	180[A]	GLU	CG-CD-OE2	-38.95	40.40	118.30
3	F	180[B]	GLU	CG-CD-OE2	-38.95	40.40	118.30
3	F	180[A]	GLU	CG-CD-OE1	-29.66	58.98	118.30
3	F	180[B]	GLU	CG-CD-OE1	-29.66	58.98	118.30
3	F	180[A]	GLU	CB-CG-CD	-18.86	63.28	114.20
3	F	180[B]	GLU	CB-CG-CD	-18.86	63.28	114.20
1	A	2[A]	LYS	CD-CE-NZ	-10.05	88.58	111.70
1	A	2[B]	LYS	CD-CE-NZ	-10.05	88.58	111.70
3	F	102	PRO	N-CA-C	-5.60	97.55	112.10
3	C	102	PRO	N-CA-C	-5.58	97.60	112.10
1	D	397	TRP	N-CA-C	-5.19	96.98	111.00
1	A	397	TRP	N-CA-C	-5.17	97.05	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	180[A]	GLU	Sidechain
3	F	180[A]	GLU	Sidechain

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	5145	0	5124	126	0
1	D	5125	0	5100	128	0
2	B	1902	0	1869	44	0
2	E	1902	0	1869	49	0
3	C	2099	0	2111	56	0
3	F	2099	0	2111	67	0
4	A	53	0	29	3	0
4	D	53	0	29	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	2	0	0
5	D	8	0	2	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
8	B	7	0	0	0	0
8	E	7	0	0	0	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
10	C	86	0	60	1	0
10	F	86	0	60	1	0
11	C	35	0	46	8	0
11	F	35	0	46	9	0
12	A	273	0	0	9	0
12	B	155	0	0	3	0
12	C	55	0	0	1	0
12	D	287	0	0	5	0
12	E	164	0	0	2	0
12	F	56	0	0	1	0
All	All	19666	0	18458	444	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 (444) 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)
3:F:180[B]:GLU:CG	3:F:180[B]:GLU:CD	1.80	1.47
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:OE1	1.70	1.31
3:F:180[B]:GLU:HG2	3:F:180[B]:GLU:OE1	1.47	1.11
2:B:1:MET:HG2	2:B:2:GLY:H	1.24	1.01
2:E:1:MET:HG2	2:E:2:GLY:H	1.24	0.98
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:HB2	1.84	0.97
1:D:64:ASP:HB2	1:D:146:LYS:HG2	1.47	0.96
1:A:64:ASP:HB2	1:A:146:LYS:HG2	1.47	0.95
3:F:180[A]:GLU:OE2	3:F:180[A]:GLU:HG3	1.68	0.93
2:B:8:ARG:HG2	2:B:25:GLU:HG2	1.52	0.90
2:E:8:ARG:HG2	2:E:25:GLU:HG2	1.53	0.89
1:D:27:LYS:HD2	1:D:425:ALA:HB1	1.56	0.86
1:A:27:LYS:HD2	1:A:425:ALA:HB1	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:MET:SD	3:F:100:LYS:HG3	2.17	0.85
1:A:52:GLN:HG2	1:A:69:HIS:NE2	1.92	0.85
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:HG2	1.76	0.84
2:B:209:MET:SD	3:C:100:LYS:HG3	2.17	0.84
1:D:52:GLN:HG2	1:D:69:HIS:NE2	1.92	0.83
1:A:535:LYS:HG3	1:A:578:LEU:HD11	1.60	0.83
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:CB	2.49	0.81
1:D:535:LYS:HG3	1:D:578:LEU:HD11	1.61	0.81
3:F:131:MET:HG2	11:F:1257:LMT:H123	1.63	0.80
1:A:330:ILE:HD11	1:A:357:PRO:HB2	1.63	0.80
3:F:103:ILE:H	3:F:107:GLN:NE2	1.80	0.80
3:C:131:MET:HG2	11:C:1257:LMT:H123	1.63	0.79
1:D:330:ILE:HD11	1:D:357:PRO:HB2	1.63	0.79
1:D:112:LYS:H	1:D:133:HIS:HD2	1.31	0.79
2:E:180:VAL:HG11	2:E:227:LYS:HG3	1.65	0.78
3:C:103:ILE:H	3:C:107:GLN:NE2	1.82	0.78
1:A:611:LYS:NZ	1:A:611:LYS:HB3	2.00	0.76
1:D:611:LYS:NZ	1:D:611:LYS:HB3	2.00	0.76
1:D:628:LYS:HG3	1:D:632:ALA:HB3	1.68	0.76
1:A:628:LYS:HG3	1:A:632:ALA:HB3	1.67	0.76
2:E:238:VAL:O	2:E:239:ASN:HB2	1.85	0.75
1:A:112:LYS:H	1:A:133:HIS:HD2	1.32	0.75
2:B:180:VAL:HG11	2:B:227:LYS:HG3	1.67	0.75
3:C:180[B]:GLU:HG3	3:C:180[B]:GLU:OE2	1.87	0.74
1:D:268:LEU:HD22	1:D:345:VAL:HG23	1.70	0.74
1:A:346:GLN:HA	1:A:357:PRO:HG3	1.70	0.74
2:E:1:MET:HG2	2:E:2:GLY:N	2.02	0.74
2:B:238:VAL:O	2:B:239:ASN:HB2	1.86	0.74
1:D:179:LYS:HG3	1:D:196:VAL:HG11	1.70	0.73
1:D:112:LYS:HG3	1:D:130:ASP:HA	1.70	0.73
1:D:482:ARG:HH11	1:D:547:HIS:HD2	1.36	0.73
1:D:346:GLN:HA	1:D:357:PRO:HG3	1.69	0.73
1:A:179:LYS:HG3	1:A:196:VAL:HG11	1.70	0.72
1:A:268:LEU:HD22	1:A:345:VAL:HG23	1.70	0.72
1:A:112:LYS:HG3	1:A:130:ASP:HA	1.70	0.72
1:A:482:ARG:HH11	1:A:547:HIS:HD2	1.36	0.72
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:CG	2.38	0.72
1:A:179:LYS:HG3	1:A:196:VAL:CG1	2.20	0.71
1:D:179:LYS:HG3	1:D:196:VAL:CG1	2.20	0.71
3:C:4:GLU:H	3:C:4:GLU:CD	1.94	0.71
2:B:1:MET:HG2	2:B:2:GLY:N	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:GLU:CD	3:F:4:GLU:H	1.94	0.70
3:F:180[A]:GLU:CG	3:F:180[A]:GLU:OE2	2.38	0.70
3:F:180[A]:GLU:CG	3:F:180[A]:GLU:OE1	2.39	0.70
3:C:95:PHE:HE1	11:F:1257:LMT:H101	1.58	0.69
3:F:131:MET:HG2	11:F:1257:LMT:C12	2.23	0.68
3:C:131:MET:HG2	11:C:1257:LMT:C12	2.23	0.67
1:D:320:SER:HB3	1:D:323:GLY:O	1.94	0.67
1:A:386:LYS:HG3	12:A:2164:HOH:O	1.95	0.66
1:D:386:LYS:HG3	12:D:2164:HOH:O	1.95	0.66
1:A:320:SER:HB3	1:A:323:GLY:O	1.94	0.66
1:D:121:ALA:O	1:D:122:GLN:HG3	1.96	0.66
1:A:64:ASP:CB	1:A:146:LYS:HG2	2.25	0.66
2:E:191:THR:OG1	2:E:193:GLU:HG2	1.96	0.65
1:D:64:ASP:CB	1:D:146:LYS:HG2	2.25	0.65
1:D:540:ARG:HH22	1:D:562:ASN:ND2	1.95	0.65
1:A:540:ARG:HH22	1:A:562:ASN:ND2	1.93	0.65
2:B:126:LYS:HG2	12:B:2083:HOH:O	1.96	0.65
1:A:342:LEU:HB3	1:A:345:VAL:HG12	1.79	0.64
3:C:69:PHE:CD1	3:C:70:ILE:HG13	2.32	0.64
3:F:69:PHE:HD1	3:F:70:ILE:HG13	1.62	0.64
2:E:68:MET:HB2	2:E:92:LEU:HB2	1.79	0.64
1:A:121:ALA:O	1:A:122:GLN:HG3	1.97	0.64
2:B:191:THR:OG1	2:B:193:GLU:HG2	1.97	0.64
2:B:119:GLU:OE1	2:B:123:HIS:HE1	1.80	0.64
2:B:68:MET:HB2	2:B:92:LEU:HB2	1.80	0.64
2:E:119:GLU:OE1	2:E:123:HIS:HE1	1.81	0.64
1:A:342:LEU:HB3	1:A:345:VAL:CG1	2.29	0.63
3:F:69:PHE:CD1	3:F:70:ILE:HG13	2.32	0.63
1:D:342:LEU:HB3	1:D:345:VAL:CG1	2.28	0.63
1:D:342:LEU:HB3	1:D:345:VAL:HG12	1.79	0.63
1:D:115[A]:ARG:HD2	1:D:117:ALA:HB2	1.81	0.63
1:D:64:ASP:HB2	1:D:146:LYS:CG	2.27	0.63
3:C:69:PHE:HD1	3:C:70:ILE:HG13	1.62	0.63
1:A:540:ARG:HH22	1:A:562:ASN:HD22	1.45	0.63
1:D:221:ARG:HD2	1:D:226:THR:HG21	1.81	0.63
1:D:540:ARG:HH22	1:D:562:ASN:HD22	1.46	0.62
3:C:1:MET:HE3	3:C:6:ILE:HD11	1.82	0.62
1:A:342:LEU:O	1:A:345:VAL:HG12	2.00	0.62
1:A:27:LYS:HD2	1:A:425:ALA:CB	2.29	0.61
1:A:651:GLU:OE2	2:B:133:LEU:HD23	2.01	0.61
1:D:224:LYS:HB3	1:D:475:ASP:OD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HG2	2:B:3:ARG:H	1.66	0.61
3:C:103:ILE:H	3:C:107:GLN:HE21	1.48	0.61
2:B:2:GLY:O	2:B:30:GLU:HB3	2.01	0.61
1:D:342:LEU:O	1:D:345:VAL:HG12	2.00	0.61
3:F:103:ILE:H	3:F:107:GLN:HE21	1.48	0.61
2:E:2:GLY:O	2:E:30:GLU:HB3	2.01	0.61
3:F:180[B]:GLU:CB	3:F:180[B]:GLU:CD	2.63	0.61
1:A:64:ASP:HB2	1:A:146:LYS:CG	2.26	0.61
1:D:295:LYS:HG2	1:D:299:ALA:HA	1.83	0.60
3:F:180[B]:GLU:CG	3:F:180[B]:GLU:OE1	2.38	0.60
1:D:651:GLU:OE2	2:E:133:LEU:HD23	2.00	0.60
2:E:1:MET:HG2	2:E:3:ARG:H	1.66	0.60
1:D:27:LYS:HD2	1:D:425:ALA:CB	2.30	0.60
2:E:180:VAL:HG11	2:E:227:LYS:CG	2.32	0.59
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:OE1	2.19	0.59
1:A:221:ARG:HD2	1:A:226:THR:HG21	1.84	0.59
3:F:180[A]:GLU:OE1	3:F:180[A]:GLU:OE2	2.20	0.59
2:E:13:ASP:HA	2:E:101:LYS:HG3	1.84	0.59
3:F:233:LYS:O	3:F:237:GLU:HG3	2.03	0.59
3:C:17:ARG:NH1	2:E:16:SER:O	2.35	0.59
1:A:295:LYS:HG2	1:A:299:ALA:HA	1.83	0.59
2:B:13:ASP:HA	2:B:101:LYS:HG3	1.84	0.59
1:D:257:HIS:HD2	1:D:259:THR:H	1.51	0.59
11:C:1257:LMT:H101	3:F:95:PHE:HE1	1.68	0.59
2:B:180:VAL:HG11	2:B:227:LYS:CG	2.33	0.58
1:D:92:THR:O	1:D:95:LYS:HG3	2.03	0.58
3:C:233:LYS:O	3:C:237:GLU:HG3	2.03	0.58
2:E:2:GLY:O	2:E:3:ARG:HG2	2.04	0.58
2:B:2:GLY:O	2:B:3:ARG:HG2	2.03	0.58
1:A:332:ILE:HD12	1:A:333:LEU:N	2.19	0.58
1:A:224:LYS:HB3	1:A:475:ASP:OD2	2.03	0.58
1:A:562:ASN:HD22	1:A:562:ASN:C	2.07	0.58
1:A:92:THR:O	1:A:95:LYS:HG3	2.04	0.58
1:D:562:ASN:C	1:D:562:ASN:HD22	2.06	0.57
1:A:257:HIS:HD2	1:A:259:THR:H	1.51	0.57
1:A:257:HIS:CE1	1:A:267:LEU:HD11	2.39	0.57
1:D:257:HIS:CE1	1:D:267:LEU:HD11	2.39	0.57
3:F:207:ALA:O	3:F:211:LYS:HG3	2.04	0.57
1:A:498:TYR:HA	1:A:527:LEU:HD13	1.87	0.57
3:C:206:ARG:O	3:C:210:LYS:HG3	2.04	0.57
1:D:464:PHE:CD1	2:E:45:GLU:HG2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:ASN:O	1:D:573:GLN:HG2	2.05	0.57
1:A:455:VAL:O	1:A:509:LYS:HD2	2.04	0.57
3:C:207:ALA:O	3:C:211:LYS:HG3	2.05	0.57
3:F:206:ARG:O	3:F:210:LYS:HG3	2.04	0.57
1:D:455:VAL:O	1:D:509:LYS:HD2	2.05	0.57
1:D:332:ILE:HD12	1:D:333:LEU:N	2.19	0.56
1:A:8:SER:HB2	1:A:31:THR:HB	1.87	0.56
3:F:102:PRO:O	11:F:1257:LMT:H62	2.05	0.56
3:C:102:PRO:O	11:C:1257:LMT:H62	2.06	0.56
3:C:95:PHE:CE1	11:F:1257:LMT:H51	2.42	0.55
2:E:121:TRP:O	2:E:123:HIS:HD2	1.89	0.55
1:A:306:ARG:HD2	12:A:2241:HOH:O	2.07	0.55
1:D:498:TYR:HA	1:D:527:LEU:HD13	1.87	0.55
1:A:611:LYS:HZ3	1:A:611:LYS:HB3	1.72	0.54
2:B:85:GLU:O	2:B:86:ASP:HB2	2.07	0.54
2:E:85:GLU:O	2:E:86:ASP:HB2	2.07	0.54
3:F:248:PHE:HE2	3:F:252:ARG:HH21	1.55	0.54
3:C:211:LYS:O	3:C:215:LEU:HD23	2.07	0.54
3:C:217:SER:O	3:C:221:ILE:HG12	2.08	0.54
1:A:570:ASN:O	1:A:573:GLN:HG2	2.06	0.54
2:E:10:PHE:HB2	2:E:92:LEU:HD23	1.90	0.54
3:F:217:SER:O	3:F:221:ILE:HG12	2.07	0.54
1:A:464:PHE:CD1	2:B:45:GLU:HG2	2.42	0.54
3:F:180[B]:GLU:OE2	3:F:180[B]:GLU:CD	2.46	0.54
1:A:114:ASP:HB3	1:A:125:THR:HG21	1.89	0.54
2:B:121:TRP:O	2:B:123:HIS:HD2	1.91	0.53
2:B:197:GLU:OE1	3:C:19:LYS:HG3	2.08	0.53
2:E:197:GLU:O	3:F:19:LYS:HD2	2.09	0.53
1:A:260:PRO:HD2	1:A:365:LEU:O	2.07	0.53
3:C:169:TRP:N	3:C:170:PRO:HD2	2.24	0.53
1:D:114:ASP:HB3	1:D:125:THR:HG21	1.89	0.53
3:F:211:LYS:O	3:F:215:LEU:HD23	2.09	0.53
2:B:10:PHE:HB2	2:B:92:LEU:HD23	1.90	0.53
3:C:248:PHE:HE2	3:C:252:ARG:HH21	1.56	0.53
3:C:145:TYR:OH	3:F:170:PRO:HG2	2.09	0.53
2:B:197:GLU:O	3:C:19:LYS:HD2	2.09	0.53
2:B:158:ILE:HG23	2:B:164:LYS:HD3	1.91	0.53
1:D:8:SER:HB2	1:D:31:THR:HB	1.91	0.53
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:CG	2.77	0.52
1:A:112:LYS:HG3	1:A:130:ASP:CA	2.40	0.52
1:D:140:ASP:HB2	1:D:147:TRP:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:PRO:HD2	1:D:365:LEU:O	2.08	0.52
3:F:169:TRP:N	3:F:170:PRO:HD2	2.24	0.52
1:A:140:ASP:HB2	1:A:147:TRP:CE2	2.45	0.52
1:D:482:ARG:NH1	1:D:547:HIS:HD2	2.06	0.52
1:D:257:HIS:CD2	1:D:259:THR:H	2.28	0.52
3:C:170:PRO:HG2	3:F:145:TYR:OH	2.09	0.52
1:A:434:ASP:OD1	1:D:434:ASP:OD1	2.28	0.51
1:D:24:THR:OG1	1:D:31:THR:HG21	2.10	0.51
2:E:158:ILE:HG23	2:E:164:LYS:HD3	1.91	0.51
1:A:24:THR:OG1	1:A:31:THR:HG21	2.11	0.51
3:F:1:MET:CE	3:F:6:ILE:HD11	2.41	0.51
1:D:255:GLN:HE21	1:D:403:ASN:ND2	2.08	0.51
2:E:197:GLU:OE1	3:F:19:LYS:HG3	2.10	0.51
1:A:245:ILE:O	1:A:384:LYS:HE2	2.10	0.51
1:A:467:LYS:O	1:A:471:LYS:HG3	2.11	0.51
1:D:122:GLN:O	1:D:124:THR:N	2.36	0.51
1:D:524:PRO:O	1:D:528:LYS:HG3	2.10	0.51
1:A:295:LYS:CG	1:A:299:ALA:HA	2.41	0.51
1:A:52:GLN:HG3	1:A:148:ARG:HD2	1.94	0.51
2:B:61:ILE:HG23	12:B:2038:HOH:O	2.10	0.51
3:C:168:MET:HE2	12:C:2043:HOH:O	2.10	0.51
1:D:295:LYS:CG	1:D:299:ALA:HA	2.41	0.51
1:A:64:ASP:HA	1:A:68:LEU:HD12	1.94	0.50
1:A:257:HIS:CD2	1:A:259:THR:H	2.28	0.50
1:A:325:HIS:HD2	1:A:326:LEU:O	1.94	0.50
3:C:17:ARG:HD2	2:E:19:SER:O	2.11	0.50
3:C:1:MET:CE	3:C:6:ILE:HD11	2.40	0.50
1:A:482:ARG:HH11	1:A:547:HIS:CD2	2.23	0.50
1:D:482:ARG:HH11	1:D:547:HIS:CD2	2.23	0.50
3:F:101:PHE:HB3	11:F:1257:LMT:H71	1.93	0.50
1:A:270:GLU:HG3	1:A:273[A]:ARG:HH22	1.76	0.50
1:A:611:LYS:HZ2	1:A:611:LYS:HB3	1.75	0.50
3:C:16[B]:GLU:HA	2:E:20:LYS:CE	2.42	0.50
3:C:175:LEU:O	3:C:179:VAL:HG12	2.12	0.50
2:E:52:ASN:OD1	2:E:101:LYS:HE3	2.11	0.50
3:C:16[B]:GLU:HA	2:E:20:LYS:HE3	1.92	0.50
2:E:1:MET:CG	2:E:2:GLY:H	2.09	0.50
1:A:255:GLN:HE21	1:A:403:ASN:ND2	2.10	0.50
1:A:482:ARG:NH1	1:A:547:HIS:HD2	2.06	0.50
1:A:257:HIS:O	1:A:366:PRO:HA	2.12	0.50
1:D:245:ILE:O	1:D:384:LYS:HE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:239:ASN:CG	3:F:21:ARG:HE	2.15	0.50
3:C:62:THR:O	3:C:66:GLU:HG3	2.12	0.50
3:F:1:MET:HE1	3:F:6:ILE:HD11	1.93	0.50
1:D:452:LYS:NZ	12:D:2200:HOH:O	2.45	0.49
1:D:281:ASP:HB2	1:D:316:LYS:HG3	1.93	0.49
1:D:64:ASP:HA	1:D:68:LEU:HD12	1.93	0.49
2:E:52:ASN:CG	2:E:101:LYS:HE3	2.33	0.49
2:B:1:MET:CG	2:B:2:GLY:H	2.09	0.49
1:D:467:LYS:O	1:D:471:LYS:HG3	2.11	0.49
3:F:62:THR:O	3:F:66:GLU:HG3	2.12	0.49
1:A:111:HIS:HA	1:A:133:HIS:CD2	2.48	0.49
1:A:631:HIS:O	1:A:635:GLU:HG3	2.12	0.49
1:D:112:LYS:HG3	1:D:130:ASP:CA	2.40	0.49
1:A:228:ASN:HD22	1:A:228:ASN:N	2.10	0.49
1:A:427:HIS:O	1:A:431:THR:HG22	2.13	0.49
1:D:325:HIS:HD2	1:D:326:LEU:O	1.95	0.49
1:D:341:ASN:C	1:D:342:LEU:HD12	2.33	0.49
1:A:281:ASP:HB2	1:A:316:LYS:HG3	1.93	0.49
1:D:651:GLU:HG2	2:E:133:LEU:CD2	2.43	0.49
1:A:524:PRO:O	1:A:528:LYS:HG3	2.12	0.49
1:A:651:GLU:HG2	2:B:133:LEU:CD2	2.43	0.49
2:B:239:ASN:CG	3:C:21:ARG:HE	2.15	0.49
1:D:111:HIS:HA	1:D:133:HIS:CD2	2.48	0.49
3:C:101:PHE:HB3	11:C:1257:LMT:H71	1.94	0.48
1:D:52:GLN:HG3	1:D:148:ARG:HD2	1.94	0.48
3:C:99:ARG:HG2	11:F:1257:LMT:H32	1.95	0.48
3:F:175:LEU:O	3:F:179:VAL:HG12	2.13	0.48
1:A:462:ASP:HB3	1:A:465:LYS:HD3	1.94	0.48
2:B:52:ASN:CG	2:B:101:LYS:HE3	2.33	0.48
1:D:259:THR:N	1:D:260:PRO:HD3	2.29	0.48
1:D:611:LYS:HZ2	1:D:611:LYS:HB3	1.74	0.48
1:A:341:ASN:C	1:A:342:LEU:HD12	2.33	0.48
1:A:384:LYS:NZ	12:A:2166:HOH:O	2.44	0.48
1:D:427:HIS:O	1:D:431:THR:HG22	2.13	0.48
1:D:462:ASP:HB3	1:D:465:LYS:HD3	1.95	0.48
1:D:631:HIS:O	1:D:635:GLU:HG3	2.12	0.48
1:D:228:ASN:N	1:D:228:ASN:HD22	2.12	0.48
1:D:257:HIS:O	1:D:366:PRO:HA	2.13	0.48
1:D:190:LYS:HE3	12:D:2069:HOH:O	2.14	0.48
1:D:342:LEU:HD12	1:D:342:LEU:N	2.29	0.48
1:A:179:LYS:CG	1:A:196:VAL:HG11	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LYS:CG	1:D:196:VAL:HG11	2.42	0.47
3:F:2:THR:OG1	3:F:4:GLU:HG2	2.15	0.47
1:A:410:VAL:HG13	4:A:1656:FAD:C2	2.44	0.47
1:D:384:LYS:NZ	12:D:2165:HOH:O	2.43	0.47
1:D:309:ILE:O	1:D:313:ARG:HG3	2.14	0.47
11:C:1257:LMT:H32	3:F:99:ARG:HG2	1.97	0.47
1:A:342:LEU:HD12	1:A:342:LEU:N	2.30	0.47
1:D:67:ASP:OD2	1:D:630:ARG:HD2	2.14	0.47
1:A:120:ASN:HB3	1:A:298:LEU:CD1	2.45	0.47
1:A:25:GLN:OE1	1:A:31:THR:HG23	2.14	0.47
2:B:130:ILE:HG12	12:B:2087:HOH:O	2.14	0.47
3:C:16[A]:GLU:HA	2:E:20:LYS:HE3	1.95	0.47
3:C:16[A]:GLU:HA	2:E:20:LYS:CE	2.45	0.47
1:D:410:VAL:HG13	4:D:1656:FAD:C2	2.45	0.47
1:D:120:ASN:HB3	1:D:298:LEU:CD1	2.45	0.47
1:A:259:THR:N	1:A:260:PRO:HD3	2.30	0.47
1:D:120:ASN:HB3	1:D:298:LEU:HD13	1.97	0.47
1:D:66:GLU:HG2	1:D:91:ASN:HD22	1.79	0.47
1:A:120:ASN:HB3	1:A:298:LEU:HD13	1.97	0.47
2:B:2:GLY:O	2:B:3:ARG:CG	2.64	0.47
3:F:108:TYR:CD2	11:F:1257:LMT:H52	2.50	0.47
1:A:270:GLU:HG3	1:A:273[A]:ARG:NH2	2.30	0.46
1:A:607:PRO:HG2	1:A:608:LEU:HD12	1.97	0.46
3:C:108:TYR:CD2	11:C:1257:LMT:H52	2.50	0.46
3:C:176:LEU:O	3:C:180[B]:GLU:HB2	2.15	0.46
1:D:607:PRO:HG2	1:D:608:LEU:HD12	1.96	0.46
1:A:115[B]:ARG:HB2	12:A:2055:HOH:O	2.15	0.46
2:E:57:CYS:O	2:E:58:ARG:HG3	2.14	0.46
1:A:554:LYS:HG2	1:A:602:ASN:ND2	2.31	0.46
1:A:273[A]:ARG:NH1	1:A:273[A]:ARG:HB2	2.30	0.46
1:A:67:ASP:OD2	1:A:630:ARG:HD2	2.15	0.46
1:D:261:LEU:HD21	1:D:353:ALA:HB2	1.97	0.46
1:D:611:LYS:HZ3	1:D:611:LYS:HB3	1.75	0.46
1:A:410:VAL:HG13	4:A:1656:FAD:N1	2.31	0.46
2:B:52:ASN:OD1	2:B:101:LYS:HE3	2.15	0.46
3:C:2:THR:OG1	3:C:4:GLU:HG2	2.15	0.46
1:A:122:GLN:O	1:A:124:THR:N	2.37	0.46
1:D:187:GLN:HB3	1:D:192:TYR:HE2	1.81	0.46
2:B:57:CYS:O	2:B:58:ARG:HG3	2.16	0.46
1:A:13:GLY:HA3	1:A:39:VAL:HG12	1.98	0.45
1:A:540:ARG:NH2	1:A:562:ASN:ND2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:GLY:O	2:E:3:ARG:CG	2.64	0.45
3:F:171:LEU:HD23	3:F:171:LEU:C	2.37	0.45
1:A:187:GLN:HB3	1:A:192:TYR:HE2	1.81	0.45
1:A:309:ILE:O	1:A:313:ARG:HG3	2.16	0.45
1:A:261:LEU:HD21	1:A:353:ALA:HB2	1.98	0.45
1:A:297:GLU:CD	1:A:297:GLU:H	2.19	0.45
1:A:5:TYR:CD1	1:A:5:TYR:C	2.89	0.45
1:A:66:GLU:HG2	1:A:91:ASN:HD22	1.80	0.45
3:C:59:LEU:HD22	3:C:252:ARG:NH1	2.32	0.45
4:D:1656:FAD:H1'1	4:D:1656:FAD:H9	1.61	0.45
3:C:171:LEU:HD23	3:C:171:LEU:C	2.36	0.45
3:F:59:LEU:HD22	3:F:252:ARG:NH1	2.32	0.45
1:D:13:GLY:HA3	1:D:39:VAL:HG12	1.98	0.45
1:D:410:VAL:HG13	4:D:1656:FAD:N1	2.32	0.45
2:E:125:GLN:HG2	12:E:2094:HOH:O	2.16	0.45
1:D:5:TYR:CD1	1:D:5:TYR:C	2.89	0.45
1:D:554:LYS:HG2	1:D:602:ASN:ND2	2.31	0.45
2:E:52:ASN:OD1	2:E:101:LYS:CE	2.64	0.45
3:F:176:LEU:O	3:F:180[B]:GLU:HB2	2.17	0.45
2:B:193:GLU:H	2:B:193:GLU:CD	2.21	0.44
2:B:35:THR:HG22	2:B:80:LEU:HD23	1.98	0.44
11:C:1257:LMT:H51	3:F:95:PHE:CE1	2.52	0.44
1:D:221:ARG:HD3	1:D:229:ALA:O	2.17	0.44
1:D:540:ARG:NH2	1:D:562:ASN:ND2	2.64	0.44
1:A:455:VAL:CG1	1:A:509:LYS:HG3	2.48	0.44
1:A:554:LYS:HG2	1:A:602:ASN:HD22	1.83	0.44
2:E:193:GLU:CD	2:E:193:GLU:H	2.20	0.44
2:E:35:THR:HG22	2:E:80:LEU:HD23	2.00	0.44
1:A:608:LEU:HD12	1:A:608:LEU:N	2.33	0.44
1:D:25:GLN:OE1	1:D:31:THR:HG23	2.18	0.44
1:D:422:GLU:HG2	12:D:2177:HOH:O	2.18	0.44
1:D:49:GLY:HA2	1:D:139[A]:ARG:HH21	1.82	0.44
1:A:34:LEU:HD22	1:A:179:LYS:HG2	2.00	0.44
1:A:2[A]:LYS:HE3	12:A:2108:HOH:O	2.18	0.44
2:B:85:GLU:HA	2:B:85:GLU:OE2	2.18	0.43
3:F:247:TYR:O	3:F:251:LYS:HG3	2.18	0.43
3:F:8:GLU:HA	3:F:13:VAL:O	2.18	0.43
2:E:210:THR:HG22	2:E:210:THR:O	2.18	0.43
3:F:82:LEU:HD12	10:F:1256:HEM:CBB	2.49	0.43
1:A:497:LEU:HA	1:A:497:LEU:HD12	1.86	0.43
1:A:52:GLN:HE21	1:A:52:GLN:HB2	1.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:THR:HB	3:C:4:GLU:OE2	2.18	0.43
1:D:554:LYS:HG2	1:D:602:ASN:HD22	1.83	0.43
3:F:2:THR:HB	3:F:4:GLU:OE2	2.19	0.43
2:B:164:LYS:HG2	2:B:170:PHE:HD2	1.84	0.43
2:E:5:LEU:HD11	2:E:30:GLU:HB2	2.01	0.43
1:A:318:VAL:HG21	1:A:327:TRP:NE1	2.33	0.43
1:D:314:LYS:NZ	1:D:314:LYS:HB3	2.34	0.43
2:E:164:LYS:HG2	2:E:170:PHE:HD2	1.83	0.43
2:B:16:SER:O	3:F:17:ARG:NH1	2.45	0.42
1:D:124:THR:OG1	1:D:125:THR:N	2.52	0.42
1:A:584:ASP:OD1	1:A:586:ASN:HB2	2.19	0.42
3:F:29:TRP:O	3:F:33:THR:HG23	2.19	0.42
1:A:254:VAL:CG1	1:A:368:GLN:HG2	2.49	0.42
1:D:455:VAL:HG13	1:D:509:LYS:HG3	2.02	0.42
2:E:95:PRO:HD2	2:E:159:ALA:HB1	2.01	0.42
3:F:126:TRP:O	3:F:129:GLN:HB2	2.19	0.42
1:A:335:ARG:NH1	1:A:358:ALA:HB3	2.35	0.42
3:C:200:GLU:C	3:C:202:PRO:HD3	2.40	0.42
2:E:85:GLU:OE2	2:E:85:GLU:HA	2.19	0.42
1:A:115[A]:ARG:HB2	12:A:2055:HOH:O	2.20	0.42
1:A:608:LEU:HD12	1:A:608:LEU:H	1.84	0.42
3:C:59:LEU:O	3:C:63:LYS:HG3	2.20	0.42
2:B:52:ASN:OD1	2:B:101:LYS:CE	2.67	0.42
1:D:286:ARG:NH2	1:D:296:LYS:HE2	2.35	0.42
1:D:254:VAL:CG1	1:D:368:GLN:HG2	2.50	0.42
3:C:247:TYR:O	3:C:251:LYS:HG3	2.19	0.42
3:C:63:LYS:HE2	3:C:68:ASP:OD2	2.20	0.42
1:D:584:ASP:OD1	1:D:586:ASN:HB2	2.19	0.42
2:E:121:TRP:O	2:E:123:HIS:CD2	2.72	0.42
1:A:95:LYS:HE3	1:A:95:LYS:HB3	1.91	0.42
1:D:34:LEU:HD22	1:D:179:LYS:HG2	2.01	0.42
1:D:455:VAL:CG1	1:D:509:LYS:HG3	2.49	0.42
1:D:224:LYS:HD3	1:D:472:ASP:OD1	2.20	0.42
1:A:349:CYS:HB3	1:A:355:ILE:HG13	2.00	0.42
3:C:161:PHE:CD2	3:C:246:LYS:HE3	2.55	0.42
2:B:232:ARG:CZ	3:C:193:LYS:HD2	2.50	0.42
3:C:29:TRP:O	3:C:33:THR:HG23	2.20	0.42
1:D:565:LEU:HD11	1:D:581:GLU:HB2	2.01	0.42
1:D:612:ARG:O	1:D:616:ILE:HG13	2.19	0.42
3:F:200:GLU:C	3:F:202:PRO:HD3	2.40	0.42
3:F:59:LEU:O	3:F:63:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ARG:O	1:A:616:ILE:HG13	2.20	0.41
2:B:210:THR:HG22	2:B:210:THR:O	2.19	0.41
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.85	0.41
1:D:512:HIS:O	1:D:513:ALA:C	2.58	0.41
2:E:50:ASP:HA	12:E:2035:HOH:O	2.20	0.41
3:F:161:PHE:CD2	3:F:246:LYS:HE3	2.55	0.41
1:A:512:HIS:O	1:A:513:ALA:C	2.58	0.41
3:C:82:LEU:HD13	3:C:82:LEU:O	2.20	0.41
1:D:349:CYS:HB3	1:D:355:ILE:HG13	2.01	0.41
1:D:455:VAL:HG13	1:D:509:LYS:CD	2.50	0.41
1:D:606:ASN:OD1	1:D:608:LEU:HD13	2.20	0.41
1:D:608:LEU:N	1:D:608:LEU:HD12	2.34	0.41
1:A:111:HIS:HB3	2:B:139:PRO:HG3	2.03	0.41
1:A:224:LYS:HD3	1:A:472:ASP:OD1	2.21	0.41
1:A:455:VAL:HG13	1:A:509:LYS:HG3	2.01	0.41
2:B:5:LEU:HD11	2:B:30:GLU:HB2	2.01	0.41
3:C:82:LEU:HD12	10:C:1256:HEM:CBB	2.49	0.41
3:F:60:TRP:CZ2	3:F:64:LYS:HD2	2.55	0.41
1:A:455:VAL:HG13	1:A:509:LYS:CD	2.50	0.41
1:A:565:LEU:HD11	1:A:581:GLU:HB2	2.02	0.41
1:A:71:MET:HE2	12:A:2027:HOH:O	2.21	0.41
1:D:268:LEU:HD22	1:D:345:VAL:CG2	2.47	0.41
1:D:300:SER:HB3	1:D:303:VAL:HG23	2.03	0.41
1:A:314:LYS:HB3	1:A:314:LYS:NZ	2.35	0.41
1:A:29:LEU:O	1:A:31:THR:HG22	2.19	0.41
1:D:27:LYS:HB3	1:D:27:LYS:HE3	1.89	0.41
1:D:335:ARG:NH1	1:D:358:ALA:HB3	2.35	0.41
1:D:608:LEU:HD12	1:D:608:LEU:H	1.85	0.41
1:A:221:ARG:HD3	1:A:229:ALA:O	2.21	0.41
1:A:606:ASN:OD1	1:A:608:LEU:HD13	2.20	0.41
1:D:318:VAL:HG21	1:D:327:TRP:NE1	2.35	0.41
3:F:75:LYS:HE2	12:F:2021:HOH:O	2.21	0.41
1:A:224:LYS:NZ	12:A:2207:HOH:O	2.54	0.41
1:A:301:ARG:HH12	1:A:404:ARG:NH1	2.19	0.41
3:C:222:VAL:O	3:C:226:LEU:HG	2.21	0.41
1:D:40:LYS:HE2	2:E:153:GLU:CD	2.41	0.41
1:D:49:GLY:HA2	1:D:139[A]:ARG:NH2	2.35	0.41
1:D:52:GLN:HG2	1:D:69:HIS:CE1	2.54	0.41
2:E:146:PHE:O	2:E:150:ARG:HG3	2.21	0.41
3:F:17:ARG:O	3:F:17:ARG:HG2	2.21	0.41
4:A:1656:FAD:H1'1	4:A:1656:FAD:H9	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:HB2	12:A:2023:HOH:O	2.20	0.41
2:B:227:LYS:HD3	2:B:227:LYS:HA	1.95	0.41
3:F:222:VAL:O	3:F:226:LEU:HG	2.21	0.41
1:A:483:ASP:CG	1:A:486:HIS:HD1	2.25	0.41
3:C:60:TRP:CZ2	3:C:64:LYS:HD2	2.55	0.41
1:D:455:VAL:HG13	1:D:509:LYS:HD3	2.03	0.41
3:F:63:LYS:HE2	3:F:68:ASP:OD2	2.20	0.41
1:D:496:GLU:O	1:D:500:LYS:HG3	2.21	0.40
1:D:52:GLN:HB3	1:D:408:ASN:HD22	1.87	0.40
2:B:20:LYS:HE3	3:F:16[B]:GLU:HA	2.03	0.40
3:C:169:TRP:N	3:C:170:PRO:CD	2.84	0.40
3:C:189:ARG:HA	3:C:192:VAL:HG22	2.02	0.40
1:D:531:LEU:O	1:D:535:LYS:HB3	2.21	0.40
2:E:220:LYS:HE2	2:E:220:LYS:HA	2.03	0.40
1:A:22:VAL:O	1:A:26:GLN:HG2	2.21	0.40
1:D:489:LYS:HB3	1:D:489:LYS:HE2	1.95	0.40
1:A:52:GLN:HG2	1:A:69:HIS:CE1	2.56	0.40
1:D:29:LEU:O	1:D:31:THR:HG22	2.21	0.40
1:D:341:ASN:HB2	1:D:342:LEU:HD12	2.04	0.40
1:D:398:ASP:OD2	1:D:563:ARG:NE	2.47	0.40
3:F:108:TYR:HD2	11:F:1257:LMT:H52	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	659/660 (100%)	634 (96%)	21 (3%)	4 (1%)	25	11
1	D	657/660 (100%)	631 (96%)	22 (3%)	4 (1%)	25	11
2	B	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	9	2
2	E	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	9	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	34	19
3	F	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	34	19
All	All	2304/2314 (100%)	2213 (96%)	73 (3%)	18 (1%)	19	7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
2	B	86	ASP
3	C	72	GLU
1	D	121	ALA
2	E	86	ASP
3	F	72	GLU
1	A	123	LYS
2	B	3	ARG
1	D	123	LYS
2	E	3	ARG
1	A	269	THR
2	B	239	ASN
1	D	269	THR
2	E	2	GLY
2	E	239	ASN
1	A	122	GLN
2	B	2	GLY
1	D	122	GLN

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	537/537 (100%)	519 (97%)	18 (3%)	37	20
1	D	535/537 (100%)	518 (97%)	17 (3%)	39	22
2	B	212/213 (100%)	208 (98%)	4 (2%)	57	43
2	E	212/213 (100%)	208 (98%)	4 (2%)	57	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	223/223 (100%)	218 (98%)	5 (2%)	52	36
3	F	223/223 (100%)	218 (98%)	5 (2%)	52	36
All	All	1942/1946 (100%)	1889 (97%)	53 (3%)	44	28

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2[A]	LYS
1	A	2[B]	LYS
1	A	31	THR
1	A	52	GLN
1	A	95	LYS
1	A	137	HIS
1	A	275	ASP
1	A	295	LYS
1	A	386	LYS
1	A	403	ASN
1	A	404	ARG
1	A	408	ASN
1	A	475	ASP
1	A	497	LEU
1	A	509	LYS
1	A	562	ASN
1	A	602	ASN
1	A	641	GLU
2	B	58	ARG
2	B	164	LYS
2	B	181	ARG
2	B	227	LYS
3	C	18	LYS
3	C	82	LEU
3	C	87	PHE
3	C	100	LYS
3	C	106	ARG
1	D	31	THR
1	D	52	GLN
1	D	95	LYS
1	D	137	HIS
1	D	263	PRO
1	D	275	ASP
1	D	295	LYS

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Mol	Chain	Res	Type
1	D	386	LYS
1	D	403	ASN
1	D	404	ARG
1	D	408	ASN
1	D	475	ASP
1	D	497	LEU
1	D	509	LYS
1	D	562	ASN
1	D	602	ASN
1	D	641	GLU
2	E	58	ARG
2	E	164	LYS
2	E	181	ARG
2	E	227	LYS
3	F	18	LYS
3	F	82	LEU
3	F	87	PHE
3	F	100	LYS
3	F	106	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	48	GLN
1	A	57	ASN
1	A	91	ASN
1	A	133	HIS
1	A	225	ASN
1	A	228	ASN
1	A	257	HIS
1	A	325	HIS
1	A	403	ASN
1	A	408	ASN
1	A	430	ASN
1	A	468	ASN
1	A	547	HIS
1	A	562	ASN
1	A	586	ASN
1	A	602	ASN
2	B	116	GLN
2	B	123	HIS

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Mol	Chain	Res	Type
2	B	177	ASN
3	C	107	GLN
1	D	26	GLN
1	D	48	GLN
1	D	57	ASN
1	D	91	ASN
1	D	133	HIS
1	D	225	ASN
1	D	228	ASN
1	D	257	HIS
1	D	325	HIS
1	D	403	ASN
1	D	408	ASN
1	D	430	ASN
1	D	468	ASN
1	D	547	HIS
1	D	562	ASN
1	D	586	ASN
1	D	602	ASN
2	E	116	GLN
2	E	123	HIS
2	E	177	ASN
3	F	107	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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$
10	HEM	F	1255	3	27,50,50	1.58	6 (22%)	17,82,82	1.01	2 (11%)
11	LMT	F	1257	-	36,36,36	1.11	2 (5%)	47,47,47	1.27	4 (8%)
4	FAD	D	1656	1	51,58,58	2.14	13 (25%)	60,89,89	2.27	11 (18%)
9	SF4	E	1242	2	0,12,12	0.00	-	-		
7	FES	E	1240	2	0,4,4	0.00	-	-		
5	FUM	D	1657	-	1,7,7	1.49	0	2,8,8	1.02	0
9	SF4	B	1242	2	0,12,12	0.00	-	-		
8	F3S	E	1241	2	0,9,9	0.00	-	-		
5	FUM	A	1657	-	1,7,7	1.50	0	2,8,8	1.06	0
8	F3S	B	1241	2	0,9,9	0.00	-	-		
7	FES	B	1240	2	0,4,4	0.00	-	-		
10	HEM	C	1255	3	27,50,50	1.60	6 (22%)	17,82,82	0.86	0
11	LMT	C	1257	-	36,36,36	1.11	2 (5%)	47,47,47	1.27	4 (8%)
10	HEM	F	1256	3	27,50,50	1.65	6 (22%)	17,82,82	1.19	1 (5%)
4	FAD	A	1656	1	51,58,58	2.30	15 (29%)	60,89,89	2.28	12 (20%)
10	HEM	C	1256	3	27,50,50	1.64	6 (22%)	17,82,82	1.20	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	F	1255	3	-	0/6/54/54	-
9	SF4	B	1242	2	-	-	0/6/5/5
4	FAD	D	1656	1	-	4/30/50/50	0/6/6/6
9	SF4	E	1242	2	-	-	0/6/5/5
7	FES	E	1240	2	-	-	0/1/1/1
5	FUM	D	1657	-	-	0/0/5/5	-
11	LMT	F	1257	-	-	11/21/61/61	0/2/2/2
8	F3S	E	1241	2	-	-	0/3/3/3
5	FUM	A	1657	-	-	0/0/5/5	-
8	F3S	B	1241	2	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	B	1240	2	-	-	0/1/1/1
10	HEM	C	1255	3	-	0/6/54/54	-
11	LMT	C	1257	-	-	11/21/61/61	0/2/2/2
10	HEM	F	1256	3	-	0/6/54/54	-
4	FAD	A	1656	1	-	4/30/50/50	0/6/6/6
10	HEM	C	1256	3	-	0/6/54/54	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1656	FAD	C4X-C10	9.14	1.48	1.38
4	D	1656	FAD	C4X-C10	8.63	1.47	1.38
4	A	1656	FAD	C9A-N10	4.80	1.45	1.38
4	A	1656	FAD	O4B-C1B	4.55	1.47	1.41
4	D	1656	FAD	O4B-C1B	4.38	1.47	1.41
10	F	1256	HEM	C3B-CAB	-4.10	1.39	1.47
10	C	1256	HEM	C3B-CAB	-3.98	1.39	1.47
4	A	1656	FAD	PA-O2A	-3.83	1.37	1.55
4	D	1656	FAD	C9A-N10	3.81	1.43	1.38
4	D	1656	FAD	PA-O2A	-3.79	1.37	1.55
4	A	1656	FAD	O5'-C5'	3.69	1.59	1.44
10	C	1256	HEM	C3C-CAC	-3.62	1.40	1.47
4	D	1656	FAD	O5'-C5'	3.60	1.58	1.44
10	C	1255	HEM	C3B-CAB	-3.59	1.40	1.47
10	F	1256	HEM	C3C-CAC	-3.57	1.40	1.47
10	C	1255	HEM	C3C-CAC	-3.55	1.40	1.47
10	F	1255	HEM	C3C-CAC	-3.53	1.40	1.47
4	A	1656	FAD	C2B-C1B	-3.50	1.48	1.53
4	A	1656	FAD	P-O2P	-3.36	1.39	1.55
11	F	1257	LMT	O5B-C1B	3.34	1.50	1.41
10	F	1256	HEM	C3B-C2B	-3.32	1.35	1.40
11	C	1257	LMT	O5B-C1B	3.30	1.50	1.41
10	C	1256	HEM	C3B-C2B	-3.25	1.35	1.40
10	F	1255	HEM	C3B-CAB	-3.17	1.41	1.47
4	A	1656	FAD	C4-N3	3.16	1.38	1.33
10	C	1256	HEM	C3C-C2C	-3.09	1.36	1.40
4	D	1656	FAD	C2B-C1B	-3.06	1.49	1.53
10	F	1256	HEM	C3C-C2C	-3.03	1.36	1.40
10	F	1255	HEM	C3C-C2C	-3.00	1.36	1.40
10	C	1255	HEM	C3C-C2C	-3.00	1.36	1.40
4	D	1656	FAD	P-O2P	-2.99	1.41	1.55
4	D	1656	FAD	C4-N3	2.96	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	1257	LMT	C3'-C4'	2.94	1.60	1.52
10	F	1255	HEM	C3B-C2B	-2.91	1.36	1.40
11	C	1257	LMT	C3'-C4'	2.90	1.60	1.52
10	C	1255	HEM	C3B-C2B	-2.90	1.36	1.40
4	A	1656	FAD	C2-N3	2.65	1.43	1.38
4	D	1656	FAD	C10-N1	2.59	1.36	1.33
4	A	1656	FAD	C10-N1	2.54	1.36	1.33
4	D	1656	FAD	C2-N3	2.54	1.43	1.38
10	F	1255	HEM	CBC-CAC	2.52	1.46	1.29
10	C	1256	HEM	CBC-CAC	2.52	1.46	1.29
10	C	1255	HEM	CBC-CAC	2.47	1.45	1.29
4	A	1656	FAD	C4A-N3A	2.46	1.39	1.35
10	F	1256	HEM	CBB-CAB	2.44	1.45	1.29
10	F	1255	HEM	CBB-CAB	2.43	1.45	1.29
10	F	1256	HEM	CBC-CAC	2.42	1.45	1.29
10	C	1256	HEM	CBB-CAB	2.40	1.45	1.29
10	C	1255	HEM	CBB-CAB	2.37	1.44	1.29
4	A	1656	FAD	C2-N1	-2.27	1.33	1.38
4	D	1656	FAD	C4A-N3A	2.24	1.38	1.35
4	D	1656	FAD	C4X-N5	2.22	1.36	1.33
4	A	1656	FAD	C8-C7	2.19	1.46	1.40
4	A	1656	FAD	C2A-N1A	2.11	1.37	1.33
4	A	1656	FAD	C2A-N3A	2.09	1.35	1.32
4	D	1656	FAD	C4-C4X	2.08	1.44	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1656	FAD	C1'-N10-C10	8.69	126.19	118.41
4	D	1656	FAD	C1'-N10-C10	8.47	126.00	118.41
4	D	1656	FAD	C4-N3-C2	8.02	121.91	115.14
4	A	1656	FAD	C4-N3-C2	7.88	121.80	115.14
4	D	1656	FAD	C1'-N10-C9A	-7.70	112.23	118.29
4	A	1656	FAD	C1'-N10-C9A	-7.65	112.27	118.29
11	F	1257	LMT	C1-O1'-C1'	4.99	122.11	113.84
11	C	1257	LMT	C1-O1'-C1'	4.93	122.02	113.84
4	D	1656	FAD	C4X-C4-N3	-4.63	117.10	123.43
4	A	1656	FAD	C4X-C4-N3	-4.61	117.12	123.43
10	C	1256	HEM	CBA-CAA-C2A	3.54	119.01	112.49
11	C	1257	LMT	C3'-C4'-C5'	-3.28	103.41	110.93
11	F	1257	LMT	C3'-C4'-C5'	-3.27	103.43	110.93
10	F	1256	HEM	CBA-CAA-C2A	3.26	118.51	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1656	FAD	C5'-C4'-C3'	-3.18	106.06	112.20
4	D	1656	FAD	C5'-C4'-C3'	-3.09	106.24	112.20
4	A	1656	FAD	C4-C4X-C10	-2.88	118.04	119.95
4	D	1656	FAD	C4-C4X-C10	-2.69	118.17	119.95
11	C	1257	LMT	O1'-C1'-C2'	-2.62	104.21	108.30
11	F	1257	LMT	O1'-C1'-C2'	-2.61	104.23	108.30
4	A	1656	FAD	C4X-C10-N10	-2.49	117.75	120.30
4	D	1656	FAD	C2A-N1A-C6A	2.46	122.96	118.75
4	D	1656	FAD	C5A-C6A-N6A	2.43	124.05	120.35
4	A	1656	FAD	C5A-C6A-N1A	-2.43	114.85	120.35
4	D	1656	FAD	C5A-C6A-N1A	-2.42	114.86	120.35
4	A	1656	FAD	C2A-N1A-C6A	2.40	122.86	118.75
4	D	1656	FAD	C4X-C10-N10	-2.39	117.85	120.30
4	A	1656	FAD	C5A-C6A-N6A	2.36	123.94	120.35
4	D	1656	FAD	O4B-C1B-C2B	-2.22	103.68	106.93
10	F	1255	HEM	CMB-C2B-C3B	2.17	128.74	124.68
4	A	1656	FAD	O4B-C1B-C2B	-2.11	103.84	106.93
10	F	1255	HEM	CBD-CAD-C3D	-2.05	108.70	112.48
11	C	1257	LMT	O1B-C4'-C3'	2.04	112.72	107.28
11	F	1257	LMT	O1B-C4'-C3'	2.03	112.69	107.28
4	A	1656	FAD	O3'-C3'-C2'	2.03	113.71	108.81

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	1257	LMT	C2'-C1'-O1'-C1
4	D	1656	FAD	PA-O3P-P-O5'
11	C	1257	LMT	C2'-C1'-O1'-C1
4	A	1656	FAD	PA-O3P-P-O5'
11	F	1257	LMT	O5'-C1'-O1'-C1
11	C	1257	LMT	O5'-C1'-O1'-C1
11	F	1257	LMT	C4'-C5'-C6'-O6'
11	C	1257	LMT	C4'-C5'-C6'-O6'
11	F	1257	LMT	O5'-C5'-C6'-O6'
11	C	1257	LMT	O5'-C5'-C6'-O6'
11	F	1257	LMT	O1'-C1-C2-C3
11	C	1257	LMT	O1'-C1-C2-C3
11	F	1257	LMT	C7-C8-C9-C10
11	C	1257	LMT	C7-C8-C9-C10
11	F	1257	LMT	C11-C10-C9-C8
11	C	1257	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	D	1656	FAD	P-O3P-PA-O2A
4	A	1656	FAD	P-O3P-PA-O2A
11	F	1257	LMT	C5'-C4'-O1B-C1B
11	C	1257	LMT	C5'-C4'-O1B-C1B
4	D	1656	FAD	P-O3P-PA-O1A
11	F	1257	LMT	C2B-C1B-O1B-C4'
11	C	1257	LMT	C2B-C1B-O1B-C4'
11	F	1257	LMT	C9-C10-C11-C12
11	C	1257	LMT	C9-C10-C11-C12
11	F	1257	LMT	O5B-C1B-O1B-C4'
11	C	1257	LMT	O5B-C1B-O1B-C4'
4	A	1656	FAD	P-O3P-PA-O1A
4	D	1656	FAD	O4B-C4B-C5B-O5B
4	A	1656	FAD	O4B-C4B-C5B-O5B

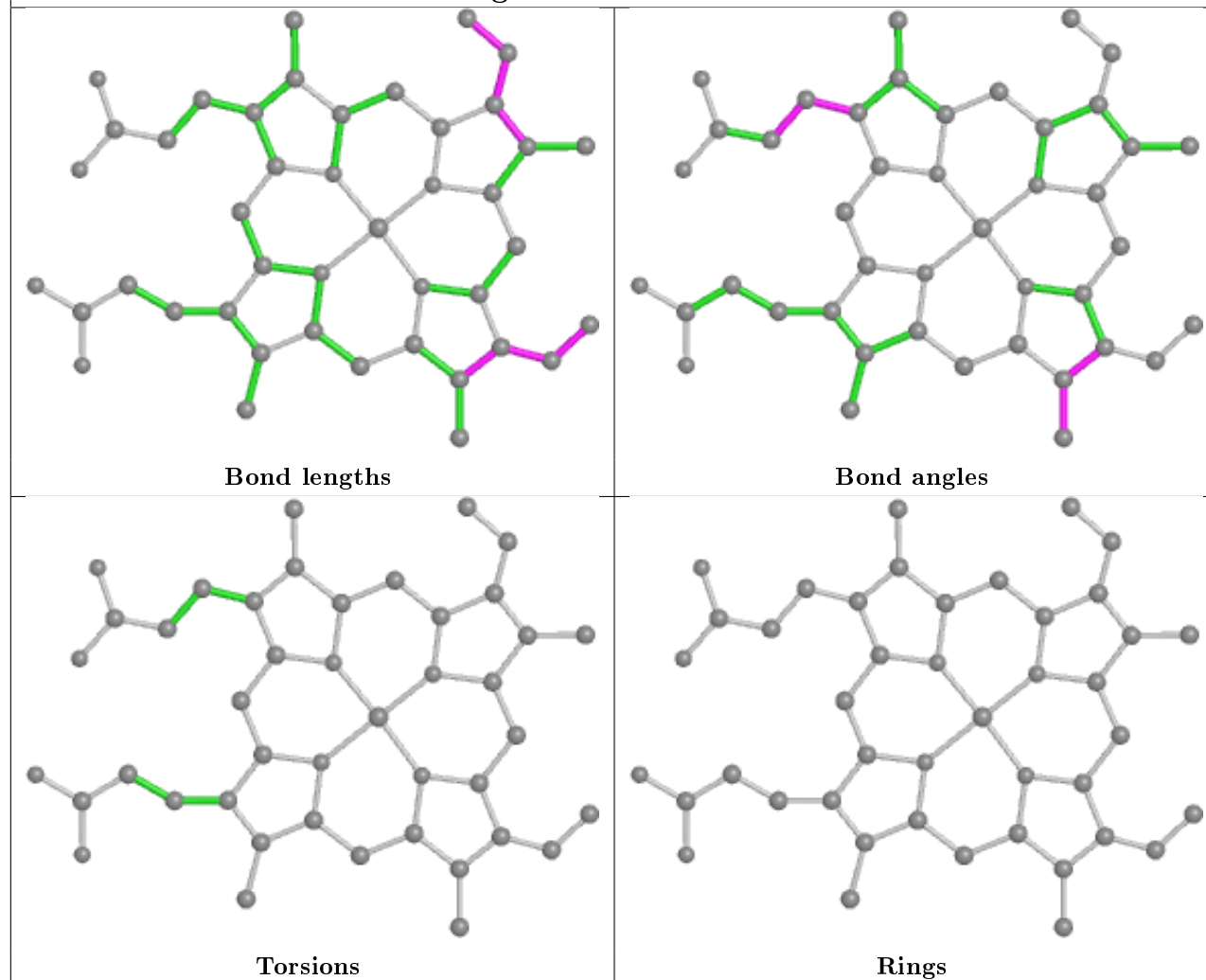
There are no ring outliers.

6 monomers are involved in 25 short contacts:

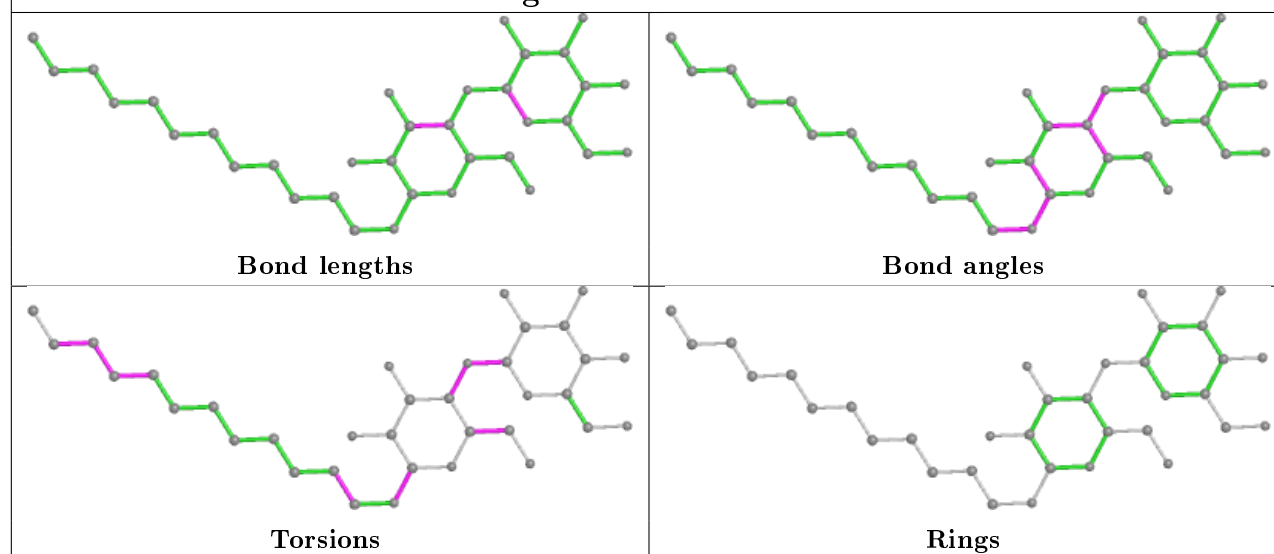
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	1257	LMT	9	0
4	D	1656	FAD	3	0
11	C	1257	LMT	8	0
10	F	1256	HEM	1	0
4	A	1656	FAD	3	0
10	C	1256	HEM	1	0

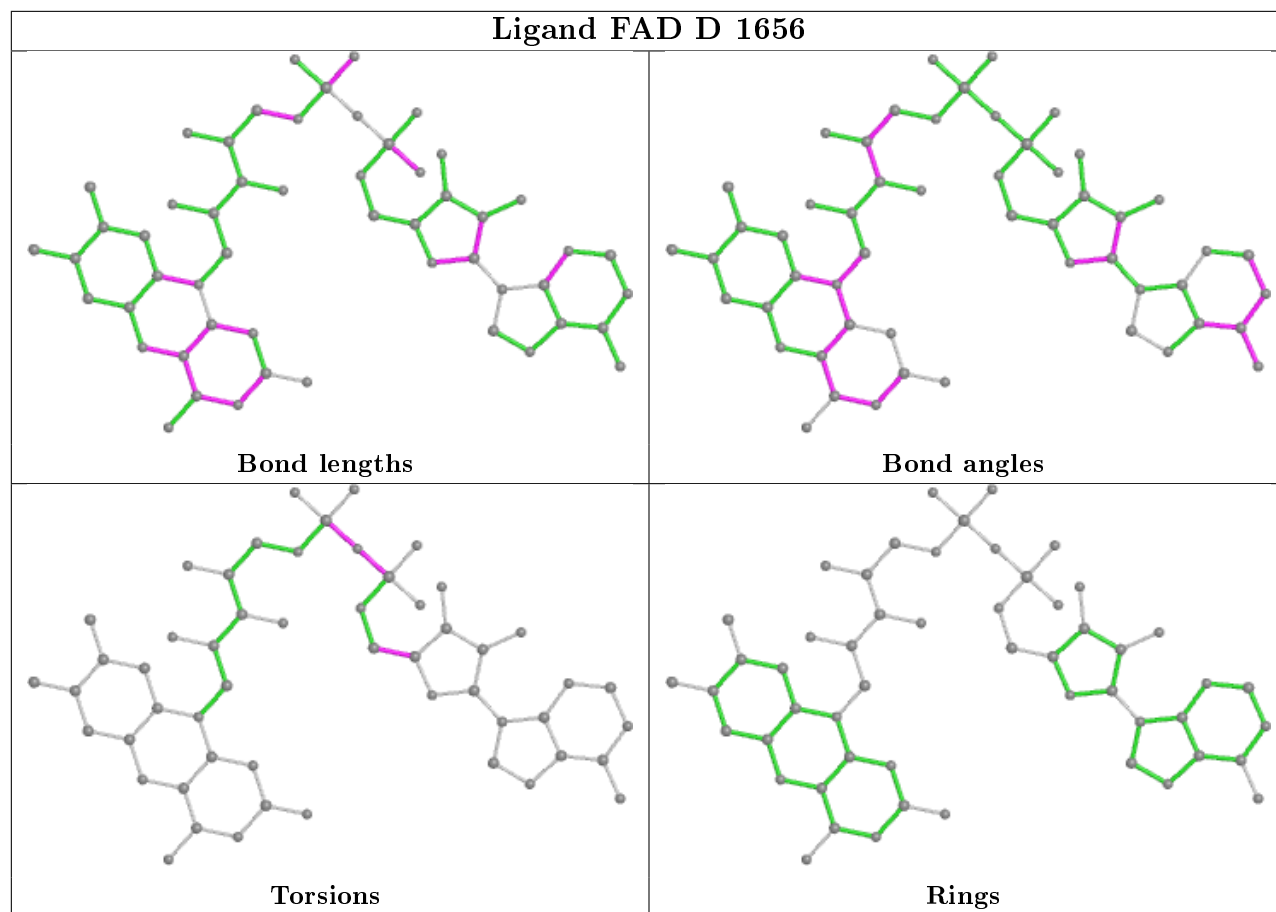
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 HEM F 1255

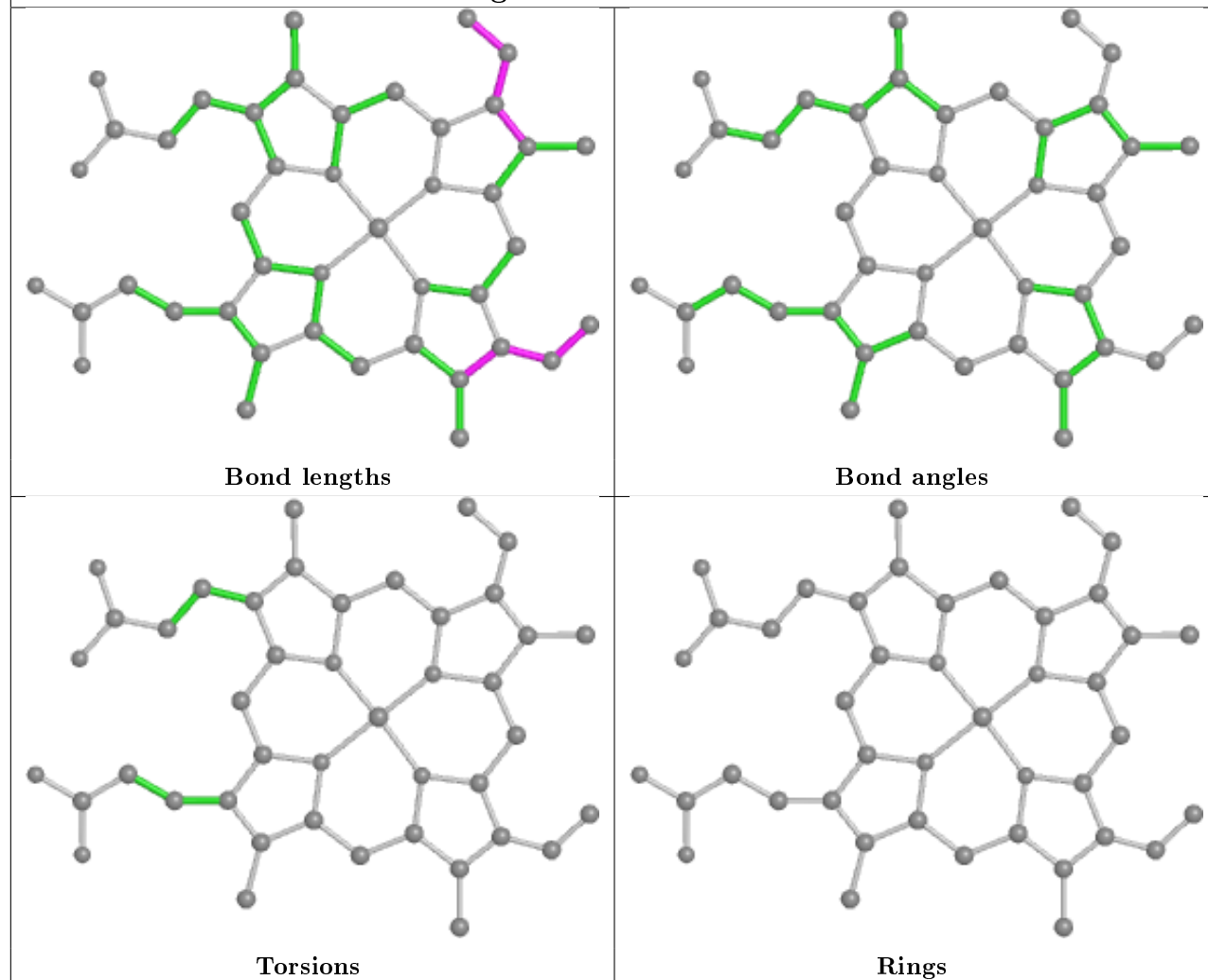


Ligand LMT F 1257

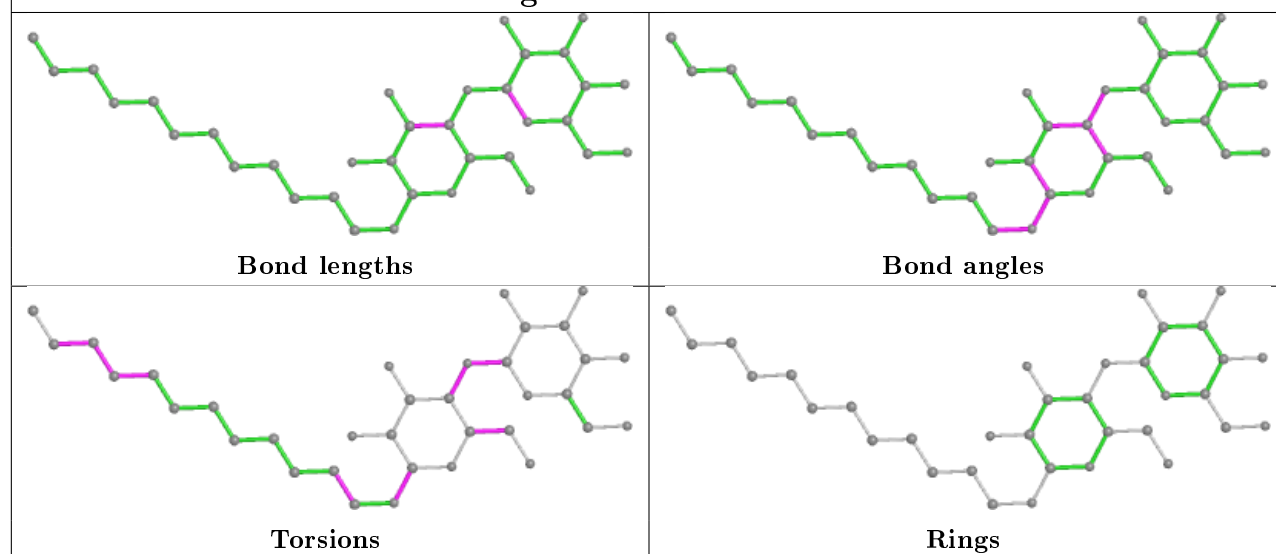


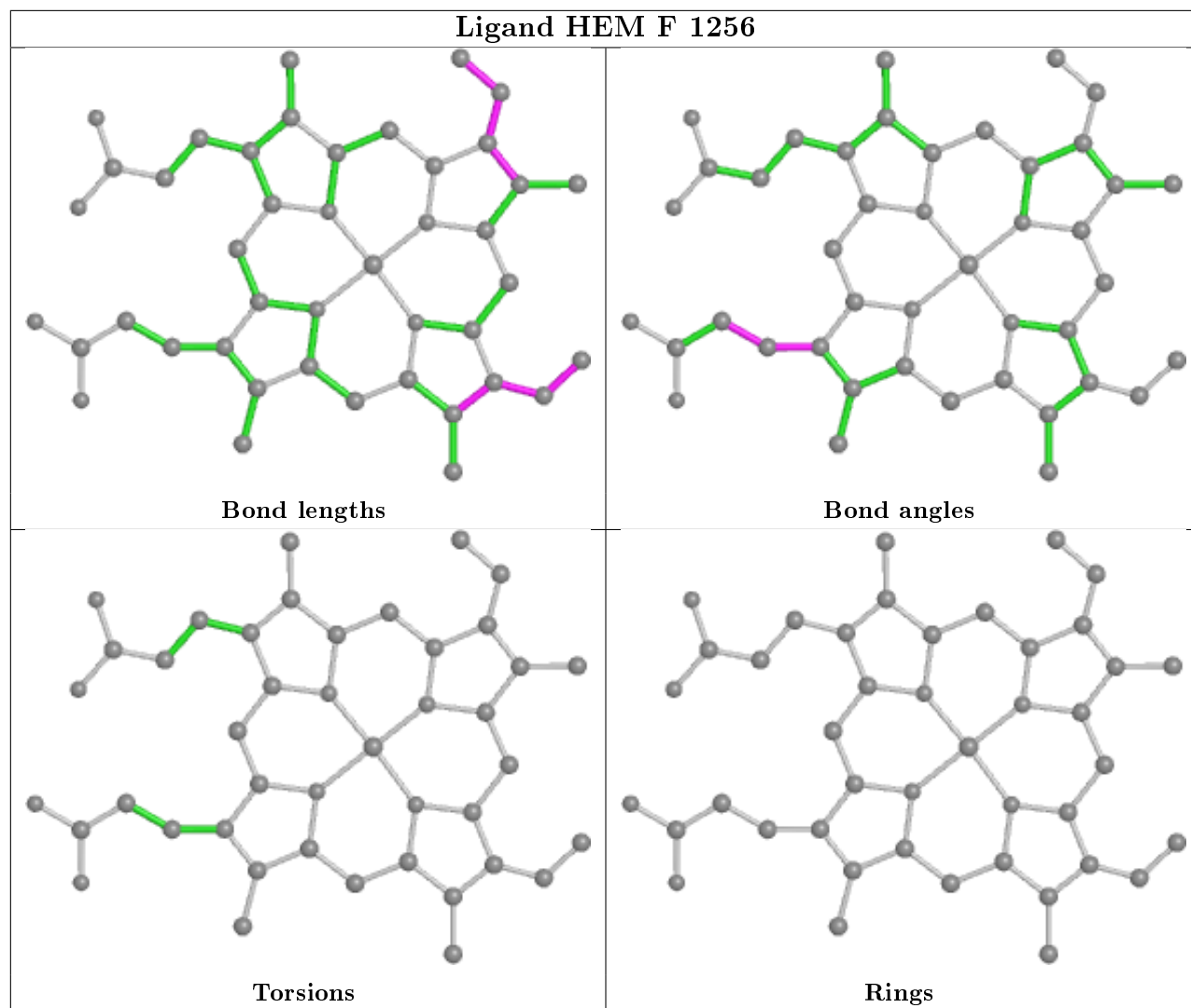


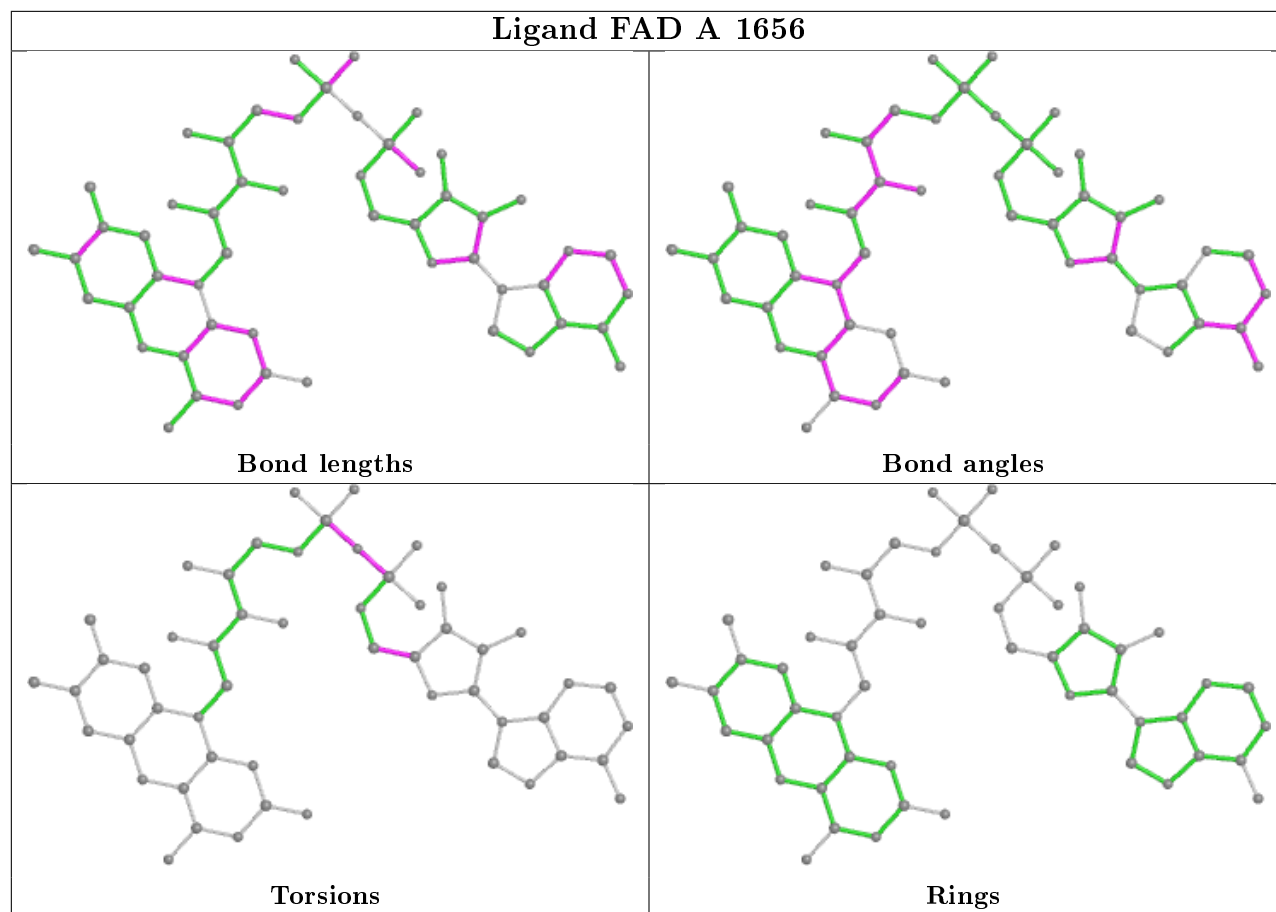
Ligand HEM C 1255

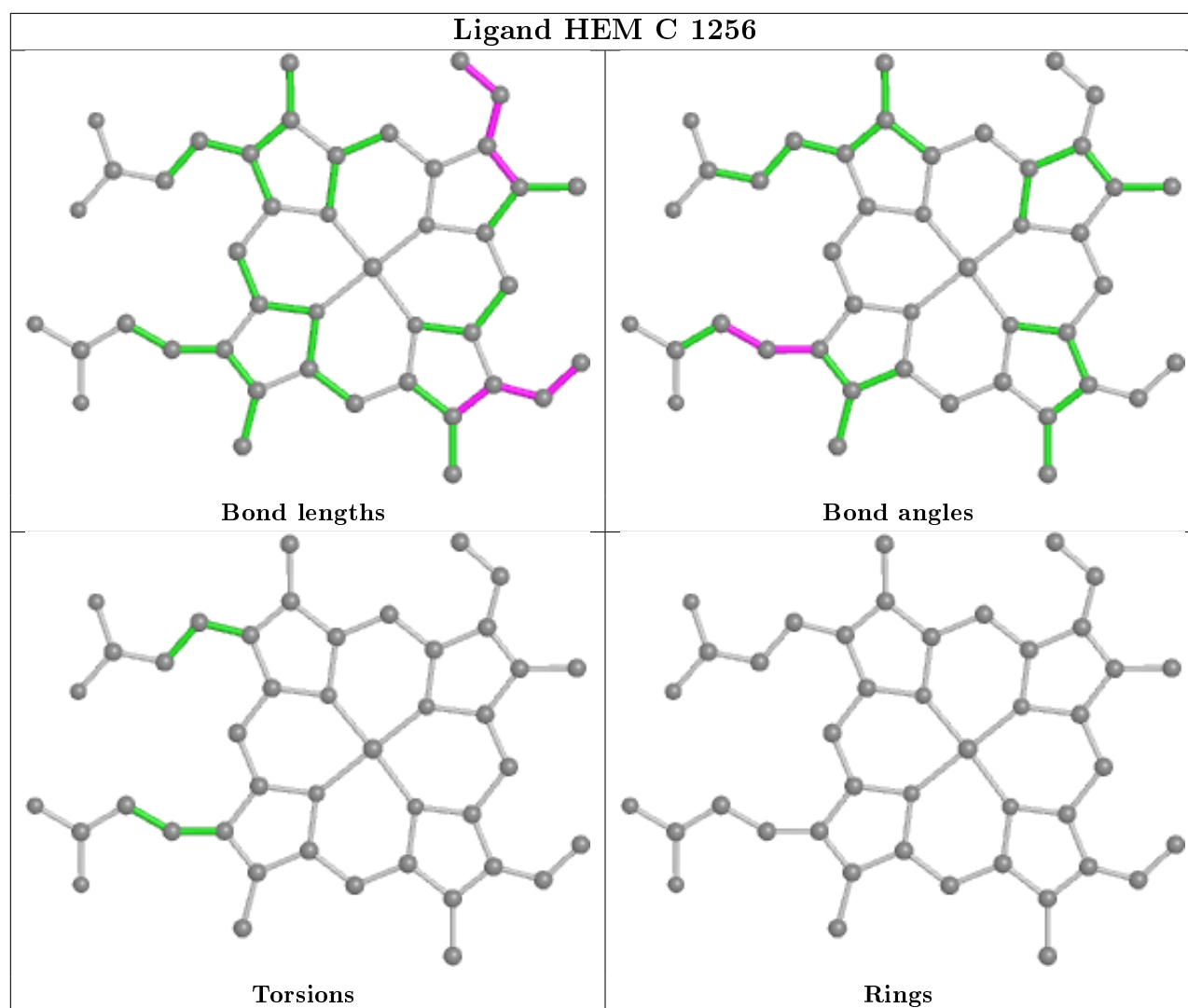


Ligand LMT C 1257









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	656/660 (99%)	0.49	54 (8%)	11 11	19, 33, 69, 80	14 (2%)
1	D	656/660 (99%)	0.57	65 (9%)	7 7	19, 33, 69, 80	16 (2%)
2	B	240/241 (99%)	0.33	14 (5%)	23 22	21, 29, 50, 74	2 (0%)
2	E	240/241 (99%)	0.37	11 (4%)	32 31	20, 28, 51, 74	2 (0%)
3	C	255/256 (99%)	1.02	47 (18%)	1 1	26, 44, 77, 91	11 (4%)
3	F	255/256 (99%)	0.86	36 (14%)	2 2	25, 43, 76, 90	10 (3%)
All	All	2302/2314 (99%)	0.58	227 (9%)	7 7	19, 34, 70, 91	55 (2%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	121	ALA	13.8
2	B	1	MET	11.8
3	C	254	HIS	11.1
1	A	121	ALA	10.3
1	D	122	GLN	10.2
1	A	122	GLN	10.2
1	A	124	THR	9.2
2	E	1	MET	9.2
1	D	599	ALA	8.8
1	D	338	ILE	8.4
2	B	240	MET	8.3
3	F	243	ILE	8.1
1	A	123	LYS	8.1
3	C	255	GLU	8.0
1	D	342	LEU	8.0
3	C	253	THR	7.9
3	C	243	ILE	7.7
3	C	69	PHE	7.6
1	D	124	THR	7.5

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Mol	Chain	Res	Type	RSRZ
3	F	253	THR	7.2
1	A	625	ALA	7.1
3	C	71	PHE	7.1
1	D	341	ASN	7.0
1	A	597	TYR	6.9
3	C	60	TRP	6.9
1	D	116	MET	6.9
1	D	623	LEU	6.8
3	F	74	GLY	6.7
1	A	118	ILE	6.5
3	C	248	PHE	6.5
3	F	69	PHE	6.4
1	A	627	GLY	6.3
3	C	239	THR	6.3
1	A	120	ASN	6.1
3	C	242	ASN	6.1
1	D	337	HIS	6.0
1	D	600	LYS	5.9
3	C	72	GLU	5.9
3	F	72	GLU	5.8
2	E	240	MET	5.8
1	D	123	LYS	5.7
3	F	60	TRP	5.7
1	A	117	ALA	5.6
3	C	236	LEU	5.6
1	A	116	MET	5.5
3	C	67	LEU	5.4
2	E	4	MET	5.3
2	B	85	GLU	5.3
1	D	119	ILE	5.2
1	A	623	LEU	5.2
3	F	254	HIS	5.2
1	A	624	GLU	5.2
3	F	215	LEU	5.1
1	D	117	ALA	5.1
2	B	2	GLY	5.1
3	C	74	GLY	5.0
1	D	340	THR	5.0
1	A	334	GLY	5.0
1	D	626	ALA	4.9
3	C	250	TYR	4.9
3	F	1	MET	4.9

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Mol	Chain	Res	Type	RSRZ
3	F	81	PHE	4.8
1	A	336	LYS	4.8
1	A	337	HIS	4.8
1	A	600	LYS	4.7
1	D	627	GLY	4.7
1	A	340	THR	4.7
1	A	341	ASN	4.7
1	D	597	TYR	4.6
1	A	351	TYR	4.6
1	D	335	ARG	4.5
3	C	200	GLU	4.5
1	D	358	ALA	4.4
1	D	656	LYS	4.4
3	C	77	ILE	4.4
3	F	71	PHE	4.3
1	A	125	THR	4.3
1	A	339	GLU	4.3
3	C	73	GLY	4.2
1	D	625	ALA	4.2
3	C	70	ILE	4.2
3	F	241	PRO	4.1
3	C	64	LYS	4.1
1	D	336	LYS	4.0
1	D	343	ARG	3.9
1	D	339	GLU	3.9
1	A	654	GLY	3.9
2	B	31	ALA	3.9
1	A	621	SER	3.9
3	C	146	ILE	3.8
3	F	77	ILE	3.8
3	C	1	MET	3.8
1	A	353	ALA	3.8
3	C	68	ASP	3.7
1	D	598	GLY	3.7
1	A	656	LYS	3.6
3	C	65	PHE	3.6
3	C	245	TYR	3.6
1	D	624	GLU	3.6
1	A	338	ILE	3.6
3	C	81	PHE	3.5
3	F	73	GLY	3.5
3	F	200	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	53	LEU	3.4
1	D	628	LYS	3.4
1	D	611	LYS	3.4
2	B	47	TYR	3.4
1	A	342	LEU	3.4
1	A	333	LEU	3.4
3	F	53	LEU	3.4
1	A	601	GLY	3.3
1	A	599	ALA	3.3
1	A	628	LYS	3.3
1	D	118	ILE	3.3
3	F	233	LYS	3.3
1	A	632	ALA	3.3
3	F	242	ASN	3.3
1	D	601	GLY	3.2
3	C	247	TYR	3.2
3	F	68	ASP	3.2
1	D	354	GLY	3.2
1	D	294	GLU	3.2
1	D	322	TYR	3.2
1	D	619	ILE	3.2
3	C	251	LYS	3.2
1	A	620	GLN	3.2
2	E	85	GLU	3.2
1	A	295	LYS	3.1
2	E	2	GLY	3.1
1	A	611	LYS	3.1
3	C	233	LYS	3.1
1	D	125	THR	3.0
1	A	294	GLU	3.0
2	B	205	VAL	3.0
1	A	602	ASN	3.0
3	C	201	THR	3.0
3	F	240	ASP	3.0
3	F	75	LYS	3.0
3	F	76	PRO	2.9
1	D	293	PRO	2.9
3	C	240	ASP	2.9
3	C	75	LYS	2.9
1	D	654	GLY	2.9
3	F	52	LEU	2.9
1	D	346	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
3	F	146	ILE	2.9
3	F	70	ILE	2.9
1	D	655	ASP	2.8
1	D	614	GLU	2.8
1	A	119	ILE	2.8
1	D	620	GLN	2.8
3	C	199	GLY	2.8
3	F	211	LYS	2.8
2	B	125	GLN	2.8
1	A	614	GLU	2.7
3	F	251	LYS	2.7
3	C	241	PRO	2.7
3	F	201	THR	2.7
3	C	157	VAL	2.6
1	A	358	ALA	2.6
1	A	586	ASN	2.6
3	C	197	PHE	2.6
1	D	356	ASP	2.6
1	D	602	ASN	2.5
3	C	161	PHE	2.5
3	F	197	PHE	2.5
3	F	57	VAL	2.5
3	C	59	LEU	2.5
3	F	239	THR	2.5
1	D	319	GLN	2.5
1	D	622	GLU	2.5
3	F	236	LEU	2.5
3	C	252	ARG	2.4
1	D	344	ASP	2.4
1	A	345	VAL	2.4
1	D	348	ILE	2.4
3	C	238	GLN	2.4
1	A	343	ARG	2.4
2	B	239	ASN	2.4
3	C	61	VAL	2.4
1	A	655	ASP	2.4
3	F	219	PHE	2.4
1	D	350	GLU	2.4
1	A	572	GLU	2.4
2	E	211	LEU	2.3
1	A	296	LYS	2.3
1	A	335	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	32	PRO	2.3
1	D	635	GLU	2.3
2	E	103	LEU	2.3
1	D	355	ILE	2.3
1	D	632	ALA	2.3
1	A	618	LYS	2.3
1	A	332	ILE	2.3
3	C	214	THR	2.3
3	F	222	VAL	2.2
1	A	271	GLY	2.2
2	B	206	PHE	2.2
3	C	219	PHE	2.2
1	D	616	ILE	2.2
1	D	295	LYS	2.2
3	C	142	VAL	2.2
3	F	142	VAL	2.2
2	B	103	LEU	2.2
3	C	212	LEU	2.2
3	F	171	LEU	2.2
2	E	239	ASN	2.2
1	A	616	ILE	2.2
2	B	86	ASP	2.2
1	D	351	TYR	2.1
2	E	53	PHE	2.1
2	B	5	LEU	2.1
1	D	120	ASN	2.1
1	D	586	ASN	2.1
2	B	32	PRO	2.1
1	A	162	PHE	2.1
1	D	321	PRO	2.1
1	D	277	GLY	2.1
1	D	314	LYS	2.1
1	A	316	LYS	2.1
1	D	296	LYS	2.1
1	D	271	GLY	2.1
2	E	94	LEU	2.0
3	C	190	LEU	2.0
1	D	357	PRO	2.0
1	D	615	GLU	2.0
1	D	653	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

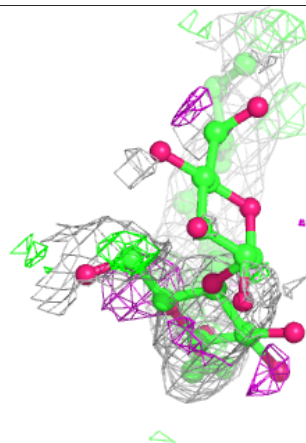
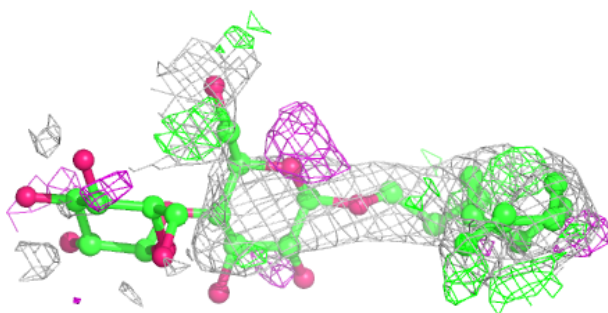
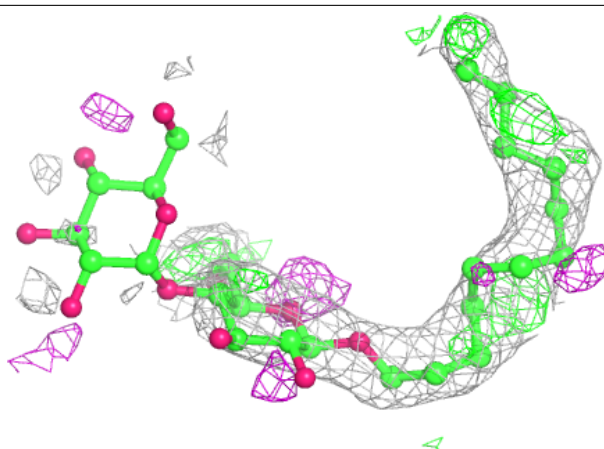
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	LMT	C	1257	35/35	0.55	0.33	59,63,68,69	16
11	LMT	F	1257	35/35	0.73	0.25	59,63,69,69	16
5	FUM	A	1657	8/8	0.76	0.17	42,46,48,50	0
5	FUM	D	1657	8/8	0.79	0.18	43,46,47,48	0
10	HEM	C	1256	43/43	0.96	0.13	38,40,43,45	0
6	NA	D	1658	1/1	0.96	0.08	26,26,26,26	0
10	HEM	F	1256	43/43	0.96	0.13	36,40,43,45	0
10	HEM	C	1255	43/43	0.96	0.10	26,31,34,38	0
4	FAD	D	1656	53/53	0.97	0.09	18,22,25,25	0
10	HEM	F	1255	43/43	0.97	0.10	26,32,35,38	0
4	FAD	A	1656	53/53	0.98	0.08	16,22,25,27	0
7	FES	B	1240	4/4	0.99	0.06	22,22,23,24	0
6	NA	A	1658	1/1	0.99	0.03	26,26,26,26	0
9	SF4	B	1242	8/8	0.99	0.05	22,24,25,25	0
9	SF4	E	1242	8/8	0.99	0.06	21,23,23,24	0
8	F3S	E	1241	7/7	0.99	0.09	23,24,25,25	0
7	FES	E	1240	4/4	0.99	0.06	21,21,21,23	0
8	F3S	B	1241	7/7	0.99	0.07	24,25,26,27	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.

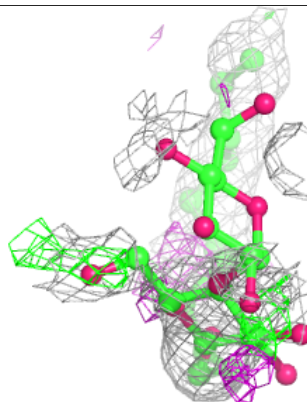
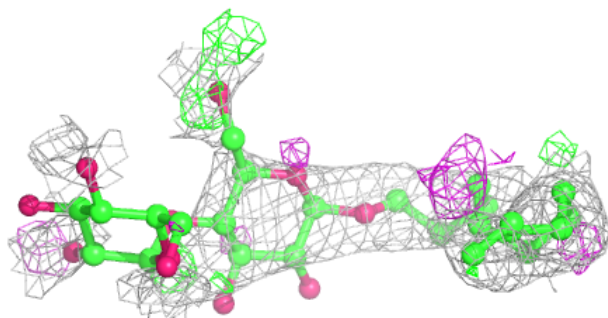
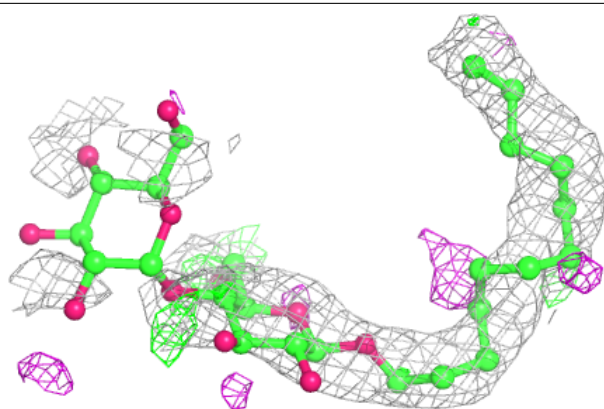
Electron density around LMT C 1257:

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



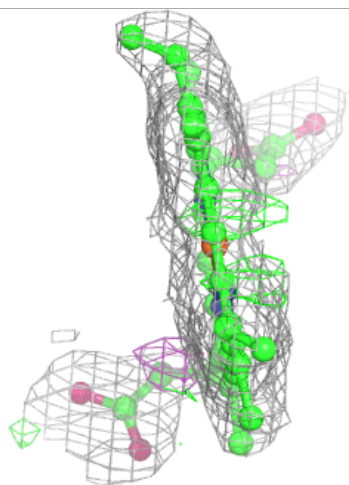
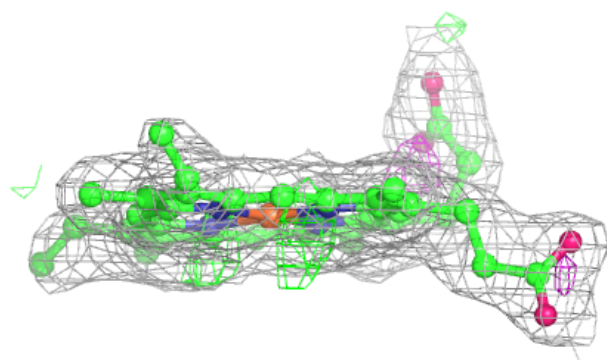
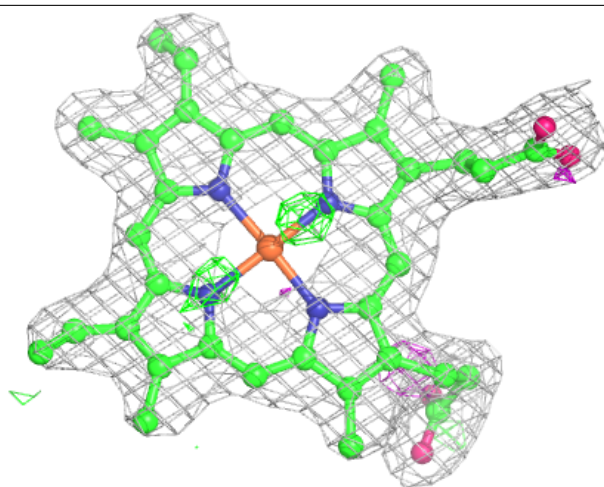
Electron density around LMT F 1257:

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



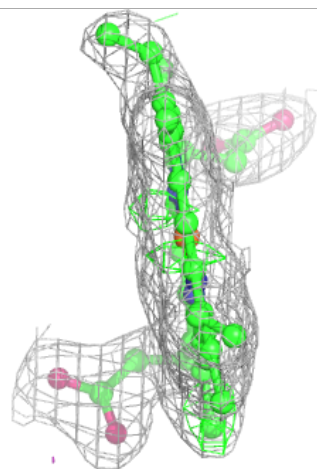
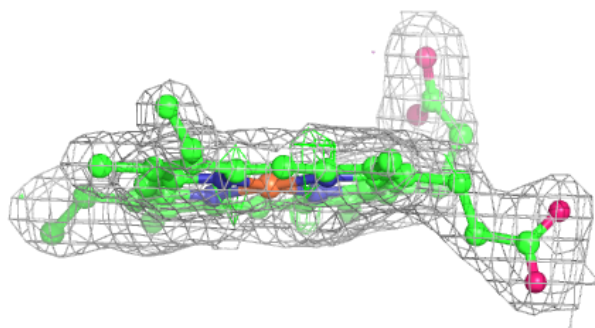
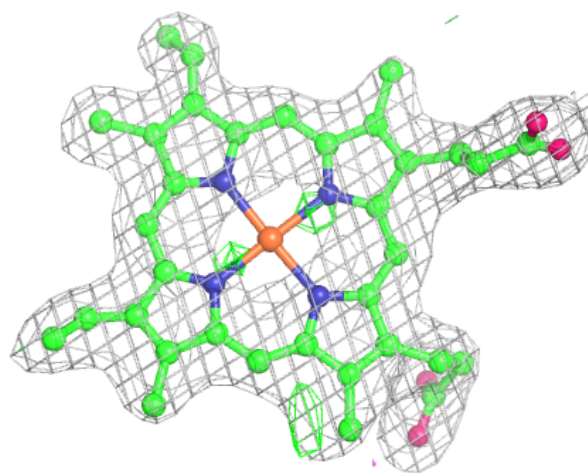
Electron density around HEM C 1256:

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



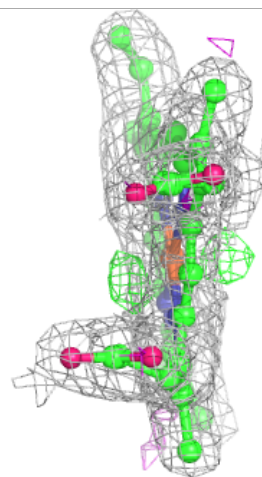
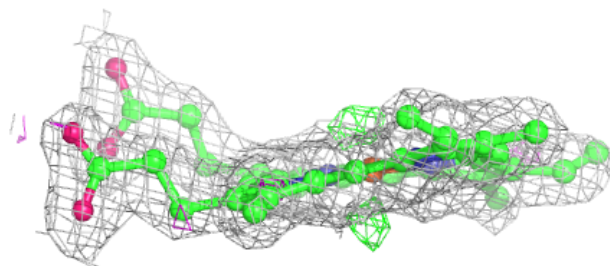
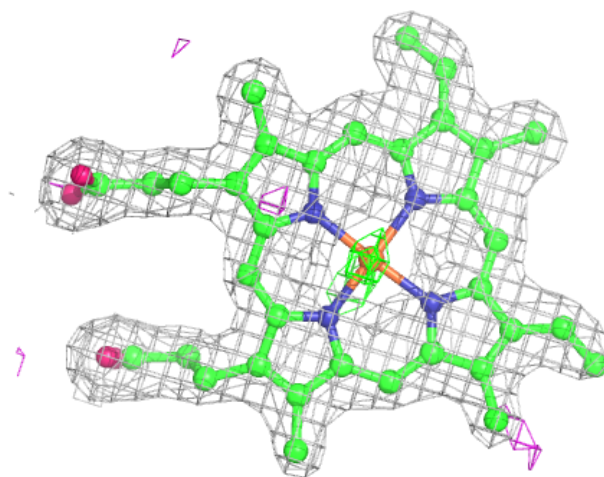
Electron density around HEM F 1256:

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



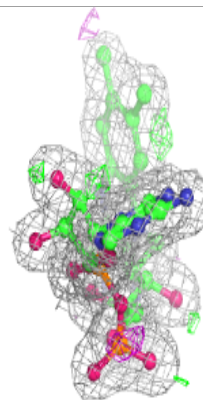
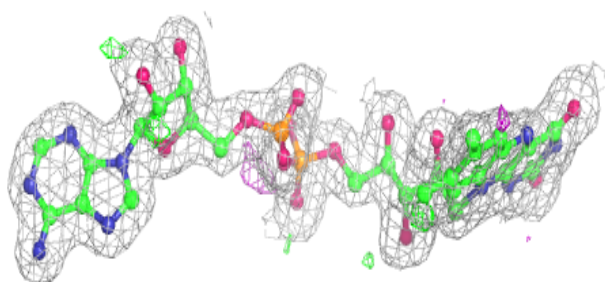
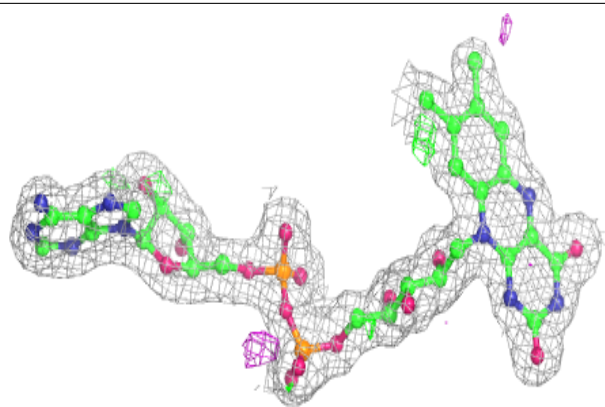
Electron density around HEM C 1255:

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



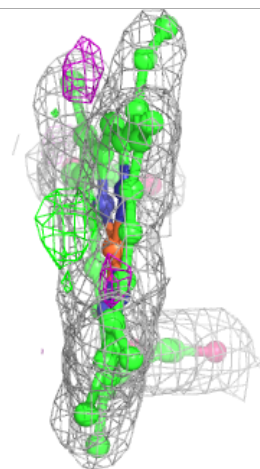
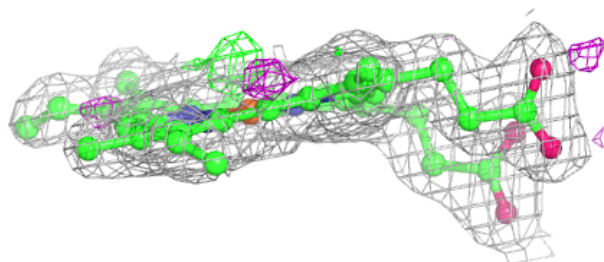
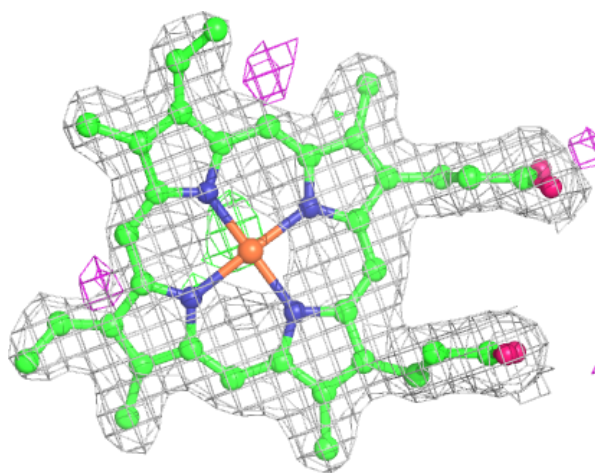
Electron density around FAD D 1656:

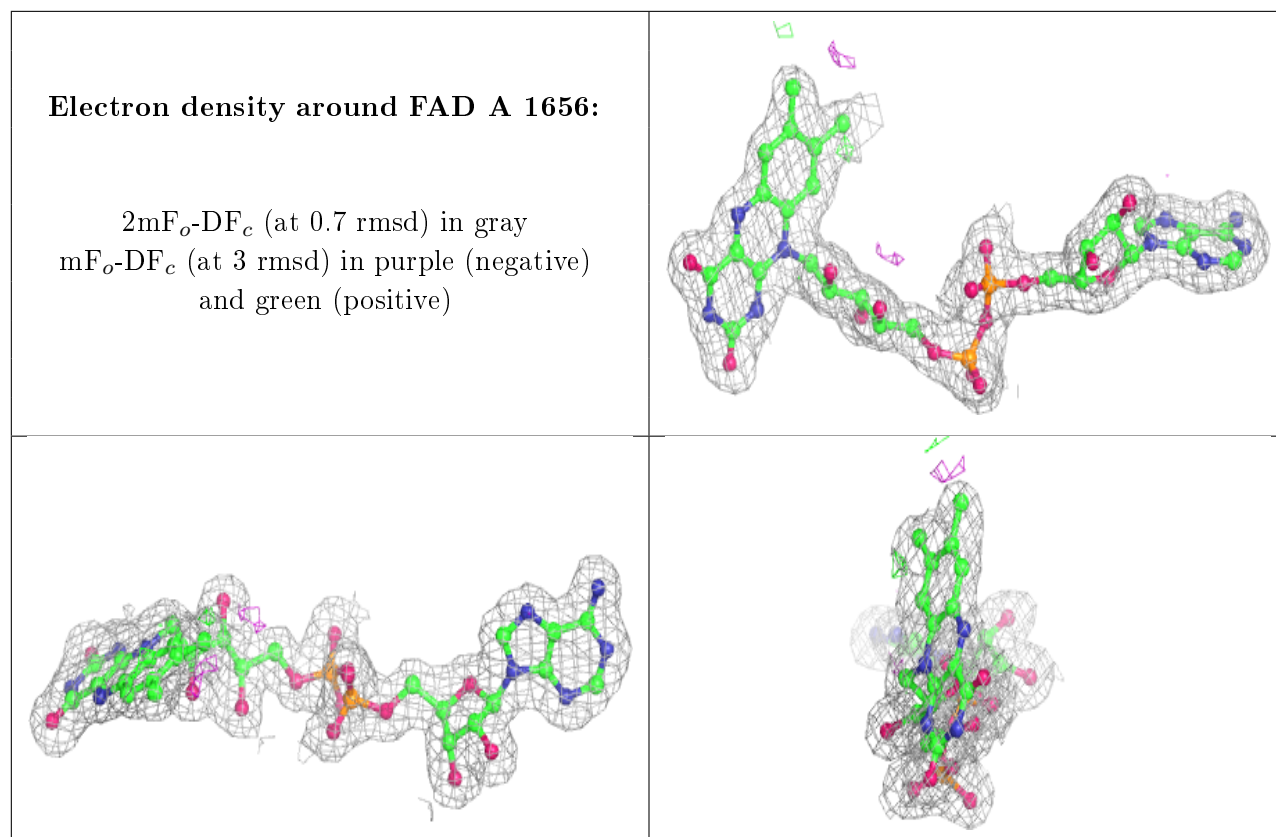
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM F 1255:

$2mF_o-DF_c$ (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.