Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2024 – 10:08 PM EST

PDB ID	:	5W6S
Title	:	Crystal structure of Bacteriophage CBA120 tailspike protein 2 enzymatically active domain (TSP2dN, orf211) complex with Escherichia Coli O157-antigen
Authors	:	Plattner, M.; Shneider, M.M.; Leiman, P.G.
Deposited on	:	2017-06-16
Resolution	:	2.26 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:

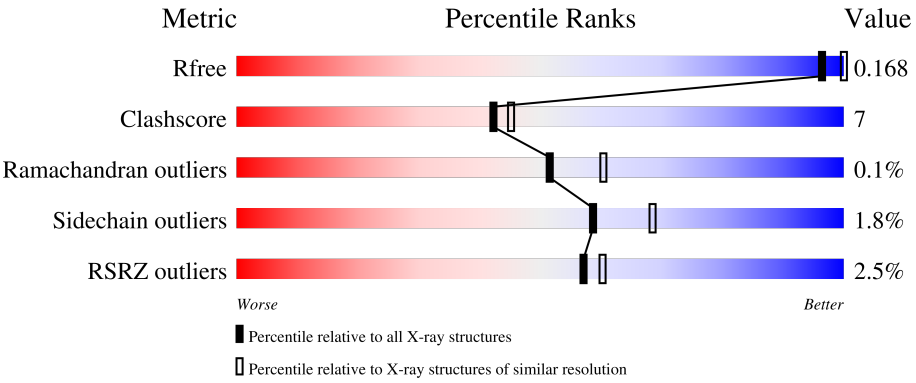
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	680	2% 89% 10%
2	B	4	75% 25%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5764 atoms, of which 6 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.

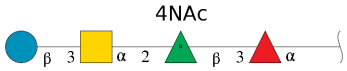
- Molecule 1 is a protein called tailspike protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	676	5059	3165	868	1005	21	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

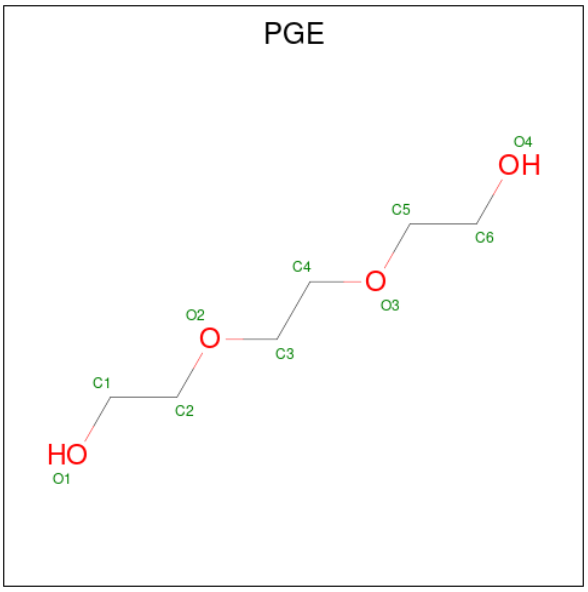
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	expression tag	UNP G3M190
A	243	SER	-	expression tag	UNP G3M190
A	244	GLY	-	expression tag	UNP G3M190
A	245	SER	-	expression tag	UNP G3M190

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-2)-4-acetamido-4,6-dideoxy-beta-D-mannopyranose-(1-3)-alpha-L-fucopyranose.



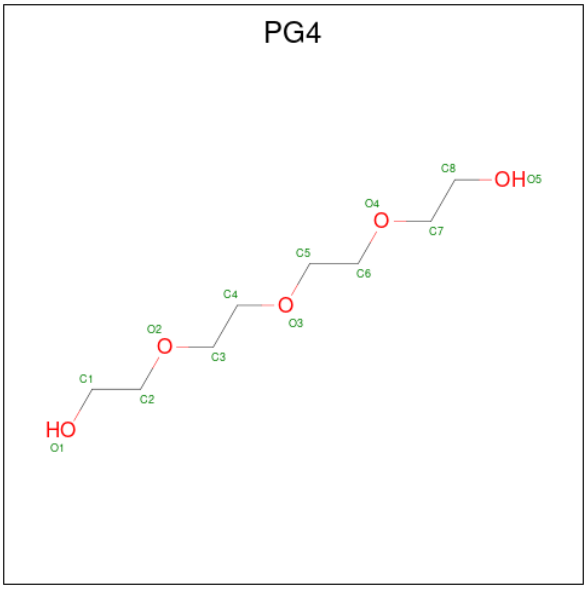
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	4	49	28	2	19	0	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



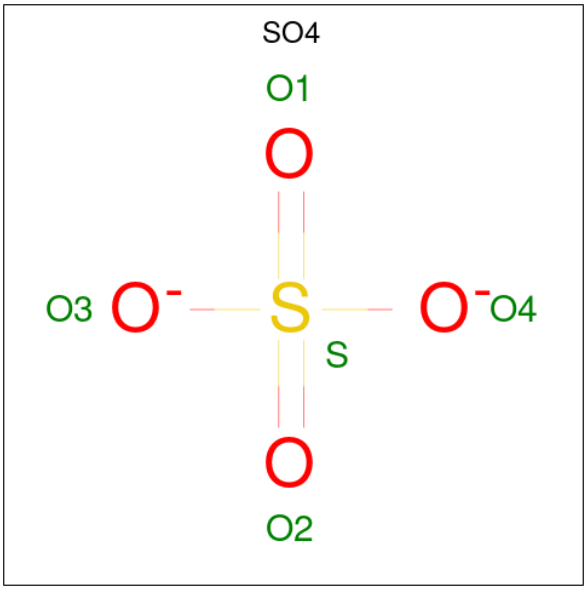
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 10 6 4	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



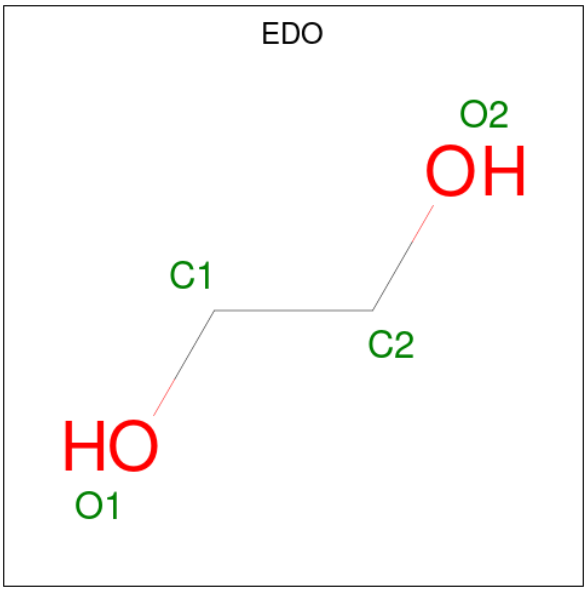
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C H O 10 2 6 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total Cl 3 3	0	0

- Molecule 10 is water.

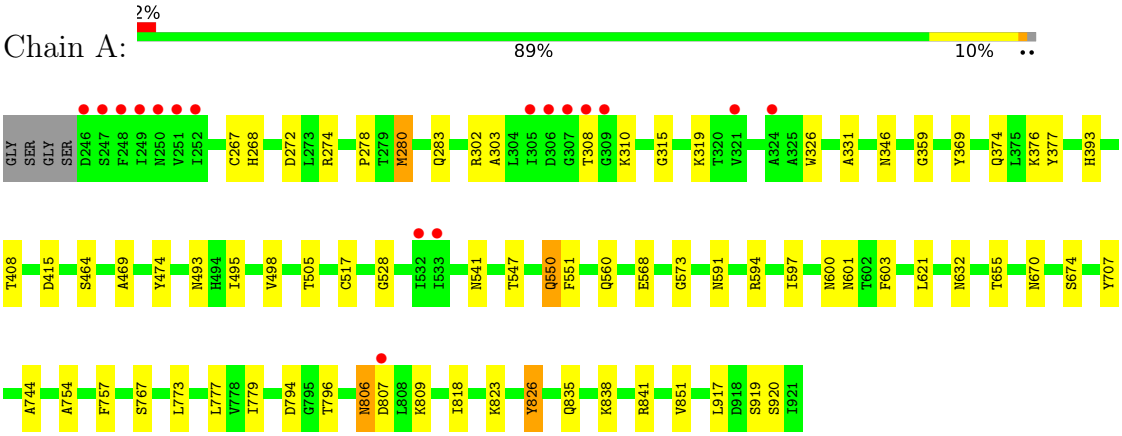
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	540	Total O 540 540	0	0

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.

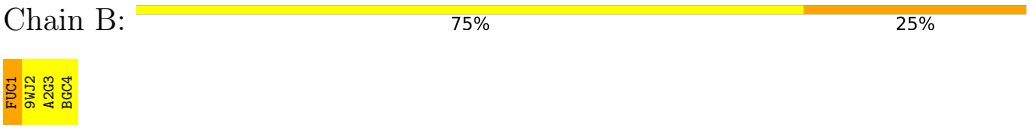
• Molecule 1: tailspike protein 2

Chain A:



• Molecule 2: beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-2)-4-acetamido-4,6-dideoxy-beta-D-mannopyranose-(1-3)-alpha-L-fucopyranose

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	185.23Å 185.23Å 185.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.26 49.50 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.50-2.26) 99.3 (49.50-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.27Å)	Xtriage
Refinement program	PHENIX (dev_2666: ???)	Depositor
R, R_{free}	0.133 , 0.164 0.136 , 0.168	Depositor DCC
R_{free} test set	2535 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5764	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BGC, PGE, EDO, K, PG4, SO4, 9WJ, A2G, NA, CL

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	0.33	0/5156	0.53	0/7014

There are no bond length outliers.

There are no bond angle outliers.

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	5059	0	4914	59	0
2	B	49	0	32	1	0
3	A	50	0	70	10	0
4	A	26	0	36	6	0
5	A	5	0	0	1	0
6	A	24	6	36	6	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	3	0	0	2	0
10	A	540	0	0	23	2
All	All	5758	6	5088	71	2

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 7.

All (71) 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)
6:A:1013:EDO:O2	10:A:1101:HOH:O	1.79	0.98
6:A:1017:EDO:O2	10:A:1103:HOH:O	1.97	0.81
3:A:1006:PGE:H22	10:A:1481:HOH:O	1.79	0.80
3:A:1009:PGE:O1	10:A:1104:HOH:O	1.99	0.79
1:A:346:ASN:HB2	10:A:1417:HOH:O	1.85	0.76
5:A:1012:SO4:O1	10:A:1106:HOH:O	2.03	0.74
1:A:600:ASN:HD22	4:A:1011:PG4:H72	1.52	0.74
1:A:268:HIS:NE2	9:A:1023:CL:CL	2.58	0.72
1:A:807:ASP:OD1	10:A:1107:HOH:O	2.06	0.72
1:A:796:THR:HG22	10:A:1109:HOH:O	1.88	0.71
1:A:806:ASN:ND2	10:A:1111:HOH:O	2.23	0.70
1:A:601:ASN:HD22	4:A:1011:PG4:H61	1.65	0.59
1:A:670:ASN:OD1	3:A:1006:PGE:H12	2.04	0.57
1:A:757:PHE:HE1	1:A:779:ILE:HD13	1.68	0.57
3:A:1005:PGE:H22	10:A:1483:HOH:O	2.03	0.57
1:A:331:ALA:HB1	10:A:1491:HOH:O	2.03	0.57
1:A:376:LYS:HD3	10:A:1600:HOH:O	2.04	0.56
1:A:310:LYS:NZ	10:A:1115:HOH:O	2.33	0.56
3:A:1008:PGE:H52	10:A:1576:HOH:O	2.05	0.55
3:A:1009:PGE:H42	10:A:1585:HOH:O	2.07	0.55
1:A:376:LYS:NZ	10:A:1105:HOH:O	2.02	0.54
10:A:1182:HOH:O	2:B:1:FUC:H1	2.09	0.52
1:A:568:GLU:HA	1:A:591:ASN:O	2.09	0.52
1:A:377:TYR:CD1	3:A:1008:PGE:H5	2.44	0.52
1:A:838:LYS:NZ	4:A:1011:PG4:H11	2.25	0.52
1:A:274:ARG:HD2	10:A:1496:HOH:O	2.09	0.52
1:A:600:ASN:ND2	4:A:1011:PG4:H72	2.24	0.52
1:A:757:PHE:CE1	1:A:779:ILE:HD13	2.45	0.51
1:A:359:GLY:HA2	3:A:1008:PGE:H32	1.92	0.51
1:A:369:TYR:HA	1:A:393:HIS:O	2.11	0.51
1:A:469:ALA:HA	1:A:493:ASN:O	2.11	0.50
1:A:835:GLN:NE2	9:A:1022:CL:CL	2.82	0.50
1:A:547:THR:HG21	1:A:551:PHE:CE1	2.46	0.50
1:A:838:LYS:HZ2	4:A:1011:PG4:H11	1.76	0.50
1:A:547:THR:HG22	1:A:547:THR:O	2.11	0.50
1:A:474:TYR:HA	1:A:498:VAL:O	2.12	0.49
1:A:528:GLY:HA2	1:A:560:GLN:O	2.12	0.49
1:A:374:GLN:HG2	10:A:1204:HOH:O	2.13	0.49
1:A:823:LYS:HG2	1:A:826:TYR:HB3	1.94	0.49
1:A:303:ALA:HB2	1:A:326:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1010:PG4:H31	10:A:1297:HOH:O	2.13	0.48
1:A:268:HIS:HB3	1:A:272:ASP:OD2	2.13	0.48
6:A:1016:EDO:H22	10:A:1470:HOH:O	2.14	0.48
1:A:773:LEU:C	1:A:773:LEU:HD23	2.34	0.47
1:A:280:MET:CE	1:A:283:GLN:HG3	2.44	0.47
1:A:806:ASN:HA	1:A:809:LYS:HD2	1.97	0.47
1:A:310:LYS:O	1:A:319:LYS:HD2	2.14	0.46
1:A:794:ASP:O	10:A:1109:HOH:O	2.20	0.46
1:A:278:PRO:HG3	1:A:303:ALA:HB1	1.96	0.46
1:A:600:ASN:HB2	1:A:632:ASN:OD1	2.16	0.45
1:A:550:GLN:HG3	1:A:603:PHE:CE1	2.52	0.45
1:A:621:LEU:C	1:A:621:LEU:HD23	2.37	0.45
1:A:707:TYR:CG	1:A:919:SER:HA	2.51	0.45
1:A:621:LEU:HD12	1:A:655:THR:HG21	1.98	0.45
1:A:777:LEU:HG	1:A:779:ILE:CD1	2.47	0.45
6:A:1014:EDO:O2	10:A:1110:HOH:O	2.21	0.45
1:A:917:LEU:HA	1:A:920:SER:O	2.17	0.44
1:A:280:MET:HE2	1:A:283:GLN:CB	2.48	0.43
1:A:377:TYR:HB3	3:A:1008:PGE:H5	2.00	0.43
1:A:280:MET:HE1	1:A:283:GLN:HG3	2.00	0.43
1:A:794:ASP:HB2	1:A:851:VAL:HG21	2.01	0.42
1:A:415:ASP:HA	1:A:464:SER:O	2.20	0.42
1:A:495:ILE:O	1:A:517:CYS:HA	2.19	0.42
1:A:547:THR:CG2	1:A:551:PHE:CE1	3.03	0.42
1:A:744:ALA:HA	1:A:818:ILE:O	2.19	0.42
1:A:408:THR:HB	6:A:1014:EDO:H22	2.02	0.41
1:A:754:ALA:HA	1:A:779:ILE:O	2.20	0.41
1:A:283:GLN:O	1:A:302:ARG:HA	2.21	0.41
1:A:767:SER:OG	6:A:1017:EDO:H12	2.20	0.41
1:A:505:THR:HG21	3:A:1005:PGE:H3	2.03	0.41
1:A:573:GLY:HA2	1:A:597:ILE:HG12	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1320:HOH:O	10:A:1521:HOH:O[9_555]	1.98	0.22
10:A:1534:HOH:O	10:A:1534:HOH:O[22_445]	2.00	0.20

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	675/680 (99%)	639 (95%)	35 (5%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLY

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	555/556 (100%)	545 (98%)	10 (2%)	59 68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	CYS
1	A	280	MET
1	A	308	THR
1	A	541	ASN
1	A	550	GLN
1	A	594	ARG
1	A	674	SER
1	A	806	ASN
1	A	826	TYR
1	A	841	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	565	ASN
1	A	588	ASN
1	A	650	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)

There are no non-standard protein/DNA/RNA residues in this entry.

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	FUC	B	1	2	11,11,11	0.90	0	15,16,16	1.61	3 (20%)
2	9WJ	B	2	2	12,13,14	0.53	0	15,18,20	2.81	7 (46%)
2	A2G	B	3	2	14,14,15	1.69	2 (14%)	17,19,21	1.81	5 (29%)
2	BGC	B	4	2	11,11,12	1.78	3 (27%)	15,15,17	1.11	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
2	FUC	B	1	2	-	-	0/1/1/1
2	9WJ	B	2	2	-	0/4/21/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2G	B	3	2	-	1/6/23/26	0/1/1/1
2	BGC	B	4	2	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	BGC	O5-C1	4.59	1.51	1.43
2	B	3	A2G	C7-N2	3.20	1.45	1.34
2	B	4	BGC	O5-C5	2.34	1.48	1.43
2	B	3	A2G	O3-C3	2.34	1.48	1.43
2	B	4	BGC	C2-C3	-2.30	1.49	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	9WJ	C1-C2-C3	-6.96	101.11	109.67
2	B	2	9WJ	C1-O5-C5	-4.89	101.69	112.78
2	B	3	A2G	C2-N2-C7	-4.45	116.56	122.90
2	B	2	9WJ	O5-C1-C2	-3.59	105.24	110.77
2	B	1	FUC	C3-C4-C5	-3.20	104.79	109.77
2	B	1	FUC	O3-C3-C4	3.00	117.28	110.35
2	B	3	A2G	C1-O5-C5	-2.90	108.26	112.19
2	B	2	9WJ	C2-C3-C4	-2.79	108.17	110.63
2	B	2	9WJ	O2-C2-C1	2.75	114.77	109.15
2	B	2	9WJ	O2-C2-C3	-2.73	104.67	110.14
2	B	3	A2G	C8-C7-N2	2.51	120.36	116.10
2	B	1	FUC	C1-C2-C3	-2.20	105.75	110.31
2	B	3	A2G	O5-C1-C2	-2.20	107.82	111.29
2	B	2	9WJ	C4-N4-C7	-2.10	118.08	123.18
2	B	3	A2G	C3-C4-C5	2.06	113.91	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

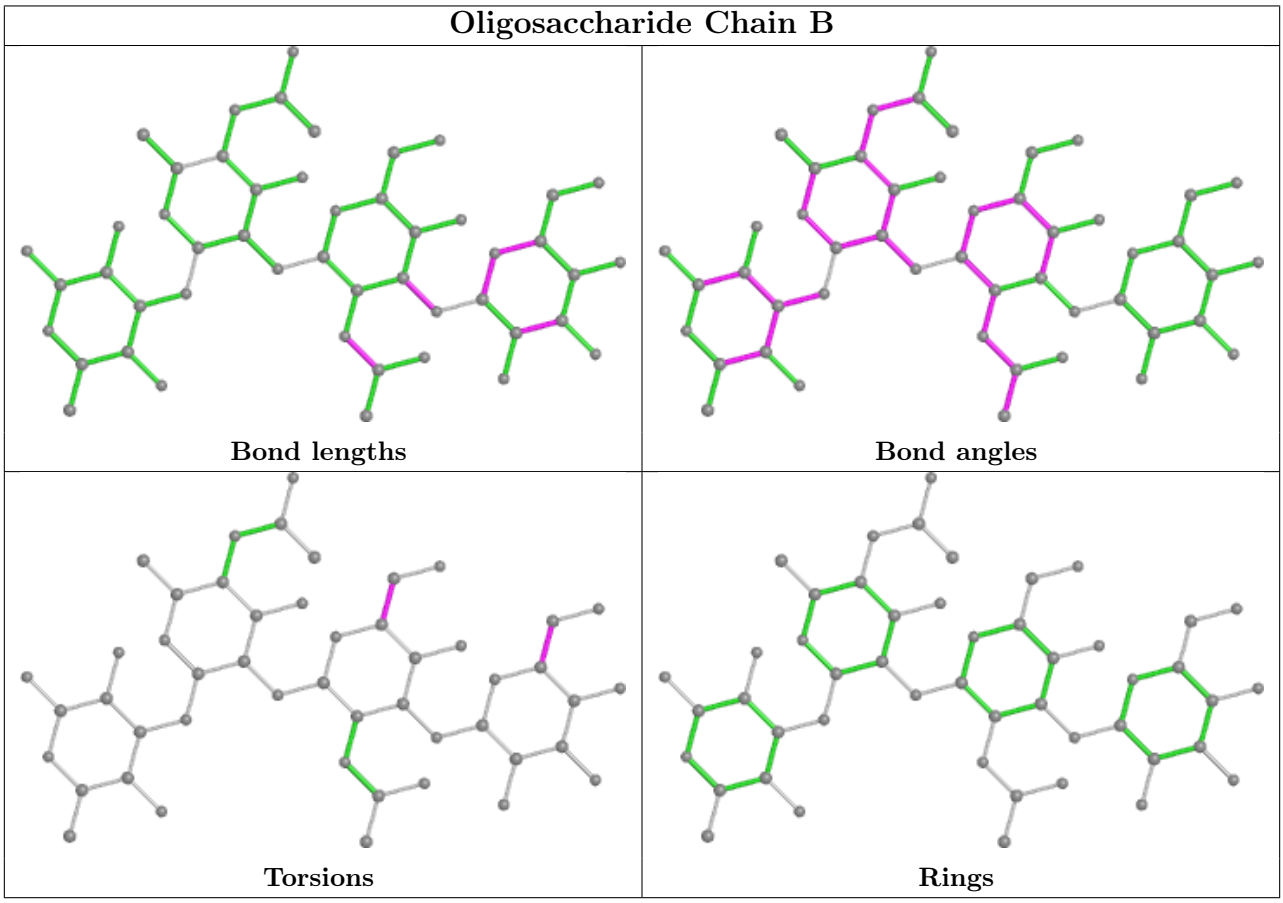
Mol	Chain	Res	Type	Atoms
2	B	4	BGC	O5-C5-C6-O6
2	B	4	BGC	C4-C5-C6-O6
2	B	3	A2G	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FUC	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.



5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
6	EDO	A	1016	-	3,3,3	0.48	0	2,2,2	0.25	0
6	EDO	A	1017	-	3,3,3	0.47	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	1018	-	3,3,3	0.48	0	2,2,2	0.23	0
3	PGE	A	1008	-	9,9,9	0.35	0	8,8,8	0.31	0
4	PG4	A	1011	-	12,12,12	0.53	0	11,11,11	0.33	0
3	PGE	A	1006	-	9,9,9	0.30	0	8,8,8	0.34	0
6	EDO	A	1014	-	3,3,3	0.48	0	2,2,2	0.28	0
4	PG4	A	1010	-	12,12,12	0.51	0	11,11,11	0.28	0
6	EDO	A	1015	-	3,3,3	0.46	0	2,2,2	0.36	0
3	PGE	A	1007	-	9,9,9	0.31	0	8,8,8	0.29	0
3	PGE	A	1009	-	9,9,9	0.33	0	8,8,8	0.30	0
6	EDO	A	1013	-	3,3,3	0.40	0	2,2,2	0.42	0
3	PGE	A	1005	-	9,9,9	0.30	0	8,8,8	0.32	0
5	SO4	A	1012	-	4,4,4	0.14	0	6,6,6	0.07	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
6	EDO	A	1016	-	-	1/1/1/1	-
6	EDO	A	1017	-	-	1/1/1/1	-
6	EDO	A	1018	-	-	0/1/1/1	-
3	PGE	A	1008	-	-	5/7/7/7	-
4	PG4	A	1011	-	-	3/10/10/10	-
3	PGE	A	1006	-	-	3/7/7/7	-
6	EDO	A	1014	-	-	0/1/1/1	-
4	PG4	A	1010	-	-	5/10/10/10	-
6	EDO	A	1015	-	-	0/1/1/1	-
3	PGE	A	1007	-	-	1/7/7/7	-
3	PGE	A	1009	-	-	5/7/7/7	-
6	EDO	A	1013	-	-	1/1/1/1	-
3	PGE	A	1005	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1006	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	A	1008	PGE	O2-C3-C4-O3
4	A	1010	PG4	O3-C5-C6-O4
3	A	1006	PGE	O3-C5-C6-O4
3	A	1008	PGE	O3-C5-C6-O4
4	A	1011	PG4	O1-C1-C2-O2
3	A	1009	PGE	O1-C1-C2-O2
4	A	1010	PG4	O1-C1-C2-O2
4	A	1010	PG4	O2-C3-C4-O3
3	A	1009	PGE	C6-C5-O3-C4
3	A	1005	PGE	C4-C3-O2-C2
3	A	1009	PGE	C3-C4-O3-C5
3	A	1005	PGE	C3-C4-O3-C5
3	A	1006	PGE	O1-C1-C2-O2
3	A	1005	PGE	C1-C2-O2-C3
6	A	1016	EDO	O1-C1-C2-O2
3	A	1008	PGE	C1-C2-O2-C3
4	A	1010	PG4	C5-C6-O4-C7
3	A	1007	PGE	O1-C1-C2-O2
3	A	1008	PGE	C4-C3-O2-C2
4	A	1010	PG4	C6-C5-O3-C4
4	A	1011	PG4	C5-C6-O4-C7
3	A	1005	PGE	O2-C3-C4-O3
3	A	1008	PGE	C3-C4-O3-C5
6	A	1013	EDO	O1-C1-C2-O2
6	A	1017	EDO	O1-C1-C2-O2
3	A	1009	PGE	C4-C3-O2-C2
3	A	1005	PGE	O3-C5-C6-O4
4	A	1011	PG4	O3-C5-C6-O4
3	A	1009	PGE	O2-C3-C4-O3

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1016	EDO	1	0
6	A	1017	EDO	2	0
3	A	1008	PGE	4	0
4	A	1011	PG4	5	0
3	A	1006	PGE	2	0
6	A	1014	EDO	2	0
4	A	1010	PG4	1	0
3	A	1009	PGE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1013	EDO	1	0
3	A	1005	PGE	2	0
5	A	1012	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	676/680 (99%)	-0.34	17 (2%) 57 60	23, 33, 59, 108	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	SER	5.3
1	A	248	PHE	4.8
1	A	251	VAL	4.3
1	A	308	THR	4.1
1	A	249	ILE	3.5
1	A	324	ALA	3.3
1	A	307	GLY	2.9
1	A	305	ILE	2.8
1	A	250	ASN	2.7
1	A	309	GLY	2.7
1	A	807	ASP	2.5
1	A	533	ILE	2.4
1	A	246	ASP	2.3
1	A	306	ASP	2.2
1	A	252	ILE	2.2
1	A	532	ILE	2.2
1	A	321	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

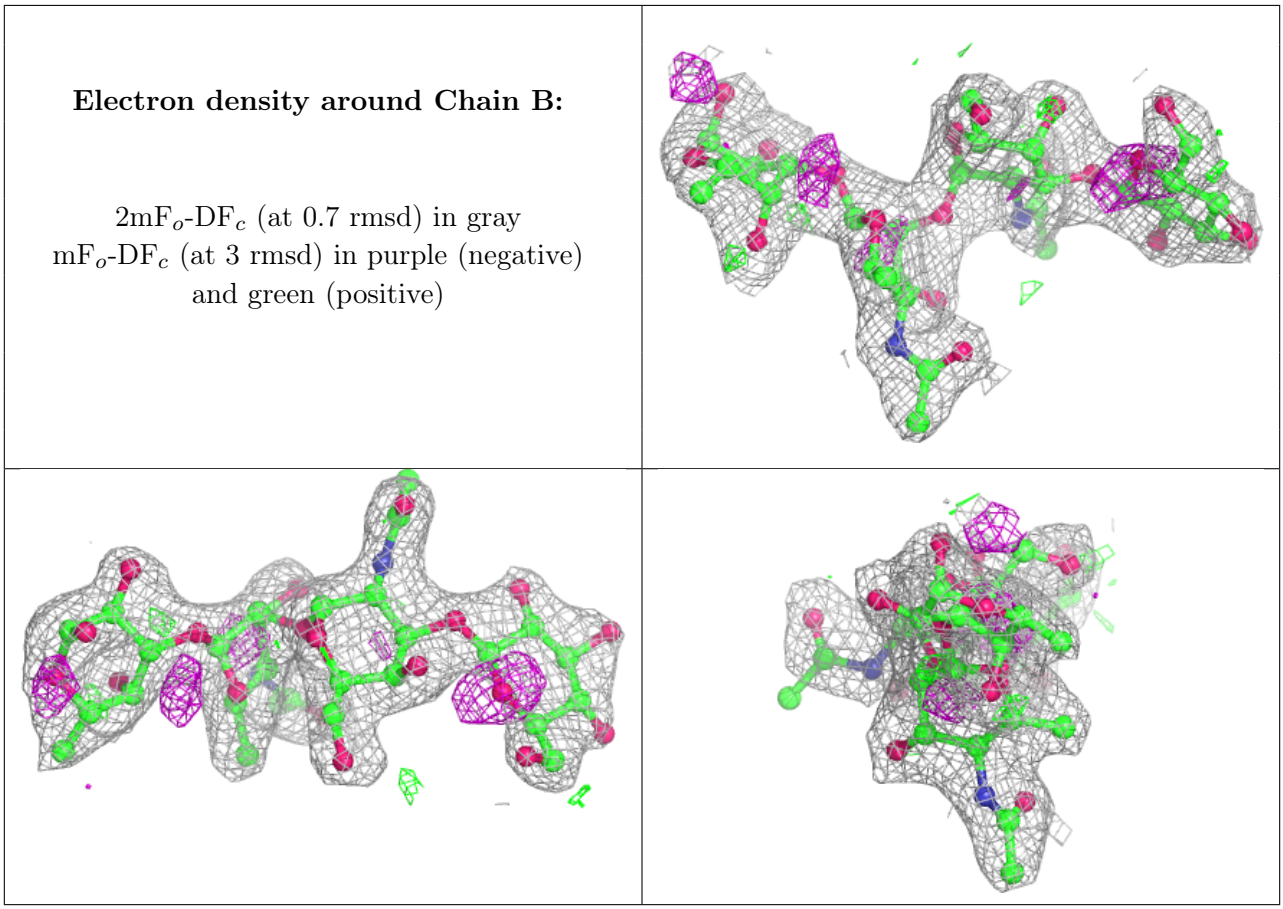
6.3 Carbohydrates

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, 95^{th} 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	BGC	B	4	11/12	0.82	0.39	74,77,78,78	0
2	A2G	B	3	14/15	0.93	0.24	50,55,67,68	0
2	FUC	B	1	11/11	0.93	0.15	38,43,51,52	0
2	9WJ	B	2	13/14	0.94	0.18	37,41,46,48	0

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



6.4 Ligands (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGE	A	1008	10/10	0.81	0.19	44,61,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG4	A	1011	13/13	0.86	0.27	67,70,75,75	0
3	PGE	A	1009	10/10	0.88	0.20	60,62,76,79	0
6	EDO	A	1015	4/4	0.88	0.12	65,65,66,67	0
6	EDO	A	1016	4/4	0.88	0.18	74,75,75,75	0
4	PG4	A	1010	13/13	0.89	0.15	54,61,66,68	0
3	PGE	A	1005	10/10	0.89	0.20	48,50,75,77	0
3	PGE	A	1006	10/10	0.92	0.22	60,66,71,72	0
9	CL	A	1023	1/1	0.92	0.11	71,71,71,71	0
6	EDO	A	1017	4/4	0.93	0.12	46,52,54,55	0
6	EDO	A	1014	4/4	0.93	0.24	50,52,53,53	0
6	EDO	A	1013	4/4	0.95	0.12	42,44,48,51	0
6	EDO	A	1018	4/4	0.95	0.11	62,75,75,76	0
3	PGE	A	1007	10/10	0.95	0.15	57,59,69,70	0
9	CL	A	1022	1/1	0.97	0.11	65,65,65,65	0
9	CL	A	1021	1/1	0.97	0.03	67,67,67,67	0
7	NA	A	1019	1/1	0.99	0.06	39,39,39,39	1
5	SO4	A	1012	5/5	0.99	0.09	57,58,61,62	0
8	K	A	1020	1/1	1.00	0.14	33,33,33,33	1

6.5 Other polymers (i)

There are no such residues in this entry.