



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:13 AM BST

PDB ID : 5XSX
Title : Crystal structure of an archaeal chitinase in the substrate-complex form (P212121)
Authors : Nishitani, Y.; Miki, K.
Deposited on : 2017-06-15
Resolution : 2.64 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 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	:	2.13.1
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)	:	2.13.1

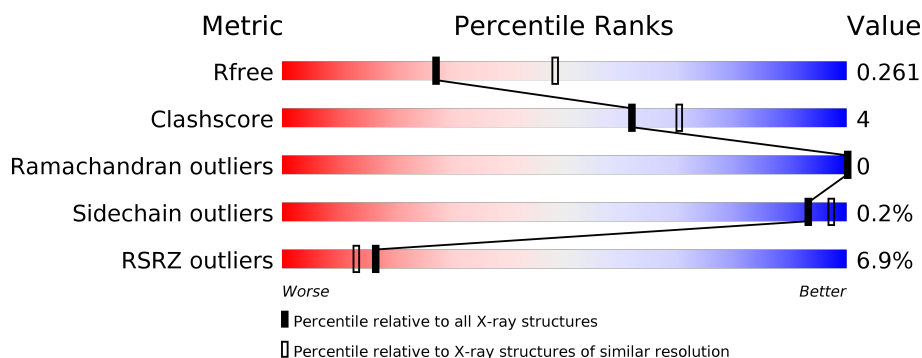
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 on 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	486	<div> <div>8%</div> <div>91%</div> <div>9%</div> </div>
1	B	486	<div> <div>6%</div> <div>84%</div> <div>16%</div> </div>
2	C	5	<div> <div>100%</div> </div>
2	D	5	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8232 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 Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3968	2578	646	731	13			
1	B	485	Total	C	N	O	S	0	0	0
			3968	2578	646	731	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	MET	-	initiating methionine	UNP A0A161KIT4
B	320	MET	-	initiating methionine	UNP A0A161KIT4

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			71	40	5	26			
2	D	5	Total	C	N	O	0	0	0
			71	40	5	26			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

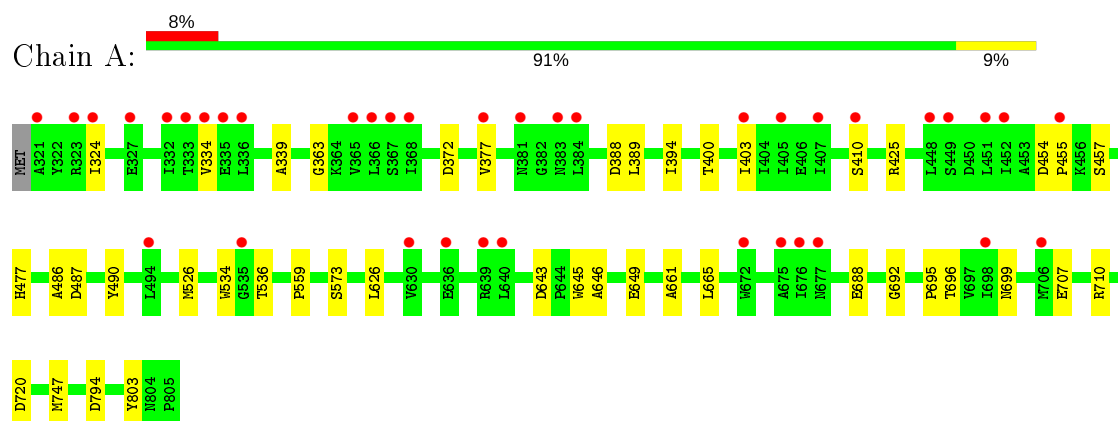
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	39	Total	O	0	0
			39	39		

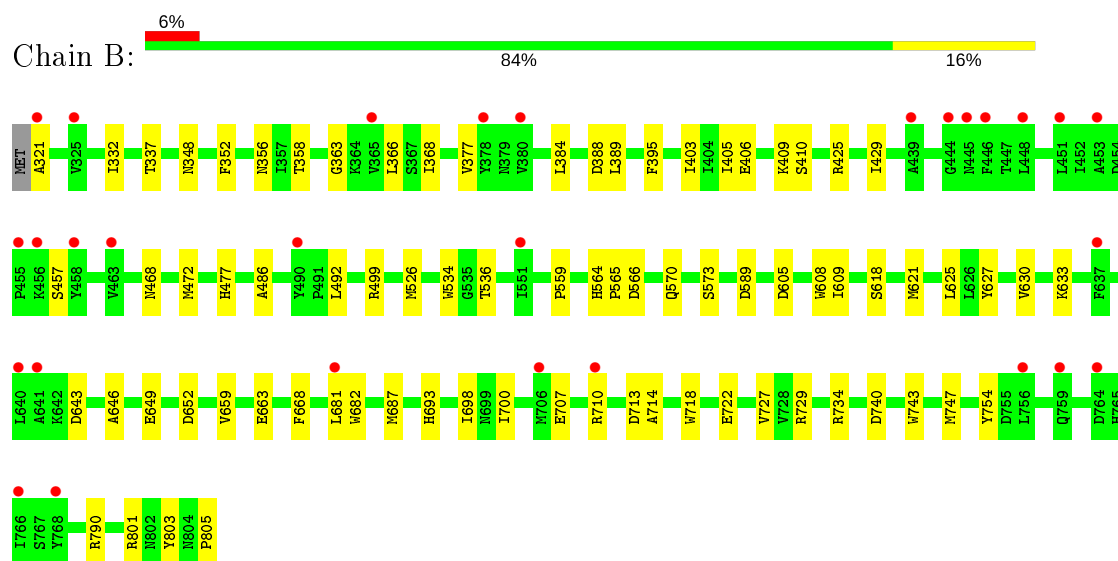
3 Residue-property plots

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: Chitinase



• Molecule 1: Chitinase



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



MAG1
MAG2
MAG3
MAG4
MAG5

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

Chain D:

100%

MAG1
MAG2
MAG3
MAG4
MAG5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.93Å 145.20Å 152.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.64 49.63 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.63-2.64) 99.5 (49.63-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.259 0.234 , 0.261	Depositor DCC
R_{free} test set	2547 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8232	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2104e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, PO4, NAG

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	0.21	0/4099	0.37	0/5596
1	B	0.21	0/4099	0.37	0/5596
All	All	0.21	0/8198	0.37	0/11192

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	3968	0	3791	25	0
1	B	3968	0	3791	45	0
2	C	71	0	63	0	0
2	D	71	0	63	0	0
3	A	24	0	32	2	0
3	B	18	0	24	3	0
4	A	15	0	0	0	0
4	B	20	0	0	0	0
5	A	38	0	0	0	0
5	B	39	0	0	0	0
All	All	8232	0	7764	70	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 4.

All (70) 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:468:ASN:ND2	1:B:472:MET:SD	2.67	0.67
1:B:790:ARG:HH12	3:B:1004:GOL:H31	1.58	0.67
1:B:630:VAL:HG12	1:B:633:LYS:HB3	1.77	0.66
1:B:573:SER:H	3:B:1003:GOL:H32	1.63	0.64
1:B:649:GLU:HG2	1:B:698:ILE:HD11	1.81	0.63
1:B:358:THR:HB	1:B:384:LEU:HD11	1.80	0.63
1:A:695:PRO:O	1:A:699:ASN:ND2	2.29	0.63
1:A:486:ALA:HB2	1:A:707:GLU:HB2	1.82	0.62
1:A:573:SER:H	3:A:1003:GOL:H2	1.65	0.62
1:B:321:ALA:HB3	1:B:337:THR:HB	1.82	0.60
1:B:363:GLY:HA2	1:B:410:SER:HB2	1.84	0.59
1:A:363:GLY:HA2	1:A:410:SER:HB3	1.85	0.59
1:B:388:ASP:OD2	1:B:801:ARG:NH2	2.36	0.59
1:B:643:ASP:HB3	1:B:646:ALA:HB2	1.87	0.55
1:B:718:TRP:NE1	1:B:722:GLU:OE1	2.39	0.55
1:B:499:ARG:HE	1:B:710:ARG:NH1	2.05	0.55
1:B:486:ALA:HB2	1:B:707:GLU:HB2	1.89	0.54
1:B:713:ASP:OD1	1:B:714:ALA:N	2.39	0.54
1:B:368:ILE:HG12	1:B:405:ILE:HG23	1.92	0.51
1:A:747:MET:HA	1:A:747:MET:HE2	1.93	0.50
1:A:324:ILE:HD13	1:A:334:VAL:HG22	1.93	0.50
1:B:803:TYR:CE2	1:B:805:PRO:HG3	2.46	0.50
1:A:490:TYR:HE1	1:A:696:THR:HG22	1.77	0.49
1:B:534:TRP:CD2	1:B:559:PRO:HG2	2.47	0.49
1:A:688:GLU:HG2	1:A:692:GLY:HA2	1.94	0.49
1:A:526:MET:O	1:A:536:THR:OG1	2.31	0.49
1:A:487:ASP:OD1	1:A:710:ARG:NH2	2.46	0.49
1:B:747:MET:HA	1:B:747:MET:HE2	1.94	0.48
1:B:425:ARG:HD2	1:B:790:ARG:HG2	1.95	0.48
1:A:534:TRP:CG	1:A:559:PRO:HG2	2.50	0.47
1:A:645:TRP:O	1:A:649:GLU:HG3	2.13	0.47
1:B:457:SER:O	1:B:477:HIS:NE2	2.42	0.47
1:B:366:LEU:HD12	1:B:406:GLU:HG2	1.95	0.47
1:A:394:ILE:HD13	1:A:794:ASP:HA	1.95	0.47
1:B:534:TRP:CG	1:B:559:PRO:HG2	2.50	0.47
1:B:566:ASP:HB3	1:B:570:GLN:HA	1.98	0.46
1:B:729:ARG:HB2	1:B:743:TRP:CZ2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:TRP:HA	1:B:687:MET:HB2	1.98	0.45
1:B:609:ILE:HD12	1:B:727:VAL:HG21	1.98	0.45
1:A:372:ASP:N	1:A:372:ASP:OD1	2.49	0.45
1:B:564:HIS:HA	1:B:565:PRO:HD3	1.88	0.45
1:B:652:ASP:OD2	1:B:693:HIS:ND1	2.44	0.45
1:A:720:ASP:OD1	3:A:1005:GOL:O1	2.32	0.44
1:A:534:TRP:CD2	1:A:559:PRO:HG2	2.52	0.44
1:B:729:ARG:NH1	1:B:740:ASP:OD1	2.52	0.43
1:B:348:ASN:HD22	3:B:1004:GOL:H2	1.83	0.43
1:A:626:LEU:HD23	1:A:803:TYR:HE2	1.85	0.42
1:A:490:TYR:CE1	1:A:696:THR:HG22	2.54	0.42
1:B:377:VAL:HB	1:B:388:ASP:HB3	2.01	0.42
1:A:661:ALA:O	1:A:665:LEU:HG	2.20	0.42
1:B:718:TRP:HB2	1:B:754:TYR:CE2	2.55	0.42
1:B:625:LEU:HD23	1:B:659:VAL:HG11	2.01	0.42
1:A:339:ALA:HB2	1:A:400:THR:HG23	2.01	0.42
1:B:630:VAL:HG11	1:B:668:PHE:CD1	2.55	0.42
1:B:389:LEU:HD21	1:B:403:ILE:HD11	2.00	0.42
1:A:377:VAL:HB	1:A:388:ASP:HB3	2.02	0.41
1:B:646:ALA:HB1	1:B:681:LEU:HD22	2.02	0.41
1:B:589:ASP:OD1	1:B:734:ARG:NH1	2.53	0.41
1:A:457:SER:O	1:A:477:HIS:NE2	2.41	0.41
1:B:605:ASP:HB3	1:B:608:TRP:CD1	2.55	0.41
1:B:526:MET:O	1:B:536:THR:OG1	2.38	0.41
1:B:618:SER:O	1:B:621:MET:HB3	2.20	0.41
1:B:492:LEU:HD13	1:B:700:ILE:HD11	2.02	0.41
1:B:429:ILE:HA	1:B:627:TYR:CE1	2.55	0.41
1:A:643:ASP:HB3	1:A:646:ALA:HB2	2.03	0.41
1:B:332:ILE:HD11	1:B:409:LYS:HG2	2.02	0.41
1:B:663:GLU:HB2	1:B:803:TYR:CE1	2.56	0.40
1:A:389:LEU:HD21	1:A:403:ILE:HD11	2.01	0.40
1:B:352:PHE:HB2	1:B:395:PHE:HB2	2.03	0.40
1:A:454:ASP:HA	1:A:455:PRO:HD3	1.88	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	483/486 (99%)	466 (96%)	17 (4%)	0	100	100
1	B	483/486 (99%)	464 (96%)	19 (4%)	0	100	100
All	All	966/972 (99%)	930 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	420/421 (100%)	419 (100%)	1 (0%)	93	97
1	B	420/421 (100%)	419 (100%)	1 (0%)	93	97
All	All	840/842 (100%)	838 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	ARG
1	B	356	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	2	15,15,15	1.53	3 (20%)	21,21,21	1.83	5 (23%)
2	NAG	C	2	2	14,14,15	1.71	3 (21%)	17,19,21	0.95	0
2	NAG	C	3	2	14,14,15	2.12	3 (21%)	17,19,21	1.15	2 (11%)
2	NAG	C	4	2	14,14,15	1.73	2 (14%)	17,19,21	1.22	2 (11%)
2	NAG	C	5	2	14,14,15	1.90	4 (28%)	17,19,21	1.17	2 (11%)
2	NAG	D	1	2	15,15,15	1.56	4 (26%)	21,21,21	1.59	4 (19%)
2	NAG	D	2	2	14,14,15	1.67	3 (21%)	17,19,21	1.19	1 (5%)
2	NAG	D	3	2	14,14,15	2.12	3 (21%)	17,19,21	1.11	2 (11%)
2	NAG	D	4	2	14,14,15	1.77	2 (14%)	17,19,21	1.14	2 (11%)
2	NAG	D	5	2	14,14,15	1.91	4 (28%)	17,19,21	1.18	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	3	2	-	0/6/23/26	0/1/1/1
2	NAG	C	4	2	-	0/6/23/26	0/1/1/1
2	NAG	C	5	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	3	2	-	2/6/23/26	0/1/1/1
2	NAG	D	4	2	-	0/6/23/26	0/1/1/1
2	NAG	D	5	2	-	0/6/23/26	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	NAG	O5-C1	5.04	1.51	1.43
2	C	3	NAG	O5-C1	4.94	1.51	1.43
2	C	5	NAG	O5-C1	4.76	1.51	1.43
2	D	5	NAG	O5-C1	4.74	1.51	1.43
2	D	4	NAG	O5-C1	4.34	1.50	1.43
2	C	4	NAG	O5-C1	4.19	1.50	1.43
2	C	3	NAG	C7-N2	3.93	1.47	1.34
2	D	3	NAG	C7-N2	3.89	1.47	1.34
2	C	2	NAG	O5-C1	3.61	1.49	1.43
2	D	2	NAG	O5-C1	3.58	1.49	1.43
2	D	1	NAG	C7-N2	3.41	1.46	1.34
2	C	1	NAG	C7-N2	3.38	1.46	1.34
2	D	4	NAG	C7-N2	3.29	1.45	1.34
2	C	4	NAG	C7-N2	3.28	1.45	1.34
2	D	5	NAG	C7-N2	3.19	1.45	1.34
2	C	5	NAG	C7-N2	3.18	1.45	1.34
2	C	2	NAG	O5-C5	2.70	1.48	1.43
2	C	2	NAG	C7-N2	2.69	1.43	1.34
2	D	2	NAG	C7-N2	2.67	1.43	1.34
2	D	1	NAG	O5-C1	2.66	1.49	1.42
2	C	3	NAG	C8-C7	2.56	1.55	1.50
2	D	3	NAG	C8-C7	2.53	1.55	1.50
2	D	2	NAG	O5-C5	2.51	1.48	1.43
2	C	1	NAG	O5-C1	2.47	1.49	1.42
2	D	1	NAG	C3-C2	-2.44	1.48	1.53
2	C	1	NAG	C3-C2	-2.32	1.48	1.53
2	D	5	NAG	O5-C5	2.30	1.48	1.43
2	C	5	NAG	O5-C5	2.16	1.47	1.43
2	C	5	NAG	C8-C7	2.15	1.55	1.50
2	D	5	NAG	C8-C7	2.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C8-C7	2.02	1.54	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C4-C3-C2	4.57	117.04	110.34
2	C	1	NAG	C3-C4-C5	3.94	117.27	110.24
2	D	1	NAG	C4-C3-C2	3.86	116.00	110.34
2	D	1	NAG	C3-C4-C5	3.20	115.95	110.24
2	D	5	NAG	C2-N2-C7	-2.62	119.17	122.90
2	C	3	NAG	C8-C7-N2	2.48	120.30	116.10
2	D	1	NAG	O5-C5-C4	2.41	114.08	109.69
2	D	5	NAG	C8-C7-N2	2.40	120.16	116.10
2	D	3	NAG	C2-N2-C7	-2.38	119.52	122.90
2	C	5	NAG	C8-C7-N2	2.37	120.12	116.10
2	C	1	NAG	O5-C5-C4	2.36	113.98	109.69
2	D	3	NAG	C8-C7-N2	2.34	120.06	116.10
2	C	4	NAG	C4-C3-C2	2.33	114.43	111.02
2	D	1	NAG	C8-C7-N2	2.27	119.94	116.10
2	C	4	NAG	C8-C7-N2	2.26	119.93	116.10
2	C	1	NAG	C8-C7-N2	2.26	119.92	116.10
2	D	4	NAG	C8-C7-N2	2.22	119.86	116.10
2	C	3	NAG	C2-N2-C7	-2.20	119.78	122.90
2	D	2	NAG	C2-N2-C7	-2.17	119.81	122.90
2	C	5	NAG	C2-N2-C7	-2.16	119.83	122.90
2	C	1	NAG	C1-C2-N2	-2.13	108.26	110.73
2	D	4	NAG	C2-N2-C7	-2.12	119.88	122.90

There are no chirality outliers.

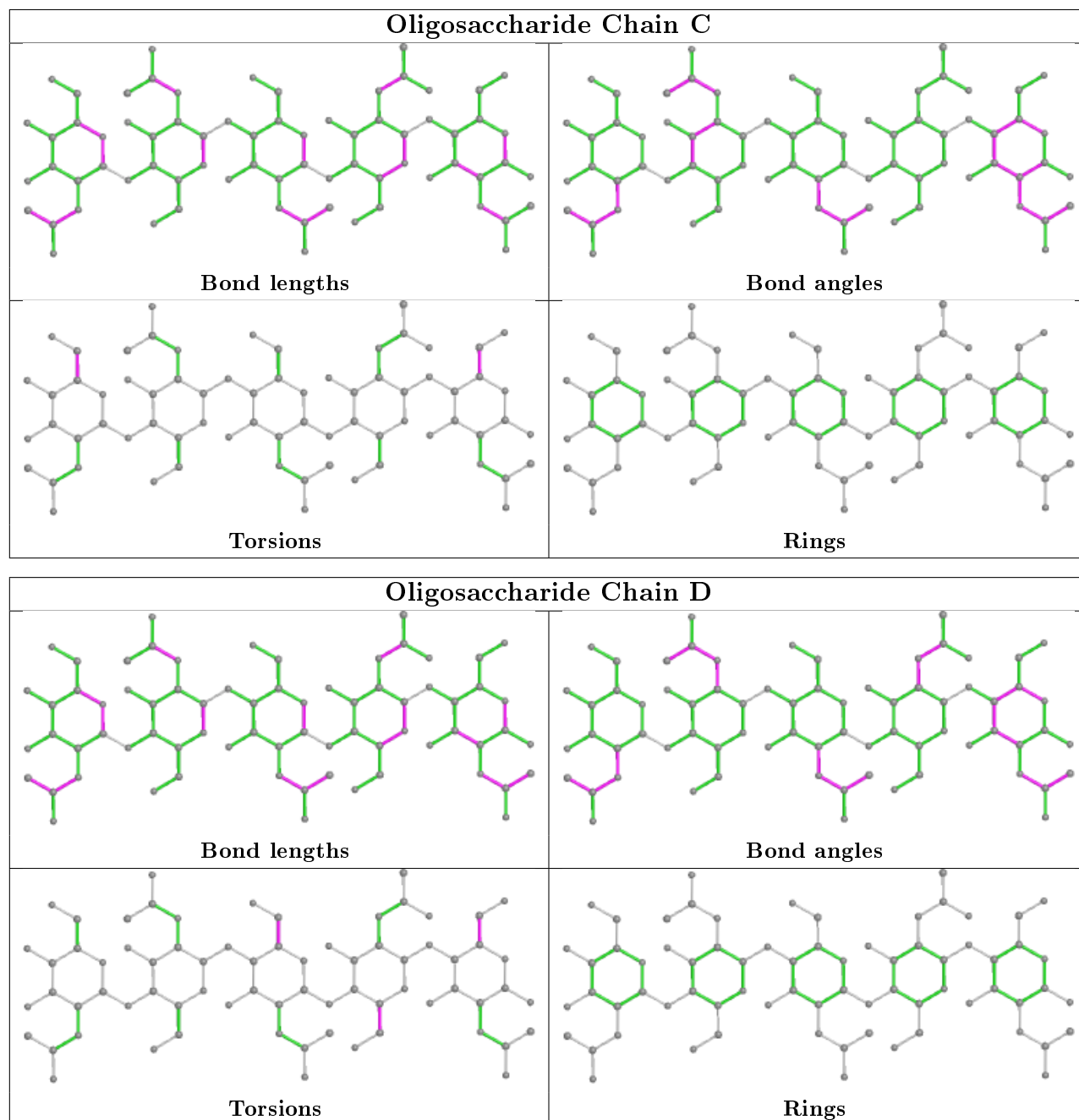
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	3	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	3	NAG	C4-C5-C6-O6
2	C	5	NAG	C4-C5-C6-O6
2	C	5	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

14 ligands 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
4	PO4	A	1007	-	4,4,4	0.92	0	6,6,6	0.40	0
3	GOL	A	1004	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	B	1003	-	5,5,5	0.38	0	5,5,5	0.27	0
3	GOL	B	1004	-	5,5,5	0.37	0	5,5,5	0.22	0
4	PO4	B	1008	-	4,4,4	0.93	0	6,6,6	0.42	0
3	GOL	A	1005	-	5,5,5	0.36	0	5,5,5	0.27	0
4	PO4	A	1009	-	4,4,4	0.91	0	6,6,6	0.45	0
4	PO4	B	1009	-	4,4,4	0.89	0	6,6,6	0.45	0
4	PO4	B	1006	-	4,4,4	0.90	0	6,6,6	0.45	0
3	GOL	A	1006	-	5,5,5	0.37	0	5,5,5	0.26	0
4	PO4	A	1008	-	4,4,4	0.89	0	6,6,6	0.48	0
3	GOL	A	1003	-	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	B	1005	-	5,5,5	0.38	0	5,5,5	0.27	0
4	PO4	B	1007	-	4,4,4	0.92	0	6,6,6	0.41	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
3	GOL	A	1004	-	-	2/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-
3	GOL	B	1004	-	-	2/4/4/4	-
3	GOL	A	1005	-	-	2/4/4/4	-
3	GOL	A	1006	-	-	2/4/4/4	-
3	GOL	A	1003	-	-	2/4/4/4	-
3	GOL	B	1005	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	GOL	O1-C1-C2-C3
3	B	1004	GOL	O1-C1-C2-O2
3	B	1004	GOL	O1-C1-C2-C3
3	A	1005	GOL	O1-C1-C2-O2
3	B	1005	GOL	O1-C1-C2-C3
3	B	1003	GOL	O1-C1-C2-O2
3	B	1003	GOL	O1-C1-C2-C3
3	A	1005	GOL	O1-C1-C2-C3
3	A	1006	GOL	O1-C1-C2-C3
3	A	1003	GOL	O1-C1-C2-C3
3	A	1003	GOL	O1-C1-C2-O2
3	A	1004	GOL	O1-C1-C2-O2
3	A	1006	GOL	O1-C1-C2-O2
3	B	1005	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	GOL	1	0
3	B	1004	GOL	2	0
3	A	1005	GOL	1	0
3	A	1003	GOL	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, 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	485/486 (99%)	0.55	38 (7%) 13 10	41, 69, 105, 120	0
1	B	485/486 (99%)	0.47	29 (5%) 21 19	41, 68, 103, 120	0
All	All	970/972 (99%)	0.51	67 (6%) 16 13	41, 69, 104, 120	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	ILE	5.6
1	A	403	ILE	5.0
1	B	444	GLY	4.9
1	A	336	LEU	4.6
1	B	455	PRO	4.4
1	B	453	ALA	4.4
1	A	334	VAL	4.3
1	A	640	LEU	4.2
1	B	490	TYR	4.1
1	A	367	SER	3.9
1	A	405	ILE	3.7
1	A	365	VAL	3.6
1	B	448	LEU	3.4
1	A	407	ILE	3.3
1	A	449	SER	3.2
1	A	384	LEU	3.2
1	A	333	THR	3.2
1	B	759	GLN	3.2
1	A	377	VAL	3.2
1	B	325	VAL	3.1
1	B	637	PHE	3.1
1	B	451	LEU	3.0
1	B	380	VAL	3.0
1	B	463	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	706	MET	3.0
1	A	327	GLU	2.9
1	B	321	ALA	2.9
1	A	494	LEU	2.9
1	B	445	ASN	2.9
1	B	446	PHE	2.8
1	A	368	ILE	2.8
1	A	672	TRP	2.8
1	A	366	LEU	2.7
1	A	676	ILE	2.7
1	A	332	ILE	2.7
1	B	456	LYS	2.7
1	A	321	ALA	2.6
1	A	381	ASN	2.6
1	B	764	ASP	2.5
1	A	452	ILE	2.5
1	B	640	LEU	2.5
1	A	383	ASN	2.5
1	B	756	LEU	2.5
1	A	675	ALA	2.4
1	B	439	ALA	2.4
1	B	706	MET	2.4
1	A	455	PRO	2.4
1	B	551	ILE	2.4
1	A	677	ASN	2.4
1	B	641	ALA	2.3
1	B	681	LEU	2.3
1	B	710	ARG	2.3
1	A	410	SER	2.3
1	A	448	LEU	2.3
1	A	639	ARG	2.3
1	A	636	GLU	2.3
1	B	378	TYR	2.3
1	B	458	TYR	2.2
1	B	766	ILE	2.2
1	A	451	LEU	2.2
1	A	698	ILE	2.2
1	A	323	ARG	2.1
1	A	335	GLU	2.1
1	B	768	TYR	2.0
1	A	535	GLY	2.0
1	A	630	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	365	VAL	2.0

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](#)

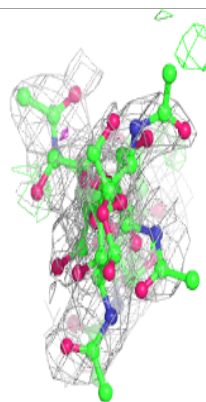
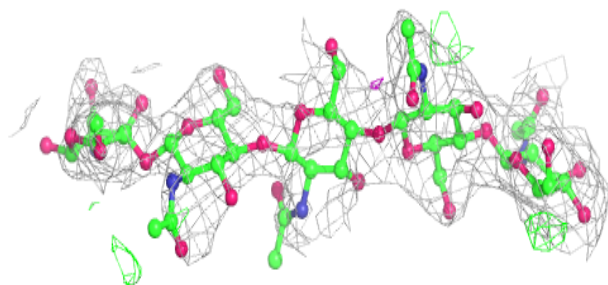
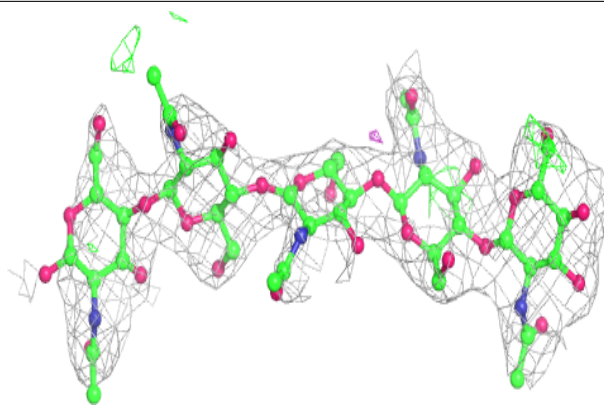
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	D	2	14/15	0.80	0.28	86,96,102,111	0
2	NAG	C	2	14/15	0.81	0.28	87,96,102,103	14
2	NAG	C	1	15/15	0.82	0.28	77,90,106,106	15
2	NAG	C	3	14/15	0.87	0.24	74,91,109,109	0
2	NAG	D	1	15/15	0.87	0.21	73,94,106,108	0
2	NAG	C	5	14/15	0.91	0.18	61,71,79,84	0
2	NAG	D	3	14/15	0.91	0.19	72,79,94,95	0
2	NAG	C	4	14/15	0.93	0.20	64,71,73,76	0
2	NAG	D	5	14/15	0.94	0.14	53,67,77,88	0
2	NAG	D	4	14/15	0.96	0.15	51,56,64,67	0

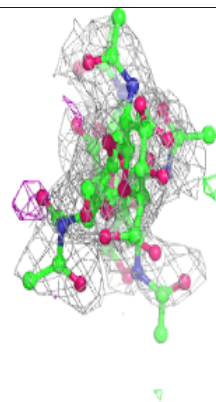
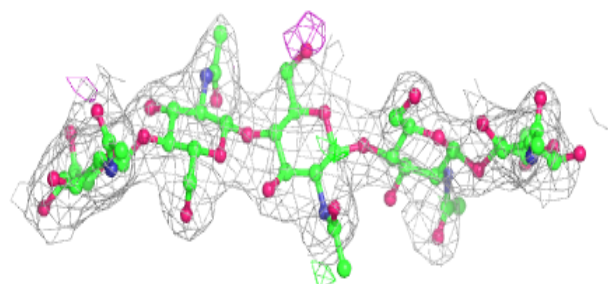
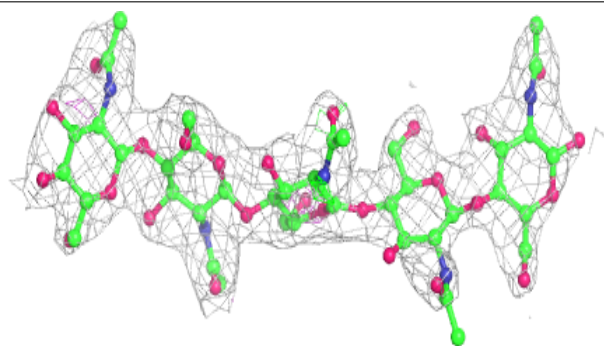
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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
3	GOL	A	1003	6/6	0.66	0.21	64,72,77,83	0
3	GOL	B	1003	6/6	0.72	0.20	74,80,81,83	0
3	GOL	B	1005	6/6	0.74	0.21	80,87,94,95	0
3	GOL	A	1004	6/6	0.80	0.19	92,102,105,105	0
4	PO4	B	1006	5/5	0.84	0.15	83,85,94,112	5
3	GOL	A	1006	6/6	0.84	0.31	68,74,83,91	0
4	PO4	B	1007	5/5	0.87	0.25	91,94,127,128	0
4	PO4	B	1009	5/5	0.89	0.13	72,73,98,123	0
3	GOL	B	1004	6/6	0.90	0.22	52,54,77,77	0
4	PO4	B	1008	5/5	0.90	0.17	60,75,83,94	5
3	GOL	A	1005	6/6	0.91	0.19	75,76,87,91	0
4	PO4	A	1009	5/5	0.91	0.22	77,86,97,110	5
4	PO4	A	1007	5/5	0.93	0.16	84,86,89,109	0
4	PO4	A	1008	5/5	0.95	0.22	58,79,85,101	5

6.5 Other polymers [i](#)

There are no such residues in this entry.