Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 10:56 PM EDT

PDB ID	:	1Y5N
Title	:	The crystal structure of the NarGHI mutant NarI-K86A in complex with pentachlorophenol
Authors	:	Bertero, M.G.; Rothery, R.A.; Boroumand, N.; Palak, M.; Blasco, F.; Ginet, N.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on	:	2004-12-02
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

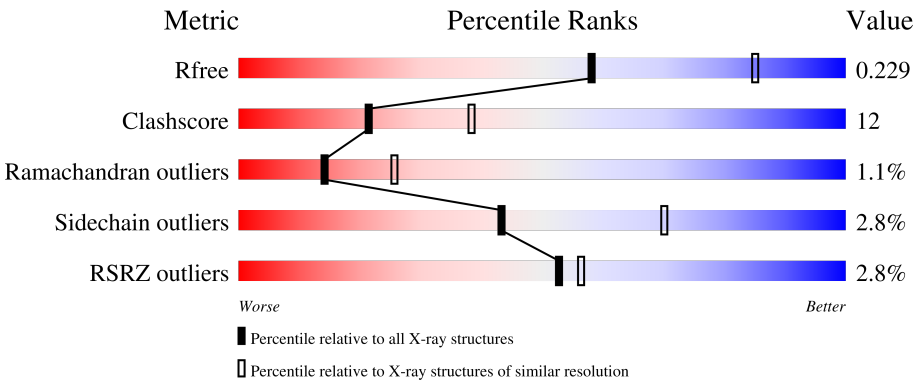
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	1246	3% 70% 28%
2	B	512	2% 83% 16%
3	C	225	3% 64% 30%

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	A	1801	-	-	X	-
8	3PH	B	1806	X	-	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 15972 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
			Total	C	N	O	S			
1	A	1244	9869	6232	1731	1858	48	0	0	0

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

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

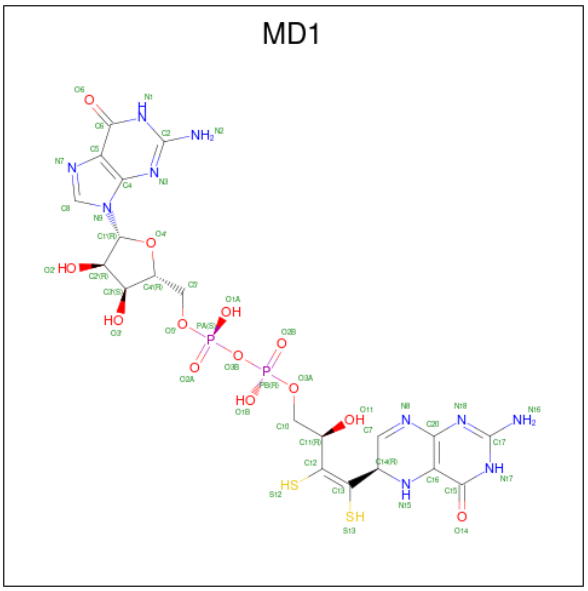
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	217	1719	1138	290	278	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	MET	modified residue	UNP P11350
C	86	ALA	LYS	engineered mutation	UNP P11350

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

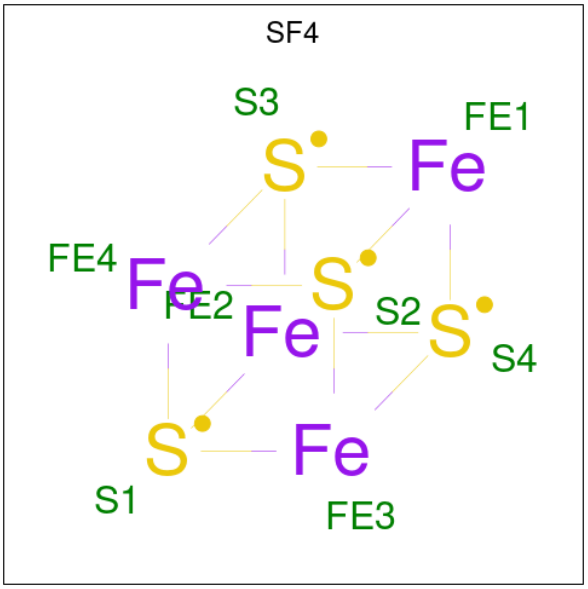


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
4	A	1	47	20	10	13	2	2	0	0

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

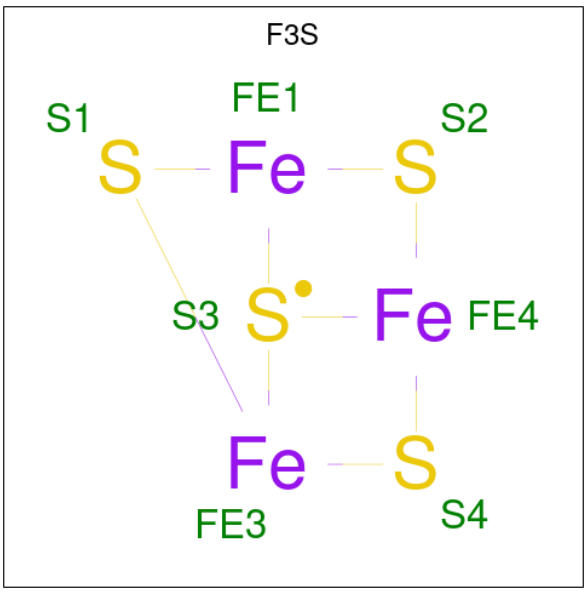
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
5	A	1	1	1	0	0

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



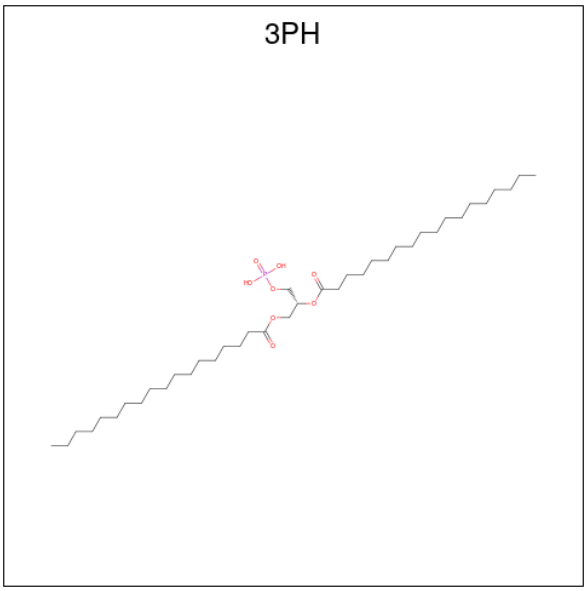
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	A	1	8	4	4	0	0
6	B	1	8	4	4	0	0
6	B	1	8	4	4	0	0
6	B	1	8	4	4	0	0

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



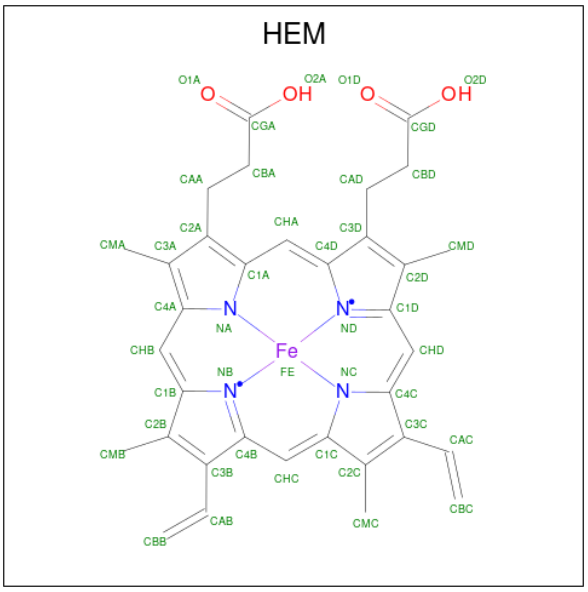
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	7	3	4	0	0

- Molecule 8 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



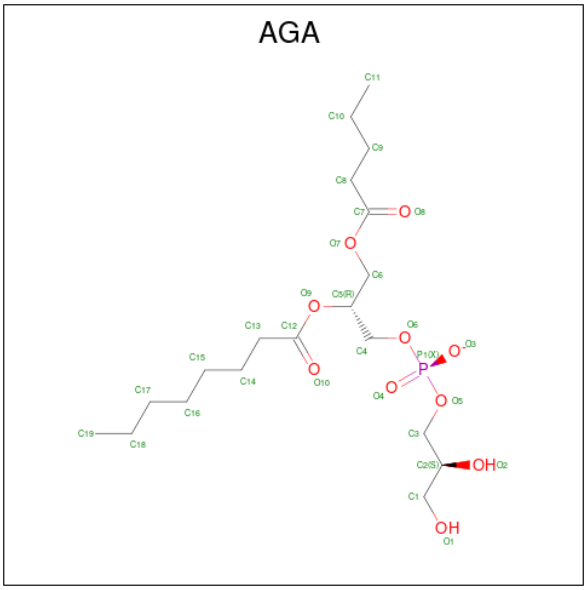
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
8	B	1	18	9	8	1	0	0

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



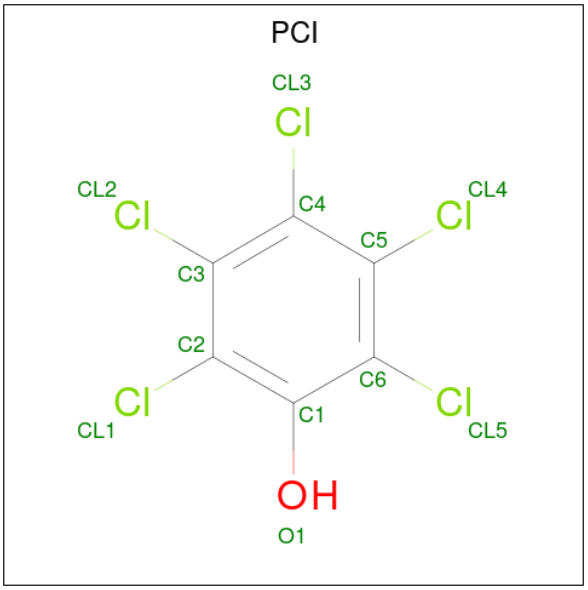
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
9	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
9	C	1	43	34	1	4	4	0	0

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



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

- Molecule 11 is PENTACHLOROPHENOL (three-letter code: PCI) (formula: C_6HCl_5O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
11	C	1	12	6	5	1	0	0

- Molecule 12 is water.

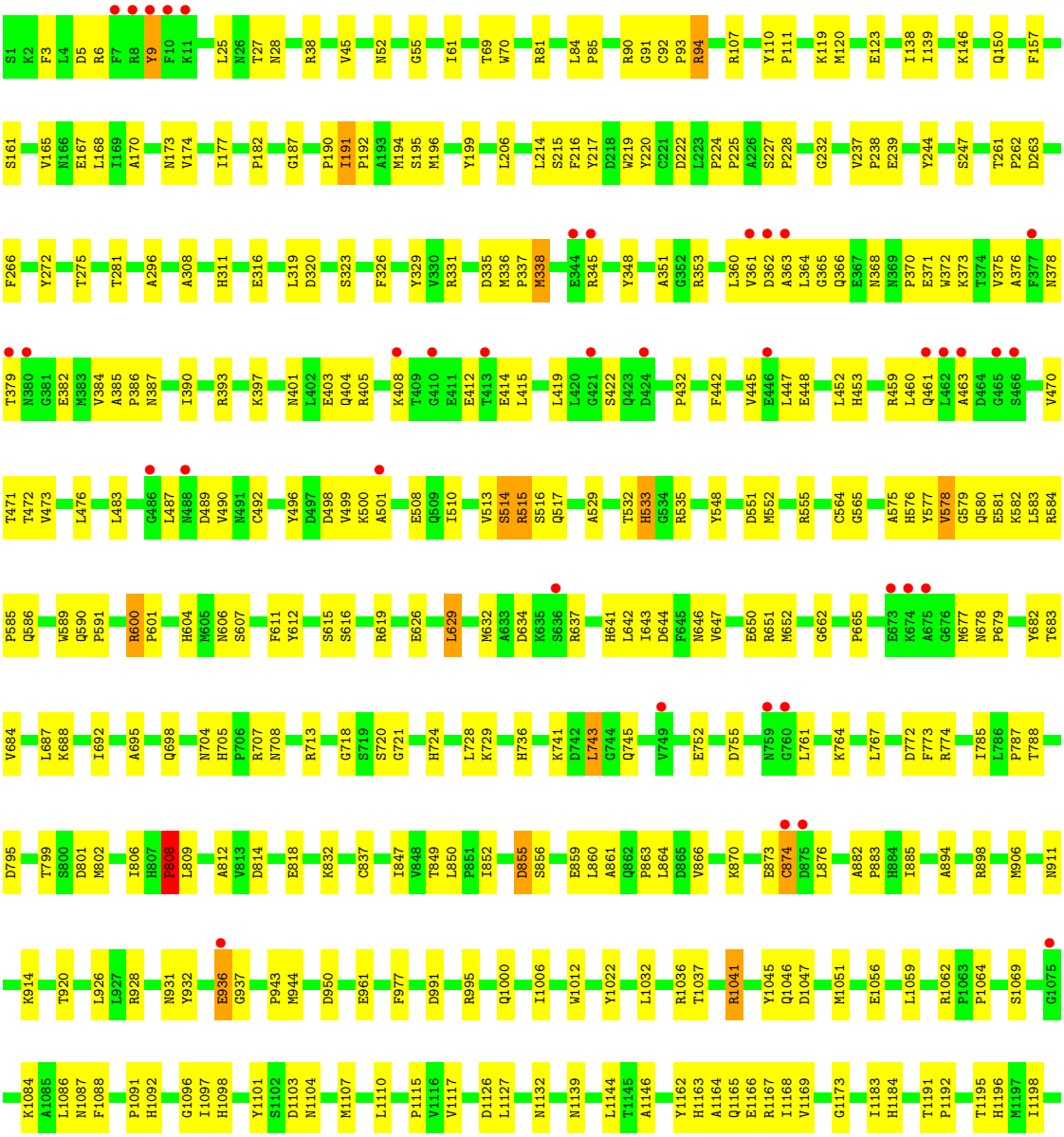
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	23	23	23	0	0
			Total	O		
12	B	29	29	29	0	0
			Total	O		
12	C	2	2	2	0	0

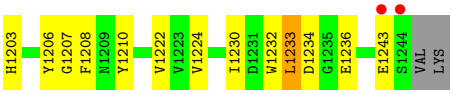
3 Residue-property plots (i)

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

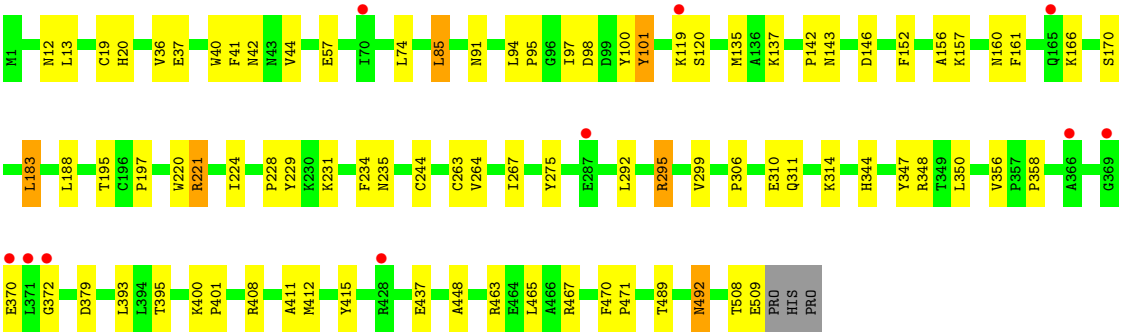
Chain A: 3% 70% 28%





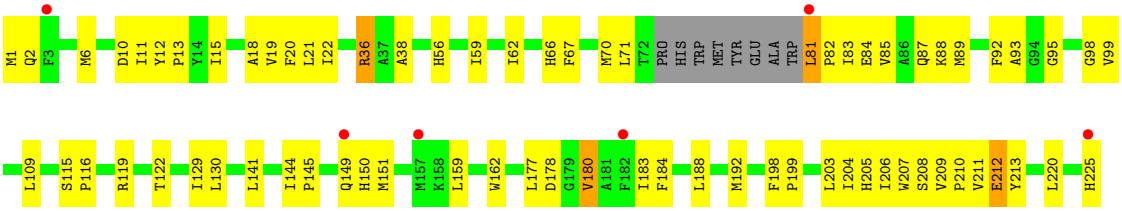
• Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B:



• Molecule 3: Respiratory nitrate reductase 1 gamma chain

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	154.26Å 241.96Å 140.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 2.50 24.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.4 (24.84-2.50) 81.5 (24.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.238 0.181 , 0.229	Depositor DCC
R_{free} test set	6007 reflections (8.16%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15972	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, HEM, MD1, AGA, 6MO, FME, SF4, 3PH, PCI

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	0.36	0/10128	0.62	0/13749
2	B	0.39	0/4146	0.65	0/5609
3	C	0.39	0/1754	0.58	0/2370
All	All	0.37	0/16028	0.62	0/21728

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	9869	0	9527	277	0
2	B	4050	0	3973	60	0
3	C	1719	0	1764	47	0
4	A	94	0	42	8	0
5	A	1	0	0	0	0
6	A	8	0	0	2	0
6	B	24	0	0	0	0
7	B	7	0	0	0	0
8	B	18	0	10	0	0
9	C	86	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	30	0	36	1	0
11	C	12	0	1	0	0
12	A	23	0	0	0	0
12	B	29	0	0	0	0
12	C	2	0	0	0	0
All	All	15972	0	15413	375	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (375) 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:928:ARG:HG2	1:A:943:PRO:HG3	1.62	0.81
1:A:578:VAL:HG23	1:A:579:GLY:H	1.46	0.80
1:A:1086:LEU:HD12	1:A:1224:VAL:HG21	1.67	0.77
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.68	0.75
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	1.86	0.73
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.04	0.73
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.71	0.72
3:C:81:LEU:N	3:C:81:LEU:HD23	2.03	0.72
1:A:471:THR:HG23	1:A:476:LEU:HD11	1.70	0.72
1:A:387:ASN:ND2	1:A:405:ARG:HB2	2.05	0.72
1:A:378:ASN:HD21	1:A:382:GLU:HB2	1.54	0.71
1:A:225:PRO:HB2	1:A:551:ASP:OD1	1.91	0.70
1:A:371:GLU:N	1:A:371:GLU:OE1	2.25	0.69
3:C:95:GLY:O	3:C:99:VAL:HG23	1.93	0.69
2:B:91:ASN:HB3	2:B:94:LEU:HB2	1.76	0.67
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.79	0.64
2:B:157:LYS:NZ	2:B:157:LYS:HB3	2.12	0.64
3:C:6:MET:O	3:C:10:ASP:HB2	1.98	0.64
1:A:196:MET:CE	1:A:799:THR:HG23	2.29	0.63
1:A:52:ASN:CG	1:A:191:ILE:HG13	2.19	0.63
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.18	0.63
1:A:1069:SER:O	1:A:1139:ASN:HB2	1.99	0.63
1:A:110:TYR:HD1	1:A:818:GLU:HG3	1.64	0.62
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.81	0.62
1:A:578:VAL:HG23	1:A:579:GLY:N	2.15	0.62
1:A:774:ARG:HH11	4:A:1800:MD1:H3'	1.64	0.61
1:A:1098:HIS:CE1	4:A:1800:MD1:S12	2.93	0.61
2:B:94:LEU:HD12	2:B:95:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:PRO:HB2	2:B:347:TYR:CD2	2.35	0.61
1:A:93:PRO:HG2	1:A:94:ARG:HD3	1.83	0.61
1:A:1163:HIS:HD2	1:A:1184:HIS:NE2	1.98	0.61
1:A:168:LEU:HD23	1:A:168:LEU:O	2.01	0.61
1:A:906:MET:HE3	1:A:911:ASN:HB2	1.81	0.61
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.82	0.60
3:C:12:TYR:N	3:C:13:PRO:HD2	2.16	0.60
1:A:25:LEU:HD11	3:C:220:LEU:HD22	1.84	0.60
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.01	0.60
1:A:584:ARG:HD3	1:A:1006:ILE:HD13	1.84	0.60
1:A:272:TYR:HB3	2:B:412:MET:CE	2.32	0.60
1:A:508:GLU:OE1	1:A:515:ARG:HD2	2.00	0.60
3:C:159:LEU:HD21	3:C:180:VAL:HG21	1.84	0.59
1:A:894:ALA:O	1:A:898:ARG:HG3	2.02	0.59
1:A:1059:LEU:HD23	1:A:1059:LEU:H	1.67	0.59
1:A:1084:LYS:HB2	1:A:1127:LEU:HD21	1.84	0.59
1:A:384:VAL:HG22	1:A:385:ALA:N	2.17	0.59
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.83	0.59
1:A:27:THR:HG22	1:A:28:ASN:N	2.17	0.59
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.82	0.59
1:A:5:ASP:OD2	2:B:489:THR:HG23	2.02	0.59
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.84	0.59
1:A:366:GLN:O	1:A:370:PRO:HB3	2.02	0.59
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.68	0.59
1:A:3:PHE:CE1	10:C:309:AGA:H161	2.39	0.58
1:A:361:VAL:HA	1:A:463:ALA:HB2	1.85	0.58
1:A:360:LEU:N	1:A:360:LEU:HD22	2.19	0.58
1:A:490:VAL:O	1:A:500:LYS:HE2	2.03	0.58
1:A:432:PRO:HD3	1:A:632:MET:HE1	1.86	0.58
1:A:107:ARG:HD2	1:A:773:PHE:O	2.04	0.58
2:B:220:TRP:O	2:B:221:ARG:NH1	2.36	0.58
1:A:684:VAL:HG13	1:A:876:LEU:HD22	1.86	0.58
1:A:110:TYR:CD1	1:A:818:GLU:HG3	2.38	0.58
1:A:498:ASP:OD1	1:A:500:LYS:HG2	2.02	0.58
1:A:353:ARG:CZ	1:A:864:LEU:HD12	2.34	0.57
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.86	0.57
3:C:204:ILE:HD12	3:C:205:HIS:N	2.18	0.57
1:A:772:ASP:C	1:A:788:THR:HG22	2.24	0.57
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.04	0.57
3:C:109:LEU:HD13	3:C:130:LEU:HD23	1.85	0.57
1:A:365:GLY:HA3	1:A:408:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:ILE:O	1:A:647:VAL:HG23	2.03	0.57
1:A:336:MET:HA	1:A:473:VAL:HB	1.86	0.57
1:A:219:TRP:HB2	1:A:607:SER:HB2	1.87	0.57
1:A:225:PRO:O	1:A:228:PRO:HD2	2.05	0.57
1:A:859:GLU:HG3	1:A:860:LEU:HD12	1.86	0.57
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.87	0.56
1:A:61:ILE:N	1:A:61:ILE:HD12	2.19	0.56
1:A:360:LEU:C	1:A:463:ALA:HB2	2.26	0.56
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.53	0.56
1:A:471:THR:CG2	1:A:476:LEU:HD11	2.34	0.56
1:A:366:GLN:HG3	1:A:373:LYS:HZ3	1.69	0.56
4:A:1800:MD1:H7	4:A:1800:MD1:C11	2.36	0.56
1:A:1098:HIS:CE1	4:A:2800:MD1:S13	2.99	0.56
1:A:191:ILE:HD13	1:A:216:PHE:CE1	2.41	0.55
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.41	0.55
1:A:345:ARG:HB2	1:A:348:TYR:O	2.06	0.55
1:A:487:LEU:HD12	1:A:487:LEU:N	2.20	0.55
1:A:646:ASN:O	1:A:650:GLU:HG3	2.06	0.55
1:A:1056:GLU:HG3	1:A:1195:THR:HG21	1.89	0.55
3:C:67:PHE:CE2	3:C:71:LEU:HD12	2.41	0.55
1:A:247:SER:C	1:A:275:THR:HG23	2.27	0.55
1:A:806:ILE:HG23	1:A:806:ILE:O	2.06	0.54
1:A:860:LEU:HD12	1:A:860:LEU:N	2.22	0.54
1:A:931:ASN:O	1:A:932:TYR:HB2	2.07	0.54
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.88	0.54
3:C:83:ILE:HG23	3:C:84:GLU:N	2.22	0.54
1:A:873:GLU:O	1:A:874:CYS:HB3	2.07	0.54
1:A:634:ASP:HB3	1:A:637:ARG:HD3	1.90	0.54
3:C:198:PHE:HB3	3:C:199:PRO:CD	2.37	0.54
3:C:62:ILE:HG23	3:C:66:HIS:CE1	2.43	0.54
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.42	0.54
1:A:272:TYR:HB3	2:B:412:MET:HE3	1.89	0.54
1:A:489:ASP:HB3	1:A:492:CYS:HB2	1.89	0.54
1:A:453:HIS:HA	1:A:489:ASP:OD1	2.08	0.54
1:A:460:LEU:HD12	1:A:470:VAL:HG11	1.89	0.54
2:B:465:LEU:O	2:B:467:ARG:HG3	2.08	0.54
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.72	0.53
3:C:119:ARG:O	3:C:122:THR:HG22	2.07	0.53
3:C:198:PHE:CE1	3:C:203:LEU:HB3	2.43	0.53
1:A:856:SER:O	1:A:859:GLU:HG2	2.07	0.53
1:A:146:LYS:O	1:A:150:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASP:O	1:A:338:MET:HB2	2.08	0.53
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.44	0.53
1:A:936:GLU:HG2	1:A:937:GLY:N	2.23	0.53
1:A:351:ALA:HB1	1:A:1045:TYR:OH	2.09	0.53
1:A:170:ALA:O	1:A:174:VAL:HG23	2.09	0.53
1:A:687:LEU:HD23	1:A:692:ILE:O	2.09	0.53
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.09	0.52
1:A:191:ILE:HG23	1:A:580:GLN:O	2.09	0.52
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.73	0.52
1:A:419:LEU:HD11	1:A:471:THR:HA	1.91	0.52
1:A:432:PRO:HD3	1:A:632:MET:CE	2.38	0.52
1:A:1101:TYR:HB3	1:A:1107:MET:HG3	1.91	0.52
2:B:19:CYS:O	2:B:20:HIS:HB2	2.08	0.52
2:B:292:LEU:HD11	2:B:348:ARG:HG2	1.90	0.52
1:A:601:PRO:HG3	1:A:850:LEU:HD22	1.92	0.52
1:A:662:GLY:HA2	1:A:704:ASN:ND2	2.25	0.52
3:C:20:PHE:CD2	3:C:21:LEU:HD23	2.45	0.52
1:A:190:PRO:HD2	1:A:713:ARG:O	2.08	0.52
3:C:198:PHE:HB3	3:C:199:PRO:HD3	1.91	0.52
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.90	0.52
1:A:447:LEU:O	1:A:448:GLU:HG2	2.08	0.52
1:A:626:GLU:HA	1:A:629:LEU:HD23	1.92	0.52
1:A:1230:ILE:N	1:A:1230:ILE:HD12	2.24	0.52
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.92	0.52
1:A:119:LYS:O	1:A:123:GLU:HG3	2.10	0.51
1:A:724:HIS:NE2	1:A:1167:ARG:NH1	2.57	0.51
3:C:70:MET:O	3:C:71:LEU:HD23	2.09	0.51
1:A:239:GLU:HG2	1:A:1022:TYR:HB3	1.92	0.51
2:B:40:TRP:O	2:B:41:PHE:C	2.48	0.51
1:A:360:LEU:HD22	1:A:360:LEU:H	1.75	0.51
1:A:387:ASN:HD22	1:A:405:ARG:HB2	1.72	0.51
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.91	0.51
1:A:552:MET:HE2	1:A:555:ARG:HD3	1.93	0.51
2:B:12:ASN:HA	2:B:356:VAL:HB	1.93	0.51
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.76	0.51
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.92	0.51
1:A:445:VAL:HG23	1:A:510:ILE:HD11	1.93	0.51
1:A:1088:PHE:HB2	1:A:1222:VAL:HG22	1.93	0.51
3:C:56:HIS:HA	3:C:59:ILE:HG22	1.92	0.51
1:A:517:GLN:HA	1:A:517:GLN:NE2	2.26	0.50
2:B:94:LEU:HD22	2:B:221:ARG:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG22	1:A:70:TRP:HE3	1.77	0.50
1:A:582:LYS:HD3	1:A:801:ASP:HA	1.93	0.50
2:B:57:GLU:OE2	2:B:344:HIS:NE2	2.41	0.50
1:A:191:ILE:O	1:A:194:MET:HG2	2.11	0.50
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.47	0.50
2:B:160:ASN:OD1	2:B:393:LEU:HD13	2.11	0.50
1:A:361:VAL:HA	1:A:463:ALA:CB	2.41	0.50
1:A:906:MET:CE	1:A:911:ASN:HB2	2.42	0.50
2:B:275:TYR:HB2	2:B:299:VAL:HG12	1.94	0.50
2:B:306:PRO:O	2:B:310:GLU:HG3	2.12	0.50
1:A:1059:LEU:HD23	1:A:1059:LEU:N	2.27	0.50
2:B:228:PRO:HG2	2:B:229:TYR:CD1	2.47	0.49
1:A:551:ASP:OD2	1:A:1196:HIS:NE2	2.38	0.49
1:A:45:VAL:HG21	1:A:812:ALA:HA	1.94	0.49
3:C:183:ILE:HG23	3:C:184:PHE:N	2.27	0.49
3:C:56:HIS:O	3:C:59:ILE:HG22	2.13	0.49
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.43	0.49
2:B:415:TYR:CE2	2:B:437:GLU:HG2	2.47	0.49
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.48	0.49
1:A:729:LYS:HB2	1:A:736:HIS:CG	2.48	0.49
3:C:83:ILE:HG23	3:C:84:GLU:H	1.78	0.49
1:A:157:PHE:CZ	1:A:785:ILE:HD11	2.48	0.48
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.95	0.48
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.48	0.48
1:A:1098:HIS:C	1:A:1164:ALA:CB	2.82	0.48
3:C:13:PRO:HB3	3:C:192:MET:SD	2.52	0.48
1:A:168:LEU:HD23	1:A:168:LEU:C	2.34	0.48
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.82	0.48
1:A:28:ASN:HA	3:C:225:HIS:CD2	2.48	0.48
1:A:69:THR:HG22	1:A:70:TRP:CE3	2.49	0.48
1:A:263:ASP:OD2	1:A:802:MET:HG3	2.13	0.48
3:C:2:GLN:O	3:C:6:MET:HG3	2.12	0.48
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.34	0.48
1:A:1167:ARG:HB2	1:A:1183:ILE:CG2	2.44	0.48
1:A:196:MET:HE1	1:A:799:THR:HG23	1.96	0.47
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.95	0.47
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.49	0.47
1:A:225:PRO:C	1:A:228:PRO:HD2	2.34	0.47
1:A:476:LEU:N	1:A:476:LEU:HD12	2.29	0.47
1:A:308:ALA:O	1:A:311:HIS:HB3	2.14	0.47
1:A:761:LEU:O	1:A:764:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.49	0.47
2:B:157:LYS:HB3	2:B:157:LYS:HZ3	1.79	0.47
3:C:89:MET:O	3:C:93:ALA:N	2.47	0.47
1:A:55:GLY:HA3	6:A:1801:SF4:S3	2.54	0.47
1:A:372:TRP:NE1	1:A:860:LEU:HB3	2.30	0.47
1:A:487:LEU:N	1:A:487:LEU:CD1	2.77	0.47
1:A:707:ARG:C	1:A:708:ASN:HD22	2.18	0.47
4:A:1800:MD1:H7	4:A:1800:MD1:H11	1.95	0.47
2:B:183:LEU:HD23	2:B:183:LEU:N	2.30	0.47
1:A:419:LEU:CD1	1:A:471:THR:HA	2.44	0.47
1:A:372:TRP:CE2	1:A:863:PRO:HB3	2.50	0.47
1:A:214:LEU:HB3	1:A:607:SER:OG	2.15	0.46
1:A:515:ARG:HG2	1:A:516:SER:N	2.29	0.46
2:B:370:GLU:OE2	2:B:370:GLU:HA	2.14	0.46
2:B:508:THR:O	2:B:509:GLU:HB3	2.15	0.46
3:C:11:ILE:C	3:C:13:PRO:HD2	2.35	0.46
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.50	0.46
1:A:384:VAL:CG2	1:A:385:ALA:N	2.78	0.46
1:A:61:ILE:N	1:A:61:ILE:CD1	2.78	0.46
1:A:323:SER:HB3	1:A:326:PHE:HB2	1.98	0.46
1:A:405:ARG:HH12	1:A:412:GLU:HG3	1.80	0.46
1:A:517:GLN:HA	1:A:517:GLN:HE21	1.80	0.46
2:B:220:TRP:C	2:B:221:ARG:HG3	2.35	0.46
1:A:677:MET:HG3	1:A:682:TYR:HB2	1.97	0.46
1:A:220:TYR:CE2	4:A:1800:MD1:H101	2.51	0.46
1:A:473:VAL:HG13	1:A:1045:TYR:HB2	1.96	0.46
1:A:679:PRO:HB2	1:A:847:ILE:HD11	1.96	0.46
1:A:876:LEU:C	1:A:876:LEU:HD23	2.34	0.46
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.51	0.46
1:A:991:ASP:CG	1:A:991:ASP:O	2.54	0.46
1:A:173:ASN:O	1:A:177:ILE:HG13	2.15	0.46
1:A:1097:ILE:O	1:A:1098:HIS:HB2	2.16	0.46
1:A:215:SER:OG	1:A:606:ASN:HA	2.16	0.46
1:A:795:ASP:HA	1:A:809:LEU:O	2.16	0.46
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.31	0.46
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.30	0.46
1:A:232:GLY:HA2	1:A:1210:TYR:OH	2.17	0.46
1:A:1051:MET:HG2	1:A:1198:ILE:CD1	2.46	0.46
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.51	0.45
1:A:1041:ARG:HG2	1:A:1041:ARG:HH21	1.80	0.45
2:B:492:ASN:N	2:B:492:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.97	0.45
1:A:1098:HIS:HE1	4:A:2800:MD1:S13	2.39	0.45
1:A:120:MET:O	1:A:138:ILE:HD11	2.16	0.45
1:A:27:THR:CG2	1:A:28:ASN:N	2.79	0.45
1:A:261:THR:HB	1:A:262:PRO:CD	2.46	0.45
1:A:472:THR:O	1:A:476:LEU:HD13	2.16	0.45
1:A:651:ARG:NH1	1:A:870:LYS:HD3	2.32	0.45
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.51	0.45
2:B:311:GLN:NE2	2:B:314:LYS:HE2	2.32	0.45
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.45
3:C:211:VAL:HG23	3:C:212:GLU:N	2.32	0.45
1:A:641:HIS:ND1	1:A:642:LEU:N	2.65	0.45
1:A:928:ARG:CG	1:A:943:PRO:HG3	2.41	0.45
3:C:177:LEU:O	3:C:178:ASP:C	2.55	0.45
1:A:91:GLY:HA2	6:A:1801:SF4:S4	2.57	0.44
1:A:644:ASP:OD1	1:A:752:GLU:HG2	2.17	0.44
1:A:774:ARG:HH11	4:A:1800:MD1:C3'	2.29	0.44
3:C:15:ILE:O	3:C:19:VAL:HG23	2.17	0.44
1:A:1092:HIS:HA	1:A:1163:HIS:HB3	1.98	0.44
2:B:395:THR:HG21	2:B:401:PRO:CG	2.44	0.44
3:C:198:PHE:HE2	3:C:207:TRP:NE1	2.15	0.44
1:A:90:ARG:HG2	1:A:90:ARG:HH11	1.81	0.44
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.47	0.44
1:A:513:VAL:O	1:A:514:SER:C	2.53	0.44
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.38	0.44
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.31	0.44
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.18	0.44
2:B:101:TYR:CD2	2:B:142:PRO:HD3	2.53	0.44
1:A:6:ARG:HG2	1:A:6:ARG:HH21	1.83	0.44
1:A:139:ILE:HD12	1:A:139:ILE:HA	1.81	0.44
1:A:182:PRO:HD2	1:A:665:PRO:HG2	2.00	0.44
1:A:316:GLU:HG3	1:A:496:TYR:OH	2.18	0.44
1:A:81:ARG:NH2	1:A:84:LEU:HD11	2.32	0.43
1:A:338:MET:HE1	1:A:386:PRO:CG	2.48	0.43
1:A:582:LYS:HB2	1:A:801:ASP:OD2	2.18	0.43
1:A:611:PHE:O	1:A:615:SER:HB3	2.19	0.43
1:A:364:LEU:HD13	1:A:385:ALA:HB2	2.00	0.43
1:A:688:LYS:HE3	1:A:876:LEU:HB3	2.00	0.43
1:A:220:TYR:CE1	1:A:720:SER:HB2	2.54	0.43
1:A:629:LEU:HD13	1:A:629:LEU:HA	1.86	0.43
1:A:743:LEU:HD13	1:A:743:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:GLN:NE2	3:C:151:MET:HA	2.33	0.43
1:A:401:ASN:CG	1:A:403:GLU:HG3	2.39	0.43
1:A:914:LYS:O	1:A:914:LYS:HG2	2.18	0.43
1:A:1132:ASN:ND2	2:B:137:LYS:HE3	2.33	0.43
2:B:195:THR:O	2:B:197:PRO:HD3	2.19	0.43
3:C:115:SER:HA	3:C:116:PRO:HD2	1.83	0.43
1:A:272:TYR:HB3	2:B:412:MET:HE1	1.98	0.43
1:A:353:ARG:NE	1:A:864:LEU:HD12	2.33	0.43
1:A:362:ASP:O	1:A:363:ALA:HB3	2.18	0.43
1:A:393:ARG:NH1	1:A:855:ASP:HA	2.33	0.43
1:A:403:GLU:HG2	1:A:1032:LEU:HD23	1.99	0.43
1:A:199:TYR:CE1	1:A:589:TRP:HZ2	2.36	0.43
1:A:1144:LEU:HD22	1:A:1184:HIS:HA	2.00	0.43
1:A:199:TYR:CD1	1:A:589:TRP:HZ2	2.36	0.43
1:A:393:ARG:HH12	1:A:855:ASP:HA	1.84	0.43
1:A:548:TYR:HE2	1:A:1191:THR:HG22	1.82	0.43
2:B:400:LYS:HB3	2:B:401:PRO:HD3	2.01	0.43
1:A:379:THR:HG21	1:A:414:GLU:CD	2.39	0.43
1:A:499:VAL:O	1:A:499:VAL:HG12	2.19	0.43
1:A:532:THR:OG1	1:A:535:ARG:HB2	2.19	0.43
1:A:1041:ARG:HG2	1:A:1041:ARG:NH2	2.33	0.43
2:B:157:LYS:NZ	2:B:157:LYS:CB	2.81	0.43
1:A:590:GLN:N	1:A:591:PRO:HD2	2.34	0.42
1:A:611:PHE:O	1:A:615:SER:CB	2.67	0.42
3:C:208:SER:O	3:C:209:VAL:C	2.58	0.42
1:A:1233:LEU:HB3	2:B:120:SER:OG	2.19	0.42
2:B:263:CYS:SG	2:B:267:ILE:HG12	2.59	0.42
1:A:220:TYR:CE1	1:A:720:SER:CB	3.02	0.42
1:A:626:GLU:O	1:A:629:LEU:HB2	2.19	0.42
2:B:224:ILE:HD11	2:B:234:PHE:HB2	2.01	0.42
1:A:161:SER:O	1:A:165:VAL:HG22	2.18	0.42
1:A:529:ALA:CB	1:A:564:CYS:HB3	2.49	0.42
2:B:156:ALA:HB1	2:B:166:LYS:HD2	2.00	0.42
2:B:463:ARG:O	2:B:467:ARG:HD3	2.19	0.42
1:A:167:GLU:HG3	1:A:832:LYS:CE	2.50	0.42
1:A:683:THR:CG2	1:A:885:ILE:HD13	2.49	0.42
2:B:36:VAL:HG13	2:B:235:ASN:ND2	2.34	0.42
1:A:375:VAL:HG12	1:A:376:ALA:N	2.34	0.42
1:A:612:TYR:CE1	1:A:1192:PRO:HG3	2.55	0.42
1:A:852:ILE:HD12	1:A:852:ILE:H	1.83	0.42
1:A:331:ARG:NH1	1:A:415:LEU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ARG:HH11	1:A:459:ARG:HG3	1.85	0.42
2:B:188:LEU:HB2	2:B:350:LEU:HB2	2.02	0.42
1:A:192:PRO:HB2	1:A:583:LEU:HD12	2.01	0.42
1:A:329:TYR:CZ	1:A:565:GLY:HA2	2.55	0.42
1:A:920:THR:O	1:A:920:THR:HG23	2.20	0.42
3:C:18:ALA:O	3:C:22:ILE:HG22	2.19	0.42
2:B:231:LYS:HE2	2:B:231:LYS:HA	2.01	0.41
2:B:295:ARG:CG	2:B:295:ARG:HH21	2.32	0.41
3:C:12:TYR:N	3:C:13:PRO:CD	2.82	0.41
1:A:192:PRO:HG2	1:A:583:LEU:HD12	2.02	0.41
1:A:729:LYS:HB2	1:A:736:HIS:CD2	2.55	0.41
1:A:774:ARG:NH2	1:A:1103:ASP:OD1	2.52	0.41
1:A:1232:TRP:O	1:A:1233:LEU:HB2	2.19	0.41
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.85	0.41
2:B:224:ILE:CD1	2:B:234:PHE:HB2	2.49	0.41
3:C:88:LYS:O	3:C:92:PHE:HD1	2.02	0.41
2:B:100:TYR:O	2:B:101:TYR:HB3	2.20	0.41
1:A:600:ARG:HA	1:A:601:PRO:HA	1.88	0.41
3:C:89:MET:O	3:C:93:ALA:HB3	2.19	0.41
1:A:336:MET:N	1:A:337:PRO:HD2	2.35	0.41
1:A:338:MET:HE1	1:A:386:PRO:HG3	2.02	0.41
1:A:167:GLU:HG3	1:A:832:LYS:HE2	2.03	0.41
1:A:532:THR:O	1:A:533:HIS:HB2	2.20	0.41
2:B:408:ARG:O	2:B:411:ALA:HB3	2.21	0.41
1:A:677:MET:CE	1:A:682:TYR:HA	2.51	0.41
1:A:695:ALA:HB1	1:A:704:ASN:HB3	2.02	0.41
1:A:808:PRO:HG3	1:A:1000:GLN:HA	2.01	0.41
1:A:1101:TYR:O	1:A:1104:ASN:HB3	2.20	0.41
1:A:1117:VAL:HG23	1:A:1146:ALA:HB3	2.02	0.41
3:C:36:ARG:HG2	3:C:38:ALA:H	1.85	0.41
1:A:705:HIS:HD2	1:A:764:LYS:HB3	1.84	0.41
1:A:1046:GLN:HG3	1:A:1051:MET:CE	2.51	0.41
3:C:149:GLN:HB2	3:C:150:HIS:HD2	1.86	0.41
1:A:52:ASN:ND2	1:A:191:ILE:HG13	2.35	0.41
1:A:90:ARG:HG2	1:A:90:ARG:NH1	2.35	0.41
1:A:368:ASN:O	1:A:373:LYS:HE3	2.21	0.41
2:B:13:LEU:HB2	2:B:356:VAL:O	2.21	0.41
2:B:372:GLY:HA3	2:B:379:ASP:OD1	2.21	0.41
3:C:81:LEU:N	3:C:81:LEU:CD2	2.75	0.41
1:A:244:TYR:OH	2:B:448:ALA:HB1	2.21	0.41
1:A:578:VAL:CG2	1:A:579:GLY:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:TRP:CZ3	3:C:188:LEU:HD13	2.56	0.41
1:A:111:PRO:HA	1:A:787:PRO:HD3	2.03	0.40
1:A:237:VAL:HG11	1:A:576:HIS:H	1.86	0.40
1:A:604:HIS:HB3	1:A:1208:PHE:CD2	2.56	0.40
1:A:1096:GLY:HA2	1:A:1101:TYR:HB2	2.03	0.40
1:A:1144:LEU:CD2	1:A:1184:HIS:HA	2.51	0.40
2:B:97:ILE:HG23	2:B:98:ASP:N	2.36	0.40
1:A:38:ARG:HD2	1:A:38:ARG:O	2.21	0.40
1:A:397:LYS:HE3	1:A:977:PHE:CE1	2.56	0.40
1:A:445:VAL:HG23	1:A:510:ILE:CD1	2.50	0.40
1:A:583:LEU:HD23	1:A:585:PRO:HD2	2.03	0.40
1:A:995:ARG:HA	1:A:995:ARG:HD3	1.89	0.40
1:A:1173:GLY:HA3	1:A:1233:LEU:HD22	2.01	0.40
1:A:1234:ASP:OD1	1:A:1236:GLU:HB2	2.21	0.40
2:B:152:PHE:CE2	2:B:170:SER:HB3	2.57	0.40
3:C:82:PRO:HG2	3:C:85:VAL:CG2	2.50	0.40
1:A:1167:ARG:HG2	1:A:1167:ARG:O	2.21	0.40
3:C:98:GLY:HA3	3:C:141:LEU:HD21	2.03	0.40
1:A:281:THR:O	1:A:296:ALA:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1242/1246 (100%)	1127 (91%)	97 (8%)	18 (1%)	11	20
2	B	507/512 (99%)	483 (95%)	23 (4%)	1 (0%)	47	68
3	C	213/225 (95%)	193 (91%)	18 (8%)	2 (1%)	17	31
All	All	1962/1983 (99%)	1803 (92%)	138 (7%)	21 (1%)	14	26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	1166	GLU
1	A	195	SER
1	A	320	ASP
1	A	501	ALA
1	A	586	GLN
1	A	578	VAL
1	A	718	GLY
1	A	855	ASP
1	A	861	ALA
1	A	874	CYS
1	A	9	TYR
1	A	191	ILE
1	A	1036	ARG
2	B	101	TYR
1	A	224	PRO
1	A	721	GLY
3	C	180	VAL
1	A	390	ILE
1	A	808	PRO
3	C	210	PRO

5.3.2 Protein sidechains (i)

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	1039/1043 (100%)	1010 (97%)	29 (3%)	43	70
2	B	436/439 (99%)	423 (97%)	13 (3%)	41	68
3	C	178/185 (96%)	174 (98%)	4 (2%)	52	77
All	All	1653/1667 (99%)	1607 (97%)	46 (3%)	43	70

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	94	ARG

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Mol	Chain	Res	Type
1	A	319	LEU
1	A	338	MET
1	A	452	LEU
1	A	461	GLN
1	A	514	SER
1	A	515	ARG
1	A	533	HIS
1	A	581	GLU
1	A	600	ARG
1	A	629	LEU
1	A	728	LEU
1	A	743	LEU
1	A	767	LEU
1	A	808	PRO
1	A	814	ASP
1	A	837	CYS
1	A	849	THR
1	A	926	LEU
1	A	936	GLU
1	A	944	MET
1	A	1041	ARG
1	A	1062	ARG
1	A	1087	ASN
1	A	1110	LEU
1	A	1126	ASP
1	A	1233	LEU
1	A	1243	GLU
2	B	37	GLU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU
2	B	119	LYS
2	B	135	MET
2	B	161	PHE
2	B	183	LEU
2	B	221	ARG
2	B	244	CYS
2	B	295	ARG
2	B	358	PRO
2	B	492	ASN
3	C	36	ARG
3	C	81	LEU

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Mol	Chain	Res	Type
3	C	129	ILE
3	C	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	37	GLN
1	A	173	ASN
1	A	234	GLN
1	A	245	ASN
1	A	258	GLN
1	A	311	HIS
1	A	369	ASN
1	A	387	ASN
1	A	461	GLN
1	A	517	GLN
1	A	599	GLN
1	A	704	ASN
1	A	705	HIS
1	A	708	ASN
1	A	946	ASN
1	A	1049	GLN
1	A	1076	GLN
1	A	1082	GLN
1	A	1087	ASN
1	A	1098	HIS
1	A	1163	HIS
2	B	20	HIS
2	B	110	ASN
2	B	143	ASN
2	B	160	ASN
2	B	311	GLN
2	B	414	HIS
2	B	451	ASN
3	C	149	GLN
3	C	164	GLN
3	C	175	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1.58	3 (37%)	7,9,11	1.61	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	-	6/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-3.26	1.47	1.53
3	C	1	FME	CB-CG	2.15	1.59	1.51
3	C	1	FME	CA-N	-2.06	1.43	1.46

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	3.16	127.69	122.82

There are no chirality outliers.

All (6) 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	C-CA-CB-CG
3	C	1	FME	O-C-CA-CB
3	C	1	FME	CA-CB-CG-SD
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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\#\|Z\| > 2$
9	HEM	C	807	3	41,50,50	1.99	14 (34%)	45,82,82	1.40	9 (20%)
8	3PH	B	1806	-	17,17,47	0.97	1 (5%)	19,21,52	1.94	4 (21%)
4	MD1	A	2800	5	39,51,51	3.47	9 (23%)	38,78,78	2.29	14 (36%)
7	F3S	B	1805	2	0,9,9	-	-	-		
6	SF4	B	1803	2	0,12,12	-	-	-		
6	SF4	A	1801	1	0,12,12	-	-	-		
4	MD1	A	1800	5	39,51,51	3.64	9 (23%)	38,78,78	2.36	11 (28%)
6	SF4	B	1802	2	0,12,12	-	-	-		
9	HEM	C	806	3	41,50,50	1.96	15 (36%)	45,82,82	1.36	7 (15%)
6	SF4	B	1804	2	0,12,12	-	-	-		
10	AGA	C	309	-	29,29,29	0.80	1 (3%)	32,35,35	1.57	3 (9%)
11	PCI	C	808	-	12,12,12	9.50	11 (91%)	18,18,18	1.15	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	C	807	3	-	6/12/54/54	-
8	3PH	B	1806	-	1/1/3/4	5/18/18/49	-
4	MD1	A	2800	5	-	2/18/59/59	0/5/5/5
7	F3S	B	1805	2	-	-	0/3/3/3
6	SF4	B	1803	2	-	-	0/6/5/5
6	SF4	A	1801	1	-	-	0/6/5/5
4	MD1	A	1800	5	-	6/18/59/59	0/5/5/5
6	SF4	B	1802	2	-	-	0/6/5/5
9	HEM	C	806	3	-	4/12/54/54	-
6	SF4	B	1804	2	-	-	0/6/5/5
10	AGA	C	309	-	-	12/34/34/34	-
11	PCI	C	808	-	-	-	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	MD1	C7-N8	19.22	1.50	1.27
4	A	2800	MD1	C7-N8	17.74	1.48	1.27
11	C	808	PCI	C2-CL1	-15.18	1.40	1.72
11	C	808	PCI	C6-CL5	-14.56	1.41	1.72
11	C	808	PCI	C5-CL4	-13.93	1.42	1.72
11	C	808	PCI	C4-CL3	-13.64	1.43	1.72
11	C	808	PCI	C3-CL2	-13.44	1.43	1.72
4	A	2800	MD1	C6-N1	5.90	1.43	1.33
4	A	1800	MD1	C15-N17	5.74	1.43	1.33
4	A	2800	MD1	C15-N17	5.36	1.42	1.33
4	A	1800	MD1	C6-N1	4.82	1.41	1.33
9	C	806	HEM	C3C-CAC	4.51	1.57	1.47
9	C	807	HEM	CAB-C3B	4.38	1.59	1.47
9	C	806	HEM	CAB-C3B	4.35	1.59	1.47
9	C	807	HEM	C3C-CAC	4.17	1.56	1.47
11	C	808	PCI	C5-C4	4.11	1.49	1.39
4	A	2800	MD1	C16-C15	4.10	1.47	1.41
11	C	808	PCI	C4-C3	3.99	1.48	1.39
4	A	1800	MD1	C17-N17	3.90	1.42	1.35
4	A	1800	MD1	C20-N18	3.88	1.40	1.34
9	C	806	HEM	C3C-C2C	-3.87	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	807	HEM	CAA-C2A	3.74	1.57	1.52
11	C	808	PCI	C6-C5	3.70	1.48	1.39
11	C	808	PCI	C3-C2	3.64	1.48	1.39
4	A	2800	MD1	C20-N18	3.40	1.39	1.34
4	A	2800	MD1	C2-N1	3.19	1.41	1.35
4	A	1800	MD1	C4-N3	3.19	1.40	1.35
11	C	808	PCI	C1-C2	3.15	1.44	1.39
9	C	807	HEM	C3C-C2C	-3.11	1.36	1.40
4	A	2800	MD1	C17-N17	3.09	1.40	1.35
4	A	1800	MD1	C14-C13	3.08	1.54	1.51
9	C	806	HEM	CMB-C2B	2.92	1.57	1.50
11	C	808	PCI	C1-C6	2.89	1.44	1.39
9	C	807	HEM	CMB-C2B	2.86	1.56	1.50
9	C	807	HEM	CMD-C2D	2.85	1.56	1.50
4	A	1800	MD1	C2-N1	2.82	1.40	1.35
9	C	806	HEM	CMD-C2D	2.74	1.56	1.50
4	A	1800	MD1	C12-C13	2.69	1.42	1.34
9	C	807	HEM	CAD-C3D	2.60	1.58	1.51
9	C	806	HEM	CMA-C3A	2.60	1.57	1.51
9	C	806	HEM	CMC-C2C	2.59	1.57	1.51
9	C	807	HEM	CMC-C2C	2.49	1.57	1.51
9	C	807	HEM	CBA-CGA	2.37	1.56	1.50
10	C	309	AGA	C8-C7	2.33	1.57	1.50
4	A	2800	MD1	C5-C6	2.32	1.45	1.41
9	C	807	HEM	C1D-C2D	2.28	1.49	1.44
9	C	807	HEM	CMA-C3A	2.26	1.56	1.51
9	C	806	HEM	CAD-C3D	2.24	1.57	1.51
9	C	806	HEM	O1D-CGD	2.20	1.29	1.22
9	C	806	HEM	CAA-C2A	2.18	1.55	1.52
9	C	806	HEM	C4D-ND	-2.18	1.36	1.40
9	C	806	HEM	C2C-C1C	2.16	1.47	1.42
9	C	806	HEM	C1B-C2B	2.12	1.48	1.44
9	C	807	HEM	C1B-C2B	2.11	1.48	1.44
9	C	807	HEM	CHB-C1B	2.08	1.40	1.35
9	C	807	HEM	O1D-CGD	2.08	1.29	1.22
8	B	1806	3PH	C32-C31	2.07	1.56	1.50
4	A	2800	MD1	O11-C11	2.07	1.47	1.42
9	C	806	HEM	C4D-C3D	2.04	1.48	1.45
9	C	806	HEM	CHA-C4D	2.04	1.40	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1800	MD1	C5-C6-N1	-6.15	115.02	123.43
10	C	309	AGA	C14-C13-C12	6.00	135.43	113.62
4	A	2800	MD1	N3-C2-N1	-5.88	119.37	127.22
4	A	1800	MD1	C2-N1-C6	5.67	124.93	115.93
4	A	2800	MD1	C5-C6-N1	-5.54	115.85	123.43
4	A	1800	MD1	C17-N17-C15	5.02	123.91	115.93
10	C	309	AGA	C9-C8-C7	4.93	131.55	113.62
8	B	1806	3PH	C3-C2-C1	4.69	122.87	111.79
8	B	1806	3PH	C33-C32-C31	4.65	130.53	113.62
4	A	2800	MD1	C2-N1-C6	4.64	123.30	115.93
4	A	1800	MD1	N18-C17-N17	-4.63	118.15	125.42
4	A	1800	MD1	N3-C2-N1	-4.60	121.09	127.22
9	C	806	HEM	C4B-CHC-C1C	4.59	128.62	122.56
9	C	807	HEM	C4B-CHC-C1C	4.54	128.56	122.56
4	A	2800	MD1	C17-N17-C15	4.35	122.84	115.93
11	C	808	PCI	C6-C1-C2	3.93	121.74	117.81
4	A	2800	MD1	C4-C5-C6	-3.93	117.04	120.80
4	A	1800	MD1	C4-C5-C6	-3.81	117.16	120.80
4	A	2800	MD1	N18-C17-N17	-3.62	119.75	125.42
8	B	1806	3PH	O21-C2-C3	3.48	121.01	108.40
9	C	807	HEM	CMA-C3A-C4A	-3.27	123.44	128.46
4	A	1800	MD1	N16-C17-N18	3.16	122.17	117.25
9	C	806	HEM	CMA-C3A-C4A	-3.00	123.86	128.46
4	A	2800	MD1	C16-C15-N17	-2.69	116.36	124.01
4	A	2800	MD1	C15-C16-N15	2.66	121.36	119.12
9	C	807	HEM	CAD-C3D-C4D	-2.66	120.01	124.66
4	A	1800	MD1	N2-C2-N3	2.64	122.09	117.79
9	C	807	HEM	CMA-C3A-C2A	2.60	129.84	124.94
4	A	1800	MD1	O3A-C10-C11	-2.59	100.46	107.94
9	C	806	HEM	CMA-C3A-C2A	2.55	129.75	124.94
10	C	309	AGA	C5-O9-C12	2.53	124.01	117.79
4	A	2800	MD1	PA-O3B-PB	2.51	141.46	132.83
4	A	2800	MD1	C2-N3-C4	2.47	118.18	115.36
9	C	806	HEM	CAD-C3D-C4D	-2.44	120.39	124.66
4	A	1800	MD1	C16-C15-N17	-2.43	117.09	124.01
4	A	1800	MD1	C15-C16-N15	2.38	121.12	119.12
4	A	2800	MD1	N2-C2-N1	2.36	120.93	117.25
4	A	2800	MD1	N16-C17-N17	2.28	120.79	117.25
9	C	806	HEM	O2D-CGD-O1D	2.27	128.97	123.30
9	C	807	HEM	CAD-C3D-C2D	2.26	132.08	127.88
9	C	806	HEM	O1D-CGD-CBD	-2.19	116.05	123.08
8	B	1806	3PH	O21-C2-C1	2.13	116.11	108.40
4	A	2800	MD1	C1'-N9-C4	-2.11	122.93	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	807	HEM	CMC-C2C-C3C	2.10	128.61	124.68
9	C	807	HEM	O2D-CGD-O1D	2.08	128.49	123.30
9	C	807	HEM	O1D-CGD-CBD	-2.07	116.44	123.08
4	A	2800	MD1	N18-C20-N8	2.02	120.86	116.00
9	C	806	HEM	CAD-C3D-C2D	2.01	131.62	127.88
9	C	807	HEM	C4C-CHD-C1D	2.00	125.20	122.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	1806	3PH	C2

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1800	MD1	C5'-O5'-PA-O2A
8	B	1806	3PH	O22-C21-O21-C2
10	C	309	AGA	O1-C1-C2-C3
10	C	309	AGA	C3-O5-P1-O3
4	A	1800	MD1	O4'-C4'-C5'-O5'
4	A	1800	MD1	C3'-C4'-C5'-O5'
8	B	1806	3PH	C32-C31-O31-C3
8	B	1806	3PH	O32-C31-O31-C3
10	C	309	AGA	O2-C2-C3-O5
10	C	309	AGA	C3-O5-P1-O6
10	C	309	AGA	C1-C2-C3-O5
10	C	309	AGA	C13-C14-C15-C16
10	C	309	AGA	O1-C1-C2-O2
10	C	309	AGA	C8-C7-O7-C6
10	C	309	AGA	C12-C13-C14-C15
10	C	309	AGA	O8-C7-O7-C6
8	B	1806	3PH	C1-C2-C3-O31
8	B	1806	3PH	O11-C1-C2-O21
9	C	807	HEM	C2B-C3B-CAB-CBB
4	A	1800	MD1	PA-O3B-PB-O2B
4	A	2800	MD1	PA-O3B-PB-O2B
4	A	1800	MD1	C5'-O5'-PA-O1A
9	C	806	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAA-CBA-CGA-O1A
10	C	309	AGA	O6-C4-C5-C6
9	C	806	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
9	C	806	HEM	CAD-CBD-CGD-O2D
9	C	807	HEM	CAD-CBD-CGD-O2D
9	C	807	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAD-CBD-CGD-O1D
9	C	807	HEM	C4B-C3B-CAB-CBB
4	A	1800	MD1	C5'-O5'-PA-O3B
4	A	2800	MD1	O3A-C10-C11-O11
10	C	309	AGA	O7-C7-C8-C9

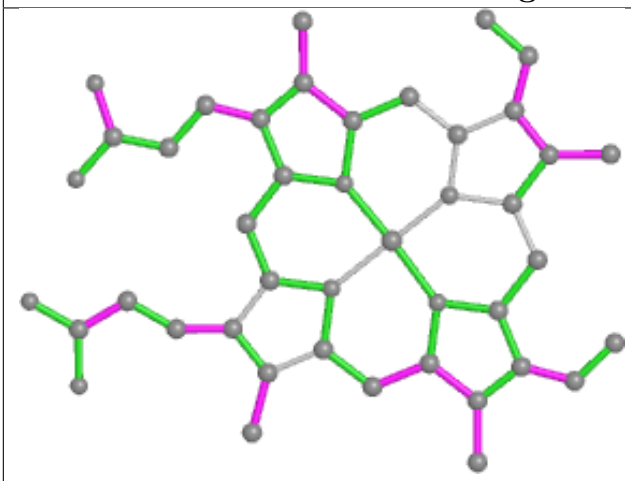
There are no ring outliers.

5 monomers are involved in 12 short contacts:

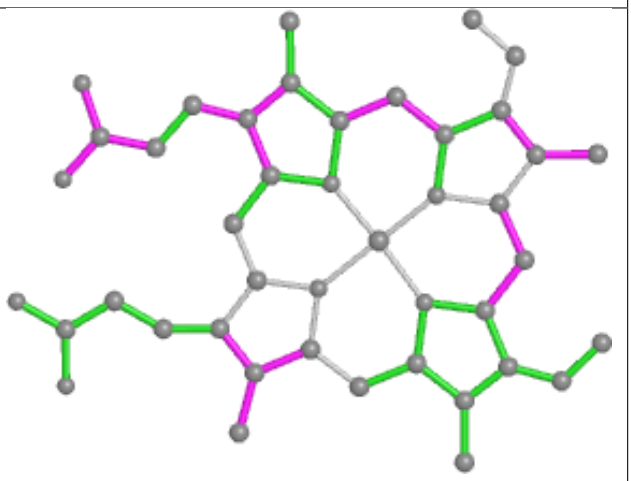
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2800	MD1	2	0
6	A	1801	SF4	2	0
4	A	1800	MD1	6	0
9	C	806	HEM	1	0
10	C	309	AGA	1	0

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 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.

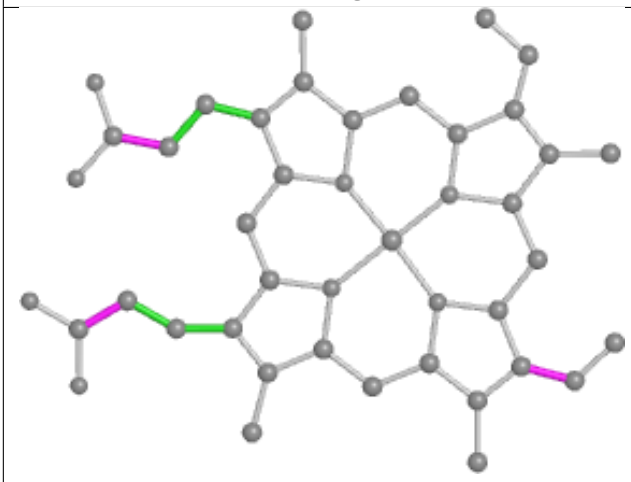
Ligand HEM C 807



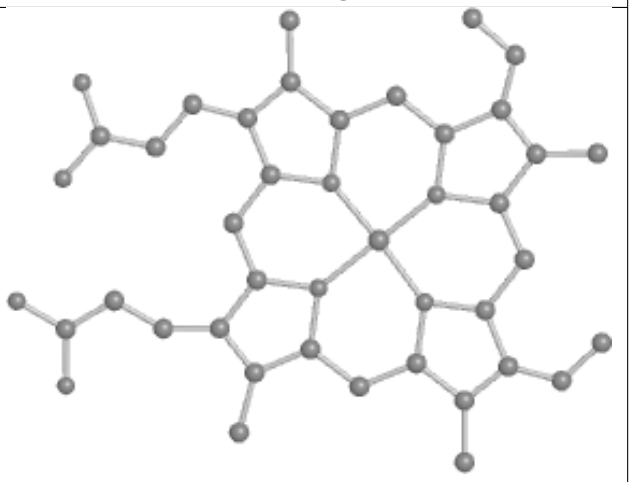
Bond lengths



Bond angles

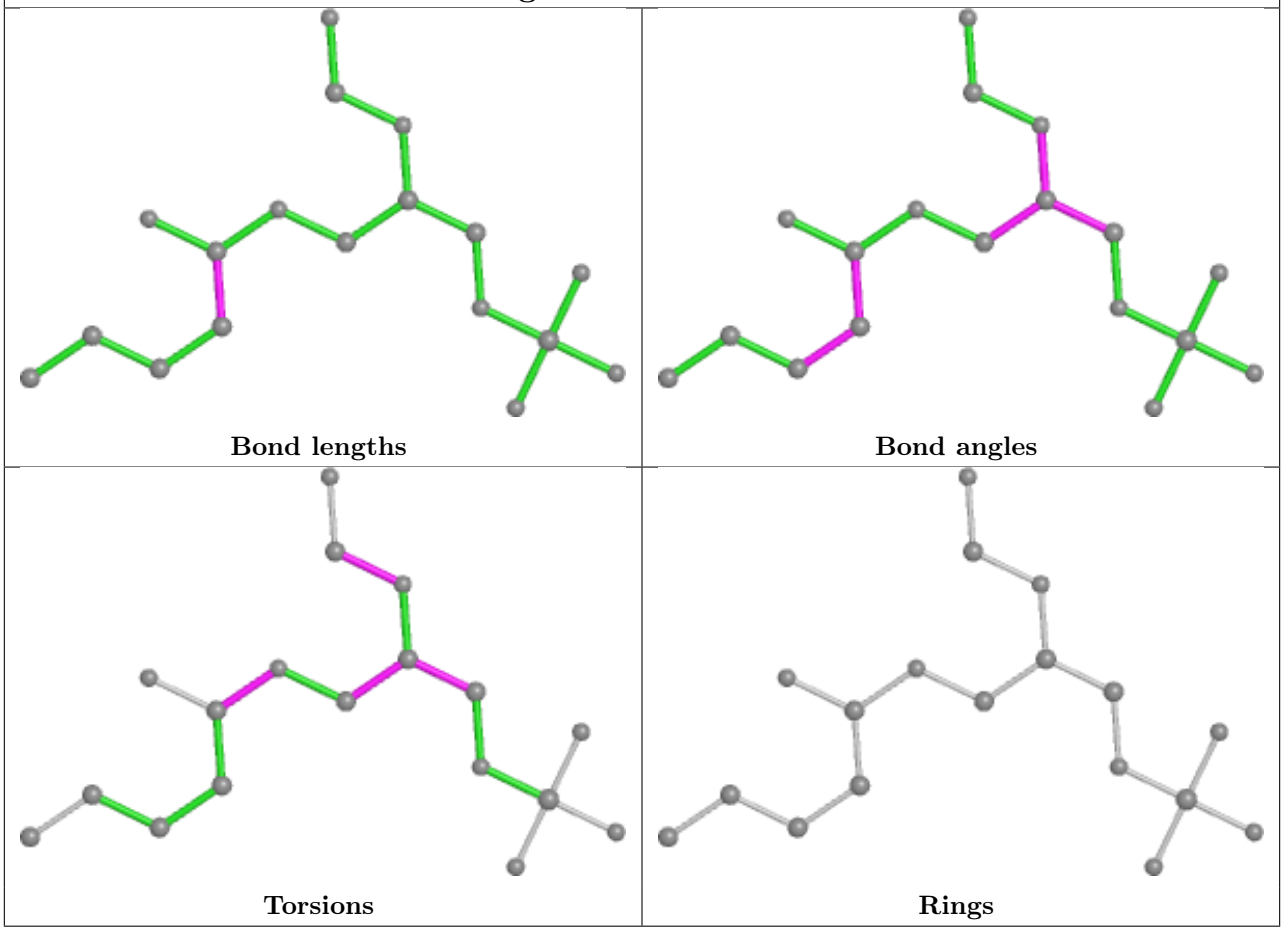


Torsions

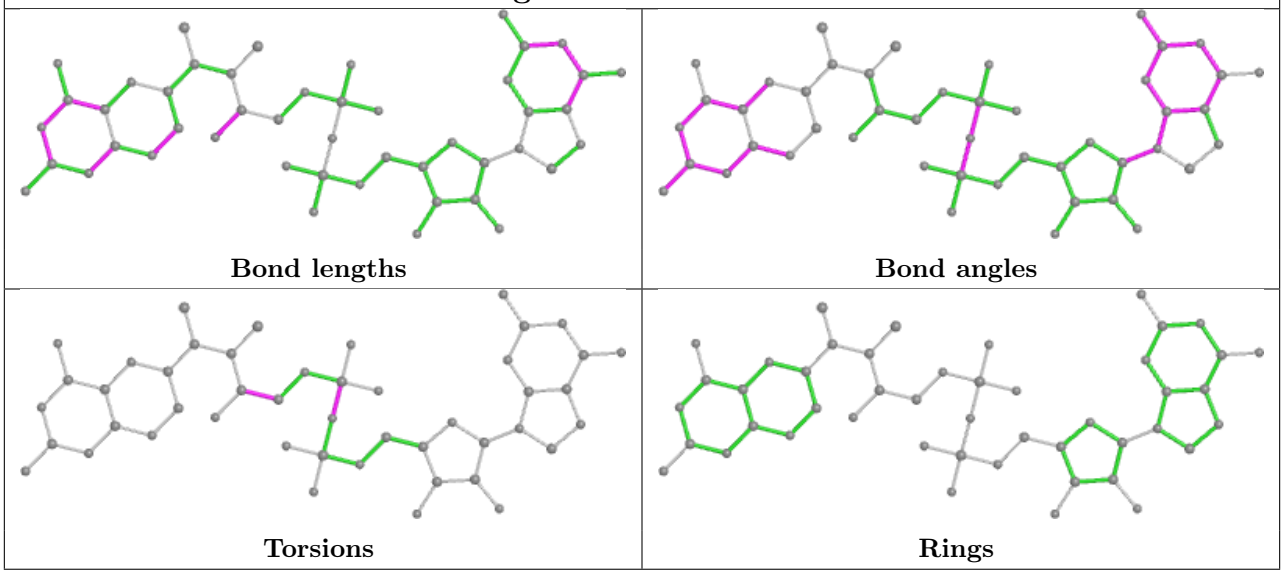


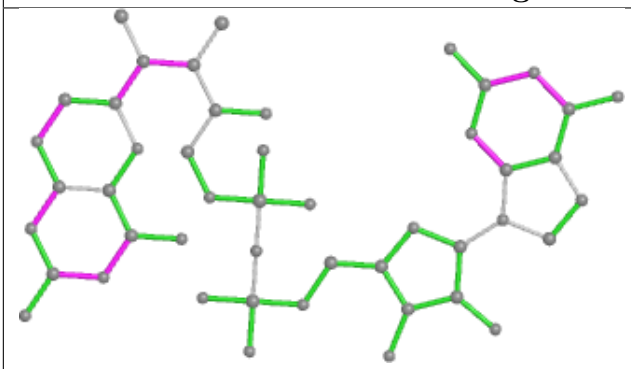
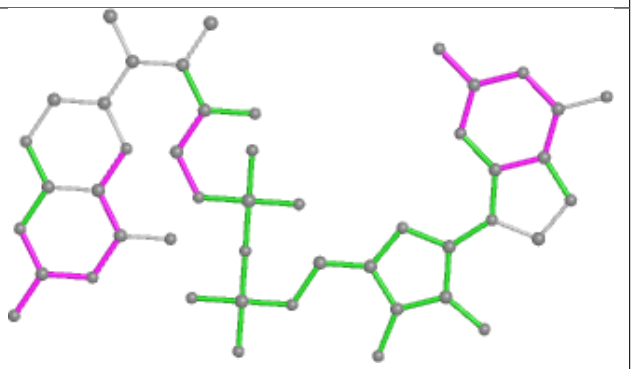
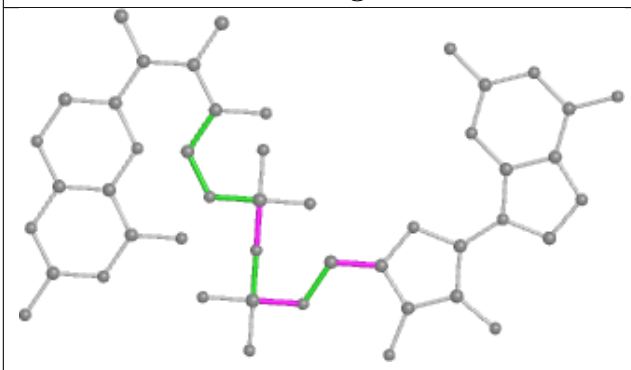
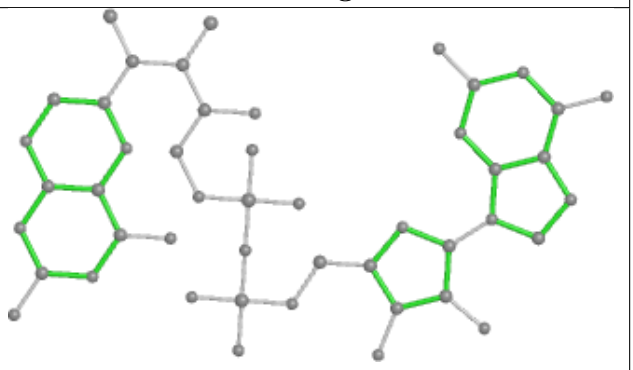
Rings

Ligand 3PH B 1806

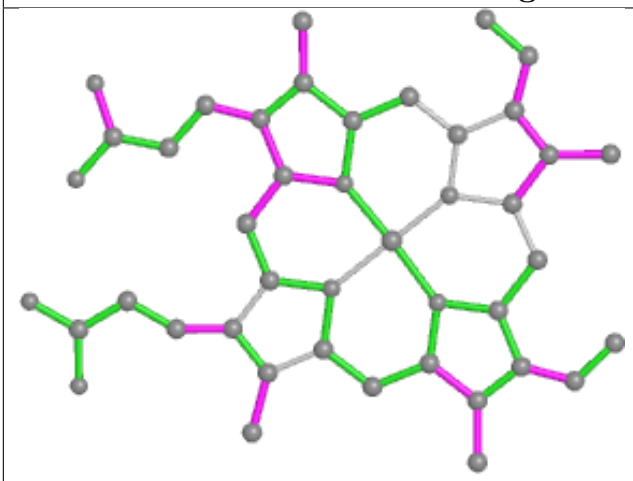


Ligand MD1 A 2800

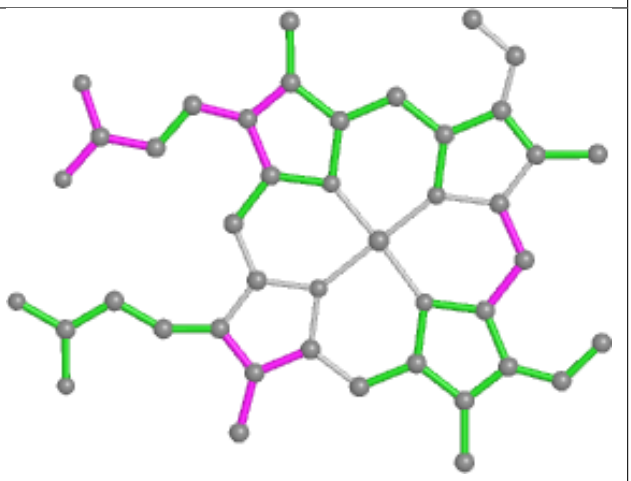


Ligand MD1 A 1800	
 Bond lengths	 Bond angles
 Torsions	 Rings

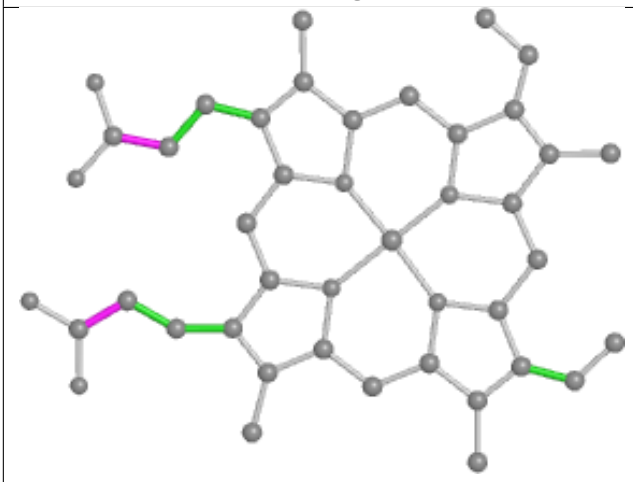
Ligand HEM C 806



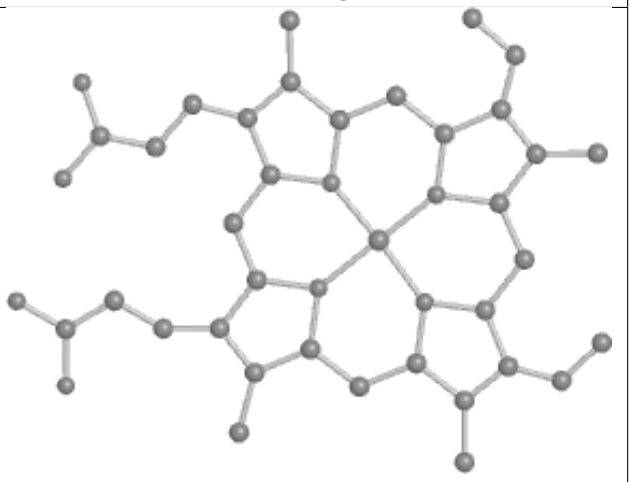
Bond lengths



Bond angles

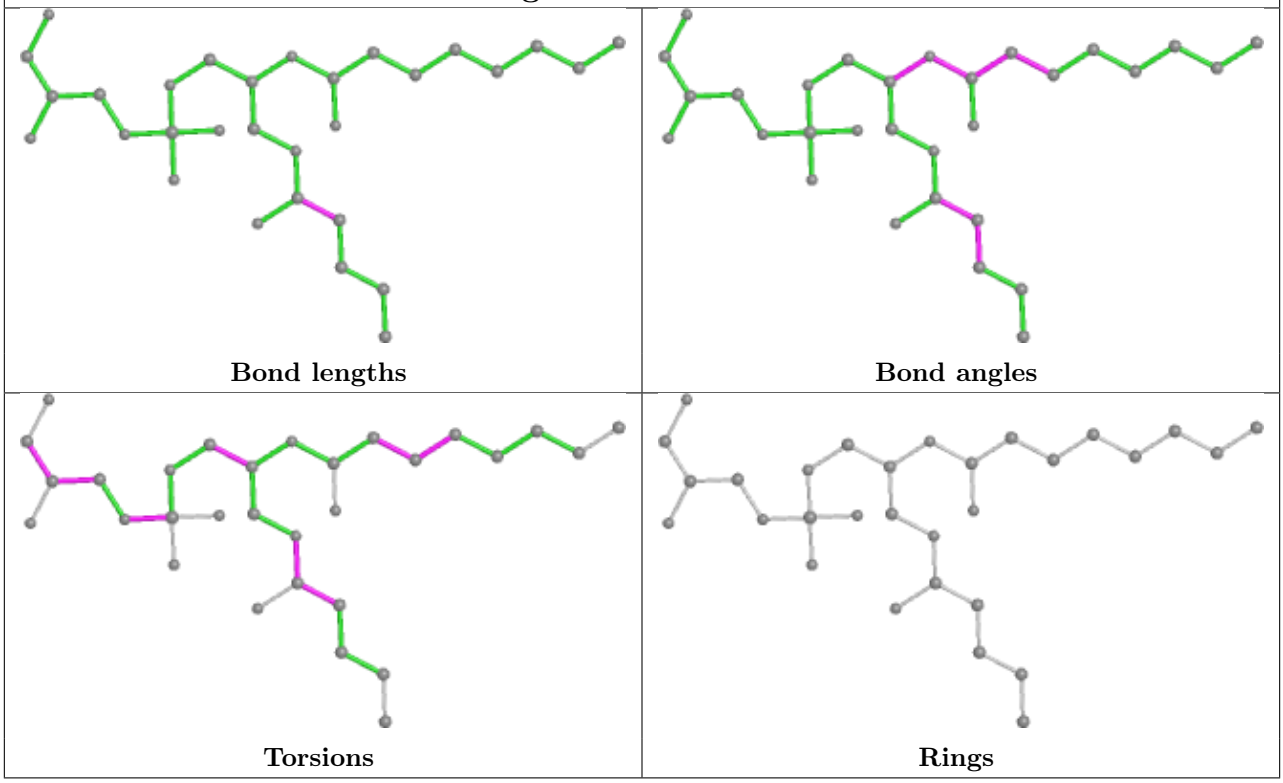


Torsions

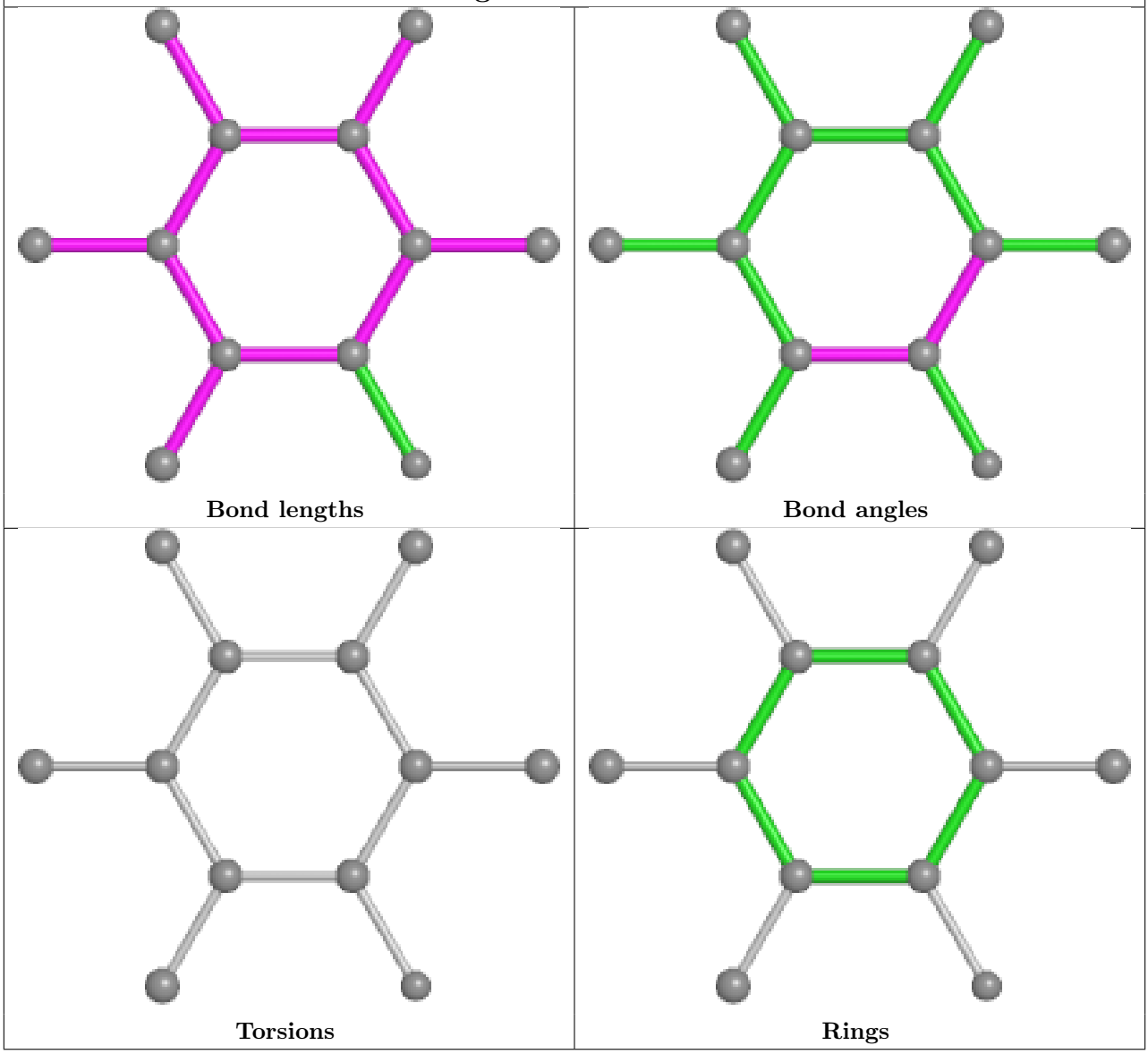


Rings

Ligand AGA C 309



Ligand PCI C 808



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	1244/1246 (99%)	-0.19	40 (3%)	47	51	25, 51, 80, 107	0
2	B	509/512 (99%)	-0.43	10 (1%)	65	68	23, 41, 66, 97	0
3	C	216/225 (96%)	-0.23	6 (2%)	53	56	32, 57, 83, 95	0
All	All	1969/1983 (99%)	-0.26	56 (2%)	53	56	23, 48, 78, 107	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	7.0
1	A	10	PHE	5.2
2	B	371	LEU	4.3
1	A	8	ARG	3.7
1	A	1244	SER	3.2
3	C	157	MET	3.2
1	A	421	GLY	3.1
1	A	11	LYS	3.0
2	B	70	ILE	3.0
1	A	1243	GLU	3.0
2	B	372	GLY	3.0
1	A	361	VAL	3.0
1	A	380	ASN	3.0
1	A	936	GLU	2.8
1	A	463	ALA	2.8
1	A	446	GLU	2.8
2	B	370	GLU	2.8
1	A	424	ASP	2.8
1	A	462	LEU	2.8
1	A	488	ASN	2.7
1	A	486	GLY	2.6
1	A	675	ALA	2.5
1	A	674	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	673	GLU	2.5
1	A	749	VAL	2.4
1	A	759	ASN	2.4
1	A	461	GLN	2.4
2	B	119	LYS	2.4
1	A	465	GLY	2.4
1	A	466	SER	2.4
1	A	760	GLY	2.3
3	C	149	GLN	2.3
1	A	408	LYS	2.3
2	B	165	GLN	2.3
1	A	363	ALA	2.3
1	A	377	PHE	2.3
1	A	379	THR	2.3
1	A	7	PHE	2.2
1	A	413	THR	2.2
3	C	3	PHE	2.2
2	B	366	ALA	2.2
1	A	1075	GLY	2.2
1	A	344	GLU	2.2
1	A	410	GLY	2.2
1	A	345	ARG	2.2
2	B	369	GLY	2.1
3	C	81	LEU	2.1
3	C	182	PHE	2.1
1	A	362	ASP	2.0
1	A	501	ALA	2.0
1	A	636	SER	2.0
1	A	875	ASP	2.0
2	B	287	GLU	2.0
1	A	874	CYS	2.0
3	C	225	HIS	2.0
2	B	428	ARG	2.0

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	0.29	82,84,96,98	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

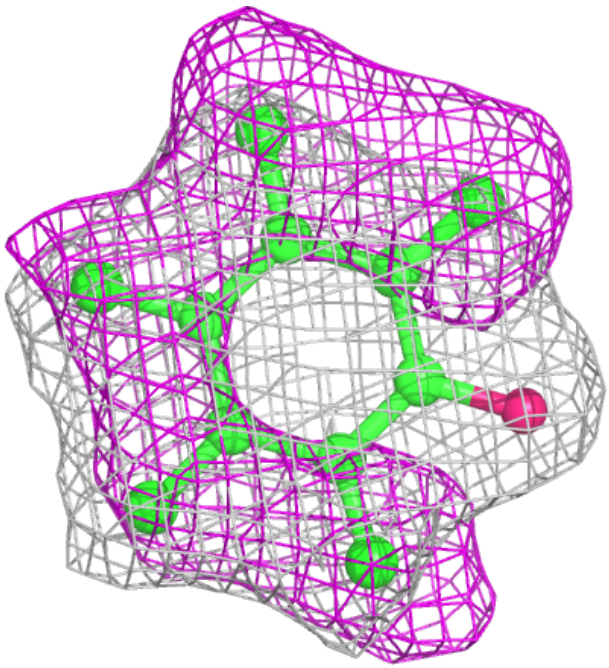
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

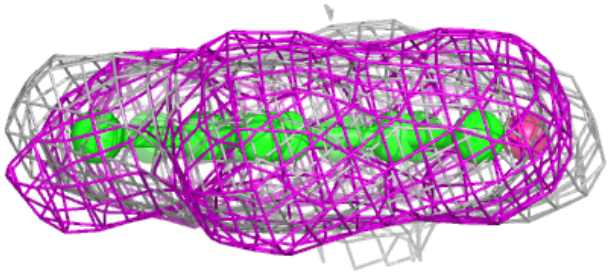
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	PCI	C	808	12/12	0.71	0.39	59,69,74,76	0
8	3PH	B	1806	18/48	0.85	0.28	59,82,111,111	0
10	AGA	C	309	30/30	0.95	0.15	30,54,85,95	0
4	MD1	A	2800	47/47	0.96	0.12	32,45,61,64	0
4	MD1	A	1800	47/47	0.97	0.11	35,50,66,71	0
9	HEM	C	807	43/43	0.97	0.16	60,68,89,92	0
6	SF4	B	1802	8/8	0.98	0.09	37,40,43,44	0
5	6MO	A	3800	1/1	0.98	0.05	72,72,72,72	0
9	HEM	C	806	43/43	0.98	0.13	27,40,51,55	0
6	SF4	B	1803	8/8	0.99	0.10	22,27,30,33	0
6	SF4	B	1804	8/8	0.99	0.10	31,38,38,39	0
7	F3S	B	1805	7/7	0.99	0.10	30,33,34,37	0
6	SF4	A	1801	8/8	0.99	0.05	34,39,46,47	0

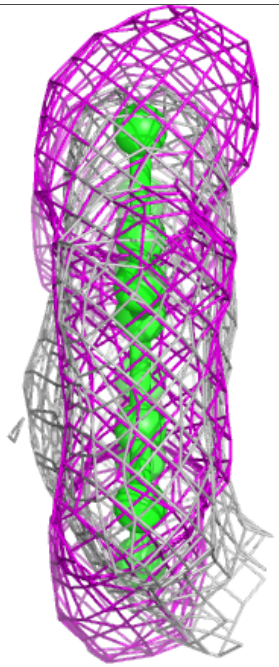
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PCI C 808:

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

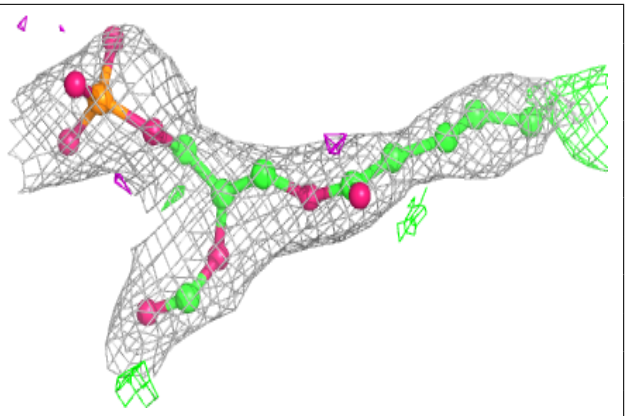


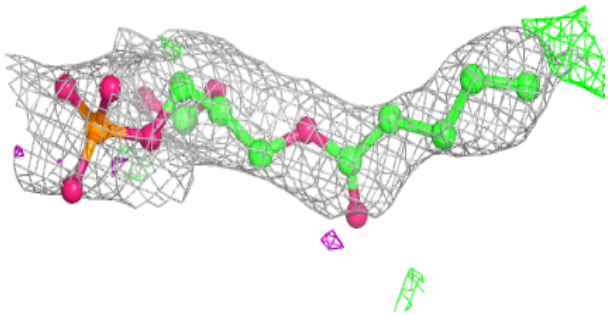


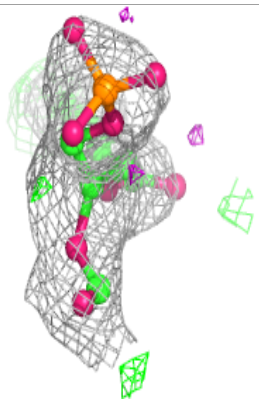


Electron density around 3PH B 1806:

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

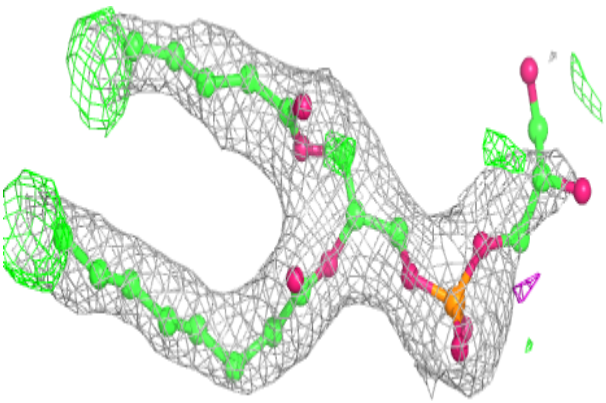


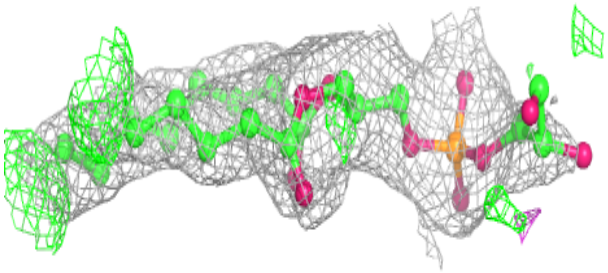


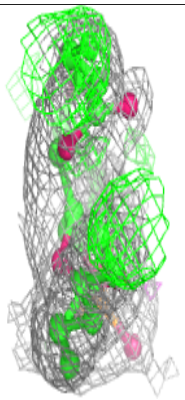


Electron density around AGA C 309:

$2mF_o$-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 2800:

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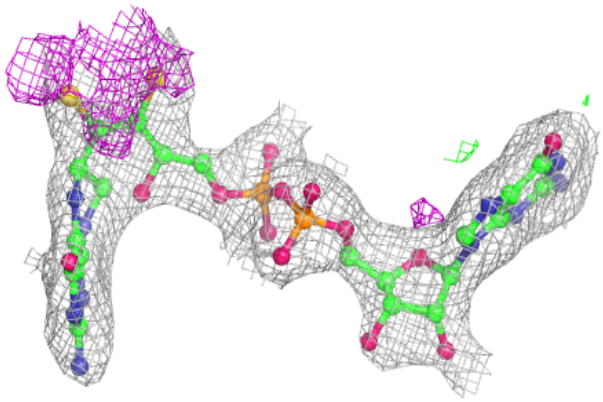
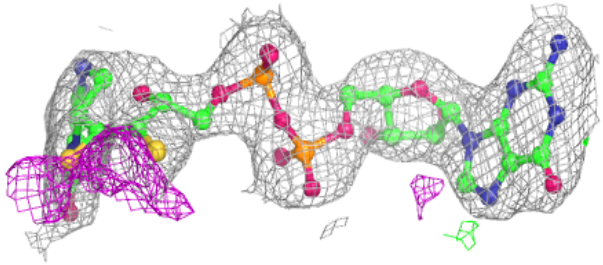
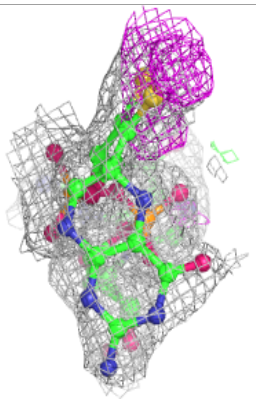
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

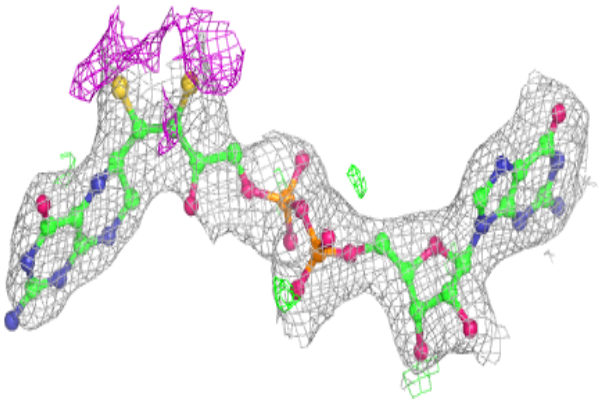


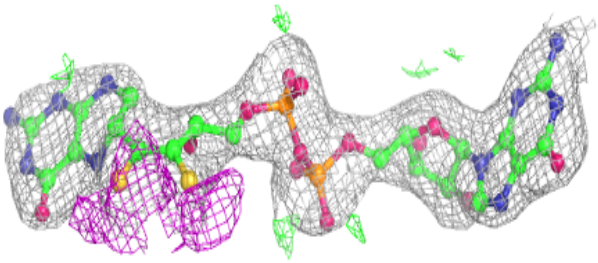


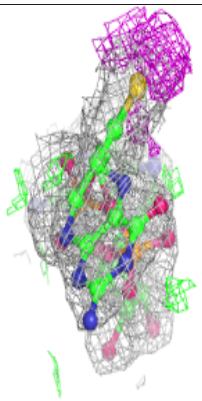


Electron density around MD1 A 1800:

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

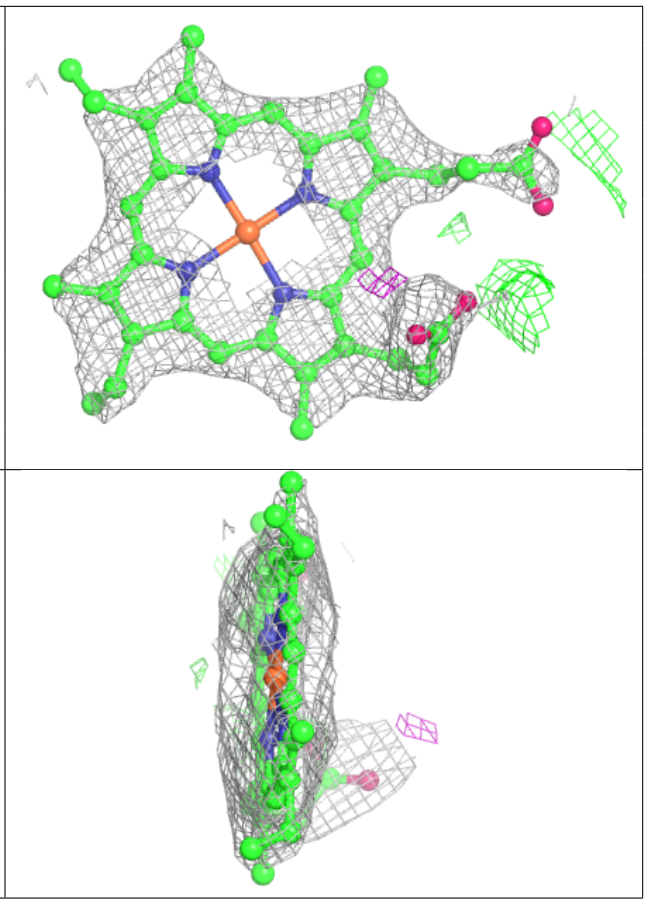






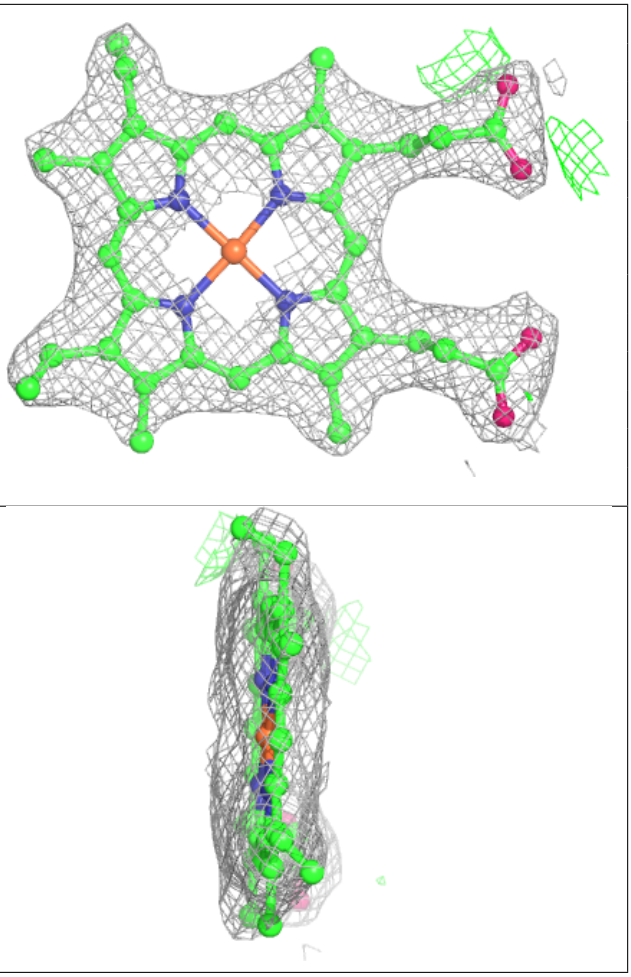
Electron density around HEM C 807:

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



Electron density around 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 (i)

There are no such residues in this entry.