



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:11 AM JST

PDB ID : 5C3J / pdb_00005c3j
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with Ubiquinone-1
Authors : Harada, S.; Shiba, T.; Sato, D.; Yamamoto, A.; Nagahama, M.; Yone, A.; Inaoka, D.K.; Sakamoto, K.; Inoue, M.; Honma, T.; Kita, K.
Deposited on : 2015-06-17
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

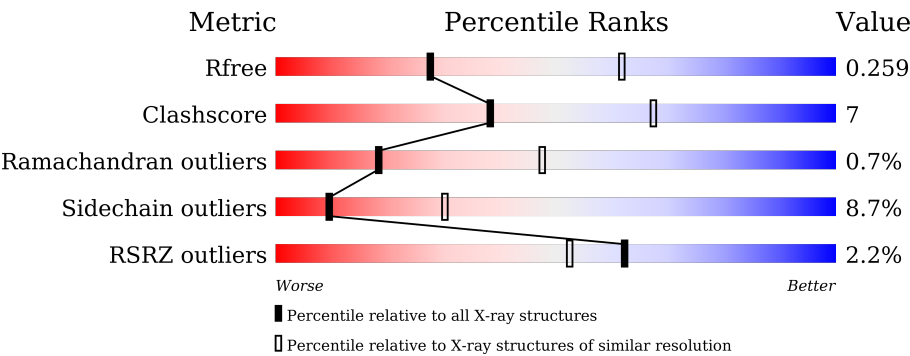
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	645	73%21%••
1	E	645	75%19%••
2	B	282	% 72%15%•11%
2	F	282	72%15%•11%
3	C	188	% 65%15%•19%

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Mol	Chain	Length	Quality of chain
3	G	188	16% 62% 14% 5% • 19%
4	D	156	2% 61% 21% • 17%
4	H	156	4% 63% 17% • 17%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18342 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			
1	E	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1985	1263	338	361	23			
2	F	250	Total	C	N	O	S	0	0	0
			1985	1263	338	361	23			

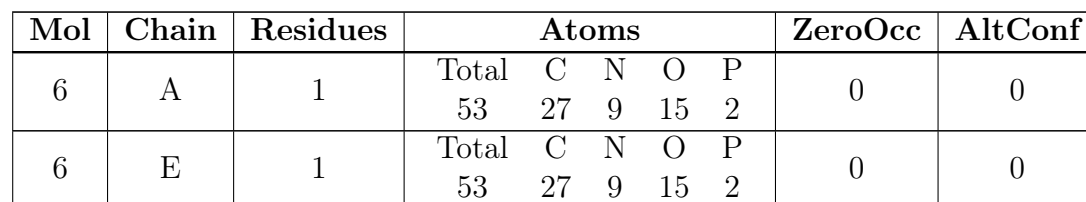
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			

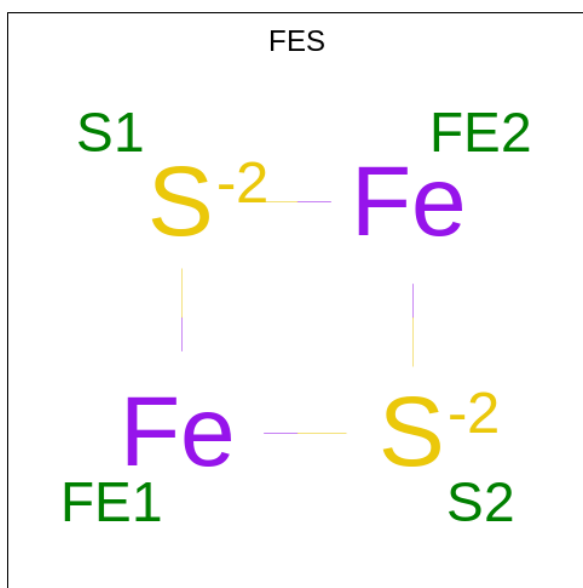
- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).

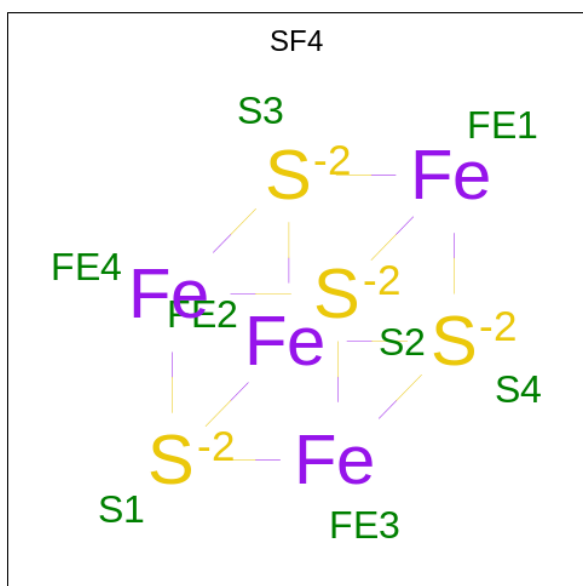


- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



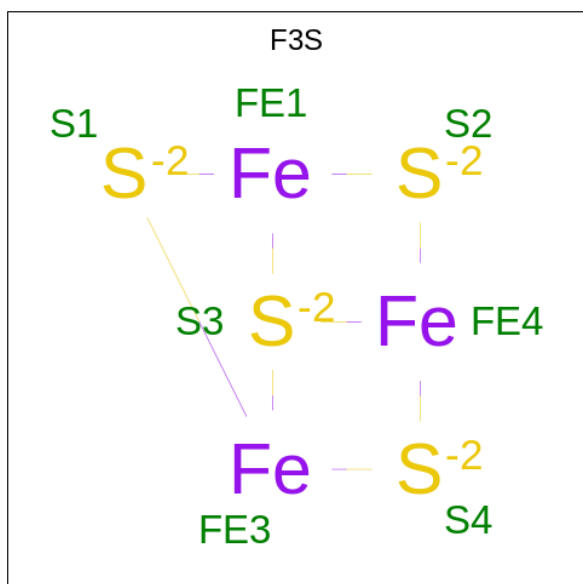
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

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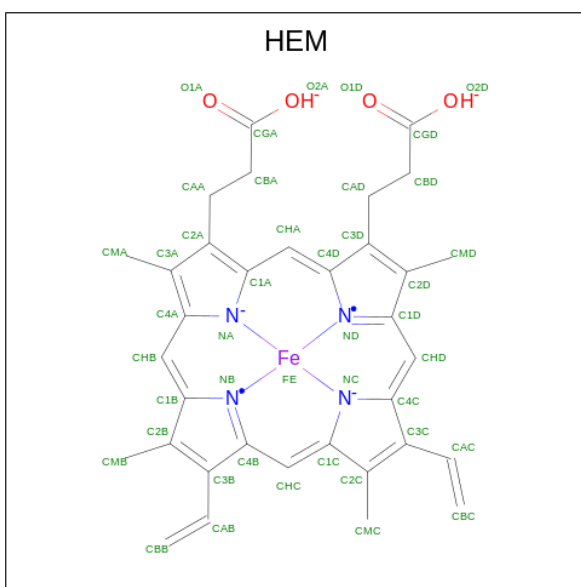
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



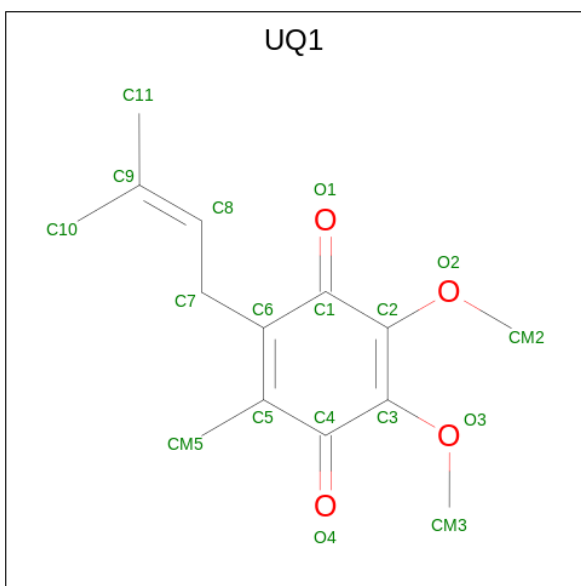
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



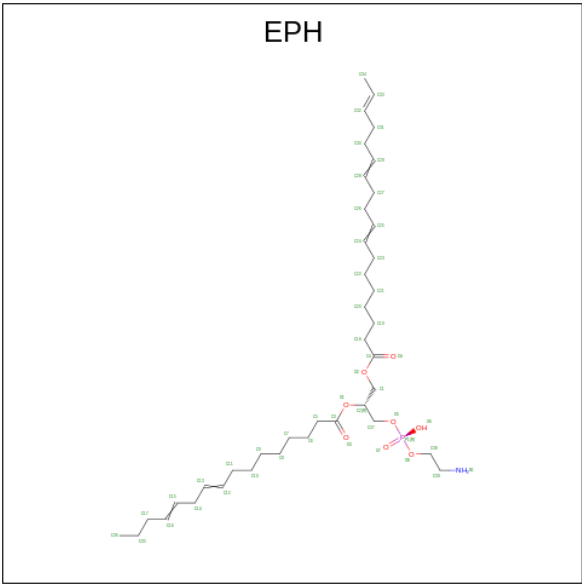
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



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

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: C₃₉H₆₈NO₈P).

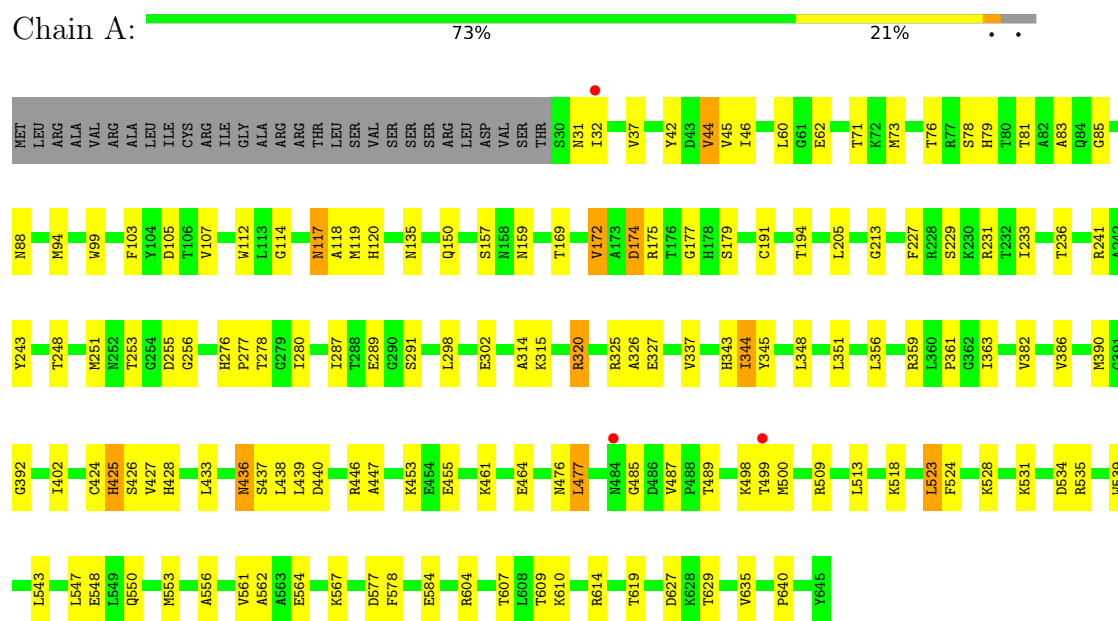


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

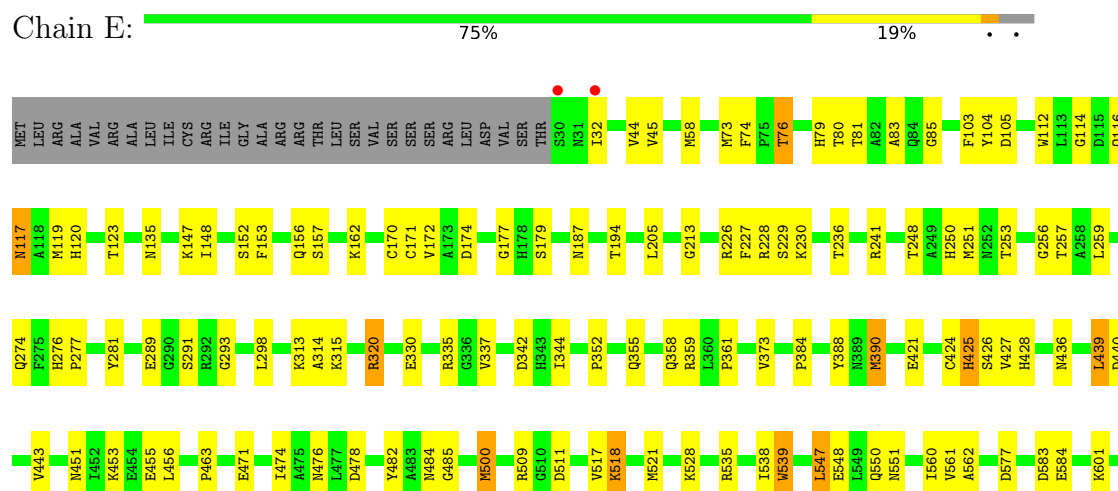
3 Residue-property plots

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

- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

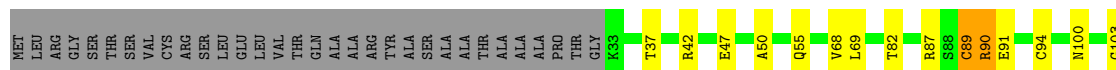


- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

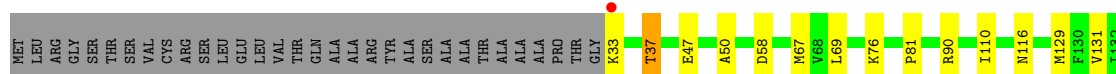




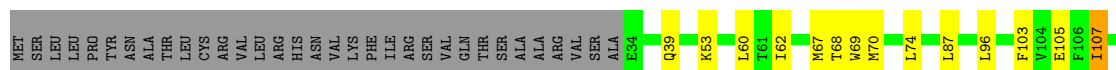
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



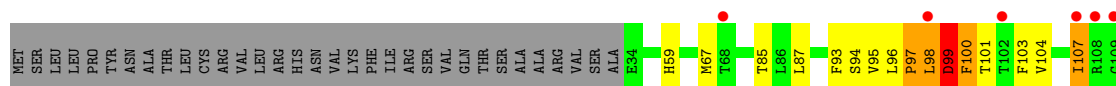
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



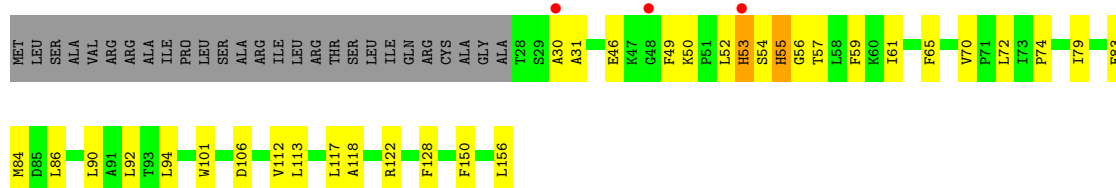
- Molecule 3: Cytochrome b-large subunit



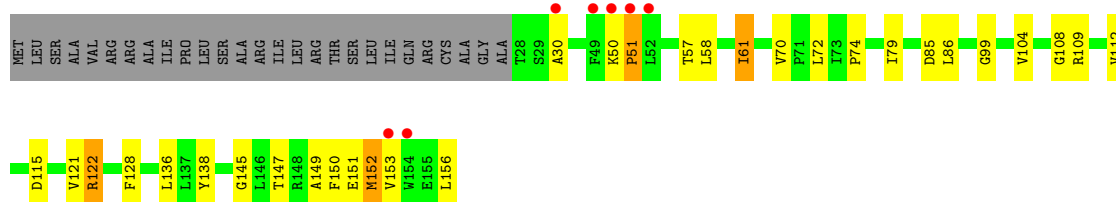
- Molecule 3: Cytochrome b-large subunit



- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.75Å 126.83Å 220.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (20.00-2.80) 88.7 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.260 0.204 , 0.259	Depositor DCC
R_{free} test set	3841 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18342	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, HEM, UQ1, FAD, SF4, F3S, FES, EPH

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	0.67	3/4889 (0.1%)	0.93	7/6605 (0.1%)
1	E	0.67	2/4889 (0.0%)	0.90	5/6605 (0.1%)
2	B	0.64	0/2029	0.86	1/2739 (0.0%)
2	F	0.69	0/2029	0.86	2/2739 (0.1%)
3	C	0.60	0/1255	0.84	0/1709
3	G	0.68	0/1255	0.87	1/1709 (0.1%)
4	D	0.71	1/1030 (0.1%)	0.88	2/1406 (0.1%)
4	H	0.60	0/1030	0.87	1/1406 (0.1%)
All	All	0.66	6/18406 (0.0%)	0.89	19/24918 (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
2	F	0	1
4	D	0	1
4	H	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	172	VAL	C-O	-6.75	1.16	1.24
4	D	55	HIS	CG-ND1	-5.57	1.32	1.38
1	E	539	TRP	NE1-CE2	-5.50	1.31	1.37
1	A	539	TRP	NE1-CE2	-5.49	1.31	1.37
1	A	539	TRP	CA-C	-5.29	1.46	1.53
1	A	172	VAL	C-O	-5.05	1.18	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	55	HIS	N-CA-C	-7.85	97.41	109.65
4	D	53	HIS	N-CA-C	-7.39	100.30	110.35
1	A	31	ASN	N-CA-C	6.54	118.49	111.36
4	H	115	ASP	N-CA-C	6.46	118.86	111.11
1	A	425	HIS	N-CA-C	6.22	119.34	111.69
1	E	171	CYS	N-CA-C	5.80	117.78	109.14
1	E	315	LYS	CB-CA-C	-5.73	109.98	116.63
3	G	100	PHE	N-CA-C	-5.65	105.02	111.07
1	A	85	GLY	N-CA-C	5.44	119.73	112.77
2	B	161	LEU	N-CA-C	5.43	116.88	111.07
1	A	276	HIS	CA-C-N	5.34	124.79	119.24
1	A	276	HIS	C-N-CA	5.34	124.79	119.24
1	A	174	ASP	N-CA-C	-5.23	105.57	112.94
1	A	392	GLY	N-CA-C	5.23	117.07	110.38
1	E	112	TRP	N-CA-C	5.20	118.76	111.90
2	F	164	LYS	N-CA-C	5.12	116.63	108.79
1	E	85	GLY	N-CA-C	5.11	118.42	112.50
1	E	425	HIS	N-CA-C	5.10	117.96	111.69
2	F	163	GLU	N-CA-C	5.08	117.20	111.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	ALA	Peptide
2	F	162	GLY	Peptide
4	H	30	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4787	0	4722	74	0
1	E	4787	0	4722	65	0
2	B	1985	0	2001	23	0
2	F	1985	0	2001	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1217	0	1265	19	0
3	G	1217	0	1265	32	0
4	D	998	0	985	17	0
4	H	998	0	985	16	0
5	A	7	0	2	1	0
5	E	7	0	2	1	0
6	A	53	0	31	9	0
6	E	53	0	31	8	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	2	0
10	G	43	0	30	4	0
11	C	18	0	18	4	0
11	G	18	0	18	1	0
12	D	44	0	53	1	0
12	H	44	0	53	1	0
All	All	18342	0	18214	252	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 7.

All (252) 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)
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.30	1.41
3:G:96:LEU:O	3:G:98:LEU:HD12	1.41	1.17
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.14	1.11
3:G:98:LEU:HD13	3:G:98:LEU:H	1.12	1.09
1:E:79:HIS:NE2	6:E:702:FAD:HM83	1.68	1.07
3:G:98:LEU:H	3:G:98:LEU:CD1	1.69	1.02
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.27	0.96
3:G:98:LEU:CD1	3:G:98:LEU:N	2.29	0.94
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.03	0.92
3:G:95:VAL:HG13	3:G:96:LEU:HD13	1.58	0.83
3:G:95:VAL:HG13	3:G:96:LEU:CD1	2.11	0.80
3:G:96:LEU:O	3:G:98:LEU:CD1	2.30	0.77
3:G:96:LEU:C	3:G:98:LEU:HD12	2.10	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:LYS:HG3	1:E:314:ALA:N	2.01	0.74
1:A:241:ARG:NH2	1:A:248:THR:O	2.24	0.71
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.71	0.71
1:E:274:GLN:HB2	1:E:390:MET:HE1	1.73	0.69
3:G:95:VAL:CG1	3:G:96:LEU:HD13	2.21	0.69
2:B:232:ASP:HB3	4:D:52:LEU:HD12	1.74	0.68
3:G:98:LEU:HD12	3:G:98:LEU:N	2.09	0.68
1:E:79:HIS:NE2	6:E:702:FAD:HM81	2.10	0.66
3:G:96:LEU:O	3:G:98:LEU:N	2.29	0.66
1:E:425:HIS:N	1:E:426:SER:HA	2.12	0.65
1:E:152:SER:O	1:E:293:GLY:HA3	1.96	0.65
1:A:425:HIS:N	1:A:426:SER:HA	2.11	0.65
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.44	0.65
1:A:291:SER:HB3	1:A:348:LEU:HD21	1.79	0.64
3:C:60:LEU:HD21	11:C:202:UQ1:C7	2.27	0.64
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.79	0.64
2:F:116:ASN:C	2:F:116:ASN:HD22	2.06	0.63
1:A:135:ASN:ND2	2:B:161:LEU:O	2.31	0.63
1:E:83:ALA:HA	6:E:702:FAD:C6	2.29	0.62
3:G:104:VAL:HG13	4:H:156:LEU:HD21	1.82	0.61
1:E:103:PHE:HA	1:E:123:THR:HG21	1.81	0.61
3:G:100:PHE:O	3:G:103:PHE:N	2.34	0.61
3:C:133:LEU:HB3	3:C:159:VAL:HG22	1.83	0.60
1:E:105:ASP:OD2	1:E:157:SER:N	2.34	0.60
3:G:184:LEU:HG	3:G:185:PRO:HD2	1.82	0.60
4:D:52:LEU:O	4:D:53:HIS:C	2.42	0.60
3:G:184:LEU:O	3:G:186:THR:N	2.35	0.59
4:D:70:VAL:O	4:D:74:PRO:HD2	2.01	0.59
1:A:103:PHE:O	1:A:107:VAL:HG23	2.03	0.59
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.83	0.59
1:E:439:LEU:HD22	1:E:443:VAL:HG23	1.85	0.59
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.85	0.59
1:A:117:ASN:HD22	1:A:118:ALA:H	1.51	0.58
2:B:238:LYS:NZ	4:D:106:ASP:OD1	2.26	0.58
3:C:74:LEU:HD23	3:C:130:PHE:CZ	2.38	0.58
10:G:201:HEM:HAD1	4:H:99:GLY:CA	2.33	0.58
3:C:70:MET:HE2	3:C:70:MET:HA	1.84	0.58
4:D:56:GLY:HA2	4:D:59:PHE:HB3	1.86	0.58
3:G:93:PHE:O	3:G:98:LEU:HB3	2.04	0.58
1:A:477:LEU:HD11	1:A:543:LEU:HD21	1.86	0.58
1:E:518:LYS:HE2	1:E:518:LYS:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:LEU:HD21	11:C:202:UQ1:H72	1.86	0.58
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.86	0.57
1:E:120:HIS:HD2	1:E:630:LEU:H	1.51	0.57
1:A:79:HIS:CD2	6:A:702:FAD:HM82	2.30	0.57
1:E:135:ASN:ND2	2:F:161:LEU:O	2.37	0.57
10:C:201:HEM:HHC	10:C:201:HEM:HBB2	1.86	0.57
1:E:551:ASN:N	1:E:551:ASN:HD22	2.03	0.57
2:F:67:MET:HE3	2:F:110:ILE:HA	1.86	0.57
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.86	0.56
3:C:179:HIS:O	3:C:183:THR:HG22	2.05	0.56
2:F:47:GLU:HG3	2:F:50:ALA:HB2	1.86	0.56
1:A:174:ASP:OD2	1:A:363:ILE:N	2.35	0.56
1:A:83:ALA:HA	6:A:702:FAD:C6	2.35	0.56
2:F:47:GLU:CG	2:F:50:ALA:HB2	2.36	0.56
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.86	0.56
3:G:98:LEU:HD13	3:G:98:LEU:N	1.94	0.56
4:D:150:PHE:HB3	12:D:201:EPH:H2	1.87	0.56
1:E:320:ARG:HH12	5:E:701:MLI:C2	2.19	0.56
1:E:289:GLU:OE2	1:E:320:ARG:HD2	2.05	0.56
4:H:109:ARG:HB2	4:H:112:VAL:HG12	1.89	0.55
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.89	0.54
1:E:538:ILE:O	1:E:539:TRP:C	2.49	0.54
3:G:93:PHE:O	3:G:98:LEU:HG	2.07	0.54
10:G:201:HEM:HHC	10:G:201:HEM:HBB2	1.89	0.54
1:E:500:MET:HE1	1:E:560:ILE:HB	1.88	0.54
1:E:451:ASN:O	1:E:455:GLU:HG3	2.07	0.54
1:A:500:MET:HE1	1:A:556:ALA:O	2.08	0.53
2:F:37:THR:HB	2:F:58:ASP:OD2	2.09	0.53
3:G:133:LEU:O	3:G:136:ILE:HG13	2.09	0.53
1:A:477:LEU:CD1	1:A:543:LEU:HD21	2.39	0.53
1:A:604:ARG:NH2	1:A:627:ASP:OD1	2.42	0.53
3:C:60:LEU:HD21	11:C:202:UQ1:H71	1.90	0.53
1:A:253:THR:HG21	1:A:548:GLU:HB3	1.91	0.52
1:E:604:ARG:NH2	1:E:627:ASP:OD1	2.42	0.52
1:E:213:GLY:HA3	1:E:227:PHE:O	2.08	0.52
1:A:325:ARG:O	1:A:326:ALA:C	2.53	0.52
1:E:228:ARG:NH1	1:E:463:PRO:O	2.43	0.51
1:E:277:PRO:CD	1:E:320:ARG:HG3	2.41	0.51
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.92	0.51
2:F:145:GLN:NE2	2:F:195:TYR:OH	2.43	0.51
2:B:105:ASN:HD21	2:B:127:PRO:CD	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:ILE:O	2:B:266:LEU:HB2	2.11	0.51
4:H:57:THR:O	4:H:61:ILE:HG23	2.10	0.51
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.24	0.51
3:G:96:LEU:O	3:G:97:PRO:C	2.53	0.51
3:G:87:LEU:HD22	4:H:128:PHE:CE1	2.46	0.50
3:G:98:LEU:O	3:G:99:ASP:O	2.30	0.50
3:G:107:ILE:HD11	4:H:156:LEU:HD22	1.92	0.50
3:G:112:ILE:HG22	3:G:113:PRO:HD2	1.93	0.50
1:E:424:CYS:SG	1:E:426:SER:HB2	2.51	0.50
1:E:114:GLY:C	1:E:119:MET:HE2	2.37	0.50
2:F:191:SER:O	2:F:193:PRO:HD3	2.11	0.50
2:B:188:CYS:SG	2:B:189:SER:N	2.85	0.50
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.94	0.50
3:C:180:LYS:O	3:C:184:LEU:N	2.45	0.50
4:H:50:LYS:N	4:H:51:PRO:CD	2.75	0.50
1:A:427:VAL:HG23	1:A:428:HIS:CE1	2.46	0.50
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.94	0.50
3:C:126:PHE:HB3	3:C:127:PRO:HD3	1.94	0.50
3:C:178:ARG:NH2	4:D:156:LEU:OXT	2.45	0.50
2:F:197:TRP:NE1	11:G:202:UQ1:O1	2.39	0.49
2:F:212:TYR:OH	2:F:261:GLU:HG2	2.13	0.49
1:A:567:LYS:HB3	1:A:578:PHE:CD1	2.47	0.49
4:D:118:ALA:HB1	4:D:122:ARG:HH21	1.77	0.49
1:A:477:LEU:HD12	1:A:477:LEU:C	2.38	0.49
1:E:79:HIS:CD2	6:E:702:FAD:HM83	2.44	0.49
1:E:32:ILE:HG22	1:E:478:ASP:OD1	2.13	0.49
3:G:112:ILE:HG22	3:G:113:PRO:CD	2.43	0.48
1:A:83:ALA:HA	6:A:702:FAD:C5X	2.43	0.48
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.14	0.48
1:E:439:LEU:HD22	1:E:443:VAL:CG2	2.43	0.48
3:G:143:MET:O	3:G:144:ALA:HB3	2.14	0.48
1:A:37:VAL:O	4:D:31:ALA:HB1	2.14	0.48
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.48	0.48
1:A:231:ARG:NH2	1:A:455:GLU:OE1	2.46	0.48
3:G:118:ASP:OD2	3:G:121:LYS:NZ	2.43	0.48
1:E:79:HIS:CE1	6:E:702:FAD:HM81	2.49	0.48
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.49	0.48
10:C:201:HEM:HBC2	10:C:201:HEM:HHD	1.95	0.48
1:E:32:ILE:HG23	1:E:482:TYR:CD1	2.49	0.48
1:A:78:SER:O	1:A:81:THR:HG22	2.14	0.47
1:E:241:ARG:NH1	1:E:250:HIS:CE1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:VAL:HG23	1:E:428:HIS:CE1	2.49	0.47
1:E:241:ARG:NH2	1:E:248:THR:O	2.45	0.47
1:A:45:VAL:HG23	1:A:229:SER:HB3	1.95	0.47
1:A:105:ASP:OD2	1:A:157:SER:N	2.39	0.47
1:A:44:VAL:HG21	1:A:60:LEU:HD13	1.95	0.47
2:B:47:GLU:O	2:B:50:ALA:HB2	2.15	0.47
4:D:65:PHE:CE2	4:D:94:LEU:HD23	2.49	0.47
1:E:509:ARG:HD2	1:E:511:ASP:OD2	2.14	0.47
1:A:289:GLU:OE2	1:A:320:ARG:HD2	2.15	0.47
3:G:85:THR:HG21	12:H:201:EPH:H272	1.96	0.47
1:E:105:ASP:OD2	1:E:156:GLN:HA	2.14	0.46
4:H:108:GLY:O	4:H:122:ARG:NH2	2.48	0.46
1:A:213:GLY:HA3	1:A:227:PHE:O	2.15	0.46
1:A:280:ILE:HD11	1:A:287:ILE:HD11	1.97	0.46
2:B:168:GLN:HE21	2:B:172:GLU:HB3	1.79	0.46
4:H:70:VAL:O	4:H:74:PRO:HD2	2.16	0.46
1:A:243:TYR:CG	1:A:386:VAL:HG21	2.51	0.46
1:A:277:PRO:CD	1:A:320:ARG:HG3	2.45	0.46
1:A:278:THR:HG22	1:A:382:VAL:HG21	1.97	0.46
2:B:42:ARG:HG3	2:B:55:GLN:HE21	1.80	0.46
2:F:76:LYS:HG2	2:F:81:PRO:HA	1.96	0.46
1:A:99:TRP:CH2	1:A:120:HIS:CE1	3.04	0.46
1:A:437:SER:HB3	6:A:702:FAD:N1	2.30	0.46
1:A:604:ARG:HH22	1:A:627:ASP:CG	2.24	0.46
2:F:227:LEU:HD22	2:F:266:LEU:CD1	2.46	0.46
2:B:239:CYS:SG	2:B:259:ILE:HG21	2.56	0.45
1:A:99:TRP:HH2	1:A:120:HIS:CE1	2.34	0.45
1:E:117:ASN:N	1:E:117:ASN:HD22	2.14	0.45
1:A:94:MET:HG2	1:A:150:GLN:HB2	1.99	0.45
1:A:424:CYS:SG	1:A:426:SER:HB2	2.56	0.45
1:A:567:LYS:HB3	1:A:578:PHE:CE1	2.52	0.45
2:B:90:ARG:HG3	2:B:90:ARG:HH11	1.82	0.45
1:A:343:HIS:HB2	1:A:382:VAL:O	2.17	0.45
1:A:88:ASN:ND2	1:A:169:THR:OG1	2.47	0.45
1:A:534:ASP:HB2	2:B:82:THR:HG22	1.98	0.45
3:C:74:LEU:HD23	3:C:130:PHE:CE1	2.52	0.45
1:A:251:MET:HE2	2:B:87:ARG:O	2.17	0.44
2:B:100:ASN:HD21	2:B:103:GLY:HA2	1.80	0.44
10:G:201:HEM:HHD	10:G:201:HEM:HBC2	1.99	0.44
1:A:534:ASP:CB	2:B:82:THR:HG22	2.46	0.44
1:E:74:PHE:CD2	1:E:76:THR:HB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ILE:H	2:F:165:GLN:HE22	1.65	0.44
1:E:577:ASP:OD2	1:E:577:ASP:N	2.48	0.44
3:G:100:PHE:O	3:G:101:THR:C	2.60	0.44
4:D:54:SER:OG	4:D:55:HIS:O	2.30	0.44
4:D:112:VAL:HG13	4:D:113:LEU:HG	2.00	0.44
4:D:55:HIS:CD2	4:D:56:GLY:H	2.35	0.44
1:E:83:ALA:HA	6:E:702:FAD:C5X	2.47	0.44
1:A:42:TYR:O	1:A:229:SER:HA	2.18	0.44
1:E:547:LEU:HD12	1:E:550:GLN:OE1	2.18	0.44
2:B:243:MET:HE3	3:C:141:PHE:CG	2.53	0.44
3:G:178:ARG:HA	3:G:181:LYS:HB2	2.00	0.44
1:E:73:MET:SD	1:E:251:MET:HG3	2.58	0.43
2:F:282:PHE:C	2:F:282:PHE:CD2	2.96	0.43
1:E:116:GLN:HA	1:E:119:MET:HE3	2.00	0.43
1:A:577:ASP:O	1:A:578:PHE:CD2	2.71	0.43
2:B:105:ASN:HD21	2:B:127:PRO:HD3	1.84	0.43
1:E:517:VAL:O	1:E:521:MET:HG2	2.18	0.43
4:H:85:ASP:OD2	4:H:147:THR:HG23	2.19	0.43
2:B:89:CYS:HB3	2:B:94:CYS:HB3	2.01	0.43
1:E:45:VAL:HG23	1:E:229:SER:HB3	2.00	0.43
1:E:276:HIS:O	1:E:384:PRO:HA	2.19	0.43
4:H:145:GLY:O	4:H:149:ALA:HB2	2.18	0.43
1:A:46:ILE:HG12	1:A:233:ILE:HD12	2.00	0.43
1:A:73:MET:SD	1:A:251:MET:HG3	2.59	0.43
1:A:236:THR:HA	6:A:702:FAD:O4B	2.19	0.43
1:E:174:ASP:HB2	1:E:361:PRO:HD2	2.01	0.42
1:A:117:ASN:HD22	1:A:118:ALA:N	2.16	0.42
3:C:87:LEU:HD22	4:D:128:PHE:CE1	2.55	0.42
1:A:114:GLY:C	1:A:119:MET:HE2	2.45	0.42
1:E:147:LYS:HD3	2:F:282:PHE:CE1	2.55	0.42
1:A:314:ALA:O	1:A:315:LYS:C	2.62	0.42
3:C:62:ILE:HD12	3:C:62:ILE:C	2.45	0.42
1:A:524:PHE:HA	1:A:553:MET:HE2	2.02	0.42
2:B:68:VAL:HG23	2:B:111:CYS:O	2.19	0.42
1:A:344:ILE:HG12	1:A:345:TYR:N	2.34	0.42
2:F:155:LYS:NZ	2:F:219:ARG:O	2.53	0.42
1:E:610:LYS:O	1:E:618:ILE:HA	2.20	0.42
3:G:94:SER:HB2	4:H:138:TYR:CD2	2.55	0.42
1:A:236:THR:OG1	1:A:256:GLY:HA3	2.20	0.41
1:A:253:THR:OG1	1:A:255:ASP:OD1	2.24	0.41
3:C:69:TRP:HE3	11:C:202:UQ1:HM53	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:O	1:A:447:ALA:C	2.62	0.41
1:E:313:LYS:CG	1:E:314:ALA:N	2.79	0.41
4:H:150:PHE:O	4:H:153:VAL:HG22	2.20	0.41
1:A:172:VAL:O	1:A:172:VAL:HG12	2.19	0.41
1:E:104:TYR:HA	1:E:638:ILE:HD13	2.01	0.41
1:E:330:GLU:OE1	1:E:335:ARG:NH2	2.53	0.41
2:F:133:LYS:O	2:F:134:ASP:C	2.63	0.41
1:E:58:MET:HE3	1:E:187:ASN:HB3	2.03	0.41
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.67	0.41
2:F:227:LEU:HD22	2:F:266:LEU:HD13	2.02	0.41
1:E:352:PRO:HD2	1:E:355:GLN:HE21	1.85	0.41
1:E:583:ASP:OD1	1:E:604:ARG:HG3	2.21	0.41
1:A:344:ILE:HD13	1:A:382:VAL:HG23	2.03	0.41
3:C:103:PHE:O	3:C:107:ILE:HG23	2.20	0.41
1:E:281:TYR:OH	1:E:342:ASP:OD2	2.31	0.41
1:A:523:LEU:HD12	1:A:523:LEU:HA	1.95	0.41
1:A:629:THR:HG21	1:A:635:VAL:HG13	2.02	0.41
1:E:253:THR:HG21	1:E:548:GLU:HB3	2.02	0.41
3:G:101:THR:HA	4:H:152:MET:HE1	2.03	0.41
1:A:498:LYS:O	1:A:499:THR:C	2.62	0.41
2:B:135:LEU:O	2:B:137:PRO:HD3	2.20	0.41
2:B:191:SER:O	2:B:193:PRO:HD3	2.21	0.41
3:C:74:LEU:HD23	3:C:130:PHE:CE2	2.55	0.41
4:D:52:LEU:C	4:D:53:HIS:O	2.57	0.41
1:A:327:GLU:OE2	1:A:344:ILE:HD11	2.21	0.40
1:A:438:LEU:HG	6:A:702:FAD:C2	2.51	0.40
2:F:116:ASN:C	2:F:116:ASN:ND2	2.77	0.40
1:A:433:LEU:O	1:A:436:ASN:HB2	2.21	0.40
1:E:79:HIS:O	1:E:80:THR:C	2.65	0.40
4:H:150:PHE:O	4:H:151:GLU:C	2.63	0.40
2:B:116:ASN:C	2:B:116:ASN:HD22	2.30	0.40
4:D:101:TRP:CH2	4:D:122:ARG:HG2	2.57	0.40
1:E:236:THR:HA	6:E:702:FAD:O4B	2.22	0.40
2:F:188:CYS:SG	2:F:206:ALA:HB2	2.61	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	614/645 (95%)	577 (94%)	35 (6%)	2 (0%)	36	66
1	E	614/645 (95%)	577 (94%)	36 (6%)	1 (0%)	43	72
2	B	248/282 (88%)	231 (93%)	15 (6%)	2 (1%)	16	44
2	F	248/282 (88%)	233 (94%)	14 (6%)	1 (0%)	30	60
3	C	151/188 (80%)	141 (93%)	9 (6%)	1 (1%)	18	47
3	G	151/188 (80%)	134 (89%)	10 (7%)	7 (5%)	2	6
4	D	127/156 (81%)	121 (95%)	6 (5%)	0	100	100
4	H	127/156 (81%)	119 (94%)	7 (6%)	1 (1%)	16	44
All	All	2280/2542 (90%)	2133 (94%)	132 (6%)	15 (1%)	18	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	185	PRO
1	A	485	GLY
2	B	116	ASN
1	E	485	GLY
3	G	97	PRO
3	G	99	ASP
3	G	173	TYR
1	A	489	THR
3	C	185	PRO
3	G	111	GLY
3	G	113	PRO
3	G	183	THR
4	H	51	PRO
2	B	89	CYS
2	F	273	PRO

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	502/527 (95%)	459 (91%)	43 (9%)	10	31
1	E	502/527 (95%)	463 (92%)	39 (8%)	11	35
2	B	220/242 (91%)	204 (93%)	16 (7%)	13	38
2	F	220/242 (91%)	202 (92%)	18 (8%)	10	33
3	C	127/158 (80%)	114 (90%)	13 (10%)	7	23
3	G	127/158 (80%)	113 (89%)	14 (11%)	6	20
4	D	98/119 (82%)	85 (87%)	13 (13%)	4	14
4	H	98/119 (82%)	90 (92%)	8 (8%)	10	33
All	All	1894/2092 (90%)	1730 (91%)	164 (9%)	9	30

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	44	VAL
1	A	62	GLU
1	A	71	THR
1	A	76	THR
1	A	117	ASN
1	A	159	ASN
1	A	175	ARG
1	A	179	SER
1	A	191	CYS
1	A	194	THR
1	A	205	LEU
1	A	298	LEU
1	A	302	GLU
1	A	320	ARG
1	A	337	VAL
1	A	344	ILE
1	A	351	LEU
1	A	356	LEU

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Mol	Chain	Res	Type
1	A	359	ARG
1	A	390	MET
1	A	402	ILE
1	A	436	ASN
1	A	439	LEU
1	A	440	ASP
1	A	453	LYS
1	A	461	LYS
1	A	464	GLU
1	A	477	LEU
1	A	487	VAL
1	A	509	ARG
1	A	518	LYS
1	A	523	LEU
1	A	528	LYS
1	A	531	LYS
1	A	535	ARG
1	A	547	LEU
1	A	561	VAL
1	A	584	GLU
1	A	609	THR
1	A	610	LYS
1	A	614	ARG
1	A	619	THR
2	B	37	THR
2	B	69	LEU
2	B	90	ARG
2	B	91	GLU
2	B	115	GLN
2	B	131	VAL
2	B	148	SER
2	B	156	LYS
2	B	171	LYS
2	B	173	GLN
2	B	176	LEU
2	B	183	ILE
2	B	184	LEU
2	B	216	ILE
2	B	238	LYS
2	B	278	THR
3	C	53	LYS
3	C	67	MET

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Mol	Chain	Res	Type
3	C	68	THR
3	C	96	LEU
3	C	105	GLU
3	C	107	ILE
3	C	133	LEU
3	C	136	ILE
3	C	159	VAL
3	C	165	LEU
3	C	170	VAL
3	C	172	VAL
3	C	175	ARG
4	D	46	GLU
4	D	49	PHE
4	D	50	LYS
4	D	57	THR
4	D	61	ILE
4	D	72	LEU
4	D	79	ILE
4	D	83	GLU
4	D	84	MET
4	D	86	LEU
4	D	90	LEU
4	D	92	LEU
4	D	117	LEU
1	E	44	VAL
1	E	76	THR
1	E	81	THR
1	E	117	ASN
1	E	153	PHE
1	E	162	LYS
1	E	170	CYS
1	E	179	SER
1	E	194	THR
1	E	205	LEU
1	E	226	ARG
1	E	230	LYS
1	E	257	THR
1	E	259	LEU
1	E	291	SER
1	E	298	LEU
1	E	320	ARG
1	E	337	VAL

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Mol	Chain	Res	Type
1	E	344	ILE
1	E	358	GLN
1	E	359	ARG
1	E	373	VAL
1	E	390	MET
1	E	436	ASN
1	E	439	LEU
1	E	440	ASP
1	E	453	LYS
1	E	456	LEU
1	E	471	GLU
1	E	474	ILE
1	E	484	ASN
1	E	500	MET
1	E	518	LYS
1	E	528	LYS
1	E	535	ARG
1	E	547	LEU
1	E	561	VAL
1	E	584	GLU
1	E	601	LYS
2	F	33	LYS
2	F	37	THR
2	F	69	LEU
2	F	90	ARG
2	F	129	MET
2	F	131	VAL
2	F	148	SER
2	F	156	LYS
2	F	159	ILE
2	F	173	GLN
2	F	176	LEU
2	F	179	LEU
2	F	184	LEU
2	F	194	SER
2	F	216	ILE
2	F	218	SER
2	F	266	LEU
2	F	278	THR
3	G	59	HIS
3	G	67	MET
3	G	98	LEU

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Mol	Chain	Res	Type
3	G	99	ASP
3	G	107	ILE
3	G	110	LEU
3	G	112	ILE
3	G	117	LEU
3	G	133	LEU
3	G	158	LEU
3	G	160	LEU
3	G	162	LEU
3	G	181	LYS
3	G	186	THR
4	H	58	LEU
4	H	61	ILE
4	H	72	LEU
4	H	79	ILE
4	H	86	LEU
4	H	122	ARG
4	H	136	LEU
4	H	152	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	125	ASN
1	A	159	ASN
1	A	250	HIS
1	A	349	HIS
1	A	358	GLN
1	A	436	ASN
1	A	451	ASN
1	A	497	GLN
1	A	550	GLN
1	A	551	ASN
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	112	ASN
2	B	116	ASN

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Mol	Chain	Res	Type
2	B	154	GLN
2	B	168	GLN
4	D	55	HIS
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN
1	E	120	HIS
1	E	182	HIS
1	E	250	HIS
1	E	252	ASN
1	E	347	GLN
1	E	349	HIS
1	E	355	GLN
1	E	358	GLN
1	E	436	ASN
1	E	497	GLN
1	E	503	HIS
1	E	551	ASN
1	E	573	HIS
1	E	594	GLN
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	112	ASN
2	F	116	ASN
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
4	H	53	HIS
4	H	140	ASN
4	H	142	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
12	EPH	H	201	-	43,43,48	1.11	2 (4%)	45,48,53	1.16	5 (11%)
9	F3S	B	303	2	0,9,9	-	-	-	-	-
10	HEM	G	201	4,3	50,50,50	1.56	6 (12%)	66,82,82	1.87	16 (24%)
11	UQ1	C	202	-	18,18,18	2.13	5 (27%)	22,25,25	1.28	3 (13%)
9	F3S	F	303	2	0,9,9	-	-	-	-	-
6	FAD	A	702	-	56,58,58	1.38	10 (17%)	81,89,89	1.93	23 (28%)
10	HEM	C	201	4,3	50,50,50	1.61	7 (14%)	66,82,82	1.70	14 (21%)
5	MLI	E	701	-	6,6,6	1.00	0	7,7,7	1.44	1 (14%)
6	FAD	E	702	-	56,58,58	1.50	9 (16%)	81,89,89	1.93	21 (25%)
12	EPH	D	201	-	43,43,48	1.08	2 (4%)	45,48,53	1.16	5 (11%)
7	FES	F	301	2	0,4,4	-	-	-	-	-
8	SF4	B	302	2	0,12,12	-	-	-	-	-
11	UQ1	G	202	-	18,18,18	2.16	6 (33%)	22,25,25	1.09	2 (9%)
7	FES	B	301	2	0,4,4	-	-	-	-	-
8	SF4	F	302	2	0,12,12	-	-	-	-	-
5	MLI	A	701	-	6,6,6	1.08	0	7,7,7	1.34	1 (14%)

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
12	EPH	H	201	-	-	29/47/47/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	F3S	B	303	2	-	-	0/3/3/3
10	HEM	G	201	4,3	-	6/14/54/54	-
11	UQ1	C	202	-	-	4/9/33/33	0/1/1/1
9	F3S	F	303	2	-	-	0/3/3/3
6	FAD	A	702	-	-	7/34/50/50	0/6/6/6
10	HEM	C	201	4,3	-	3/14/54/54	-
5	MLI	E	701	-	-	0/4/4/4	-
6	FAD	E	702	-	-	4/34/50/50	0/6/6/6
12	EPH	D	201	-	-	24/47/47/52	-
7	FES	F	301	2	-	-	0/1/1/1
8	SF4	B	302	2	-	-	0/6/5/5
11	UQ1	G	202	-	-	0/9/33/33	0/1/1/1
7	FES	B	301	2	-	-	0/1/1/1
8	SF4	F	302	2	-	-	0/6/5/5
5	MLI	A	701	-	-	0/4/4/4	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	FE-NB	5.55	2.12	1.94
10	C	201	HEM	FE-NB	5.35	2.11	1.94
11	C	202	UQ1	CM5-C5	-5.35	1.39	1.50
6	E	702	FAD	C9A-C5X	5.26	1.50	1.41
12	H	201	EPH	O1-C3	4.67	1.47	1.34
11	G	202	UQ1	CM5-C5	-4.63	1.41	1.50
12	D	201	EPH	O2-C4	4.61	1.46	1.33
12	H	201	EPH	O2-C4	4.55	1.46	1.33
6	A	702	FAD	C9A-C5X	4.49	1.48	1.41
12	D	201	EPH	O1-C3	4.36	1.46	1.34
6	E	702	FAD	C5A-C4A	4.12	1.46	1.39
10	C	201	HEM	FE-NC	4.06	2.08	1.95
10	G	201	HEM	FE-NC	4.04	2.08	1.95
11	G	202	UQ1	C7-C8	3.60	1.55	1.50
10	C	201	HEM	C1B-NB	-3.59	1.34	1.40
11	G	202	UQ1	C6-C5	3.48	1.41	1.35
11	C	202	UQ1	C7-C8	3.31	1.55	1.50
10	G	201	HEM	C1B-NB	-3.30	1.34	1.40
11	G	202	UQ1	C6-C1	3.11	1.55	1.46
10	C	201	HEM	C4D-ND	-3.09	1.35	1.40
6	E	702	FAD	C8-C7	3.05	1.48	1.40
6	A	702	FAD	C5A-C4A	3.04	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	202	UQ1	C6-C1	2.91	1.54	1.46
6	A	702	FAD	C8-C7	2.91	1.48	1.40
11	G	202	UQ1	C7-C6	2.86	1.56	1.51
11	C	202	UQ1	C7-C6	2.82	1.56	1.51
11	C	202	UQ1	C6-C5	2.81	1.40	1.35
10	G	201	HEM	C3B-C4B	2.76	1.50	1.44
6	A	702	FAD	C5X-N5	-2.71	1.34	1.39
6	A	702	FAD	C4A-N9A	-2.70	1.31	1.37
10	C	201	HEM	C1C-C2C	-2.66	1.40	1.45
6	E	702	FAD	C8A-N7A	2.60	1.36	1.31
10	C	201	HEM	C3B-C4B	2.59	1.50	1.44
6	E	702	FAD	C4-N3	-2.56	1.34	1.38
6	A	702	FAD	C8M-C8	-2.56	1.45	1.51
6	A	702	FAD	C5A-N7A	-2.50	1.34	1.39
6	A	702	FAD	C4-N3	-2.49	1.34	1.38
6	E	702	FAD	C5A-N7A	-2.42	1.34	1.39
6	E	702	FAD	C5X-N5	-2.35	1.34	1.39
6	A	702	FAD	C8A-N7A	2.26	1.35	1.31
6	E	702	FAD	C5A-C6A	2.23	1.47	1.41
10	G	201	HEM	C1C-C2C	-2.23	1.40	1.45
10	G	201	HEM	C4D-ND	-2.19	1.36	1.40
10	C	201	HEM	FE-ND	-2.16	1.88	1.94
6	E	702	FAD	C8M-C8	-2.14	1.46	1.51
11	G	202	UQ1	C5-C4	2.13	1.54	1.47
6	A	702	FAD	C5A-C6A	2.03	1.46	1.41

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FAD	C5A-C4A-N3A	-6.36	118.45	126.75
6	A	702	FAD	C5A-C4A-N3A	-5.33	119.80	126.75
10	G	201	HEM	CAD-C3D-C4D	5.26	133.86	124.66
6	E	702	FAD	N3A-C4A-N9A	5.21	135.67	127.08
6	E	702	FAD	N3A-C2A-N1A	-4.60	121.41	128.60
6	E	702	FAD	C2A-N3A-C4A	4.52	122.43	111.75
12	H	201	EPH	O1-C3-C5	4.34	120.86	111.50
10	C	201	HEM	CHA-C4D-ND	4.30	129.68	124.37
10	G	201	HEM	CBD-CAD-C3D	4.30	124.57	112.63
12	D	201	EPH	O1-C3-C5	4.12	120.37	111.50
6	A	702	FAD	N3A-C4A-N9A	4.06	133.78	127.08
10	C	201	HEM	C1B-NB-C4B	4.05	109.25	105.07
6	A	702	FAD	N3A-C2A-N1A	-4.02	122.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	C2A-N3A-C4A	4.02	121.24	111.75
10	G	201	HEM	C1B-NB-C4B	3.92	109.12	105.07
6	A	702	FAD	O4-C4-C4X	-3.91	116.21	126.60
10	G	201	HEM	C4C-NC-C1C	3.90	109.17	105.35
10	C	201	HEM	C4C-NC-C1C	3.87	109.14	105.35
12	D	201	EPH	O2-C4-C18	3.86	124.01	111.91
10	G	201	HEM	CHD-C1D-ND	3.84	128.59	124.42
10	G	201	HEM	CAC-C3C-C4C	3.83	134.14	124.90
6	E	702	FAD	O2-C2-N1	-3.78	115.57	121.83
6	A	702	FAD	C4A-N9A-C8A	3.77	109.81	105.73
12	H	201	EPH	O2-C4-C18	3.63	123.30	111.91
10	C	201	HEM	CHD-C1D-ND	3.58	128.31	124.42
10	C	201	HEM	CAC-C3C-C4C	3.48	133.31	124.90
6	A	702	FAD	N9A-C8A-N7A	-3.42	109.24	113.91
6	A	702	FAD	O2-C2-N1	-3.38	116.22	121.83
6	A	702	FAD	C4A-C5A-N7A	-3.30	106.59	110.62
6	A	702	FAD	C9-C8-C7	3.25	124.33	119.67
10	C	201	HEM	CHB-C1B-NB	3.22	128.34	124.37
10	C	201	HEM	CHA-C4D-C3D	-3.19	119.34	125.33
6	A	702	FAD	C4X-C10-N1	-3.18	117.36	124.73
6	E	702	FAD	C4X-C10-N1	-3.14	117.45	124.73
10	G	201	HEM	CAD-C3D-C2D	-3.12	122.07	127.88
6	A	702	FAD	C5A-N7A-C8A	3.11	107.92	103.51
6	E	702	FAD	O4-C4-C4X	-3.10	118.38	126.60
6	E	702	FAD	C4A-N9A-C8A	3.06	109.04	105.73
10	G	201	HEM	CAC-C3C-C2C	-2.99	118.75	128.60
6	E	702	FAD	C5A-N7A-C8A	2.99	107.76	103.51
6	E	702	FAD	C4A-C5A-N7A	-2.98	106.98	110.62
10	C	201	HEM	C4B-C3B-C2B	-2.91	104.81	107.11
10	C	201	HEM	CAC-C3C-C2C	-2.91	119.03	128.60
10	G	201	HEM	CHB-C1B-NB	2.90	127.95	124.37
12	D	201	EPH	O2-C4-O4	-2.86	116.37	123.59
11	C	202	UQ1	CM3-O3-C3	-2.80	106.55	116.47
6	E	702	FAD	C4X-C10-N10	2.74	120.48	116.48
6	E	702	FAD	C10-N1-C2	2.72	122.34	116.90
11	C	202	UQ1	CM5-C5-C6	-2.68	120.02	124.40
6	E	702	FAD	C9-C8-C7	2.68	123.50	119.67
6	E	702	FAD	C1'-C2'-C3'	2.65	117.19	109.79
11	G	202	UQ1	CM3-O3-C3	-2.65	107.09	116.47
6	A	702	FAD	O4-C4-N3	2.63	125.17	120.12
6	A	702	FAD	C6A-C5A-N7A	2.62	136.91	132.02
10	C	201	HEM	CHC-C4B-NB	2.62	127.27	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	702	FAD	N9A-C8A-N7A	-2.62	110.33	113.91
6	A	702	FAD	C6-C5X-C9A	2.61	122.62	118.94
12	D	201	EPH	C1-O2-C4	2.56	126.59	117.12
6	A	702	FAD	O4B-C1B-N9A	2.51	113.00	108.06
6	A	702	FAD	C4-N3-C2	-2.50	121.02	125.64
6	A	702	FAD	C8M-C8-C7	-2.49	115.63	120.74
6	A	702	FAD	C10-N1-C2	2.48	121.85	116.90
10	G	201	HEM	CHA-C4D-ND	2.46	127.41	124.37
10	G	201	HEM	CHD-C1D-C2D	-2.44	121.17	124.98
12	H	201	EPH	C1-O2-C4	2.42	126.09	117.12
10	G	201	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
6	E	702	FAD	C9A-N10-C10	-2.38	117.06	120.77
10	G	201	HEM	CHC-C4B-NB	2.38	127.00	124.42
10	G	201	HEM	CHC-C1C-NC	2.37	127.01	124.44
12	H	201	EPH	O2-C4-O4	-2.37	117.60	123.59
6	E	702	FAD	C2A-N1A-C6A	2.35	122.80	118.77
6	A	702	FAD	C1'-N10-C9A	2.29	124.33	120.51
5	A	701	MLI	O7-C2-C1	2.24	121.69	114.54
10	G	201	HEM	C4B-C3B-C2B	-2.23	105.34	107.11
6	E	702	FAD	C4-N3-C2	-2.21	121.55	125.64
6	E	702	FAD	C6A-C5A-N7A	2.20	136.11	132.02
6	A	702	FAD	C4'-C3'-C2'	-2.19	108.80	113.36
10	C	201	HEM	CMD-C2D-C1D	2.19	128.37	125.04
10	C	201	HEM	CBD-CAD-C3D	-2.17	106.58	112.63
6	E	702	FAD	O4B-C1B-N9A	2.15	112.30	108.06
5	E	701	MLI	O7-C2-C1	2.15	121.40	114.54
10	C	201	HEM	CHD-C1D-C2D	-2.15	121.62	124.98
11	G	202	UQ1	CM5-C5-C6	-2.14	120.92	124.40
6	A	702	FAD	C4X-C4-N3	2.13	118.61	113.19
6	E	702	FAD	C1'-N10-C9A	2.13	124.06	120.51
10	G	201	HEM	CAB-C3B-C2B	-2.11	121.65	128.60
10	C	201	HEM	CHC-C1C-NC	2.09	126.70	124.44
12	H	201	EPH	O1-C3-O3	-2.02	118.82	123.70
11	C	202	UQ1	C11-C9-C10	2.02	119.06	114.60
12	D	201	EPH	O1-C3-O3	-2.02	118.83	123.70
6	A	702	FAD	C6-C7-C8	-2.01	116.79	119.67

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-C3'
6	A	702	FAD	PA-O3P-P-O5'
6	E	702	FAD	N10-C1'-C2'-O2'
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
11	C	202	UQ1	C1-C6-C7-C8
11	C	202	UQ1	C5-C6-C7-C8
12	D	201	EPH	O4-C4-O2-C1
12	D	201	EPH	C18-C4-O2-C1
12	D	201	EPH	C25-C26-C27-C28
12	D	201	EPH	C37-O5-P1-O7
12	D	201	EPH	C5-C3-O1-C2
12	D	201	EPH	C38-O8-P1-O6
12	D	201	EPH	C38-O8-P1-O7
12	H	201	EPH	O4-C4-O2-C1
12	H	201	EPH	C18-C4-O2-C1
12	H	201	EPH	C37-O5-P1-O7
12	H	201	EPH	O3-C3-O1-C2
12	H	201	EPH	C38-O8-P1-O6
12	H	201	EPH	C39-C38-O8-P1
12	D	201	EPH	O3-C3-O1-C2
12	H	201	EPH	C5-C3-O1-C2
12	H	201	EPH	C3-C5-C6-C7
12	D	201	EPH	C38-O8-P1-O5
12	H	201	EPH	C37-O5-P1-O8
12	H	201	EPH	C38-O8-P1-O5
12	D	201	EPH	C20-C21-C22-C23
12	D	201	EPH	C6-C7-C8-C9
12	D	201	EPH	C11-C10-C9-C8
12	H	201	EPH	C9-C10-C11-C12
12	H	201	EPH	C4-C18-C19-C20
10	C	201	HEM	C4B-C3B-CAB-CBB
10	G	201	HEM	C4B-C3B-CAB-CBB
12	D	201	EPH	C9-C10-C11-C12
12	H	201	EPH	C21-C22-C23-C24
12	H	201	EPH	C7-C8-C9-C10
12	H	201	EPH	C11-C10-C9-C8
12	H	201	EPH	C6-C7-C8-C9
12	D	201	EPH	C37-O5-P1-O8
12	D	201	EPH	C13-C14-C15-C16
12	H	201	EPH	C12-C13-C14-C15
12	H	201	EPH	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
12	D	201	EPH	C28-C29-C30-C31
12	H	201	EPH	C28-C29-C30-C31
12	H	201	EPH	C1-C2-C37-O5
12	D	201	EPH	C37-C2-O1-C3
12	H	201	EPH	O1-C2-C37-O5
10	C	201	HEM	C4C-C3C-CAC-CBC
10	G	201	HEM	C4C-C3C-CAC-CBC
6	A	702	FAD	P-O3P-PA-O2A
6	E	702	FAD	P-O3P-PA-O1A
12	D	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C38-O8-P1-O7
12	D	201	EPH	C39-C38-O8-P1
12	D	201	EPH	C5-C6-C7-C8
12	H	201	EPH	C37-C2-O1-C3
12	D	201	EPH	O2-C1-C2-C37
11	C	202	UQ1	C1-C2-O2-CM2
12	H	201	EPH	O8-C38-C39-N1
12	H	201	EPH	C10-C11-C12-C13
12	H	201	EPH	O2-C1-C2-C37
10	C	201	HEM	C2A-CAA-CBA-CGA
6	A	702	FAD	P-O3P-PA-O1A
12	D	201	EPH	C18-C19-C20-C21
12	D	201	EPH	C10-C11-C12-C13
12	H	201	EPH	C24-C25-C26-C27
6	A	702	FAD	O4B-C4B-C5B-O5B
6	E	702	FAD	O4B-C4B-C5B-O5B
12	D	201	EPH	C7-C8-C9-C10
6	E	702	FAD	P-O3P-PA-O2A
11	C	202	UQ1	C4-C3-O3-CM3
10	G	201	HEM	CAD-CBD-CGD-O2D
10	G	201	HEM	CAD-CBD-CGD-O1D
6	A	702	FAD	O4'-C4'-C5'-O5'
12	H	201	EPH	C19-C18-C4-O2

There are no ring outliers.

10 monomers are involved in 32 short contacts:

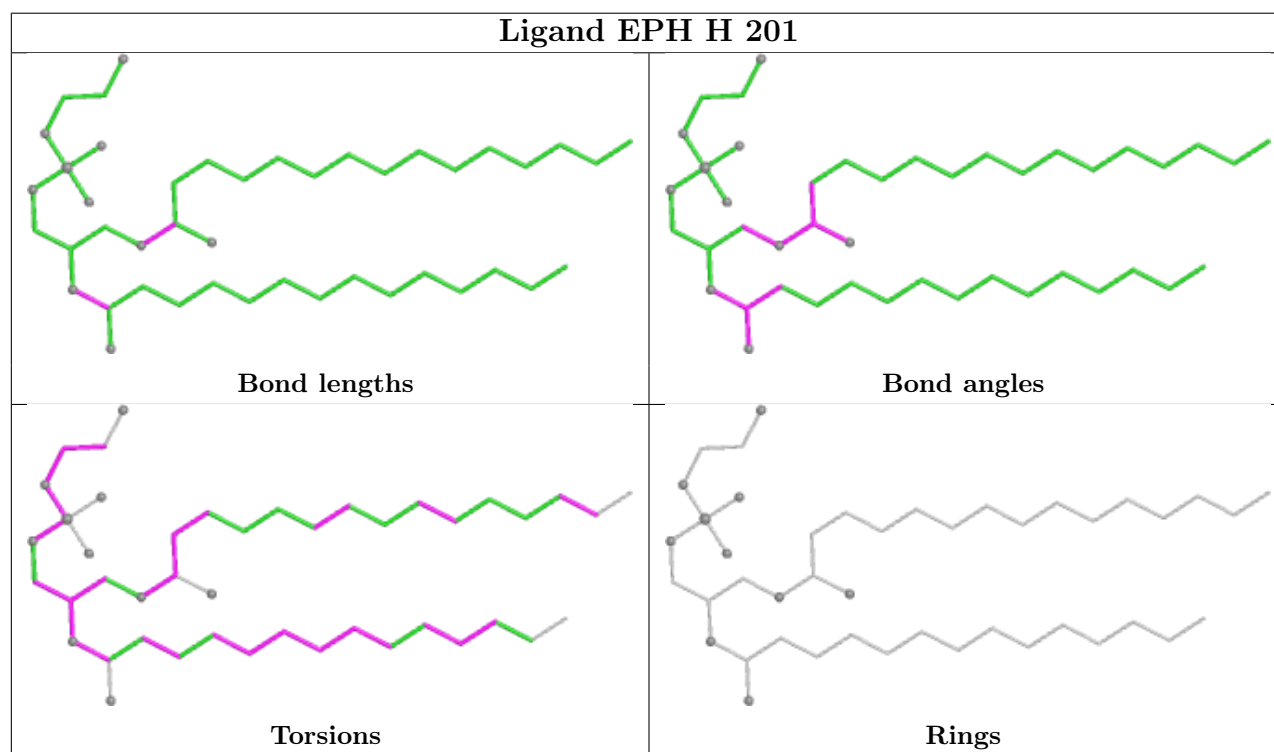
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	201	EPH	1	0
10	G	201	HEM	4	0
11	C	202	UQ1	4	0

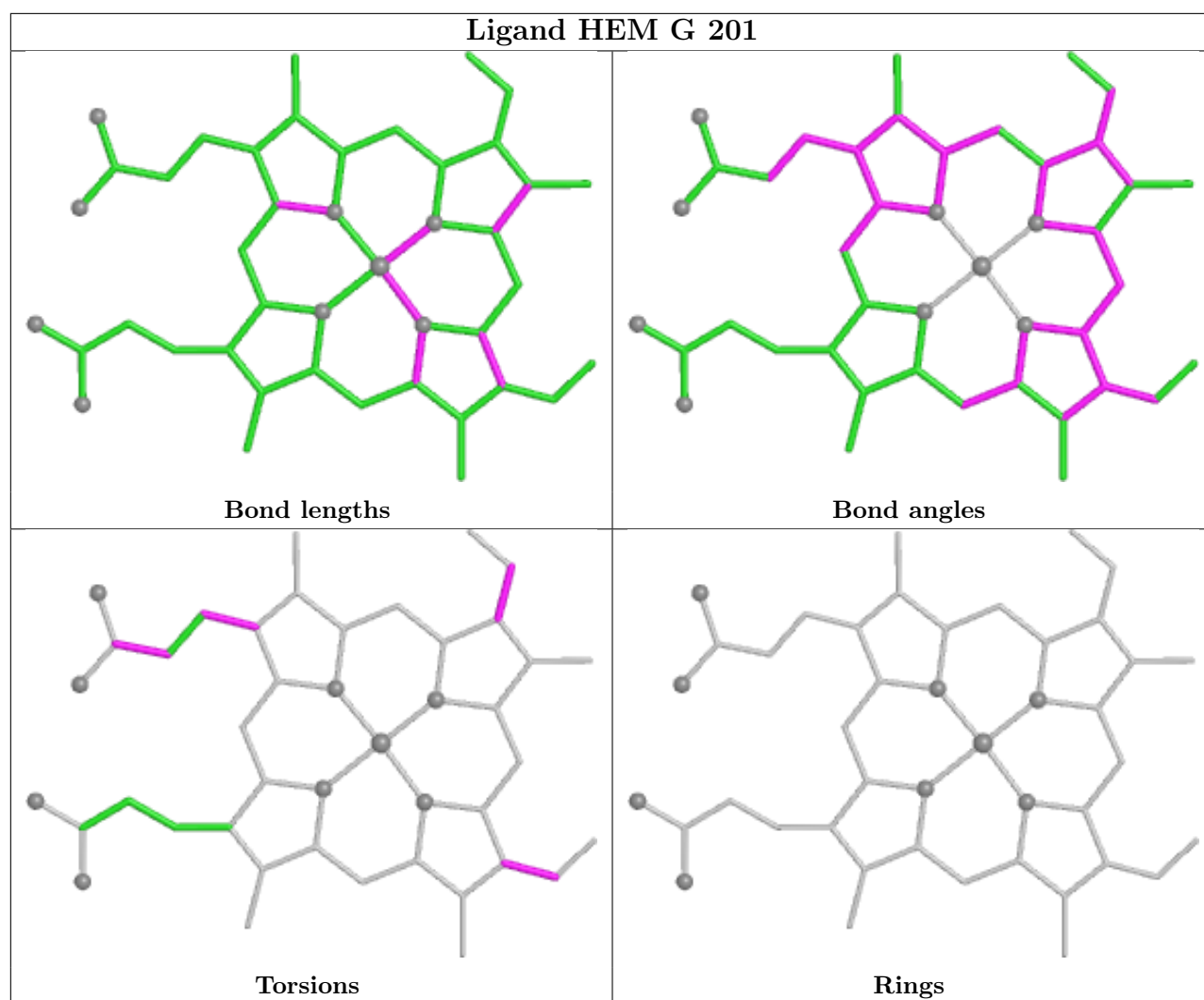
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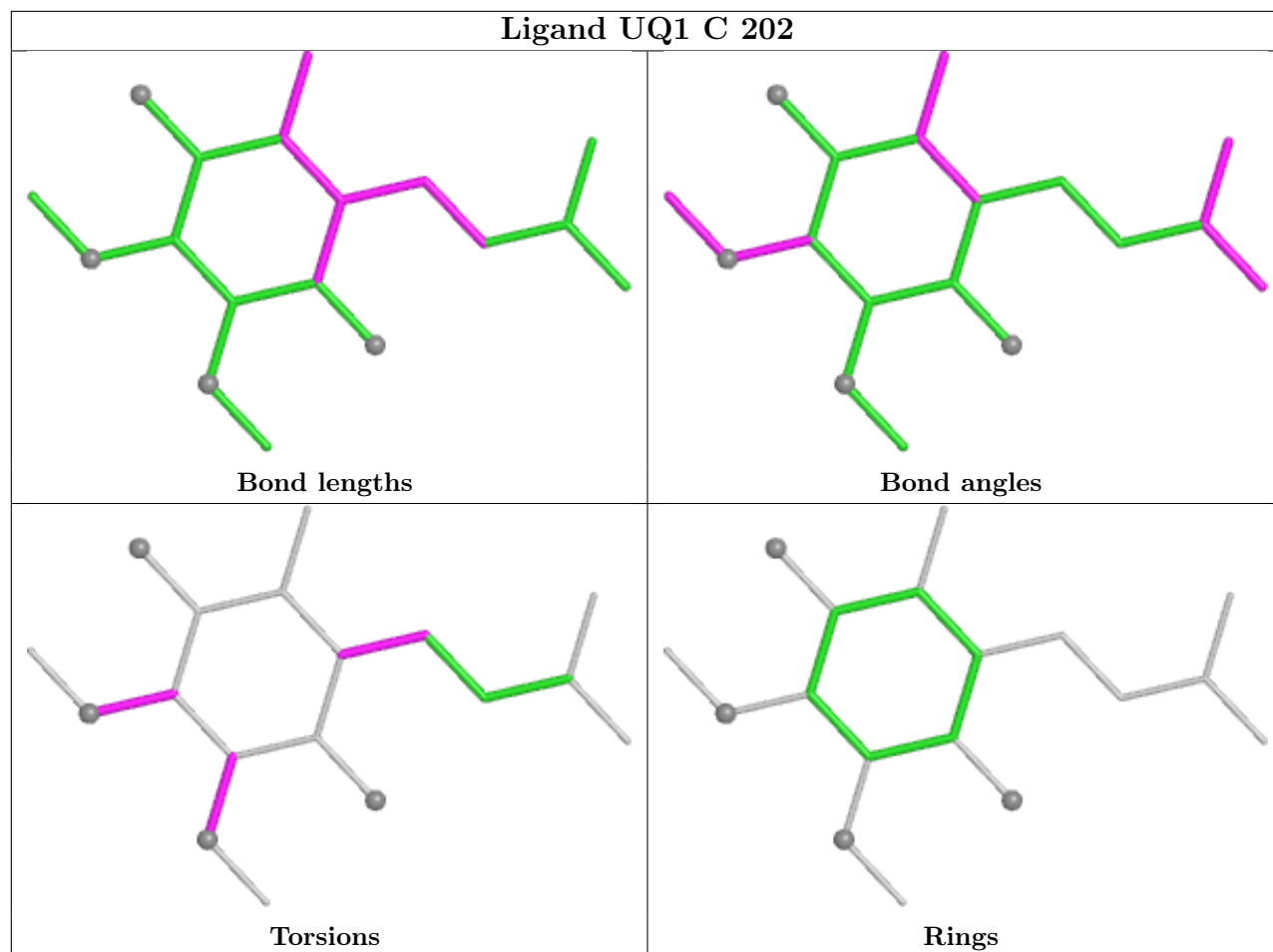
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	FAD	9	0
10	C	201	HEM	2	0
5	E	701	MLI	1	0
6	E	702	FAD	8	0
12	D	201	EPH	1	0
11	G	202	UQ1	1	0
5	A	701	MLI	1	0

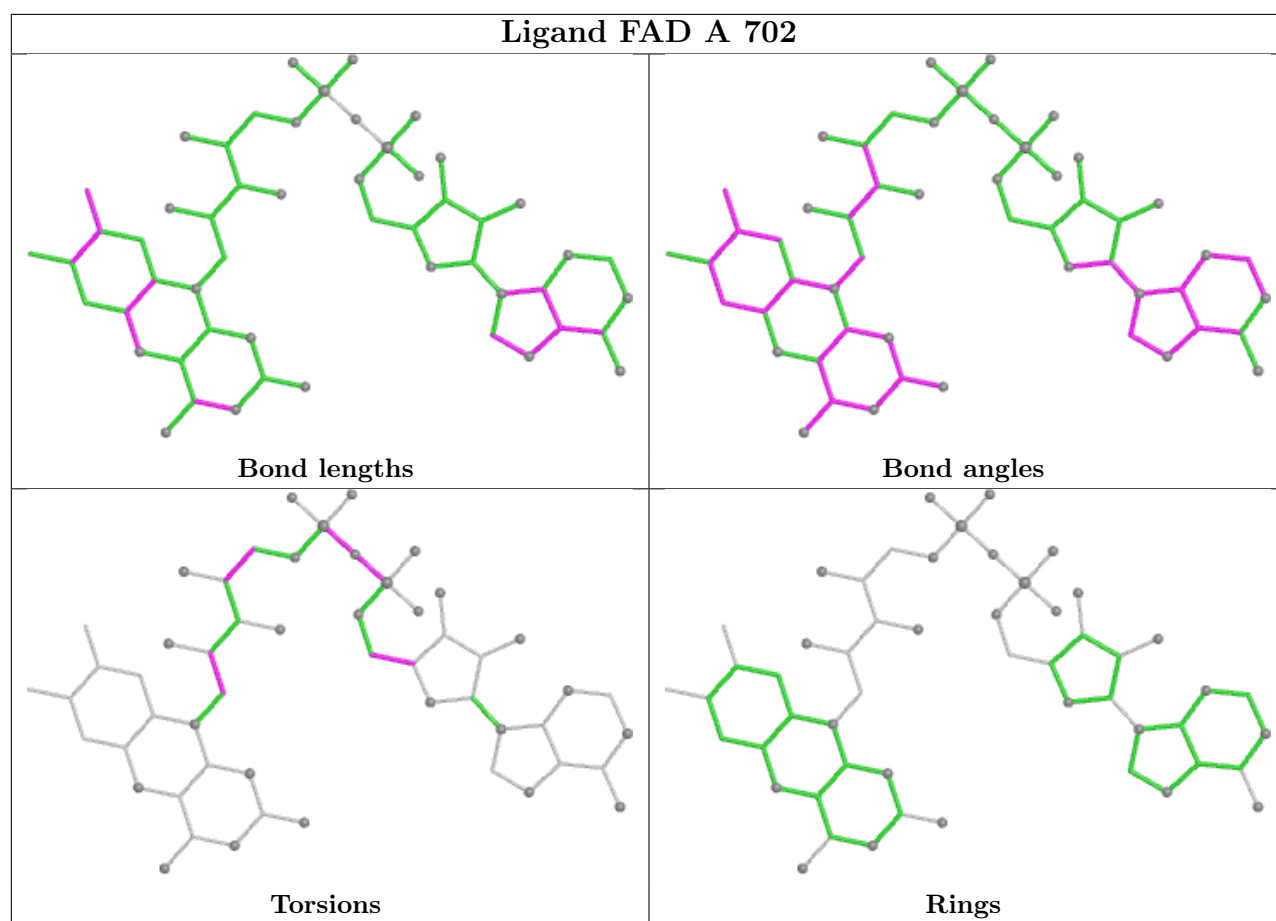
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

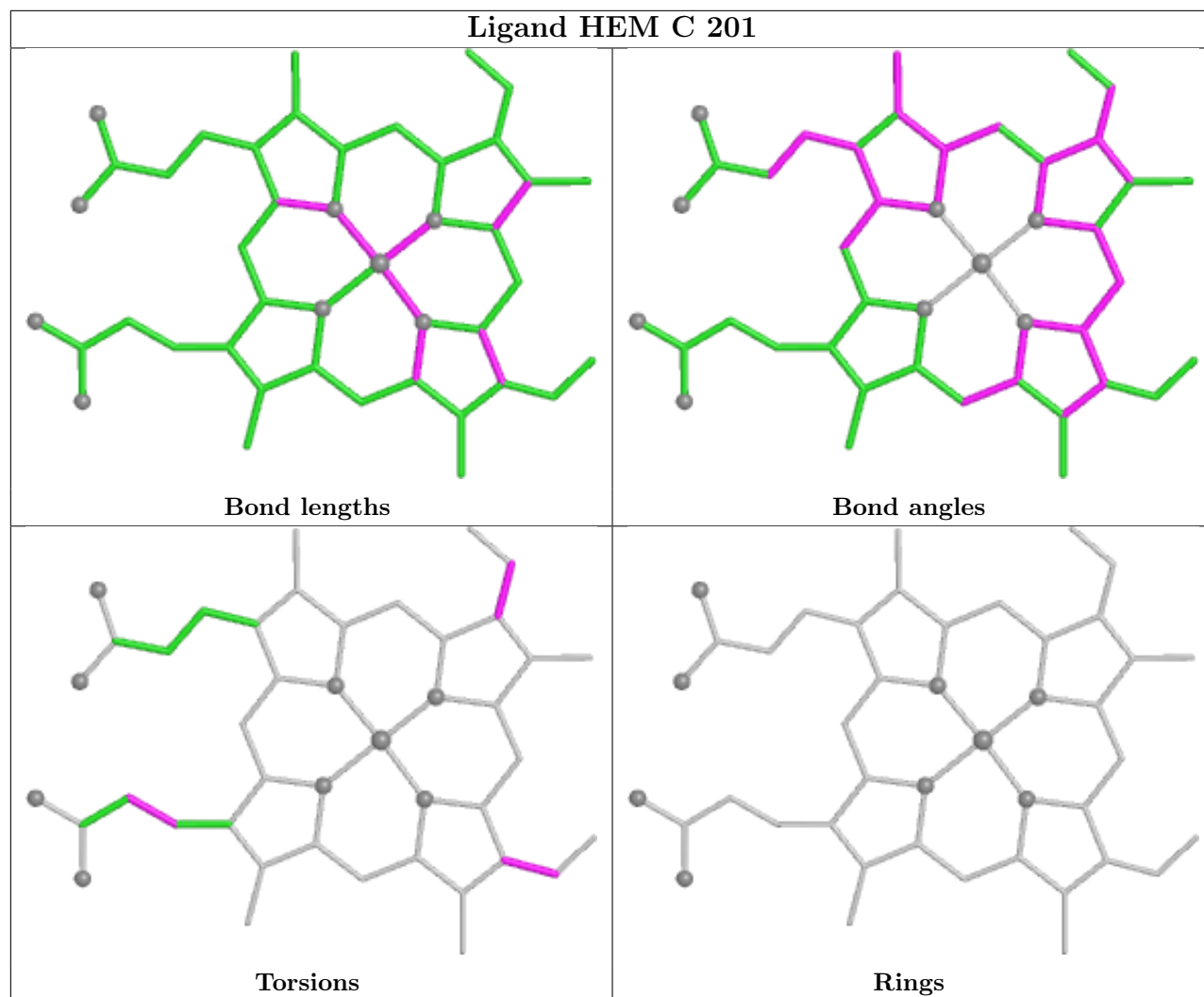




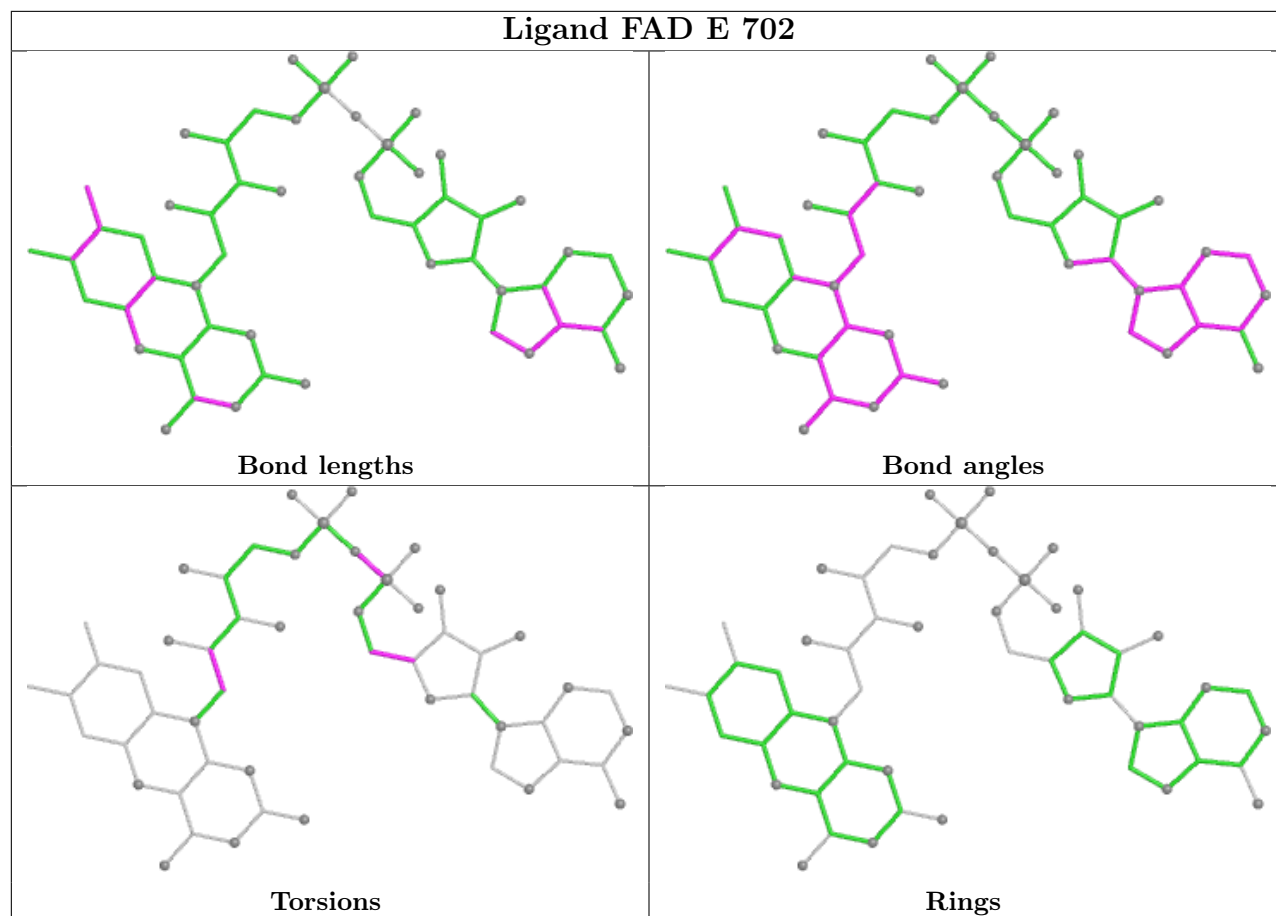
Ligand UQ1 C 202



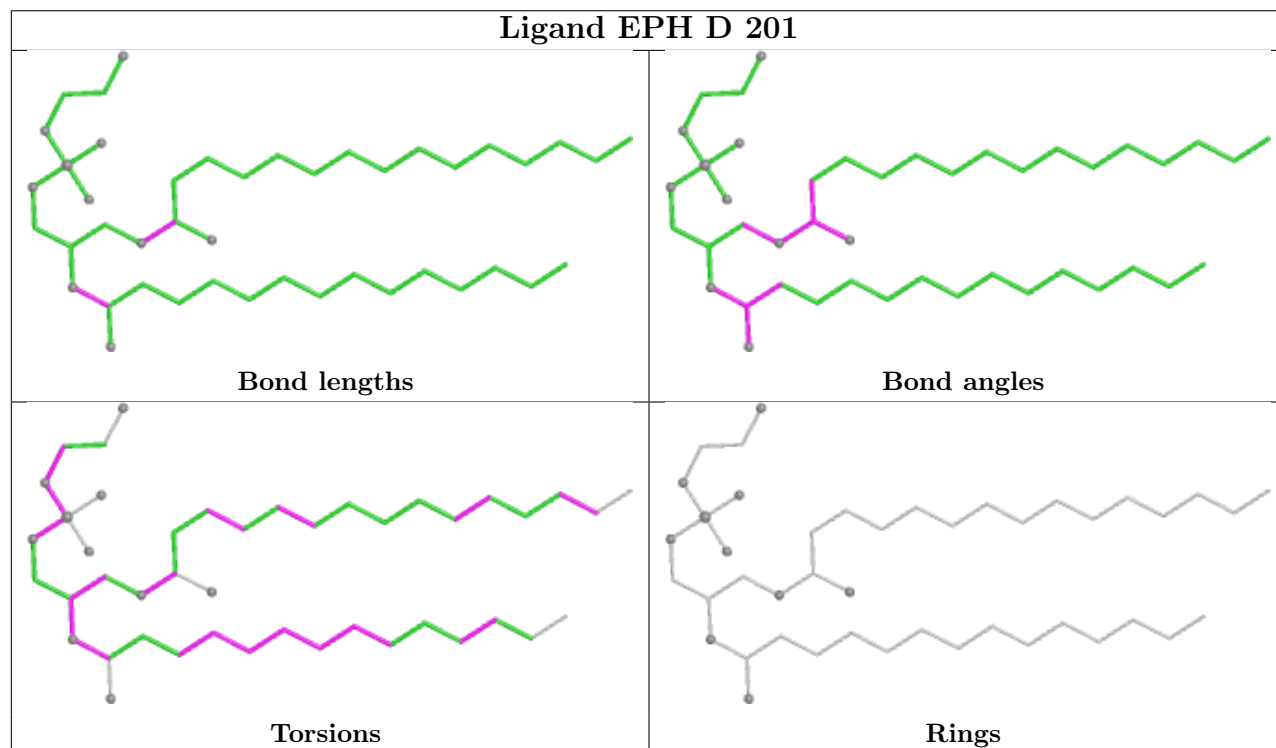


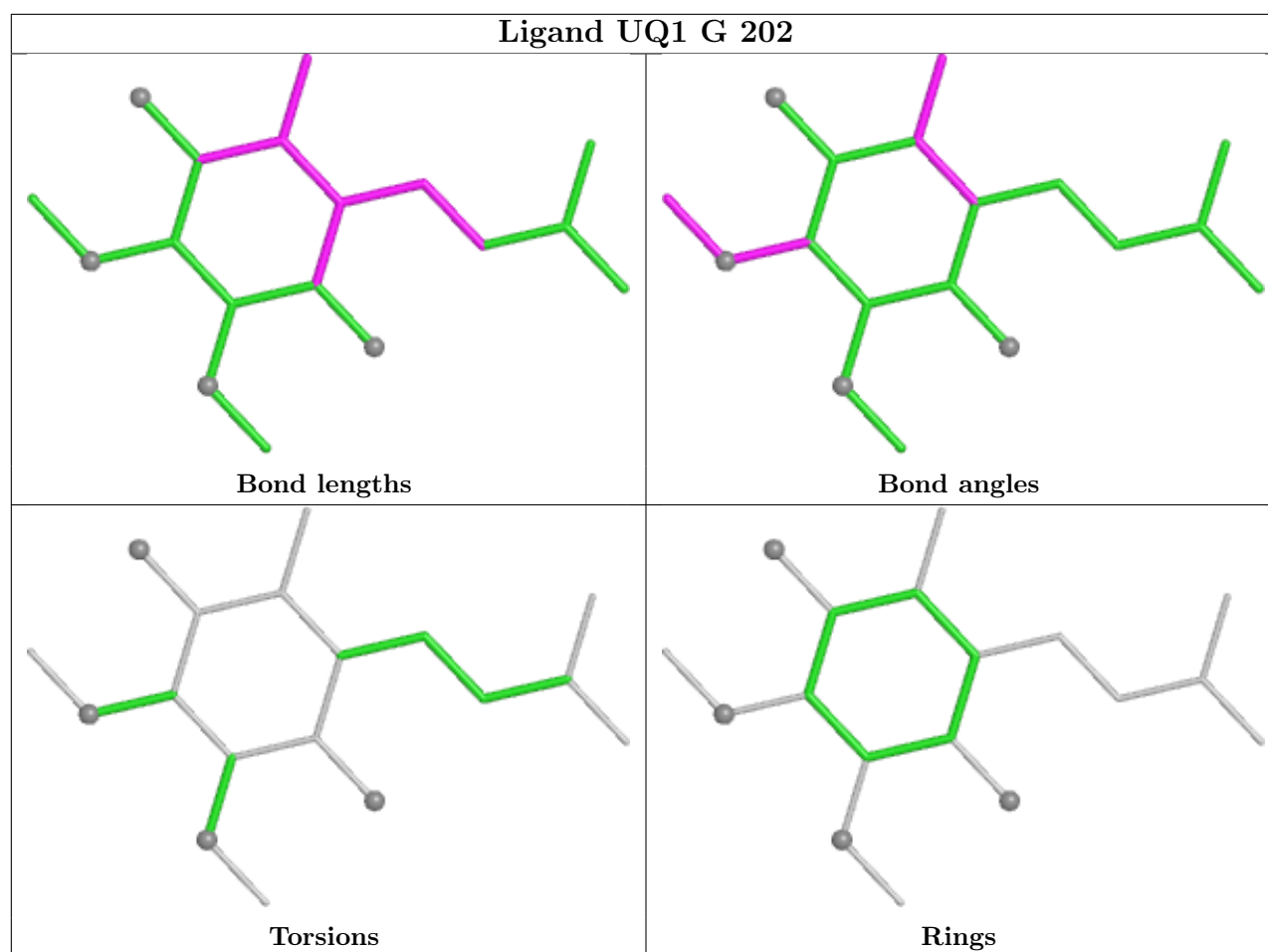


Ligand FAD E 702



Ligand EPH D 201





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	616/645 (95%)	-0.25	3 (0%) 87 82	18, 46, 71, 98	1 (0%)
1	E	616/645 (95%)	-0.29	2 (0%) 90 86	24, 45, 71, 98	1 (0%)
2	B	250/282 (88%)	-0.17	2 (0%) 82 75	28, 44, 74, 93	0
2	F	250/282 (88%)	-0.30	1 (0%) 88 84	24, 42, 66, 83	0
3	C	153/188 (81%)	0.16	2 (1%) 75 66	36, 59, 89, 121	0
3	G	153/188 (81%)	0.73	30 (19%) 3 2	34, 64, 153, 181	0
4	D	129/156 (82%)	0.29	3 (2%) 61 51	45, 60, 96, 118	0
4	H	129/156 (82%)	0.29	7 (5%) 31 24	38, 59, 104, 131	0
All	All	2296/2542 (90%)	-0.10	50 (2%) 62 52	18, 48, 84, 181	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	115	VAL	6.5
1	A	499	THR	5.9
3	G	114	TRP	5.8
3	G	185	PRO	5.4
3	G	184	LEU	5.1
3	G	176	TRP	5.0
3	G	181	LYS	5.0
3	G	182	ALA	4.9
4	D	30	ALA	4.8
4	H	52	LEU	4.7
3	G	110	LEU	4.5
3	G	178	ARG	4.5
3	G	102	THR	4.1
4	H	49	PHE	4.0
3	G	179	HIS	3.8
3	C	186	THR	3.8

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Mol	Chain	Res	Type	RSRZ
3	G	116	ILE	3.4
3	G	186	THR	3.2
4	D	53	HIS	3.2
2	B	159	ILE	3.2
3	G	120	PHE	3.0
4	H	30	ALA	2.9
1	A	32	ILE	2.9
1	E	32	ILE	2.9
3	G	174	PRO	2.8
3	G	109	GLY	2.8
1	A	484	ASN	2.8
2	F	33	LYS	2.7
1	E	30	SER	2.6
3	G	168	LEU	2.6
3	G	183	THR	2.5
3	G	175	ARG	2.5
3	G	111	GLY	2.5
3	G	173	TYR	2.4
2	B	280	ALA	2.3
3	G	180	LYS	2.3
3	G	177	GLU	2.2
3	G	98	LEU	2.2
3	G	107	ILE	2.2
4	H	154	TRP	2.2
4	H	153	VAL	2.2
4	D	48	GLY	2.2
3	G	108	ARG	2.1
4	H	50	LYS	2.1
3	G	68	THR	2.1
3	C	185	PRO	2.0
3	G	171	VAL	2.0
3	G	113	PRO	2.0
4	H	51	PRO	2.0
3	G	112	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

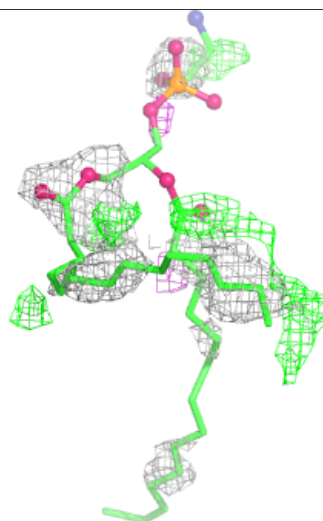
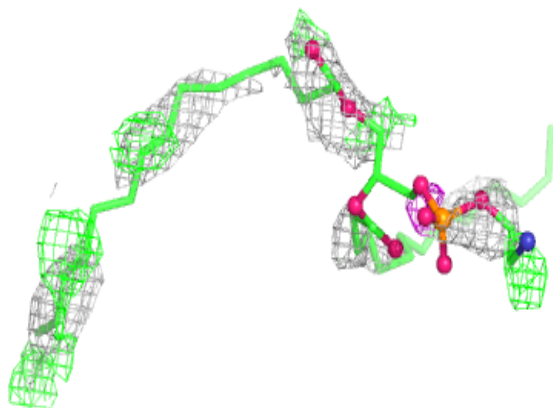
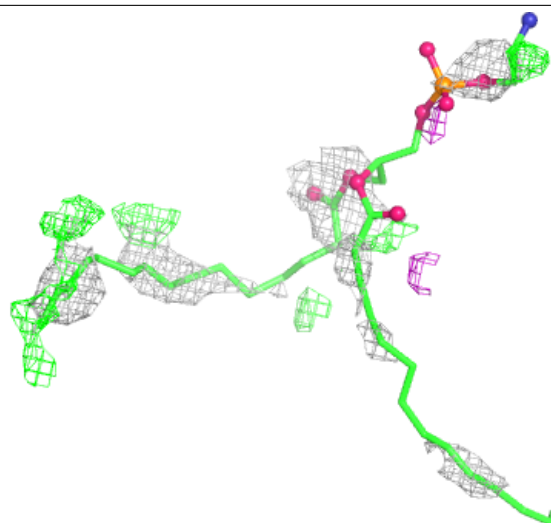
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	EPH	H	201	44/49	0.69	0.39	56,72,103,105	44
11	UQ1	C	202	18/18	0.72	0.28	63,68,71,72	18
12	EPH	D	201	44/49	0.76	0.30	42,56,72,75	44
11	UQ1	G	202	18/18	0.76	0.24	52,63,67,68	18
5	MLI	E	701	7/7	0.93	0.09	31,33,34,35	0
10	HEM	G	201	43/43	0.94	0.12	50,66,75,84	0
10	HEM	C	201	43/43	0.96	0.12	49,65,74,83	0
6	FAD	E	702	53/53	0.96	0.07	25,28,33,35	0
9	F3S	F	303	7/7	0.96	0.06	30,37,43,47	0
5	MLI	A	701	7/7	0.97	0.07	42,43,44,44	0
9	F3S	B	303	7/7	0.97	0.05	36,40,46,46	0
6	FAD	A	702	53/53	0.97	0.06	21,24,31,33	0
8	SF4	F	302	8/8	0.98	0.05	25,27,30,30	0
7	FES	B	301	4/4	0.98	0.04	29,30,33,33	0
8	SF4	B	302	8/8	0.98	0.04	27,29,31,33	0
7	FES	F	301	4/4	0.99	0.04	29,29,32,34	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.

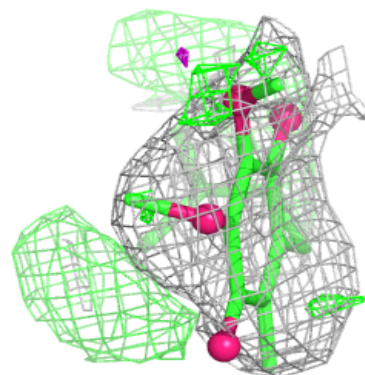
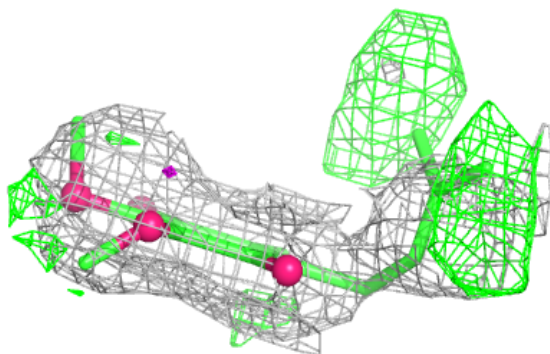
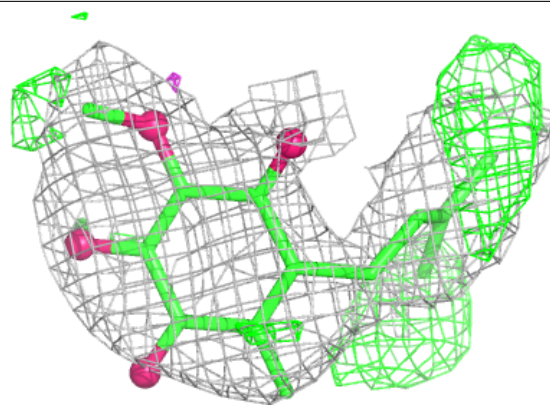
Electron density around EPH H 201:

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



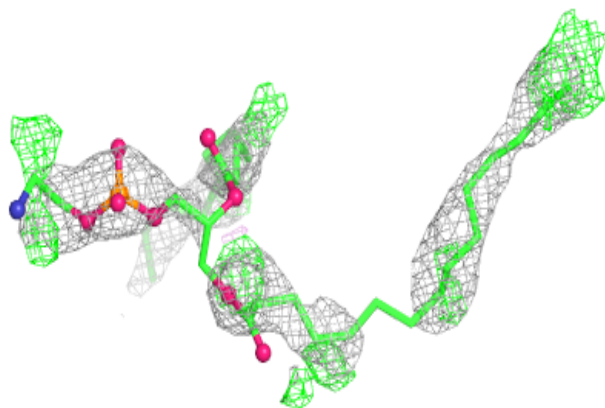
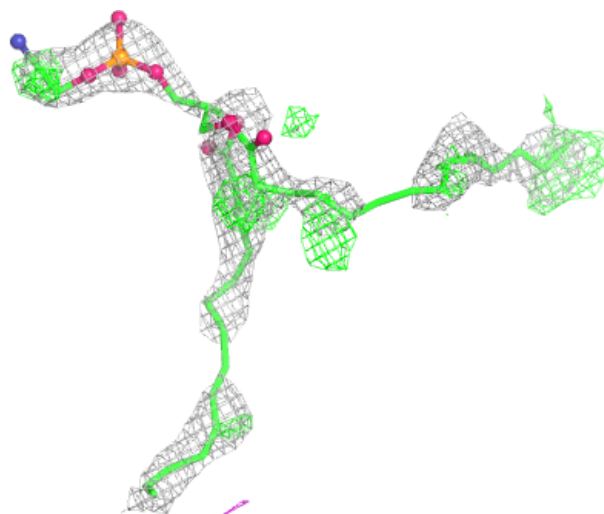
Electron density around UQ1 C 202:

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



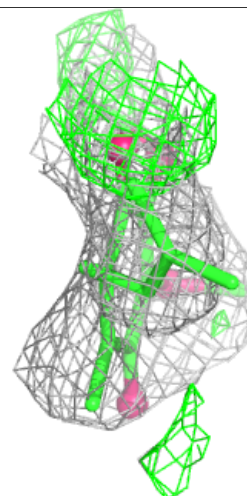
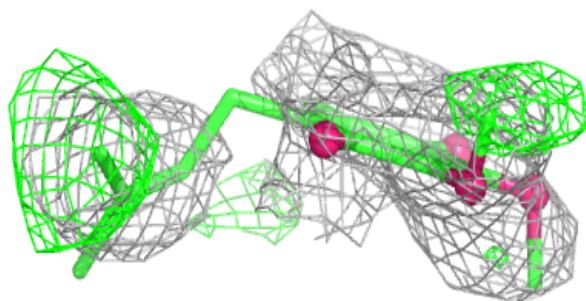
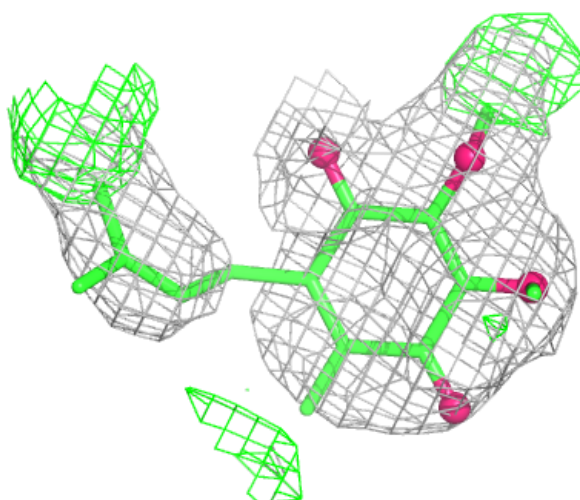
Electron density around EPH D 201:

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



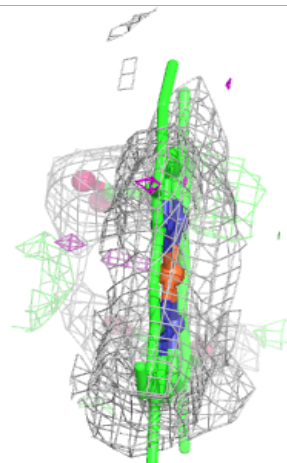
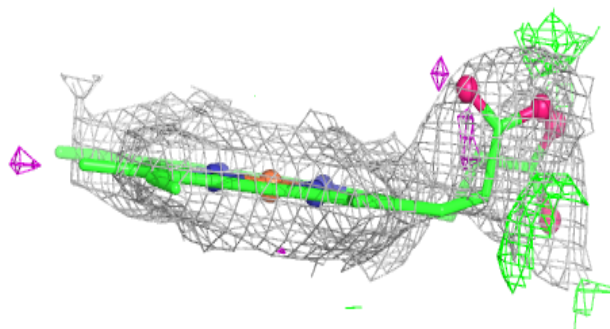
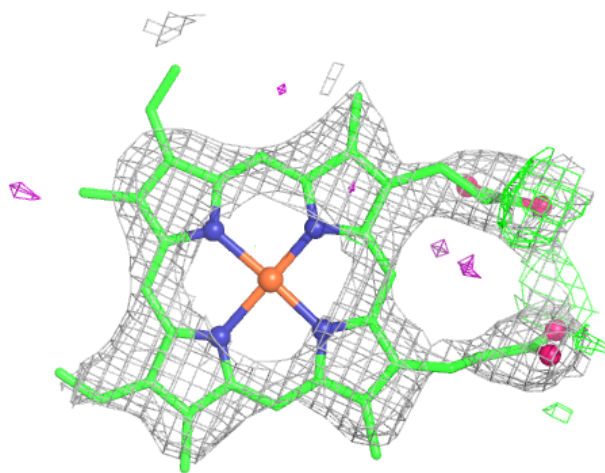
Electron density around UQ1 G 202:

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



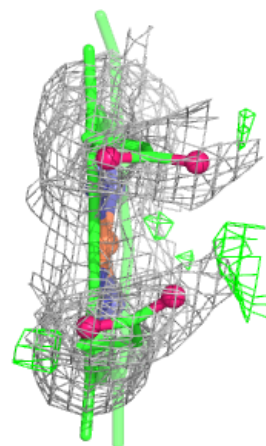
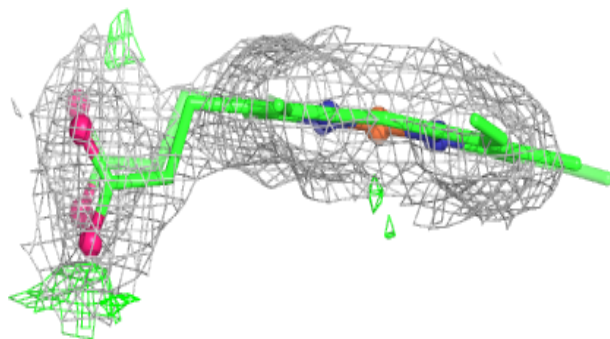
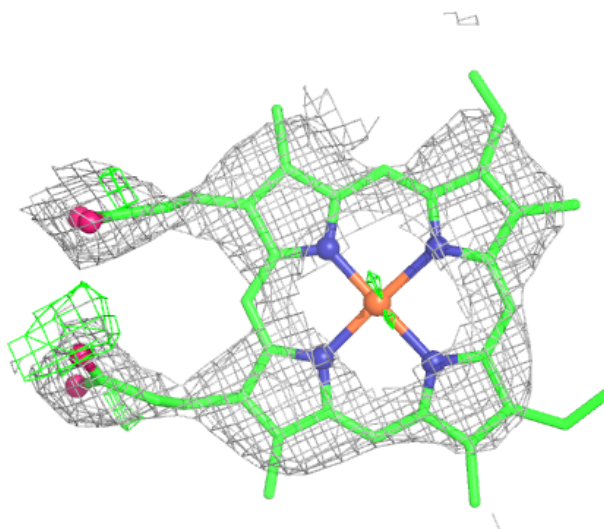
Electron density around HEM G 201:

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



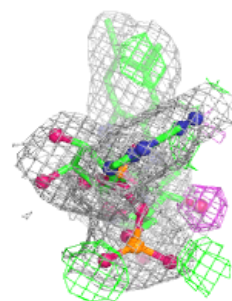
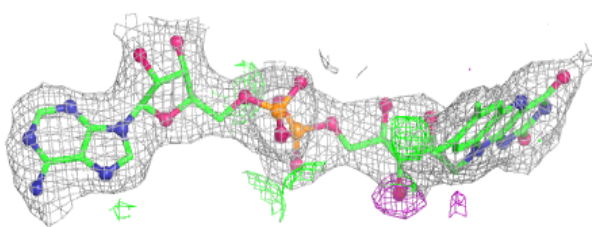
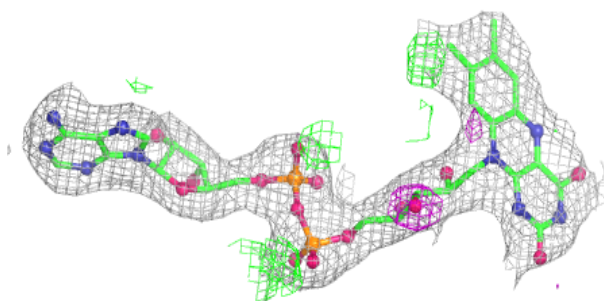
Electron density around HEM C 201:

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

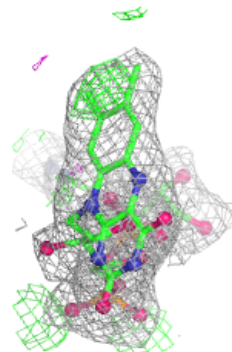
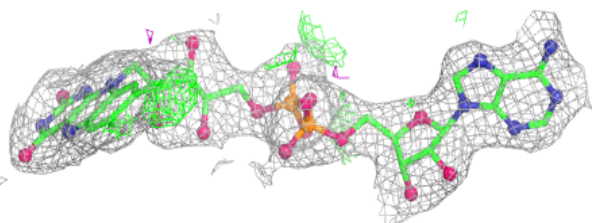
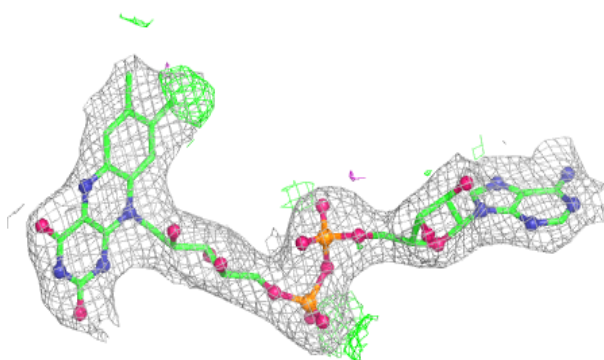


Electron density around FAD E 702:

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

**Electron density around FAD A 702:**

$2mF_o-DF_c$ (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.