



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 06:35 AM EDT

PDB ID : 6B9B / pdb_00006b9b
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 ⓘ 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

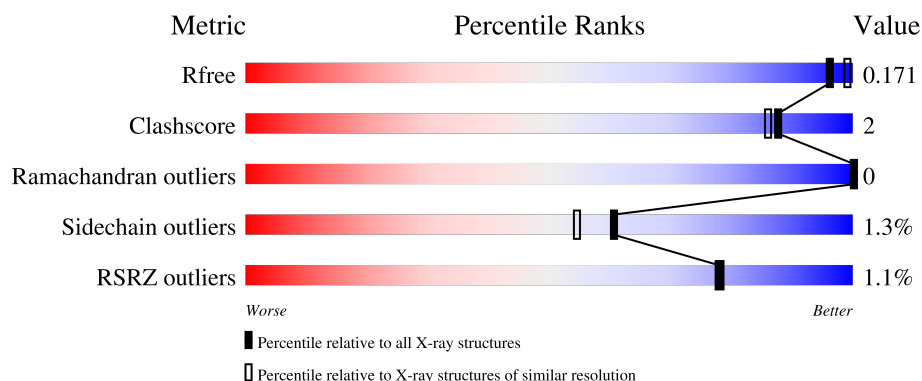
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	728	% 85% 13% .
1	B	728	% 85% 12% ..
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
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.

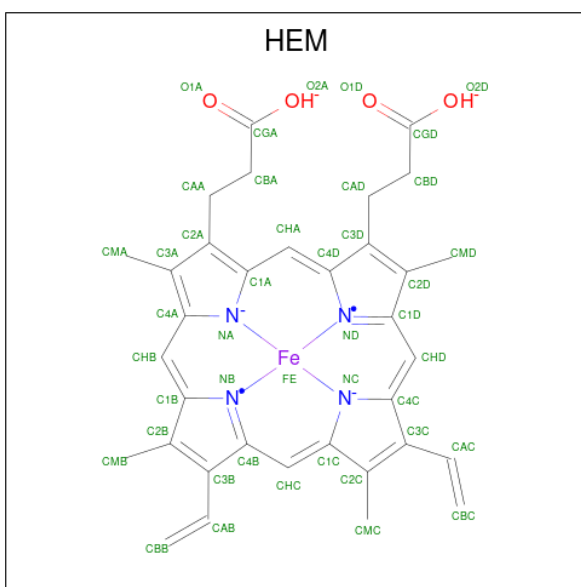
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	6	0
			5550	3502	990	1044	14			
1	B	713	Total	C	N	O	S	0	11	0
			5589	3525	994	1056	14			

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



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

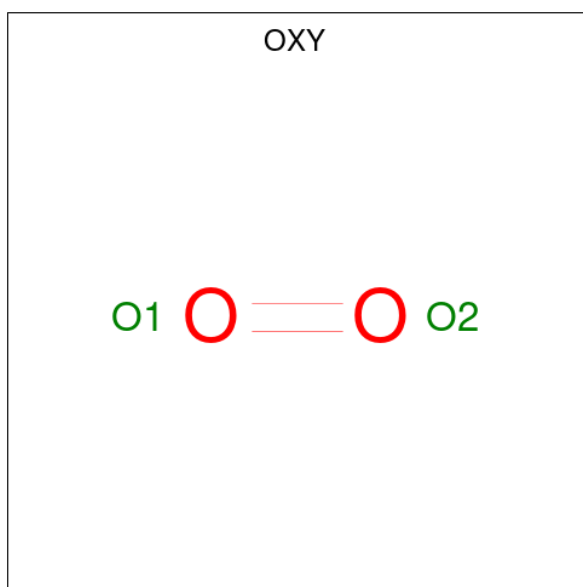
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

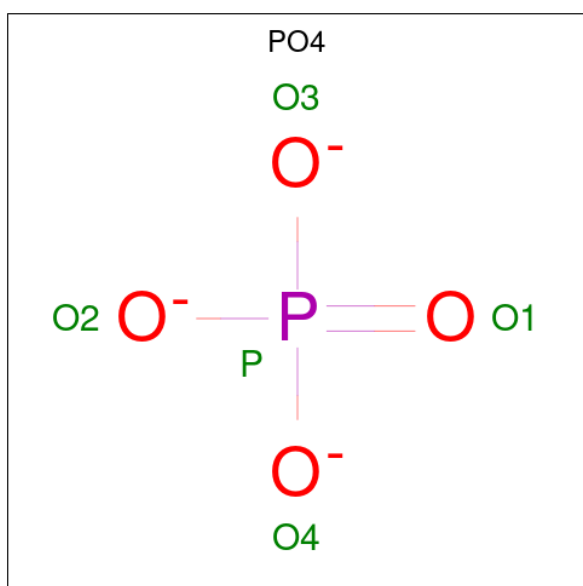
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



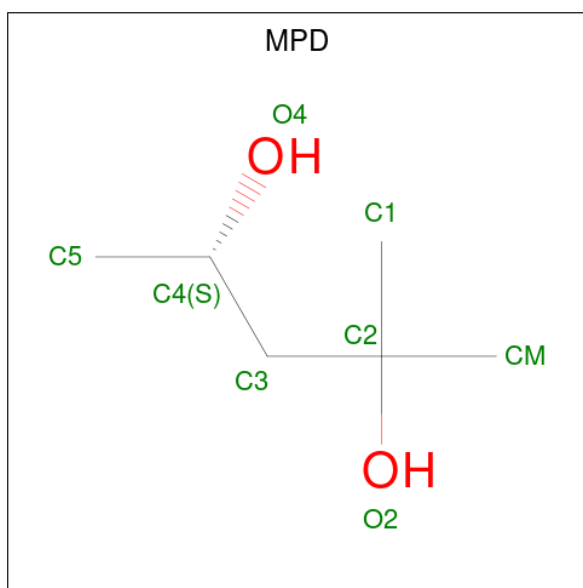
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			2	2		
6	B	1	Total	O	0	0
			2	2		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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



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

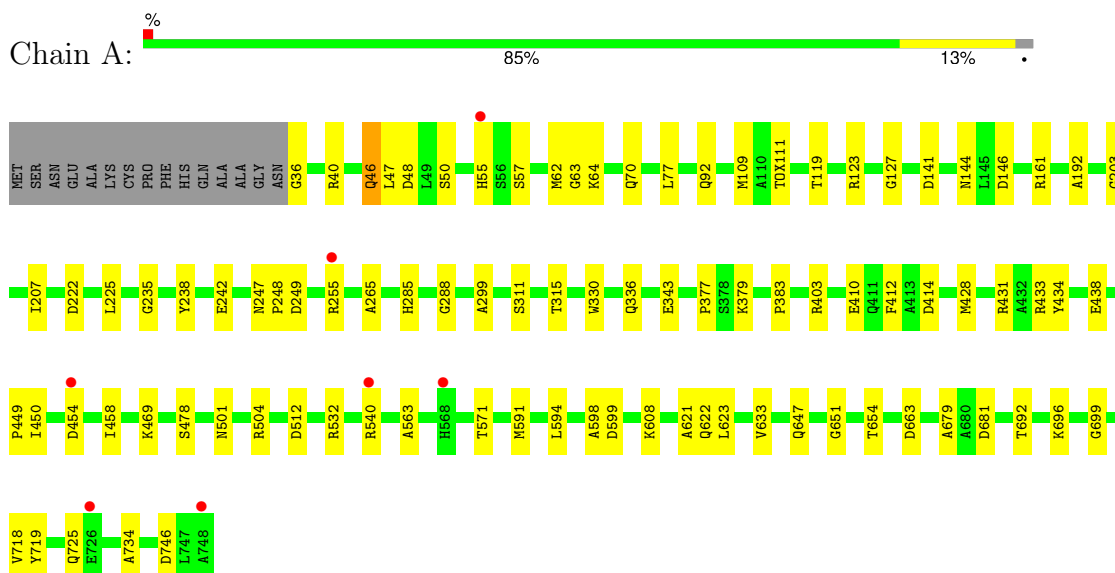
- Molecule 9 is water.

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

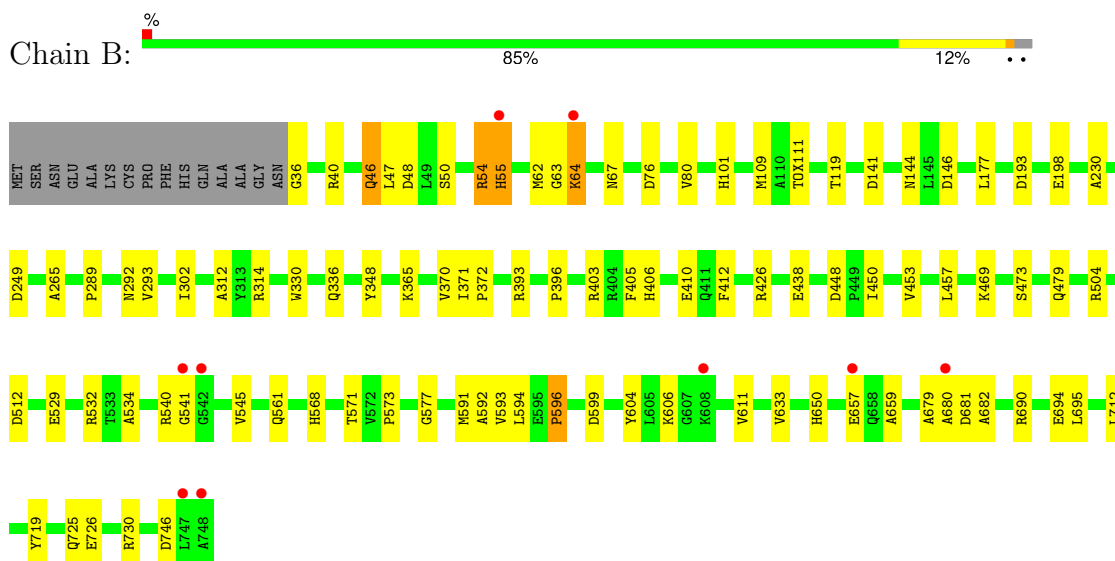
3 Residue-property plots [i](#)

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



- Molecule 1: Catalase-peroxidase



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

Chain C:  100%

GLC1
GLC2

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

Chain D:  50%  50%

GLC1
GLC2

4 Data and refinement statistics

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 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-1.80) 98.4 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ 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	9226 reflections (4.92%)	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 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: PO4, GLC, NA, HEM, OXY, CL, TOX, 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	1.76	62/5675 (1.1%)	1.31	14/7712 (0.2%)
1	B	1.74	61/5720 (1.1%)	1.32	17/7772 (0.2%)
All	All	1.75	123/11395 (1.1%)	1.31	31/15484 (0.2%)

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	448	ASP	N-CA	8.98	1.52	1.46
1	B	596	PRO	CA-CB	-8.20	1.45	1.54
1	A	63	GLY	N-CA	7.92	1.55	1.45
1	B	694	GLU	CA-C	7.44	1.62	1.52
1	B	63	GLY	N-CA	7.35	1.55	1.45
1	A	431	ARG	CD-NE	6.95	1.55	1.46
1	A	127	GLY	C-O	6.93	1.31	1.24
1	A	192	ALA	N-CA	6.93	1.54	1.46
1	B	479	GLN	CA-C	6.92	1.61	1.52
1	B	289	PRO	N-CA	-6.88	1.38	1.47
1	B	47	LEU	CB-CG	-6.83	1.39	1.53
1	B	348	TYR	C-O	6.75	1.32	1.23
1	B	561	GLN	CA-C	6.64	1.61	1.52
1	B	606	LYS	N-CA	6.64	1.54	1.46
1	A	501	ASN	CA-C	6.62	1.61	1.52
1	B	453	VAL	C-O	-6.44	1.16	1.24
1	B	690	ARG	CD-NE	-6.44	1.37	1.46
1	A	679	ALA	N-CA	6.43	1.54	1.46
1	B	438	GLU	CA-CB	6.43	1.62	1.53
1	B	177	LEU	N-CA	-6.42	1.38	1.46
1	B	573	PRO	CA-C	6.39	1.60	1.52
1	A	725	GLN	CD-OE1	6.38	1.35	1.23
1	A	699	GLY	N-CA	6.37	1.52	1.45
1	A	57	SER	CA-C	6.36	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	647	GLN	CA-C	6.21	1.61	1.53
1	B	403	ARG	CA-C	-6.20	1.44	1.52
1	A	57	SER	CB-OG	6.18	1.54	1.42
1	A	681	ASP	CA-C	6.16	1.59	1.52
1	B	457	LEU	C-O	6.16	1.31	1.23
1	A	433	ARG	C-N	6.15	1.41	1.33
1	B	64	LYS	C-O	-6.13	1.16	1.24
1	A	623	LEU	C-O	6.10	1.31	1.24
1	B	592	ALA	CA-C	-6.09	1.44	1.52
1	A	734	ALA	N-CA	-6.07	1.39	1.46
1	B	746	ASP	C-O	-6.05	1.16	1.24
1	A	725	GLN	N-CA	6.00	1.53	1.46
1	B	681	ASP	CA-C	5.98	1.59	1.52
1	A	249	ASP	CA-C	5.96	1.60	1.52
1	B	611	VAL	C-O	-5.89	1.16	1.24
1	B	109	MET	CA-C	5.88	1.60	1.52
1	B	599	ASP	C-O	-5.87	1.17	1.23
1	B	406	HIS	CA-C	5.85	1.60	1.52
1	A	36	GLY	N-CA	5.84	1.54	1.45
1	B	448	ASP	C-O	5.81	1.26	1.23
1	A	532	ARG	CA-C	5.79	1.60	1.52
1	B	371	ILE	N-CA	5.77	1.53	1.46
1	A	692	THR	CA-C	-5.76	1.45	1.52
1	A	540	ARG	C-O	5.74	1.31	1.23
1	B	650	HIS	CA-C	5.74	1.60	1.52
1	A	123	ARG	C-O	-5.71	1.16	1.23
1	B	679	ALA	N-CA	5.71	1.53	1.46
1	B	67	ASN	CA-C	5.68	1.59	1.52
1	A	235	GLY	CA-C	5.68	1.59	1.51
1	A	222	ASP	CA-C	5.65	1.59	1.53
1	B	193	ASP	C-O	5.62	1.30	1.23
1	B	101	HIS	CA-C	5.61	1.58	1.52
1	B	712	LEU	C-O	5.59	1.30	1.24
1	A	47	LEU	CB-CG	-5.59	1.42	1.53
1	A	247	ASN	CG-ND2	-5.58	1.21	1.33
1	A	438	GLU	CA-CB	5.57	1.61	1.53
1	A	203	GLY	CA-C	5.55	1.57	1.52
1	B	577	GLY	C-O	-5.54	1.18	1.24
1	B	695	LEU	C-O	-5.51	1.17	1.24
1	B	403	ARG	CD-NE	5.48	1.53	1.46
1	B	370	VAL	CA-C	5.44	1.60	1.52
1	A	225	LEU	CA-CB	5.43	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	LEU	N-CA	-5.42	1.39	1.46
1	A	46	GLN	CA-CB	5.42	1.62	1.53
1	B	659	ALA	CA-C	5.41	1.59	1.52
1	B	682	ALA	CA-C	5.41	1.60	1.52
1	A	92	GLN	CD-NE2	-5.40	1.22	1.33
1	A	207	ILE	N-CA	-5.38	1.39	1.46
1	B	393	ARG	N-CA	5.38	1.53	1.46
1	A	311	SER	CA-C	5.38	1.59	1.52
1	B	312	ALA	N-CA	5.37	1.53	1.46
1	A	377	PRO	C-O	-5.36	1.16	1.24
1	B	230	ALA	N-CA	-5.35	1.40	1.46
1	B	596	PRO	C-N	-5.35	1.27	1.34
1	A	599	ASP	CA-C	-5.33	1.47	1.53
1	B	62	MET	N-CA	-5.33	1.38	1.45
1	A	410	GLU	C-N	-5.33	1.26	1.33
1	B	680	ALA	N-CA	5.32	1.52	1.46
1	A	109	MET	N-CA	5.30	1.52	1.46
1	A	403	ARG	CA-C	-5.30	1.45	1.52
1	B	365	LYS	N-CA	5.29	1.52	1.46
1	A	428	MET	CG-SD	-5.28	1.67	1.80
1	A	663	ASP	CA-C	5.27	1.59	1.52
1	A	718	VAL	C-O	5.27	1.30	1.24
1	B	372	PRO	C-O	5.25	1.29	1.23
1	B	314	ARG	CA-C	-5.25	1.48	1.53
1	A	621	ALA	N-CA	-5.24	1.40	1.46
1	B	46	GLN	N-CA	5.22	1.52	1.45
1	B	534	ALA	N-CA	-5.22	1.40	1.46
1	B	504	ARG	CZ-NH1	-5.20	1.25	1.32
1	A	288	GLY	N-CA	5.20	1.51	1.44
1	A	621	ALA	CA-C	5.20	1.59	1.52
1	B	293	VAL	C-O	-5.20	1.18	1.24
1	A	383	PRO	CA-C	-5.19	1.46	1.52
1	A	285	HIS	C-O	5.18	1.29	1.23
1	A	449	PRO	C-N	-5.18	1.29	1.33
1	B	396	PRO	CA-CB	5.17	1.61	1.53
1	A	299	ALA	CA-C	-5.17	1.46	1.52
1	B	604	TYR	C-O	5.15	1.30	1.24
1	A	449	PRO	CA-C	5.15	1.59	1.52
1	B	292	ASN	CA-C	5.13	1.59	1.52
1	A	431	ARG	C-N	-5.12	1.27	1.33
1	A	654	THR	CA-C	5.11	1.58	1.52
1	A	598	ALA	CA-C	5.10	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	473	SER	C-O	-5.10	1.17	1.24
1	A	622	GLN	CA-C	5.09	1.59	1.52
1	A	563	ALA	N-CA	-5.09	1.40	1.46
1	A	343	GLU	CA-C	-5.08	1.46	1.52
1	B	36	GLY	N-CA	5.07	1.53	1.45
1	B	568	HIS	CA-C	5.07	1.58	1.52
1	A	336	GLN	CD-NE2	5.06	1.43	1.33
1	B	730	ARG	CZ-NH1	5.05	1.39	1.32
1	A	651	GLY	C-N	5.05	1.37	1.33
1	A	458	ILE	CA-CB	-5.03	1.49	1.54
1	A	414	ASP	CG-OD1	-5.03	1.15	1.25
1	A	746	ASP	C-O	-5.03	1.17	1.24
1	B	593	VAL	CA-C	-5.02	1.46	1.52
1	A	315	THR	C-O	-5.01	1.17	1.24
1	B	336	GLN	CA-C	-5.00	1.46	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	725	GLN	CB-CG-CD	7.83	125.91	112.60
1	A	48	ASP	N-CA-C	7.24	120.58	108.20
1	B	48	ASP	N-CA-C	7.22	120.55	108.20
1	B	46	GLN	CB-CG-CD	6.94	124.40	112.60
1	B	46	GLN	N-CA-C	-6.86	101.47	110.53
1	A	47	LEU	N-CA-CB	-6.55	100.34	109.97
1	A	46	GLN	N-CA-C	-6.31	102.20	110.53
1	A	330	TRP	N-CA-C	6.24	119.37	111.69
1	B	330	TRP	N-CA-C	6.20	119.32	111.69
1	A	55	HIS	CB-CA-C	6.09	120.82	111.39
1	A	62	MET	CA-C-N	-5.91	112.61	121.01
1	A	62	MET	C-N-CA	-5.91	112.61	121.01
1	B	450	ILE	CA-CB-CG1	-5.91	100.35	110.40
1	A	412	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	46	GLN	CG-CD-NE2	5.68	124.91	116.40
1	A	571	THR	OG1-CB-CG2	-5.63	98.04	109.30
1	A	450	ILE	CB-CA-C	-5.57	104.72	110.13
1	B	410	GLU	CB-CG-CD	5.54	122.01	112.60
1	B	47	LEU	N-CA-CB	-5.39	102.05	109.97
1	B	62	MET	CA-C-N	-5.37	113.39	121.01
1	B	62	MET	C-N-CA	-5.37	113.39	121.01
1	A	70	GLN	CA-CB-CG	5.27	124.64	114.10
1	B	50	SER	CA-CB-OG	-5.23	100.65	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	HIS	CB-CA-C	5.21	119.46	111.39
1	A	50	SER	CA-CB-OG	-5.19	100.72	111.10
1	B	80	VAL	N-CA-CB	5.18	116.61	110.55
1	A	478	SER	N-CA-C	5.04	116.77	111.28
1	B	541	GLY	N-CA-C	-5.03	103.12	112.37
1	B	46	GLN	CA-CB-CG	5.02	124.14	114.10
1	B	571	THR	O-C-N	-5.02	117.37	123.29
1	A	512	ASP	CA-CB-CG	-5.00	107.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5550	0	5353	14	0
1	B	5589	0	5382	21	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
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	5	0
9	B	741	0	0	9	0
All	All	12762	0	10878	44	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 (44) 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:B:726[B]:GLU:CD	1:B:726[B]:GLU:H	2.08	0.61
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: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:657[A]:GLU:CD	9:B:1236:HOH:O	2.56	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:696:LYS:NZ	9:A:925:HOH:O	2.49	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
1:B:726[B]:GLU:CD	1:B:726[B]:GLU:N	2.75	0.43
8:A:807:MPD:H11	8:A:807:MPD:C5	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLU:O	1:A:248:PRO:HA	2.21	0.41
1:A:591:MET:HB2	1:A:591:MET:HE2	1.88	0.41
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.91	0.40
1:B:249:ASP:OD1	1:B:249:ASP:C	2.64	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%)	59	52
1	B	559/560 (100%)	553 (99%)	6 (1%)	65	60
All	All	1113/1120 (99%)	1099 (99%)	14 (1%)	61	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	64	LYS
1	A	141	ASP
1	A	161	ARG
1	A	379	LYS
1	A	469	LYS
1	A	608	LYS
1	B	40	ARG
1	B	46	GLN
1	B	54	ARG
1	B	64	LYS
1	B	141	ASP
1	B	469	LYS

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	70	GLN
1	A	247	ASN
1	A	520	GLN
1	A	568	HIS
1	A	737	ASN
1	B	46	GLN
1	B	227	ASN
1	B	406	HIS
1	B	725	GLN
1	B	737	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	14,17,18	2.24	6 (42%)	12,23,25	3.24	5 (41%)
1	TOX	B	111[B]	-	14,17,18	1.88	5 (35%)	12,23,25	1.95	5 (41%)
1	TOX	B	111[A]	3	14,17,18	1.88	5 (35%)	12,23,25	1.95	5 (41%)
1	TOX	A	111[B]	-	14,17,18	2.24	6 (42%)	12,23,25	3.24	5 (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
1	TOX	A	111[A]	3	-	2/5/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	B	111[A]	3	-	2/5/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/5/8/10	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	CE2-NE1	-4.40	1.32	1.39
1	A	111[B]	TOX	CE2-NE1	-4.40	1.32	1.39
1	A	111[A]	TOX	CD2-CE2	4.36	1.46	1.41
1	A	111[B]	TOX	CD2-CE2	4.36	1.46	1.41
1	B	111[A]	TOX	CD2-CE2	3.55	1.45	1.41
1	B	111[B]	TOX	CD2-CE2	3.55	1.45	1.41
1	B	111[A]	TOX	O-C	3.01	1.31	1.20
1	B	111[B]	TOX	O-C	3.01	1.31	1.20
1	A	111[A]	TOX	CA-N	-2.83	1.40	1.48
1	A	111[B]	TOX	CA-N	-2.83	1.40	1.48
1	B	111[A]	TOX	CA-N	-2.59	1.40	1.48
1	B	111[B]	TOX	CA-N	-2.59	1.40	1.48
1	B	111[A]	TOX	CD1-CG	2.58	1.42	1.36
1	B	111[B]	TOX	CD1-CG	2.58	1.42	1.36
1	A	111[A]	TOX	CD2-CG	2.35	1.47	1.44
1	A	111[B]	TOX	CD2-CG	2.35	1.47	1.44
1	A	111[A]	TOX	CH2-CZ2	2.35	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[B]	TOX	CH2-CZ2	2.35	1.42	1.38
1	A	111[A]	TOX	CZ2-CE2	-2.33	1.36	1.39
1	A	111[B]	TOX	CZ2-CE2	-2.33	1.36	1.39
1	B	111[A]	TOX	CB-CA	-2.17	1.49	1.53
1	B	111[B]	TOX	CB-CA	-2.17	1.49	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-CD2	-7.47	113.61	121.95
1	A	111[B]	TOX	CZ2-CE2-CD2	-7.47	113.61	121.95
1	A	111[A]	TOX	CE2-CD2-CG	-4.79	102.98	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-4.79	102.98	107.39
1	A	111[A]	TOX	CZ2-CE2-NE1	4.67	136.80	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	4.67	136.80	129.37
1	B	111[A]	TOX	CZ2-CE2-CD2	-3.04	118.55	121.95
1	B	111[B]	TOX	CZ2-CE2-CD2	-3.04	118.55	121.95
1	A	111[A]	TOX	CH2-CZ3-CE3	-3.00	116.54	120.24
1	A	111[B]	TOX	CH2-CZ3-CE3	-3.00	116.54	120.24
1	A	111[A]	TOX	CH2-CZ2-CE2	2.97	124.28	118.28
1	A	111[B]	TOX	CH2-CZ2-CE2	2.97	124.28	118.28
1	B	111[A]	TOX	CZ3-CH2-CZ2	2.79	123.69	120.24
1	B	111[B]	TOX	CZ3-CH2-CZ2	2.79	123.69	120.24
1	B	111[A]	TOX	CD2-CG-CD1	-2.65	103.94	106.34
1	B	111[B]	TOX	CD2-CG-CD1	-2.65	103.94	106.34
1	B	111[A]	TOX	CE3-CD2-CE2	2.51	122.13	119.24
1	B	111[B]	TOX	CE3-CD2-CE2	2.51	122.13	119.24
1	B	111[A]	TOX	CE3-CD2-CG	-2.16	130.63	133.85
1	B	111[B]	TOX	CE3-CD2-CG	-2.16	130.63	133.85

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

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	1.67	4 (33%)	17,17,17	1.82	5 (29%)
2	GLC	C	2	2	11,11,12	0.54	0	15,15,17	2.70	7 (46%)
2	GLC	D	1	2	12,12,12	1.69	4 (33%)	17,17,17	3.15	8 (47%)
2	GLC	D	2	2	11,11,12	1.88	2 (18%)	15,15,17	2.32	6 (40%)

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	3.99	1.61	1.52
2	D	1	GLC	O4-C4	3.06	1.50	1.43
2	D	2	GLC	C2-C3	2.98	1.57	1.52
2	D	1	GLC	C4-C3	2.56	1.59	1.52
2	D	1	GLC	C1-C2	2.51	1.58	1.52
2	C	1	GLC	O4-C4	2.43	1.49	1.43
2	C	1	GLC	C3-C2	2.41	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	C4-C5	2.32	1.58	1.53
2	C	1	GLC	C4-C3	2.27	1.58	1.52
2	C	1	GLC	O1-C1	2.25	1.46	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	O4-C4-C5	5.97	124.02	109.32
2	C	2	GLC	O5-C1-C2	-5.63	97.36	110.79
2	D	1	GLC	O2-C2-C1	4.83	120.40	109.25
2	D	1	GLC	C4-C3-C2	-4.64	102.68	110.83
2	D	1	GLC	O3-C3-C4	4.63	121.29	110.38
2	D	1	GLC	C6-C5-C4	4.54	124.17	113.02
2	C	2	GLC	C1-C2-C3	-4.44	103.18	109.64
2	D	1	GLC	C3-C4-C5	-4.11	102.78	110.23
2	D	2	GLC	O3-C3-C2	4.08	118.38	110.05
2	C	2	GLC	O4-C4-C5	-3.80	99.97	109.32
2	D	2	GLC	C1-C2-C3	3.47	114.69	109.64
2	D	2	GLC	C1-O5-C5	-3.42	107.60	112.19
2	C	1	GLC	O4-C4-C3	3.42	118.43	110.38
2	C	2	GLC	C2-C3-C4	-3.34	104.98	110.86
2	D	2	GLC	O5-C5-C4	3.34	118.95	110.83
2	C	2	GLC	O3-C3-C4	3.10	117.68	110.38
2	D	1	GLC	O1-C1-C2	3.09	117.96	108.98
2	D	2	GLC	O4-C4-C3	-2.99	103.33	110.38
2	C	1	GLC	O5-C1-C2	-2.95	105.11	110.30
2	C	1	GLC	O5-C5-C4	2.93	114.98	109.70
2	C	1	GLC	O1-C1-C2	2.92	117.47	108.98
2	C	1	GLC	C3-C4-C5	-2.72	105.30	110.23
2	D	1	GLC	O4-C4-C3	2.70	116.75	110.38
2	C	2	GLC	C1-O5-C5	2.67	115.77	112.19
2	C	2	GLC	O3-C3-C2	2.52	115.19	110.05
2	D	2	GLC	O3-C3-C4	-2.34	104.86	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

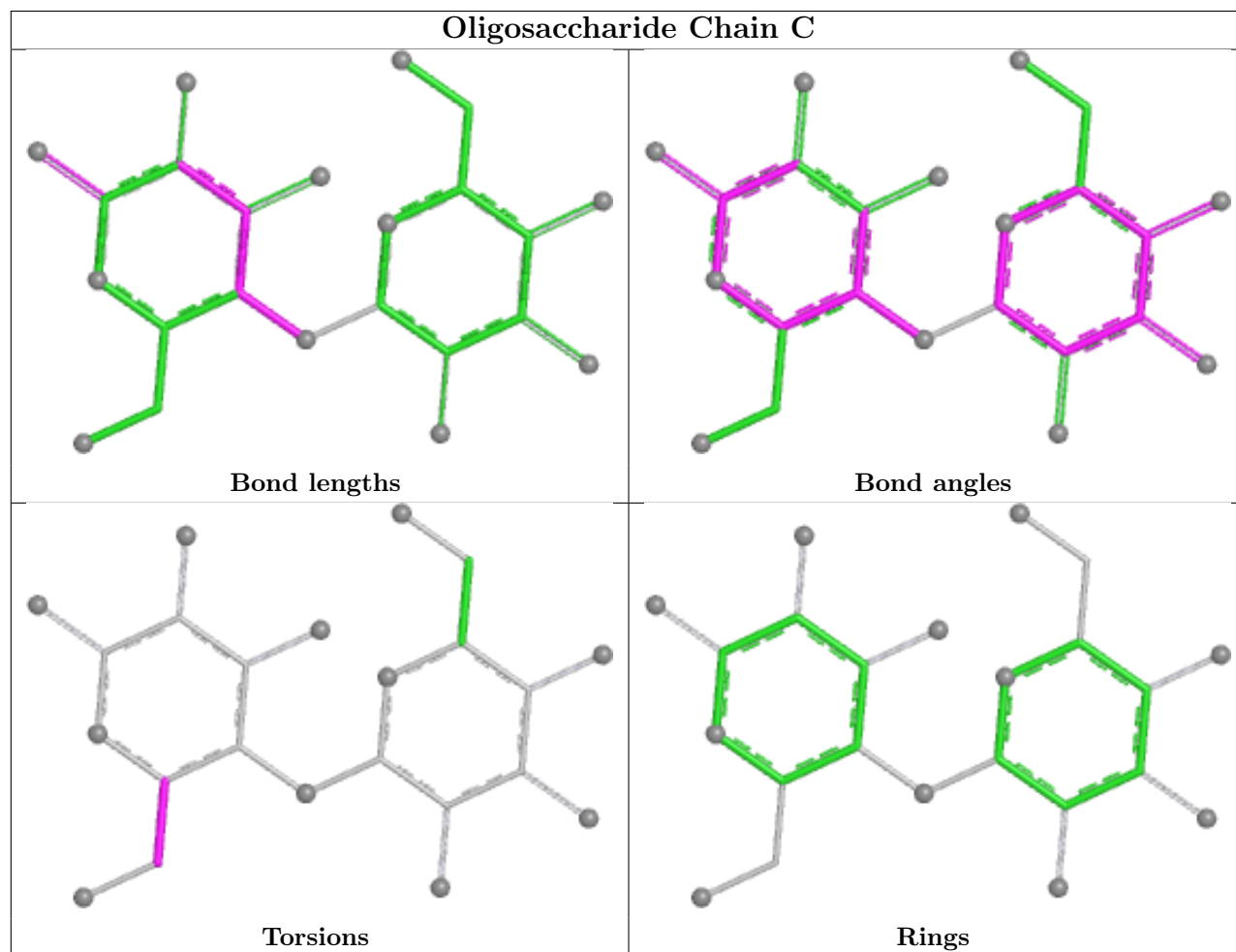
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6

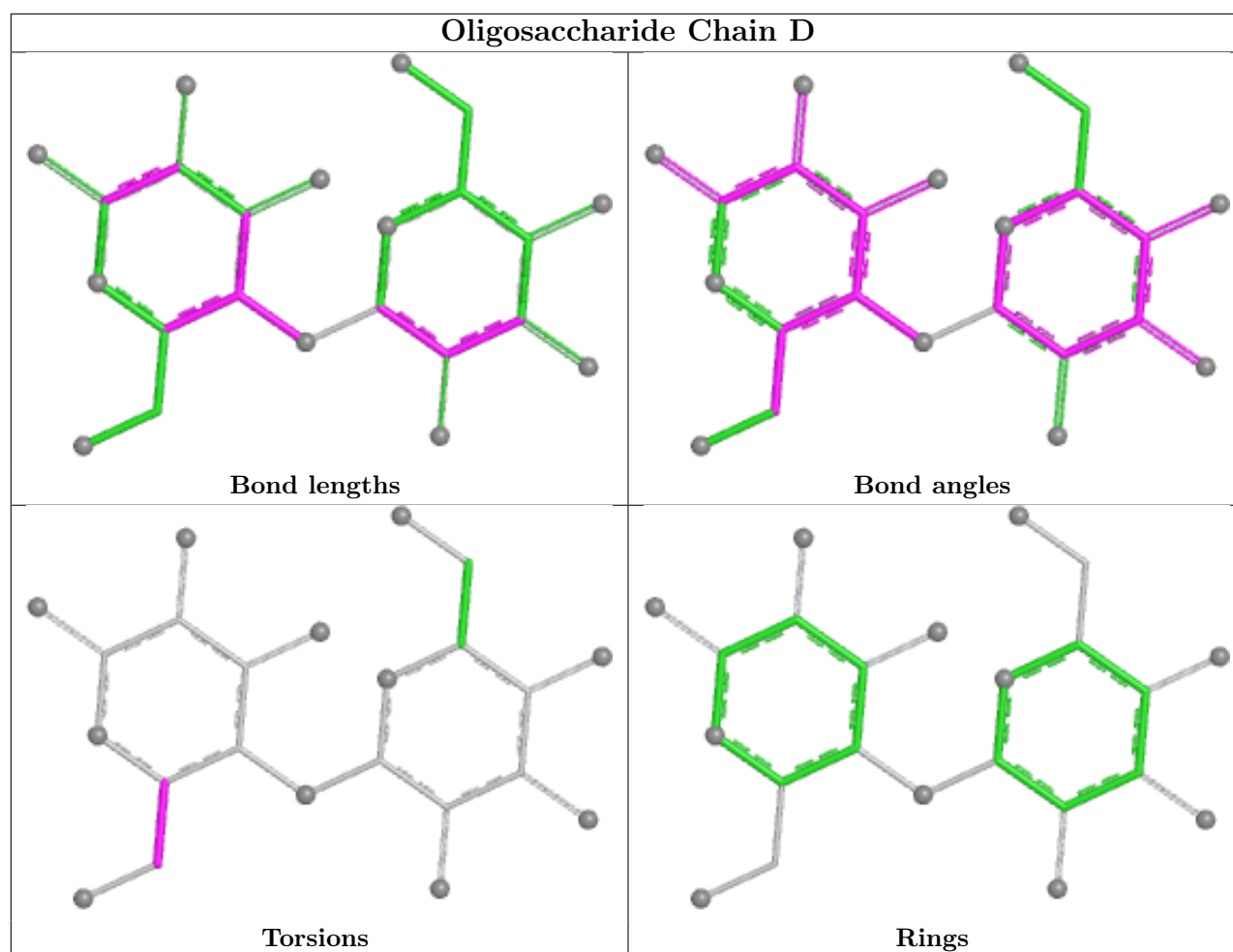
There are no ring outliers.

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.





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	A	805	-	4,4,4	1.16	0	6,6,6	2.68	4 (66%)
8	MPD	A	806	-	7,7,7	1.20	0	9,10,10	1.64	3 (33%)
8	MPD	B	806	-	7,7,7	0.54	0	9,10,10	1.99	3 (33%)
6	OXY	B	804	-	1,1,1	0.86	0	-		
8	MPD	A	807	-	7,7,7	1.01	0	9,10,10	2.05	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	801	1	50,50,50	1.58	8 (16%)	67,82,82	1.42	10 (14%)
6	OXY	A	804	-	1,1,1	0.38	0	-		
7	PO4	B	805	-	4,4,4	0.91	0	6,6,6	1.69	2 (33%)
3	HEM	B	801	1	50,50,50	1.53	10 (20%)	67,82,82	1.42	10 (14%)

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	806	-	-	3/5/5/5	-
8	MPD	B	806	-	-	3/5/5/5	-
8	MPD	A	807	-	-	4/5/5/5	-
3	HEM	A	801	1	-	2/14/54/54	-
3	HEM	B	801	1	-	3/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	FE-NB	4.35	2.08	1.94
3	B	801	HEM	C1C-NC	-3.80	1.32	1.39
3	A	801	HEM	FE-NC	3.42	2.06	1.95
3	B	801	HEM	C2A-C3A	-3.23	1.30	1.38
3	A	801	HEM	C1B-NB	-3.18	1.34	1.40
3	A	801	HEM	CHB-C4A	3.14	1.46	1.39
3	B	801	HEM	C4B-NB	-3.07	1.32	1.38
3	B	801	HEM	C1B-NB	-2.92	1.35	1.40
3	A	801	HEM	C1A-C2A	-2.84	1.38	1.44
3	B	801	HEM	FE-NB	2.79	2.03	1.94
3	A	801	HEM	FE-NA	2.63	2.03	1.95
3	B	801	HEM	CHB-C1B	2.61	1.43	1.38
3	B	801	HEM	O1D-CGD	2.59	1.30	1.22
3	A	801	HEM	CBA-CGA	2.48	1.56	1.50
3	B	801	HEM	O1A-CGA	2.45	1.30	1.22
3	B	801	HEM	FE-NC	2.31	2.02	1.95
3	B	801	HEM	C1A-NA	-2.27	1.35	1.39
3	A	801	HEM	CMA-C3A	2.16	1.55	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	HEM	C4B-C3B-C2B	-4.57	103.08	107.28
3	B	801	HEM	CHD-C4C-NC	4.28	129.12	124.45
8	A	807	MPD	C5-C4-C3	3.93	129.91	111.67
7	A	805	PO4	O3-P-O1	-3.88	97.22	110.95
3	B	801	HEM	C4B-C3B-C2B	-3.58	103.99	107.28
8	A	807	MPD	CM-C2-C1	-3.45	102.89	110.63
7	A	805	PO4	O4-P-O1	3.33	122.73	110.95
3	A	801	HEM	O2A-CGA-CBA	3.17	124.03	114.00
8	B	806	MPD	C1-C2-C3	3.17	123.87	110.20
3	B	801	HEM	CHC-C4B-NB	3.02	127.67	124.42
3	A	801	HEM	O1A-CGA-CBA	-2.96	113.70	123.09
3	A	801	HEM	CAA-CBA-CGA	-2.83	106.17	113.67
7	B	805	PO4	O2-P-O1	-2.77	101.15	110.95
8	B	806	MPD	O2-C2-CM	2.67	116.32	107.99
3	B	801	HEM	CAA-CBA-CGA	-2.60	106.76	113.67
7	B	805	PO4	O3-P-O1	2.60	120.15	110.95
7	A	805	PO4	O4-P-O2	-2.60	99.83	107.91
3	A	801	HEM	C4C-C3C-C2C	2.51	108.99	106.81
3	B	801	HEM	CHD-C4C-C3C	-2.51	120.98	125.21
3	A	801	HEM	C3B-C2B-C1B	2.49	108.28	106.41
3	B	801	HEM	C3C-C2C-C1C	-2.49	104.69	107.05
3	A	801	HEM	CAC-C3C-C4C	-2.48	118.90	124.82
7	A	805	PO4	O4-P-O3	2.46	115.56	107.91
8	A	806	MPD	O4-C4-C5	2.41	119.82	109.45
8	A	806	MPD	CM-C2-C3	2.38	120.45	110.20
3	B	801	HEM	O2A-CGA-CBA	2.31	121.30	114.00
3	B	801	HEM	C4A-C3A-C2A	2.25	109.39	106.82
3	B	801	HEM	CBA-CAA-C2A	2.23	118.69	112.53
8	B	806	MPD	O4-C4-C5	2.17	118.78	109.45
3	A	801	HEM	CMA-C3A-C2A	2.13	130.14	125.62
3	B	801	HEM	O1D-CGD-CBD	-2.07	116.53	123.09
8	A	806	MPD	CM-C2-C1	2.06	115.24	110.63
3	A	801	HEM	CHA-C4D-ND	2.05	126.90	124.37
8	A	807	MPD	O4-C4-C3	-2.05	103.21	111.35
3	A	801	HEM	C3C-C2C-C1C	-2.05	105.11	107.05

There are no chirality outliers.

All (15) 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

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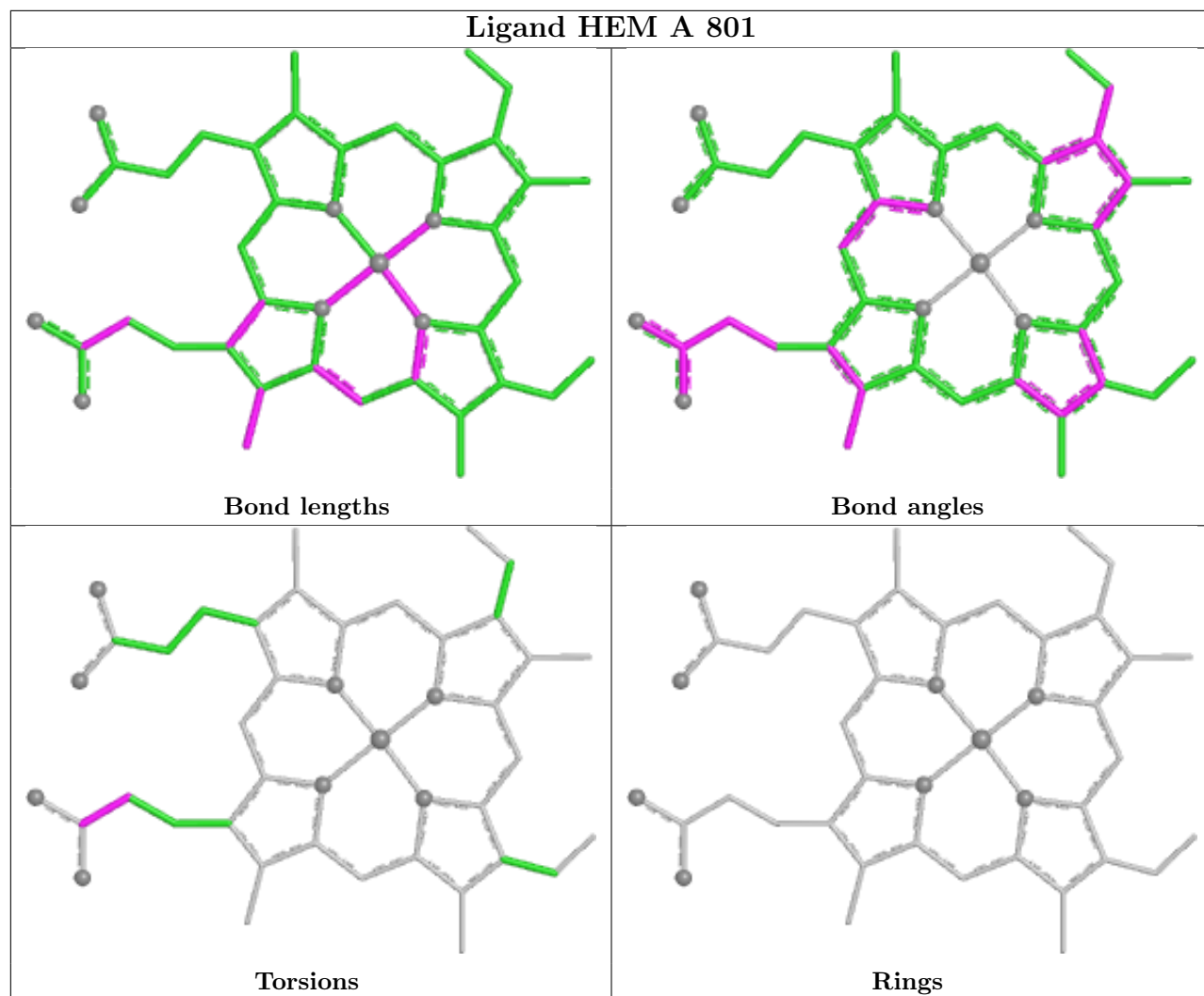
Mol	Chain	Res	Type	Atoms
8	A	807	MPD	C2-C3-C4-C5
8	B	806	MPD	C1-C2-C3-C4
8	B	806	MPD	O2-C2-C3-C4
8	A	806	MPD	C1-C2-C3-C4
8	A	807	MPD	CM-C2-C3-C4
8	B	806	MPD	CM-C2-C3-C4
3	B	801	HEM	CAA-CBA-CGA-O2A
3	A	801	HEM	CAA-CBA-CGA-O2A
3	A	801	HEM	CAA-CBA-CGA-O1A
3	B	801	HEM	CAA-CBA-CGA-O1A
8	A	807	MPD	C2-C3-C4-O4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

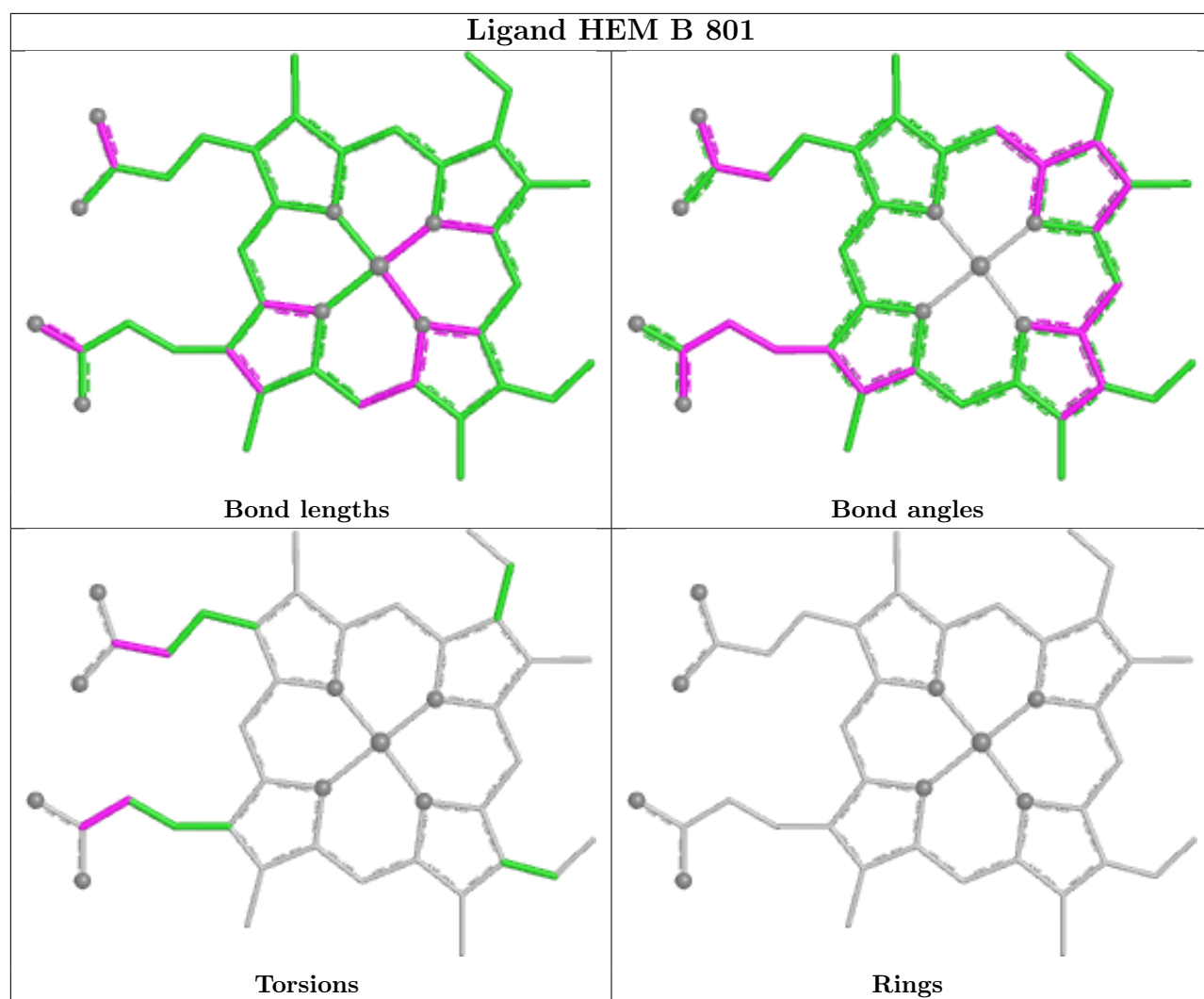
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	806	MPD	2	0
8	B	806	MPD	1	0
6	B	804	OXY	1	0
8	A	807	MPD	2	0
6	A	804	OXY	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 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 [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%)	-0.43	7 (0%) 79 80	9, 22, 40, 80	5 (0%)
1	B	712/728 (97%)	-0.48	9 (1%) 75 75	9, 22, 40, 85	10 (1%)
All	All	1424/1456 (97%)	-0.46	16 (1%) 78 78	9, 22, 40, 85	15 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.4
1	B	748	ALA	5.1
1	B	55	HIS	3.4
1	A	454	ASP	3.1
1	A	726[A]	GLU	2.7
1	A	568	HIS	2.7
1	A	55	HIS	2.6
1	B	657[A]	GLU	2.6
1	B	542	GLY	2.5
1	B	541	GLY	2.4
1	B	608	LYS	2.4
1	B	747	LEU	2.1
1	A	255[A]	ARG	2.1
1	B	64	LYS	2.0
1	B	680	ALA	2.0
1	A	540	ARG	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($\text{\AA}^2$)	Q<0.9
1	TOX	A	111[A]	16/17	0.98	0.05	15,16,20,22	2
1	TOX	A	111[B]	16/17	0.98	0.05	15,16,19,22	2
1	TOX	B	111[A]	16/17	0.98	0.04	14,17,22,23	1
1	TOX	B	111[B]	16/17	0.98	0.04	14,17,19,23	1

6.3 Carbohydrates

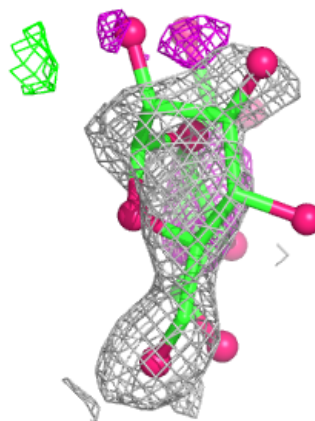
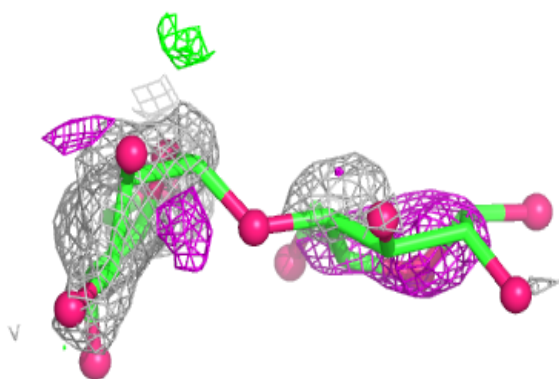
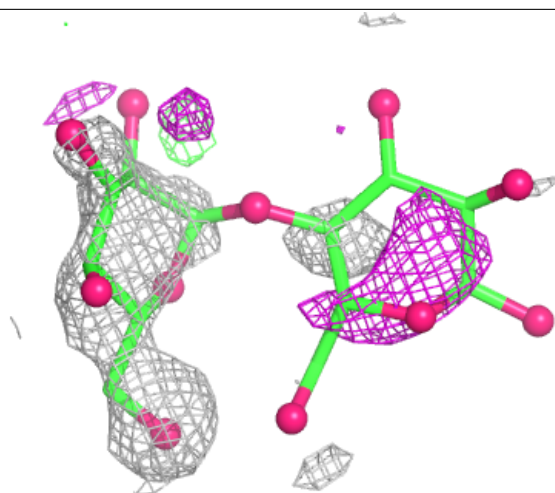
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

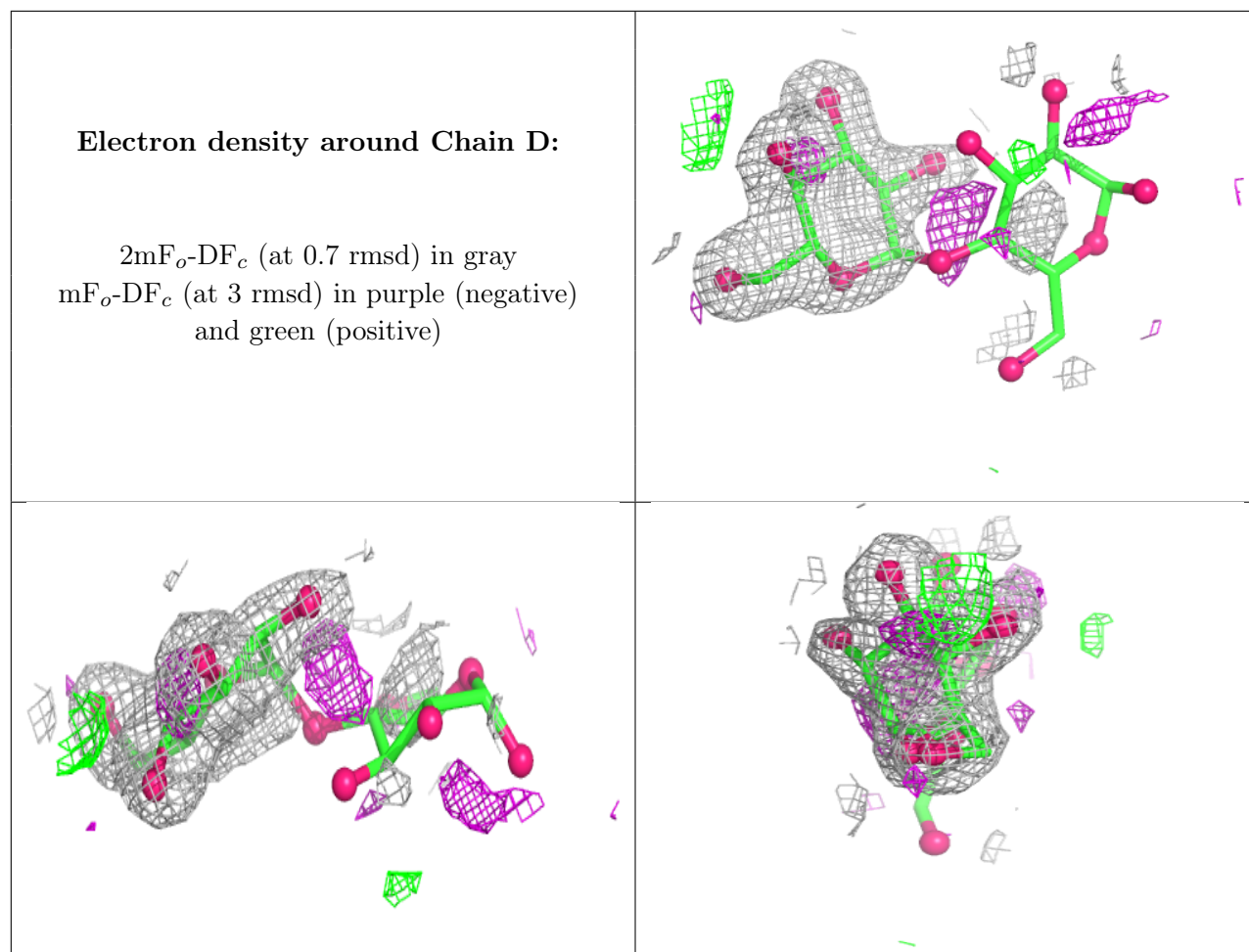
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	1	12/12	0.59	0.21	102,123,132,139	0
2	GLC	D	1	12/12	0.73	0.21	97,137,148,159	0
2	GLC	C	2	11/12	0.85	0.17	60,88,103,104	0
2	GLC	D	2	11/12	0.92	0.10	39,54,64,72	0

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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MPD	A	806	8/8	0.82	0.28	49,59,74,74	0
8	MPD	B	806	8/8	0.86	0.22	50,55,61,61	0
8	MPD	A	807	8/8	0.89	0.15	38,44,58,66	0
7	PO4	B	805	5/5	0.89	0.10	39,59,64,64	0
6	OXY	A	804	2/2	0.90	0.20	35,35,35,40	0
7	PO4	A	805	5/5	0.90	0.10	45,56,66,67	0
6	OXY	B	804	2/2	0.94	0.20	30,30,30,35	0
5	CL	B	803	1/1	0.96	0.09	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	0.04	14,17,18,20	0
3	HEM	A	801	43/43	0.99	0.04	15,18,21,21	0

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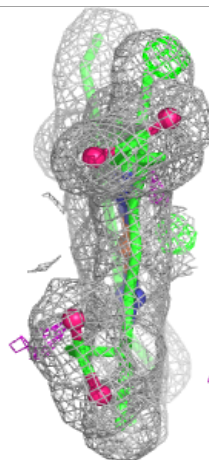
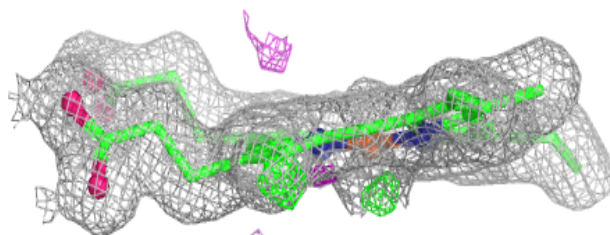
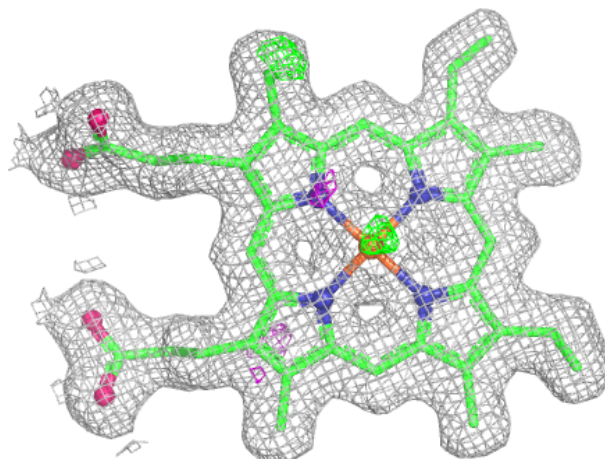
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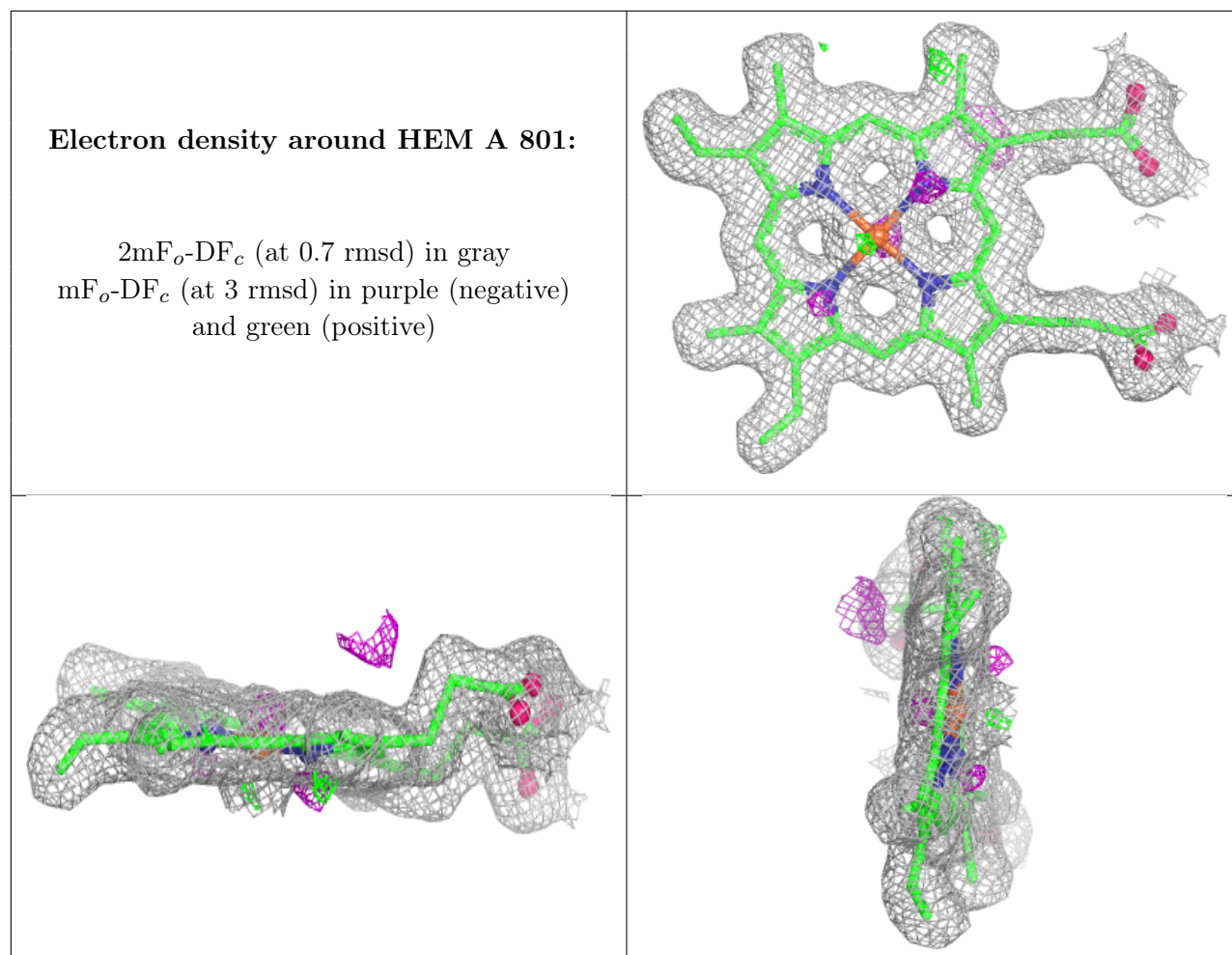
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	B	802	1/1	1.00	0.04	19,19,19,19	0
4	NA	A	802	1/1	1.00	0.03	19,19,19,19	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.