



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2024 – 10:59 PM EDT

PDB ID : 2PN5
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

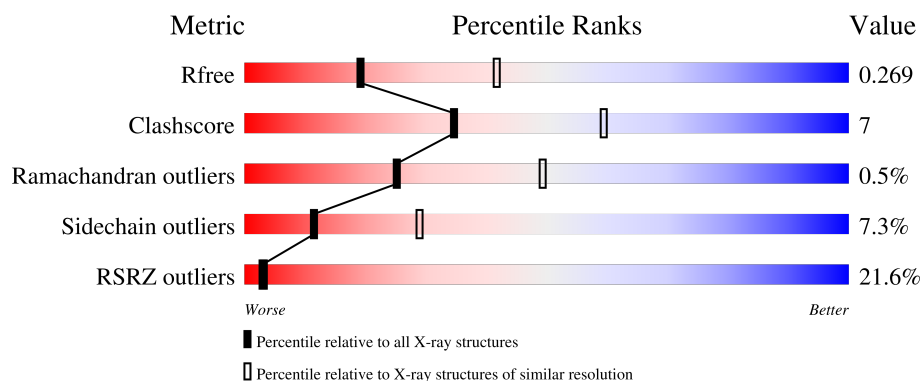
1 Overall quality at a glance

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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	
2	B	2	

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.

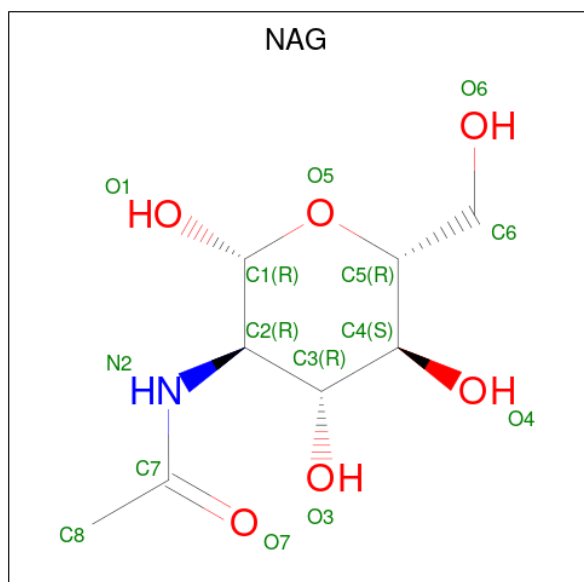
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1283	Total	C	N	O	S	0	7	0
			10333	6618	1724	1945	46			

- 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 (three-letter code: 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 (three-letter code: NA) (formula: Na).

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

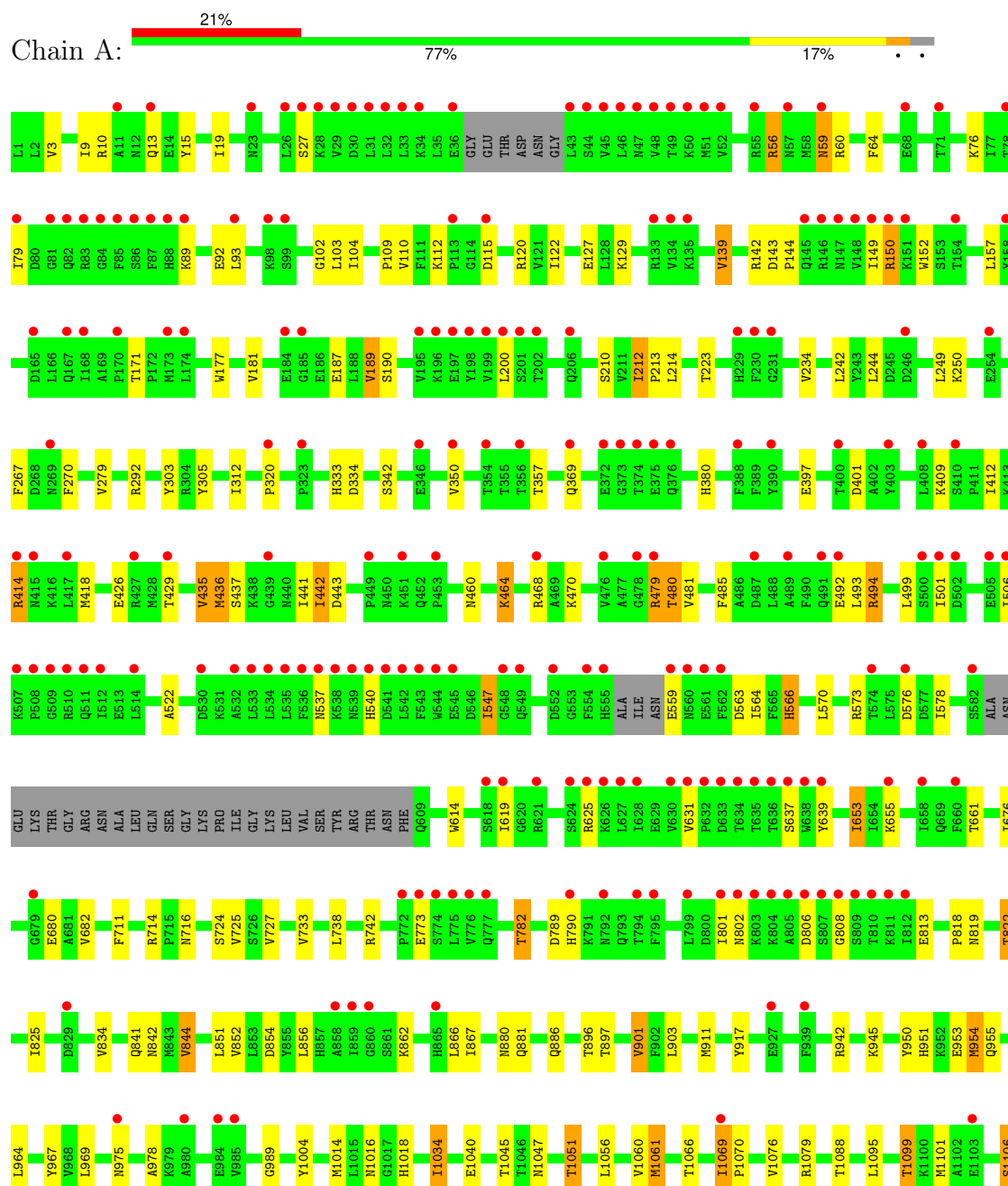
- Molecule 5 is water.

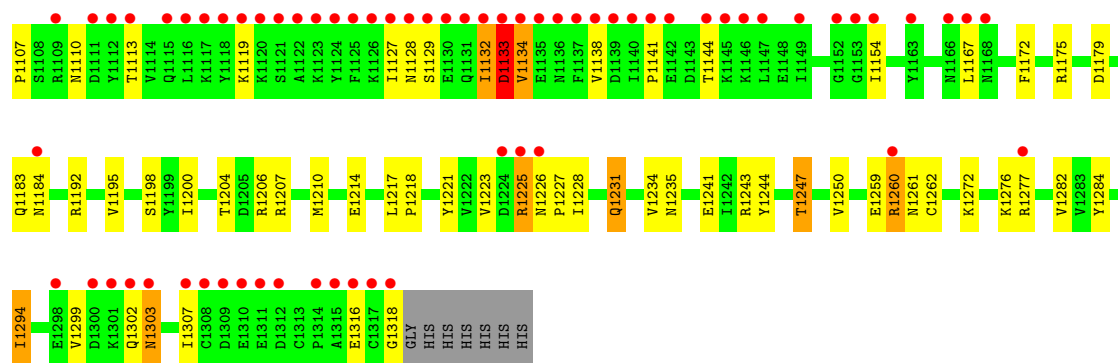
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total	O	0	0
			140	140		

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

Chain B:



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 [i](#)

5.1 Standard geometry [i](#)

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	0.46	1/10543 (0.0%)	0.59	1/14272 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1318	GLY	C-O	12.94	1.44	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1318	GLY	CA-C-O	-7.01	107.97	120.60

There are no chirality outliers.

There are no planarity outliers.

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	A	10333	0	10327	154	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	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (154) 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: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:1056:LEU:HD11	1:A:1101:MET:CE	2.23	0.68
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:436:MET:HE2	1:A:441:ILE:HG12	1.77	0.67
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:1056:LEU:HD11	1:A:1101:MET:HE3	1.78	0.65
1:A:951:HIS:H	1:A:955:GLN:HE21	1.45	0.65
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:LEU:HD11	1:A:1101:MET:HE2	1.92	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:59:ASN:C	1:A:59:ASN:HD22	2.15	0.50
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:954:MET:HE1	1:A:967:TYR:HB2	1.95	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1076:VAL:O	1:A:1079:ARG:HD3	2.19	0.42
1:A:1129:SER:HG	1:A:1132:ILE:HG23	1.84	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:485:PHE:HB3	1:A:564:ILE:HD11	2.02	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
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%)	25	49

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 [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	1147/1173 (98%)	1063 (93%)	84 (7%)	11	29

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	59	ASN
1	A	60	ARG
1	A	76	LYS

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Mol	Chain	Res	Type
1	A	92	GLU
1	A	139	VAL
1	A	142	ARG
1	A	150	ARG
1	A	157	LEU
1	A	189	VAL
1	A	212	ILE
1	A	234	VAL
1	A	250	LYS
1	A	312	ILE
1	A	334	ASP
1	A	369	GLN
1	A	380	HIS
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	470	LYS
1	A	479	ARG
1	A	480	THR
1	A	494	ARG
1	A	499	LEU
1	A	501	ILE
1	A	540	HIS
1	A	547	ILE
1	A	559	GLU
1	A	566	HIS
1	A	570	LEU
1	A	576	ASP
1	A	625	ARG
1	A	639	TYR
1	A	653	ILE
1	A	738	LEU
1	A	782	THR
1	A	789	ASP
1	A	790	HIS
1	A	801	ILE
1	A	802	ASN
1	A	806	ASP
1	A	822	THR

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Mol	Chain	Res	Type
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	942	ARG
1	A	945	LYS
1	A	954	MET
1	A	1034	ILE
1	A	1051	THR
1	A	1061	MET
1	A	1069	ILE
1	A	1099	THR
1	A	1106	SER
1	A	1113	THR
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	1184	ASN
1	A	1204	THR
1	A	1206	ARG
1	A	1207	ARG
1	A	1225	ARG
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	1316	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	59	ASN
1	A	227	ASN
1	A	333	HIS
1	A	369	GLN
1	A	458	GLN
1	A	540	HIS
1	A	716	ASN
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
1	A	1047	ASN
1	A	1128	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.

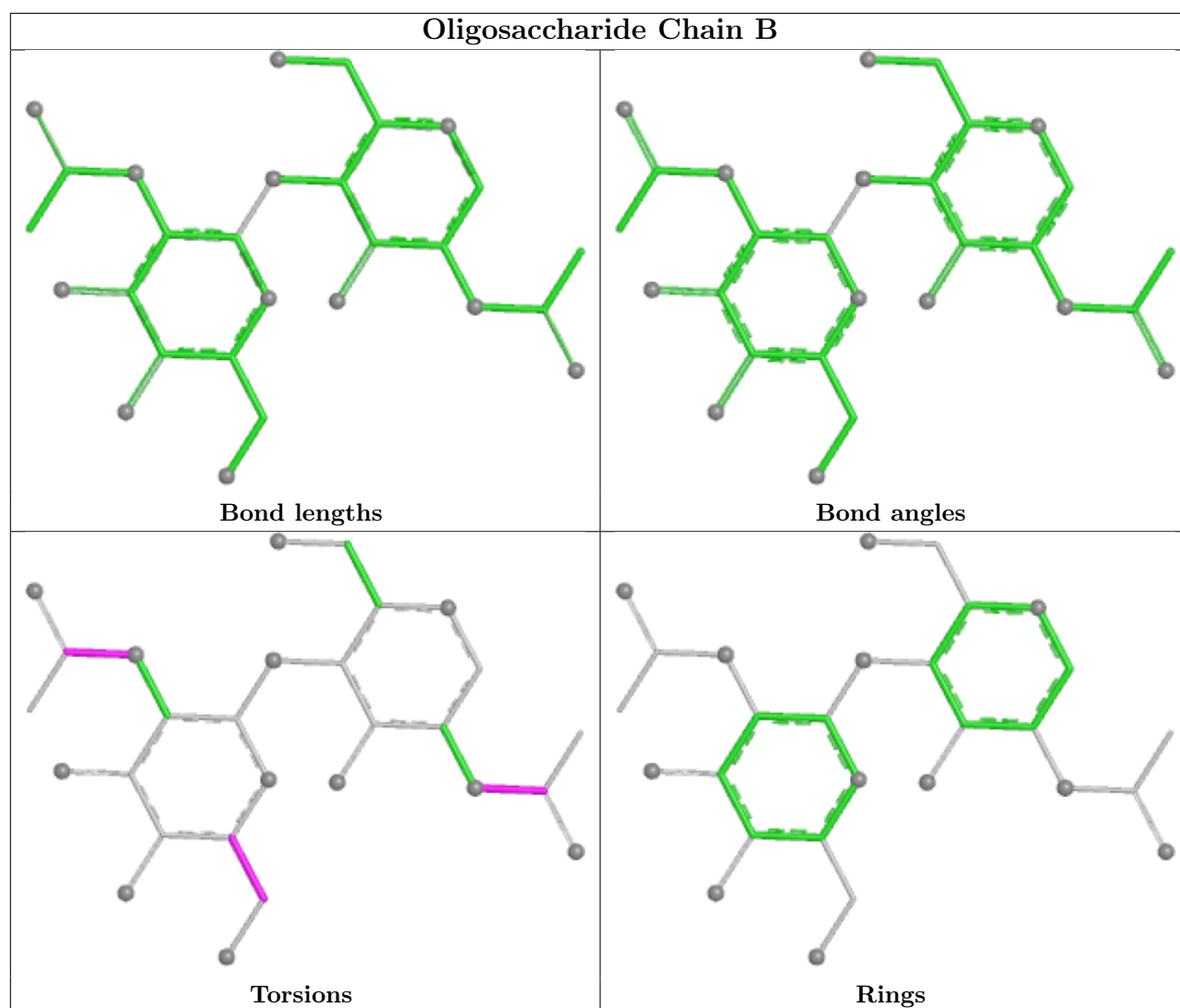
All (6) torsion outliers are listed below:

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	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%)
3	NAG	A	1327	1	14,14,15	0.43	0	17,19,21	1.30	4 (23%)

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	1328	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1326	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1327	1	-	0/6/23/26	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

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%)	1.04	277 (21%) 3 3	15, 58, 109, 147	7 (0%)

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	LEU	9.7
1	A	199	VAL	8.2
1	A	230	PHE	8.1
1	A	198	TYR	7.5
1	A	635	THR	6.7
1	A	492	GLU	6.5
1	A	200	LEU	6.5
1	A	554	PHE	6.1
1	A	506	ILE	6.1
1	A	1122	ALA	5.8
1	A	1140	ILE	5.8
1	A	1139	ASP	5.7
1	A	27	SER	5.6
1	A	801	ILE	5.5
1	A	1135	GLU	5.4
1	A	540	HIS	5.3
1	A	542	LEU	5.2
1	A	45	VAL	5.0
1	A	1314	PRO	5.0
1	A	773	GLU	4.9
1	A	805	ALA	4.8
1	A	535	LEU	4.6
1	A	507	LYS	4.6
1	A	536	PHE	4.6
1	A	1134	VAL	4.5
1	A	491	GLN	4.5
1	A	196	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	808	GLY	4.4
1	A	1318	GLY	4.4
1	A	1144	THR	4.4
1	A	510	ARG	4.4
1	A	1141	PRO	4.2
1	A	1137	PHE	4.1
1	A	533	LEU	4.1
1	A	1225	ARG	4.1
1	A	173[A]	MET	4.1
1	A	1317	CYS	4.0
1	A	32	LEU	4.0
1	A	775	LEU	4.0
1	A	812	ILE	4.0
1	A	201	SER	4.0
1	A	1138	VAL	4.0
1	A	51	MET	4.0
1	A	388	PHE	3.9
1	A	1316	GLU	3.9
1	A	44	SER	3.9
1	A	1166	ASN	3.8
1	A	1119	LYS	3.8
1	A	146	ARG	3.8
1	A	776	VAL	3.8
1	A	637	SER	3.8
1	A	792	ASN	3.7
1	A	29	VAL	3.7
1	A	1124	TYR	3.7
1	A	57	ASN	3.6
1	A	1126	LYS	3.6
1	A	46	LEU	3.6
1	A	632	PRO	3.6
1	A	167	GLN	3.6
1	A	1315	ALA	3.6
1	A	532	ALA	3.6
1	A	1120	LYS	3.5
1	A	530	ASP	3.5
1	A	1133	ASP	3.5
1	A	555	HIS	3.5
1	A	810	THR	3.5
1	A	501	ILE	3.5
1	A	84	GLY	3.5
1	A	562	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	634	THR	3.5
1	A	231	GLY	3.4
1	A	1125	PHE	3.4
1	A	202	THR	3.4
1	A	772	PRO	3.4
1	A	86	SER	3.4
1	A	1123	LYS	3.4
1	A	806	ASP	3.4
1	A	1132	ILE	3.4
1	A	1168	ASN	3.4
1	A	1117	LYS	3.4
1	A	34	LYS	3.4
1	A	552	ASP	3.3
1	A	534	LEU	3.3
1	A	1128	ASN	3.3
1	A	197	GLU	3.3
1	A	559	GLU	3.3
1	A	1145	LYS	3.3
1	A	98	LYS	3.3
1	A	512	ILE	3.3
1	A	626	LYS	3.3
1	A	799	LEU	3.3
1	A	660	PHE	3.3
1	A	479	ARG	3.3
1	A	1303	ASN	3.3
1	A	168	ILE	3.2
1	A	229	HIS	3.2
1	A	1311	GLU	3.2
1	A	638	TRP	3.2
1	A	487	ASP	3.2
1	A	1312	ASP	3.2
1	A	807	SER	3.2
1	A	1226	ASN	3.1
1	A	451	LYS	3.1
1	A	1301	LYS	3.1
1	A	809	SER	3.1
1	A	49	THR	3.1
1	A	158	TYR	3.1
1	A	539	ASN	3.1
1	A	802	ASN	3.1
1	A	468	ARG	3.1
1	A	508	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	576	ASP	3.0
1	A	83	ARG	3.0
1	A	414	ARG	3.0
1	A	1118	TYR	3.0
1	A	538	LYS	3.0
1	A	1130	GLU	3.0
1	A	30	ASP	3.0
1	A	1146	LYS	3.0
1	A	865	HIS	3.0
1	A	373	GLY	3.0
1	A	375	GLU	2.9
1	A	78	THR	2.9
1	A	13	GLN	2.9
1	A	633	ASP	2.9
1	A	500	SER	2.9
1	A	28	LYS	2.9
1	A	390	TYR	2.9
1	A	548	GLY	2.9
1	A	346	GLU	2.9
1	A	1310	GLU	2.9
1	A	82	GLN	2.9
1	A	1131	GLN	2.9
1	A	415	ASN	2.9
1	A	1103	GLU	2.8
1	A	48	VAL	2.8
1	A	939	PHE	2.8
1	A	184	GLU	2.8
1	A	11	ALA	2.8
1	A	150	ARG	2.8
1	A	195	VAL	2.8
1	A	376	GLN	2.8
1	A	1115	GLN	2.8
1	A	804	LYS	2.8
1	A	625	ARG	2.8
1	A	151	LYS	2.8
1	A	803	LYS	2.8
1	A	246	ASP	2.8
1	A	1184	ASN	2.7
1	A	145	GLN	2.7
1	A	1129	SER	2.7
1	A	87	PHE	2.7
1	A	81	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1127	ILE	2.7
1	A	1113	THR	2.7
1	A	1136	ASN	2.7
1	A	170	PRO	2.7
1	A	509	GLY	2.7
1	A	639	TYR	2.7
1	A	36	GLU	2.7
1	A	269	ASN	2.7
1	A	630	VAL	2.7
1	A	85	PHE	2.7
1	A	93	LEU	2.7
1	A	582	SER	2.7
1	A	323	PRO	2.6
1	A	453	PRO	2.6
1	A	549	GLN	2.6
1	A	1109	ARG	2.6
1	A	544	TRP	2.6
1	A	1121	SER	2.6
1	A	777	GLN	2.6
1	A	1142	GLU	2.6
1	A	627	LEU	2.6
1	A	1147	LEU	2.6
1	A	369	GLN	2.6
1	A	71	THR	2.6
1	A	89	LYS	2.6
1	A	545	GLU	2.6
1	A	541	ASP	2.6
1	A	658	ILE	2.6
1	A	774	SER	2.5
1	A	1300	ASP	2.5
1	A	537	ASN	2.5
1	A	560	ASN	2.5
1	A	980	ALA	2.5
1	A	628	ILE	2.5
1	A	794	THR	2.5
1	A	33	LEU	2.5
1	A	50	LYS	2.5
1	A	26	LEU	2.5
1	A	511	GLN	2.5
1	A	1224	ASP	2.5
1	A	47	ASN	2.5
1	A	149	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	514	LEU	2.5
1	A	1116	LEU	2.5
1	A	1302	GLN	2.5
1	A	811	LYS	2.5
1	A	655	LYS	2.4
1	A	79	ILE	2.4
1	A	147	ASN	2.4
1	A	859	ILE	2.4
1	A	31	LEU	2.4
1	A	52	VAL	2.4
1	A	543	PHE	2.4
1	A	858	ALA	2.4
1	A	1154	ILE	2.4
1	A	1307	ILE	2.4
1	A	829	ASP	2.4
1	A	1167	LEU	2.4
1	A	133	ARG	2.4
1	A	790	HIS	2.4
1	A	59	ASN	2.4
1	A	427	ARG	2.4
1	A	134	VAL	2.4
1	A	185	GLY	2.4
1	A	403	TYR	2.4
1	A	1152	GLY	2.4
1	A	374	THR	2.3
1	A	148	VAL	2.3
1	A	618	SER	2.3
1	A	439	GLY	2.3
1	A	679	GLY	2.3
1	A	68	GLU	2.3
1	A	621	ARG	2.3
1	A	860	GLY	2.3
1	A	1277	ARG	2.2
1	A	410	SER	2.2
1	A	1260[A]	ARG	2.2
1	A	400	THR	2.2
1	A	574	THR	2.2
1	A	1112	TYR	2.2
1	A	985	VAL	2.2
1	A	619	ILE	2.2
1	A	174	LEU	2.2
1	A	113	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	320	PRO	2.2
1	A	354	THR	2.2
1	A	206	GLN	2.2
1	A	795	PHE	2.2
1	A	1308	CYS	2.2
1	A	55	ARG	2.2
1	A	1153	GLY	2.2
1	A	505	GLU	2.2
1	A	88	HIS	2.2
1	A	478	GLY	2.2
1	A	254	GLU	2.1
1	A	927	GLU	2.1
1	A	975	ASN	2.1
1	A	350	VAL	2.1
1	A	1069	ILE	2.1
1	A	636	THR	2.1
1	A	23	ASN	2.1
1	A	115	ASP	2.1
1	A	165	ASP	2.1
1	A	476	VAL	2.1
1	A	449	PRO	2.1
1	A	429	THR	2.1
1	A	99	SER	2.1
1	A	624	SER	2.1
1	A	417	LEU	2.1
1	A	489	ALA	2.1
1	A	372	GLU	2.1
1	A	984	GLU	2.1
1	A	1298	GLU	2.1
1	A	135	LYS	2.1
1	A	1149	ILE	2.1
1	A	408	LEU	2.1
1	A	502	ASP	2.1
1	A	1111	ASP	2.1
1	A	356	THR	2.0
1	A	631	VAL	2.0
1	A	561	GLU	2.0
1	A	154	THR	2.0
1	A	1163	TYR	2.0
1	A	1309	ASP	2.0

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

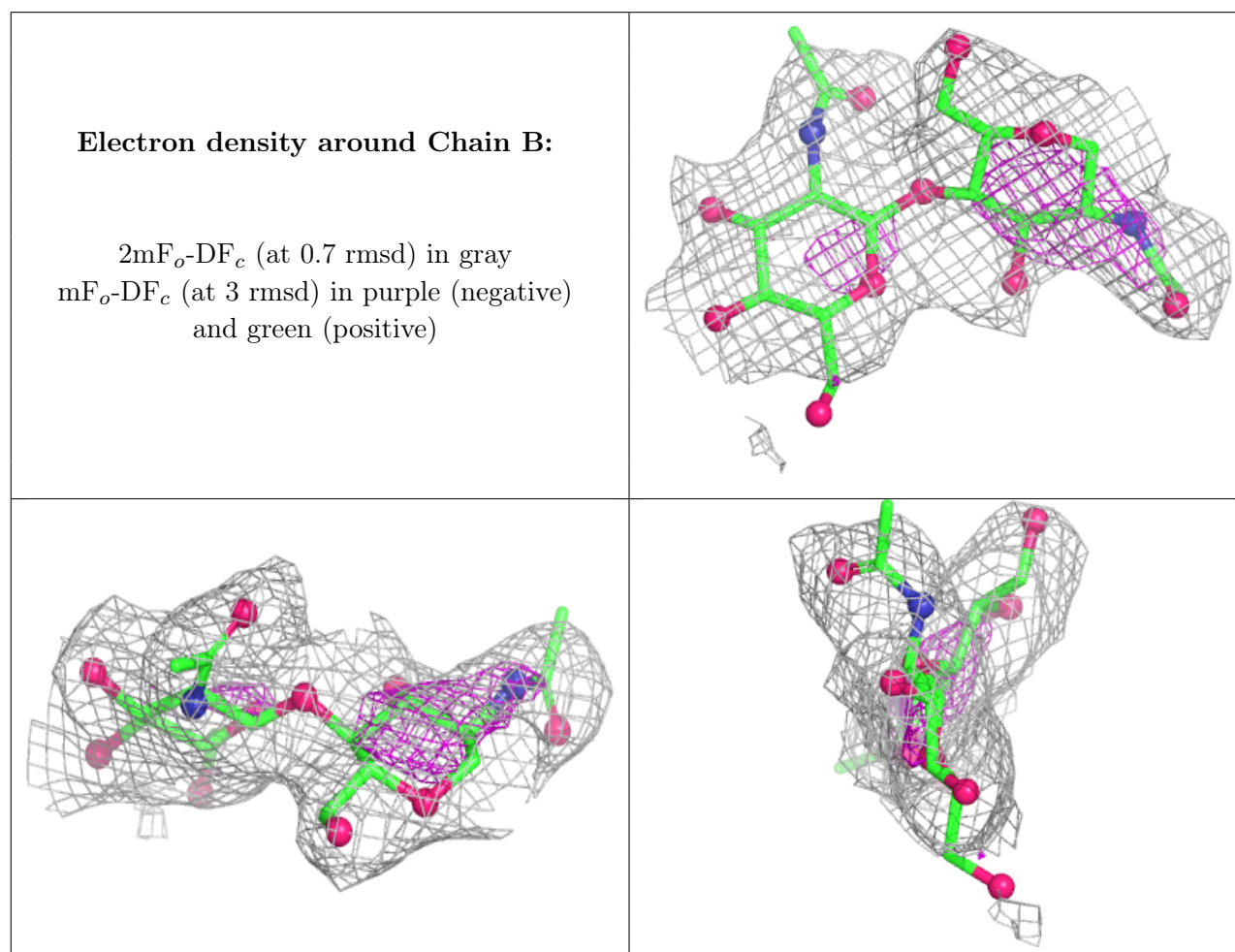
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^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(\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	0.82	0.17	53,53,53,53	0
4	NA	A	1332	1/1	0.97	0.18	43,43,43,43	0
4	NA	A	1331	1/1	0.98	0.10	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.