Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 04:24 PM EST

PDB ID	:	6B9B
Title	:	Crystal structure of the catalase-peroxidase from B. pseudomallei with maltose bound
Authors	:	Loewen, P.C.
Deposited on	:	2017-10-10
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

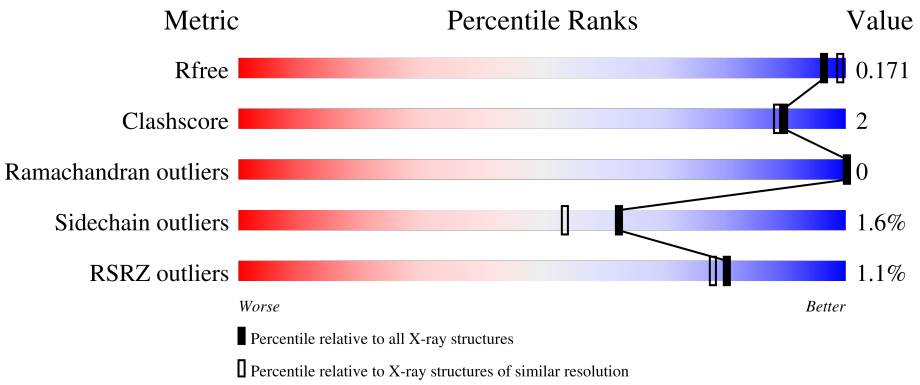
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	728	% 90% 8% •
1	B	728	% 90% 7% • •
2	C	2	100%
2	D	2	50% 50%

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
2	GLC	C	1	-	-	-	X
2	GLC	D	1	-	-	-	X
7	PO4	A	805	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12762 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.

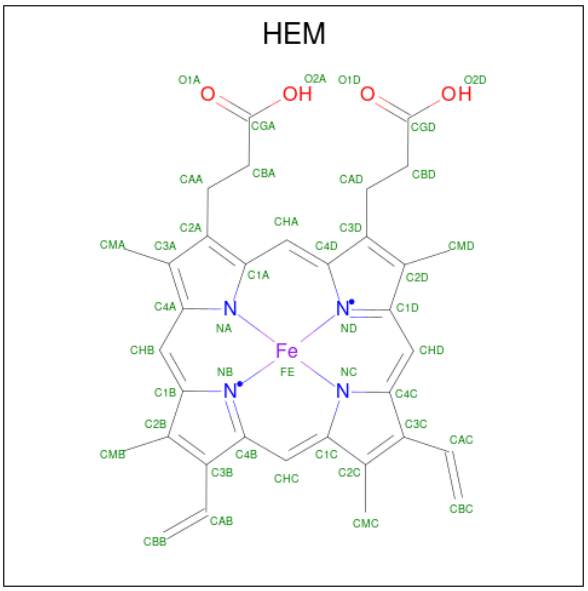
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	713	5550	3502	990	1044	14	0	6	0
1	B	713	5589	3525	994	1056	14	0	11	0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	2	23	12	11	0	0	0
2	D	2	23	12	11	0	0	0

- Molecule 3 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		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0

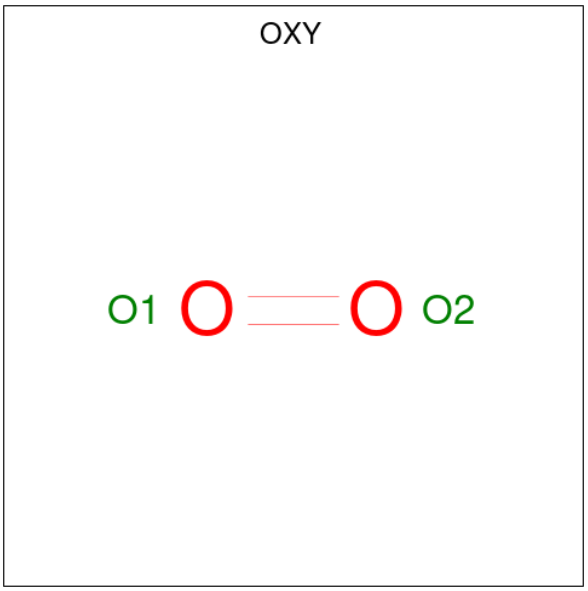
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0
			Total	Na		
4	B	1	1	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

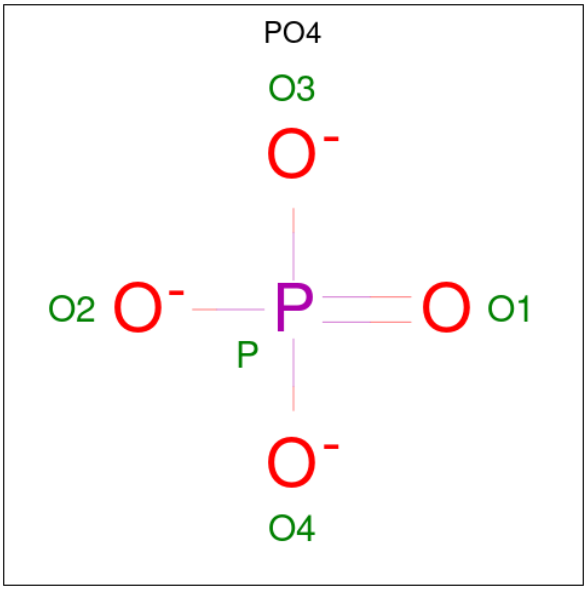
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
			Total	Cl		
5	B	1	1	1	0	0

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



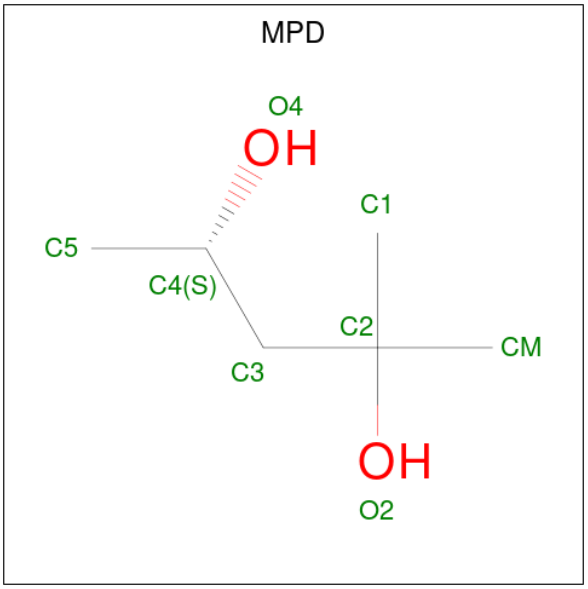
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	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
			Total	C	O		
8	A	1	8	6	2	0	0
			Total	C	O		
8	B	1	8	6	2	0	0

- Molecule 9 is water.

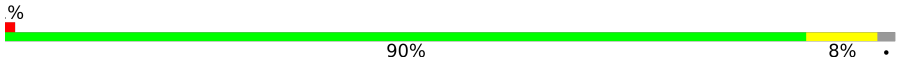
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	708	708	708	0	1
			Total	O		
9	B	741	741	741	0	2

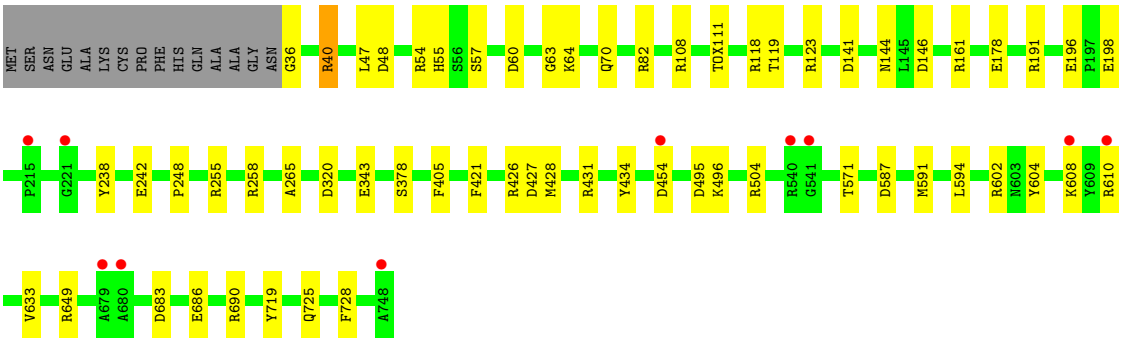
3 Residue-property plots (i)

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: Catalase-peroxidase

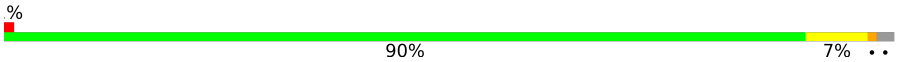
Chain A:

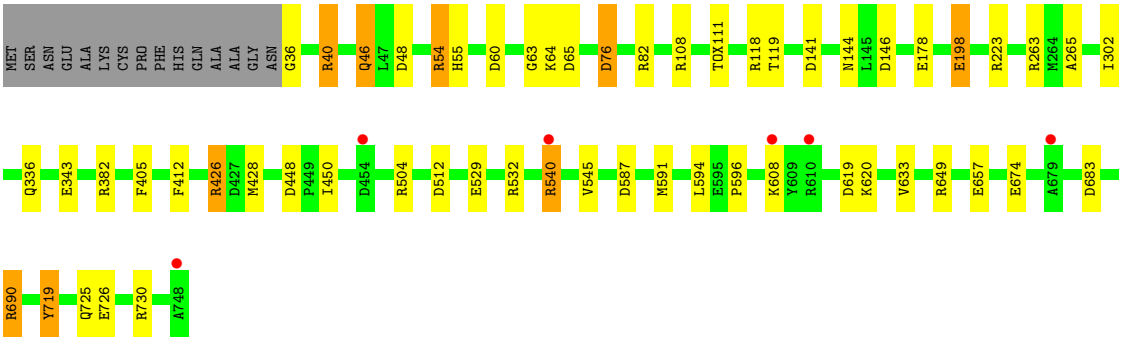




• Molecule 1: Catalase-peroxidase

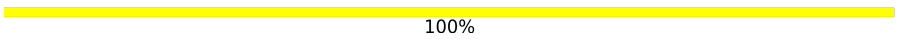
Chain B:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.42Å 115.09Å 174.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 48.26 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-1.80) 98.4 (48.26-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.135 , 0.162 0.148 , 0.171	Depositor DCC
R_{free} test set	9225 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12762	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: OXY, CL, NA, MPD, HEM, PO4, TOX, GLC

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	1.40	19/5675 (0.3%)	1.16	22/7712 (0.3%)
1	B	1.38	16/5720 (0.3%)	1.19	22/7772 (0.3%)
All	All	1.39	35/11395 (0.3%)	1.17	44/15484 (0.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	SER	CB-OG	9.44	1.54	1.42
1	A	63	GLY	N-CA	6.56	1.55	1.46
1	B	63	GLY	N-CA	6.04	1.55	1.46
1	A	36	GLY	N-CA	5.90	1.54	1.46
1	B	178	GLU	CD-OE2	5.87	1.32	1.25
1	B	504	ARG	CZ-NH1	-5.83	1.25	1.33
1	B	46	GLN	CG-CD	5.81	1.64	1.51
1	A	426[A]	ARG	CZ-NH1	-5.73	1.25	1.33
1	A	426[B]	ARG	CZ-NH1	-5.73	1.25	1.33
1	A	178	GLU	CD-OE1	-5.66	1.19	1.25
1	A	431	ARG	CD-NE	5.61	1.55	1.46
1	A	198	GLU	CG-CD	5.59	1.60	1.51
1	A	604	TYR	CE1-CZ	-5.59	1.31	1.38
1	A	496	LYS	CE-NZ	-5.58	1.35	1.49
1	A	123	ARG	CZ-NH1	-5.48	1.25	1.33
1	A	343	GLU	CG-CD	5.47	1.60	1.51
1	B	719	TYR	CE1-CZ	5.46	1.45	1.38
1	B	198	GLU	CD-OE2	-5.44	1.19	1.25
1	B	336	GLN	CG-CD	5.43	1.63	1.51
1	B	674	GLU	CD-OE2	-5.43	1.19	1.25
1	B	690	ARG	CD-NE	-5.42	1.37	1.46
1	A	728	PHE	CG-CD2	-5.37	1.30	1.38
1	B	178	GLU	CG-CD	5.34	1.59	1.51
1	A	378	SER	CB-OG	5.34	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	GLN	CD-OE1	5.33	1.35	1.24
1	A	686	GLU	CG-CD	5.24	1.59	1.51
1	B	223	ARG	CG-CD	-5.24	1.38	1.51
1	A	196	GLU	CB-CG	-5.24	1.42	1.52
1	A	428	MET	CG-SD	-5.23	1.67	1.81
1	B	730	ARG	CZ-NH1	5.21	1.39	1.33
1	B	426[A]	ARG	CZ-NH2	5.16	1.39	1.33
1	B	426[B]	ARG	CZ-NH2	5.16	1.39	1.33
1	B	343	GLU	CG-CD	5.12	1.59	1.51
1	B	36	GLY	N-CA	5.08	1.53	1.46
1	A	690	ARG	CZ-NH1	-5.02	1.26	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	48	ASP	CB-CG-OD1	9.99	127.29	118.30
1	B	60	ASP	CB-CG-OD2	-9.41	109.83	118.30
1	B	65	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	A	48	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	76	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	B	108	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	54	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	108	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	60	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	48	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	40	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	60	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	82	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	40	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	320	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	263	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	448	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	450	ILE	CA-CB-CG1	-5.61	100.35	111.00
1	A	587	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	587	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	725	GLN	CB-CG-CD	5.50	125.91	111.60
1	A	602	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	683	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	421	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	A	82	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	619	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	428	MET	CA-CB-CG	-5.38	104.15	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	683	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	730	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	A	191	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	427	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	55	HIS	CB-CA-C	5.21	120.82	110.40
1	A	587	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	571	THR	OG1-CB-CG2	-5.20	98.04	110.00
1	B	382	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	719	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	70	GLN	CA-CB-CG	5.11	124.64	113.40
1	A	495	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	198	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	A	405	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	B	48	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	258	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	47	LEU	N-CA-CB	-5.03	100.34	110.40
1	B	620	LYS	CD-CE-NZ	-5.00	100.19	111.70

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	5550	0	5353	12	0
1	B	5589	0	5382	19	0
2	C	23	0	21	0	0
2	D	23	0	20	3	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	1	0
6	B	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	16	0	28	4	0
8	B	8	0	14	1	0
9	A	708	0	0	4	0
9	B	741	0	0	9	0
All	All	12762	0	10878	40	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 2.

All (40) 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:B:119[B]:THR:HG21	9:B:1088:HOH:O	1.69	0.91
1:A:119[B]:THR:HG21	9:A:995:HOH:O	1.72	0.90
1:B:540:ARG:NE	1:B:540:ARG:HA	1.99	0.75
6:B:804:OXY:O2	9:B:901:HOH:O	2.12	0.66
1:A:255[A]:ARG:NH2	9:A:904:HOH:O	2.25	0.58
1:A:504:ARG:HD2	9:A:985:HOH:O	2.05	0.57
1:B:726[B]:GLU:CD	1:B:726[B]:GLU:H	2.08	0.56
1:B:512:ASP:OD1	9:B:903:HOH:O	2.18	0.55
1:B:512:ASP:HB2	9:B:1451:HOH:O	2.07	0.55
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.93	0.52
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.45	0.52
9:B:910:HOH:O	2:D:1:GLC:H62	2.10	0.51
8:A:806:MPD:O4	8:A:806:MPD:CM	2.59	0.51
1:B:405:PHE:HB3	1:B:412:PHE:HB2	1.93	0.51
6:A:804:OXY:O2	9:A:902:HOH:O	2.20	0.48
9:B:910:HOH:O	2:D:1:GLC:C6	2.60	0.48
1:B:596:PRO:HG3	9:B:1526:HOH:O	2.13	0.47
1:B:529[B]:GLU:OE1	2:D:1:GLC:H2	2.14	0.47
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.14	0.47
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.14	0.46
1:B:76:ASP:OD1	9:B:904:HOH:O	2.21	0.46
1:A:434:TYR:CD1	1:A:434:TYR:N	2.84	0.46
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.99	0.45
8:A:807:MPD:H53	8:A:807:MPD:H11	1.99	0.45
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.47	0.45
1:B:591:MET:SD	1:B:594:LEU:HD12	2.58	0.44
8:B:806:MPD:O4	8:B:806:MPD:H12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:807:MPD:H11	8:A:807:MPD:C5	2.48	0.43
1:B:657[A]:GLU:CD	9:B:1236:HOH:O	2.56	0.43
1:A:591:MET:SD	1:A:594:LEU:HD12	2.59	0.43
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.49	0.43
8:A:806:MPD:O4	8:A:806:MPD:HM2	2.18	0.43
1:A:434:TYR:N	1:A:434:TYR:HD1	2.17	0.42
1:B:198:GLU:OE1	1:B:198:GLU:HA	2.19	0.42
1:A:454:ASP:OD1	1:A:454:ASP:N	2.50	0.42
1:B:532:ARG:HG3	1:B:545:VAL:HG13	2.03	0.41
1:A:242:GLU:O	1:A:248:PRO:HA	2.21	0.41
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.91	0.40
1:B:302:ILE:HD13	1:B:302:ILE:HG21	1.85	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	715/728 (98%)	706 (99%)	9 (1%)	0	100	100
1	B	720/728 (99%)	709 (98%)	11 (2%)	0	100	100
All	All	1435/1456 (99%)	1415 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	554/560 (99%)	546 (99%)	8 (1%)	67	59
1	B	559/560 (100%)	549 (98%)	10 (2%)	59	48
All	All	1113/1120 (99%)	1095 (98%)	18 (2%)	62	54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	118	ARG
1	A	141	ASP
1	A	161	ARG
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	46	GLN
1	B	54	ARG
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	540	ARG
1	B	608	LYS
1	B	649	ARG
1	B	690	ARG

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	70	GLN
1	A	247	ASN
1	A	568	HIS
1	B	46	GLN
1	B	227	ASN
1	B	406	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TOX	A	111[A]	3	10,17,18	1.79	4 (40%)	10,23,25	2.28	3 (30%)
1	TOX	B	111[B]	-	10,17,18	1.69	4 (40%)	10,23,25	1.91	6 (60%)
1	TOX	A	111[B]	-	10,17,18	1.79	4 (40%)	10,23,25	2.28	3 (30%)
1	TOX	B	111[A]	3	10,17,18	1.69	4 (40%)	10,23,25	1.91	6 (60%)

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	TOX	A	111[A]	3	-	2/4/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	B	111[A]	3	-	2/4/8/10	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	O-C	2.88	1.31	1.19
1	B	111[B]	TOX	O-C	2.88	1.31	1.19
1	A	111[A]	TOX	CD1-NE1	-2.84	1.36	1.39
1	A	111[B]	TOX	CD1-NE1	-2.84	1.36	1.39
1	A	111[A]	TOX	CH2-CZ2	2.74	1.42	1.36
1	A	111[B]	TOX	CH2-CZ2	2.74	1.42	1.36
1	A	111[A]	TOX	CA-N	-2.66	1.40	1.48
1	A	111[B]	TOX	CA-N	-2.66	1.40	1.48
1	A	111[A]	TOX	CZ2-CE2	-2.55	1.36	1.41
1	A	111[B]	TOX	CZ2-CE2	-2.55	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CA-N	-2.43	1.40	1.48
1	B	111[B]	TOX	CA-N	-2.43	1.40	1.48
1	B	111[A]	TOX	CZ2-CE2	-2.16	1.36	1.41
1	B	111[B]	TOX	CZ2-CE2	-2.16	1.36	1.41
1	B	111[A]	TOX	CB-CA	-2.07	1.49	1.53
1	B	111[B]	TOX	CB-CA	-2.07	1.49	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111[A]	TOX	CZ2-CE2-CD2	-5.39	113.61	120.94
1	A	111[B]	TOX	CZ2-CE2-CD2	-5.39	113.61	120.94
1	A	111[A]	TOX	CH2-CZ3-CE3	-2.78	116.54	120.44
1	A	111[B]	TOX	CH2-CZ3-CE3	-2.78	116.54	120.44
1	B	111[A]	TOX	CB-CG-CD2	2.58	130.26	126.25
1	B	111[B]	TOX	CB-CG-CD2	2.58	130.26	126.25
1	A	111[A]	TOX	CH2-CZ2-CE2	2.52	124.28	119.44
1	A	111[B]	TOX	CH2-CZ2-CE2	2.52	124.28	119.44
1	B	111[A]	TOX	CZ3-CE3-CD2	-2.37	117.61	120.89
1	B	111[B]	TOX	CZ3-CE3-CD2	-2.37	117.61	120.89
1	B	111[A]	TOX	CZ3-CH2-CZ2	2.32	123.69	120.44
1	B	111[B]	TOX	CZ3-CH2-CZ2	2.32	123.69	120.44
1	B	111[A]	TOX	CB-CG-CD1	-2.23	125.21	127.97
1	B	111[B]	TOX	CB-CG-CD1	-2.23	125.21	127.97
1	B	111[A]	TOX	CB-CA-C	2.13	115.46	111.47
1	B	111[B]	TOX	CB-CA-C	2.13	115.46	111.47
1	B	111[A]	TOX	CE3-CD2-CG	-2.06	130.63	134.42
1	B	111[B]	TOX	CE3-CD2-CG	-2.06	130.63	134.42

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

4 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	GLC	C	1	2	12,12,12	1.69	4 (33%)	17,17,17	1.84	5 (29%)
2	GLC	C	2	2	11,11,12	0.55	0	15,15,17	3.32	7 (46%)
2	GLC	D	1	2	12,12,12	1.72	4 (33%)	17,17,17	3.19	8 (47%)
2	GLC	D	2	2	11,11,12	1.95	2 (18%)	15,15,17	2.50	7 (46%)

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	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	C1-C2	4.19	1.61	1.52
2	D	1	GLC	O4-C4	3.21	1.50	1.43
2	D	2	GLC	C2-C3	3.08	1.57	1.52
2	D	1	GLC	C4-C3	2.61	1.59	1.52
2	C	1	GLC	O4-C4	2.55	1.49	1.43
2	C	1	GLC	C3-C2	2.46	1.58	1.52
2	D	1	GLC	C1-C2	2.44	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	C4-C5	2.34	1.58	1.53
2	C	1	GLC	C4-C3	2.32	1.58	1.52
2	C	1	GLC	O1-C1	2.21	1.46	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	GLC	O5-C1-C2	-8.69	97.36	110.77
2	D	1	GLC	O4-C4-C5	5.93	124.02	109.30
2	C	2	GLC	C1-C2-C3	-5.28	103.18	109.67
2	D	1	GLC	O2-C2-C1	4.85	120.40	109.16
2	D	1	GLC	C6-C5-C4	4.77	124.17	113.00
2	D	1	GLC	O3-C3-C4	4.73	121.29	110.35
2	D	1	GLC	C4-C3-C2	-4.66	102.68	110.82
2	D	2	GLC	O3-C3-C2	4.38	118.38	109.99
2	D	1	GLC	C3-C4-C5	-4.18	102.78	110.24
2	D	2	GLC	C1-C2-C3	4.09	114.69	109.67
2	C	2	GLC	O4-C4-C5	-3.76	99.97	109.30
2	C	1	GLC	O4-C4-C3	3.49	118.43	110.35
2	C	2	GLC	C2-C3-C4	-3.42	104.98	110.89
2	D	2	GLC	C1-O5-C5	-3.39	107.60	112.19
2	D	2	GLC	O5-C5-C4	3.34	118.95	110.83
2	C	2	GLC	O3-C3-C4	3.17	117.68	110.35
2	D	1	GLC	O1-C1-C2	3.17	117.96	109.03
2	D	2	GLC	O4-C4-C3	-3.04	103.33	110.35
2	C	1	GLC	O1-C1-C2	3.00	117.47	109.03
2	C	1	GLC	O5-C5-C4	2.91	114.98	109.69
2	C	1	GLC	O5-C1-C2	-2.90	105.11	110.28
2	D	2	GLC	O5-C1-C2	-2.78	106.47	110.77
2	D	1	GLC	O4-C4-C3	2.77	116.75	110.35
2	C	1	GLC	C3-C4-C5	-2.77	105.30	110.24
2	C	2	GLC	O3-C3-C2	2.71	115.19	109.99
2	C	2	GLC	C1-O5-C5	2.64	115.77	112.19
2	D	2	GLC	O3-C3-C4	-2.38	104.86	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	1	GLC	C4-C5-C6-O6

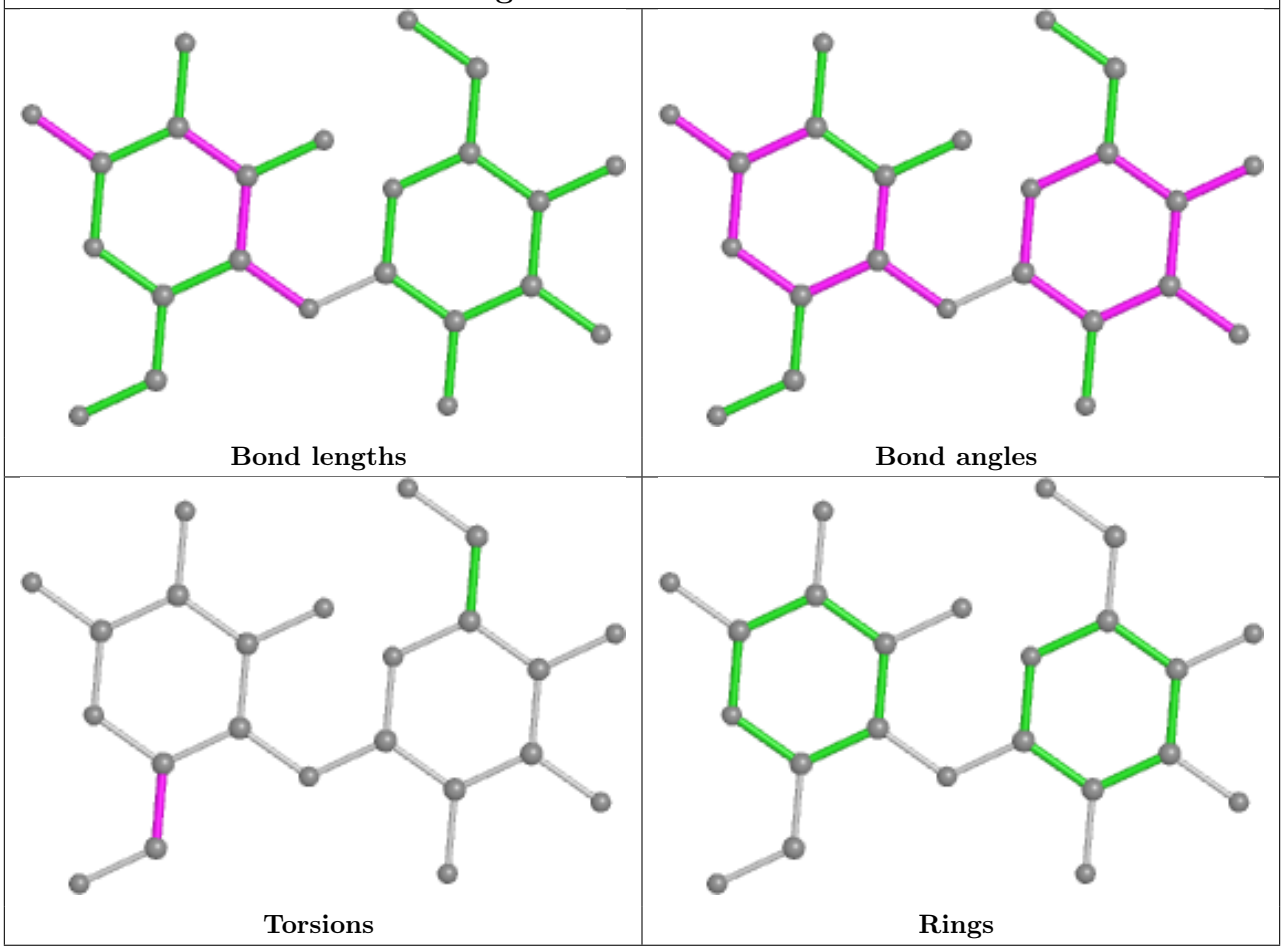
There are no ring outliers.

1 monomer is involved in 3 short contacts:

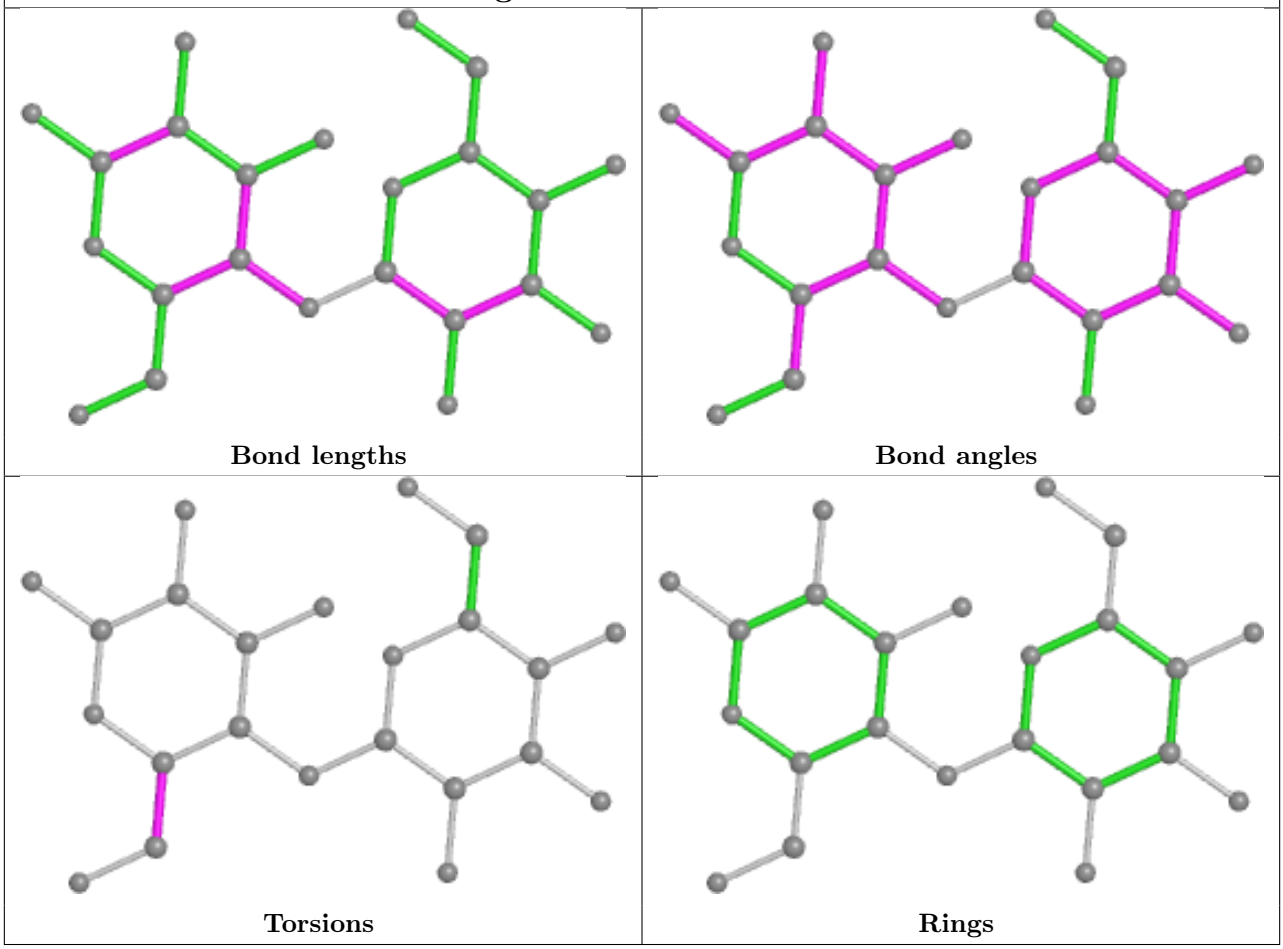
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	3	0

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 C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	PO4	B	805	-	4,4,4	0.87	0	6,6,6	1.63	2 (33%)
7	PO4	A	805	-	4,4,4	1.11	0	6,6,6	2.59	4 (66%)
6	OXY	B	804	-	1,1,1	1.01	0	-		
8	MPD	A	807	-	7,7,7	0.98	0	9,10,10	2.08	3 (33%)
8	MPD	A	806	-	7,7,7	1.15	0	9,10,10	1.63	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	OXY	A	804	-	1,1,1	0.47	0	-		
3	HEM	B	801	1	41,50,50	1.47	7 (17%)	45,82,82	1.53	9 (20%)
3	HEM	A	801	1	41,50,50	1.49	8 (19%)	45,82,82	1.91	15 (33%)
8	MPD	B	806	-	7,7,7	0.50	0	9,10,10	1.94	3 (33%)

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	MPD	A	807	-	-	5/5/5/5	-
8	MPD	A	806	-	-	3/5/5/5	-
3	HEM	B	801	1	-	3/12/54/54	-
3	HEM	A	801	1	-	2/12/54/54	-
8	MPD	B	806	-	-	3/5/5/5	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	HEM	CHB-C1B	3.41	1.43	1.35
3	A	801	HEM	C3C-C2C	-3.32	1.35	1.40
3	A	801	HEM	C1B-NB	-3.23	1.34	1.40
3	B	801	HEM	C1B-NB	-2.97	1.35	1.40
3	B	801	HEM	C4B-NB	-2.90	1.32	1.38
3	A	801	HEM	C2C-C1C	2.62	1.48	1.42
3	B	801	HEM	O1D-CGD	2.54	1.30	1.22
3	A	801	HEM	CBA-CGA	2.46	1.56	1.50
3	B	801	HEM	C2A-C3A	-2.42	1.30	1.37
3	B	801	HEM	O1A-CGA	2.40	1.30	1.22
3	A	801	HEM	C1A-NA	2.39	1.41	1.36
3	A	801	HEM	FE-NB	2.31	2.08	1.96
3	B	801	HEM	C4A-NA	2.30	1.40	1.36
3	A	801	HEM	CHA-C4D	2.24	1.40	1.35
3	A	801	HEM	C3C-CAC	2.12	1.52	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	HEM	C4B-C3B-C2B	-5.09	103.08	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	801	HEM	C4B-C3B-C2B	-3.94	103.99	107.11
8	A	807	MPD	C5-C4-C3	3.87	129.91	111.69
7	A	805	PO4	O3-P-O1	-3.74	97.22	110.89
8	A	807	MPD	CM-C2-C1	-3.69	102.89	110.57
3	A	801	HEM	CMC-C2C-C3C	3.69	131.57	124.68
3	B	801	HEM	CBA-CAA-C2A	3.56	118.69	112.62
3	B	801	HEM	C4A-C3A-C2A	3.45	109.39	107.00
7	A	805	PO4	O4-P-O1	3.23	122.73	110.89
3	A	801	HEM	CMA-C3A-C4A	-3.19	123.56	128.46
3	A	801	HEM	O2A-CGA-CBA	3.11	124.03	114.03
3	A	801	HEM	C2C-C3C-C4C	3.00	108.99	106.90
8	B	806	MPD	C1-C2-C3	2.99	123.87	109.96
3	B	801	HEM	CHC-C4B-NB	2.99	127.67	124.43
3	A	801	HEM	C4B-CHC-C1C	2.94	126.44	122.56
3	A	801	HEM	O1A-CGA-CBA	-2.92	113.70	123.08
3	A	801	HEM	CBA-CAA-C2A	2.77	117.35	112.62
3	A	801	HEM	CMA-C3A-C2A	2.76	130.14	124.94
3	A	801	HEM	CAA-CBA-CGA	-2.71	106.17	113.76
7	B	805	PO4	O2-P-O1	-2.66	101.15	110.89
3	A	801	HEM	C4C-CHD-C1D	2.64	126.04	122.56
8	B	806	MPD	O2-C2-CM	2.57	116.32	108.08
7	A	805	PO4	O4-P-O2	-2.53	99.83	107.97
7	B	805	PO4	O3-P-O1	2.53	120.15	110.89
3	B	801	HEM	CMC-C2C-C3C	2.53	129.41	124.68
3	B	801	HEM	CAA-CBA-CGA	-2.50	106.76	113.76
3	A	801	HEM	C3B-C2B-C1B	2.42	108.28	106.49
8	A	806	MPD	O4-C4-C5	2.41	119.82	109.38
3	A	801	HEM	C1B-NB-C4B	2.39	107.54	105.07
7	A	805	PO4	O4-P-O3	2.36	115.56	107.97
3	B	801	HEM	O2A-CGA-CBA	2.26	121.30	114.03
8	A	806	MPD	CM-C2-C3	2.25	120.45	109.96
8	A	806	MPD	CM-C2-C1	2.24	115.24	110.57
8	B	806	MPD	O4-C4-C5	2.17	118.78	109.38
3	B	801	HEM	CHC-C4B-C3B	-2.12	121.32	124.57
3	A	801	HEM	CHA-C4D-ND	2.04	126.90	124.38
3	B	801	HEM	O1D-CGD-CBD	-2.04	116.53	123.08
8	A	807	MPD	O4-C4-C3	-2.02	103.21	111.36
3	A	801	HEM	CMB-C2B-C1B	-2.01	121.98	125.04

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	806	MPD	O2-C2-C3-C4
8	A	806	MPD	CM-C2-C3-C4
8	A	807	MPD	C1-C2-C3-C4
8	A	807	MPD	C2-C3-C4-C5
8	B	806	MPD	C1-C2-C3-C4
8	B	806	MPD	O2-C2-C3-C4
8	A	807	MPD	O2-C2-C3-C4
8	A	806	MPD	C1-C2-C3-C4
8	A	807	MPD	CM-C2-C3-C4
8	B	806	MPD	CM-C2-C3-C4
3	A	801	HEM	CAA-CBA-CGA-O2A
3	A	801	HEM	CAA-CBA-CGA-O1A
3	B	801	HEM	CAA-CBA-CGA-O2A
3	B	801	HEM	CAA-CBA-CGA-O1A
3	B	801	HEM	CAD-CBD-CGD-O2D
8	A	807	MPD	C2-C3-C4-O4

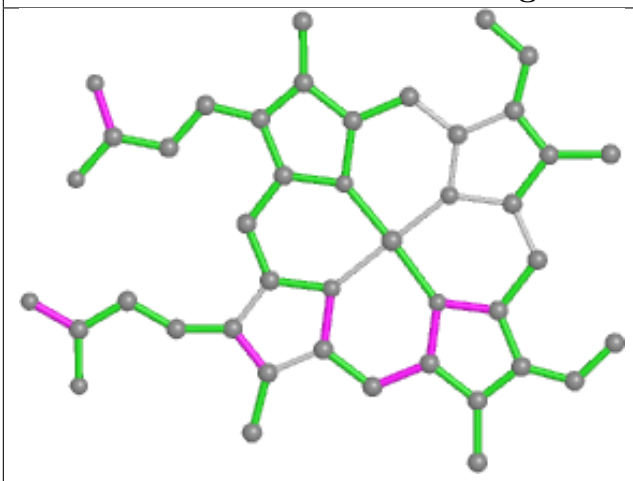
There are no ring outliers.

5 monomers are involved in 7 short contacts:

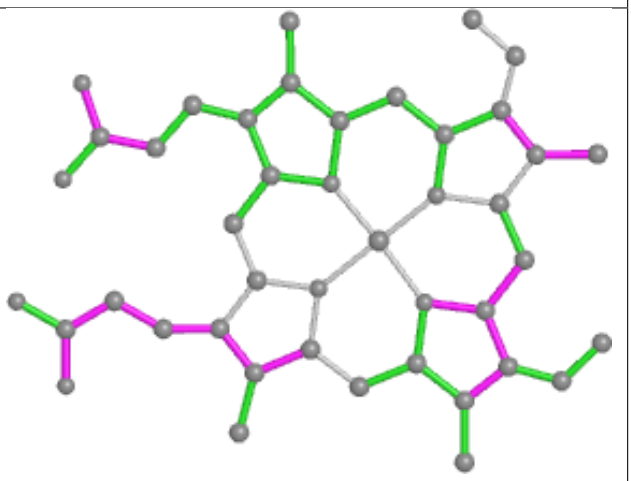
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	804	OXY	1	0
8	A	807	MPD	2	0
8	A	806	MPD	2	0
6	A	804	OXY	1	0
8	B	806	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

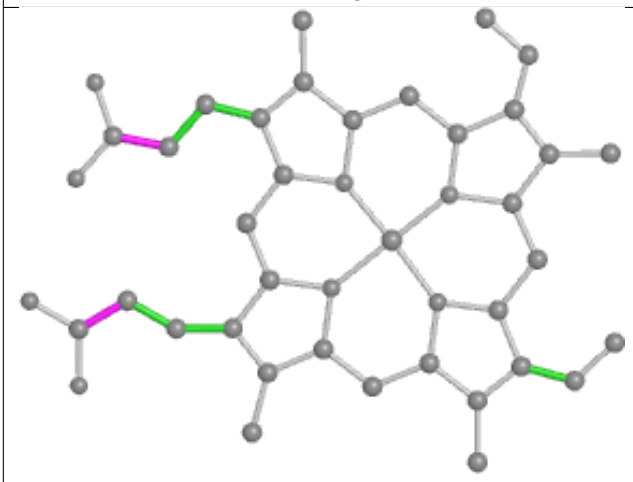
Ligand HEM B 801



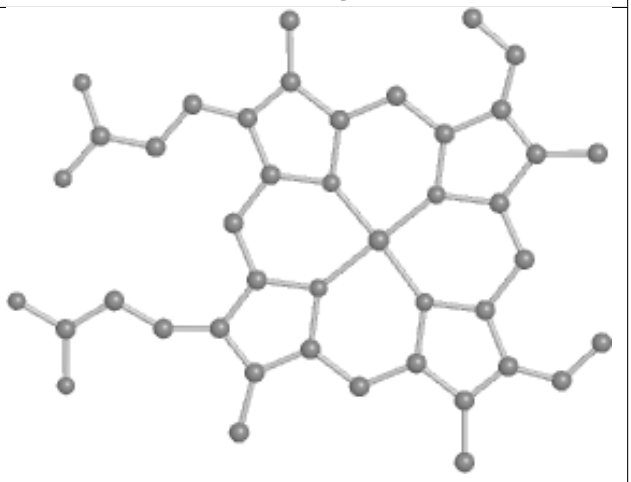
Bond lengths



Bond angles

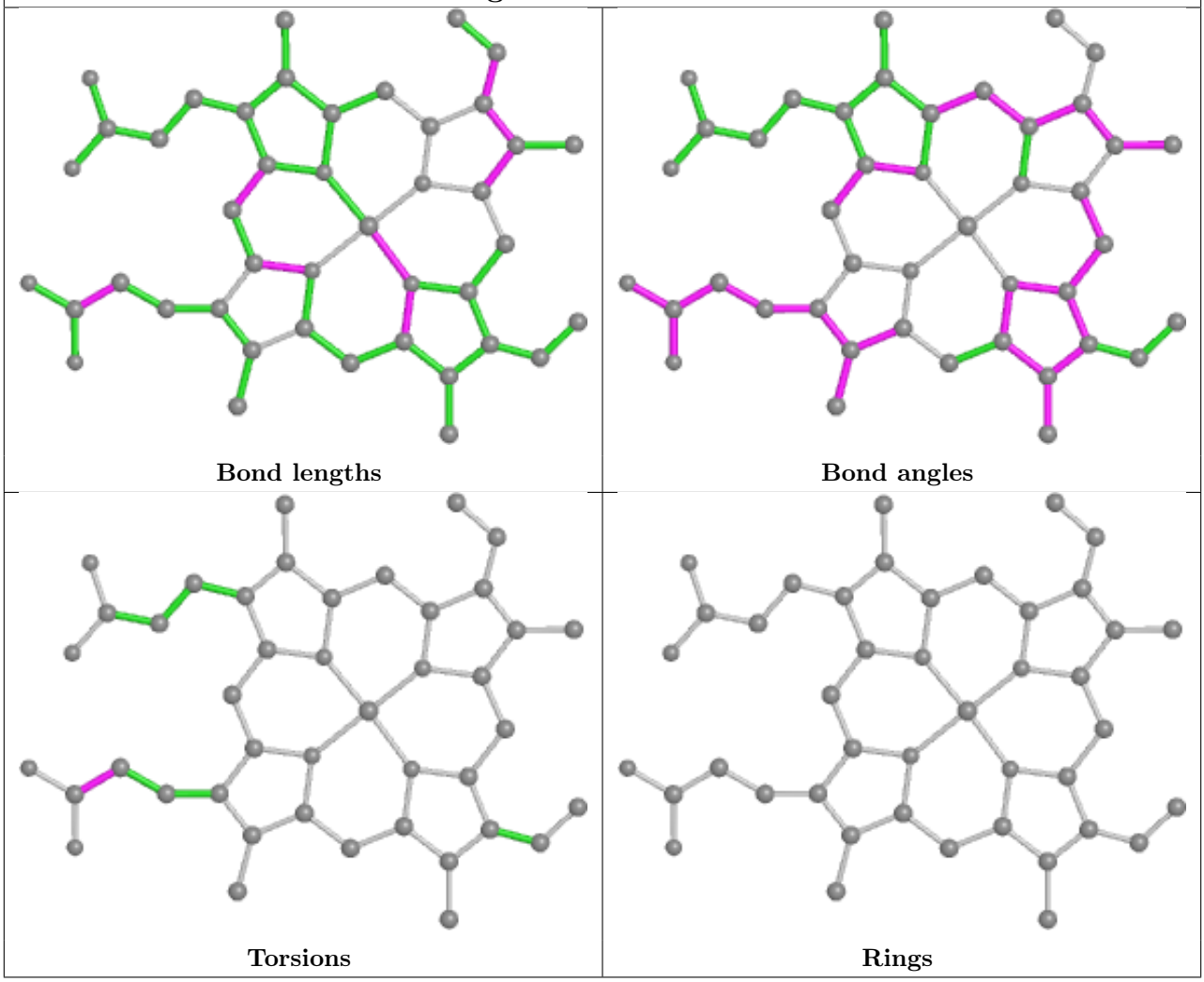


Torsions



Rings

Ligand HEM A 801



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	712/728 (97%)	-0.53	10 (1%)	75	72	15, 22, 40, 80	0
1	B	712/728 (97%)	-0.60	6 (0%)	86	84	15, 22, 40, 85	0
All	All	1424/1456 (97%)	-0.57	16 (1%)	80	78	15, 22, 40, 85	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	4.3
1	A	540	ARG	3.9
1	A	541	GLY	3.5
1	B	540	ARG	3.3
1	B	610	ARG	3.2
1	A	748	ALA	3.2
1	A	610	ARG	3.0
1	B	679	ALA	3.0
1	A	608	LYS	2.9
1	A	221	GLY	2.8
1	A	680	ALA	2.6
1	A	679	ALA	2.5
1	A	454	ASP	2.3
1	A	215	PRO	2.1
1	B	454	ASP	2.1
1	B	608	LYS	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TOX	A	111[A]	16/17	0.97	0.10	15,16,20,22	2
1	TOX	A	111[B]	16/17	0.97	0.10	15,16,19,22	2
1	TOX	B	111[A]	16/17	0.98	0.11	14,17,22,23	1
1	TOX	B	111[B]	16/17	0.98	0.11	14,17,19,23	1

6.3 Carbohydrates (i)

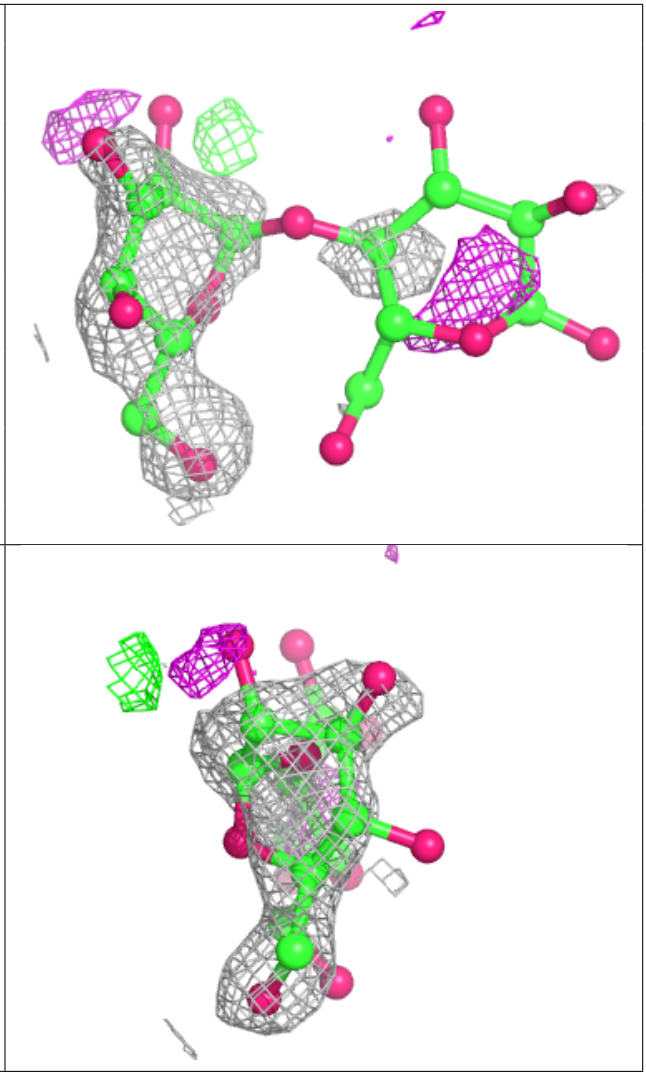
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GLC	C	1	12/12	0.15	0.82	102,123,132,139	0
2	GLC	D	1	12/12	0.65	0.86	97,137,148,159	0
2	GLC	C	2	11/12	0.78	0.37	60,88,103,104	0
2	GLC	D	2	11/12	0.92	0.26	39,54,64,72	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.

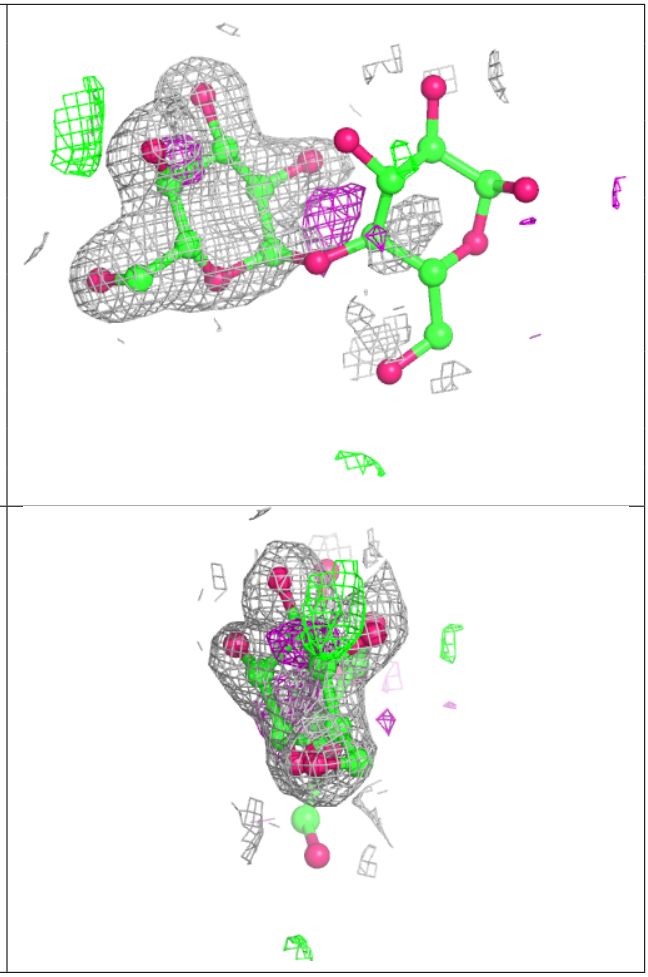
Electron density around Chain C:

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



Electron density around Chain D:

$2mF_o$-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
8	MPD	B	806	8/8	0.85	0.19	50,55,61,61	0
8	MPD	A	806	8/8	0.90	0.20	49,59,74,74	0
8	MPD	A	807	8/8	0.92	0.16	38,44,58,66	0
6	OXY	A	804	2/2	0.93	0.16	35,35,35,40	0
6	OXY	B	804	2/2	0.93	0.12	30,30,30,35	0
7	PO4	B	805	5/5	0.93	0.29	39,59,64,64	0
7	PO4	A	805	5/5	0.94	0.17	45,56,66,67	0
5	CL	B	803	1/1	0.97	0.07	38,38,38,38	0
5	CL	A	803	1/1	0.97	0.08	36,36,36,36	0
3	HEM	B	801	43/43	0.99	0.10	14,17,18,20	0
3	HEM	A	801	43/43	0.99	0.08	15,18,21,21	0

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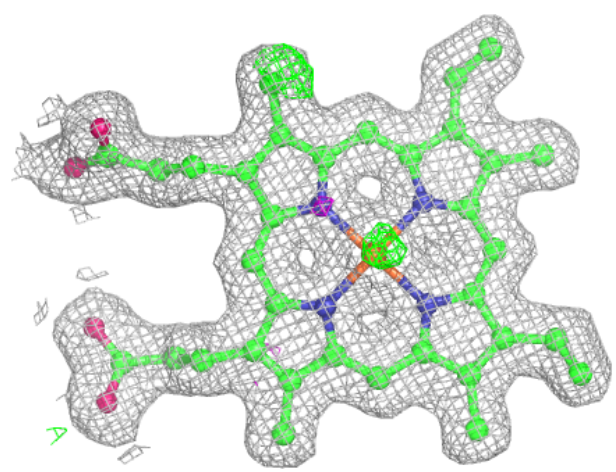
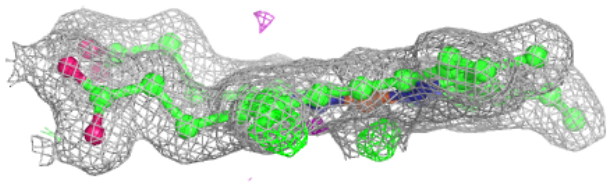
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	B	802	1/1	1.00	0.03	19,19,19,19	0
4	NA	A	802	1/1	1.00	0.06	19,19,19,19	0

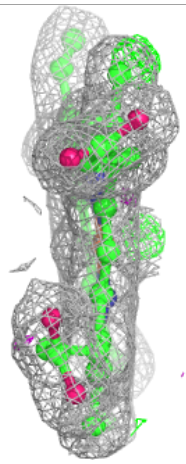
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM B 801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

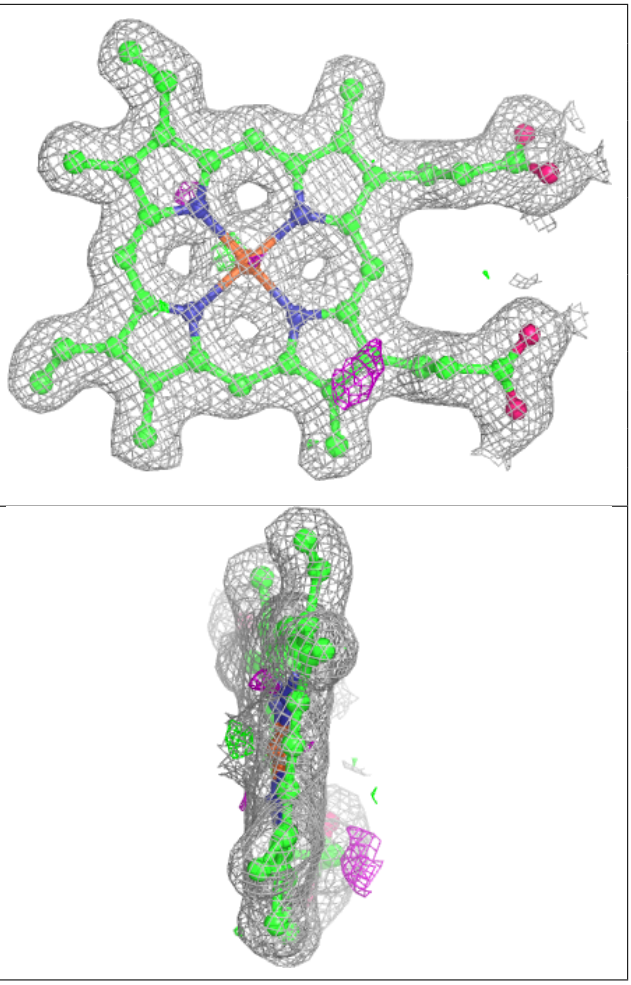






Electron density around HEM A 801:

$2mF_o$-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.