



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:19 PM EDT

PDB ID : 1SIW / pdb_00001siw
Title : Crystal structure of the apomolybdo-NarGHI
Authors : Rothery, R.A.; Bertero, M.G.; Cammack, R.; Palak, M.; Blasco, F.; Strynadka, N.C.; Weiner, J.H.
Deposited on : 2004-03-01
Resolution : 2.20 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

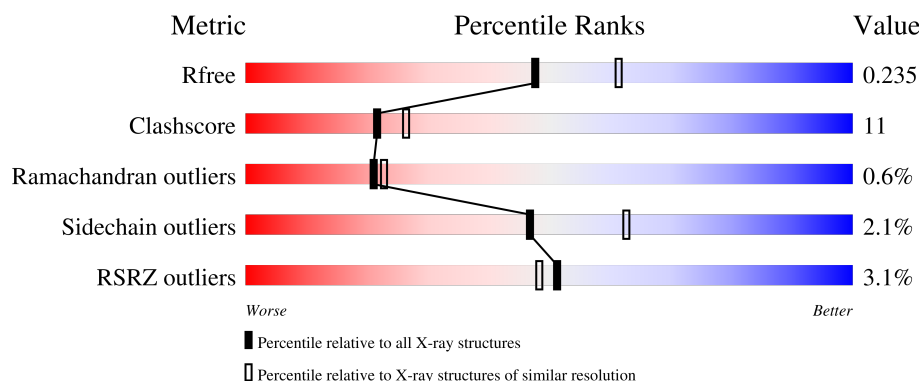
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

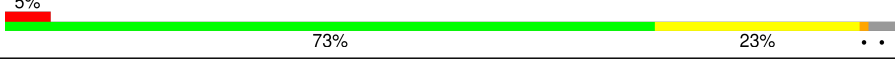
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1246	
2	B	512	
3	C	225	

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
5	SF4	B	803	-	-	X	-
6	3PH	B	1310	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16430 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	1240	Total	C	N	O	S	0	0	0
			9851	6225	1726	1853	47			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	508	Total	C	N	O	S	0	0	0
			4041	2557	700	752	32			

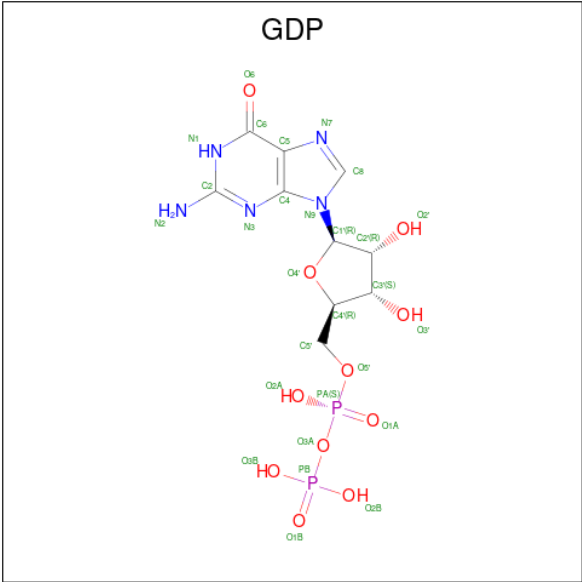
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1742	1155	294	280	13			

There is a discrepancy between the modelled and reference sequences:

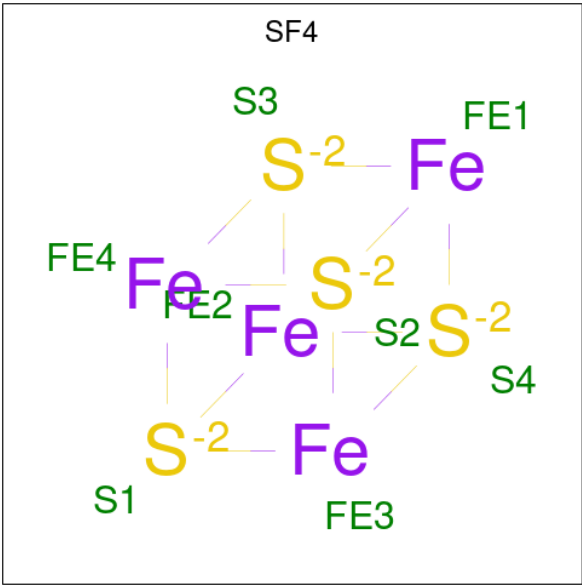
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	MET	modified residue	UNP P11350

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



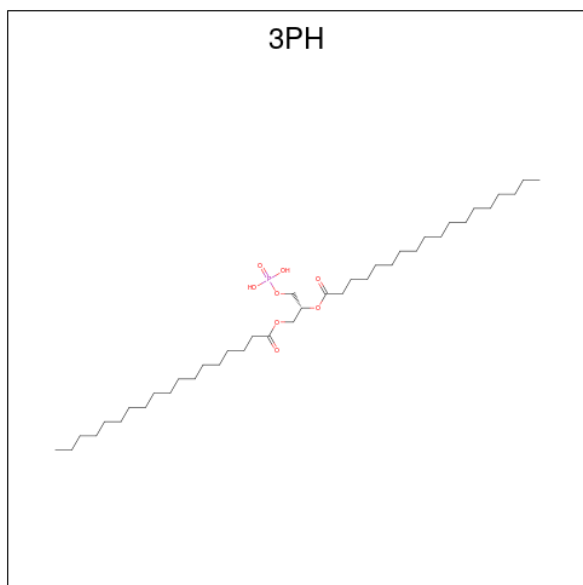
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	Fe 4	S 4	0	0
5	B	1	Total 8	Fe 4	S 4	0	0
5	B	1	Total 8	Fe 4	S 4	0	0

Continued on next page...

Continued from previous page...

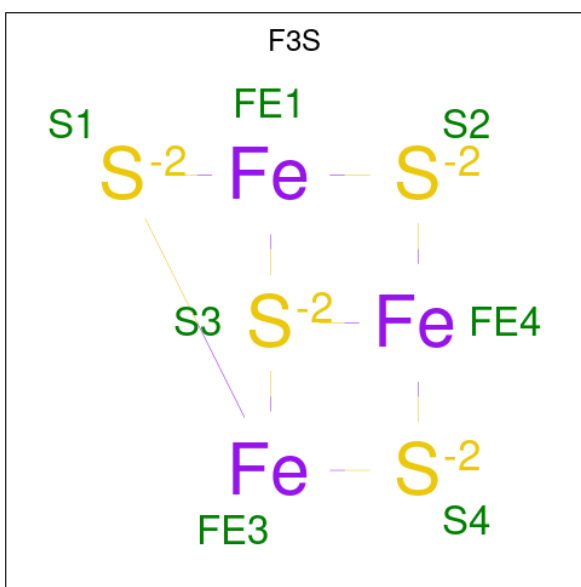
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



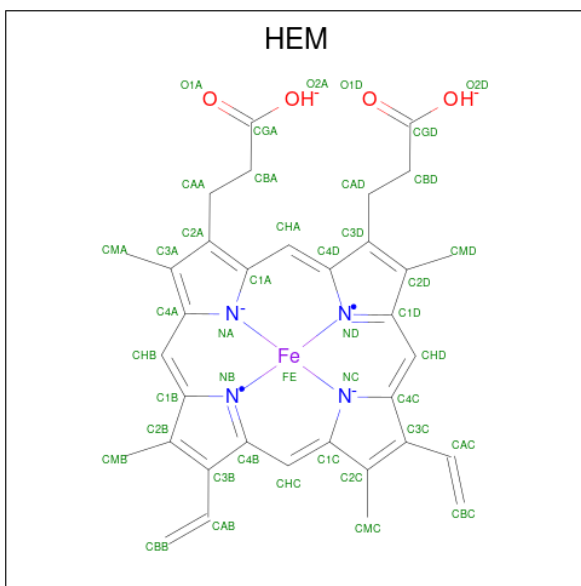
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			27	18	8	1		
6	B	1	Total	C	O	P	0	0
			18	9	8	1		

- Molecule 7 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

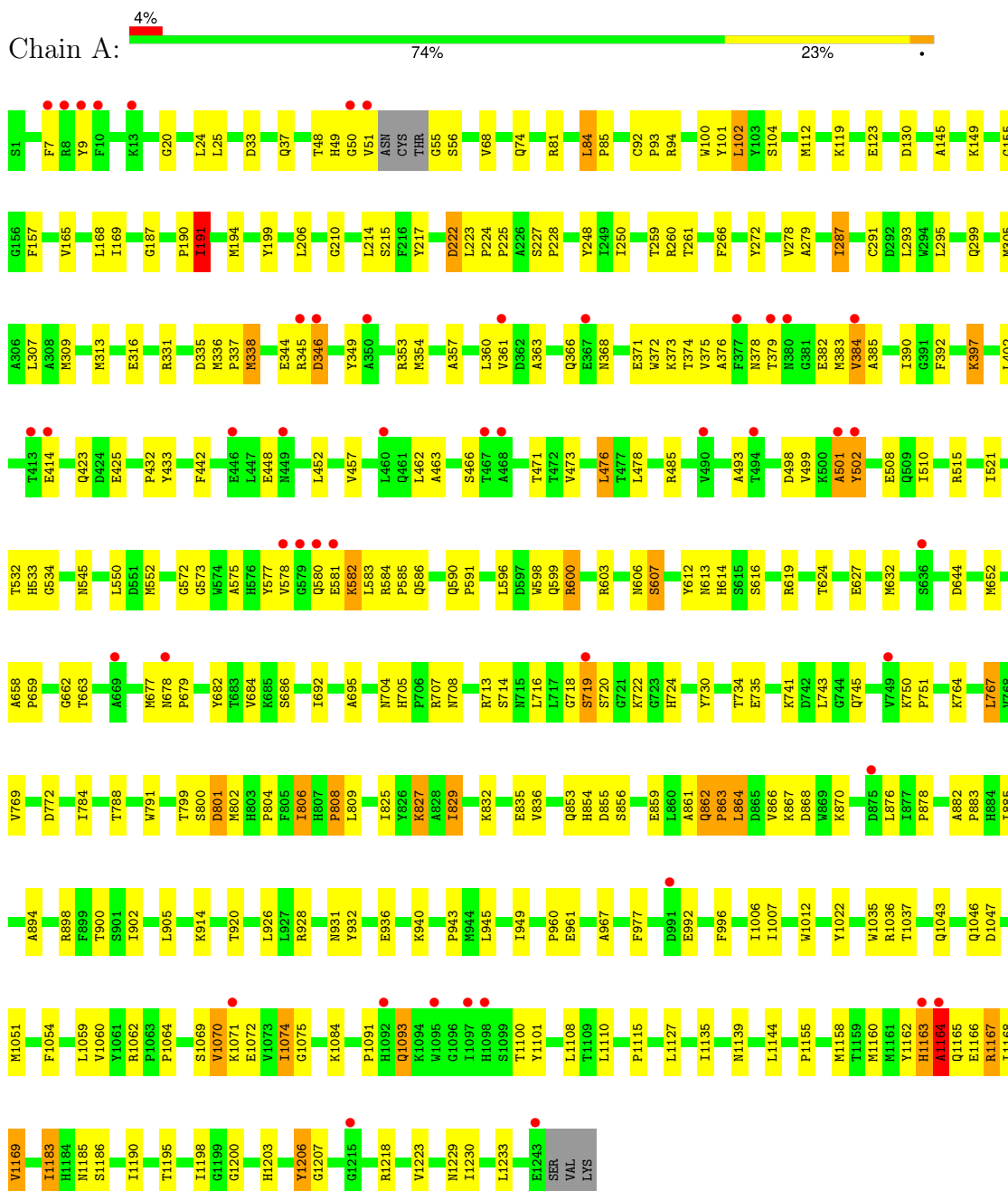
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	328	Total 328	O 328	0	0
9	B	228	Total 228	O 228	0	0
9	C	42	Total 42	O 42	0	0

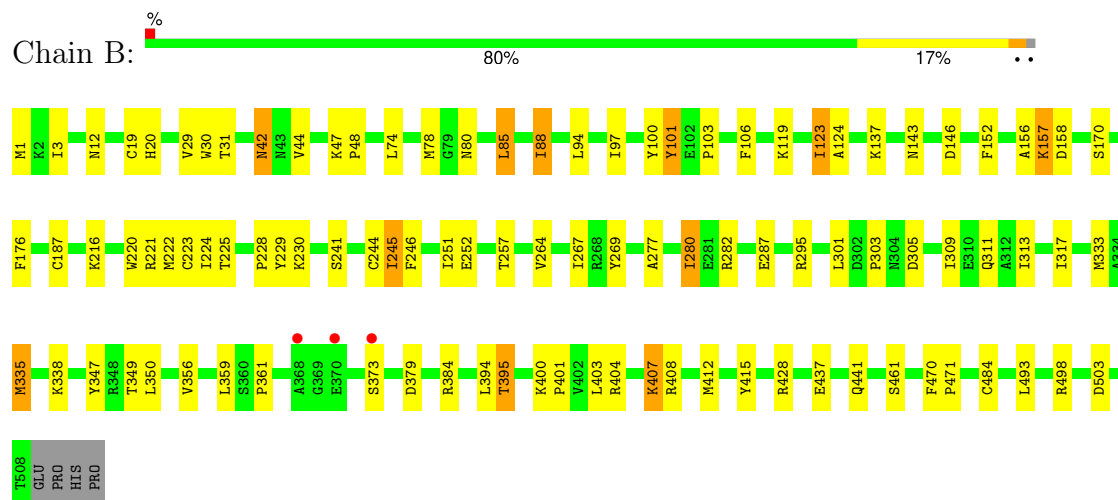
3 Residue-property plots

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

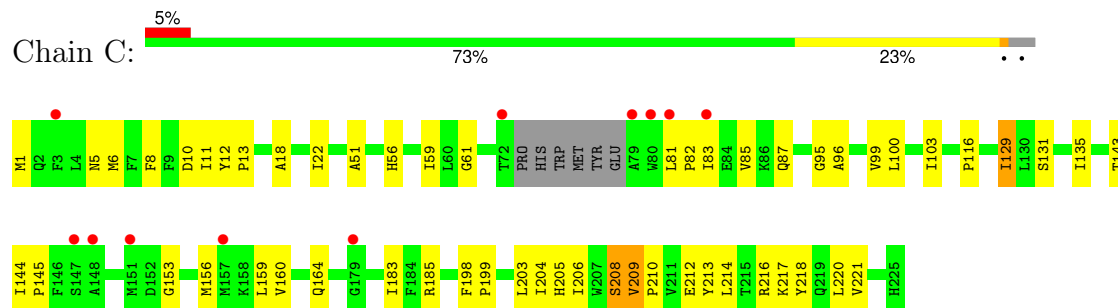
- Molecule 1: Respiratory nitrate reductase 1 alpha chain



- Molecule 2: Respiratory nitrate reductase 1 beta chain



- Molecule 3: Respiratory nitrate reductase 1 gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.00Å 241.28Å 140.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.20 29.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.73-2.20) 97.3 (29.73-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.244 0.195 , 0.235	Depositor DCC
R_{free} test set	6475 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16430	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, FME, 3PH, SF4, F3S, GDP

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	0.40	0/10110	0.94	42/13722 (0.3%)
2	B	0.41	0/4137	0.93	15/5597 (0.3%)
3	C	0.39	0/1779	0.88	7/2404 (0.3%)
All	All	0.40	0/16026	0.93	64/21723 (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	0	3

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	CA-C-N	15.24	150.66	121.54
1	A	1163	HIS	C-N-CA	15.24	150.66	121.54
1	A	502	TYR	CA-C-O	10.52	135.55	120.51
1	A	501	ALA	CA-C-O	-9.59	110.26	122.63
1	A	1070	VAL	N-CA-C	9.29	119.42	111.90
1	A	501	ALA	CA-C-N	9.18	139.08	121.54
1	A	501	ALA	C-N-CA	9.18	139.08	121.54
2	B	30	TRP	N-CA-C	7.98	123.15	113.41
1	A	607	SER	N-CA-C	7.91	120.90	111.33
1	A	809	LEU	N-CA-C	-7.56	97.42	109.59
1	A	1163	HIS	CB-CA-C	7.12	121.01	109.90
3	C	209	VAL	CA-C-N	7.11	128.73	119.84
3	C	209	VAL	C-N-CA	7.11	128.73	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	862	GLN	CA-C-N	6.74	126.19	118.85
1	A	862	GLN	C-N-CA	6.74	126.19	118.85
1	A	502	TYR	O-C-N	-6.73	113.64	122.59
1	A	1169	VAL	N-CA-C	6.72	117.53	108.11
2	B	88	ILE	N-CA-C	6.68	117.44	110.62
1	A	102	LEU	N-CA-C	6.65	119.09	111.11
1	A	1164	ALA	N-CA-C	6.46	124.55	110.80
2	B	359	LEU	N-CA-C	-6.33	101.40	110.59
1	A	74	GLN	N-CA-C	-6.28	101.19	110.48
2	B	31	THR	N-CA-C	6.21	118.84	110.88
1	A	614	HIS	N-CA-C	6.21	119.03	111.82
1	A	1035	TRP	N-CA-C	-6.19	101.12	110.28
1	A	222	ASP	N-CA-C	-6.17	105.91	113.50
1	A	863	PRO	N-CA-C	6.14	121.63	113.40
1	A	1167	ARG	N-CA-C	6.14	120.08	112.59
1	A	1206	TYR	N-CA-C	6.10	118.58	110.53
1	A	573	GLY	N-CA-C	5.98	119.35	111.52
1	A	853	GLN	N-CA-C	5.97	118.98	109.24
1	A	501	ALA	N-CA-CB	5.90	117.72	110.53
2	B	395	THR	N-CA-C	5.81	117.87	110.61
1	A	101	TYR	N-CA-C	5.77	118.52	111.82
1	A	583	LEU	N-CA-C	-5.77	97.02	107.75
1	A	384	VAL	N-CA-C	5.67	115.70	107.88
2	B	287	GLU	N-CA-C	5.66	117.12	111.07
2	B	216	LYS	N-CA-C	5.60	119.38	112.54
1	A	1163	HIS	CA-C-O	5.55	127.25	120.92
1	A	1071	LYS	N-CA-C	5.41	117.94	111.71
2	B	94	LEU	N-CA-C	5.41	116.22	109.57
2	B	29	VAL	N-CA-C	5.39	116.05	110.82
2	B	280	ILE	N-CA-C	5.39	116.02	110.36
3	C	208	SER	N-CA-C	5.37	118.95	112.93
1	A	808	PRO	N-CA-C	5.37	123.52	112.47
1	A	316	GLU	N-CA-C	5.36	119.88	113.23
1	A	502	TYR	CB-CA-C	5.34	121.05	110.42
1	A	612	TYR	N-CA-C	-5.32	105.48	111.28
1	A	730	TYR	N-CA-C	5.28	118.88	112.23
2	B	157	LYS	N-CA-C	-5.25	106.70	113.01
3	C	61	GLY	N-CA-C	-5.19	106.48	112.50
2	B	222	MET	N-CA-C	-5.15	107.12	113.41
3	C	51	ALA	N-CA-C	5.15	116.58	111.07
1	A	582	LYS	N-CA-C	5.12	117.65	108.17
1	A	1043	GLN	N-CA-C	5.11	116.59	108.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	379	ASP	N-CA-C	-5.08	101.87	109.95
1	A	1093	GLN	N-CA-C	5.08	116.66	110.41
2	B	394	LEU	N-CA-C	5.07	120.31	113.72
1	A	84	LEU	CA-C-N	-5.05	115.03	120.03
1	A	84	LEU	C-N-CA	-5.05	115.03	120.03
3	C	218	TYR	N-CA-C	5.03	116.46	111.07
3	C	8	PHE	N-CA-C	5.02	117.49	111.71
2	B	493	LEU	N-CA-C	5.02	116.75	111.28
1	A	829	ILE	N-CA-C	-5.01	105.82	110.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9851	0	9513	241	0
2	B	4041	0	3967	74	0
3	C	1742	0	1787	31	0
4	A	28	0	12	4	0
5	A	8	0	0	1	0
5	B	24	0	0	3	0
6	A	27	0	27	0	0
6	B	18	0	10	0	0
7	B	7	0	0	0	0
8	C	86	0	60	1	0
9	A	328	0	0	4	2
9	B	228	0	0	7	0
9	C	42	0	0	1	0
All	All	16430	0	15376	338	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 11.

All (338) 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:552:MET:HE1	1:A:1059:LEU:HA	1.43	0.96
1:A:552:MET:HE2	1:A:1060:VAL:H	1.33	0.92
1:A:378:ASN:HD21	1:A:382:GLU:HB2	1.41	0.84
2:B:407:LYS:HD3	9:B:1482:HOH:O	1.77	0.83
3:C:129:ILE:HD11	3:C:203:LEU:HD11	1.62	0.82
1:A:663:THR:HG21	1:A:692:ILE:HD12	1.62	0.80
1:A:724:HIS:HE1	1:A:1167:ARG:HH11	1.29	0.80
1:A:191:ILE:H	1:A:191:ILE:HD12	1.47	0.80
1:A:1168:ILE:HD13	1:A:1169:VAL:HG23	1.63	0.77
1:A:902:ILE:HD13	1:A:943:PRO:HB2	1.68	0.76
1:A:165:VAL:O	1:A:169:ILE:HG12	1.86	0.75
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.68	0.74
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.69	0.74
2:B:123:ILE:HD13	2:B:124:ALA:H	1.52	0.73
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.71	0.72
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.72	0.71
1:A:508:GLU:OE1	1:A:515:ARG:HD2	1.91	0.71
1:A:719:SER:HB2	1:A:1164:ALA:CB	2.21	0.70
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.73	0.70
3:C:99:VAL:O	3:C:103:ILE:HG12	1.91	0.70
1:A:552:MET:CE	1:A:1060:VAL:H	2.05	0.69
2:B:3:ILE:HD13	2:B:311:GLN:HG3	1.74	0.68
1:A:1168:ILE:CD1	1:A:1169:VAL:HG23	2.24	0.67
1:A:378:ASN:ND2	1:A:382:GLU:HB2	2.10	0.67
2:B:245:ILE:HD13	2:B:245:ILE:H	1.60	0.66
1:A:1183:ILE:HD13	1:A:1183:ILE:H	1.60	0.66
2:B:223:CYS:SG	2:B:224:ILE:HD12	2.36	0.66
2:B:303:PRO:O	2:B:309:ILE:HD11	1.96	0.66
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.78	0.65
1:A:338:MET:HB3	1:A:354:MET:HE2	1.78	0.65
2:B:123:ILE:HD13	2:B:124:ALA:N	2.13	0.64
1:A:287:ILE:HD13	1:A:287:ILE:O	1.97	0.64
3:C:96:ALA:O	3:C:100:LEU:HD13	1.97	0.63
1:A:1218:ARG:HH21	1:A:1218:ARG:HG3	1.63	0.63
1:A:686:SER:HB3	1:A:692:ILE:HG12	1.79	0.62
1:A:695:ALA:HB1	1:A:704:ASN:HB3	1.80	0.62
1:A:50:GLY:O	1:A:51:VAL:HG22	1.99	0.62
1:A:397:LYS:HE3	1:A:397:LYS:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:CD2	1:A:521:ILE:HD11	2.31	0.61
1:A:1135:ILE:HD12	1:A:1135:ILE:C	2.25	0.61
1:A:799:THR:CG2	1:A:806:ILE:HG12	2.31	0.61
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.82	0.61
1:A:619:ARG:O	1:A:743:LEU:HD13	2.00	0.61
2:B:224:ILE:HD12	2:B:224:ILE:H	1.65	0.60
2:B:428:ARG:NH2	2:B:428:ARG:HB3	2.17	0.60
1:A:825:ILE:O	1:A:829:ILE:HG12	2.02	0.60
1:A:596:LEU:O	1:A:600:ARG:HD2	2.01	0.59
2:B:309:ILE:O	2:B:313:ILE:HG12	2.02	0.59
1:A:55:GLY:HA3	5:A:1248:SF4:S3	2.42	0.59
1:A:190:PRO:HD3	1:A:714:SER:HB2	1.84	0.59
1:A:1074:ILE:HD13	1:A:1075:GLY:N	2.17	0.59
1:A:720:SER:HB2	4:A:1247:GDP:O2B	2.03	0.59
2:B:19:CYS:O	2:B:20:HIS:HB2	2.02	0.58
3:C:6:MET:O	3:C:10:ASP:HB2	2.02	0.58
1:A:707:ARG:C	1:A:708:ASN:HD22	2.11	0.58
3:C:56:HIS:HA	3:C:59:ILE:HG22	1.85	0.57
2:B:1:MET:SD	2:B:3:ILE:HD11	2.44	0.57
1:A:360:LEU:HG	1:A:383:MET:HE3	1.85	0.57
2:B:3:ILE:HD13	2:B:311:GLN:CG	2.34	0.57
1:A:360:LEU:N	1:A:360:LEU:HD22	2.20	0.57
1:A:20:GLY:O	3:C:217:LYS:HD2	2.05	0.56
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.37	0.56
1:A:1100:THR:O	1:A:1101:TYR:HB2	2.06	0.56
1:A:24:LEU:HD12	3:C:221:VAL:O	2.06	0.56
1:A:713:ARG:HA	4:A:1247:GDP:C4	2.40	0.56
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.87	0.56
1:A:191:ILE:HD12	1:A:191:ILE:N	2.17	0.56
1:A:55:GLY:N	1:A:580:GLN:NE2	2.53	0.56
1:A:295:LEU:HD11	1:A:521:ILE:CD1	2.36	0.56
1:A:652:MET:HE3	1:A:867:LYS:O	2.05	0.56
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.41	0.56
1:A:462:LEU:HD12	1:A:466:SER:OG	2.06	0.55
1:A:652:MET:HE1	1:A:866:VAL:CG1	2.37	0.55
1:A:1195:THR:HA	1:A:1198:ILE:CD1	2.36	0.55
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.89	0.55
1:A:552:MET:CE	1:A:1059:LEU:HA	2.29	0.55
1:A:336:MET:N	1:A:337:PRO:HD2	2.22	0.55
1:A:662:GLY:HA2	1:A:704:ASN:OD1	2.07	0.55
1:A:49:HIS:HB3	1:A:791:TRP:CZ3	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:TYR:HB3	1:A:448:GLU:O	2.07	0.54
2:B:441:GLN:HG3	9:B:1520:HOH:O	2.06	0.54
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.43	0.54
1:A:1093:GLN:HB3	1:A:1162:TYR:HB3	1.89	0.54
1:A:145:ALA:O	1:A:149:LYS:HG3	2.07	0.54
2:B:220:TRP:C	2:B:221:ARG:HG3	2.33	0.54
1:A:724:HIS:HE1	1:A:1167:ARG:NH1	2.01	0.54
3:C:18:ALA:O	3:C:22:ILE:HG22	2.07	0.54
2:B:224:ILE:HD12	2:B:224:ILE:N	2.23	0.54
2:B:305:ASP:O	2:B:309:ILE:HG12	2.08	0.54
3:C:206:ILE:HD11	8:C:806:HEM:HBC2	1.90	0.54
1:A:295:LEU:HD11	1:A:521:ILE:HD12	1.89	0.54
1:A:992:GLU:HG2	1:A:1007:ILE:HD11	1.90	0.53
2:B:280:ILE:HG23	2:B:350:LEU:HD12	1.89	0.53
2:B:282:ARG:HG2	2:B:295:ARG:NH2	2.23	0.53
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.89	0.53
1:A:345:ARG:HH21	1:A:345:ARG:HG3	1.72	0.53
1:A:894:ALA:O	1:A:898:ARG:HG3	2.07	0.53
3:C:81:LEU:N	3:C:81:LEU:HD23	2.24	0.53
1:A:168:LEU:HD23	1:A:168:LEU:C	2.34	0.52
1:A:168:LEU:HD23	1:A:168:LEU:O	2.10	0.52
1:A:344:GLU:HG2	1:A:349:TYR:HE1	1.74	0.52
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.10	0.52
1:A:1168:ILE:HD12	1:A:1169:VAL:N	2.24	0.52
3:C:129:ILE:HD13	3:C:129:ILE:O	2.10	0.52
1:A:94:ARG:HB3	1:A:1101:TYR:CE1	2.45	0.52
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.91	0.52
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.91	0.52
3:C:12:TYR:N	3:C:13:PRO:HD2	2.25	0.52
1:A:338:MET:HG3	1:A:374:THR:HB	1.90	0.52
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.91	0.52
2:B:245:ILE:HD13	5:B:803:SF4:S3	2.49	0.52
2:B:187:CYS:HB3	2:B:349:THR:O	2.10	0.52
1:A:856:SER:O	1:A:859:GLU:HG2	2.10	0.52
1:A:1183:ILE:HG12	1:A:1185:ASN:H	1.74	0.52
2:B:269:TYR:CD1	2:B:333:MET:HE1	2.45	0.52
1:A:718:GLY:O	1:A:719:SER:HB3	2.10	0.51
1:A:876:LEU:C	1:A:876:LEU:HD23	2.35	0.51
2:B:277:ALA:O	2:B:280:ILE:HG12	2.10	0.51
1:A:33:ASP:O	1:A:37:GLN:HG3	2.10	0.51
1:A:293:LEU:HD23	1:A:521:ILE:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:GLN:CB	1:A:1162:TYR:HB3	2.40	0.51
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.09	0.51
2:B:137:LYS:HA	9:B:1476:HOH:O	2.10	0.51
1:A:155:GLY:HA2	9:B:1440:HOH:O	2.11	0.51
2:B:3:ILE:N	2:B:3:ILE:HD12	2.25	0.51
2:B:246:PHE:HA	5:B:803:SF4:S4	2.50	0.51
1:A:582:LYS:HG2	1:A:584:ARG:HG2	1.93	0.51
1:A:305:MET:O	1:A:309:MET:HG3	2.10	0.51
1:A:471:THR:HG21	1:A:476:LEU:HD13	1.92	0.50
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.93	0.50
1:A:1093:GLN:NE2	1:A:1164:ALA:O	2.44	0.50
1:A:194:MET:HE3	1:A:580:GLN:CB	2.42	0.50
1:A:532:THR:O	1:A:533:HIS:HB2	2.11	0.50
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.37	0.50
1:A:1229:ASN:C	1:A:1230:ILE:HD12	2.37	0.50
2:B:317:ILE:HD12	2:B:317:ILE:N	2.27	0.50
1:A:931:ASN:O	1:A:932:TYR:HB2	2.10	0.50
3:C:11:ILE:C	3:C:13:PRO:HD2	2.37	0.50
1:A:309:MET:O	1:A:313:MET:HG3	2.12	0.50
1:A:68:VAL:HB	1:A:102:LEU:HD22	1.94	0.49
1:A:1007:ILE:N	1:A:1007:ILE:HD12	2.27	0.49
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.94	0.49
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.46	0.49
1:A:260:ARG:HD2	1:A:802:MET:SD	2.52	0.49
1:A:767:LEU:HD13	1:A:769:VAL:HG23	1.93	0.49
1:A:225:PRO:O	1:A:228:PRO:HD2	2.13	0.49
1:A:336:MET:HA	1:A:473:VAL:HB	1.94	0.49
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.47	0.49
1:A:1036:ARG:HD3	9:A:1439:HOH:O	2.13	0.49
1:A:335:ASP:O	1:A:338:MET:HB2	2.12	0.49
2:B:157:LYS:NZ	2:B:157:LYS:HB3	2.28	0.49
1:A:684:VAL:HG13	1:A:876:LEU:HD22	1.95	0.49
1:A:51:VAL:H	1:A:194:MET:HB3	1.78	0.49
2:B:119:LYS:HD2	2:B:119:LYS:N	2.28	0.49
1:A:750:LYS:HD2	1:A:750:LYS:N	2.28	0.49
1:A:452:LEU:N	1:A:452:LEU:HD12	2.27	0.49
1:A:677:MET:HG3	1:A:682:TYR:HB2	1.95	0.49
1:A:827:LYS:HD2	1:A:900:THR:HG22	1.95	0.49
1:A:582:LYS:HD2	1:A:801:ASP:HA	1.95	0.48
1:A:724:HIS:CE1	1:A:1167:ARG:HH11	2.20	0.48
1:A:835:GLU:HG3	1:A:836:VAL:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:SER:O	3:C:135:ILE:HG12	2.14	0.48
1:A:720:SER:HB2	4:A:1247:GDP:PB	2.53	0.48
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.48	0.48
1:A:425:GLU:HG3	1:A:457:VAL:CG2	2.44	0.47
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.49	0.47
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.13	0.47
1:A:864:LEU:HD22	1:A:864:LEU:N	2.29	0.47
1:A:722:LYS:HB2	1:A:1190:ILE:HD11	1.97	0.47
1:A:1074:ILE:HD13	1:A:1074:ILE:C	2.39	0.47
1:A:112:MET:HE3	1:A:157:PHE:HB3	1.97	0.47
1:A:432:PRO:HD3	1:A:632:MET:CE	2.43	0.47
1:A:478:LEU:HD23	1:A:485:ARG:HD2	1.96	0.47
1:A:299:GLN:NE2	1:A:1158:MET:HE2	2.29	0.47
1:A:878:PRO:HB3	1:A:885:ILE:HG12	1.97	0.47
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.95	0.47
1:A:652:MET:CE	1:A:862:GLN:HE22	2.28	0.47
1:A:902:ILE:HD12	1:A:945:LEU:HG	1.95	0.47
2:B:80:ASN:HB2	9:B:1426:HOH:O	2.14	0.47
1:A:493:ALA:HA	1:A:498:ASP:OD2	2.14	0.47
1:A:719:SER:O	1:A:1185:ASN:ND2	2.48	0.47
2:B:373:SER:HB3	2:B:428:ARG:NH1	2.29	0.47
1:A:390:ILE:HD11	1:A:859:GLU:OE1	2.14	0.47
1:A:423:GLN:HB2	1:A:457:VAL:O	2.14	0.47
1:A:868:ASP:OD1	1:A:870:LYS:HB3	2.14	0.47
1:A:772:ASP:C	1:A:788:THR:HG22	2.40	0.47
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.30	0.47
3:C:160:VAL:O	3:C:164:GLN:HG3	2.15	0.47
2:B:224:ILE:HD11	2:B:241:SER:OG	2.14	0.47
1:A:81:ARG:CZ	1:A:84:LEU:HD11	2.45	0.46
1:A:250:ILE:CD1	1:A:278:VAL:HB	2.45	0.46
1:A:914:LYS:O	1:A:914:LYS:HG2	2.15	0.46
1:A:1195:THR:O	1:A:1198:ILE:HD13	2.15	0.46
1:A:222:ASP:HB3	1:A:578:VAL:HG23	1.96	0.46
1:A:1070:VAL:HG13	1:A:1223:VAL:CG2	2.46	0.46
1:A:169:ILE:HD11	1:A:784:ILE:HD12	1.97	0.46
1:A:293:LEU:HD21	1:A:521:ILE:HD11	1.96	0.46
1:A:658:ALA:HA	1:A:659:PRO:C	2.40	0.46
2:B:1:MET:SD	2:B:3:ILE:CD1	3.04	0.46
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.51	0.46
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.84	0.46
2:B:78:MET:HG2	2:B:225:THR:HG22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:HD12	1:A:769:VAL:HG21	1.97	0.46
2:B:428:ARG:HB3	2:B:428:ARG:HH21	1.81	0.46
1:A:223:LEU:O	1:A:225:PRO:HD3	2.15	0.46
1:A:591:PRO:HA	1:A:596:LEU:HB2	1.96	0.46
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.97	0.46
1:A:279:ALA:HB2	1:A:291:CYS:SG	2.56	0.45
1:A:832:LYS:O	1:A:836:VAL:HG23	2.17	0.45
1:A:225:PRO:C	1:A:228:PRO:HD2	2.42	0.45
1:A:949:ILE:HD12	1:A:996:PHE:CE2	2.51	0.45
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.82	0.45
2:B:245:ILE:H	2:B:245:ILE:CD1	2.27	0.45
2:B:97:ILE:HD11	2:B:103:PRO:HD2	1.98	0.45
1:A:217:TYR:CZ	1:A:581:GLU:HG2	2.52	0.45
2:B:143:ASN:CG	2:B:146:ASP:HB2	2.41	0.45
1:A:194:MET:HE3	1:A:580:GLN:HB3	2.00	0.44
1:A:861:ALA:HB3	1:A:1200:GLY:O	2.17	0.44
1:A:960:PRO:O	1:A:967:ALA:HB2	2.16	0.44
1:A:373:LYS:HD3	1:A:392:PHE:CE1	2.53	0.44
2:B:282:ARG:HG2	2:B:295:ARG:HH22	1.82	0.44
1:A:678:ASN:HB2	1:A:679:PRO:HD2	2.00	0.44
3:C:95:GLY:O	3:C:99:VAL:HG23	2.18	0.44
1:A:199:TYR:CD1	1:A:199:TYR:C	2.95	0.44
1:A:272:TYR:HB3	2:B:412:MET:HE3	1.99	0.44
2:B:85:LEU:HD22	3:C:214:LEU:HD21	1.99	0.44
1:A:259:THR:HG21	9:A:1540:HOH:O	2.16	0.44
2:B:176:PHE:CD1	2:B:176:PHE:C	2.95	0.44
2:B:230:LYS:HA	9:B:1326:HOH:O	2.17	0.44
1:A:248:TYR:HE2	1:A:250:ILE:HD11	1.83	0.44
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.53	0.44
2:B:404:ARG:O	2:B:408:ARG:HG3	2.17	0.44
3:C:143:THR:HG22	3:C:183:ILE:HG12	1.99	0.44
1:A:50:GLY:O	1:A:51:VAL:CG2	2.66	0.44
1:A:50:GLY:HA2	1:A:194:MET:HB3	2.00	0.44
1:A:287:ILE:HD13	1:A:287:ILE:C	2.42	0.44
1:A:7:PHE:N	1:A:7:PHE:CD1	2.86	0.44
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.18	0.44
1:A:25:LEU:HD11	3:C:220:LEU:HD22	2.00	0.43
1:A:734:THR:HG23	1:A:735:GLU:O	2.18	0.43
1:A:936:GLU:HA	1:A:940:LYS:HD2	1.99	0.43
2:B:12:ASN:HA	2:B:356:VAL:HB	1.99	0.43
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:PRO:HG2	2:B:229:TYR:CD1	2.52	0.43
2:B:335:MET:O	2:B:338:LYS:HE3	2.18	0.43
3:C:144:ILE:N	3:C:145:PRO:HD2	2.33	0.43
2:B:100:TYR:O	2:B:101:TYR:HB3	2.17	0.43
1:A:344:GLU:HG2	1:A:349:TYR:CE1	2.53	0.43
2:B:251:ILE:HD11	2:B:257:THR:HG22	2.00	0.43
3:C:208:SER:O	3:C:209:VAL:C	2.61	0.43
3:C:204:ILE:HD12	3:C:205:HIS:N	2.33	0.43
1:A:307:LEU:HD21	1:A:1059:LEU:HG	1.99	0.43
2:B:484:CYS:HB2	2:B:498:ARG:HG2	2.01	0.43
1:A:100:TRP:O	1:A:104:SER:HB3	2.18	0.43
1:A:586:GLN:O	1:A:590:GLN:HG3	2.19	0.43
1:A:799:THR:HG22	1:A:806:ILE:HG12	2.01	0.43
2:B:228:PRO:HB2	2:B:347:TYR:CD2	2.53	0.43
3:C:83:ILE:HD11	3:C:156:MET:HG2	2.01	0.43
1:A:51:VAL:HG13	1:A:194:MET:HB2	2.00	0.43
1:A:384:VAL:HG22	1:A:385:ALA:N	2.33	0.43
2:B:415:TYR:CE2	2:B:437:GLU:HG2	2.54	0.43
2:B:335:MET:HE3	2:B:335:MET:HA	2.00	0.43
1:A:600:ARG:HD3	1:A:905:LEU:HD13	2.01	0.43
2:B:3:ILE:HG13	2:B:301:LEU:CD1	2.49	0.43
2:B:156:ALA:C	2:B:158:ASP:H	2.27	0.43
1:A:1160:MET:HE2	1:A:1162:TYR:OH	2.19	0.42
2:B:224:ILE:H	2:B:224:ILE:CD1	2.32	0.42
1:A:346:ASP:O	1:A:346:ASP:CG	2.62	0.42
1:A:552:MET:HE1	1:A:1059:LEU:CA	2.31	0.42
1:A:584:ARG:HD3	1:A:1006:ILE:HD13	2.01	0.42
1:A:863:PRO:HG2	1:A:864:LEU:CD2	2.45	0.42
2:B:156:ALA:C	2:B:158:ASP:N	2.77	0.42
1:A:56:SER:HB2	1:A:800:SER:HB2	2.00	0.42
1:A:345:ARG:HH21	1:A:345:ARG:CG	2.32	0.42
1:A:371:GLU:OE1	1:A:371:GLU:N	2.39	0.42
1:A:598:TRP:C	1:A:599:GLN:HG3	2.44	0.42
1:A:713:ARG:HG2	4:A:1247:GDP:C6	2.54	0.42
1:A:854:HIS:O	1:A:855:ASP:HB2	2.19	0.42
3:C:159:LEU:HD22	3:C:159:LEU:H	1.85	0.42
1:A:379:THR:HG21	1:A:414:GLU:OE2	2.20	0.42
1:A:1183:ILE:HD13	1:A:1186:SER:OG	2.19	0.42
1:A:360:LEU:C	1:A:463:ALA:HB2	2.45	0.42
2:B:42:ASN:HB2	5:B:803:SF4:S1	2.59	0.42
1:A:471:THR:CG2	1:A:476:LEU:HD13	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:GLN:CA	1:A:1162:TYR:HB3	2.50	0.42
2:B:403:LEU:O	2:B:407:LYS:HB2	2.19	0.42
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.49	0.42
1:A:56:SER:CB	1:A:800:SER:HB2	2.50	0.42
1:A:210:GLY:O	1:A:603:ARG:HD2	2.20	0.42
1:A:372:TRP:CE2	1:A:863:PRO:HB3	2.54	0.42
1:A:624:THR:OG1	1:A:627:GLU:HG2	2.20	0.42
2:B:252:GLU:HA	2:B:461:SER:HB2	2.01	0.42
9:B:1355:HOH:O	3:C:216:ARG:HD3	2.19	0.42
1:A:260:ARG:CG	1:A:802:MET:HE2	2.50	0.42
1:A:724:HIS:CE1	1:A:1167:ARG:NH1	2.84	0.42
1:A:48:THR:OG1	1:A:49:HIS:N	2.53	0.42
1:A:215:SER:OG	1:A:606:ASN:HA	2.20	0.42
1:A:373:LYS:HD3	1:A:392:PHE:CZ	2.54	0.42
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	2.01	0.41
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.55	0.41
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.53	0.41
1:A:119:LYS:O	1:A:123:GLU:HG3	2.21	0.41
1:A:214:LEU:HB3	1:A:607:SER:OG	2.20	0.41
1:A:338:MET:HE2	1:A:374:THR:OG1	2.20	0.41
1:A:584:ARG:C	1:A:586:GLN:H	2.28	0.41
1:A:397:LYS:HE2	1:A:977:PHE:HA	2.02	0.41
1:A:1070:VAL:HG13	1:A:1223:VAL:HG22	2.02	0.41
1:A:1100:THR:O	1:A:1101:TYR:CB	2.68	0.41
2:B:245:ILE:HD13	2:B:245:ILE:N	2.32	0.41
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.50	0.41
1:A:169:ILE:HD11	1:A:784:ILE:CD1	2.51	0.41
1:A:599:GLN:HE21	1:A:599:GLN:HB2	1.65	0.41
1:A:190:PRO:HB2	1:A:191:ILE:HD12	2.03	0.41
1:A:368:ASN:O	1:A:373:LYS:HE3	2.20	0.41
2:B:269:TYR:CG	2:B:333:MET:HE1	2.56	0.41
1:A:644:ASP:OD2	1:A:751:PRO:HB2	2.21	0.41
1:A:928:ARG:CG	1:A:943:PRO:HG3	2.50	0.41
1:A:130:ASP:OD2	1:A:130:ASP:C	2.64	0.41
1:A:936:GLU:HB2	9:A:1504:HOH:O	2.20	0.41
1:A:949:ILE:HD12	1:A:996:PHE:CD2	2.56	0.41
1:A:1062:ARG:HD2	9:A:1529:HOH:O	2.20	0.41
1:A:7:PHE:N	1:A:7:PHE:HD1	2.19	0.41
1:A:375:VAL:HG12	1:A:376:ALA:N	2.34	0.41
1:A:534:GLY:O	1:A:572:GLY:HA3	2.20	0.41
1:A:613:ASN:C	1:A:613:ASN:ND2	2.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:LYS:HB2	1:A:1127:LEU:HD21	2.02	0.41
2:B:3:ILE:N	2:B:3:ILE:CD1	2.83	0.41
2:B:47:LYS:HA	2:B:48:PRO:C	2.46	0.41
1:A:250:ILE:HD12	1:A:278:VAL:HB	2.03	0.40
1:A:545:ASN:O	1:A:550:LEU:HD13	2.21	0.40
1:A:920:THR:O	1:A:920:THR:HG23	2.21	0.40
3:C:87:GLN:OE1	3:C:153:GLY:HA2	2.21	0.40
1:A:336:MET:N	1:A:337:PRO:CD	2.83	0.40
1:A:750:LYS:N	1:A:750:LYS:CD	2.85	0.40
3:C:116:PRO:HG2	9:C:833:HOH:O	2.22	0.40
3:C:198:PHE:HB3	3:C:199:PRO:HD3	2.03	0.40
1:A:397:LYS:HE2	1:A:977:PHE:CG	2.57	0.40
1:A:357:ALA:O	1:A:363:ALA:HA	2.21	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)
9:A:1535:HOH:O	9:A:1535:HOH:O[3_354]	1.23	0.97
9:A:1536:HOH:O	9:A:1536:HOH:O[3_354]	1.54	0.66

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1236/1246 (99%)	1157 (94%)	69 (6%)	10 (1%)	16	16
2	B	506/512 (99%)	489 (97%)	16 (3%)	1 (0%)	43	51
3	C	215/225 (96%)	206 (96%)	8 (4%)	1 (0%)	24	27
All	All	1957/1983 (99%)	1852 (95%)	93 (5%)	12 (1%)	21	23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1164	ALA
1	A	1166	GLU
1	A	9	TYR
1	A	719	SER
1	A	502	TYR
1	A	361	VAL
1	A	191	ILE
2	B	101	TYR
1	A	716	LEU
1	A	224	PRO
1	A	499	VAL
3	C	210	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1037/1043 (99%)	1015 (98%)	22 (2%)	47	63
2	B	435/439 (99%)	424 (98%)	11 (2%)	42	56
3	C	180/186 (97%)	178 (99%)	2 (1%)	65	79
All	All	1652/1668 (99%)	1617 (98%)	35 (2%)	47	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	ILE
1	A	287	ILE
1	A	338	MET
1	A	346	ASP
1	A	397	LYS
1	A	402	LEU
1	A	476	LEU
1	A	510	ILE
1	A	600	ARG
1	A	767	LEU
1	A	801	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	804	PRO
1	A	806	ILE
1	A	808	PRO
1	A	827	LYS
1	A	864	LEU
1	A	926	LEU
1	A	1072	GLU
1	A	1074	ILE
1	A	1110	LEU
1	A	1183	ILE
1	A	1233	LEU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU
2	B	88	ILE
2	B	123	ILE
2	B	244	CYS
2	B	245	ILE
2	B	267	ILE
2	B	335	MET
2	B	407	LYS
2	B	503	ASP
3	C	129	ILE
3	C	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	40	GLN
1	A	65	ASN
1	A	173	ASN
1	A	234	GLN
1	A	321	ASN
1	A	368	ASN
1	A	441	HIS
1	A	480	ASN
1	A	559	ASN
1	A	586	GLN
1	A	590	GLN
1	A	599	GLN
1	A	613	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	704	ASN
1	A	708	ASN
1	A	724	HIS
1	A	942	GLN
1	A	946	ASN
1	A	1023	ASN
1	A	1087	ASN
1	A	1093	GLN
1	A	1098	HIS
1	A	1184	HIS
2	B	294	GLN
2	B	485	HIS
3	C	53	ASN
3	C	149	GLN
3	C	175	GLN
3	C	225	HIS

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	1.31	2 (25%)	8,9,11	1.67	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-2.22	1.48	1.53
3	C	1	FME	CB-CG	2.20	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	3.06	127.52	122.82
3	C	1	FME	CB-CA-N	2.34	114.79	110.52

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	CB-CA-N-CN
3	C	1	FME	N-CA-CB-CG
3	C	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	B	802	2	0,12,12	-	-	-		
5	SF4	B	804	2	0,12,12	-	-	-		
7	F3S	B	805	2	0,9,9	-	-	-		
5	SF4	B	803	2	0,12,12	-	-	-		
5	SF4	A	1248	1,9	0,12,12	-	-	-		
4	GDP	A	1247	-	29,30,30	1.52	5 (17%)	45,47,47	1.11	3 (6%)
8	HEM	C	807	3	50,50,50	1.83	14 (28%)	67,82,82	0.95	5 (7%)
6	3PH	B	1310	-	17,17,47	0.90	0	18,21,52	2.02	5 (27%)
8	HEM	C	806	3	50,50,50	1.77	12 (24%)	67,82,82	0.87	2 (2%)
6	3PH	A	1309	-	26,26,47	0.74	1 (3%)	29,31,52	1.56	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	B	802	2	-	-	0/6/5/5
5	SF4	B	804	2	-	-	0/6/5/5
7	F3S	B	805	2	-	-	1/3/3/3
5	SF4	B	803	2	-	-	0/6/5/5
8	HEM	C	807	3	-	7/14/54/54	-
4	GDP	A	1247	-	-	1/16/32/32	0/3/3/3
5	SF4	A	1248	1,9	-	-	0/6/5/5
6	3PH	B	1310	-	1/1/3/4	5/18/18/49	-
8	HEM	C	806	3	-	8/14/54/54	-
6	3PH	A	1309	-	-	5/28/28/49	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	807	HEM	CAB-C3B	4.69	1.59	1.47
8	C	806	HEM	CAB-C3B	4.39	1.59	1.47
4	A	1247	GDP	C4-N3	3.96	1.43	1.34
8	C	806	HEM	CAC-C3C	3.69	1.57	1.47
4	A	1247	GDP	PB-O1B	3.59	1.61	1.50
8	C	807	HEM	FE-NC	3.49	2.06	1.95
8	C	806	HEM	FE-NC	3.41	2.06	1.95
8	C	807	HEM	CMC-C2C	3.30	1.57	1.50
8	C	807	HEM	CAC-C3C	3.28	1.56	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	806	HEM	CMC-C2C	3.19	1.57	1.50
8	C	806	HEM	CMD-C2D	3.10	1.57	1.50
8	C	807	HEM	CMB-C2B	3.03	1.57	1.50
8	C	807	HEM	CMD-C2D	3.01	1.56	1.50
8	C	806	HEM	CMB-C2B	2.95	1.56	1.50
8	C	806	HEM	CMA-C3A	2.92	1.56	1.50
4	A	1247	GDP	C6-N1	2.88	1.44	1.38
8	C	807	HEM	FE-NB	2.82	2.03	1.94
8	C	807	HEM	CAD-C3D	2.74	1.58	1.51
8	C	807	HEM	CMA-C3A	2.64	1.56	1.50
8	C	806	HEM	CAD-C3D	2.64	1.58	1.51
8	C	807	HEM	CBA-CAA	2.44	1.60	1.51
4	A	1247	GDP	PB-O3B	-2.42	1.45	1.54
8	C	806	HEM	FE-NB	2.42	2.02	1.94
4	A	1247	GDP	C2-N3	2.29	1.38	1.33
6	A	1309	3PH	C32-C31	2.27	1.57	1.50
8	C	807	HEM	C1D-C2D	2.22	1.49	1.44
8	C	807	HEM	CBD-CAD	2.16	1.59	1.51
8	C	807	HEM	CBD-CGD	2.15	1.55	1.50
8	C	806	HEM	CBA-CAA	2.14	1.59	1.51
8	C	807	HEM	CAA-C2A	2.12	1.56	1.51
8	C	806	HEM	CBD-CAD	2.10	1.59	1.51
8	C	806	HEM	CBA-CGA	2.02	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1309	3PH	C23-C22-C21	5.09	132.34	113.69
6	A	1309	3PH	C33-C32-C31	4.79	131.24	113.69
6	B	1310	3PH	C3-C2-C1	4.72	122.80	111.78
6	B	1310	3PH	C33-C32-C31	4.55	130.38	113.69
6	B	1310	3PH	O21-C2-C3	3.48	120.84	108.34
8	C	807	HEM	CAD-C3D-C4D	-2.74	119.92	124.70
4	A	1247	GDP	PA-O5'-C5'	2.46	135.43	121.35
8	C	807	HEM	CAD-C3D-C2D	2.26	132.10	127.87
6	B	1310	3PH	O21-C2-C1	2.23	116.36	108.34
6	B	1310	3PH	O13-P-O11	2.22	112.46	106.67
8	C	806	HEM	CAD-C3D-C4D	-2.21	120.84	124.70
8	C	806	HEM	O1D-CGD-CBD	-2.13	116.34	123.09
4	A	1247	GDP	O3B-PB-O2B	2.10	115.69	107.80
8	C	807	HEM	O1D-CGD-CBD	-2.03	116.65	123.09
4	A	1247	GDP	O4'-C1'-N9	-2.02	103.78	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	807	HEM	CMA-C3A-C2A	2.01	129.89	125.62
8	C	807	HEM	O1A-CGA-CBA	-2.00	116.74	123.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1310	3PH	C2

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1310	3PH	O22-C21-O21-C2
8	C	806	HEM	C2C-C3C-CAC-CBC
8	C	807	HEM	C2C-C3C-CAC-CBC
8	C	806	HEM	C4C-C3C-CAC-CBC
8	C	807	HEM	C4C-C3C-CAC-CBC
6	B	1310	3PH	C1-C2-C3-O31
6	A	1309	3PH	C32-C31-O31-C3
6	A	1309	3PH	O32-C31-O31-C3
8	C	807	HEM	C2A-CAA-CBA-CGA
6	B	1310	3PH	C32-C31-O31-C3
8	C	806	HEM	C2B-C3B-CAB-CBB
6	B	1310	3PH	O32-C31-O31-C3
6	B	1310	3PH	O11-C1-C2-O21
6	A	1309	3PH	C26-C27-C28-C29
6	A	1309	3PH	C33-C34-C35-C36
8	C	806	HEM	CAA-CBA-CGA-O2A
8	C	806	HEM	CAD-CBD-CGD-O1D
8	C	806	HEM	CAD-CBD-CGD-O2D
8	C	807	HEM	CAA-CBA-CGA-O2A
8	C	807	HEM	CAA-CBA-CGA-O1A
8	C	807	HEM	CAD-CBD-CGD-O2D
8	C	806	HEM	CAA-CBA-CGA-O1A
6	A	1309	3PH	O11-C1-C2-C3
8	C	807	HEM	CAD-CBD-CGD-O1D
8	C	806	HEM	C4B-C3B-CAB-CBB
4	A	1247	GDP	PB-O3A-PA-O2A

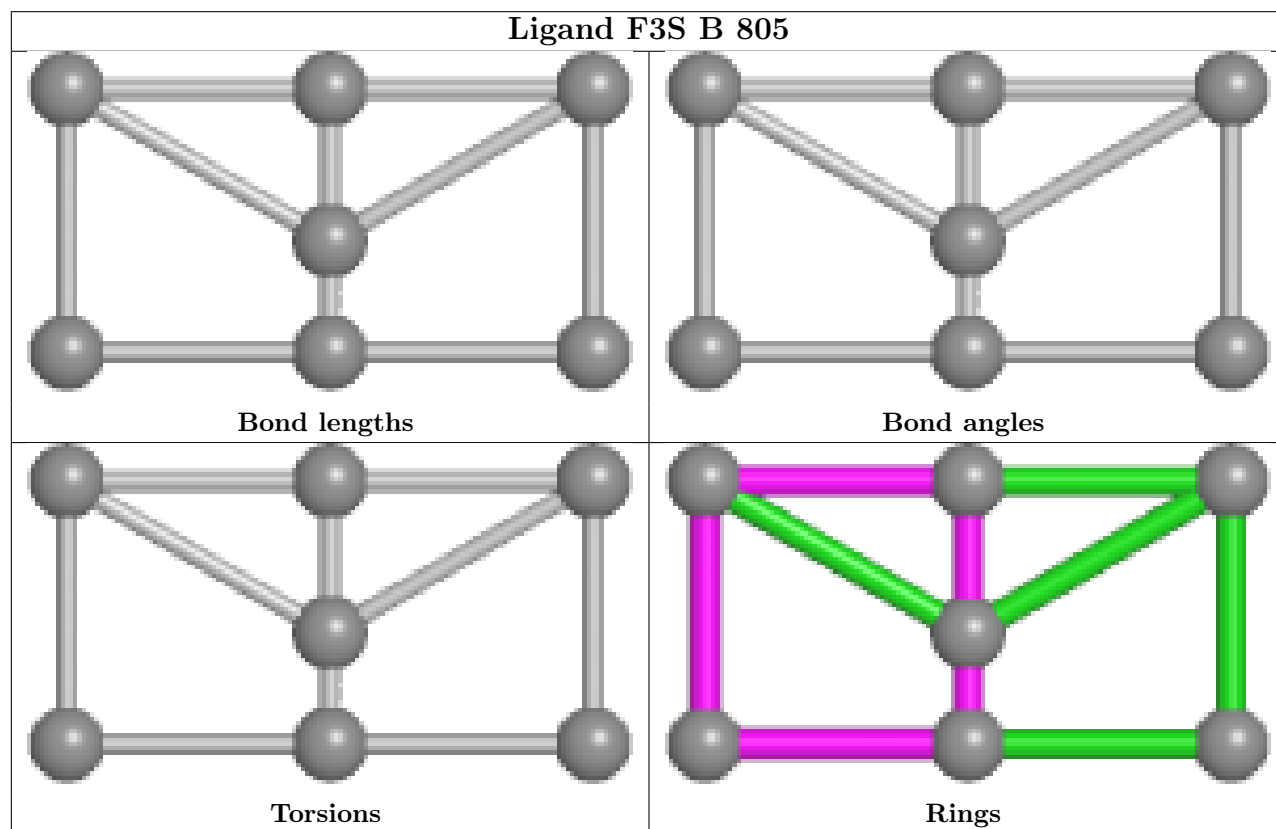
All (1) ring outliers are listed below:

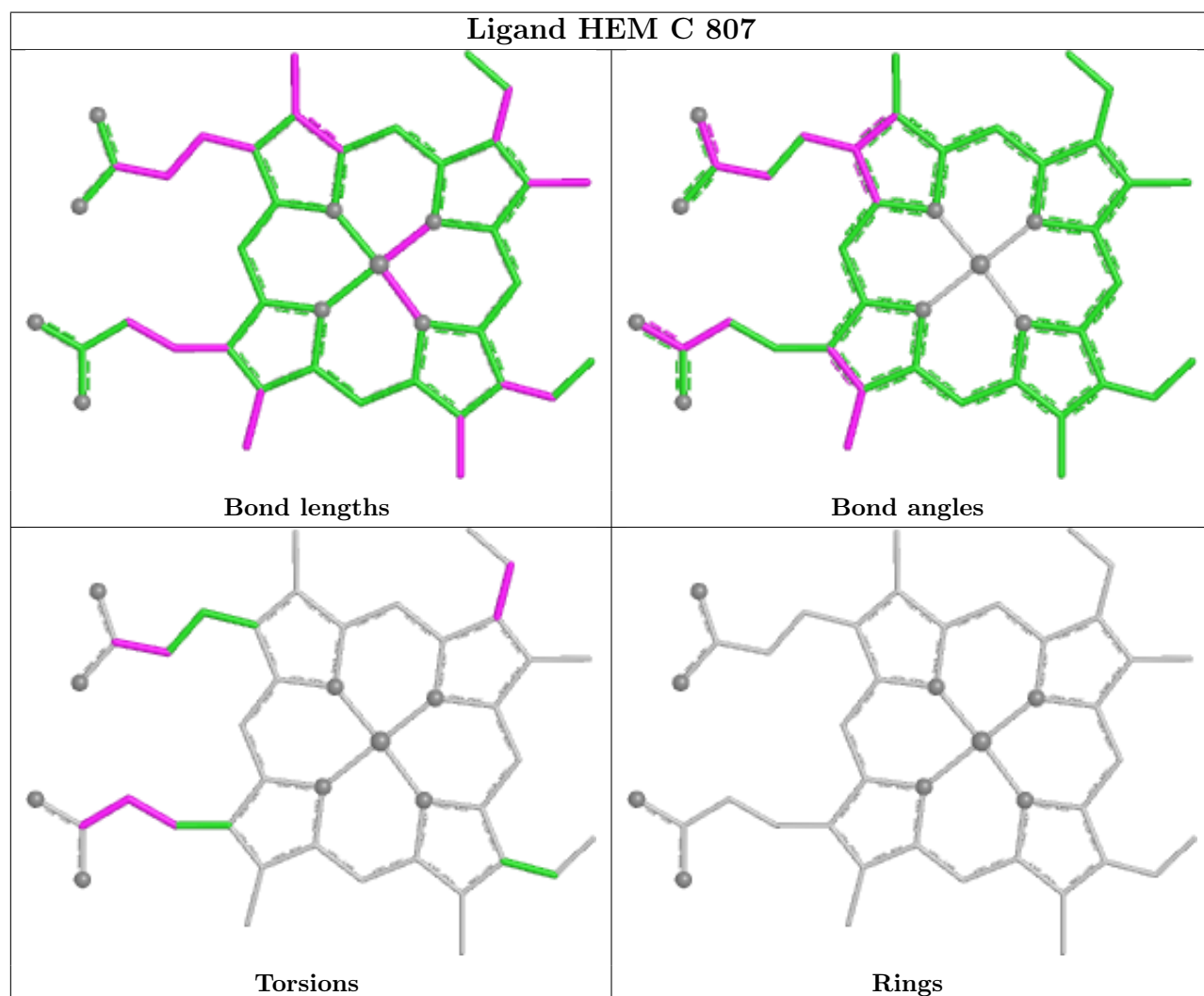
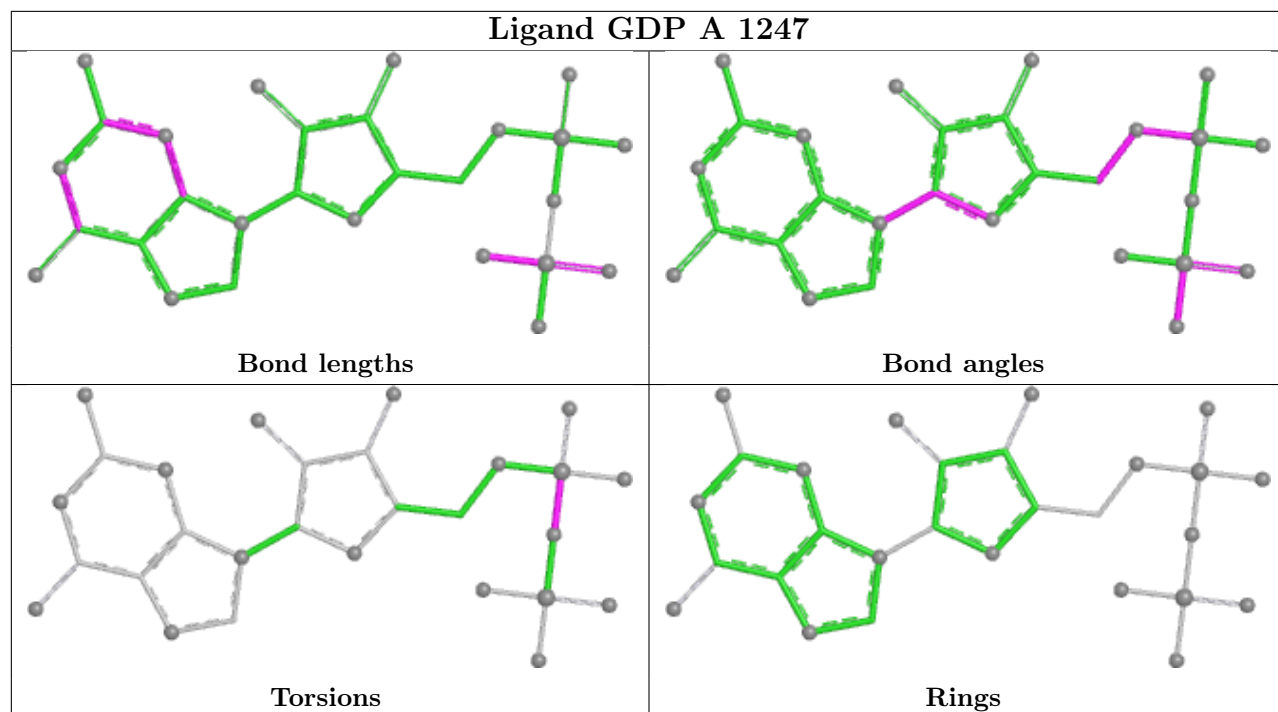
Mol	Chain	Res	Type	Atoms
7	B	805	F3S	FE1-FE3-S1-S3

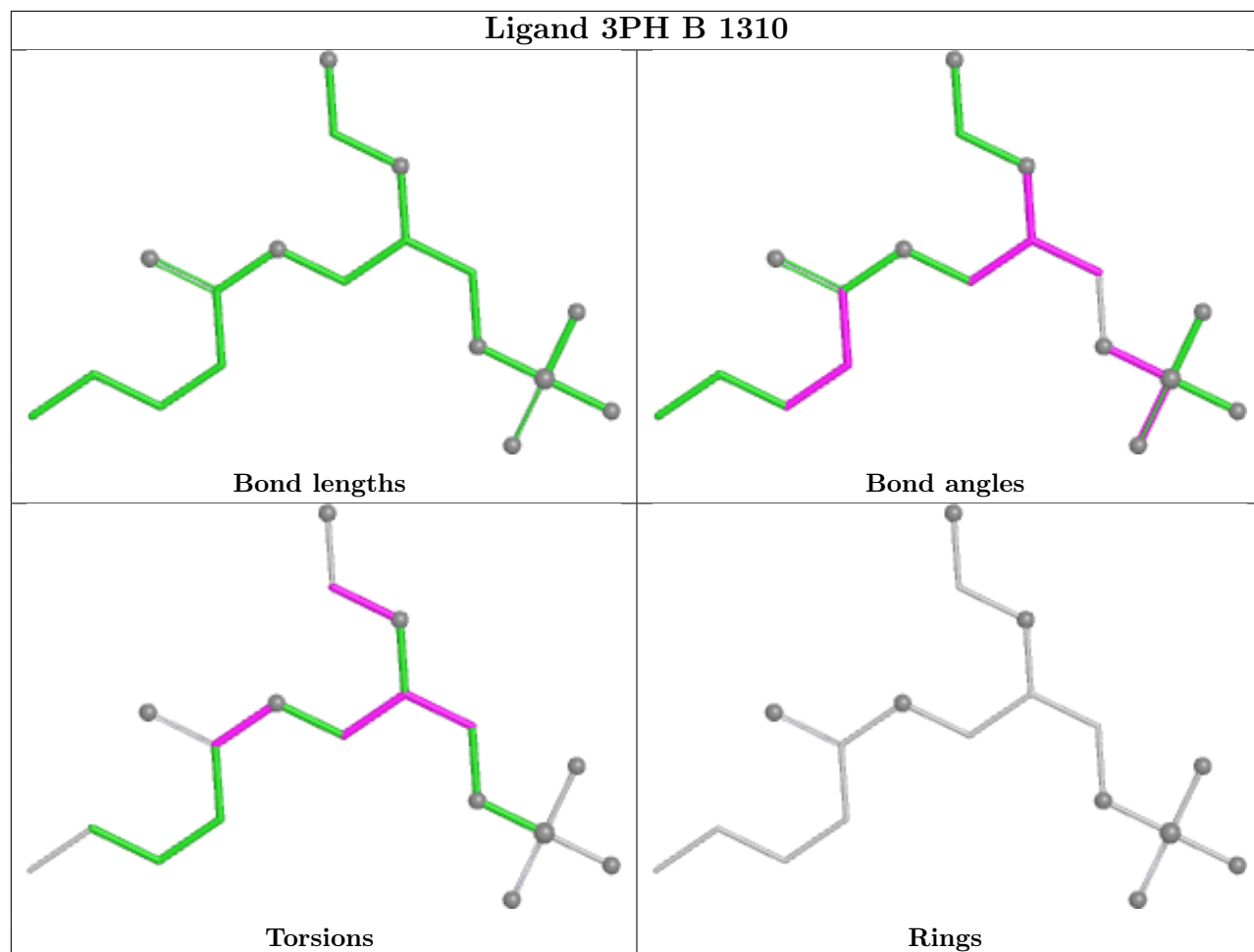
4 monomers are involved in 9 short contacts:

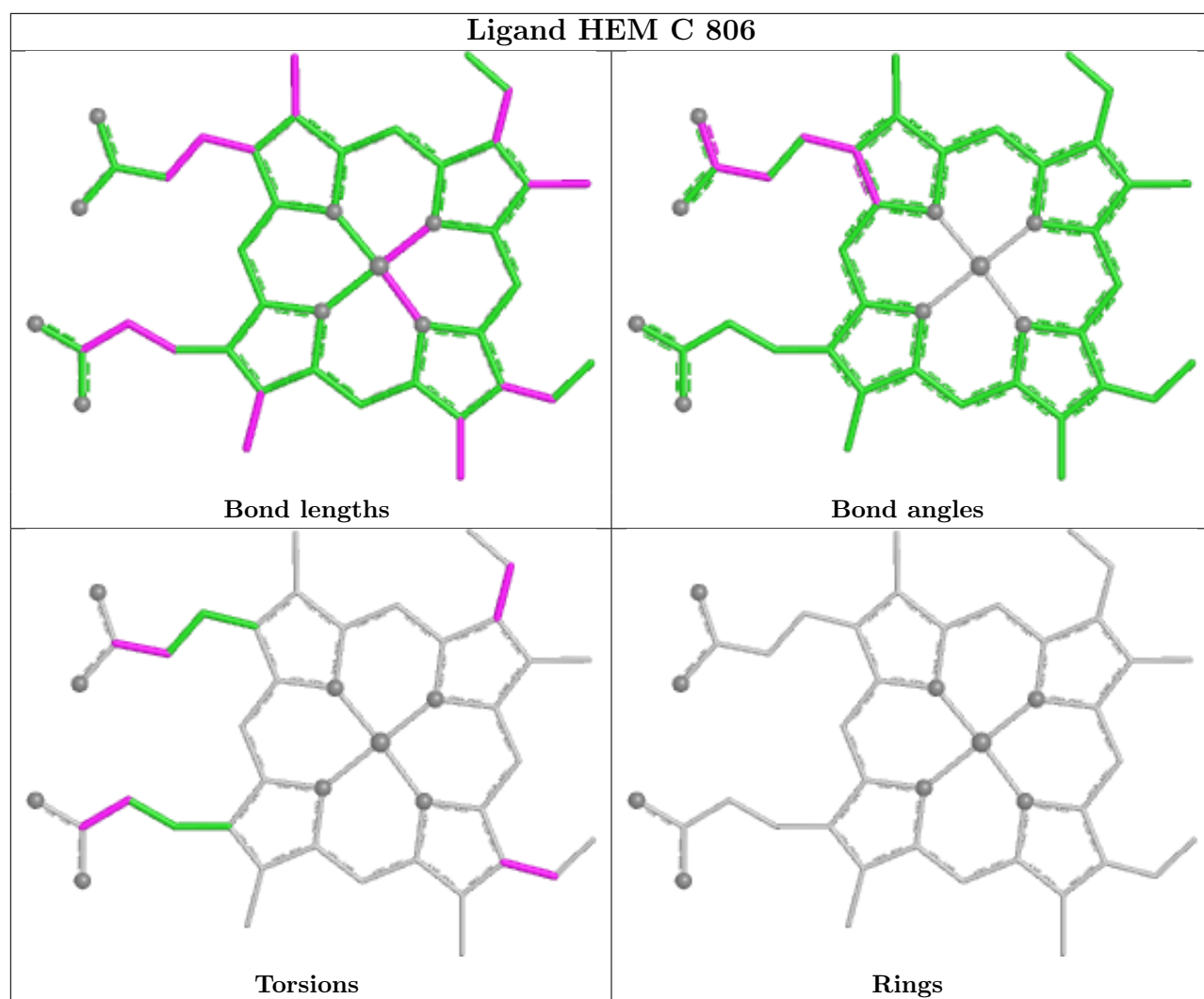
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	SF4	3	0
5	A	1248	SF4	1	0
4	A	1247	GDP	4	0
8	C	806	HEM	1	0

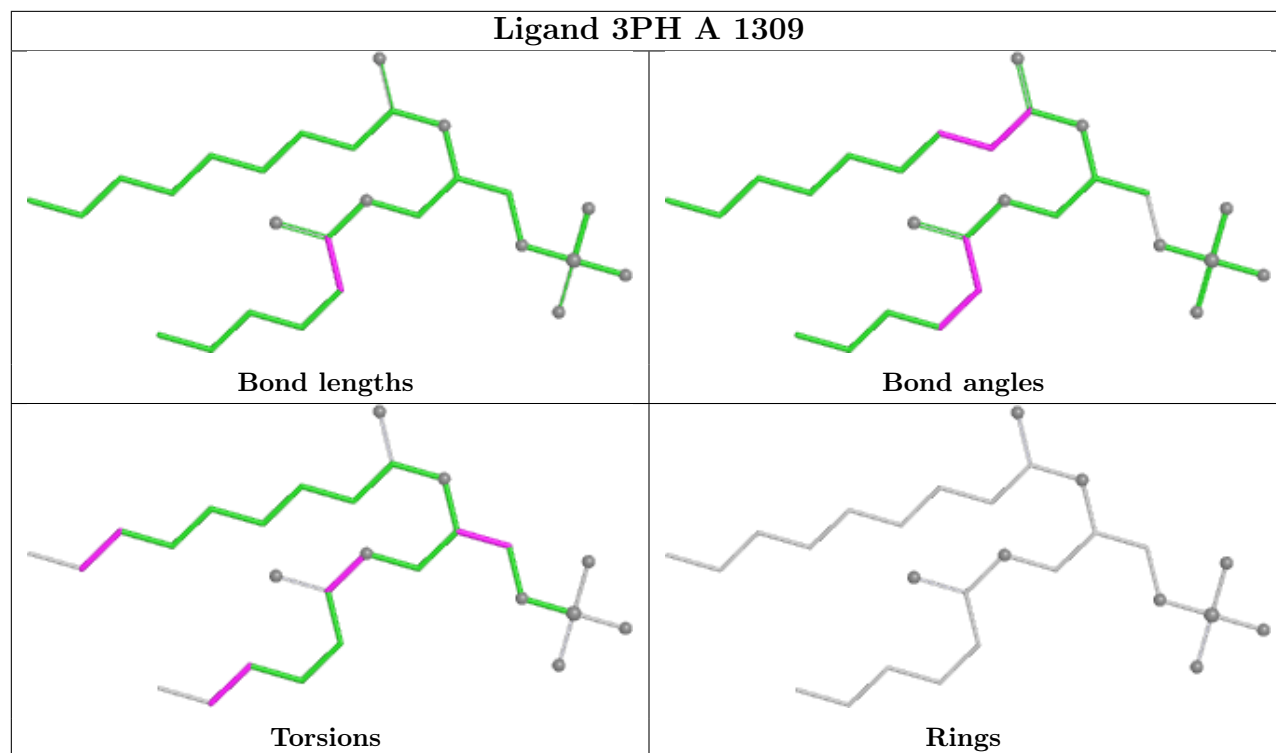
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	1240/1246 (99%)	0.26	47 (3%) 44 41	16, 35, 63, 80	0
2	B	508/512 (99%)	-0.29	3 (0%) 85 83	16, 27, 46, 82	0
3	C	218/225 (96%)	0.46	11 (5%) 34 31	19, 38, 64, 86	0
All	All	1966/1983 (99%)	0.14	61 (3%) 51 48	16, 33, 61, 86	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	5.5
1	A	749	VAL	5.1
1	A	719	SER	4.7
1	A	580	GLN	4.6
1	A	579	GLY	4.4
1	A	10	PHE	4.4
1	A	9	TYR	4.1
1	A	50	GLY	3.8
3	C	80	TRP	3.7
1	A	1097	ILE	3.2
1	A	1243	GLU	3.1
1	A	7	PHE	3.1
3	C	72	THR	3.1
3	C	83	ILE	3.0
1	A	1095	TRP	2.9
3	C	81	LEU	2.9
1	A	501	ALA	2.8
1	A	467	THR	2.8
1	A	1215	GLY	2.7
1	A	581	GLU	2.6
1	A	350	ALA	2.6
1	A	449	ASN	2.6
1	A	413	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1098	HIS	2.6
1	A	875	ASP	2.5
3	C	179	GLY	2.5
1	A	1163	HIS	2.5
1	A	991	ASP	2.5
1	A	1164	ALA	2.5
1	A	460	LEU	2.5
1	A	346	ASP	2.5
1	A	8	ARG	2.4
1	A	361	VAL	2.4
1	A	490	VAL	2.4
1	A	494	THR	2.4
1	A	377	PHE	2.4
2	B	370	GLU	2.4
3	C	79	ALA	2.3
1	A	446	GLU	2.3
1	A	502	TYR	2.3
1	A	384	VAL	2.3
1	A	367	GLU	2.3
1	A	578	VAL	2.3
1	A	379	THR	2.2
1	A	13	LYS	2.2
1	A	1092	HIS	2.2
1	A	468	ALA	2.2
2	B	368	ALA	2.2
1	A	678	ASN	2.2
3	C	3	PHE	2.2
3	C	151	MET	2.2
1	A	669	ALA	2.2
1	A	345	ARG	2.1
3	C	157	MET	2.1
1	A	1071	LYS	2.1
3	C	148	ALA	2.1
1	A	380	ASN	2.1
3	C	147	SER	2.1
1	A	414	GLU	2.1
2	B	373	SER	2.1
1	A	636	SER	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	0.85	0.15	60,69,80,82	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

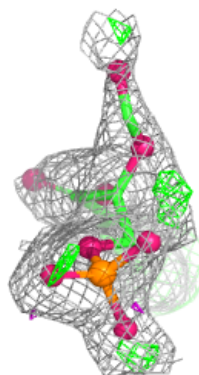
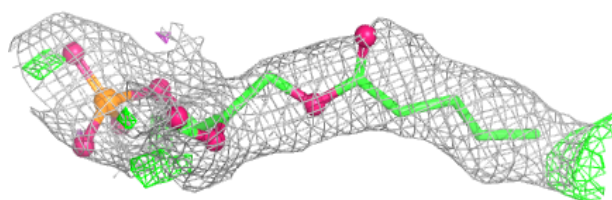
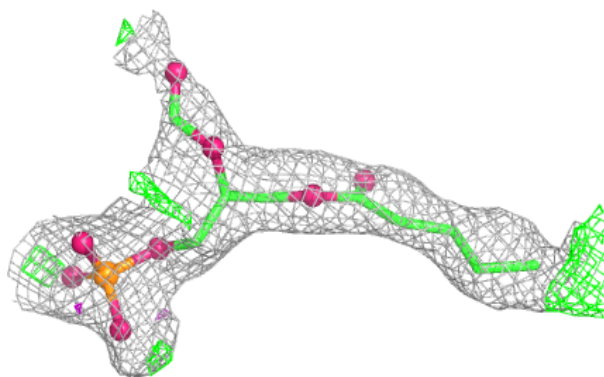
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	3PH	B	1310	18/48	0.71	0.20	54,76,91,92	0
4	GDP	A	1247	28/28	0.84	0.14	49,57,74,78	0
5	SF4	A	1248	8/8	0.90	0.14	20,28,31,42	8
6	3PH	A	1309	27/48	0.94	0.10	27,37,49,53	0
8	HEM	C	807	43/43	0.95	0.12	33,46,64,79	0
8	HEM	C	806	43/43	0.97	0.07	14,26,31,43	0
5	SF4	B	802	8/8	0.97	0.04	21,27,30,30	0
7	F3S	B	805	7/7	0.99	0.05	19,22,25,26	0
5	SF4	B	803	8/8	0.99	0.04	15,16,18,20	0
5	SF4	B	804	8/8	0.99	0.03	22,24,28,28	0

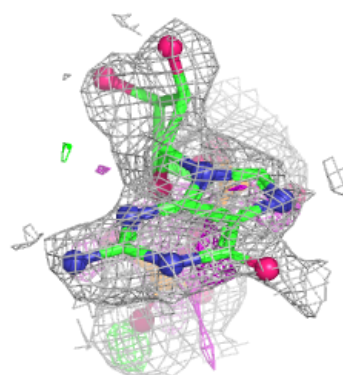
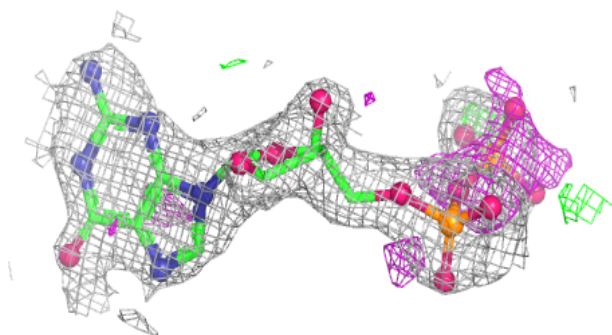
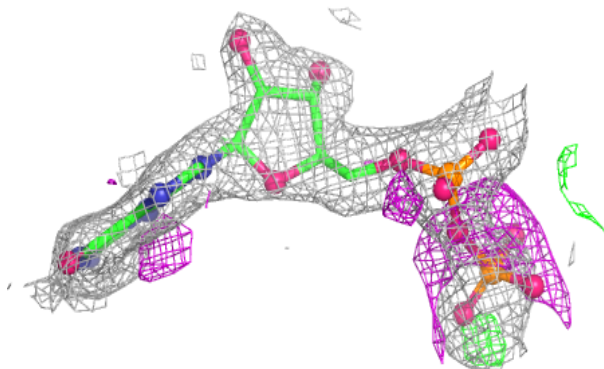
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3PH B 1310:

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

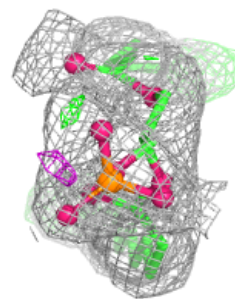
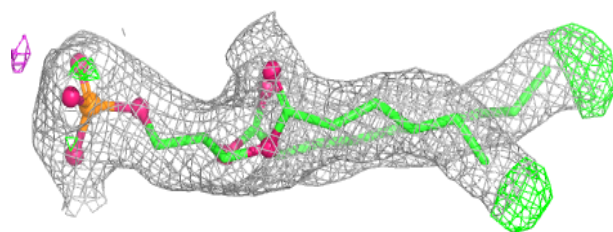
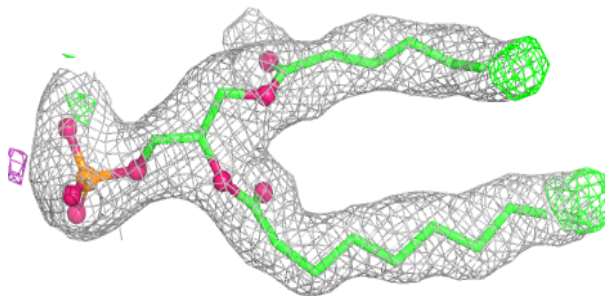
**Electron density around GDP A 1247:**

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



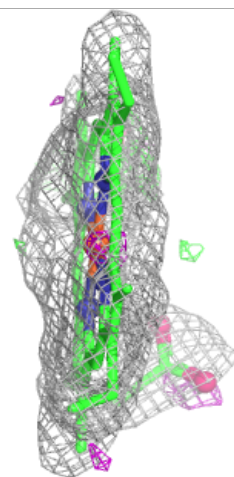
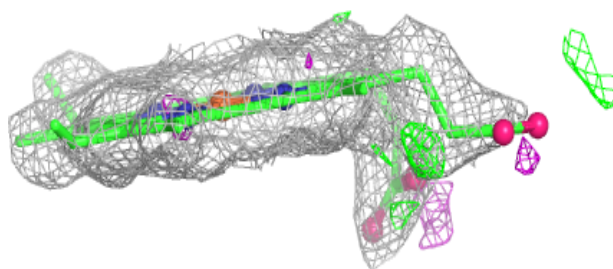
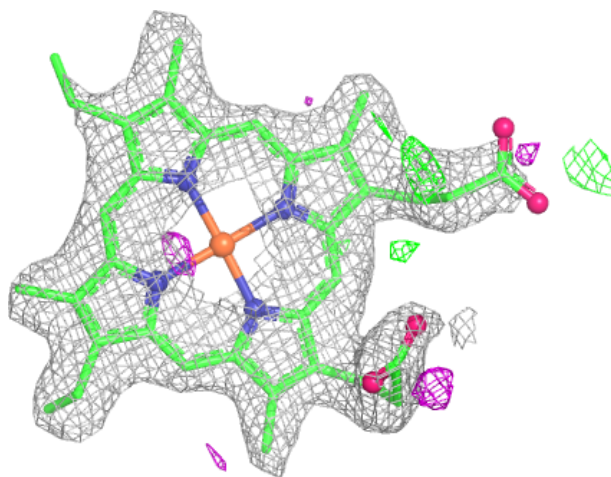
Electron density around 3PH A 1309:

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



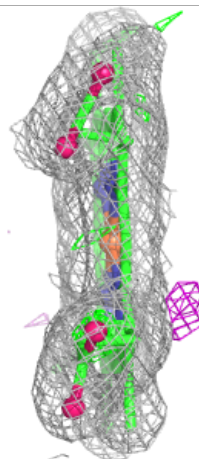
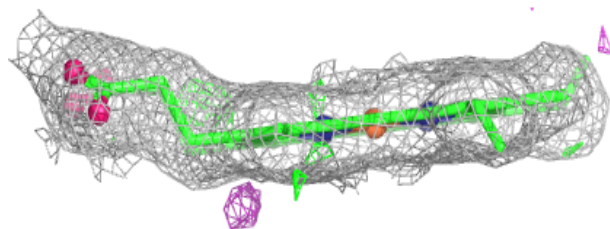
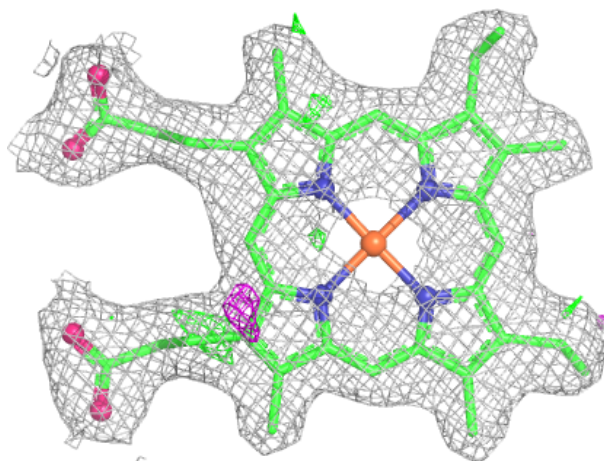
Electron density around HEM C 807:

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



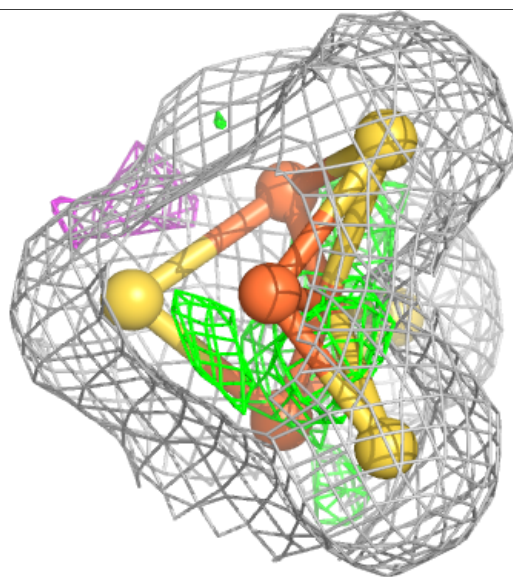
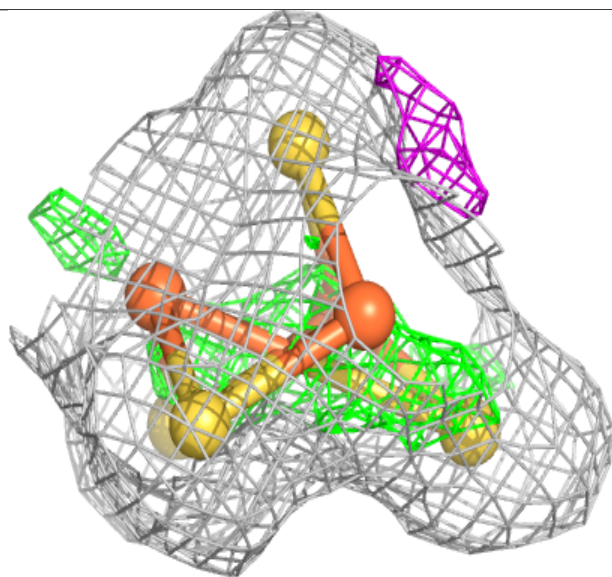
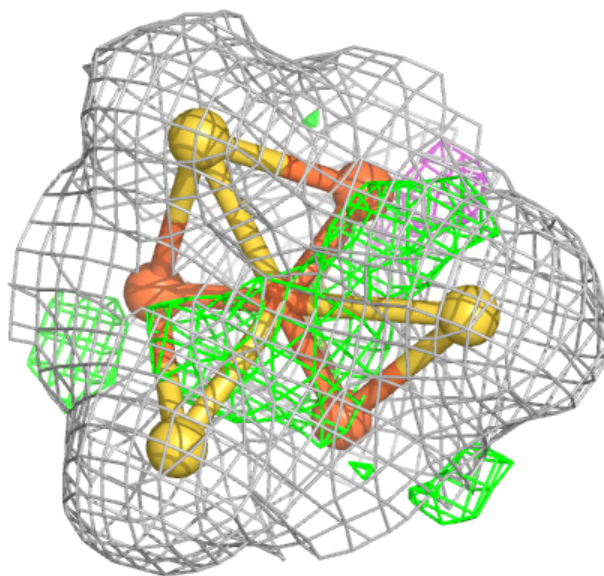
Electron density around HEM C 806:

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



Electron density around F3S B 805:

$2mF_o-DF_c$ (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.