



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:45 AM JST

PDB ID : 5GLS / pdb_00005gls
Title : Structure of bovine Lactoperoxidase with a partially modified covalent bond with heme moiety
Authors : Tiwari, P.; Singh, P.K.; Sirohi, H.V.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-07-12
Resolution : 1.93 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

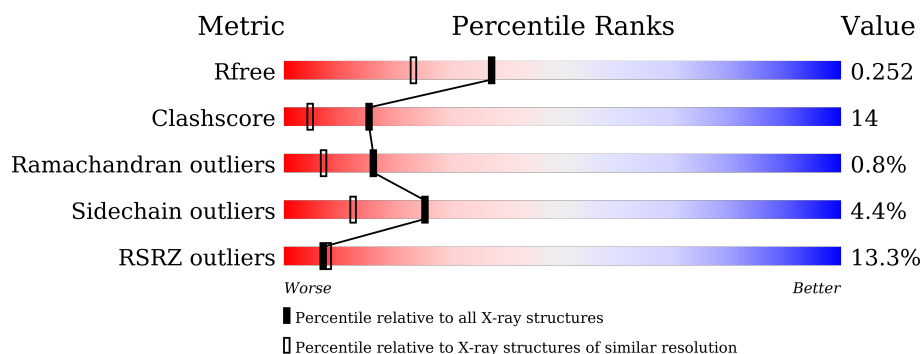
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	595	13% 77% 18% ..
2	B	2	100%

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
7	IOD	A	709	-	-	X	-
7	IOD	A	713	-	-	X	-
7	IOD	A	716	-	-	X	-
7	IOD	A	719	-	-	X	-
7	IOD	A	723	-	-	X	-
8	OSM	A	727	-	-	X	-
8	OSM	A	728	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5270 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 Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	1	0
			4775	3035	848	864	1	27			

There are 3 discrepancies between the modelled and reference sequences:

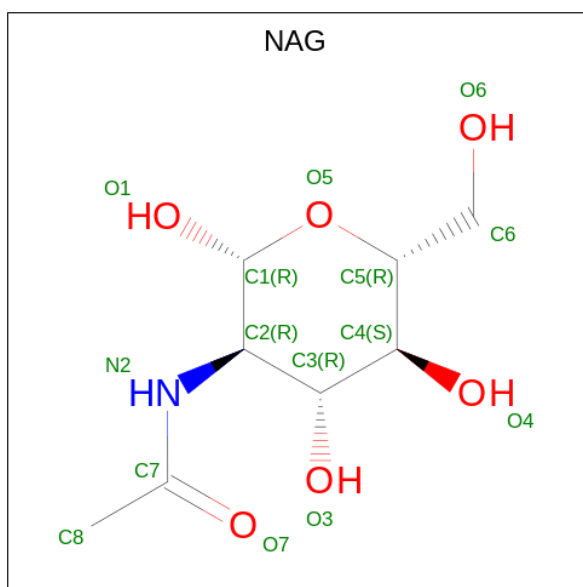
Chain	Residue	Modelled	Actual	Comment	Reference
A	254	SER	PHE	conflict	UNP P80025
A	410	LYS	ASP	conflict	UNP P80025
A	547	MET	VAL	conflict	UNP P80025

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

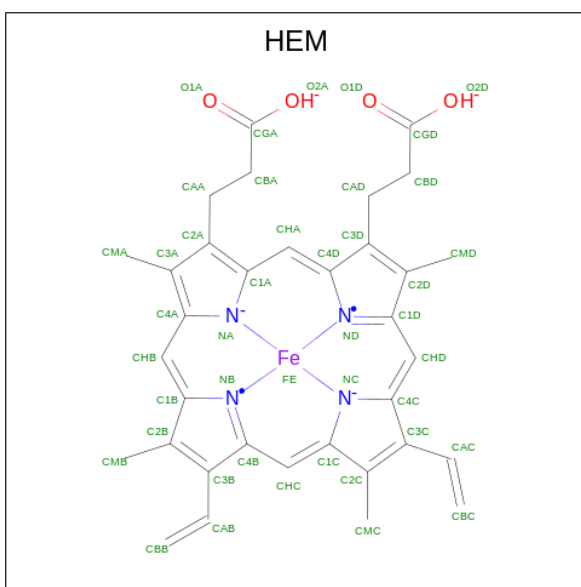


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

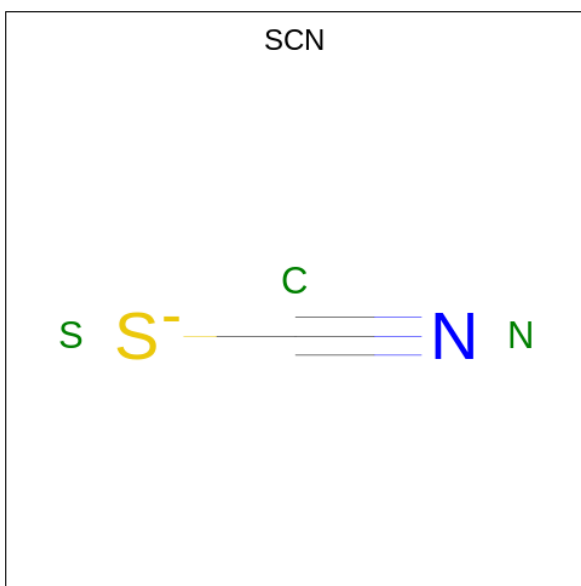
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).

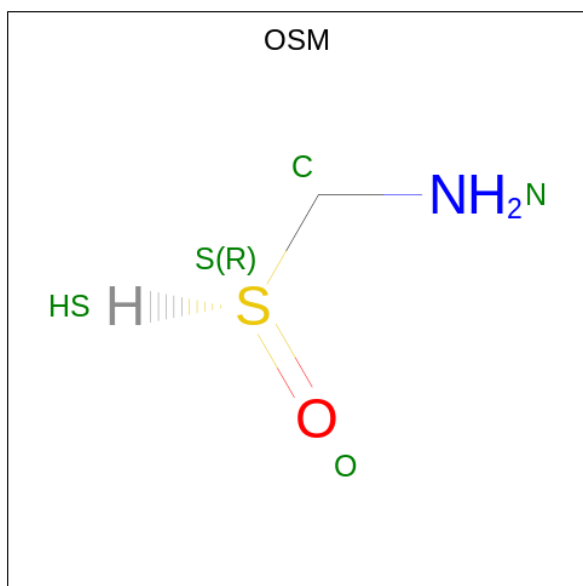


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is IODIDE ION (CCD ID: IOD) (formula: I).

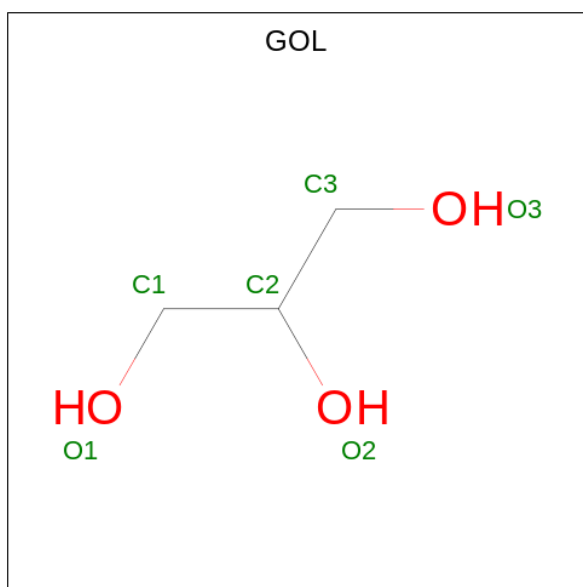
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	18	Total I 18 18	0	0

- Molecule 8 is 1-(OXIDOSULFANYL)METHANAMINE (CCD ID: OSM) (formula: CH₅NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
8	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

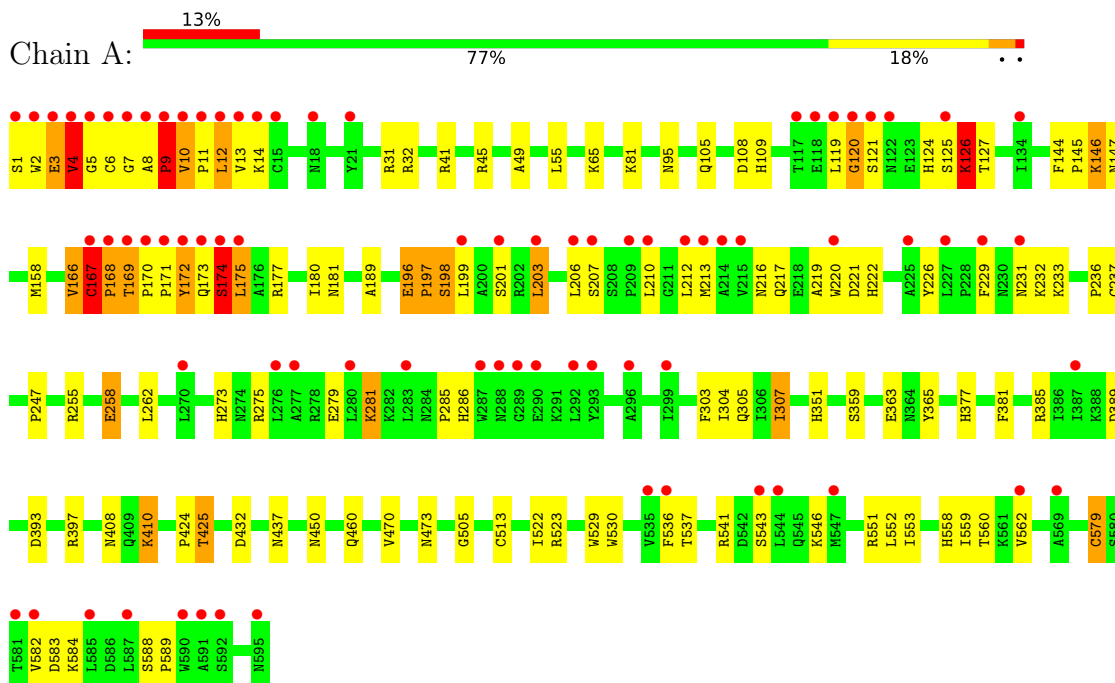
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	346	Total	O	0	0
			346	346		

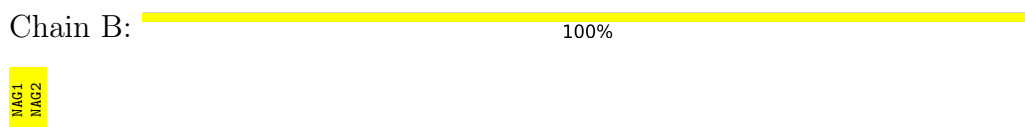
3 Residue-property plots [i](#)

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: Lactoperoxidase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.01Å 79.83Å 76.13Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	50.00 – 1.93 50.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.93) 100.0 (50.00-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.245 0.204 , 0.252	Depositor DCC
R_{free} test set	2406 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.2	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	5270	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 5.68% 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: SCN, SEP, CA, GOL, NAG, IOD, OSM, 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	1.20	13/4896 (0.3%)	1.19	24/6638 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	460	GLN	N-CA	-7.76	1.38	1.46
1	A	174	SER	C-N	-7.63	1.23	1.33
1	A	470	VAL	N-CA	6.33	1.53	1.46
1	A	258[A]	GLU	C-O	-6.17	1.16	1.24
1	A	258[B]	GLU	C-O	-6.17	1.16	1.24
1	A	255	ARG	C-O	-6.13	1.15	1.24
1	A	168	PRO	N-CD	5.85	1.55	1.47
1	A	505	GLY	N-CA	5.54	1.50	1.45
1	A	513	CYS	CA-C	5.39	1.59	1.52
1	A	177	ARG	CD-NE	-5.29	1.38	1.46
1	A	305	GLN	CA-C	-5.22	1.46	1.52
1	A	9	PRO	N-CD	5.19	1.55	1.47
1	A	562	VAL	C-O	5.12	1.28	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	VAL	O-C-N	11.20	134.08	122.54
1	A	258[A]	GLU	CA-CB-CG	9.46	133.02	114.10
1	A	258[B]	GLU	CA-CB-CG	9.46	133.02	114.10
1	A	167	CYS	CA-C-N	7.60	129.34	119.84
1	A	167	CYS	C-N-CA	7.60	129.34	119.84
1	A	3	GLU	N-CA-C	-6.66	98.81	109.39
1	A	171	PRO	N-CA-C	6.62	122.74	113.53
1	A	450	ASN	N-CA-C	6.62	119.50	111.82
1	A	579	CYS	N-CA-C	6.41	119.08	111.71
1	A	8	ALA	CA-C-N	-6.01	112.33	119.84
1	A	8	ALA	C-N-CA	-6.01	112.33	119.84
1	A	10	VAL	CA-C-N	-5.89	112.47	119.84
1	A	10	VAL	C-N-CA	-5.89	112.47	119.84
1	A	231	ASN	N-CA-C	5.86	118.61	111.82
1	A	168	PRO	CA-N-CD	-5.76	103.93	112.00
1	A	4	VAL	N-CA-C	-5.74	100.22	108.48
1	A	95	ASN	N-CA-C	5.62	119.31	111.56
1	A	119	LEU	N-CA-C	5.47	119.80	113.18
1	A	126	LYS	N-CA-C	-5.37	105.08	111.69
1	A	120	GLY	N-CA-C	5.36	120.56	113.37
1	A	144	PHE	N-CA-C	5.22	116.41	109.93
1	A	553	ILE	N-CA-C	-5.13	105.60	110.42
1	A	146	LYS	N-CA-C	-5.12	103.73	110.43
1	A	212	LEU	N-CA-C	-5.11	102.95	110.52

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	CYS	Peptide
1	A	4	VAL	Peptide
1	A	5	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4775	0	4693	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	25	0	0
3	A	42	0	39	0	0
4	A	1	0	0	0	0
5	A	43	0	30	12	0
6	A	3	0	0	0	0
7	A	18	0	0	20	0
8	A	8	0	10	8	0
9	A	6	0	8	1	0
10	A	346	0	0	8	0
All	All	5270	0	4805	132	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 (132) 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:108:ASP:OD2	5:A:707:HEM:CMD	1.74	1.35
1:A:258[A]:GLU:OE2	5:A:707:HEM:CMB	1.77	1.31
1:A:2:TRP:HB3	1:A:4:VAL:CG1	1.60	1.31
1:A:258[A]:GLU:OE2	5:A:707:HEM:HMB1	1.19	1.26
1:A:2:TRP:CB	1:A:4:VAL:HG12	1.83	1.08
1:A:172:TYR:HB2	1:A:173:GLN:HB2	1.02	1.02
1:A:108:ASP:OD2	5:A:707:HEM:HMD1	0.80	0.98
1:A:108:ASP:CG	5:A:707:HEM:HMD1	1.90	0.96
1:A:172:TYR:CB	1:A:173:GLN:HB2	1.96	0.95
1:A:172:TYR:HB2	1:A:173:GLN:CB	1.96	0.94
1:A:2:TRP:HB3	1:A:4:VAL:HG12	0.95	0.93
1:A:169:THR:HB	1:A:170:PRO:HD3	1.49	0.92
1:A:166:VAL:O	1:A:167:CYS:HB2	1.71	0.90
7:A:720:IOD:I	10:A:1120:HOH:O	2.62	0.88
1:A:120:GLY:O	1:A:126:LYS:HD2	1.75	0.87
1:A:173:GLN:O	1:A:174:SER:OG	1.92	0.86
1:A:109:HIS:NE2	7:A:709:IOD:I	2.79	0.85
1:A:10:VAL:CG1	1:A:11:PRO:HD2	2.08	0.84
7:A:713:IOD:I	10:A:1138:HOH:O	2.65	0.83
1:A:10:VAL:HG12	1:A:11:PRO:HD2	1.60	0.81
7:A:719:IOD:I	10:A:937:HOH:O	2.70	0.80
1:A:9:PRO:CB	1:A:10:VAL:HA	2.13	0.79
7:A:709:IOD:I	10:A:801:HOH:O	2.69	0.79
1:A:258[A]:GLU:OE2	5:A:707:HEM:HMB2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.66	0.77
1:A:2:TRP:CB	1:A:4:VAL:CG1	2.51	0.76
1:A:9:PRO:HD3	1:A:168:PRO:HD3	1.67	0.75
1:A:169:THR:HB	1:A:170:PRO:CD	2.17	0.72
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.71	0.71
1:A:126:LYS:HE3	1:A:127:THR:OG1	1.92	0.70
1:A:31:ARG:HD2	7:A:716:IOD:I	2.63	0.69
1:A:559:ILE:HA	8:A:727:OSM:O	1.93	0.69
1:A:169:THR:CB	1:A:170:PRO:HD3	2.21	0.68
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.40	0.68
1:A:2:TRP:C	1:A:4:VAL:H	2.02	0.68
1:A:9:PRO:HB3	1:A:10:VAL:HA	1.77	0.66
1:A:258[A]:GLU:HG2	10:A:1004:HOH:O	1.94	0.66
1:A:559:ILE:HG23	8:A:727:OSM:H2	1.78	0.65
1:A:124:HIS:O	1:A:127:THR:N	2.29	0.64
1:A:10:VAL:O	1:A:12:LEU:N	2.30	0.64
1:A:10:VAL:HG12	1:A:11:PRO:CD	2.29	0.63
1:A:172:TYR:HD2	1:A:172:TYR:H	1.48	0.61
1:A:410:LYS:HE2	1:A:473:ASN:HD21	1.66	0.60
1:A:10:VAL:HG13	1:A:11:PRO:HD2	1.83	0.60
1:A:258[B]:GLU:HG2	1:A:262:LEU:HD23	1.84	0.60
1:A:10:VAL:O	1:A:11:PRO:C	2.44	0.59
1:A:530:TRP:NE1	7:A:710:IOD:I	3.04	0.59
1:A:2:TRP:HB3	1:A:4:VAL:CB	2.33	0.58
1:A:1:SER:O	1:A:2:TRP:C	2.44	0.58
1:A:108:ASP:CG	5:A:707:HEM:CMD	2.62	0.58
1:A:175:LEU:HD12	10:A:830:HOH:O	2.03	0.58
1:A:410:LYS:CE	1:A:473:ASN:HD21	2.17	0.57
1:A:216:ASN:HA	8:A:728:OSM:HN2	1.69	0.57
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.40	0.56
1:A:2:TRP:C	1:A:4:VAL:N	2.60	0.56
1:A:169:THR:CB	1:A:170:PRO:CD	2.82	0.55
1:A:303:PHE:CZ	1:A:307:ILE:CD1	2.89	0.55
5:A:707:HEM:HBC2	5:A:707:HEM:HMC1	1.87	0.55
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.41	0.55
1:A:281:LYS:HD3	1:A:285:PRO:HA	1.87	0.55
1:A:166:VAL:HA	1:A:168:PRO:HB3	1.89	0.55
1:A:258[A]:GLU:OE2	5:A:707:HEM:C2B	2.59	0.55
1:A:424:PRO:O	1:A:425:THR:HB	2.08	0.54
1:A:303:PHE:CZ	1:A:307:ILE:HD13	2.43	0.54
1:A:210:LEU:CD2	1:A:281:LYS:HG3	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.53
5:A:707:HEM:HMB2	5:A:707:HEM:HBB2	1.91	0.52
1:A:31:ARG:CD	7:A:716:IOD:I	3.28	0.51
1:A:359:SER:OG	7:A:719:IOD:I	2.97	0.51
1:A:2:TRP:O	1:A:4:VAL:HG12	2.10	0.51
1:A:229:PHE:HB2	8:A:728:OSM:S	2.51	0.51
1:A:551:ARG:HD3	1:A:583:ASP:O	2.11	0.50
1:A:377:HIS:CD2	7:A:723:IOD:I	3.34	0.50
1:A:560:THR:HA	1:A:579:CYS:SG	2.52	0.50
1:A:172:TYR:HD2	1:A:172:TYR:N	2.09	0.50
1:A:172:TYR:N	1:A:172:TYR:CD2	2.79	0.49
1:A:236:PRO:HA	7:A:724:IOD:I	2.82	0.49
1:A:120:GLY:CA	1:A:126:LYS:HB3	2.42	0.49
1:A:10:VAL:CG1	1:A:11:PRO:CD	2.85	0.49
1:A:145:PRO:HG2	7:A:714:IOD:I	2.83	0.49
1:A:196:GLU:HG2	1:A:198:SEP:O1P	2.13	0.49
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.94	0.49
1:A:216:ASN:HA	8:A:728:OSM:N	2.28	0.49
7:A:716:IOD:I	10:A:926:HOH:O	2.90	0.49
1:A:425:THR:N	7:A:725:IOD:I	3.11	0.48
1:A:543:SER:O	1:A:546:LYS:HB2	2.14	0.48
1:A:124:HIS:O	1:A:126:LYS:N	2.47	0.48
1:A:237:CYS:HA	1:A:381:PHE:O	2.14	0.47
1:A:197:PRO:HG3	7:A:718:IOD:I	2.85	0.47
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.50	0.47
1:A:229:PHE:HD2	8:A:728:OSM:HS	1.63	0.47
1:A:206:LEU:O	1:A:207:SER:C	2.57	0.47
1:A:124:HIS:C	1:A:126:LYS:N	2.72	0.47
1:A:11:PRO:HG2	1:A:11:PRO:O	2.15	0.46
1:A:551:ARG:NH1	1:A:582:VAL:O	2.46	0.46
1:A:2:TRP:HB3	1:A:4:VAL:HG11	1.82	0.46
1:A:536:PHE:O	1:A:541:ARG:NH1	2.48	0.46
1:A:377:HIS:NE2	7:A:723:IOD:I	3.18	0.46
1:A:219:ALA:C	1:A:220:TRP:CD1	2.93	0.46
1:A:9:PRO:CB	1:A:10:VAL:CA	2.85	0.45
1:A:180:ILE:HG22	1:A:181:ASN:N	2.31	0.45
1:A:2:TRP:C	1:A:4:VAL:HG12	2.40	0.45
1:A:303:PHE:CE1	1:A:307:ILE:CD1	3.00	0.45
1:A:222:HIS:HB2	1:A:558:HIS:NE2	2.32	0.45
1:A:281:LYS:CD	1:A:285:PRO:HA	2.47	0.44
5:A:707:HEM:C4A	7:A:709:IOD:I	3.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLN:H	8:A:728:OSM:HN2	1.62	0.44
1:A:551:ARG:CD	1:A:583:ASP:O	2.66	0.44
1:A:365:TYR:CE2	1:A:397:ARG:HB3	2.52	0.44
1:A:55:LEU:HD13	1:A:173:GLN:CD	2.44	0.43
1:A:9:PRO:CD	1:A:168:PRO:HD3	2.44	0.43
1:A:81:LYS:HE3	7:A:713:IOD:I	2.89	0.43
1:A:303:PHE:CE1	1:A:307:ILE:HD11	2.54	0.43
1:A:385:ARG:O	1:A:389:ASP:HB3	2.19	0.42
1:A:363:GLU:HA	8:A:727:OSM:HS	1.84	0.42
5:A:707:HEM:C1A	7:A:709:IOD:I	3.41	0.42
1:A:6:CYS:SG	1:A:7:GLY:CA	3.08	0.42
1:A:258[B]:GLU:HG2	1:A:262:LEU:CD2	2.47	0.42
1:A:146:LYS:O	1:A:147:ASN:HB2	2.20	0.41
1:A:275:ARG:O	1:A:279:GLU:HB2	2.19	0.41
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.50	0.41
1:A:10:VAL:HB	1:A:41:ARG:CZ	2.51	0.41
1:A:105:GLN:NE2	7:A:709:IOD:I	3.11	0.41
1:A:124:HIS:C	1:A:126:LYS:H	2.29	0.41
1:A:126:LYS:HG2	1:A:127:THR:N	2.36	0.41
1:A:232:LYS:O	1:A:232:LYS:CG	2.68	0.41
1:A:393:ASP:O	1:A:397:ARG:HG3	2.21	0.41
1:A:408:ASN:HB2	10:A:925:HOH:O	2.20	0.41
1:A:158:MET:HE1	1:A:432:ASP:HB3	2.03	0.41
1:A:199:LEU:N	9:A:729:GOL:H2	2.37	0.40
1:A:168:PRO:O	1:A:169:THR:CB	2.70	0.40
1:A:588:SER:HB2	1:A:589:PRO:HD3	2.04	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	593/595 (100%)	557 (94%)	31 (5%)	5 (1%)	16 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	169	THR
1	A	174	SER
1	A	125	SER
1	A	9	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	518/517 (100%)	495 (96%)	23 (4%)	25 12

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	12	LEU
1	A	13	VAL
1	A	14	LYS
1	A	32	ARG
1	A	65	LYS
1	A	121	SER
1	A	126	LYS
1	A	172	TYR
1	A	175	LEU
1	A	196	GLU
1	A	197	PRO
1	A	201	SER
1	A	203	LEU
1	A	233	LYS
1	A	281	LYS

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	307	ILE
1	A	410	LYS
1	A	425	THR
1	A	522	ILE
1	A	537	THR
1	A	552	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	273	HIS
1	A	288	ASN
1	A	329	GLN
1	A	468	GLN
1	A	473	ASN

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	$\# Z > 2$
1	SEP	A	198	1	8,9,10	1.76	2 (25%)	8,12,14	4.01	6 (75%)

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
1	SEP	A	198	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O2P	-2.51	1.45	1.54
1	A	198	SEP	P-OG	2.51	1.68	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-OG	5.31	120.87	106.73
1	A	198	SEP	OG-CB-CA	5.26	113.26	108.14
1	A	198	SEP	OG-P-O1P	-5.09	92.20	106.47
1	A	198	SEP	P-OG-CB	4.69	131.22	118.30
1	A	198	SEP	O3P-P-O1P	3.64	124.92	110.68
1	A	198	SEP	O3P-P-O2P	-3.01	96.14	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	1	0

5.5 Carbohydrates [i](#)

2 monosaccharides 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
2	NAG	B	1	2,1	14,14,15	0.64	0	17,19,21	2.02	4 (23%)
2	NAG	B	2	2	14,14,15	0.86	0	17,19,21	2.58	4 (23%)

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
2	NAG	B	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.90	122.90	112.19
2	B	2	NAG	C1-C2-N2	4.21	117.68	110.49
2	B	1	NAG	C1-O5-C5	-3.93	106.87	112.19
2	B	1	NAG	O5-C1-C2	-3.82	105.25	111.29
2	B	1	NAG	C6-C5-C4	3.60	121.42	113.00
2	B	1	NAG	O5-C5-C4	-3.39	102.59	110.83
2	B	2	NAG	C4-C3-C2	-3.29	106.20	111.02
2	B	2	NAG	O5-C5-C6	2.71	111.46	107.20

There are no chirality outliers.

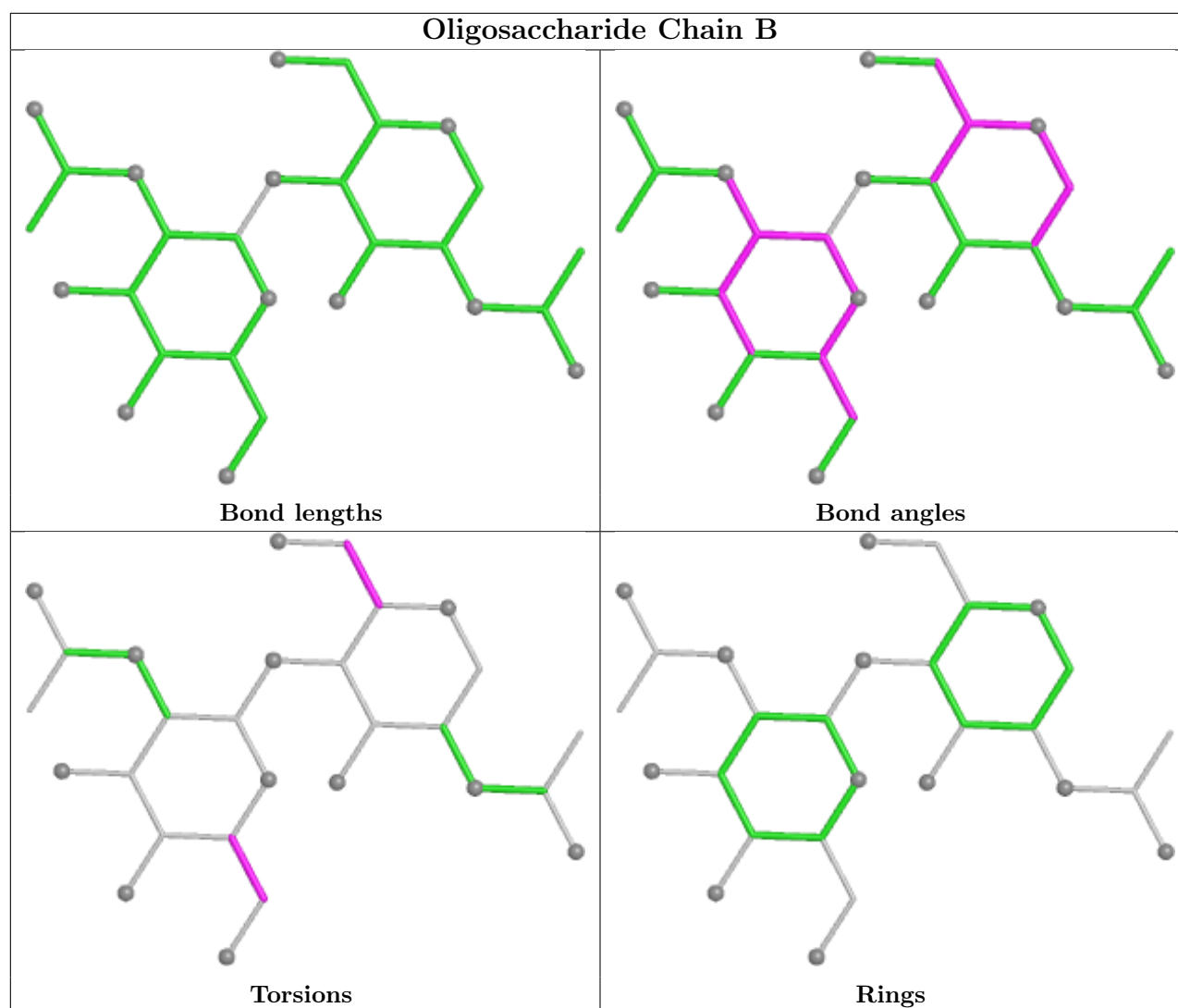
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 19 are monoatomic - leaving 8 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	$\# Z > 2$
8	OSM	A	727	-	1,3,3	0.05	0	0,2,2	-	-
8	OSM	A	728	-	1,3,3	0.05	0	0,2,2	-	-
3	NAG	A	701	1	14,14,15	0.75	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	705	1	14,14,15	0.58	0	17,19,21	1.04	1 (5%)
9	GOL	A	729	-	5,5,5	0.25	0	5,5,5	0.28	0
3	NAG	A	702	1	14,14,15	0.58	0	17,19,21	1.67	2 (11%)
5	HEM	A	707	1	50,50,50	1.97	12 (24%)	66,82,82	1.54	13 (19%)
6	SCN	A	708	-	1,2,2	0.05	0	0,1,1	-	-

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	OSM	A	727	-	-	0/0/1/1	-
8	OSM	A	728	-	-	0/0/1/1	-
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1	-	2/6/23/26	0/1/1/1
9	GOL	A	729	-	-	2/4/4/4	-
3	NAG	A	702	1	-	0/6/23/26	0/1/1/1
5	HEM	A	707	1	-	4/14/54/54	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	707	HEM	FE-NB	5.70	2.12	1.94
5	A	707	HEM	FE-NC	4.25	2.09	1.95
5	A	707	HEM	C4C-NC	-3.66	1.32	1.39
5	A	707	HEM	C4D-ND	-3.63	1.34	1.40
5	A	707	HEM	CMB-C2B	3.53	1.58	1.50
5	A	707	HEM	FE-NA	3.28	2.06	1.95
5	A	707	HEM	CHB-C1B	3.18	1.45	1.38
5	A	707	HEM	C1B-NB	-2.71	1.35	1.40
5	A	707	HEM	CBD-CAD	2.62	1.60	1.52
5	A	707	HEM	C3D-C2D	-2.40	1.31	1.36
5	A	707	HEM	C2A-C3A	-2.29	1.32	1.38
5	A	707	HEM	O2D-CGD	-2.17	1.23	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAG	C1-C2-N2	4.77	118.64	110.49
5	A	707	HEM	C4C-NC-C1C	3.68	108.95	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	707	HEM	CMD-C2D-C1D	3.66	130.62	125.04
5	A	707	HEM	O2D-CGD-O1D	-3.61	114.31	123.30
5	A	707	HEM	CAD-CBD-CGD	-3.48	106.12	113.60
3	A	705	NAG	O5-C5-C6	3.20	112.22	107.20
3	A	702	NAG	O4-C4-C5	3.17	117.18	109.30
5	A	707	HEM	CBD-CAD-C3D	-3.10	104.01	112.63
3	A	701	NAG	C6-C5-C4	3.02	120.07	113.00
5	A	707	HEM	CAD-C3D-C4D	2.74	129.45	124.66
3	A	701	NAG	O5-C5-C6	-2.73	102.92	107.20
5	A	707	HEM	CHA-C4D-C3D	-2.72	120.23	125.33
5	A	707	HEM	CMA-C3A-C4A	2.64	129.39	125.37
5	A	707	HEM	C3C-C2C-C1C	-2.44	104.75	107.08
5	A	707	HEM	O2A-CGA-O1A	-2.38	117.38	123.30
5	A	707	HEM	CBA-CAA-C2A	-2.27	106.32	112.63
5	A	707	HEM	C3D-C4D-ND	2.27	112.69	110.17
5	A	707	HEM	CHA-C4D-ND	2.04	126.89	124.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	729	GOL	C1-C2-C3-O3
9	A	729	GOL	O2-C2-C3-O3
3	A	705	NAG	C4-C5-C6-O6
3	A	705	NAG	O5-C5-C6-O6
5	A	707	HEM	CAA-CBA-CGA-O2A
5	A	707	HEM	CAD-CBD-CGD-O2D
5	A	707	HEM	CAD-CBD-CGD-O1D
5	A	707	HEM	CAA-CBA-CGA-O1A

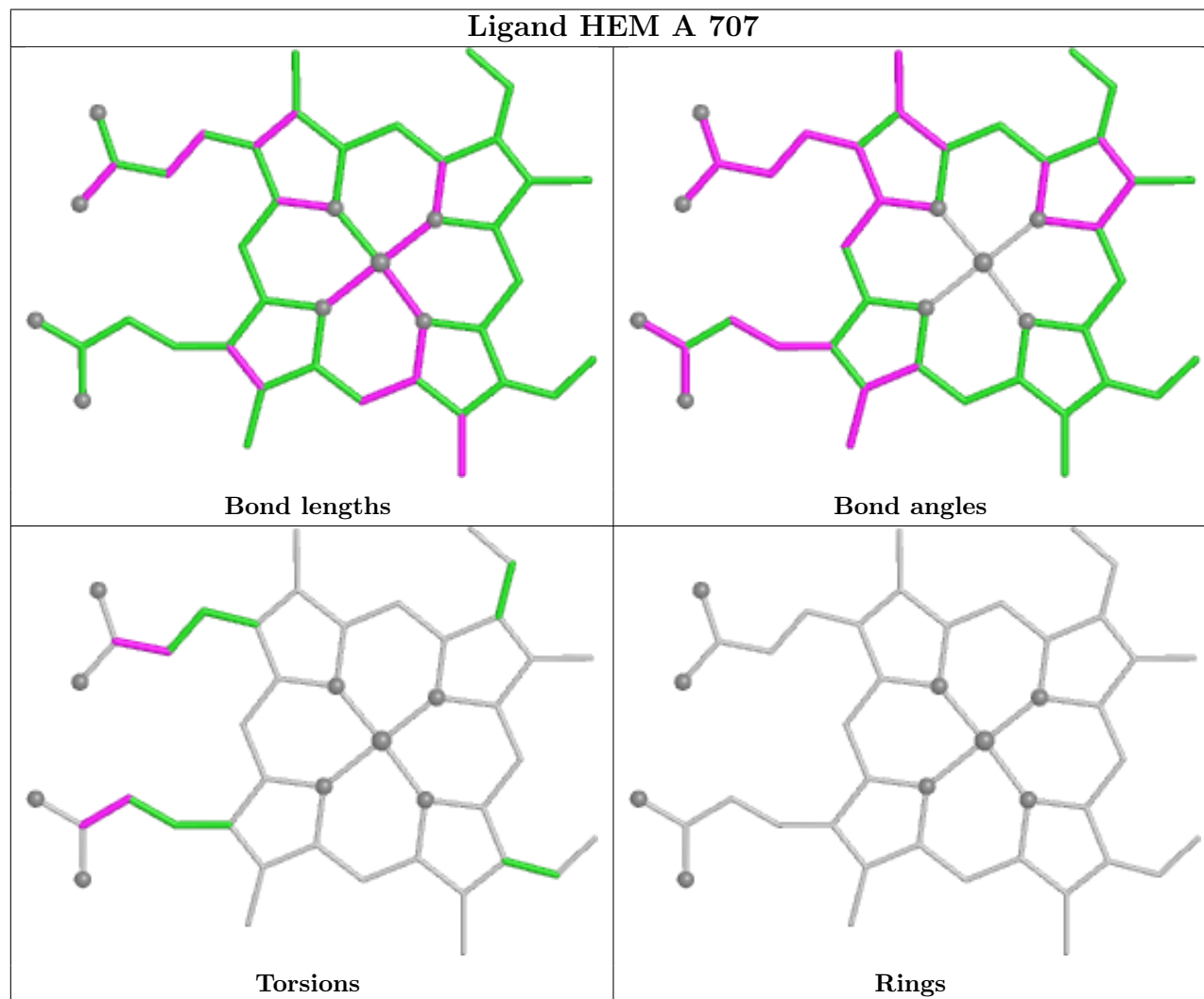
There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	727	OSM	3	0
8	A	728	OSM	5	0
9	A	729	GOL	1	0
5	A	707	HEM	12	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 ⓘ

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	594/595 (99%)	0.71	79 (13%) 7 8	14, 34, 85, 162	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	9.4
1	A	2	TRP	7.3
1	A	119	LEU	5.8
1	A	4	VAL	5.5
1	A	10	VAL	5.5
1	A	172	TYR	5.4
1	A	171	PRO	5.3
1	A	8	ALA	5.3
1	A	11	PRO	5.3
1	A	5	GLY	5.0
1	A	9	PRO	4.9
1	A	6	CYS	4.9
1	A	168	PRO	4.9
1	A	173	GLN	4.8
1	A	174	SER	4.8
1	A	170	PRO	4.5
1	A	287	TRP	4.1
1	A	167	CYS	3.9
1	A	280	LEU	3.9
1	A	169	THR	3.8
1	A	220	TRP	3.8
1	A	209	PRO	3.8
1	A	581	THR	3.7
1	A	12	LEU	3.6
1	A	587	LEU	3.6
1	A	121	SER	3.6
1	A	206	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	3.5
1	A	1	SER	3.5
1	A	229	PHE	3.4
1	A	120	GLY	3.3
1	A	296	ALA	3.3
1	A	215	VAL	3.2
1	A	276	LEU	3.1
1	A	13	VAL	3.0
1	A	283	LEU	3.0
1	A	293	TYR	3.0
1	A	231	ASN	3.0
1	A	175	LEU	2.9
1	A	591	ALA	2.8
1	A	595	ASN	2.8
1	A	125	SER	2.8
1	A	292	LEU	2.8
1	A	21	TYR	2.8
1	A	210	LEU	2.7
1	A	212	LEU	2.5
1	A	289	GLY	2.4
1	A	199	LEU	2.4
1	A	536	PHE	2.4
1	A	134	ILE	2.4
1	A	213	MET	2.4
1	A	535	VAL	2.4
1	A	585	LEU	2.3
1	A	18	ASN	2.3
1	A	225	ALA	2.3
1	A	543	SER	2.3
1	A	270	LEU	2.3
1	A	118	GLU	2.2
1	A	387	ILE	2.2
1	A	582	VAL	2.2
1	A	117	THR	2.2
1	A	3	GLU	2.2
1	A	544	LEU	2.2
1	A	14	LYS	2.2
1	A	277	ALA	2.2
1	A	562	VAL	2.2
1	A	592	SER	2.2
1	A	590	TRP	2.1
1	A	15	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	122	ASN	2.1
1	A	299	ILE	2.1
1	A	207	SER	2.1
1	A	290	GLU	2.1
1	A	227	LEU	2.1
1	A	569	ALA	2.1
1	A	547	MET	2.1
1	A	288	ASN	2.1
1	A	203	LEU	2.1
1	A	201	SER	2.0

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

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

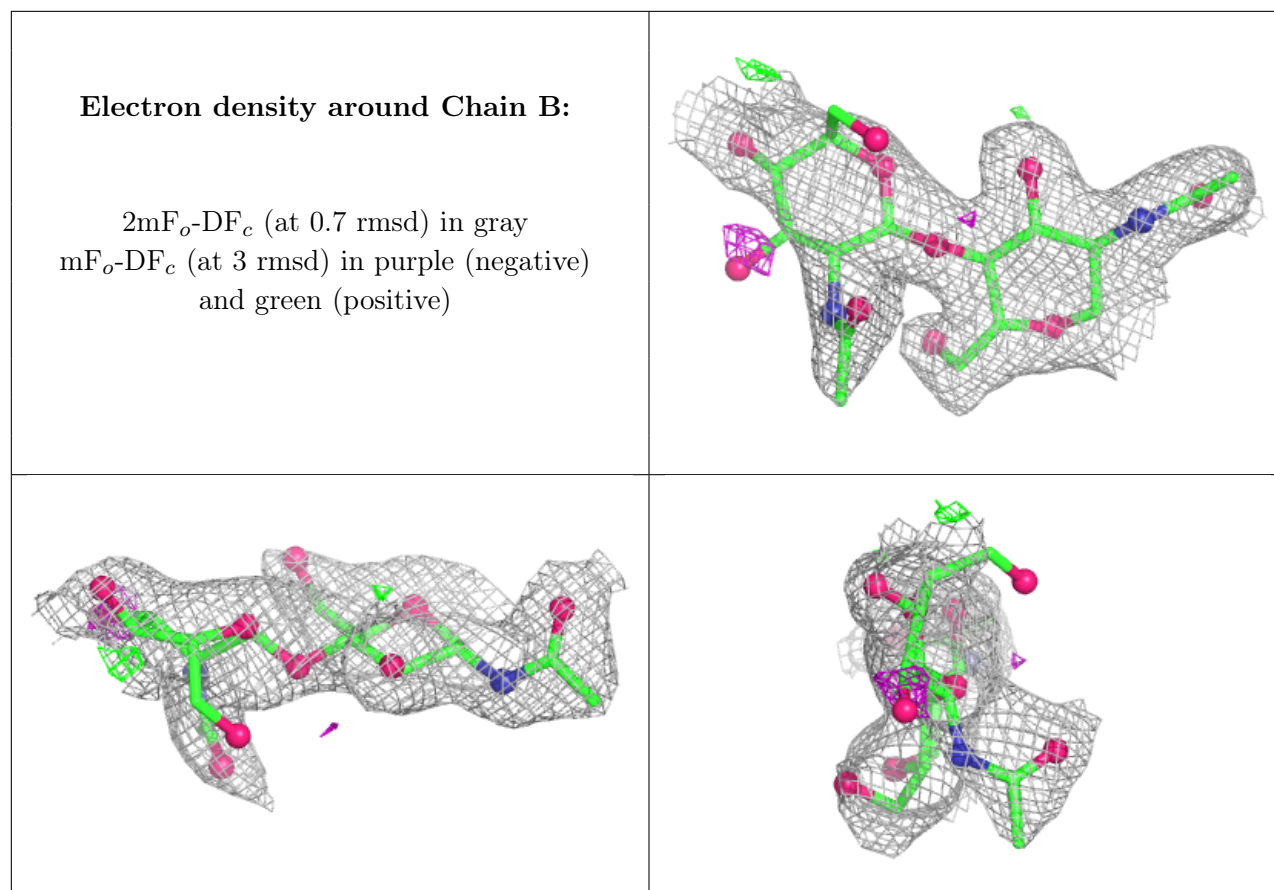
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.85	0.16	34,45,57,58	0

6.3 Carbohydrates [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
2	NAG	B	2	14/15	0.65	0.15	58,69,86,86	0
2	NAG	B	1	14/15	0.91	0.08	32,40,49,54	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

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

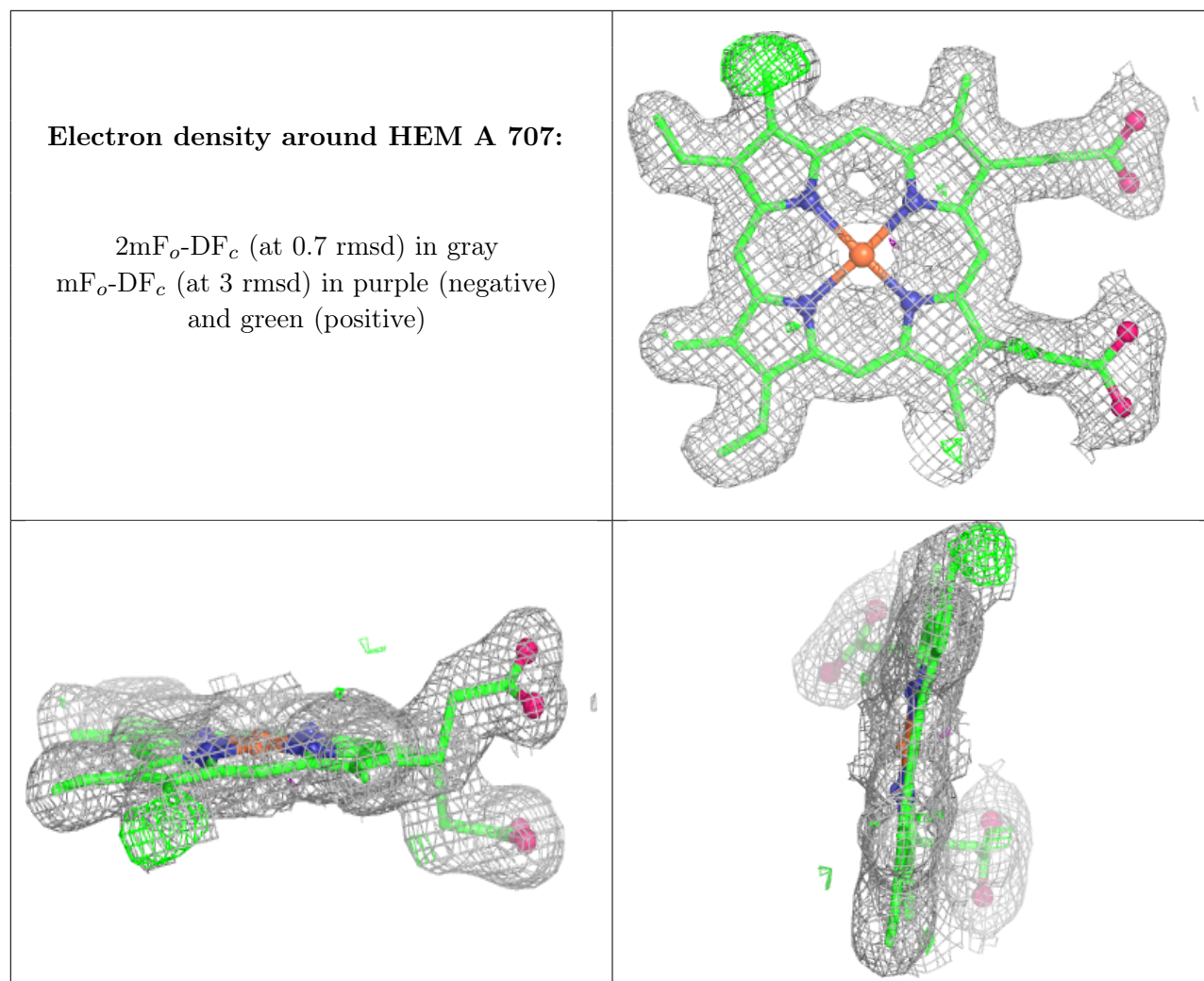
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	701	14/15	0.61	0.16	62,71,80,80	0
3	NAG	A	702	14/15	0.66	0.15	54,72,75,78	0
9	GOL	A	729	6/6	0.67	0.17	19,23,29,31	0
3	NAG	A	705	14/15	0.71	0.13	56,66,71,73	0
8	OSM	A	728	4/4	0.78	0.15	20,23,36,36	0
8	OSM	A	727	4/4	0.83	0.17	16,19,26,27	0
7	IOD	A	720	1/1	0.87	0.13	64,64,64,64	1
7	IOD	A	716	1/1	0.89	0.12	62,62,62,62	1
7	IOD	A	709	1/1	0.91	0.12	66,66,66,66	1
7	IOD	A	726	1/1	0.92	0.10	44,44,44,44	1
7	IOD	A	718	1/1	0.93	0.10	63,63,63,63	1
7	IOD	A	717	1/1	0.94	0.09	54,54,54,54	1
7	IOD	A	723	1/1	0.94	0.10	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SCN	A	708	3/3	0.95	0.09	31,31,32,45	0
5	HEM	A	707	43/43	0.97	0.07	16,20,25,30	0
7	IOD	A	719	1/1	0.98	0.06	50,50,50,50	1
7	IOD	A	725	1/1	0.98	0.06	38,38,38,38	1
7	IOD	A	722	1/1	0.98	0.09	41,41,41,41	1
7	IOD	A	710	1/1	0.99	0.04	34,34,34,34	1
7	IOD	A	724	1/1	0.99	0.04	36,36,36,36	1
7	IOD	A	711	1/1	0.99	0.05	35,35,35,35	1
7	IOD	A	712	1/1	0.99	0.02	20,20,20,20	1
7	IOD	A	713	1/1	0.99	0.02	30,30,30,30	1
7	IOD	A	721	1/1	0.99	0.05	37,37,37,37	1
4	CA	A	706	1/1	0.99	0.03	23,23,23,23	0
7	IOD	A	714	1/1	1.00	0.01	28,28,28,28	1
7	IOD	A	715	1/1	1.00	0.01	18,18,18,18	1

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.



6.5 Other polymers ⓘ

There are no such residues in this entry.