Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 08:09 PM EDT

PDB ID	:	3R5O
Title	:	Crystal structure of the complex of bovine lactoperoxidase with 4-allyl-2-methoxyphenol at 2.6 A resolution
Authors	:	Pandey, N.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2011-03-19
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

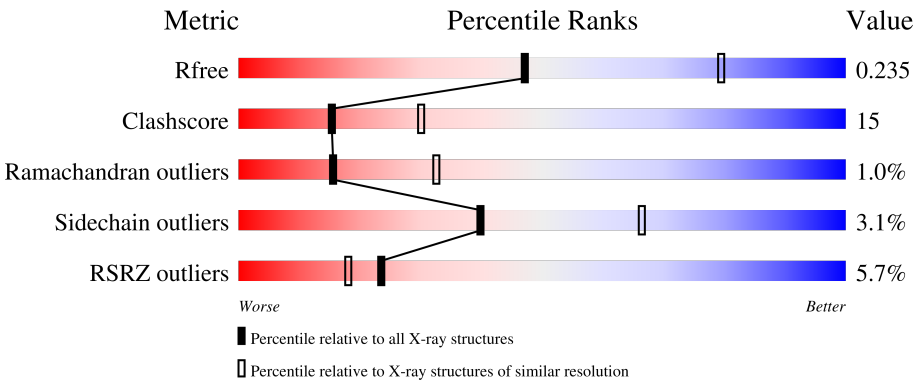
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	6% 76% 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
6	IOD	A	612	-	-	X	-
7	EUG	A	597	-	X	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 5085 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
			Total	C	N	O	P	S			
1	A	595	4775	3037	847	864	1	26	0	0	0

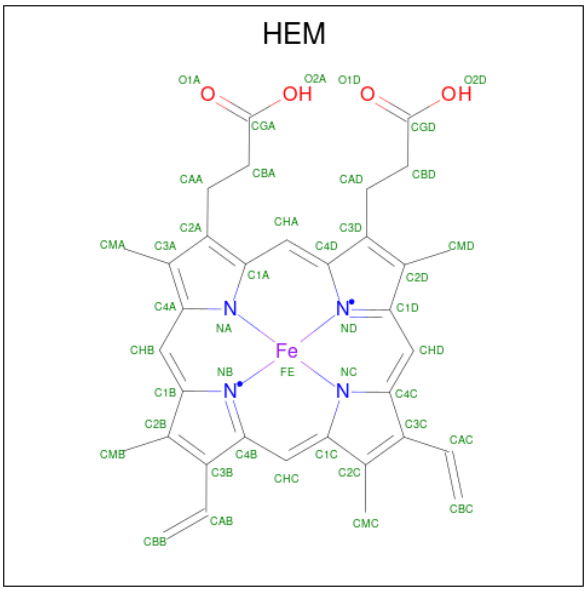
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

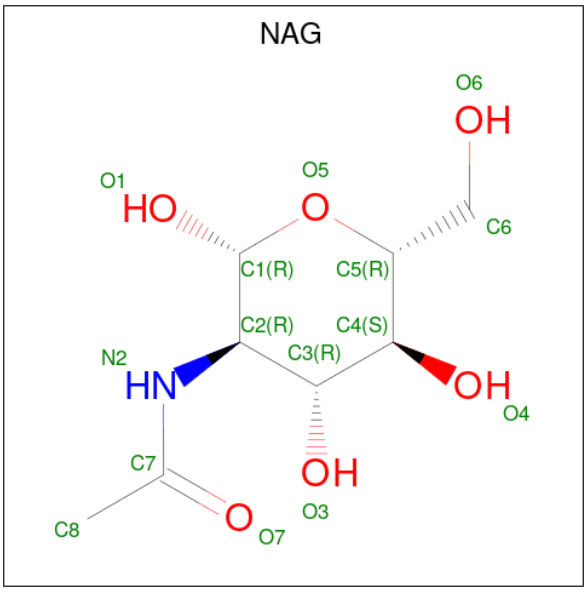
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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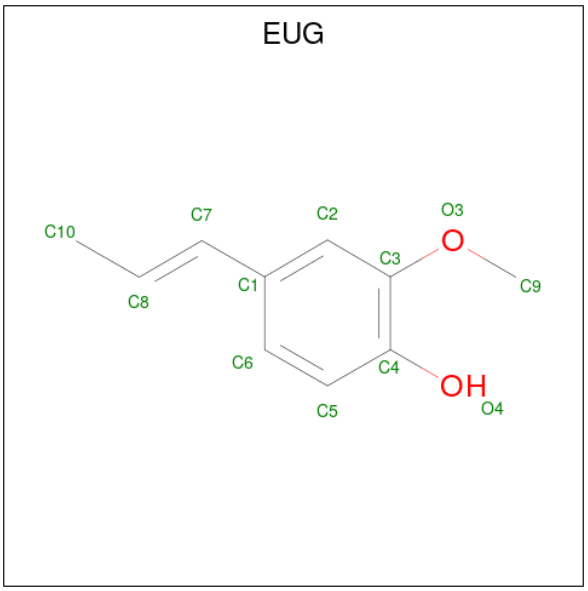
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

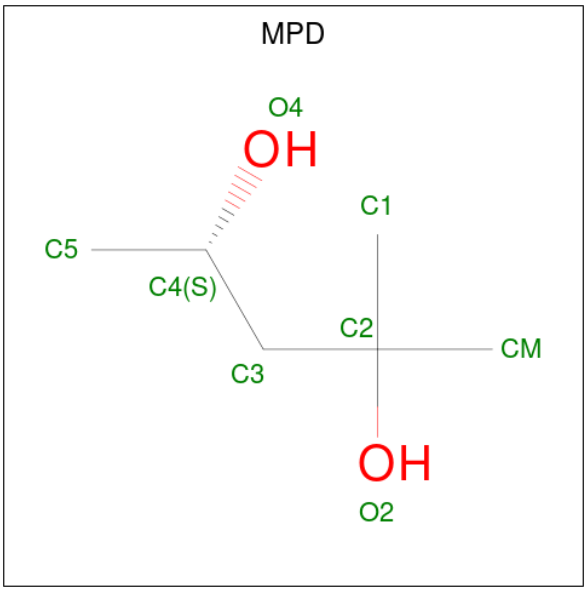
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
6	A	10	10	10	0	0

- Molecule 7 is 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (three-letter code: EUG) (formula: $C_{10}H_{12}O_2$).



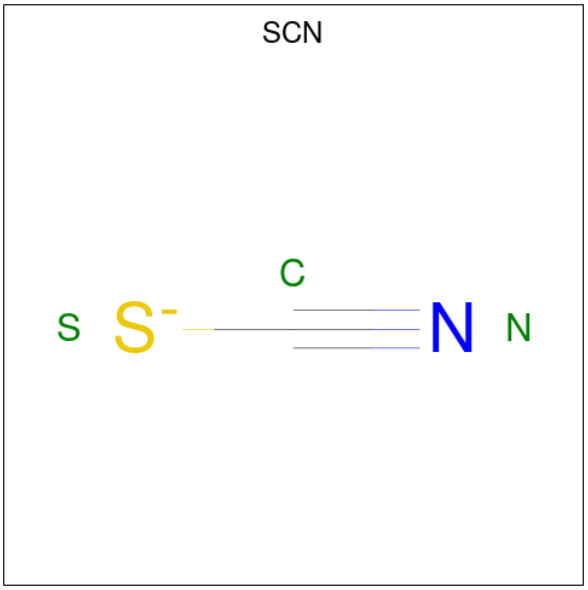
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	11	9	2	0	0

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



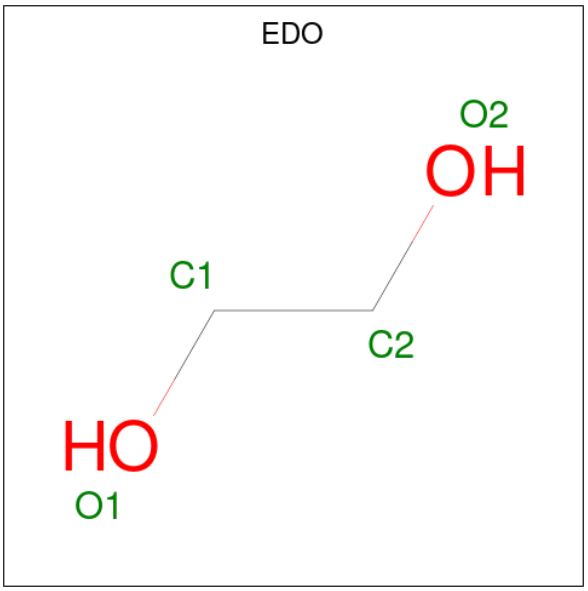
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
8	A	1	8	6	2		0	0

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



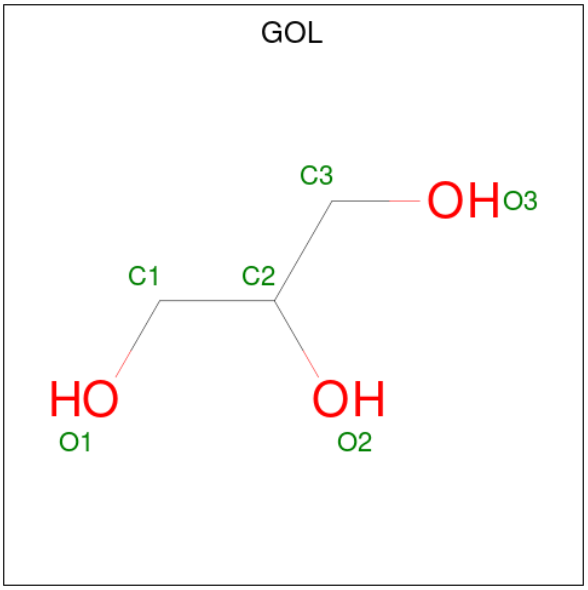
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
9	A	1	3	1	1	1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 12 is water.

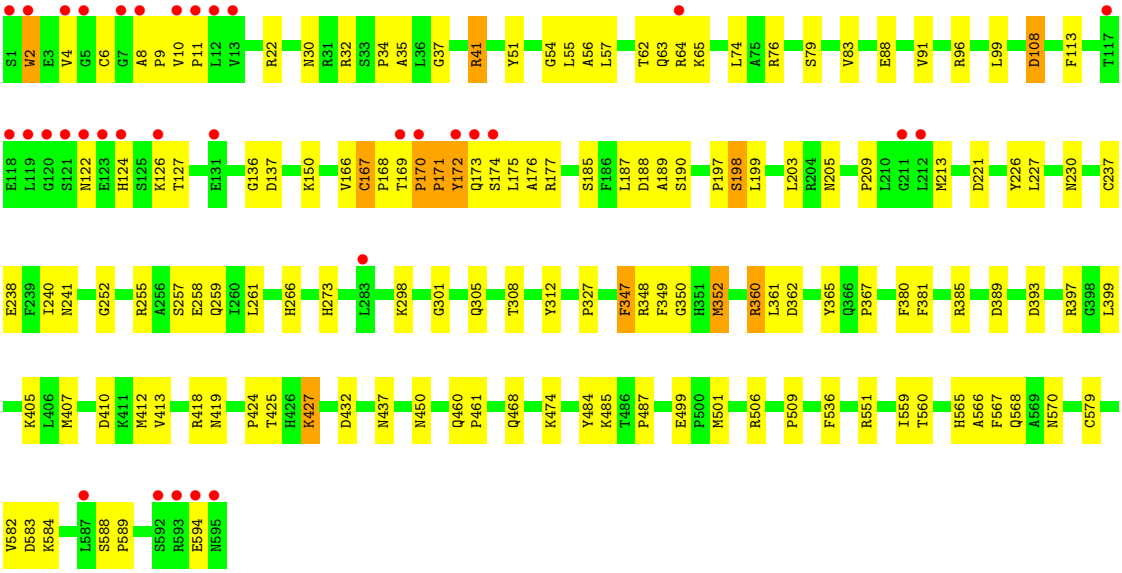
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	A	150	150	150	0	0

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

Chain A:



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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.01Å 80.05Å 75.68Å 90.00° 102.98° 90.00°	Depositor
Resolution (Å)	24.00 – 2.60 43.98 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.00-2.60) 98.6 (43.98-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.09 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.245 0.215 , 0.235	Depositor DCC
R_{free} test set	944 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.979	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, HEM, IOD, EUG, SEP, EDO, NAG, GOL, CA, MPD

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	0.46	0/4892	0.68	2/6634 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	6	CYS	N-CA-C	-5.68	95.67	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4775	0	4687	141	0
2	B	28	0	25	1	0
3	A	1	0	0	0	0
4	A	43	0	30	5	0
5	A	42	0	39	0	0
6	A	10	0	0	4	0
7	A	11	0	8	4	0
8	A	8	0	13	1	0
9	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	8	0	12	0	0
11	A	6	0	8	0	0
12	A	150	0	0	10	0
All	All	5085	0	4822	145	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 15.

All (145) 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:150:LYS:HE2	1:A:419:ASN:HD22	1.17	1.10
1:A:170:PRO:CG	1:A:171:PRO:HD3	1.82	1.10
1:A:170:PRO:CD	1:A:171:PRO:HD3	1.88	1.02
1:A:168:PRO:HG3	1:A:172:TYR:CG	1.97	1.00
1:A:168:PRO:HG3	1:A:172:TYR:HB2	1.44	0.98
1:A:170:PRO:HG2	1:A:171:PRO:HD3	1.45	0.97
1:A:168:PRO:HG3	1:A:172:TYR:CB	2.00	0.92
1:A:76:ARG:HH22	1:A:419:ASN:HD21	1.18	0.90
1:A:360:ARG:O	1:A:361:LEU:HD23	1.71	0.90
1:A:170:PRO:HD2	1:A:171:PRO:HD3	1.55	0.89
1:A:150:LYS:HE2	1:A:419:ASN:ND2	1.92	0.84
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.12	0.84
1:A:197:PRO:HD2	1:A:198:SEP:O3P	1.78	0.83
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.60	0.82
1:A:150:LYS:CE	1:A:419:ASN:HD22	1.94	0.80
1:A:360:ARG:C	1:A:361:LEU:HD23	2.02	0.79
1:A:167:CYS:CB	1:A:168:PRO:CD	2.62	0.77
1:A:170:PRO:HD2	1:A:171:PRO:CD	2.13	0.77
1:A:425:THR:HG22	1:A:425:THR:O	1.84	0.76
1:A:91:VAL:HG22	1:A:405:LYS:HG3	1.70	0.74
1:A:551:ARG:HD3	1:A:583:ASP:O	1.91	0.71
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.88	0.71
1:A:170:PRO:CD	1:A:171:PRO:CD	2.67	0.70
1:A:2:TRP:HB3	1:A:175:LEU:CD1	2.22	0.70
1:A:76:ARG:HH22	1:A:419:ASN:ND2	1.90	0.68
1:A:51:TYR:HD2	1:A:57:LEU:O	1.76	0.68
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.24	0.67
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.26	0.66
1:A:168:PRO:HB2	1:A:171:PRO:O	1.97	0.64
1:A:168:PRO:CB	1:A:171:PRO:O	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:CG	1:A:172:TYR:HB2	2.21	0.64
1:A:4:VAL:HG23	1:A:4:VAL:O	1.97	0.63
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.47	0.62
1:A:205:ASN:HA	12:A:719:HOH:O	1.99	0.62
1:A:227:LEU:HD11	1:A:266:HIS:HB3	1.83	0.61
1:A:168:PRO:CG	1:A:172:TYR:CD1	2.81	0.61
1:A:83:VAL:HG12	1:A:413:VAL:HB	1.83	0.60
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.84	0.60
1:A:172:TYR:O	1:A:173:GLN:HG3	2.03	0.59
1:A:450:ASN:ND2	1:A:487:PRO:HB2	2.17	0.59
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.85	0.58
1:A:51:TYR:CD2	1:A:57:LEU:O	2.55	0.58
1:A:2:TRP:CD1	1:A:175:LEU:HD11	2.38	0.58
1:A:169:THR:HB	1:A:170:PRO:HD3	1.86	0.57
1:A:30:ASN:O	1:A:34:PRO:HA	2.03	0.57
1:A:237:CYS:HA	1:A:381:PHE:O	2.04	0.57
1:A:385:ARG:O	1:A:389:ASP:HB3	2.04	0.57
1:A:259:GLN:OE1	1:A:261:LEU:HB2	2.04	0.57
1:A:425:THR:O	1:A:425:THR:CG2	2.53	0.56
1:A:63:GLN:OE1	1:A:63:GLN:N	2.30	0.56
4:A:605:HEM:HMC2	4:A:605:HEM:HBC2	1.88	0.56
1:A:407:MET:HB3	1:A:501:MET:CE	2.36	0.55
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.72	0.55
1:A:301:GLY:O	1:A:305:GLN:HG3	2.07	0.55
1:A:427:LYS:HD3	1:A:427:LYS:H	1.72	0.54
1:A:32:ARG:HD3	12:A:742:HOH:O	2.08	0.54
1:A:230:ASN:C	1:A:230:ASN:OD1	2.46	0.54
1:A:461:PRO:O	1:A:487:PRO:HG2	2.07	0.54
1:A:255:ARG:HB3	7:A:597:EUG:C5	2.38	0.53
1:A:32:ARG:HD2	12:A:675:HOH:O	2.07	0.53
1:A:170:PRO:HG2	1:A:171:PRO:CD	2.31	0.53
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.89	0.53
1:A:168:PRO:CG	1:A:172:TYR:CG	2.85	0.53
1:A:2:TRP:HD1	1:A:175:LEU:HD11	1.75	0.52
4:A:605:HEM:HMB2	4:A:605:HEM:HBB2	1.91	0.52
1:A:484:TYR:O	1:A:485:LYS:HB2	2.09	0.52
1:A:188:ASP:O	1:A:189:ALA:HB3	2.11	0.51
1:A:2:TRP:HB3	1:A:175:LEU:HD12	1.93	0.51
1:A:582:VAL:HA	12:A:768:HOH:O	2.09	0.51
1:A:177:ARG:HA	12:A:634:HOH:O	2.10	0.51
1:A:361:LEU:O	1:A:397:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:MET:HB3	1:A:407:MET:HG2	1.93	0.50
1:A:91:VAL:HG22	1:A:91:VAL:O	2.11	0.50
1:A:124:HIS:CD2	12:A:749:HOH:O	2.64	0.50
1:A:74:LEU:HB3	12:A:722:HOH:O	2.12	0.50
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.47	0.49
1:A:568:GLN:HE21	1:A:570:ASN:HD21	1.61	0.49
1:A:551:ARG:CD	1:A:583:ASP:O	2.60	0.49
1:A:240:ILE:HG13	1:A:241:ASN:H	1.77	0.49
1:A:559:ILE:HA	6:A:612:IOD:I	2.83	0.49
1:A:175:LEU:HD23	1:A:176:ALA:O	2.12	0.49
1:A:352:MET:CB	1:A:407:MET:HG2	2.43	0.49
1:A:393:ASP:HB2	12:A:686:HOH:O	2.12	0.49
4:A:605:HEM:HBB2	4:A:605:HEM:CMB	2.42	0.49
1:A:62:THR:HG21	1:A:65:LYS:HG3	1.95	0.48
1:A:175:LEU:HD23	1:A:176:ALA:N	2.28	0.48
1:A:258:GLU:HB2	7:A:597:EUG:H6	1.97	0.47
1:A:362:ASP:O	1:A:365:TYR:N	2.40	0.47
1:A:560:THR:HA	1:A:579:CYS:SG	2.54	0.47
1:A:168:PRO:CG	1:A:171:PRO:O	2.63	0.47
1:A:484:TYR:O	1:A:485:LYS:CB	2.62	0.47
1:A:2:TRP:HD1	1:A:175:LEU:CD1	2.27	0.47
1:A:427:LYS:H	1:A:427:LYS:CD	2.26	0.47
1:A:565:HIS:HB3	6:A:614:IOD:I	2.84	0.47
1:A:199:LEU:HB2	8:A:598:MPD:HM1	1.97	0.47
1:A:367:PRO:HG3	6:A:621:IOD:I	2.85	0.47
1:A:113:PHE:HE1	7:A:597:EUG:H93	1.79	0.46
1:A:10:VAL:HG11	1:A:41:ARG:HE	1.81	0.46
1:A:54:GLY:C	1:A:55:LEU:HD12	2.37	0.45
1:A:169:THR:HG23	12:A:758:HOH:O	2.15	0.45
1:A:79:SER:HA	1:A:83:VAL:HG23	1.98	0.45
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.98	0.45
1:A:238:GLU:O	1:A:241:ASN:O	2.35	0.45
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.47	0.44
1:A:99:LEU:HG	1:A:567:PHE:CE1	2.52	0.44
1:A:136:GLY:O	1:A:137:ASP:C	2.53	0.44
1:A:308:THR:HA	1:A:312:TYR:HB3	2.00	0.44
1:A:240:ILE:HG13	1:A:241:ASN:N	2.33	0.44
1:A:88:GLU:O	1:A:91:VAL:HG12	2.18	0.44
1:A:258:GLU:O	1:A:380:PHE:HA	2.18	0.43
1:A:348:ARG:NH2	4:A:605:HEM:HAD1	2.32	0.43
1:A:559:ILE:HG23	6:A:612:IOD:I	2.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:HB3	1:A:174:SER:HA	2.01	0.43
1:A:203:LEU:HD11	1:A:252:GLY:HA2	2.00	0.43
1:A:113:PHE:CE1	7:A:597:EUG:H93	2.52	0.43
1:A:418:ARG:O	1:A:432:ASP:HA	2.18	0.43
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.54	0.43
1:A:2:TRP:HB3	1:A:175:LEU:HD11	2.00	0.42
1:A:79:SER:HA	1:A:83:VAL:CG2	2.49	0.42
1:A:257:SER:O	1:A:381:PHE:HA	2.19	0.42
1:A:350:GLY:HA3	4:A:605:HEM:CBC	2.49	0.42
1:A:424:PRO:O	1:A:425:THR:HB	2.19	0.42
1:A:261:LEU:HD22	1:A:399:LEU:HG	2.02	0.42
1:A:568:GLN:HE21	1:A:570:ASN:ND2	2.18	0.42
1:A:8:ALA:N	1:A:9:PRO:CD	2.82	0.42
1:A:37:GLY:HA2	1:A:185:SER:HB2	2.02	0.42
1:A:588:SER:N	1:A:589:PRO:CD	2.83	0.41
1:A:96:ARG:HG3	1:A:506:ARG:HE	1.85	0.41
1:A:187:LEU:HD23	1:A:305:GLN:HA	2.02	0.41
1:A:499:GLU:OE2	1:A:509:PRO:HD2	2.19	0.41
2:B:1:NAG:H61	2:B:2:NAG:N2	2.35	0.41
1:A:56:ALA:HB1	1:A:177:ARG:NE	2.35	0.41
1:A:298:LYS:HG2	1:A:536:PHE:CZ	2.55	0.41
1:A:62:THR:CG2	1:A:65:LYS:HG3	2.49	0.41
1:A:347:PHE:C	1:A:349:PHE:H	2.24	0.41
1:A:63:GLN:HA	12:A:743:HOH:O	2.20	0.41
1:A:2:TRP:CD1	1:A:175:LEU:CD1	3.02	0.41
1:A:35:ALA:HB1	1:A:41:ARG:CD	2.51	0.41
1:A:126:LYS:HE3	1:A:126:LYS:HB2	1.94	0.41
1:A:166:VAL:O	1:A:167:CYS:HB2	2.21	0.41
1:A:460:GLN:HA	1:A:461:PRO:HD2	1.89	0.41
1:A:76:ARG:NH2	1:A:419:ASN:ND2	2.63	0.41
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.44	0.40
1:A:57:LEU:HD23	1:A:57:LEU:HA	1.92	0.40
1:A:348:ARG:NH1	1:A:437:ASN:HD22	2.16	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	592/595 (100%)	565 (95%)	21 (4%)	6 (1%)	15 32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	167	CYS
1	A	170	PRO
1	A	171	PRO
1	A	327	PRO
1	A	209	PRO

5.3.2 Protein sidechains (i)

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%)	501 (97%)	16 (3%)	40 66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	22	ARG
1	A	41	ARG
1	A	64	ARG
1	A	108	ASP

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Mol	Chain	Res	Type
1	A	122	ASN
1	A	127	THR
1	A	172	TYR
1	A	190	SER
1	A	347	PHE
1	A	352	MET
1	A	360	ARG
1	A	410	ASP
1	A	412	MET
1	A	427	LYS
1	A	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	122	ASN
1	A	128	GLN
1	A	138	ASN
1	A	147	ASN
1	A	364	ASN
1	A	419	ASN
1	A	437	ASN
1	A	497	ASN
1	A	570	ASN
1	A	595	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.69	0	8,12,14	2.23	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
1	SEP	A	198	1	-	3/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	OG-CB-CA	4.92	112.94	108.14
1	A	198	SEP	O3P-P-OG	-2.17	100.95	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	CA-CB-OG-P
1	A	198	SEP	CB-OG-P-O1P
1	A	198	SEP	CB-OG-P-O2P

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	1.66	3 (21%)	17,19,21	2.13	8 (47%)
2	NAG	B	2	2	14,14,15	1.13	2 (14%)	17,19,21	1.69	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	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O4-C4	-3.61	1.34	1.43
2	B	1	NAG	C4-C5	-3.27	1.46	1.53
2	B	2	NAG	C1-C2	-2.87	1.48	1.52
2	B	1	NAG	O5-C5	-2.77	1.37	1.43
2	B	2	NAG	C3-C2	-2.28	1.47	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O4-C4-C5	-4.54	98.04	109.30
2	B	1	NAG	C1-O5-C5	-4.29	106.38	112.19
2	B	2	NAG	O5-C1-C2	3.96	117.54	111.29
2	B	2	NAG	C3-C4-C5	3.19	115.94	110.24
2	B	2	NAG	C1-O5-C5	2.78	115.95	112.19
2	B	1	NAG	C3-C4-C5	2.64	114.94	110.24
2	B	2	NAG	C4-C3-C2	-2.56	107.27	111.02
2	B	1	NAG	C4-C3-C2	-2.25	107.73	111.02
2	B	1	NAG	O5-C5-C4	-2.20	105.48	110.83
2	B	1	NAG	C6-C5-C4	2.09	117.91	113.00
2	B	1	NAG	O4-C4-C3	-2.06	105.59	110.35
2	B	1	NAG	O5-C1-C2	2.01	114.46	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

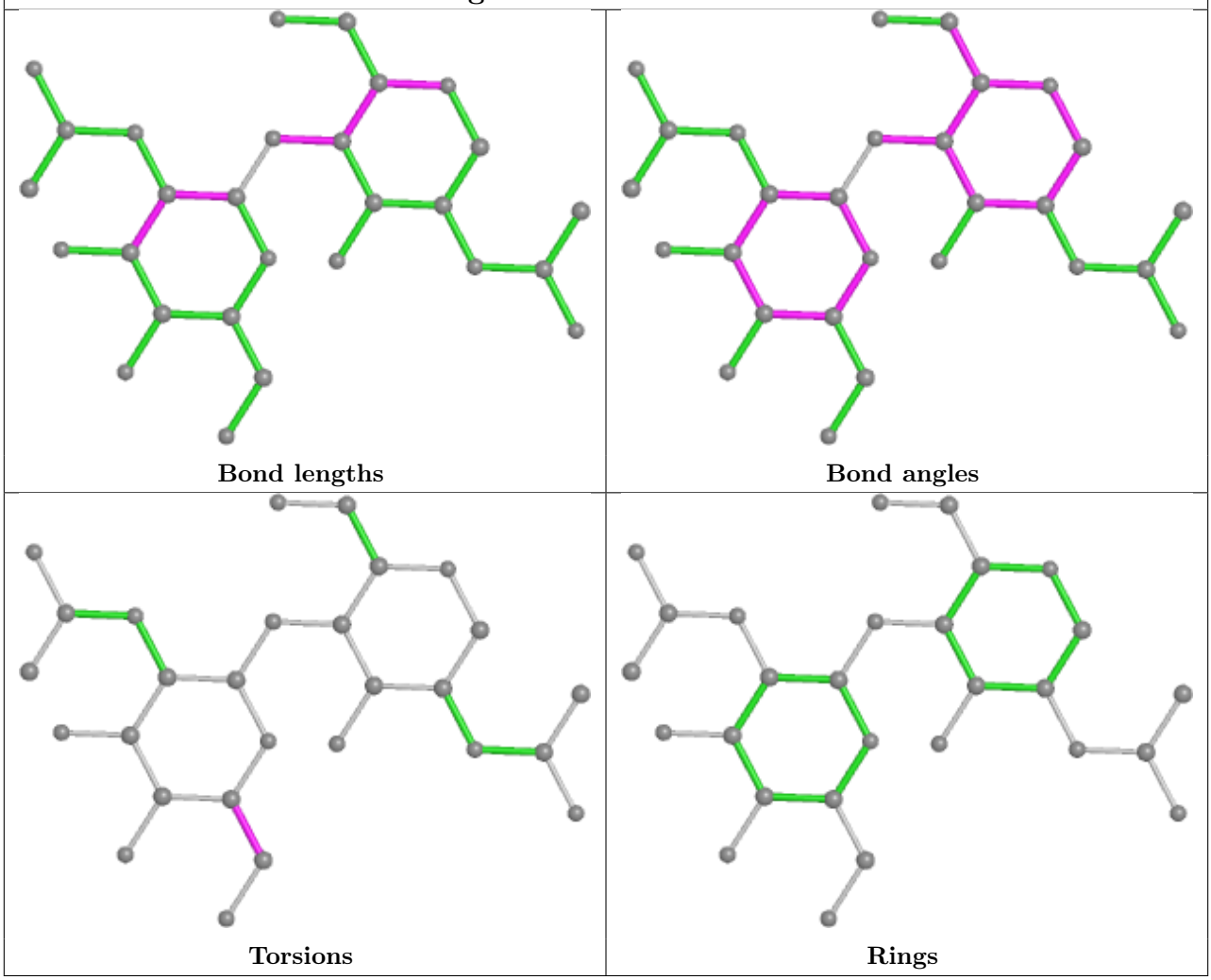
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NAG	1	0

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	599	1	14,14,15	0.92	1 (7%)	17,19,21	0.91	1 (5%)
8	MPD	A	598	-	7,7,7	2.34	1 (14%)	9,10,10	1.20	2 (22%)
5	NAG	A	604	1	14,14,15	0.62	0	17,19,21	0.98	1 (5%)
10	EDO	A	603	-	3,3,3	0.45	0	2,2,2	0.34	0
5	NAG	A	596	1	14,14,15	0.94	1 (7%)	17,19,21	0.99	0
4	HEM	A	605	12,1	41,50,50	2.14	12 (29%)	45,82,82	2.09	9 (20%)
9	SCN	A	700	-	1,2,2	1.55	0	0,1,1	-	-
10	EDO	A	600	-	3,3,3	0.30	0	2,2,2	0.16	0
7	EUG	A	597	-	11,11,12	2.96	4 (36%)	14,14,15	2.05	4 (28%)
11	GOL	A	610	-	5,5,5	0.50	0	5,5,5	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	599	1	-	0/6/23/26	0/1/1/1
8	MPD	A	598	-	-	1/5/5/5	-
5	NAG	A	604	1	-	0/6/23/26	0/1/1/1
10	EDO	A	603	-	-	1/1/1/1	-
5	NAG	A	596	1	-	0/6/23/26	0/1/1/1
4	HEM	A	605	12,1	-	2/12/54/54	-
10	EDO	A	600	-	-	1/1/1/1	-
7	EUG	A	597	-	-	4/4/4/5	0/1/1/1
11	GOL	A	610	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	597	EUG	C4-C3	6.52	1.52	1.40
8	A	598	MPD	O2-C2	-5.64	1.30	1.44
7	A	597	EUG	C5-C4	-5.10	1.30	1.39
4	A	605	HEM	FE-NB	4.99	2.21	1.96
4	A	605	HEM	C3D-C2D	4.90	1.47	1.36
4	A	605	HEM	C4D-ND	-4.66	1.32	1.40
4	A	605	HEM	C3C-CAC	4.25	1.56	1.47
4	A	605	HEM	CMC-C2C	3.88	1.60	1.51
4	A	605	HEM	CAB-C3B	3.70	1.57	1.47
7	A	597	EUG	O3-C3	3.53	1.42	1.37
7	A	597	EUG	O4-C4	2.95	1.42	1.36
4	A	605	HEM	CAA-C2A	2.42	1.55	1.52
4	A	605	HEM	O1A-CGA	2.38	1.30	1.22
4	A	605	HEM	CHC-C4B	-2.23	1.34	1.41
4	A	605	HEM	C3C-C2C	-2.22	1.37	1.40
4	A	605	HEM	C1B-NB	-2.07	1.36	1.40
4	A	605	HEM	C3B-C2B	-2.05	1.33	1.37
5	A	599	NAG	O5-C1	-2.03	1.40	1.43
5	A	596	NAG	O5-C1	-2.02	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	605	HEM	CMD-C2D-C1D	6.81	135.40	125.04
4	A	605	HEM	C4B-CHC-C1C	5.82	130.23	122.56
4	A	605	HEM	CAD-C3D-C4D	5.66	134.54	124.66
7	A	597	EUG	C5-C6-C1	4.89	127.63	121.25
4	A	605	HEM	C4D-ND-C1D	4.22	109.43	105.07
4	A	605	HEM	CAD-C3D-C2D	-3.77	120.85	127.88
7	A	597	EUG	C6-C5-C4	-3.19	117.22	120.50
5	A	604	NAG	C1-O5-C5	-2.67	108.58	112.19
7	A	597	EUG	C9-O3-C3	2.65	121.53	117.53
4	A	605	HEM	C4C-CHD-C1D	2.54	125.90	122.56
7	A	597	EUG	O3-C3-C4	2.49	118.17	114.57
8	A	598	MPD	O2-C2-CM	-2.33	100.59	108.08
4	A	605	HEM	CMD-C2D-C3D	-2.31	119.83	126.12
5	A	599	NAG	O5-C1-C2	2.27	114.86	111.29
8	A	598	MPD	O2-C2-C3	2.23	118.19	109.80
4	A	605	HEM	O1D-CGD-CBD	-2.15	116.17	123.08
4	A	605	HEM	C1D-C2D-C3D	-2.10	104.75	106.96

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	598	MPD	C2-C3-C4-O4
7	A	597	EUG	C2-C3-O3-C9
7	A	597	EUG	C4-C3-O3-C9
10	A	603	EDO	O1-C1-C2-O2
7	A	597	EUG	C2-C1-C7-C8
7	A	597	EUG	C6-C1-C7-C8
10	A	600	EDO	O1-C1-C2-O2
11	A	610	GOL	C1-C2-C3-O3
11	A	610	GOL	O2-C2-C3-O3
4	A	605	HEM	CAD-CBD-CGD-O1D
4	A	605	HEM	CAD-CBD-CGD-O2D

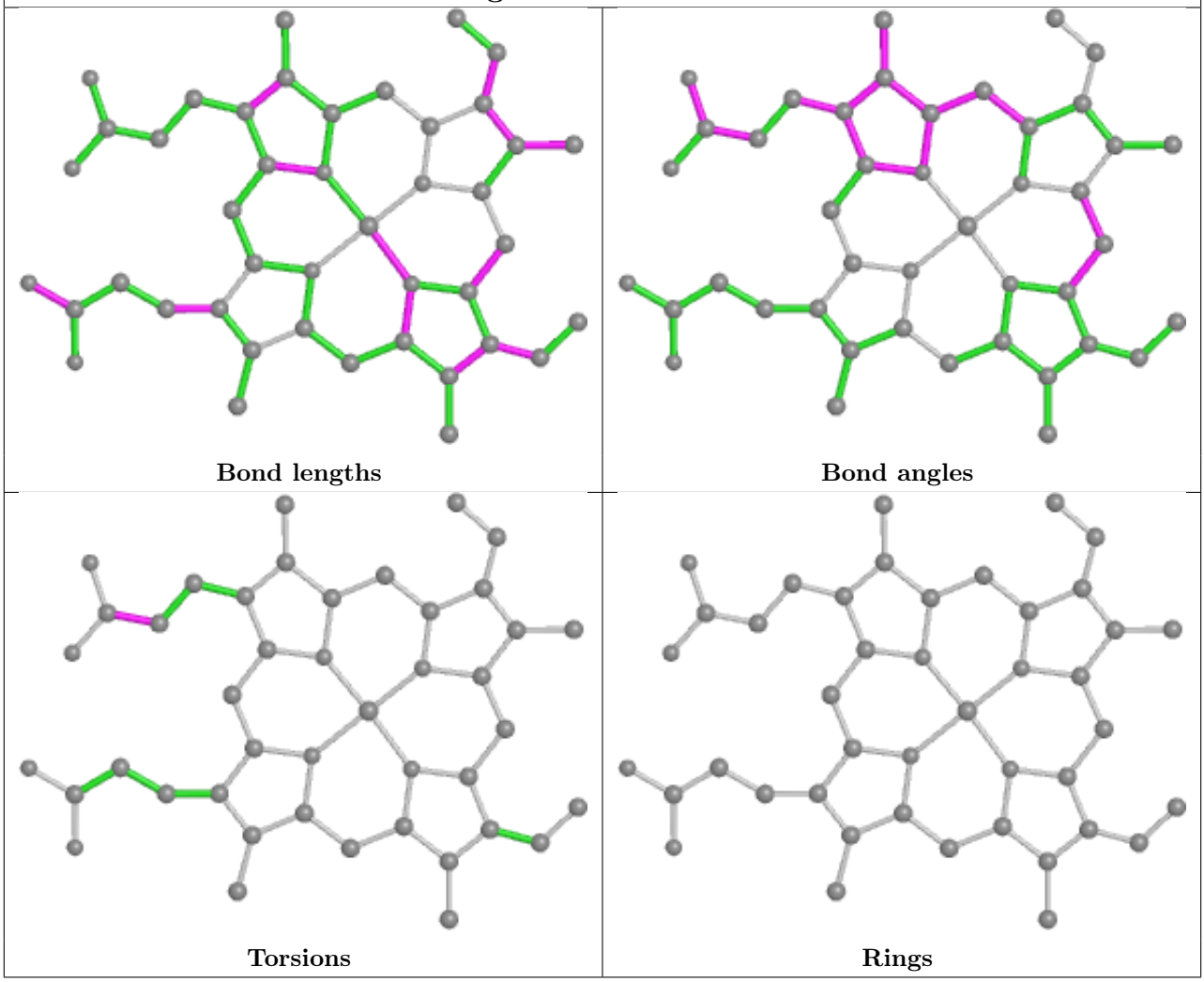
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	598	MPD	1	0
4	A	605	HEM	5	0
7	A	597	EUG	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 then 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.

Ligand HEM A 605



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	594/595 (99%)	0.09	34 (5%) 23 18	33, 56, 97, 100	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	SER	11.4
1	A	174	SER	9.8
1	A	173	GLN	9.5
1	A	120	GLY	8.6
1	A	122	ASN	7.9
1	A	7	GLY	6.9
1	A	2	TRP	6.0
1	A	119	LEU	5.8
1	A	595	ASN	5.6
1	A	10	VAL	5.0
1	A	13	VAL	4.6
1	A	12	LEU	4.5
1	A	1	SER	4.3
1	A	172	TYR	3.7
1	A	124	HIS	3.6
1	A	4	VAL	3.5
1	A	592	SER	3.4
1	A	587	LEU	3.3
1	A	594	GLU	3.3
1	A	5	GLY	3.1
1	A	64	ARG	3.0
1	A	211	GLY	3.0
1	A	126	LYS	2.8
1	A	169	THR	2.8
1	A	123	GLU	2.8
1	A	283	LEU	2.7
1	A	170	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	118	GLU	2.4
1	A	131	GLU	2.3
1	A	593	ARG	2.3
1	A	11	PRO	2.1
1	A	212	LEU	2.1
1	A	117	THR	2.1
1	A	8	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	A	198	10/11	0.94	0.14	51,54,58,58	0

6.3 Carbohydrates (i)

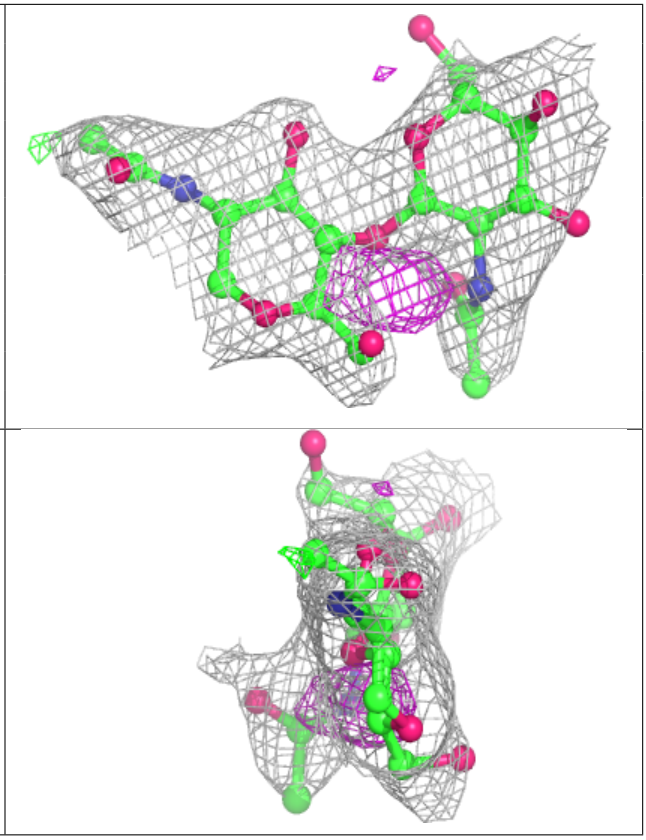
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1	14/15	0.83	0.21	65,69,71,71	0
2	NAG	B	2	14/15	0.85	0.29	73,79,81,84	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.

Electron density around Chain B:

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



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(Å^2)	Q<0.9
7	EUG	A	597	11/12	0.68	0.50	30,42,45,45	11
5	NAG	A	596	14/15	0.82	0.32	78,79,80,81	0
11	GOL	A	610	6/6	0.83	0.23	74,76,77,78	6
10	EDO	A	603	4/4	0.84	0.26	75,75,75,77	4
5	NAG	A	604	14/15	0.86	0.22	89,92,94,94	0
9	SCN	A	700	3/3	0.88	0.35	61,61,62,64	3
5	NAG	A	599	14/15	0.89	0.12	63,75,77,77	0
6	IOD	A	609	1/1	0.92	0.14	84,84,84,84	1
10	EDO	A	600	4/4	0.92	0.11	74,74,76,76	0
6	IOD	A	621	1/1	0.94	0.12	91,91,91,91	1
8	MPD	A	598	8/8	0.94	0.22	24,32,41,46	0
6	IOD	A	624	1/1	0.94	0.05	95,95,95,95	1
6	IOD	A	614	1/1	0.95	0.11	79,79,79,79	1
6	IOD	A	623	1/1	0.96	0.06	88,88,88,88	1

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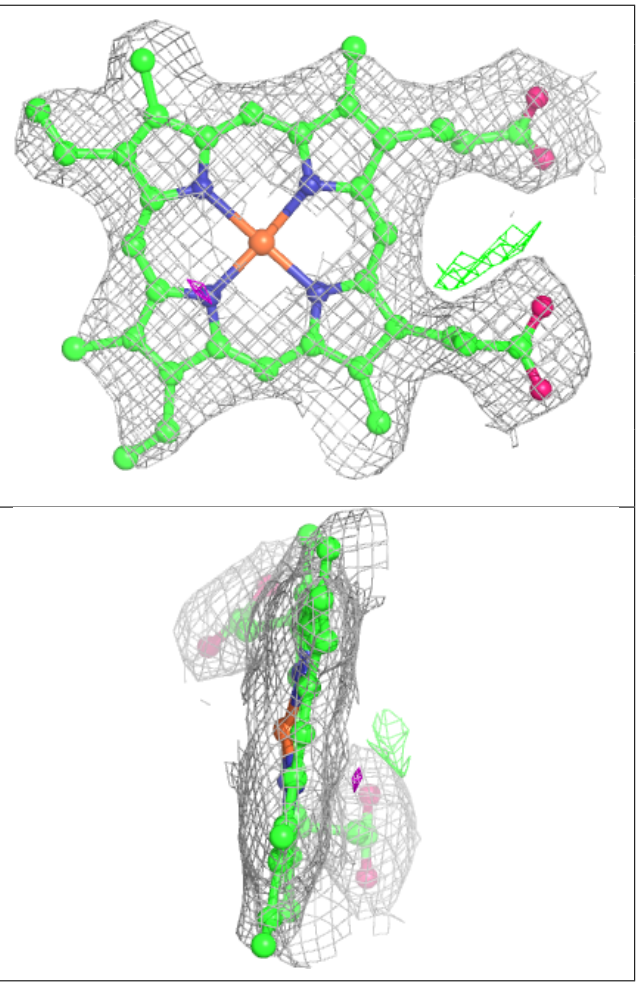
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HEM	A	605	43/43	0.97	0.20	30,37,43,48	0
6	IOD	A	612	1/1	0.97	0.07	97,97,97,97	0
3	CA	A	606	1/1	0.97	0.18	54,54,54,54	0
6	IOD	A	608	1/1	0.98	0.04	84,84,84,84	0
6	IOD	A	622	1/1	0.99	0.03	75,75,75,75	0
6	IOD	A	611	1/1	0.99	0.07	74,74,74,74	0
6	IOD	A	607	1/1	0.99	0.09	56,56,56,56	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 HEM A 605:

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.