



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:39 AM UTC

PDB ID : 5HOF / pdb_00005hof
Title : Crystal structure of AbnA, a GH43 extracellular arabinanase from *Geobacillus stearothermophilus*, in complex with arabinopentaose
Authors : Lansky, S.; Shwartstien, O.; Salama, R.; Shoham, Y.; Shoham, G.
Deposited on : 2016-01-19
Resolution : 2.96 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

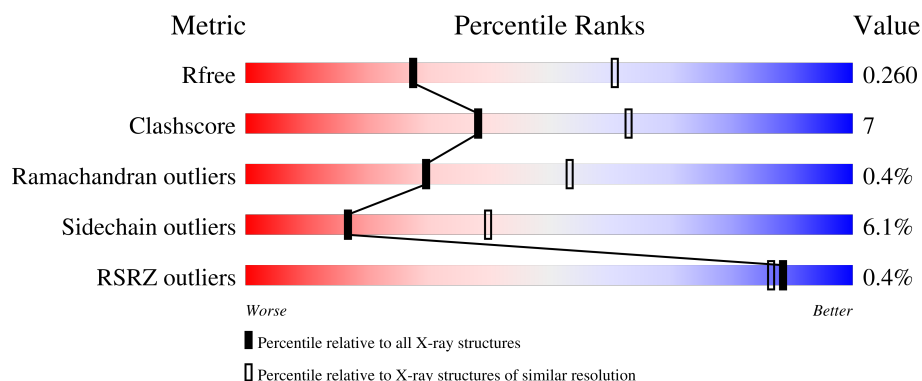
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

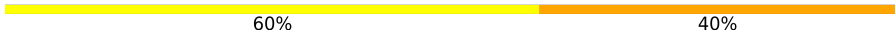
The reported resolution of this entry is 2.96 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	848	 77% 16% • 5%
2	B	5	 60% 40%

2 Entry composition

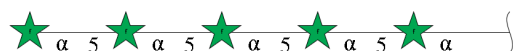
There are 7 unique types of molecules in this entry. The entry contains 6568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Extracellular arabinanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	803	Total	C	N	O	S	0	8	0
			6359	4055	1063	1230	11			

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose.

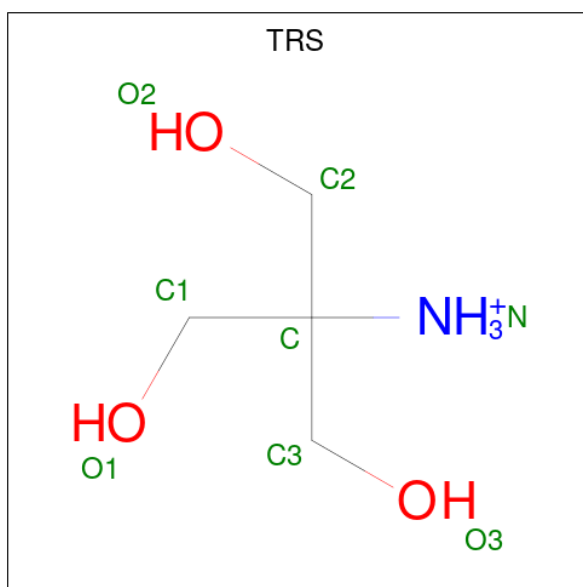


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	5	Total	C	O	0	0	0
			46	25	21			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

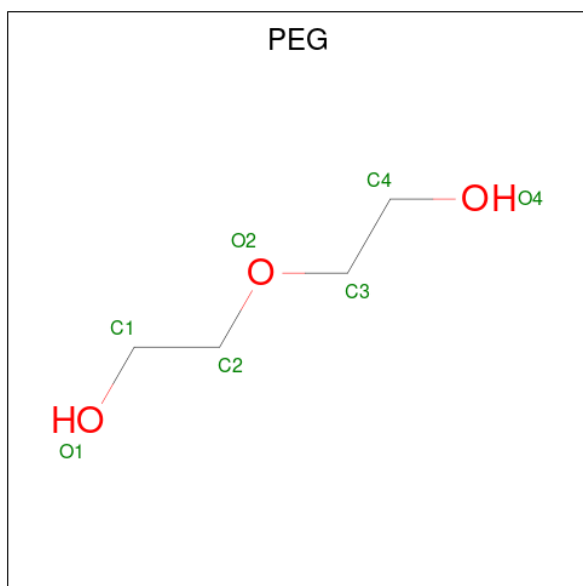
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

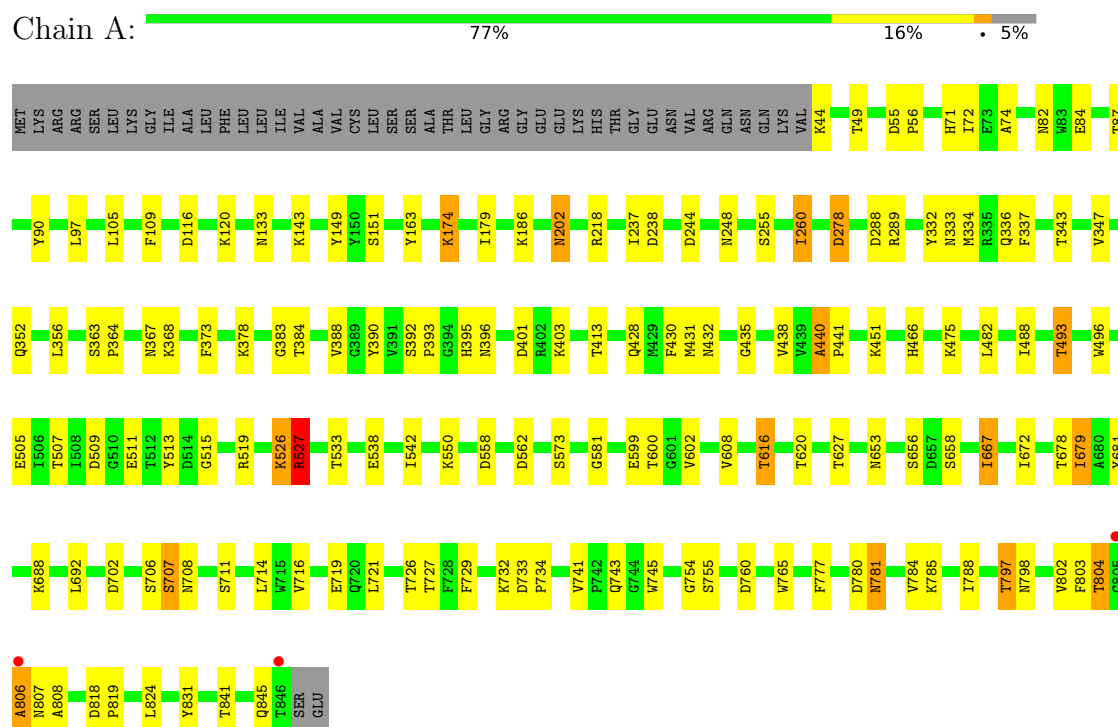
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	142	Total	O	0	0
			142	142		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Extracellular arabinanase



- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.46Å 87.79Å 129.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 2.96 47.80 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.80-2.96) 99.8 (47.80-2.96)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.168 , 0.259 0.172 , 0.260	Depositor DCC
R_{free} test set	879 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6568	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: CA, ACT, PEG, AHR, TRS

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	0.90	2/6565 (0.0%)	1.03	13/8934 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	ARG	C-O	-5.51	1.17	1.23
1	A	754	GLY	N-CA	5.32	1.50	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ILE	CB-CA-C	-7.41	103.67	110.63
1	A	440	ALA	CA-C-N	7.17	126.79	119.19
1	A	440	ALA	C-N-CA	7.17	126.79	119.19
1	A	179	ILE	N-CA-C	7.04	120.39	113.71
1	A	356	LEU	CA-C-N	6.72	126.31	119.19
1	A	356	LEU	C-N-CA	6.72	126.31	119.19
1	A	667	ILE	N-CA-C	6.23	117.09	107.99
1	A	538	GLU	N-CA-C	-5.38	106.76	113.38
1	A	741	VAL	CA-C-N	5.15	124.94	119.28
1	A	741	VAL	C-N-CA	5.15	124.94	119.28
1	A	466	HIS	N-CA-C	5.08	118.74	112.54
1	A	777	PHE	N-CA-C	5.03	117.35	108.75
1	A	581	GLY	N-CA-C	-5.02	105.88	112.81

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	6359	0	6061	84	0
2	B	46	0	0	4	0
3	A	2	0	0	0	0
4	A	8	0	12	2	0
5	A	7	0	10	1	0
6	A	4	0	3	0	0
7	A	142	0	0	9	0
All	All	6568	0	6086	86	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 7.

All (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ARG:HG2	1:A:527:ARG:HH11	1.27	0.96
1:A:120:LYS:HE2	7:A:1067:HOH:O	1.85	0.75
1:A:526:LYS:O	1:A:527:ARG:HG2	1.91	0.71
1:A:733:ASP:HB2	1:A:734:PRO:HD2	1.72	0.71
1:A:527:ARG:HG2	1:A:527:ARG:NH1	2.00	0.70
1:A:526:LYS:O	1:A:527:ARG:NH1	2.26	0.69
1:A:755:SER:HB3	2:B:4:AHR:O2	1.94	0.68
1:A:732:LYS:HD3	1:A:802:VAL:O	1.98	0.64
1:A:336:GLN:HG2	1:A:367:ASN:HB2	1.80	0.63
1:A:72:ILE:HG23	1:A:97:LEU:HD12	1.80	0.63
1:A:599:GLU:H	1:A:599:GLU:CD	2.10	0.60
1:A:401:ASP:OD1	1:A:401:ASP:C	2.45	0.59
1:A:120:LYS:CE	7:A:1067:HOH:O	2.48	0.58
1:A:428:GLN:HG2	1:A:430:PHE:CZ	2.39	0.58
1:A:526:LYS:C	1:A:527:ARG:HG2	2.29	0.57
1:A:244:ASP:OD2	1:A:248:ASN:HB2	2.06	0.55
1:A:509:ASP:HB3	7:A:1128:HOH:O	2.06	0.55
1:A:784:VAL:HG13	1:A:784:VAL:O	2.08	0.54
1:A:44:LYS:HD3	1:A:526:LYS:HE2	1.90	0.53
1:A:678:THR:O	1:A:679:ILE:HD12	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:CZ	1:A:278:ASP:OD2	2.57	0.52
1:A:616:THR:HG22	7:A:1049:HOH:O	2.08	0.52
5:A:904:PEG:H42	7:A:1126:HOH:O	2.09	0.52
1:A:714:LEU:CD1	1:A:716:VAL:HG13	2.39	0.51
1:A:721:LEU:HD22	1:A:743:GLN:HB2	1.92	0.51
1:A:218:ARG:NH1	1:A:288:ASP:OD1	2.42	0.51
1:A:507:THR:HA	1:A:511:GLU:O	2.11	0.51
1:A:519:ARG:HD2	7:A:1062:HOH:O	2.11	0.50
1:A:488:ILE:O	1:A:493:THR:HA	2.12	0.49
1:A:334:MET:SD	1:A:396:ASN:HB3	2.52	0.49
1:A:797:THR:HG23	1:A:798:ASN:ND2	2.28	0.49
1:A:692:LEU:HD12	1:A:692:LEU:N	2.28	0.49
1:A:732:LYS:HE3	1:A:806:ALA:HB3	1.95	0.48
1:A:336:GLN:CG	1:A:367:ASN:HD22	2.27	0.47
1:A:440:ALA:HA	1:A:441:PRO:HD3	1.73	0.47
1:A:707:SER:HA	1:A:804:THR:HG23	1.97	0.47
1:A:74:ALA:HB3	1:A:87:THR:HG23	1.97	0.47
1:A:802:VAL:O	1:A:802:VAL:HG12	2.14	0.47
1:A:55:ASP:HB3	1:A:395:HIS:CD2	2.50	0.46
1:A:432:ASN:OD1	1:A:432:ASN:C	2.59	0.46
1:A:87:THR:HB	7:A:1014:HOH:O	2.14	0.46
1:A:390:TYR:HB3	1:A:413:THR:OG1	2.16	0.46
1:A:527:ARG:NH1	1:A:527:ARG:CG	2.73	0.45
1:A:706:SER:HA	1:A:803:PHE:O	2.16	0.45
1:A:237:ILE:HD12	4:A:903:TRS:O1	2.16	0.45
1:A:72:ILE:CG2	1:A:97:LEU:HD12	2.45	0.45
1:A:392:SER:N	1:A:393:PRO:CD	2.80	0.44
1:A:438:VAL:HA	7:A:1070:HOH:O	2.18	0.44
1:A:726:THR:HG21	1:A:729:PHE:HB2	1.98	0.44
1:A:238:ASP:OD1	4:A:903:TRS:O1	2.35	0.44
1:A:202:ASN:HD22	1:A:202:ASN:N	2.16	0.43
1:A:667:ILE:HD13	1:A:679:ILE:HB	2.01	0.43
1:A:780:ASP:O	1:A:781:ASN:C	2.62	0.43
1:A:133:ASN:OD1	1:A:133:ASN:C	2.60	0.43
1:A:760:ASP:OD1	2:B:1:AHR:O1	2.36	0.43
1:A:765:TRP:CE3	1:A:788:ILE:HD13	2.54	0.43
1:A:383:GLY:C	1:A:384:THR:CG2	2.92	0.43
1:A:550:LYS:HE3	1:A:558:ASP:OD2	2.19	0.43
7:A:1103:HOH:O	2:B:1:AHR:C5	2.66	0.43
1:A:71:HIS:HA	1:A:90:TYR:CZ	2.54	0.43
1:A:174:LYS:NZ	1:A:174:LYS:HB3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:SER:HB2	1:A:831:TYR:HB2	2.01	0.42
1:A:260:ILE:N	1:A:260:ILE:HD13	2.34	0.42
1:A:347:VAL:HA	1:A:352:GLN:O	2.20	0.42
1:A:653:ASN:HA	1:A:681:TYR:CD2	2.55	0.42
1:A:714:LEU:C	1:A:714:LEU:HD12	2.45	0.42
1:A:600:THR:OG1	1:A:602:VAL:HG23	2.20	0.42
1:A:653:ASN:HD21	1:A:688:LYS:HD2	1.84	0.42
1:A:702:ASP:HA	1:A:808:ALA:O	2.19	0.42
1:A:745:TRP:NE1	2:B:1:AHR:O1	2.53	0.42
1:A:515:GLY:HA3	1:A:533:THR:O	2.19	0.42
1:A:55:ASP:N	1:A:56:PRO:HD3	2.35	0.41
1:A:149:TYR:CD2	1:A:163:TYR:HB3	2.55	0.41
1:A:818:ASP:HB3	1:A:819:PRO:HD2	2.03	0.41
1:A:105:LEU:HB2	1:A:109:PHE:CE2	2.55	0.41
1:A:373:PHE:HA	1:A:475:LYS:O	2.20	0.41
1:A:278:ASP:N	1:A:278:ASP:OD1	2.53	0.41
1:A:513:TYR:CD2	1:A:542:ILE:HG12	2.56	0.41
1:A:363:SER:HB2	1:A:364:PRO:HD3	2.01	0.41
1:A:496:TRP:HA	1:A:505:GLU:O	2.21	0.40
1:A:49:THR:HB	1:A:82:ASN:HA	2.04	0.40
1:A:656:SER:H	1:A:656:SER:HG	1.67	0.40
1:A:802:VAL:O	1:A:802:VAL:CG1	2.69	0.40
1:A:337:PHE:CD1	1:A:337:PHE:N	2.89	0.40
1:A:726:THR:OG1	1:A:727:THR:N	2.54	0.40
1:A:431:MET:SD	1:A:435:GLY:C	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	809/848 (95%)	743 (92%)	63 (8%)	3 (0%)	30 53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	A	781	ASN
1	A	806	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	677/707 (96%)	636 (94%)	41 (6%)	17	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	116	ASP
1	A	143	LYS
1	A	151	SER
1	A	174	LYS
1	A	186	LYS
1	A	202	ASN
1	A	255	SER
1	A	260	ILE
1	A	278	ASP
1	A	332	TYR
1	A	333	ASN
1	A	343	THR
1	A	368	LYS
1	A	378	LYS
1	A	388	VAL
1	A	403	LYS
1	A	451	LYS
1	A	482	LEU
1	A	493	THR
1	A	526	LYS
1	A	527	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	562	ASP
1	A	573	SER
1	A	608	VAL
1	A	616	THR
1	A	620	THR
1	A	627	THR
1	A	658	SER
1	A	672	ILE
1	A	679	ILE
1	A	707	SER
1	A	708	ASN
1	A	719	GLU
1	A	785	LYS
1	A	797	THR
1	A	804	THR
1	A	807	ASN
1	A	824	LEU
1	A	841	THR
1	A	845	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	333	ASN
1	A	352	GLN
1	A	406	GLN
1	A	428	GLN
1	A	434	ASN
1	A	462	GLN
1	A	501	HIS
1	A	653	ASN
1	A	661	ASN
1	A	708	ASN
1	A	735	ASN
1	A	736	HIS
1	A	789	ASN
1	A	798	ASN
1	A	845	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 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	AHR	B	1	2	10,10,10	0.55	0	13,14,14	1.35	3 (23%)
2	AHR	B	2	2	9,9,10	0.69	0	11,12,14	1.31	2 (18%)
2	AHR	B	3	2	9,9,10	0.70	0	11,12,14	1.52	3 (27%)
2	AHR	B	4	2	9,9,10	0.59	0	11,12,14	1.57	2 (18%)
2	AHR	B	5	2	9,9,10	0.50	0	11,12,14	1.16	1 (9%)

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	AHR	B	1	2	-	2/2/18/18	0/1/1/1
2	AHR	B	2	2	-	2/2/15/18	0/1/1/1
2	AHR	B	3	2	-	0/2/15/18	0/1/1/1
2	AHR	B	4	2	-	2/2/15/18	0/1/1/1
2	AHR	B	5	2	-	0/2/15/18	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	AHR	C1-C2-C3	3.04	106.49	101.63
2	B	4	AHR	O4-C4-C3	2.89	107.30	104.63
2	B	3	AHR	C1-C2-C3	2.88	106.23	101.63
2	B	1	AHR	O1-C1-O4	-2.85	107.49	111.12
2	B	2	AHR	O4-C4-C5	2.75	114.37	109.36
2	B	5	AHR	C1-C2-C3	2.69	105.92	101.63
2	B	2	AHR	O2-C2-C3	2.38	116.11	111.43
2	B	3	AHR	O4-C4-C3	2.14	106.61	104.63
2	B	1	AHR	O4-C1-C2	2.09	107.57	104.67
2	B	1	AHR	C1-C2-C3	2.07	104.83	102.29
2	B	3	AHR	C1-O4-C4	2.02	112.51	108.06

There are no chirality outliers.

All (6) torsion outliers are listed below:

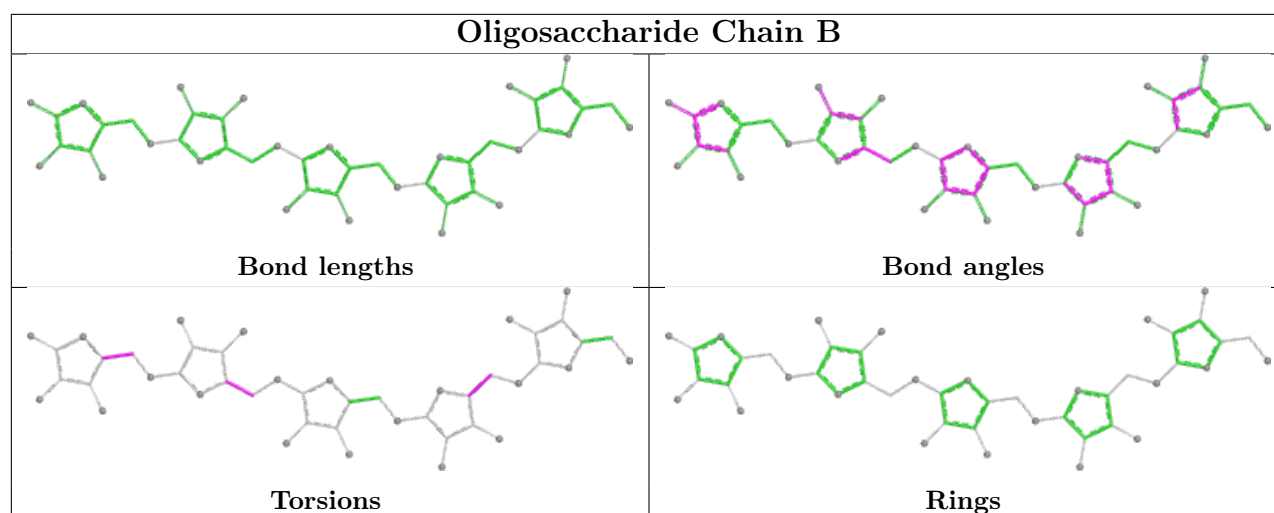
Mol	Chain	Res	Type	Atoms
2	B	2	AHR	O4-C4-C5-O5
2	B	2	AHR	C3-C4-C5-O5
2	B	4	AHR	O4-C4-C5-O5
2	B	1	AHR	C3-C4-C5-O5
2	B	4	AHR	C3-C4-C5-O5
2	B	1	AHR	O4-C4-C5-O5

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	AHR	3	0
2	B	4	AHR	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	ACT	A	905	-	3,3,3	0.85	0	3,3,3	1.04	0
5	PEG	A	904	-	6,6,6	0.46	0	5,5,5	0.57	0
4	TRS	A	903	-	7,7,7	0.45	0	9,9,9	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	904	-	-	3/4/4/4	-
4	TRS	A	903	-	-	4/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	TRS	C3-C-C1-O1
4	A	903	TRS	N-C-C1-O1
5	A	904	PEG	C1-C2-O2-C3
4	A	903	TRS	C2-C-C1-O1
5	A	904	PEG	C4-C3-O2-C2
4	A	903	TRS	C1-C-C2-O2
5	A	904	PEG	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	904	PEG	1	0
4	A	903	TRS	2	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 [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	803/848 (94%)	-0.42	3 (0%) 88 86	14, 31, 51, 81	8 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	806	ALA	3.9
1	A	846	THR	3.9
1	A	805	GLY	2.3

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

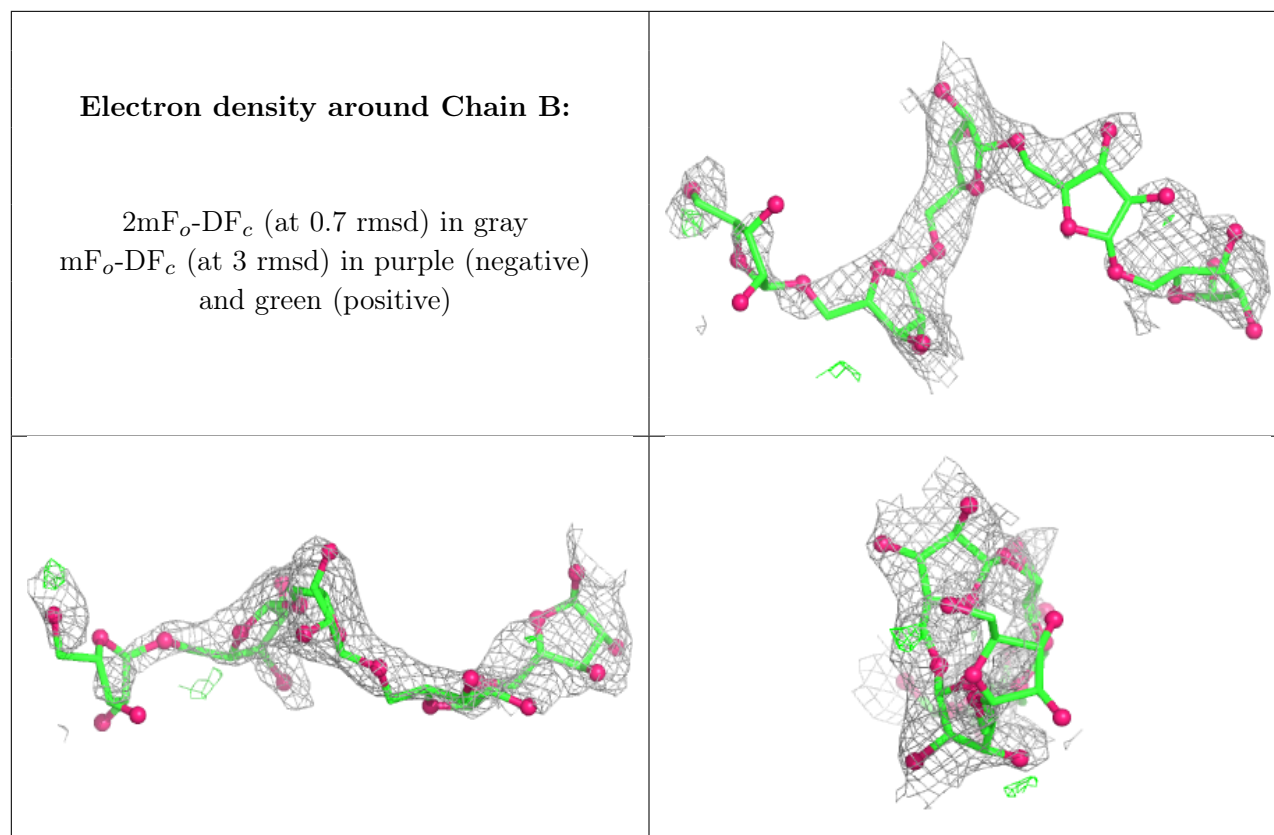
There are no non-standard protein/DNA/RNA residues in this entry.

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	AHR	B	5	9/10	0.74	0.21	46,57,61,62	9
2	AHR	B	2	9/10	0.79	0.18	46,55,58,59	9
2	AHR	B	1	10/10	0.79	0.17	53,59,62,62	10
2	AHR	B	4	9/10	0.85	0.14	41,44,52,56	9
2	AHR	B	3	9/10	0.88	0.13	35,38,42,43	9

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	A	905	4/4	0.75	0.17	46,50,50,52	0
5	PEG	A	904	7/7	0.88	0.15	38,40,45,48	0
4	TRS	A	903	8/8	0.93	0.09	28,30,31,31	0
3	CA	A	902	1/1	0.99	0.03	37,37,37,37	0
3	CA	A	901	1/1	1.00	0.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.