



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:11 PM UTC

PDB ID : 1Y5I / pdb_00001y5i
Title : The crystal structure of the NarGHI mutant NarI-K86A
Authors : Bertero, M.G.; Rothery, R.A.; Boroumand, N.; Palak, M.; Blasco, F.; Ginet, N.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2004-12-02
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

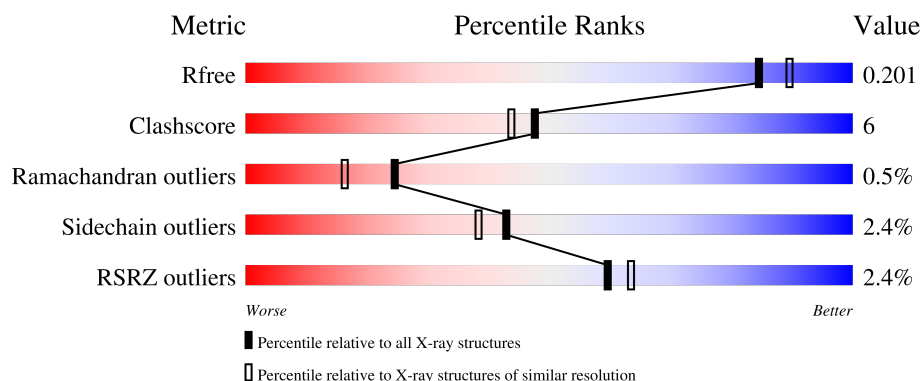
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1246	3% 82% 15% .
2	B	512	% 89% 10% ..
3	C	225	2% 83% 12% ..

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
8	3PH	B	1310	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17019 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
			9869	6232	1731	1858	48			

- 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			

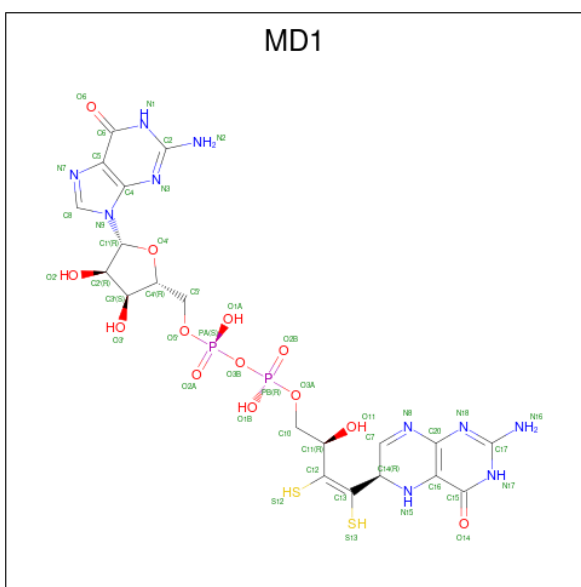
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (CCD ID: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

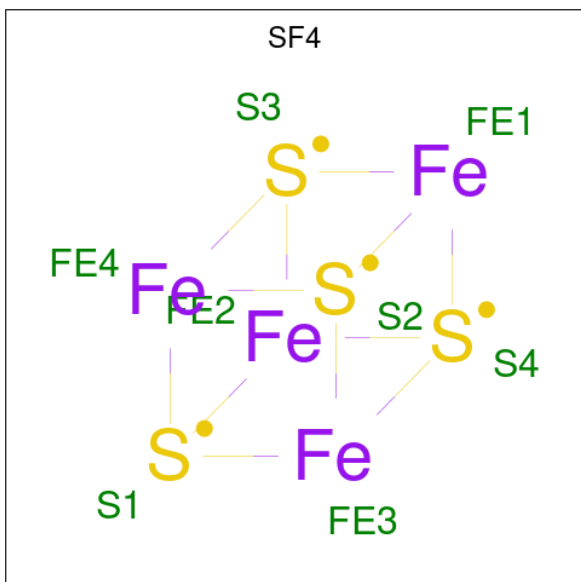


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

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

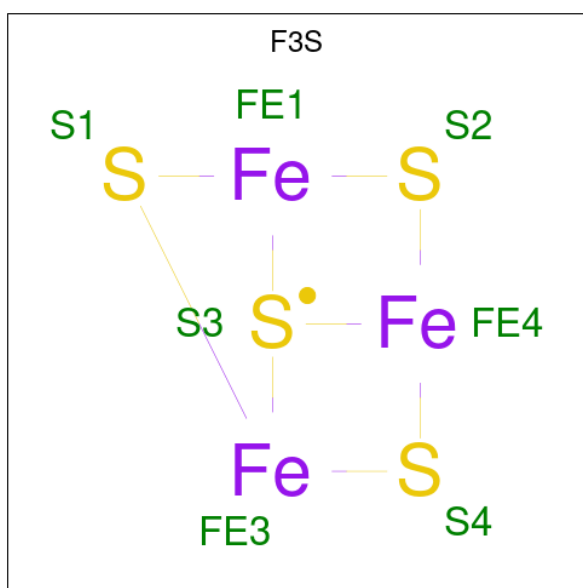
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mo 1 1	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



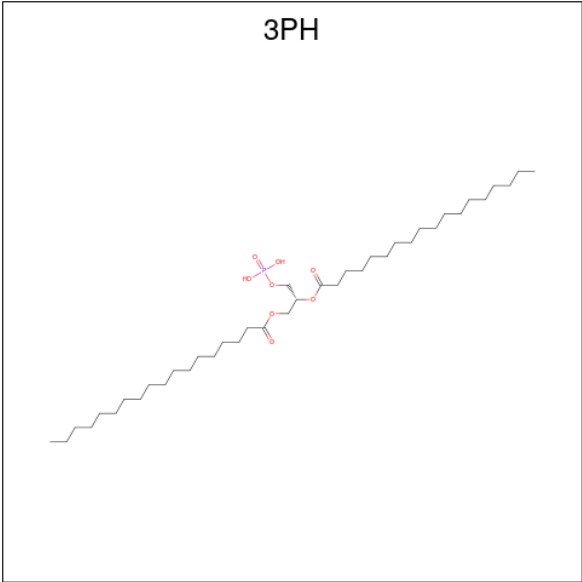
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

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



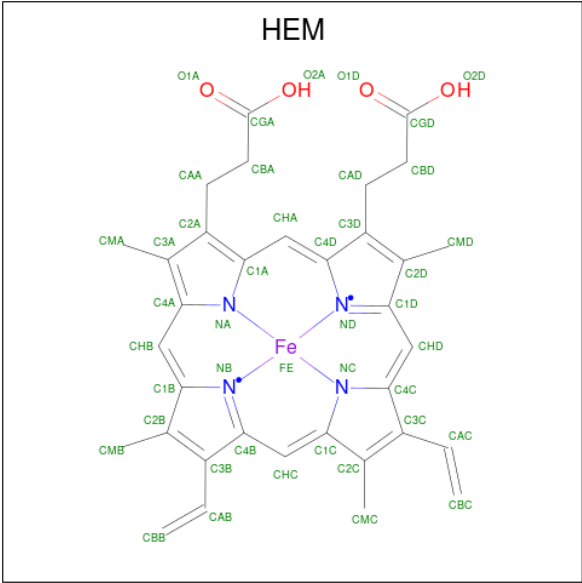
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 8 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $\text{C}_{39}\text{H}_{77}\text{O}_8\text{P}$).



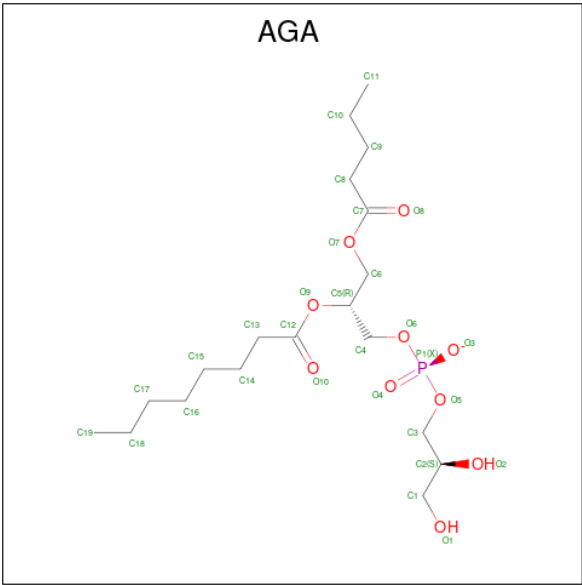
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	P	0	0
			18	9	8	1		

- 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	0
			43	34	1	4	4	
9	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 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
10	C	1	Total	C	O	P	0	0
			25	16	8	1		

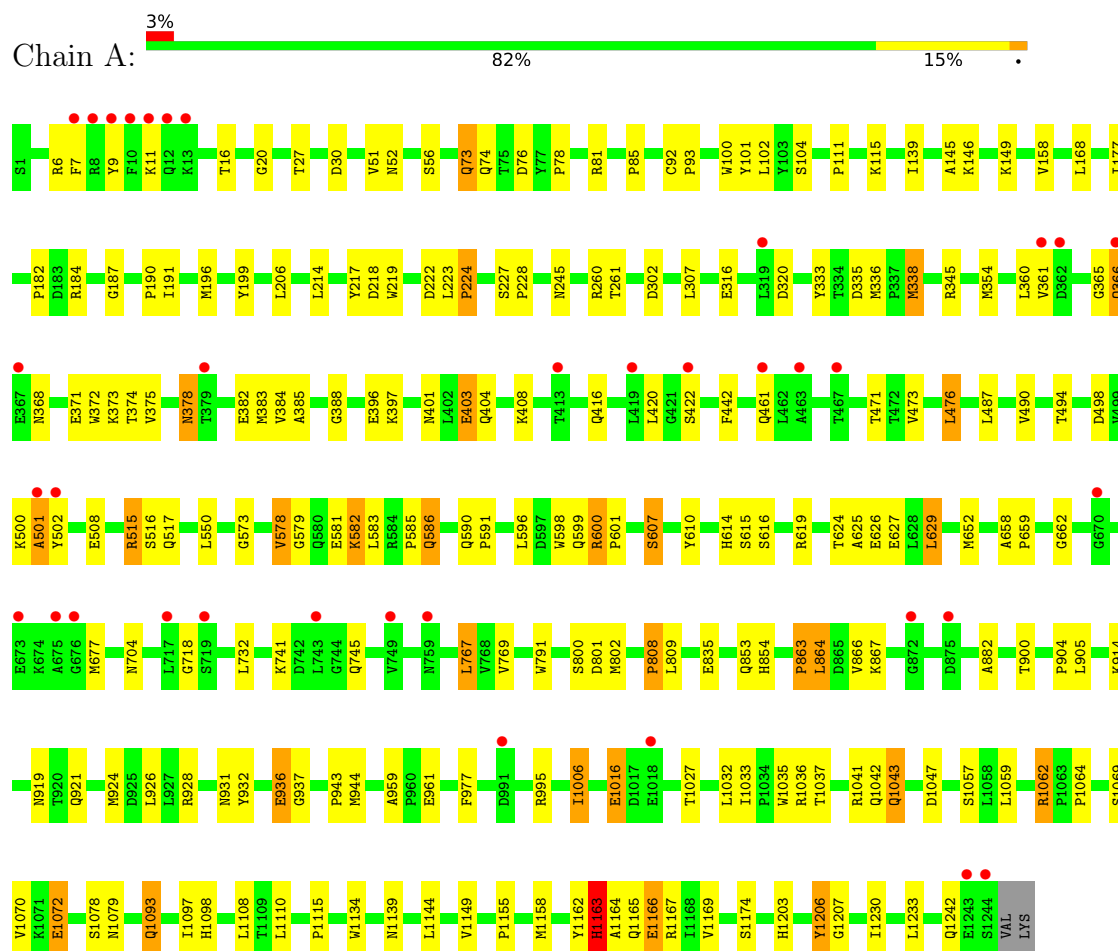
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	641	Total	O	0	0
			641	641		
11	B	400	Total	O	0	0
			400	400		
11	C	77	Total	O	0	0
			77	77		

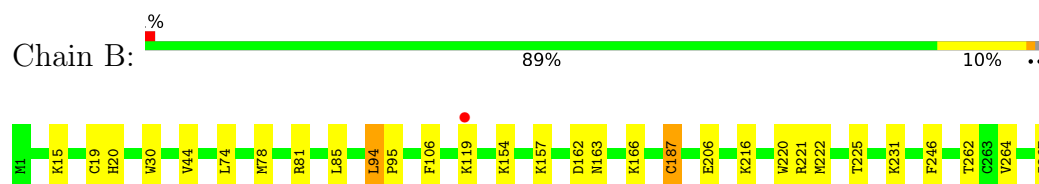
3 Residue-property plots [i](#)

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

- Molecule 1: Respiratory nitrate reductase 1 alpha chain

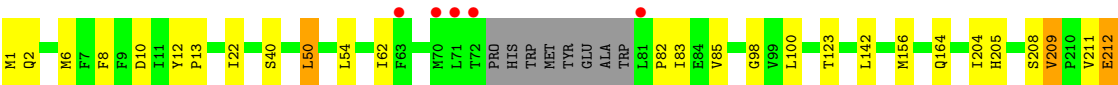
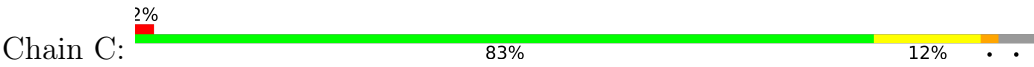


- Molecule 2: Respiratory nitrate reductase 1 beta chain





● 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	154.59Å 242.40Å 139.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 1.90 29.74 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.74-1.90) 96.2 (29.74-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.176 , 0.208 0.171 , 0.201	Depositor DCC
R_{free} test set	9740 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17019	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: F3S, 6MO, FME, SF4, HEM, 3PH, MD1, AGA

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	0.72	3/10128 (0.0%)	1.10	67/13749 (0.5%)
2	B	0.79	0/4146	1.04	16/5609 (0.3%)
3	C	0.70	0/1754	0.95	7/2370 (0.3%)
All	All	0.74	3/16028 (0.0%)	1.07	90/21728 (0.4%)

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	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1163	HIS	C-N	-6.19	1.25	1.33
1	A	501	ALA	C-N	-5.87	1.25	1.33
1	A	501	ALA	C-O	5.15	1.29	1.23

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	CA-C-N	15.77	151.66	121.54
1	A	1163	HIS	C-N-CA	15.77	151.66	121.54
1	A	501	ALA	CA-C-N	15.22	150.61	121.54
1	A	501	ALA	C-N-CA	15.22	150.61	121.54
1	A	1163	HIS	CA-C-O	-10.80	109.31	121.19
1	A	501	ALA	CA-C-O	-10.09	110.16	122.36
1	A	1070	VAL	N-CA-C	9.61	119.82	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	SER	N-CA-C	9.08	122.15	111.71
1	A	224	PRO	N-CA-C	-8.70	100.08	110.70
1	A	809	LEU	N-CA-C	-7.94	96.75	109.76
2	B	30	TRP	N-CA-C	7.88	123.03	113.41
1	A	1206	TYR	N-CA-C	7.42	120.96	110.50
1	A	1149	VAL	N-CA-C	-7.05	97.45	107.75
1	A	1093	GLN	N-CA-C	7.05	119.83	110.53
1	A	320	ASP	N-CA-C	7.03	118.94	111.28
1	A	863	PRO	N-CA-C	6.88	122.58	113.57
1	A	1097	ILE	N-CA-C	-6.82	96.44	107.28
1	A	1035	TRP	N-CA-C	-6.79	100.43	110.48
2	B	379	ASP	N-CA-C	-6.79	99.24	110.17
1	A	388	GLY	N-CA-C	6.78	123.15	115.08
1	A	573	GLY	N-CA-C	6.69	120.29	111.52
2	B	166	LYS	N-CA-C	6.61	121.35	113.16
1	A	74	GLN	N-CA-C	-6.46	102.00	110.53
1	A	1043	GLN	N-CA-C	6.43	119.31	107.99
2	B	216	LYS	N-CA-C	6.41	120.36	112.54
1	A	854	HIS	N-CA-C	-6.38	101.67	110.35
1	A	808	PRO	N-CA-C	6.34	125.53	112.47
1	A	102	LEU	N-CA-C	6.30	118.67	111.11
2	B	287	GLU	N-CA-C	6.28	118.65	111.11
1	A	1167	ARG	N-CA-C	6.27	120.24	112.59
1	A	260	ARG	N-CA-C	-6.18	102.88	110.61
1	A	900	THR	N-CA-C	6.16	119.83	112.93
1	A	1016	GLU	N-CA-C	-6.16	97.67	108.20
1	A	614	HIS	N-CA-C	6.11	118.90	111.82
2	B	94	LEU	N-CA-C	6.03	118.16	109.48
1	A	1169	VAL	N-CA-C	6.01	116.53	108.11
2	B	458	VAL	CA-C-N	-6.01	114.36	120.85
2	B	458	VAL	C-N-CA	-6.01	114.36	120.85
2	B	359	LEU	N-CA-C	-5.98	101.09	110.36
1	A	582	LYS	N-CA-C	5.98	119.23	108.17
2	B	157	LYS	N-CA-C	-5.97	105.84	113.01
2	B	206	GLU	N-CA-C	5.95	119.80	112.54
1	A	1164	ALA	N-CA-C	5.94	123.46	110.80
1	A	1079	ASN	N-CA-C	-5.89	105.29	112.88
1	A	302	ASP	N-CA-C	5.88	117.69	111.28
3	C	8	PHE	N-CA-C	5.86	118.45	111.71
1	A	959	ALA	N-CA-C	5.81	117.13	109.93
2	B	280	ILE	N-CA-C	5.77	116.41	110.36
2	B	81	ARG	N-CA-C	5.76	117.24	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	MET	N-CA-C	5.68	117.95	111.02
1	A	802	MET	N-CA-C	5.66	118.39	111.82
1	A	184	ARG	N-CA-C	-5.65	105.97	112.92
1	A	583	LEU	N-CA-C	-5.60	98.14	107.99
1	A	403	GLU	N-CA-C	-5.59	102.00	110.28
1	A	101	TYR	N-CA-C	5.59	118.31	111.82
3	C	209	VAL	CA-C-N	5.59	126.83	119.84
3	C	209	VAL	C-N-CA	5.59	126.83	119.84
1	A	85	PRO	N-CA-C	-5.59	103.03	111.41
1	A	1163	HIS	N-CA-CB	5.58	118.26	109.83
1	A	76	ASP	N-CA-C	5.56	118.85	112.57
1	A	1042	GLN	N-CA-C	-5.49	101.52	109.59
3	C	40	SER	N-CA-C	-5.47	105.22	112.94
1	A	1162	TYR	CA-C-N	5.45	128.44	120.71
1	A	1162	TYR	C-N-CA	5.45	128.44	120.71
1	A	199	TYR	N-CA-C	-5.38	105.33	111.14
1	A	904	PRO	N-CA-C	5.36	120.63	114.03
1	A	937	GLY	CA-C-N	5.32	125.38	119.32
1	A	937	GLY	C-N-CA	5.32	125.38	119.32
1	A	494	THR	N-CA-C	-5.31	106.80	113.28
1	A	16	THR	N-CA-C	-5.28	102.94	110.59
1	A	615	SER	N-CA-C	-5.27	106.69	113.02
2	B	222	MET	N-CA-C	-5.27	106.98	113.41
3	C	123	THR	N-CA-C	-5.27	101.98	110.14
1	A	853	GLN	N-CA-C	5.26	118.19	109.46
3	C	217	LYS	N-CA-C	-5.25	103.10	110.50
1	A	378	ASN	N-CA-C	-5.22	103.79	110.53
2	B	394	LEU	N-CA-C	5.21	121.04	114.31
2	B	187	CYS	N-CA-C	5.18	117.22	110.43
1	A	1163	HIS	CA-CB-CG	5.17	118.97	113.80
1	A	1166	GLU	N-CA-C	5.16	121.78	110.80
1	A	1047	ASP	N-CA-C	5.14	119.54	113.16
1	A	111	PRO	N-CA-C	-5.11	103.16	111.14
1	A	316	GLU	N-CA-C	5.09	119.57	112.90
1	A	1057	SER	N-CA-C	-5.09	105.85	111.71
1	A	1078	SER	N-CA-C	5.07	117.58	110.23
1	A	882	ALA	CA-C-N	-5.06	115.35	120.31
1	A	882	ALA	C-N-CA	-5.06	115.35	120.31
3	C	218	TYR	N-CA-C	5.06	116.49	111.07
1	A	333	TYR	N-CA-C	5.03	120.04	113.30
1	A	586	GLN	N-CA-C	5.02	117.13	111.11

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Mainchain,Peptide
1	A	501	ALA	Mainchain,Peptide
1	A	610	TYR	Sidechain

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	9869	0	9525	135	0
2	B	4050	0	3973	27	0
3	C	1719	0	1764	17	0
4	A	94	0	42	7	0
5	A	1	0	0	0	0
6	A	8	0	0	0	0
6	B	24	0	0	1	0
7	B	7	0	0	0	0
8	B	18	0	10	0	0
9	C	86	0	60	0	0
10	C	25	0	29	0	0
11	A	641	0	0	8	0
11	B	400	0	0	7	0
11	C	77	0	0	1	1
All	All	17019	0	15403	175	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (175) 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:73:GLN:H	1:A:73:GLN:HE21	1.20	0.86
1:A:371:GLU:OE1	1:A:371:GLU:N	2.08	0.86
1:A:586:GLN:HE21	1:A:590:GLN:CD	1.85	0.84
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.59	0.82
1:A:1134:TRP:CD1	1:A:1230:ILE:HD13	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:GLU:OE1	1:A:515:ARG:HD2	1.86	0.76
1:A:378:ASN:HD21	1:A:382:GLU:HB2	1.53	0.74
2:B:78:MET:HG3	11:B:1871:HOH:O	1.87	0.74
1:A:586:GLN:HE21	1:A:590:GLN:CG	2.02	0.73
1:A:338:MET:HE2	1:A:374:THR:OG1	1.90	0.72
1:A:1062:ARG:HD2	11:A:4321:HOH:O	1.89	0.71
1:A:652:MET:HE3	1:A:867:LYS:O	1.88	0.71
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.73	0.70
1:A:619:ARG:NH1	11:A:4302:HOH:O	2.23	0.70
1:A:1098:HIS:CE1	4:A:2800:MD1:S13	2.88	0.66
1:A:578:VAL:HG23	1:A:579:GLY:H	1.59	0.66
1:A:20:GLY:O	3:C:217:LYS:HD2	1.96	0.65
1:A:1230:ILE:HD11	1:A:1242:GLN:HG3	1.78	0.64
1:A:73:GLN:HE21	1:A:73:GLN:N	1.94	0.64
2:B:78:MET:HG2	2:B:225:THR:HG22	1.79	0.64
1:A:579:GLY:HA3	11:A:4441:HOH:O	1.97	0.64
2:B:361:PRO:HG2	2:B:384:ARG:HD3	1.79	0.63
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.81	0.63
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.45	0.62
11:B:2126:HOH:O	3:C:212:GLU:HG2	1.98	0.62
1:A:1098:HIS:CE1	4:A:1800:MD1:S12	2.94	0.61
4:A:1800:MD1:O11	4:A:1800:MD1:H7	2.00	0.61
1:A:365:GLY:HA3	1:A:408:LYS:HG3	1.81	0.61
1:A:11:LYS:NZ	1:A:11:LYS:HB3	2.16	0.61
1:A:335:ASP:O	1:A:338:MET:HB2	2.00	0.60
4:A:1800:MD1:H7	4:A:1800:MD1:C11	2.32	0.59
1:A:73:GLN:H	1:A:73:GLN:NE2	1.98	0.59
1:A:366:GLN:HG3	1:A:373:LYS:HD2	1.84	0.58
1:A:924:MET:HE2	11:A:4168:HOH:O	2.02	0.58
1:A:177:ILE:HG12	1:A:182:PRO:HA	1.86	0.58
3:C:82:PRO:HG2	3:C:85:VAL:CG2	2.34	0.57
1:A:360:LEU:HD22	1:A:360:LEU:N	2.19	0.57
1:A:1174:SER:HB2	11:A:4182:HOH:O	2.04	0.57
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.35	0.56
1:A:578:VAL:HG23	1:A:579:GLY:N	2.20	0.56
1:A:73:GLN:HE22	2:B:262:THR:HB	1.70	0.56
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.41	0.56
1:A:652:MET:HE1	1:A:866:VAL:CG1	2.34	0.55
2:B:295:ARG:NH1	2:B:298:ASP:OD1	2.39	0.55
1:A:626:GLU:HA	1:A:629:LEU:HD23	1.88	0.55
1:A:338:MET:HG3	1:A:374:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:LYS:HD3	11:B:2075:HOH:O	2.06	0.55
1:A:378:ASN:ND2	1:A:382:GLU:HB2	2.20	0.55
2:B:508:THR:O	2:B:509:GLU:HB3	2.06	0.54
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.89	0.54
1:A:338:MET:HE2	1:A:374:THR:CB	2.36	0.54
1:A:931:ASN:O	1:A:932:TYR:HB2	2.06	0.54
1:A:936:GLU:HB2	11:A:4070:HOH:O	2.07	0.54
1:A:1072:GLU:HB2	11:A:4310:HOH:O	2.07	0.54
2:B:187:CYS:HB3	2:B:349:THR:O	2.08	0.54
1:A:168:LEU:HD23	1:A:168:LEU:C	2.33	0.53
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.90	0.53
1:A:586:GLN:NE2	1:A:590:GLN:CG	2.70	0.53
2:B:289:GLU:HG2	11:B:2078:HOH:O	2.08	0.53
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.91	0.53
3:C:83:ILE:HD11	3:C:156:MET:HG2	1.91	0.53
1:A:919:ASN:ND2	1:A:921:GLN:H	2.06	0.53
1:A:372:TRP:CE2	1:A:863:PRO:HB3	2.43	0.52
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.44	0.52
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.92	0.51
4:A:1800:MD1:O11	4:A:1800:MD1:C7	2.59	0.51
1:A:1006:ILE:CD1	1:A:1016:GLU:HG3	2.41	0.51
3:C:62:ILE:HD11	3:C:98:GLY:HA2	1.93	0.50
1:A:1098:HIS:HE1	4:A:2800:MD1:S13	2.32	0.50
1:A:222:ASP:OD1	11:A:4441:HOH:O	2.20	0.49
1:A:1098:HIS:CG	4:A:1800:MD1:H102	2.48	0.49
2:B:441:GLN:HG2	11:B:2004:HOH:O	2.13	0.49
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.94	0.49
1:A:596:LEU:O	1:A:600:ARG:HD2	2.13	0.49
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.78	0.49
1:A:1037:THR:HB	1:A:1043:GLN:HG3	1.94	0.49
2:B:154:LYS:HE3	11:B:2011:HOH:O	2.12	0.48
1:A:498:ASP:OD2	1:A:500:LYS:NZ	2.46	0.48
1:A:6:ARG:HG2	1:A:6:ARG:HH21	1.79	0.48
1:A:490:VAL:O	1:A:500:LYS:HE2	2.14	0.48
1:A:624:THR:O	1:A:627:GLU:HG2	2.14	0.48
1:A:11:LYS:HB3	1:A:11:LYS:HZ3	1.79	0.48
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.82	0.47
1:A:625:ALA:O	1:A:629:LEU:HD22	2.14	0.47
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.95	0.47
1:A:7:PHE:N	1:A:7:PHE:CD1	2.83	0.47
1:A:336:MET:HA	1:A:473:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LYS:N	2:B:119:LYS:HD2	2.30	0.47
1:A:338:MET:HB3	1:A:354:MET:HE2	1.97	0.47
1:A:115:LYS:HD3	1:A:158:VAL:HG11	1.97	0.46
1:A:658:ALA:HA	1:A:659:PRO:C	2.40	0.46
1:A:56:SER:HB2	1:A:800:SER:HB2	1.97	0.46
1:A:586:GLN:O	1:A:590:GLN:HG3	2.16	0.46
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.16	0.46
2:B:19:CYS:O	2:B:20:HIS:HB2	2.16	0.46
2:B:246:PHE:HA	6:B:1803:SF4:S4	2.56	0.46
1:A:7:PHE:N	1:A:7:PHE:HD1	2.14	0.45
1:A:1006:ILE:HD13	1:A:1016:GLU:HG3	1.99	0.45
1:A:401:ASN:OD1	1:A:403:GLU:HB2	2.16	0.45
1:A:586:GLN:HE21	1:A:590:GLN:NE2	2.12	0.45
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.16	0.45
1:A:307:LEU:HD21	1:A:1059:LEU:HG	1.98	0.45
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.41	0.45
1:A:81:ARG:HH22	1:A:245:ASN:HD21	1.64	0.45
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.99	0.45
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.82	0.45
1:A:145:ALA:O	1:A:149:LYS:HG3	2.16	0.45
1:A:420:LEU:HD11	1:A:487:LEU:HD11	1.99	0.45
1:A:73:GLN:HE22	2:B:262:THR:CB	2.29	0.45
3:C:2:GLN:HA	3:C:2:GLN:OE1	2.17	0.45
1:A:600:ARG:HD3	1:A:905:LEU:HD13	1.99	0.44
1:A:100:TRP:O	1:A:104:SER:HB3	2.17	0.44
1:A:581:GLU:OE2	1:A:801:ASP:OD2	2.36	0.44
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.17	0.44
3:C:12:TYR:N	3:C:13:PRO:HD2	2.33	0.44
1:A:51:VAL:HB	1:A:791:TRP:CH2	2.52	0.44
1:A:214:LEU:HB3	1:A:607:SER:OG	2.16	0.44
1:A:338:MET:HE3	1:A:375:VAL:C	2.43	0.44
1:A:626:GLU:HA	1:A:629:LEU:CD2	2.47	0.44
1:A:1027:THR:HB	1:A:1033:ILE:HD12	2.00	0.44
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.98	0.43
3:C:6:MET:O	3:C:10:ASP:HB2	2.18	0.43
1:A:191:ILE:O	1:A:191:ILE:HG22	2.17	0.43
1:A:52:ASN:CG	1:A:191:ILE:HG13	2.43	0.43
1:A:146:LYS:HB2	1:A:146:LYS:HE3	1.79	0.43
3:C:83:ILE:HG22	11:C:1370:HOH:O	2.18	0.43
1:A:338:MET:HB3	1:A:354:MET:CE	2.48	0.43
1:A:219:TRP:HB2	1:A:607:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASN:O	1:A:373:LYS:HE3	2.19	0.43
2:B:295:ARG:NE	2:B:295:ARG:HA	2.34	0.43
1:A:261:THR:HG22	2:B:264:VAL:HG11	2.01	0.42
3:C:22:ILE:HD12	3:C:22:ILE:HA	1.88	0.42
1:A:1093:GLN:HG2	1:A:1163:HIS:O	2.18	0.42
2:B:162:ASP:O	2:B:163:ASN:HB2	2.19	0.42
3:C:204:ILE:HD12	3:C:205:HIS:N	2.33	0.42
1:A:92:CYS:HB2	1:A:93:PRO:HD2	2.02	0.42
1:A:767:LEU:HD13	1:A:769:VAL:HG23	2.01	0.42
2:B:231:LYS:HA	2:B:231:LYS:HD3	1.86	0.42
1:A:366:GLN:HE21	1:A:373:LYS:NZ	2.18	0.42
1:A:586:GLN:NE2	1:A:590:GLN:NE2	2.68	0.42
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.54	0.42
3:C:208:SER:O	3:C:209:VAL:C	2.62	0.42
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.54	0.42
1:A:471:THR:HG21	1:A:476:LEU:HD13	2.01	0.42
1:A:30:ASP:HB2	2:B:486:GLY:HA2	2.02	0.42
1:A:396:GLU:O	1:A:397:LYS:HG2	2.20	0.42
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.35	0.42
1:A:27:THR:HG23	3:C:222:ARG:HD3	2.02	0.42
1:A:222:ASP:HB3	1:A:578:VAL:HG21	2.01	0.41
1:A:1144:LEU:C	1:A:1144:LEU:HD12	2.45	0.41
1:A:168:LEU:HD23	1:A:168:LEU:O	2.20	0.41
1:A:550:LEU:HD23	1:A:550:LEU:H	1.85	0.41
1:A:384:VAL:HG22	1:A:385:ALA:N	2.34	0.41
1:A:218:ASP:OD2	1:A:218:ASP:N	2.53	0.41
11:B:2126:HOH:O	3:C:212:GLU:CG	2.63	0.41
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.36	0.41
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.21	0.41
1:A:914:LYS:HE3	1:A:1036:ARG:NH1	2.35	0.41
2:B:94:LEU:HA	2:B:95:PRO:HD3	1.89	0.41
3:C:50:LEU:HD13	3:C:54:LEU:HD12	2.03	0.41
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.84	0.41
1:A:487:LEU:N	1:A:487:LEU:CD1	2.84	0.41
1:A:81:ARG:NH2	1:A:245:ASN:HD21	2.19	0.41
1:A:598:TRP:C	1:A:599:GLN:HG3	2.46	0.41
1:A:1230:ILE:CD1	1:A:1242:GLN:HG3	2.48	0.41
2:B:327:GLN:HG3	2:B:457:VAL:HG11	2.03	0.40
1:A:442:PHE:CZ	1:A:1064:PRO:HG2	2.57	0.40
1:A:397:LYS:HD3	1:A:977:PHE:HA	2.03	0.40
2:B:220:TRP:C	2:B:221:ARG:HG3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:HG2	1:A:516:SER:N	2.37	0.40
3:C:211:VAL:HG23	3:C:212:GLU:N	2.36	0.40
1:A:366:GLN:HG2	1:A:373:LYS:HD2	2.03	0.40
1:A:517:GLN:HA	1:A:517:GLN:HE21	1.85	0.40
1:A:578:VAL:CG2	1:A:579:GLY:H	2.26	0.40
1:A:590:GLN:N	1:A:591:PRO:HD2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:1386:HOH:O	11:C:1386:HOH:O[3_354]	1.38	0.82

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1242/1246 (100%)	1182 (95%)	51 (4%)	9 (1%)	18	10
2	B	507/512 (99%)	496 (98%)	11 (2%)	0	100	100
3	C	213/225 (95%)	209 (98%)	4 (2%)	0	100	100
All	All	1962/1983 (99%)	1887 (96%)	66 (3%)	9 (0%)	24	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	578	VAL
1	A	502	TYR
1	A	1166	GLU
1	A	9	TYR
1	A	190	PRO

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Mol	Chain	Res	Type
1	A	361	VAL
1	A	224	PRO
1	A	718	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1039/1043 (100%)	1010 (97%)	29 (3%)	38	32
2	B	436/439 (99%)	430 (99%)	6 (1%)	59	59
3	C	178/185 (96%)	173 (97%)	5 (3%)	38	32
All	All	1653/1667 (99%)	1613 (98%)	40 (2%)	43	38

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

Mol	Chain	Res	Type
1	A	73	GLN
1	A	78	PRO
1	A	139	ILE
1	A	338	MET
1	A	366	GLN
1	A	383	MET
1	A	416	GLN
1	A	461	GLN
1	A	476	LEU
1	A	515	ARG
1	A	600	ARG
1	A	601	PRO
1	A	629	LEU
1	A	677	MET
1	A	732	LEU
1	A	767	LEU
1	A	808	PRO
1	A	835	GLU
1	A	864	LEU

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Mol	Chain	Res	Type
1	A	926	LEU
1	A	936	GLU
1	A	944	MET
1	A	995	ARG
1	A	1006	ILE
1	A	1032	LEU
1	A	1062	ARG
1	A	1072	GLU
1	A	1110	LEU
1	A	1233	LEU
2	B	74	LEU
2	B	85	LEU
2	B	267	ILE
2	B	335	MET
2	B	428	ARG
2	B	473	LYS
3	C	50	LEU
3	C	100	LEU
3	C	142	LEU
3	C	164	GLN
3	C	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	73	GLN
1	A	150	GLN
1	A	173	ASN
1	A	179	ASN
1	A	234	GLN
1	A	245	ASN
1	A	258	GLN
1	A	366	GLN
1	A	369	ASN
1	A	404	GLN
1	A	461	GLN
1	A	517	GLN
1	A	559	ASN
1	A	586	GLN
1	A	590	GLN
1	A	604	HIS

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Mol	Chain	Res	Type
1	A	704	ASN
1	A	708	ASN
1	A	919	ASN
1	A	942	GLN
1	A	1000	GLN
1	A	1023	ASN
1	A	1076	GLN
1	A	1082	GLN
1	A	1238	ASN
2	B	109	GLN
2	B	110	ASN
2	B	160	ASN
2	B	451	ASN
3	C	149	GLN
3	C	164	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	1.24	1 (12%)	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	-	5/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CG	2.19	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	3.31	127.91	122.82
3	C	1	FME	CB-CA-N	2.35	114.79	110.52

There are no chirality outliers.

All (5) 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	CB-CA-N-CN
3	C	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEM	C	806	3	50,50,50	1.78	12 (24%)	67,82,82	0.90	1 (1%)
6	SF4	A	1801	1	0,12,12	-	-	-		
6	SF4	B	1803	2	0,12,12	-	-	-		
10	AGA	C	1309	-	24,24,29	0.78	1 (4%)	27,29,35	1.59	2 (7%)
8	3PH	B	1310	-	17,17,47	1.16	2 (11%)	18,21,52	2.00	5 (27%)
4	MD1	A	2800	5	47,51,51	2.88	8 (17%)	56,78,78	1.40	7 (12%)
4	MD1	A	1800	5	47,51,51	2.64	8 (17%)	56,78,78	1.43	8 (14%)
6	SF4	B	1802	2	0,12,12	-	-	-		
7	F3S	B	1805	2	0,9,9	-	-	-		
9	HEM	C	807	3	50,50,50	1.88	18 (36%)	67,82,82	0.93	4 (5%)
6	SF4	B	1804	2	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	C	806	3	-	4/14/54/54	-
6	SF4	A	1801	1	-	-	0/6/5/5
6	SF4	B	1803	2	-	-	0/6/5/5
10	AGA	C	1309	-	-	3/26/26/34	-
8	3PH	B	1310	-	1/1/3/4	8/18/18/49	-
4	MD1	A	2800	5	-	1/22/59/59	0/5/5/5
4	MD1	A	1800	5	-	7/22/59/59	0/5/5/5
6	SF4	B	1802	2	-	-	0/6/5/5
7	F3S	B	1805	2	-	-	0/3/3/3
9	HEM	C	807	3	-	6/14/54/54	-
6	SF4	B	1804	2	-	-	0/6/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2800	MD1	C7-N8	17.06	1.49	1.28
4	A	1800	MD1	C7-N8	15.41	1.47	1.28
4	A	2800	MD1	PA-O3B	-5.07	1.54	1.59
9	C	807	HEM	CAB-C3B	4.50	1.59	1.47
9	C	806	HEM	CAB-C3B	4.10	1.58	1.47
9	C	807	HEM	FE-NC	3.97	2.08	1.95
9	C	806	HEM	CAC-C3C	3.94	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	806	HEM	CMA-C3A	3.90	1.58	1.50
4	A	1800	MD1	C16-C20	3.74	1.49	1.39
9	C	806	HEM	CMB-C2B	3.66	1.58	1.50
9	C	807	HEM	CMC-C2C	3.51	1.58	1.50
9	C	807	HEM	CMB-C2B	3.45	1.57	1.50
9	C	806	HEM	FE-NC	3.20	2.05	1.95
9	C	806	HEM	CMC-C2C	3.18	1.57	1.50
4	A	1800	MD1	C4-N3	3.12	1.41	1.34
9	C	806	HEM	CMD-C2D	3.12	1.57	1.50
9	C	807	HEM	CAC-C3C	3.04	1.55	1.47
4	A	1800	MD1	C12-C13	3.00	1.43	1.34
4	A	1800	MD1	PA-O3B	-2.93	1.56	1.59
4	A	2800	MD1	C20-N8	2.79	1.41	1.36
4	A	1800	MD1	C6-N1	2.76	1.44	1.38
4	A	2800	MD1	C14-N15	2.70	1.51	1.46
9	C	807	HEM	CAD-C3D	2.57	1.58	1.51
4	A	2800	MD1	C4-N3	2.53	1.40	1.34
9	C	807	HEM	CMA-C3A	2.52	1.55	1.50
9	C	806	HEM	C4D-C3D	2.47	1.49	1.45
9	C	806	HEM	CBD-CAD	2.41	1.60	1.51
9	C	807	HEM	CBD-CGD	2.35	1.56	1.50
9	C	807	HEM	O1A-CGA	2.33	1.29	1.22
9	C	807	HEM	CBA-CAA	2.32	1.60	1.51
10	C	1309	AGA	C8-C7	2.31	1.57	1.50
9	C	807	HEM	C1D-C2D	2.29	1.49	1.44
9	C	807	HEM	FE-NB	2.26	2.01	1.94
4	A	1800	MD1	C15-N17	2.25	1.43	1.38
9	C	807	HEM	FE-ND	2.23	2.01	1.94
9	C	807	HEM	C4A-C3A	2.22	1.48	1.43
9	C	806	HEM	CBA-CAA	2.21	1.59	1.51
9	C	807	HEM	CAA-C2A	2.21	1.57	1.51
8	B	1310	3PH	O21-C21	2.21	1.38	1.33
8	B	1310	3PH	P-O14	2.18	1.62	1.54
9	C	807	HEM	CBA-CGA	2.17	1.55	1.50
4	A	1800	MD1	PB-O3B	2.15	1.61	1.59
9	C	807	HEM	CBD-CAD	2.10	1.59	1.51
9	C	806	HEM	CAD-C3D	2.09	1.56	1.51
4	A	2800	MD1	C12-C13	2.08	1.40	1.34
4	A	2800	MD1	O11-C11	2.06	1.47	1.42
4	A	2800	MD1	O6-C6	2.04	1.27	1.23
9	C	806	HEM	O1A-CGA	2.02	1.28	1.22
9	C	807	HEM	CMD-C2D	2.02	1.54	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2800	MD1	C17-N18-C20	6.06	122.59	114.20
4	A	1800	MD1	C17-N18-C20	5.87	122.33	114.20
10	C	1309	AGA	C9-C8-C7	5.46	133.69	113.69
8	B	1310	3PH	C3-C2-C1	4.82	123.03	111.78
8	B	1310	3PH	C33-C32-C31	4.52	130.27	113.69
10	C	1309	AGA	C14-C13-C12	4.27	129.34	113.69
8	B	1310	3PH	O21-C2-C3	3.61	121.30	108.34
4	A	1800	MD1	O14-C15-C16	-2.67	120.82	127.26
4	A	1800	MD1	N17-C17-N18	-2.62	118.52	123.32
4	A	2800	MD1	C2-N3-C4	2.57	116.73	112.30
4	A	1800	MD1	O3B-PA-O2A	-2.53	103.09	110.70
4	A	1800	MD1	O3A-C10-C11	-2.49	100.96	107.96
4	A	2800	MD1	O1B-PB-O2B	2.44	123.78	112.44
9	C	807	HEM	CAD-C3D-C4D	-2.29	120.71	124.70
9	C	806	HEM	CMA-C3A-C2A	2.28	130.46	125.62
4	A	2800	MD1	N17-C17-N18	-2.27	119.17	123.32
9	C	807	HEM	CMA-C3A-C2A	2.25	130.39	125.62
4	A	1800	MD1	C15-C16-N15	2.25	122.39	116.27
8	B	1310	3PH	O11-P-O12	2.22	112.45	106.44
9	C	807	HEM	O1D-CGD-CBD	-2.21	116.10	123.09
4	A	2800	MD1	C1'-N9-C8	2.15	132.82	126.73
4	A	2800	MD1	N16-C17-N17	2.12	121.23	116.76
4	A	1800	MD1	N16-C17-N17	2.06	121.11	116.76
4	A	1800	MD1	C1'-N9-C8	2.05	132.55	126.73
4	A	2800	MD1	N1-C2-N3	-2.05	119.57	123.32
9	C	807	HEM	O1A-CGA-CBA	-2.05	116.59	123.09
8	B	1310	3PH	O21-C2-C1	2.03	115.61	108.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	1310	3PH	C2

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1800	MD1	C5'-O5'-PA-O3B
4	A	1800	MD1	C5'-O5'-PA-O2A
8	B	1310	3PH	O22-C21-O21-C2
4	A	1800	MD1	O4'-C4'-C5'-O5'
4	A	1800	MD1	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	B	1310	3PH	C1-C2-C3-O31
8	B	1310	3PH	C31-C32-C33-C34
10	C	1309	AGA	C11-C10-C9-C8
9	C	807	HEM	C2C-C3C-CAC-CBC
8	B	1310	3PH	O11-C1-C2-O21
4	A	1800	MD1	PA-O3B-PB-O2B
4	A	1800	MD1	C5'-O5'-PA-O1A
8	B	1310	3PH	O32-C31-O31-C3
8	B	1310	3PH	C32-C31-O31-C3
9	C	807	HEM	C4C-C3C-CAC-CBC
10	C	1309	AGA	C8-C7-O7-C6
9	C	807	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAD-CBD-CGD-O2D
10	C	1309	AGA	O8-C7-O7-C6
9	C	807	HEM	CAD-CBD-CGD-O2D
9	C	806	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAA-CBA-CGA-O2A
8	B	1310	3PH	C3-C2-O21-C21
9	C	806	HEM	CAA-CBA-CGA-O1A
9	C	807	HEM	CAA-CBA-CGA-O1A
4	A	1800	MD1	PA-O3B-PB-O1B
4	A	2800	MD1	PA-O3B-PB-O2B
8	B	1310	3PH	C32-C33-C34-C35

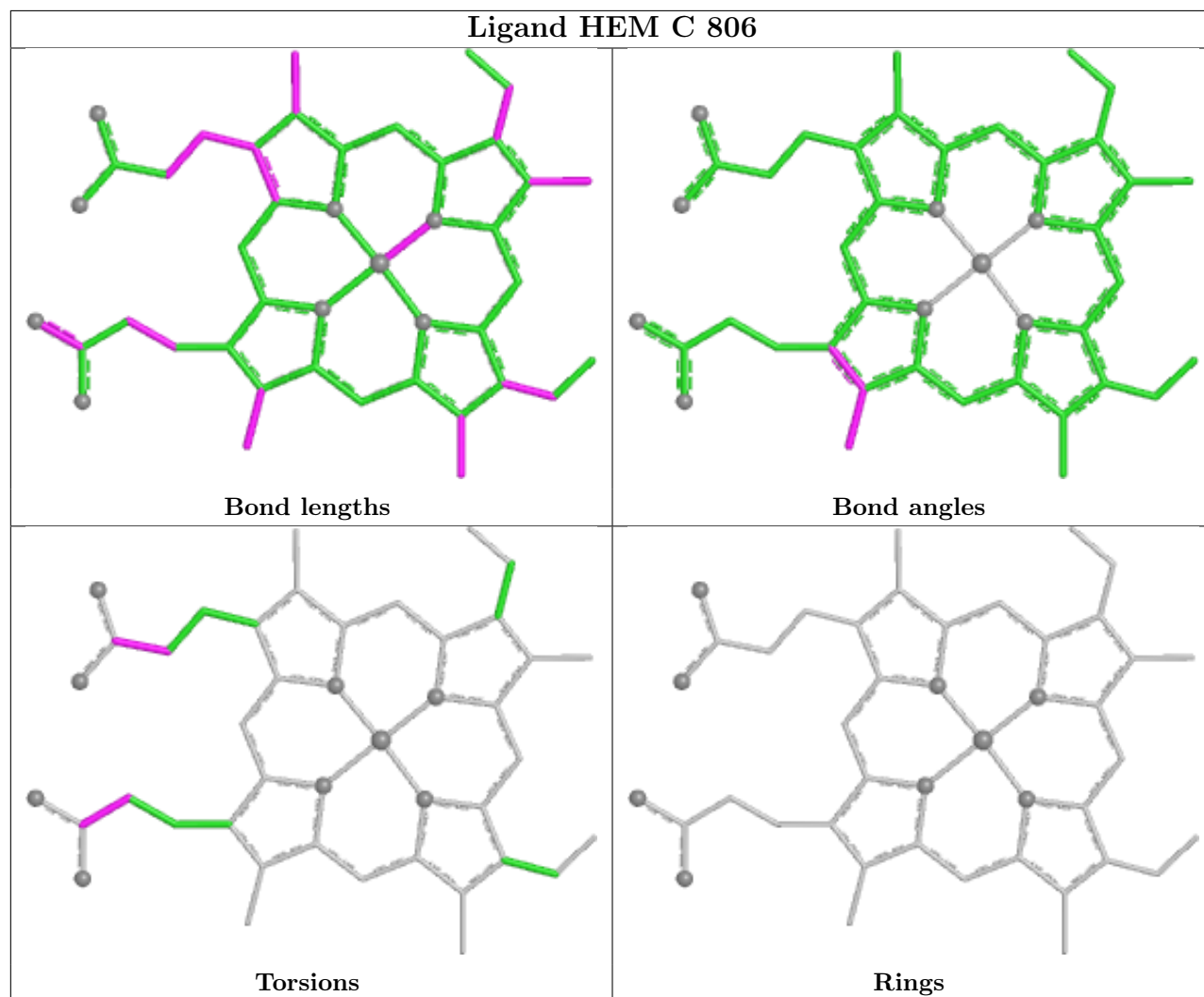
There are no ring outliers.

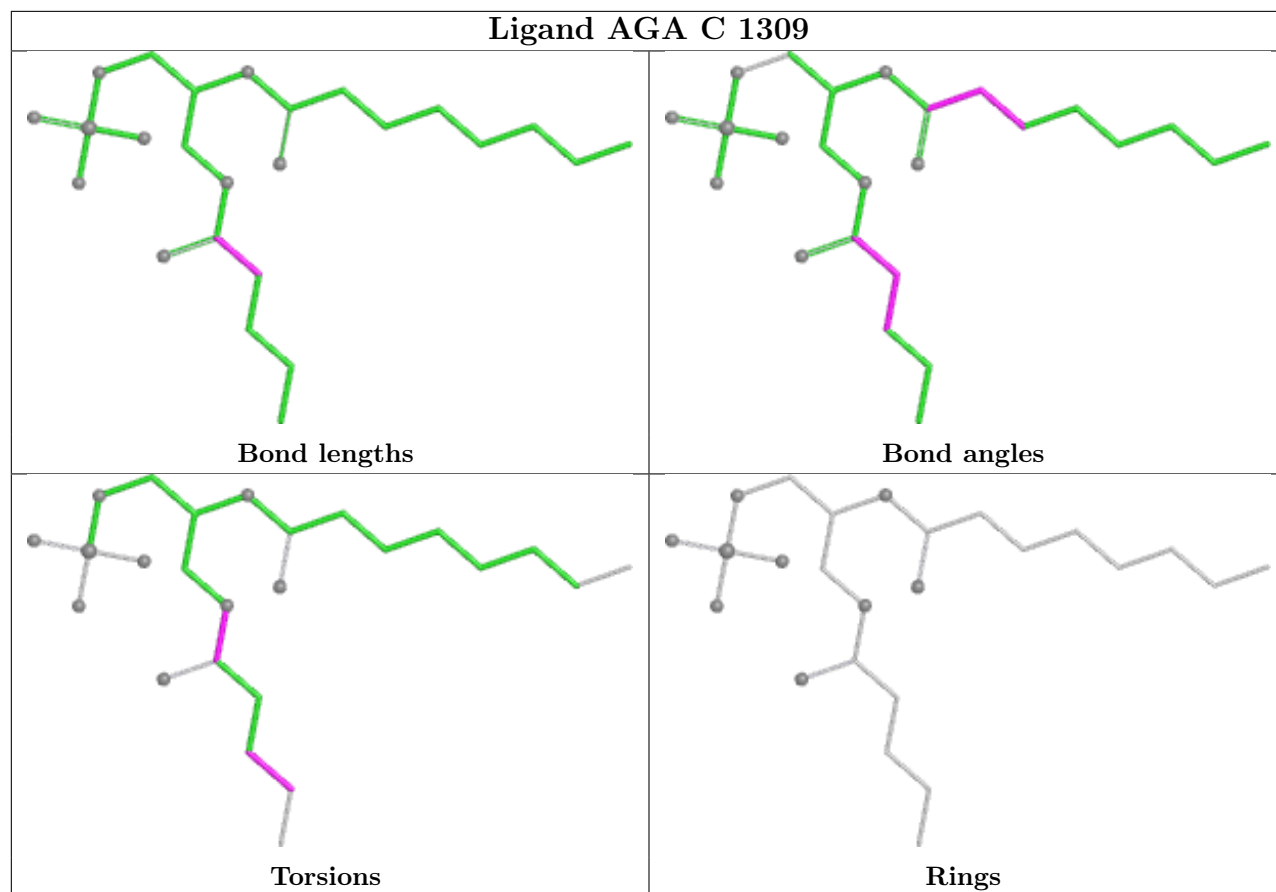
3 monomers are involved in 8 short contacts:

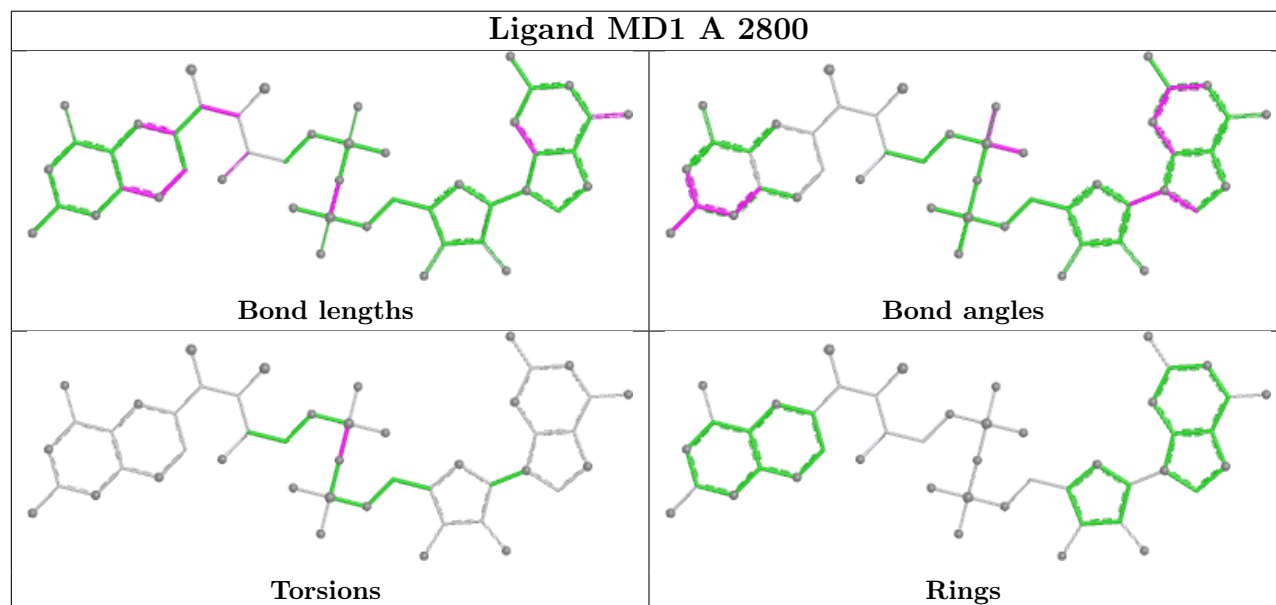
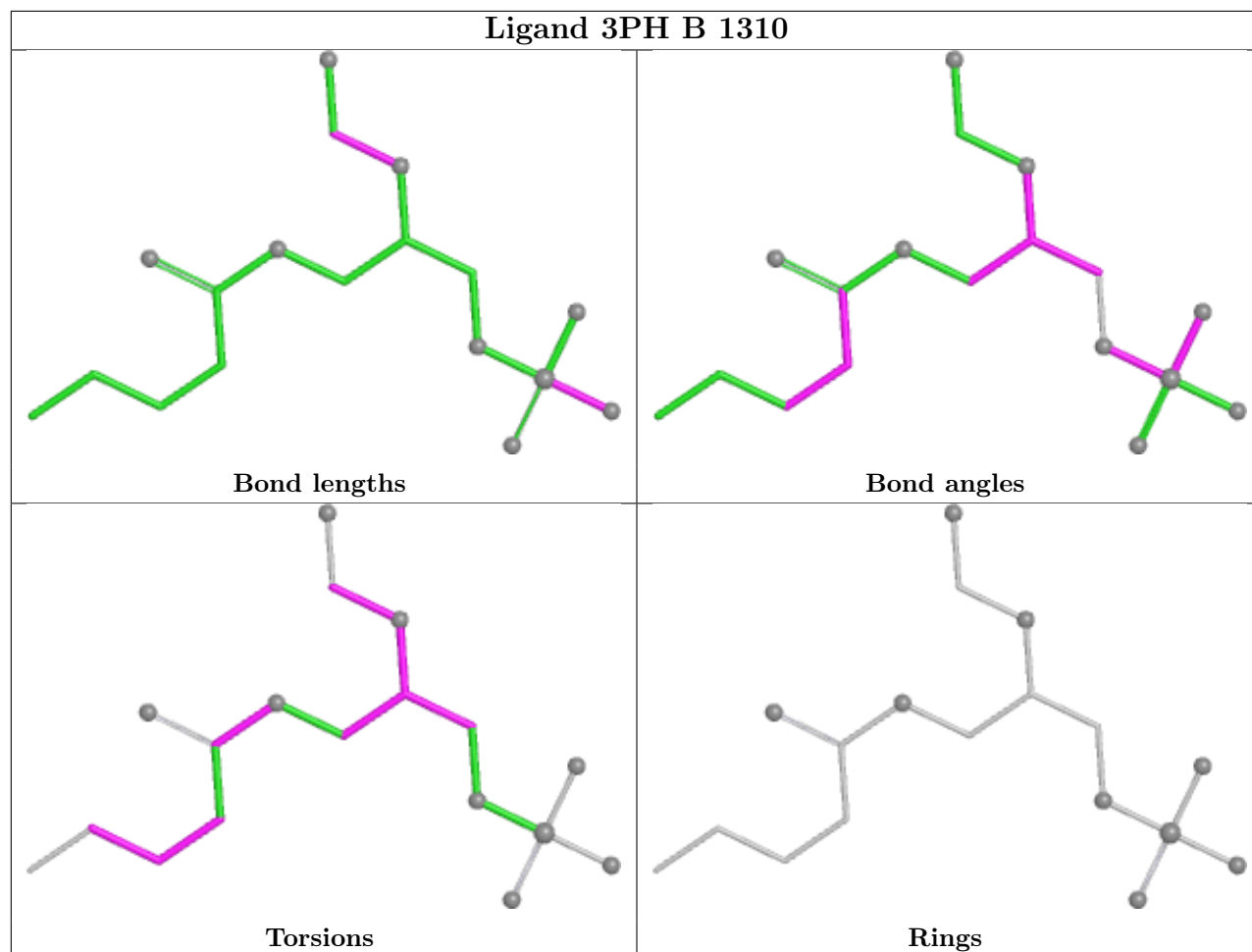
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1803	SF4	1	0
4	A	2800	MD1	2	0
4	A	1800	MD1	5	0

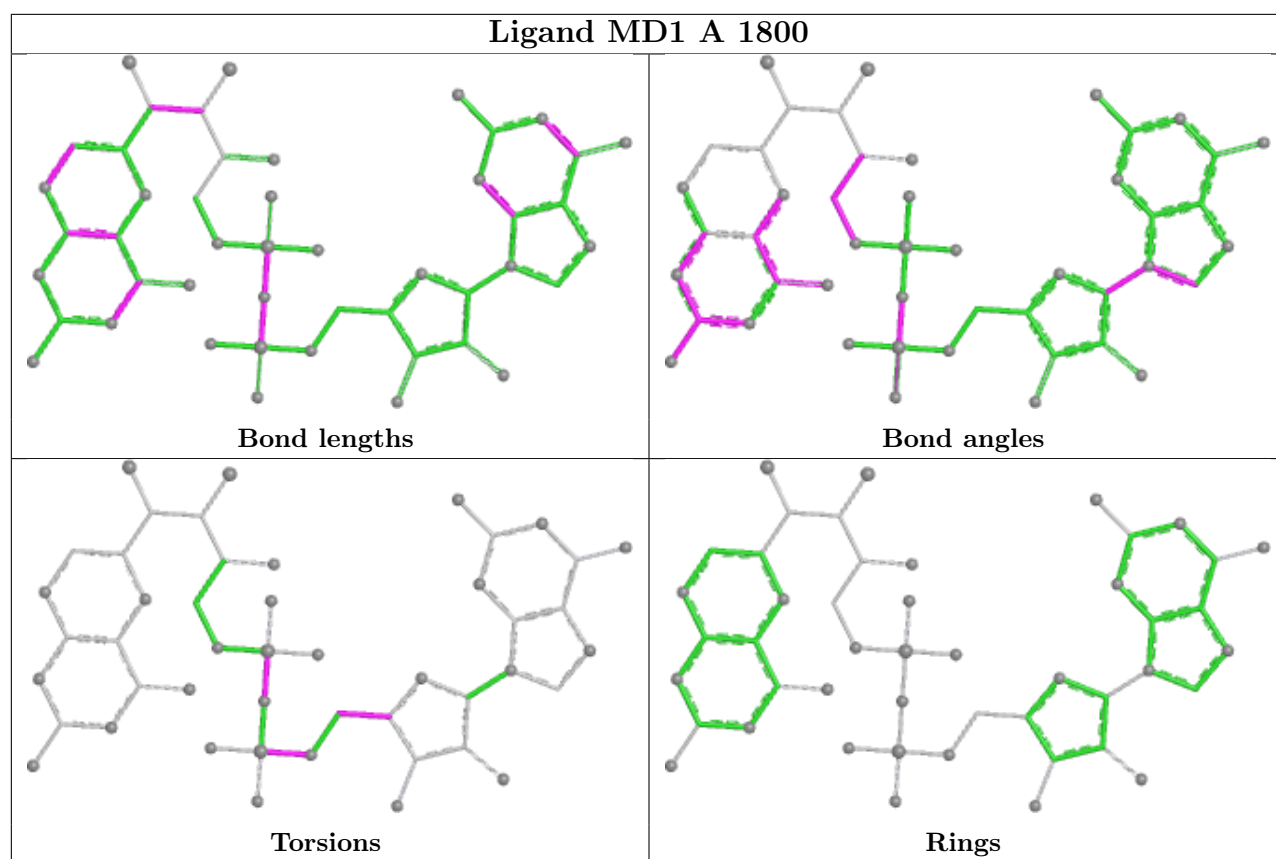
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

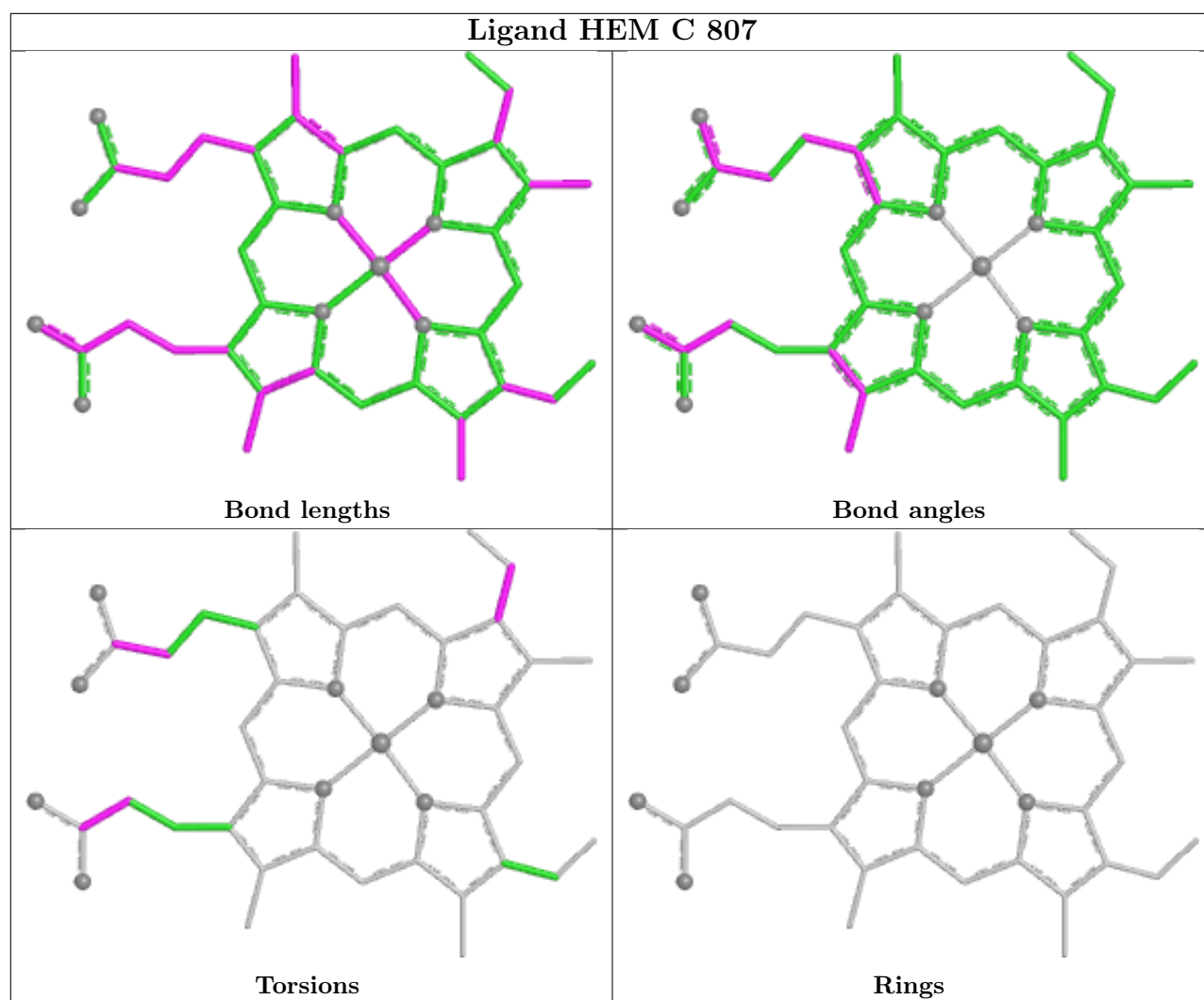
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	1244/1246 (99%)	-0.03	36 (2%) 53 57	10, 23, 43, 58	0
2	B	509/512 (99%)	-0.59	6 (1%) 76 79	10, 17, 30, 51	0
3	C	216/225 (96%)	0.01	5 (2%) 61 65	12, 23, 40, 53	0
All	All	1969/1983 (99%)	-0.17	47 (2%) 59 63	10, 21, 41, 58	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	6.9
1	A	10	PHE	4.8
1	A	749	VAL	4.5
1	A	501	ALA	4.0
1	A	1244	SER	3.5
1	A	367	GLU	3.5
1	A	362	ASP	3.4
3	C	72	THR	3.1
1	A	463	ALA	2.9
1	A	8	ARG	2.9
1	A	467	THR	2.8
1	A	13	LYS	2.8
1	A	1243	GLU	2.6
1	A	361	VAL	2.6
1	A	673	GLU	2.6
1	A	719	SER	2.6
1	A	413	THR	2.6
1	A	7	PHE	2.5
1	A	759	ASN	2.5
1	A	12	GLN	2.5
1	A	502	TYR	2.5
1	A	743	LEU	2.5
1	A	676	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	71	LEU	2.4
1	A	379	THR	2.4
2	B	366	ALA	2.4
2	B	365	ALA	2.3
1	A	875	ASP	2.3
1	A	991	ASP	2.3
1	A	319	LEU	2.2
1	A	422	SER	2.2
2	B	364	SER	2.2
3	C	63	PHE	2.2
1	A	366	GLN	2.2
1	A	11	LYS	2.2
3	C	70	MET	2.1
1	A	1018	GLU	2.1
1	A	670	GLY	2.1
2	B	119	LYS	2.1
3	C	81	LEU	2.1
2	B	509	GLU	2.1
1	A	461	GLN	2.1
2	B	371	LEU	2.1
1	A	419	LEU	2.0
1	A	717	LEU	2.0
1	A	675	ALA	2.0
1	A	872	GLY	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	0.92	0.10	40,45,55,56	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

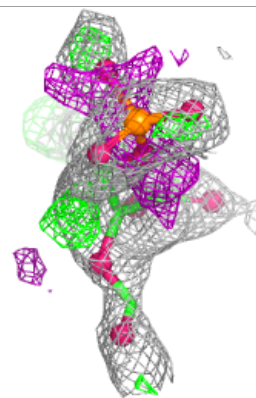
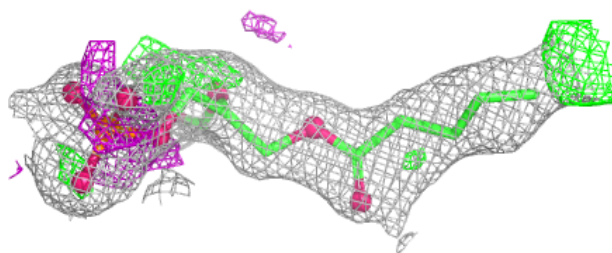
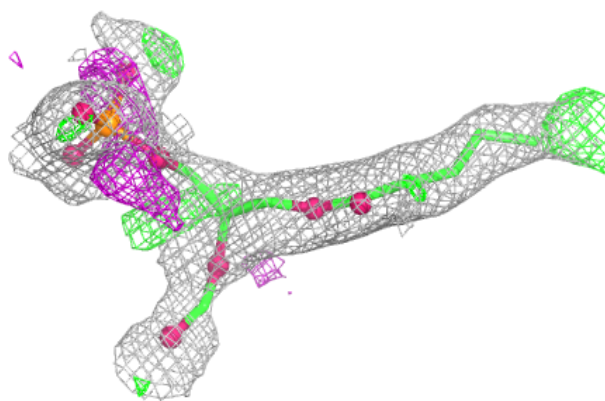
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	3PH	B	1310	18/48	0.69	0.22	46,54,60,61	0
4	MD1	A	2800	47/47	0.96	0.06	15,21,29,33	0
4	MD1	A	1800	47/47	0.96	0.07	12,19,32,36	0
10	AGA	C	1309	25/30	0.96	0.08	15,20,39,41	0
9	HEM	C	807	43/43	0.97	0.09	22,27,40,47	0
9	HEM	C	806	43/43	0.98	0.05	10,15,18,30	0
6	SF4	A	1801	8/8	0.98	0.06	18,20,24,24	0
5	6MO	A	3800	1/1	0.98	0.15	40,40,40,40	0
6	SF4	B	1802	8/8	0.99	0.04	17,19,20,21	0
6	SF4	B	1804	8/8	0.99	0.02	16,17,19,20	0
6	SF4	B	1803	8/8	1.00	0.02	11,12,13,13	0
7	F3S	B	1805	7/7	1.00	0.02	11,13,14,14	0

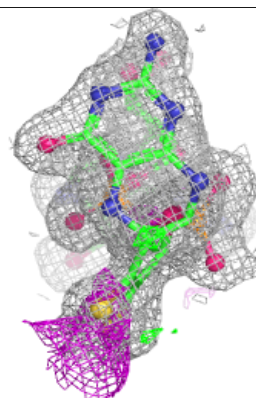
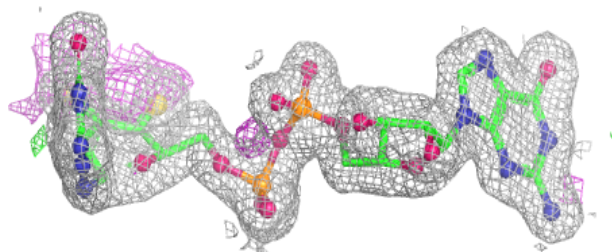
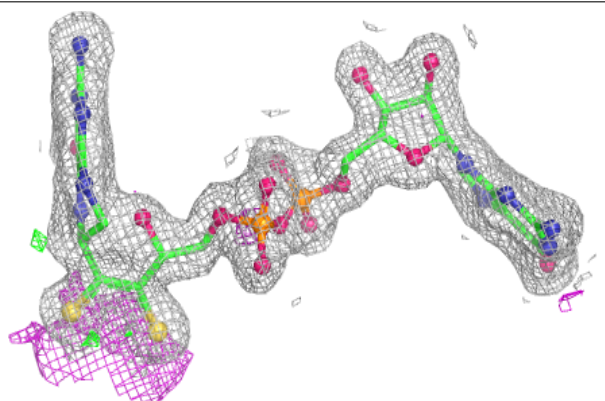
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3PH B 1310:

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

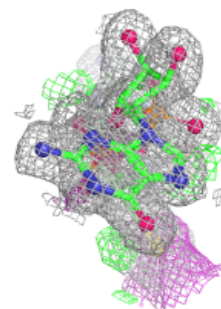
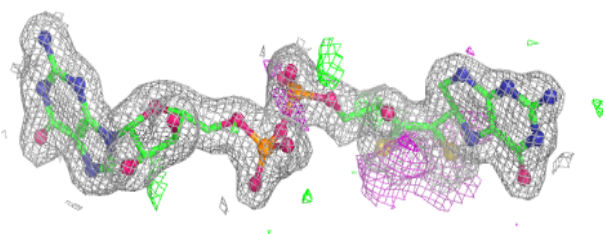
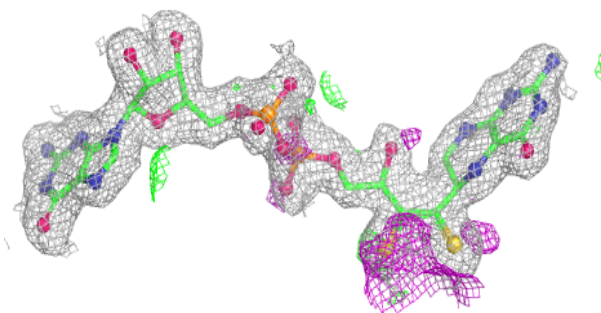
**Electron density around MD1 A 2800:**

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

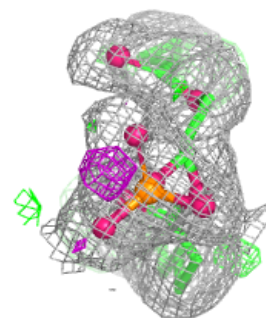
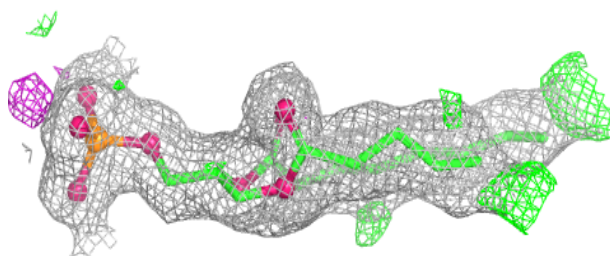
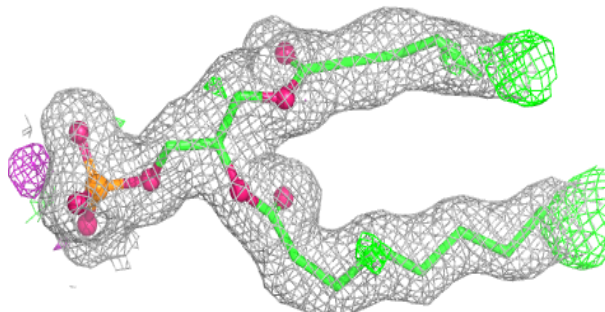


Electron density around MD1 A 1800:

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

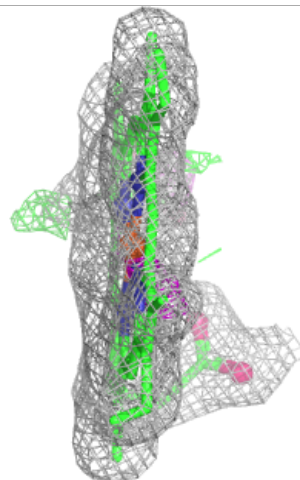
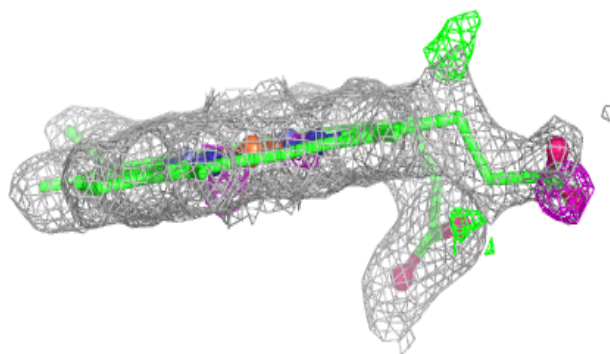
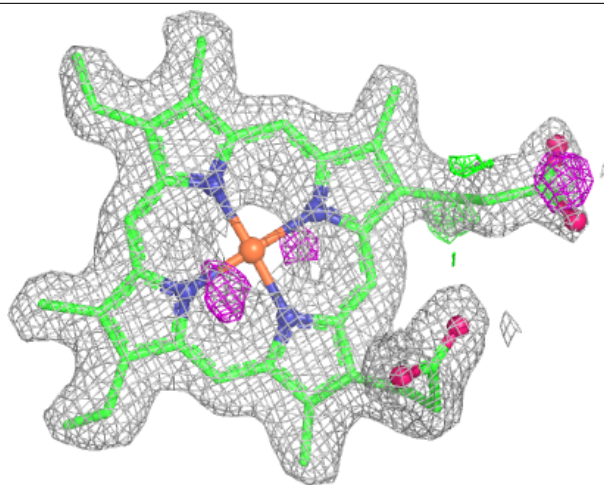
**Electron density around AGA C 1309:**

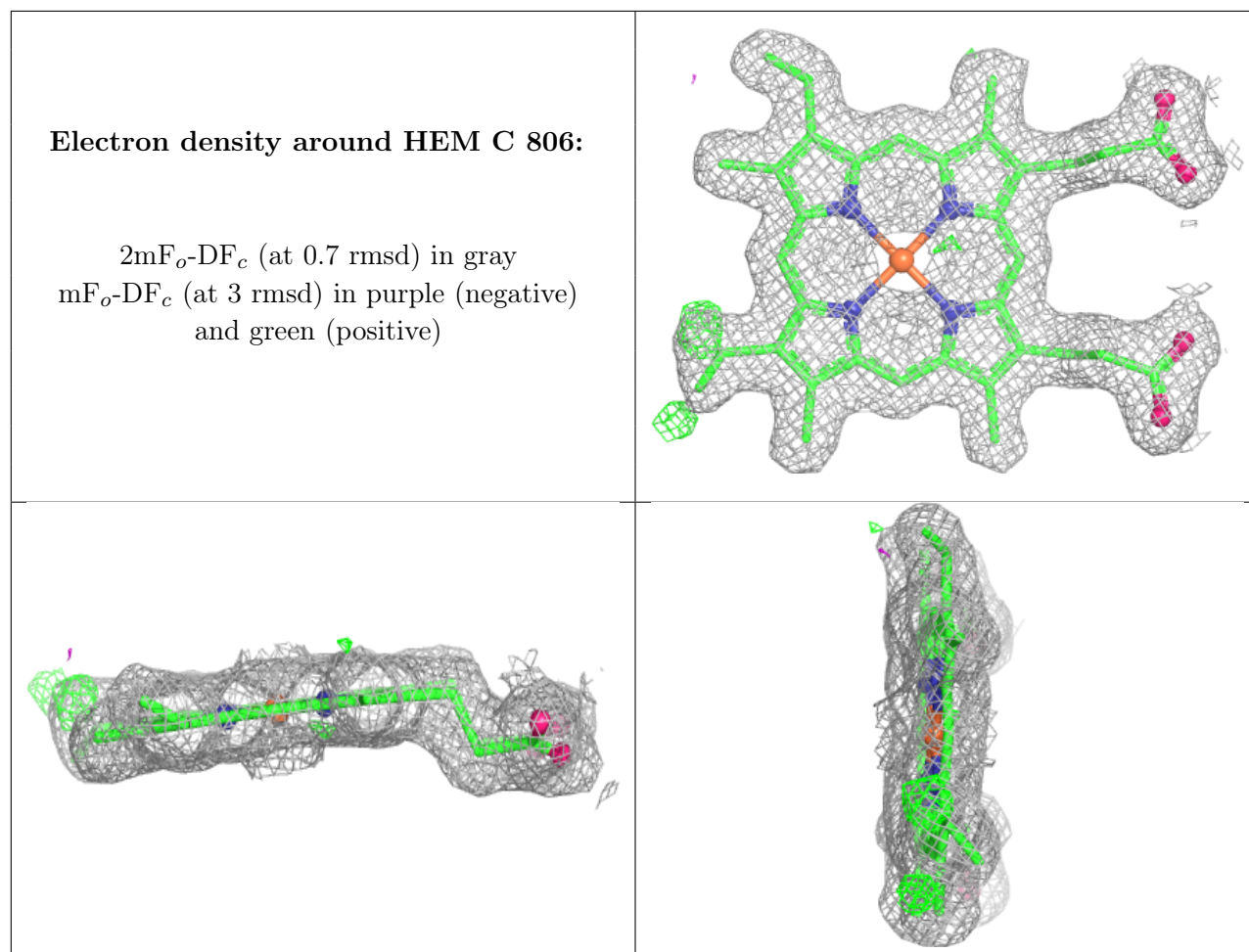
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.