



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:15 AM UTC

PDB ID : 1MDQ / pdb_00001mdq
Title : REFINED STRUCTURES OF TWO INSERTION(SLASH)DELETION MUTANTS PROBE FUNCTION OF THE MALTODEXTRIN BINDING PROTEIN
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Deposited on : 1994-08-10
Resolution : 1.90 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

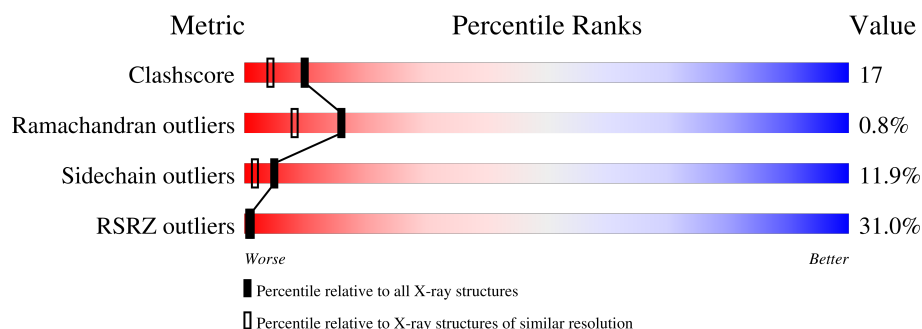
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	371	31% 51% 39% 9% .
2	B	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	B	1	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2998 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 MALTODEXTRIN BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2867	1845	469	547	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	GLY	-	insertion	UNP P02928
A	302	SER	ALA	conflict	UNP P02928

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



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

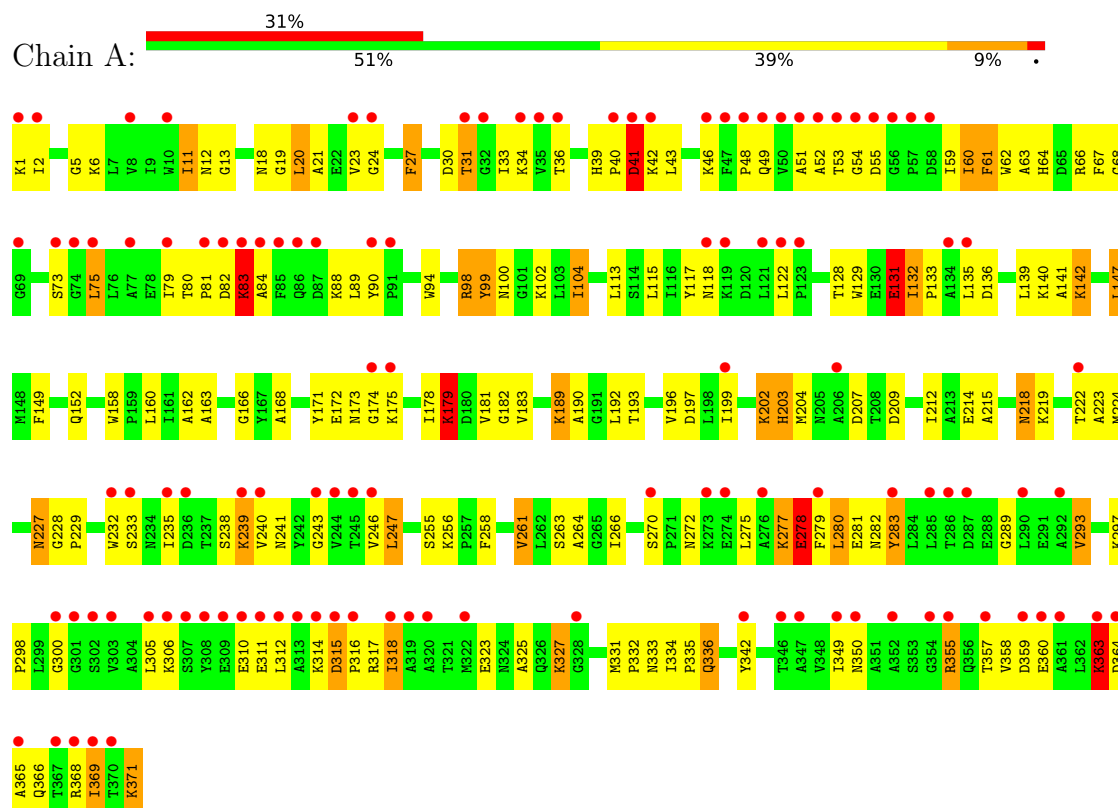
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	108	Total	O	0	0
			108	108		

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: MALTODEXTRIN BINDING PROTEIN



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.01Å 66.46Å 57.75Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 84.3 (10.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.85Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.220 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 37.3	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	0.92	EDS
Total number of atoms	2998	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	2/2936 (0.1%)	1.94	87/3985 (2.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ILE	CA-CB	6.44	1.58	1.53
1	A	243	GLY	N-CA	5.45	1.50	1.44

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	41	ASP	CA-CB-CG	11.85	124.45	112.60
1	A	61	PHE	CA-CB-CG	9.20	123.00	113.80
1	A	363	LYS	N-CA-CB	9.17	123.37	110.07
1	A	30	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	131	GLU	CA-C-N	7.71	125.09	120.24
1	A	131	GLU	C-N-CA	7.71	125.09	120.24
1	A	270	SER	O-C-N	7.67	128.41	121.35
1	A	270	SER	N-CA-C	-7.21	99.21	109.24
1	A	189	LYS	CA-C-O	-7.18	113.28	120.82
1	A	314	LYS	CA-C-N	6.95	130.36	120.49
1	A	314	LYS	C-N-CA	6.95	130.36	120.49
1	A	31	THR	N-CA-C	6.83	121.48	112.13
1	A	80	THR	N-CA-C	6.74	120.20	108.75
1	A	240	VAL	N-CA-C	-6.60	98.86	108.89
1	A	152	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	A	11	ILE	CB-CA-C	6.58	121.43	110.30
1	A	218	ASN	CB-CA-C	6.42	121.77	110.85
1	A	41	ASP	N-CA-CB	6.39	120.16	110.45
1	A	27	PHE	CA-C-N	6.28	129.33	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	PHE	C-N-CA	6.28	129.33	120.28
1	A	315	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	264	ALA	CA-C-N	6.24	126.49	122.18
1	A	264	ALA	C-N-CA	6.24	126.49	122.18
1	A	364	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	318	ILE	N-CA-C	-6.21	104.46	110.42
1	A	99	TYR	CA-C-O	-6.11	113.98	120.40
1	A	283	TYR	CB-CA-C	6.09	119.61	109.56
1	A	166	GLY	N-CA-C	-6.00	104.41	112.14
1	A	255	SER	N-CA-C	-5.99	101.42	110.28
1	A	261	VAL	CA-C-O	-5.97	113.91	120.48
1	A	241	ASN	O-C-N	5.93	130.04	122.93
1	A	90	TYR	CA-C-N	5.88	125.08	118.97
1	A	90	TYR	C-N-CA	5.88	125.08	118.97
1	A	332	PRO	CA-C-O	-5.80	114.65	122.08
1	A	261	VAL	O-C-N	5.80	129.20	122.99
1	A	135	LEU	O-C-N	5.76	128.22	122.12
1	A	63	ALA	N-CA-C	-5.74	102.41	110.50
1	A	158	TRP	CA-C-N	5.74	125.86	119.32
1	A	158	TRP	C-N-CA	5.74	125.86	119.32
1	A	190	ALA	CA-C-N	5.74	126.19	119.94
1	A	190	ALA	C-N-CA	5.74	126.19	119.94
1	A	240	VAL	CA-C-O	-5.70	114.16	121.40
1	A	98	ARG	N-CA-CB	5.70	119.72	110.43
1	A	196	VAL	CA-C-O	-5.69	114.48	120.57
1	A	238	SER	N-CA-C	-5.64	105.65	112.54
1	A	270	SER	CA-C-O	-5.61	115.17	119.32
1	A	21	ALA	CA-C-N	5.58	127.76	120.28
1	A	21	ALA	C-N-CA	5.58	127.76	120.28
1	A	222	THR	N-CA-CB	5.58	121.11	111.00
1	A	163	ALA	N-CA-C	5.58	117.36	111.28
1	A	325	ALA	O-C-N	5.55	128.00	122.12
1	A	179	LYS	CA-CB-CG	5.50	125.09	114.10
1	A	277	LYS	CA-C-N	5.45	127.84	120.65
1	A	277	LYS	C-N-CA	5.45	127.84	120.65
1	A	129	TRP	O-C-N	5.43	128.34	122.15
1	A	293	VAL	CA-C-N	5.41	127.53	120.28
1	A	293	VAL	C-N-CA	5.41	127.53	120.28
1	A	197	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	12	ASN	CA-C-N	5.39	126.87	120.14
1	A	12	ASN	C-N-CA	5.39	126.87	120.14
1	A	189	LYS	N-CA-CB	5.37	117.79	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	PHE	CA-C-O	-5.36	115.54	121.33
1	A	41	ASP	O-C-N	5.35	128.95	122.85
1	A	355	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	13	GLY	N-CA-C	5.30	120.19	113.24
1	A	214	GLU	CA-C-N	5.30	127.33	120.44
1	A	214	GLU	C-N-CA	5.30	127.33	120.44
1	A	325	ALA	CA-C-N	5.29	127.32	120.44
1	A	325	ALA	C-N-CA	5.29	127.32	120.44
1	A	363	LYS	N-CA-C	-5.28	105.44	111.14
1	A	147	LEU	N-CA-C	5.26	117.06	108.76
1	A	203	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	19	GLY	N-CA-C	-5.25	106.36	113.24
1	A	278	GLU	CB-CG-CD	5.25	121.52	112.60
1	A	369	ILE	N-CA-C	5.24	117.64	111.09
1	A	42	LYS	CA-C-N	5.21	127.52	120.38
1	A	42	LYS	C-N-CA	5.21	127.52	120.38
1	A	196	VAL	O-C-N	5.21	127.13	121.87
1	A	255	SER	CA-C-O	-5.20	115.33	121.16
1	A	241	ASN	CA-C-O	-5.19	115.03	120.58
1	A	266	ILE	N-CA-C	5.19	115.56	107.99
1	A	363	LYS	O-C-N	5.18	127.68	122.09
1	A	73	SER	CA-C-N	5.16	131.01	120.80
1	A	73	SER	C-N-CA	5.16	131.01	120.80
1	A	118	ASN	OD1-CG-ND2	5.06	127.66	122.60
1	A	349	ILE	CA-C-O	-5.01	115.86	121.17
1	A	24	GLY	N-CA-C	-5.00	106.70	112.50

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	2867	0	2831	96	11
2	B	23	0	20	4	0
3	A	108	0	0	4	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2998	0	2851	100	11

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 17.

All (100) 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)
2:B:1:GLC:O5	2:B:1:GLC:C1	1.72	1.37
2:B:1:GLC:O5	2:B:1:GLC:O1	1.76	1.02
2:B:1:GLC:C1	2:B:1:GLC:C5	2.39	0.99
1:A:202:LYS:HA	1:A:202:LYS:HE3	1.49	0.92
1:A:199:ILE:HD13	1:A:204:MET:HB3	1.59	0.85
1:A:64:HIS:HD2	1:A:261:VAL:H	1.30	0.80
1:A:229:PRO:HG2	1:A:300:GLY:HA2	1.65	0.77
1:A:122:LEU:HD12	1:A:223:ALA:HB1	1.70	0.73
1:A:27:PHE:HD1	1:A:283:TYR:HD2	1.37	0.72
1:A:189:LYS:O	1:A:193:THR:HG23	1.90	0.72
1:A:23:VAL:HG12	1:A:279:PHE:HE1	1.55	0.71
1:A:5:GLY:O	1:A:33:ILE:HG23	1.90	0.71
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.55	0.71
1:A:359:ASP:O	1:A:363:LYS:HG3	1.91	0.71
2:B:1:GLC:O5	2:B:1:GLC:C2	2.40	0.69
1:A:202:LYS:HA	1:A:202:LYS:CE	2.25	0.65
1:A:64:HIS:CD2	1:A:261:VAL:H	2.17	0.60
1:A:277:LYS:O	1:A:281:GLU:HG3	2.02	0.60
1:A:48:PRO:HA	1:A:75:LEU:HD13	1.83	0.60
1:A:41:ASP:O	1:A:46:LYS:HD2	2.02	0.59
1:A:64:HIS:HE1	1:A:331:MET:O	1.85	0.59
1:A:68:GLY:HA3	1:A:333:ASN:O	2.02	0.59
1:A:52:ALA:C	1:A:54:GLY:H	2.11	0.59
1:A:23:VAL:HG12	1:A:279:PHE:CE1	2.36	0.58
1:A:82:ASP:O	1:A:84:ALA:N	2.36	0.58
1:A:182:GLY:HA2	3:A:489:HOH:O	2.05	0.57
1:A:6:LYS:HZ3	1:A:6:LYS:HB2	1.71	0.56
1:A:136:ASP:HB3	1:A:203:HIS:HD2	1.71	0.56
1:A:27:PHE:HD1	1:A:283:TYR:CD2	2.20	0.56
1:A:199:ILE:CD1	1:A:204:MET:HB3	2.34	0.55
1:A:27:PHE:CD1	1:A:283:TYR:HD2	2.23	0.54
1:A:67:PHE:CE2	1:A:263:SER:HB2	2.42	0.54
1:A:79:ILE:HD12	1:A:81:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:O	1:A:83:LYS:HG3	2.08	0.54
1:A:278:GLU:O	1:A:282:ASN:HB2	2.08	0.54
1:A:246:VAL:HG12	1:A:247:LEU:O	2.08	0.53
1:A:128:THR:OG1	1:A:131:GLU:HG2	2.08	0.52
1:A:178:ILE:HG13	1:A:179:LYS:HD2	1.91	0.52
1:A:141:ALA:O	1:A:142:LYS:HG2	2.09	0.52
1:A:59:ILE:HD13	1:A:280:LEU:HD13	1.92	0.52
1:A:67:PHE:HB3	1:A:104:ILE:HD12	1.92	0.51
1:A:209:ASP:OD1	1:A:212:ILE:HG13	2.10	0.51
1:A:136:ASP:O	1:A:140:LYS:HB2	2.11	0.50
1:A:162:ALA:O	1:A:256:LYS:HD2	2.12	0.50
1:A:360:GLU:HA	1:A:363:LYS:HE3	1.92	0.49
1:A:365:ALA:O	1:A:369:ILE:HG13	2.12	0.49
1:A:147:LEU:HD23	1:A:204:MET:HE1	1.94	0.49
1:A:132:ILE:N	1:A:133:PRO:CD	2.75	0.49
1:A:360:GLU:HA	1:A:363:LYS:CE	2.43	0.48
1:A:1:LYS:HA	1:A:55:ASP:HB3	1.96	0.48
1:A:334:ILE:HD12	1:A:336:GLN:HG2	1.94	0.48
1:A:60:ILE:HD12	1:A:61:PHE:N	2.29	0.48
1:A:122:LEU:HD12	1:A:223:ALA:CB	2.41	0.48
1:A:117:TYR:HB3	1:A:224:MET:HG2	1.96	0.48
1:A:11:ILE:HG21	1:A:20:LEU:HD12	1.96	0.47
1:A:172:GLU:O	1:A:173:ASN:HB2	2.13	0.47
1:A:136:ASP:HB3	1:A:203:HIS:CD2	2.49	0.47
1:A:88:LYS:O	1:A:306:LYS:HG3	2.15	0.47
1:A:48:PRO:HA	1:A:75:LEU:CD1	2.44	0.47
1:A:256:LYS:HE2	3:A:393:HOH:O	2.14	0.47
1:A:272:ASN:HB2	1:A:275:LEU:HD13	1.97	0.47
1:A:34:LYS:HE2	1:A:36:THR:OG1	2.15	0.46
1:A:82:ASP:C	1:A:84:ALA:N	2.72	0.46
1:A:300:GLY:O	1:A:318:ILE:HD12	2.15	0.46
1:A:89:LEU:HD22	1:A:94:TRP:CZ2	2.51	0.46
1:A:297:LYS:HE2	3:A:457:HOH:O	2.14	0.46
1:A:6:LYS:NZ	1:A:34:LYS:HG3	2.31	0.46
1:A:18:ASN:HD22	1:A:18:ASN:HA	1.62	0.46
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.15	0.46
1:A:168:ALA:O	1:A:181:VAL:HA	2.15	0.45
1:A:239:LYS:NZ	1:A:239:LYS:HB3	2.30	0.45
1:A:51:ALA:HA	1:A:55:ASP:O	2.17	0.45
1:A:215:ALA:O	1:A:219:LYS:HB2	2.16	0.45
1:A:11:ILE:O	1:A:39:HIS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:OD2	1:A:203:HIS:HD2	2.00	0.44
1:A:371:LYS:HA	1:A:371:LYS:HD2	1.59	0.44
1:A:82:ASP:OD2	1:A:84:ALA:HB3	2.17	0.44
1:A:31:THR:HG22	1:A:33:ILE:H	1.83	0.43
1:A:289:GLY:O	1:A:293:VAL:HG23	2.18	0.43
1:A:315:ASP:OD1	1:A:316:PRO:HD2	2.18	0.43
1:A:132:ILE:HD12	1:A:224:MET:HE1	1.99	0.43
1:A:323:GLU:O	1:A:327:LYS:HD3	2.19	0.43
1:A:342:TYR:CE2	1:A:368:ARG:NH2	2.86	0.43
1:A:62:TRP:CD1	1:A:66:ARG:HG3	2.54	0.43
1:A:227:ASN:HD22	1:A:228:GLY:H	1.66	0.42
1:A:336:GLN:HB3	3:A:441:HOH:O	2.19	0.42
1:A:39:HIS:N	1:A:40:PRO:HD3	2.35	0.42
1:A:98:ARG:HA	1:A:102:LYS:O	2.20	0.42
1:A:202:LYS:HE3	1:A:202:LYS:CA	2.32	0.42
1:A:147:LEU:O	1:A:204:MET:HE2	2.20	0.41
1:A:193:THR:HG23	1:A:358:VAL:HG11	2.02	0.41
1:A:357:THR:OG1	1:A:360:GLU:HG3	2.20	0.41
1:A:6:LYS:HZ3	1:A:34:LYS:HG3	1.86	0.41
1:A:342:TYR:HE2	1:A:368:ARG:NH2	2.18	0.41
1:A:59:ILE:HD13	1:A:280:LEU:CD1	2.51	0.41
1:A:60:ILE:HD12	1:A:61:PHE:H	1.85	0.41
1:A:334:ILE:HA	1:A:335:PRO:HD3	1.91	0.41
1:A:232:TRP:HB2	1:A:298:PRO:HG2	2.02	0.41
1:A:79:ILE:O	1:A:79:ILE:HG13	2.21	0.40
1:A:323:GLU:HG3	1:A:327:LYS:HE2	2.04	0.40

All (11) 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)
1:A:140:LYS:NZ	3:A:488:HOH:O[4_556]	1.36	0.84
1:A:239:LYS:CA	1:A:355:ARG:NH2[4_546]	1.38	0.82
1:A:239:LYS:CD	1:A:350:ASN:ND2[4_546]	1.44	0.76
1:A:239:LYS:CE	1:A:350:ASN:ND2[4_546]	1.63	0.57
1:A:100:ASN:ND2	1:A:310:GLU:OE1[4_557]	1.67	0.53
1:A:235:ILE:O	1:A:355:ARG:NH1[4_546]	1.72	0.48
1:A:99:TYR:OH	1:A:310:GLU:OE2[4_557]	1.91	0.29
1:A:239:LYS:NZ	1:A:350:ASN:ND2[4_546]	2.04	0.16
1:A:239:LYS:C	1:A:355:ARG:NH2[4_546]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:NZ	3:A:433:HOH:O[4_547]	2.17	0.03
1:A:207:ASP:CG	1:A:316:PRO:CG[4_556]	2.18	0.02

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	369/371 (100%)	349 (95%)	17 (5%)	3 (1%)	16 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	83	LYS
1	A	53	THR

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	293/298 (98%)	258 (88%)	35 (12%)	5 2

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU

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Mol	Chain	Res	Type
1	A	41	ASP
1	A	43	LEU
1	A	49	GLN
1	A	60	ILE
1	A	75	LEU
1	A	83	LYS
1	A	104	ILE
1	A	113	LEU
1	A	115	LEU
1	A	131	GLU
1	A	139	LEU
1	A	142	LYS
1	A	160	LEU
1	A	175	LYS
1	A	179	LYS
1	A	183	VAL
1	A	192	LEU
1	A	202	LYS
1	A	227	ASN
1	A	233	SER
1	A	239	LYS
1	A	247	LEU
1	A	258	PHE
1	A	278	GLU
1	A	280	LEU
1	A	305	LEU
1	A	311	GLU
1	A	312	LEU
1	A	317	ARG
1	A	327	LYS
1	A	336	GLN
1	A	363	LYS
1	A	366	GLN
1	A	371	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	18	ASN
1	A	64	HIS
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	203	HIS
1	A	205	ASN
1	A	218	ASN
1	A	227	ASN
1	A	356	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 ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	B	1	2	12,12,12	3.68	2 (16%)	17,17,17	4.64	7 (41%)
2	GLC	B	2	2	11,11,12	0.81	0	15,15,17	1.16	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	1	2	1/1/5/5	2/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	O5-C1	12.08	1.72	1.42
2	B	1	GLC	O1-C1	-3.14	1.29	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O1-C1-O5	-13.58	70.07	110.41
2	B	1	GLC	O5-C1-C2	-8.88	94.68	110.30
2	B	1	GLC	C1-O5-C5	-7.91	98.34	113.65
2	B	1	GLC	C1-C2-C3	-3.93	102.35	110.36
2	B	2	GLC	C1-O5-C5	3.42	116.77	112.19
2	B	1	GLC	O1-C1-C2	-3.16	99.80	108.98
2	B	1	GLC	O2-C2-C3	2.32	115.85	110.38
2	B	1	GLC	O4-C4-C3	-2.16	105.29	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	GLC	C1

All (2) torsion outliers are listed below:

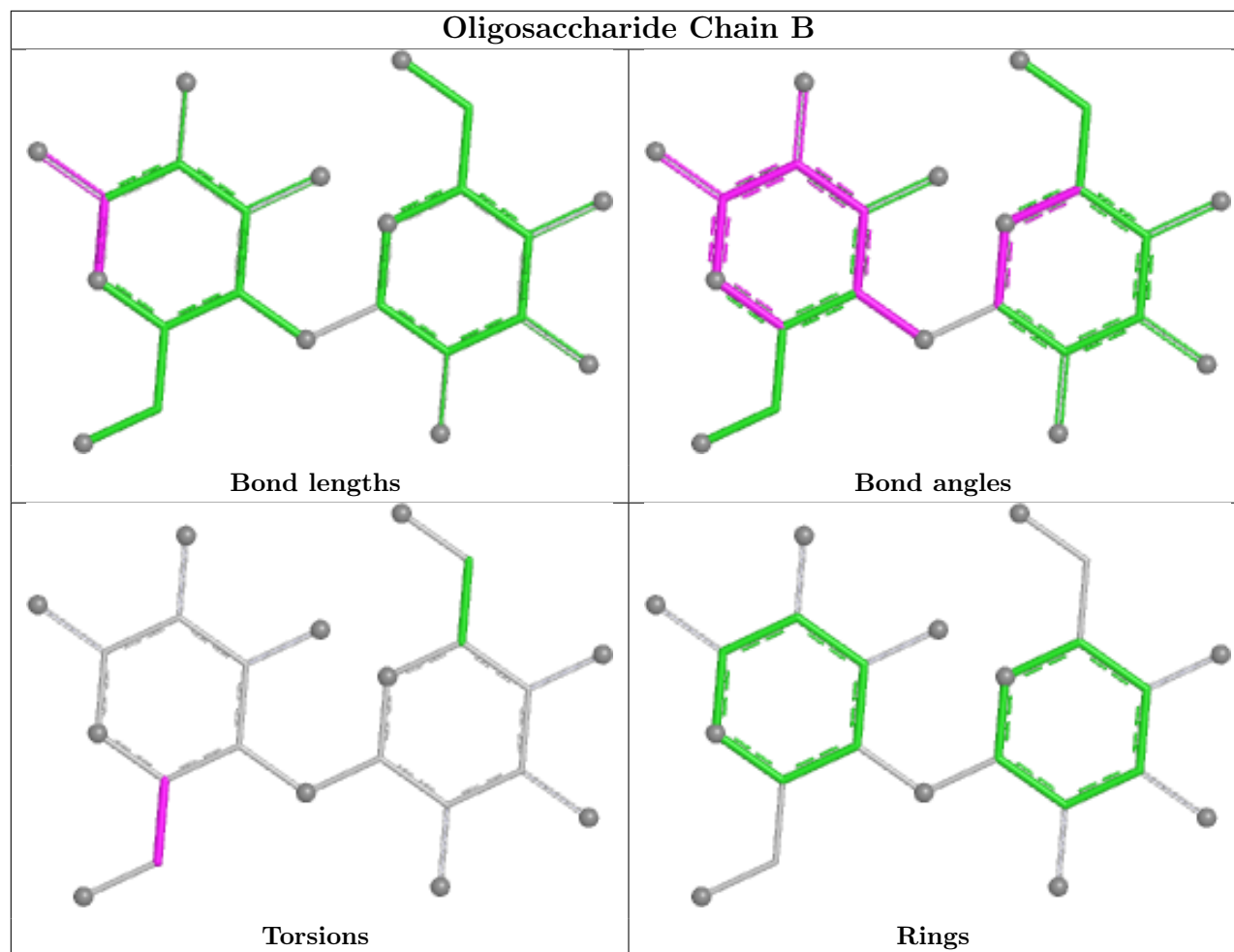
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GLC	4	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](#)

There are no ligands in this entry.

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	371/371 (100%)	1.46	115 (30%) 1 1	14, 32, 60, 92	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ALA	7.5
1	A	316	PRO	6.4
1	A	365	ALA	6.0
1	A	313	ALA	5.8
1	A	319	ALA	5.2
1	A	50	VAL	5.2
1	A	1	LYS	5.0
1	A	367	THR	4.8
1	A	244	VAL	4.5
1	A	355	ARG	4.2
1	A	361	ALA	4.2
1	A	73	SER	4.1
1	A	307	SER	3.8
1	A	308	TYR	3.7
1	A	54	GLY	3.7
1	A	123	PRO	3.7
1	A	286	THR	3.6
1	A	52	ALA	3.3
1	A	77	ALA	3.3
1	A	283	TYR	3.2
1	A	31	THR	3.2
1	A	312	LEU	3.2
1	A	90	TYR	3.2
1	A	302	SER	3.2
1	A	41	ASP	3.1
1	A	357	THR	3.1
1	A	40	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	3.0
1	A	23	VAL	3.0
1	A	354	GLY	3.0
1	A	363	LYS	3.0
1	A	236	ASP	3.0
1	A	342	TYR	3.0
1	A	55	ASP	3.0
1	A	85	PHE	3.0
1	A	370	THR	2.9
1	A	51	ALA	2.9
1	A	364	ASP	2.9
1	A	35	VAL	2.9
1	A	82	ASP	2.9
1	A	292	ALA	2.9
1	A	274	GLU	2.9
1	A	239	LYS	2.8
1	A	87	ASP	2.8
1	A	303	VAL	2.8
1	A	240	VAL	2.8
1	A	245	THR	2.7
1	A	350	ASN	2.7
1	A	49	GLN	2.7
1	A	310	GLU	2.7
1	A	32	GLY	2.7
1	A	222	THR	2.7
1	A	122	LEU	2.7
1	A	83	LYS	2.7
1	A	24	GLY	2.6
1	A	34	LYS	2.6
1	A	270	SER	2.6
1	A	47	PHE	2.6
1	A	318	ILE	2.6
1	A	243	GLY	2.6
1	A	246	VAL	2.6
1	A	135	LEU	2.6
1	A	235	ILE	2.6
1	A	311	GLU	2.6
1	A	306	LYS	2.6
1	A	53	THR	2.6
1	A	346	THR	2.5
1	A	81	PRO	2.5
1	A	232	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	349	ILE	2.5
1	A	301	GLY	2.5
1	A	322	MET	2.5
1	A	174	GLY	2.4
1	A	279	PHE	2.4
1	A	315	ASP	2.4
1	A	290	LEU	2.4
1	A	36	THR	2.4
1	A	352	ALA	2.4
1	A	309	GLU	2.4
1	A	56	GLY	2.4
1	A	199	ILE	2.4
1	A	368	ARG	2.4
1	A	42	LYS	2.3
1	A	233	SER	2.3
1	A	75	LEU	2.3
1	A	305	LEU	2.3
1	A	10	TRP	2.2
1	A	91	PRO	2.2
1	A	206	ALA	2.2
1	A	48	PRO	2.2
1	A	347	ALA	2.2
1	A	314	LYS	2.2
1	A	300	GLY	2.2
1	A	320	ALA	2.2
1	A	359	ASP	2.2
1	A	57	PRO	2.2
1	A	46	LYS	2.2
1	A	369	ILE	2.1
1	A	74	GLY	2.1
1	A	86	GLN	2.1
1	A	79	ILE	2.1
1	A	58	ASP	2.1
1	A	119	LYS	2.1
1	A	118	ASN	2.1
1	A	121	LEU	2.1
1	A	69	GLY	2.1
1	A	328	GLY	2.1
1	A	134	ALA	2.1
1	A	276	ALA	2.1
1	A	175	LYS	2.0
1	A	273	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	360	GLU	2.0
1	A	285	LEU	2.0
1	A	287	ASP	2.0
1	A	8	VAL	2.0

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

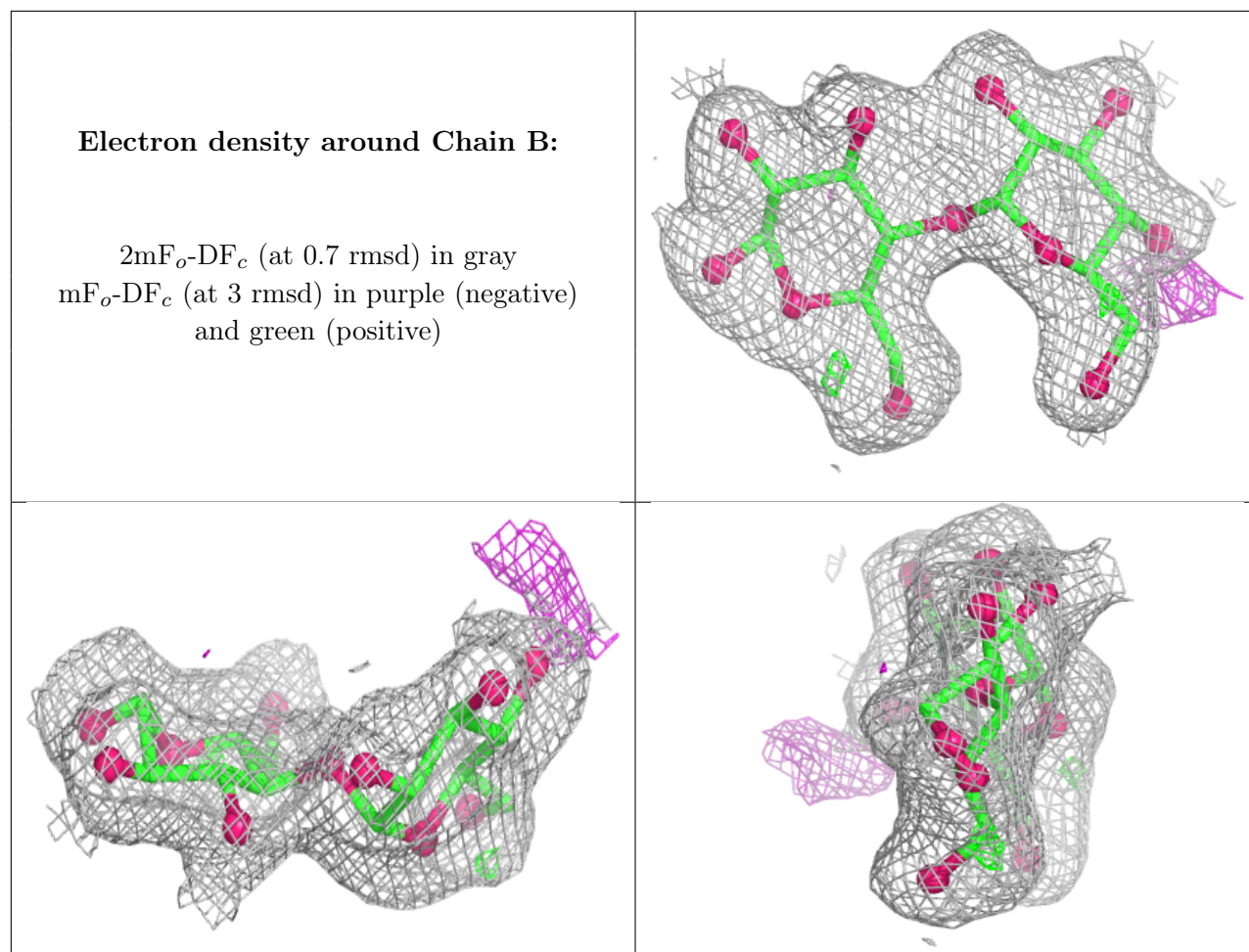
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	GLC	B	1	12/12	0.83	0.09	18,19,22,24	0
2	GLC	B	2	11/12	0.89	0.08	16,16,18,18	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.