



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 12:56 AM UTC

PDB ID : 3IR6 / pdb_00003ir6
Title : Crystal structure of NarGHI mutant NarG-H49S
Authors : Bertero, M.G.; Rothery, R.A.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2009-08-21
Resolution : 2.80 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

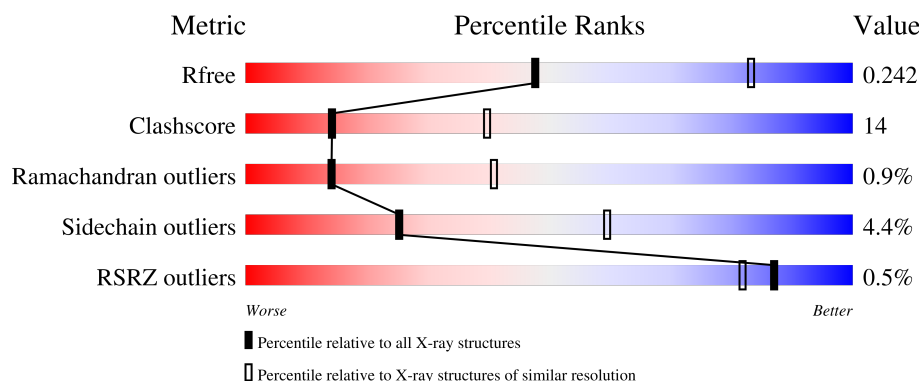
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	% 62% 33% ..
2	B	512	74% 23% ..
3	C	225	76% 20% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SF4	B	803	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15892 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	1233	Total	C	N	O	S	0	0	0
			9770	6173	1710	1840	47			

There is a discrepancy between the modelled and reference sequences:

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

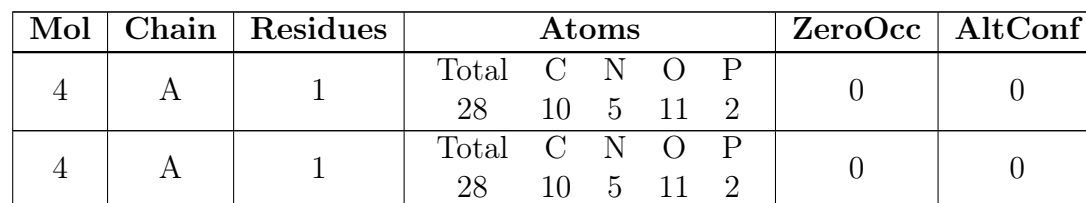
- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

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

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

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

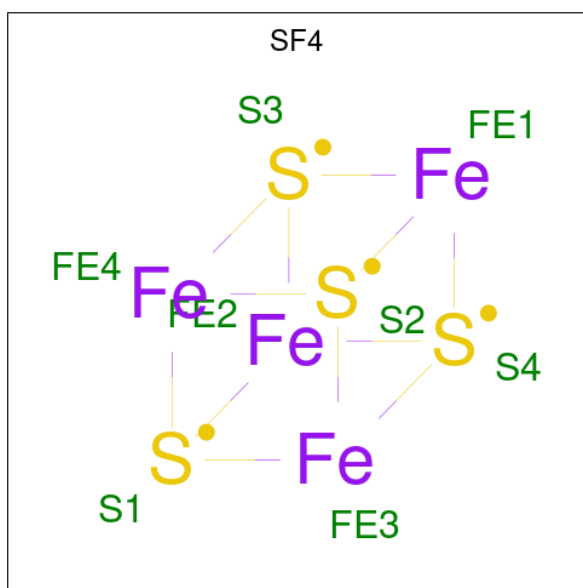
- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



- # AGA

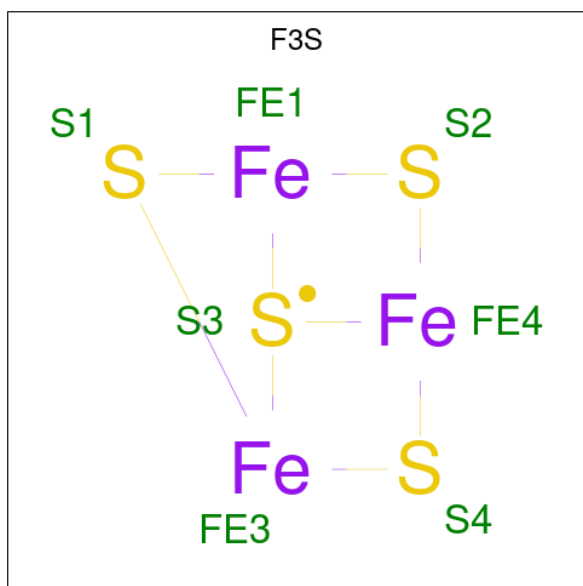
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			25	16	8	1		

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



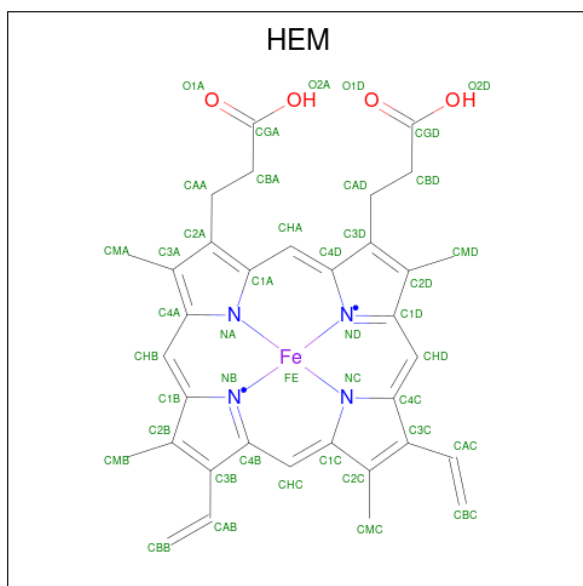
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

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

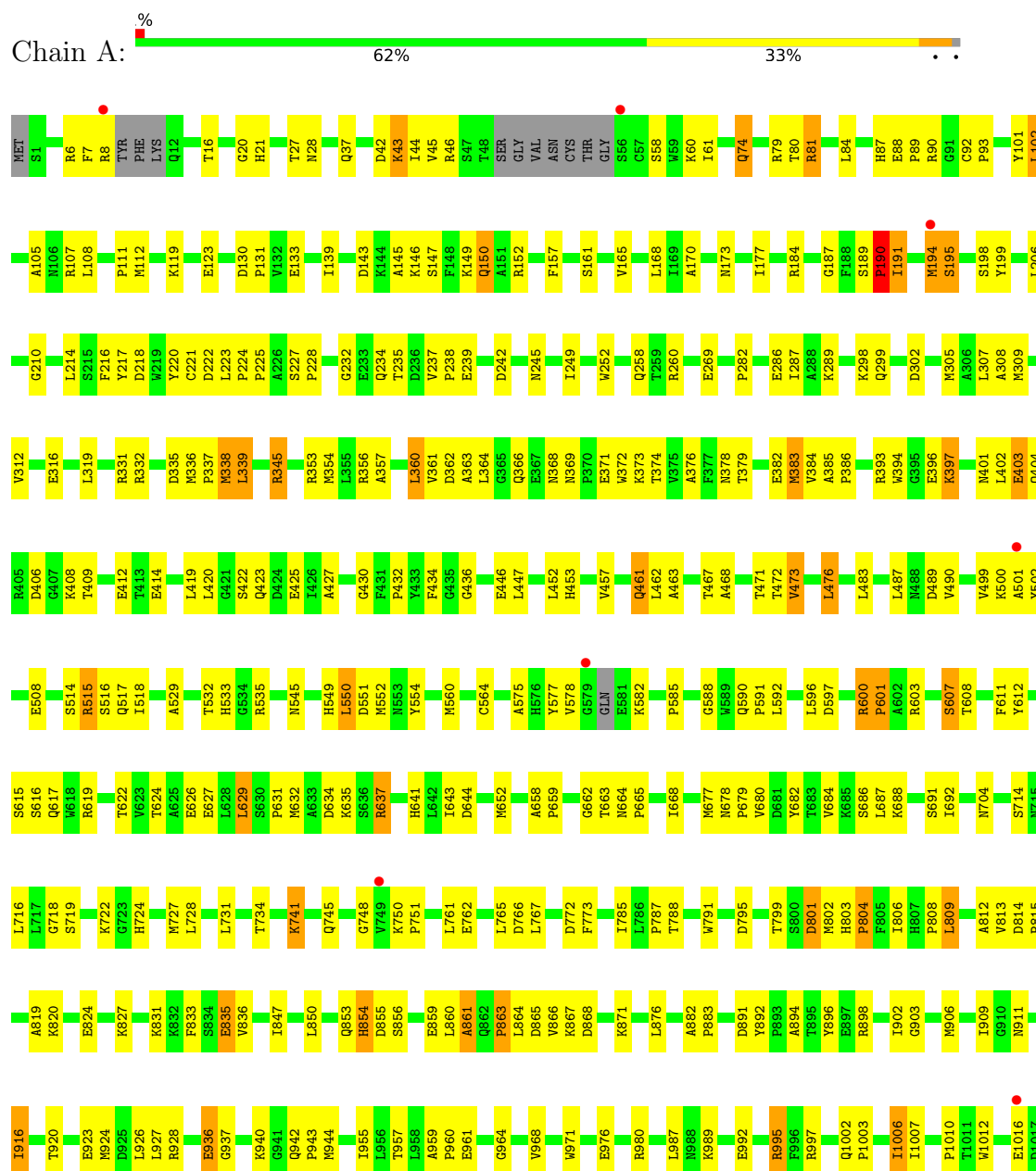
- Molecule 9 is water.

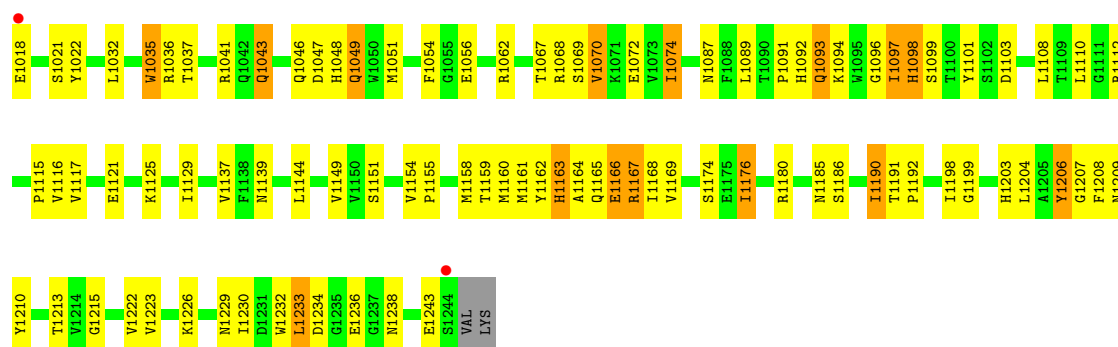
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	43	Total	O	0	0
			43	43		
9	B	29	Total	O	0	0
			29	29		
9	C	11	Total	O	0	0
			11	11		

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.

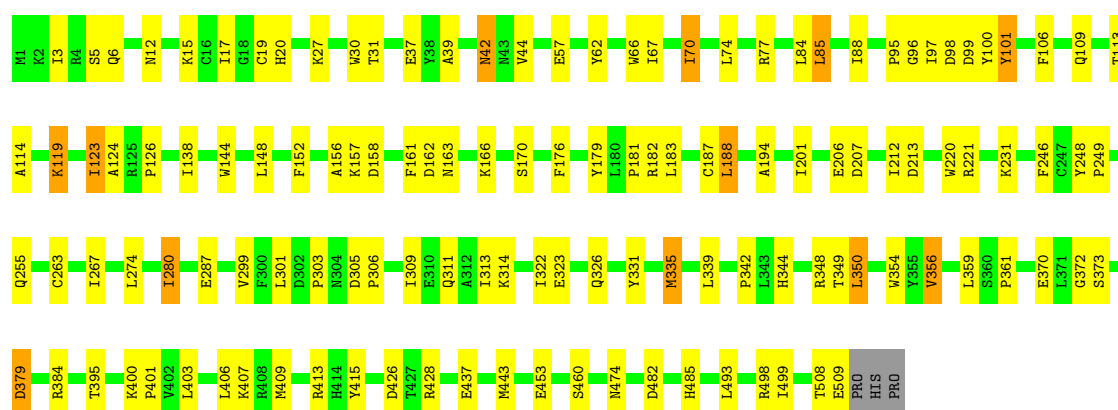
- Molecule 1: Respiratory nitrate reductase 1 alpha chain





• Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B: 74% 23%



• Molecule 3: Respiratory nitrate reductase 1 gamma chain

Chain C: 76% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.14Å 239.82Å 139.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.80 29.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.87-2.80) 99.8 (29.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.249 0.183 , 0.242	Depositor DCC
R_{free} test set	3849 reflections (6.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15892	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: GDP, SF4, HEM, AGA, F3S, FME

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	0.50	0/10024	1.00	45/13607 (0.3%)
2	B	0.53	0/4146	1.02	16/5609 (0.3%)
3	C	0.51	0/1833	0.94	3/2481 (0.1%)
All	All	0.50	0/16003	1.00	64/21697 (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	8.89	121.93	111.71
1	A	1167	ARG	N-CA-C	8.66	123.57	112.92
2	B	88	ILE	N-CA-C	8.51	119.31	110.72
1	A	1163	HIS	N-CA-C	7.88	122.12	110.30
2	B	350	LEU	CA-C-N	7.66	127.67	119.78
2	B	350	LEU	C-N-CA	7.66	127.67	119.78
2	B	30	TRP	N-CA-C	7.65	122.93	112.90
1	A	1093	GLN	N-CA-C	7.50	119.49	110.19
1	A	809	LEU	N-CA-C	-7.21	97.14	108.90
1	A	1070	VAL	N-CA-C	6.94	117.11	111.62
1	A	302	ASP	N-CA-C	6.83	118.72	111.28
2	B	287	GLU	N-CA-C	6.76	118.65	111.28
1	A	615	SER	N-CA-C	-6.58	105.13	113.02
1	A	1206	TYR	N-CA-C	6.54	119.16	110.53
1	A	987	LEU	N-CA-C	6.52	119.22	111.33
1	A	1191	THR	CA-C-N	6.48	126.44	120.03
1	A	1191	THR	C-N-CA	6.48	126.44	120.03
1	A	316	GLU	N-CA-C	6.46	120.42	112.54
2	B	31	THR	N-CA-C	6.42	120.92	111.87
2	B	493	LEU	N-CA-C	6.22	118.86	111.71
1	A	1043	GLN	N-CA-C	6.14	118.79	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	854	HIS	N-CA-C	-6.06	102.72	110.53
1	A	21	HIS	N-CA-C	-5.99	105.80	113.23
2	B	206	GLU	N-CA-C	5.98	118.75	111.82
1	A	892	TYR	CA-C-N	-5.92	113.59	119.56
1	A	892	TYR	C-N-CA	-5.92	113.59	119.56
1	A	473	VAL	N-CA-C	-5.88	104.62	110.62
1	A	1166	GLU	N-CA-C	5.83	123.22	110.80
1	A	222	ASP	N-CA-C	-5.82	105.28	112.90
3	C	74	HIS	N-CA-C	5.80	117.28	111.07
1	A	397	LYS	N-CA-C	5.79	117.40	109.18
1	A	101	TYR	N-CA-C	5.76	118.30	111.33
2	B	379	ASP	N-CA-C	-5.73	100.94	110.17
1	A	84	LEU	CA-C-N	-5.72	114.36	120.03
1	A	84	LEU	C-N-CA	-5.72	114.36	120.03
1	A	863	PRO	N-CA-C	5.63	120.95	113.40
2	B	474	ASN	N-CA-C	5.63	117.42	111.28
1	A	16	THR	N-CA-C	-5.53	102.28	110.46
3	C	208	SER	N-CA-C	5.51	119.71	113.15
2	B	335	MET	N-CA-C	5.47	119.92	112.04
3	C	8	PHE	N-CA-C	5.44	117.97	111.71
2	B	144	TRP	N-CA-C	5.39	118.66	111.75
1	A	812	ALA	N-CA-C	-5.34	105.63	111.82
1	A	1098	HIS	CB-CA-C	-5.34	110.44	116.63
1	A	74	GLN	N-CA-C	-5.28	101.86	110.20
1	A	1169	VAL	N-CA-C	5.27	115.49	108.11
1	A	937	GLY	CA-C-N	5.22	125.52	119.47
1	A	937	GLY	C-N-CA	5.22	125.52	119.47
1	A	102	LEU	N-CA-C	5.21	119.96	111.37
1	A	339	LEU	N-CA-C	5.20	117.22	108.96
1	A	363	ALA	N-CA-C	-5.20	105.59	112.24
1	A	249	ILE	N-CA-C	5.19	116.19	108.46
1	A	853	GLN	N-CA-C	5.17	118.37	110.20
2	B	356	VAL	N-CA-C	-5.17	101.98	107.77
2	B	280	ILE	N-CA-C	5.17	115.60	110.23
1	A	1097	ILE	N-CA-C	-5.16	99.07	107.28
1	A	403	GLU	N-CA-C	-5.13	101.60	109.76
1	A	1186	SER	N-CA-C	-5.13	106.97	113.18
2	B	182	ARG	N-CA-C	5.07	117.09	109.23
1	A	1035	TRP	N-CA-C	-5.07	100.91	108.96
1	A	959	ALA	N-CA-C	5.05	116.19	109.93
2	B	188	LEU	N-CA-C	-5.04	106.29	112.90
1	A	622	THR	N-CA-C	-5.03	107.82	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	LYS	N-CA-C	-5.01	102.63	110.10

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	9770	0	9423	334	0
2	B	4050	0	3973	85	0
3	C	1791	0	1825	38	0
4	A	56	0	24	2	0
5	A	25	0	29	0	0
6	B	24	0	0	3	0
7	B	7	0	0	0	0
8	C	86	0	60	5	0
9	A	43	0	0	0	0
9	B	29	0	0	1	0
9	C	11	0	0	0	0
All	All	15892	0	15334	442	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 14.

All (442) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:ARG:HG2	1:A:943:PRO:HG3	1.49	0.95
2:B:70:ILE:HD12	2:B:70:ILE:H	1.42	0.84
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.42	0.82
1:A:992:GLU:HG2	1:A:1007:ILE:HD11	1.62	0.82
1:A:361:VAL:HG13	1:A:362:ASP:H	1.46	0.81
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.61	0.79
1:A:727:MET:HG3	1:A:731:LEU:HD12	1.64	0.79
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:O	1:A:408:LYS:HG3	1.86	0.75
1:A:686:SER:HB3	1:A:691:SER:HB2	1.70	0.74
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.67	0.74
1:A:686:SER:HB3	1:A:692:ILE:HG12	1.69	0.73
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.71	0.71
1:A:361:VAL:HG13	1:A:362:ASP:N	2.04	0.71
1:A:378:ASN:HD21	1:A:382:GLU:HB2	1.56	0.70
1:A:1099:SER:HB3	4:A:1247:GDP:O1A	1.92	0.70
2:B:70:ILE:HD12	2:B:70:ILE:N	2.06	0.70
1:A:225:PRO:HB2	1:A:551:ASP:OD1	1.91	0.69
1:A:624:THR:O	1:A:627:GLU:HG2	1.91	0.69
1:A:423:GLN:HB2	1:A:457:VAL:O	1.92	0.69
1:A:1155:PRO:HG2	1:A:1158:MET:HG2	1.74	0.68
2:B:188:LEU:HB3	2:B:280:ILE:HD12	1.76	0.68
1:A:368:ASN:O	1:A:373:LYS:HE3	1.94	0.68
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	1.94	0.68
3:C:209:VAL:HG22	3:C:211:VAL:HG13	1.75	0.68
1:A:662:GLY:HA2	1:A:704:ASN:ND2	2.09	0.66
1:A:338:MET:HE1	1:A:386:PRO:HG3	1.78	0.66
1:A:168:LEU:HD23	1:A:168:LEU:O	1.96	0.65
1:A:684:VAL:HG12	1:A:688:LYS:HE3	1.79	0.65
2:B:156:ALA:HB1	2:B:166:LYS:HD2	1.76	0.65
1:A:772:ASP:C	1:A:788:THR:HG22	2.21	0.65
1:A:663:THR:HG21	1:A:692:ILE:HD12	1.80	0.64
1:A:336:MET:HA	1:A:473:VAL:HB	1.79	0.64
1:A:406:ASP:OD1	1:A:409:THR:HG23	1.97	0.64
1:A:305:MET:HG3	1:A:518:ILE:HD12	1.78	0.64
1:A:161:SER:O	1:A:165:VAL:HG22	1.97	0.64
2:B:372:GLY:HA3	2:B:379:ASP:OD1	1.98	0.64
1:A:617:GLN:OE1	1:A:1190:ILE:HG12	1.98	0.63
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.80	0.63
3:C:87:GLN:O	3:C:91:MET:HG3	1.99	0.62
1:A:592:LEU:HD23	1:A:955:ILE:HD11	1.81	0.62
1:A:366:GLN:HG2	1:A:373:LYS:HD2	1.82	0.62
2:B:3:ILE:HG12	2:B:301:LEU:CD1	2.29	0.61
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.81	0.61
3:C:143:THR:HG22	3:C:183:ILE:HG13	1.81	0.61
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.83	0.61
1:A:338:MET:HB3	1:A:354:MET:HE2	1.83	0.60
2:B:70:ILE:H	2:B:70:ILE:CD1	2.14	0.60
1:A:1006:ILE:HD11	1:A:1016:GLU:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.34	0.60
3:C:6:MET:O	3:C:10:ASP:HB2	2.01	0.60
1:A:1074:ILE:HG12	1:A:1223:VAL:CG2	2.32	0.60
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.83	0.59
1:A:368:ASN:HD22	1:A:396:GLU:CD	2.09	0.59
1:A:928:ARG:HH11	1:A:942:GLN:NE2	2.00	0.59
1:A:601:PRO:HG3	1:A:850:LEU:HD22	1.83	0.59
1:A:750:LYS:HD2	1:A:750:LYS:N	2.18	0.59
1:A:43:LYS:HE2	1:A:45:VAL:HG23	1.85	0.59
1:A:860:LEU:HD12	1:A:860:LEU:N	2.18	0.59
1:A:906:MET:HB2	1:A:924:MET:HE2	1.84	0.58
1:A:891:ASP:HB3	1:A:894:ALA:HB3	1.86	0.58
1:A:369:ASN:O	1:A:373:LYS:HG3	2.04	0.58
1:A:906:MET:HE3	1:A:911:ASN:HB2	1.85	0.58
1:A:105:ALA:O	2:B:109:GLN:NE2	2.37	0.57
1:A:596:LEU:O	1:A:600:ARG:HD2	2.03	0.57
1:A:989:LYS:O	1:A:992:GLU:HB3	2.04	0.57
1:A:1098:HIS:O	1:A:1164:ALA:HB3	2.04	0.57
1:A:1117:VAL:HG22	1:A:1161:MET:HB2	1.86	0.57
1:A:430:GLY:O	1:A:632:MET:HE1	2.05	0.57
1:A:223:LEU:O	1:A:225:PRO:HD3	2.04	0.57
2:B:220:TRP:C	2:B:221:ARG:HG3	2.29	0.57
1:A:111:PRO:HA	1:A:787:PRO:HD3	1.86	0.57
1:A:368:ASN:ND2	1:A:396:GLU:HG2	2.20	0.57
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.73	0.57
1:A:550:LEU:H	1:A:550:LEU:HD23	1.68	0.56
1:A:652:MET:HE1	1:A:866:VAL:CG1	2.33	0.56
2:B:373:SER:HB3	2:B:428:ARG:NH1	2.20	0.56
1:A:332:ARG:HG2	1:A:404:GLN:HG3	1.87	0.56
1:A:928:ARG:CG	1:A:943:PRO:HG3	2.31	0.56
2:B:19:CYS:O	2:B:20:HIS:HB2	2.05	0.56
2:B:306:PRO:HA	2:B:309:ILE:HG13	1.88	0.56
2:B:322:ILE:O	2:B:326:GLN:HG3	2.05	0.56
3:C:206:ILE:HD11	8:C:806:HEM:HBC2	1.88	0.56
2:B:361:PRO:HD2	2:B:384:ARG:HD3	1.86	0.56
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.30	0.56
3:C:13:PRO:HB3	3:C:192:MET:SD	2.45	0.56
1:A:588:GLY:O	1:A:955:ILE:HA	2.06	0.56
1:A:916:ILE:HD13	1:A:916:ILE:H	1.71	0.56
1:A:258:GLN:HB2	1:A:286:GLU:OE2	2.06	0.56
1:A:928:ARG:HH11	1:A:942:GLN:HE22	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:ALA:O	1:A:863:PRO:HD3	2.06	0.56
2:B:508:THR:O	2:B:509:GLU:HB3	2.05	0.56
1:A:1093:GLN:HB3	1:A:1162:TYR:HB3	1.88	0.55
2:B:305:ASP:O	2:B:309:ILE:HG12	2.06	0.55
1:A:722:LYS:HB2	1:A:1190:ILE:CD1	2.36	0.55
1:A:590:GLN:N	1:A:591:PRO:HD2	2.21	0.55
1:A:964:GLY:O	1:A:968:VAL:HG23	2.06	0.55
1:A:997:ARG:HH21	1:A:997:ARG:HG3	1.71	0.55
1:A:119:LYS:O	1:A:123:GLU:HG3	2.06	0.55
1:A:1035:TRP:O	1:A:1037:THR:N	2.39	0.55
1:A:835:GLU:HG3	1:A:836:VAL:N	2.21	0.55
2:B:309:ILE:O	2:B:313:ILE:HG12	2.07	0.55
1:A:393:ARG:HH12	1:A:855:ASP:HA	1.71	0.55
1:A:686:SER:CB	1:A:692:ILE:HG12	2.37	0.55
1:A:1180:ARG:HD2	2:B:123:ILE:HG13	1.87	0.55
1:A:677:MET:HE2	1:A:682:TYR:HA	1.88	0.55
1:A:863:PRO:HG2	1:A:864:LEU:CD2	2.37	0.55
1:A:508:GLU:OE1	1:A:515:ARG:HD2	2.07	0.54
1:A:686:SER:CB	1:A:691:SER:HB2	2.36	0.54
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.07	0.54
1:A:906:MET:CE	1:A:911:ASN:HB2	2.36	0.54
2:B:44:VAL:HA	2:B:181:PRO:HA	1.89	0.54
3:C:12:TYR:N	3:C:13:PRO:HD2	2.23	0.54
1:A:145:ALA:O	1:A:149:LYS:HG3	2.07	0.54
1:A:1121:GLU:O	1:A:1125:LYS:HG3	2.07	0.54
1:A:722:LYS:HE2	1:A:1215:GLY:O	2.07	0.54
1:A:27:THR:CG2	3:C:222:ARG:HD3	2.38	0.54
1:A:338:MET:HE1	1:A:386:PRO:CG	2.38	0.53
1:A:865:ASP:OD1	1:A:867:LYS:HE3	2.07	0.53
1:A:1074:ILE:HG12	1:A:1223:VAL:HG21	1.89	0.53
1:A:199:TYR:CD1	1:A:199:TYR:C	2.86	0.53
1:A:372:TRP:CE2	1:A:863:PRO:HB3	2.43	0.53
1:A:1092:HIS:HA	1:A:1163:HIS:HB3	1.90	0.53
1:A:42:ASP:O	1:A:43:LYS:HB3	2.07	0.53
1:A:626:GLU:HA	1:A:629:LEU:HD23	1.90	0.53
2:B:331:TYR:CE2	2:B:335:MET:HG3	2.43	0.53
1:A:552:MET:HE3	1:A:1056:GLU:OE1	2.09	0.53
1:A:1199:GLY:HA2	1:A:1204:LEU:O	2.09	0.53
2:B:42:ASN:HB2	6:B:803:SF4:S1	2.49	0.53
1:A:1190:ILE:HD13	1:A:1190:ILE:N	2.22	0.53
3:C:1:FME:O1	3:C:3:PHE:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:N	1:A:371:GLU:OE1	2.39	0.53
1:A:1046:GLN:HG3	1:A:1051:MET:CE	2.39	0.53
1:A:107:ARG:HD2	1:A:773:PHE:O	2.08	0.53
1:A:644:ASP:OD2	1:A:751:PRO:HB2	2.08	0.53
1:A:1112:ARG:HB2	1:A:1116:VAL:HG11	1.89	0.53
2:B:201:ILE:HG12	2:B:212:ILE:HG12	1.91	0.53
1:A:214:LEU:HB3	1:A:607:SER:OG	2.09	0.52
1:A:361:VAL:CG1	1:A:362:ASP:H	2.19	0.52
1:A:378:ASN:ND2	1:A:382:GLU:HB2	2.22	0.52
1:A:585:PRO:HD3	1:A:799:THR:HG21	1.91	0.52
1:A:856:SER:O	1:A:859:GLU:HG2	2.09	0.52
1:A:824:GLU:OE2	1:A:827:LYS:HE3	2.09	0.52
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.44	0.52
9:B:541:HOH:O	3:C:212:GLU:HG2	2.08	0.52
1:A:876:LEU:C	1:A:876:LEU:HD23	2.35	0.52
1:A:1069:SER:O	1:A:1139:ASN:HB2	2.10	0.52
1:A:366:GLN:HG2	1:A:373:LYS:CD	2.40	0.52
1:A:684:VAL:CG1	1:A:688:LYS:HE3	2.39	0.52
3:C:159:LEU:HG	8:C:807:HEM:HMA3	1.92	0.52
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.75	0.52
1:A:427:ALA:HB3	1:A:457:VAL:HG11	1.92	0.52
1:A:1093:GLN:CB	1:A:1162:TYR:HB3	2.40	0.52
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.91	0.52
1:A:269:GLU:HG3	2:B:15:LYS:HE3	1.92	0.52
1:A:168:LEU:HD23	1:A:168:LEU:C	2.35	0.51
1:A:360:LEU:C	1:A:463:ALA:HB2	2.35	0.51
1:A:831:LYS:HA	1:A:896:TYR:HB2	1.91	0.51
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.46	0.51
2:B:220:TRP:O	2:B:221:ARG:HG3	2.10	0.51
1:A:360:LEU:HD11	1:A:383:MET:HE1	1.92	0.51
1:A:1098:HIS:C	1:A:1164:ALA:CB	2.83	0.51
1:A:194:MET:HE1	1:A:791:TRP:CE2	2.44	0.51
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.91	0.51
1:A:1087:ASN:O	1:A:1159:THR:HG22	2.10	0.51
1:A:1137:VAL:CG1	1:A:1222:VAL:HG21	2.41	0.51
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.46	0.51
1:A:902:ILE:CD1	1:A:927:LEU:HD13	2.41	0.51
1:A:957:THR:OG1	1:A:995:ARG:NH1	2.40	0.51
2:B:66:TRP:HB2	2:B:348:ARG:HB2	1.92	0.51
1:A:234:GLN:HG3	1:A:235:THR:N	2.25	0.51
1:A:1137:VAL:HG13	1:A:1222:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:TYR:OH	2:B:437:GLU:HG2	2.11	0.51
3:C:83:ILE:HD11	3:C:156:MET:HG2	1.93	0.51
1:A:305:MET:O	1:A:309:MET:HG3	2.11	0.51
1:A:80:THR:O	1:A:81:ARG:C	2.53	0.50
1:A:393:ARG:NH1	1:A:855:ASP:HA	2.25	0.50
1:A:239:GLU:HG2	1:A:1022:TYR:HB3	1.93	0.50
1:A:1112:ARG:NH1	1:A:1149:VAL:HG22	2.26	0.50
1:A:43:LYS:HE2	1:A:45:VAL:CG2	2.40	0.50
1:A:684:VAL:HG13	1:A:876:LEU:HD22	1.93	0.50
1:A:795:ASP:HA	1:A:809:LEU:O	2.11	0.50
2:B:359:LEU:HD23	2:B:406:LEU:HD22	1.94	0.50
1:A:143:ASP:O	1:A:147:SER:HB3	2.12	0.50
1:A:146:LYS:C	1:A:146:LYS:HD2	2.36	0.50
1:A:394:TRP:CD1	1:A:860:LEU:HD11	2.47	0.50
3:C:73:PRO:HG2	3:C:76:MET:HG3	1.94	0.50
1:A:61:ILE:HD13	1:A:61:ILE:N	2.26	0.49
1:A:108:LEU:CD2	1:A:785:ILE:HG21	2.41	0.49
1:A:1151:SER:HB2	2:B:148:LEU:O	2.11	0.49
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.92	0.49
1:A:353:ARG:CZ	1:A:864:LEU:HD12	2.43	0.49
1:A:1168:ILE:O	2:B:123:ILE:HD13	2.13	0.49
1:A:372:TRP:NE1	1:A:860:LEU:HB3	2.27	0.49
1:A:864:LEU:HD22	1:A:864:LEU:N	2.28	0.49
1:A:868:ASP:HB3	1:A:871:LYS:HB2	1.93	0.49
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.94	0.49
1:A:102:LEU:HD12	1:A:102:LEU:H	1.77	0.49
1:A:1067:THR:O	1:A:1068:ARG:C	2.56	0.49
1:A:677:MET:HE2	1:A:682:TYR:CA	2.43	0.49
1:A:1234:ASP:OD1	1:A:1236:GLU:HB2	2.12	0.49
1:A:225:PRO:O	1:A:228:PRO:HD2	2.13	0.48
1:A:462:LEU:HD11	1:A:468:ALA:HB2	1.94	0.48
1:A:28:ASN:HA	3:C:225:HIS:CD2	2.48	0.48
1:A:20:GLY:O	3:C:217:LYS:HD2	2.13	0.48
1:A:403:GLU:HG2	1:A:1032:LEU:HD23	1.95	0.48
1:A:1070:VAL:HG13	1:A:1223:VAL:CG2	2.43	0.48
1:A:190:PRO:HD3	1:A:714:SER:HB2	1.95	0.48
1:A:372:TRP:CE2	1:A:860:LEU:HB3	2.49	0.48
2:B:428:ARG:HH21	2:B:428:ARG:HB3	1.78	0.48
3:C:98:GLY:HA3	3:C:141:LEU:HD21	1.96	0.48
3:C:183:ILE:HG23	3:C:184:PHE:N	2.28	0.48
1:A:6:ARG:C	1:A:8:ARG:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASN:HD22	1:A:396:GLU:CG	2.26	0.48
2:B:280:ILE:HG23	2:B:350:LEU:HD12	1.95	0.48
1:A:419:LEU:HD11	1:A:471:THR:HA	1.95	0.48
1:A:803:HIS:HB2	1:A:804:PRO:HD2	1.95	0.48
1:A:909:ILE:O	1:A:909:ILE:HG22	2.13	0.48
3:C:119:ARG:O	3:C:122:THR:HG22	2.13	0.48
1:A:668:ILE:HB	1:A:847:ILE:HD13	1.96	0.48
1:A:1089:LEU:O	1:A:1160:MET:HA	2.14	0.48
2:B:57:GLU:OE2	2:B:344:HIS:NE2	2.39	0.48
1:A:425:GLU:HG3	1:A:457:VAL:CG2	2.44	0.48
2:B:113:THR:O	2:B:114:ALA:C	2.57	0.47
2:B:428:ARG:HB3	2:B:428:ARG:NH2	2.29	0.47
3:C:11:ILE:C	3:C:13:PRO:HD2	2.39	0.47
3:C:159:LEU:HD12	3:C:188:LEU:HD11	1.96	0.47
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.95	0.47
1:A:338:MET:HB3	1:A:354:MET:CE	2.44	0.47
1:A:514:SER:OG	1:A:517:GLN:HG2	2.13	0.47
2:B:126:PRO:CB	2:B:138:ILE:HD11	2.43	0.47
3:C:56:HIS:O	3:C:59:ILE:HG22	2.14	0.47
3:C:83:ILE:CD1	3:C:156:MET:HG2	2.43	0.47
1:A:60:LYS:HG2	1:A:74:GLN:CD	2.39	0.47
1:A:46:ARG:HG3	1:A:58:SER:OG	2.14	0.47
1:A:384:VAL:CG2	1:A:385:ALA:N	2.78	0.47
1:A:1112:ARG:CB	1:A:1116:VAL:HG11	2.44	0.47
1:A:44:ILE:CG2	1:A:60:LYS:HB3	2.43	0.47
1:A:634:ASP:O	1:A:637:ARG:N	2.47	0.47
3:C:202:ARG:CZ	8:C:806:HEM:HAD2	2.44	0.47
1:A:360:LEU:HD11	1:A:383:MET:CE	2.45	0.47
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.80	0.47
1:A:419:LEU:CD1	1:A:471:THR:HA	2.45	0.47
1:A:1016:GLU:HA	1:A:1016:GLU:OE2	2.15	0.47
2:B:188:LEU:HB3	2:B:280:ILE:CD1	2.42	0.47
1:A:89:PRO:O	1:A:90:ARG:HB2	2.15	0.47
1:A:112:MET:HE3	1:A:157:PHE:HB3	1.97	0.47
1:A:308:ALA:O	1:A:312:VAL:HG23	2.15	0.47
1:A:552:MET:HE3	1:A:1056:GLU:CD	2.39	0.47
3:C:25:TRP:CD1	3:C:25:TRP:C	2.93	0.47
1:A:515:ARG:HG2	1:A:516:SER:N	2.29	0.47
1:A:750:LYS:N	1:A:750:LYS:CD	2.78	0.47
2:B:162:ASP:O	2:B:163:ASN:HB2	2.15	0.47
3:C:56:HIS:HA	3:C:59:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:THR:HG23	1:A:414:GLU:HG2	1.96	0.46
1:A:87:HIS:O	1:A:88:GLU:C	2.57	0.46
1:A:634:ASP:HB3	1:A:637:ARG:HB2	1.96	0.46
1:A:309:MET:HB3	1:A:560:MET:HE3	1.97	0.46
1:A:1048:HIS:O	1:A:1049:GLN:C	2.57	0.46
2:B:248:TYR:CG	2:B:249:PRO:HD3	2.50	0.46
1:A:361:VAL:CG1	1:A:362:ASP:N	2.74	0.46
2:B:12:ASN:HA	2:B:356:VAL:HB	1.97	0.46
3:C:125:ALA:O	3:C:129:ILE:HB	2.16	0.46
1:A:232:GLY:HA2	1:A:1210:TYR:OH	2.16	0.46
1:A:338:MET:HG3	1:A:374:THR:HB	1.97	0.46
1:A:368:ASN:ND2	1:A:396:GLU:OE2	2.36	0.46
2:B:482:ASP:OD1	2:B:499:ILE:HG13	2.16	0.46
2:B:187:CYS:HB3	2:B:349:THR:O	2.16	0.46
2:B:409:MET:O	2:B:413:ARG:HG3	2.16	0.46
1:A:339:LEU:HD23	1:A:472:THR:HG22	1.98	0.46
1:A:419:LEU:O	1:A:420:LEU:C	2.58	0.46
1:A:1198:ILE:HG21	1:A:1204:LEU:CD1	2.46	0.46
1:A:384:VAL:HG22	1:A:385:ALA:N	2.30	0.46
1:A:81:ARG:HD3	1:A:1018:GLU:O	2.16	0.45
1:A:242:ASP:OD1	1:A:1021:SER:HB2	2.15	0.45
1:A:814:ASP:O	1:A:815:PRO:C	2.59	0.45
1:A:289:LYS:HD3	1:A:289:LYS:C	2.41	0.45
1:A:335:ASP:O	1:A:338:MET:HB2	2.15	0.45
1:A:658:ALA:HA	1:A:659:PRO:C	2.40	0.45
1:A:1099:SER:CB	4:A:1247:GDP:O1A	2.63	0.45
1:A:79:ARG:NH1	2:B:453:GLU:OE2	2.48	0.45
2:B:119:LYS:HD2	2:B:119:LYS:N	2.32	0.45
2:B:263:CYS:SG	2:B:267:ILE:HG12	2.57	0.45
1:A:1094:LYS:O	1:A:1094:LYS:HG2	2.17	0.45
1:A:719:SER:O	1:A:1185:ASN:ND2	2.50	0.45
1:A:1096:GLY:HA2	1:A:1101:TYR:HB2	1.99	0.45
2:B:306:PRO:HA	2:B:309:ILE:CG1	2.46	0.45
1:A:286:GLU:HG2	2:B:179:TYR:OH	2.16	0.45
1:A:545:ASN:HB2	1:A:554:TYR:OH	2.16	0.45
1:A:210:GLY:O	1:A:603:ARG:HD2	2.16	0.45
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.42	0.45
1:A:108:LEU:HD13	1:A:785:ILE:CG2	2.46	0.45
1:A:532:THR:O	1:A:533:HIS:HB2	2.17	0.45
1:A:787:PRO:O	1:A:819:ALA:HA	2.17	0.45
1:A:1074:ILE:HG12	1:A:1223:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ASP:OD2	2:B:426:ASP:C	2.60	0.45
1:A:397:LYS:HD2	1:A:976:GLU:HB3	1.99	0.44
1:A:1232:TRP:O	1:A:1233:LEU:HB2	2.16	0.44
2:B:157:LYS:HE2	2:B:157:LYS:HB3	1.81	0.44
1:A:936:GLU:HA	1:A:940:LYS:CG	2.48	0.44
1:A:1137:VAL:HG13	1:A:1222:VAL:CG2	2.47	0.44
1:A:184:ARG:HH21	1:A:704:ASN:HD22	1.64	0.44
1:A:299:GLN:CD	1:A:1158:MET:HE2	2.41	0.44
1:A:430:GLY:HA2	1:A:452:LEU:HD12	1.99	0.44
1:A:446:GLU:O	1:A:447:LEU:HD23	2.18	0.44
3:C:208:SER:O	3:C:209:VAL:C	2.59	0.44
1:A:532:THR:OG1	1:A:535:ARG:HB2	2.17	0.44
1:A:1041:ARG:HG2	1:A:1041:ARG:HH21	1.83	0.44
1:A:139:ILE:HD11	1:A:766:ASP:OD2	2.18	0.44
1:A:806:ILE:HG23	1:A:806:ILE:O	2.17	0.44
1:A:173:ASN:O	1:A:177:ILE:HG13	2.17	0.44
1:A:1229:ASN:C	1:A:1230:ILE:HD12	2.42	0.44
3:C:72:THR:HG23	3:C:76:MET:HE3	2.00	0.44
1:A:687:LEU:HD23	1:A:692:ILE:O	2.18	0.44
1:A:1230:ILE:HD12	1:A:1230:ILE:N	2.33	0.44
1:A:245:ASN:O	1:A:535:ARG:HD2	2.18	0.44
2:B:97:ILE:HG23	2:B:98:ASP:N	2.33	0.44
3:C:59:ILE:HG12	8:C:806:HEM:HAC	1.99	0.44
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.99	0.43
2:B:246:PHE:HA	6:B:803:SF4:S4	2.58	0.43
1:A:356:ARG:O	1:A:357:ALA:C	2.61	0.43
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.53	0.43
1:A:517:GLN:HE21	1:A:517:GLN:HA	1.82	0.43
1:A:724:HIS:NE2	1:A:1167:ARG:NH1	2.66	0.43
2:B:126:PRO:HB3	2:B:138:ILE:HD11	1.99	0.43
1:A:289:LYS:HD3	1:A:289:LYS:O	2.18	0.43
1:A:471:THR:HG21	1:A:476:LEU:HD13	2.01	0.43
1:A:1154:VAL:HG22	1:A:1160:MET:CE	2.48	0.43
2:B:339:LEU:HD11	2:B:443:MET:HE3	1.99	0.43
1:A:130:ASP:HA	1:A:131:PRO:HD2	1.90	0.43
2:B:213:ASP:OD2	2:B:213:ASP:C	2.62	0.43
1:A:260:ARG:HD2	1:A:802:MET:SD	2.59	0.43
1:A:637:ARG:HH12	1:A:1049:GLN:HE22	1.66	0.43
2:B:67:ILE:HG23	2:B:77:ARG:HB2	2.00	0.43
1:A:831:LYS:HB2	1:A:896:TYR:CD1	2.54	0.43
1:A:894:ALA:O	1:A:898:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HD13	1:A:502:TYR:CD2	2.54	0.43
1:A:364:LEU:HD13	1:A:385:ALA:HB2	2.00	0.43
1:A:453:HIS:HA	1:A:489:ASP:OD1	2.18	0.43
1:A:529:ALA:CB	1:A:564:CYS:HB3	2.48	0.43
3:C:42:MET:HE2	3:C:42:MET:HB3	1.94	0.43
1:A:146:LYS:HG2	1:A:150:GLN:NE2	2.34	0.43
1:A:597:ASP:O	1:A:903:GLY:HA3	2.18	0.43
1:A:611:PHE:CD2	1:A:727:MET:HE2	2.53	0.43
2:B:96:GLY:O	2:B:99:ASP:HB2	2.19	0.43
1:A:339:LEU:HG	1:A:376:ALA:HA	2.00	0.43
1:A:1198:ILE:HG21	1:A:1204:LEU:HD13	2.01	0.43
2:B:100:TYR:O	2:B:101:TYR:HB3	2.19	0.43
1:A:549:HIS:CD2	1:A:1062:ARG:HB3	2.54	0.42
1:A:626:GLU:HA	1:A:629:LEU:CD2	2.48	0.42
2:B:17:ILE:HG12	6:B:802:SF4:S2	2.58	0.42
3:C:70:MET:HG2	3:C:160:VAL:HG22	2.01	0.42
1:A:971:TRP:CZ3	1:A:1010:PRO:HB3	2.54	0.42
1:A:1097:ILE:O	1:A:1098:HIS:HB2	2.18	0.42
1:A:1176:ILE:O	1:A:1176:ILE:HG22	2.19	0.42
2:B:415:TYR:CZ	2:B:437:GLU:HG2	2.54	0.42
2:B:485:HIS:CD2	2:B:498:ARG:NH1	2.87	0.42
1:A:27:THR:HG22	3:C:222:ARG:HD3	2.00	0.42
1:A:612:TYR:CE1	1:A:1192:PRO:HG3	2.54	0.42
1:A:722:LYS:HB2	1:A:1190:ILE:HD11	2.01	0.42
2:B:342:PRO:HB3	2:B:354:TRP:CE2	2.54	0.42
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.49	0.42
1:A:170:ALA:HB1	1:A:833:PHE:HA	2.01	0.42
1:A:617:GLN:CD	1:A:1190:ILE:HG12	2.44	0.42
1:A:997:ARG:HG3	1:A:997:ARG:NH2	2.34	0.42
1:A:195:SER:HB2	1:A:198:SER:HB2	2.02	0.42
1:A:336:MET:N	1:A:337:PRO:HD2	2.35	0.42
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.85	0.42
1:A:804:PRO:O	1:A:1006:ILE:HG23	2.20	0.42
1:A:108:LEU:HD22	1:A:785:ILE:HG21	2.01	0.42
1:A:305:MET:HG3	1:A:518:ILE:CD1	2.48	0.42
1:A:1041:ARG:HG2	1:A:1041:ARG:NH2	2.34	0.42
2:B:403:LEU:O	2:B:407:LYS:HB2	2.20	0.42
1:A:218:ASP:HA	1:A:223:LEU:HB3	2.02	0.42
1:A:345:ARG:HG2	1:A:345:ARG:NH1	2.34	0.42
1:A:403:GLU:OE2	1:A:980:ARG:NH1	2.52	0.42
1:A:1208:PHE:O	1:A:1209:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LYS:HD2	2:B:119:LYS:H	1.85	0.42
1:A:854:HIS:CE1	1:A:1203:HIS:HA	2.55	0.41
2:B:303:PRO:HB2	2:B:326:GLN:HG2	2.01	0.41
1:A:216:PHE:CD1	1:A:217:TYR:N	2.88	0.41
1:A:332:ARG:HG2	1:A:404:GLN:CG	2.48	0.41
1:A:461:GLN:C	1:A:461:GLN:HE21	2.28	0.41
1:A:471:THR:CG2	1:A:476:LEU:HD13	2.50	0.41
1:A:582:LYS:HB2	1:A:801:ASP:OD2	2.19	0.41
1:A:641:HIS:HB3	1:A:643:ILE:HG22	2.02	0.41
1:A:641:HIS:O	1:A:644:ASP:HB2	2.20	0.41
1:A:960:PRO:HG2	1:A:961:GLU:CD	2.46	0.41
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.21	0.41
2:B:5:SER:HB3	2:B:274:LEU:CD2	2.51	0.41
3:C:128:LEU:O	3:C:132:LEU:HG	2.20	0.41
1:A:190:PRO:O	1:A:191:ILE:C	2.63	0.41
1:A:282:PRO:CG	1:A:1158:MET:HE1	2.50	0.41
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.56	0.41
1:A:1129:ILE:HG12	1:A:1226:LYS:HB2	2.03	0.41
2:B:6:GLN:HG3	2:B:207:ASP:O	2.20	0.41
2:B:311:GLN:NE2	2:B:314:LYS:HE2	2.35	0.41
3:C:188:LEU:HD22	8:C:807:HEM:HMB3	2.02	0.41
2:B:27:LYS:NZ	2:B:39:ALA:O	2.50	0.41
2:B:84:LEU:C	2:B:84:LEU:HD23	2.45	0.41
2:B:123:ILE:HG23	2:B:124:ALA:N	2.34	0.41
2:B:156:ALA:C	2:B:158:ASP:N	2.77	0.41
2:B:194:ALA:HB1	3:C:218:TYR:CD2	2.56	0.41
2:B:85:LEU:HD12	2:B:85:LEU:HA	1.79	0.41
1:A:499:VAL:O	1:A:499:VAL:HG12	2.21	0.41
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.20	0.41
1:A:928:ARG:NH1	1:A:942:GLN:HE22	2.17	0.41
1:A:1043:GLN:HE21	1:A:1043:GLN:HB3	1.69	0.41
2:B:370:GLU:OE2	2:B:370:GLU:HA	2.20	0.41
3:C:139:LEU:O	3:C:143:THR:HG23	2.20	0.41
1:A:368:ASN:HD22	1:A:396:GLU:HG2	1.86	0.41
1:A:637:ARG:NH1	1:A:1049:GLN:NE2	2.69	0.41
1:A:665:PRO:HA	1:A:668:ILE:HD12	2.02	0.41
1:A:432:PRO:HB3	1:A:631:PRO:HD2	2.02	0.41
1:A:500:LYS:O	1:A:502:TYR:N	2.54	0.41
1:A:608:THR:HB	1:A:1213:THR:OG1	2.20	0.41
1:A:1168:ILE:C	2:B:123:ILE:HD13	2.46	0.41
2:B:231:LYS:HA	2:B:231:LYS:HD3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:HE2	1:A:765:LEU:O	2.21	0.41
1:A:252:TRP:CZ2	1:A:305:MET:HE2	2.56	0.41
1:A:663:THR:O	1:A:664:ASN:C	2.64	0.41
1:A:727:MET:O	1:A:731:LEU:HB2	2.20	0.41
1:A:859:GLU:HG3	1:A:860:LEU:HD12	2.03	0.41
1:A:1070:VAL:HG13	1:A:1223:VAL:HG23	2.03	0.41
2:B:373:SER:HB3	2:B:428:ARG:HH11	1.85	0.41
1:A:225:PRO:C	1:A:228:PRO:HD2	2.45	0.40
1:A:1101:TYR:C	1:A:1103:ASP:H	2.29	0.40
1:A:220:TYR:O	1:A:221:CYS:CB	2.69	0.40
1:A:1002:GLN:HA	1:A:1003:PRO:HD3	1.96	0.40
2:B:176:PHE:CD1	2:B:176:PHE:C	2.98	0.40
1:A:152:ARG:O	1:A:734:THR:HG21	2.21	0.40
1:A:487:LEU:N	1:A:487:LEU:CD1	2.84	0.40
1:A:677:MET:HE2	1:A:682:TYR:N	2.36	0.40
1:A:920:THR:OG1	1:A:923:GLU:HB2	2.21	0.40
1:A:1198:ILE:HG22	1:A:1204:LEU:HB3	2.03	0.40
1:A:46:ARG:HG3	1:A:58:SER:HG	1.86	0.40
1:A:420:LEU:HD11	1:A:487:LEU:HD11	2.03	0.40
1:A:434:PHE:C	1:A:436:GLY:H	2.30	0.40
1:A:663:THR:HG21	1:A:692:ILE:CD1	2.47	0.40
1:A:80:THR:O	1:A:81:ARG:O	2.39	0.40
1:A:761:LEU:HD12	1:A:762:GLU:N	2.37	0.40
2:B:62:TYR:CE2	2:B:95:PRO:HB3	2.56	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	1225/1247 (98%)	1115 (91%)	93 (8%)	17 (1%)	9 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	507/512 (99%)	483 (95%)	23 (4%)	1 (0%)	43	72
3	C	223/225 (99%)	209 (94%)	14 (6%)	0	100	100
All	All	1955/1984 (98%)	1807 (92%)	130 (7%)	18 (1%)	14	41

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	501	ALA
1	A	1036	ARG
1	A	1166	GLU
1	A	7	PHE
1	A	578	VAL
1	A	716	LEU
1	A	748	GLY
1	A	635	LYS
1	A	861	ALA
1	A	43	LYS
1	A	1049	GLN
2	B	101	TYR
1	A	190	PRO
1	A	191	ILE
1	A	81	ARG
1	A	718	GLY
1	A	224	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	1027/1044 (98%)	976 (95%)	51 (5%)	22	54
2	B	436/439 (99%)	423 (97%)	13 (3%)	36	72
3	C	184/186 (99%)	176 (96%)	8 (4%)	26	60
All	All	1647/1669 (99%)	1575 (96%)	72 (4%)	25	59

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	133	GLU
1	A	150	GLN
1	A	189	SER
1	A	190	PRO
1	A	194	MET
1	A	195	SER
1	A	287	ILE
1	A	319	LEU
1	A	338	MET
1	A	345	ARG
1	A	360	LEU
1	A	383	MET
1	A	402	LEU
1	A	412	GLU
1	A	461	GLN
1	A	467	THR
1	A	476	LEU
1	A	483	LEU
1	A	490	VAL
1	A	515	ARG
1	A	550	LEU
1	A	600	ARG
1	A	601	PRO
1	A	629	LEU
1	A	637	ARG
1	A	680	VAL
1	A	728	LEU
1	A	741	LYS
1	A	767	LEU
1	A	801	ASP
1	A	804	PRO
1	A	808	PRO
1	A	813	VAL
1	A	820	LYS
1	A	835	GLU
1	A	916	ILE
1	A	926	LEU
1	A	936	GLU
1	A	944	MET
1	A	995	ARG
1	A	1006	ILE

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Mol	Chain	Res	Type
1	A	1072	GLU
1	A	1074	ILE
1	A	1110	LEU
1	A	1174	SER
1	A	1176	ILE
1	A	1190	ILE
1	A	1233	LEU
1	A	1238	ASN
1	A	1243	GLU
2	B	37	GLU
2	B	42	ASN
2	B	70	ILE
2	B	74	LEU
2	B	85	LEU
2	B	119	LYS
2	B	123	ILE
2	B	161	PHE
2	B	183	LEU
2	B	255	GLN
2	B	299	VAL
2	B	323	GLU
2	B	460	SER
3	C	76	MET
3	C	83	ILE
3	C	110	LYS
3	C	129	ILE
3	C	142	LEU
3	C	204	ILE
3	C	209	VAL
3	C	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	150	GLN
1	A	173	ASN
1	A	179	ASN
1	A	229	GLN
1	A	423	GLN
1	A	461	GLN
1	A	480	ASN

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Mol	Chain	Res	Type
1	A	517	GLN
1	A	559	ASN
1	A	586	GLN
1	A	599	GLN
1	A	660	GLN
1	A	698	GLN
1	A	704	ASN
1	A	705	HIS
1	A	708	ASN
1	A	759	ASN
1	A	942	GLN
1	A	1049	GLN
1	A	1076	GLN
1	A	1082	GLN
1	A	1141	ASN
1	A	1217	ASN
1	A	1229	ASN
2	B	143	ASN
2	B	294	GLN
2	B	296	GLN
2	B	304	ASN
2	B	311	GLN
2	B	327	GLN
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	1.36	2 (25%)	8,9,11	1.74	3 (37%)

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-CG	2.46	1.61	1.51
3	C	1	FME	CB-CA	-2.11	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	3.03	127.49	122.82
3	C	1	FME	CB-CA-N	2.55	115.16	110.52
3	C	1	FME	O-C-CA	-2.08	119.43	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	O1-CN-N-CA
3	C	1	FME	N-CA-CB-CG
3	C	1	FME	C-CA-CB-CG
3	C	1	FME	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](#)

9 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	$\# Z > 2$
8	HEM	C	806	3	50,50,50	1.69	11 (22%)	67,82,82	0.98	5 (7%)
7	F3S	B	805	2	0,9,9	-	-	-		
4	GDP	A	1247	-	29,30,30	1.40	5 (17%)	45,47,47	1.01	1 (2%)
6	SF4	B	803	2	0,12,12	-	-	-		
8	HEM	C	807	3	50,50,50	1.79	16 (32%)	67,82,82	0.96	5 (7%)
4	GDP	A	1248	-	29,30,30	1.50	6 (20%)	45,47,47	1.04	2 (4%)
6	SF4	B	804	2	0,12,12	-	-	-		
6	SF4	B	802	2	0,12,12	-	-	-		
5	AGA	A	1249	-	24,24,29	0.92	1 (4%)	27,29,35	1.61	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	C	806	3	-	6/14/54/54	-
7	F3S	B	805	2	-	-	0/3/3/3
4	GDP	A	1247	-	-	0/16/32/32	0/3/3/3
6	SF4	B	803	2	-	-	0/6/5/5
8	HEM	C	807	3	-	7/14/54/54	-
4	GDP	A	1248	-	-	5/16/32/32	0/3/3/3
6	SF4	B	804	2	-	-	0/6/5/5
6	SF4	B	802	2	-	-	0/6/5/5
5	AGA	A	1249	-	-	3/26/26/34	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	807	HEM	CAB-C3B	4.66	1.59	1.47
8	C	806	HEM	CAB-C3B	4.57	1.59	1.47
4	A	1248	GDP	C4-N3	4.40	1.44	1.34
4	A	1247	GDP	C4-N3	3.86	1.43	1.34
8	C	806	HEM	CMC-C2C	3.54	1.58	1.50
8	C	807	HEM	FE-NC	3.52	2.06	1.95
8	C	807	HEM	CMC-C2C	3.45	1.57	1.50
8	C	807	HEM	CAC-C3C	3.33	1.56	1.47
8	C	806	HEM	CAC-C3C	3.30	1.56	1.47
4	A	1248	GDP	C6-N1	3.29	1.45	1.38
8	C	806	HEM	FE-NC	3.10	2.05	1.95
8	C	807	HEM	CMB-C2B	3.09	1.57	1.50
8	C	806	HEM	CMA-C3A	3.01	1.57	1.50
8	C	806	HEM	CMB-C2B	2.86	1.56	1.50
8	C	807	HEM	CMD-C2D	2.78	1.56	1.50
5	A	1249	AGA	C8-C7	2.75	1.58	1.50
4	A	1247	GDP	C6-N1	2.73	1.44	1.38
8	C	807	HEM	CMA-C3A	2.71	1.56	1.50
8	C	806	HEM	C4D-ND	-2.64	1.35	1.40
8	C	806	HEM	CMD-C2D	2.62	1.56	1.50
8	C	806	HEM	FE-NB	2.54	2.02	1.94
8	C	807	HEM	FE-NB	2.43	2.02	1.94
8	C	807	HEM	CBD-CGD	2.41	1.56	1.50
4	A	1248	GDP	PB-O2B	-2.38	1.46	1.54
8	C	807	HEM	CAD-C3D	2.33	1.57	1.51
8	C	807	HEM	O1D-CGD	2.31	1.29	1.22
8	C	807	HEM	C4D-ND	-2.24	1.36	1.40
8	C	806	HEM	O1D-CGD	2.23	1.29	1.22
4	A	1247	GDP	PB-O2B	-2.22	1.46	1.54
8	C	807	HEM	CBA-CAA	2.14	1.59	1.51
4	A	1247	GDP	PB-O3B	2.13	1.62	1.54
4	A	1248	GDP	C2-N3	2.12	1.38	1.33
8	C	807	HEM	CBD-CAD	2.12	1.59	1.51
4	A	1247	GDP	C2-N3	2.10	1.38	1.33
8	C	807	HEM	C1D-C2D	2.09	1.48	1.44
8	C	806	HEM	C2A-C3A	-2.04	1.33	1.38
8	C	807	HEM	O1A-CGA	2.02	1.28	1.22
4	A	1248	GDP	C2-N1	2.02	1.42	1.37
4	A	1248	GDP	PB-O3B	2.00	1.62	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1249	AGA	C14-C13-C12	5.18	132.66	113.69
5	A	1249	AGA	C9-C8-C7	4.89	131.61	113.69
8	C	807	HEM	CAD-C3D-C4D	-2.88	119.68	124.70
8	C	806	HEM	CAD-C3D-C4D	-2.71	119.97	124.70
4	A	1247	GDP	PA-O5'-C5'	2.53	135.87	121.35
8	C	807	HEM	CAD-C3D-C2D	2.42	132.40	127.87
4	A	1248	GDP	PA-O5'-C5'	2.36	134.88	121.35
8	C	807	HEM	O1A-CGA-CBA	-2.32	115.74	123.09
8	C	806	HEM	O1D-CGD-CBD	-2.20	116.10	123.09
8	C	806	HEM	O2D-CGD-O1D	2.19	128.97	123.33
8	C	806	HEM	CAD-C3D-C2D	2.17	131.93	127.87
8	C	807	HEM	CMA-C3A-C2A	2.14	130.16	125.62
4	A	1248	GDP	C1'-N9-C8	2.14	132.80	126.73
5	A	1249	AGA	C6-O7-C7	2.05	124.63	117.12
5	A	1249	AGA	C5-O9-C12	2.05	122.70	117.80
8	C	807	HEM	O1D-CGD-CBD	-2.01	116.71	123.09
8	C	806	HEM	O1A-CGA-CBA	-2.01	116.71	123.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

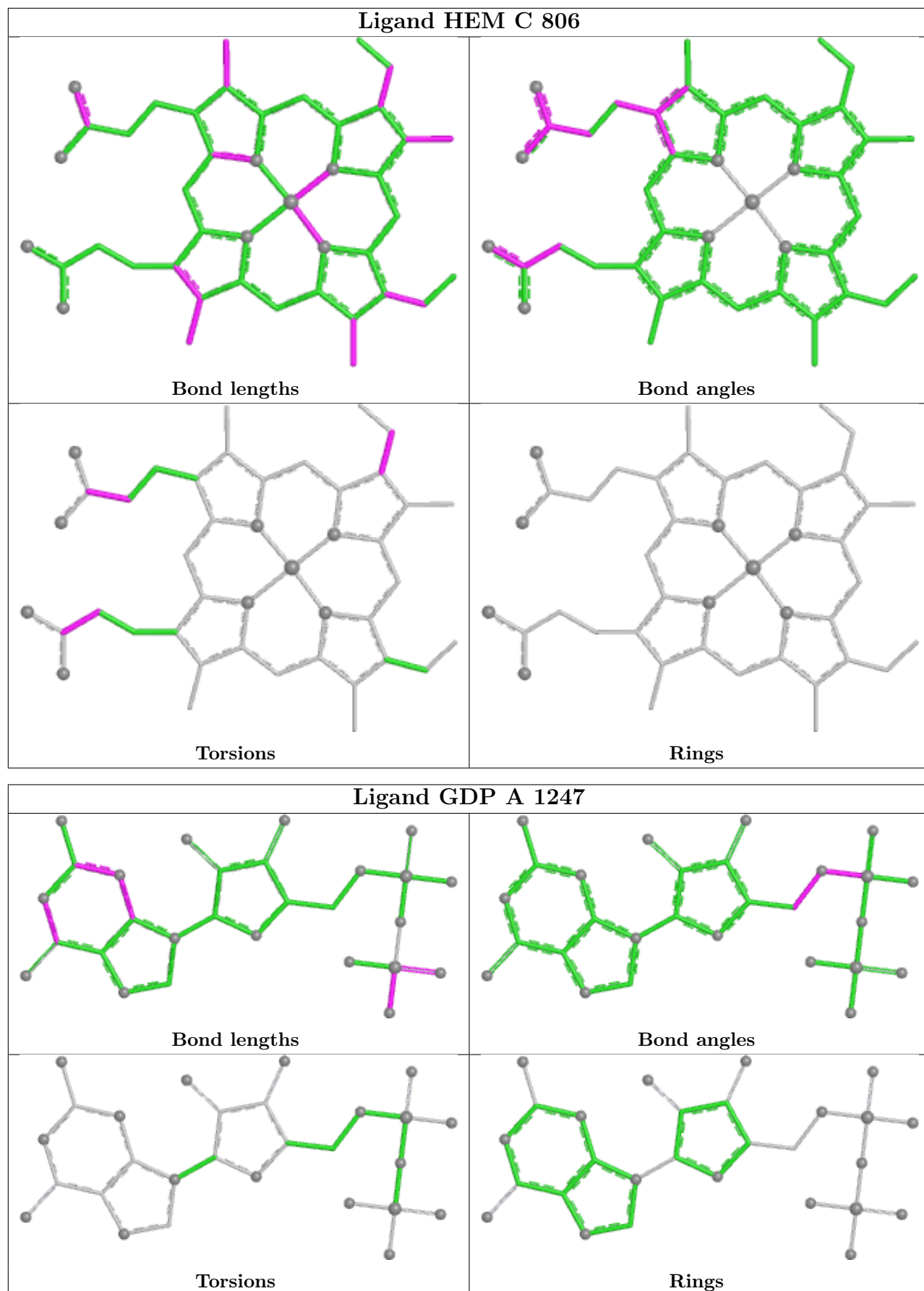
Mol	Chain	Res	Type	Atoms
4	A	1248	GDP	C5'-O5'-PA-O1A
8	C	806	HEM	C2C-C3C-CAC-CBC
8	C	806	HEM	C4C-C3C-CAC-CBC
8	C	807	HEM	C2C-C3C-CAC-CBC
8	C	807	HEM	C4C-C3C-CAC-CBC
4	A	1248	GDP	O4'-C4'-C5'-O5'
8	C	807	HEM	C2A-CAA-CBA-CGA
4	A	1248	GDP	C3'-C4'-C5'-O5'
5	A	1249	AGA	C8-C7-O7-C6
5	A	1249	AGA	O8-C7-O7-C6
4	A	1248	GDP	C5'-O5'-PA-O3A
4	A	1248	GDP	C5'-O5'-PA-O2A
5	A	1249	AGA	O6-C4-C5-C6
8	C	807	HEM	CAA-CBA-CGA-O2A
8	C	806	HEM	CAA-CBA-CGA-O2A
8	C	807	HEM	CAD-CBD-CGD-O2D
8	C	806	HEM	CAA-CBA-CGA-O1A
8	C	806	HEM	CAD-CBD-CGD-O1D
8	C	806	HEM	CAD-CBD-CGD-O2D
8	C	807	HEM	CAA-CBA-CGA-O1A
8	C	807	HEM	CAD-CBD-CGD-O1D

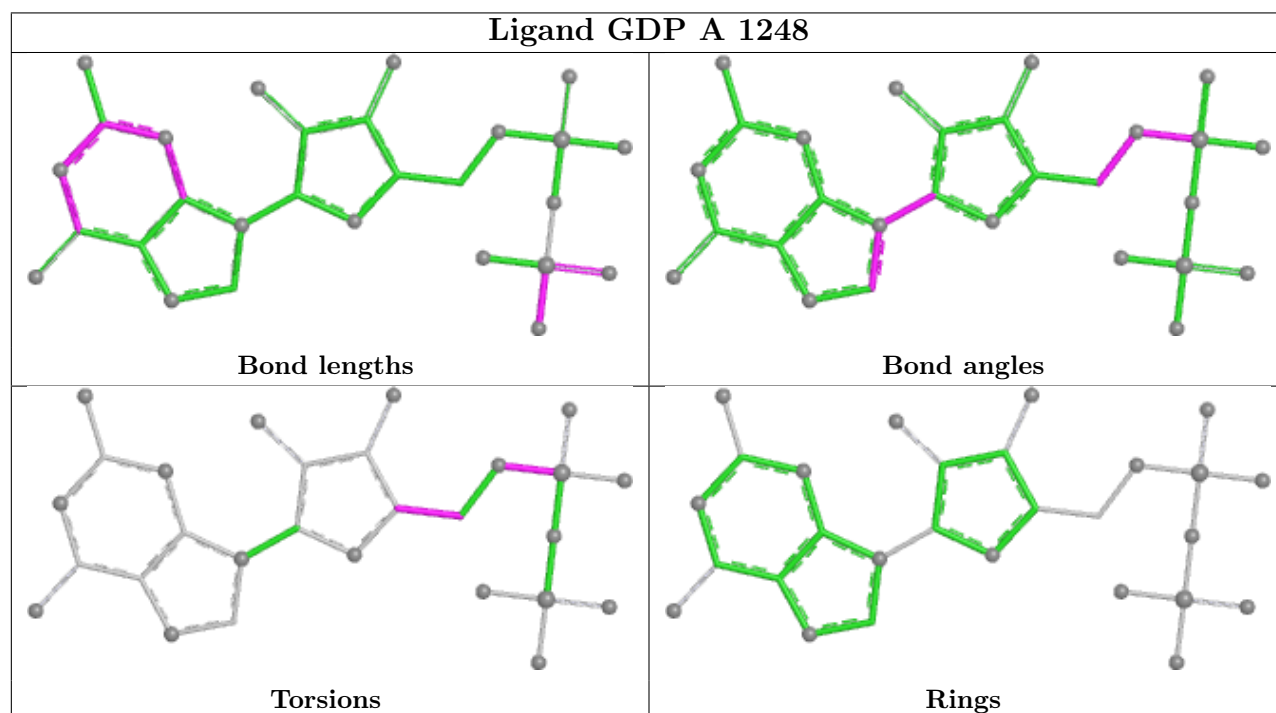
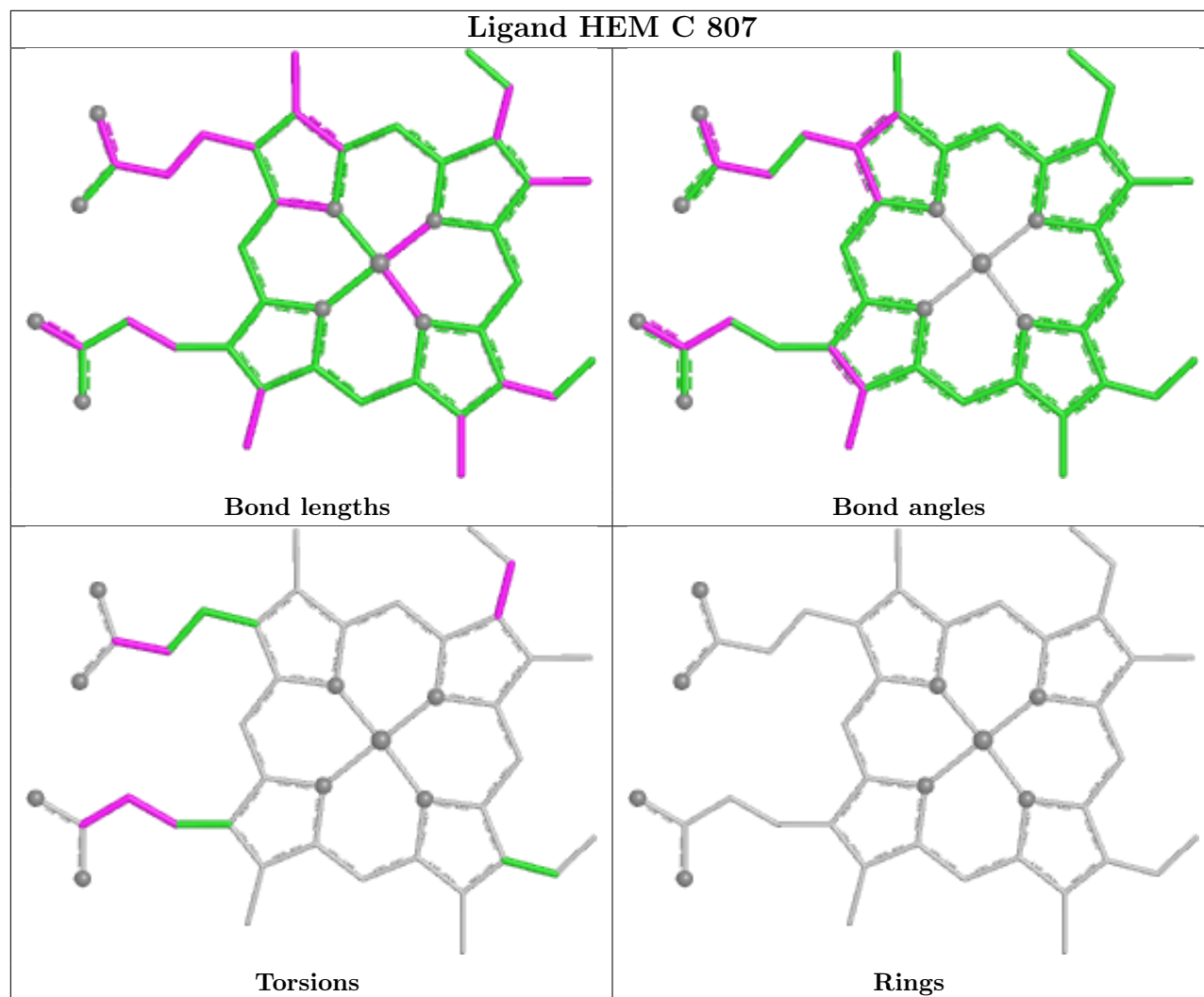
There are no ring outliers.

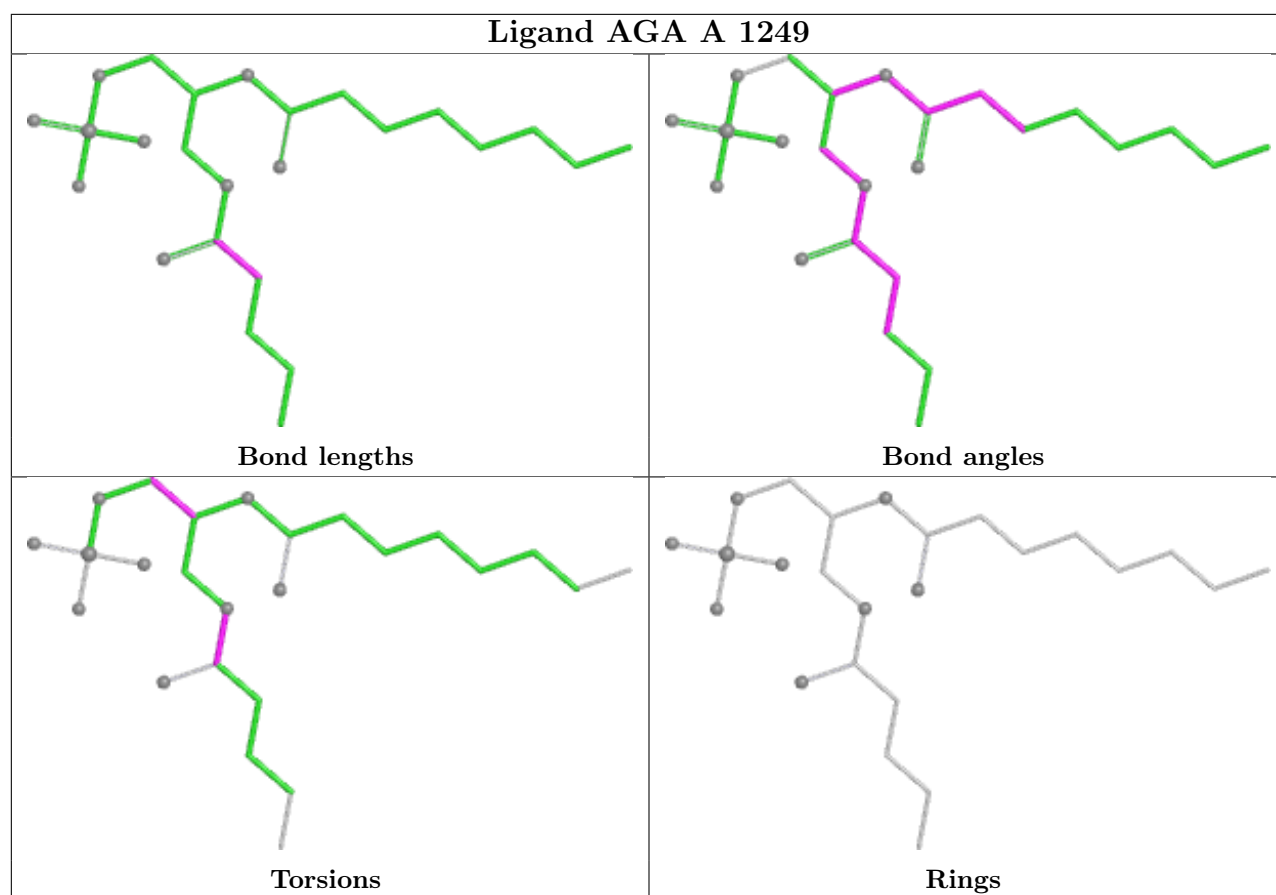
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	806	HEM	3	0
4	A	1247	GDP	2	0
6	B	803	SF4	2	0
8	C	807	HEM	2	0
6	B	802	SF4	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 [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	1233/1247 (98%)	-0.37	9 (0%) 84 77	20, 41, 68, 103	0
2	B	509/512 (99%)	-0.65	0 100 100	16, 31, 54, 98	0
3	C	224/225 (99%)	-0.42	0 100 100	23, 39, 62, 98	0
All	All	1966/1984 (99%)	-0.45	9 (0%) 87 82	16, 38, 65, 103	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	GLY	5.0
1	A	194	MET	3.1
1	A	56	SER	2.9
1	A	1016	GLU	2.7
1	A	1244	SER	2.4
1	A	8	ARG	2.4
1	A	501	ALA	2.4
1	A	749	VAL	2.3
1	A	1018	GLU	2.1

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	0.88	0.13	40,40,40,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

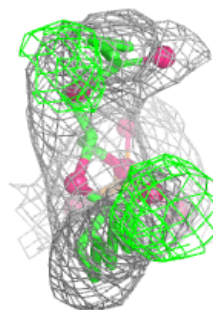
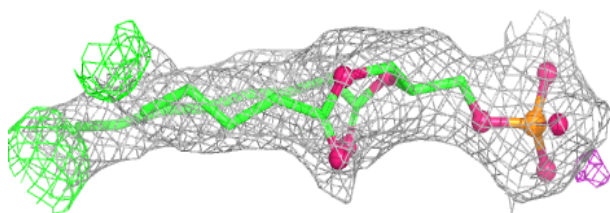
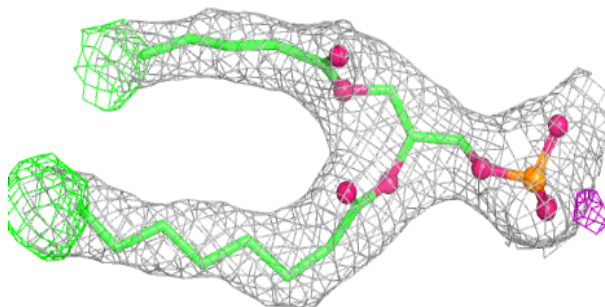
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	AGA	A	1249	25/30	0.90	0.11	44,44,44,44	0
4	GDP	A	1247	28/28	0.92	0.10	56,56,56,56	0
4	GDP	A	1248	28/28	0.94	0.08	49,49,49,49	0
8	HEM	C	807	43/43	0.94	0.10	45,45,45,45	0
8	HEM	C	806	43/43	0.98	0.07	32,32,32,32	0
6	SF4	B	804	8/8	0.98	0.05	36,36,36,36	0
7	F3S	B	805	7/7	0.99	0.03	23,23,23,23	0
6	SF4	B	803	8/8	0.99	0.03	20,20,20,20	0
6	SF4	B	802	8/8	0.99	0.04	30,30,30,30	0

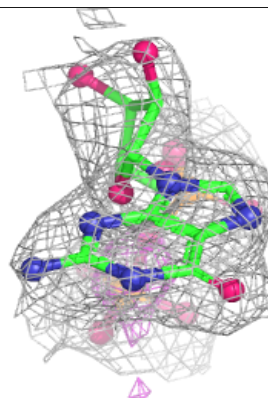
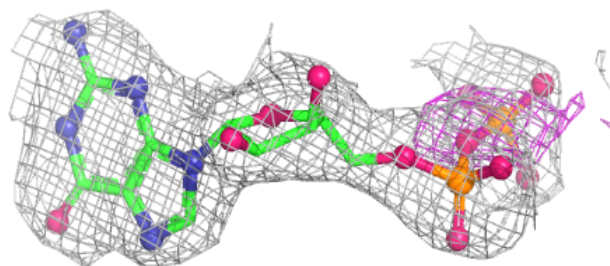
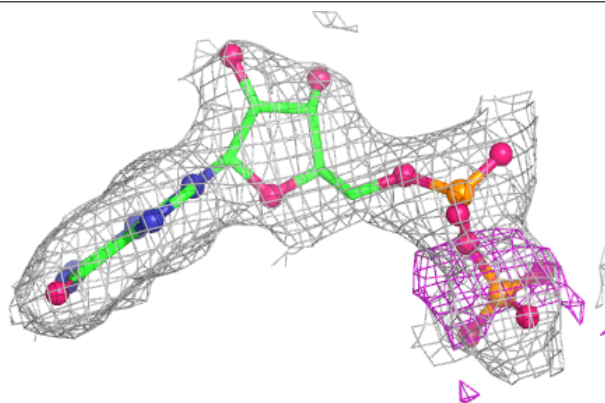
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

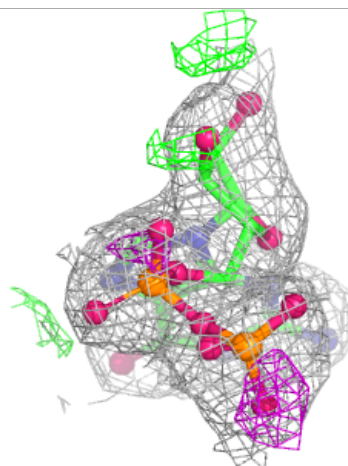
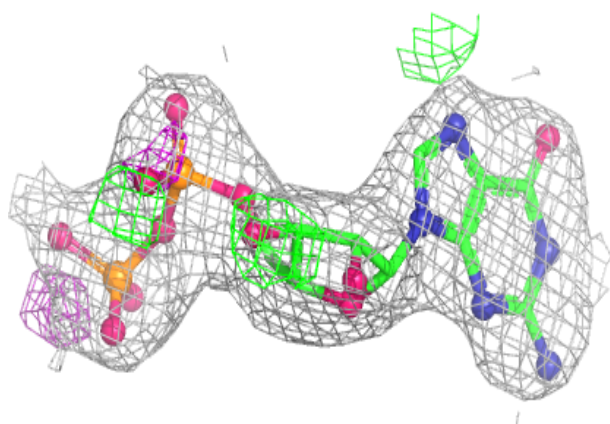
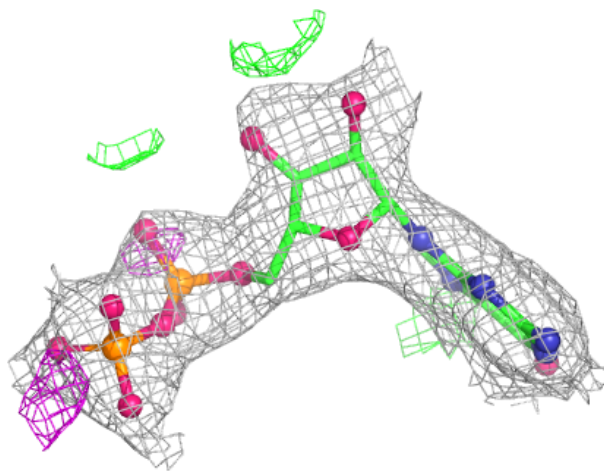
**Electron density around GDP A 1247:**

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



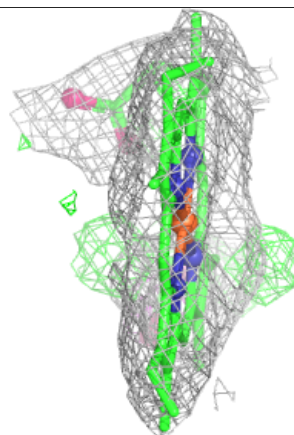
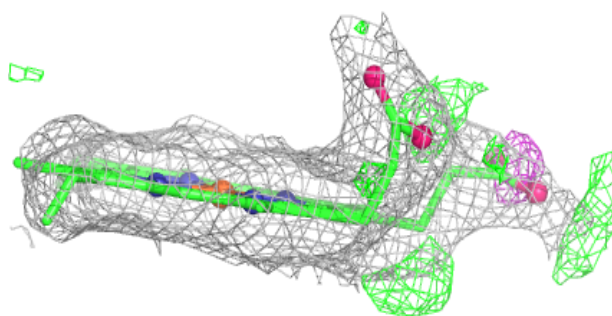
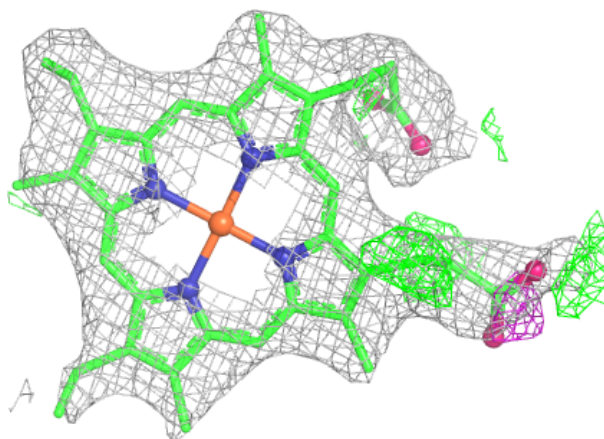
Electron density around GDP A 1248:

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

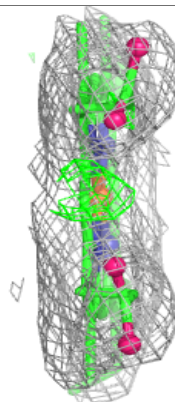
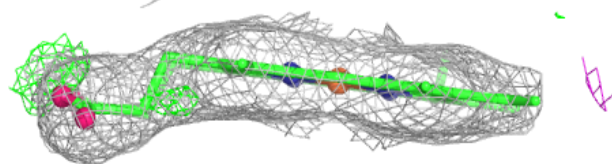
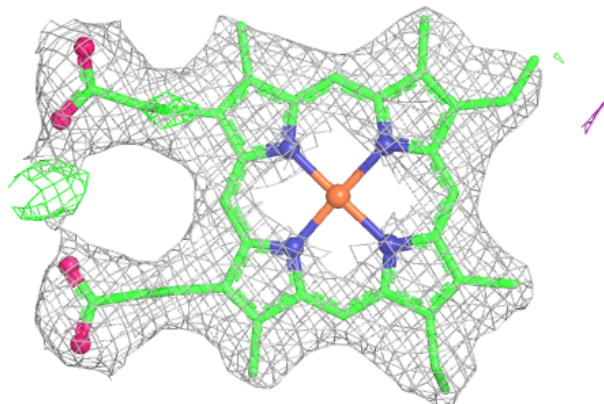


Electron density around HEM C 807:

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

**Electron density around HEM C 806:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.