



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:33 PM EDT

PDB ID : 4KSZ / pdb_00004ksz
Title : Crystal structure of bovine lactoperoxidase complexed with cystiene at 1.98Å resolution
Authors : Singh, R.P.; Singh, N.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-05-19
Resolution : 1.98 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	:	9.0.015 (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

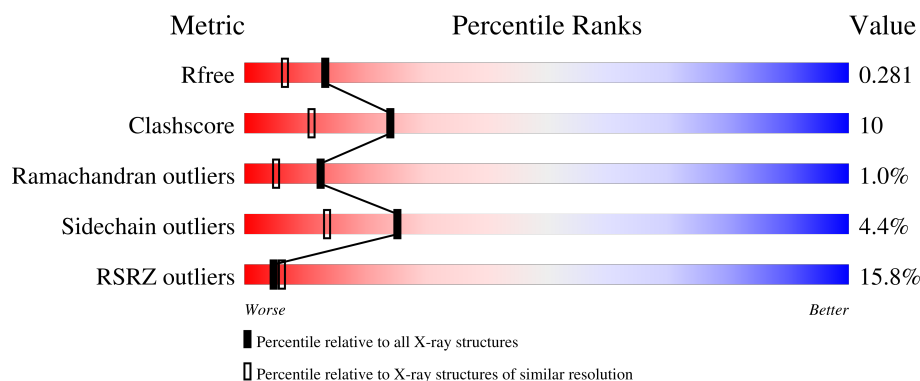
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	16% 73% 22% ..
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
8	CYS	A	620	-	X	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5209 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.

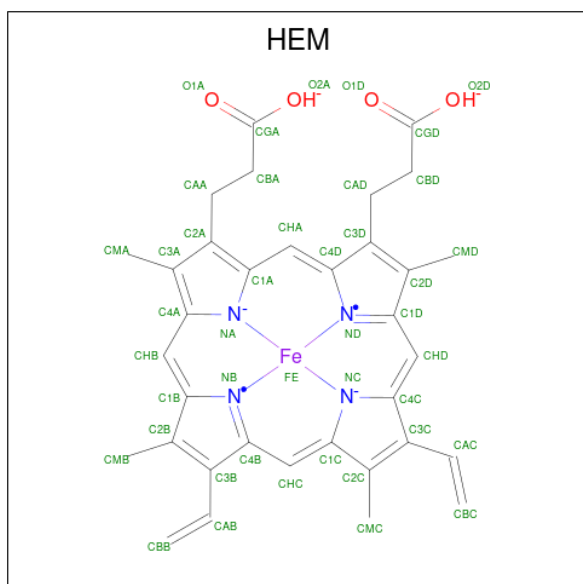
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

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



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

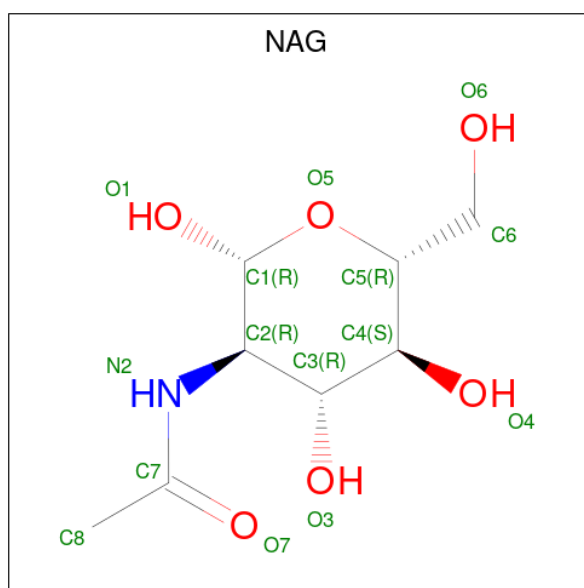
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

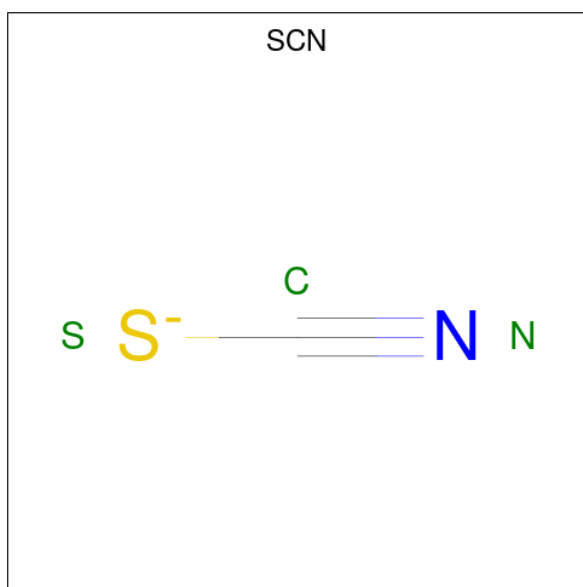
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	I		
			11	11	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



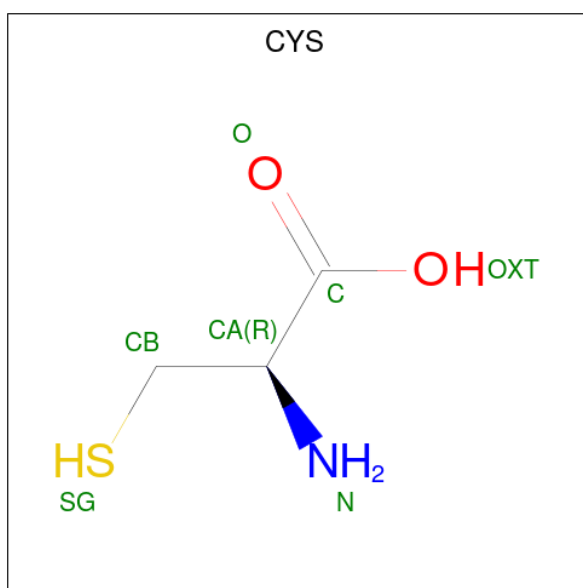
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O		
			14	8	1	5	0	0
6	A	1	Total	C	N	O		
			14	8	1	5	0	0
6	A	1	Total	C	N	O		
			14	8	1	5	0	0

- Molecule 7 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



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

- Molecule 8 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

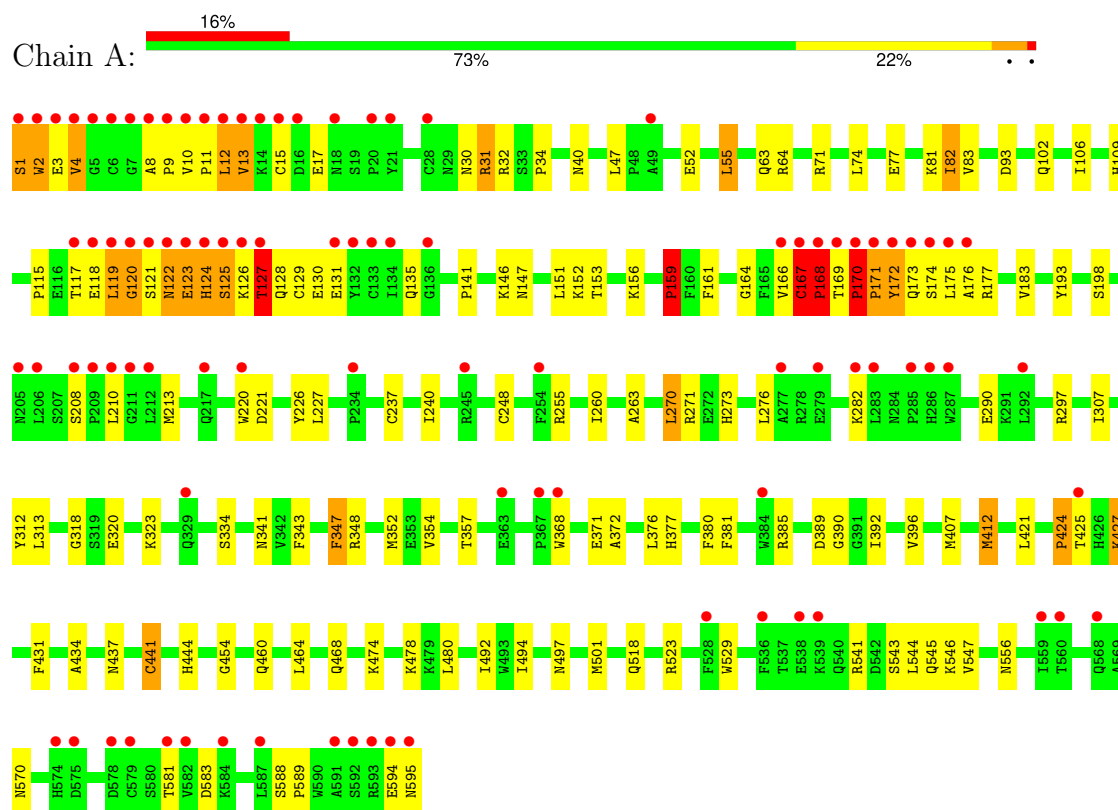
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	297	Total 297	O 297	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: 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 80.30Å 76.51Å 90.00° 102.02° 90.00°	Depositor
Resolution (Å)	74.83 – 1.98 74.83 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (74.83-1.98) 96.7 (74.83-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.252 0.235 , 0.281	Depositor DCC
R_{free} test set	2188 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5209	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 6.13% 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: HEM, IOD, CA, NAG, SCN, SEP

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	1.34	23/4891 (0.5%)	1.36	48/6634 (0.7%)

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	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	CYS	N-CA	8.43	1.58	1.46
1	A	434	ALA	CA-CB	8.41	1.66	1.53
1	A	312	TYR	C-O	-6.30	1.16	1.24
1	A	313	LEU	C-O	-6.28	1.18	1.24
1	A	372	ALA	CA-CB	-6.14	1.43	1.53
1	A	372	ALA	C-O	-5.92	1.17	1.24
1	A	492	ILE	C-O	-5.91	1.17	1.24
1	A	441	CYS	C-O	-5.84	1.17	1.24
1	A	170	PRO	CA-C	5.79	1.57	1.52
1	A	166	VAL	C-N	5.79	1.45	1.33
1	A	106	ILE	N-CA	5.60	1.53	1.46
1	A	82	ILE	C-O	-5.51	1.17	1.23
1	A	126	LYS	N-CA	-5.46	1.39	1.46
1	A	109	HIS	C-O	-5.45	1.17	1.24
1	A	494	ILE	CA-CB	5.27	1.61	1.54
1	A	121	SER	CA-C	5.23	1.55	1.52
1	A	357	THR	CA-C	5.17	1.59	1.52
1	A	248	CYS	C-O	5.14	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	HIS	CB-CG	5.08	1.57	1.50
1	A	47	LEU	CA-C	-5.06	1.47	1.52
1	A	460	GLN	N-CA	-5.02	1.41	1.46
1	A	183	VAL	CA-CB	5.01	1.62	1.54
1	A	11	PRO	N-CD	5.00	1.54	1.47

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	PRO	N-CA-C	13.27	139.81	112.47
1	A	169	THR	N-CA-C	12.07	129.16	112.75
1	A	170	PRO	N-CA-C	8.62	121.22	110.70
1	A	595	ASN	CA-CB-CG	8.27	120.87	112.60
1	A	170	PRO	C-N-CD	-7.65	93.64	125.00
1	A	125	SER	O-C-N	7.63	132.74	122.59
1	A	173	GLN	N-CA-C	7.37	120.36	109.24
1	A	125	SER	CA-C-N	7.32	135.51	121.54
1	A	125	SER	C-N-CA	7.32	135.51	121.54
1	A	127	THR	N-CA-C	7.08	121.01	109.76
1	A	240	ILE	N-CA-C	7.07	117.86	110.72
1	A	167	CYS	N-CA-C	-6.97	94.41	109.81
1	A	13	VAL	CB-CA-C	-6.93	100.84	110.96
1	A	119	LEU	CA-C-N	6.85	134.83	121.41
1	A	119	LEU	C-N-CA	6.85	134.83	121.41
1	A	13	VAL	CA-C-N	-6.67	112.39	123.33
1	A	13	VAL	C-N-CA	-6.67	112.39	123.33
1	A	125	SER	CA-C-O	6.59	129.93	120.51
1	A	122	ASN	CA-C-N	6.53	134.02	121.54
1	A	122	ASN	C-N-CA	6.53	134.02	121.54
1	A	124	HIS	CA-CB-CG	6.51	120.31	113.80
1	A	93	ASP	N-CA-C	-6.49	98.65	108.96
1	A	55	LEU	N-CA-C	6.34	120.62	112.12
1	A	412	MET	N-CA-C	6.34	118.06	111.03
1	A	125	SER	N-CA-C	6.32	124.26	110.80
1	A	31	ARG	N-CA-C	6.29	117.93	111.14
1	A	13	VAL	O-C-N	-6.20	115.85	123.10
1	A	390	GLY	N-CA-C	6.17	123.65	114.95
1	A	177	ARG	CB-CG-CD	-6.09	97.29	111.30
1	A	13	VAL	N-CA-C	6.07	116.61	107.80
1	A	82	ILE	N-CA-C	5.98	116.70	111.56
1	A	263	ALA	N-CA-C	-5.83	105.00	111.36
1	A	168	PRO	O-C-N	5.83	130.50	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLN	N-CA-C	5.77	118.04	111.11
1	A	347	PHE	N-CA-C	-5.69	106.29	113.18
1	A	81	LYS	N-CA-C	5.67	117.54	111.36
1	A	454	GLY	N-CA-C	5.55	119.36	112.64
1	A	159	PRO	CB-CA-C	5.51	118.56	111.56
1	A	427	LYS	N-CA-C	5.42	122.35	110.80
1	A	478	LYS	N-CA-C	5.40	116.85	111.07
1	A	172	TYR	N-CA-C	5.38	116.69	108.52
1	A	594	GLU	CA-C-N	5.25	131.16	121.70
1	A	594	GLU	C-N-CA	5.25	131.16	121.70
1	A	167	CYS	O-C-N	5.23	127.34	121.32
1	A	541	ARG	N-CA-C	5.21	116.96	111.28
1	A	260	ILE	N-CA-C	5.21	117.56	111.05
1	A	474	LYS	N-CA-C	5.18	116.61	111.07
1	A	570	ASN	N-CA-C	5.06	117.14	108.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	SER	Peptide
1	A	167	CYS	Peptide

5.2 Too-close contacts [i](#)

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	4774	0	4687	94	0
2	B	28	0	25	0	0
3	A	43	0	30	4	0
4	A	1	0	0	0	0
5	A	11	0	0	1	0
6	A	42	0	39	0	0
7	A	6	0	0	0	0
8	A	7	0	4	4	0
9	A	297	0	0	0	0
All	All	5209	0	4785	97	0

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

All (97) 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:170:PRO:HB2	1:A:171:PRO:CD	1.73	1.18
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.39	1.00
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.41	0.99
1:A:115:PRO:HG3	1:A:119:LEU:HD13	1.45	0.98
1:A:130:GLU:HA	1:A:159:PRO:HG3	1.58	0.85
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.58	0.83
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.05	0.82
1:A:407:MET:HB3	1:A:501:MET:HE2	1.62	0.81
1:A:407:MET:HB3	1:A:501:MET:CE	2.09	0.81
1:A:129:CYS:CB	1:A:161:PHE:HE1	1.97	0.77
1:A:127:THR:HG23	1:A:129:CYS:H	1.48	0.76
1:A:170:PRO:CB	1:A:171:PRO:CD	2.46	0.75
1:A:55:LEU:HD22	1:A:174:SER:H	1.52	0.73
1:A:115:PRO:CG	1:A:119:LEU:HD13	2.20	0.70
1:A:271:ARG:HG2	5:A:612:IOD:I	2.63	0.69
1:A:167:CYS:N	1:A:168:PRO:HD3	2.08	0.69
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.15	0.69
1:A:271:ARG:HB3	1:A:556:ASN:OD1	1.95	0.67
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.78	0.66
1:A:127:THR:HG23	1:A:129:CYS:N	2.10	0.66
1:A:129:CYS:HB3	1:A:161:PHE:HE1	1.60	0.65
1:A:255:ARG:HG2	8:A:620:CYS:HB3	1.77	0.64
1:A:543:SER:OG	1:A:589:PRO:HG2	1.99	0.63
1:A:464:LEU:O	1:A:468:GLN:HG3	1.99	0.62
1:A:352:MET:SD	1:A:407:MET:SD	2.97	0.62
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.35	0.62
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.30	0.61
1:A:129:CYS:HB3	1:A:161:PHE:CE1	2.35	0.60
1:A:129:CYS:SG	1:A:161:PHE:CE1	2.97	0.57
3:A:601:HEM:HBC2	3:A:601:HEM:HMC1	1.86	0.57
1:A:10:VAL:HG12	1:A:12:LEU:N	2.19	0.57
1:A:3:GLU:HG3	1:A:4:VAL:N	2.20	0.55
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.41	0.55
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.41	0.55
1:A:129:CYS:CB	1:A:161:PHE:CE1	2.86	0.55
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.42	0.55
1:A:10:VAL:CG1	1:A:12:LEU:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.42	0.54
1:A:13:VAL:O	1:A:13:VAL:HG12	2.07	0.53
1:A:407:MET:HE2	1:A:497:ASN:O	2.09	0.53
1:A:10:VAL:C	1:A:12:LEU:H	2.17	0.51
1:A:146:LYS:O	1:A:147:ASN:CB	2.59	0.51
1:A:118:GLU:C	1:A:120:GLY:H	2.19	0.51
1:A:385:ARG:O	1:A:389:ASP:HB3	2.10	0.50
1:A:129:CYS:SG	1:A:161:PHE:HE1	2.35	0.50
1:A:175:LEU:HD23	1:A:176:ALA:O	2.12	0.49
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.59	0.49
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.49
1:A:82:ILE:CD1	1:A:480:LEU:HD23	2.42	0.49
1:A:237:CYS:HA	1:A:381:PHE:O	2.13	0.49
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.93	0.49
1:A:341:ASN:OD1	1:A:444:HIS:ND1	2.33	0.49
1:A:17:GLU:HG2	1:A:31:ARG:HG2	1.95	0.49
1:A:3:GLU:HG3	1:A:4:VAL:H	1.78	0.49
1:A:545:GLN:O	1:A:545:GLN:HG3	2.12	0.49
1:A:122:ASN:CG	1:A:123:GLU:H	2.20	0.48
1:A:146:LYS:O	1:A:147:ASN:HB2	2.14	0.47
1:A:1:SER:O	1:A:2:TRP:C	2.56	0.47
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.50	0.46
1:A:122:ASN:CG	1:A:123:GLU:N	2.74	0.46
1:A:424:PRO:C	1:A:425:THR:HG23	2.40	0.46
1:A:10:VAL:C	1:A:12:LEU:N	2.72	0.46
1:A:546:LYS:HB3	1:A:583:ASP:HB3	1.97	0.46
1:A:30:ASN:O	1:A:34:PRO:HA	2.16	0.45
1:A:371:GLU:CD	1:A:385:ARG:HH12	2.24	0.45
1:A:128:GLN:O	1:A:131:GLU:HB2	2.16	0.45
1:A:151:LEU:CD2	1:A:156:LYS:HD3	2.46	0.45
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.14	0.45
1:A:40:ASN:HD21	1:A:119:LEU:HD21	1.82	0.45
1:A:193:TYR:CE2	1:A:297:ARG:HG3	2.52	0.45
1:A:392:ILE:O	1:A:396:VAL:HG23	2.17	0.44
1:A:74:LEU:HB2	1:A:77:GLU:HB2	1.99	0.44
1:A:3:GLU:CG	1:A:4:VAL:N	2.80	0.44
3:A:601:HEM:CMA	8:A:620:CYS:HA	2.48	0.44
1:A:83:VAL:HG12	1:A:83:VAL:O	2.17	0.43
1:A:323:LYS:HB2	1:A:323:LYS:HE3	1.54	0.43
3:A:601:HEM:HMA1	8:A:620:CYS:HA	2.00	0.42
1:A:135:GLN:HB2	1:A:141:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:TRP:HZ3	1:A:389:ASP:OD1	2.03	0.42
1:A:17:GLU:CB	1:A:31:ARG:HE	2.32	0.42
1:A:255:ARG:HG2	8:A:620:CYS:CB	2.46	0.41
1:A:421:LEU:HB3	1:A:431:PHE:HB2	2.03	0.41
1:A:544:LEU:O	1:A:547:VAL:HG22	2.20	0.41
1:A:8:ALA:CB	1:A:9:PRO:CD	2.96	0.41
1:A:117:THR:O	1:A:118:GLU:HB2	2.19	0.41
1:A:318:GLY:C	1:A:320:GLU:H	2.28	0.41
1:A:354:VAL:HG12	1:A:376:LEU:HD22	2.02	0.41
1:A:13:VAL:HG13	1:A:15:CYS:SG	2.61	0.41
1:A:118:GLU:C	1:A:120:GLY:N	2.79	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.95	0.41
1:A:290:GLU:HA	1:A:290:GLU:OE1	2.21	0.41
1:A:82:ILE:CD1	1:A:480:LEU:CD2	2.99	0.40
1:A:348:ARG:HD3	1:A:437:ASN:ND2	2.36	0.40
1:A:407:MET:HE1	1:A:412:MET:HE2	2.03	0.40
1:A:151:LEU:HD21	1:A:156:LYS:HD3	2.04	0.40
1:A:208:SER:C	1:A:210:LEU:H	2.29	0.40
1:A:347:PHE:HB3	3:A:601:HEM:HMD3	2.04	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	592/595 (100%)	558 (94%)	28 (5%)	6 (1%)	12 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLY
1	A	168	PRO

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Mol	Chain	Res	Type
1	A	171	PRO
1	A	123	GLU
1	A	170	PRO
1	A	427	LYS

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	517/517 (100%)	494 (96%)	23 (4%)	25	14

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

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	12	LEU
1	A	32	ARG
1	A	52	GLU
1	A	63	GLN
1	A	64	ARG
1	A	71	ARG
1	A	124	HIS
1	A	125	SER
1	A	127	THR
1	A	152	LYS
1	A	153	THR
1	A	159	PRO
1	A	172	TYR
1	A	220	TRP
1	A	270	LEU
1	A	282	LYS
1	A	307	ILE
1	A	334	SER
1	A	424	PRO
1	A	441	CYS

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Mol	Chain	Res	Type
1	A	581	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	40	ASN
1	A	128	GLN
1	A	138	ASN
1	A	366	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	521	GLN
1	A	568	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	$\# Z > 2$
1	SEP	A	198	1	8,9,10	1.58	2 (25%)	7,12,14	3.95	5 (71%)

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	-	3/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-N	-3.01	1.39	1.48
1	A	198	SEP	P-O2P	-2.04	1.47	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-OG	6.79	124.39	106.67
1	A	198	SEP	OG-P-O1P	-5.48	91.63	106.44
1	A	198	SEP	O3P-P-OG	4.75	119.05	106.67
1	A	198	SEP	O2P-P-O1P	-2.41	101.46	110.83
1	A	198	SEP	OG-CB-CA	2.01	110.10	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	C-CA-CB-OG
1	A	198	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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	1.02	0	17,19,21	1.59	7 (41%)
2	NAG	B	2	2	14,14,15	0.56	0	17,19,21	2.55	7 (41%)

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.88	122.75	112.19
2	B	2	NAG	C2-N2-C7	3.42	127.48	122.90
2	B	2	NAG	C3-C4-C5	2.94	115.56	110.23
2	B	1	NAG	C2-N2-C7	2.53	126.29	122.90
2	B	1	NAG	C3-C4-C5	2.52	114.80	110.23
2	B	1	NAG	C1-O5-C5	2.50	115.53	112.19
2	B	2	NAG	C4-C3-C2	2.41	114.55	111.02
2	B	2	NAG	O5-C5-C4	2.40	116.66	110.83
2	B	1	NAG	O7-C7-C8	-2.34	117.88	122.05
2	B	1	NAG	O7-C7-N2	2.31	126.07	121.98
2	B	1	NAG	O4-C4-C3	-2.31	104.93	110.38
2	B	1	NAG	C1-C2-N2	2.23	113.95	110.43
2	B	2	NAG	C6-C5-C4	-2.12	107.82	113.02
2	B	2	NAG	C1-C2-N2	2.07	113.70	110.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

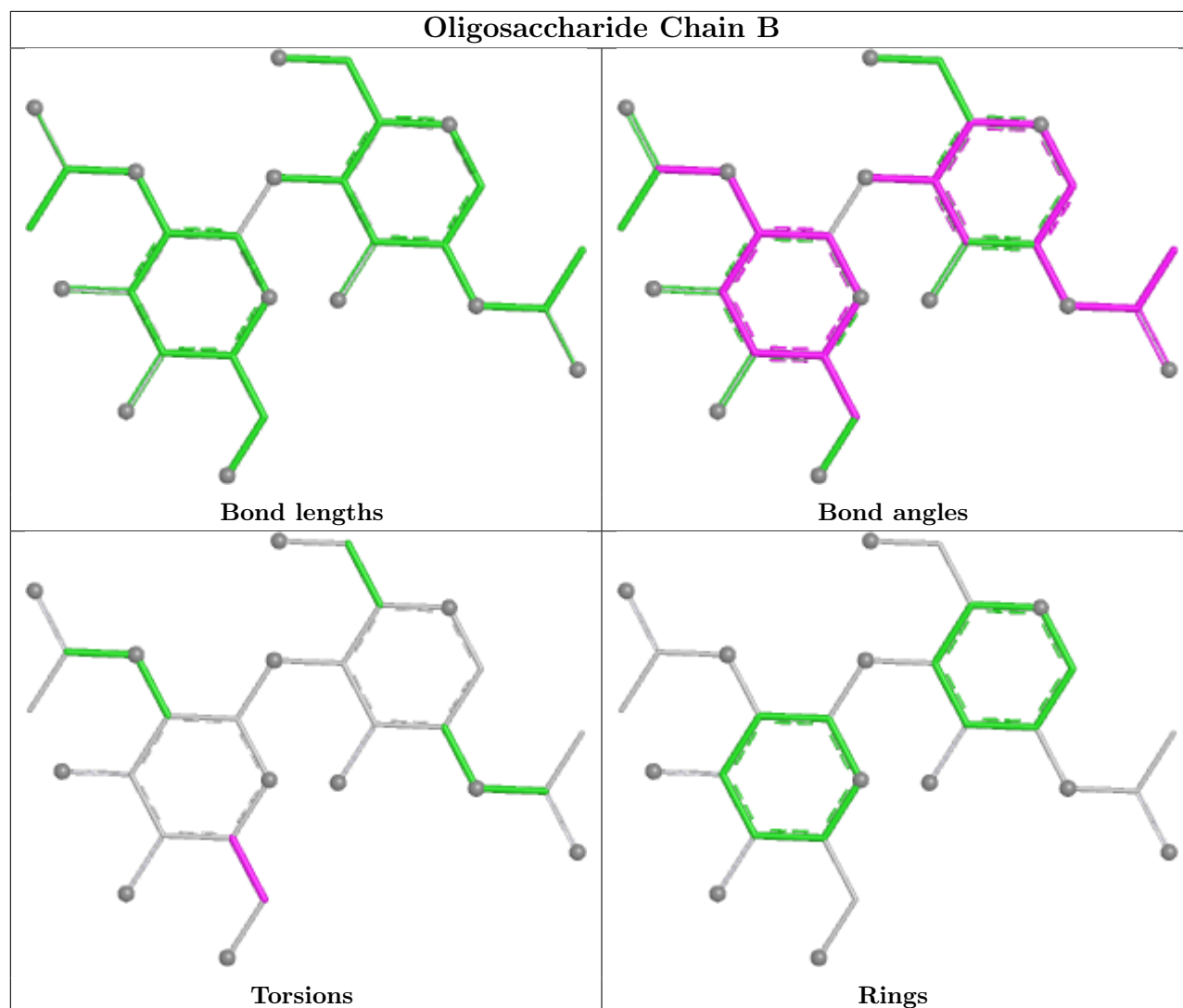
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6

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 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	$\# Z > 2$
7	SCN	A	619	-	1,2,2	0.85	0	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	617	1	14,14,15	0.64	0	17,19,21	1.49	3 (17%)
7	SCN	A	621	-	1,2,2	1.67	0	0,1,1	-	-
6	NAG	A	616	1	14,14,15	0.55	0	17,19,21	1.20	2 (11%)
3	HEM	A	601	9,1	50,50,50	2.38	18 (36%)	67,82,82	2.02	14 (20%)
8	CYS	A	620	-	5,6,6	3.10	3 (60%)	3,7,7	2.08	1 (33%)
6	NAG	A	618	1	14,14,15	0.62	0	17,19,21	1.24	1 (5%)

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
6	NAG	A	617	1	-	1/6/23/26	0/1/1/1
6	NAG	A	616	1	-	0/6/23/26	0/1/1/1
3	HEM	A	601	9,1	-	4/14/54/54	-
8	CYS	A	620	-	-	6/6/6/6	-
6	NAG	A	618	1	-	2/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	FE-ND	8.05	2.19	1.94
3	A	601	HEM	FE-NB	7.36	2.17	1.94
8	A	620	CYS	CB-SG	-5.65	1.69	1.81
3	A	601	HEM	C4D-ND	-4.89	1.31	1.40
3	A	601	HEM	C3D-C2D	4.17	1.45	1.36
3	A	601	HEM	CMC-C2C	3.22	1.57	1.50
3	A	601	HEM	CAB-C3B	3.19	1.55	1.47
3	A	601	HEM	CAC-C3C	2.89	1.55	1.47
8	A	620	CYS	CB-CA	-2.88	1.49	1.53
3	A	601	HEM	CMA-C3A	2.83	1.56	1.50
3	A	601	HEM	C3C-C2C	-2.82	1.31	1.37
3	A	601	HEM	C1B-NB	-2.71	1.35	1.40
3	A	601	HEM	O1A-CGA	2.44	1.30	1.22
3	A	601	HEM	CMD-C2D	2.43	1.55	1.50
3	A	601	HEM	C1A-NA	-2.32	1.35	1.39
3	A	601	HEM	CAD-C3D	2.28	1.57	1.51
8	A	620	CYS	O-C	2.13	1.28	1.22
3	A	601	HEM	FE-NA	2.11	2.02	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	C2A-C3A	-2.10	1.33	1.38
3	A	601	HEM	CMB-C2B	2.08	1.55	1.50
3	A	601	HEM	C1D-C2D	-2.01	1.40	1.44

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEM	C4D-ND-C1D	6.60	113.03	105.21
3	A	601	HEM	C1B-NB-C4B	6.25	112.61	105.21
3	A	601	HEM	C2B-C1B-NB	-4.07	105.16	109.84
6	A	617	NAG	C1-C2-N2	-3.84	104.39	110.43
3	A	601	HEM	CHC-C1C-NC	3.82	128.61	124.45
3	A	601	HEM	CMD-C2D-C1D	3.82	131.00	125.03
3	A	601	HEM	CHD-C4C-NC	3.76	128.54	124.45
3	A	601	HEM	C3B-C4B-NB	-3.72	106.80	109.47
3	A	601	HEM	CAD-CBD-CGD	-3.69	103.87	113.67
3	A	601	HEM	C3D-C4D-ND	-3.68	106.13	110.17
3	A	601	HEM	CHC-C4B-NB	3.57	128.26	124.42
8	A	620	CYS	CB-CA-C	-3.25	106.65	109.89
3	A	601	HEM	C2A-C1A-NA	-3.06	106.75	110.15
6	A	616	NAG	O5-C5-C6	2.90	113.31	107.66
3	A	601	HEM	CBD-CAD-C3D	-2.73	104.99	112.53
3	A	601	HEM	C3B-C2B-C1B	2.69	108.43	106.41
6	A	617	NAG	O5-C5-C6	2.63	112.78	107.66
6	A	616	NAG	C3-C4-C5	-2.63	105.46	110.23
6	A	618	NAG	C1-C2-N2	2.17	113.86	110.43
6	A	617	NAG	O5-C1-C2	-2.09	108.05	111.29
3	A	601	HEM	CHA-C4D-C3D	2.05	129.00	125.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	620	CYS	O-C-CA-CB
8	A	620	CYS	OXT-C-CA-CB
8	A	620	CYS	N-CA-CB-SG
8	A	620	CYS	C-CA-CB-SG
6	A	618	NAG	O5-C5-C6-O6
6	A	618	NAG	C4-C5-C6-O6
8	A	620	CYS	OXT-C-CA-N
8	A	620	CYS	O-C-CA-N
6	A	617	NAG	C4-C5-C6-O6

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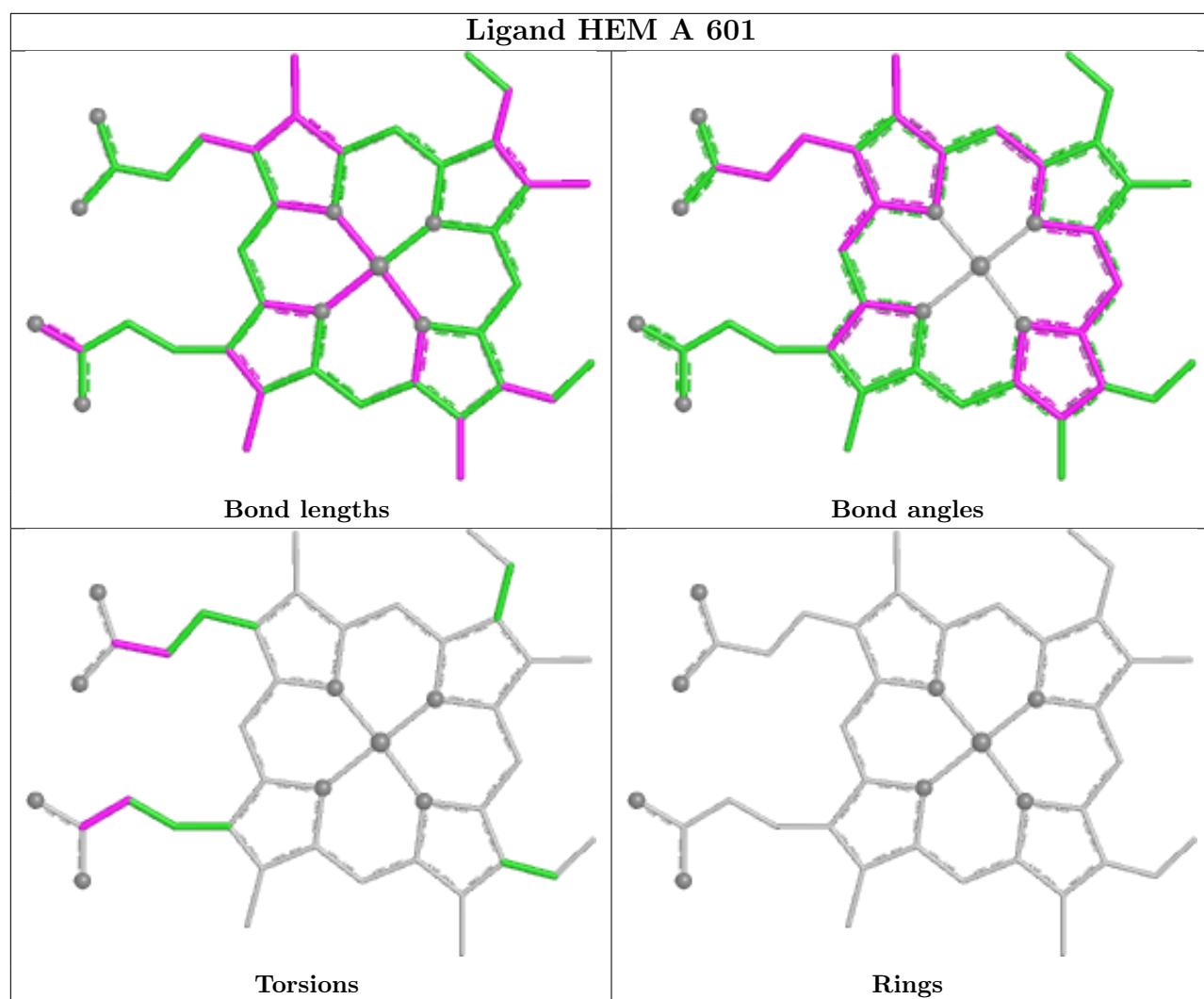
Mol	Chain	Res	Type	Atoms
3	A	601	HEM	CAA-CBA-CGA-O2A
3	A	601	HEM	CAD-CBD-CGD-O1D
3	A	601	HEM	CAD-CBD-CGD-O2D
3	A	601	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	4	0
8	A	620	CYS	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	1.02	94 (15%) 5 6	20, 37, 79, 109	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	6.9
1	A	10	VAL	6.3
1	A	2	TRP	6.1
1	A	119	LEU	6.0
1	A	7	GLY	5.8
1	A	121	SER	5.7
1	A	172	TYR	5.4
1	A	167	CYS	5.2
1	A	4	VAL	5.0
1	A	168	PRO	4.8
1	A	124	HIS	4.7
1	A	5	GLY	4.6
1	A	13	VAL	4.2
1	A	122	ASN	4.1
1	A	12	LEU	4.0
1	A	209	PRO	3.8
1	A	220	TRP	3.8
1	A	123	GLU	3.8
1	A	14	LYS	3.8
1	A	16	ASP	3.7
1	A	210	LEU	3.7
1	A	593	ARG	3.7
1	A	594	GLU	3.6
1	A	6	CYS	3.6
1	A	277	ALA	3.6
1	A	11	PRO	3.6
1	A	595	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	125	SER	3.6
1	A	9	PRO	3.5
1	A	127	THR	3.5
1	A	20	PRO	3.5
1	A	171	PRO	3.5
1	A	206	LEU	3.5
1	A	292	LEU	3.4
1	A	169	THR	3.4
1	A	170	PRO	3.3
1	A	1	SER	3.3
1	A	3	GLU	3.3
1	A	175	LEU	3.3
1	A	120	GLY	3.2
1	A	592	SER	3.2
1	A	166	VAL	3.0
1	A	559	ILE	3.0
1	A	283	LEU	2.9
1	A	579	CYS	2.9
1	A	117	THR	2.9
1	A	132	TYR	2.8
1	A	131	GLU	2.8
1	A	582	VAL	2.8
1	A	581	THR	2.7
1	A	282	LYS	2.7
1	A	591	ALA	2.6
1	A	174	SER	2.6
1	A	217	GLN	2.6
1	A	285	PRO	2.5
1	A	134	ILE	2.5
1	A	208	SER	2.5
1	A	126	LYS	2.5
1	A	18	ASN	2.5
1	A	254	PHE	2.4
1	A	176	ALA	2.4
1	A	49	ALA	2.4
1	A	363	GLU	2.4
1	A	173	GLN	2.4
1	A	286	HIS	2.4
1	A	287	TRP	2.4
1	A	584	LYS	2.4
1	A	211	GLY	2.3
1	A	279	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	28	CYS	2.3
1	A	21	TYR	2.2
1	A	560	THR	2.2
1	A	212	LEU	2.2
1	A	329	GLN	2.2
1	A	528	PHE	2.2
1	A	539	LYS	2.2
1	A	538	GLU	2.2
1	A	15	CYS	2.2
1	A	234	PRO	2.2
1	A	367	PRO	2.2
1	A	384	TRP	2.2
1	A	578	ASP	2.2
1	A	133	CYS	2.2
1	A	574	HIS	2.1
1	A	136	GLY	2.1
1	A	587	LEU	2.1
1	A	536	PHE	2.1
1	A	568	GLN	2.1
1	A	368	TRP	2.1
1	A	245	ARG	2.1
1	A	205	ASN	2.1
1	A	575	ASP	2.1
1	A	118	GLU	2.0
1	A	425	THR	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($\text{\AA}^2$)	Q<0.9
1	SEP	A	198	10/11	0.93	0.13	27,41,44,48	0

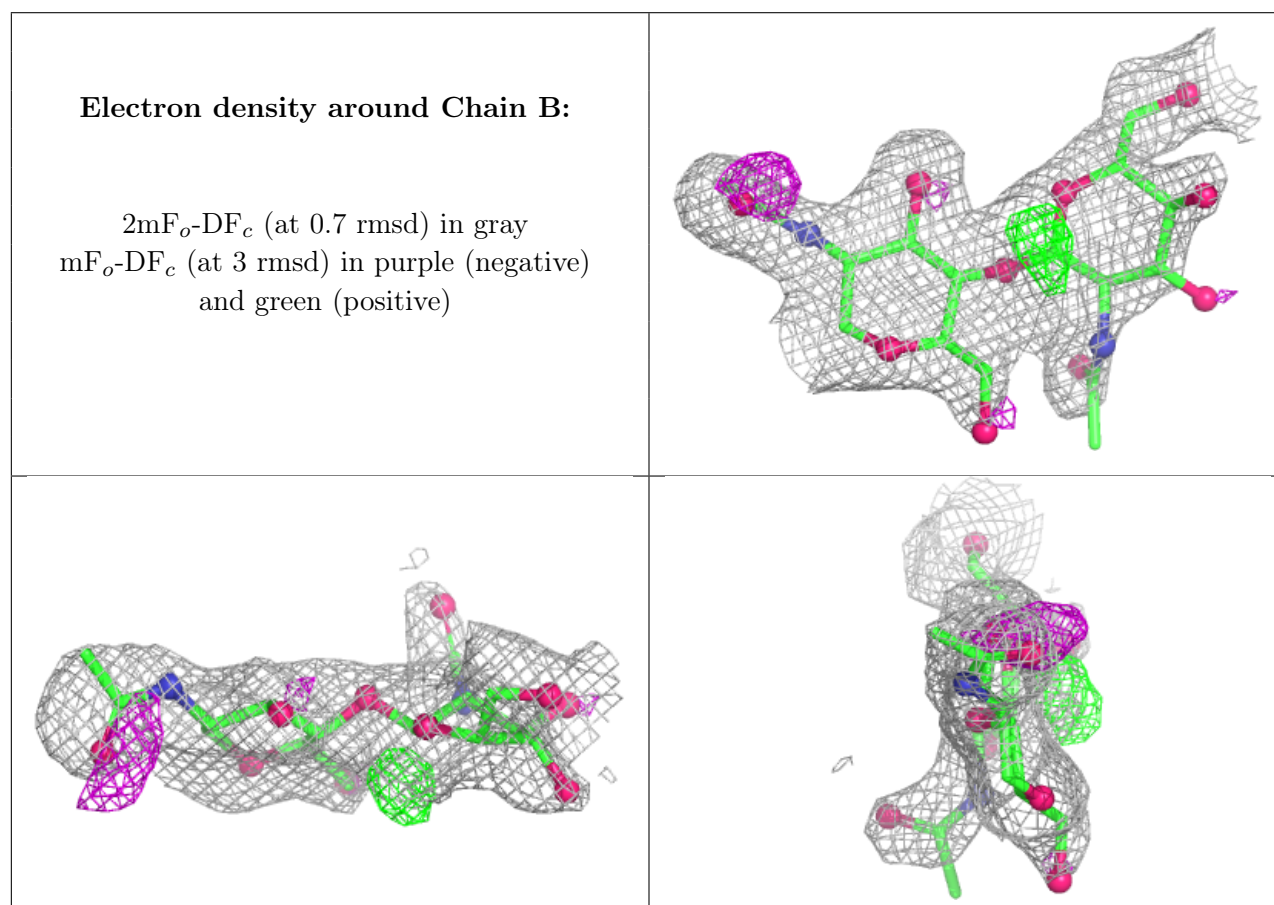
6.3 Carbohydrates ⓘ

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
2	NAG	B	2	14/15	0.61	0.16	51,59,62,63	0
2	NAG	B	1	14/15	0.84	0.10	24,29,38,38	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.

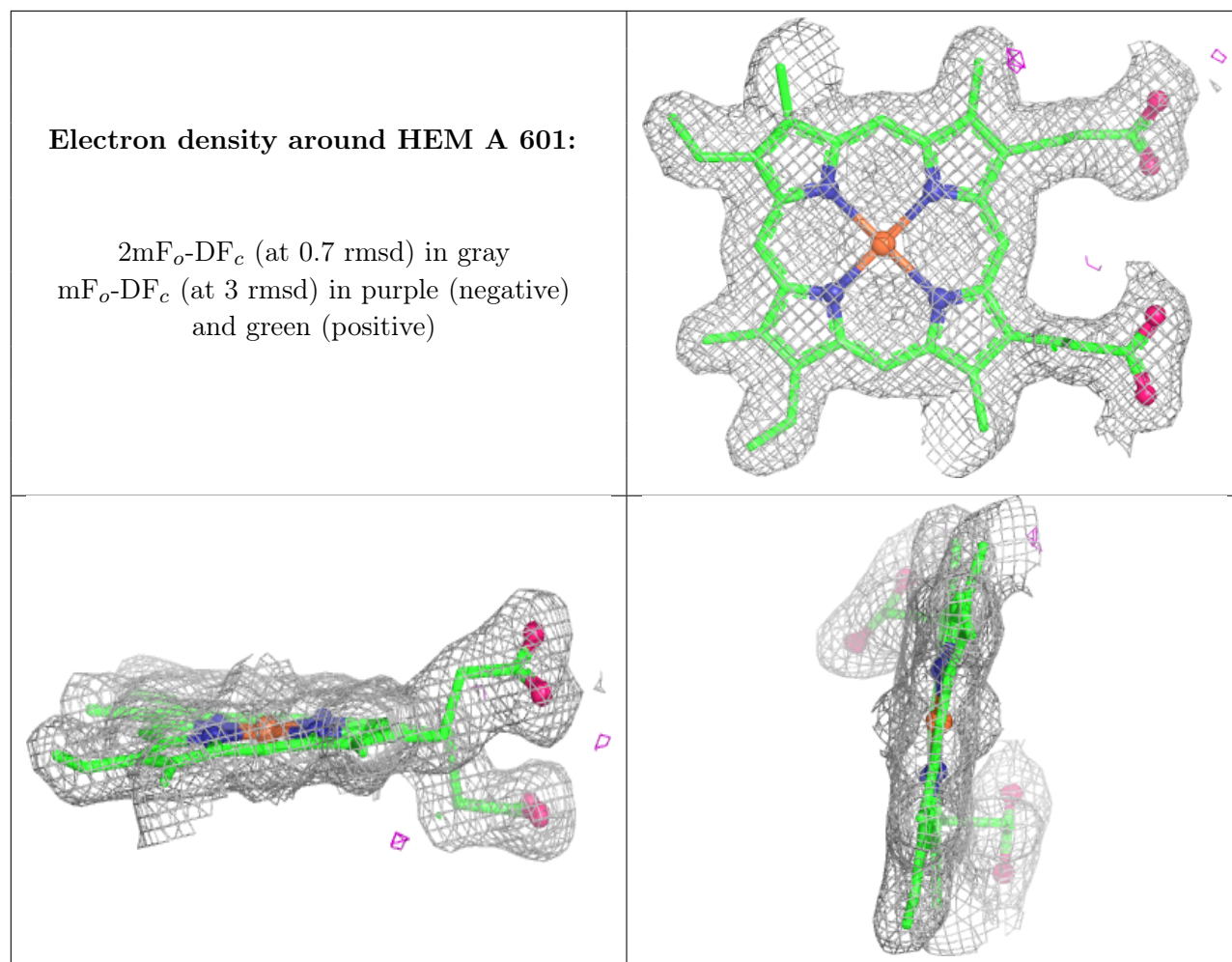
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	617	14/15	0.70	0.13	39,44,46,47	0
6	NAG	A	618	14/15	0.75	0.13	40,45,54,55	0
6	NAG	A	616	14/15	0.82	0.10	22,30,36,39	0
5	IOD	A	612	1/1	0.90	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SCN	A	621	3/3	0.92	0.15	48,48,49,49	0
5	IOD	A	611	1/1	0.93	0.24	45,45,45,45	0
5	IOD	A	609	1/1	0.93	0.16	47,47,47,47	0
5	IOD	A	608	1/1	0.94	0.20	37,37,37,37	0
5	IOD	A	613	1/1	0.95	0.20	68,68,68,68	0
8	CYS	A	620	7/7	0.95	0.17	22,36,38,40	0
5	IOD	A	607	1/1	0.97	0.09	27,27,27,27	0
3	HEM	A	601	43/43	0.97	0.05	10,15,22,24	0
7	SCN	A	619	3/3	0.97	0.08	9,9,12,14	0
5	IOD	A	605	1/1	0.97	0.16	31,31,31,31	0
5	IOD	A	610	1/1	0.97	0.15	70,70,70,70	0
5	IOD	A	604	1/1	0.98	0.12	42,42,42,42	0
4	CA	A	602	1/1	0.98	0.05	17,17,17,17	0
5	IOD	A	603	1/1	0.98	0.12	34,34,34,34	0
5	IOD	A	606	1/1	1.00	0.02	19,19,19,19	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.