Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 10:55 AM JST

PDB ID	:	5AVY
Title	:	Kinetics by X-ray crystallography: Tl+-substitution of bound K+ in the E2.MgF42-.2K+ crystal after 20 min
Authors	:	Ogawa, H.; Cornelius, F.; Hirata, A.; Toyoshima, C.
Deposited on	:	2015-07-01
Resolution	:	3.45 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 (i) 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 (i)) were used in the production of this report:

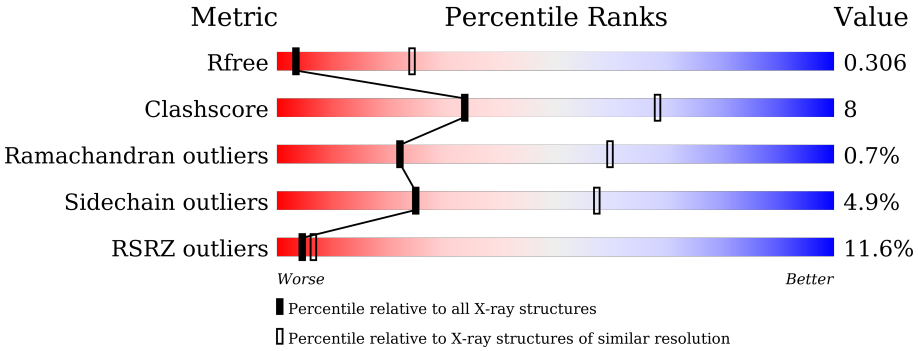
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 <=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	1028	10%; 74%; 21%; • •
2	B	305	15%; 67%; 19%; •; 12%
3	G	74	%; 35%; 18%; 47%
4	C	2	100%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	B	4021	-	-	-	X
4	NAG	C	2	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 10235 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 Na, K-ATPase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	992	7675	4886	1290	1453	46	0	0	0

- Molecule 2 is a protein called Na+,K+-ATPase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	268	2174	1409	358	396	11	0	0	0

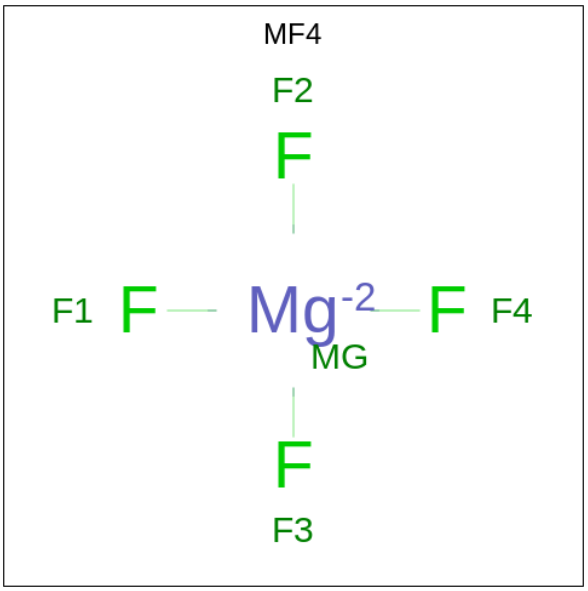
- Molecule 3 is a protein called Phospholemman-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	39	305	200	50	54	1	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	C	2	28	16	2	10	0	0	0

- Molecule 5 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total F Mg 5 4 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0

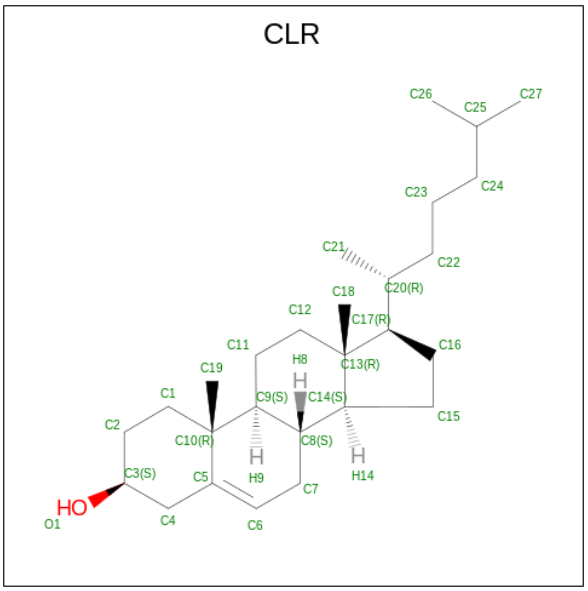
- Molecule 7 is THALLIUM (I) ION (three-letter code: TL) (formula: Tl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total Tl 3 3	0	1

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

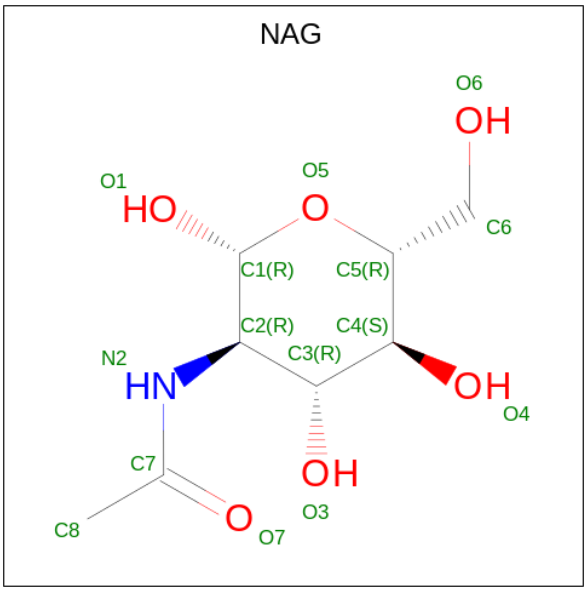
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	1

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	28	27	1	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	14	8	1	5	0	0

- Molecule 11 is water.

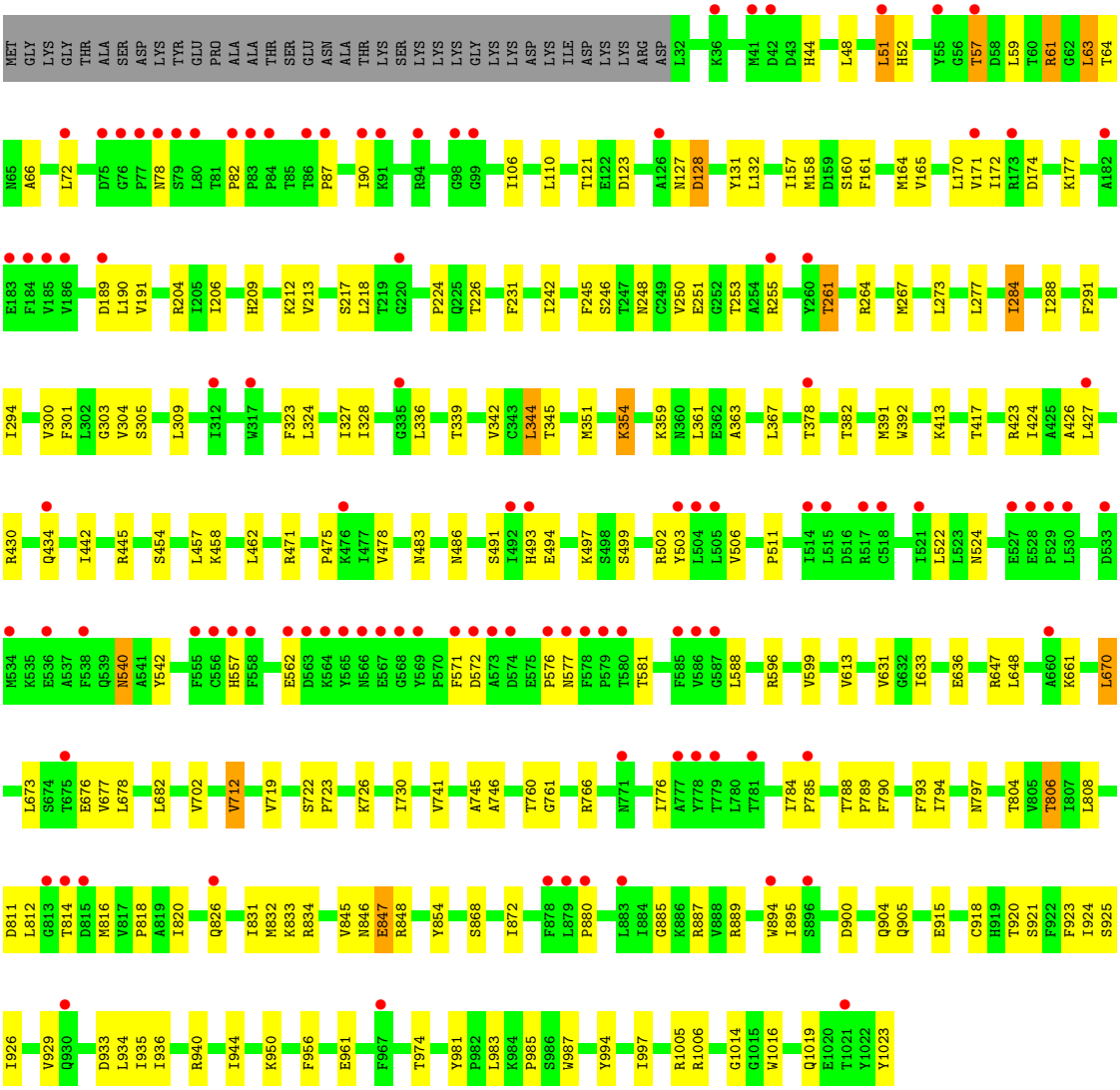
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	1	1	1	0	0

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.

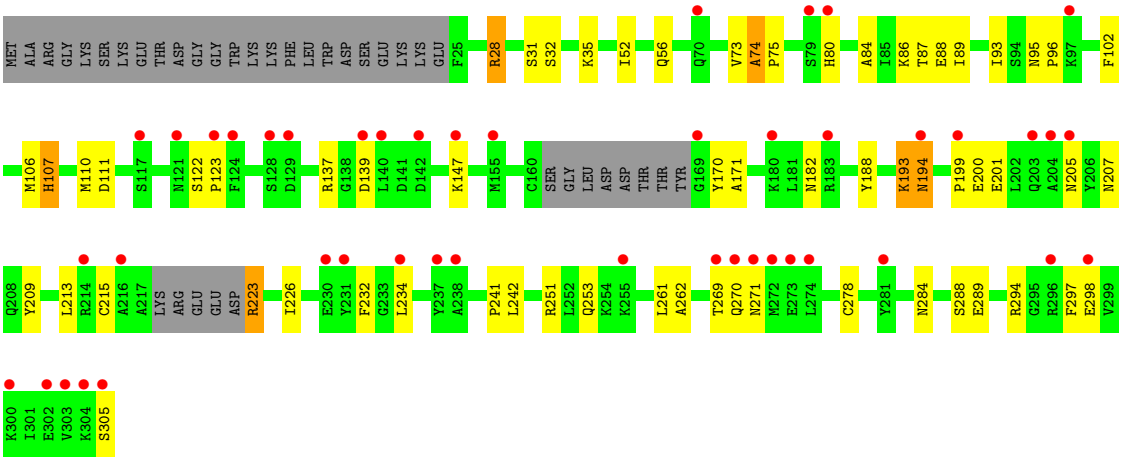
- Molecule 1: Na, K-ATPase alpha subunit

Chain A: 10% 74% 21%



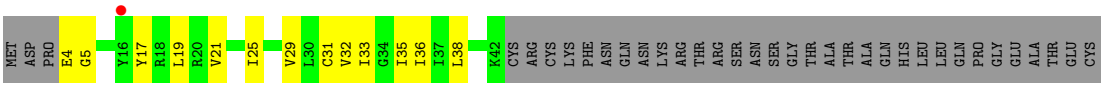
- Molecule 2: Na+,K+-ATPase beta subunit

Chain B:



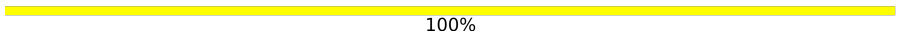
- Molecule 3: Phospholemman-like protein

Chain G:



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

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	220.59Å 50.67Å 163.92Å 90.00° 103.63° 90.00°	Depositor
Resolution (Å)	14.94 – 3.45 38.92 – 3.45	Depositor EDS
% Data completeness (in resolution range)	85.6 (14.94-3.45) 93.8 (38.92-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.308 , 0.305 0.295 , 0.306	Depositor DCC
R_{free} test set	672 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å^2)	107.2	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10235	wwPDB-VP
Average B, all atoms (Å^2)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CLR, NAG, MG, K, TL, MF4

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	0.38	0/7825	0.51	0/10616
2	B	0.36	0/2229	0.49	0/3002
3	G	0.36	0/309	0.46	0/419
All	All	0.38	0/10363	0.51	0/14037

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	7675	0	7699	125	1
2	B	2174	0	2146	45	0
3	G	305	0	318	10	0
4	C	28	0	25	0	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0
7	A	3	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	46	1	0
10	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	1	0	0	0	0
All	All	10235	0	10247	173	1

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 (173) 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:74:ALA:HB3	2:B:75:PRO:HD3	1.47	0.94
1:A:478:VAL:HG21	1:A:571:PHE:HB2	1.65	0.79
1:A:497:LYS:HE2	1:A:499:SER:HB2	1.68	0.76
1:A:868:SER:O	1:A:872:ILE:HG12	1.86	0.75
1:A:905:GLN:NE2	2:B:182:ASN:HA	2.00	0.75
1:A:61:ARG:HH11	1:A:61:ARG:HB3	1.52	0.73
1:A:261:THR:HG22	1:A:264:ARG:NH2	2.02	0.73
1:A:51:LEU:HD13	1:A:204:ARG:HG3	1.69	0.72
2:B:270:GLN:HG2	2:B:271:ASN:HD22	1.58	0.68
1:A:766:ARG:HD2	1:A:832:MET:CE	2.24	0.68
1:A:339:THR:HG23	1:A:820:ILE:HD13	1.77	0.67
2:B:213:LEU:HD11	2:B:278:CYS:HB3	1.78	0.65
1:A:935:ILE:HG23	1:A:944:ILE:HD12	1.77	0.65
1:A:78:ASN:HA	1:A:261:THR:HG23	1.79	0.64
2:B:28:ARG:NH1	9:B:3001:CLR:H22	2.12	0.64
1:A:816:MET:O	1:A:820:ILE:HG12	1.97	0.63
1:A:160:SER:HB3	1:A:741:VAL:HG22	1.80	0.63
2:B:74:ALA:CB	2:B:75:PRO:HD3	2.23	0.63
1:A:52:HIS:HA	1:A:57:THR:HG23	1.80	0.63
2:B:28:ARG:HB2	2:B:32:SER:HB3	1.81	0.63
1:A:673:LEU:HD22	1:A:677:VAL:HG11	1.80	0.62
2:B:193:LYS:HA	2:B:207:ASN:HD21	1.65	0.62
1:A:323:PHE:O	1:A:327:ILE:HG12	2.00	0.61
1:A:64:THR:HG22	1:A:66:ALA:H	1.65	0.61
3:G:29:VAL:O	3:G:33:ILE:HG12	2.00	0.61
1:A:483:ASN:HB2	1:A:486:ASN:HB2	1.82	0.60
1:A:363:ALA:HB1	1:A:730:ILE:HD12	1.83	0.60
2:B:270:GLN:HG2	2:B:271:ASN:ND2	2.16	0.60
2:B:31:SER:O	2:B:35:LYS:HG3	2.01	0.60
1:A:344:LEU:HB3	1:A:361:LEU:HG	1.85	0.59
2:B:84:ALA:HB1	2:B:88:GLU:H	1.67	0.59
1:A:392:TRP:HB3	1:A:588:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:21:VAL:O	3:G:25:ILE:HG12	2.02	0.59
1:A:106:ILE:O	1:A:110:LEU:HB2	2.03	0.59
1:A:212:LYS:HB2	1:A:251:GLU:HG2	1.85	0.59
2:B:106:MET:O	2:B:110:MET:HG2	2.03	0.58
1:A:345:THR:HA	1:A:361:LEU:HD11	1.84	0.58
1:A:1016:TRP:HE1	2:B:35:LYS:HE3	1.68	0.57
2:B:75:PRO:HG2	2:B:294:ARG:HH21	1.68	0.57
2:B:193:LYS:HA	2:B:207:ASN:ND2	2.20	0.57
1:A:491:SER:HB3	1:A:493:HIS:NE2	2.19	0.57
2:B:74:ALA:HB3	2:B:75:PRO:CD	2.29	0.56
2:B:137:ARG:HD2	2:B:147:LYS:HB3	1.87	0.56
2:B:52:ILE:O	2:B:56:GLN:HG2	2.05	0.56
1:A:818:PRO:HB3	1:A:934:LEU:HD22	1.87	0.56
1:A:172:ILE:HD13	1:A:177:LYS:HB3	1.87	0.56
1:A:933:ASP:HA	1:A:936:ILE:HG12	1.86	0.56
1:A:190:LEU:HD11	1:A:206:ILE:HD11	1.88	0.55
2:B:93:ILE:H	2:B:305:SER:HB2	1.72	0.55
1:A:157:ILE:HD11	1:A:745:ALA:HA	1.88	0.55
1:A:994:TYR:O	1:A:997:ILE:HG22	2.06	0.55
1:A:351:MET:HA	1:A:354:LYS:HG2	1.89	0.55
1:A:596:ARG:HB2	1:A:599:VAL:HG23	1.89	0.55
1:A:261:THR:HG22	1:A:264:ARG:HH21	1.71	0.54
1:A:924:ILE:HD12	1:A:983:LEU:HD12	1.89	0.54
1:A:994:TYR:HA	1:A:997:ILE:HG22	1.89	0.54
1:A:64:THR:HG22	1:A:66:ALA:N	2.23	0.54
1:A:921:SER:HA	1:A:983:LEU:HD11	1.90	0.54
1:A:51:LEU:CD1	1:A:204:ARG:HG3	2.36	0.53
1:A:424:ILE:HG23	1:A:506:VAL:HB	1.90	0.53
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.89	0.53
1:A:161:PHE:HA	1:A:164:MET:CE	2.39	0.52
1:A:324:LEU:O	1:A:328:ILE:HG12	2.09	0.52
1:A:808:LEU:O	1:A:812:LEU:HB2	2.10	0.52
1:A:956:PHE:CE1	3:G:38:LEU:HD22	2.44	0.52
1:A:212:LYS:HD3	1:A:224:PRO:HB2	1.90	0.52
1:A:766:ARG:HD2	1:A:832:MET:HE2	1.91	0.52
2:B:75:PRO:HG2	2:B:294:ARG:NH2	2.25	0.52
3:G:32:VAL:O	3:G:36:ILE:HG12	2.09	0.52
1:A:161:PHE:HA	1:A:164:MET:HE3	1.92	0.52
1:A:82:PRO:HA	1:A:158:MET:HG2	1.92	0.51
1:A:572:ASP:HB3	1:A:577:ASN:HB2	1.92	0.51
3:G:25:ILE:O	3:G:29:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:THR:N	1:A:789:PRO:HD2	2.26	0.51
1:A:417:THR:HA	1:A:522:LEU:HD22	1.93	0.51
2:B:288:SER:HB2	2:B:294:ARG:HH11	1.76	0.50
1:A:571:PHE:HA	1:A:577:ASN:HD22	1.76	0.50
1:A:359:LYS:HE2	1:A:746:ALA:O	2.12	0.49
1:A:826:GLN:HE22	1:A:950:LYS:HE3	1.78	0.49
2:B:232:PHE:HB2	2:B:262:ALA:HB3	1.93	0.49
1:A:1005:ARG:NH1	1:A:1006:ARG:HG3	2.28	0.49
2:B:209:TYR:HA	2:B:242:LEU:HD22	1.95	0.48
1:A:502:ARG:CG	1:A:503:TYR:H	2.27	0.48
1:A:442:ILE:O	1:A:445:ARG:HG2	2.14	0.48
1:A:323:PHE:CE1	1:A:793:PHE:HE2	2.32	0.47
1:A:132:LEU:HD21	1:A:804:THR:HG21	1.96	0.47
2:B:87:THR:HB	2:B:298:GLU:O	2.14	0.47
1:A:171:VAL:HG12	1:A:191:VAL:HG22	1.97	0.47
1:A:797:ASN:HD22	1:A:887:ARG:HD3	1.79	0.47
1:A:814:THR:HB	1:A:961:GLU:HG3	1.96	0.47
3:G:31:CYS:O	3:G:35:ILE:HG12	2.14	0.47
2:B:80:HIS:HB3	2:B:297:PHE:CZ	2.50	0.47
1:A:127:ASN:HB3	1:A:131:TYR:CD1	2.50	0.47
1:A:336:LEU:HD11	1:A:776:ILE:HG12	1.96	0.47
1:A:985:PRO:HD3	3:G:19:LEU:HD11	1.97	0.46
1:A:631:VAL:HG23	1:A:633:ILE:HG12	1.96	0.46
1:A:924:ILE:HD12	1:A:983:LEU:CD1	2.45	0.46
2:B:226:ILE:HG22	2:B:269:THR:HB	1.96	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.76	0.46
2:B:215:CYS:HA	2:B:278:CYS:HA	1.96	0.46
1:A:63:LEU:HD22	1:A:189:ASP:HB3	1.96	0.46
1:A:670:LEU:HD23	1:A:678:LEU:HD21	1.96	0.46
1:A:784:ILE:HD11	1:A:854:TYR:CG	2.51	0.46
1:A:209:HIS:HB3	1:A:253:THR:HG22	1.98	0.45
1:A:303:GLY:HA2	1:A:327:ILE:HG21	1.97	0.45
1:A:475:PRO:HD2	1:A:494:GLU:HB2	1.98	0.45
1:A:905:GLN:HE21	2:B:182:ASN:HA	1.78	0.45
1:A:889:ARG:HD2	1:A:895:ILE:CD1	2.46	0.45
1:A:631:VAL:CG2	1:A:633:ILE:HG12	2.46	0.45
1:A:676:GLU:H	1:A:676:GLU:CD	2.20	0.45
2:B:84:ALA:HB1	2:B:88:GLU:N	2.31	0.45
1:A:722:SER:OG	1:A:723:PRO:HD3	2.17	0.45
1:A:847:GLU:CD	1:A:847:GLU:H	2.20	0.45
1:A:52:HIS:HE2	1:A:59:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:GLU:O	1:A:918:CYS:HB2	2.17	0.44
1:A:806:THR:HG22	1:A:923:PHE:HB2	2.00	0.44
2:B:234:LEU:HG	2:B:241:PRO:HG3	1.99	0.44
2:B:194:ASN:HD22	2:B:194:ASN:N	2.15	0.44
1:A:354:LYS:HZ2	1:A:354:LYS:HB2	1.81	0.44
1:A:894:TRP:CH2	2:B:86:LYS:HG2	2.53	0.44
1:A:246:SER:OG	1:A:267:MET:HG3	2.18	0.43
2:B:107:HIS:O	2:B:111:ASP:HB2	2.18	0.43
2:B:107:HIS:ND1	2:B:170:TYR:HE1	2.17	0.43
1:A:273:LEU:O	1:A:277:LEU:HG	2.19	0.43
1:A:790:PHE:O	1:A:794:ILE:HG12	2.19	0.43
1:A:956:PHE:CD1	3:G:38:LEU:HD22	2.54	0.43
2:B:147:LYS:HB2	2:B:253:GLN:HG3	1.99	0.43
1:A:87:PRO:HD2	1:A:90:ILE:HD12	1.99	0.43
1:A:110:LEU:HD22	1:A:324:LEU:HD12	1.99	0.43
1:A:511:PRO:HG2	1:A:542:TYR:CE1	2.53	0.43
3:G:4:GLU:CD	3:G:5:GLY:H	2.23	0.43
1:A:300:VAL:O	1:A:304:VAL:HG22	2.19	0.42
1:A:64:THR:HA	1:A:174:ASP:OD1	2.19	0.42
1:A:661:LYS:HE2	1:A:661:LYS:HA	2.00	0.42
1:A:797:ASN:HB3	1:A:885:GLY:HA2	2.00	0.42
2:B:74:ALA:CB	2:B:75:PRO:CD	2.92	0.42
1:A:940:ARG:HE	1:A:1023:TYR:HB2	1.84	0.42
1:A:170:LEU:HD21	1:A:177:LYS:HD3	2.00	0.42
1:A:291:PHE:HA	1:A:294:ILE:HD12	2.01	0.42
2:B:95:ASN:HA	2:B:96:PRO:HD3	1.86	0.42
2:B:188:TYR:O	2:B:284:ASN:ND2	2.53	0.42
2:B:223:ARG:HB2	2:B:223:ARG:HH11	1.84	0.42
1:A:291:PHE:HB3	1:A:845:VAL:HB	2.02	0.42
2:B:89:ILE:HG22	2:B:102:PHE:CE2	2.55	0.42
1:A:784:ILE:N	1:A:785:PRO:HD2	2.35	0.42
1:A:378:THR:HA	1:A:382:THR:OG1	2.20	0.42
1:A:367:LEU:HD23	1:A:761:GLY:HA3	2.01	0.42
2:B:137:ARG:HB3	2:B:147:LYS:HD2	2.01	0.42
2:B:194:ASN:HB3	2:B:205:ASN:OD1	2.20	0.42
1:A:502:ARG:HE	1:A:562:GLU:HG2	1.85	0.41
1:A:48:LEU:HD23	1:A:59:LEU:HD11	2.01	0.41
1:A:846:ASN:ND2	1:A:848:ARG:HB2	2.35	0.41
1:A:920:THR:HG21	1:A:981:TYR:O	2.20	0.41
1:A:110:LEU:CD2	1:A:324:LEU:HD12	2.50	0.41
1:A:785:PRO:HB2	1:A:926:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:HB3	1:A:242:ILE:HD11	2.02	0.41
2:B:271:ASN:HD21	2:B:305:SER:N	2.19	0.41
1:A:426:ALA:O	1:A:471:ARG:HD2	2.20	0.41
1:A:342:VAL:HB	1:A:820:ILE:HD12	2.03	0.41
1:A:540:ASN:HD22	1:A:540:ASN:N	2.18	0.41
3:G:17:TYR:O	3:G:21:VAL:HG23	2.21	0.41
1:A:458:LYS:O	1:A:462:LEU:HB2	2.21	0.41
1:A:423:ARG:O	1:A:427:LEU:HB2	2.21	0.41
1:A:502:ARG:HG3	1:A:562:GLU:HG2	2.02	0.41
1:A:647:ARG:HH21	1:A:648:LEU:HD11	1.86	0.41
1:A:284:ILE:O	1:A:288:ILE:HG12	2.21	0.41
1:A:301:PHE:O	1:A:305:SER:HB2	2.20	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG21	2.03	0.41
1:A:900:ASP:OD1	1:A:904:GLN:HB2	2.21	0.40
1:A:831:ILE:O	1:A:834:ARG:HG2	2.22	0.40
1:A:354:LYS:HE2	1:A:760:THR:HB	2.02	0.40
1:A:613:VAL:HG12	1:A:633:ILE:HD12	2.04	0.40
1:A:925:SER:O	1:A:929:VAL:HG22	2.22	0.40

All (1) 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:430:ARG:NH2	1:A:648:LEU:O[1_565]	2.07	0.13

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	990/1028 (96%)	942 (95%)	43 (4%)	5 (0%)	29 66
2	B	262/305 (86%)	223 (85%)	35 (13%)	4 (2%)	10 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	37/74 (50%)	33 (89%)	4 (11%)	0	100	100
All	All	1289/1407 (92%)	1198 (93%)	82 (6%)	9 (1%)	22	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	128	ASP
1	A	576	PRO
2	B	74	ALA
2	B	171	ALA
2	B	201	GLU
1	A	123	ASP
1	A	1014	GLY
2	B	199	PRO

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	840/869 (97%)	796 (95%)	44 (5%)	23	55
2	B	234/266 (88%)	224 (96%)	10 (4%)	29	61
3	G	32/62 (52%)	32 (100%)	0	100	100
All	All	1106/1197 (92%)	1052 (95%)	54 (5%)	25	57

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	57	THR
1	A	61	ARG
1	A	63	LEU
1	A	72	LEU
1	A	128	ASP

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	213	VAL
1	A	217	SER
1	A	218	LEU
1	A	226	THR
1	A	231	PHE
1	A	245	PHE
1	A	248	ASN
1	A	250	VAL
1	A	255	ARG
1	A	261	THR
1	A	284	ILE
1	A	309	LEU
1	A	344	LEU
1	A	354	LYS
1	A	391	MET
1	A	413	LYS
1	A	434	GLN
1	A	454	SER
1	A	457	LEU
1	A	524	ASN
1	A	540	ASN
1	A	557	HIS
1	A	581	THR
1	A	636	GLU
1	A	670	LEU
1	A	682	LEU
1	A	712	VAL
1	A	719	VAL
1	A	726	LYS
1	A	806	THR
1	A	811	ASP
1	A	833	LYS
1	A	847	GLU
1	A	880	PRO
1	A	974	THR
1	A	987	TRP
1	A	1019	GLN
2	B	28	ARG
2	B	73	VAL
2	B	107	HIS
2	B	139	ASP

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Mol	Chain	Res	Type
2	B	193	LYS
2	B	194	ASN
2	B	200	GLU
2	B	223	ARG
2	B	251	ARG
2	B	289	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	129	ASN
1	A	163	ASN
1	A	225	GLN
1	A	290	HIS
1	A	434	GLN
1	A	524	ASN
1	A	540	ASN
1	A	557	HIS
1	A	577	ASN
1	A	754	ASN
1	A	797	ASN
1	A	826	GLN
1	A	905	GLN
1	A	1019	GLN
2	B	80	HIS
2	B	194	ASN
2	B	207	ASN
2	B	258	GLN
2	B	264	GLN
2	B	271	ASN
2	B	284	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)

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	$\#\|Z\| > 2$
4	NAG	C	1	4,2	14,14,15	0.51	0	17,19,21	0.92	1 (5%)
4	NAG	C	2	4	14,14,15	0.65	0	17,19,21	1.41	1 (5%)

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	C	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2	NAG	C2-N2-C7	3.95	128.52	122.90
4	C	1	NAG	C1-O5-C5	2.65	115.78	112.19

There are no chirality outliers.

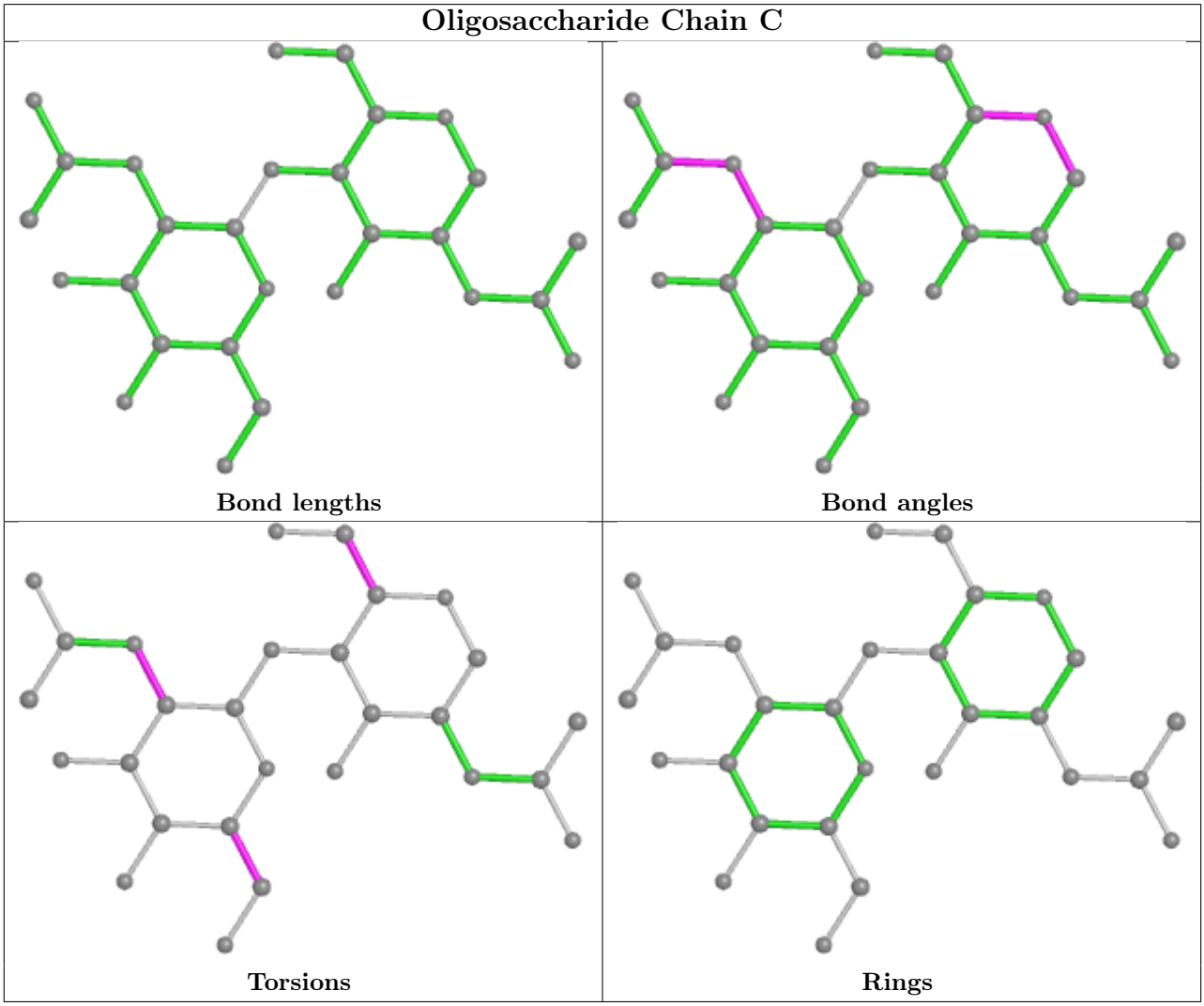
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C3-C2-N2-C7

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 8 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
9	CLR	B	3001	-	31,31,31	0.46	0	48,48,48	1.10	5 (10%)
10	NAG	B	4021	2	14,14,15	0.59	0	17,19,21	1.25	2 (11%)
5	MF4	A	2001	1	0,4,4	-	-	-		

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
10	NAG	B	4021	2	-	0/6/23/26	0/1/1/1
9	CLR	B	3001	-	-	2/10/68/68	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	3001	CLR	C15-C14-C13	3.00	107.46	103.84
10	B	4021	NAG	C1-O5-C5	2.62	115.74	112.19
9	B	3001	CLR	C1-C2-C3	2.56	113.75	110.47
9	B	3001	CLR	C4-C5-C6	-2.51	116.99	120.61
9	B	3001	CLR	C4-C5-C10	2.46	119.69	116.42
10	B	4021	NAG	C4-C3-C2	2.31	114.40	111.02
9	B	3001	CLR	C12-C11-C9	2.05	116.67	113.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	3001	CLR	C23-C24-C25-C26
9	B	3001	CLR	C23-C24-C25-C27

There are no ring outliers.

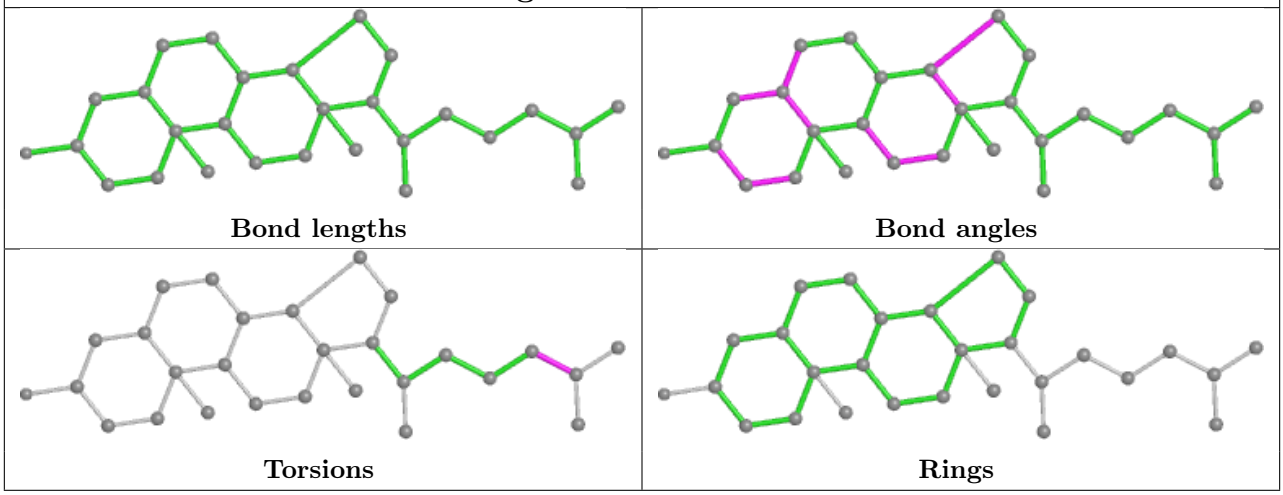
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	3001	CLR	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 all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLR B 3001



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	A	992/1028 (96%)	0.69	105 (10%) 6 8	112, 134, 175, 200	0
2	B	268/305 (87%)	0.88	45 (16%) 1 2	133, 183, 208, 218	0
3	G	39/74 (52%)	0.31	1 (2%) 56 53	129, 138, 181, 185	0
All	All	1299/1407 (92%)	0.72	151 (11%) 4 6	112, 139, 196, 218	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	PRO	8.4
1	A	260	TYR	7.3
1	A	578	PHE	6.5
1	A	580	THR	5.8
1	A	183	GLU	5.7
1	A	571	PHE	5.4
2	B	123	PRO	5.3
1	A	880	PRO	5.2
1	A	57	THR	5.1
1	A	534	MET	5.0
1	A	530	LEU	5.0
1	A	585	PHE	5.0
1	A	79	SER	4.9
1	A	563	ASP	4.9
1	A	41	MET	4.9
2	B	214	ARG	4.9
1	A	503	TYR	4.8
1	A	894	TRP	4.5
1	A	78	ASN	4.5
1	A	72	LEU	4.4
2	B	199	PRO	4.2
1	A	567	GLU	4.1
1	A	504	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	815	ASP	4.1
1	A	573	ALA	4.0
1	A	42	ASP	3.9
2	B	274	LEU	3.9
2	B	273	GLU	3.9
2	B	121	ASN	3.9
2	B	298	GLU	3.9
1	A	171	VAL	3.8
2	B	80	HIS	3.8
1	A	521	ILE	3.7
2	B	271	ASN	3.7
2	B	272	MET	3.7
2	B	270	GLN	3.6
1	A	86	THR	3.6
1	A	312	ILE	3.6
1	A	562	GLU	3.6
1	A	185	VAL	3.6
2	B	79	SER	3.6
1	A	55	TYR	3.5
1	A	660	ALA	3.4
2	B	269	THR	3.4
1	A	80	LEU	3.3
1	A	317	TRP	3.2
1	A	186	VAL	3.2
1	A	90	ILE	3.2
2	B	180	LYS	3.2
2	B	305	SER	3.2
1	A	565	TYR	3.2
1	A	883	LEU	3.2
1	A	492	ILE	3.1
2	B	155	MET	3.0
1	A	514	ILE	2.9
1	A	182	ALA	2.9
1	A	814	THR	2.9
1	A	556	CYS	2.9
2	B	238	ALA	2.9
2	B	230	GLU	2.9
1	A	91	LYS	2.9
1	A	779	THR	2.8
1	A	517	ARG	2.8
1	A	538	PHE	2.8
1	A	878	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	194	ASN	2.8
1	A	529	PRO	2.8
1	A	77	PRO	2.8
2	B	142	ASP	2.7
1	A	335	GLY	2.7
1	A	576	PRO	2.7
1	A	220	GLY	2.7
1	A	505	LEU	2.7
1	A	574	ASP	2.7
2	B	231	TYR	2.7
2	B	139	ASP	2.7
1	A	434	GLN	2.6
1	A	82	PRO	2.6
1	A	557	HIS	2.6
1	A	587	GLY	2.6
1	A	99	GLY	2.6
1	A	533	ASP	2.6
2	B	216	ALA	2.6
3	G	16	TYR	2.6
1	A	566	ASN	2.6
2	B	205	ASN	2.6
1	A	930	GLN	2.5
2	B	128	SER	2.5
2	B	303	VAL	2.5
1	A	586	VAL	2.5
2	B	281	TYR	2.5
2	B	129	ASP	2.5
1	A	94	ARG	2.5
2	B	117	SER	2.5
1	A	558	PHE	2.5
1	A	378	THR	2.4
1	A	967	PHE	2.4
2	B	147	LYS	2.4
1	A	51	LEU	2.4
1	A	98	GLY	2.4
1	A	781	THR	2.4
1	A	255	ARG	2.4
2	B	255	LYS	2.4
2	B	304	LYS	2.4
1	A	771	ASN	2.3
1	A	572	ASP	2.3
1	A	527	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	184	PHE	2.3
1	A	493	HIS	2.3
2	B	183	ARG	2.3
1	A	518	CYS	2.3
1	A	778	TYR	2.3
1	A	173	ARG	2.3
1	A	427	LEU	2.3
1	A	84	PRO	2.3
1	A	568	GLY	2.3
2	B	140	LEU	2.3
1	A	896	SER	2.2
1	A	555	PHE	2.2
1	A	76	GLY	2.2
2	B	97	LYS	2.2
2	B	237	TYR	2.2
1	A	577	ASN	2.2
1	A	879	LEU	2.2
2	B	296	ARG	2.2
1	A	476	LYS	2.2
1	A	569	TYR	2.2
2	B	302	GLU	2.2
2	B	70	GLN	2.1
1	A	813	GLY	2.1
1	A	564	LYS	2.1
1	A	515	LEU	2.1
2	B	169	GLY	2.1
1	A	36	LYS	2.1
2	B	300	LYS	2.1
1	A	536	GLU	2.1
1	A	126	ALA	2.1
1	A	1021	THR	2.1
2	B	234	LEU	2.1
2	B	124	PHE	2.1
1	A	83	PRO	2.1
1	A	777	ALA	2.1
1	A	189	ASP	2.1
1	A	75	ASP	2.1
1	A	826	GLN	2.0
1	A	87	PRO	2.0
2	B	204	ALA	2.0
1	A	785	PRO	2.0
1	A	675	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	528	GLU	2.0
2	B	203	GLN	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)

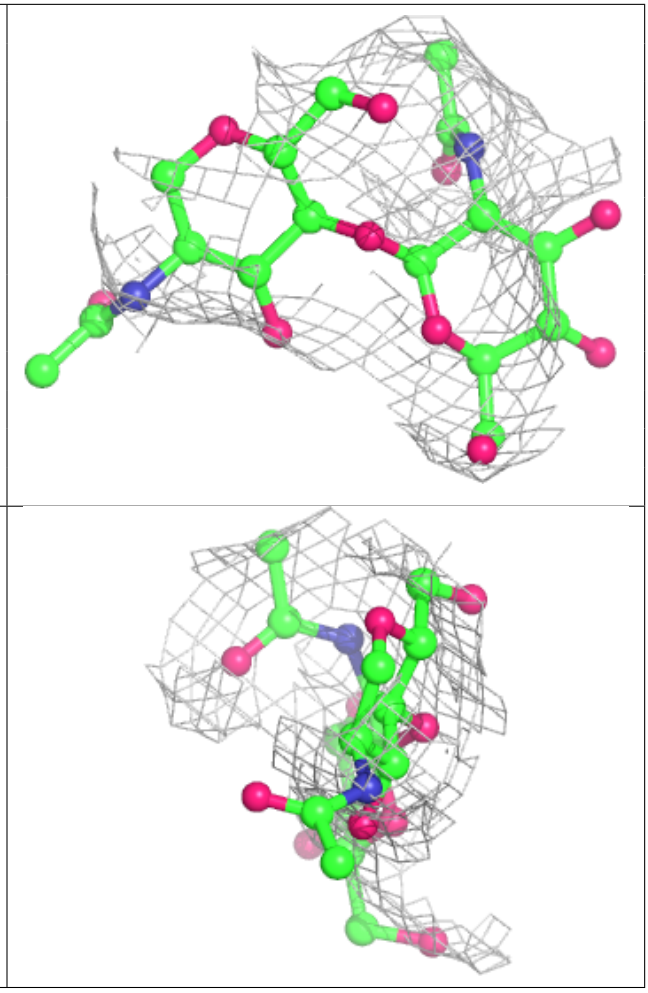
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	2	14/15	0.44	0.43	197,197,198,198	0
4	NAG	C	1	14/15	0.82	0.38	190,193,194,195	0

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

Electron density around Chain C:

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



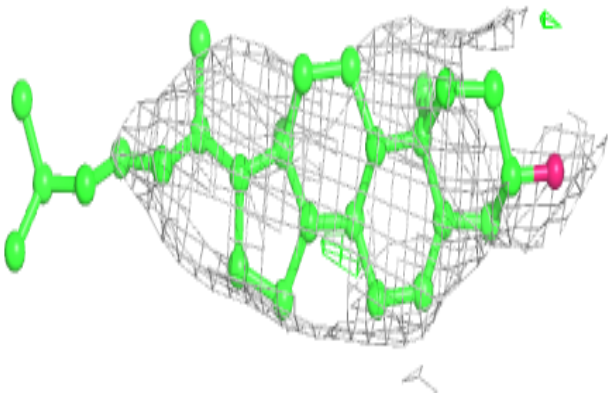
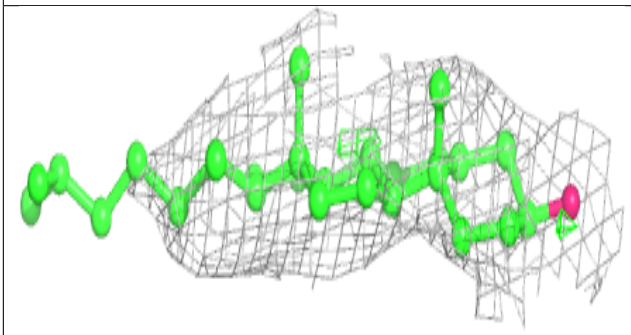
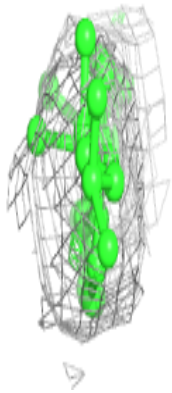
6.4 Ligands (i)

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
10	NAG	B	4021	14/15	0.69	0.49	196,197,197,197	0
6	MG	A	2002	1/1	0.81	0.51	114,114,114,114	0
9	CLR	B	3001	28/28	0.83	0.30	176,176,176,177	0
5	MF4	A	2001	5/5	0.88	0.50	117,119,120,121	0
7	TL	A	2006[B]	1/1	0.93	0.04	130,130,130,130	1
8	K	A	2005[A]	1/1	0.93	0.04	130,130,130,130	1
7	TL	A	2003	1/1	0.94	0.06	135,135,135,135	0
7	TL	A	2004	1/1	0.97	0.12	135,135,135,135	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 CLR B 3001: $2mF_o$-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.