



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:30 AM UTC

PDB ID : 6VC9 / pdb_00006vc9
Title : TB19 complex
Authors : Zhou, Y.F.; Lord, D.M.
Deposited on : 2019-12-20
Resolution : 2.25 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

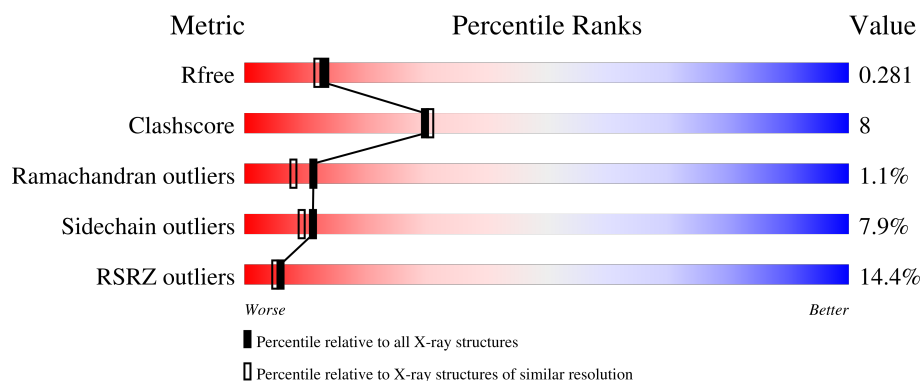
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. 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	H	233	
2	L	215	
3	A	529	
4	B	5	

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
8	EDO	A	612	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6035 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 TB19 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	118	Total	C	N	O	S	0	0	0
			899	559	155	182	3			

- Molecule 2 is a protein called TB19 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	108	Total	C	N	O	S	0	0	0
			841	533	137	168	3			

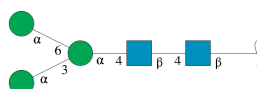
- Molecule 3 is a protein called 5'-nucleotidase, ecto (CD73), isoform CRA_a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	523	Total	C	N	O	S	0	0	0
			4074	2590	698	768	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	550	HIS	-	expression tag	UNP Q53Z63
A	551	HIS	-	expression tag	UNP Q53Z63
A	552	HIS	-	expression tag	UNP Q53Z63
A	553	HIS	-	expression tag	UNP Q53Z63
A	554	HIS	-	expression tag	UNP Q53Z63
A	555	HIS	-	expression tag	UNP Q53Z63

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

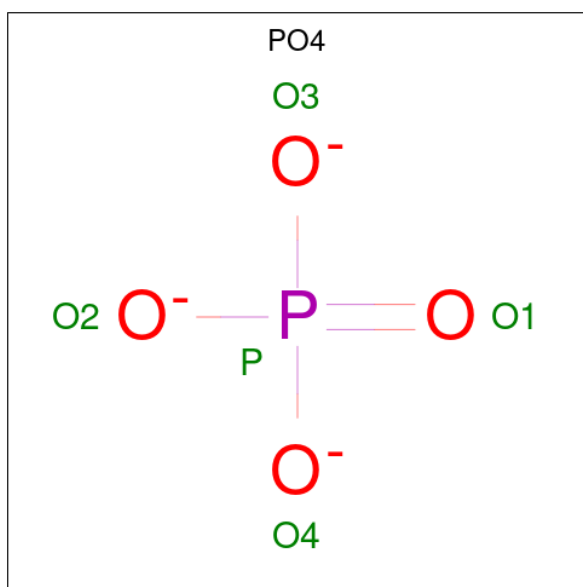


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

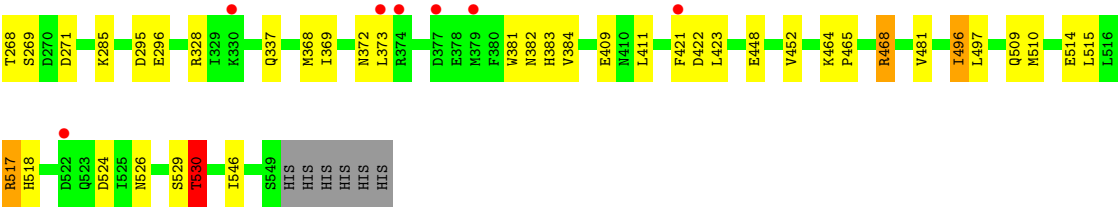
- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	9	Total 9	O 9	0	0
9	L	15	Total 15	O 15	0	0
9	A	102	Total 102	O 102	0	0



● Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.31Å 74.22Å 148.33Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25 30.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.25) 99.5 (30.00-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.237 , 0.279 0.245 , 0.281	Depositor DCC
R_{free} test set	2017 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6035	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: ZN, MAN, PO4, PG4, EDO, 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	H	2.08	20/916 (2.2%)	1.48	2/1245 (0.2%)
2	L	1.82	16/862 (1.9%)	1.52	5/1174 (0.4%)
3	A	1.22	6/4160 (0.1%)	1.45	15/5636 (0.3%)
All	All	1.48	42/5938 (0.7%)	1.46	22/8055 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
2	L	0	2
All	All	0	4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	6	GLU	CD-OE2	31.48	1.85	1.25
1	H	119	SER	C-O	13.89	1.51	1.23
2	L	106	GLU	C-O	13.56	1.40	1.24
2	L	106	GLU	CD-OE1	12.44	1.49	1.25
1	H	10	GLY	C-O	12.06	1.37	1.23
1	H	56	THR	C-O	11.04	1.36	1.23
2	L	106	GLU	CD-OE2	10.80	1.45	1.25
2	L	85	GLY	C-O	10.67	1.31	1.24
2	L	86	ILE	C-O	10.64	1.36	1.24
2	L	38	GLN	C-N	9.85	1.46	1.33
1	H	32	ASN	C-O	9.39	1.35	1.23
2	L	78	SER	C-O	8.89	1.34	1.23
1	H	7	SER	CB-OG	8.36	1.58	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	46	ARG	C-O	8.03	1.33	1.24
2	L	38	GLN	C-O	7.78	1.33	1.23
1	H	6	GLU	CD-OE1	7.47	1.39	1.25
1	H	72	ASP	CG-OD2	7.42	1.39	1.25
1	H	23	THR	C-O	7.40	1.32	1.24
1	H	50	ARG	C-O	7.28	1.32	1.23
2	L	6	GLN	CD-NE2	7.20	1.48	1.33
1	H	4	LEU	C-O	7.08	1.32	1.24
1	H	3	GLN	C-O	-6.92	1.15	1.23
3	A	176	TYR	C-O	6.34	1.31	1.23
1	H	90	THR	C-O	6.32	1.31	1.24
1	H	31	ASN	C-O	6.11	1.30	1.23
2	L	104	TYR	C-O	5.86	1.31	1.24
1	H	3	GLN	C-N	5.80	1.42	1.33
2	L	97	TYR	C-O	5.79	1.30	1.23
2	L	10	THR	C-O	5.74	1.30	1.23
2	L	5	THR	C-O	5.71	1.30	1.23
3	A	546	ILE	C-O	5.63	1.30	1.24
3	A	481	VAL	N-CA	5.45	1.50	1.46
3	A	135	ALA	C-O	5.45	1.30	1.23
1	H	103	GLY	C-O	5.42	1.31	1.23
3	A	219	GLY	C-O	5.40	1.29	1.23
2	L	71	ASP	C-O	5.38	1.30	1.24
1	H	3	GLN	CA-C	5.36	1.59	1.52
2	L	81	PRO	C-O	5.27	1.30	1.24
3	A	259	PRO	C-O	-5.23	1.18	1.23
1	H	111	GLN	C-O	5.22	1.30	1.24
1	H	116	THR	C-O	5.05	1.29	1.23
1	H	47	TRP	C-O	5.01	1.30	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	38	GLN	OE1-CD-NE2	-9.80	112.80	122.60
3	A	296	GLU	CB-CA-C	-7.78	97.88	110.79
3	A	268	THR	CA-CB-OG1	-6.69	99.57	109.60
3	A	530	THR	CB-CA-C	6.55	121.25	110.90
3	A	47	ASP	CA-CB-CG	6.45	119.05	112.60
2	L	39	GLN	OE1-CD-NE2	6.41	129.01	122.60
3	A	524	ASP	CA-CB-CG	6.03	118.63	112.60
3	A	452	VAL	CA-C-N	5.96	125.70	121.65
3	A	452	VAL	C-N-CA	5.96	125.70	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	530	THR	N-CA-C	-5.95	104.71	111.14
3	A	172	GLY	CA-C-O	-5.72	116.14	121.18
2	L	70	THR	CB-CA-C	5.66	119.59	109.29
1	H	112	GLY	CA-C-O	-5.59	118.43	122.45
1	H	6	GLU	CG-CD-OE2	-5.57	105.58	118.40
2	L	106	GLU	OE1-CD-OE2	5.43	135.93	122.90
3	A	295	ASP	CA-C-N	5.36	127.46	120.28
3	A	295	ASP	C-N-CA	5.36	127.46	120.28
2	L	38	GLN	CG-CD-NE2	5.31	124.36	116.40
3	A	85	ASP	CB-CA-C	5.24	118.52	111.82
3	A	257	GLU	CA-C-N	5.18	126.32	122.59
3	A	257	GLU	C-N-CA	5.18	126.32	122.59
3	A	180	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	6	GLU	Sidechain
1	H	91	ALA	Mainchain
2	L	45	PRO	Mainchain
2	L	50	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	899	0	880	37	0
2	L	841	0	811	24	0
3	A	4074	0	4046	40	0
4	B	61	0	52	1	0
5	A	2	0	0	0	0
6	A	15	0	0	0	0
7	A	13	0	18	5	0
8	A	4	0	6	4	0
9	A	102	0	0	8	0
9	H	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	15	0	0	2	0
All	All	6035	0	5813	99	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 8.

All (99) 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:H:6:GLU:OE2	1:H:6:GLU:CD	1.85	1.19
3:A:381:TRP:O	9:A:701:HOH:O	1.74	1.04
3:A:101:VAL:HG22	8:A:612:EDO:H11	1.44	0.98
1:H:22:CYS:O	1:H:77:GLN:HB2	1.64	0.96
3:A:381:TRP:C	9:A:701:HOH:O	2.18	0.84
3:A:101:VAL:HG22	8:A:612:EDO:C1	2.10	0.81
1:H:35:ASN:HD22	1:H:47:TRP:HE1	1.31	0.79
2:L:56:ALA:HB3	2:L:59:ILE:HD13	1.69	0.75
1:H:71:ILE:HG12	1:H:78:PHE:HB3	1.73	0.71
3:A:256:LYS:NZ	3:A:257:GLU:OE2	2.18	0.71
1:H:109:TRP:HB2	2:L:44:THR:CG2	2.23	0.68
3:A:129:GLU:O	3:A:129:GLU:OE1	2.12	0.67
3:A:269:SER:OG	3:A:271:ASP:OD1	2.08	0.66
1:H:5:GLN:HA	1:H:5:GLN:OE1	1.98	0.63
2:L:36:TRP:CE2	2:L:74:LEU:HB2	2.35	0.62
3:A:526:ASN:O	3:A:530:THR:HG23	2.01	0.60
3:A:373:LEU:HA	3:A:382:ASN:HD21	1.67	0.60
3:A:75:GLU:CD	9:A:705:HOH:O	2.45	0.59
1:H:18:LEU:O	1:H:81:LYS:HA	2.01	0.59
2:L:10:THR:HA	2:L:104:TYR:O	2.02	0.59
3:A:223:PHE:N	9:A:702:HOH:O	2.36	0.59
1:H:86:THR:O	1:H:117:VAL:HG21	2.04	0.58
2:L:27:GLN:NE2	9:A:706:HOH:O	2.37	0.57
2:L:50:TYR:C	2:L:51:GLY:O	2.44	0.57
3:A:251:GLY:H	7:A:611:PG4:H51	1.69	0.57
1:H:71:ILE:HG12	1:H:78:PHE:CB	2.36	0.56
1:H:3:GLN:O	1:H:3:GLN:CD	2.48	0.56
1:H:29:ILE:HD12	1:H:76:ASN:OD1	2.06	0.55
1:H:17:THR:O	1:H:18:LEU:HB2	2.07	0.55
1:H:29:ILE:CD1	1:H:76:ASN:OD1	2.55	0.55
2:L:34:PHE:O	2:L:51:GLY:O	2.24	0.54
3:A:175:GLY:HA2	3:A:218:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:LEU:HD23	1:H:11:LEU:O	2.07	0.54
1:H:2:GLU:HA	1:H:26:GLY:HA3	1.89	0.53
3:A:337:GLN:HA	3:A:337:GLN:OE1	2.09	0.53
2:L:21:LEU:HB3	9:L:312:HOH:O	2.08	0.53
3:A:422:ASP:OD2	3:A:518:HIS:NE2	2.41	0.53
2:L:13:LEU:C	2:L:13:LEU:HD23	2.35	0.52
1:H:6:GLU:N	1:H:6:GLU:OE1	2.43	0.52
1:H:3:GLN:CD	1:H:3:GLN:C	2.78	0.51
2:L:66:SER:HB3	2:L:73:THR:OG1	2.11	0.51
3:A:46:GLU:HA	3:A:58:MET:HE2	1.93	0.51
2:L:34:PHE:CE2	2:L:72:PHE:CD1	3.00	0.50
2:L:79:LEU:HD12	2:L:107:ILE:HG22	1.93	0.50
3:A:75:GLU:HG3	9:A:705:HOH:O	2.12	0.50
1:H:72:ASP:CG	1:H:75:LYS:HB2	2.36	0.50
1:H:68:THR:OG1	1:H:81:LYS:HB2	2.12	0.49
1:H:87:ALA:O	1:H:90:THR:HG22	2.12	0.49
3:A:262:LYS:HE2	7:A:611:PG4:O4	2.12	0.49
3:A:368:MET:HG2	3:A:421:PHE:CD2	2.48	0.49
2:L:56:ALA:HB1	9:L:314:HOH:O	2.11	0.49
3:A:58:MET:HE3	3:A:285:LYS:HG3	1.95	0.49
1:H:10:GLY:O	1:H:116:THR:HG22	2.12	0.49
1:H:49:GLY:HA3	1:H:69:MET:HE1	1.94	0.49
2:L:13:LEU:HD23	2:L:13:LEU:O	2.12	0.49
3:A:261:GLY:HA2	7:A:611:PG4:H21	1.95	0.49
2:L:95:LEU:HA	2:L:96:PRO:C	2.38	0.48
3:A:57:CYS:O	3:A:58:MET:HG2	2.12	0.48
1:H:49:GLY:HA3	1:H:69:MET:CE	2.44	0.48
2:L:12:SER:HA	2:L:106:GLU:O	2.12	0.48
3:A:231:GLN:HA	3:A:269:SER:HA	1.95	0.47
3:A:251:GLY:H	7:A:611:PG4:C5	2.27	0.47
1:H:4:LEU:HA	1:H:23:THR:O	2.14	0.47
3:A:422:ASP:O	3:A:496:ILE:HA	2.15	0.47
3:A:510:MET:O	3:A:514:GLU:HB2	2.14	0.47
1:H:49:GLY:CA	1:H:69:MET:HE1	2.45	0.46
1:H:61:PRO:HA	1:H:64:LYS:HB2	1.96	0.46
3:A:372:ASN:O	3:A:383:HIS:NE2	2.49	0.45
1:H:35:ASN:HD22	1:H:47:TRP:NE1	2.07	0.45
3:A:517:ARG:HG2	3:A:517:ARG:HH11	1.82	0.45
9:A:703:HOH:O	4:B:4:MAN:O3	2.21	0.45
1:H:29:ILE:HG12	1:H:29:ILE:O	2.16	0.45
3:A:39:SER:HA	8:A:612:EDO:C2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:79:LEU:HD13	2:L:80:GLN:N	2.32	0.44
1:H:3:GLN:NE2	1:H:25:SER:OG	2.47	0.44
1:H:6:GLU:OE2	1:H:94:TYR:HA	2.17	0.44
3:A:181:THR:N	3:A:182:PRO:CD	2.80	0.44
1:H:99:HIS:HD1	1:H:107:ASP:CG	2.26	0.44
1:H:29:ILE:HD13	1:H:29:ILE:N	2.32	0.43
3:A:75:GLU:CG	9:A:705:HOH:O	2.65	0.43
3:A:251:GLY:H	7:A:611:PG4:C6	2.31	0.43
3:A:57:CYS:C	3:A:58:MET:CG	2.91	0.43
2:L:33:TYR:O	2:L:91:GLN:HA	2.18	0.43
3:A:369:ILE:HG13	3:A:496:ILE:HD11	2.01	0.42
1:H:47:TRP:CZ3	2:L:96:PRO:HA	2.55	0.42
3:A:515:LEU:C	3:A:515:LEU:HD12	2.44	0.42
1:H:38:ARG:HG2	1:H:48:ILE:HD11	2.01	0.42
2:L:56:ALA:HB3	2:L:59:ILE:CD1	2.45	0.42
1:H:51:ILE:HA	1:H:56:THR:O	2.19	0.42
3:A:465:PRO:HA	3:A:468:ARG:HD2	2.02	0.42
2:L:97:TYR:OH	3:A:189:THR:HG22	2.20	0.41
2:L:79:LEU:CD1	2:L:107:ILE:HG22	2.50	0.41
3:A:38:HIS:CE1	3:A:85:ASP:HB3	2.56	0.41
2:L:18:ARG:HG3	2:L:77:SER:HA	2.02	0.41
2:L:35:SER:HB2	2:L:49:ILE:O	2.20	0.41
3:A:129:GLU:HB3	3:A:130:PRO:HD3	2.03	0.41
3:A:101:VAL:CG2	8:A:612:EDO:H22	2.52	0.40
1:H:4:LEU:CD2	1:H:24:VAL:HB	2.51	0.40
1:H:4:LEU:HD22	1:H:24:VAL:HB	2.03	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	H	116/233 (50%)	101 (87%)	11 (10%)	4 (3%)	3	1
2	L	106/215 (49%)	98 (92%)	6 (6%)	2 (2%)	6	3
3	A	521/529 (98%)	492 (94%)	27 (5%)	2 (0%)	30	31
All	All	743/977 (76%)	691 (93%)	44 (6%)	8 (1%)	11	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	18	LEU
1	H	76	ASN
1	H	29	ILE
1	H	118	SER
2	L	51	GLY
3	A	130	PRO
2	L	41	PRO
3	A	88	GLN

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	H	102/203 (50%)	86 (84%)	16 (16%)	2	1
2	L	94/190 (50%)	80 (85%)	14 (15%)	3	1
3	A	448/456 (98%)	427 (95%)	21 (5%)	23	26
All	All	644/849 (76%)	593 (92%)	51 (8%)	11	9

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	GLN
1	H	6	GLU
1	H	12	VAL
1	H	13	LYS
1	H	28	SER

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Mol	Chain	Res	Type
1	H	29	ILE
1	H	62	SER
1	H	63	LEU
1	H	70	SER
1	H	71	ILE
1	H	82	LEU
1	H	85	VAL
1	H	92	ILE
1	H	105	SER
1	H	114	LEU
1	H	117	VAL
2	L	3	VAL
2	L	5	THR
2	L	9	THR
2	L	10	THR
2	L	11	LEU
2	L	13	LEU
2	L	22	SER
2	L	64	SER
2	L	70	THR
2	L	77	SER
2	L	79	LEU
2	L	81	PRO
2	L	101	GLN
2	L	103	THR
3	A	47	ASP
3	A	49	SER
3	A	70	GLN
3	A	75	GLU
3	A	129	GLU
3	A	173	ILE
3	A	180	GLU
3	A	328	ARG
3	A	384	VAL
3	A	409	GLU
3	A	411	LEU
3	A	423	LEU
3	A	448	GLU
3	A	464	LYS
3	A	468	ARG
3	A	496	ILE
3	A	497	LEU

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Mol	Chain	Res	Type
3	A	509	GLN
3	A	517	ARG
3	A	529	SER
3	A	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	31	ASN
1	H	32	ASN
1	H	35	ASN
1	H	108	ASN
2	L	90	GLN
2	L	101	GLN
3	A	69	GLN
3	A	279	GLN
3	A	351	GLN
3	A	372	ASN
3	A	382	ASN
3	A	410	ASN
3	A	425	GLN
3	A	444	GLN
3	A	456	HIS
3	A	499	ASN
3	A	503	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](#)

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	$\# Z > 2$
4	NAG	B	1	3,4	14,14,15	0.42	0	17,19,21	0.73	0
4	NAG	B	2	4	14,14,15	0.33	0	17,19,21	1.08	1 (5%)
4	MAN	B	3	4	11,11,12	0.48	0	15,15,17	1.22	3 (20%)
4	MAN	B	4	4	11,11,12	0.74	0	15,15,17	1.54	3 (20%)
4	MAN	B	5	4	11,11,12	0.46	0	15,15,17	0.53	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
4	NAG	B	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	MAN	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	2/2/19/22	0/1/1/1
4	MAN	B	5	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4	MAN	C1-C2-C3	3.68	115.00	109.64
4	B	4	MAN	C2-C3-C4	3.09	116.29	110.86
4	B	3	MAN	C1-C2-C3	2.90	113.86	109.64
4	B	2	NAG	C4-C3-C2	2.29	114.38	111.02
4	B	3	MAN	O5-C5-C4	-2.15	105.59	110.83
4	B	3	MAN	O5-C5-C6	2.05	111.66	107.66
4	B	4	MAN	C3-C4-C5	2.03	113.92	110.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

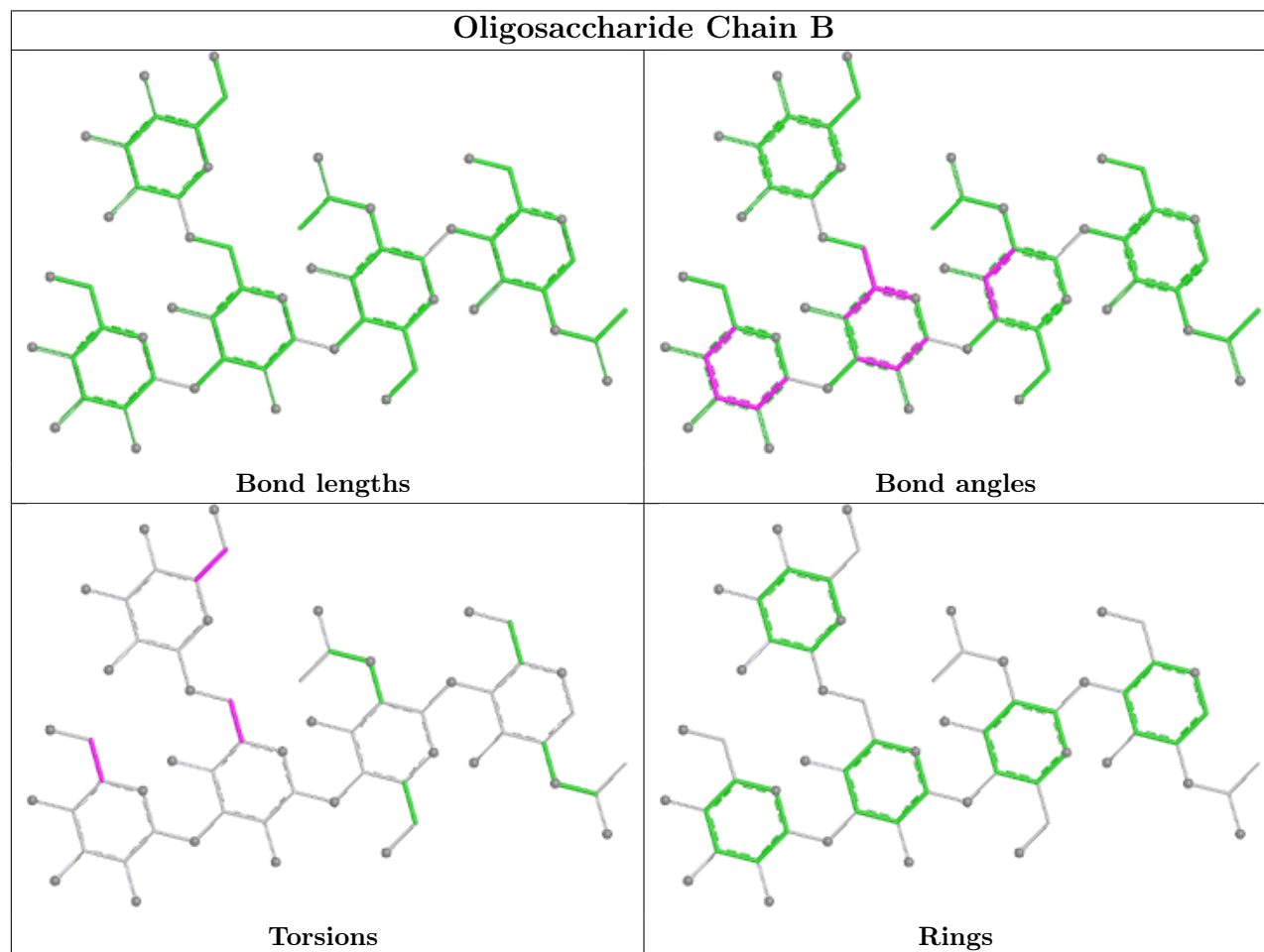
Mol	Chain	Res	Type	Atoms
4	B	4	MAN	O5-C5-C6-O6
4	B	4	MAN	C4-C5-C6-O6
4	B	3	MAN	C4-C5-C6-O6
4	B	5	MAN	O5-C5-C6-O6
4	B	3	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4	MAN	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	PG4	A	611	-	12,12,12	0.34	0	11,11,11	0.27	0
6	PO4	A	609	-	4,4,4	1.29	0	6,6,6	0.46	0
8	EDO	A	612	-	3,3,3	0.28	0	2,2,2	0.39	0
6	PO4	A	610	-	4,4,4	0.64	0	6,6,6	0.46	0
6	PO4	A	603	5	4,4,4	0.93	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
8	EDO	A	612	-	-	1/1/1/1	-
7	PG4	A	611	-	-	7/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	611	PG4	O3-C5-C6-O4
7	A	611	PG4	O4-C7-C8-O5
7	A	611	PG4	O1-C1-C2-O2
7	A	611	PG4	C3-C4-O3-C5
8	A	612	EDO	O1-C1-C2-O2
7	A	611	PG4	C1-C2-O2-C3
7	A	611	PG4	C8-C7-O4-C6
7	A	611	PG4	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	611	PG4	5	0
8	A	612	EDO	4	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	H	118/233 (50%)	1.97	55 (46%)	0 0	57, 94, 132, 148	0
2	L	108/215 (50%)	1.72	42 (38%)	1 0	51, 90, 126, 141	0
3	A	523/529 (98%)	0.34	11 (2%)	63 64	33, 53, 77, 114	0
All	All	749/977 (76%)	0.80	108 (14%)	6 5	33, 59, 116, 148	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	41	ALA	7.7
2	L	84	PHE	6.7
1	H	119	SER	6.3
1	H	11	LEU	5.7
2	L	107	ILE	5.0
2	L	12	SER	4.8
2	L	10	THR	4.5
1	H	64	LYS	4.3
2	L	43	LEU	4.3
2	L	81	PRO	4.2
1	H	9	PRO	4.1
1	H	87	ALA	4.0
1	H	16	GLU	4.0
2	L	11	LEU	3.9
2	L	13	LEU	3.8
3	A	52	VAL	3.7
1	H	13	LYS	3.7
1	H	17	THR	3.7
1	H	100	TYR	3.6
2	L	85	GLY	3.6
1	H	112	GLY	3.5
1	H	43	LYS	3.5
2	L	102	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	79	LEU	3.5
2	L	24	ARG	3.4
2	L	104	TYR	3.4
1	H	2	GLU	3.2
1	H	40	PRO	3.2
2	L	23	CYS	3.1
1	H	115	VAL	3.1
2	L	17	GLU	3.1
1	H	29	ILE	3.0
1	H	92	ILE	3.0
1	H	116	THR	3.0
1	H	86	THR	3.0
1	H	14	PRO	3.0
3	A	47	ASP	3.0
1	H	118	SER	2.9
3	A	421	PHE	2.9
1	H	114	LEU	2.9
2	L	78	SER	2.8
1	H	26	GLY	2.8
1	H	44	GLY	2.8
2	L	63	PHE	2.8
3	A	379	MET	2.8
3	A	51	CYS	2.8
1	H	74	SER	2.7
1	H	45	LEU	2.7
2	L	105	LEU	2.7
1	H	3	GLN	2.7
1	H	111	GLN	2.7
3	A	180	GLU	2.7
2	L	42	GLY	2.7
1	H	85	VAL	2.6
2	L	103	THR	2.6
2	L	76	ILE	2.6
1	H	12	VAL	2.6
2	L	1	GLU	2.6
1	H	23	THR	2.6
2	L	74	LEU	2.5
2	L	73	THR	2.5
1	H	19	SER	2.5
1	H	25	SER	2.5
2	L	77	SER	2.5
1	H	63	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	8	GLY	2.5
2	L	15	PRO	2.5
1	H	96	ALA	2.5
1	H	27	GLY	2.5
1	H	15	SER	2.4
2	L	108	LYS	2.4
2	L	18	ARG	2.4
2	L	16	GLY	2.4
1	H	117	VAL	2.4
2	L	83	ASP	2.3
2	L	87	TYR	2.3
1	H	110	GLY	2.3
2	L	67	GLY	2.3
1	H	69	MET	2.3
1	H	82	LEU	2.3
3	A	373	LEU	2.3
1	H	18	LEU	2.2
1	H	20	LEU	2.2
2	L	4	MET	2.2
2	L	46	ARG	2.2
3	A	377	ASP	2.2
2	L	8	PRO	2.2
1	H	77	GLN	2.2
1	H	88	ALA	2.2
2	L	38	GLN	2.2
2	L	5	THR	2.2
3	A	330	LYS	2.1
1	H	42	GLY	2.1
1	H	73	THR	2.1
3	A	374	ARG	2.1
2	L	3	VAL	2.1
1	H	7	SER	2.1
1	H	91	ALA	2.1
1	H	90	THR	2.1
1	H	5	GLN	2.1
2	L	39	GLN	2.1
3	A	522	ASP	2.1
1	H	62	SER	2.0
2	L	9	THR	2.0
1	H	93	TYR	2.0
2	L	19	ALA	2.0
1	H	72	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	86	ILE	2.0

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

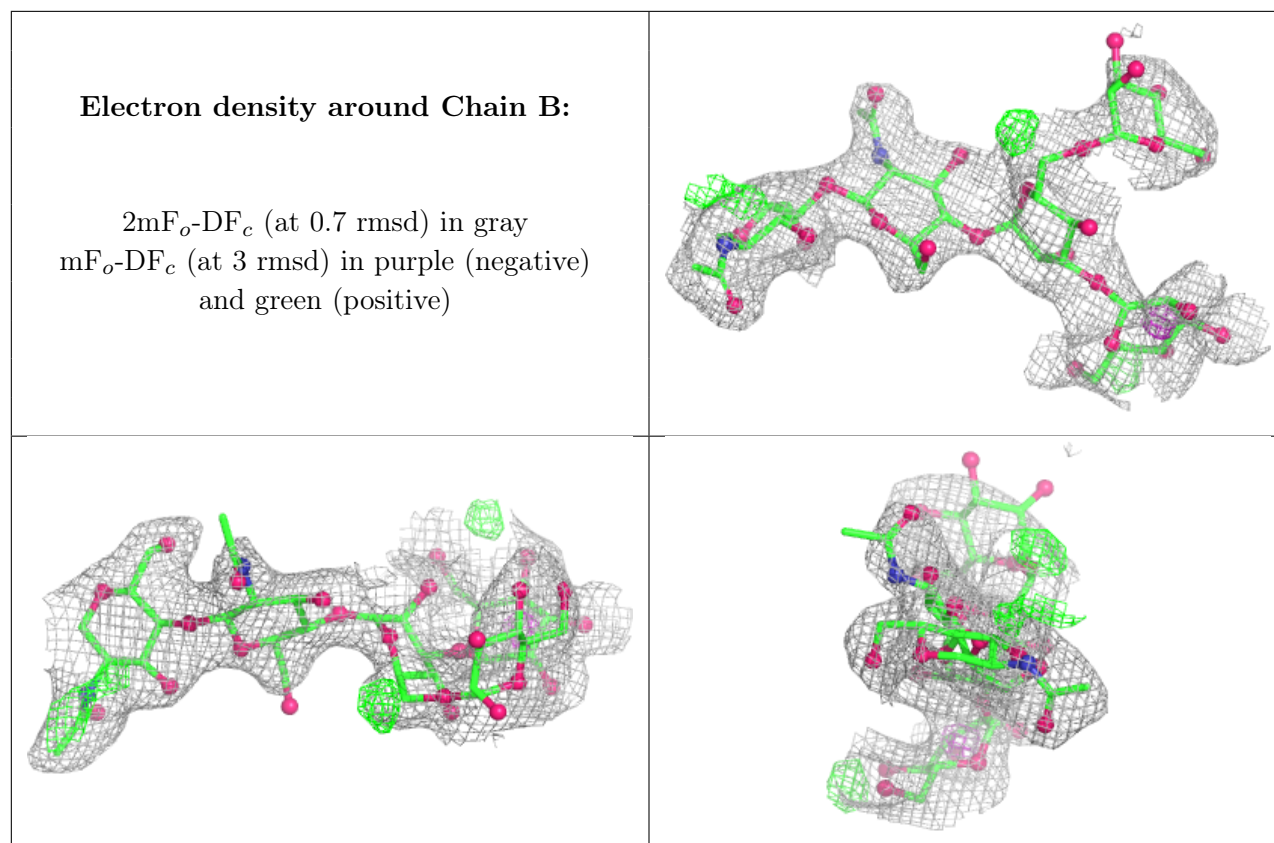
There are no non-standard protein/DNA/RNA residues in this entry.

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
4	NAG	B	1	14/15	-	-	54,59,67,75	0
4	NAG	B	2	14/15	-	-	84,95,101,110	0
4	MAN	B	3	11/12	-	-	118,132,135,145	0
4	MAN	B	4	11/12	-	-	112,118,125,128	0
4	MAN	B	5	11/12	-	-	108,120,131,133	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](#)

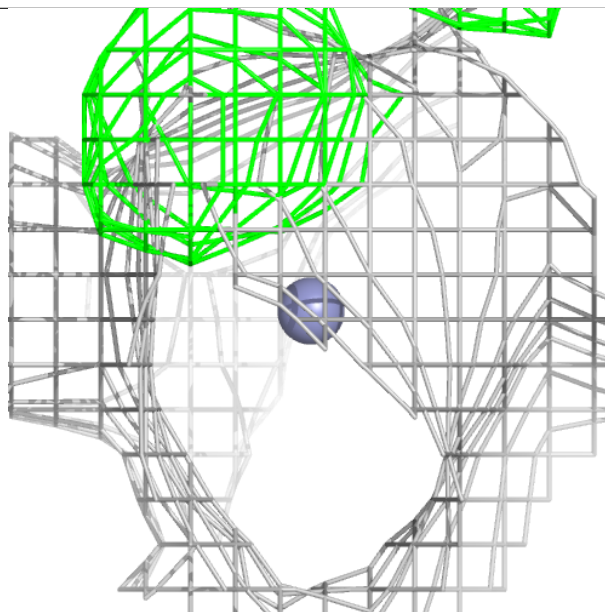
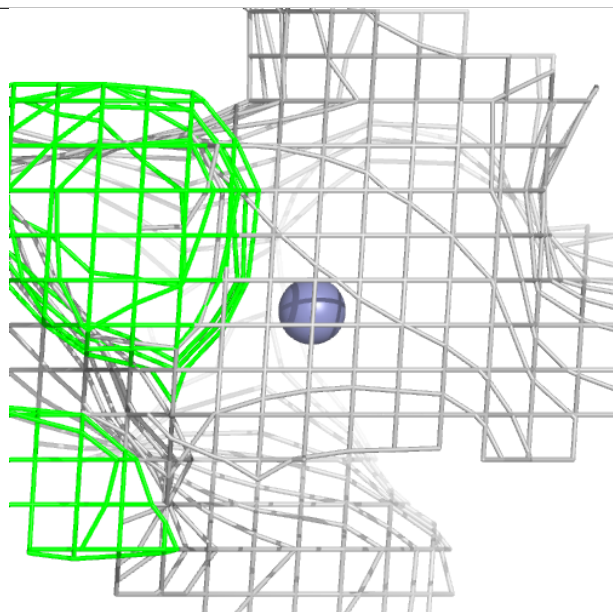
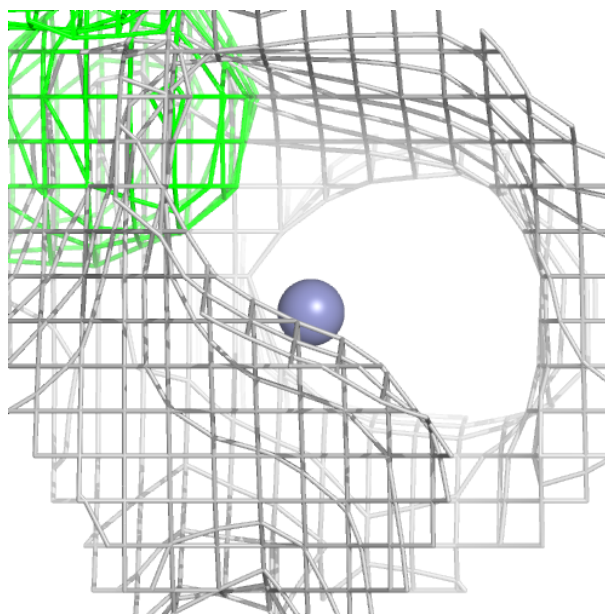
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	A	610	5/5	0.78	0.10	92,93,102,104	0
7	PG4	A	611	13/13	0.80	0.18	44,61,75,76	0
8	EDO	A	612	4/4	0.84	0.34	53,59,64,65	0
6	PO4	A	609	5/5	0.95	0.07	54,54,57,59	0
6	PO4	A	603	5/5	0.96	0.07	51,52,64,68	0
5	ZN	A	602	1/1	0.98	0.03	59,59,59,59	0
5	ZN	A	601	1/1	0.99	0.03	44,44,44,44	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.

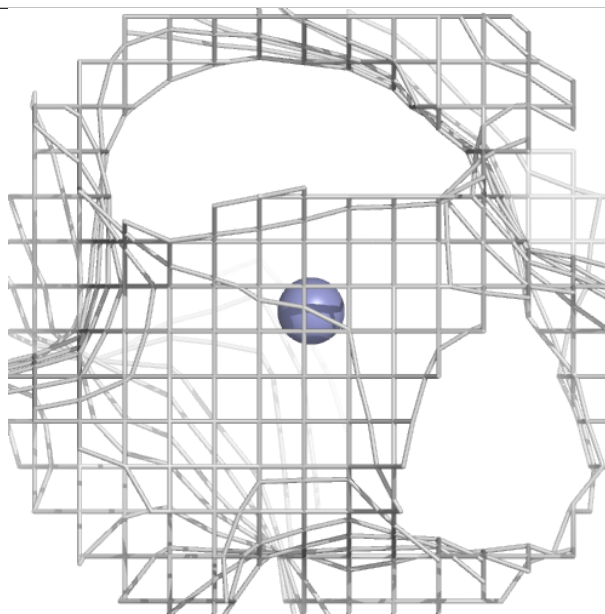
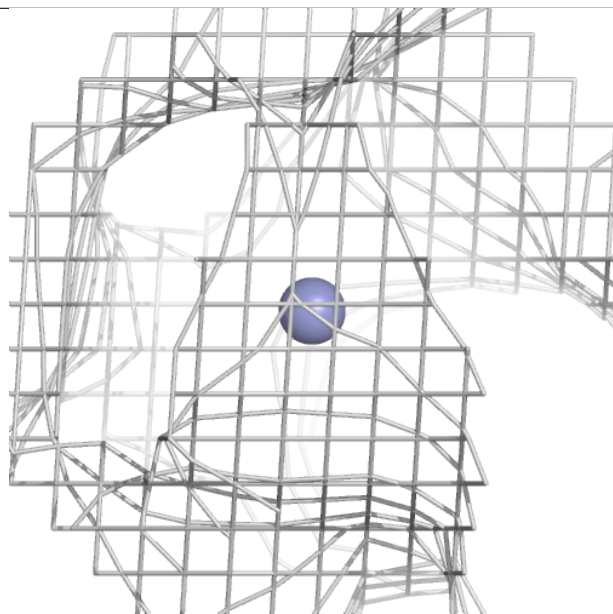
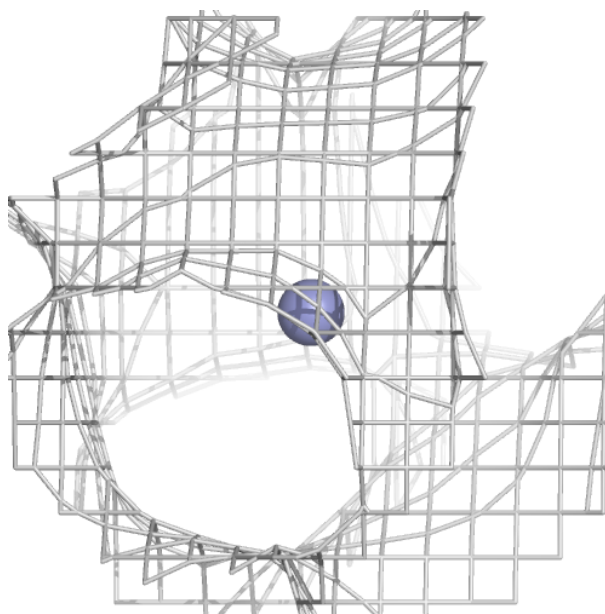
Electron density around ZN A 602:

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



Electron density around ZN A 601:

$2mF_o-DF_c$ (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.