



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 03:19 PM EDT

PDB ID : 3EGW
Title : The crystal structure of the NarGHI mutant NarH - C16A
Authors : Bertero, M.G.; Rothery, R.A.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2008-09-11
Resolution : 1.90 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 ⓘ 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 : 2.23.2
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

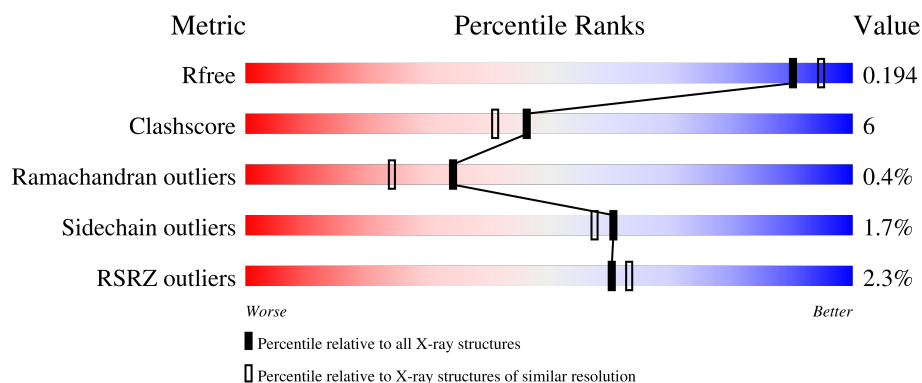
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	1244	<div> <div>2%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	B	509	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
3	C	225	<div> <div>3%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>

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
7	SF4	B	803	-	-	X	-
9	3PH	B	806	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17504 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	C	N	O	S	0	0	0
			9870	6232	1731	1859	48			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	PHE	conflict	UNP P09152
A	362	ALA	ASP	conflict	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	C	N	O	S	0	0	0
			4050	2562	701	756	31			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	ALA	CYS	engineered mutation	UNP P11349

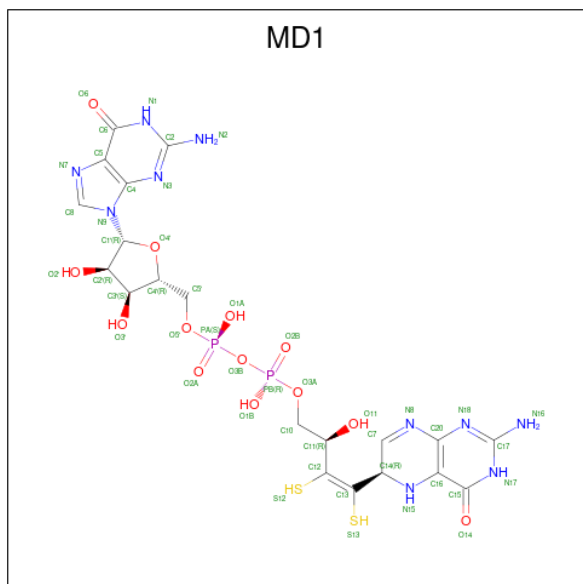
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	225	Total	C	N	O	S	0	0	0
			1791	1188	303	286	14			

There are 2 discrepancies between the modelled and reference sequences:

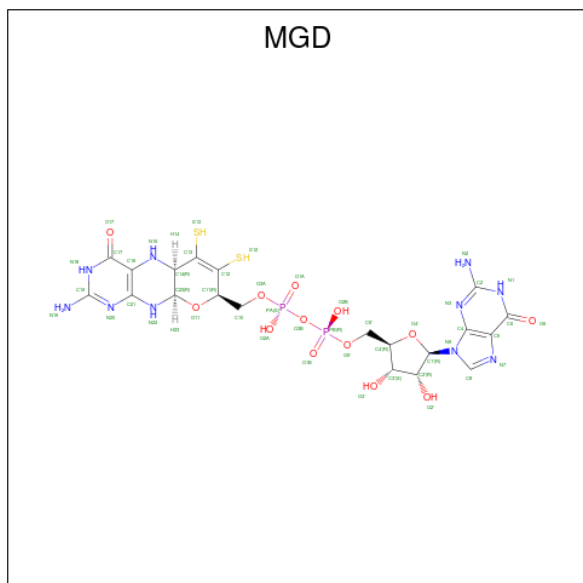
Chain	Residue	Modelled	Actual	Comment	Reference
C	77	ALA	TYR	conflict	UNP P11350
C	78	ALA	GLU	conflict	UNP P11350

- 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: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



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

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).

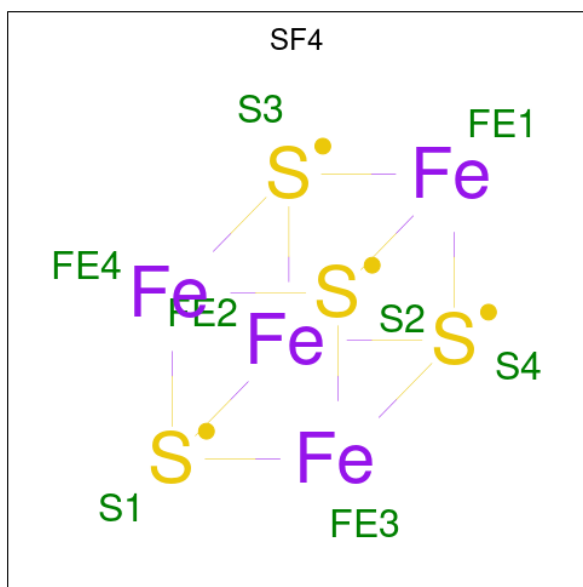


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

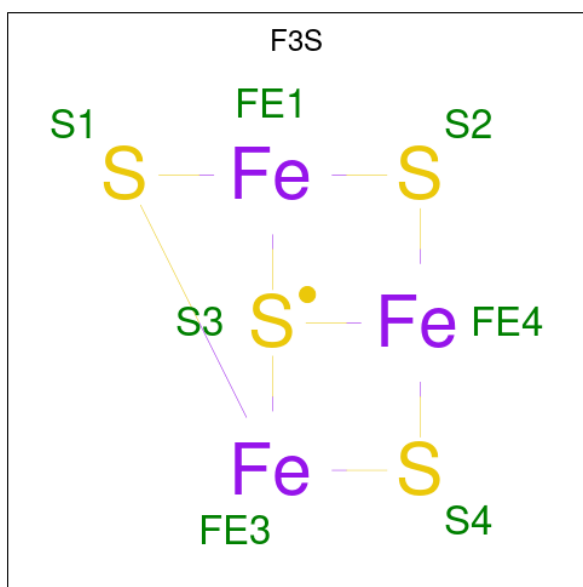
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



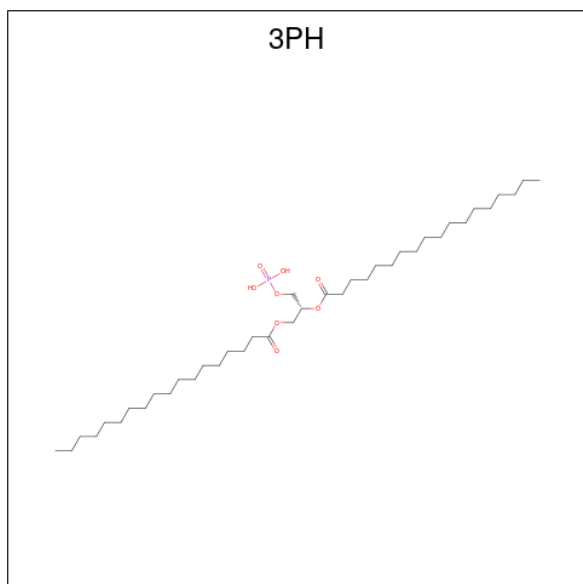
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

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



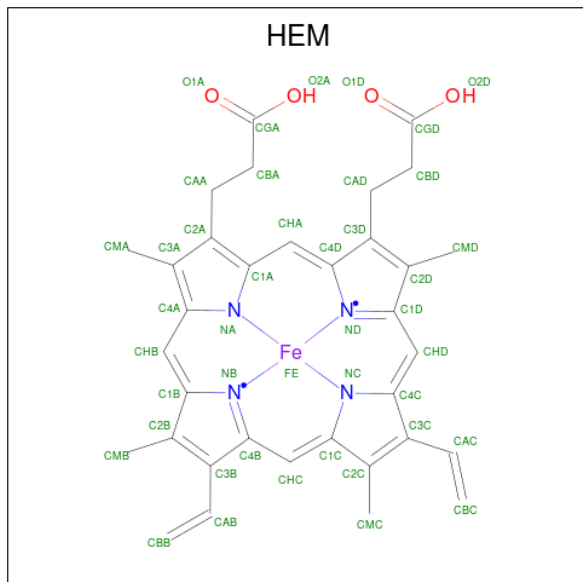
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



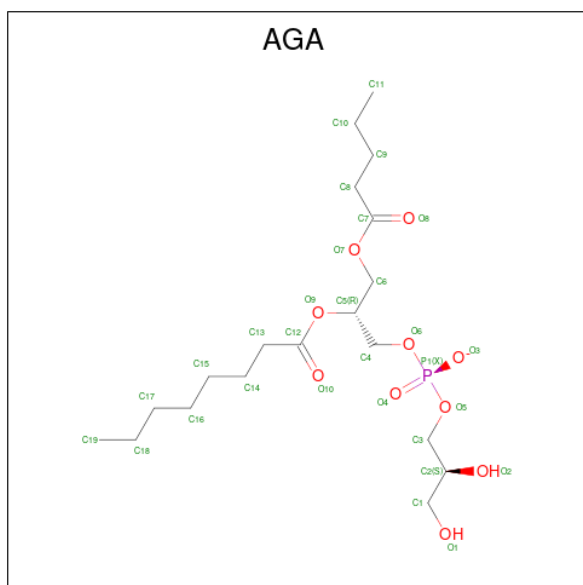
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	P	0	0
			18	9	8	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 11 is (1S)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYL OXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula: $C_{19}H_{36}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	O	P	0	0
			30	19	10	1		

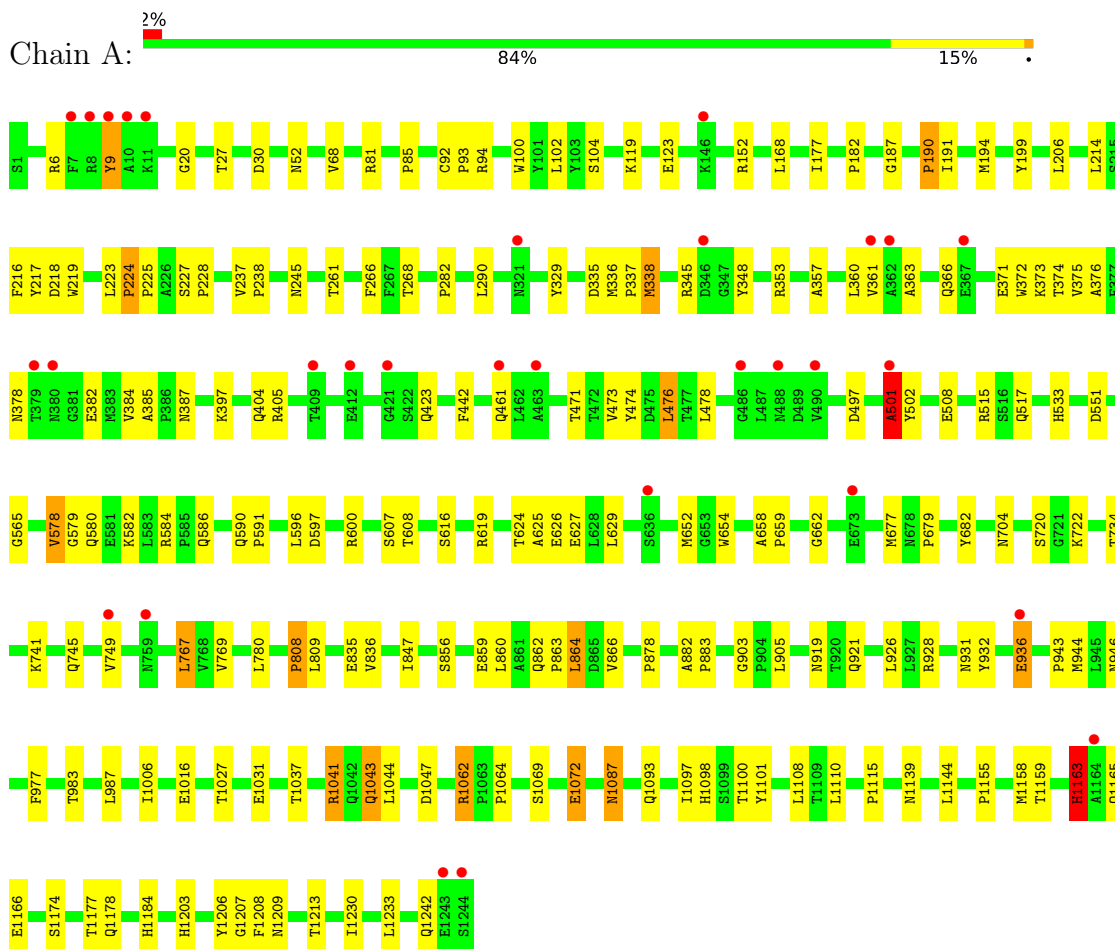
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	912	Total	O	0	0
			912	912		
12	B	512	Total	O	0	0
			512	512		
12	C	102	Total	O	0	0
			102	102		

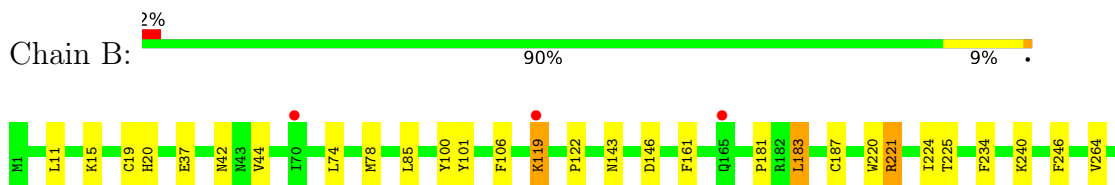
3 Residue-property plots

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

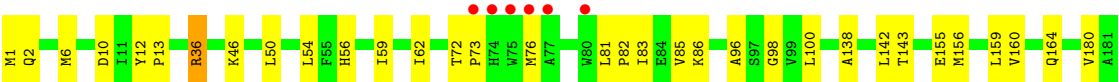
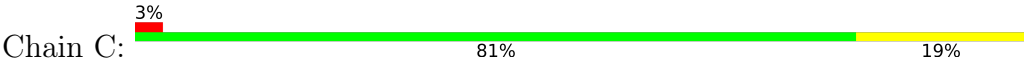


- Molecule 2: Respiratory nitrate reductase 1 beta chain





● Molecule 3: Respiratory nitrate reductase 1 gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.00Å 241.68Å 139.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.90 19.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.99-1.90) 96.2 (19.99-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.90Å)	Xtriage
Refinement program	REFMAC, CNS 1.1	Depositor
R, R_{free}	0.175 , 0.196 0.173 , 0.194	Depositor DCC
R_{free} test set	9737 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17504	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: MD1, 6MO, MGD, AGA, F3S, SF4, 3PH, HEM, FME

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	0.31	0/10129	0.63	8/13749 (0.1%)
2	B	0.32	0/4146	0.60	0/5608
3	C	0.32	0/1833	0.53	0/2481
All	All	0.31	0/16108	0.61	8/21838 (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	0	4

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	ALA	C-N-CA	12.16	152.09	121.70
1	A	1163	HIS	C-N-CA	11.64	150.80	121.70
1	A	502	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	A	501	ALA	N-CA-CB	6.20	118.78	110.10
1	A	502	TYR	CB-CG-CD2	6.01	124.61	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Peptide,Mainchain
1	A	501	ALA	Peptide,Mainchain

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	9870	0	9531	137	0
2	B	4050	0	3974	34	0
3	C	1791	0	1831	31	0
4	A	47	0	22	3	0
5	A	47	0	22	2	0
6	A	1	0	0	0	0
7	A	8	0	0	0	0
7	B	16	0	0	2	0
8	B	14	0	0	0	0
9	B	18	0	10	0	0
10	C	86	0	60	0	0
11	C	30	0	36	0	0
12	A	912	0	0	8	1
12	B	512	0	0	3	0
12	C	102	0	0	2	0
All	All	17504	0	15486	197	1

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 6.

The worst 5 of 197 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:378:ASN:HD21	1:A:382:GLU:HB2	1.27	1.00
3:C:73:PRO:HG2	3:C:76:MET:HG3	1.47	0.95
1:A:378:ASN:ND2	1:A:382:GLU:HB2	1.97	0.80
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.66	0.77
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.67	0.76

All (1) 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)
12:A:1886:HOH:O	12:A:1886:HOH:O[3_354]	1.99	0.21

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	1242/1244 (100%)	1176 (95%)	58 (5%)	8 (1%)	25	15
2	B	507/509 (100%)	493 (97%)	14 (3%)	0	100	100
3	C	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
All	All	1972/1978 (100%)	1887 (96%)	77 (4%)	8 (0%)	34	24

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	578	VAL
1	A	1166	GLU
1	A	190	PRO
1	A	361	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1039/1039 (100%)	1019 (98%)	20 (2%)	57	53
2	B	435/435 (100%)	427 (98%)	8 (2%)	59	55
3	C	184/184 (100%)	183 (100%)	1 (0%)	88	89
All	All	1658/1658 (100%)	1629 (98%)	29 (2%)	60	57

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1062	ARG
2	B	428	ARG
1	A	1110	LEU
2	B	161	PHE
1	A	1087	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	ASN
3	C	175	GLN
1	A	942	GLN
2	B	451	ASN
1	A	919	ASN

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	1.48	2 (25%)	7,9,11	1.53	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	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-2.96	1.48	1.53
3	C	1	FME	CB-CG	2.25	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	2.96	127.38	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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
5	MGD	A	1246	6	41,52,52	1.97	10 (24%)	43,81,81	2.59	18 (41%)
11	AGA	C	309	-	29,29,29	0.74	1 (3%)	32,35,35	1.48	3 (9%)
7	SF4	B	804	2	0,12,12	-	-	-		
7	SF4	B	803	2	0,12,12	-	-	-		
4	MD1	A	1245	6	38,51,51	3.82	9 (23%)	35,78,78	2.11	9 (25%)
9	3PH	B	806	-	17,17,47	1.01	1 (5%)	19,21,52	1.95	5 (26%)
10	HEM	C	806	3	27,50,50	2.28	13 (48%)	17,82,82	1.70	4 (23%)
10	HEM	C	807	3	27,50,50	2.32	13 (48%)	17,82,82	1.91	5 (29%)
7	SF4	A	1248	1	0,12,12	-	-	-		
8	F3S	B	805	2	0,9,9	-	-	-		
8	F3S	B	802	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
5	MGD	A	1246	6	-	2/18/66/66	0/6/6/6
11	AGA	C	309	-	-	6/34/34/34	-
7	SF4	B	804	2	-	-	0/6/5/5
8	F3S	B	802	2	-	-	0/3/3/3
4	MD1	A	1245	6	-	7/21/59/59	0/5/5/5
10	HEM	C	806	3	-	0/6/54/54	-
9	3PH	B	806	-	1/1/3/4	8/18/18/49	-
7	SF4	B	803	2	-	-	0/6/5/5
7	SF4	A	1248	1	-	-	0/6/5/5
8	F3S	B	805	2	-	-	0/3/3/3
10	HEM	C	807	3	-	0/6/54/54	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1245	MD1	C7-N8	18.85	1.50	1.27
4	A	1245	MD1	C4-N9	-6.82	1.38	1.47
10	C	807	HEM	C3B-CAB	5.85	1.59	1.47
4	A	1245	MD1	C6-N1	5.54	1.42	1.33
4	A	1245	MD1	C15-N17	5.46	1.42	1.33

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1245	MD1	C4-C5-N7	6.46	111.02	102.46
5	A	1246	MGD	N3-C2-N1	-5.67	119.66	127.22
5	A	1246	MGD	C5-C6-N1	-5.66	115.69	123.43
11	C	309	AGA	C14-C13-C12	5.36	133.11	113.62
5	A	1246	MGD	C17-C16-C21	5.21	119.20	114.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	806	3PH	C2

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1245	MD1	C5'-O5'-PA-O2A
9	B	806	3PH	O22-C21-O21-C2
4	A	1245	MD1	O4'-C4'-C5'-O5'
4	A	1245	MD1	C3'-C4'-C5'-O5'
9	B	806	3PH	C32-C31-O31-C3

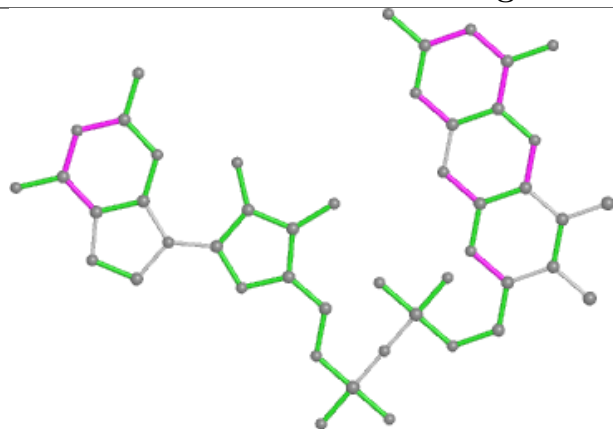
There are no ring outliers.

3 monomers are involved in 7 short contacts:

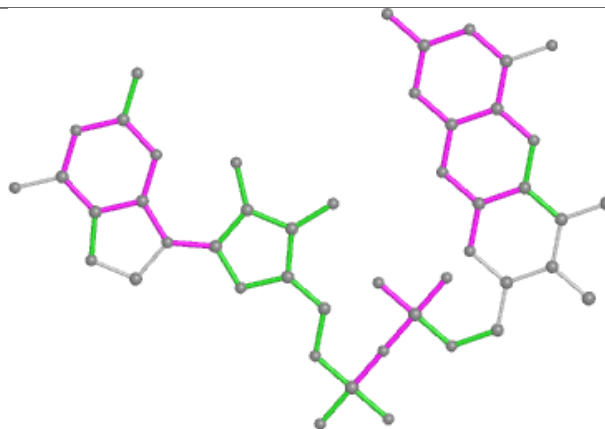
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1246	MGD	2	0
7	B	803	SF4	2	0
4	A	1245	MD1	3	0

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.

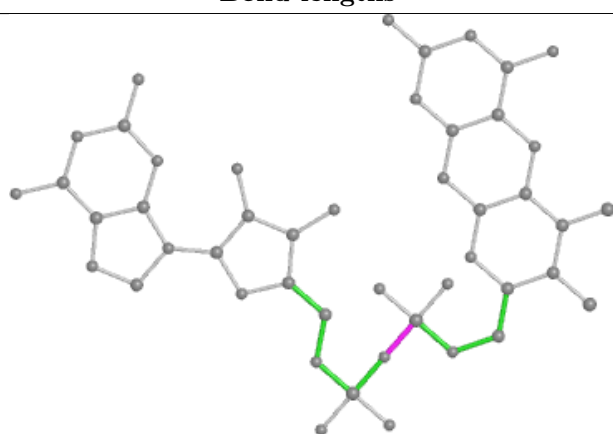
Ligand MGD A 1246



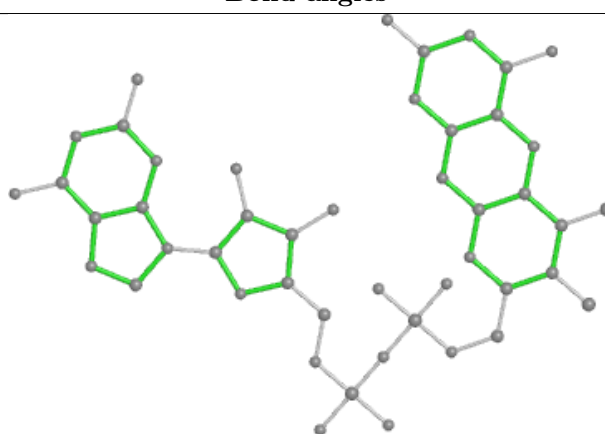
Bond lengths



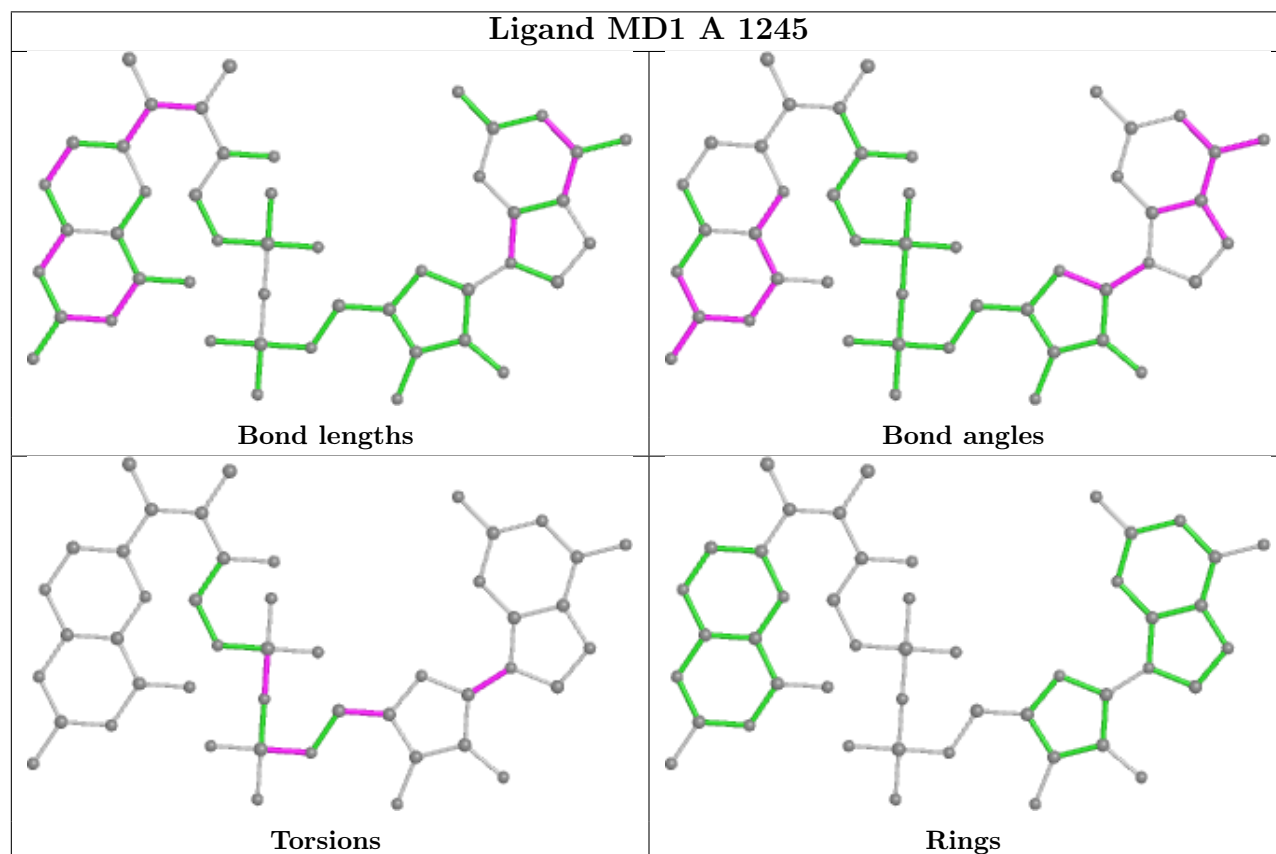
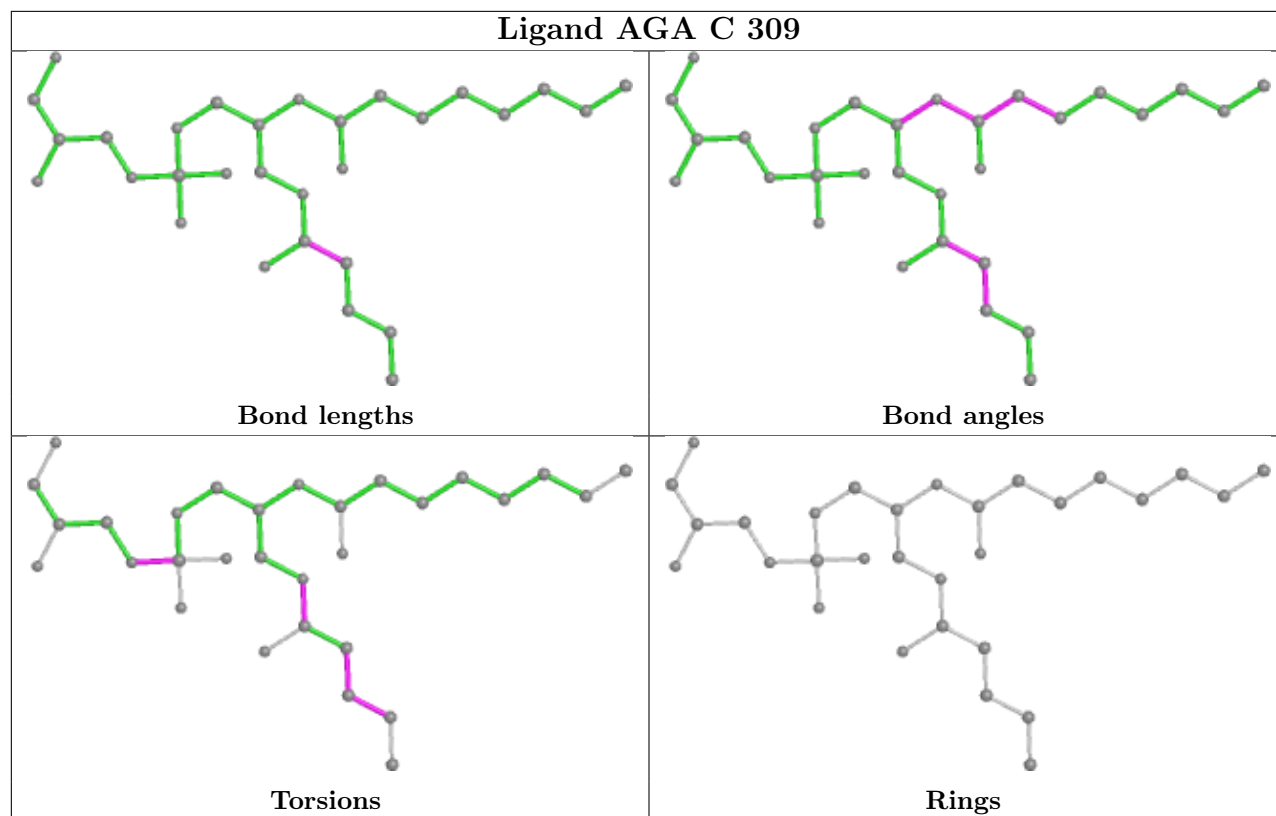
Bond angles



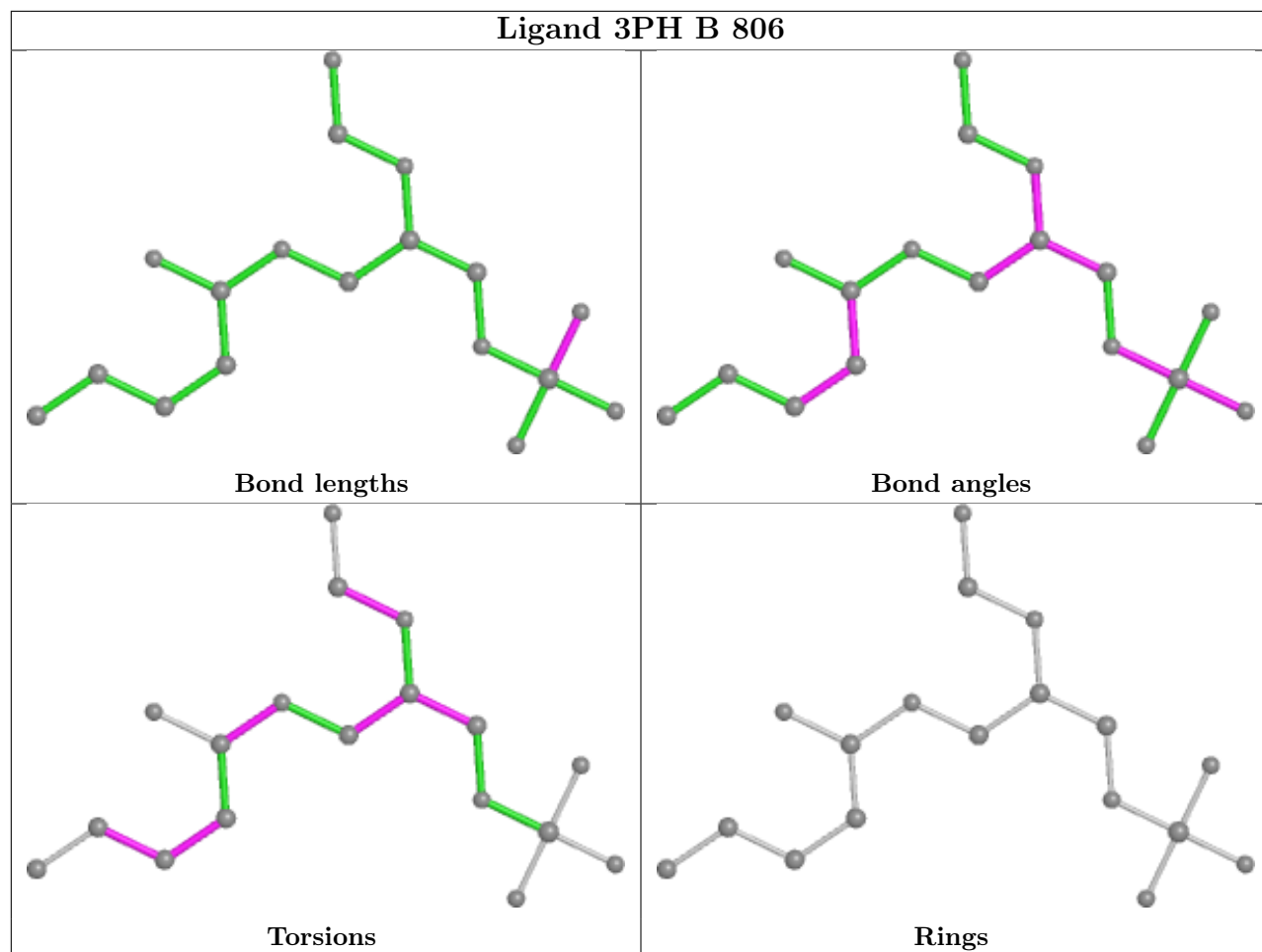
Torsions

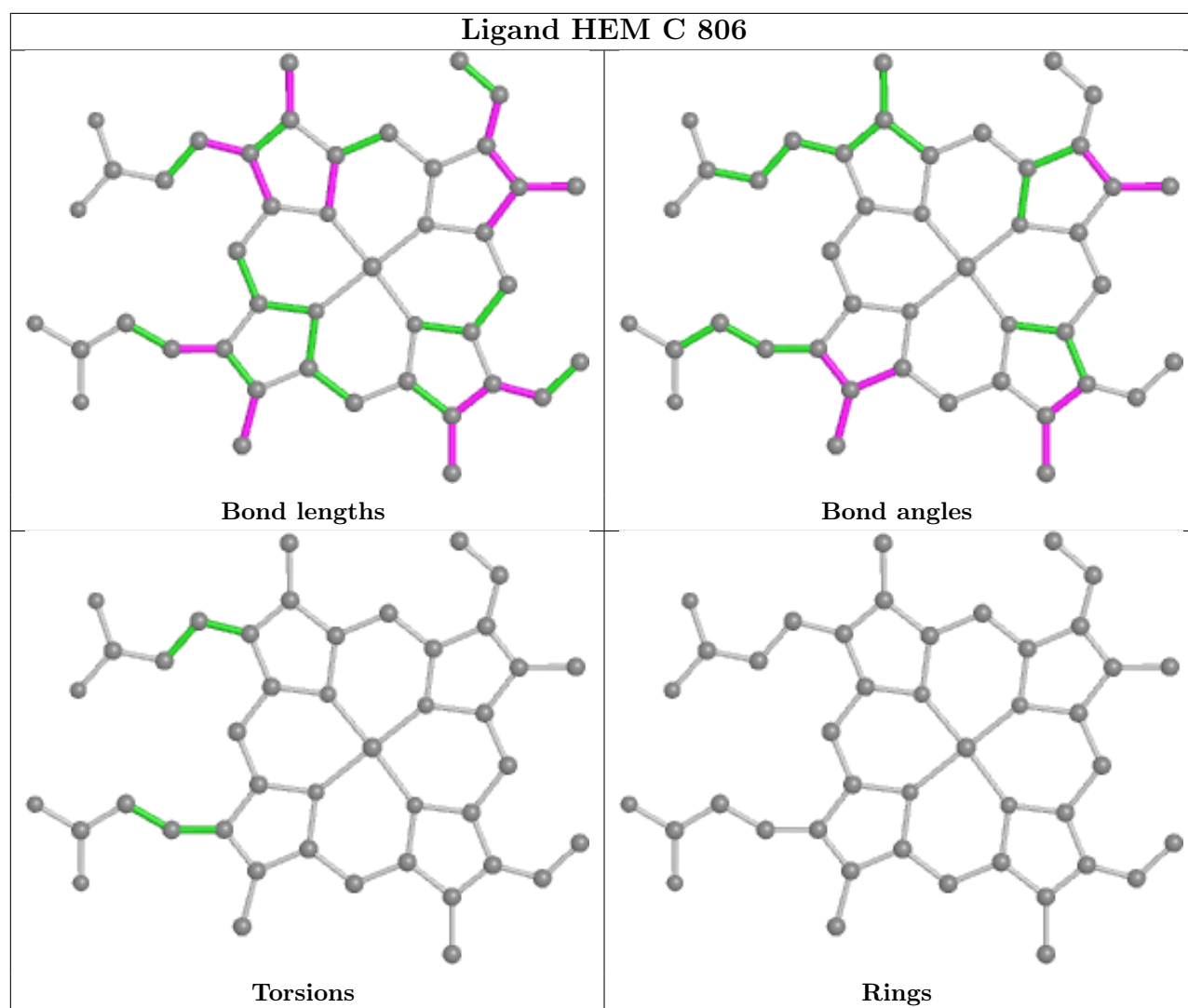


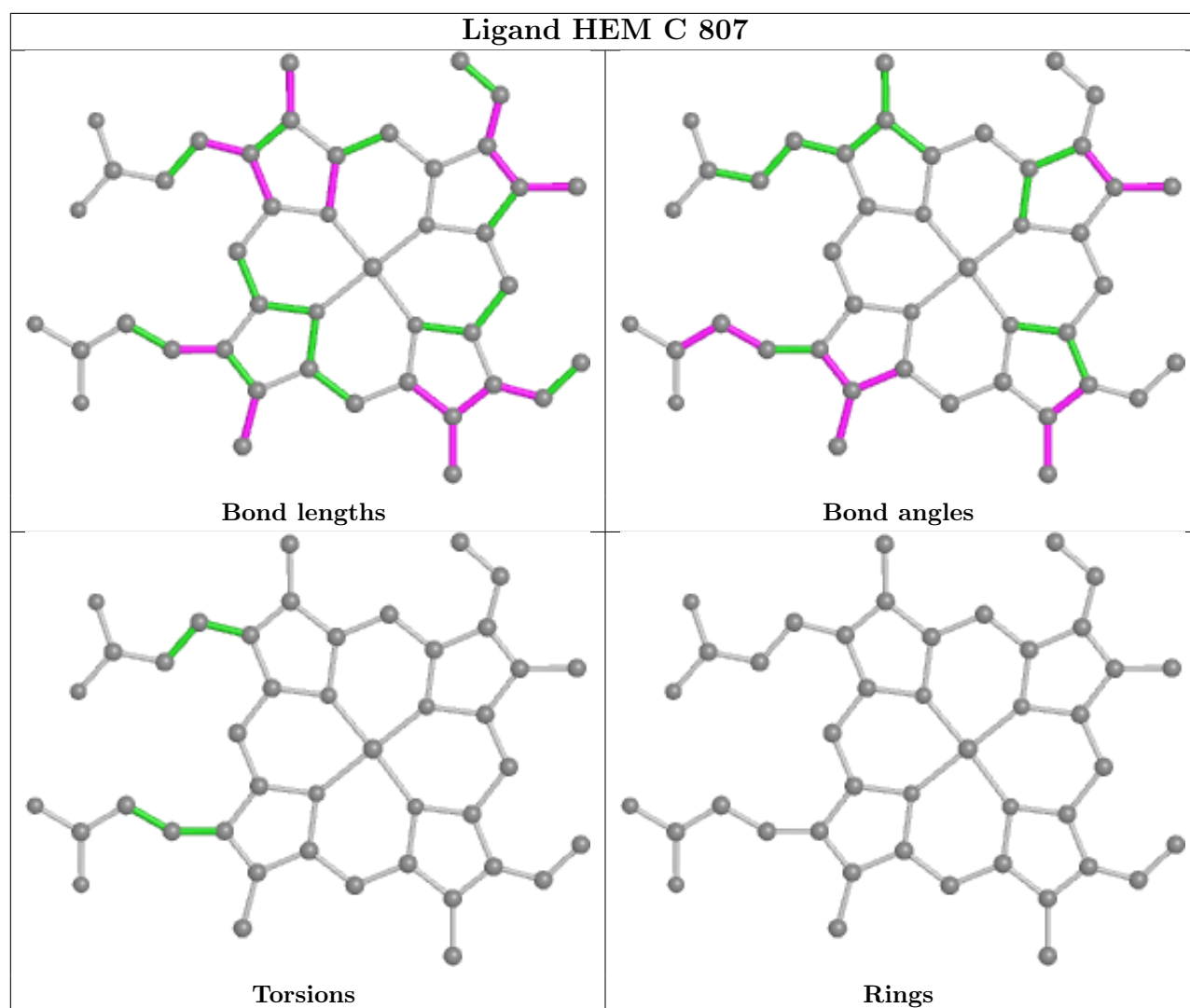
Rings



Ligand 3PH B 806







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1244/1244 (100%)	-0.11	30 (2%) 59 62	9, 20, 39, 52	0
2	B	509/509 (100%)	-0.45	9 (1%) 68 71	9, 15, 27, 46	0
3	C	224/225 (99%)	-0.12	7 (3%) 49 51	11, 19, 36, 53	0
All	All	1977/1978 (99%)	-0.20	46 (2%) 60 63	9, 18, 36, 53	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	8.6
3	C	75	TRP	7.8
1	A	10	ALA	7.4
3	C	77	ALA	4.6
3	C	76	MET	4.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	FME	C	1	10/11	0.90	0.20	31,36,45,46	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

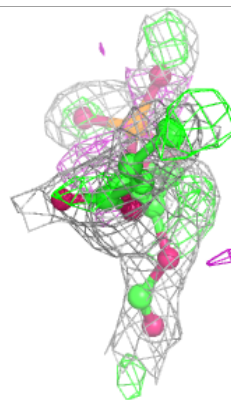
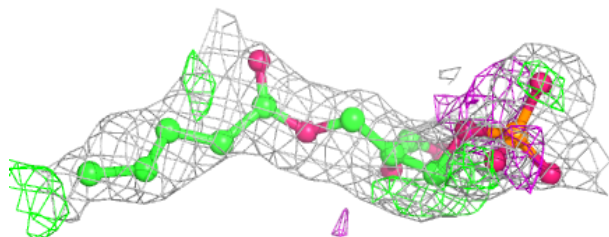
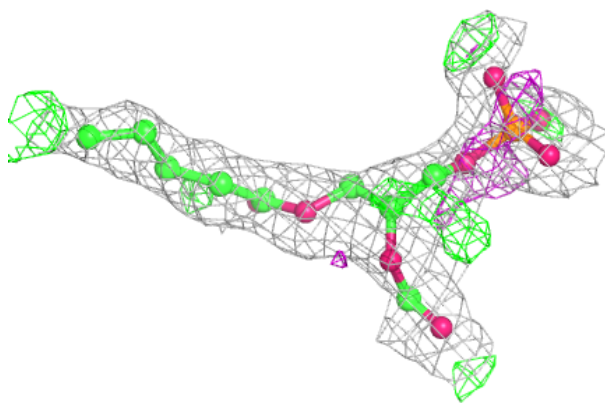
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	3PH	B	806	18/48	0.68	0.26	43,52,55,56	0
11	AGA	C	309	30/30	0.92	0.15	17,21,42,42	0
4	MD1	A	1245	47/47	0.96	0.09	9,16,20,21	0
10	HEM	C	807	43/43	0.96	0.13	17,19,32,38	0
6	6MO	A	1247	1/1	0.96	0.05	21,21,21,21	0
5	MGD	A	1246	47/47	0.97	0.08	11,15,17,20	0
10	HEM	C	806	43/43	0.98	0.10	9,13,15,23	0
7	SF4	B	804	8/8	0.99	0.04	10,11,12,13	0
8	F3S	B	802	7/7	0.99	0.04	12,13,14,14	0
7	SF4	B	803	8/8	1.00	0.04	9,10,11,11	0
8	F3S	B	805	7/7	1.00	0.04	11,11,12,12	0
7	SF4	A	1248	8/8	1.00	0.04	12,13,13,14	0

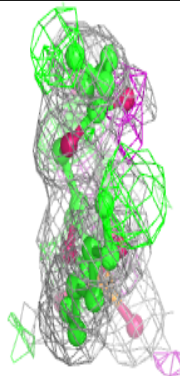
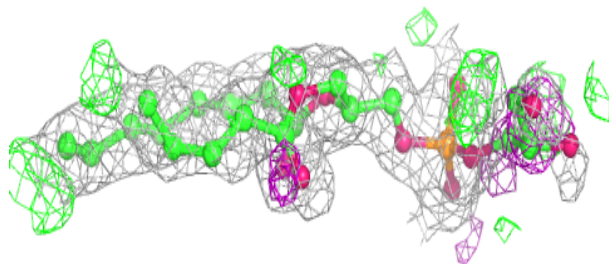
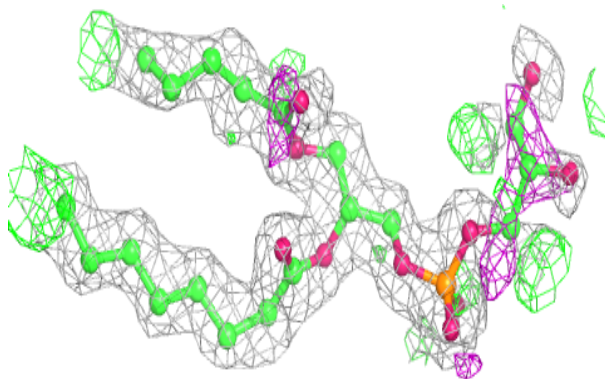
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3PH B 806:

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

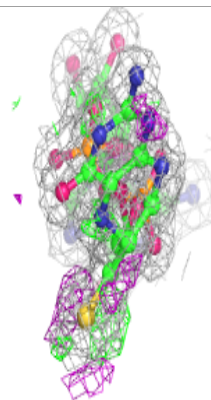
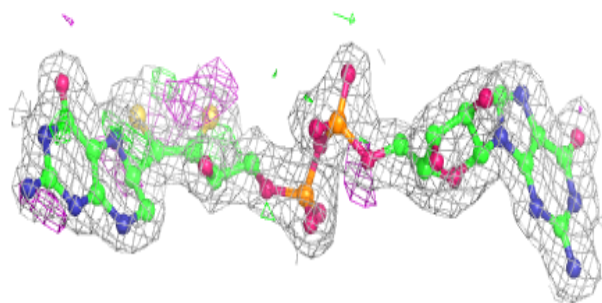
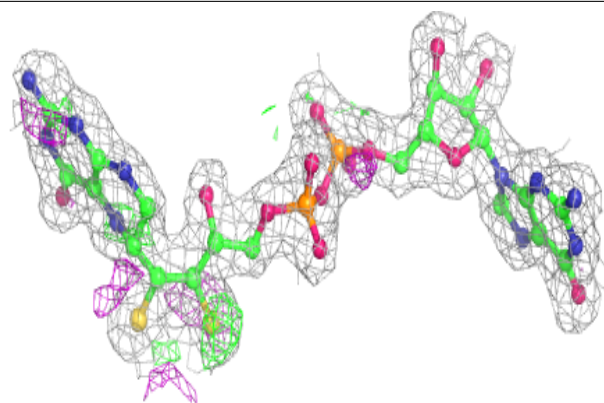
**Electron density around AGA C 309:**

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



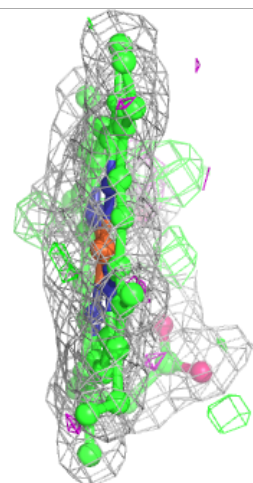
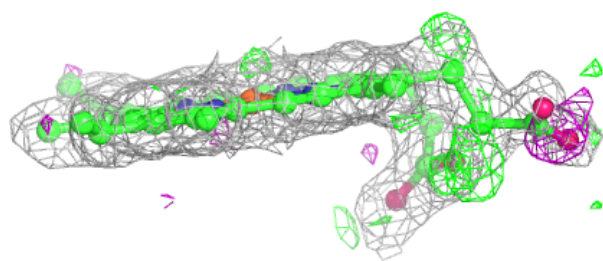
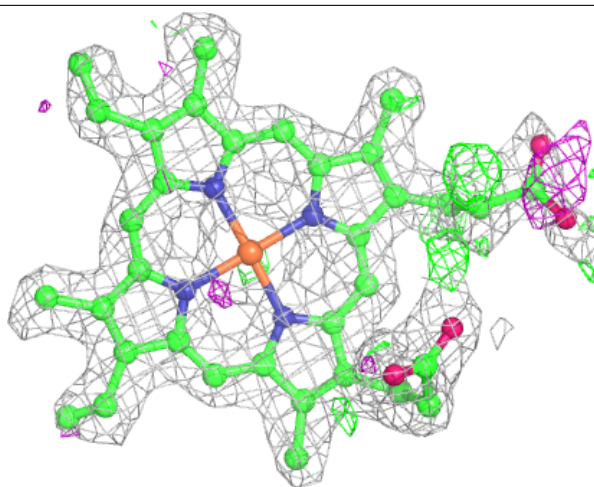
Electron density around MD1 A 1245:

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



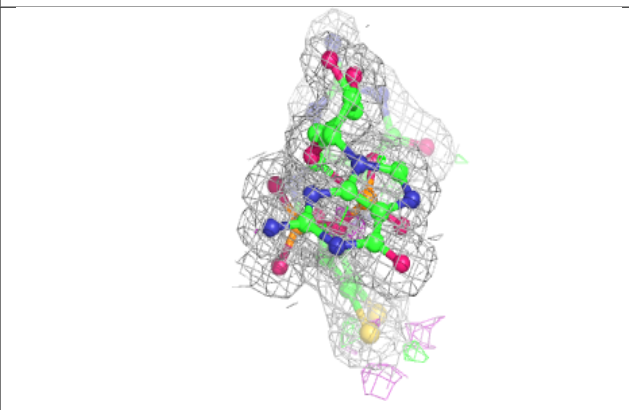
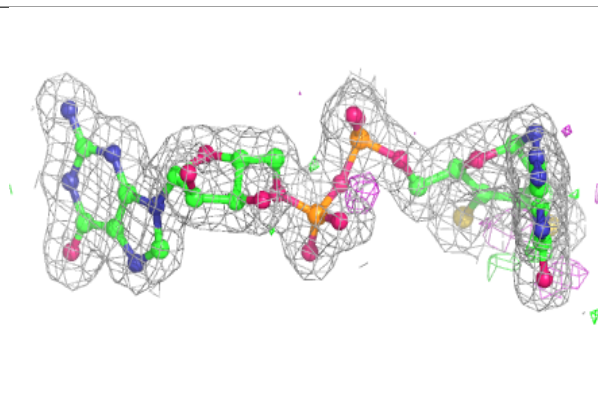
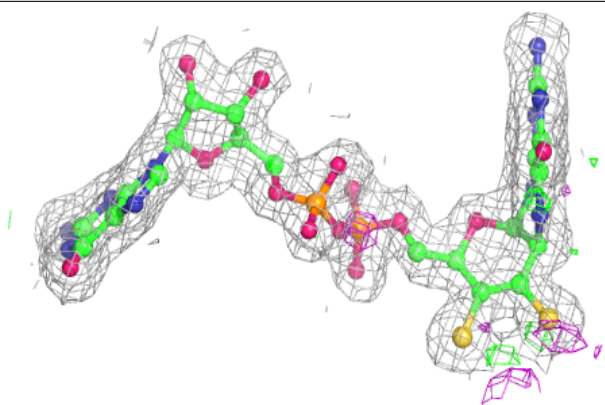
Electron density around HEM C 807:

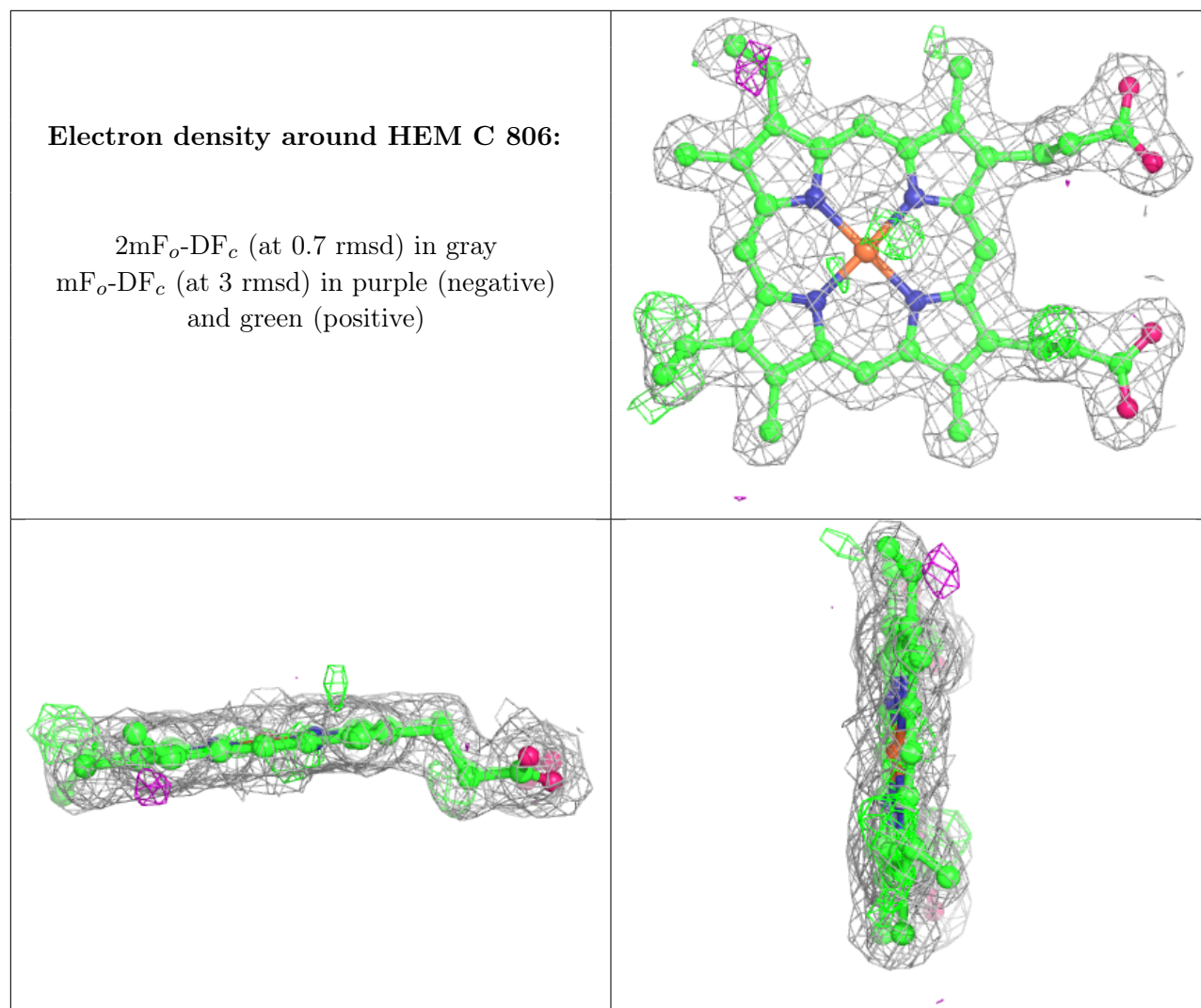
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MGD A 1246:

$2mF_o-DF_c$ (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.