



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:52 PM UTC

PDB ID : 2PN5 / pdb_00002pn5
Title : Crystal Structure of TEP1r
Authors : Baxter, R.H.G.
Deposited on : 2007-04-23
Resolution : 2.70 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

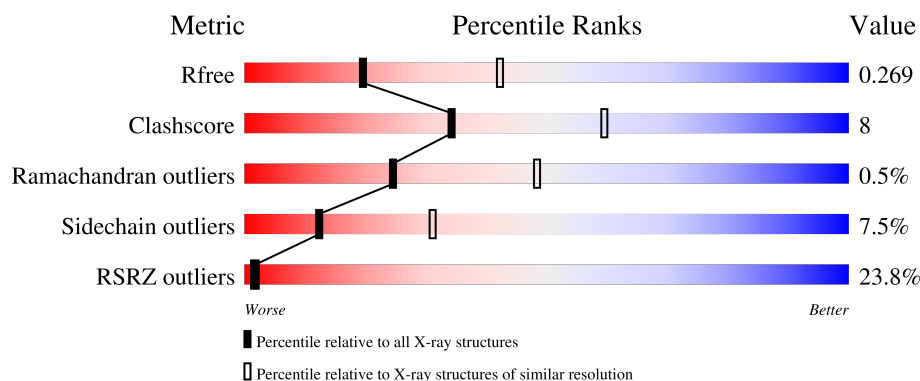
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1325	23% 77% 16% • •
2	B	2	100%

2 Entry composition [i](#)

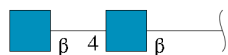
There are 5 unique types of molecules in this entry. The entry contains 10546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thioester-containing protein I.

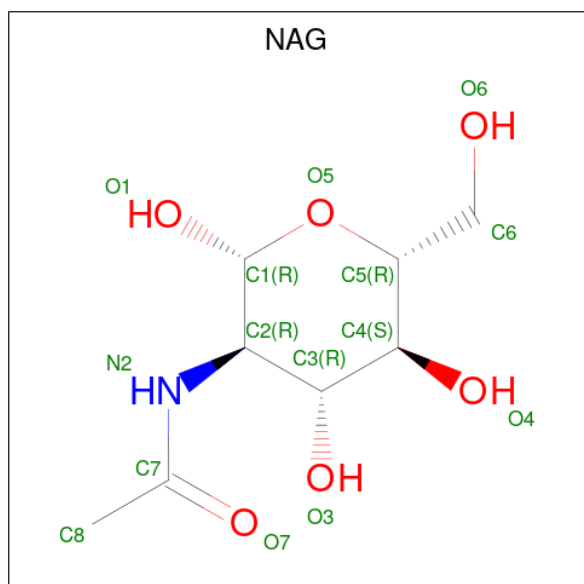
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1283	Total	C	N	O	S	0	7	0
			10333	6618	1724	1945	46			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Na	0	0
			3	3		

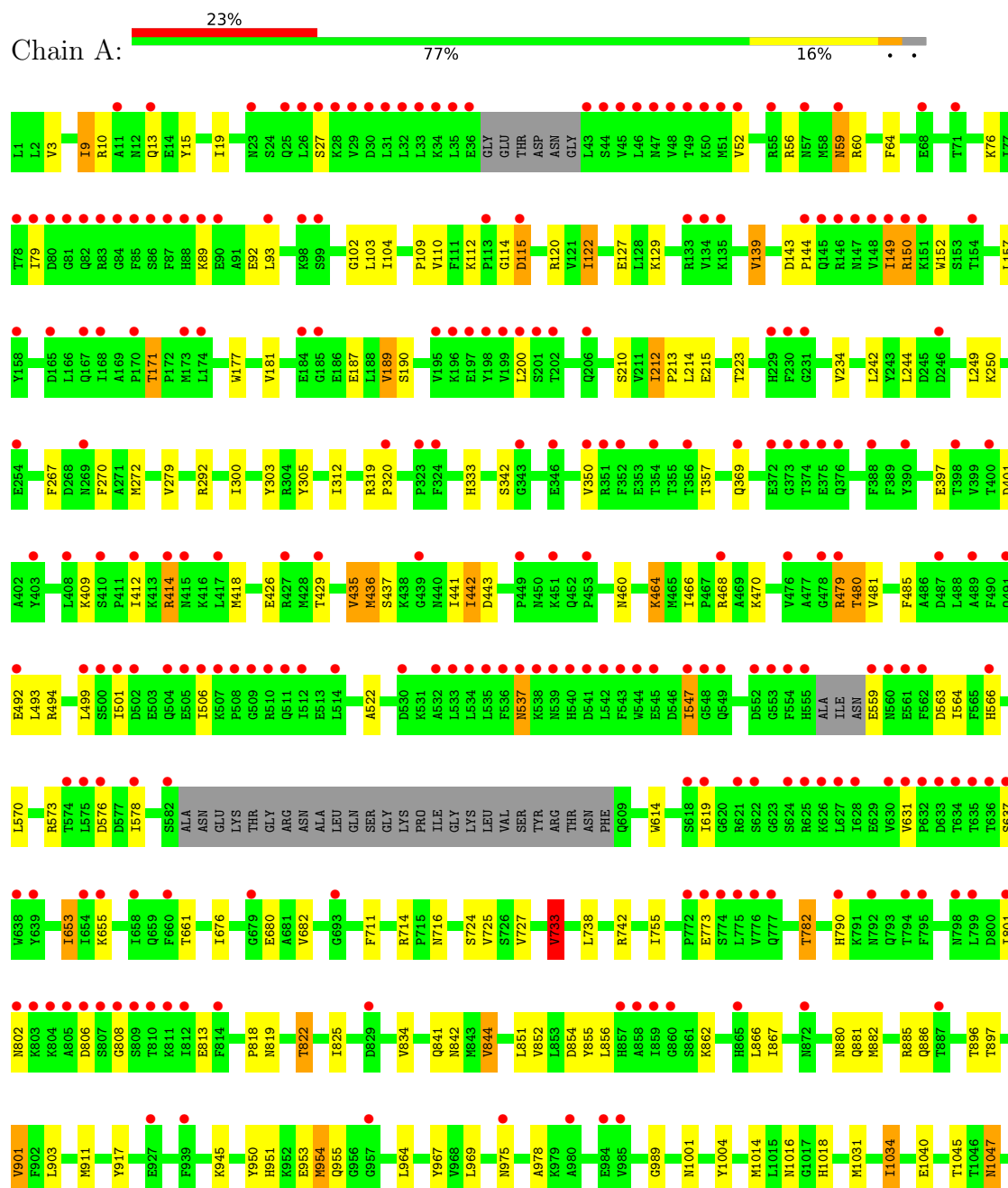
- Molecule 5 is water.

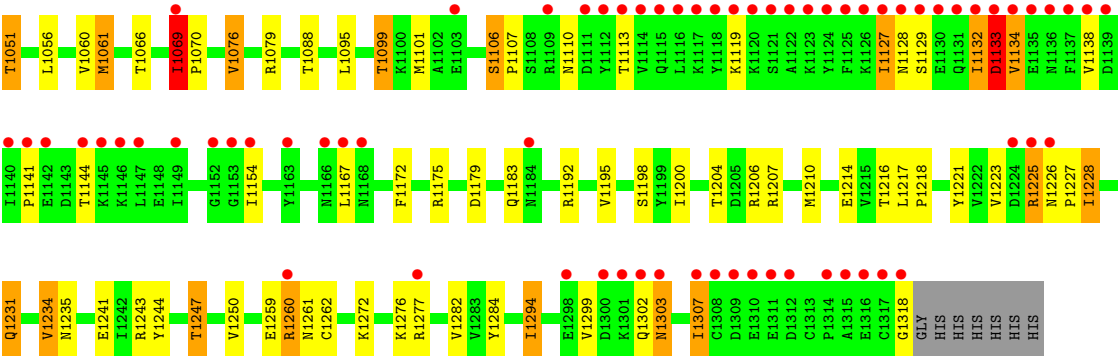
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total	O	0	0
			140	140		

3 Residue-property plots [i](#)

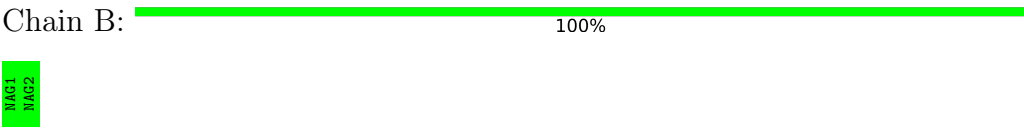
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Thioester-containing protein I





● Molecule 2: 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	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.51Å 150.51Å 226.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.70 45.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.88-2.70) 99.7 (45.88-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.275 0.240 , 0.269	Depositor DCC
R_{free} test set	3631 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10546	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: NA, 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	0.54	3/10543 (0.0%)	0.81	8/14272 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1318	GLY	C-O	10.40	1.44	1.23
1	A	1069	ILE	CA-CB	6.89	1.58	1.53
1	A	733	VAL	CA-CB	5.16	1.58	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	ILE	N-CA-C	9.95	119.48	111.62
1	A	1069	ILE	N-CA-CB	9.47	116.46	110.50
1	A	1234	VAL	CB-CA-C	-6.88	103.07	111.88
1	A	1318	GLY	CA-C-O	-6.11	107.97	120.80
1	A	115	ASP	N-CA-C	6.05	119.74	110.36
1	A	319	ARG	CA-C-N	5.89	127.21	119.84
1	A	319	ARG	C-N-CA	5.89	127.21	119.84
1	A	114	GLY	N-CA-C	5.13	118.88	112.73

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	10333	0	10327	159	0
2	B	28	0	25	0	0
3	A	42	0	39	1	0
4	A	3	0	0	0	0
5	A	140	0	0	5	0
All	All	10546	0	10391	159	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 (159) 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:1303:ASN:H	1:A:1303:ASN:ND2	1.56	1.00
1:A:1056:LEU:HD11	1:A:1101:MET:HE3	1.44	0.99
1:A:1303:ASN:HD22	1:A:1303:ASN:N	1.60	0.99
1:A:1231:GLN:HE21	1:A:1231:GLN:H	1.13	0.94
1:A:1244:TYR:O	1:A:1247:THR:HB	1.70	0.91
1:A:27:SER:HA	1:A:56:ARG:HD2	1.58	0.86
1:A:1066:THR:HG22	5:A:1440:HOH:O	1.77	0.82
1:A:637:SER:HB3	1:A:661:THR:HG22	1.62	0.81
1:A:89:LYS:HG2	1:A:573:ARG:HB3	1.65	0.78
1:A:1175:ARG:NH1	1:A:1200:ILE:O	2.17	0.78
1:A:950:TYR:H	1:A:955:GLN:HE22	1.28	0.78
1:A:1129:SER:OG	1:A:1132:ILE:HG23	1.86	0.76
1:A:1303:ASN:H	1:A:1303:ASN:HD22	0.78	0.75
1:A:1127:ILE:HG23	1:A:1132:ILE:HD13	1.68	0.74
1:A:187:GLU:OE2	3:A:1326:NAG:H62	1.89	0.73
1:A:1272:LYS:HB3	1:A:1307:ILE:HD12	1.71	0.73
1:A:9:ILE:HD13	1:A:93:LEU:HB3	1.71	0.71
1:A:1183:GLN:OE1	1:A:1192:ARG:NH1	2.24	0.70
1:A:187:GLU:OE1	1:A:190:SER:HB2	1.90	0.70
1:A:1221:TYR:OH	1:A:1299:VAL:HG11	1.91	0.69
1:A:1225:ARG:HG2	1:A:1226:ASN:HD22	1.57	0.69
1:A:1227:PRO:HG2	1:A:1228:ILE:HD12	1.75	0.68
1:A:414:ARG:HD3	1:A:493:LEU:HD11	1.75	0.68
1:A:143:ASP:HB2	1:A:144:PRO:HD2	1.76	0.66
1:A:866:LEU:HD21	1:A:1134:VAL:HG22	1.78	0.66
1:A:412:ILE:HG12	1:A:418:MET:HG2	1.78	0.66
1:A:951:HIS:H	1:A:955:GLN:HE21	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:SER:HB3	1:A:357:THR:HG22	1.81	0.63
1:A:1235:ASN:HB3	1:A:1261:ASN:HD21	1.64	0.62
1:A:1095:LEU:O	1:A:1099:THR:HB	1.99	0.62
1:A:1056:LEU:CD1	1:A:1101:MET:HE3	2.26	0.62
1:A:215:GLU:HB2	1:A:272:MET:HE2	1.81	0.61
1:A:818:PRO:HB3	1:A:1132:ILE:HD12	1.81	0.61
1:A:342:SER:CB	1:A:357:THR:HG22	2.31	0.60
1:A:1235:ASN:HB3	1:A:1261:ASN:ND2	2.17	0.60
1:A:436:MET:HE2	1:A:441:ILE:HG12	1.82	0.60
1:A:1056:LEU:HD11	1:A:1101:MET:CE	2.23	0.60
1:A:350:VAL:HG12	1:A:350:VAL:O	2.02	0.60
1:A:813:GLU:HA	1:A:1141:PRO:HD2	1.84	0.60
1:A:109:PRO:HB2	1:A:537:ASN:ND2	2.16	0.59
1:A:818:PRO:CB	1:A:1132:ILE:HD12	2.32	0.59
1:A:819:ASN:HB3	1:A:822:THR:HG22	1.85	0.59
1:A:1045:THR:OG1	1:A:1051:THR:HG21	2.03	0.58
1:A:171:THR:HB	1:A:880:ASN:HD21	1.68	0.58
1:A:292:ARG:NH2	1:A:1225:ARG:HD2	2.18	0.58
1:A:436:MET:CE	1:A:441:ILE:HG12	2.33	0.58
1:A:856:LEU:HD13	1:A:867:ILE:HG12	1.85	0.58
1:A:547:ILE:HD12	1:A:653:ILE:HD11	1.86	0.58
1:A:822:THR:HB	1:A:1133:ASP:O	2.04	0.57
1:A:1231:GLN:H	1:A:1231:GLN:NE2	1.94	0.57
1:A:1217:LEU:HD11	1:A:1223:VAL:HG13	1.87	0.57
1:A:143:ASP:HB2	1:A:144:PRO:CD	2.34	0.57
1:A:563:ASP:HB3	1:A:566:HIS:HB2	1.87	0.57
1:A:841:GLN:HA	1:A:1088:THR:HG21	1.86	0.57
1:A:244:LEU:HB2	1:A:249:LEU:HB2	1.87	0.56
1:A:480:THR:HG22	5:A:1366:HOH:O	2.04	0.56
1:A:782:THR:HG21	1:A:1079:ARG:NH1	2.20	0.56
1:A:818:PRO:HD2	1:A:822:THR:HG21	1.88	0.56
1:A:841:GLN:O	1:A:844:VAL:HG22	2.05	0.56
1:A:825:ILE:HG21	1:A:866:LEU:HD22	1.87	0.56
1:A:676:ILE:HG21	1:A:682:VAL:HG21	1.88	0.56
1:A:1195:VAL:O	1:A:1262:CYS:HA	2.06	0.55
1:A:59:ASN:C	1:A:59:ASN:HD22	2.15	0.55
1:A:103:LEU:HB2	1:A:122:ILE:HB	1.90	0.54
1:A:856:LEU:CD1	1:A:867:ILE:HG12	2.37	0.54
1:A:120:ARG:HG3	1:A:614:TRP:CZ2	2.43	0.54
1:A:773:GLU:HG2	1:A:1277:ARG:HD3	1.90	0.54
1:A:242:LEU:HD21	1:A:279:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1223:VAL:HB	1:A:1227:PRO:HB3	1.91	0.53
1:A:3:VAL:HG11	1:A:79:ILE:HD13	1.90	0.53
1:A:292:ARG:HH22	1:A:1225:ARG:HD2	1.72	0.53
1:A:950:TYR:N	1:A:955:GLN:HE22	2.03	0.53
1:A:485:PHE:CD1	1:A:564:ILE:HD11	2.44	0.53
1:A:437:SER:HB3	1:A:442:ILE:HD13	1.90	0.53
1:A:969:LEU:HD21	1:A:989:GLY:HA3	1.90	0.53
1:A:435:VAL:HG13	1:A:443:ASP:HB3	1.91	0.53
1:A:951:HIS:H	1:A:955:GLN:NE2	2.06	0.52
1:A:150:ARG:HG2	1:A:152:TRP:CH2	2.44	0.52
1:A:10:ARG:HD2	1:A:13:GLN:HE21	1.74	0.52
1:A:109:PRO:HB2	1:A:537:ASN:HD21	1.74	0.51
1:A:139:VAL:HG13	1:A:152:TRP:HB2	1.91	0.51
1:A:954:MET:HE1	1:A:967:TYR:HB2	1.91	0.51
1:A:711:PHE:HB2	1:A:714:ARG:HG3	1.93	0.51
1:A:522:ALA:HB3	1:A:619:ILE:HD12	1.92	0.51
1:A:854:ASP:HB3	1:A:917:TYR:OH	2.10	0.51
1:A:1069:ILE:HG12	1:A:1070:PRO:HD3	1.92	0.51
1:A:305:TYR:O	1:A:333:HIS:HE1	1.95	0.50
1:A:112:LYS:HG2	1:A:115:ASP:OD2	2.11	0.50
1:A:212:ILE:HD13	1:A:333:HIS:HB2	1.94	0.50
1:A:1302:GLN:OE1	1:A:1307:ILE:HD11	2.11	0.50
1:A:468:ARG:HD2	1:A:494:ARG:NH2	2.26	0.49
1:A:1179:ASP:OD2	1:A:1260[B]:ARG:NH2	2.45	0.49
1:A:950:TYR:H	1:A:955:GLN:NE2	2.04	0.49
1:A:1016:ASN:HD22	1:A:1018:HIS:HB2	1.78	0.49
1:A:143:ASP:HB3	1:A:149:ILE:CD1	2.44	0.48
1:A:102:GLY:HA3	1:A:189:VAL:HG22	1.94	0.48
1:A:110:VAL:HG23	1:A:537:ASN:HD21	1.78	0.48
1:A:127:GLU:HB3	1:A:129:LYS:HG2	1.96	0.47
1:A:842:ASN:HB3	1:A:881:GLN:HE22	1.80	0.47
1:A:951:HIS:CD2	1:A:954:MET:HB2	2.49	0.47
1:A:886:GLN:HE22	1:A:896:THR:HA	1.80	0.46
1:A:1172:PHE:HB3	1:A:1294:ILE:HG22	1.97	0.46
1:A:1198:SER:HB3	1:A:1259:GLU:O	2.16	0.46
1:A:1001:ASN:O	1:A:1031:MET:HE1	2.15	0.46
1:A:102:GLY:HA3	1:A:189:VAL:CG2	2.45	0.46
1:A:1241:GLU:HG2	1:A:1250:VAL:HB	1.97	0.46
1:A:144:PRO:HD3	1:A:177:TRP:CD1	2.50	0.46
1:A:19:ILE:O	1:A:59:ASN:HB2	2.16	0.45
1:A:1034:ILE:HD13	1:A:1040:GLU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:TYR:HB2	1:A:1210:MET:HB2	1.97	0.45
1:A:953:GLU:HG3	1:A:1047:ASN:HD21	1.81	0.45
1:A:492:GLU:HG2	1:A:493:LEU:HG	1.99	0.45
1:A:547:ILE:HD12	1:A:653:ILE:CD1	2.47	0.44
1:A:1218:PRO:HG2	1:A:1299:VAL:HG21	1.98	0.44
1:A:819:ASN:O	1:A:822:THR:HG23	2.17	0.44
1:A:716:ASN:HD22	1:A:742:ARG:CZ	2.30	0.44
1:A:350:VAL:O	1:A:350:VAL:CG1	2.65	0.44
1:A:680:GLU:HG2	1:A:1276:LYS:HA	1.98	0.44
1:A:1045:THR:OG1	1:A:1051:THR:CG2	2.65	0.44
1:A:1214[A]:GLU:HG3	1:A:1250:VAL:HG22	1.99	0.44
1:A:481:VAL:HG23	1:A:578:ILE:CG2	2.47	0.44
1:A:724:SER:O	1:A:725:VAL:HG23	2.18	0.44
1:A:727:VAL:HG13	1:A:733:VAL:HG13	1.99	0.44
1:A:464:LYS:H	1:A:464:LYS:HG3	1.66	0.44
1:A:397:GLU:H	1:A:401:ASP:HB2	1.83	0.43
1:A:854:ASP:CB	1:A:917:TYR:OH	2.66	0.43
1:A:1127:ILE:HG23	1:A:1132:ILE:CD1	2.43	0.43
1:A:1014:MET:HB3	1:A:1061:MET:HG2	2.01	0.43
1:A:855:TYR:CD2	1:A:855:TYR:C	2.97	0.43
1:A:882:MET:HE1	1:A:885:ARG:HD2	2.01	0.42
1:A:1076:VAL:O	1:A:1079:ARG:HD3	2.19	0.42
1:A:15:TYR:HB3	1:A:64:PHE:HB2	2.02	0.42
1:A:886:GLN:NE2	1:A:897:THR:H	2.17	0.42
1:A:171:THR:O	1:A:880:ASN:ND2	2.52	0.42
1:A:506:ILE:HG23	1:A:631:VAL:HG21	2.01	0.42
1:A:210:SER:HB3	1:A:223:THR:OG1	2.20	0.42
1:A:1303:ASN:ND2	1:A:1303:ASN:N	2.32	0.42
1:A:212:ILE:HA	1:A:213:PRO:HD3	1.89	0.42
1:A:479:ARG:HG3	5:A:1366:HOH:O	2.19	0.42
1:A:1056:LEU:O	1:A:1060:VAL:HG23	2.20	0.42
1:A:1282:VAL:HG12	1:A:1284:TYR:HD1	1.84	0.42
1:A:854:ASP:OD1	1:A:854:ASP:C	2.63	0.42
1:A:485:PHE:HB3	1:A:564:ILE:HD11	2.02	0.41
1:A:1060:VAL:HG22	1:A:1101:MET:HE2	2.01	0.41
1:A:409:LYS:HD3	1:A:409:LYS:HA	1.91	0.41
1:A:852:VAL:O	1:A:856:LEU:HG	2.20	0.41
1:A:1106:SER:HA	1:A:1107:PRO:HD3	1.94	0.41
1:A:267:PHE:HB3	1:A:270:PHE:HB2	2.02	0.41
1:A:460:ASN:ND2	5:A:1364:HOH:O	2.46	0.41
1:A:214:LEU:HA	1:A:303:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:TYR:HA	1:A:1051:THR:HB	2.03	0.41
1:A:975:ASN:HD22	1:A:978:ALA:H	1.68	0.40
1:A:479:ARG:O	1:A:578:ILE:HA	2.22	0.40
1:A:901:VAL:HG22	1:A:964:LEU:HD21	2.04	0.40
1:A:782:THR:OG1	1:A:1076:VAL:HG13	2.21	0.40
1:A:1079:ARG:NH2	5:A:1399:HOH:O	2.54	0.40
1:A:104:ILE:HD11	1:A:181:VAL:HG23	2.03	0.40
1:A:903:LEU:HD12	1:A:903:LEU:HA	1.89	0.40
1:A:1110:ASN:HD22	1:A:1132:ILE:HD11	1.87	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	A	1282/1325 (97%)	1214 (95%)	61 (5%)	7 (0%)	24 48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	808	GLY
1	A	1119	LYS
1	A	200	LEU
1	A	414	ARG
1	A	1133	ASP
1	A	320	PRO
1	A	655	LYS

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	1147/1173 (98%)	1061 (92%)	86 (8%)	12	31

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	52	VAL
1	A	59	ASN
1	A	60	ARG
1	A	76	LYS
1	A	92	GLU
1	A	122	ILE
1	A	139	VAL
1	A	149	ILE
1	A	150	ARG
1	A	157	LEU
1	A	171	THR
1	A	189	VAL
1	A	212	ILE
1	A	234	VAL
1	A	250	LYS
1	A	300	ILE
1	A	312	ILE
1	A	369	GLN
1	A	426	GLU
1	A	429	THR
1	A	435	VAL
1	A	436	MET
1	A	442	ILE
1	A	464	LYS
1	A	466	ILE
1	A	470	LYS
1	A	479	ARG
1	A	480	THR
1	A	499	LEU

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Mol	Chain	Res	Type
1	A	501	ILE
1	A	537	ASN
1	A	547	ILE
1	A	559	GLU
1	A	570	LEU
1	A	576	ASP
1	A	653	ILE
1	A	733	VAL
1	A	738	LEU
1	A	782	THR
1	A	790	HIS
1	A	801	ILE
1	A	802	ASN
1	A	806	ASP
1	A	822	THR
1	A	834	VAL
1	A	844	VAL
1	A	851	LEU
1	A	862	LYS
1	A	901	VAL
1	A	911	MET
1	A	945	LYS
1	A	954	MET
1	A	1034	ILE
1	A	1047	ASN
1	A	1051	THR
1	A	1061	MET
1	A	1069	ILE
1	A	1076	VAL
1	A	1099	THR
1	A	1106	SER
1	A	1113	THR
1	A	1127	ILE
1	A	1128	ASN
1	A	1132	ILE
1	A	1133	ASP
1	A	1134	VAL
1	A	1138	VAL
1	A	1144	THR
1	A	1154	ILE
1	A	1167	LEU
1	A	1204	THR

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Mol	Chain	Res	Type
1	A	1206	ARG
1	A	1207	ARG
1	A	1216	THR
1	A	1225	ARG
1	A	1228	ILE
1	A	1231	GLN
1	A	1234	VAL
1	A	1243	ARG
1	A	1247	THR
1	A	1260[A]	ARG
1	A	1260[B]	ARG
1	A	1294	ILE
1	A	1303	ASN
1	A	1307	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	59	ASN
1	A	147	ASN
1	A	227	ASN
1	A	277	GLN
1	A	288	GLN
1	A	333	HIS
1	A	369	GLN
1	A	382	ASN
1	A	458	GLN
1	A	537	ASN
1	A	540	HIS
1	A	691	ASN
1	A	716	ASN
1	A	793	GLN
1	A	802	ASN
1	A	880	ASN
1	A	881	GLN
1	A	886	GLN
1	A	898	ASN
1	A	951	HIS
1	A	955	GLN
1	A	975	ASN
1	A	1016	ASN

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Mol	Chain	Res	Type
1	A	1047	ASN
1	A	1226	ASN
1	A	1231	GLN
1	A	1238	GLN
1	A	1261	ASN
1	A	1303	ASN

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	NAG	B	1	1,2	14,14,15	0.61	0	17,19,21	0.85	0
2	NAG	B	2	2	14,14,15	0.47	0	17,19,21	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

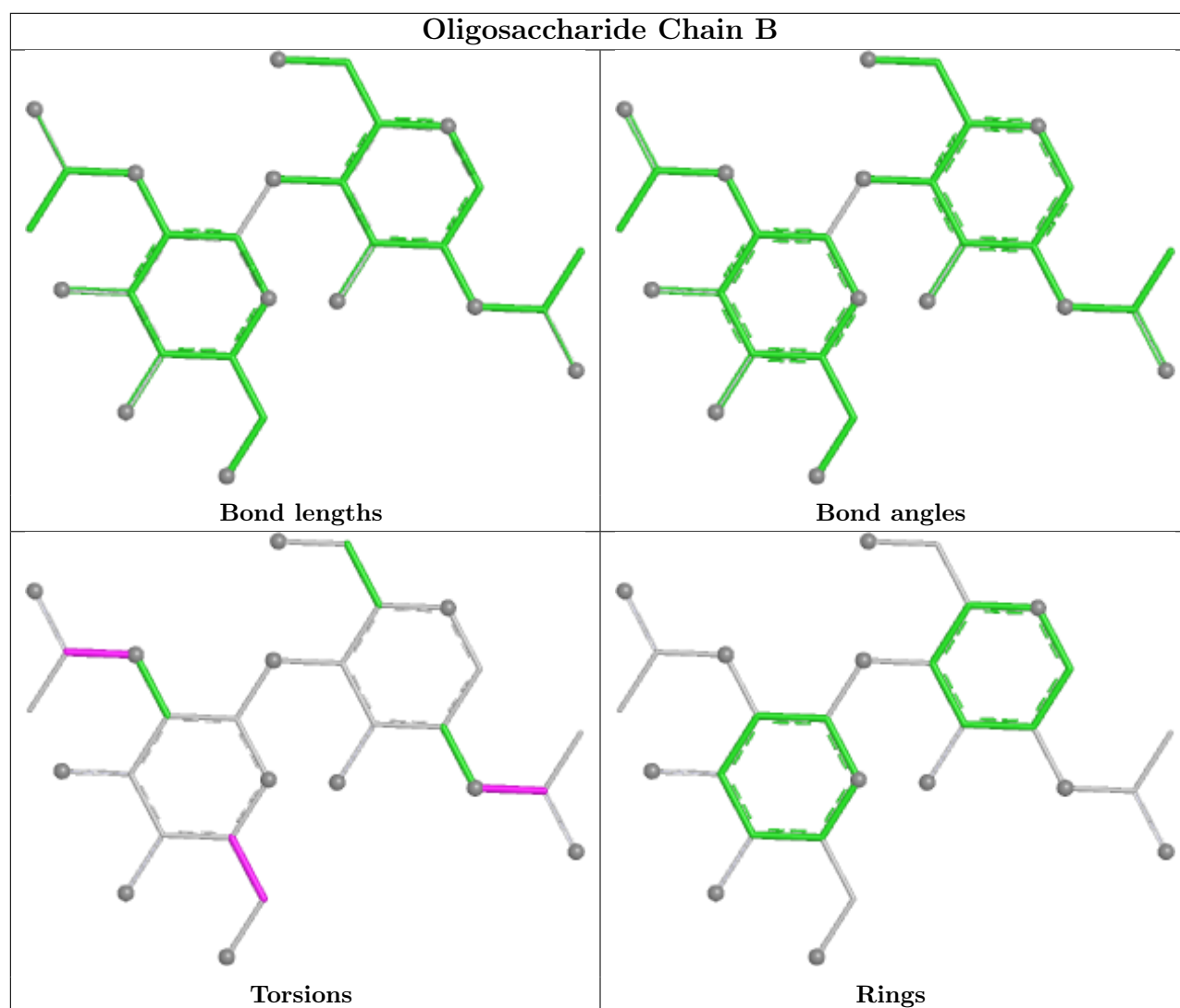
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2

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 [i](#)

Of 6 ligands modelled in this entry, 3 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	$\# Z > 2$
3	NAG	A	1327	1	14,14,15	0.43	0	17,19,21	1.30	4 (23%)
3	NAG	A	1328	1	14,14,15	0.58	0	17,19,21	0.84	0
3	NAG	A	1326	1	14,14,15	0.47	0	17,19,21	1.96	3 (17%)

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	NAG	A	1327	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1328	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1326	1	-	2/6/23/26	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(°)
3	A	1326	NAG	C1-O5-C5	5.92	120.12	112.19
3	A	1326	NAG	C3-C4-C5	3.43	116.46	110.23
3	A	1327	NAG	C1-O5-C5	2.52	115.57	112.19
3	A	1326	NAG	O5-C5-C4	2.49	116.88	110.83
3	A	1327	NAG	O5-C1-C2	-2.20	107.89	111.29
3	A	1327	NAG	O4-C4-C5	2.15	114.61	109.32
3	A	1327	NAG	C2-N2-C7	-2.14	120.03	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1326	NAG	O5-C5-C6-O6
3	A	1326	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1326	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1283/1325 (96%)	1.16	305 (23%) 2 1	15, 58, 109, 147	7 (0%)

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	LEU	9.8
1	A	230	PHE	8.3
1	A	199	VAL	8.3
1	A	198	TYR	7.6
1	A	635	THR	6.7
1	A	200	LEU	6.6
1	A	492	GLU	6.5
1	A	554	PHE	6.3
1	A	506	ILE	6.2
1	A	1122	ALA	6.0
1	A	1140	ILE	5.9
1	A	1139	ASP	5.7
1	A	801	ILE	5.6
1	A	27	SER	5.6
1	A	1135	GLU	5.4
1	A	540	HIS	5.3
1	A	542	LEU	5.3
1	A	45	VAL	5.1
1	A	1314	PRO	5.1
1	A	805	ALA	4.9
1	A	773	GLU	4.9
1	A	535	LEU	4.8
1	A	536	PHE	4.7
1	A	507	LYS	4.7
1	A	1134	VAL	4.7
1	A	491	GLN	4.6
1	A	196	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	808	GLY	4.6
1	A	1318	GLY	4.6
1	A	1144	THR	4.5
1	A	510	ARG	4.4
1	A	1137	PHE	4.3
1	A	1141	PRO	4.3
1	A	533	LEU	4.2
1	A	173[A]	MET	4.2
1	A	1317	CYS	4.1
1	A	1225	ARG	4.1
1	A	32	LEU	4.1
1	A	775	LEU	4.1
1	A	812	ILE	4.1
1	A	1138	VAL	4.1
1	A	51	MET	4.1
1	A	388	PHE	4.1
1	A	201	SER	4.0
1	A	44	SER	3.9
1	A	1166	ASN	3.9
1	A	1316	GLU	3.9
1	A	776	VAL	3.9
1	A	1119	LYS	3.9
1	A	637	SER	3.8
1	A	29	VAL	3.8
1	A	146	ARG	3.8
1	A	792	ASN	3.8
1	A	1124	TYR	3.8
1	A	46	LEU	3.8
1	A	632	PRO	3.8
1	A	1315	ALA	3.7
1	A	57	ASN	3.7
1	A	1126	LYS	3.7
1	A	167	GLN	3.7
1	A	532	ALA	3.7
1	A	562	PHE	3.6
1	A	1120	LYS	3.6
1	A	84	GLY	3.6
1	A	1125	PHE	3.6
1	A	555	HIS	3.6
1	A	501	ILE	3.6
1	A	810	THR	3.6
1	A	530	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1133	ASP	3.6
1	A	231	GLY	3.6
1	A	634	THR	3.5
1	A	772	PRO	3.5
1	A	202	THR	3.5
1	A	1132	ILE	3.5
1	A	86	SER	3.5
1	A	1123	LYS	3.5
1	A	806	ASP	3.5
1	A	1168	ASN	3.5
1	A	534	LEU	3.5
1	A	1117	LYS	3.4
1	A	34	LYS	3.4
1	A	552	ASP	3.4
1	A	1128	ASN	3.4
1	A	660	PHE	3.4
1	A	799	LEU	3.4
1	A	512	ILE	3.4
1	A	1145	LYS	3.4
1	A	197	GLU	3.4
1	A	559	GLU	3.4
1	A	168	ILE	3.3
1	A	98	LYS	3.3
1	A	229	HIS	3.3
1	A	1303	ASN	3.3
1	A	626	LYS	3.3
1	A	638	TRP	3.3
1	A	479	ARG	3.3
1	A	487	ASP	3.3
1	A	1312	ASP	3.3
1	A	1311	GLU	3.2
1	A	807	SER	3.2
1	A	1226	ASN	3.2
1	A	451	LYS	3.2
1	A	1301	LYS	3.2
1	A	158	TYR	3.2
1	A	49	THR	3.2
1	A	809	SER	3.2
1	A	508	PRO	3.2
1	A	1118	TYR	3.2
1	A	539	ASN	3.1
1	A	802	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	576	ASP	3.1
1	A	468	ARG	3.1
1	A	373	GLY	3.1
1	A	538	LYS	3.1
1	A	83	ARG	3.1
1	A	414	ARG	3.1
1	A	30	ASP	3.1
1	A	865	HIS	3.1
1	A	1146	LYS	3.1
1	A	1130	GLU	3.0
1	A	78	THR	3.0
1	A	390	TYR	3.0
1	A	13	GLN	3.0
1	A	548	GLY	3.0
1	A	375	GLU	3.0
1	A	633	ASP	3.0
1	A	939	PHE	3.0
1	A	500	SER	3.0
1	A	28	LYS	3.0
1	A	48	VAL	3.0
1	A	82	GLN	2.9
1	A	1131	GLN	2.9
1	A	415	ASN	2.9
1	A	11	ALA	2.9
1	A	346	GLU	2.9
1	A	1310	GLU	2.9
1	A	195	VAL	2.9
1	A	1103	GLU	2.9
1	A	87	PHE	2.9
1	A	184	GLU	2.9
1	A	376	GLN	2.9
1	A	1115	GLN	2.9
1	A	81	GLY	2.9
1	A	804	LYS	2.9
1	A	150	ARG	2.8
1	A	1127	ILE	2.8
1	A	1184	ASN	2.8
1	A	246	ASP	2.8
1	A	151	LYS	2.8
1	A	803	LYS	2.8
1	A	625	ARG	2.8
1	A	145	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1129	SER	2.8
1	A	509	GLY	2.8
1	A	639	TYR	2.8
1	A	1113	THR	2.8
1	A	85	PHE	2.8
1	A	170	PRO	2.8
1	A	1136	ASN	2.8
1	A	93	LEU	2.8
1	A	630	VAL	2.8
1	A	544	TRP	2.8
1	A	269	ASN	2.8
1	A	323	PRO	2.7
1	A	453	PRO	2.7
1	A	582	SER	2.7
1	A	36	GLU	2.7
1	A	549	GLN	2.7
1	A	627	LEU	2.7
1	A	1147	LEU	2.7
1	A	1121	SER	2.7
1	A	777	GLN	2.7
1	A	1109	ARG	2.7
1	A	71	THR	2.7
1	A	369	GLN	2.7
1	A	658	ILE	2.7
1	A	1142	GLU	2.7
1	A	89	LYS	2.7
1	A	980	ALA	2.7
1	A	541	ASP	2.7
1	A	628	ILE	2.6
1	A	33	LEU	2.6
1	A	545	GLU	2.6
1	A	537	ASN	2.6
1	A	560	ASN	2.6
1	A	774	SER	2.6
1	A	794	THR	2.6
1	A	1300	ASP	2.6
1	A	26	LEU	2.6
1	A	149	ILE	2.6
1	A	514	LEU	2.6
1	A	1116	LEU	2.6
1	A	50	LYS	2.6
1	A	47	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	511	GLN	2.6
1	A	1224	ASP	2.6
1	A	543	PHE	2.6
1	A	1302	GLN	2.6
1	A	79	ILE	2.5
1	A	859	ILE	2.5
1	A	31	LEU	2.5
1	A	811	LYS	2.5
1	A	52	VAL	2.5
1	A	858	ALA	2.5
1	A	147	ASN	2.5
1	A	1154	ILE	2.5
1	A	1307	ILE	2.5
1	A	655	LYS	2.5
1	A	1167	LEU	2.5
1	A	829	ASP	2.5
1	A	790	HIS	2.5
1	A	403	TYR	2.5
1	A	185	GLY	2.5
1	A	1152	GLY	2.5
1	A	134	VAL	2.5
1	A	59	ASN	2.5
1	A	133	ARG	2.4
1	A	374	THR	2.4
1	A	427	ARG	2.4
1	A	439	GLY	2.4
1	A	679	GLY	2.4
1	A	148	VAL	2.4
1	A	860	GLY	2.4
1	A	618	SER	2.4
1	A	1112	TYR	2.3
1	A	68	GLU	2.3
1	A	621	ARG	2.3
1	A	985	VAL	2.3
1	A	795	PHE	2.3
1	A	174	LEU	2.3
1	A	619	ILE	2.3
1	A	400	THR	2.3
1	A	574	THR	2.3
1	A	410	SER	2.3
1	A	113	PRO	2.3
1	A	320	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1153	GLY	2.3
1	A	1277	ARG	2.3
1	A	1308	CYS	2.3
1	A	354	THR	2.3
1	A	1260[A]	ARG	2.3
1	A	206	GLN	2.3
1	A	478	GLY	2.3
1	A	88	HIS	2.3
1	A	350	VAL	2.3
1	A	1069	ILE	2.2
1	A	505	GLU	2.2
1	A	975	ASN	2.2
1	A	55	ARG	2.2
1	A	476	VAL	2.2
1	A	254	GLU	2.2
1	A	636	THR	2.2
1	A	927	GLU	2.2
1	A	23	ASN	2.2
1	A	449	PRO	2.2
1	A	115	ASP	2.2
1	A	165	ASP	2.2
1	A	417	LEU	2.2
1	A	489	ALA	2.2
1	A	429	THR	2.2
1	A	99	SER	2.2
1	A	408	LEU	2.2
1	A	624	SER	2.2
1	A	1149	ILE	2.2
1	A	135	LYS	2.2
1	A	502	ASP	2.2
1	A	1111	ASP	2.2
1	A	631	VAL	2.2
1	A	372	GLU	2.1
1	A	984	GLU	2.1
1	A	1298	GLU	2.1
1	A	356	THR	2.1
1	A	1163	TYR	2.1
1	A	693	GLY	2.1
1	A	154	THR	2.1
1	A	144	PRO	2.1
1	A	35	LEU	2.1
1	A	957	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	578	ILE	2.1
1	A	1114	VAL	2.1
1	A	1309	ASP	2.1
1	A	561	GLU	2.1
1	A	504	GLN	2.1
1	A	412	ILE	2.1
1	A	654	ILE	2.1
1	A	80	ASP	2.1
1	A	622	SER	2.1
1	A	398	THR	2.1
1	A	25	GLN	2.1
1	A	575	LEU	2.1
1	A	798	ASN	2.1
1	A	566	HIS	2.1
1	A	324	PHE	2.1
1	A	90	GLU	2.0
1	A	499	LEU	2.0
1	A	547	ILE	2.0
1	A	352	PHE	2.0
1	A	814	PHE	2.0
1	A	887	THR	2.0
1	A	857	HIS	2.0
1	A	343	GLY	2.0
1	A	553	GLY	2.0
1	A	872	ASN	2.0
1	A	351	ARG	2.0

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

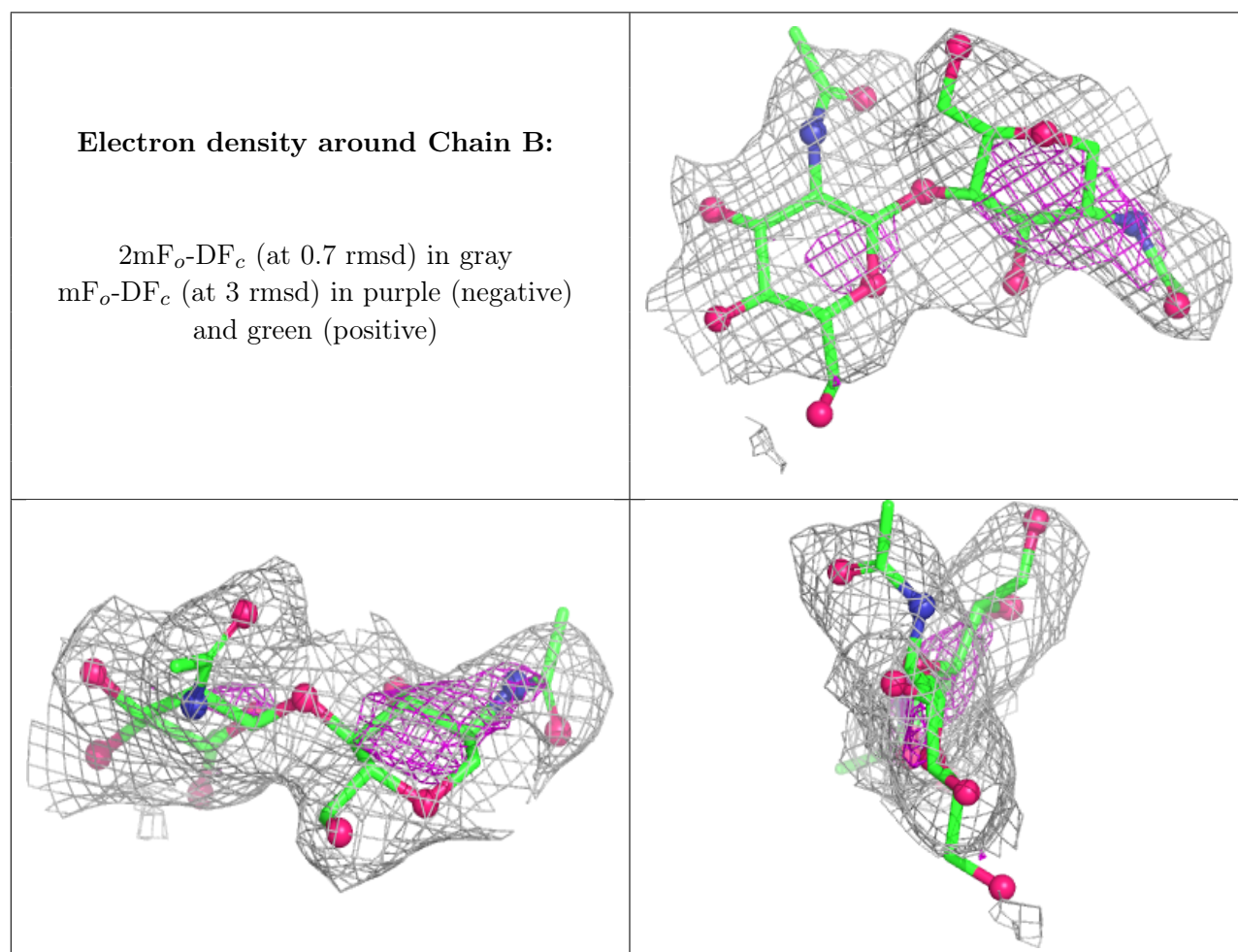
There are no non-standard protein/DNA/RNA residues in this entry.

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	B	2	14/15	0.62	0.19	89,91,92,93	0
2	NAG	B	1	14/15	0.79	0.16	79,83,85,88	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($\text{\AA}^2$)	Q<0.9
3	NAG	A	1326	14/15	0.47	0.20	66,72,74,75	0
3	NAG	A	1328	14/15	0.76	0.17	58,60,63,65	0
3	NAG	A	1327	14/15	0.79	0.14	52,55,57,58	0
4	NA	A	1333	1/1	0.81	0.16	53,53,53,53	0
4	NA	A	1332	1/1	0.96	0.17	43,43,43,43	0
4	NA	A	1331	1/1	0.99	0.10	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.