W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2021 – 03:21 PM EDT

PDB ID	:	3IR5
Title	:	Crystal structure of NarGHI mutant NarG-H49C
Authors	:	Bertero, M.G.; Rothery, R.A.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on	:	2009-08-21
Resolution	:	2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

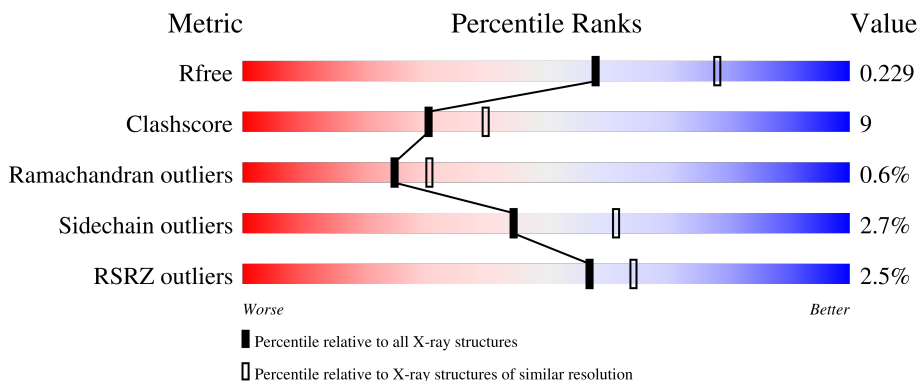|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.229
Clashscore		9
Ramachandran outliers		0.6%
Sidechain outliers		2.7%
RSRZ outliers		2.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	1247	3% / 77% / 21% / •
2	B	512	83% / 16% / ••
3	C	225	5% / 75% / 23% / •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SF4	B	803	-	-	X	-

2   Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 16376 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 Respiratory nitrate reductase 1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1244	Total 9865	C 6229	N 1729	O 1858	S 49	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	CYS	HIS	engineered mutation	UNP P09152

- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	509	Total 4050	C 2562	N 701	O 755	S 32	0	0	0

- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total 1747	C 1158	N 295	O 281	S 13	0	0	0

- Molecule 4 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).
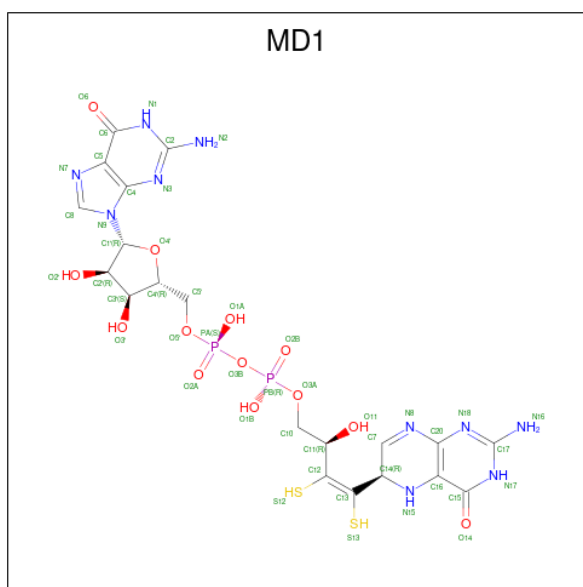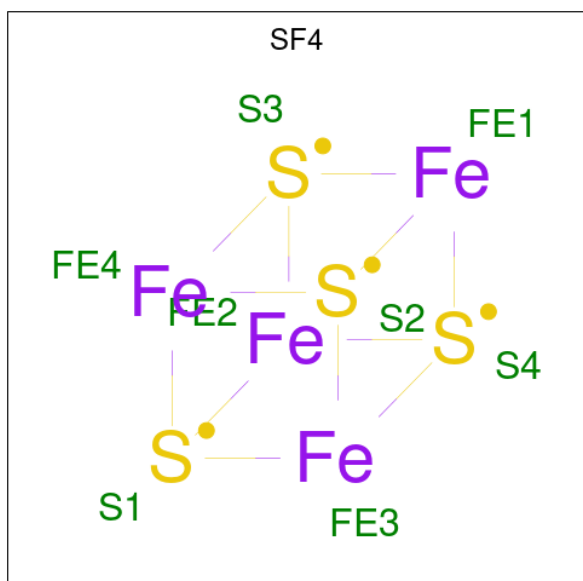
MD1

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 5 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

SF4

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

- Molecule 7 is (1S)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula: $C_{19}H_{36}O_{10}P$).
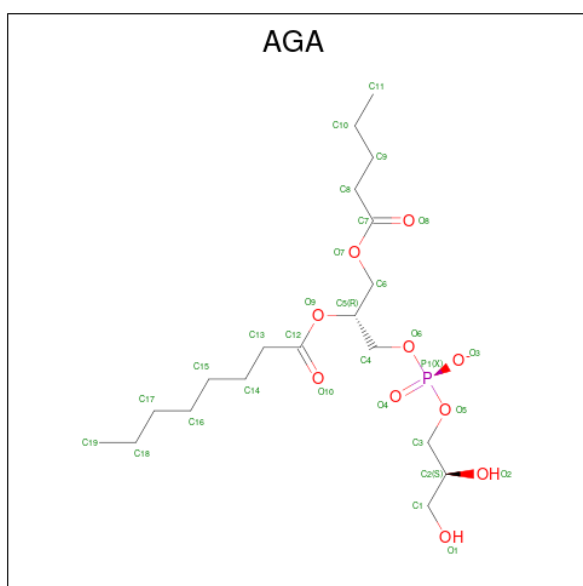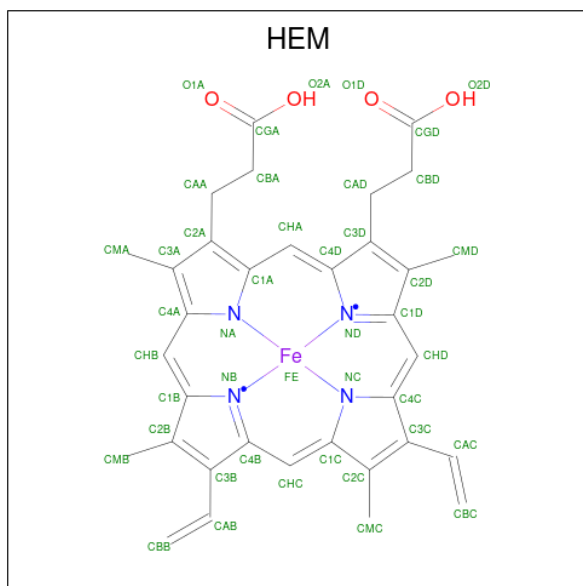

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 25	C 16	O 8	P 1	0	0

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

F3S
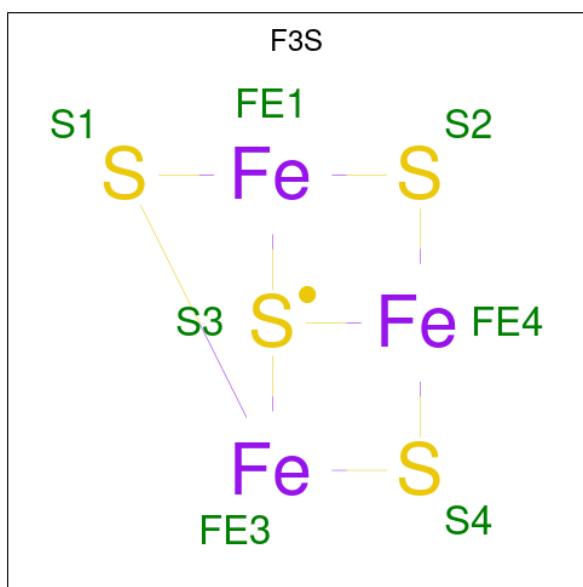
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 7	Fe 3	S 4	0	0

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM

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

- Molecule 10 is water.

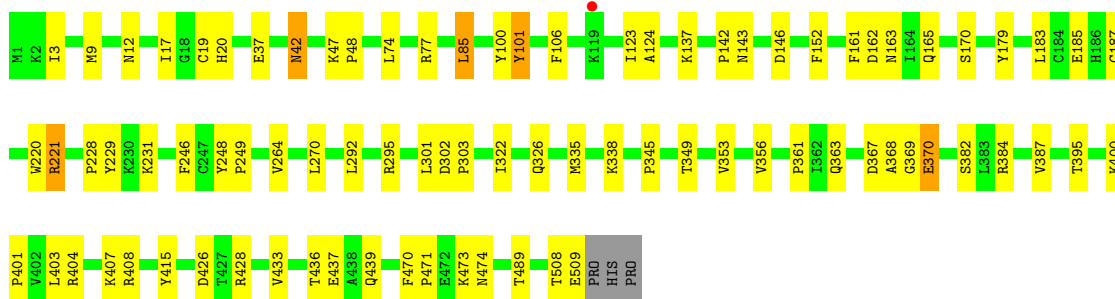| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	253	Total 253	O 253	0	0
10	B	182	Total 182	O 182	0	0
10	C	34	Total 34	O 34	0	0

3 Residue-property plots ⓘ

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

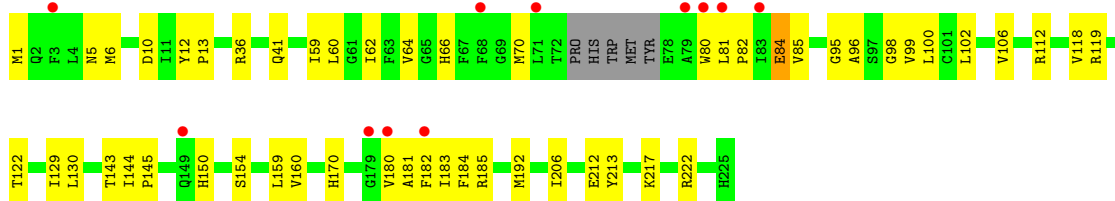• Molecule 1: Respiratory nitrate reductase 1 alpha chain
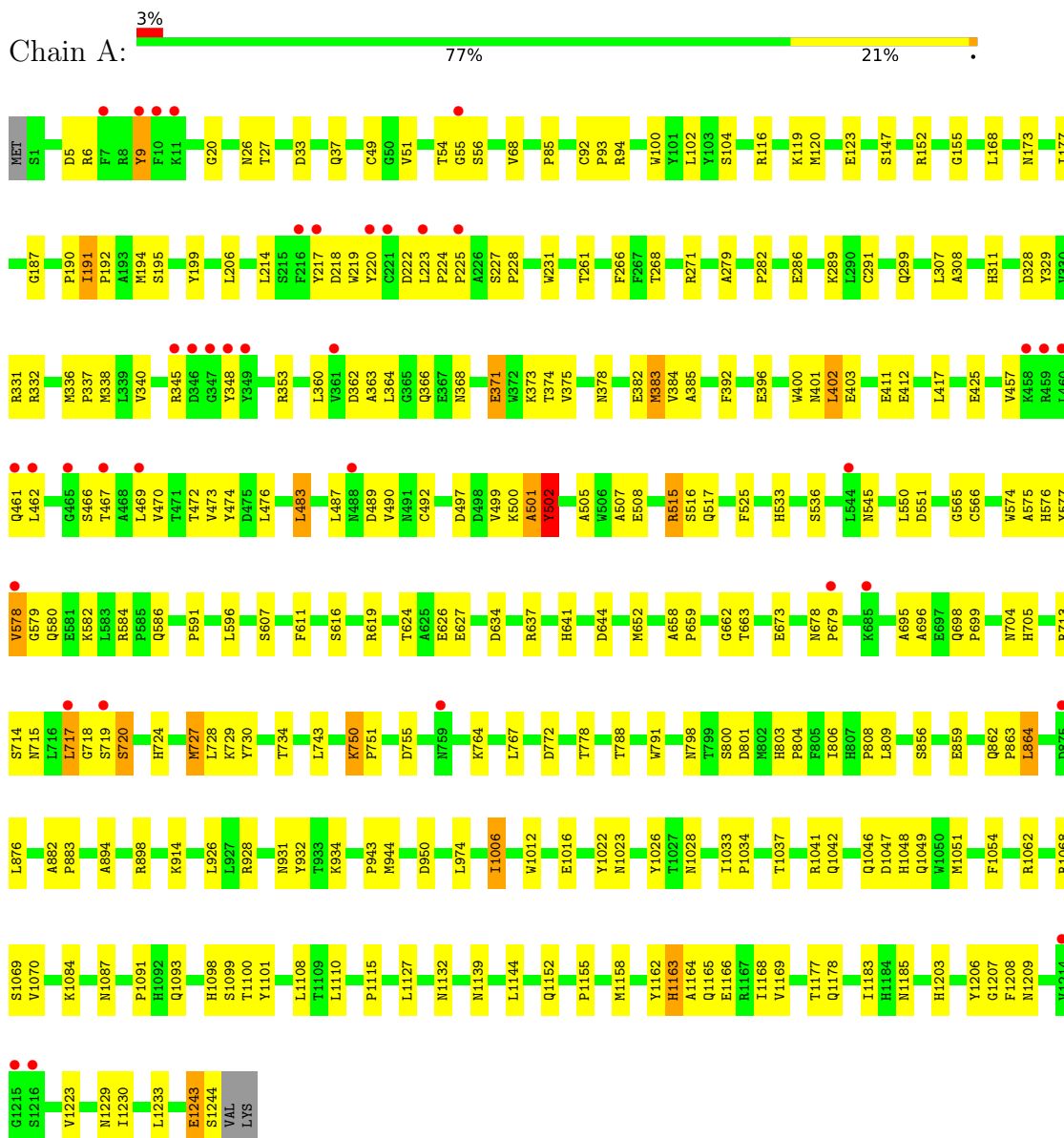
• Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B:

83%   16%   ••

M1 K2 I3 M9 N12 I17 G18 C19 H20 E37 N42 K47 P48 L74 R77 L85 Y100 Y101 F106 K119 I123 A124 K137 P142 N143 D146 F152 F161 D162 N163 I164 Q165 S170 Y179 L183 C184 E185 H186 C187

W220 R221 P228 Y229 K230 K231 F246 C247 Y248 P249 V264 L270 L292 R295 L301 D302 P303 I322 Q326 M335 K338 P345 T349 V353 V356 P361 I362 Q363 D367 A368 G369 E370 S382 L383 R384 V387 T395 K400

P401 V402 L403 R404 K407 R408 Y415 D426 T427 R428 V433 T436 E437 A438 Q439 F470 P471 E472 K473 N474 T489 T508 E509 PRO HIS PRO

• Molecule 3: Respiratory nitrate reductase 1 gamma chain

5%

Chain C:

75%   23%   •

M1 Q2 F3 L4 N5 M6 D10 I11 Y12 P13 R36 Q41 I59 L60 G61 I62 F63 V64 G65 H66 F67 F68 G69 M70 L71 T72 PRO HIS TRP MET TYR E78 A79 W80 L81 P82 I83 E84 V85 G95 A96 S97 G98 V99 L100 C101 L102 V106 R112 V118 R119

T122 I129 L130 T143 I144 P145 Q149 H150 S154 L159 V160 H170 G179 V180 A181 F182 I183 F184 R185 M192 I206 E212 Y213 K217 R222 H225

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	153.45Å 240.69Å 139.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.30 49.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.61-2.30) 99.7 (49.84-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.237 0.193 , 0.229	Depositor DCC
R_{free} test set	6895 reflections (6.04%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.976	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.5	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16376	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FME, F3S, MD1, 6MO, SF4, AGA, HEM

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	0.38	0/10123	0.66	6/13742 (0.0%)
2	B	0.36	0/4146	0.62	0/5609
3	C	0.42	0/1784	0.57	0/2411
All	All	0.38	0/16053	0.64	6/21762 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1163	HIS	C-N-CA	12.74	153.56	121.70
1	A	501	ALA	C-N-CA	9.37	145.14	121.70
1	A	1163	HIS	CA-C-N	-6.47	102.95	117.20
1	A	501	ALA	N-CA-CB	6.20	118.78	110.10
1	A	809	LEU	N-CA-C	-5.50	96.15	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	501	ALA	CA
1	A	502	TYR	CA

All (1) planarity outliers are listed below:

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Peptide

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9865	0	9522	205	0
2	B	4050	0	3973	56	0
3	C	1747	0	1789	33	0
4	A	94	0	42	11	0
5	A	1	0	0	0	0
6	A	8	0	0	1	0
6	B	24	0	0	2	0
7	A	25	0	29	0	0
8	B	7	0	0	0	0
9	C	86	0	60	3	0
10	A	253	0	0	5	2
10	B	182	0	0	4	0
10	C	34	0	0	0	0
All	All	16376	0	15415	287	2

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 9.

The worst 5 of 287 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:338:MET:HE2	1:A:374:THR:HB	1.58	0.85
1:A:360:LEU:HG	1:A:383:MET:HE3	1.59	0.81
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.66	0.78
1:A:715:ASN:O	1:A:718:GLY:O	2.02	0.77
1:A:345:ARG:HB2	1:A:348:TYR:O	1.86	0.75

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1489:HOH:O	10:A:1489:HOH:O[3_354]	1.16	1.04
10:A:1450:HOH:O	10:A:1450:HOH:O[3_354]	1.59	0.61

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	1242/1247 (100%)	1162 (94%)	71 (6%)	9 (1%)	22	26
2	B	507/512 (99%)	492 (97%)	13 (3%)	2 (0%)	34	42
3	C	216/225 (96%)	202 (94%)	14 (6%)	0	100	100
All	All	1965/1984 (99%)	1856 (94%)	98 (5%)	11 (1%)	25	31

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	A	502	TYR
1	A	1166	GLU
1	A	578	VAL
1	A	1164	ALA

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	1039/1044 (100%)	1009 (97%)	30 (3%)	42	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	436/439 (99%)	427 (98%)	9 (2%)	53	70
3	C	180/186 (97%)	175 (97%)	5 (3%)	43	60
All	All	1655/1669 (99%)	1611 (97%)	44 (3%)	44	61

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1233	LEU
2	B	165	GLN
1	A	1243	GLU
2	B	74	LEU
2	B	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	708	ASN
1	A	946	ASN
3	C	175	GLN
2	B	143	ASN
3	C	149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#|Z| > 2$
3	FME	C	1	3	8,9,10	1.66	3 (37%)	7,9,11	1.47	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
3	FME	C	1	3	-	4/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-3.35	1.47	1.53
3	C	1	FME	CA-N	-2.26	1.43	1.46
3	C	1	FME	CB-CG	2.11	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	FME	CA-N-CN	2.51	126.68	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	O1-CN-N-CA
3	C	1	FME	N-CA-CB-CG
3	C	1	FME	CA-CB-CG-SD
3	C	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
7	AGA	A	1250	-	24,24,29	0.77	1 (4%)	28,29,35	1.57	2 (7%)
6	SF4	B	803	2	0,12,12	-	-	-		
6	SF4	A	1249	1	0,12,12	-	-	-		
6	SF4	B	802	2	0,12,12	-	-	-		
9	HEM	C	806	3	27,50,50	2.26	12 (44%)	17,82,82	1.72	6 (35%)
6	SF4	B	804	2	0,12,12	-	-	-		
9	HEM	C	807	3	27,50,50	2.41	14 (51%)	17,82,82	1.82	5 (29%)
4	MD1	A	1251	5	38,51,51	3.69	12 (31%)	35,78,78	1.92	8 (22%)
4	MD1	A	1247	5	38,51,51	3.83	10 (26%)	35,78,78	2.09	9 (25%)
8	F3S	B	805	2	0,9,9	-	-	-		

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
7	AGA	A	1250	-	-	6/26/26/34	-
6	SF4	B	803	2	-	-	0/6/5/5
6	SF4	A	1249	1	-	-	0/6/5/5
6	SF4	B	802	2	-	-	0/6/5/5
9	HEM	C	806	3	-	0/6/54/54	-
6	SF4	B	804	2	-	-	0/6/5/5
9	HEM	C	807	3	-	0/6/54/54	-
4	MD1	A	1251	5	-	3/21/59/59	0/5/5/5
4	MD1	A	1247	5	-	7/21/59/59	0/5/5/5
8	F3S	B	805	2	-	-	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1247	MD1	C7-N8	19.39	1.50	1.27
4	A	1251	MD1	C7-N8	17.94	1.49	1.27
4	A	1251	MD1	C4-N9	-6.40	1.39	1.47
4	A	1247	MD1	C4-N9	-6.16	1.39	1.47
4	A	1251	MD1	C6-N1	5.84	1.42	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1247	MD1	C4-C5-N7	6.46	111.02	102.46
4	A	1251	MD1	C4-C5-N7	6.13	110.58	102.46
4	A	1247	MD1	C15-N17-C17	5.17	124.15	115.93
7	A	1250	AGA	C14-C13-C12	4.99	131.78	113.62
7	A	1250	AGA	C9-C8-C7	4.97	131.69	113.62

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1247	MD1	C5'-O5'-PA-O2A
4	A	1247	MD1	O4'-C4'-C5'-O5'
4	A	1247	MD1	C3'-C4'-C5'-O5'
7	A	1250	AGA	C8-C7-O7-C6
7	A	1250	AGA	C11-C10-C9-C8

There are no ring outliers.

5 monomers are involved in 17 short contacts:

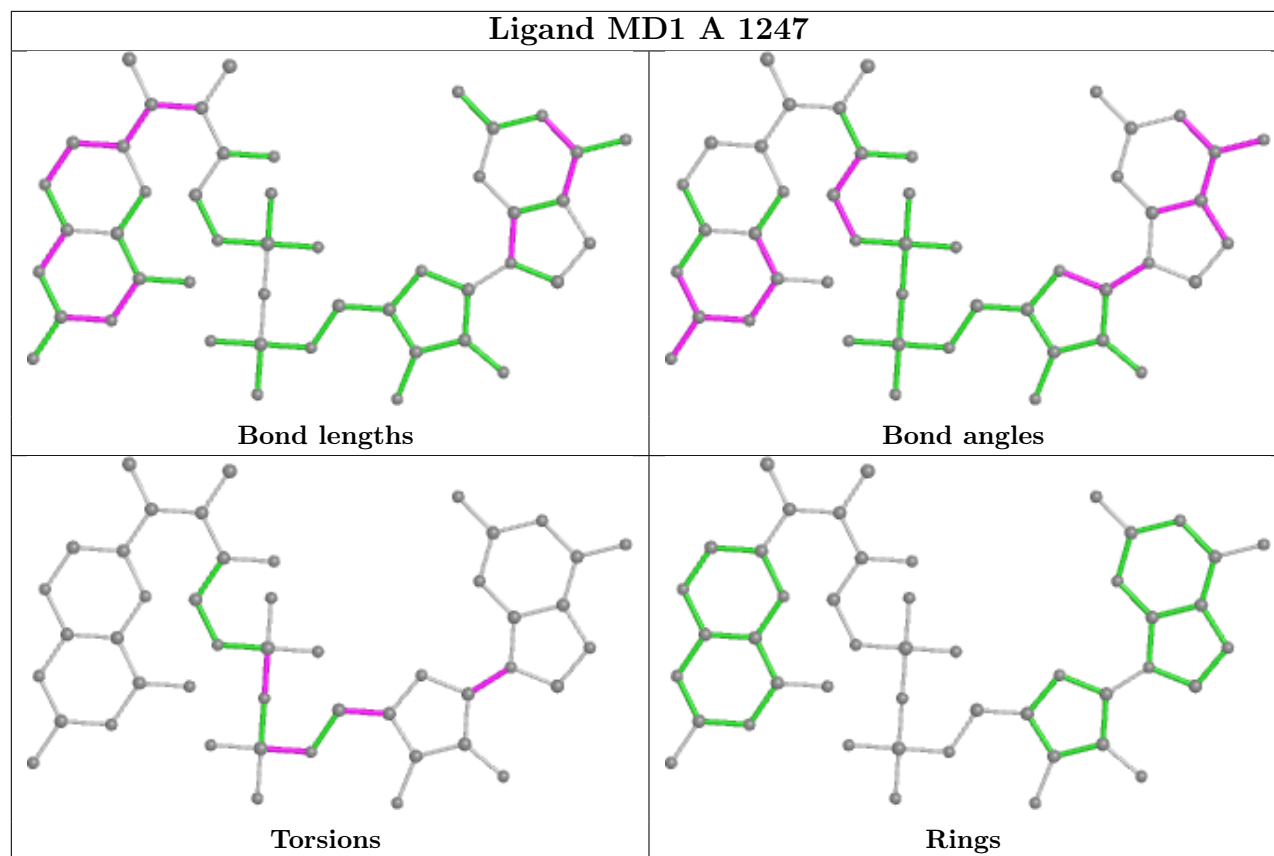| Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	803	SF4	2	0
6	A	1249	SF4	1	0
9	C	806	HEM	3	0
4	A	1251	MD1	3	0
4	A	1247	MD1	8	0

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 then 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 AGA A 1250

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 806

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 807

Bond lengths

Bond angles

Torsions

Rings

Ligand MD1 A 1251

Bond lengths

Bond angles

Torsions

Rings

Ligand MD1 A 1247

Bond lengths

Bond angles

Torsions

Rings
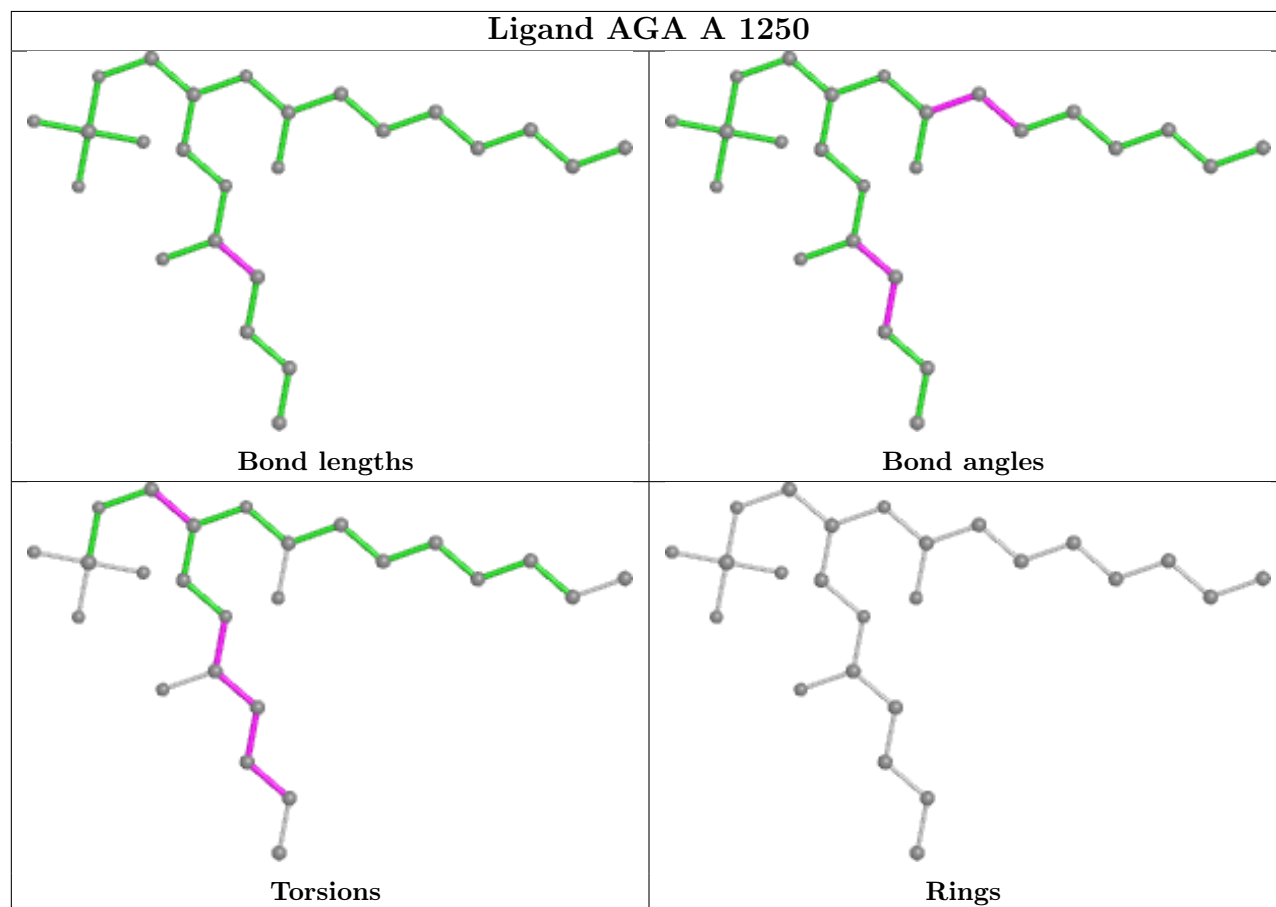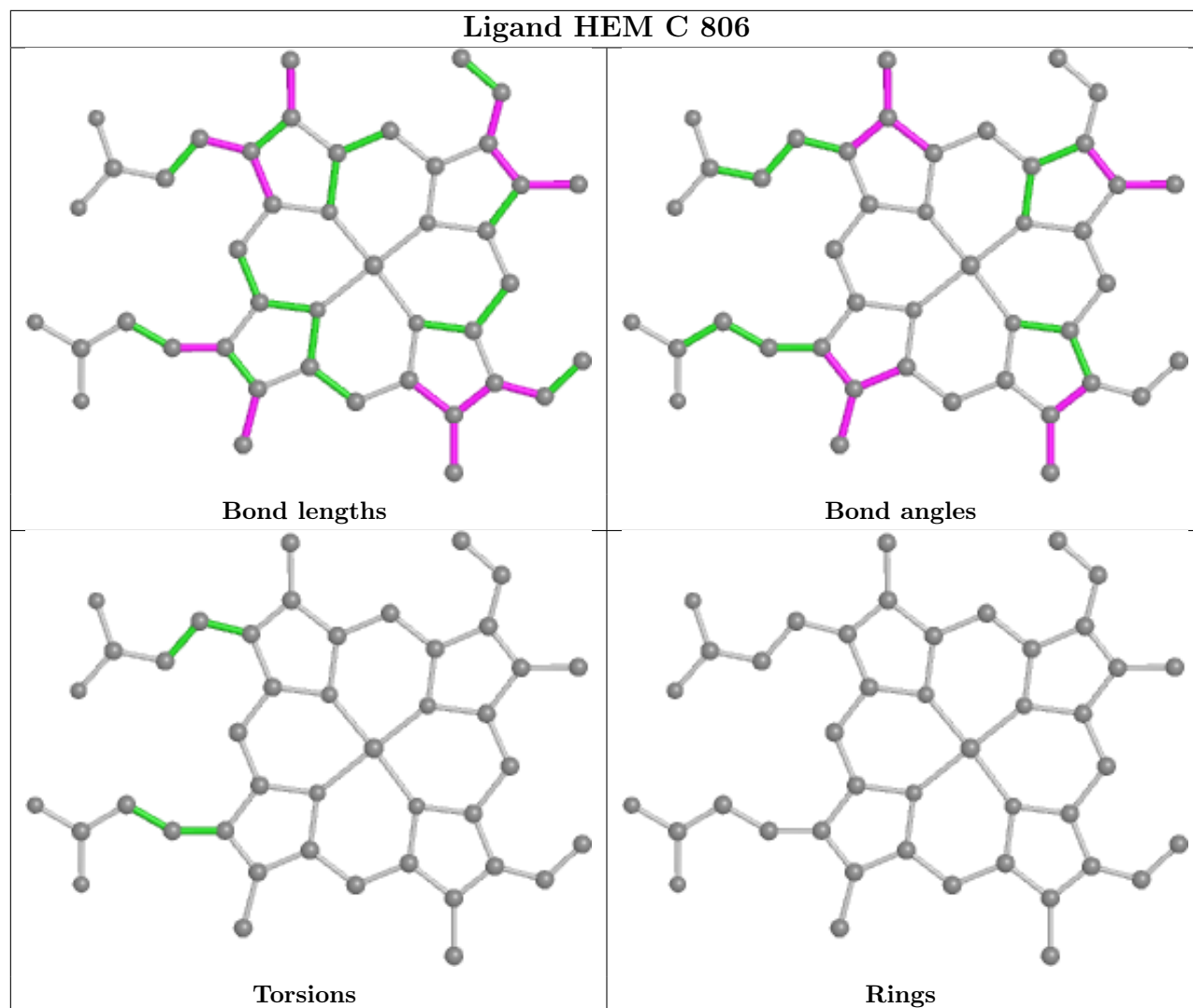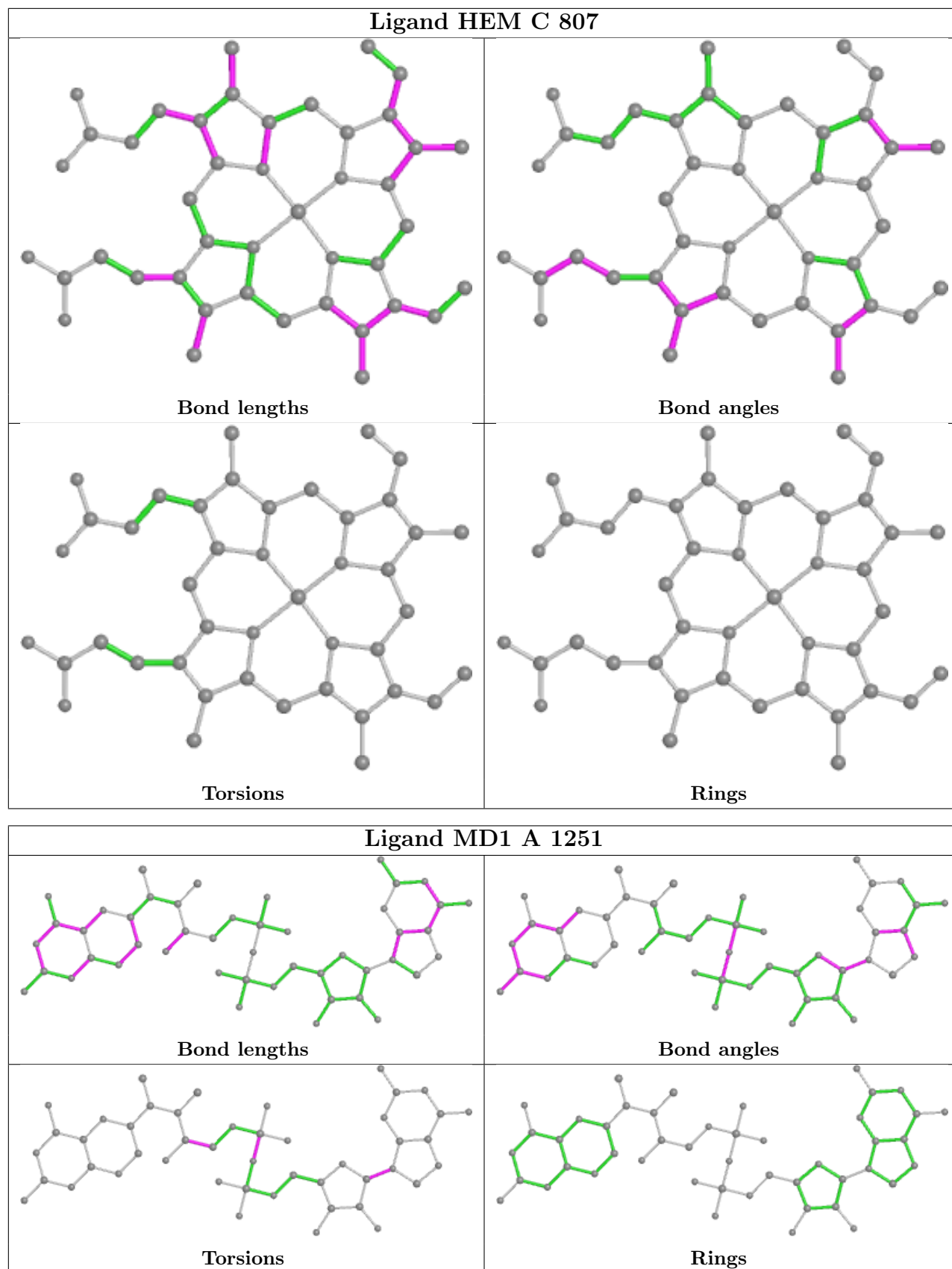
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1244/1247 (99%)	-0.10	37 (2%)	50	57	19, 34, 49, 58	0
2	B	509/512 (99%)	-0.52	1 (0%)	95	96	19, 28, 41, 57	0
3	C	219/225 (97%)	-0.11	11 (5%)	28	35	22, 39, 53, 58	0
All	All	1972/1984 (99%)	-0.21	49 (2%)	57	64	19, 33, 49, 58	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	80	TRP	5.8
1	A	9	TYR	5.4
1	A	10	PHE	5.4
3	C	79	ALA	4.3
1	A	221	CYS	3.7

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

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(Å²)	Q<0.9
3	FME	C	1	10/11	0.93	0.28	53,57,63,64	0

6.3 Carbohydrates ⓘ
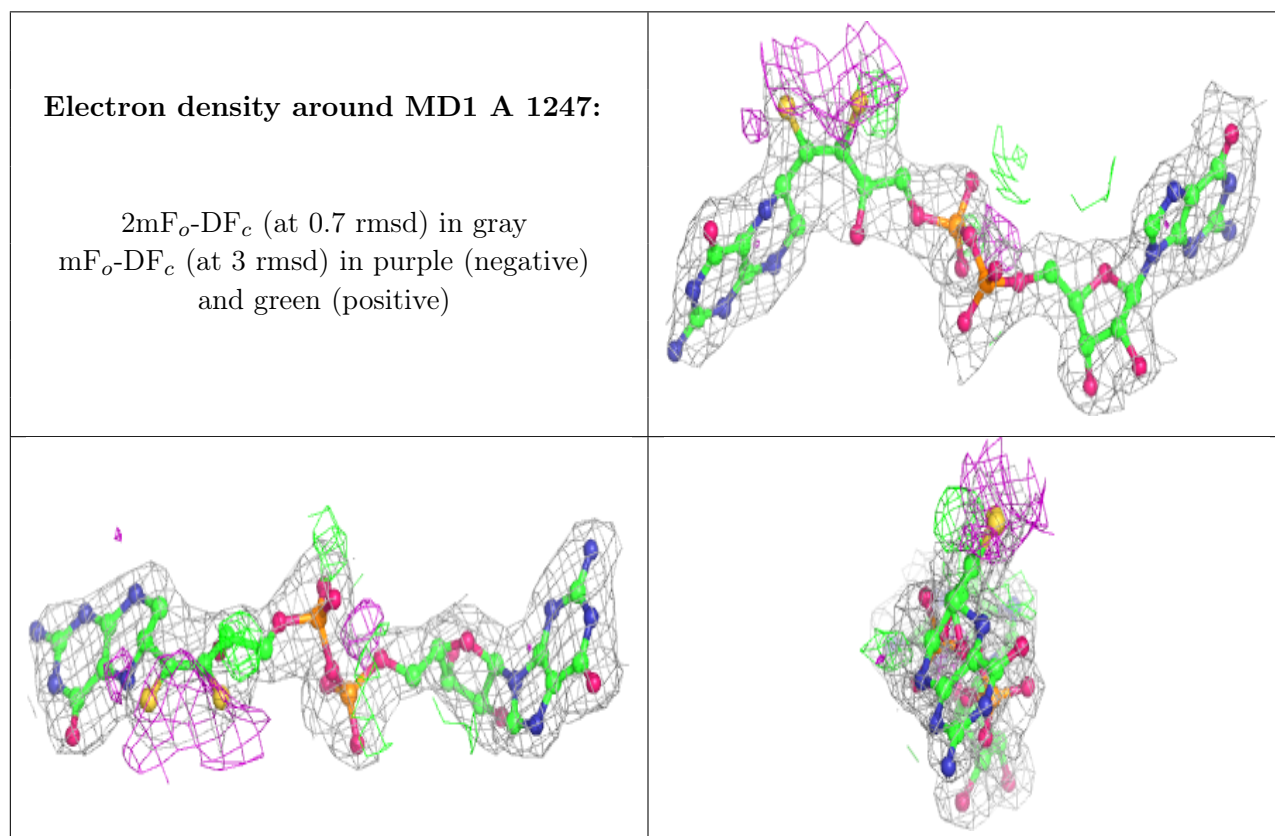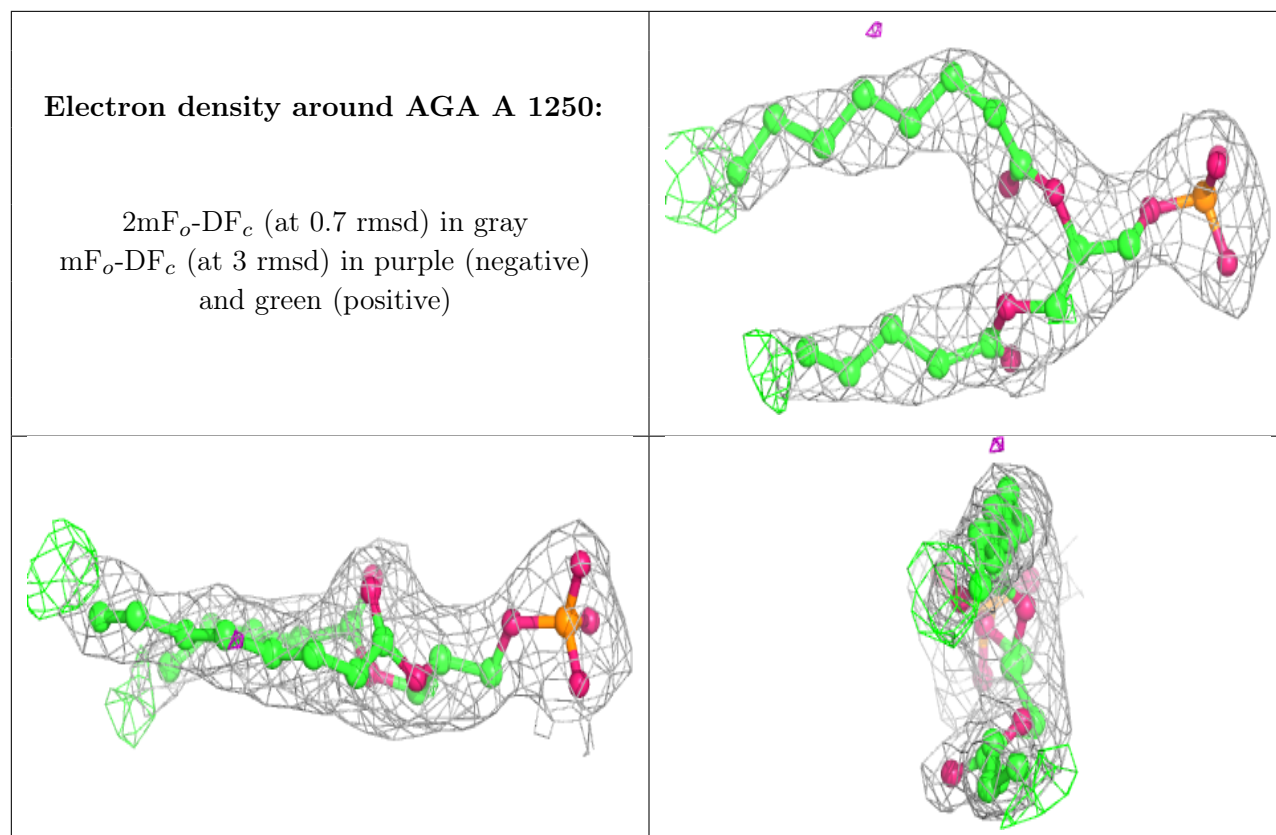
There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	MD1	A	1247	47/47	0.93	0.15	30,38,58,65	0
5	6MO	A	1248	1/1	0.93	0.16	61,61,61,61	0
6	SF4	B	804	8/8	0.94	0.08	31,35,37,37	0
7	AGA	A	1250	25/30	0.94	0.15	34,38,47,48	0
9	HEM	C	807	43/43	0.94	0.13	44,46,53,56	0
4	MD1	A	1251	47/47	0.95	0.17	26,39,53,56	0
6	SF4	A	1249	8/8	0.96	0.07	31,31,33,34	0
9	HEM	C	806	43/43	0.97	0.11	25,28,30,35	0
6	SF4	B	802	8/8	0.97	0.10	26,28,30,32	0
6	SF4	B	803	8/8	0.99	0.13	19,22,24,24	0
8	F3S	B	805	7/7	0.99	0.12	26,26,28,28	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.
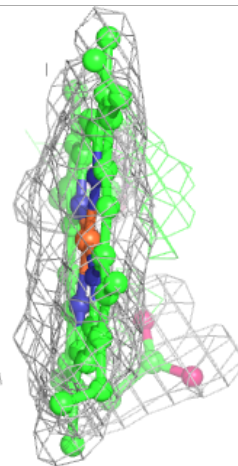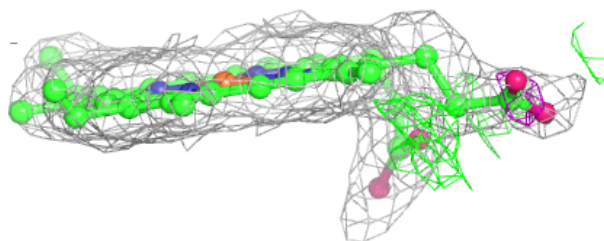

Electron density around MD1 A 1247:

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

Electron density around AGA A 1250:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
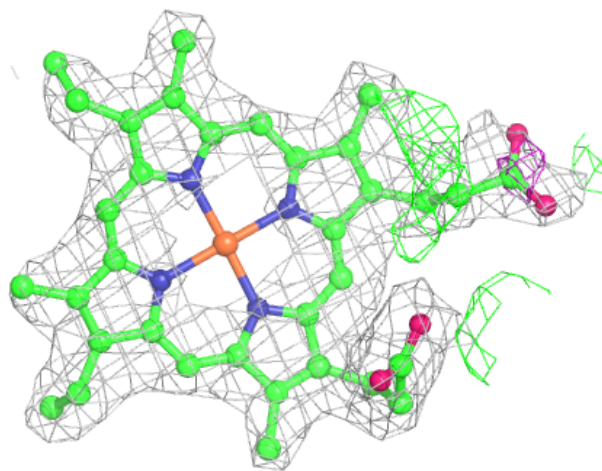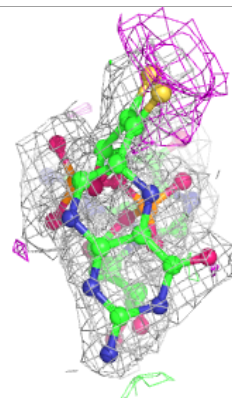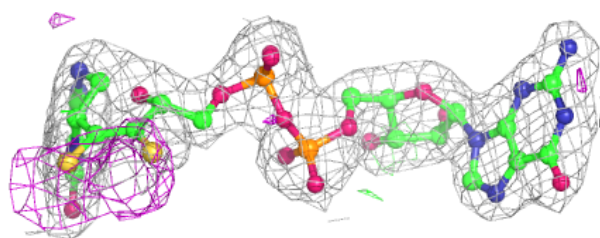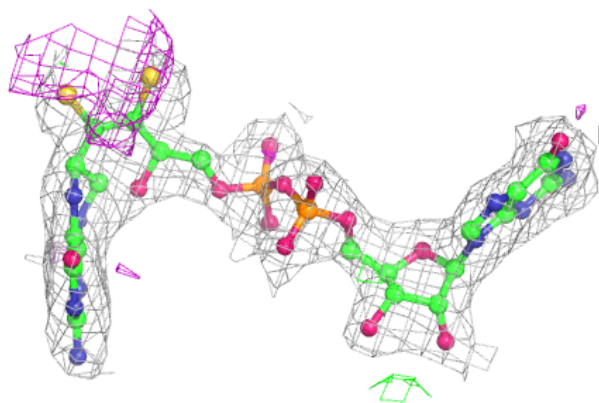$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
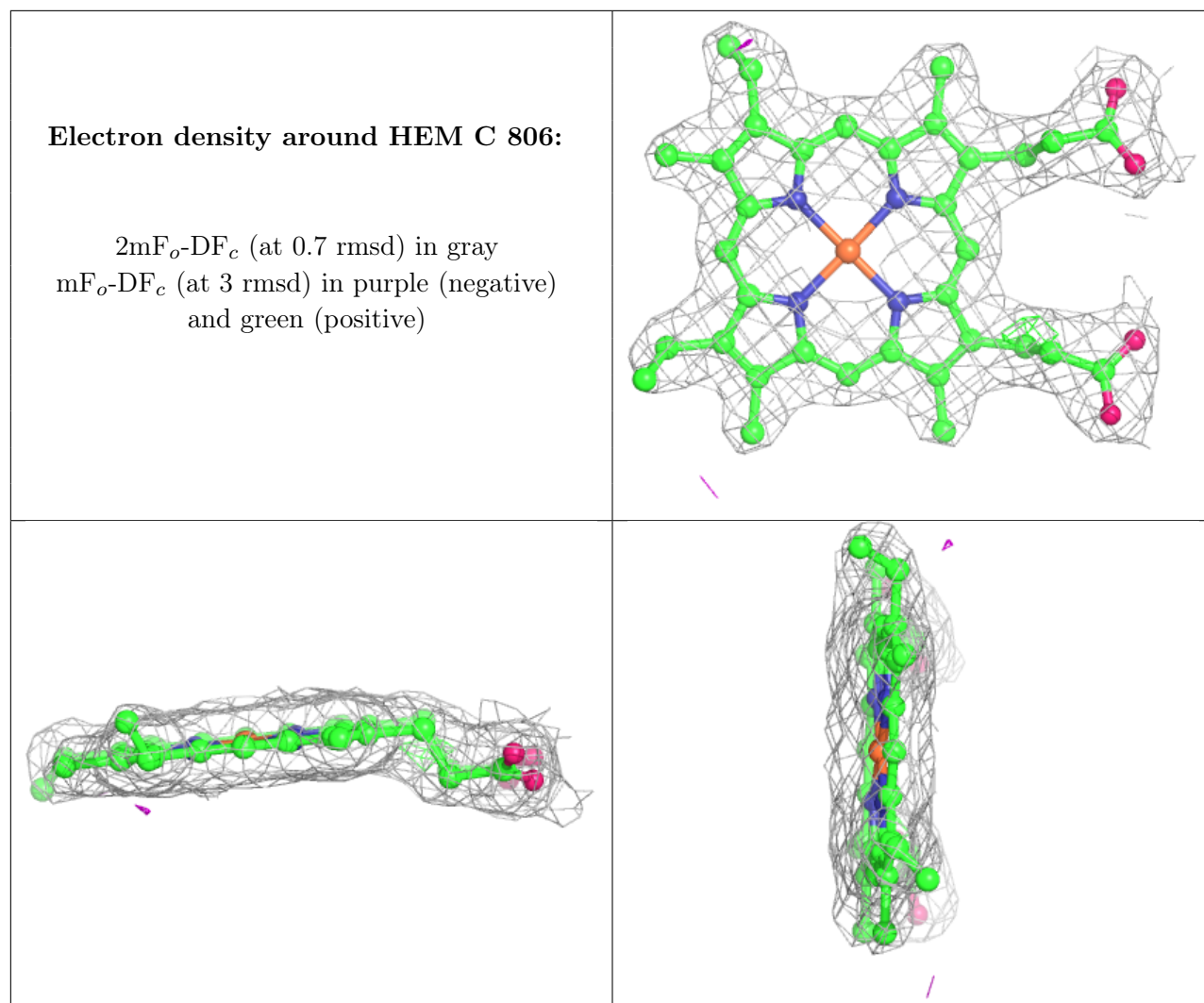
Electron density around HEM C 807:

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

Electron density around MD1 A 1251:

$2mF_o$-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 806:

$2mF_o$-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 ⓘ

There are no such residues in this entry.