Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2023 – 01:20 AM EDT

PDB ID	:	3NKN
Title	:	Crystal structure of mouse autotaxin in complex with 14:0-LPA
Authors	:	Nishimasu, H.; Ishitani, R.; Mihara, E.; Takagi, J.; Aoki, J.; Nureki, O.
Deposited on	:	2010-06-20
Resolution	:	1.80 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:

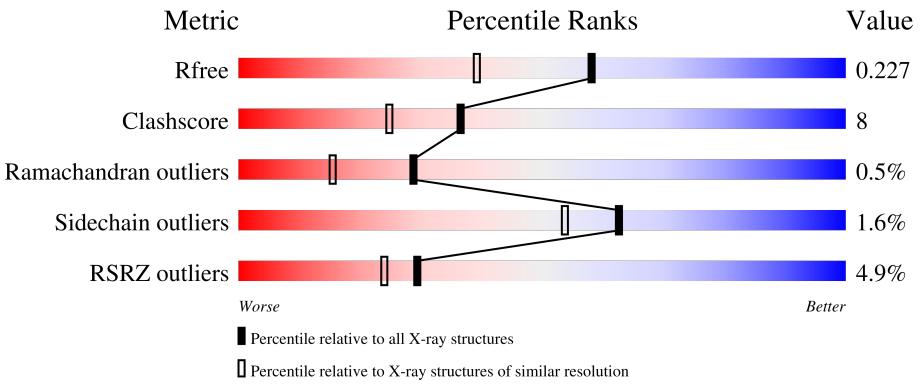
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	831	5%, 81%, 13%, • 6%
2	B	2	100%
2	D	2	50%, 50%
3	C	6	33%, 67%

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
10	EDO	A	1012	-	-	X	-
10	EDO	A	1025	-	-	X	-
10	EDO	A	1026	-	-	X	-
10	EDO	A	1027	-	-	X	-
10	EDO	A	1029	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7189 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	782	6268	3981	1068	1169	50	0	3	0

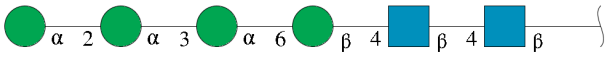
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	SEE REMARK 999	UNP Q9R1E6
A	?	-	VAL	SEE REMARK 999	UNP Q9R1E6
A	?	-	GLU	SEE REMARK 999	UNP Q9R1E6
A	?	-	PRO	SEE REMARK 999	UNP Q9R1E6
A	859	SER	-	expression tag	UNP Q9R1E6
A	860	ARG	-	expression tag	UNP Q9R1E6
A	861	GLU	-	expression tag	UNP Q9R1E6
A	862	ASN	-	expression tag	UNP Q9R1E6
A	863	LEU	-	expression tag	UNP Q9R1E6
A	864	TYR	-	expression tag	UNP Q9R1E6
A	865	PHE	-	expression tag	UNP Q9R1E6
A	866	GLN	-	expression tag	UNP Q9R1E6

- 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
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-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			
3	C	6	72	40	2	30	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	2	2	2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0

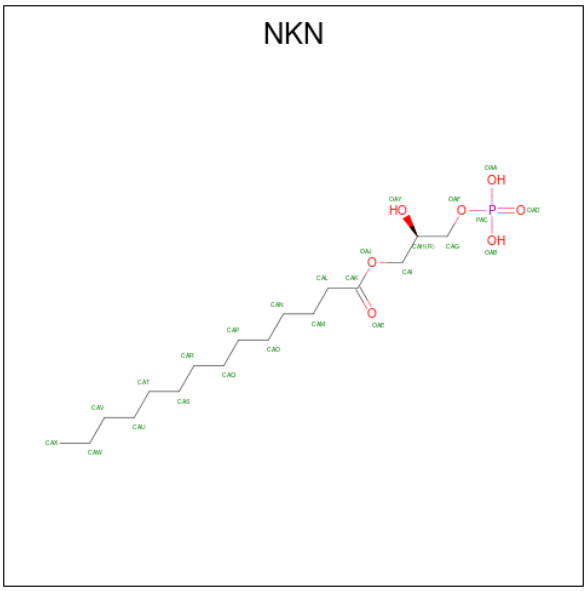
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

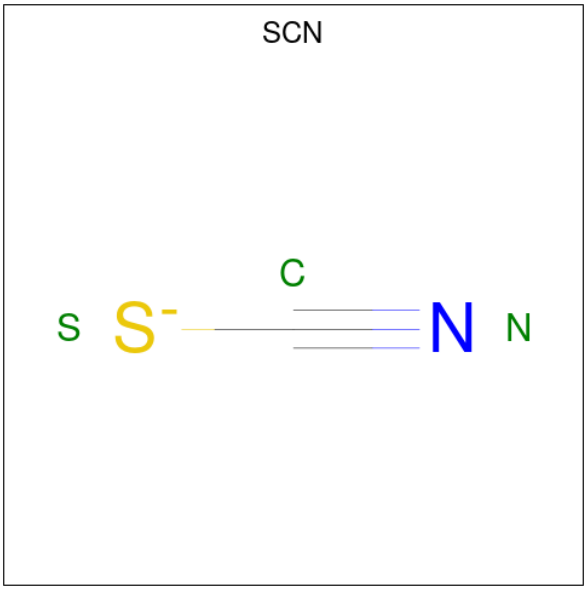
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	A	1	1	1	0	0

- Molecule 8 is (2R)-2-hydroxy-3-(phosphonooxy)propyl tetradecanoate (three-letter code: NKN) (formula: $C_{17}H_{35}O_7P$).



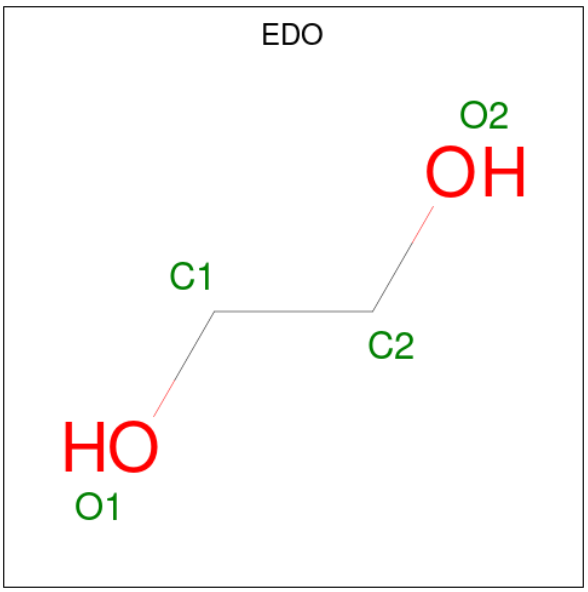
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O P 25 17 7 1	0	0
8	A	1	Total C 8 8	0	0

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N S 3 1 1 1	0	0
9	A	1	Total C N S 3 1 1 1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0
10	A	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0
			Total	C	O		
10	A	1	4	2	2	0	0

- Molecule 11 is water.

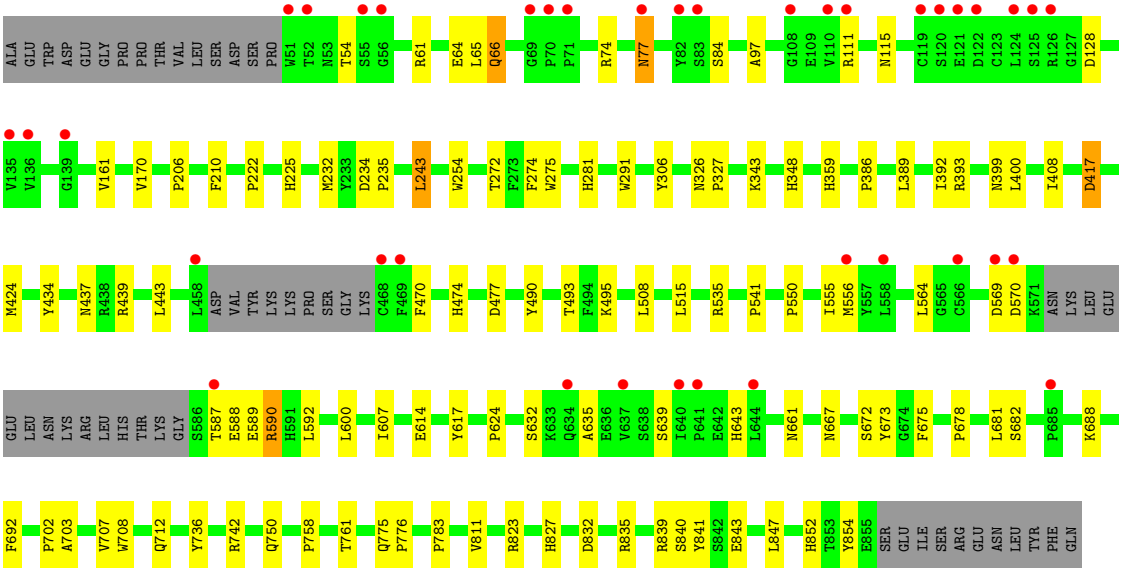
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	665	665	665	0	0

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.

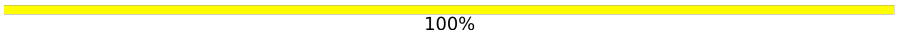
• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2

Chain A:



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

Chain B:

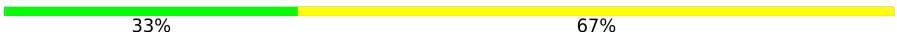


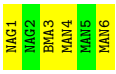
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam

ido-2-deoxy-beta-D-glucopyranose

Chain C: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.58Å 94.62Å 75.37Å 90.00° 94.86° 90.00°	Depositor
Resolution (Å)	32.85 – 1.80 43.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (32.85-1.80) 98.0 (43.94-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.184 , 0.234 0.179 , 0.227	Depositor DCC
R_{free} test set	3925 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7189	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: NKN, BMA, EDO, SCN, MAN, CA, ZN, NA, K, 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	0.47	0/6458	0.59	0/8781

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	6268	0	5949	98	0
2	B	28	0	25	1	0
2	D	28	0	25	0	0
3	C	72	0	61	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	33	0	48	2	0
9	A	6	0	0	0	0
10	A	84	0	126	36	0
11	A	665	0	0	8	0
All	All	7189	0	6234	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (101) 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:675:PHE:H	10:A:1012:EDO:H11	1.02	1.10
1:A:835:ARG:HE	10:A:1027:EDO:H22	1.11	1.07
1:A:702:PRO:HB2	10:A:1028:EDO:H22	1.42	1.00
1:A:272:THR:HG22	1:A:274:PHE:H	1.25	0.97
1:A:424:MET:HG3	11:A:1296:HOH:O	1.67	0.95
1:A:675:PHE:N	10:A:1012:EDO:H11	1.83	0.94
1:A:495:LYS:HG2	10:A:1030:EDO:H12	1.49	0.93
1:A:852:HIS:HD2	1:A:854:TYR:CZ	1.90	0.89
1:A:835:ARG:NE	10:A:1027:EDO:H22	1.92	0.81
1:A:570:ASP:HB2	1:A:643:HIS:CD2	2.17	0.79
1:A:675:PHE:H	10:A:1012:EDO:C1	1.90	0.77
1:A:742:ARG:HH21	10:A:1021:EDO:H11	1.49	0.76
1:A:437:ASN:HD21	10:A:1025:EDO:H22	1.51	0.73
1:A:667:ASN:HB2	11:A:1524:HOH:O	1.89	0.72
1:A:835:ARG:HE	10:A:1027:EDO:C2	1.98	0.70
1:A:535:ARG:CZ	10:A:1030:EDO:H22	2.23	0.68
1:A:535:ARG:NH2	10:A:1030:EDO:H22	2.08	0.68
1:A:111:ARG:NH2	1:A:128:ASP:OD2	2.27	0.68
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.78	0.66
1:A:439:ARG:CZ	10:A:1025:EDO:H21	2.27	0.65
1:A:600:LEU:HD11	1:A:832:ASP:HB2	1.79	0.64
1:A:742:ARG:NH2	10:A:1021:EDO:H11	2.12	0.64
1:A:399:ASN:HA	11:A:1399:HOH:O	1.97	0.63
1:A:570:ASP:HB2	1:A:643:HIS:HD2	1.62	0.61
1:A:852:HIS:CD2	1:A:854:TYR:CZ	2.82	0.60
1:A:417:ASP:HB3	11:A:1510:HOH:O	2.00	0.59
1:A:437:ASN:ND2	10:A:1025:EDO:H22	2.17	0.58
1:A:541:PRO:HG2	1:A:841:TYR:CD2	2.40	0.57
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.41	0.56
1:A:823:ARG:CZ	10:A:1010:EDO:H22	2.35	0.56
1:A:682:SER:OG	1:A:688:LYS:NZ	2.40	0.55
1:A:570:ASP:CB	1:A:643:HIS:CD2	2.90	0.55
1:A:77:ASN:ND2	1:A:274:PHE:O	2.41	0.54
1:A:54:THR:O	1:A:54:THR:HG22	2.08	0.54
1:A:111:ARG:HH22	1:A:128:ASP:CG	2.11	0.53
1:A:306:TYR:HB2	8:A:1006:NKN:HARA	1.89	0.53
1:A:839:ARG:HE	10:A:1029:EDO:C2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:NE	10:A:1029:EDO:H21	2.25	0.52
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.92	0.51
1:A:742:ARG:HH21	10:A:1021:EDO:C1	2.20	0.51
1:A:281:HIS:ND1	10:A:1026:EDO:C2	2.73	0.51
1:A:210:PHE:CE1	1:A:243:LEU:HD22	2.45	0.51
1:A:758:PRO:HD3	10:A:1019:EDO:H22	1.93	0.50
1:A:688:LYS:HG2	1:A:692:PHE:HE1	1.76	0.50
1:A:672:SER:OG	1:A:673:TYR:N	2.44	0.50
1:A:400:LEU:O	11:A:1498:HOH:O	2.19	0.50
1:A:437:ASN:HD21	10:A:1025:EDO:C2	2.21	0.49
1:A:493:THR:HG21	1:A:515:LEU:HD23	1.93	0.49
1:A:703:ALA:N	10:A:1028:EDO:H21	2.27	0.49
1:A:77:ASN:OD1	1:A:275:TRP:HA	2.13	0.49
1:A:281:HIS:ND1	10:A:1026:EDO:H21	2.26	0.49
1:A:97:ALA:HB3	1:A:115:ASN:HA	1.95	0.49
1:A:281:HIS:CE1	10:A:1026:EDO:H12	2.48	0.49
1:A:678:PRO:HG2	1:A:681:LEU:HD12	1.95	0.48
1:A:736:TYR:OH	1:A:750:GLN:HB3	2.13	0.48
1:A:541:PRO:HG2	1:A:841:TYR:HD2	1.78	0.48
1:A:343:LYS:HA	1:A:348:HIS:CD2	2.49	0.48
1:A:490:TYR:CD1	10:A:1011:EDO:H12	2.49	0.47
1:A:839:ARG:HE	10:A:1029:EDO:H21	1.78	0.47
1:A:840:SER:OG	1:A:843:GLU:HG3	2.14	0.47
1:A:392:ILE:HD12	1:A:443:LEU:HG	1.96	0.47
1:A:707:VAL:HG13	1:A:811:VAL:HG13	1.97	0.47
10:A:1027:EDO:H11	11:A:1419:HOH:O	2.13	0.47
1:A:65:LEU:HD21	1:A:291:TRP:CE2	2.50	0.46
1:A:272:THR:CG2	1:A:274:PHE:O	2.64	0.46
1:A:206:PRO:HB3	1:A:389:LEU:HD13	1.98	0.45
1:A:326:ASN:HB3	1:A:327:PRO:HD3	1.98	0.45
1:A:210:PHE:CD1	1:A:243:LEU:HD22	2.52	0.45
1:A:590:ARG:HH22	1:A:632:SER:HB3	1.80	0.45
1:A:61:ARG:HD2	1:A:64:GLU:OE1	2.18	0.44
1:A:272:THR:HG21	1:A:274:PHE:O	2.17	0.44
1:A:617:TYR:HA	1:A:624:PRO:HA	1.99	0.44
1:A:839:ARG:HG3	10:A:1029:EDO:H21	1.99	0.44
10:A:1027:EDO:H21	11:A:1338:HOH:O	2.17	0.44
1:A:64:GLU:OE1	1:A:66:GLN:NE2	2.50	0.44
1:A:77:ASN:ND2	1:A:272:THR:HG21	2.33	0.44
1:A:348:HIS:CD2	1:A:348:HIS:H	2.36	0.44
1:A:827:HIS:HE1	11:A:906:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:O	1:A:54:THR:CG2	2.66	0.43
1:A:470:PHE:CD1	1:A:470:PHE:C	2.91	0.43
1:A:564:LEU:O	1:A:661:ASN:HB2	2.18	0.43
1:A:761:THR:HA	10:A:1015:EDO:H12	2.01	0.43
1:A:74:ARG:HD3	1:A:84:SER:OG	2.18	0.43
1:A:588:GLU:O	1:A:589:GLU:C	2.55	0.43
1:A:783:PRO:HB3	10:A:1029:EDO:H12	2.01	0.43
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.54	0.43
1:A:359:HIS:CE1	1:A:474:HIS:CE1	3.06	0.43
1:A:852:HIS:CD2	1:A:854:TYR:CE1	3.07	0.42
1:A:847:LEU:HD12	10:A:1020:EDO:H11	2.02	0.42
1:A:708:TRP:CD1	10:A:1012:EDO:H12	2.54	0.42
1:A:775:GLN:HA	1:A:776:PRO:HD3	1.90	0.42
1:A:281:HIS:HE1	10:A:1026:EDO:H12	1.85	0.42
1:A:555:ILE:O	1:A:556:MET:HG3	2.20	0.42
1:A:592:LEU:HD23	1:A:614:GLU:OE1	2.20	0.42
1:A:708:TRP:O	1:A:712:GLN:HG2	2.20	0.41
2:B:1:NAG:H83	2:B:1:NAG:H2	1.91	0.41
1:A:508:LEU:HA	1:A:508:LEU:HD23	1.83	0.41
1:A:234:ASP:HA	1:A:235:PRO:HD3	1.93	0.41
1:A:254:TRP:HB2	8:A:1007:NKN:HATA	2.03	0.41
1:A:393:ARG:HA	10:A:1017:EDO:H21	2.02	0.41
1:A:678:PRO:CG	1:A:681:LEU:HD12	2.51	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	779/831 (94%)	745 (96%)	30 (4%)	4 (0%)	29 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	ASP
1	A	477	ASP
1	A	635	ALA
1	A	386	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	699/756 (92%)	688 (98%)	11 (2%)	62 54

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	77	ASN
1	A	161	VAL
1	A	170	VAL
1	A	232	MET
1	A	243	LEU
1	A	408	ILE
1	A	417	ASP
1	A	587	THR
1	A	590	ARG
1	A	639	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	337	GLN
1	A	348	HIS
1	A	374	ASN
1	A	378	ASN
1	A	643	HIS
1	A	646	ASN

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Mol	Chain	Res	Type
1	A	667	ASN
1	A	802	ASN
1	A	827	HIS
1	A	852	HIS

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)

10 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	0.56	0	17,19,21	0.74	0
2	NAG	B	2	2	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
3	NAG	C	1	3,1	14,14,15	0.66	0	17,19,21	1.27	1 (5%)
3	NAG	C	2	3	14,14,15	0.68	0	17,19,21	0.86	0
3	BMA	C	3	3	11,11,12	0.70	0	15,15,17	1.15	1 (6%)
3	MAN	C	4	3	11,11,12	0.61	0	15,15,17	0.99	1 (6%)
3	MAN	C	5	3	11,11,12	0.63	0	15,15,17	0.97	0
3	MAN	C	6	3	11,11,12	0.54	0	15,15,17	1.28	3 (20%)
2	NAG	D	1	1,2	14,14,15	0.67	0	17,19,21	1.06	0
2	NAG	D	2	2	14,14,15	0.76	1 (7%)	17,19,21	0.99	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
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	O5-C1	-2.01	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C1-O5-C5	3.56	117.01	112.19
3	C	6	MAN	O2-C2-C1	2.77	114.83	109.15
3	C	4	MAN	O5-C5-C6	2.72	111.47	107.20
3	C	6	MAN	O2-C2-C3	-2.33	105.47	110.14
3	C	1	NAG	C1-C2-N2	2.33	114.46	110.49
3	C	3	BMA	C2-C3-C4	-2.23	107.04	110.89
3	C	6	MAN	O5-C5-C6	2.18	110.62	107.20
2	D	2	NAG	C4-C3-C2	2.17	114.20	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

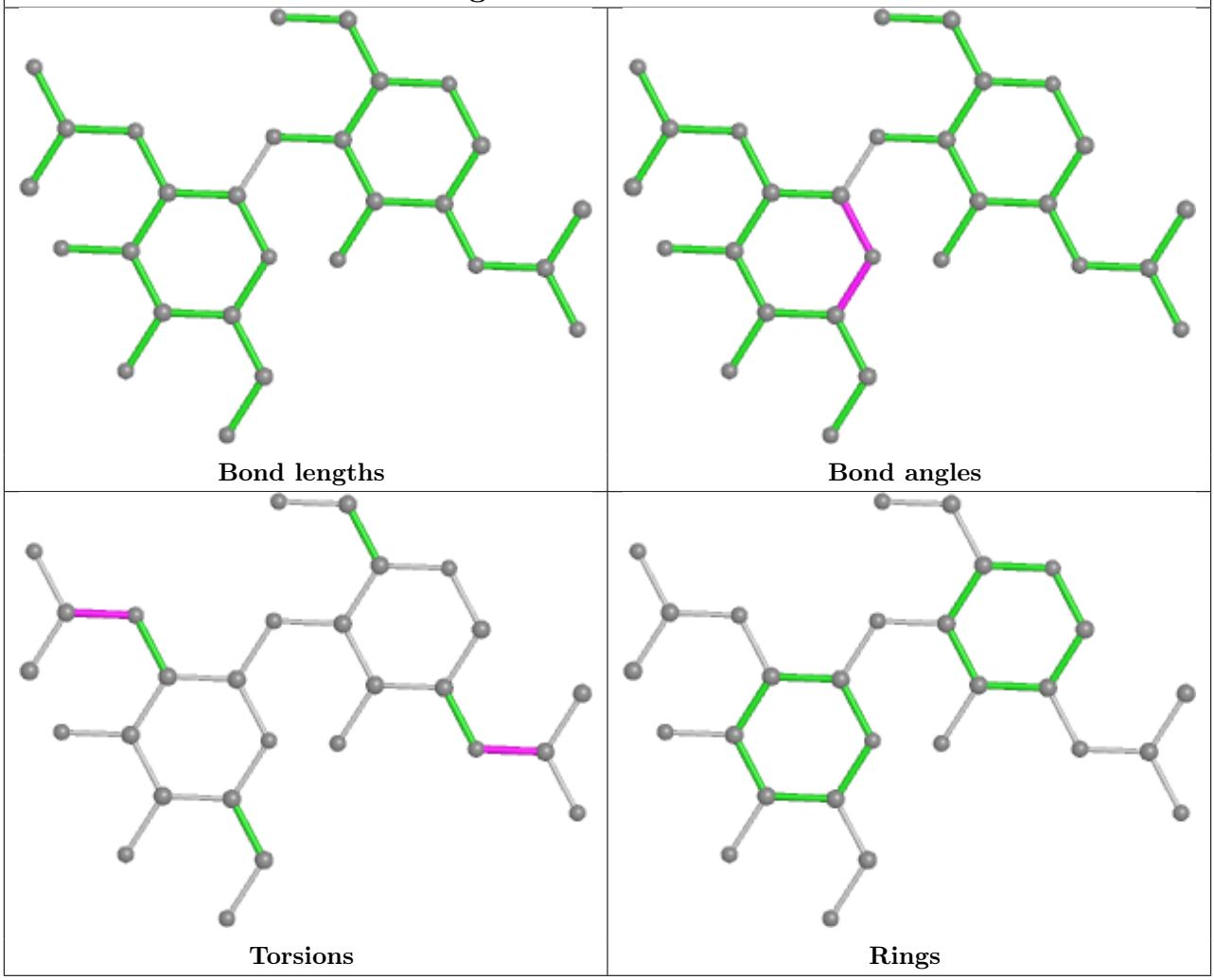
There are no ring outliers.

1 monomer is involved in 1 short contact:

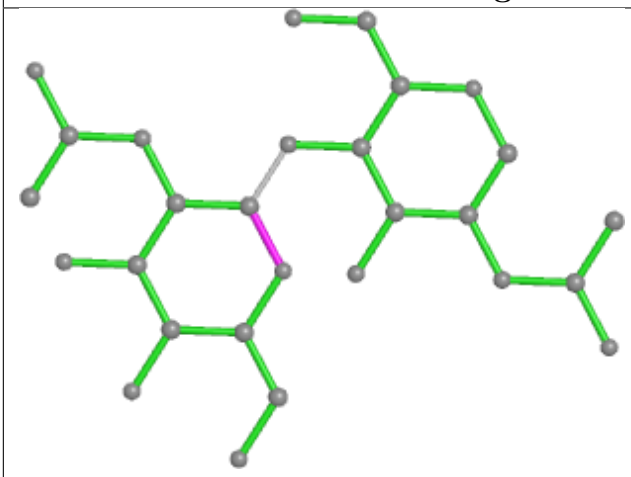
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

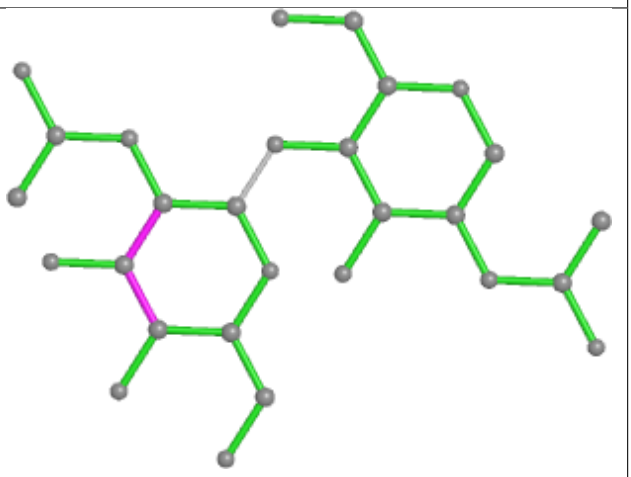
Oligosaccharide Chain B



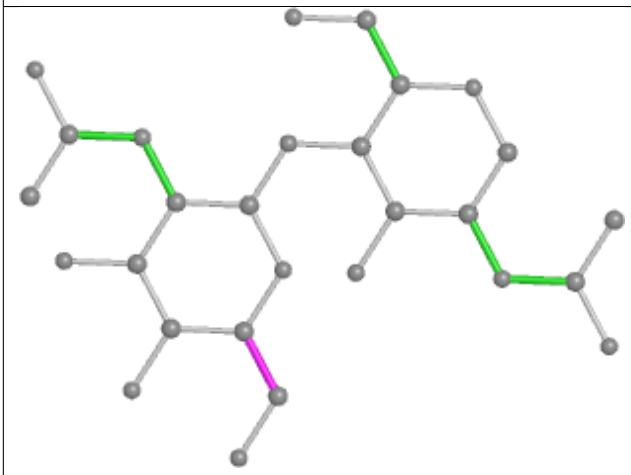
Oligosaccharide Chain D



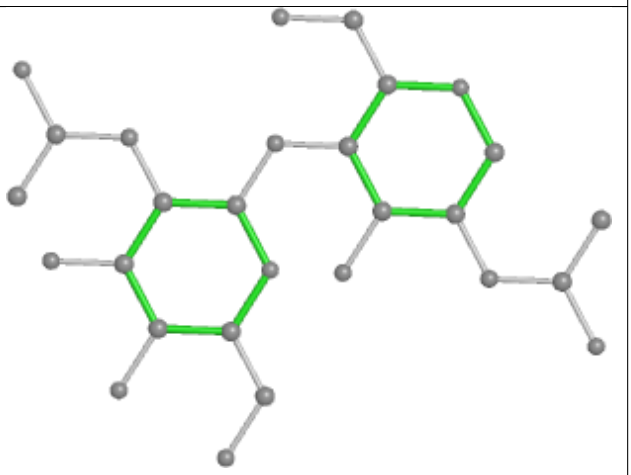
Bond lengths



Bond angles

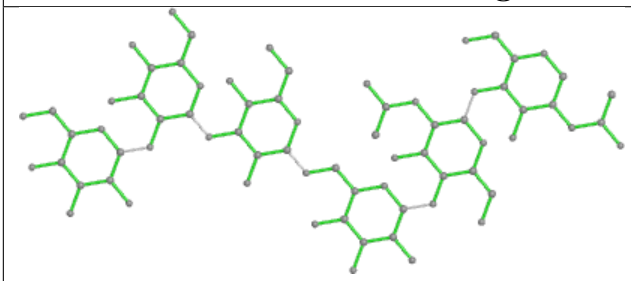


Torsions

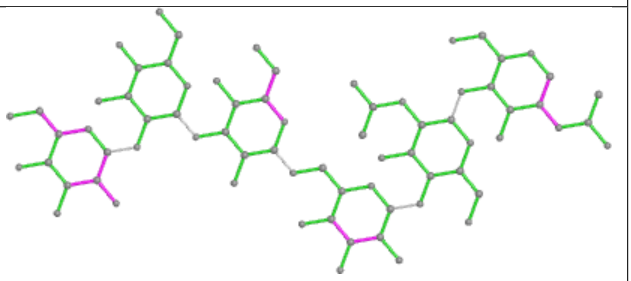


Rings

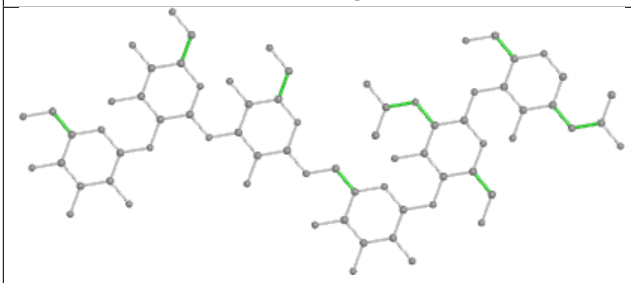
Oligosaccharide Chain C



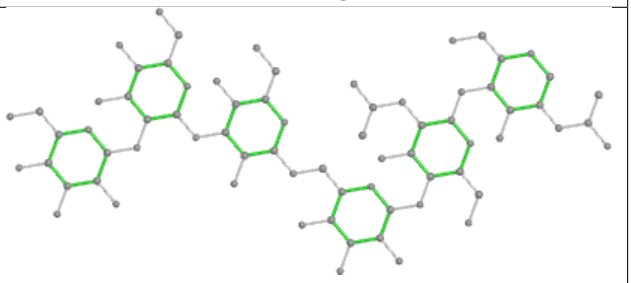
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 5 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
10	EDO	A	1013	-	3,3,3	0.52	0	2,2,2	0.44	0
10	EDO	A	1019	-	3,3,3	0.44	0	2,2,2	0.57	0
9	SCN	A	1008	-	1,2,2	1.27	0	0,1,1	-	-
9	SCN	A	1009	-	1,2,2	0.97	0	0,1,1	-	-
10	EDO	A	1026	-	3,3,3	0.45	0	2,2,2	0.65	0
10	EDO	A	1030	-	3,3,3	0.45	0	2,2,2	0.16	0
10	EDO	A	1016	-	3,3,3	0.53	0	2,2,2	0.38	0
10	EDO	A	1015	-	3,3,3	0.42	0	2,2,2	0.44	0
10	EDO	A	1025	-	3,3,3	0.45	0	2,2,2	0.27	0
10	EDO	A	1020	-	3,3,3	0.49	0	2,2,2	0.29	0
10	EDO	A	1014	-	3,3,3	0.57	0	2,2,2	0.10	0
10	EDO	A	1021	-	3,3,3	0.53	0	2,2,2	0.33	0
10	EDO	A	1023	-	3,3,3	0.49	0	2,2,2	0.64	0
10	EDO	A	1028	-	3,3,3	0.44	0	2,2,2	0.32	0
10	EDO	A	1029	-	3,3,3	0.34	0	2,2,2	0.40	0
10	EDO	A	1012	-	3,3,3	0.32	0	2,2,2	0.67	0
10	EDO	A	1027	-	3,3,3	0.53	0	2,2,2	0.18	0
10	EDO	A	1017	-	3,3,3	0.53	0	2,2,2	0.26	0
10	EDO	A	1022	-	3,3,3	0.54	0	2,2,2	0.32	0
10	EDO	A	1024	-	3,3,3	0.59	0	2,2,2	0.35	0
8	NKN	A	1007	-	7,7,24	0.24	0	6,6,28	0.85	0
10	EDO	A	1018	-	3,3,3	0.67	0	2,2,2	0.24	0
10	EDO	A	1010	-	3,3,3	0.56	0	2,2,2	0.32	0
8	NKN	A	1006	4	24,24,24	0.63	0	27,28,28	1.64	3 (11%)
10	EDO	A	1011	-	3,3,3	0.72	0	2,2,2	0.15	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
10	EDO	A	1013	-	-	0/1/1/1	-
10	EDO	A	1019	-	-	1/1/1/1	-
10	EDO	A	1026	-	-	0/1/1/1	-
10	EDO	A	1030	-	-	0/1/1/1	-
10	EDO	A	1016	-	-	0/1/1/1	-
10	EDO	A	1015	-	-	0/1/1/1	-
10	EDO	A	1025	-	-	0/1/1/1	-
10	EDO	A	1020	-	-	0/1/1/1	-
10	EDO	A	1014	-	-	0/1/1/1	-
10	EDO	A	1021	-	-	0/1/1/1	-
10	EDO	A	1023	-	-	0/1/1/1	-
10	EDO	A	1028	-	-	0/1/1/1	-
10	EDO	A	1029	-	-	0/1/1/1	-
10	EDO	A	1012	-	-	0/1/1/1	-
10	EDO	A	1027	-	-	0/1/1/1	-
10	EDO	A	1017	-	-	0/1/1/1	-
10	EDO	A	1022	-	-	0/1/1/1	-
10	EDO	A	1024	-	-	1/1/1/1	-
8	NKN	A	1007	-	-	0/5/5/24	-
10	EDO	A	1018	-	-	0/1/1/1	-
10	EDO	A	1010	-	-	1/1/1/1	-
8	NKN	A	1006	4	-	0/24/24/24	-
10	EDO	A	1011	-	-	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})
8	A	1006	NKN	OAF-PAC-OAD	4.88	120.16	106.47
8	A	1006	NKN	CAI-OAJ-CAK	-3.36	104.69	117.12
8	A	1006	NKN	CAU-CAT-CAS	-2.56	101.42	114.42

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1024	EDO	O1-C1-C2-O2
10	A	1019	EDO	O1-C1-C2-O2
10	A	1010	EDO	O1-C1-C2-O2

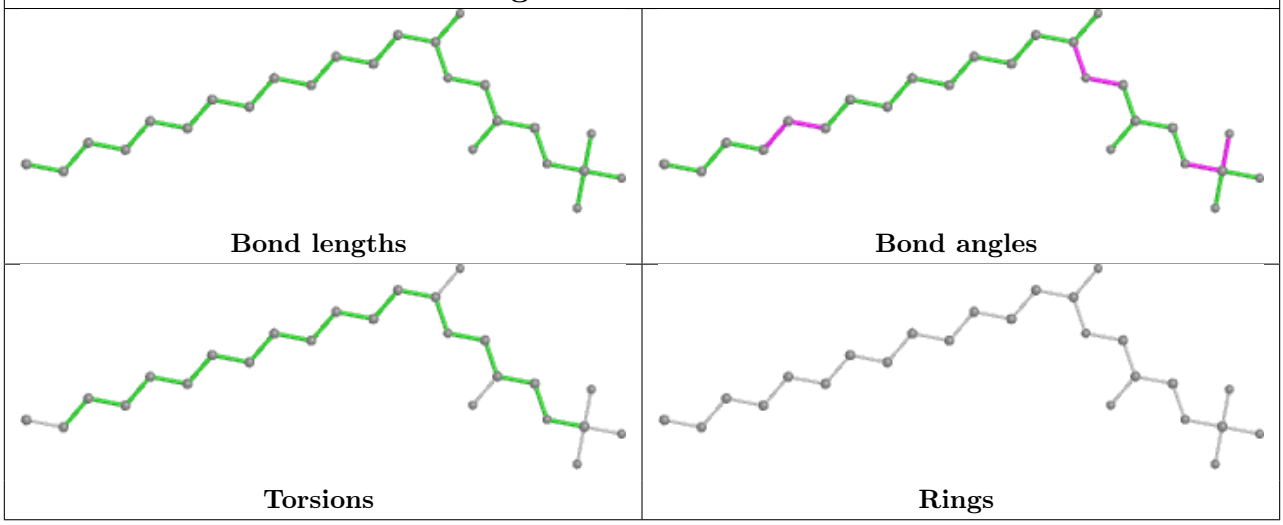
There are no ring outliers.

16 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1019	EDO	1	0
10	A	1026	EDO	4	0
10	A	1030	EDO	3	0
10	A	1015	EDO	1	0
10	A	1025	EDO	4	0
10	A	1020	EDO	1	0
10	A	1021	EDO	3	0
10	A	1028	EDO	2	0
10	A	1029	EDO	5	0
10	A	1012	EDO	4	0
10	A	1027	EDO	5	0
10	A	1017	EDO	1	0
8	A	1007	NKN	1	0
10	A	1010	EDO	1	0
8	A	1006	NKN	1	0
10	A	1011	EDO	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 NKN A 1006



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	782/831 (94%)	0.07	38 (4%) 29 24	13, 29, 56, 73	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	5.0
1	A	110	VAL	4.5
1	A	569	ASP	4.3
1	A	124	LEU	4.2
1	A	52	THR	4.1
1	A	637	VAL	4.0
1	A	587	THR	3.7
1	A	70	PRO	3.6
1	A	120	SER	3.6
1	A	56	GLY	3.6
1	A	69	GLY	3.6
1	A	83	SER	3.6
1	A	71	PRO	3.6
1	A	570	ASP	3.3
1	A	634	GLN	3.1
1	A	55	SER	3.0
1	A	644	LEU	3.0
1	A	108	GLY	3.0
1	A	458	LEU	2.7
1	A	685	PRO	2.6
1	A	125	SER	2.5
1	A	121	GLU	2.5
1	A	82	TYR	2.5
1	A	111	ARG	2.4
1	A	135	VAL	2.4
1	A	136	VAL	2.4
1	A	556	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	641	PRO	2.3
1	A	126	ARG	2.3
1	A	640	ILE	2.3
1	A	558	LEU	2.2
1	A	139	GLY	2.2
1	A	77	ASN	2.2
1	A	122	ASP	2.2
1	A	469	PHE	2.2
1	A	566	CYS	2.2
1	A	119	CYS	2.1
1	A	468	CYS	2.0

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

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

6.3 Carbohydrates (i)

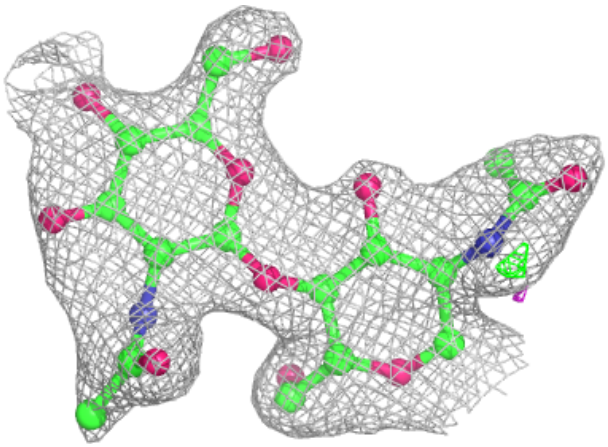
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

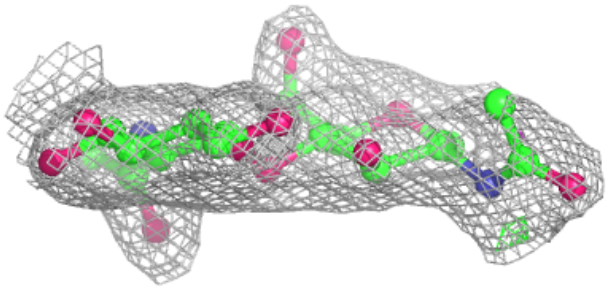
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	1	14/15	0.84	0.25	56,61,63,63	0
3	MAN	C	4	11/12	0.85	0.14	36,38,42,49	0
2	NAG	D	2	14/15	0.86	0.24	47,52,55,56	0
2	NAG	B	2	14/15	0.88	0.23	61,64,67,71	0
3	BMA	C	3	11/12	0.90	0.13	37,40,46,47	0
3	MAN	C	5	11/12	0.91	0.20	31,34,40,49	0
3	MAN	C	6	11/12	0.91	0.13	23,31,36,37	0
2	NAG	D	1	14/15	0.94	0.09	25,32,40,47	0
3	NAG	C	2	14/15	0.96	0.07	24,28,33,38	0
3	NAG	C	1	14/15	0.98	0.11	16,18,22,22	0

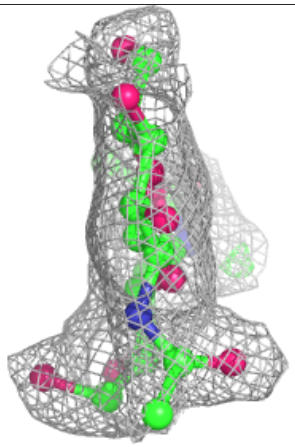
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

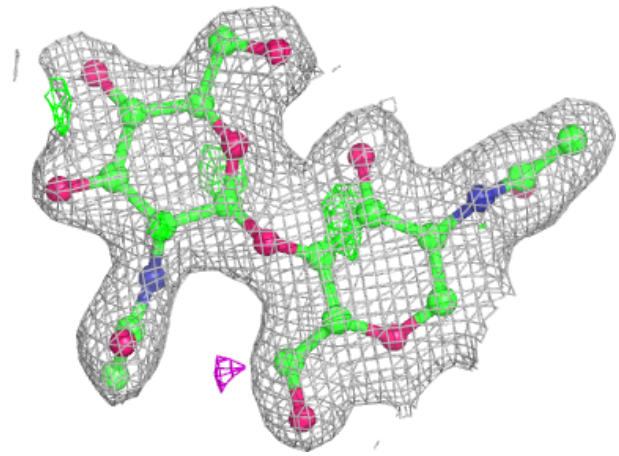


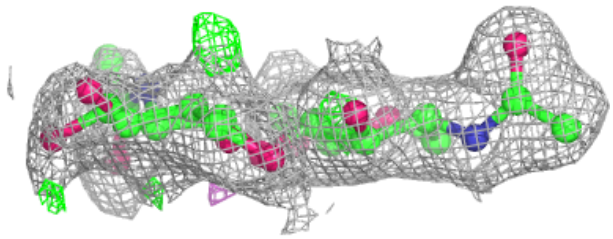


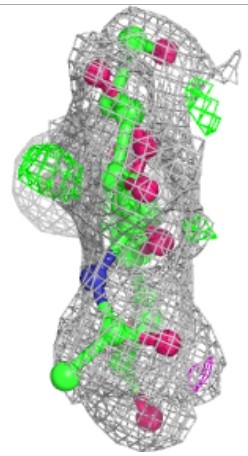


Electron density around Chain D:

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

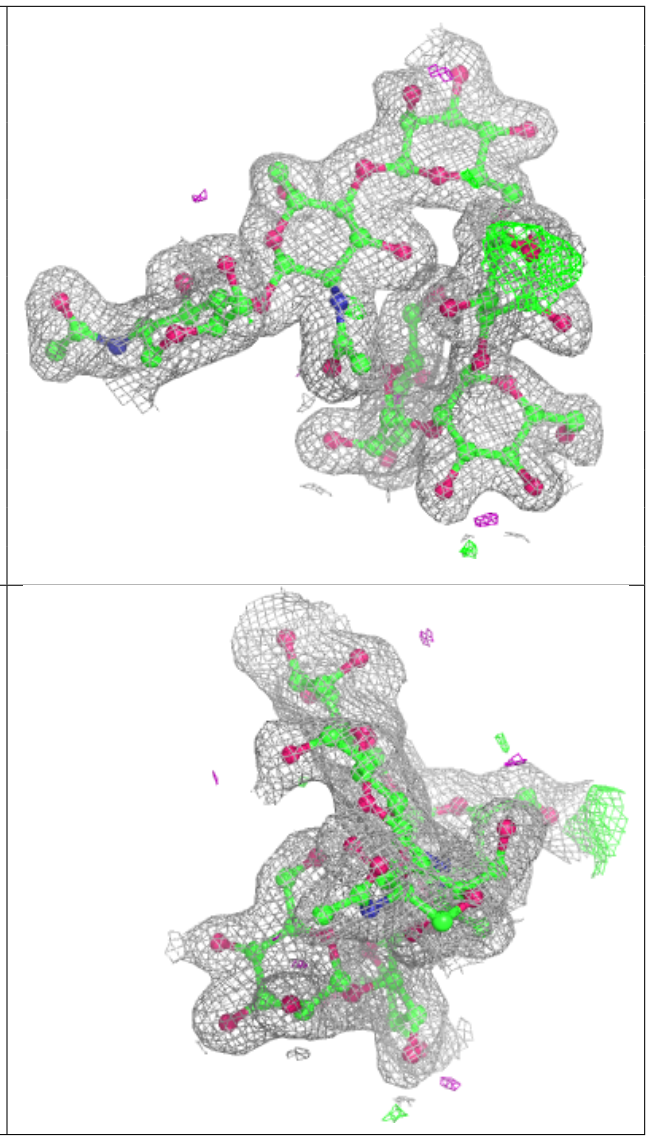






Electron density around Chain C:

$2mF_o$-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	EDO	A	1027	4/4	0.81	0.14	41,43,45,47	0
10	EDO	A	1011	4/4	0.84	0.20	26,30,30,36	0
10	EDO	A	1018	4/4	0.86	0.15	21,27,29,39	0
7	K	A	1005	1/1	0.89	0.13	46,46,46,46	0
10	EDO	A	1014	4/4	0.90	0.14	31,31,33,35	0
10	EDO	A	1022	4/4	0.91	0.10	34,36,36,45	0
10	EDO	A	1016	4/4	0.92	0.12	28,29,29,31	0

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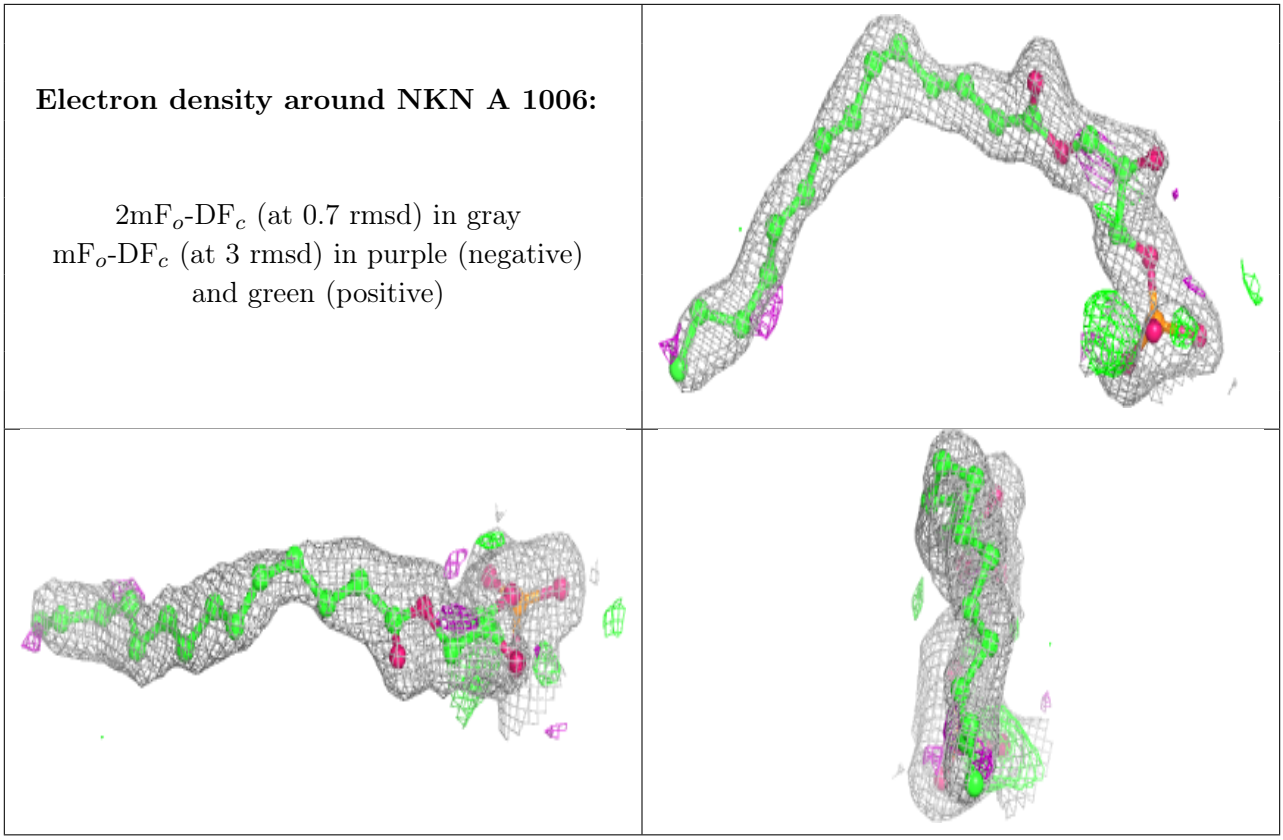
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	EDO	A	1010	4/4	0.92	0.17	34,34,34,36	0
9	SCN	A	1008	3/3	0.94	0.19	32,32,33,39	0
10	EDO	A	1020	4/4	0.94	0.15	28,31,38,41	0
10	EDO	A	1021	4/4	0.94	0.13	33,36,41,42	0
10	EDO	A	1012	4/4	0.94	0.13	33,34,36,37	0
10	EDO	A	1017	4/4	0.94	0.17	23,25,28,29	0
8	NKN	A	1007	8/25	0.95	0.12	31,33,39,41	0
10	EDO	A	1025	4/4	0.95	0.13	22,26,31,36	0
10	EDO	A	1013	4/4	0.95	0.13	29,30,31,31	0
8	NKN	A	1006	25/25	0.96	0.13	19,35,40,45	0
10	EDO	A	1024	4/4	0.96	0.08	25,26,27,34	0
10	EDO	A	1028	4/4	0.96	0.19	32,33,34,39	0
10	EDO	A	1030	4/4	0.96	0.16	33,34,35,38	0
6	NA	A	1004	1/1	0.97	0.07	25,25,25,25	0
10	EDO	A	1015	4/4	0.97	0.09	26,27,31,33	0
10	EDO	A	1029	4/4	0.97	0.11	22,31,32,38	0
10	EDO	A	1026	4/4	0.97	0.11	22,28,30,36	0
9	SCN	A	1009	3/3	0.98	0.10	23,23,33,40	0
10	EDO	A	1019	4/4	0.98	0.09	35,35,36,41	0
10	EDO	A	1023	4/4	0.99	0.07	19,22,22,24	0
4	ZN	A	1001	1/1	1.00	0.09	19,19,19,19	0
4	ZN	A	1002	1/1	1.00	0.09	17,17,17,17	0
5	CA	A	1003	1/1	1.00	0.08	22,22,22,22	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.



6.5 Other polymers (i)

There are no such residues in this entry.