Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 01:44 PM EDT

PDB ID	:	2ZXE
Title	:	Crystal structure of the sodium - potassium pump in the E2.2K+.Pi state
Authors	:	Shinoda, T.; Ogawa, H.; Cornelius, F.; Toyoshima, C.
Deposited on	:	2008-12-22
Resolution	:	2.40 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:

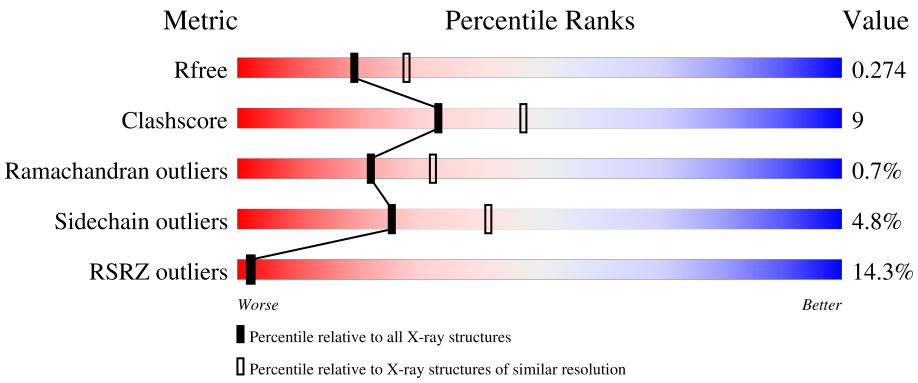
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	9%, 74%, 21%, • •
2	B	305	28%, 67%, 18%, •, 13%
3	G	74	11%, 38%, 15%, 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NDG	C	2	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10340 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	265	2151	1392	355	393	11	0	0	0

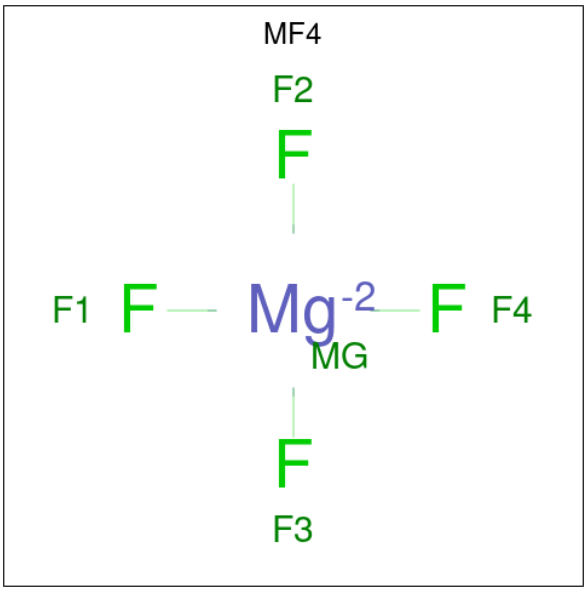
- Molecule 3 is a protein called Phospholemman-like protein.

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-alpha-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

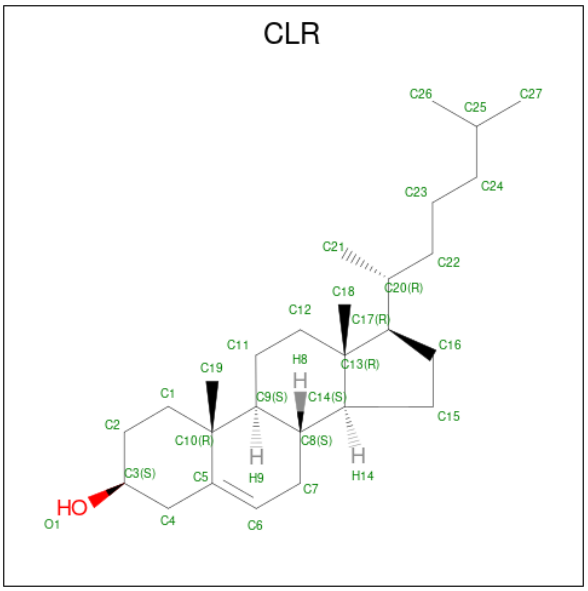
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

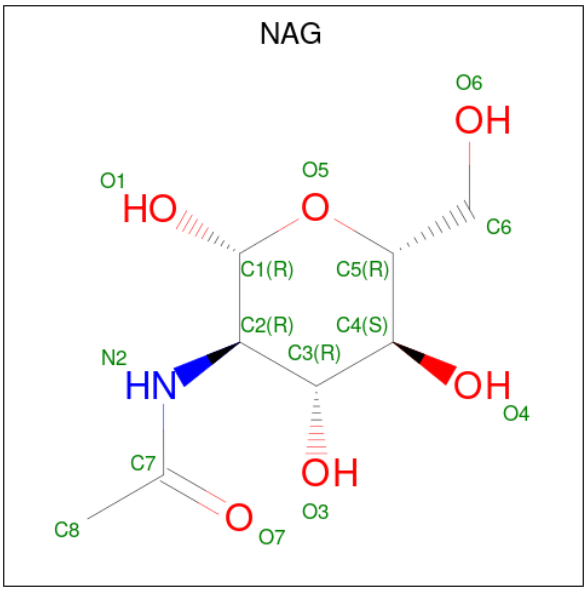
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total K 3 3	0	0

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	28	27	1	0	0

- Molecule 9 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		
9	B	1	14	8	1	5	0	0

- Molecule 10 is water.

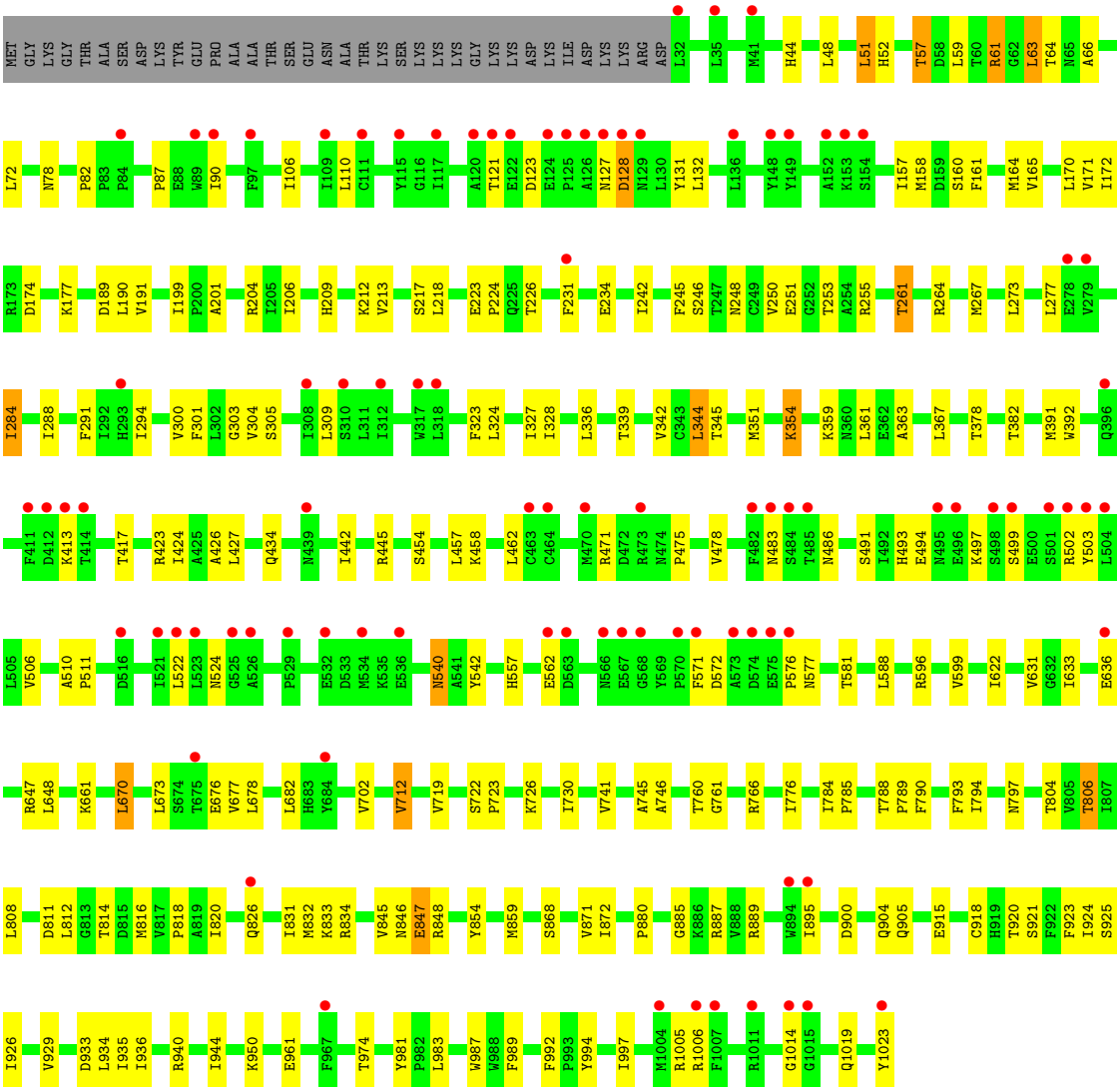
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	130	130	130	0	0

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.

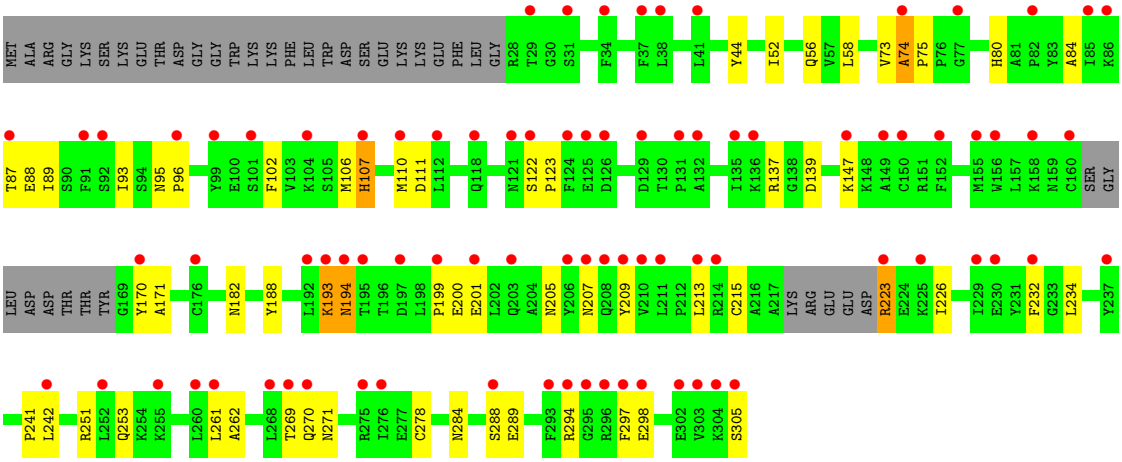
- Molecule 1: Na, K-ATPase alpha subunit

Chain A:



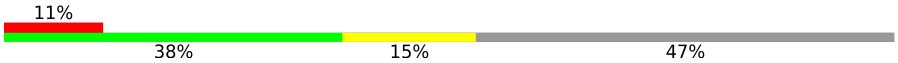
- Molecule 2: Na+,K+-ATPase beta subunit

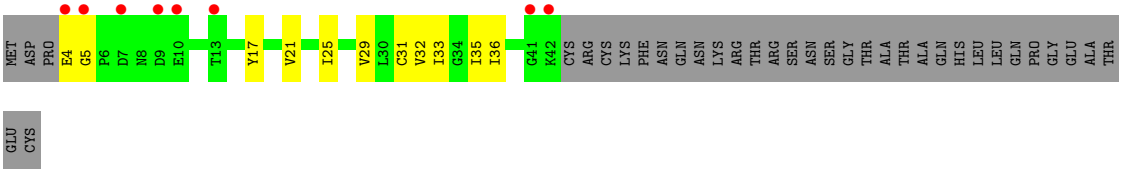
Chain B:



• Molecule 3: Phospholemman-like protein

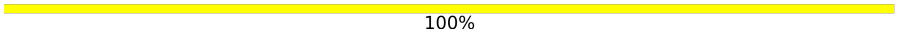
Chain G:





• Molecule 4: 2-acetamido-2-deoxy-alpha-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	223.81Å 50.91Å 163.79Å 90.00° 105.12° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 14.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.40) 99.1 (14.99-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.246 , 0.271 0.246 , 0.274	Depositor DCC
R_{free} test set	3555 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10340	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: K, CLR, NAG, NDG, MF4, MG

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	0.33	0/2205	0.48	0/2970
3	G	0.36	0/309	0.46	0/419
All	All	0.37	0/10339	0.51	0/14005

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	130	0
2	B	2151	0	2123	42	0
3	G	305	0	318	7	0
4	C	28	0	24	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	28	0	46	0	0
9	B	14	0	13	0	0
10	A	130	0	0	5	0
All	All	10340	0	10223	175	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 9.

All (175) 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:261:THR:HG21	10:A:5063:HOH:O	1.84	0.76
1:A:497:LYS:HE2	1:A:499:SER:HB2	1.69	0.76
1:A:868:SER:O	1:A:872:ILE:HG12	1.86	0.75
1:A:61:ARG:HH11	1:A:61:ARG:HB3	1.52	0.73
1:A:677:VAL:HG21	10:A:5074:HOH:O	1.87	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	0.71
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
1:A:905:GLN:NE2	2:B:182:ASN:HA	2.11	0.65
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	0.64
1:A:160:SER:HB3	1:A:741:VAL:HG22	1.80	0.64
1:A:78:ASN:HA	1:A:261:THR:HG23	1.79	0.63
1:A:816:MET:O	1:A:820:ILE:HG12	1.97	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
1:A:673:LEU:HD22	1:A:677:VAL:HG11	1.80	0.63
2:B:193:LYS:HA	2:B:207:ASN:HD21	1.65	0.62
1:A:64:THR:HG22	1:A:66:ALA:H	1.65	0.61
1:A:323:PHE:O	1:A:327:ILE:HG12	2.01	0.61
3:G:29:VAL:O	3:G:33:ILE:HG12	2.00	0.60
1:A:363:ALA:HB1	1:A:730:ILE:HD12	1.83	0.60
1:A:483:ASN:HB2	1:A:486:ASN:HB2	1.82	0.60
2:B:270:GLN:HG2	2:B:271:ASN:ND2	2.16	0.60
1:A:344:LEU:HB3	1:A:361:LEU:HG	1.84	0.60
1:A:905:GLN:HE21	2:B:182:ASN:HA	1.66	0.60
1:A:392:TRP:HB3	1:A:588:LEU:HB2	1.84	0.59
2:B:84:ALA:HB1	2:B:88:GLU:H	1.67	0.59
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	0.58
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	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:PRO:HG2	2:B:294:ARG:HH21	1.68	0.57
1:A:491:SER:HB3	1:A:493:HIS:NE2	2.20	0.57
2:B:193:LYS:HA	2:B:207:ASN:ND2	2.20	0.57
2:B:74:ALA:HB3	2:B:75:PRO:CD	2.29	0.57
1:A:818:PRO:HB3	1:A:934:LEU:HD22	1.87	0.56
2:B:52:ILE:O	2:B:56:GLN:HG2	2.05	0.56
2:B:137:ARG:HD2	2:B:147:LYS:HB3	1.88	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	0.55
1:A:190:LEU:HD11	1:A:206:ILE:HD11	1.88	0.55
1:A:157:ILE:HD11	1:A:745:ALA:HA	1.88	0.55
2:B:93:ILE:H	2:B:305:SER:HB2	1.72	0.55
1:A:351:MET:HA	1:A:354:LYS:HG2	1.88	0.55
1:A:994:TYR:O	1:A:997:ILE:HG22	2.06	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	0.55
1:A:924:ILE:HD12	1:A:983:LEU:HD12	1.89	0.54
1:A:64:THR:HG22	1:A:66:ALA:N	2.23	0.54
1:A:223:GLU:HB2	10:A:5106:HOH:O	2.07	0.54
1:A:994:TYR:HA	1:A:997:ILE:HG22	1.89	0.54
1:A:921:SER:HA	1:A:983:LEU:HD11	1.90	0.54
2:B:213:LEU:HD23	2:B:261:LEU:HD13	1.89	0.53
1:A:424:ILE:HG23	1:A:506:VAL:HB	1.90	0.53
1:A:51:LEU:CD1	1:A:204:ARG:HG3	2.36	0.53
1:A:161:PHE:HA	1:A:164:MET:HE3	1.90	0.53
1:A:324:LEU:O	1:A:328:ILE:HG12	2.09	0.53
1:A:161:PHE:HA	1:A:164:MET:CE	2.39	0.52
1:A:212:LYS:HD3	1:A:224:PRO:HB2	1.90	0.52
1:A:808:LEU:O	1:A:812:LEU:HB2	2.10	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:82:PRO:HA	1:A:158:MET:HG2	1.92	0.51
1:A:766:ARG:HD2	1:A:832:MET:HE2	1.91	0.51
3:G:25:ILE:O	3:G:29:VAL:HG23	2.11	0.51
1:A:572:ASP:HB3	1:A:577:ASN:HB2	1.92	0.51
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
2:B:232:PHE:HB2	2:B:262:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:GLN:HE22	1:A:950:LYS:HE3	1.78	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: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:132:LEU:HD21	1:A:804:THR:HG21	1.97	0.47
3:G:31:CYS:O	3:G:35:ILE:HG12	2.14	0.47
1:A:814:THR:HB	1:A:961:GLU:HG3	1.96	0.47
2:B:80:HIS:HB3	2:B:297:PHE:CZ	2.50	0.47
1:A:622:ILE:HG12	10:A:5110:HOH:O	2.14	0.47
2:B:87:THR:HB	2:B:298:GLU:O	2.14	0.47
1:A:336:LEU:HD11	1:A:776:ILE:HG12	1.96	0.46
2:B:215:CYS:HA	2:B:278:CYS:HA	1.96	0.46
1:A:127:ASN:HB3	1:A:131:TYR:CD1	2.50	0.46
1:A:924:ILE:HD12	1:A:983:LEU:CD1	2.45	0.46
1:A:63:LEU:HD22	1:A:189:ASP:HB3	1.96	0.46
2:B:226:ILE:HG22	2:B:269:THR:HB	1.96	0.46
1:A:631:VAL:HG23	1:A:633:ILE:HG12	1.96	0.46
1:A:234:GLU:HG2	10:A:5124:HOH:O	2.14	0.46
2:B:74:ALA:CB	2:B:75:PRO:CD	2.92	0.46
1:A:303:GLY:HA2	1:A:327:ILE:HG21	1.97	0.46
1:A:670:LEU:HD23	1:A:678:LEU:HD21	1.96	0.46
2:B:122:SER:HA	2:B:123:PRO:HA	1.75	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:889:ARG:HD2	1:A:895:ILE:CD1	2.46	0.45
1:A:475:PRO:HD2	1:A:494:GLU:HB2	1.99	0.45
1:A:676:GLU:H	1:A:676:GLU:CD	2.20	0.45
1:A:847:GLU:CD	1:A:847:GLU:H	2.20	0.45
2:B:84:ALA:HB1	2:B:88:GLU:N	2.32	0.45
1:A:722:SER:OG	1:A:723:PRO:HD3	2.17	0.45
1:A:631:VAL:CG2	1:A:633:ILE:HG12	2.46	0.45
1:A:52:HIS:HE2	1:A:59:LEU:HD12	1.82	0.44
1:A:915:GLU:O	1:A:918:CYS:HB2	2.17	0.44
2:B:194:ASN:HD22	2:B:194:ASN:N	2.15	0.44
1:A:806:THR:HG22	1:A:923:PHE:HB2	2.00	0.44
1:A:859:MET:HG2	2:B:44:TYR:CE2	2.53	0.44
1:A:354:LYS:HZ2	1:A:354:LYS:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LEU:HG	2:B:241:PRO:HG3	1.99	0.44
1:A:246:SER:OG	1:A:267:MET:HG3	2.18	0.44
2:B:107:HIS:O	2:B:111:ASP:HB2	2.18	0.44
1:A:273:LEU:O	1:A:277:LEU:HG	2.19	0.43
2:B:107:HIS:ND1	2:B:170:TYR:HE1	2.17	0.43
1:A:790:PHE:O	1:A:794:ILE:HG12	2.19	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
1:A:87:PRO:HD2	1:A:90:ILE:HD12	1.99	0.43
2:B:147:LYS:HB2	2:B:253:GLN:HG3	1.99	0.43
3:G:4:GLU:CD	3:G:5:GLY:H	2.23	0.43
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:766:ARG:HD2	1:A:832:MET:HE1	2.02	0.42
1:A:797:ASN:HB3	1:A:885:GLY:HA2	2.01	0.42
1:A:940:ARG:HE	1:A:1023:TYR:HB2	1.84	0.42
1:A:291:PHE:HA	1:A:294:ILE:HD12	2.01	0.42
1:A:300:VAL:O	1:A:304:VAL:HG22	2.19	0.42
2:B:188:TYR:O	2:B:284:ASN:ND2	2.53	0.42
2:B:89:ILE:HG22	2:B:102:PHE:CE2	2.55	0.42
2:B:223:ARG:HB2	2:B:223:ARG:HH11	1.84	0.42
1:A:170:LEU:HD21	1:A:177:LYS:HD3	2.00	0.42
1:A:291:PHE:HB3	1:A:845:VAL:HB	2.02	0.42
2:B:95:ASN:HA	2:B:96:PRO:HD3	1.86	0.42
1:A:48:LEU:HD23	1:A:59:LEU:HD11	2.01	0.42
1:A:510:ALA:HA	1:A:511:PRO:HD3	1.94	0.42
1:A:784:ILE:N	1:A:785:PRO:HD2	2.35	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: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
1:A:367:LEU:HD23	1:A:761:GLY:HA3	2.01	0.41
1:A:378:THR:HA	1:A:382:THR:OG1	2.20	0.41
1:A:846:ASN:ND2	1:A:848:ARG:HB2	2.35	0.41
2:B:271:ASN:HD21	2:B:305:SER:N	2.19	0.41
1:A:44:HIS:HB3	1:A:242:ILE:HD11	2.03	0.41
1:A:502:ARG:HE	1:A:562:GLU:HG2	1.85	0.41
1:A:920:THR:HG21	1:A:981:TYR:O	2.20	0.41
3:G:17:TYR:O	3:G:21:VAL:HG23	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:VAL:HG22	2:B:58:LEU:HD13	2.02	0.41
1:A:502:ARG:HG3	1:A:562:GLU:HG2	2.02	0.41
1:A:540:ASN:HD22	1:A:540:ASN:N	2.18	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:423:ARG:O	1:A:427:LEU:HB2	2.21	0.41
1:A:458:LYS:O	1:A:462:LEU:HB2	2.21	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG21	2.03	0.41
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:925:SER:O	1:A:929:VAL:HG22	2.22	0.40
1:A:199:ILE:HG22	1:A:201:ALA:O	2.22	0.40
1:A:900:ASP:OD1	1:A:904:GLN:HB2	2.21	0.40
1:A:989:PHE:HA	1:A:992:PHE:CD2	2.57	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	990/1028 (96%)	942 (95%)	43 (4%)	5 (0%)	29	41
2	B	259/305 (85%)	220 (85%)	35 (14%)	4 (2%)	10	14
3	G	37/74 (50%)	33 (89%)	4 (11%)	0	100	100
All	All	1286/1407 (91%)	1195 (93%)	82 (6%)	9 (1%)	22	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	128	ASP

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Mol	Chain	Res	Type
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	38
2	B	232/266 (87%)	223 (96%)	9 (4%)	32	50
3	G	32/62 (52%)	32 (100%)	0	100	100
All	All	1104/1197 (92%)	1051 (95%)	53 (5%)	25	41

All (53) 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
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

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Mol	Chain	Res	Type
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	73	VAL
2	B	107	HIS
2	B	139	ASP
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 (19) 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	434	GLN
1	A	524	ASN
1	A	540	ASN
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	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	1.60	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NDG	C	2	4	14,14,15	0.49	0	17,19,21	1.13	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	-	0/6/23/26	0/1/1/1
4	NDG	C	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1	NAG	C1-O5-C5	5.23	119.28	112.19
4	C	2	NDG	C1-O5-C5	2.59	115.70	112.19
4	C	1	NAG	C1-C2-N2	2.18	114.21	110.49

There are no chirality outliers.

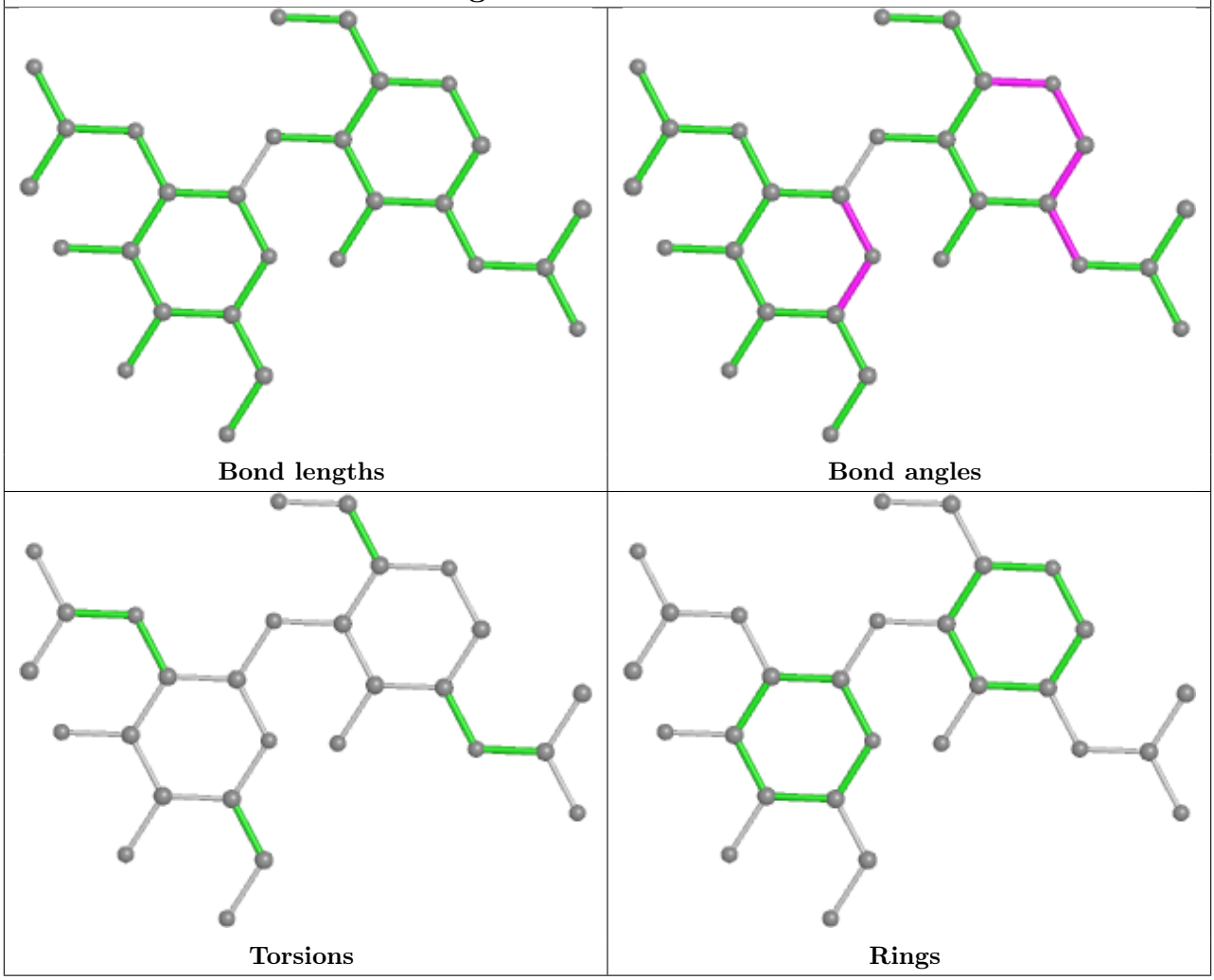
There are no torsion outliers.

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.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
8	CLR	A	3001	-	31,31,31	0.46	0	48,48,48	1.10	5 (10%)
5	MF4	A	2001	-	0,4,4	-	-	-		
9	NAG	B	4021	2	14,14,15	0.60	0	17,19,21	1.24	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	A	3001	-	-	2/10/68/68	0/4/4/4
9	NAG	B	4021	2	-	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(^{o})	Ideal(^{o})
8	A	3001	CLR	C15-C14-C13	2.97	107.42	103.84
9	B	4021	NAG	C1-O5-C5	2.62	115.74	112.19
8	A	3001	CLR	C1-C2-C3	2.58	113.78	110.47
8	A	3001	CLR	C4-C5-C6	-2.50	117.00	120.61
8	A	3001	CLR	C4-C5-C10	2.44	119.66	116.42
9	B	4021	NAG	C4-C3-C2	2.27	114.34	111.02
8	A	3001	CLR	C12-C11-C9	2.07	116.69	113.11

There are no chirality outliers.

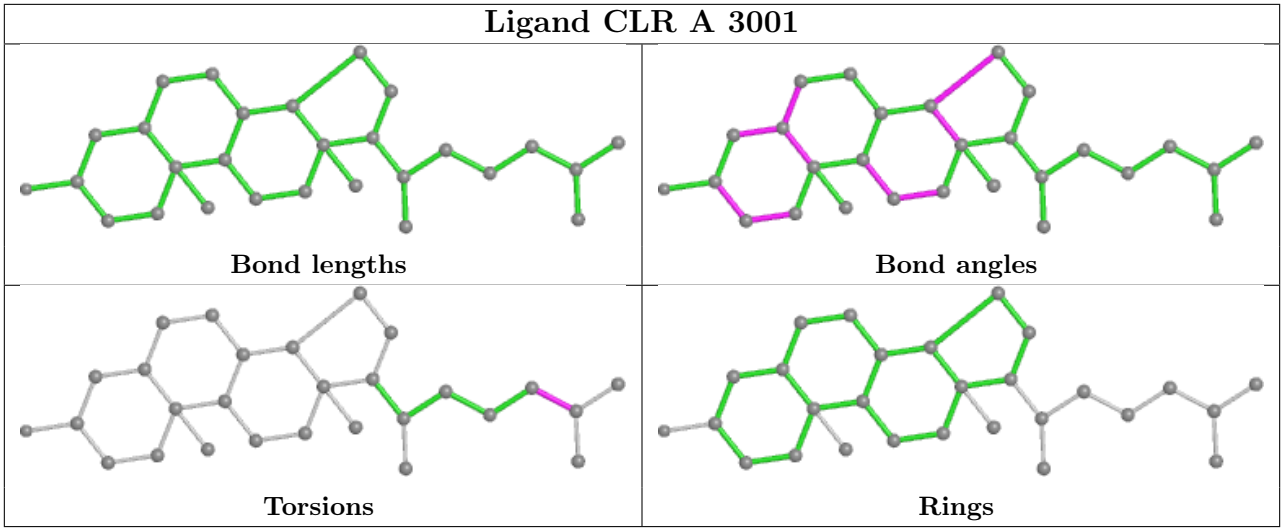
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	3001	CLR	C23-C24-C25-C26
8	A	3001	CLR	C23-C24-C25-C27

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 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.



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%)	0.32	92 (9%)	8	8	24, 46, 87, 112	0
2	B	265/305 (86%)	1.54	85 (32%)	0	0	44, 94, 120, 124	0
3	G	39/74 (52%)	0.76	8 (20%)	1	0	41, 50, 93, 97	0
All	All	1296/1407 (92%)	0.58	185 (14%)	2	2	24, 51, 108, 124	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	268	LEU	10.0
2	B	195	THR	8.5
1	A	125	PRO	6.8
1	A	126	ALA	6.8
1	A	562	GLU	6.5
1	A	563	ASP	6.4
2	B	304	LYS	6.4
3	G	41	GLY	6.1
2	B	303	VAL	5.9
1	A	501	SER	5.5
1	A	498	SER	5.4
1	A	89	TRP	5.1
2	B	149	ALA	5.0
1	A	127	ASN	5.0
1	A	574	ASP	5.0
2	B	214	ARG	4.9
1	A	894	TRP	4.7
2	B	160	CYS	4.7
1	A	32	LEU	4.7
2	B	99	TYR	4.7
1	A	121	THR	4.6
2	B	121	ASN	4.6
2	B	96	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	317	TRP	4.6
2	B	296	ARG	4.5
2	B	85	ILE	4.4
2	B	230	GLU	4.4
2	B	295	GLY	4.4
2	B	207	ASN	4.4
1	A	97	PHE	4.4
1	A	568	GLY	4.3
1	A	1007	PHE	4.3
1	A	675	THR	4.2
2	B	298	GLU	4.2
1	A	412	ASP	4.2
2	B	156	TRP	4.1
1	A	153	LYS	4.1
2	B	194	ASN	4.0
1	A	231	PHE	3.9
2	B	199	PRO	3.9
1	A	566	ASN	3.8
1	A	571	PHE	3.8
3	G	7	ASP	3.7
2	B	252	LEU	3.7
1	A	503	TYR	3.7
3	G	4	GLU	3.7
1	A	154	SER	3.7
1	A	567	GLU	3.7
1	A	414	THR	3.7
3	G	5	GLY	3.6
2	B	136	LYS	3.6
1	A	499	SER	3.6
1	A	470	MET	3.6
2	B	92	SER	3.5
2	B	155	MET	3.5
1	A	684	TYR	3.4
1	A	84	PRO	3.4
3	G	42	LYS	3.4
2	B	255	LYS	3.4
2	B	150	CYS	3.3
1	A	41	MET	3.3
1	A	115	TYR	3.3
1	A	149	TYR	3.3
2	B	237	TYR	3.3
2	B	193	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	209	TYR	3.3
1	A	318	LEU	3.3
1	A	439	ASN	3.3
2	B	124	PHE	3.2
2	B	203	GLN	3.2
2	B	176	CYS	3.2
1	A	895	ILE	3.1
1	A	279	VAL	3.1
2	B	206	TYR	3.1
3	G	13	THR	3.1
2	B	158	LYS	3.0
1	A	967	PHE	2.9
2	B	210	VAL	2.9
2	B	34	PHE	2.9
2	B	213	LEU	2.9
2	B	126	ASP	2.8
1	A	826	GLN	2.8
1	A	496	GLU	2.8
2	B	29	THR	2.8
1	A	122	GLU	2.8
1	A	570	PRO	2.8
1	A	411	PHE	2.8
2	B	232	PHE	2.8
2	B	91	PHE	2.8
1	A	523	LEU	2.7
2	B	135	ILE	2.7
2	B	122	SER	2.7
1	A	413	LYS	2.7
2	B	118	GLN	2.7
1	A	128	ASP	2.7
2	B	211	LEU	2.6
1	A	525	GLY	2.6
1	A	1006	ARG	2.6
1	A	312	ILE	2.6
2	B	74	ALA	2.6
2	B	276	ILE	2.6
1	A	109	ILE	2.6
1	A	485	THR	2.5
1	A	35	LEU	2.5
1	A	576	PRO	2.5
1	A	117	ILE	2.5
1	A	120	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	473	ARG	2.5
2	B	223	ARG	2.5
1	A	124	GLU	2.5
1	A	129	ASN	2.5
1	A	483	ASN	2.5
2	B	112	LEU	2.5
1	A	148	TYR	2.4
2	B	201	GLU	2.4
1	A	534	MET	2.4
2	B	297	PHE	2.4
1	A	396	GLN	2.4
1	A	522	LEU	2.4
2	B	38	LEU	2.4
2	B	242	LEU	2.4
2	B	288	SER	2.4
2	B	77	GLY	2.4
2	B	132	ALA	2.4
2	B	269	THR	2.4
2	B	125	GLU	2.4
2	B	104	LYS	2.4
1	A	1015	GLY	2.4
1	A	463	CYS	2.4
3	G	9	ASP	2.4
1	A	111	CYS	2.4
2	B	275	ARG	2.4
1	A	278	GLU	2.4
2	B	152	PHE	2.4
2	B	170	TYR	2.4
3	G	10	GLU	2.4
1	A	308	ILE	2.3
1	A	521	ILE	2.3
1	A	1023	TYR	2.3
1	A	136	LEU	2.3
2	B	147	LYS	2.3
2	B	41	LEU	2.3
1	A	1004	MET	2.3
2	B	101	SER	2.3
1	A	636	GLU	2.3
1	A	529	PRO	2.3
2	B	260	LEU	2.3
2	B	31	SER	2.2
2	B	261	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1014	GLY	2.2
1	A	293	HIS	2.2
2	B	86	LYS	2.2
2	B	87	THR	2.2
1	A	575	GLU	2.2
1	A	502	ARG	2.2
1	A	1011	ARG	2.2
2	B	192	LEU	2.2
1	A	484	SER	2.2
2	B	294	ARG	2.2
1	A	152	ALA	2.2
1	A	536	GLU	2.2
2	B	302	GLU	2.2
1	A	532	GLU	2.2
1	A	516	ASP	2.2
2	B	305	SER	2.2
2	B	37	PHE	2.2
2	B	293	PHE	2.2
2	B	82	PRO	2.1
2	B	131	PRO	2.1
1	A	504	LEU	2.1
1	A	310	SER	2.1
2	B	110	MET	2.1
2	B	229	ILE	2.1
2	B	107	HIS	2.1
2	B	129	ASP	2.1
2	B	197	ASP	2.1
1	A	526	ALA	2.1
1	A	573	ALA	2.1
2	B	225	LYS	2.1
1	A	495	ASN	2.1
1	A	464	CYS	2.1
2	B	208	GLN	2.0
1	A	482	PHE	2.0
2	B	270	GLN	2.0
1	A	90	ILE	2.0

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

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

6.3 Carbohydrates (i)

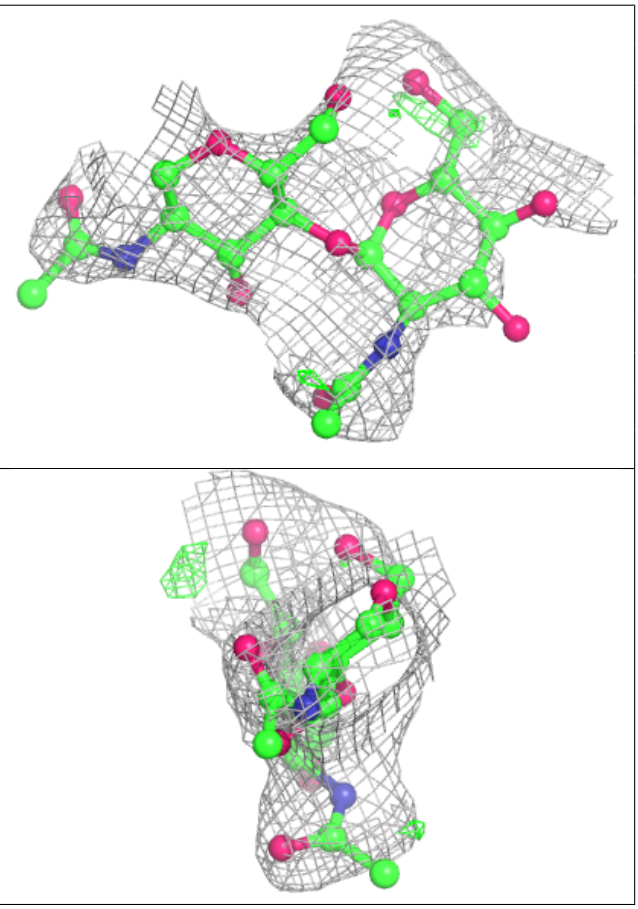
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NDG	C	2	14/15	0.56	0.43	111,111,111,111	0
4	NAG	C	1	14/15	0.79	0.25	107,108,109,110	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)

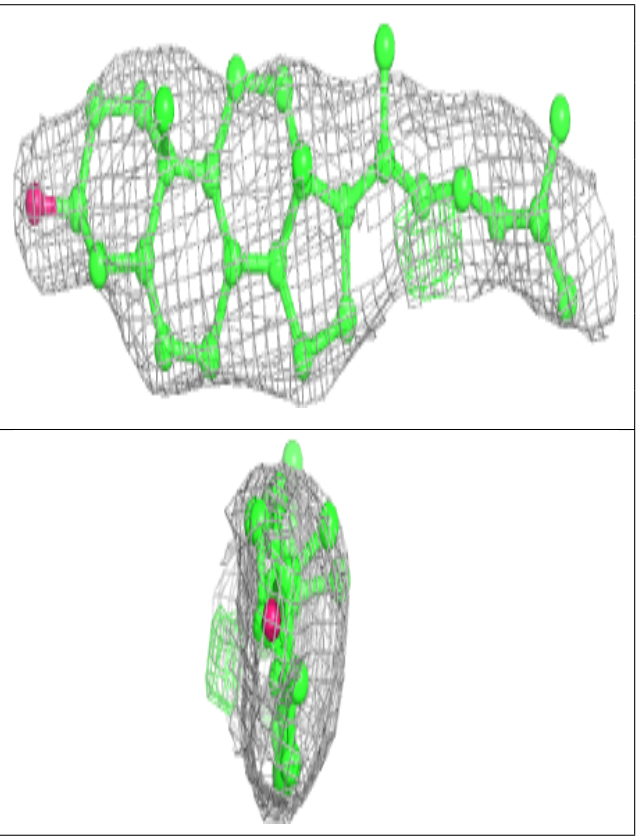
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	B	4021	14/15	0.69	0.38	108,109,109,109	0
8	CLR	A	3001	28/28	0.81	0.23	88,88,88,89	0
5	MF4	A	2001	5/5	0.95	0.18	29,31,32,33	0
7	K	A	2004	1/1	0.97	0.05	47,47,47,47	0
7	K	A	2003	1/1	0.98	0.08	47,47,47,47	0
6	MG	A	2002	1/1	0.98	0.06	26,26,26,26	0
7	K	A	2005	1/1	0.99	0.03	42,42,42,42	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 A 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.