



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:25 PM UTC

PDB ID : 1Y5N / pdb_00001y5n
Title : The crystal structure of the NarGHI mutant NarI-K86A in complex with pentachlorophenol
Authors : Bertero, M.G.; Rothery, R.A.; Boroumand, N.; Palak, M.; Blasco, F.; Ginet, N.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2004-12-02
Resolution : 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

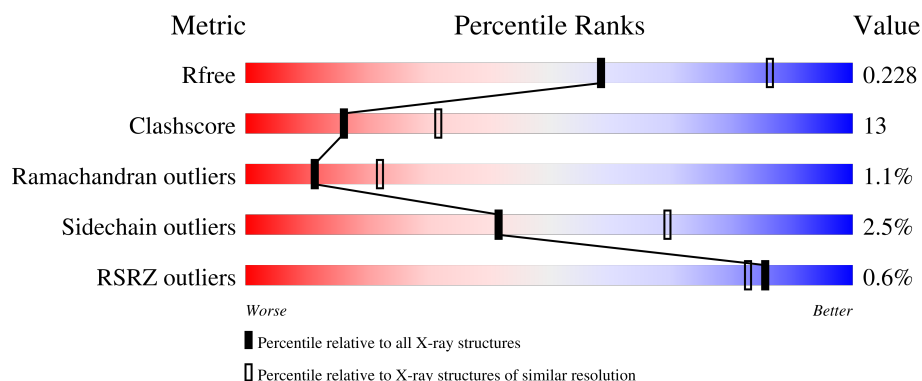
1 Overall quality at a glance

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	1246	68% 29%
2	B	512	77% 20%
3	C	225	63% 31%

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
3	FME	C	1	-	X	-	-
6	SF4	A	1801	-	-	X	-
8	3PH	B	1806	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15972 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1244	Total	C	N	O	S	0	0	0
			9869	6232	1731	1858	48			

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

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

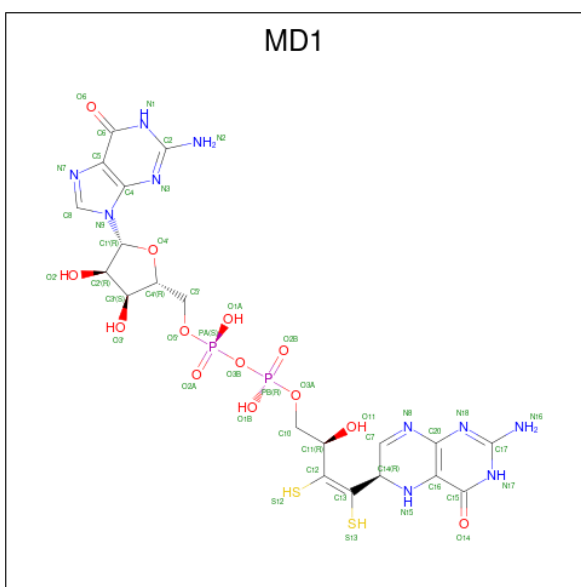
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

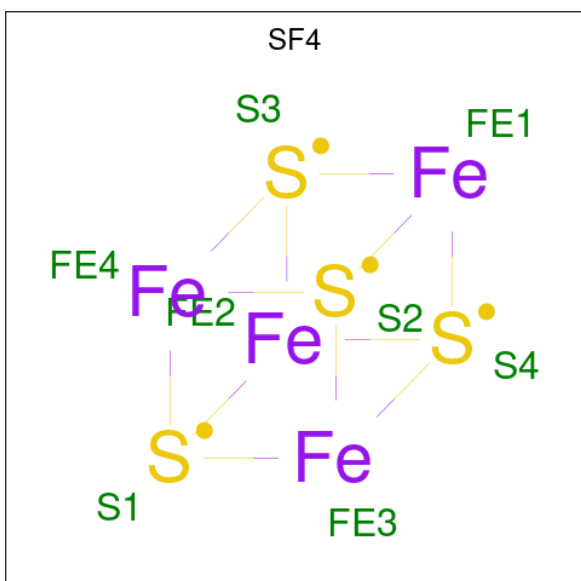


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

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

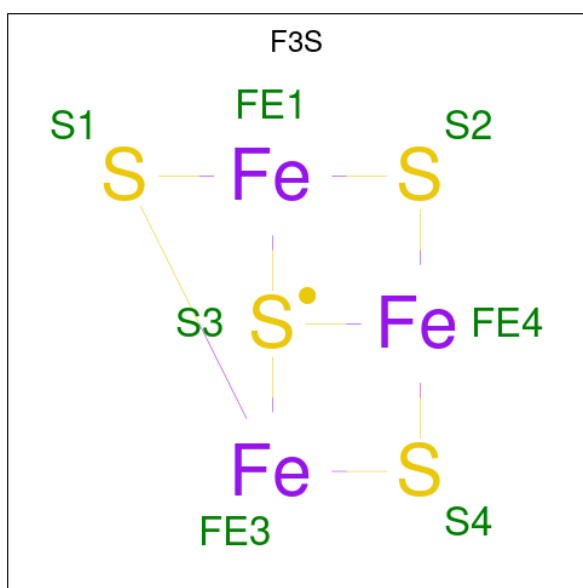
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mo 1 1	0	0

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



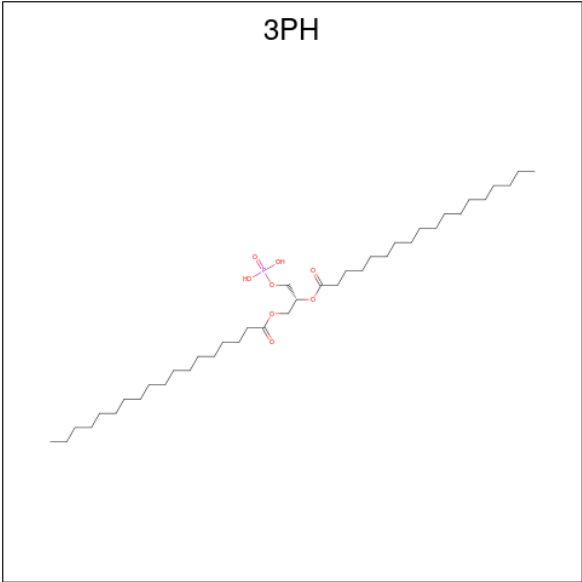
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

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



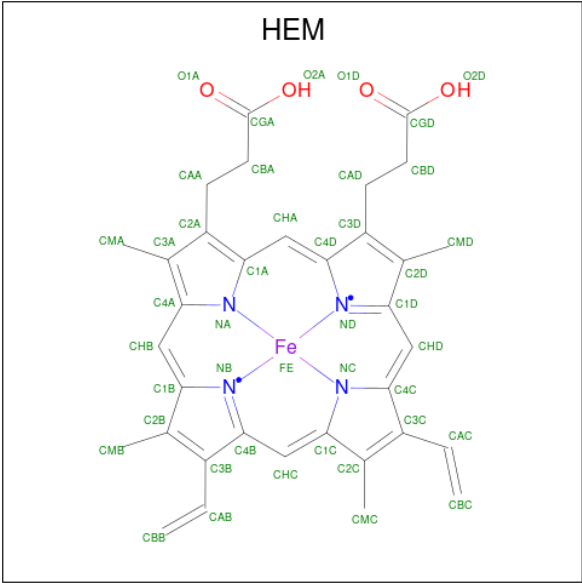
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			7	3	4		

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



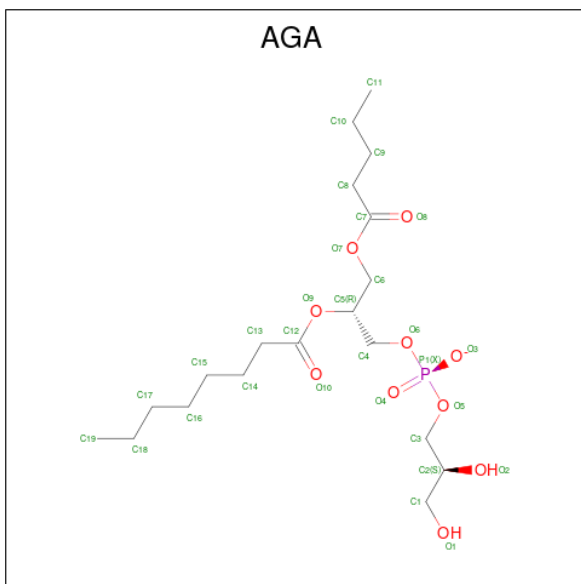
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	P	0	0
			18	9	8	1		

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



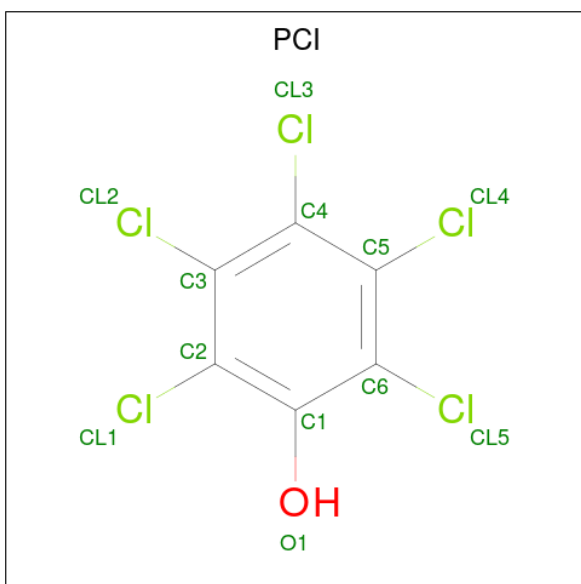
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
9	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 10 is (1S)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (CCD ID: AGA) (formula: C₁₉H₃₆O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	O	P	0	0
			30	19	10	1		

- Molecule 11 is PENTACHLOROPHENOL (CCD ID: PCI) (formula: C₆HCl₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Cl	O	0	0
			12	6	5	1		

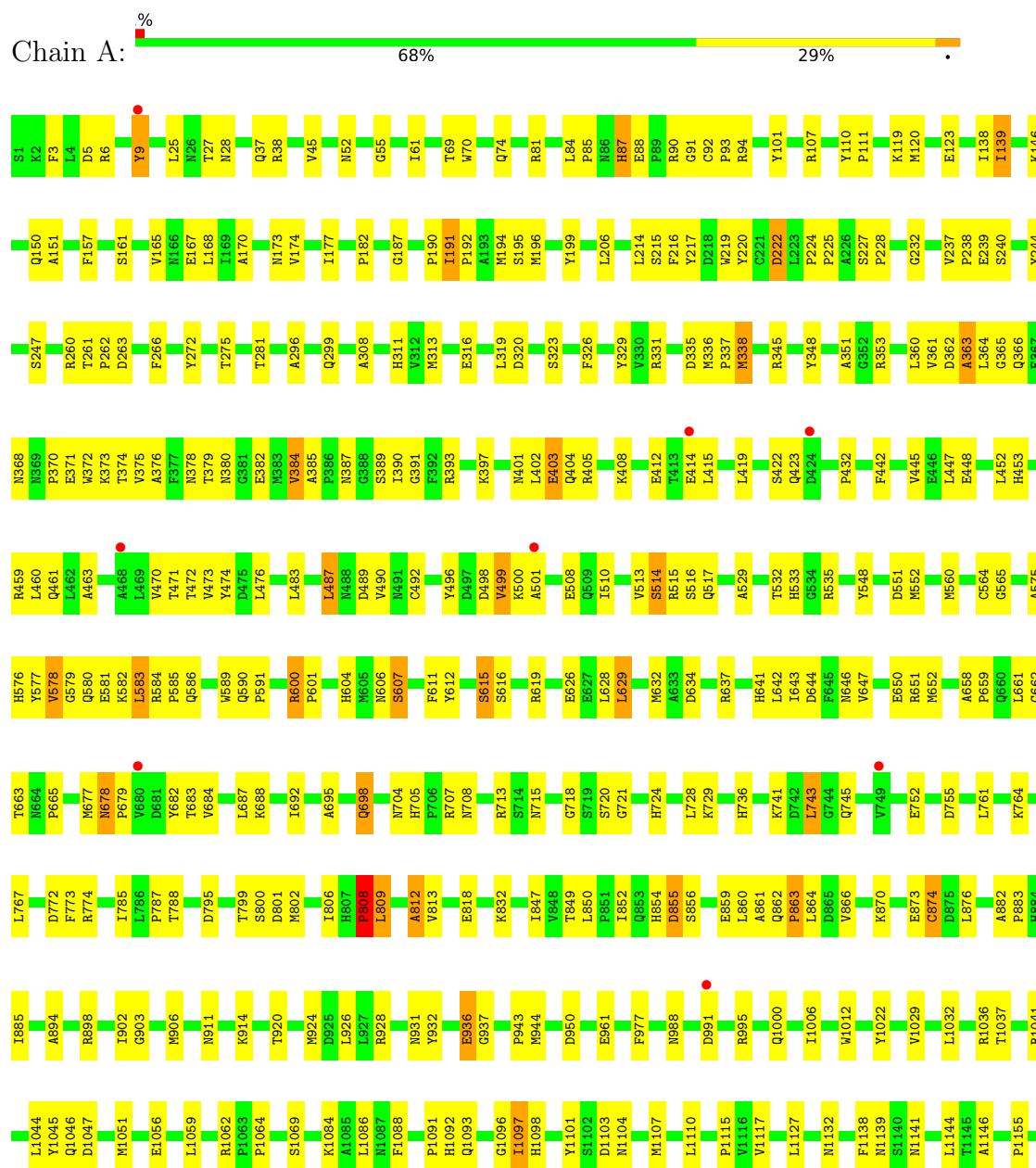
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	23	Total 23	O 23	0	0
12	B	29	Total 29	O 29	0	0
12	C	2	Total 2	O 2	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.

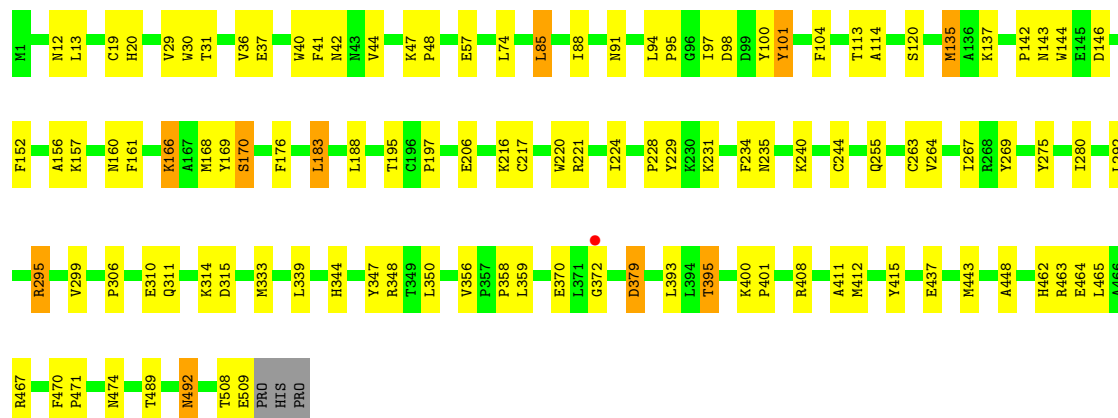
- Molecule 1: Respiratory nitrate reductase 1 alpha chain





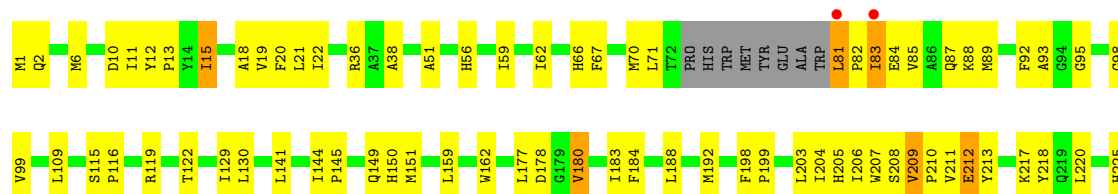
• Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B: 77% 20% ..



• Molecule 3: Respiratory nitrate reductase 1 gamma chain

Chain C: 63% 31% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.26Å 241.96Å 140.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 2.50 24.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	81.4 (24.84-2.50) 81.3 (24.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.238 0.181 , 0.228	Depositor DCC
R_{free} test set	6007 reflections (8.16%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.7	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	15972	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, SF4, AGA, F3S, FME, PCI, MD1, 6MO, 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	0.43	0/10128	0.94	40/13749 (0.3%)
2	B	0.45	0/4146	0.98	16/5609 (0.3%)
3	C	0.45	0/1754	0.95	7/2370 (0.3%)
All	All	0.44	0/16028	0.95	63/21728 (0.3%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	TRP	N-CA-C	8.52	123.80	113.41
3	C	83	ILE	N-CA-C	7.76	118.30	110.23
1	A	1093	GLN	N-CA-C	7.71	119.89	110.41
1	A	499	VAL	N-CA-C	7.63	114.38	106.21
3	C	209	VAL	CA-C-N	7.61	129.35	119.84
3	C	209	VAL	C-N-CA	7.61	129.35	119.84
2	B	29	VAL	N-CA-C	7.28	117.37	110.53
1	A	862	GLN	CA-C-N	7.00	126.48	118.85
1	A	862	GLN	C-N-CA	7.00	126.48	118.85
1	A	607	SER	N-CA-C	6.98	119.77	111.33
2	B	88	ILE	N-CA-C	6.90	119.72	111.09
1	A	1163	HIS	N-CA-C	6.86	120.59	110.30
1	A	222	ASP	N-CA-C	-6.74	104.87	113.23
2	B	280	ILE	N-CA-C	6.60	117.29	110.36
1	A	615	SER	N-CA-C	-6.44	105.17	113.16
1	A	809	LEU	N-CA-C	-6.42	98.44	108.90
1	A	678	ASN	CA-C-N	6.40	126.61	119.32
1	A	678	ASN	C-N-CA	6.40	126.61	119.32
2	B	395	THR	N-CA-C	6.29	118.93	110.88
1	A	1138	PHE	N-CA-C	6.26	117.74	108.60
1	A	903	GLY	CA-C-N	6.24	125.80	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	903	GLY	C-N-CA	6.24	125.80	119.19
2	B	144	TRP	N-CA-C	6.22	118.86	111.71
1	A	812	ALA	N-CA-C	-6.17	104.46	112.23
1	A	863	PRO	N-CA-C	6.16	121.65	113.40
1	A	101	TYR	N-CA-C	6.16	117.66	111.07
1	A	698	GLN	CA-C-N	6.08	125.78	119.82
1	A	698	GLN	C-N-CA	6.08	125.78	119.82
1	A	87	HIS	N-CA-C	6.06	117.97	111.36
1	A	1165	GLN	N-CA-C	-5.87	104.62	113.89
1	A	628	LEU	N-CA-C	-5.85	105.99	114.12
2	B	474	ASN	N-CA-C	5.84	118.59	111.82
1	A	854	HIS	N-CA-C	-5.75	103.34	110.41
1	A	1141	ASN	N-CA-C	5.75	118.48	111.82
2	B	216	LYS	N-CA-C	5.74	119.46	112.23
1	A	74	GLN	N-CA-C	-5.72	100.35	109.96
2	B	206	GLU	N-CA-C	5.62	118.34	111.82
3	C	217	LYS	N-CA-C	-5.55	102.07	110.28
1	A	1167	ARG	N-CA-C	5.52	119.55	112.26
1	A	1097	ILE	N-CA-C	-5.49	97.98	106.72
2	B	255	GLN	CA-C-N	5.49	125.48	120.21
2	B	255	GLN	C-N-CA	5.49	125.48	120.21
1	A	384	VAL	N-CA-C	5.48	115.53	107.75
1	A	363	ALA	N-CA-C	-5.43	106.61	113.23
1	A	403	GLU	N-CA-C	-5.42	102.26	110.28
1	A	583	LEU	N-CA-C	-5.39	100.01	108.63
1	A	1166	GLU	N-CA-C	5.34	122.18	110.80
2	B	359	LEU	N-CA-C	-5.33	102.87	110.59
1	A	1029	VAL	N-CA-C	5.31	116.09	110.72
1	A	151	ALA	N-CA-C	-5.26	106.70	113.23
3	C	218	TYR	N-CA-C	5.25	116.69	110.97
1	A	1186	SER	N-CA-C	-5.24	106.84	113.18
2	B	379	ASP	N-CA-C	-5.22	101.18	109.59
2	B	31	THR	N-CA-C	5.21	118.75	111.30
1	A	1191	THR	CA-C-N	5.17	125.15	120.03
1	A	1191	THR	C-N-CA	5.17	125.15	120.03
2	B	166	LYS	N-CA-C	5.17	119.58	113.28
3	C	15	ILE	N-CA-C	-5.14	105.58	110.42
1	A	800	SER	N-CA-C	5.13	116.60	108.96
1	A	715	ASN	N-CA-C	-5.12	104.33	110.88
3	C	51	ALA	N-CA-C	5.11	117.25	111.02
1	A	260	ARG	N-CA-C	-5.08	104.26	110.61
2	B	170	SER	N-CA-C	-5.04	106.91	113.16

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	9869	0	9527	299	0
2	B	4050	0	3973	70	0
3	C	1719	0	1764	49	0
4	A	94	0	42	8	0
5	A	1	0	0	0	0
6	A	8	0	0	2	0
6	B	24	0	0	0	0
7	B	7	0	0	0	0
8	B	18	0	10	0	0
9	C	86	0	60	1	0
10	C	30	0	36	1	0
11	C	12	0	1	0	0
12	A	23	0	0	0	0
12	B	29	0	0	0	0
12	C	2	0	0	0	0
All	All	15972	0	15413	410	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 13.

All (410) 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	1.62	0.81
1:A:578:VAL:HG23	1:A:579:GLY:H	1.46	0.80
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.64	0.78
1:A:1086:LEU:HD12	1:A:1224:VAL:HG21	1.67	0.77
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.68	0.75
1:A:1012:TRP:HB3	1:A:1022:TYR:OH	1.86	0.73
1:A:366:GLN:HG3	1:A:373:LYS:NZ	2.04	0.73
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:LEU:N	3:C:81:LEU:HD23	2.03	0.72
1:A:471:THR:HG23	1:A:476:LEU:HD11	1.70	0.72
1:A:387:ASN:ND2	1:A:405:ARG:HB2	2.05	0.72
1:A:378:ASN:HD21	1:A:382:GLU:HB2	1.54	0.71
1:A:225:PRO:HB2	1:A:551:ASP:OD1	1.91	0.70
1:A:371:GLU:N	1:A:371:GLU:OE1	2.25	0.69
1:A:313:MET:HE1	1:A:560:MET:HE3	1.74	0.69
1:A:366:GLN:HG3	1:A:373:LYS:HZ2	1.57	0.69
3:C:95:GLY:O	3:C:99:VAL:HG23	1.93	0.69
1:A:677:MET:HE2	1:A:682:TYR:HA	1.73	0.68
1:A:552:MET:HE3	1:A:1056:GLU:OE1	1.94	0.68
1:A:582:LYS:HB2	1:A:801:ASP:CG	2.18	0.68
1:A:52:ASN:CG	1:A:191:ILE:HG13	2.19	0.67
2:B:91:ASN:HB3	2:B:94:LEU:HB2	1.76	0.67
1:A:299:GLN:NE2	1:A:1158:MET:HE2	2.10	0.66
1:A:272:TYR:HB3	2:B:412:MET:HE3	1.78	0.65
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.79	0.64
2:B:157:LYS:NZ	2:B:157:LYS:HB3	2.12	0.64
3:C:6:MET:O	3:C:10:ASP:HB2	1.98	0.64
1:A:196:MET:CE	1:A:799:THR:HG23	2.29	0.63
1:A:1069:SER:O	1:A:1139:ASN:HB2	1.99	0.63
1:A:432:PRO:HD3	1:A:632:MET:HE2	1.79	0.63
1:A:110:TYR:HD1	1:A:818:GLU:HG3	1.64	0.62
1:A:772:ASP:C	1:A:788:THR:HG22	2.24	0.62
1:A:578:VAL:HG23	1:A:579:GLY:N	2.15	0.62
1:A:774:ARG:HH11	4:A:1800:MD1:H3'	1.64	0.61
1:A:1098:HIS:CE1	4:A:1800:MD1:S12	2.93	0.61
2:B:94:LEU:HD12	2:B:95:PRO:HD2	1.82	0.61
2:B:228:PRO:HB2	2:B:347:TYR:CD2	2.35	0.61
1:A:93:PRO:HG2	1:A:94:ARG:HD3	1.83	0.61
1:A:360:LEU:C	1:A:463:ALA:HB2	2.26	0.61
1:A:1163:HIS:HD2	1:A:1184:HIS:NE2	1.98	0.61
1:A:168:LEU:HD23	1:A:168:LEU:O	2.01	0.61
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.82	0.60
3:C:12:TYR:N	3:C:13:PRO:HD2	2.16	0.60
1:A:25:LEU:HD11	3:C:220:LEU:HD22	1.84	0.60
1:A:401:ASN:OD1	1:A:403:GLU:HG3	2.01	0.60
1:A:584:ARG:HD3	1:A:1006:ILE:HD13	1.84	0.60
1:A:272:TYR:HB3	2:B:412:MET:CE	2.32	0.60
1:A:508:GLU:OE1	1:A:515:ARG:HD2	2.00	0.60
3:C:159:LEU:HD21	3:C:180:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ALA:O	1:A:898:ARG:HG3	2.02	0.59
1:A:247:SER:C	1:A:275:THR:HG23	2.27	0.59
1:A:1059:LEU:HD23	1:A:1059:LEU:H	1.67	0.59
1:A:1084:LYS:HB2	1:A:1127:LEU:HD21	1.84	0.59
1:A:384:VAL:HG22	1:A:385:ALA:N	2.17	0.59
1:A:1037:THR:HA	1:A:1203:HIS:HB3	1.83	0.59
1:A:27:THR:HG22	1:A:28:ASN:N	2.17	0.59
1:A:741:LYS:HB3	1:A:745:GLN:HB2	1.82	0.59
1:A:5:ASP:OD2	2:B:489:THR:HG23	2.02	0.59
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.84	0.59
1:A:366:GLN:O	1:A:370:PRO:HB3	2.02	0.59
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.68	0.59
1:A:3:PHE:CE1	10:C:309:AGA:H161	2.39	0.58
1:A:361:VAL:HA	1:A:463:ALA:HB2	1.85	0.58
1:A:360:LEU:N	1:A:360:LEU:HD22	2.19	0.58
1:A:490:VAL:O	1:A:500:LYS:HE2	2.03	0.58
1:A:107:ARG:HD2	1:A:773:PHE:O	2.04	0.58
2:B:220:TRP:O	2:B:221:ARG:NH1	2.36	0.58
1:A:684:VAL:HG13	1:A:876:LEU:HD22	1.86	0.58
1:A:110:TYR:CD1	1:A:818:GLU:HG3	2.38	0.58
1:A:498:ASP:OD1	1:A:500:LYS:HG2	2.02	0.58
1:A:353:ARG:CZ	1:A:864:LEU:HD12	2.34	0.57
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.86	0.57
3:C:204:ILE:HD12	3:C:205:HIS:N	2.18	0.57
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.04	0.57
3:C:109:LEU:HD13	3:C:130:LEU:HD23	1.85	0.57
1:A:365:GLY:HA3	1:A:408:LYS:HG3	1.85	0.57
1:A:643:ILE:O	1:A:647:VAL:HG23	2.03	0.57
1:A:196:MET:HE1	1:A:799:THR:HG23	1.87	0.57
1:A:336:MET:HA	1:A:473:VAL:HB	1.86	0.57
1:A:219:TRP:HB2	1:A:607:SER:HB2	1.87	0.57
1:A:225:PRO:O	1:A:228:PRO:HD2	2.05	0.57
1:A:338:MET:HE2	1:A:374:THR:OG1	2.05	0.57
1:A:859:GLU:HG3	1:A:860:LEU:HD12	1.86	0.57
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.87	0.56
1:A:61:ILE:N	1:A:61:ILE:HD12	2.19	0.56
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.53	0.56
1:A:471:THR:CG2	1:A:476:LEU:HD11	2.34	0.56
2:B:40:TRP:O	2:B:41:PHE:C	2.48	0.56
4:A:1800:MD1:H7	4:A:1800:MD1:C11	2.36	0.56
1:A:1098:HIS:CE1	4:A:2800:MD1:S13	2.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HD13	1:A:216:PHE:CE1	2.41	0.55
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.41	0.55
1:A:345:ARG:HB2	1:A:348:TYR:O	2.06	0.55
1:A:487:LEU:HD12	1:A:487:LEU:N	2.20	0.55
1:A:646:ASN:O	1:A:650:GLU:HG3	2.06	0.55
1:A:677:MET:HE2	1:A:682:TYR:CA	2.36	0.55
1:A:1056:GLU:HG3	1:A:1195:THR:HG21	1.89	0.55
3:C:67:PHE:CE2	3:C:71:LEU:HD12	2.41	0.55
2:B:269:TYR:CG	2:B:333:MET:HE1	2.42	0.55
1:A:806:ILE:HG23	1:A:806:ILE:O	2.06	0.54
1:A:860:LEU:HD12	1:A:860:LEU:N	2.22	0.54
1:A:931:ASN:O	1:A:932:TYR:HB2	2.07	0.54
3:C:206:ILE:HD11	9:C:806:HEM:HBC2	1.88	0.54
3:C:83:ILE:HG23	3:C:84:GLU:N	2.22	0.54
1:A:873:GLU:O	1:A:874:CYS:HB3	2.07	0.54
1:A:634:ASP:HB3	1:A:637:ARG:HD3	1.90	0.54
3:C:198:PHE:HB3	3:C:199:PRO:CD	2.37	0.54
3:C:62:ILE:HG23	3:C:66:HIS:CE1	2.43	0.54
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.42	0.54
1:A:489:ASP:HB3	1:A:492:CYS:HB2	1.89	0.54
1:A:453:HIS:HA	1:A:489:ASP:OD1	2.08	0.54
1:A:460:LEU:HD12	1:A:470:VAL:HG11	1.89	0.54
2:B:465:LEU:O	2:B:467:ARG:HG3	2.08	0.54
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.72	0.53
1:A:240:SER:HB3	1:A:802:MET:HE3	1.90	0.53
3:C:119:ARG:O	3:C:122:THR:HG22	2.07	0.53
3:C:198:PHE:CE1	3:C:203:LEU:HB3	2.43	0.53
1:A:856:SER:O	1:A:859:GLU:HG2	2.07	0.53
1:A:146:LYS:O	1:A:150:GLN:HG3	2.08	0.53
1:A:335:ASP:O	1:A:338:MET:HB2	2.08	0.53
1:A:1098:HIS:C	1:A:1164:ALA:CB	2.82	0.53
2:B:152:PHE:CD2	2:B:170:SER:HB3	2.44	0.53
1:A:168:LEU:HD23	1:A:168:LEU:C	2.34	0.53
1:A:936:GLU:HG2	1:A:937:GLY:N	2.23	0.53
1:A:1107:MET:HA	1:A:1107:MET:HE2	1.89	0.53
1:A:351:ALA:HB1	1:A:1045:TYR:OH	2.09	0.53
1:A:170:ALA:O	1:A:174:VAL:HG23	2.09	0.53
1:A:687:LEU:HD23	1:A:692:ILE:O	2.09	0.53
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.09	0.52
1:A:191:ILE:HG23	1:A:580:GLN:O	2.09	0.52
1:A:225:PRO:C	1:A:228:PRO:HD2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:HIS:C	1:A:1164:ALA:HB3	2.34	0.52
1:A:419:LEU:HD11	1:A:471:THR:HA	1.91	0.52
1:A:432:PRO:HD3	1:A:632:MET:CE	2.38	0.52
1:A:1101:TYR:HB3	1:A:1107:MET:HG3	1.91	0.52
2:B:19:CYS:O	2:B:20:HIS:HB2	2.08	0.52
2:B:292:LEU:HD11	2:B:348:ARG:HG2	1.90	0.52
1:A:601:PRO:HG3	1:A:850:LEU:HD22	1.92	0.52
1:A:662:GLY:HA2	1:A:704:ASN:ND2	2.25	0.52
3:C:20:PHE:CD2	3:C:21:LEU:HD23	2.45	0.52
1:A:190:PRO:HD2	1:A:713:ARG:O	2.08	0.52
3:C:198:PHE:HB3	3:C:199:PRO:HD3	1.91	0.52
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.90	0.52
1:A:447:LEU:O	1:A:448:GLU:HG2	2.08	0.52
1:A:626:GLU:HA	1:A:629:LEU:HD23	1.92	0.52
1:A:876:LEU:C	1:A:876:LEU:HD23	2.34	0.52
1:A:1230:ILE:N	1:A:1230:ILE:HD12	2.24	0.52
1:A:707:ARG:C	1:A:708:ASN:HD22	2.18	0.52
1:A:678:ASN:HB2	1:A:679:PRO:HD2	1.92	0.52
1:A:119:LYS:O	1:A:123:GLU:HG3	2.10	0.51
1:A:724:HIS:NE2	1:A:1167:ARG:NH1	2.57	0.51
3:C:70:MET:O	3:C:71:LEU:HD23	2.09	0.51
1:A:239:GLU:HG2	1:A:1022:TYR:HB3	1.92	0.51
1:A:360:LEU:HD22	1:A:360:LEU:H	1.75	0.51
1:A:387:ASN:HD22	1:A:405:ARG:HB2	1.72	0.51
3:C:11:ILE:C	3:C:13:PRO:HD2	2.35	0.51
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.91	0.51
2:B:220:TRP:C	2:B:221:ARG:HG3	2.35	0.51
1:A:902:ILE:HG22	1:A:924:MET:HE1	1.93	0.51
2:B:12:ASN:HA	2:B:356:VAL:HB	1.93	0.51
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.76	0.51
1:A:991:ASP:CG	1:A:991:ASP:O	2.54	0.51
1:A:1168:ILE:HG13	1:A:1169:VAL:HG23	1.92	0.51
1:A:445:VAL:HG23	1:A:510:ILE:HD11	1.93	0.51
1:A:1088:PHE:HB2	1:A:1222:VAL:HG22	1.93	0.51
3:C:56:HIS:HA	3:C:59:ILE:HG22	1.92	0.51
1:A:517:GLN:HA	1:A:517:GLN:NE2	2.26	0.50
2:B:94:LEU:HD22	2:B:221:ARG:HD3	1.93	0.50
2:B:339:LEU:HD11	2:B:443:MET:HE3	1.93	0.50
2:B:168:MET:HE2	2:B:169:TYR:CE2	2.45	0.50
1:A:69:THR:HG22	1:A:70:TRP:HE3	1.77	0.50
1:A:582:LYS:HD3	1:A:801:ASP:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:TYR:CD1	2:B:333:MET:HE1	2.46	0.50
2:B:57:GLU:OE2	2:B:344:HIS:NE2	2.41	0.50
1:A:191:ILE:O	1:A:194:MET:HG2	2.11	0.50
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.47	0.50
2:B:160:ASN:OD1	2:B:393:LEU:HD13	2.11	0.50
1:A:313:MET:CE	1:A:560:MET:HE3	2.40	0.50
1:A:361:VAL:HA	1:A:463:ALA:CB	2.41	0.50
1:A:906:MET:CE	1:A:911:ASN:HB2	2.42	0.50
2:B:275:TYR:HB2	2:B:299:VAL:HG12	1.94	0.50
2:B:306:PRO:O	2:B:310:GLU:HG3	2.12	0.50
1:A:1059:LEU:HD23	1:A:1059:LEU:N	2.27	0.50
2:B:228:PRO:HG2	2:B:229:TYR:CD1	2.47	0.49
1:A:551:ASP:OD2	1:A:1196:HIS:NE2	2.38	0.49
1:A:45:VAL:HG21	1:A:812:ALA:HA	1.94	0.49
3:C:177:LEU:O	3:C:178:ASP:C	2.55	0.49
3:C:183:ILE:HG23	3:C:184:PHE:N	2.27	0.49
3:C:56:HIS:O	3:C:59:ILE:HG22	2.13	0.49
1:A:513:VAL:O	1:A:514:SER:C	2.53	0.49
2:B:400:LYS:HB3	2:B:401:PRO:CD	2.43	0.49
2:B:415:TYR:CE2	2:B:437:GLU:HG2	2.47	0.49
1:A:705:HIS:CD2	1:A:764:LYS:HB3	2.48	0.49
1:A:729:LYS:HB2	1:A:736:HIS:CG	2.48	0.49
3:C:83:ILE:HG23	3:C:84:GLU:H	1.78	0.49
1:A:157:PHE:CZ	1:A:785:ILE:HD11	2.48	0.48
1:A:1155:PRO:HG2	1:A:1158:MET:HE3	1.95	0.48
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.48	0.48
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.38	0.48
3:C:13:PRO:HB3	3:C:192:MET:SD	2.52	0.48
1:A:1206:TYR:CG	1:A:1207:GLY:N	2.82	0.48
1:A:28:ASN:HA	3:C:225:HIS:CD2	2.48	0.48
1:A:69:THR:HG22	1:A:70:TRP:CE3	2.49	0.48
1:A:336:MET:HE2	1:A:474:TYR:HA	1.96	0.48
1:A:263:ASP:OD2	1:A:802:MET:HG3	2.13	0.48
1:A:1046:GLN:HG3	1:A:1051:MET:HE2	1.96	0.48
1:A:1155:PRO:CG	1:A:1158:MET:HE3	2.44	0.48
3:C:2:GLN:O	3:C:6:MET:HG3	2.12	0.48
1:A:379:THR:HG21	1:A:414:GLU:CD	2.39	0.48
1:A:1167:ARG:HB2	1:A:1183:ILE:CG2	2.44	0.48
1:A:261:THR:HG22	2:B:264:VAL:HG11	1.95	0.47
1:A:401:ASN:CG	1:A:403:GLU:HG3	2.39	0.47
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:N	1:A:476:LEU:HD12	2.29	0.47
1:A:308:ALA:O	1:A:311:HIS:HB3	2.14	0.47
1:A:761:LEU:O	1:A:764:LYS:HE3	2.14	0.47
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.49	0.47
3:C:208:SER:O	3:C:209:VAL:C	2.58	0.47
2:B:157:LYS:HB3	2:B:157:LYS:HZ3	1.79	0.47
3:C:89:MET:O	3:C:93:ALA:N	2.47	0.47
1:A:55:GLY:HA3	6:A:1801:SF4:S3	2.54	0.47
1:A:372:TRP:NE1	1:A:860:LEU:HB3	2.30	0.47
1:A:487:LEU:N	1:A:487:LEU:CD1	2.77	0.47
4:A:1800:MD1:H7	4:A:1800:MD1:H11	1.95	0.47
2:B:183:LEU:HD23	2:B:183:LEU:N	2.30	0.47
1:A:419:LEU:CD1	1:A:471:THR:HA	2.44	0.47
1:A:372:TRP:CE2	1:A:863:PRO:HB3	2.50	0.47
1:A:214:LEU:HB3	1:A:607:SER:OG	2.15	0.46
1:A:515:ARG:HG2	1:A:516:SER:N	2.29	0.46
2:B:370:GLU:OE2	2:B:370:GLU:HA	2.14	0.46
1:A:85:PRO:HG2	1:A:266:PHE:CE2	2.50	0.46
1:A:384:VAL:CG2	1:A:385:ALA:N	2.78	0.46
1:A:61:ILE:N	1:A:61:ILE:CD1	2.78	0.46
1:A:323:SER:HB3	1:A:326:PHE:HB2	1.98	0.46
1:A:405:ARG:HH12	1:A:412:GLU:HG3	1.80	0.46
1:A:517:GLN:HA	1:A:517:GLN:HE21	1.80	0.46
1:A:677:MET:HG3	1:A:682:TYR:HB2	1.97	0.46
1:A:220:TYR:CE2	4:A:1800:MD1:H101	2.51	0.46
1:A:473:VAL:HG13	1:A:1045:TYR:HB2	1.96	0.46
1:A:679:PRO:HB2	1:A:847:ILE:HD11	1.96	0.46
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.51	0.46
2:B:508:THR:O	2:B:509:GLU:HB3	2.15	0.46
1:A:173:ASN:O	1:A:177:ILE:HG13	2.15	0.46
1:A:1097:ILE:O	1:A:1098:HIS:HB2	2.16	0.46
1:A:215:SER:OG	1:A:606:ASN:HA	2.16	0.46
1:A:795:ASP:HA	1:A:809:LEU:O	2.16	0.46
1:A:931:ASN:ND2	1:A:950:ASP:HB3	2.31	0.46
2:B:143:ASN:ND2	2:B:146:ASP:HB2	2.30	0.46
1:A:232:GLY:HA2	1:A:1210:TYR:OH	2.17	0.46
1:A:1051:MET:HG2	1:A:1198:ILE:CD1	2.46	0.46
1:A:217:TYR:CE1	1:A:222:ASP:HB3	2.51	0.45
1:A:1041:ARG:HG2	1:A:1041:ARG:HH21	1.80	0.45
2:B:492:ASN:N	2:B:492:ASN:HD22	2.14	0.45
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:HIS:HE1	4:A:2800:MD1:S13	2.39	0.45
2:B:104:PHE:HB3	2:B:135:MET:HE1	1.98	0.45
1:A:120:MET:O	1:A:138:ILE:HD11	2.16	0.45
1:A:261:THR:HB	1:A:262:PRO:CD	2.46	0.45
1:A:472:THR:O	1:A:476:LEU:HD13	2.16	0.45
1:A:581:GLU:CD	1:A:581:GLU:C	2.85	0.45
1:A:651:ARG:NH1	1:A:870:LYS:HD3	2.32	0.45
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.51	0.45
2:B:311:GLN:NE2	2:B:314:LYS:HE2	2.32	0.45
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.45
3:C:211:VAL:HG23	3:C:212:GLU:N	2.32	0.45
1:A:313:MET:HE1	1:A:560:MET:CE	2.46	0.45
1:A:583:LEU:C	1:A:583:LEU:HD23	2.42	0.45
1:A:641:HIS:ND1	1:A:642:LEU:N	2.65	0.45
1:A:928:ARG:CG	1:A:943:PRO:HG3	2.41	0.45
1:A:27:THR:CG2	1:A:28:ASN:N	2.79	0.44
1:A:91:GLY:HA2	6:A:1801:SF4:S4	2.57	0.44
1:A:644:ASP:OD1	1:A:752:GLU:HG2	2.17	0.44
1:A:774:ARG:HH11	4:A:1800:MD1:C3'	2.29	0.44
3:C:15:ILE:O	3:C:19:VAL:HG23	2.17	0.44
1:A:1092:HIS:HA	1:A:1163:HIS:HB3	1.98	0.44
2:B:395:THR:HG21	2:B:401:PRO:CG	2.44	0.44
3:C:188:LEU:O	3:C:192:MET:HE2	2.18	0.44
3:C:198:PHE:HE2	3:C:207:TRP:NE1	2.15	0.44
1:A:90:ARG:HG2	1:A:90:ARG:HH11	1.81	0.44
2:B:470:PHE:HB3	2:B:471:PRO:CD	2.47	0.44
1:A:299:GLN:CD	1:A:1158:MET:HE2	2.42	0.44
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.31	0.44
1:A:698:GLN:HG2	1:A:755:ASP:OD1	2.18	0.44
2:B:101:TYR:CD2	2:B:142:PRO:HD3	2.53	0.44
1:A:6:ARG:HG2	1:A:6:ARG:HH21	1.83	0.44
1:A:139:ILE:HD12	1:A:139:ILE:HA	1.81	0.44
1:A:182:PRO:HD2	1:A:665:PRO:HG2	2.00	0.44
1:A:316:GLU:HG3	1:A:496:TYR:OH	2.18	0.44
1:A:81:ARG:NH2	1:A:84:LEU:HD11	2.32	0.43
1:A:582:LYS:HB2	1:A:801:ASP:OD2	2.18	0.43
1:A:611:PHE:O	1:A:615:SER:HB3	2.19	0.43
1:A:364:LEU:HD13	1:A:385:ALA:HB2	2.00	0.43
1:A:688:LYS:HE3	1:A:876:LEU:HB3	2.00	0.43
2:B:462:HIS:C	2:B:464:GLU:H	2.26	0.43
1:A:220:TYR:CE1	1:A:720:SER:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LEU:HD13	1:A:629:LEU:HA	1.86	0.43
1:A:743:LEU:HD13	1:A:743:LEU:H	1.83	0.43
2:B:217:CYS:O	2:B:240:LYS:NZ	2.51	0.43
3:C:87:GLN:NE2	3:C:151:MET:HA	2.33	0.43
1:A:914:LYS:O	1:A:914:LYS:HG2	2.18	0.43
1:A:1132:ASN:ND2	2:B:137:LYS:HE3	2.33	0.43
2:B:195:THR:O	2:B:197:PRO:HD3	2.19	0.43
3:C:115:SER:HA	3:C:116:PRO:HD2	1.83	0.43
1:A:353:ARG:NE	1:A:864:LEU:HD12	2.33	0.43
1:A:362:ASP:O	1:A:363:ALA:HB3	2.18	0.43
1:A:393:ARG:NH1	1:A:855:ASP:HA	2.33	0.43
1:A:403:GLU:HG2	1:A:1032:LEU:HD23	1.99	0.43
1:A:199:TYR:CE1	1:A:589:TRP:HZ2	2.36	0.43
1:A:1144:LEU:HD22	1:A:1184:HIS:HA	2.00	0.43
3:C:149:GLN:C	3:C:150:HIS:CD2	2.96	0.43
1:A:199:TYR:CD1	1:A:589:TRP:HZ2	2.36	0.43
1:A:393:ARG:HH12	1:A:855:ASP:HA	1.84	0.43
1:A:548:TYR:HE2	1:A:1191:THR:HG22	1.82	0.43
2:B:400:LYS:HB3	2:B:401:PRO:HD3	2.01	0.43
2:B:176:PHE:CD1	2:B:176:PHE:C	2.96	0.43
1:A:499:VAL:O	1:A:499:VAL:HG12	2.19	0.43
1:A:532:THR:OG1	1:A:535:ARG:HB2	2.19	0.43
1:A:906:MET:HE3	1:A:911:ASN:HB2	2.00	0.43
1:A:1041:ARG:HG2	1:A:1041:ARG:NH2	2.33	0.43
2:B:157:LYS:NZ	2:B:157:LYS:CB	2.81	0.43
1:A:590:GLN:N	1:A:591:PRO:HD2	2.34	0.42
1:A:611:PHE:O	1:A:615:SER:CB	2.67	0.42
1:A:1233:LEU:HB3	2:B:120:SER:OG	2.19	0.42
2:B:263:CYS:SG	2:B:267:ILE:HG12	2.59	0.42
1:A:220:TYR:CE1	1:A:720:SER:CB	3.02	0.42
1:A:626:GLU:O	1:A:629:LEU:HB2	2.19	0.42
2:B:224:ILE:HD11	2:B:234:PHE:HB2	2.01	0.42
1:A:161:SER:O	1:A:165:VAL:HG22	2.18	0.42
1:A:529:ALA:CB	1:A:564:CYS:HB3	2.49	0.42
2:B:156:ALA:HB1	2:B:166:LYS:HD2	2.00	0.42
1:A:661:LEU:C	1:A:663:THR:H	2.27	0.42
2:B:463:ARG:O	2:B:467:ARG:HD3	2.19	0.42
1:A:167:GLU:HG3	1:A:832:LYS:CE	2.50	0.42
1:A:683:THR:CG2	1:A:885:ILE:HD13	2.49	0.42
2:B:36:VAL:HG13	2:B:235:ASN:ND2	2.34	0.42
1:A:423:GLN:CD	1:A:423:GLN:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:TYR:CE1	1:A:1192:PRO:HG3	2.55	0.42
1:A:852:ILE:HD12	1:A:852:ILE:H	1.83	0.42
1:A:331:ARG:NH1	1:A:415:LEU:O	2.53	0.42
1:A:459:ARG:HH11	1:A:459:ARG:HG3	1.85	0.42
1:A:552:MET:HE2	1:A:552:MET:HA	2.01	0.42
2:B:188:LEU:HB2	2:B:350:LEU:HB2	2.02	0.42
1:A:192:PRO:HB2	1:A:583:LEU:HD12	2.01	0.42
1:A:329:TYR:CZ	1:A:565:GLY:HA2	2.55	0.42
1:A:658:ALA:HA	1:A:659:PRO:C	2.45	0.42
2:B:311:GLN:HE21	2:B:315:ASP:CG	2.28	0.42
3:C:18:ALA:O	3:C:22:ILE:HG22	2.19	0.42
2:B:231:LYS:HE2	2:B:231:LYS:HA	2.01	0.41
2:B:295:ARG:CG	2:B:295:ARG:HH21	2.32	0.41
3:C:12:TYR:N	3:C:13:PRO:CD	2.82	0.41
1:A:192:PRO:HG2	1:A:583:LEU:HD12	2.02	0.41
1:A:729:LYS:HB2	1:A:736:HIS:CD2	2.55	0.41
1:A:774:ARG:NH2	1:A:1103:ASP:OD1	2.52	0.41
1:A:1232:TRP:O	1:A:1233:LEU:HB2	2.19	0.41
2:B:85:LEU:HD13	3:C:213:TYR:HD1	1.85	0.41
2:B:224:ILE:CD1	2:B:234:PHE:HB2	2.49	0.41
3:C:88:LYS:O	3:C:92:PHE:HD1	2.02	0.41
1:A:389:SER:C	1:A:391:GLY:N	2.79	0.41
2:B:100:TYR:O	2:B:101:TYR:HB3	2.20	0.41
1:A:375:VAL:HG12	1:A:376:ALA:N	2.34	0.41
1:A:600:ARG:HA	1:A:601:PRO:HA	1.88	0.41
3:C:89:MET:O	3:C:93:ALA:HB3	2.19	0.41
1:A:336:MET:N	1:A:337:PRO:HD2	2.35	0.41
1:A:902:ILE:CG2	1:A:924:MET:HE1	2.50	0.41
1:A:167:GLU:HG3	1:A:832:LYS:HE2	2.03	0.41
1:A:532:THR:O	1:A:533:HIS:HB2	2.20	0.41
2:B:47:LYS:HA	2:B:48:PRO:C	2.46	0.41
2:B:408:ARG:O	2:B:411:ALA:HB3	2.21	0.41
1:A:695:ALA:HB1	1:A:704:ASN:HB3	2.02	0.41
1:A:808:PRO:HG3	1:A:1000:GLN:HA	2.01	0.41
1:A:1101:TYR:O	1:A:1104:ASN:HB3	2.20	0.41
1:A:1117:VAL:HG23	1:A:1146:ALA:HB3	2.02	0.41
3:C:36:ARG:HG2	3:C:38:ALA:H	1.85	0.41
1:A:705:HIS:HD2	1:A:764:LYS:HB3	1.84	0.41
1:A:1046:GLN:HG3	1:A:1051:MET:CE	2.51	0.41
3:C:149:GLN:HB2	3:C:150:HIS:HD2	1.86	0.41
1:A:52:ASN:ND2	1:A:191:ILE:HG13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HG2	1:A:90:ARG:NH1	2.35	0.41
1:A:368:ASN:O	1:A:373:LYS:HE3	2.21	0.41
2:B:13:LEU:HB2	2:B:356:VAL:O	2.21	0.41
2:B:372:GLY:HA3	2:B:379:ASP:OD1	2.21	0.41
3:C:81:LEU:N	3:C:81:LEU:CD2	2.75	0.41
1:A:244:TYR:OH	2:B:448:ALA:HB1	2.21	0.41
1:A:380:ASN:C	1:A:382:GLU:H	2.29	0.41
1:A:578:VAL:CG2	1:A:579:GLY:N	2.81	0.41
3:C:162:TRP:CZ3	3:C:188:LEU:HD13	2.56	0.41
1:A:87:HIS:O	1:A:88:GLU:C	2.64	0.40
1:A:111:PRO:HA	1:A:787:PRO:HD3	2.03	0.40
1:A:237:VAL:HG11	1:A:576:HIS:H	1.86	0.40
1:A:920:THR:O	1:A:920:THR:HG23	2.20	0.40
1:A:604:HIS:HB3	1:A:1208:PHE:CD2	2.56	0.40
1:A:1096:GLY:HA2	1:A:1101:TYR:HB2	2.03	0.40
1:A:1144:LEU:CD2	1:A:1184:HIS:HA	2.51	0.40
2:B:97:ILE:HG23	2:B:98:ASP:N	2.36	0.40
1:A:38:ARG:HD2	1:A:38:ARG:O	2.21	0.40
1:A:389:SER:C	1:A:391:GLY:H	2.30	0.40
1:A:397:LYS:HE3	1:A:977:PHE:CE1	2.56	0.40
1:A:445:VAL:HG23	1:A:510:ILE:CD1	2.50	0.40
1:A:583:LEU:HD23	1:A:585:PRO:HD2	2.03	0.40
1:A:995:ARG:HA	1:A:995:ARG:HD3	1.89	0.40
1:A:1173:GLY:HA3	1:A:1233:LEU:HD22	2.01	0.40
1:A:1234:ASP:OD1	1:A:1236:GLU:HB2	2.21	0.40
2:B:152:PHE:CE2	2:B:170:SER:HB3	2.57	0.40
3:C:82:PRO:HG2	3:C:85:VAL:CG2	2.50	0.40
1:A:906:MET:HE1	1:A:911:ASN:HB2	2.04	0.40
1:A:1167:ARG:HG2	1:A:1167:ARG:O	2.21	0.40
2:B:113:THR:O	2:B:114:ALA:C	2.65	0.40
3:C:98:GLY:HA3	3:C:141:LEU:HD21	2.03	0.40
1:A:281:THR:O	1:A:296:ALA:HA	2.22	0.40
1:A:366:GLN:HG3	1:A:373:LYS:HZ3	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1242/1246 (100%)	1127 (91%)	97 (8%)	18 (1%)	9	17
2	B	507/512 (99%)	483 (95%)	23 (4%)	1 (0%)	43	63
3	C	213/225 (95%)	193 (91%)	18 (8%)	2 (1%)	14	27
All	All	1962/1983 (99%)	1803 (92%)	138 (7%)	21 (1%)	11	22

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	1166	GLU
1	A	195	SER
1	A	320	ASP
1	A	501	ALA
1	A	586	GLN
1	A	578	VAL
1	A	718	GLY
1	A	855	ASP
1	A	861	ALA
1	A	874	CYS
1	A	9	TYR
1	A	191	ILE
1	A	1036	ARG
2	B	101	TYR
1	A	224	PRO
1	A	721	GLY
3	C	180	VAL
1	A	390	ILE
1	A	808	PRO
3	C	210	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1039/1043 (100%)	1012 (97%)	27 (3%)	40	68
2	B	436/439 (99%)	425 (98%)	11 (2%)	42	69
3	C	178/185 (96%)	175 (98%)	3 (2%)	53	78
All	All	1653/1667 (99%)	1612 (98%)	41 (2%)	42	69

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	37	GLN
1	A	139	ILE
1	A	319	LEU
1	A	338	MET
1	A	402	LEU
1	A	452	LEU
1	A	461	GLN
1	A	487	LEU
1	A	514	SER
1	A	600	ARG
1	A	629	LEU
1	A	728	LEU
1	A	743	LEU
1	A	767	LEU
1	A	808	PRO
1	A	813	VAL
1	A	849	THR
1	A	926	LEU
1	A	936	GLU
1	A	944	MET
1	A	988	ASN
1	A	1044	LEU
1	A	1062	ARG
1	A	1110	LEU
1	A	1233	LEU

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Mol	Chain	Res	Type
1	A	1243	GLU
2	B	37	GLU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU
2	B	135	MET
2	B	161	PHE
2	B	183	LEU
2	B	244	CYS
2	B	295	ARG
2	B	358	PRO
2	B	492	ASN
3	C	81	LEU
3	C	129	ILE
3	C	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	37	GLN
1	A	87	HIS
1	A	173	ASN
1	A	234	GLN
1	A	245	ASN
1	A	258	GLN
1	A	311	HIS
1	A	366	GLN
1	A	369	ASN
1	A	453	HIS
1	A	461	GLN
1	A	480	ASN
1	A	517	GLN
1	A	590	GLN
1	A	599	GLN
1	A	646	ASN
1	A	678	ASN
1	A	704	ASN
1	A	708	ASN
1	A	921	GLN
1	A	942	GLN
1	A	1049	GLN

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Mol	Chain	Res	Type
1	A	1076	GLN
1	A	1082	GLN
1	A	1087	ASN
1	A	1098	HIS
1	A	1163	HIS
2	B	110	ASN
2	B	143	ASN
2	B	160	ASN
2	B	311	GLN
2	B	414	HIS
2	B	451	ASN
3	C	87	GLN
3	C	149	GLN
3	C	164	GLN
3	C	175	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FME	C	1	3	8,9,10	1.39	3 (37%)	8,9,11	1.73	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	-	6/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CA	-2.45	1.47	1.53
3	C	1	FME	CA-N	-2.17	1.43	1.46
3	C	1	FME	CB-CG	2.07	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	3.16	127.69	122.82
3	C	1	FME	CB-CA-N	2.40	114.89	110.52

There are no chirality outliers.

All (6) 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	O-C-CA-CB
3	C	1	FME	CA-CB-CG-SD
3	C	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MD1	A	2800	5	47,51,51	2.77	5 (10%)	56,78,78	1.43	5 (8%)
6	SF4	B	1803	2	0,12,12	-	-	-		
6	SF4	B	1804	2	0,12,12	-	-	-		
9	HEM	C	806	3	50,50,50	1.77	13 (26%)	67,82,82	0.93	4 (5%)
10	AGA	C	309	-	29,29,29	0.83	1 (3%)	32,35,35	1.57	3 (9%)
8	3PH	B	1806	-	17,17,47	0.97	1 (5%)	18,21,52	1.97	5 (27%)
11	PCI	C	808	-	12,12,12	9.74	11 (91%)	18,18,18	1.11	1 (5%)
7	F3S	B	1805	2	0,9,9	-	-	-		
6	SF4	B	1802	2	0,12,12	-	-	-		
9	HEM	C	807	3	50,50,50	1.84	17 (34%)	67,82,82	0.94	4 (5%)
4	MD1	A	1800	5	47,51,51	2.88	7 (14%)	56,78,78	1.34	4 (7%)
6	SF4	A	1801	1	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
4	MD1	A	2800	5	-	2/22/59/59	0/5/5/5
6	SF4	B	1803	2	-	-	0/6/5/5
6	SF4	B	1804	2	-	-	0/6/5/5
9	HEM	C	806	3	-	7/14/54/54	-
10	AGA	C	309	-	-	11/34/34/34	-
8	3PH	B	1806	-	1/1/3/4	5/18/18/49	-
11	PCI	C	808	-	-	-	0/1/1/1
9	HEM	C	807	3	-	8/14/54/54	-
6	SF4	B	1802	2	-	-	0/6/5/5
7	F3S	B	1805	2	-	-	0/3/3/3
4	MD1	A	1800	5	-	7/22/59/59	0/5/5/5
6	SF4	A	1801	1	-	-	0/6/5/5

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	MD1	C7-N8	17.57	1.50	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2800	MD1	C7-N8	16.21	1.48	1.28
11	C	808	PCI	C2-CL1	-15.56	1.40	1.72
11	C	808	PCI	C6-CL5	-14.93	1.41	1.72
11	C	808	PCI	C5-CL4	-14.28	1.42	1.72
11	C	808	PCI	C4-CL3	-13.98	1.43	1.72
11	C	808	PCI	C3-CL2	-13.78	1.43	1.72
4	A	2800	MD1	PA-O3B	-5.11	1.54	1.59
9	C	807	HEM	CAB-C3B	4.49	1.59	1.47
9	C	806	HEM	CAB-C3B	4.45	1.59	1.47
11	C	808	PCI	C5-C4	4.20	1.49	1.39
11	C	808	PCI	C4-C3	4.08	1.48	1.39
11	C	808	PCI	C6-C5	3.78	1.48	1.39
11	C	808	PCI	C3-C2	3.71	1.48	1.39
9	C	806	HEM	CAC-C3C	3.62	1.57	1.47
9	C	806	HEM	FE-NC	3.51	2.06	1.95
9	C	807	HEM	FE-NC	3.45	2.06	1.95
9	C	806	HEM	CMC-C2C	3.40	1.57	1.50
9	C	807	HEM	CAC-C3C	3.36	1.56	1.47
9	C	807	HEM	CMC-C2C	3.28	1.57	1.50
4	A	1800	MD1	C14-C13	3.21	1.54	1.51
11	C	808	PCI	C1-C2	3.19	1.44	1.39
4	A	1800	MD1	C16-C20	3.16	1.47	1.39
9	C	806	HEM	CMA-C3A	3.06	1.57	1.50
9	C	806	HEM	CMB-C2B	3.03	1.57	1.50
9	C	807	HEM	CMB-C2B	2.97	1.56	1.50
9	C	807	HEM	CMD-C2D	2.95	1.56	1.50
11	C	808	PCI	C1-C6	2.93	1.44	1.39
4	A	2800	MD1	C20-N8	2.91	1.41	1.36
9	C	806	HEM	CMD-C2D	2.84	1.56	1.50
9	C	807	HEM	FE-NB	2.83	2.03	1.94
4	A	1800	MD1	C4-N3	2.80	1.40	1.34
9	C	807	HEM	CMA-C3A	2.72	1.56	1.50
4	A	1800	MD1	C12-C13	2.69	1.42	1.34
9	C	807	HEM	CAD-C3D	2.60	1.58	1.51
9	C	807	HEM	CBA-CAA	2.55	1.60	1.51
4	A	1800	MD1	C20-N8	2.51	1.40	1.36
9	C	806	HEM	FE-NB	2.49	2.02	1.94
9	C	807	HEM	CAA-C2A	2.41	1.57	1.51
4	A	2800	MD1	C6-N1	2.39	1.43	1.38
9	C	807	HEM	CBA-CGA	2.38	1.56	1.50
10	C	309	AGA	C8-C7	2.35	1.57	1.50
9	C	806	HEM	O1D-CGD	2.24	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	806	HEM	CAD-C3D	2.24	1.57	1.51
4	A	1800	MD1	C15-N17	2.23	1.43	1.38
9	C	807	HEM	C1D-C2D	2.19	1.49	1.44
9	C	806	HEM	C4D-ND	-2.13	1.36	1.40
9	C	807	HEM	O1D-CGD	2.12	1.29	1.22
9	C	807	HEM	FE-ND	2.11	2.01	1.94
9	C	807	HEM	C4A-C3A	2.11	1.48	1.43
8	B	1806	3PH	C32-C31	2.09	1.56	1.50
9	C	806	HEM	C4D-C3D	2.07	1.48	1.45
9	C	806	HEM	C1B-C2B	2.04	1.48	1.44
9	C	807	HEM	C1B-C2B	2.03	1.48	1.44
4	A	2800	MD1	O11-C11	2.01	1.47	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	309	AGA	C14-C13-C12	5.93	135.43	113.69
4	A	1800	MD1	C17-N18-C20	5.72	122.12	114.20
4	A	2800	MD1	C17-N18-C20	5.65	122.03	114.20
10	C	309	AGA	C9-C8-C7	4.87	131.55	113.69
8	B	1806	3PH	C3-C2-C1	4.75	122.87	111.78
8	B	1806	3PH	C33-C32-C31	4.59	130.53	113.69
11	C	808	PCI	C6-C1-C2	3.70	121.74	117.78
8	B	1806	3PH	O21-C2-C3	3.53	121.01	108.34
4	A	2800	MD1	C2-N3-C4	3.42	118.18	112.30
4	A	1800	MD1	N17-C17-N18	-2.82	118.15	123.32
4	A	1800	MD1	O14-C15-C16	-2.73	120.67	127.26
9	C	807	HEM	CAD-C3D-C4D	-2.69	120.01	124.70
4	A	1800	MD1	O3A-C10-C11	-2.66	100.46	107.96
10	C	309	AGA	C5-O9-C12	2.60	124.01	117.80
9	C	806	HEM	CAD-C3D-C4D	-2.47	120.39	124.70
4	A	2800	MD1	O4'-C1'-N9	2.27	113.51	108.36
9	C	807	HEM	CAD-C3D-C2D	2.25	132.08	127.87
9	C	806	HEM	O1D-CGD-CBD	-2.22	116.05	123.09
9	C	806	HEM	O2D-CGD-O1D	2.19	128.97	123.33
8	B	1806	3PH	O21-C2-C1	2.16	116.11	108.34
4	A	2800	MD1	N1-C2-N3	-2.16	119.37	123.32
9	C	807	HEM	O1D-CGD-CBD	-2.10	116.44	123.09
4	A	2800	MD1	C1'-N9-C8	2.09	132.67	126.73
8	B	1806	3PH	O11-P-O12	2.01	111.88	106.44
9	C	807	HEM	O2D-CGD-O1D	2.01	128.49	123.33
9	C	806	HEM	CAD-C3D-C2D	2.00	131.62	127.87

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	1806	3PH	C2

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1800	MD1	C5'-O5'-PA-O3B
4	A	1800	MD1	C5'-O5'-PA-O2A
8	B	1806	3PH	O22-C21-O21-C2
9	C	806	HEM	C2C-C3C-CAC-CBC
9	C	806	HEM	C4C-C3C-CAC-CBC
9	C	807	HEM	C2C-C3C-CAC-CBC
9	C	807	HEM	C4C-C3C-CAC-CBC
10	C	309	AGA	O1-C1-C2-C3
10	C	309	AGA	C3-O5-P1-O3
10	C	309	AGA	C3-O5-P1-O6
8	B	1806	3PH	C32-C31-O31-C3
4	A	1800	MD1	O4'-C4'-C5'-O5'
8	B	1806	3PH	O32-C31-O31-C3
10	C	309	AGA	O2-C2-C3-O5
10	C	309	AGA	C1-C2-C3-O5
10	C	309	AGA	O1-C1-C2-O2
4	A	1800	MD1	C3'-C4'-C5'-O5'
10	C	309	AGA	C8-C7-O7-C6
10	C	309	AGA	C13-C14-C15-C16
10	C	309	AGA	O8-C7-O7-C6
10	C	309	AGA	C12-C13-C14-C15
8	B	1806	3PH	C1-C2-C3-O31
8	B	1806	3PH	O11-C1-C2-O21
9	C	807	HEM	C2B-C3B-CAB-CBB
4	A	1800	MD1	PA-O3B-PB-O2B
4	A	2800	MD1	PA-O3B-PB-O2B
4	A	1800	MD1	C5'-O5'-PA-O1A
9	C	806	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAA-CBA-CGA-O1A
9	C	807	HEM	CAD-CBD-CGD-O2D
9	C	806	HEM	CAA-CBA-CGA-O1A
9	C	807	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAD-CBD-CGD-O2D
10	C	309	AGA	O6-C4-C5-C6
9	C	807	HEM	C4B-C3B-CAB-CBB
9	C	806	HEM	CAD-CBD-CGD-O1D

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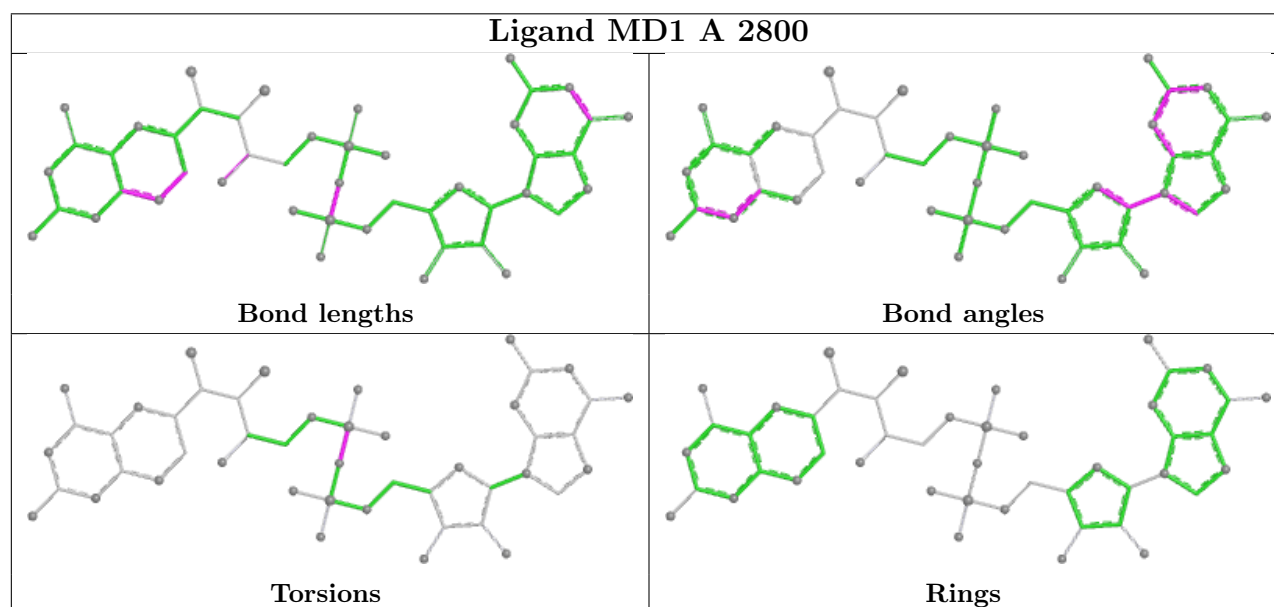
Mol	Chain	Res	Type	Atoms
9	C	806	HEM	C2B-C3B-CAB-CBB
4	A	1800	MD1	PA-O3B-PB-O1B
4	A	2800	MD1	PA-O3B-PB-O1B

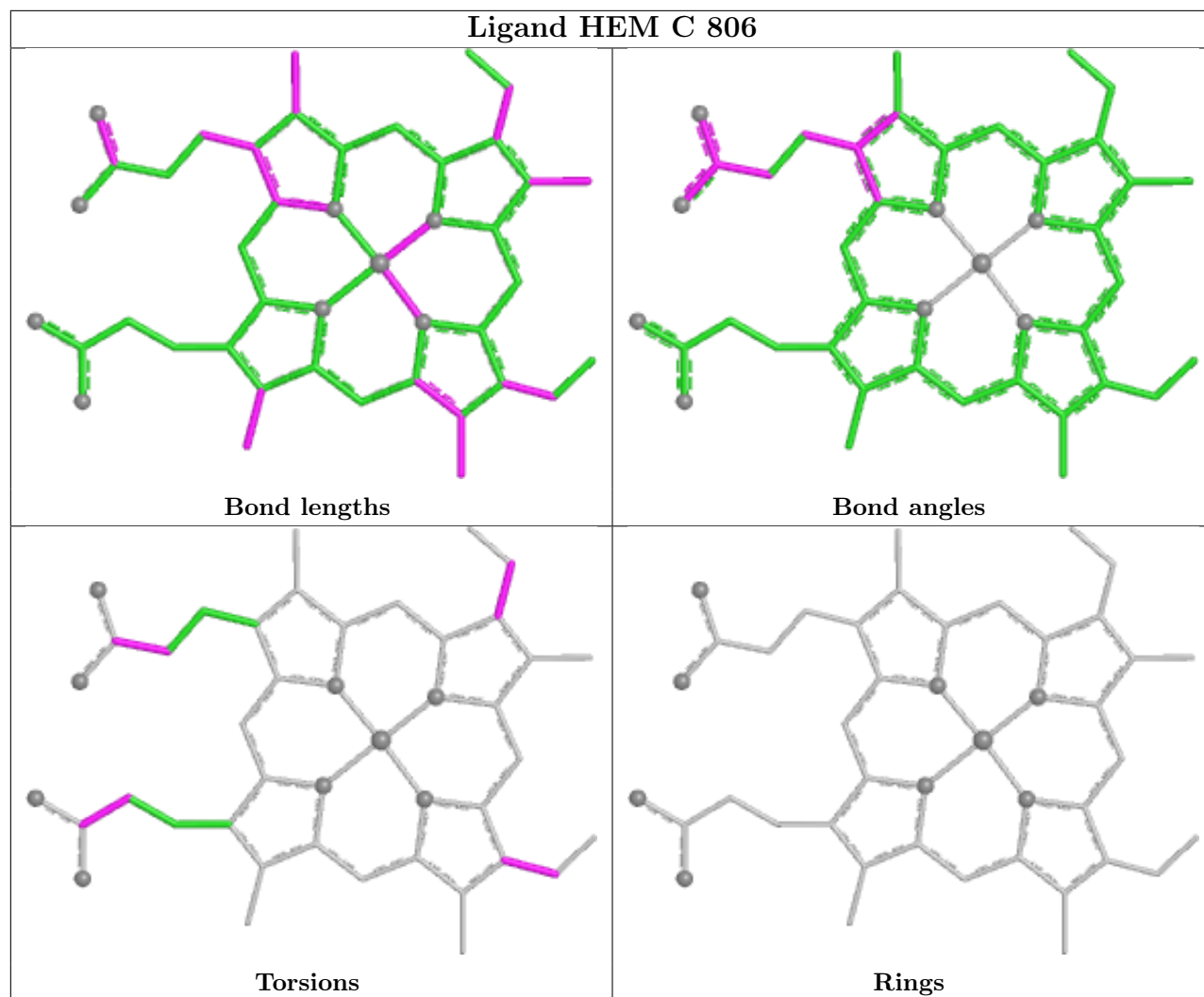
There are no ring outliers.

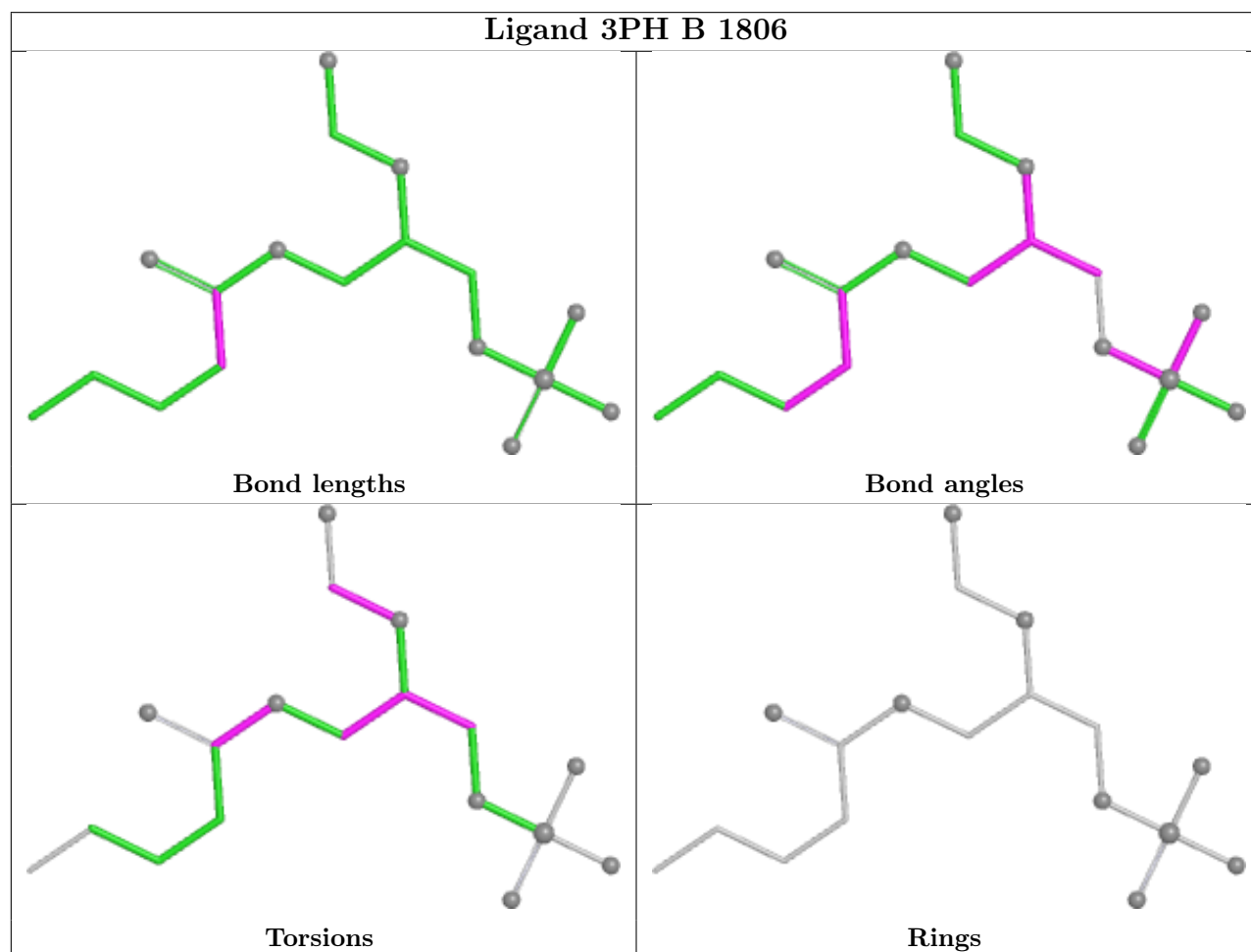
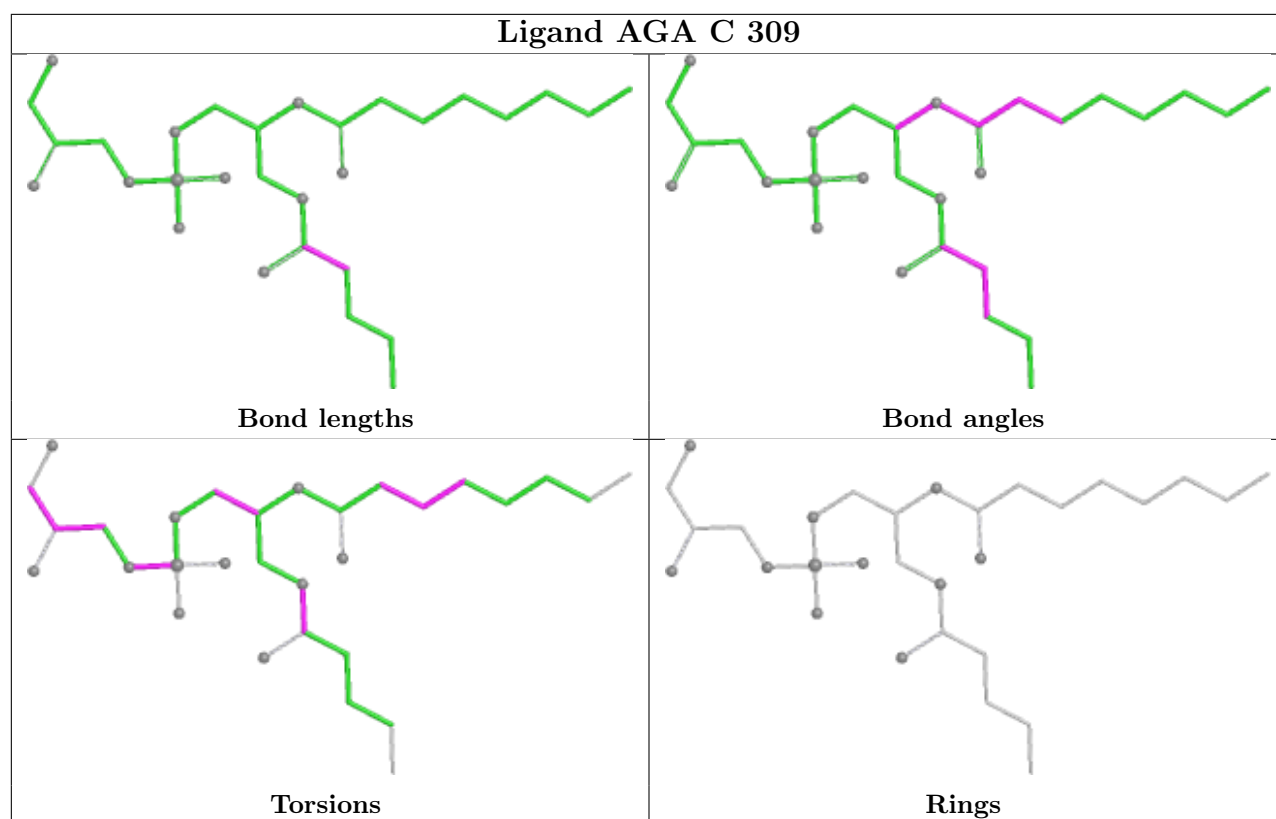
5 monomers are involved in 12 short contacts:

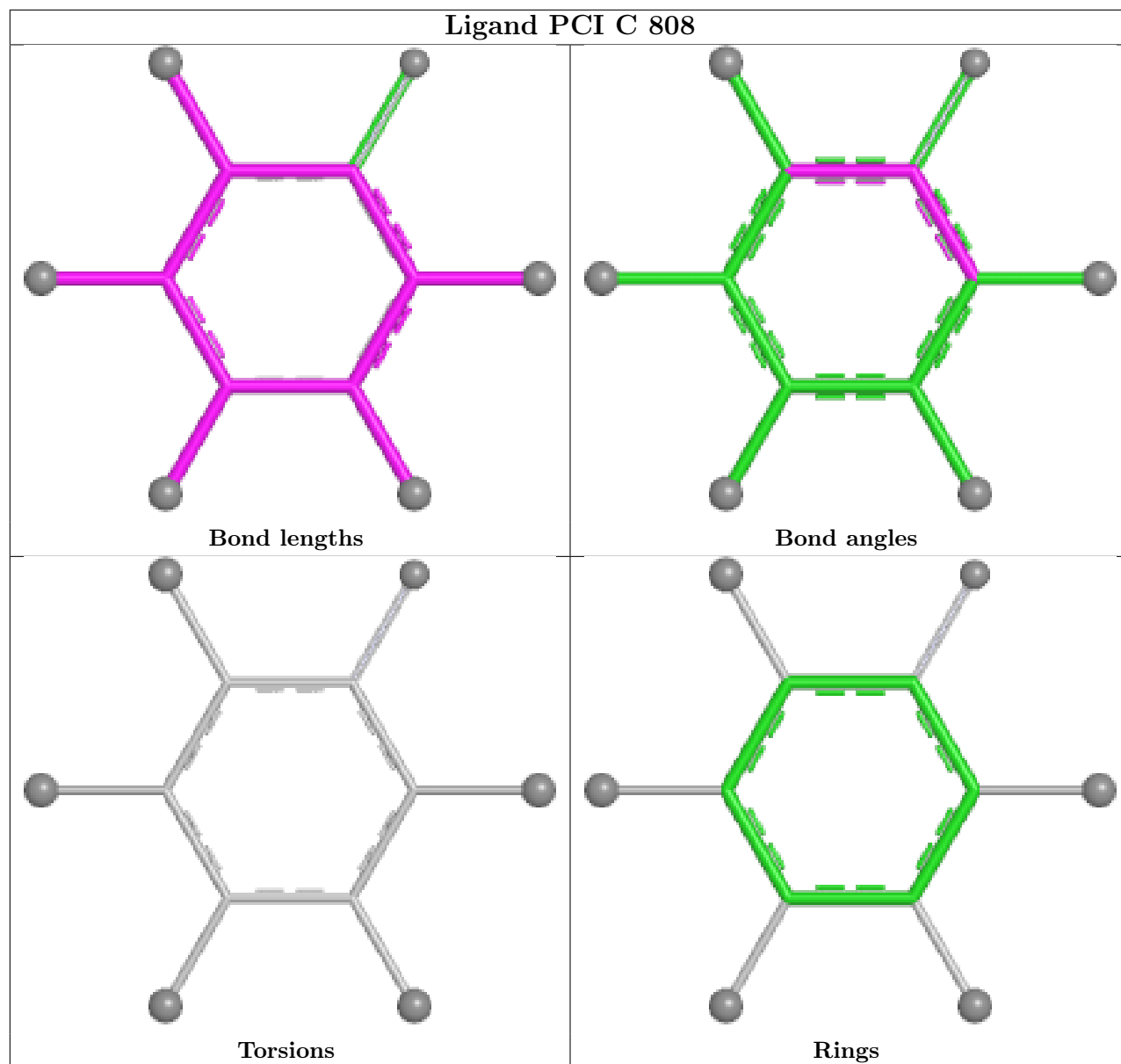
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2800	MD1	2	0
9	C	806	HEM	1	0
10	C	309	AGA	1	0
4	A	1800	MD1	6	0
6	A	1801	SF4	2	0

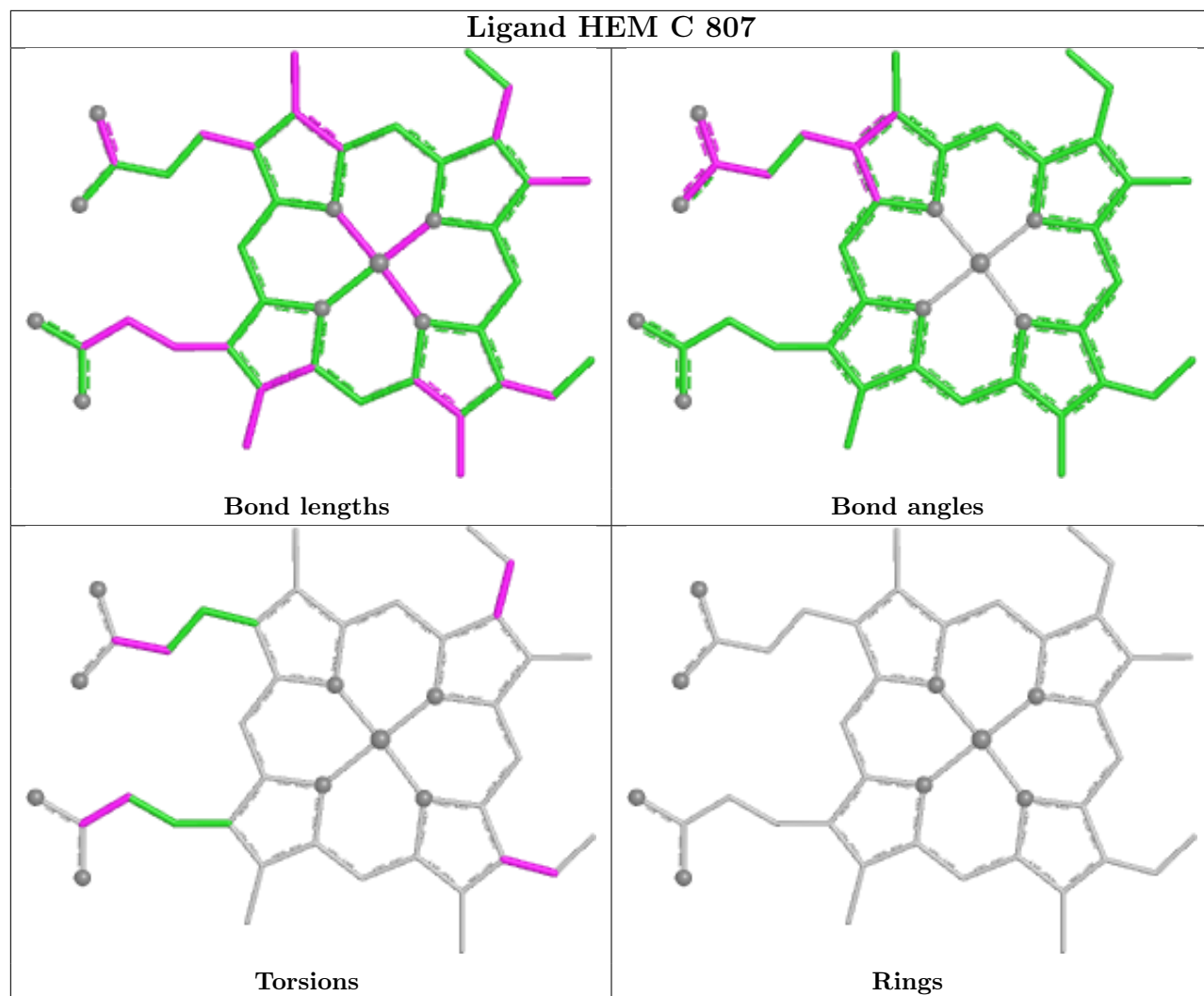
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

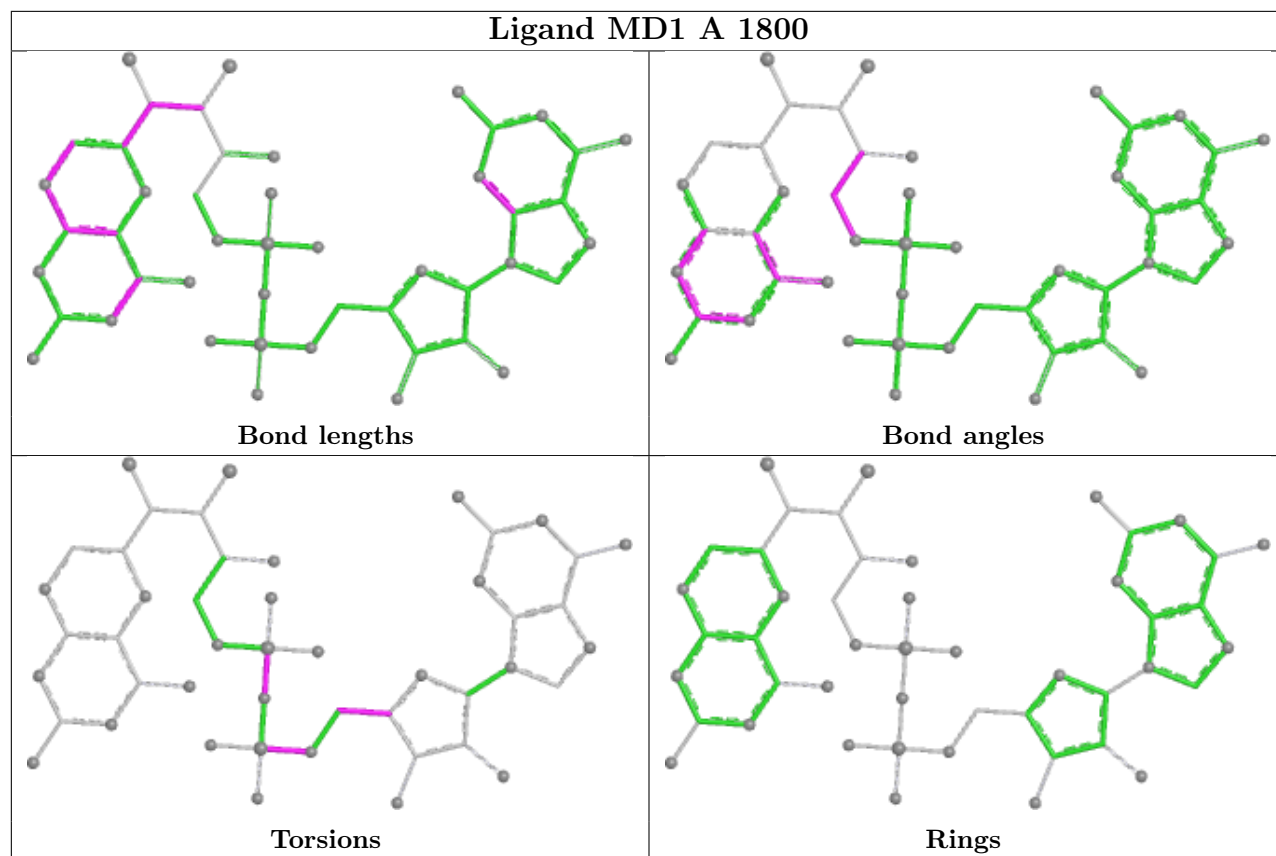












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1244/1246 (99%)	-0.11	9 (0%) 84 81	25, 51, 80, 107	0
2	B	509/512 (99%)	-0.41	1 (0%) 91 89	23, 41, 66, 97	0
3	C	216/225 (96%)	0.13	2 (0%) 81 78	32, 57, 83, 95	0
All	All	1969/1983 (99%)	-0.16	12 (0%) 85 83	23, 48, 78, 107	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	3.2
1	A	501	ALA	3.2
1	A	1244	SER	2.8
3	C	81	LEU	2.8
1	A	991	ASP	2.7
3	C	83	ILE	2.6
2	B	372	GLY	2.6
1	A	749	VAL	2.6
1	A	414	GLU	2.5
1	A	680	VAL	2.1
1	A	424	ASP	2.1
1	A	468	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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	0.79	0.13	82,84,96,98	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

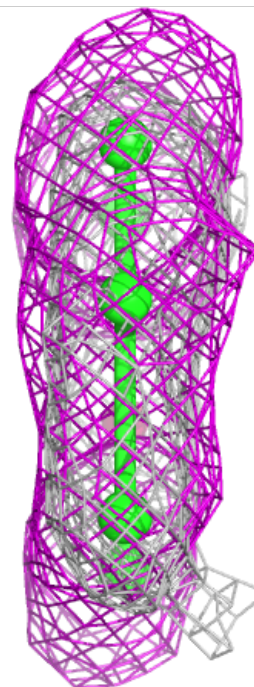
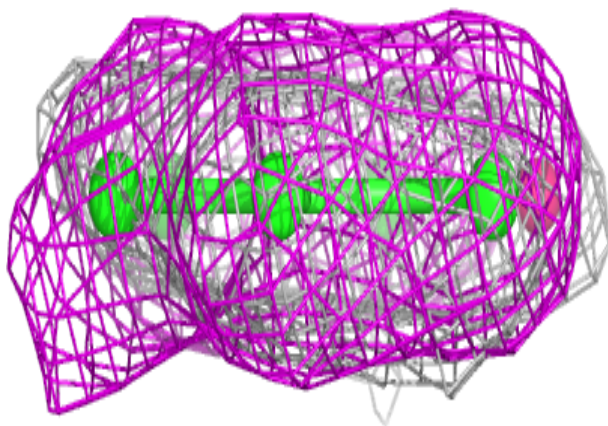
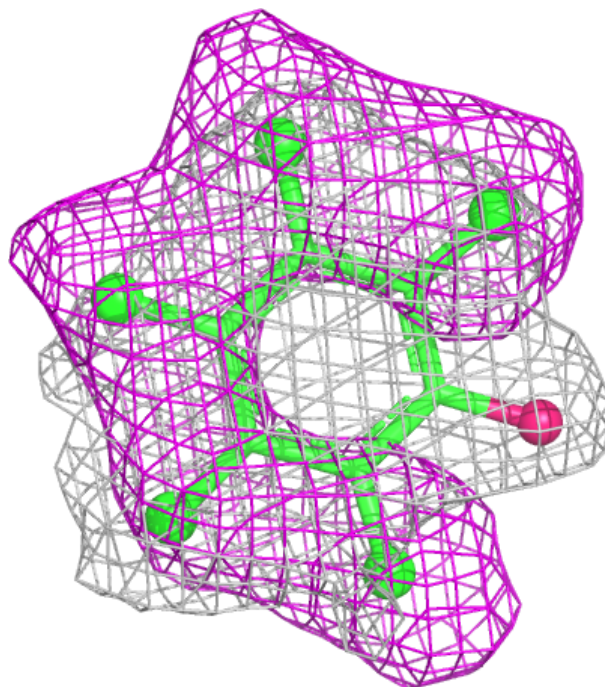
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
11	PCI	C	808	12/12	0.74	0.14	59,69,74,76	0
8	3PH	B	1806	18/48	0.75	0.15	59,82,111,111	0
10	AGA	C	309	30/30	0.91	0.12	30,54,85,95	0
9	HEM	C	807	43/43	0.95	0.12	60,68,89,92	0
4	MD1	A	2800	47/47	0.95	0.07	32,45,61,64	0
4	MD1	A	1800	47/47	0.95	0.08	35,50,66,71	0
6	SF4	B	1804	8/8	0.98	0.04	31,38,38,39	0
6	SF4	B	1802	8/8	0.98	0.04	37,40,43,44	0
9	HEM	C	806	43/43	0.98	0.07	27,40,51,55	0
6	SF4	B	1803	8/8	0.99	0.04	22,27,30,33	0
6	SF4	A	1801	8/8	0.99	0.04	34,39,46,47	0
7	F3S	B	1805	7/7	0.99	0.04	30,33,34,37	0
5	6MO	A	3800	1/1	0.99	0.10	72,72,72,72	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.

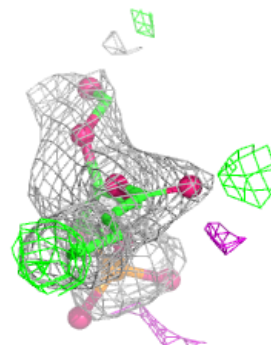
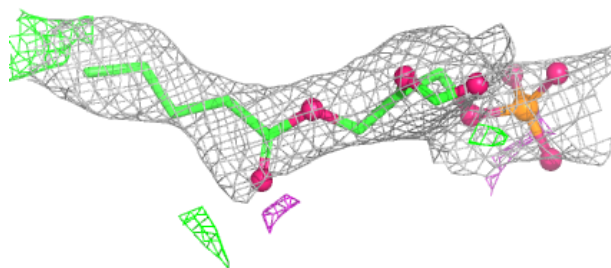
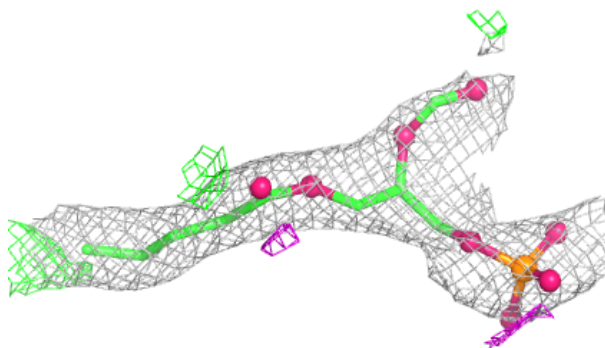
Electron density around PCI C 808:

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

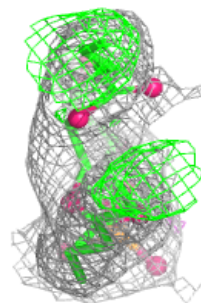
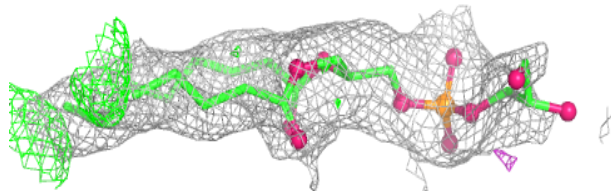
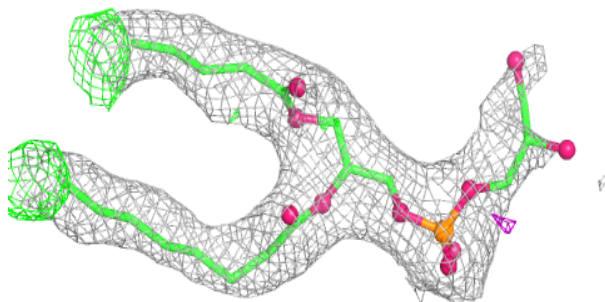


Electron density around 3PH B 1806:

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

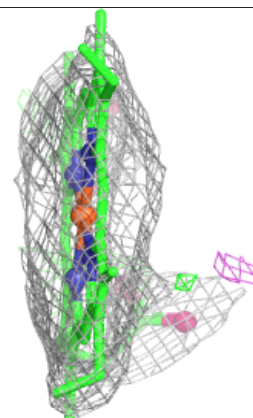
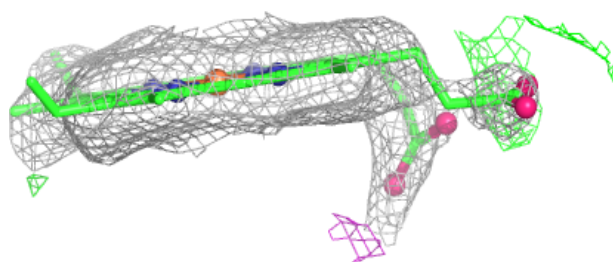
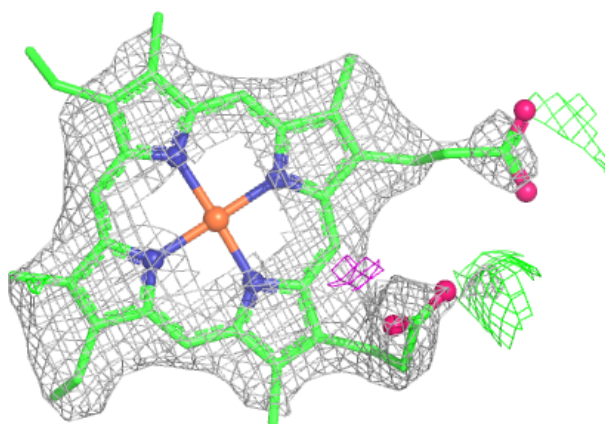
**Electron density around AGA C 309:**

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

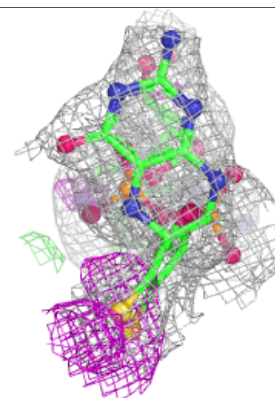
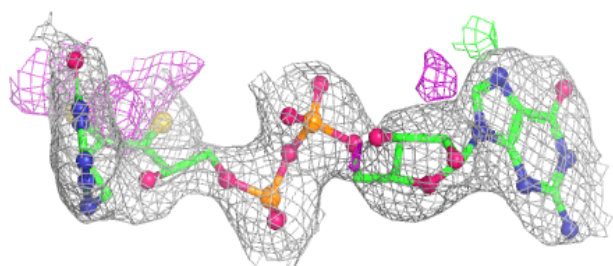
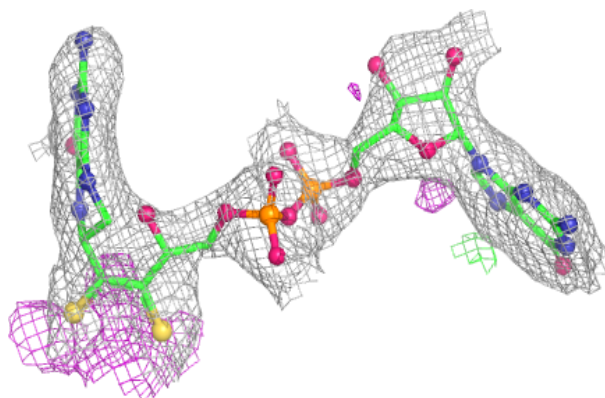


Electron density around HEM C 807:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

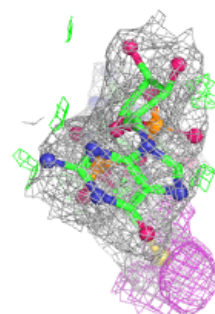
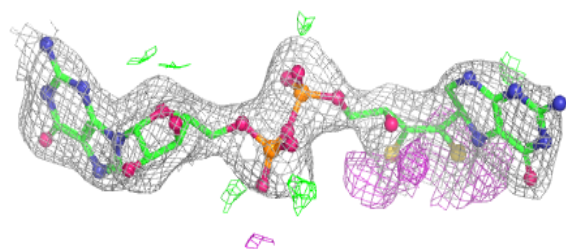
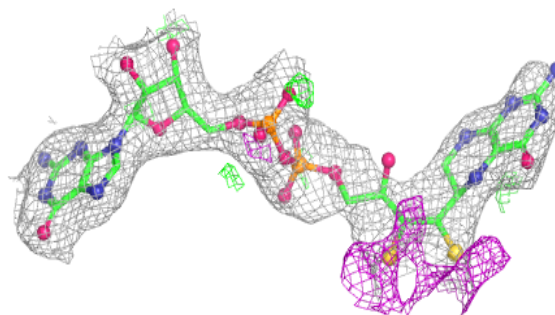
**Electron density around MD1 A 2800:**

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

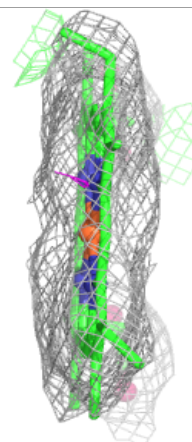
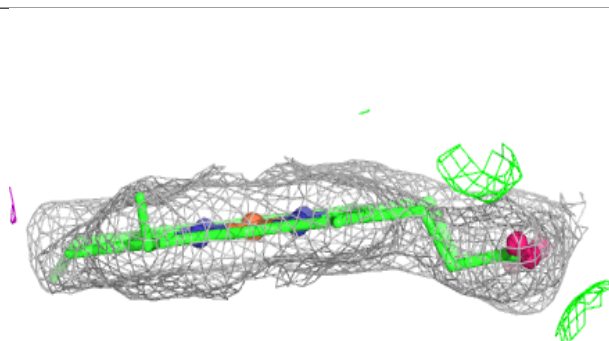
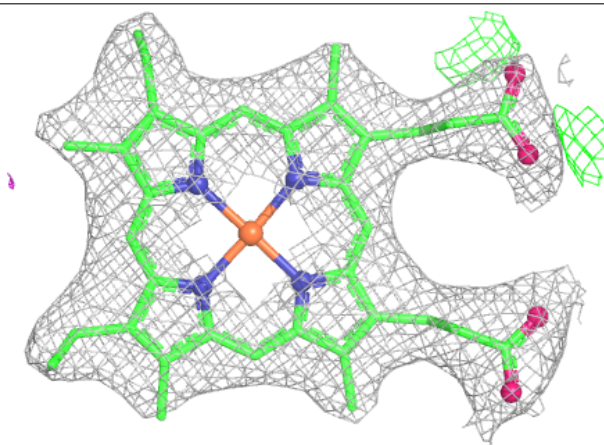


Electron density around MD1 A 1800:

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

**Electron density around 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.