



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 3IR7 / pdb_00003ir7
Title : Crystal structure of NarGHI mutant NarG-R94S
Authors : Bertero, M.G.; Rothery, R.A.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2009-08-21
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

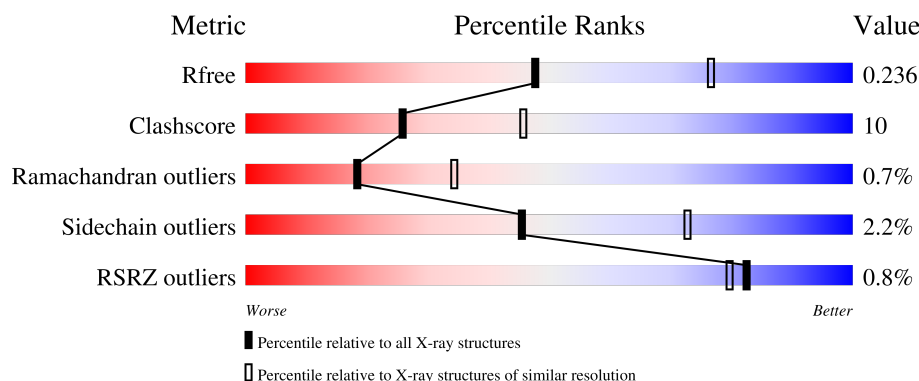
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	1247	76% 22% .
2	B	512	81% 17% ..
3	C	225	4% 74% 24% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16102 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	1242	Total	C	N	O	S	0	0	0
			9840	6214	1723	1855	48			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	SER	ARG	engineered mutation	UNP P09152

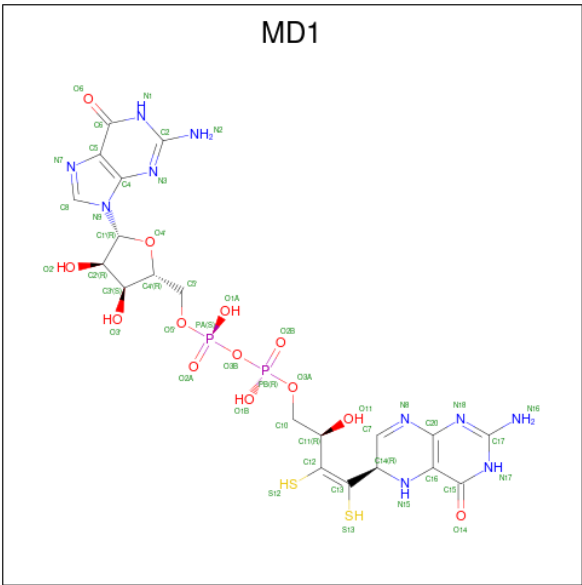
- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

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

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

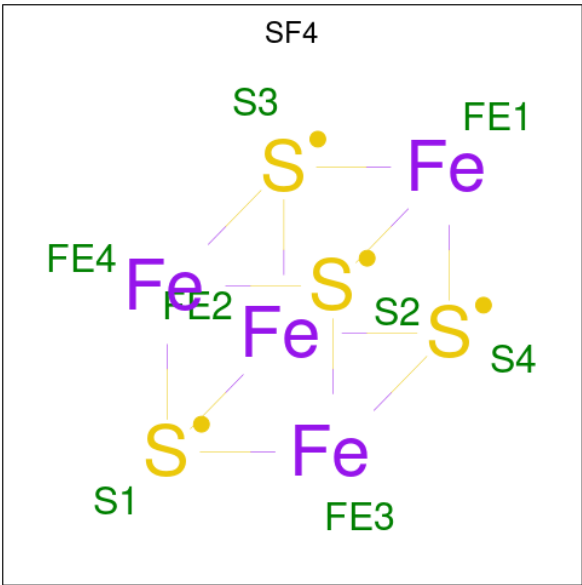
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	225	Total	C	N	O	S	0	0	0
			1791	1188	303	286	14			

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



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

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



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

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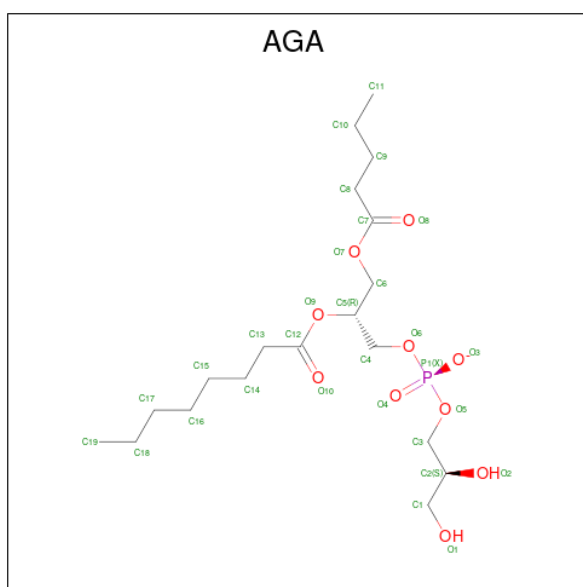
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

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

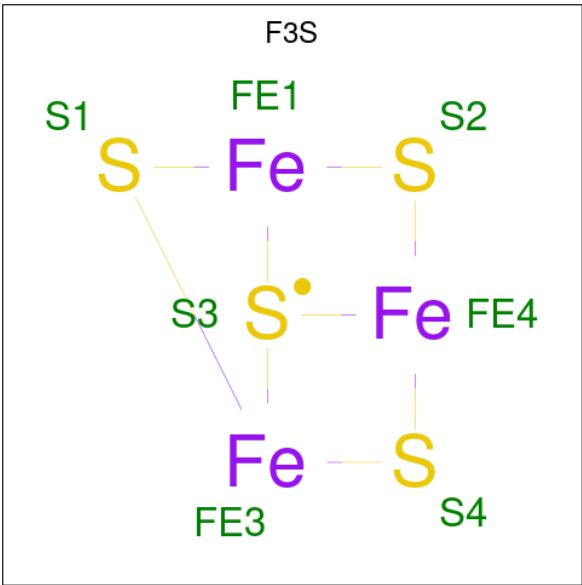
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		

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



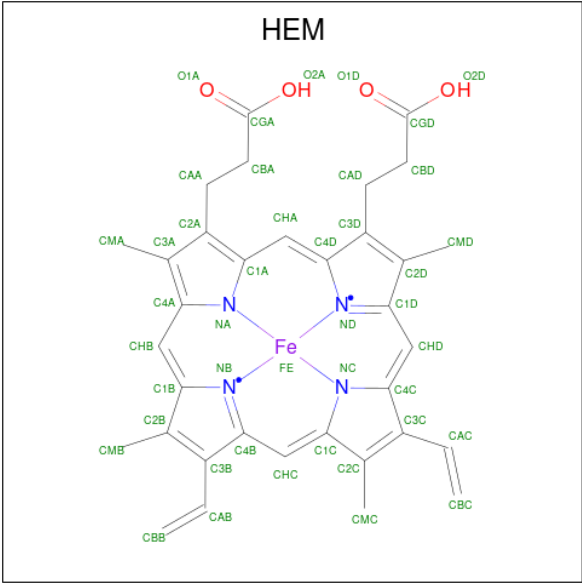
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			25	16	8	1		

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



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

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



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

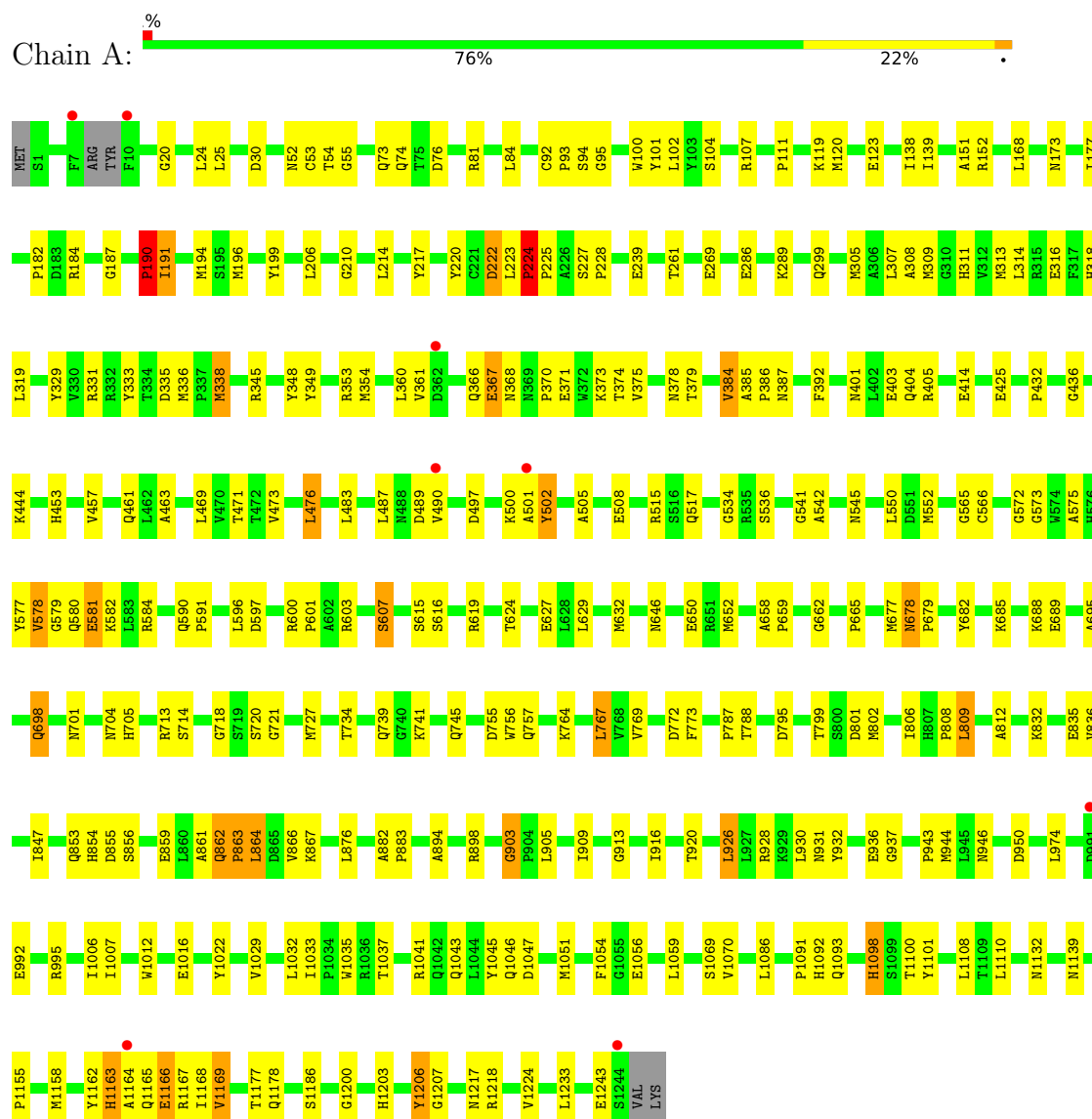
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	86	Total 86	O 86	0	0
10	B	82	Total 82	O 82	0	0
10	C	8	Total 8	O 8	0	0

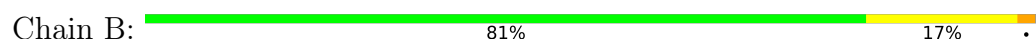
3 Residue-property plots

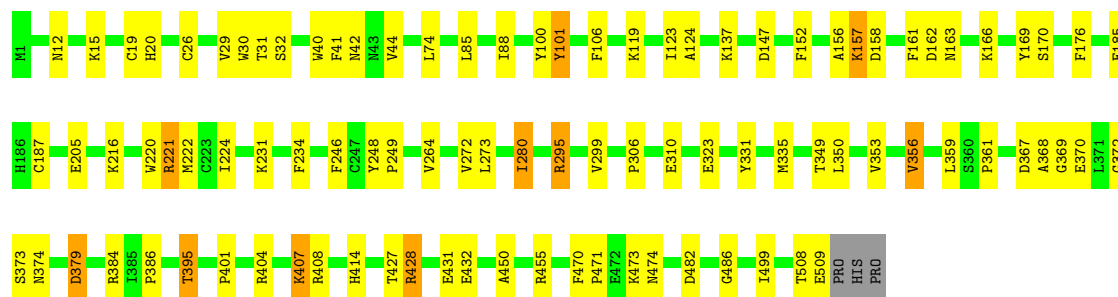
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

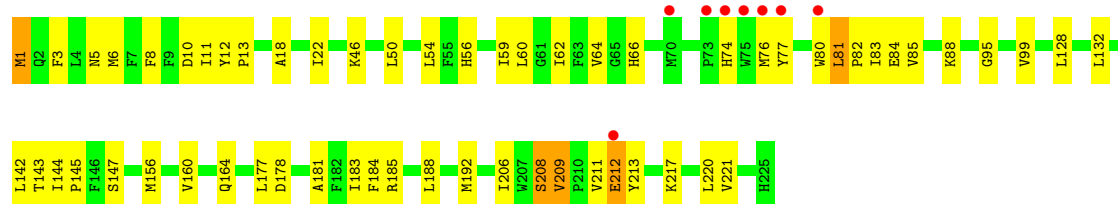
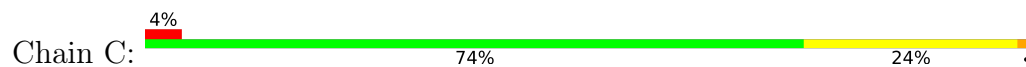


- Molecule 2: Respiratory nitrate reductase 1 beta chain





• 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	153.85Å 241.15Å 139.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.96 – 2.50 24.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.96-2.50) 99.8 (24.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.243 0.194 , 0.236	Depositor DCC
R_{free} test set	7209 reflections (8.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.2	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	0.95	EDS
Total number of atoms	16102	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, AGA, MD1, SF4, 6MO, FME, HEM

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	0.41	0/10097	0.94	45/13707 (0.3%)
2	B	0.42	0/4146	0.96	15/5609 (0.3%)
3	C	0.42	0/1833	0.86	4/2481 (0.2%)
All	All	0.42	0/16076	0.94	64/21797 (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	607	SER	N-CA-C	9.05	123.34	111.75
2	B	30	TRP	N-CA-C	8.28	123.51	113.41
1	A	809	LEU	N-CA-C	-7.80	96.52	109.07
1	A	1163	HIS	N-CA-C	7.71	122.05	110.64
1	A	1167	ARG	N-CA-C	7.38	121.59	112.59
2	B	280	ILE	N-CA-C	7.30	118.03	110.36
1	A	1093	GLN	N-CA-C	7.03	119.06	110.41
1	A	1070	VAL	N-CA-C	6.85	117.45	111.56
2	B	407	LYS	CB-CA-C	6.78	121.53	110.88
2	B	88	ILE	N-CA-C	6.76	119.50	111.05
1	A	812	ALA	N-CA-C	-6.53	104.24	111.36
2	B	29	VAL	N-CA-C	6.40	117.03	110.82
2	B	379	ASP	N-CA-C	-6.39	100.51	110.42
1	A	1043	GLN	N-CA-C	6.37	118.55	108.67
1	A	802	MET	N-CA-C	6.19	118.03	111.28
1	A	316	GLU	N-CA-C	6.16	119.99	112.23
1	A	1165	GLN	N-CA-C	-6.12	104.43	113.61
1	A	1206	TYR	N-CA-C	6.05	118.35	110.43
2	B	216	LYS	N-CA-C	6.04	119.91	112.54
2	B	359	LEU	N-CA-C	-6.03	101.02	110.36
1	A	615	SER	N-CA-C	-5.87	105.98	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	209	VAL	CA-C-N	5.82	127.11	119.84
3	C	209	VAL	C-N-CA	5.82	127.11	119.84
1	A	1035	TRP	N-CA-C	-5.81	101.03	110.20
1	A	937	GLY	CA-C-N	5.81	125.67	119.28
1	A	937	GLY	C-N-CA	5.81	125.67	119.28
1	A	101	TYR	N-CA-C	5.77	117.25	111.07
2	B	356	VAL	N-CA-C	-5.76	101.31	107.77
1	A	1186	SER	N-CA-C	-5.71	105.80	112.89
2	B	221	ARG	N-CA-C	5.70	119.06	111.30
1	A	224	PRO	N-CA-C	-5.68	103.77	110.70
1	A	903	GLY	CA-C-N	5.63	125.24	119.56
1	A	903	GLY	C-N-CA	5.63	125.24	119.56
1	A	1169	VAL	N-CA-C	5.62	116.04	108.17
1	A	573	GLY	N-CA-C	5.60	118.85	111.52
1	A	678	ASN	CA-C-N	5.54	125.00	119.24
1	A	678	ASN	C-N-CA	5.54	125.00	119.24
1	A	76	ASP	N-CA-C	5.54	119.14	112.93
1	A	863	PRO	N-CA-C	5.53	121.22	113.53
2	B	157	LYS	N-CA-C	-5.52	106.39	113.01
1	A	184	ARG	N-CA-C	-5.51	105.91	113.30
1	A	74	GLN	N-CA-C	-5.49	101.53	110.20
2	B	205	GLU	N-CA-C	5.47	117.05	111.14
3	C	8	PHE	N-CA-C	5.47	118.00	111.71
1	A	151	ALA	N-CA-C	-5.43	106.70	113.38
1	A	333	TYR	N-CA-C	5.38	120.51	113.30
3	C	208	SER	N-CA-C	5.32	119.40	113.02
1	A	222	ASP	N-CA-C	-5.31	106.94	113.41
1	A	1166	GLU	N-CA-C	5.28	122.04	110.80
1	A	1054	PHE	N-CA-C	-5.16	106.83	112.72
1	A	1098	HIS	CB-CA-C	-5.16	110.65	116.63
2	B	31	THR	N-CA-C	5.14	118.66	111.30
1	A	698	GLN	CA-C-N	5.14	124.86	119.82
1	A	698	GLN	C-N-CA	5.14	124.86	119.82
1	A	73	GLN	N-CA-C	5.11	117.65	110.23
2	B	395	THR	N-CA-C	5.11	118.62	111.56
1	A	853	GLN	N-CA-C	5.11	117.94	109.46
1	A	862	GLN	CA-C-N	5.10	124.71	119.05
1	A	862	GLN	C-N-CA	5.10	124.71	119.05
1	A	713	ARG	N-CA-C	-5.10	105.72	112.24
2	B	222	MET	N-CA-C	-5.08	106.77	113.12
1	A	1029	VAL	N-CA-C	5.06	115.83	110.72
1	A	384	VAL	N-CA-C	5.04	114.83	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1016	GLU	N-CA-C	-5.02	98.42	107.75

There are no chirality outliers.

There are no planarity outliers.

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	9840	0	9496	209	0
2	B	4050	0	3973	57	0
3	C	1791	0	1825	39	0
4	A	94	0	42	8	0
5	A	8	0	0	1	0
5	B	24	0	0	1	0
6	A	1	0	0	0	0
7	A	25	0	29	0	0
8	B	7	0	0	0	0
9	C	86	0	60	2	0
10	A	86	0	0	6	0
10	B	82	0	0	4	0
10	C	8	0	0	0	0
All	All	16102	0	15425	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (298) 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:508:GLU:OE1	1:A:515:ARG:HD2	1.75	0.86
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.62	0.81
1:A:584:ARG:HD3	1:A:1006:ILE:HD13	1.62	0.80
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.67	0.77
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.65	0.77
1:A:1218:ARG:HD2	10:A:1319:HOH:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:LYS:NZ	2:B:432:GLU:HG2	2.07	0.70
1:A:578:VAL:HG23	1:A:579:GLY:H	1.56	0.69
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.74	0.69
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.75	0.69
3:C:6:MET:O	3:C:10:ASP:HB2	1.94	0.68
1:A:1098:HIS:CE1	4:A:1251:MD1:S13	2.88	0.66
2:B:407:LYS:HZ3	2:B:432:GLU:HG2	1.60	0.66
1:A:677:MET:HG3	1:A:682:TYR:HB2	1.77	0.66
1:A:1098:HIS:HE1	4:A:1251:MD1:S13	2.18	0.66
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.78	0.65
1:A:335:ASP:O	1:A:338:MET:HB2	1.96	0.65
1:A:387:ASN:ND2	1:A:405:ARG:HB2	2.11	0.65
1:A:225:PRO:O	1:A:228:PRO:HD2	1.97	0.65
1:A:652:MET:HE2	1:A:862:GLN:HE22	1.62	0.65
3:C:95:GLY:O	3:C:99:VAL:HG23	1.96	0.64
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.79	0.63
1:A:338:MET:HB3	1:A:354:MET:HE2	1.81	0.63
1:A:338:MET:HE2	1:A:374:THR:OG1	1.99	0.62
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.35	0.62
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.64	0.62
1:A:168:LEU:HD23	1:A:168:LEU:O	2.00	0.62
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.82	0.62
1:A:336:MET:HA	1:A:473:VAL:HB	1.81	0.61
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.80	0.61
1:A:652:MET:HE3	1:A:867:LYS:O	2.01	0.60
2:B:187:CYS:HB3	2:B:349:THR:O	2.01	0.60
1:A:552:MET:HE3	1:A:1056:GLU:OE1	2.01	0.60
3:C:143:THR:HG22	3:C:183:ILE:HG13	1.84	0.59
1:A:517:GLN:HA	1:A:517:GLN:NE2	2.18	0.59
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.83	0.59
1:A:1098:HIS:CE1	4:A:1247:MD1:S12	2.96	0.59
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.85	0.59
2:B:373:SER:HB3	2:B:428:ARG:NH1	2.19	0.58
2:B:508:THR:O	2:B:509:GLU:HB3	2.03	0.58
1:A:191:ILE:O	1:A:194:MET:HG2	2.04	0.57
1:A:345:ARG:HB2	1:A:348:TYR:O	2.04	0.57
1:A:1092:HIS:HA	1:A:1163:HIS:HB3	1.85	0.57
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.28	0.57
3:C:84:GLU:O	3:C:88:LYS:HG2	2.04	0.57
1:A:487:LEU:HD12	1:A:487:LEU:N	2.20	0.57
3:C:12:TYR:N	3:C:13:PRO:HD2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:O	1:A:123:GLU:HG3	2.04	0.57
1:A:360:LEU:N	1:A:360:LEU:HD22	2.20	0.57
1:A:677:MET:HE2	1:A:682:TYR:HA	1.86	0.56
1:A:578:VAL:HG23	1:A:579:GLY:N	2.20	0.56
1:A:652:MET:HE1	1:A:866:VAL:CG1	2.33	0.56
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.40	0.56
1:A:338:MET:HG3	1:A:374:THR:HB	1.87	0.56
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.30	0.56
1:A:214:LEU:HB3	1:A:607:SER:OG	2.05	0.56
3:C:50:LEU:HD13	3:C:54:LEU:HD12	1.88	0.56
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.74	0.56
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.88	0.56
1:A:931:ASN:O	1:A:932:TYR:HB2	2.05	0.55
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.88	0.55
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.88	0.55
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.87	0.55
4:A:1247:MD1:H7	4:A:1247:MD1:C11	2.37	0.55
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.88	0.55
2:B:372:GLY:HA3	2:B:379:ASP:OD1	2.07	0.55
1:A:52:ASN:CG	1:A:191:ILE:HG13	2.32	0.55
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.42	0.55
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.42	0.55
3:C:1:FME:O1	3:C:3:PHE:HB3	2.07	0.55
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.42	0.55
1:A:1155:PRO:HG2	1:A:1158:MET:HE3	1.89	0.55
1:A:220:TYR:CE1	1:A:720:SER:HB2	2.42	0.55
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.88	0.54
1:A:220:TYR:CE2	4:A:1247:MD1:H101	2.43	0.54
1:A:309:MET:O	1:A:313:MET:HG3	2.06	0.54
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.07	0.54
3:C:128:LEU:O	3:C:132:LEU:HG	2.08	0.54
1:A:581:GLU:OE2	1:A:801:ASP:OD2	2.25	0.54
1:A:662:GLY:HA2	1:A:704:ASN:OD1	2.07	0.54
1:A:1132:ASN:ND2	2:B:137:LYS:HE3	2.22	0.54
3:C:83:ILE:HD11	3:C:156:MET:HG2	1.89	0.54
2:B:220:TRP:C	2:B:221:ARG:HG3	2.33	0.53
2:B:370:GLU:OE2	2:B:370:GLU:HA	2.07	0.53
1:A:1086:LEU:HD12	1:A:1224:VAL:HG21	1.90	0.53
3:C:80:TRP:C	3:C:81:LEU:HD23	2.34	0.53
1:A:225:PRO:C	1:A:228:PRO:HD2	2.34	0.53
1:A:1006:ILE:CD1	10:A:1323:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:ALA:HB1	2:B:455:ARG:HD3	1.91	0.53
1:A:795:ASP:HA	1:A:809:LEU:O	2.10	0.52
1:A:223:LEU:O	1:A:225:PRO:HD3	2.09	0.52
1:A:299:GLN:CD	1:A:1158:MET:HE2	2.35	0.52
1:A:453:HIS:HA	1:A:489:ASP:OD1	2.10	0.52
3:C:181:ALA:HB3	3:C:184:PHE:CD2	2.45	0.52
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.10	0.51
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.46	0.51
1:A:767:LEU:HD13	1:A:769:VAL:HG23	1.93	0.51
1:A:679:PRO:HB2	1:A:847:ILE:HD11	1.93	0.51
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.22	0.51
1:A:490:VAL:O	1:A:500:LYS:HE2	2.11	0.50
1:A:856:SER:O	1:A:859:GLU:HG2	2.11	0.50
3:C:81:LEU:HD23	3:C:81:LEU:N	2.27	0.50
1:A:652:MET:CE	1:A:862:GLN:HE22	2.25	0.50
1:A:739:GLN:NE2	1:A:1177:THR:HG22	2.27	0.50
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.47	0.50
2:B:137:LYS:HA	10:B:585:HOH:O	2.11	0.50
2:B:119:LYS:HD2	2:B:119:LYS:N	2.26	0.50
1:A:269:GLU:HG3	2:B:15:LYS:HE3	1.94	0.50
1:A:473:VAL:HG13	1:A:1045:TYR:HB2	1.93	0.50
1:A:624:THR:O	1:A:627:GLU:HG2	2.12	0.50
1:A:338:MET:HE1	1:A:386:PRO:HG3	1.94	0.49
2:B:185:GLU:OE1	2:B:353:VAL:HB	2.12	0.49
1:A:1218:ARG:HG3	10:A:1319:HOH:O	2.11	0.49
1:A:920:THR:O	1:A:920:THR:HG23	2.12	0.49
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.43	0.49
1:A:373:LYS:HD3	1:A:392:PHE:CZ	2.47	0.49
1:A:835:GLU:HG3	1:A:836:VAL:N	2.27	0.49
3:C:160:VAL:O	3:C:164:GLN:HG3	2.12	0.49
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.78	0.49
2:B:306:PRO:O	2:B:310:GLU:HG3	2.13	0.49
1:A:338:MET:HE1	1:A:386:PRO:CG	2.42	0.49
1:A:368:ASN:O	1:A:373:LYS:HE3	2.13	0.49
1:A:1155:PRO:CG	1:A:1158:MET:HE3	2.42	0.49
2:B:137:LYS:HE2	10:B:591:HOH:O	2.12	0.49
3:C:18:ALA:O	3:C:22:ILE:HG22	2.13	0.49
1:A:107:ARG:HD2	1:A:773:PHE:O	2.12	0.49
1:A:378:ASN:HA	1:A:414:GLU:O	2.13	0.49
1:A:102:LEU:HD12	1:A:102:LEU:H	1.78	0.48
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ALA:HB1	1:A:704:ASN:HB3	1.95	0.48
3:C:50:LEU:CD1	3:C:54:LEU:HD12	2.43	0.48
3:C:11:ILE:C	3:C:13:PRO:HD2	2.38	0.48
1:A:534:GLY:O	1:A:572:GLY:HA3	2.12	0.48
1:A:974:LEU:HD21	1:A:1033:ILE:HD13	1.94	0.48
2:B:427:THR:O	2:B:431:GLU:HG3	2.13	0.48
3:C:56:HIS:HA	3:C:59:ILE:HG22	1.94	0.48
1:A:497:ASP:HA	1:A:505:ALA:HB2	1.96	0.48
1:A:658:ALA:HA	1:A:659:PRO:C	2.38	0.48
1:A:152:ARG:HB2	1:A:734:THR:CG2	2.43	0.48
3:C:83:ILE:HG23	3:C:84:GLU:N	2.28	0.48
1:A:926:LEU:HD22	1:A:930:LEU:CD1	2.44	0.48
1:A:436:GLY:O	1:A:444:LYS:HD3	2.13	0.48
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.96	0.48
1:A:168:LEU:HD23	1:A:168:LEU:C	2.39	0.47
4:A:1247:MD1:H7	4:A:1247:MD1:H11	1.94	0.47
1:A:864:LEU:HD22	1:A:864:LEU:N	2.29	0.47
2:B:404:ARG:O	2:B:408:ARG:HG3	2.14	0.47
1:A:387:ASN:HD22	1:A:405:ARG:HB2	1.77	0.47
2:B:331:TYR:CE2	2:B:335:MET:HG3	2.49	0.47
1:A:894:ALA:O	1:A:898:ARG:HG3	2.14	0.47
2:B:152:PHE:CE2	2:B:170:SER:HB3	2.49	0.47
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.50	0.47
1:A:373:LYS:HD3	1:A:392:PHE:CE1	2.49	0.47
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.29	0.47
1:A:1100:THR:O	1:A:1101:TYR:HB2	2.14	0.47
1:A:552:MET:HE3	1:A:1056:GLU:CD	2.39	0.47
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.96	0.46
1:A:582:LYS:NZ	1:A:584:ARG:NH1	2.63	0.46
1:A:597:ASP:O	1:A:903:GLY:HA3	2.15	0.46
1:A:199:TYR:CD1	1:A:199:TYR:C	2.93	0.46
1:A:384:VAL:HG22	1:A:385:ALA:N	2.29	0.46
1:A:210:GLY:O	1:A:603:ARG:HD2	2.16	0.46
1:A:20:GLY:O	3:C:217:LYS:HD2	2.14	0.46
1:A:54:THR:HA	1:A:580:GLN:HG3	1.96	0.46
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.16	0.46
1:A:24:LEU:HD12	3:C:221:VAL:O	2.16	0.46
1:A:95:GLY:HA3	5:A:1248:SF4:S4	2.55	0.46
1:A:289:LYS:HD3	1:A:289:LYS:C	2.41	0.46
1:A:338:MET:HB3	1:A:354:MET:CE	2.45	0.46
1:A:366:GLN:O	1:A:370:PRO:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:CYS:O	2:B:20:HIS:HB2	2.16	0.46
1:A:100:TRP:O	1:A:104:SER:HB3	2.15	0.46
1:A:220:TYR:CE1	1:A:720:SER:CB	2.99	0.46
2:B:224:ILE:HD11	2:B:234:PHE:HB2	1.98	0.46
1:A:289:LYS:HD3	1:A:289:LYS:O	2.16	0.45
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.51	0.45
1:A:30:ASP:HB2	2:B:486:GLY:HA2	1.98	0.45
1:A:102:LEU:HD12	1:A:102:LEU:N	2.31	0.45
1:A:308:ALA:O	1:A:311:HIS:HB3	2.16	0.45
3:C:211:VAL:HG23	3:C:212:GLU:N	2.30	0.45
1:A:832:LYS:O	1:A:836:VAL:HG23	2.17	0.45
2:B:162:ASP:O	2:B:163:ASN:HB2	2.16	0.45
1:A:584:ARG:HD3	1:A:1006:ILE:CD1	2.39	0.45
2:B:26:CYS:SG	2:B:41:PHE:HB2	2.56	0.45
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.46	0.45
2:B:123:ILE:HG13	2:B:124:ALA:H	1.82	0.45
1:A:338:MET:HE3	1:A:375:VAL:C	2.41	0.45
1:A:677:MET:HE2	1:A:682:TYR:CA	2.46	0.45
1:A:196:MET:HE1	1:A:799:THR:HG23	1.98	0.45
1:A:944:MET:HE3	1:A:946:ASN:HD21	1.82	0.45
2:B:12:ASN:HA	2:B:356:VAL:HB	1.99	0.45
2:B:295:ARG:HE	2:B:295:ARG:HA	1.82	0.45
1:A:120:MET:O	1:A:138:ILE:HD11	2.17	0.44
1:A:191:ILE:HG23	1:A:580:GLN:O	2.17	0.44
1:A:239:GLU:HG2	1:A:1022:TYR:HB3	1.98	0.44
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.52	0.44
3:C:50:LEU:HD13	3:C:50:LEU:C	2.43	0.44
1:A:81:ARG:CZ	1:A:84:LEU:HD11	2.47	0.44
1:A:349:TYR:CZ	1:A:469:LEU:HD12	2.52	0.44
1:A:471:THR:HG21	1:A:476:LEU:HD13	1.99	0.44
2:B:156:ALA:HB1	2:B:166:LYS:HD2	1.99	0.44
2:B:482:ASP:OD1	2:B:499:ILE:HG13	2.17	0.44
1:A:1059:LEU:N	1:A:1059:LEU:HD23	2.33	0.44
1:A:1098:HIS:C	1:A:1164:ALA:CB	2.91	0.44
1:A:578:VAL:CG2	1:A:579:GLY:H	2.21	0.44
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.98	0.44
1:A:1218:ARG:CD	10:A:1319:HOH:O	2.57	0.44
1:A:905:LEU:HD22	1:A:909:ILE:HD12	1.99	0.44
3:C:62:ILE:HG23	3:C:66:HIS:CE1	2.53	0.44
1:A:360:LEU:C	1:A:463:ALA:HB2	2.42	0.43
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:HB3	1:A:1101:TYR:CD1	2.53	0.43
1:A:425:GLU:O	1:A:457:VAL:HG22	2.18	0.43
2:B:156:ALA:C	2:B:158:ASP:N	2.75	0.43
1:A:582:LYS:HB2	1:A:801:ASP:OD2	2.19	0.43
1:A:913:GLY:O	1:A:916:ILE:HG12	2.19	0.43
2:B:176:PHE:CD1	2:B:176:PHE:C	2.96	0.43
1:A:1218:ARG:CG	10:A:1319:HOH:O	2.66	0.43
2:B:231:LYS:HD3	2:B:231:LYS:HA	1.82	0.43
2:B:100:TYR:O	2:B:101:TYR:HB3	2.18	0.43
2:B:123:ILE:HG13	2:B:124:ALA:N	2.34	0.43
1:A:854:HIS:O	1:A:855:ASP:HB2	2.18	0.43
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.84	0.42
1:A:926:LEU:HD22	1:A:930:LEU:HD11	2.00	0.42
3:C:208:SER:O	3:C:209:VAL:C	2.61	0.42
1:A:314:LEU:O	1:A:318:HIS:HB2	2.19	0.42
2:B:169:TYR:OH	2:B:386:PRO:HB3	2.19	0.42
1:A:190:PRO:HD3	1:A:714:SER:HB2	2.01	0.42
1:A:545:ASN:OD1	1:A:550:LEU:HD12	2.18	0.42
1:A:487:LEU:N	1:A:487:LEU:CD1	2.82	0.42
1:A:541:GLY:HA3	4:A:1251:MD1:O1B	2.20	0.42
1:A:305:MET:O	1:A:309:MET:HG3	2.19	0.42
1:A:876:LEU:C	1:A:876:LEU:HD23	2.44	0.42
2:B:374:ASN:HA	2:B:414:HIS:CD2	2.55	0.42
1:A:432:PRO:HD3	1:A:632:MET:CE	2.50	0.42
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.34	0.42
2:B:508:THR:O	2:B:509:GLU:CB	2.67	0.42
1:A:371:GLU:H	1:A:371:GLU:CD	2.26	0.42
3:C:212:GLU:HG3	3:C:213:TYR:N	2.35	0.42
1:A:196:MET:CE	1:A:799:THR:HG23	2.50	0.42
1:A:861:ALA:HB3	1:A:1200:GLY:O	2.19	0.42
1:A:54:THR:HA	1:A:580:GLN:CG	2.50	0.41
1:A:862:GLN:HA	1:A:863:PRO:HD2	1.93	0.41
2:B:137:LYS:CE	10:B:591:HOH:O	2.66	0.41
3:C:13:PRO:HB3	3:C:192:MET:SD	2.60	0.41
1:A:701:ASN:ND2	1:A:704:ASN:ND2	2.68	0.41
2:B:40:TRP:O	2:B:41:PHE:C	2.63	0.41
3:C:74:HIS:C	3:C:76:MET:H	2.27	0.41
3:C:188:LEU:HD22	9:C:807:HEM:HMB3	2.02	0.41
1:A:360:LEU:HD22	1:A:360:LEU:H	1.84	0.41
1:A:685:LYS:O	1:A:689:GLU:HG3	2.20	0.41
1:A:767:LEU:CD1	1:A:769:VAL:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:TYR:CG	2:B:249:PRO:HD3	2.55	0.41
1:A:992:GLU:HG2	1:A:1007:ILE:HD11	2.02	0.41
1:A:1177:THR:O	1:A:1178:GLN:HB2	2.19	0.41
1:A:182:PRO:HD2	1:A:665:PRO:HG2	2.02	0.41
1:A:1059:LEU:HD23	1:A:1059:LEU:H	1.85	0.41
2:B:280:ILE:HG23	2:B:350:LEU:HD12	2.03	0.41
3:C:144:ILE:N	3:C:145:PRO:HD2	2.35	0.41
1:A:542:ALA:HB3	4:A:1251:MD1:O3B	2.21	0.41
1:A:806:ILE:O	1:A:806:ILE:HG23	2.21	0.41
1:A:329:TYR:CD1	1:A:565:GLY:HA2	2.55	0.41
1:A:764:LYS:CE	10:A:1328:HOH:O	2.67	0.41
2:B:246:PHE:HA	5:B:803:SF4:S4	2.60	0.41
2:B:272:VAL:CG1	2:B:273:LEU:N	2.83	0.41
3:C:184:PHE:O	3:C:188:LEU:HG	2.21	0.41
1:A:286:GLU:OE1	2:B:147:ASP:OD1	2.39	0.41
1:A:756:TRP:CG	1:A:757:GLN:N	2.89	0.41
2:B:157:LYS:HE2	2:B:157:LYS:HB3	1.78	0.41
3:C:77:TYR:CB	3:C:81:LEU:HD21	2.51	0.41
1:A:367:GLU:HG3	1:A:368:ASN:N	2.35	0.41
1:A:403:GLU:O	1:A:405:ARG:N	2.54	0.41
1:A:590:GLN:N	1:A:591:PRO:HD2	2.36	0.41
1:A:591:PRO:HA	1:A:596:LEU:HB2	2.01	0.41
1:A:772:ASP:C	1:A:788:THR:HG22	2.46	0.41
2:B:367:ASP:C	2:B:369:GLY:N	2.77	0.41
3:C:60:LEU:O	3:C:64:VAL:HG23	2.21	0.41
1:A:227:SER:HB3	1:A:228:PRO:CD	2.46	0.41
1:A:536:SER:HB2	1:A:566:CYS:SG	2.61	0.41
2:B:367:ASP:C	2:B:369:GLY:H	2.29	0.41
1:A:111:PRO:HA	1:A:787:PRO:HD3	2.03	0.40
1:A:992:GLU:CG	1:A:1007:ILE:HD11	2.50	0.40
1:A:53:CYS:C	1:A:55:GLY:H	2.30	0.40
1:A:222:ASP:O	1:A:224:PRO:HD3	2.21	0.40
3:C:177:LEU:O	3:C:178:ASP:C	2.64	0.40
1:A:307:LEU:HD13	1:A:502:TYR:CD2	2.56	0.40
1:A:379:THR:HG21	1:A:414:GLU:OE2	2.21	0.40
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.21	0.40
2:B:32:SER:HB2	10:B:556:HOH:O	2.22	0.40
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.54	0.40
3:C:50:LEU:CD1	3:C:54:LEU:CD1	3.00	0.40
3:C:74:HIS:C	3:C:76:MET:N	2.79	0.40
1:A:25:LEU:HD11	3:C:220:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:O	1:A:177:ILE:HG13	2.21	0.40
1:A:307:LEU:HD13	1:A:502:TYR:CE2	2.56	0.40
1:A:646:ASN:O	1:A:650:GLU:HG3	2.22	0.40
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.56	0.40
1:A:190:PRO:O	1:A:191:ILE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1238/1247 (99%)	1149 (93%)	78 (6%)	11 (1%)	14	27
2	B	507/512 (99%)	486 (96%)	19 (4%)	2 (0%)	30	49
3	C	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
All	All	1968/1984 (99%)	1845 (94%)	110 (6%)	13 (1%)	18	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	A	721	GLY
1	A	1166	GLU
1	A	578	VAL
2	B	101	TYR
1	A	190	PRO
1	A	224	PRO
1	A	361	VAL
1	A	502	TYR
1	A	718	GLY
1	A	1217	ASN
2	B	368	ALA

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Mol	Chain	Res	Type
1	A	191	ILE

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	1037/1044 (99%)	1014 (98%)	23 (2%)	45	73
2	B	436/439 (99%)	428 (98%)	8 (2%)	51	77
3	C	184/186 (99%)	179 (97%)	5 (3%)	39	67
All	All	1657/1669 (99%)	1621 (98%)	36 (2%)	45	73

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	190	PRO
1	A	319	LEU
1	A	338	MET
1	A	367	GLU
1	A	461	GLN
1	A	476	LEU
1	A	581	GLU
1	A	600	ARG
1	A	601	PRO
1	A	629	LEU
1	A	688	LYS
1	A	727	MET
1	A	767	LEU
1	A	808	PRO
1	A	864	LEU
1	A	926	LEU
1	A	936	GLU
1	A	995	ARG
1	A	1032	LEU
1	A	1110	LEU

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Mol	Chain	Res	Type
1	A	1233	LEU
1	A	1243	GLU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU
2	B	161	PHE
2	B	295	ARG
2	B	299	VAL
2	B	323	GLU
2	B	428	ARG
3	C	46	LYS
3	C	81	LEU
3	C	142	LEU
3	C	147	SER
3	C	212	GLU

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	26	ASN
1	A	37	GLN
1	A	173	ASN
1	A	179	ASN
1	A	229	GLN
1	A	234	GLN
1	A	368	ASN
1	A	461	GLN
1	A	480	ASN
1	A	517	GLN
1	A	559	ASN
1	A	586	GLN
1	A	590	GLN
1	A	704	ASN
1	A	708	ASN
1	A	759	ASN
1	A	946	ASN
1	A	1000	GLN
1	A	1023	ASN
1	A	1076	GLN
1	A	1082	GLN
1	A	1098	HIS

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Mol	Chain	Res	Type
1	A	1179	GLN
2	B	20	HIS
2	B	160	ASN
2	B	294	GLN
2	B	414	HIS
2	B	451	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	1.29	2 (25%)	8,9,11	1.68	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CG	2.23	1.60	1.51
3	C	1	FME	CB-CA	-2.05	1.48	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	3.21	127.75	122.82
3	C	1	FME	CB-CA-N	2.15	114.44	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	CB-CG-SD-CE
3	C	1	FME	C-CA-CB-CG
3	C	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	B	803	2	0,12,12	-	-	-		
8	F3S	B	805	2	0,9,9	-	-	-		
9	HEM	C	806	3	50,50,50	1.77	11 (22%)	67,82,82	0.88	3 (4%)
5	SF4	B	802	2	0,12,12	-	-	-		
7	AGA	A	1249	-	24,24,29	0.87	1 (4%)	27,29,35	1.56	2 (7%)
4	MD1	A	1247	6	47,51,51	2.94	7 (14%)	56,78,78	1.31	4 (7%)
9	HEM	C	807	3	50,50,50	1.90	19 (38%)	67,82,82	0.96	3 (4%)
5	SF4	A	1248	1	0,12,12	-	-	-		
4	MD1	A	1251	6	47,51,51	2.83	6 (12%)	56,78,78	1.41	5 (8%)
5	SF4	B	804	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
5	SF4	B	803	2	-	-	0/6/5/5
9	HEM	C	806	3	-	8/14/54/54	-
8	F3S	B	805	2	-	-	0/3/3/3
5	SF4	B	802	2	-	-	0/6/5/5
7	AGA	A	1249	-	-	4/26/26/34	-
4	MD1	A	1247	6	-	7/22/59/59	0/5/5/5
9	HEM	C	807	3	-	4/14/54/54	-
5	SF4	A	1248	1	-	-	0/6/5/5
4	MD1	A	1251	6	-	2/22/59/59	0/5/5/5
5	SF4	B	804	2	-	-	0/6/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1247	MD1	C7-N8	17.86	1.50	1.28
4	A	1251	MD1	C7-N8	16.88	1.49	1.28
9	C	807	HEM	CAB-C3B	4.77	1.60	1.47
9	C	806	HEM	CAB-C3B	4.24	1.58	1.47
4	A	1251	MD1	PA-O3B	-3.90	1.55	1.59
9	C	806	HEM	CAC-C3C	3.67	1.57	1.47
4	A	1247	MD1	C14-C13	3.66	1.55	1.51
9	C	807	HEM	CMC-C2C	3.53	1.58	1.50
9	C	807	HEM	FE-NC	3.51	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	807	HEM	CAC-C3C	3.50	1.56	1.47
9	C	806	HEM	FE-NC	3.48	2.06	1.95
9	C	806	HEM	CMC-C2C	3.39	1.57	1.50
4	A	1251	MD1	C20-N8	3.39	1.41	1.36
4	A	1247	MD1	C16-C20	3.35	1.48	1.39
9	C	806	HEM	CMA-C3A	3.19	1.57	1.50
9	C	807	HEM	CMB-C2B	3.15	1.57	1.50
9	C	806	HEM	CMD-C2D	2.99	1.56	1.50
9	C	807	HEM	CMD-C2D	2.93	1.56	1.50
4	A	1247	MD1	C12-C13	2.91	1.43	1.34
4	A	1247	MD1	C20-N8	2.87	1.41	1.36
9	C	806	HEM	CMB-C2B	2.81	1.56	1.50
9	C	807	HEM	CBA-CAA	2.76	1.61	1.51
4	A	1247	MD1	C4-N3	2.76	1.40	1.34
9	C	807	HEM	CAD-C3D	2.73	1.58	1.51
9	C	807	HEM	CMA-C3A	2.70	1.56	1.50
9	C	807	HEM	FE-NB	2.65	2.03	1.94
7	A	1249	AGA	C8-C7	2.60	1.58	1.50
4	A	1251	MD1	O11-C11	2.52	1.48	1.42
9	C	806	HEM	FE-NB	2.51	2.02	1.94
9	C	807	HEM	CBA-CGA	2.44	1.56	1.50
9	C	806	HEM	CAD-C3D	2.39	1.57	1.51
4	A	1251	MD1	C6-N1	2.34	1.43	1.38
9	C	806	HEM	C4D-C3D	2.32	1.49	1.45
9	C	807	HEM	CAA-C2A	2.32	1.57	1.51
9	C	807	HEM	C1D-C2D	2.30	1.49	1.44
9	C	807	HEM	CBD-CGD	2.27	1.55	1.50
4	A	1251	MD1	C4-N3	2.25	1.39	1.34
9	C	807	HEM	CBD-CAD	2.22	1.59	1.51
9	C	807	HEM	O1D-CGD	2.14	1.29	1.22
4	A	1247	MD1	C14-C7	2.13	1.55	1.50
9	C	807	HEM	FE-ND	2.12	2.01	1.94
9	C	806	HEM	CBD-CAD	2.09	1.59	1.51
9	C	807	HEM	C4A-C3A	2.06	1.48	1.43
9	C	807	HEM	O1A-CGA	2.02	1.28	1.22

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1247	MD1	C17-N18-C20	5.75	122.17	114.20
4	A	1251	MD1	C17-N18-C20	5.50	121.82	114.20
7	A	1249	AGA	C9-C8-C7	5.07	132.28	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1249	AGA	C14-C13-C12	4.85	131.45	113.69
4	A	1251	MD1	C2-N3-C4	3.34	118.06	112.30
9	C	807	HEM	CAD-C3D-C4D	-2.79	119.84	124.70
4	A	1247	MD1	N17-C17-N18	-2.70	118.39	123.32
4	A	1247	MD1	O14-C15-C16	-2.54	121.13	127.26
9	C	807	HEM	CAD-C3D-C2D	2.33	132.22	127.87
4	A	1251	MD1	N1-C2-N3	-2.30	119.11	123.32
4	A	1247	MD1	O3A-C10-C11	-2.25	101.64	107.96
9	C	806	HEM	O1D-CGD-CBD	-2.17	116.21	123.09
9	C	806	HEM	CAD-C3D-C4D	-2.09	121.05	124.70
9	C	807	HEM	O1D-CGD-CBD	-2.08	116.50	123.09
4	A	1251	MD1	C1'-N9-C8	2.06	132.59	126.73
4	A	1251	MD1	O14-C15-C16	-2.02	122.39	127.26
9	C	806	HEM	CMA-C3A-C2A	2.00	129.87	125.62

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1247	MD1	C5'-O5'-PA-O3B
4	A	1247	MD1	C5'-O5'-PA-O2A
9	C	806	HEM	C2C-C3C-CAC-CBC
9	C	807	HEM	C2C-C3C-CAC-CBC
9	C	807	HEM	C4C-C3C-CAC-CBC
4	A	1247	MD1	O4'-C4'-C5'-O5'
7	A	1249	AGA	C7-C8-C9-C10
4	A	1247	MD1	C3'-C4'-C5'-O5'
7	A	1249	AGA	C8-C7-O7-C6
9	C	806	HEM	C4C-C3C-CAC-CBC
7	A	1249	AGA	O8-C7-O7-C6
7	A	1249	AGA	C11-C10-C9-C8
9	C	806	HEM	C2B-C3B-CAB-CBB
4	A	1247	MD1	PA-O3B-PB-O2B
4	A	1251	MD1	PA-O3B-PB-O2B
4	A	1247	MD1	C5'-O5'-PA-O1A
9	C	806	HEM	C4B-C3B-CAB-CBB
9	C	806	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAD-CBD-CGD-O2D
9	C	806	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAD-CBD-CGD-O2D
9	C	807	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAA-CBA-CGA-O1A

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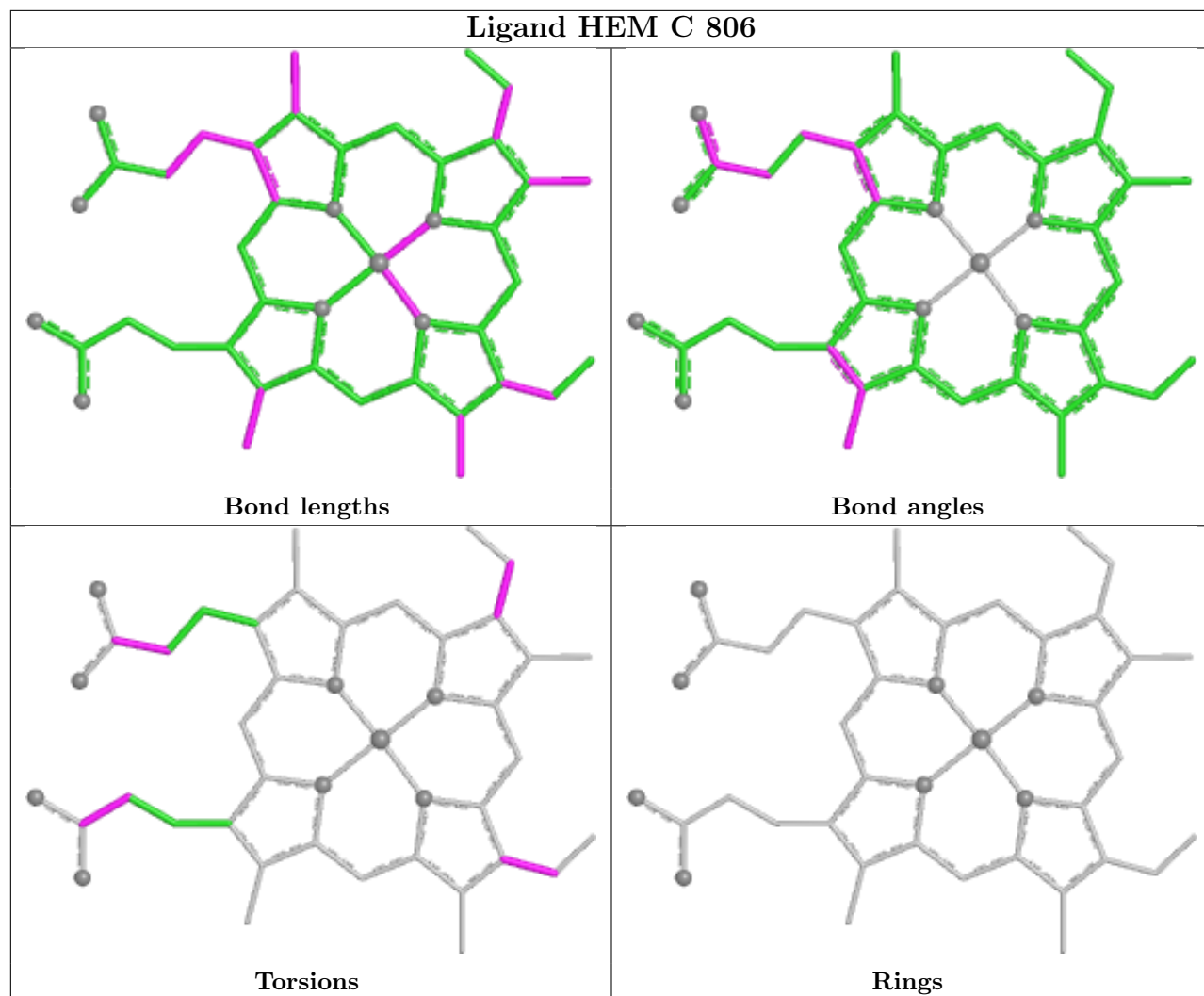
Mol	Chain	Res	Type	Atoms
4	A	1247	MD1	PA-O3B-PB-O1B
4	A	1251	MD1	PA-O3B-PB-O1B

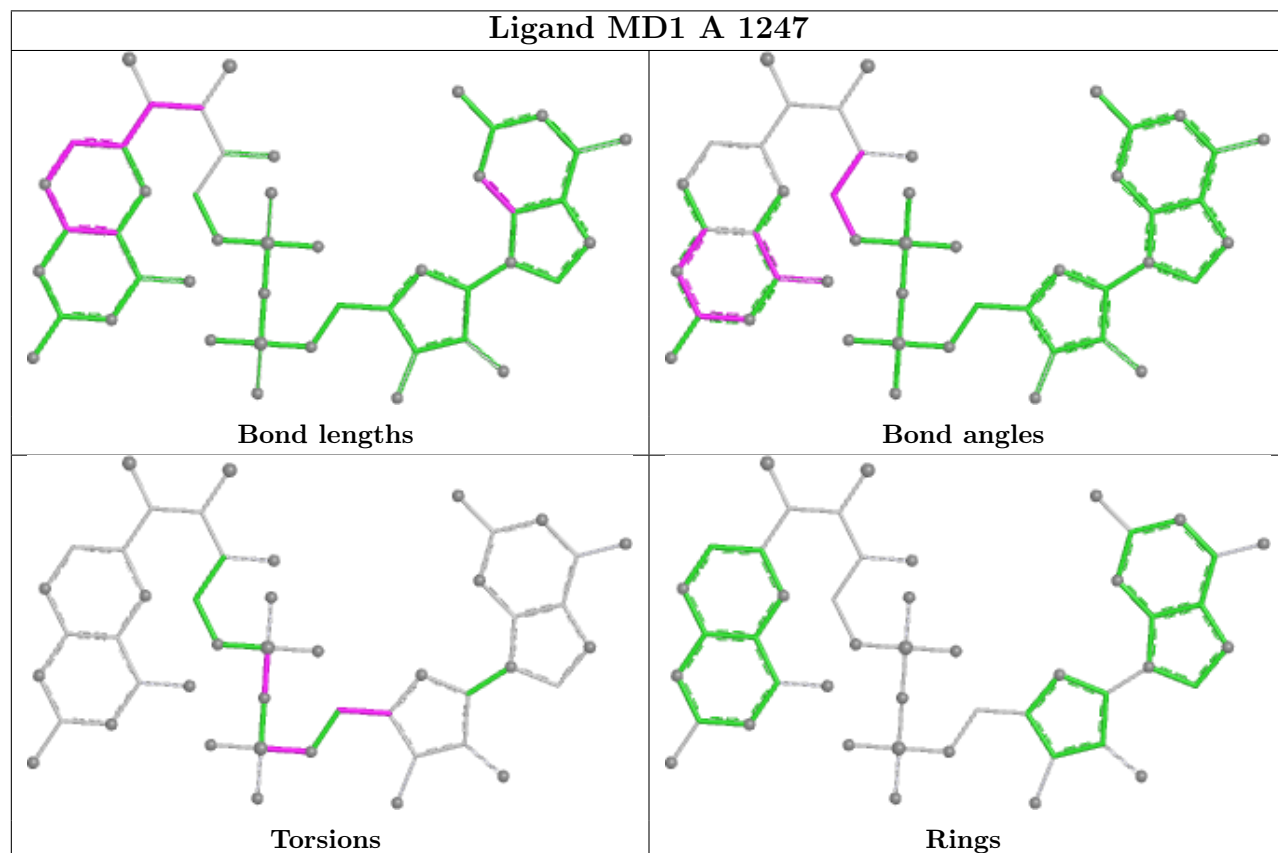
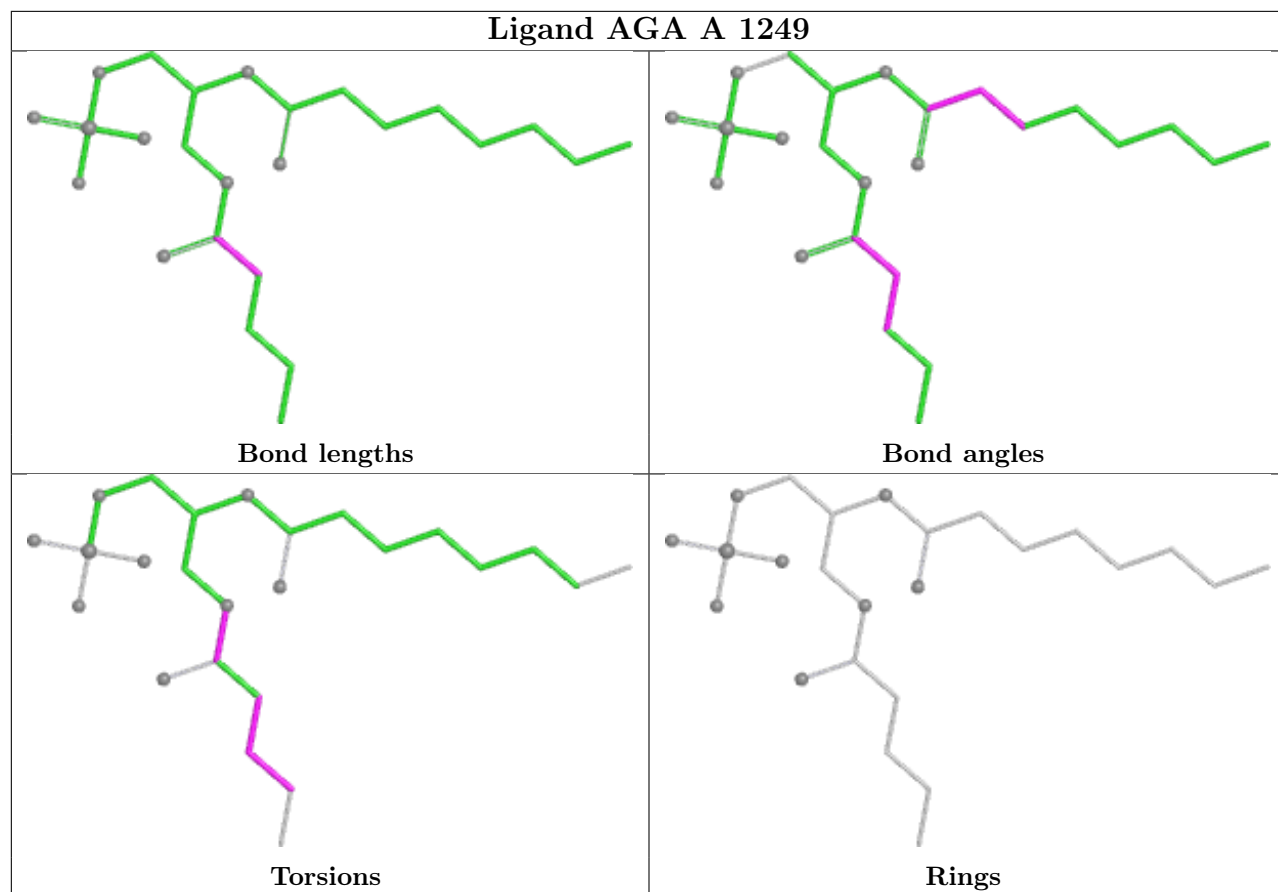
There are no ring outliers.

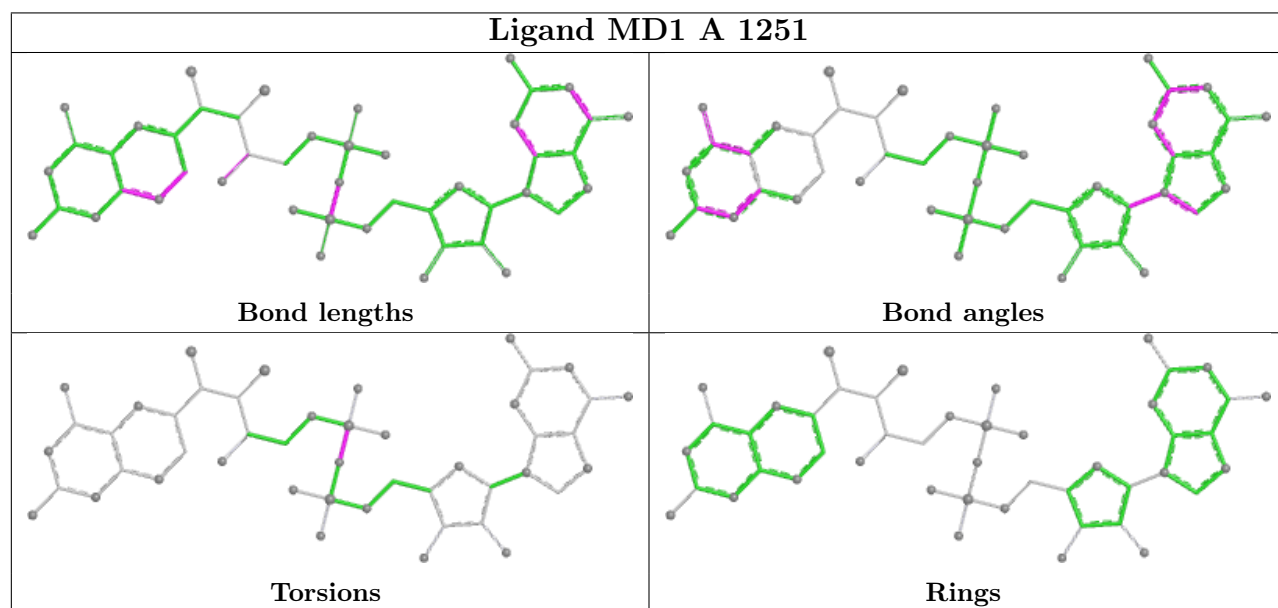
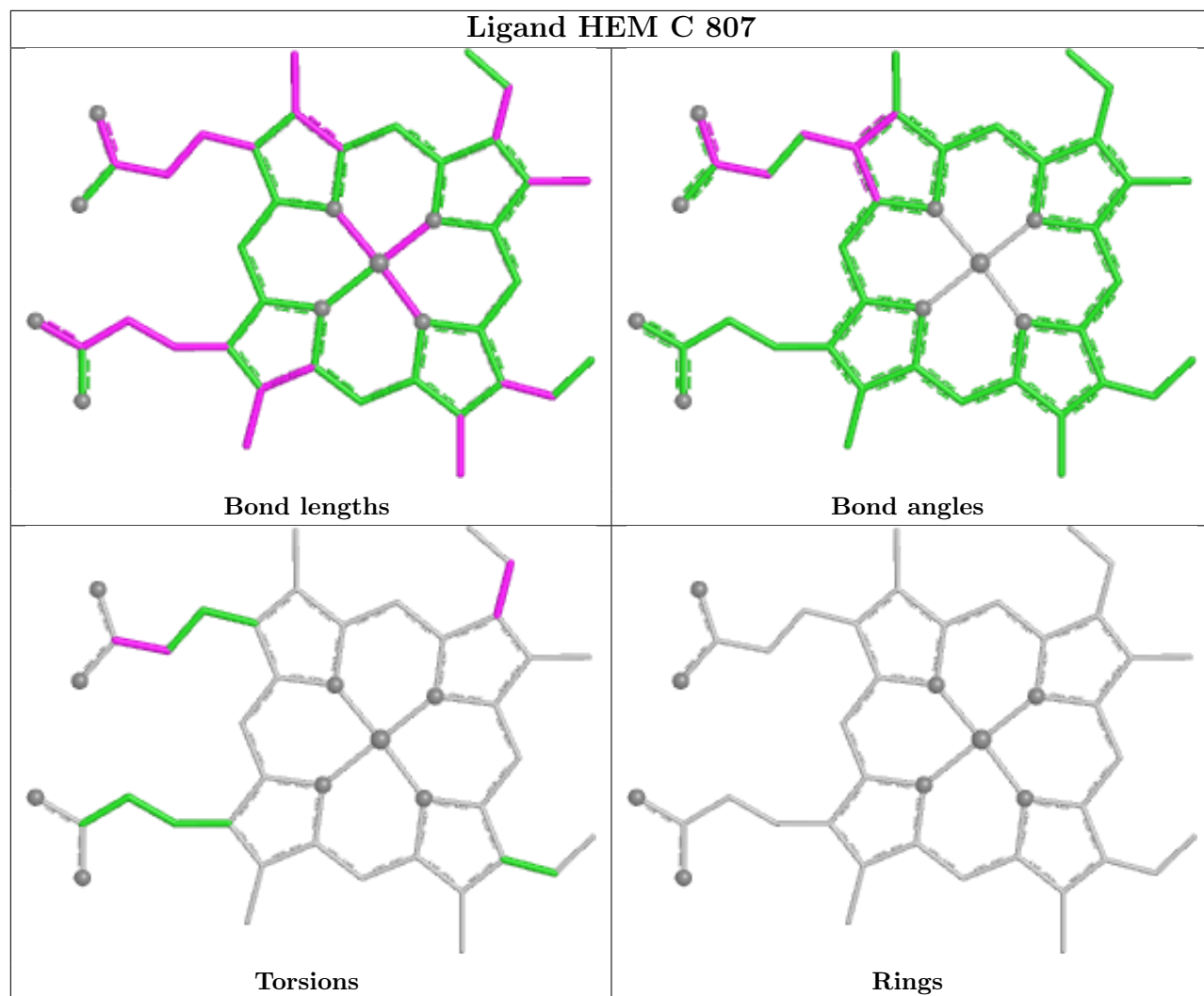
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	SF4	1	0
9	C	806	HEM	1	0
4	A	1247	MD1	4	0
9	C	807	HEM	1	0
5	A	1248	SF4	1	0
4	A	1251	MD1	4	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1242/1247 (99%)	-0.17	8 (0%) 85 83	20, 36, 56, 73	0
2	B	509/512 (99%)	-0.44	0 100 100	18, 30, 45, 68	0
3	C	224/225 (99%)	0.14	8 (3%) 46 41	26, 41, 67, 87	0
All	All	1975/1984 (99%)	-0.20	16 (0%) 82 80	18, 35, 57, 87	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	77	TYR	4.1
1	A	7	PHE	4.1
3	C	75	TRP	3.9
3	C	80	TRP	3.2
3	C	76	MET	2.9
1	A	362	ASP	2.8
1	A	501	ALA	2.6
1	A	1244	SER	2.6
1	A	991	ASP	2.5
1	A	10	PHE	2.5
3	C	74	HIS	2.3
3	C	70	MET	2.3
3	C	212	GLU	2.3
3	C	73	PRO	2.3
1	A	490	VAL	2.1
1	A	1164	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FME	C	1	10/11	0.90	0.10	60,64,72,72	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

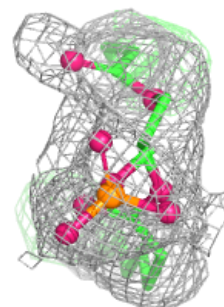
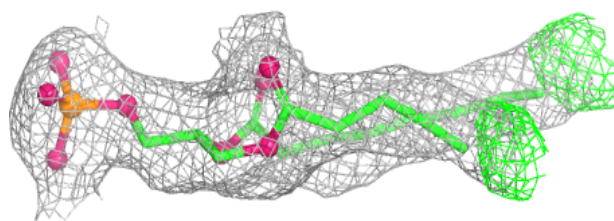
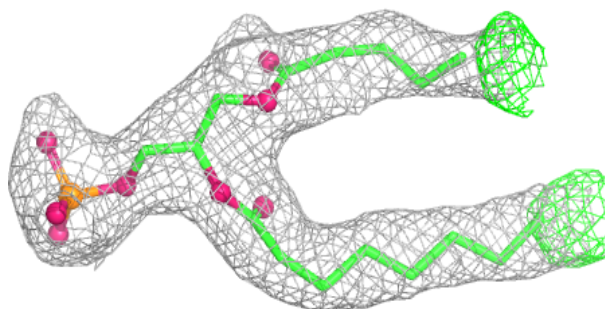
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	AGA	A	1249	25/30	0.90	0.12	39,42,55,56	0
4	MD1	A	1247	47/47	0.93	0.10	33,44,62,65	0
4	MD1	A	1251	47/47	0.94	0.09	31,47,60,63	0
9	HEM	C	807	43/43	0.94	0.12	49,52,61,66	0
5	SF4	B	804	8/8	0.96	0.06	30,35,36,37	0
6	6MO	A	1250	1/1	0.96	0.20	67,67,67,67	0
9	HEM	C	806	43/43	0.97	0.08	26,31,35,43	0
5	SF4	B	803	8/8	0.99	0.04	20,22,23,24	0
8	F3S	B	805	7/7	0.99	0.03	25,26,28,30	0
5	SF4	A	1248	8/8	0.99	0.03	30,31,31,34	0
5	SF4	B	802	8/8	0.99	0.03	25,26,27,27	0

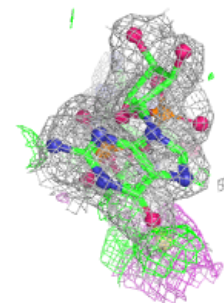
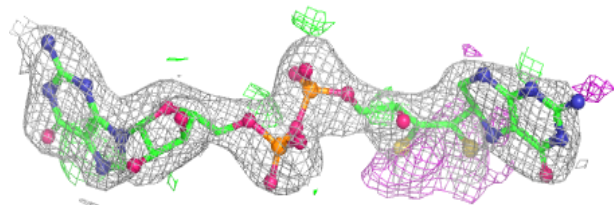
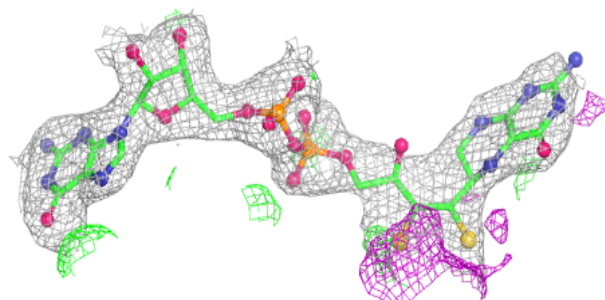
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGA A 1249:

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

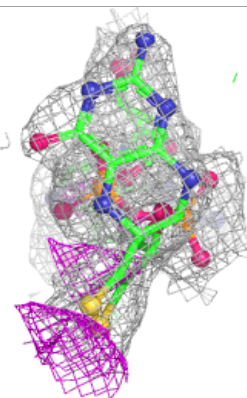
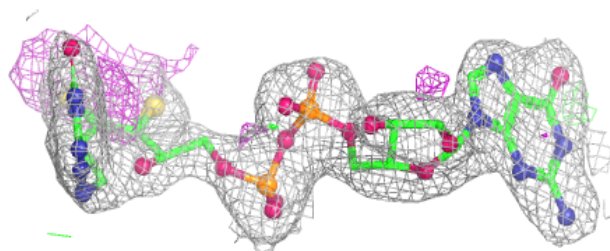
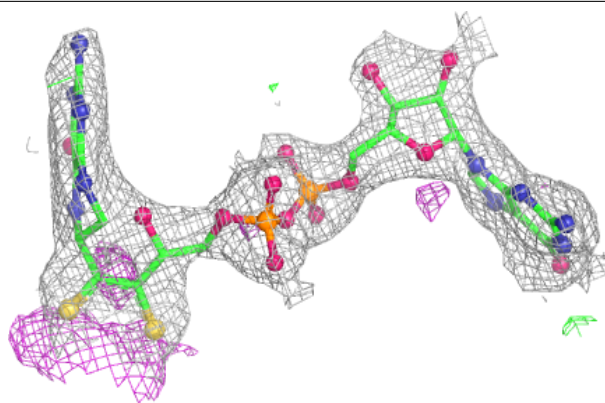
**Electron density around MD1 A 1247:**

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

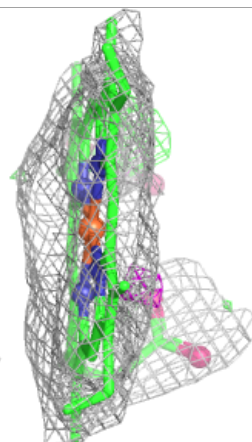
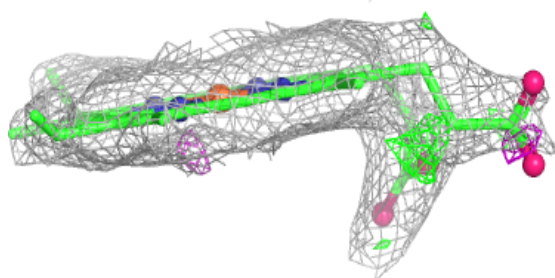
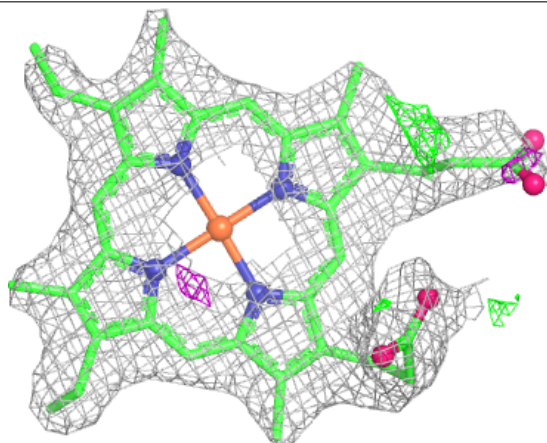


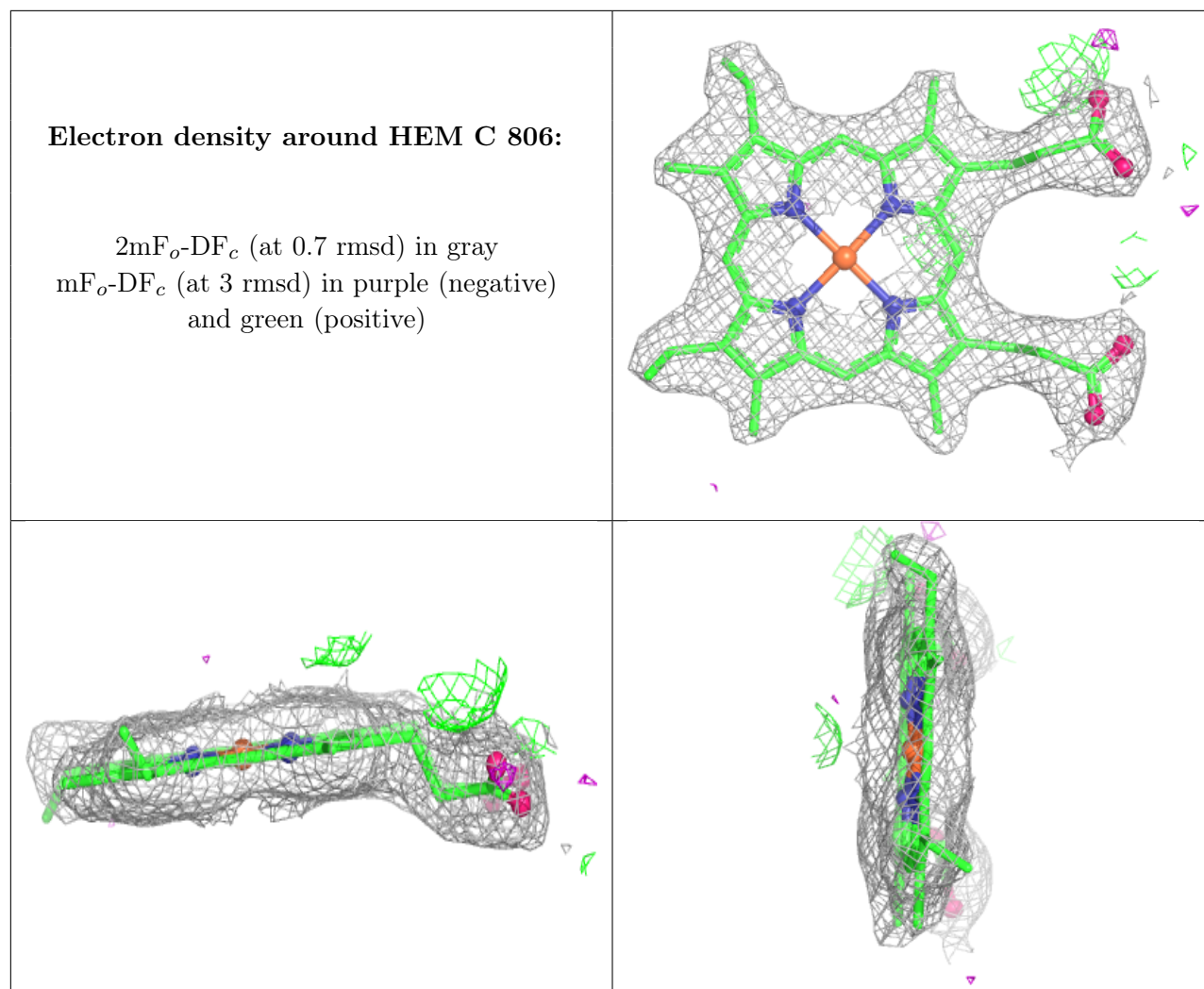
Electron density around MD1 A 1251:

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

**Electron density around HEM C 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.