



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:58 AM EDT

PDB ID : 3IR5 / pdb_00003ir5
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

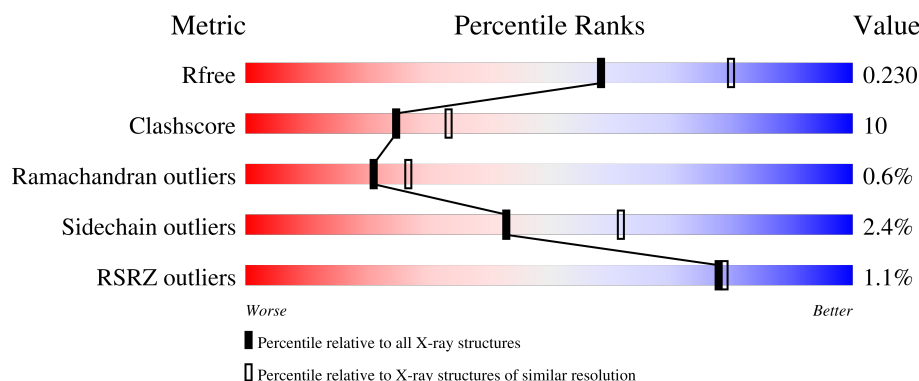
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	1247	0% 74% 23% •
2	B	512	81% 17% ••
3	C	225	3% 71% 27% •

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	C	N	O	S	0	0	0
			9865	6229	1729	1858	49			

There is a discrepancy between the modelled and reference sequences:

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

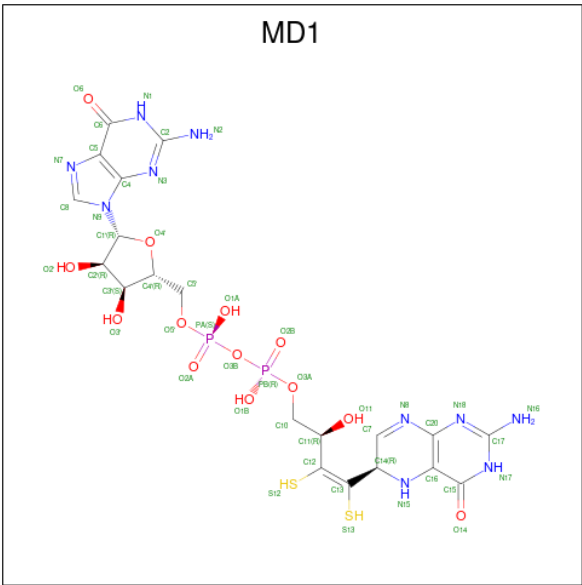
- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

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

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

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

- 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 (CCD ID: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

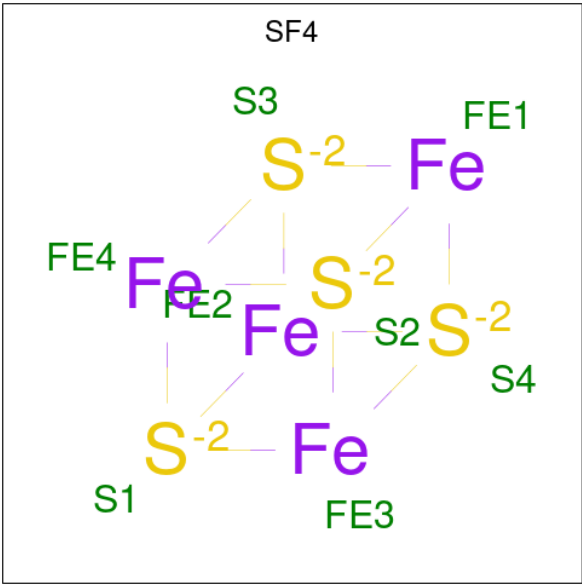


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 5 is MOLYBDENUM(VI) ION (CCD ID: 6MO) (formula: Mo).

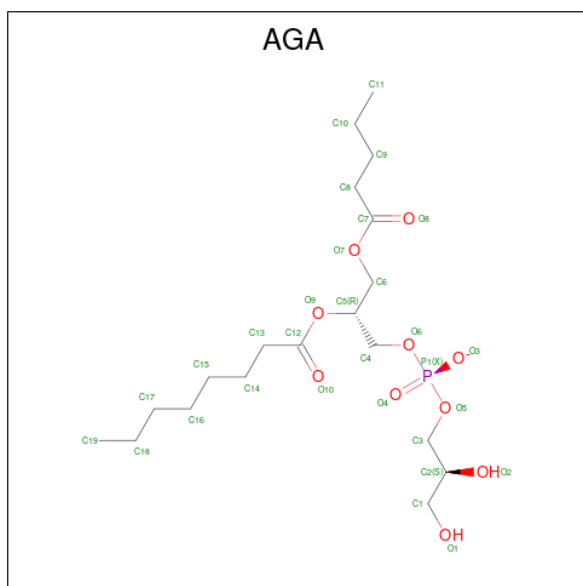
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



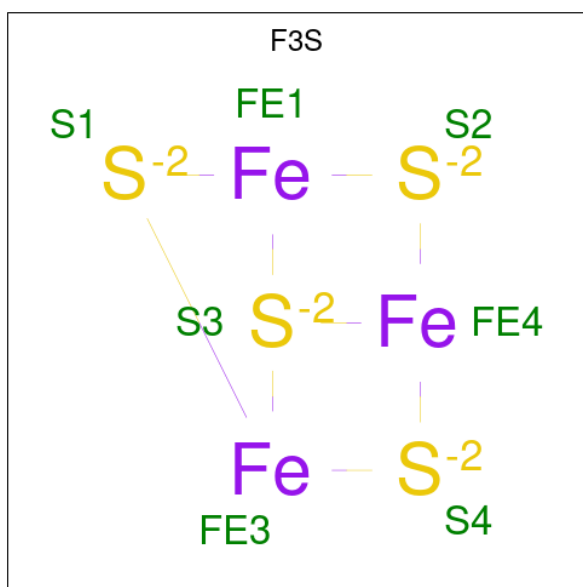
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is (1S)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (CCD ID: AGA) (formula: C₁₉H₃₆O₁₀P).



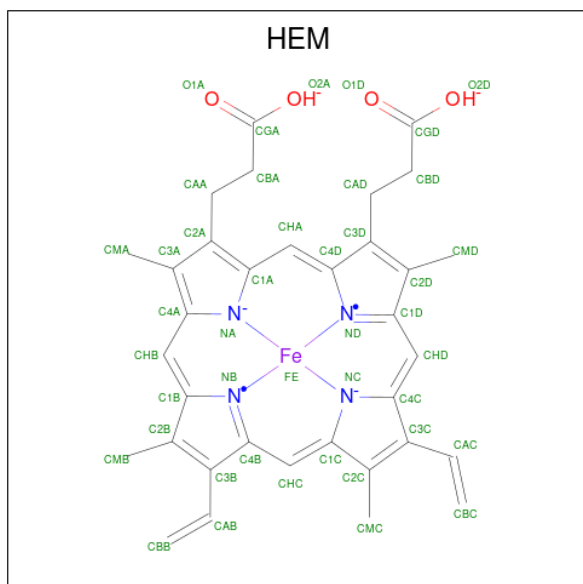
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			25	16	8	1		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



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

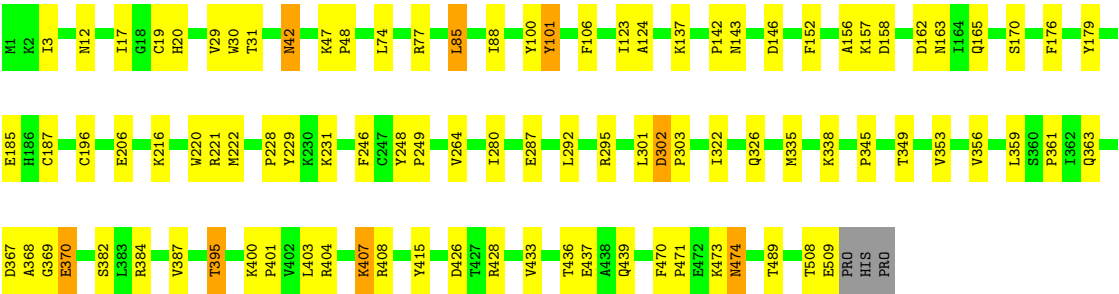
- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



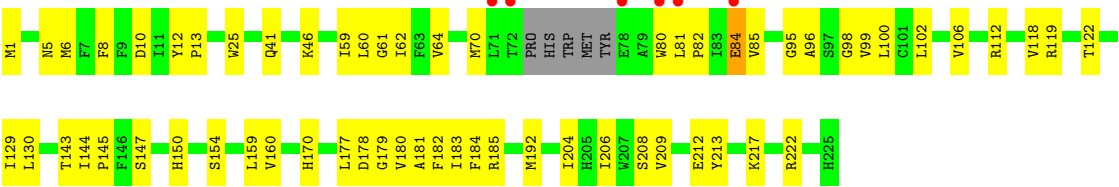
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
9	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- 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



• 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	153.45Å 240.69Å 139.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.30 29.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.61-2.30) 99.7 (29.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.237 0.194 , 0.230	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)	0.31 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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: HEM, AGA, FME, F3S, SF4, 6MO, MD1

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	0.44	0/10123	1.00	51/13742 (0.4%)
2	B	0.43	0/4146	0.96	17/5609 (0.3%)
3	C	0.45	0/1784	0.90	7/2411 (0.3%)
All	All	0.44	0/16053	0.98	75/21762 (0.3%)

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.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	CA-C-N	16.76	153.56	121.54
1	A	1163	HIS	C-N-CA	16.76	153.56	121.54
1	A	501	ALA	CA-C-N	12.35	145.14	121.54
1	A	501	ALA	C-N-CA	12.35	145.14	121.54
1	A	718	GLY	CA-C-O	-11.61	111.78	121.77
1	A	363	ALA	N-CA-C	-9.56	101.20	112.86
1	A	1093	GLN	N-CA-C	8.17	120.87	110.33
1	A	809	LEU	N-CA-C	-8.13	96.15	109.40
1	A	607	SER	N-CA-C	8.10	121.02	111.71
2	B	30	TRP	N-CA-C	8.03	123.20	113.41
1	A	586	GLN	N-CA-C	7.71	120.43	111.02
1	A	1167	ARG	N-CA-C	7.52	122.18	112.26
1	A	1070	VAL	N-CA-C	7.51	117.99	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	LEU	N-CA-C	7.02	119.53	111.11
1	A	862	GLN	CA-C-N	6.89	126.70	119.05
1	A	862	GLN	C-N-CA	6.89	126.70	119.05
1	A	720	SER	N-CA-C	6.59	124.84	110.80
1	A	863	PRO	N-CA-C	6.58	122.68	113.53
1	A	1169	VAL	N-CA-C	6.57	117.31	108.11
3	C	8	PHE	N-CA-C	6.55	119.24	111.71
1	A	74	GLN	N-CA-C	-6.33	101.11	110.48
2	B	359	LEU	N-CA-C	-6.32	100.56	110.36
2	B	88	ILE	N-CA-C	6.31	118.94	111.05
2	B	216	LYS	N-CA-C	6.24	119.05	111.82
1	A	151	ALA	N-CA-C	-6.17	105.76	113.28
3	C	209	VAL	CA-C-N	6.12	127.49	119.84
3	C	209	VAL	C-N-CA	6.12	127.49	119.84
2	B	302	ASP	CA-C-N	6.08	125.78	119.82
2	B	302	ASP	C-N-CA	6.08	125.78	119.82
1	A	719	SER	CB-CA-C	-6.07	109.56	116.54
1	A	473	VAL	N-CA-C	-6.04	103.51	111.05
1	A	101	TYR	N-CA-C	6.01	118.62	111.71
1	A	583	LEU	N-CA-C	-5.96	97.50	107.99
2	B	287	GLU	N-CA-C	5.89	117.39	110.97
2	B	31	THR	N-CA-C	5.89	118.42	110.88
1	A	612	TYR	N-CA-C	-5.86	104.90	111.28
3	C	208	SER	N-CA-C	5.83	119.45	112.93
1	A	937	GLY	CA-C-N	5.82	126.22	119.47
1	A	937	GLY	C-N-CA	5.82	126.22	119.47
2	B	395	THR	N-CA-C	5.81	118.32	110.88
1	A	302	ASP	N-CA-C	5.76	118.30	111.33
1	A	16	THR	N-CA-C	-5.74	102.27	110.59
1	A	424	ASP	N-CA-C	-5.65	106.55	113.50
1	A	1206	TYR	N-CA-C	5.64	117.97	110.53
1	A	184	ARG	N-CA-C	-5.50	106.25	113.17
1	A	1164	ALA	N-CA-C	5.50	122.51	110.80
1	A	1163	HIS	O-C-N	5.49	129.58	122.89
1	A	1043	GLN	N-CA-C	5.48	117.16	108.67
1	A	339	LEU	N-CA-C	5.48	118.55	109.46
1	A	403	GLU	N-CA-C	-5.47	101.75	109.96
2	B	280	ILE	N-CA-C	5.43	115.57	110.30
2	B	29	VAL	N-CA-C	5.38	116.04	110.82
2	B	196	CYS	CA-C-N	5.38	125.19	119.28
2	B	196	CYS	C-N-CA	5.38	125.19	119.28
1	A	384	VAL	N-CA-C	5.37	115.29	107.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	61	GLY	N-CA-C	-5.33	106.05	112.49
1	A	1071	LYS	N-CA-C	5.32	118.86	112.38
2	B	157	LYS	N-CA-C	-5.28	106.67	113.01
2	B	206	GLU	N-CA-C	5.26	117.76	111.71
2	B	222	MET	N-CA-C	-5.25	107.01	113.41
1	A	1163	HIS	CA-C-O	5.24	127.03	121.16
1	A	1054	PHE	N-CA-C	-5.22	106.77	112.72
2	B	474	ASN	N-CA-C	5.21	117.04	111.36
1	A	503	THR	N-CA-C	5.18	116.53	110.31
1	A	614	HIS	N-CA-C	5.18	117.83	111.82
1	A	1029	VAL	N-CA-C	5.18	115.95	110.72
1	A	316	GLU	N-CA-C	5.17	119.67	112.90
3	C	179	GLY	N-CA-C	5.15	122.72	115.30
1	A	853	GLN	N-CA-C	5.14	118.19	109.76
1	A	554	TYR	N-CA-C	5.12	116.67	111.14
1	A	582	LYS	N-CA-C	5.10	117.60	108.17
3	C	147	SER	N-CA-C	-5.09	106.58	112.89
1	A	615	SER	N-CA-C	-5.09	106.91	113.02
1	A	903	GLY	CA-C-N	5.01	124.70	119.64
1	A	903	GLY	C-N-CA	5.01	124.70	119.64

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:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9865	0	9524	222	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4050	0	3973	57	0
3	C	1747	0	1789	34	0
4	A	94	0	42	10	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	15417	306	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 10.

All (306) 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	1.36	1.04
1:A:338:MET:HE2	1:A:374:THR:CB	2.03	0.88
1:A:360:LEU:HG	1:A:383:MET:HE3	1.60	0.83
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
2:B:426:ASP:OD2	2:B:428:ARG:HD3	1.88	0.74
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.70	0.72
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.70	0.71
2:B:407:LYS:HD2	10:B:693:HOH:O	1.91	0.70
1:A:1098:HIS:CE1	4:A:1251:MD1:S13	2.85	0.69
1:A:582:LYS:HZ2	1:A:584:ARG:NH1	1.92	0.67
1:A:401:ASN:HA	1:A:1034:PRO:HD3	1.77	0.67
1:A:402:LEU:HD13	1:A:1034:PRO:HB3	1.77	0.66
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.78	0.66
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.78	0.66
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.77	0.65
1:A:462:LEU:HD12	1:A:466:SER:OG	1.97	0.65
2:B:407:LYS:HG2	2:B:433:VAL:HG11	1.80	0.64
1:A:214:LEU:HB3	1:A:607:SER:OG	1.96	0.64
1:A:1229:ASN:C	1:A:1230:ILE:HD12	2.22	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:LYS:HD2	1:A:750:LYS:N	2.13	0.63
1:A:856:SER:O	1:A:859:GLU:HG2	1.98	0.63
1:A:578:VAL:HG23	1:A:579:GLY:H	1.64	0.63
1:A:552:MET:HE3	1:A:1056:GLU:CD	2.24	0.63
1:A:611:PHE:CD2	1:A:727:MET:HE1	2.35	0.62
1:A:652:MET:HE3	1:A:867:LYS:O	1.99	0.62
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.15	0.62
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.80	0.62
3:C:80:TRP:C	3:C:81:LEU:HG	2.24	0.61
1:A:1098:HIS:HE1	4:A:1251:MD1:S13	2.24	0.61
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.82	0.61
2:B:137:LYS:HA	10:B:667:HOH:O	2.00	0.61
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.01	0.61
1:A:191:ILE:H	1:A:191:ILE:HD12	1.65	0.60
2:B:187:CYS:HB3	2:B:349:THR:O	2.02	0.60
2:B:370:GLU:OE1	2:B:370:GLU:HA	2.02	0.60
1:A:223:LEU:O	1:A:225:PRO:HD3	2.00	0.60
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.27	0.60
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.84	0.60
2:B:407:LYS:HG2	2:B:433:VAL:CG1	2.31	0.59
1:A:49:CYS:HB3	1:A:791:TRP:CZ3	2.37	0.59
1:A:371:GLU:OE1	1:A:371:GLU:N	2.28	0.59
2:B:367:ASP:C	2:B:369:GLY:H	2.10	0.59
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.85	0.58
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.03	0.58
1:A:20:GLY:O	3:C:217:LYS:HD2	2.04	0.58
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.86	0.58
2:B:404:ARG:O	2:B:408:ARG:HG3	2.02	0.57
1:A:360:LEU:CG	1:A:383:MET:HE3	2.33	0.57
1:A:582:LYS:HD2	10:A:1497:HOH:O	2.04	0.57
1:A:190:PRO:HD3	1:A:714:SER:HB2	1.85	0.57
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.34	0.57
1:A:719:SER:HB2	1:A:1099:SER:HB3	1.87	0.57
1:A:508:GLU:OE1	1:A:515:ARG:HD2	2.04	0.56
1:A:116:ARG:HE	1:A:147:SER:CB	2.19	0.56
3:C:6:MET:O	3:C:10:ASP:HB2	2.06	0.56
1:A:515:ARG:HG2	1:A:516:SER:N	2.20	0.56
3:C:96:ALA:O	3:C:100:LEU:HD13	2.06	0.56
1:A:336:MET:HA	1:A:473:VAL:HB	1.88	0.55
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.40	0.55
1:A:750:LYS:N	1:A:750:LYS:CD	2.69	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:H	1:A:371:GLU:CD	2.12	0.55
3:C:180:VAL:HG22	3:C:184:PHE:CD2	2.42	0.55
1:A:220:TYR:HD1	10:A:1469:HOH:O	1.90	0.55
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.89	0.55
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.88	0.55
1:A:1098:HIS:CE1	4:A:1247:MD1:S12	3.00	0.54
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.90	0.54
1:A:974:LEU:HD21	1:A:1033:ILE:HD13	1.88	0.54
1:A:417:LEU:O	1:A:472:THR:HG21	2.06	0.54
1:A:225:PRO:HB2	1:A:551:ASP:OD1	2.07	0.54
4:A:1247:MD1:H7	4:A:1247:MD1:C11	2.38	0.54
1:A:362:ASP:C	1:A:364:LEU:N	2.58	0.54
1:A:328:ASP:CG	1:A:332:ARG:HE	2.16	0.54
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.88	0.54
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.90	0.54
3:C:13:PRO:HG3	3:C:192:MET:SD	2.48	0.53
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.77	0.53
1:A:299:GLN:NE2	1:A:1158:MET:HB3	2.24	0.53
1:A:457:VAL:HG21	1:A:469:LEU:HD22	1.90	0.53
1:A:499:VAL:O	1:A:500:LYS:HG2	2.07	0.53
1:A:402:LEU:CD1	1:A:1034:PRO:HB3	2.38	0.53
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.44	0.53
3:C:181:ALA:HB3	3:C:184:PHE:CD2	2.43	0.53
1:A:368:ASN:ND2	1:A:396:GLU:HG2	2.24	0.53
1:A:191:ILE:O	1:A:194:MET:HG2	2.07	0.53
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.42	0.53
3:C:60:LEU:O	3:C:64:VAL:HG23	2.09	0.53
2:B:246:PHE:HA	6:B:803:SF4:S4	2.48	0.52
1:A:457:VAL:CG2	1:A:469:LEU:HD22	2.39	0.52
2:B:220:TRP:C	2:B:221:ARG:HG3	2.34	0.52
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.90	0.52
1:A:1163:HIS:CG	1:A:1164:ALA:H	2.26	0.52
3:C:181:ALA:HB3	3:C:184:PHE:CE2	2.44	0.52
1:A:54:THR:HA	1:A:580:GLN:HG3	1.91	0.52
1:A:68:VAL:HB	1:A:102:LEU:HD22	1.91	0.52
1:A:652:MET:HE1	1:A:866:VAL:CG1	2.40	0.51
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.76	0.51
1:A:578:VAL:HG23	1:A:579:GLY:N	2.25	0.51
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.10	0.51
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.45	0.51
1:A:804:PRO:O	1:A:1006:ILE:HG13	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.91	0.51
1:A:119:LYS:O	1:A:123:GLU:HG3	2.10	0.51
2:B:19:CYS:O	2:B:20:HIS:HB2	2.10	0.51
2:B:367:ASP:C	2:B:369:GLY:N	2.69	0.51
1:A:191:ILE:O	1:A:191:ILE:HG22	2.10	0.51
1:A:662:GLY:HA2	1:A:704:ASN:OD1	2.11	0.51
1:A:1100:THR:O	1:A:1101:TYR:HB2	2.10	0.51
1:A:100:TRP:O	1:A:104:SER:HB3	2.10	0.51
1:A:864:LEU:HD22	1:A:864:LEU:N	2.25	0.50
1:A:914:LYS:O	1:A:914:LYS:HG2	2.11	0.50
1:A:1243:GLU:O	1:A:1244:SER:O	2.29	0.50
1:A:299:GLN:CD	1:A:1158:MET:HE2	2.35	0.50
3:C:119:ARG:O	3:C:122:THR:HG22	2.11	0.50
4:A:1247:MD1:H7	4:A:1247:MD1:O11	2.12	0.50
1:A:500:LYS:O	1:A:502:TYR:N	2.41	0.50
1:A:400:TRP:CE2	1:A:1034:PRO:HG2	2.47	0.50
1:A:634:ASP:OD1	1:A:637:ARG:HG3	2.12	0.50
1:A:515:ARG:HG2	1:A:516:SER:H	1.77	0.50
1:A:49:CYS:HA	1:A:791:TRP:CE3	2.46	0.49
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.47	0.49
1:A:582:LYS:NZ	1:A:584:ARG:NH1	2.60	0.49
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.37	0.49
1:A:931:ASN:O	1:A:932:TYR:HB2	2.11	0.49
1:A:1093:GLN:HB3	1:A:1162:TYR:HB3	1.93	0.49
3:C:12:TYR:HB3	3:C:13:PRO:HD3	1.94	0.49
2:B:100:TYR:O	2:B:101:TYR:HB3	2.11	0.49
1:A:116:ARG:HE	1:A:147:SER:HB2	1.76	0.49
1:A:168:LEU:HD23	1:A:168:LEU:O	2.13	0.49
1:A:652:MET:CE	1:A:862:GLN:HE22	2.26	0.49
3:C:183:ILE:HG23	3:C:184:PHE:N	2.28	0.49
1:A:411:GLU:HG3	1:A:412:GLU:N	2.27	0.49
1:A:487:LEU:CD1	1:A:487:LEU:N	2.76	0.49
1:A:362:ASP:C	1:A:364:LEU:H	2.20	0.48
1:A:624:THR:O	1:A:627:GLU:HG2	2.12	0.48
3:C:102:LEU:O	3:C:106:VAL:HG23	2.14	0.48
1:A:220:TYR:CE1	4:A:1247:MD1:H101	2.49	0.48
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.96	0.48
1:A:490:VAL:O	1:A:500:LYS:HE2	2.14	0.48
1:A:876:LEU:C	1:A:876:LEU:HD23	2.39	0.48
2:B:363:GLN:HG2	2:B:382:SER:O	2.14	0.48
3:C:70:MET:HG2	3:C:160:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:THR:OG1	4:A:1247:MD1:H5'1	2.14	0.47
3:C:59:ILE:HD13	9:C:806:HEM:HAC	1.95	0.47
1:A:116:ARG:HG3	1:A:120:MET:HE2	1.95	0.47
1:A:695:ALA:HB1	1:A:704:ASN:HB3	1.96	0.47
1:A:1177:THR:O	1:A:1178:GLN:HB2	2.15	0.47
1:A:1132:ASN:ND2	2:B:137:LYS:HE2	2.28	0.47
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.15	0.47
1:A:378:ASN:OD1	1:A:382:GLU:HB2	2.15	0.47
1:A:173:ASN:O	1:A:177:ILE:HG13	2.14	0.47
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.29	0.47
1:A:1098:HIS:CE1	4:A:1251:MD1:H15	2.33	0.47
3:C:84:GLU:HG3	3:C:85:VAL:N	2.29	0.47
1:A:578:VAL:CG2	1:A:579:GLY:H	2.26	0.47
1:A:772:ASP:C	1:A:788:THR:HG22	2.40	0.47
1:A:1062:ARG:HD2	10:A:1476:HOH:O	2.14	0.47
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.50	0.47
2:B:3:ILE:HG12	2:B:301:LEU:CD1	2.45	0.47
1:A:1006:ILE:CD1	1:A:1016:GLU:CD	2.88	0.46
1:A:1070:VAL:HG13	1:A:1223:VAL:CG2	2.45	0.46
2:B:248:TYR:CG	2:B:249:PRO:HD3	2.50	0.46
1:A:430:GLY:O	1:A:632:MET:HE1	2.15	0.46
1:A:33:ASP:O	1:A:37:GLN:HG3	2.16	0.46
1:A:199:TYR:CD1	1:A:199:TYR:C	2.92	0.46
1:A:1183:ILE:HG13	1:A:1185:ASN:H	1.79	0.46
2:B:335:MET:O	2:B:338:LYS:HE3	2.15	0.46
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.51	0.46
2:B:162:ASP:O	2:B:163:ASN:HB2	2.16	0.46
3:C:150:HIS:HB3	3:C:154:SER:OG	2.15	0.46
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.50	0.46
2:B:47:LYS:HA	2:B:48:PRO:C	2.41	0.46
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.46	0.46
1:A:658:ALA:HA	1:A:659:PRO:C	2.40	0.46
1:A:279:ALA:HB2	1:A:291:CYS:SG	2.56	0.45
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.50	0.45
1:A:536:SER:HB2	1:A:566:CYS:SG	2.57	0.45
1:A:1048:HIS:O	1:A:1049:GLN:C	2.59	0.45
1:A:373:LYS:HD3	1:A:392:PHE:CE1	2.52	0.45
1:A:644:ASP:OD2	1:A:751:PRO:HB2	2.17	0.45
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.82	0.45
1:A:1230:ILE:HD12	1:A:1230:ILE:N	2.32	0.45
3:C:182:PHE:O	3:C:185:ARG:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ASP:OD2	1:A:466:SER:OG	2.27	0.45
2:B:228:PRO:HG2	2:B:229:TYR:CD1	2.52	0.45
2:B:295:ARG:HA	2:B:295:ARG:HD2	1.81	0.45
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.52	0.44
1:A:307:LEU:HD13	1:A:502:TYR:CD2	2.52	0.44
3:C:143:THR:HB	3:C:184:PHE:CE1	2.51	0.44
3:C:177:LEU:O	3:C:178:ASP:C	2.61	0.44
1:A:1084:LYS:HB2	1:A:1127:LEU:HD21	1.99	0.44
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.17	0.44
1:A:384:VAL:HG22	1:A:385:ALA:N	2.33	0.44
1:A:487:LEU:N	1:A:487:LEU:HD12	2.33	0.44
1:A:641:HIS:O	1:A:644:ASP:HB2	2.17	0.44
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.44
1:A:1067:THR:O	1:A:1068:ARG:C	2.61	0.44
1:A:1068:ARG:HG3	1:A:1068:ARG:HH21	1.82	0.44
1:A:425:GLU:O	1:A:457:VAL:HG22	2.18	0.44
1:A:336:MET:N	1:A:337:PRO:HD2	2.33	0.44
1:A:729:LYS:HD3	1:A:730:TYR:CE1	2.53	0.44
1:A:6:ARG:O	1:A:9:TYR:N	2.49	0.44
1:A:894:ALA:O	1:A:898:ARG:HG3	2.16	0.43
2:B:302:ASP:HA	2:B:303:PRO:HD2	1.88	0.43
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.47	0.43
1:A:168:LEU:HD23	1:A:168:LEU:C	2.43	0.43
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.18	0.43
1:A:1152:GLN:OE1	2:B:170:SER:HA	2.19	0.43
1:A:53:CYS:C	1:A:54:THR:HG23	2.44	0.43
1:A:56:SER:HB2	1:A:800:SER:HB2	1.99	0.43
1:A:584:ARG:HD3	1:A:1006:ILE:HG12	1.99	0.43
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.54	0.43
3:C:95:GLY:O	3:C:99:VAL:HG23	2.19	0.43
1:A:868:ASP:OD1	1:A:868:ASP:C	2.62	0.43
1:A:1028:ASN:HA	1:A:1033:ILE:O	2.18	0.43
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.83	0.43
2:B:42:ASN:HB2	6:B:803:SF4:S1	2.59	0.42
1:A:155:GLY:HA2	10:B:619:HOH:O	2.18	0.42
1:A:286:GLU:HG2	2:B:179:TYR:OH	2.19	0.42
1:A:308:ALA:HB2	1:A:507:ALA:HB2	2.00	0.42
1:A:591:PRO:HA	1:A:596:LEU:HB2	2.00	0.42
1:A:26:ASN:HB3	10:A:1496:HOH:O	2.18	0.42
2:B:176:PHE:CD1	2:B:176:PHE:C	2.96	0.42
1:A:219:TRP:HB2	1:A:607:SER:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HA	1:A:271:ARG:HD3	2.00	0.42
1:A:289:LYS:HD3	1:A:289:LYS:C	2.44	0.42
1:A:55:GLY:HA3	6:A:1249:SF4:S3	2.59	0.42
1:A:360:LEU:C	1:A:463:ALA:HB2	2.44	0.42
2:B:12:ASN:HA	2:B:356:VAL:HB	2.01	0.42
2:B:387:VAL:HG21	2:B:403:LEU:HG	2.01	0.42
2:B:508:THR:O	2:B:509:GLU:CB	2.67	0.42
1:A:1208:PHE:O	1:A:1209:ASN:HB2	2.19	0.42
3:C:41:GLN:HB2	9:C:806:HEM:O1A	2.20	0.42
1:A:5:ASP:OD2	2:B:489:THR:HG23	2.19	0.42
1:A:634:ASP:CG	1:A:637:ARG:HG3	2.45	0.42
3:C:129:ILE:CG2	3:C:130:LEU:N	2.82	0.42
1:A:340:VAL:O	1:A:470:VAL:HA	2.19	0.42
1:A:525:PHE:CZ	1:A:536:SER:HB3	2.55	0.42
1:A:1023:ASN:O	1:A:1026:TYR:HB2	2.20	0.42
1:A:225:PRO:C	1:A:228:PRO:HD2	2.45	0.42
1:A:803:HIS:HB2	1:A:804:PRO:HD2	2.01	0.42
1:A:862:GLN:HA	1:A:863:PRO:HD2	1.85	0.42
1:A:1037:THR:HA	1:A:1203:HIS:HB3	2.02	0.42
1:A:27:THR:HG23	3:C:222:ARG:HD3	2.01	0.41
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.55	0.41
1:A:313:MET:HE1	1:A:560:MET:HE3	2.02	0.41
1:A:705:HIS:HD2	1:A:764:LYS:HB3	1.83	0.41
1:A:401:ASN:CG	1:A:403:GLU:HG3	2.45	0.41
1:A:552:MET:HE3	1:A:1056:GLU:OE1	2.20	0.41
1:A:724:HIS:O	1:A:728:LEU:HD13	2.20	0.41
2:B:292:LEU:HD13	2:B:345:PRO:O	2.20	0.41
1:A:194:MET:HA	1:A:798:ASN:ND2	2.35	0.41
1:A:1006:ILE:HD13	1:A:1016:GLU:HG3	2.01	0.41
1:A:51:VAL:HB	1:A:791:TRP:CZ2	2.55	0.41
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.45	0.41
1:A:1091:PRO:O	1:A:1162:TYR:HA	2.20	0.41
2:B:400:LYS:HB3	2:B:401:PRO:HD3	2.03	0.41
1:A:54:THR:HA	1:A:580:GLN:CG	2.51	0.41
1:A:934:LYS:HD3	1:A:944:MET:SD	2.60	0.41
1:A:489:ASP:HB3	1:A:492:CYS:SG	2.60	0.41
1:A:574:TRP:CZ2	1:A:576:HIS:HB2	2.55	0.41
1:A:1068:ARG:HG3	1:A:1068:ARG:NH2	2.35	0.41
2:B:185:GLU:OE1	2:B:353:VAL:HB	2.21	0.41
1:A:338:MET:HE2	1:A:374:THR:OG1	2.19	0.41
1:A:497:ASP:HA	1:A:505:ALA:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ASN:OD1	1:A:550:LEU:HD12	2.20	0.41
1:A:634:ASP:HB3	1:A:637:ARG:HG3	2.02	0.41
2:B:77:ARG:HH11	2:B:77:ARG:HB2	1.86	0.41
2:B:123:ILE:HG13	2:B:124:ALA:H	1.85	0.41
2:B:156:ALA:C	2:B:158:ASP:N	2.78	0.41
2:B:407:LYS:HG3	10:B:639:HOH:O	2.21	0.41
2:B:415:TYR:CE2	2:B:437:GLU:HG2	2.55	0.41
1:A:218:ASP:OD2	1:A:218:ASP:N	2.54	0.41
1:A:289:LYS:HD3	1:A:289:LYS:O	2.21	0.41
1:A:336:MET:HB3	1:A:474:TYR:HB2	2.02	0.41
4:A:1247:MD1:O11	4:A:1247:MD1:C7	2.69	0.41
1:A:51:VAL:C	1:A:194:MET:SD	3.04	0.41
1:A:231:TRP:CD1	1:A:1042:GLN:HG2	2.56	0.41
1:A:261:THR:HG23	2:B:17:ILE:HD12	2.02	0.41
1:A:338:MET:HE3	1:A:375:VAL:O	2.21	0.41
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.55	0.41
1:A:338:MET:HE3	1:A:338:MET:HA	2.02	0.41
3:C:159:LEU:HD22	3:C:159:LEU:H	1.86	0.41
1:A:378:ASN:OD1	1:A:382:GLU:N	2.54	0.40
2:B:101:TYR:CZ	2:B:142:PRO:HD3	2.56	0.40
2:B:508:THR:O	2:B:509:GLU:HB3	2.20	0.40
1:A:152:ARG:HB2	1:A:734:THR:CG2	2.51	0.40
1:A:517:GLN:HA	1:A:517:GLN:NE2	2.36	0.40
2:B:231:LYS:HA	2:B:231:LYS:HD3	1.73	0.40
2:B:436:THR:OG1	2:B:439:GLN:HG3	2.21	0.40
2:B:322:ILE:O	2:B:326:GLN:HG3	2.22	0.40
3:C:12:TYR:N	3:C:13:PRO:CD	2.84	0.40
1:A:37:GLN:HB3	10:A:1450:HOH:O	2.22	0.40
1:A:191:ILE:HA	1:A:192:PRO:HD2	1.97	0.40
1:A:406:ASP:C	1:A:408:LYS:H	2.30	0.40
1:A:717:LEU:HG	1:A:778:THR:HG23	2.03	0.40
1:A:806:ILE:O	1:A:806:ILE:HG23	2.21	0.40
3:C:112:ARG:HA	3:C:118:VAL:CG1	2.51	0.40
1:A:307:LEU:HD13	1:A:502:TYR:CE2	2.56	0.40
1:A:363:ALA:O	1:A:366:GLN:HB2	2.22	0.40
1:A:696:ALA:O	1:A:699:PRO:HD3	2.22	0.40
1:A:713:ARG:HA	4:A:1247:MD1:C4	2.51	0.40
3:C:25:TRP:C	3:C:25:TRP:CD1	2.97	0.40
3:C:62:ILE:HD11	3:C:98:GLY:HA2	2.03	0.40

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 [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	1242/1247 (100%)	1162 (94%)	71 (6%)	9 (1%)	18	23
2	B	507/512 (99%)	492 (97%)	13 (3%)	2 (0%)	30	38
3	C	216/225 (96%)	202 (94%)	14 (6%)	0	100	100
All	All	1965/1984 (99%)	1856 (94%)	98 (5%)	11 (1%)	21	27

All (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
1	A	720	SER
2	B	101	TYR
1	A	191	ILE
1	A	224	PRO
2	B	368	ALA
1	A	195	SER

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	1039/1044 (100%)	1010 (97%)	29 (3%)	38	56
2	B	436/439 (99%)	430 (99%)	6 (1%)	59	76
3	C	180/186 (97%)	175 (97%)	5 (3%)	38	56
All	All	1655/1669 (99%)	1615 (98%)	40 (2%)	43	62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	GLU
1	A	383	MET
1	A	402	LEU
1	A	461	GLN
1	A	467	THR
1	A	476	LEU
1	A	483	LEU
1	A	502	TYR
1	A	515	ARG
1	A	586	GLN
1	A	600	ARG
1	A	626	GLU
1	A	629	LEU
1	A	663	THR
1	A	673	GLU
1	A	717	LEU
1	A	727	MET
1	A	743	LEU
1	A	767	LEU
1	A	808	PRO
1	A	864	LEU
1	A	926	LEU
1	A	1006	ILE
1	A	1062	ARG
1	A	1072	GLU
1	A	1110	LEU
1	A	1228	LYS
1	A	1233	LEU
1	A	1243	GLU
2	B	42	ASN
2	B	74	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	85	LEU
2	B	165	GLN
2	B	370	GLU
2	B	407	LYS
3	C	46	LYS
3	C	84	GLU
3	C	170	HIS
3	C	204	ILE
3	C	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	128	HIS
1	A	173	ASN
1	A	179	ASN
1	A	245	ASN
1	A	258	GLN
1	A	366	GLN
1	A	368	ASN
1	A	369	ASN
1	A	461	GLN
1	A	517	GLN
1	A	559	ASN
1	A	704	ASN
1	A	708	ASN
1	A	745	GLN
1	A	946	ASN
1	A	1000	GLN
1	A	1023	ASN
1	A	1048	HIS
1	A	1082	GLN
1	A	1229	ASN
2	B	294	GLN
2	B	304	ASN
2	B	414	HIS
2	B	451	ASN
3	C	149	GLN
3	C	175	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	1.46	3 (37%)	8,9,11	1.63	2 (25%)

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	-2.52	1.47	1.53
3	C	1	FME	CA-N	-2.36	1.43	1.46
3	C	1	FME	CB-CG	2.04	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CB-CA-N	2.53	115.12	110.52
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	C-CA-CB-CG
3	C	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	MD1	A	1247	5	47,51,51	2.95	8 (17%)	56,78,78	1.32	5 (8%)
9	HEM	C	807	3	50,50,50	1.90	19 (38%)	67,82,82	0.95	4 (5%)
6	SF4	B	804	2	0,12,12	-	-	-		
6	SF4	A	1249	1	0,12,12	-	-	-		
6	SF4	B	802	2	0,12,12	-	-	-		
8	F3S	B	805	2	0,9,9	-	-	-		
9	HEM	C	806	3	50,50,50	1.68	11 (22%)	67,82,82	0.90	2 (2%)
4	MD1	A	1251	5	47,51,51	2.82	9 (19%)	56,78,78	1.40	3 (5%)
6	SF4	B	803	2	0,12,12	-	-	-		
7	AGA	A	1250	-	24,24,29	0.79	1 (4%)	27,29,35	1.58	2 (7%)

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
4	MD1	A	1247	5	-	7/22/59/59	0/5/5/5
9	HEM	C	807	3	-	9/14/54/54	-
6	SF4	B	804	2	-	-	0/6/5/5
6	SF4	A	1249	1	-	-	0/6/5/5
6	SF4	B	802	2	-	-	0/6/5/5
8	F3S	B	805	2	-	-	0/3/3/3
9	HEM	C	806	3	-	7/14/54/54	-
4	MD1	A	1251	5	-	2/22/59/59	0/5/5/5
6	SF4	B	803	2	-	-	0/6/5/5
7	AGA	A	1250	-	-	6/26/26/34	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1247	MD1	C7-N8	17.73	1.50	1.28
4	A	1251	MD1	C7-N8	16.40	1.49	1.28
4	A	1251	MD1	PA-O3B	-5.30	1.53	1.59
9	C	807	HEM	CAB-C3B	4.52	1.59	1.47
9	C	806	HEM	CAB-C3B	4.30	1.58	1.47
4	A	1247	MD1	C16-C20	3.55	1.48	1.39
9	C	807	HEM	FE-NC	3.50	2.06	1.95
9	C	806	HEM	CAC-C3C	3.50	1.56	1.47
9	C	807	HEM	CAC-C3C	3.48	1.56	1.47
9	C	806	HEM	CMC-C2C	3.31	1.57	1.50
9	C	807	HEM	CMC-C2C	3.20	1.57	1.50
4	A	1247	MD1	PB-O3B	3.17	1.62	1.59
9	C	807	HEM	CMD-C2D	3.16	1.57	1.50
9	C	806	HEM	FE-NC	3.13	2.05	1.95
4	A	1247	MD1	C20-N8	2.99	1.41	1.36
9	C	806	HEM	CMB-C2B	2.95	1.56	1.50
9	C	807	HEM	CMB-C2B	2.94	1.56	1.50
9	C	806	HEM	CMA-C3A	2.94	1.56	1.50
4	A	1251	MD1	C20-N8	2.93	1.41	1.36
4	A	1247	MD1	C4-N3	2.90	1.40	1.34
9	C	807	HEM	CMA-C3A	2.90	1.56	1.50
9	C	806	HEM	CMD-C2D	2.83	1.56	1.50
9	C	807	HEM	CAD-C3D	2.77	1.58	1.51
4	A	1247	MD1	C12-C13	2.74	1.42	1.34
9	C	807	HEM	CBA-CAA	2.57	1.60	1.51
4	A	1251	MD1	O11-C11	2.53	1.48	1.42
4	A	1247	MD1	C14-C7	2.49	1.56	1.50
9	C	807	HEM	CBA-CGA	2.48	1.56	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1250	AGA	C8-C7	2.47	1.57	1.50
9	C	806	HEM	FE-NB	2.43	2.02	1.94
9	C	807	HEM	FE-NB	2.43	2.02	1.94
9	C	807	HEM	CAA-C2A	2.42	1.57	1.51
9	C	807	HEM	CBD-CGD	2.41	1.56	1.50
9	C	807	HEM	C1D-C2D	2.41	1.49	1.44
4	A	1251	MD1	C14-N15	2.32	1.51	1.46
4	A	1247	MD1	C14-C13	2.30	1.53	1.51
9	C	807	HEM	CBD-CAD	2.29	1.59	1.51
9	C	807	HEM	C4A-C3A	2.23	1.48	1.43
9	C	807	HEM	FE-ND	2.22	2.01	1.94
4	A	1251	MD1	C4-N3	2.21	1.39	1.34
9	C	806	HEM	CAD-C3D	2.20	1.57	1.51
4	A	1251	MD1	C14-C7	2.20	1.56	1.50
9	C	807	HEM	O1A-CGA	2.17	1.29	1.22
9	C	806	HEM	C4D-ND	-2.17	1.36	1.40
9	C	807	HEM	O1D-CGD	2.11	1.29	1.22
9	C	806	HEM	CBA-CAA	2.04	1.59	1.51
4	A	1251	MD1	C16-C20	2.04	1.45	1.39
4	A	1251	MD1	C6-N1	2.03	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1247	MD1	C17-N18-C20	5.75	122.16	114.20
4	A	1251	MD1	C17-N18-C20	5.62	121.99	114.20
7	A	1250	AGA	C14-C13-C12	4.93	131.78	113.69
7	A	1250	AGA	C9-C8-C7	4.91	131.69	113.69
4	A	1251	MD1	C2-N3-C4	3.22	117.85	112.30
9	C	807	HEM	CAD-C3D-C4D	-2.75	119.90	124.70
4	A	1247	MD1	N17-C17-N18	-2.66	118.46	123.32
4	A	1247	MD1	O14-C15-C16	-2.60	120.98	127.26
4	A	1247	MD1	O3A-C10-C11	-2.44	101.09	107.96
9	C	806	HEM	CAD-C3D-C4D	-2.32	120.66	124.70
9	C	807	HEM	CAD-C3D-C2D	2.23	132.05	127.87
9	C	807	HEM	CMA-C3A-C2A	2.23	130.36	125.62
9	C	806	HEM	O1D-CGD-CBD	-2.20	116.12	123.09
9	C	807	HEM	O1D-CGD-CBD	-2.13	116.33	123.09
4	A	1251	MD1	N1-C2-N3	-2.11	119.45	123.32
4	A	1247	MD1	C1'-N9-C8	2.02	132.48	126.73

There are no chirality outliers.

All (31) torsion outliers are listed below:

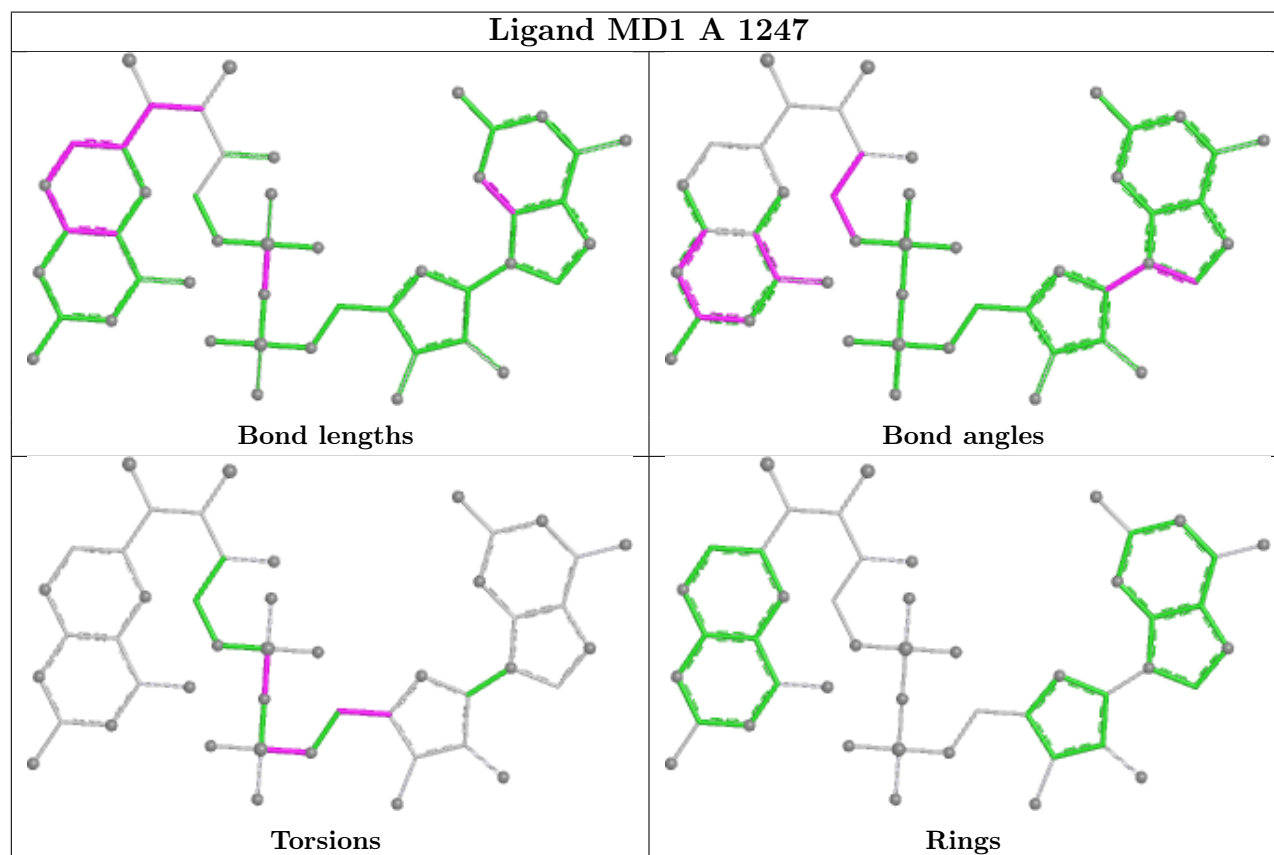
Mol	Chain	Res	Type	Atoms
4	A	1247	MD1	C5'-O5'-PA-O3B
4	A	1247	MD1	C5'-O5'-PA-O2A
9	C	806	HEM	C2C-C3C-CAC-CBC
9	C	807	HEM	C2C-C3C-CAC-CBC
9	C	807	HEM	C4C-C3C-CAC-CBC
4	A	1247	MD1	O4'-C4'-C5'-O5'
4	A	1247	MD1	C3'-C4'-C5'-O5'
9	C	806	HEM	C4C-C3C-CAC-CBC
7	A	1250	AGA	C8-C7-O7-C6
7	A	1250	AGA	O8-C7-O7-C6
7	A	1250	AGA	C11-C10-C9-C8
4	A	1247	MD1	PA-O3B-PB-O2B
4	A	1251	MD1	PA-O3B-PB-O2B
4	A	1247	MD1	C5'-O5'-PA-O1A
9	C	807	HEM	C2A-CAA-CBA-CGA
9	C	806	HEM	CAD-CBD-CGD-O2D
7	A	1250	AGA	O6-C4-C5-C6
9	C	806	HEM	CAA-CBA-CGA-O1A
9	C	806	HEM	CAA-CBA-CGA-O2A
9	C	806	HEM	CAD-CBD-CGD-O1D
9	C	807	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAD-CBD-CGD-O2D
9	C	807	HEM	C2B-C3B-CAB-CBB
7	A	1250	AGA	C7-C8-C9-C10
9	C	807	HEM	CAA-CBA-CGA-O1A
9	C	807	HEM	C4B-C3B-CAB-CBB
9	C	807	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	C2B-C3B-CAB-CBB
7	A	1250	AGA	O7-C7-C8-C9
4	A	1247	MD1	PA-O3B-PB-O1B
4	A	1251	MD1	PA-O3B-PB-O1B

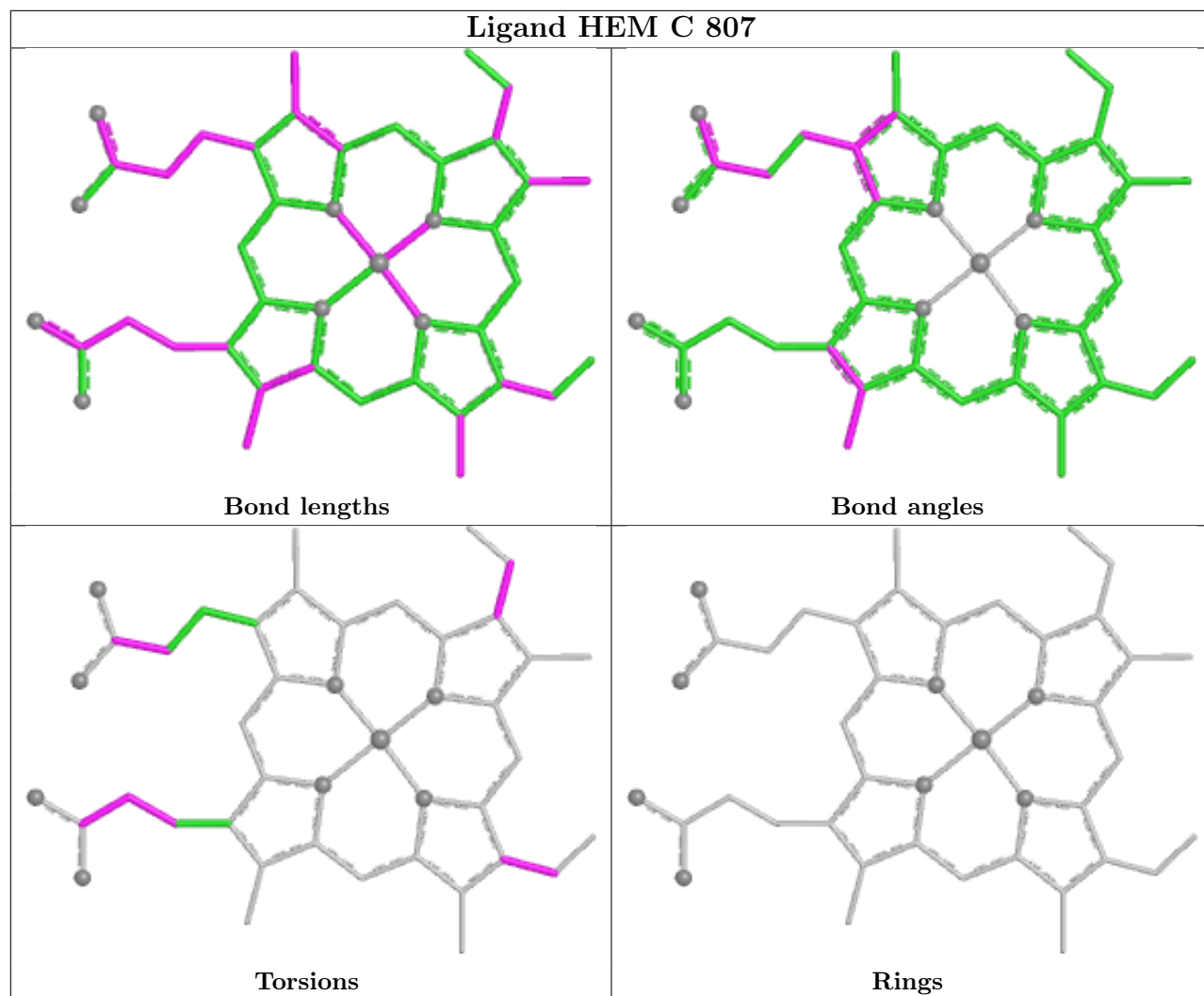
There are no ring outliers.

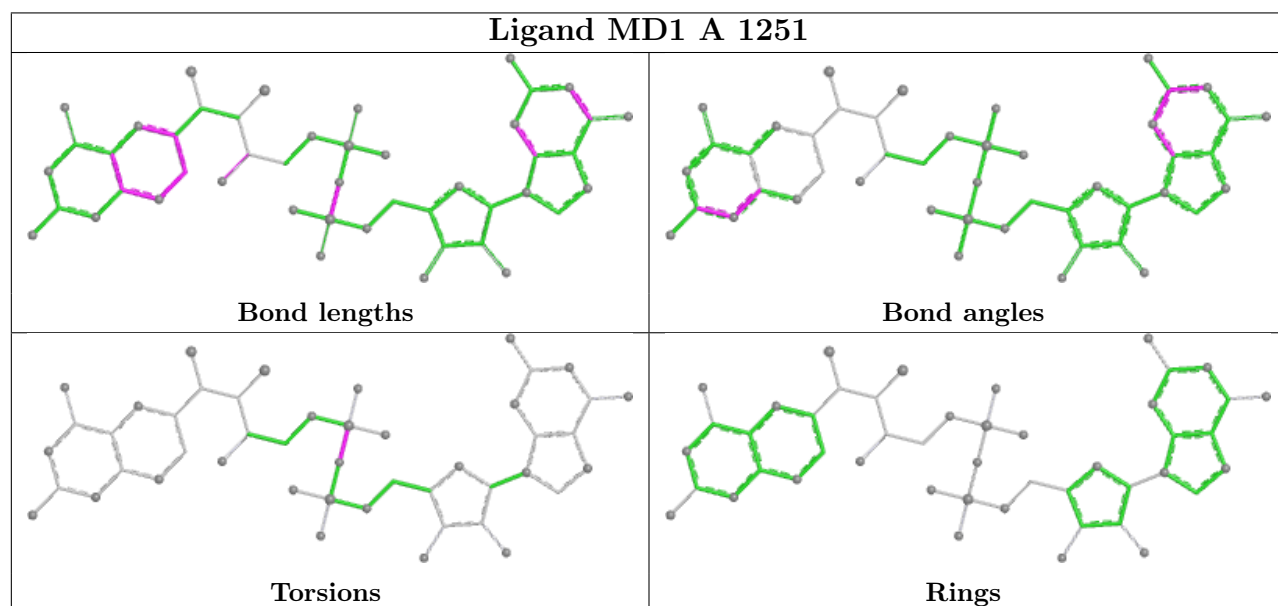
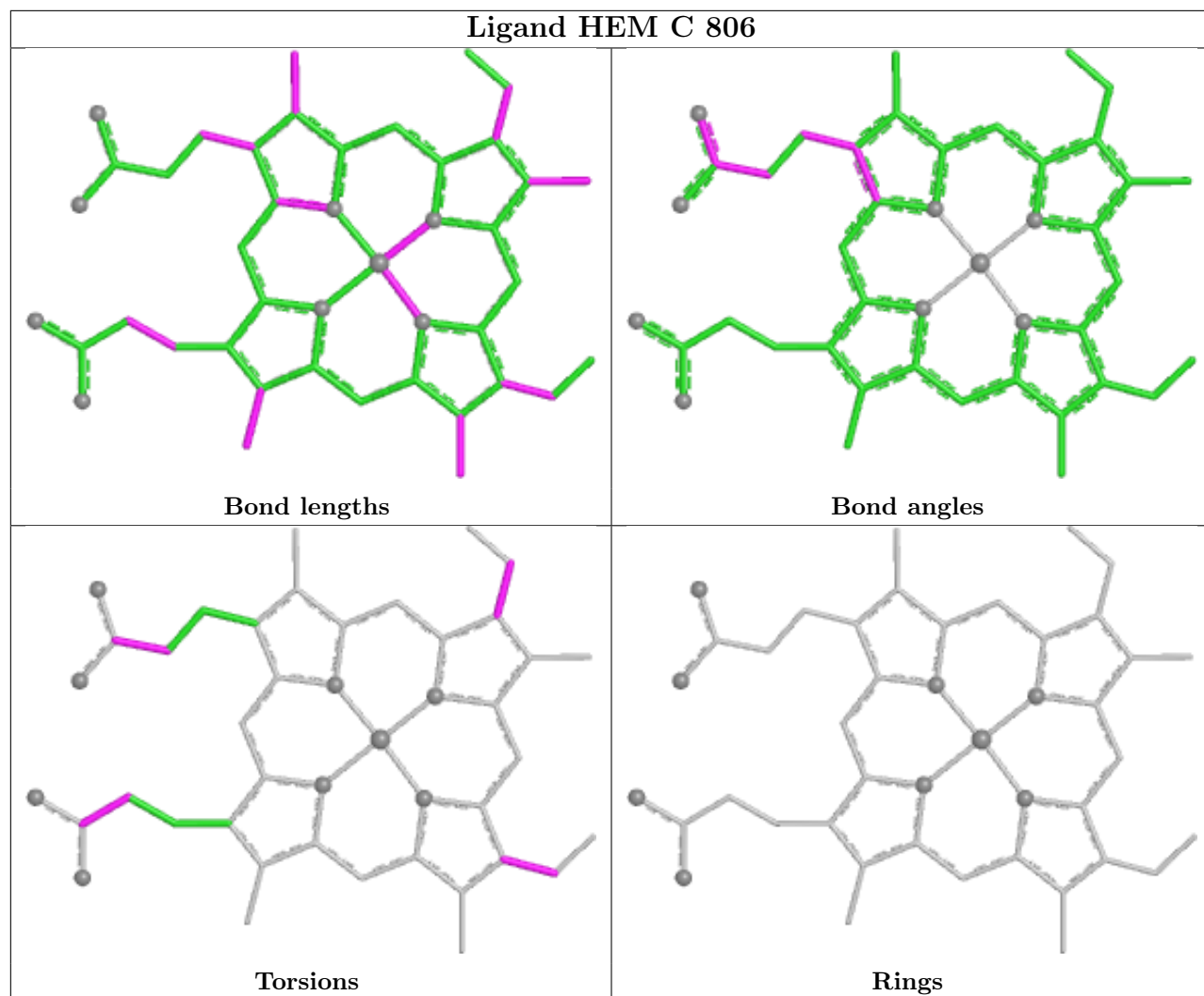
5 monomers are involved in 16 short contacts:

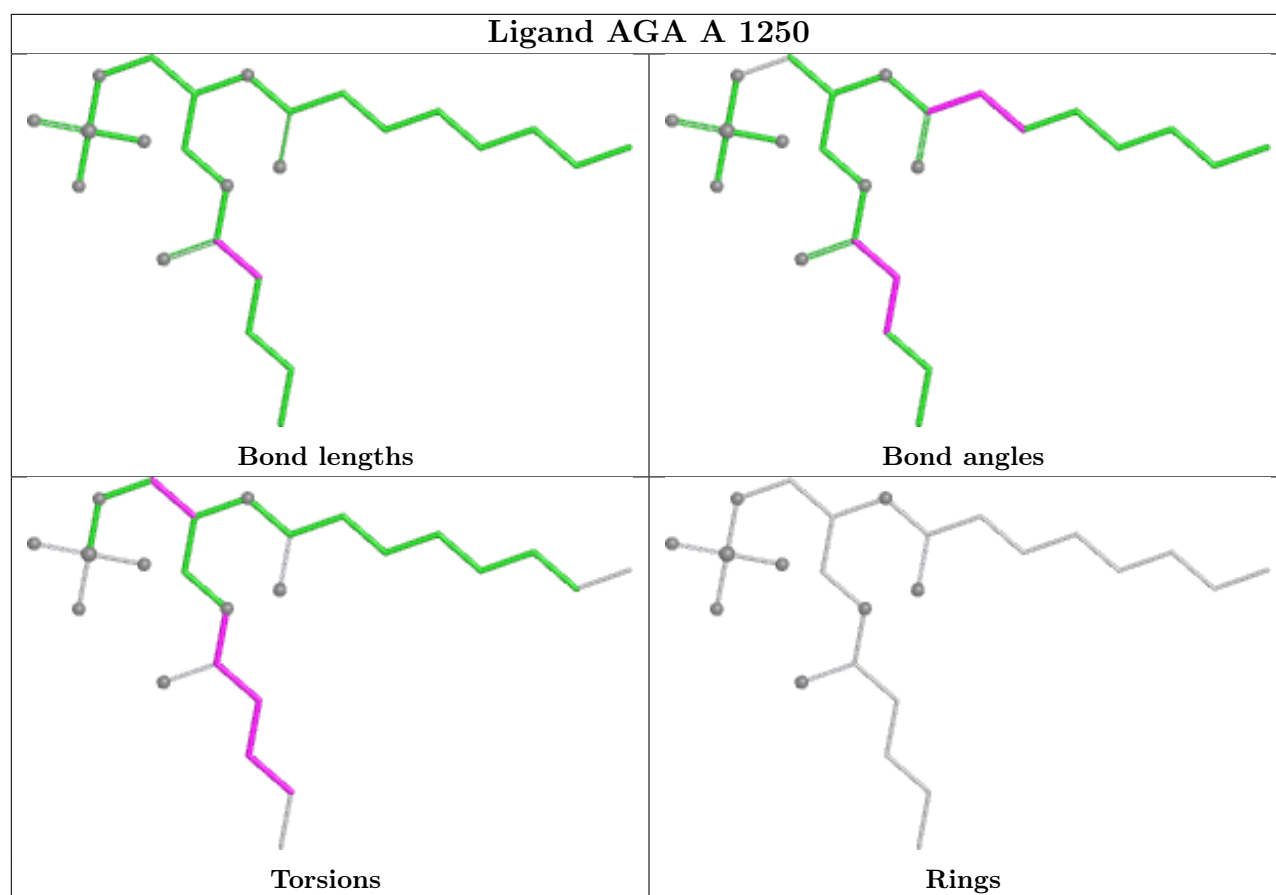
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1247	MD1	7	0
6	A	1249	SF4	1	0
9	C	806	HEM	3	0
4	A	1251	MD1	3	0
6	B	803	SF4	2	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1244/1247 (99%)	-0.00	16 (1%) 75 76	19, 34, 49, 58	0
2	B	509/512 (99%)	-0.36	0 100 100	19, 28, 41, 57	0
3	C	219/225 (97%)	0.26	6 (2%) 56 58	22, 39, 53, 58	0
All	All	1972/1984 (99%)	-0.07	22 (1%) 78 79	19, 33, 49, 58	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	4.7
1	A	717	LEU	4.2
1	A	719	SER	3.7
1	A	749	VAL	3.3
3	C	80	TRP	3.2
1	A	362	ASP	3.1
1	A	718	GLY	3.0
1	A	991	ASP	2.5
3	C	81	LEU	2.4
1	A	220	TYR	2.4
1	A	467	THR	2.3
3	C	72	THR	2.3
1	A	1244	SER	2.3
1	A	874	CYS	2.3
1	A	10	PHE	2.2
1	A	875	ASP	2.2
3	C	71	LEU	2.2
1	A	52	ASN	2.1
1	A	460	LEU	2.0
3	C	78	GLU	2.0
3	C	84	GLU	2.0
1	A	449	ASN	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($\text{\AA}^2$)	Q<0.9
3	FME	C	1	10/11	0.89	0.12	53,57,63,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

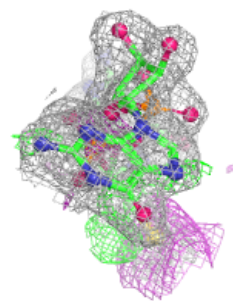
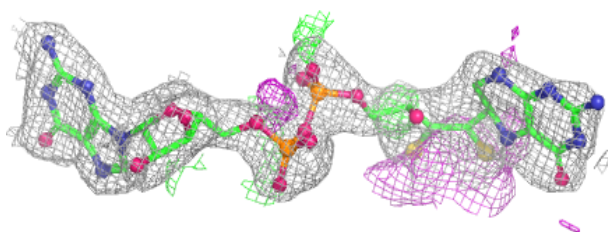
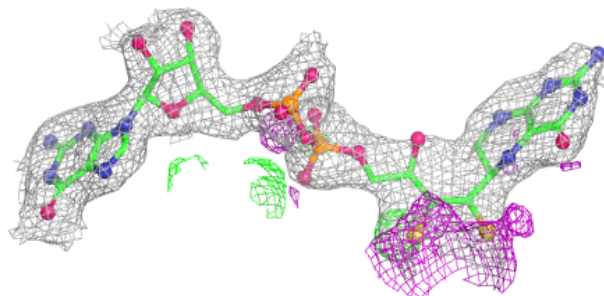
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MD1	A	1247	47/47	0.90	0.10	30,38,58,65	0
7	AGA	A	1250	25/30	0.91	0.12	34,38,47,48	0
9	HEM	C	807	43/43	0.92	0.12	44,46,53,56	0
4	MD1	A	1251	47/47	0.93	0.09	26,39,53,56	0
6	SF4	B	804	8/8	0.95	0.06	31,35,37,37	0
5	6MO	A	1248	1/1	0.96	0.25	61,61,61,61	0
6	SF4	B	802	8/8	0.97	0.04	26,28,30,32	0
6	SF4	A	1249	8/8	0.97	0.06	31,31,33,34	0
9	HEM	C	806	43/43	0.98	0.07	25,28,30,35	0
6	SF4	B	803	8/8	0.99	0.05	19,22,24,24	0
8	F3S	B	805	7/7	0.99	0.05	26,26,28,28	0

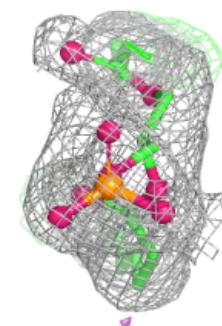
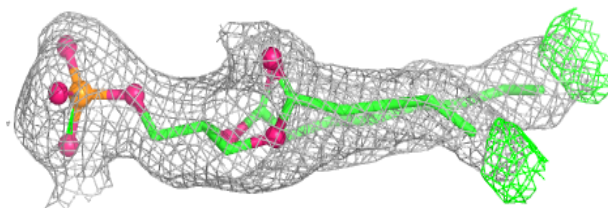
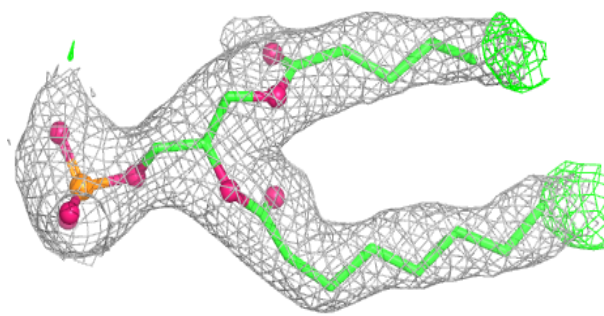
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

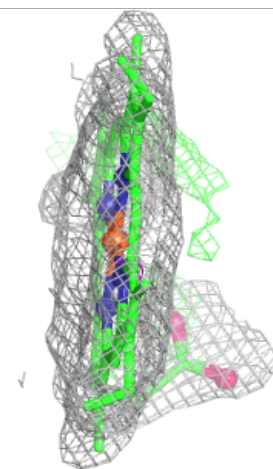
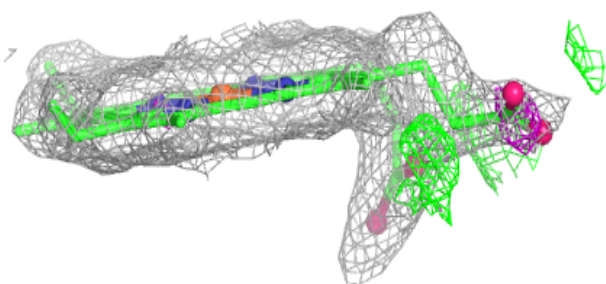
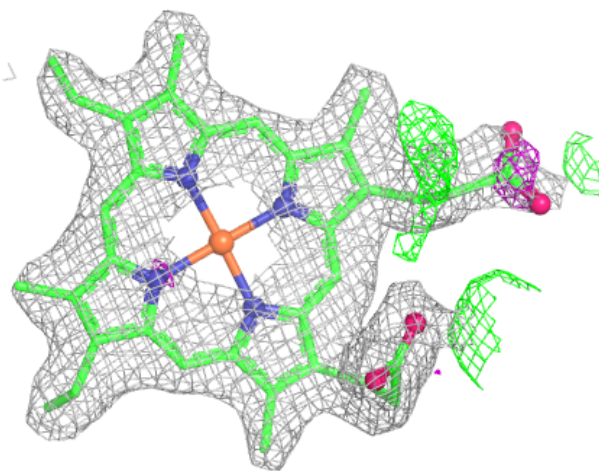
**Electron density around AGA A 1250:**

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



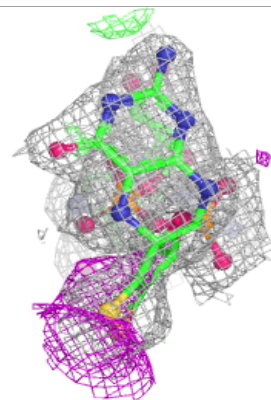
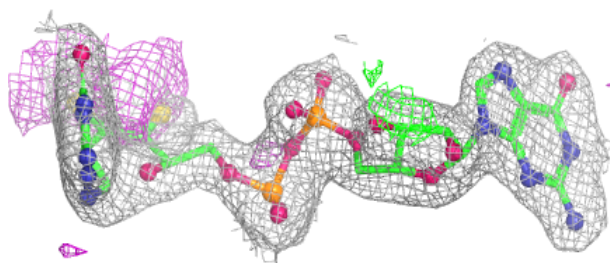
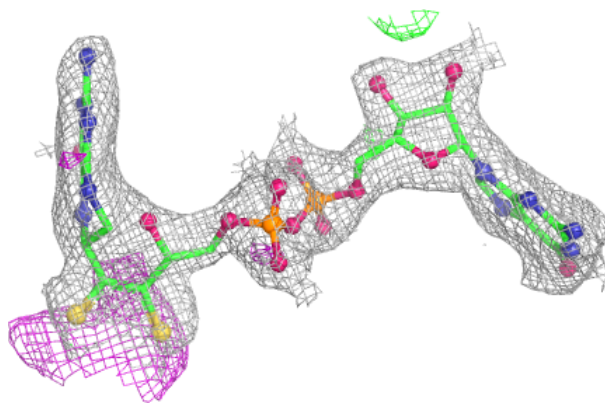
Electron density around HEM C 807:

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

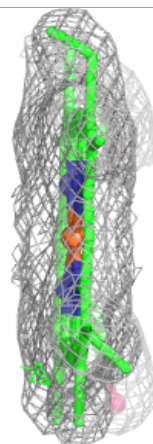
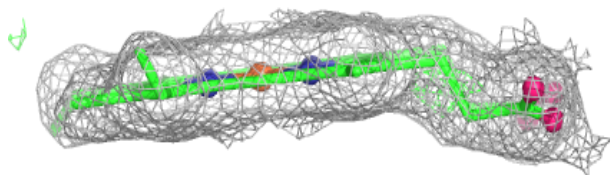
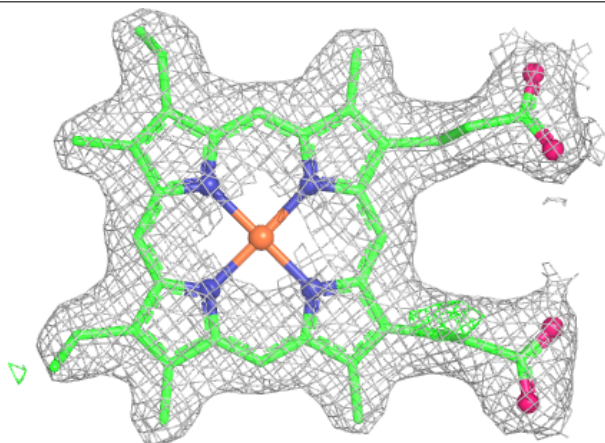


Electron density around MD1 A 1251:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.