Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 08:50 AM EDT

PDB ID	:	3NKQ
Title	:	Crystal structure of mouse autotaxin in complex with 18:3-LPA
Authors	:	Nishimasu, H.; Ishitani, R.; Mihara, E.; Takagi, J.; Aoki, J.; Nureki, O.
Deposited on	:	2010-06-20
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

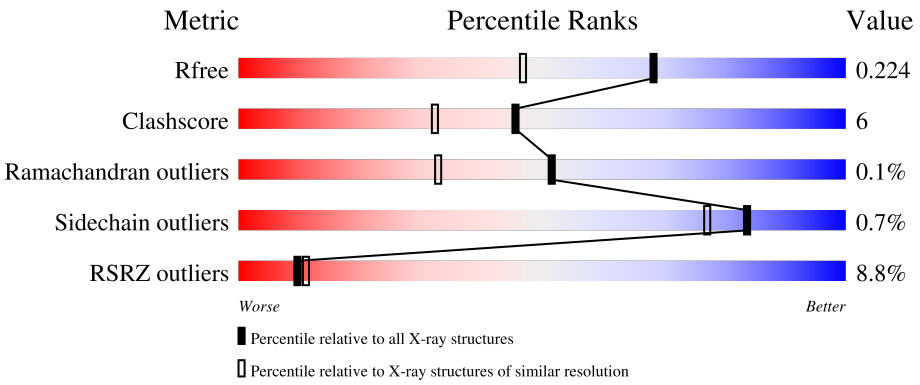
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	8%, 84%, 10%, 6%
2	B	2	50%, 50%
2	D	2	50%, 50%
3	C	6	17%, 83%

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	1024	-	-	X	-
10	EDO	A	1026	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7216 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	6260	3975	1068	1167	50	0	3	0

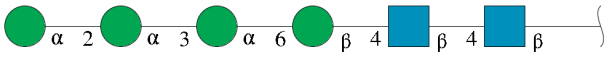
There are 12 discrepancies between the modelled and reference sequences:

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

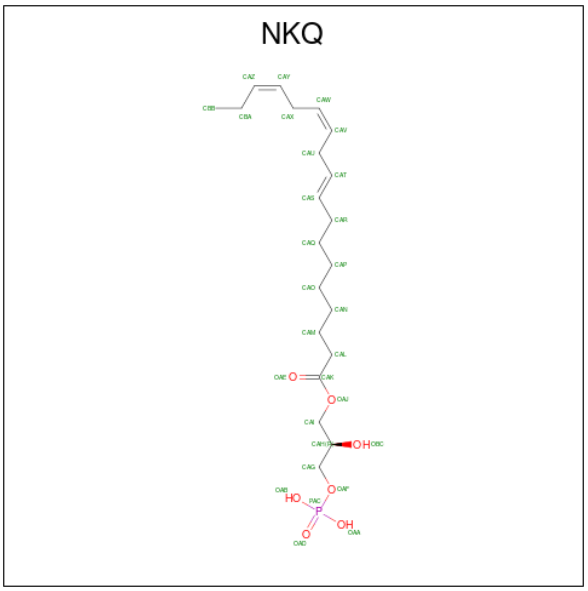
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

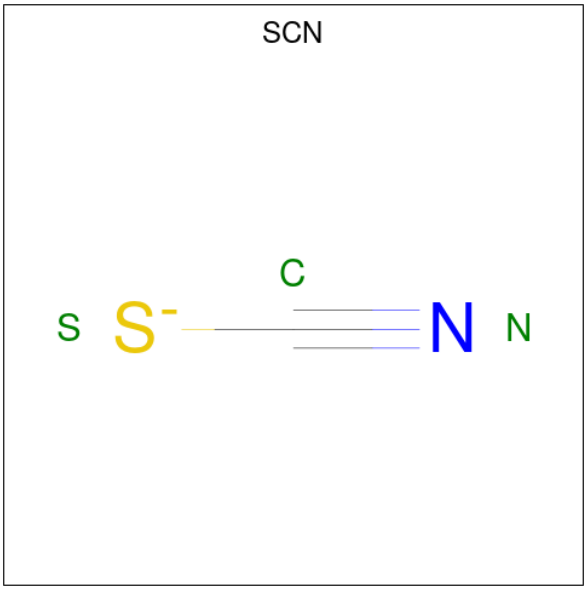
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	A	1	1	1	0	0

- Molecule 8 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E,12Z,15Z)-octadeca-9,12,15-trienoate (three-letter code: NKQ) (formula: $C_{21}H_{37}O_7P$).



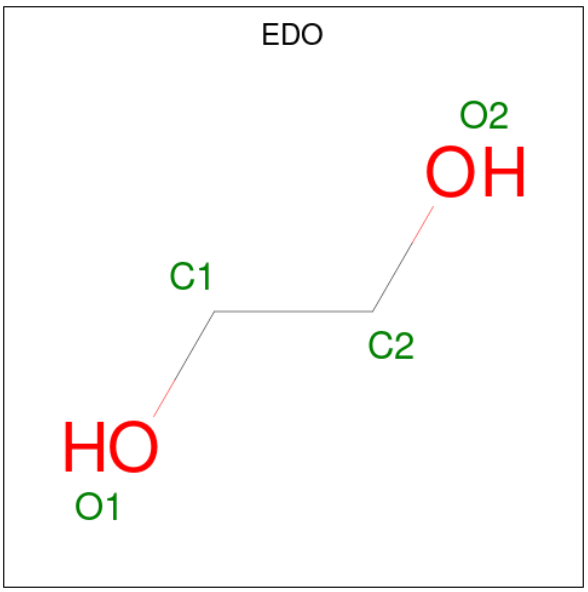
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O P 29 21 7 1	0	0
8	A	1	Total C 8 8	0	0

- 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.

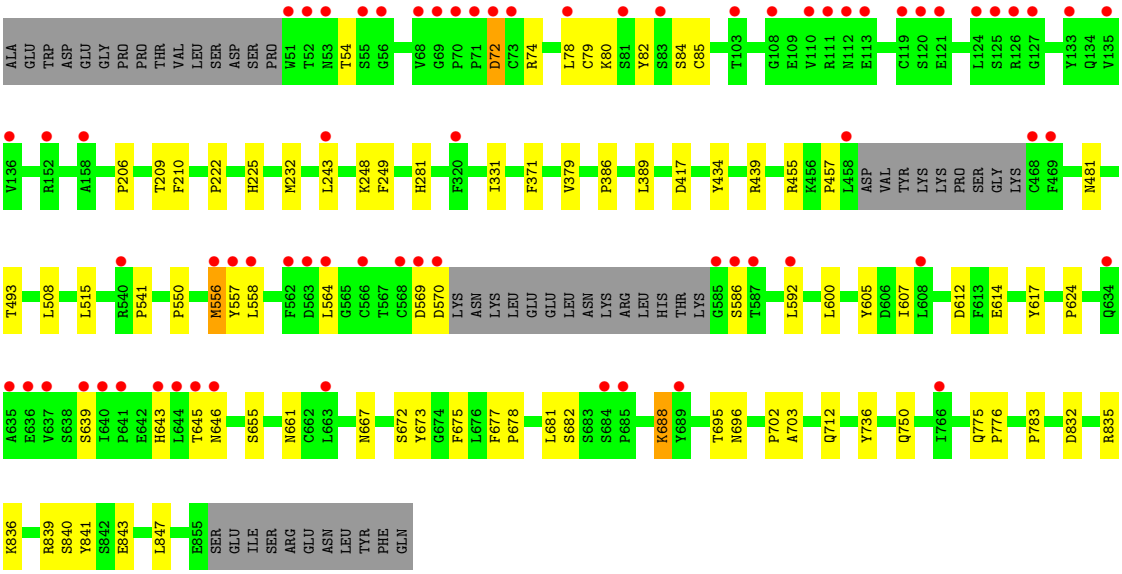
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	696	696	696	0	0

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

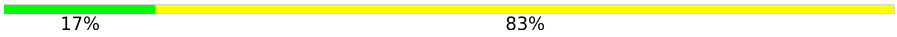
Chain B:

• 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	61.52Å 94.53Å 75.58Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	25.89 – 1.70 41.15 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.89-1.70) 99.5 (41.15-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.190 , 0.228 0.186 , 0.224	Depositor DCC
R_{free} test set	4722 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.8	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	7216	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: SCN, CA, EDO, MAN, NA, NKQ, BMA, ZN, 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	0/6450	0.61	0/8770

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	6260	0	5938	77	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	37	0	46	2	0
9	A	6	0	0	0	0
10	A	84	0	126	23	0
11	A	696	0	0	9	0
All	All	7216	0	6221	81	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 6.

All (81) 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	0.96	1.12
1:A:675:PHE:N	10:A:1012:EDO:H11	1.77	0.99
1:A:835:ARG:HE	10:A:1024:EDO:H22	1.39	0.86
1:A:481:ASN:OD1	11:A:1519:HOH:O	1.92	0.85
1:A:639:SER:O	1:A:688:LYS:NZ	2.12	0.83
1:A:439:ARG:CZ	10:A:1030:EDO:H21	2.11	0.81
1:A:675:PHE:H	10:A:1012:EDO:C1	1.88	0.77
1:A:210:PHE:CE1	1:A:243:LEU:HD23	2.21	0.76
1:A:389:LEU:CD1	11:A:1525:HOH:O	2.35	0.73
1:A:702:PRO:HB2	10:A:1025:EDO:H22	1.69	0.73
1:A:682:SER:OG	1:A:688:LYS:HD3	1.88	0.73
10:A:1011:EDO:H22	11:A:974:HOH:O	1.89	0.72
1:A:281:HIS:ND1	10:A:1023:EDO:H21	2.06	0.70
1:A:835:ARG:HE	10:A:1024:EDO:C2	2.05	0.69
1:A:835:ARG:NE	10:A:1024:EDO:H22	2.09	0.67
1:A:74:ARG:HH22	1:A:78:LEU:CB	2.07	0.67
10:A:1024:EDO:H11	11:A:1513:HOH:O	1.95	0.67
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.77	0.66
1:A:783:PRO:HB3	10:A:1026:EDO:H21	1.79	0.64
1:A:600:LEU:HD11	1:A:832:ASP:HB2	1.84	0.57
1:A:281:HIS:ND1	10:A:1023:EDO:C2	2.66	0.57
1:A:243:LEU:CD1	11:A:1476:HOH:O	2.53	0.56
1:A:586:SER:HA	11:A:881:HOH:O	2.05	0.55
1:A:389:LEU:HD12	11:A:1525:HOH:O	2.01	0.55
1:A:840:SER:OG	1:A:843:GLU:HG3	2.08	0.53
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.43	0.53
1:A:569:ASP:O	1:A:570:ASP:HB2	2.07	0.53
1:A:243:LEU:HD11	11:A:1476:HOH:O	2.09	0.53
1:A:72:ASP:N	1:A:72:ASP:OD1	2.42	0.53
1:A:675:PHE:HB3	1:A:696:ASN:ND2	2.24	0.53
1:A:541:PRO:HG2	1:A:841:TYR:CD2	2.44	0.52
1:A:592:LEU:HD23	1:A:614:GLU:OE1	2.10	0.51
1:A:74:ARG:NH2	1:A:78:LEU:CB	2.73	0.51
1:A:836:LYS:HE2	10:A:1024:EDO:H21	1.93	0.51
1:A:210:PHE:HE1	1:A:243:LEU:HD23	1.72	0.50
1:A:645:THR:HG22	1:A:646:ASN:ND2	2.27	0.50
1:A:54:THR:O	1:A:54:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:THR:HG21	1:A:515:LEU:HD23	1.94	0.49
1:A:80:LYS:N	1:A:85:CYS:SG	2.86	0.49
1:A:839:ARG:HG3	10:A:1026:EDO:H22	1.94	0.48
1:A:558:LEU:HD12	1:A:558:LEU:N	2.28	0.48
1:A:556:MET:HB3	1:A:557:TYR:CD1	2.49	0.48
1:A:783:PRO:CB	10:A:1026:EDO:H21	2.43	0.48
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.49	0.48
1:A:667:ASN:HB2	11:A:15:HOH:O	2.13	0.48
1:A:54:THR:O	1:A:54:THR:CG2	2.62	0.47
1:A:550:PRO:HB3	1:A:605:TYR:CE1	2.50	0.47
1:A:74:ARG:HD3	1:A:84:SER:OG	2.15	0.47
1:A:612:ASP:HB3	1:A:677:PHE:CZ	2.51	0.46
1:A:703:ALA:N	10:A:1025:EDO:H21	2.31	0.46
8:A:1006:NKQ:HBAA	8:A:1006:NKQ:HAX	1.67	0.45
2:B:1:NAG:H83	2:B:1:NAG:H2	1.79	0.45
1:A:570:ASP:CB	1:A:643:HIS:HD2	2.29	0.45
1:A:678:PRO:HG2	1:A:681:LEU:HD12	1.99	0.45
1:A:783:PRO:HA	10:A:1026:EDO:H21	1.99	0.45
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.99	0.44
1:A:541:PRO:HG2	1:A:841:TYR:HD2	1.82	0.44
1:A:556:MET:HB3	1:A:557:TYR:CE1	2.53	0.44
1:A:439:ARG:NE	10:A:1030:EDO:H21	2.32	0.44
1:A:79:CYS:O	1:A:80:LYS:C	2.55	0.43
1:A:78:LEU:O	1:A:82:TYR:HD1	2.02	0.43
1:A:331:ILE:CG1	10:A:1023:EDO:H11	2.48	0.43
1:A:672:SER:OG	1:A:673:TYR:N	2.50	0.43
1:A:617:TYR:CE1	1:A:695:THR:HG22	2.53	0.43
1:A:612:ASP:OD2	1:A:682:SER:HA	2.19	0.42
1:A:847:LEU:HD12	10:A:1020:EDO:H22	2.01	0.42
1:A:209:THR:OG1	8:A:1006:NKQ:HAG	2.19	0.42
1:A:703:ALA:CA	10:A:1025:EDO:H21	2.50	0.42
1:A:678:PRO:CG	1:A:681:LEU:HD12	2.50	0.42
1:A:617:TYR:HA	1:A:624:PRO:HA	2.01	0.42
1:A:839:ARG:NE	10:A:1026:EDO:H22	2.35	0.42
1:A:210:PHE:CD1	1:A:243:LEU:HD23	2.56	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.92	0.41
1:A:775:GLN:HA	1:A:776:PRO:HD3	1.87	0.41
1:A:417:ASP:OD1	1:A:417:ASP:N	2.53	0.41
1:A:379:VAL:HB	1:A:455:ARG:HG2	2.03	0.41
1:A:736:TYR:OH	1:A:750:GLN:HB3	2.20	0.41
1:A:550:PRO:HB3	1:A:605:TYR:CZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.56	0.40
1:A:248:LYS:HE2	1:A:249:PHE:CE2	2.57	0.40
1:A:564:LEU:O	1:A:661:ASN:HB2	2.21	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%)	755 (97%)	23 (3%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	697/756 (92%)	692 (99%)	5 (1%)	84 77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	232	MET
1	A	556	MET
1	A	655	SER
1	A	688	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	134	GLN
1	A	290	GLN
1	A	337	GLN
1	A	374	ASN
1	A	643	HIS
1	A	646	ASN
1	A	667	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)

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	0.75	0	17,19,21	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	2	2	14,14,15	0.51	0	17,19,21	1.18	3 (17%)
3	NAG	C	1	1,3	14,14,15	0.57	0	17,19,21	1.25	2 (11%)
3	NAG	C	2	3	14,14,15	0.68	1 (7%)	17,19,21	1.14	1 (5%)
3	BMA	C	3	3	11,11,12	0.80	1 (9%)	15,15,17	0.84	0
3	MAN	C	4	3	11,11,12	0.60	0	15,15,17	0.92	1 (6%)
3	MAN	C	5	3	11,11,12	0.69	0	15,15,17	0.89	1 (6%)
3	MAN	C	6	3	11,11,12	0.55	0	15,15,17	0.93	0
2	NAG	D	1	1,2	14,14,15	0.62	0	17,19,21	0.99	0
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	2.35	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	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	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	-2.14	1.40	1.43
3	C	3	BMA	O5-C1	-2.00	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	C1-O5-C5	7.89	122.89	112.19
2	B	2	NAG	C1-O5-C5	3.13	116.43	112.19
2	D	2	NAG	O5-C1-C2	3.02	116.06	111.29
2	B	1	NAG	C2-N2-C7	-3.01	118.62	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	C1-C2-N2	-2.31	106.54	110.49
3	C	1	NAG	O4-C4-C3	-2.30	105.04	110.35
3	C	1	NAG	O5-C1-C2	-2.21	107.80	111.29
2	B	2	NAG	O5-C5-C6	2.20	110.65	107.20
3	C	4	MAN	O5-C5-C6	2.16	110.59	107.20
3	C	2	NAG	O7-C7-C8	-2.11	118.14	122.06
2	D	2	NAG	C2-N2-C7	2.09	125.88	122.90
2	B	2	NAG	C4-C3-C2	2.06	114.04	111.02
2	B	1	NAG	C1-O5-C5	2.03	114.95	112.19
3	C	5	MAN	O5-C5-C6	2.02	110.37	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

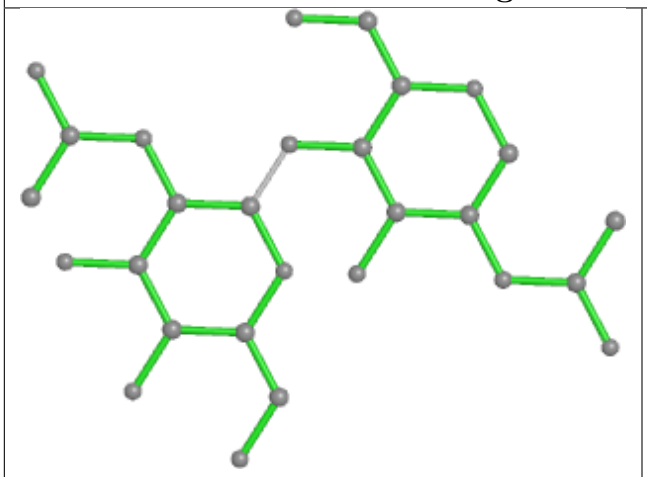
There are no ring outliers.

1 monomer is involved in 1 short contact:

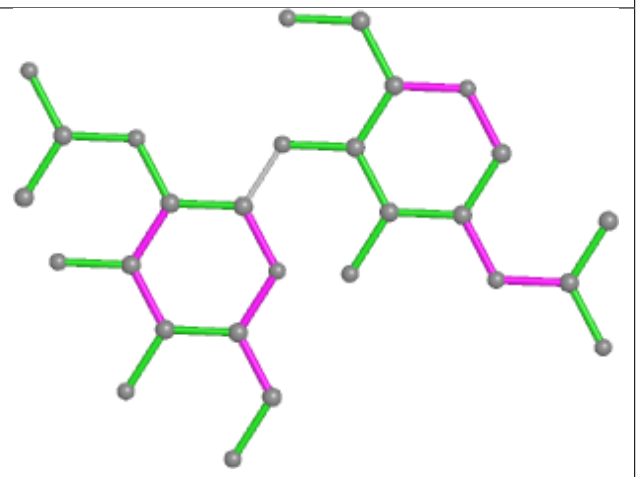
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0

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

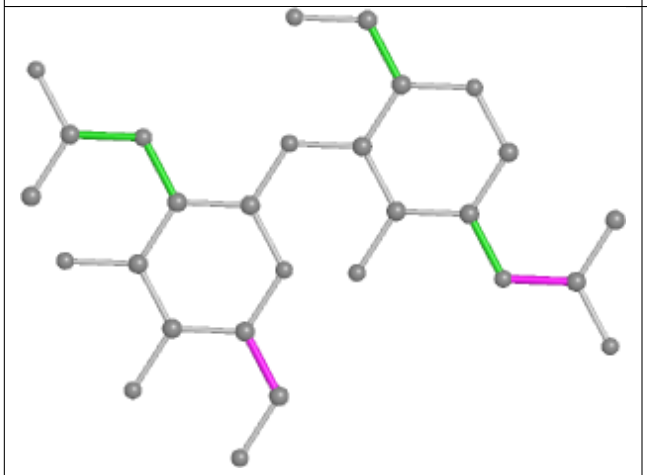
Oligosaccharide Chain B



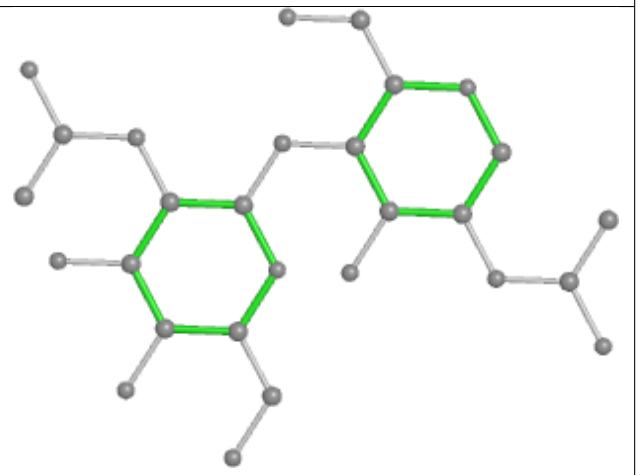
Bond lengths



Bond angles

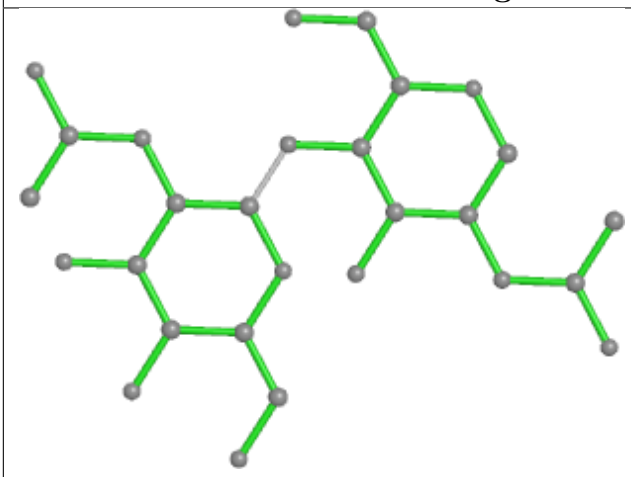


Torsions

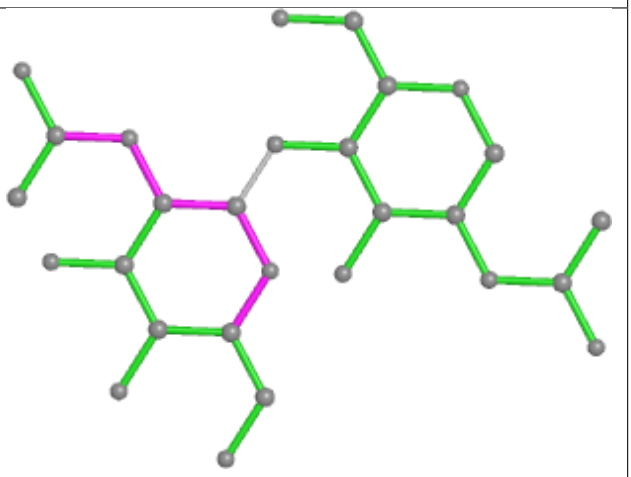


Rings

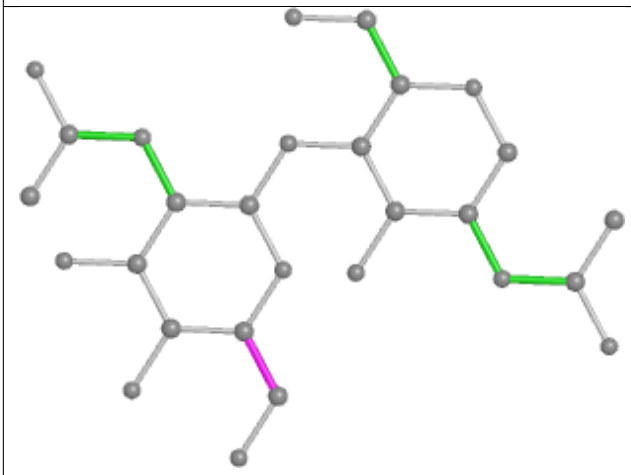
Oligosaccharide Chain D



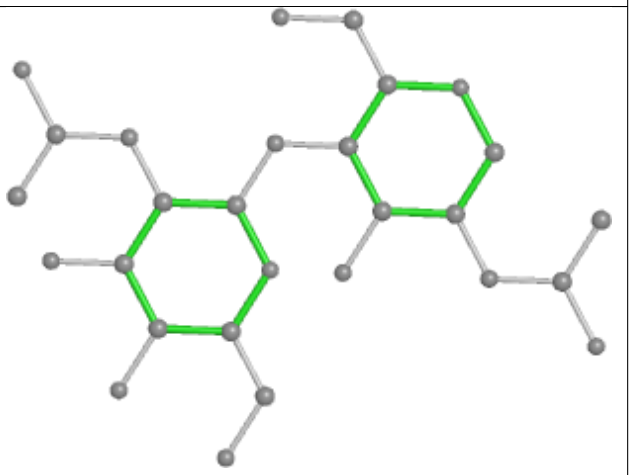
Bond lengths



Bond angles

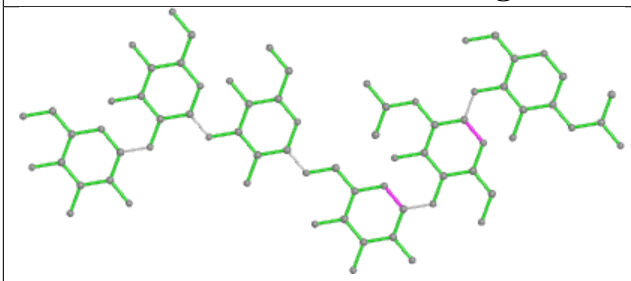


Torsions

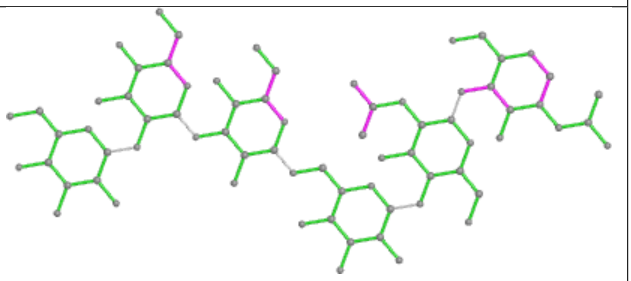


Rings

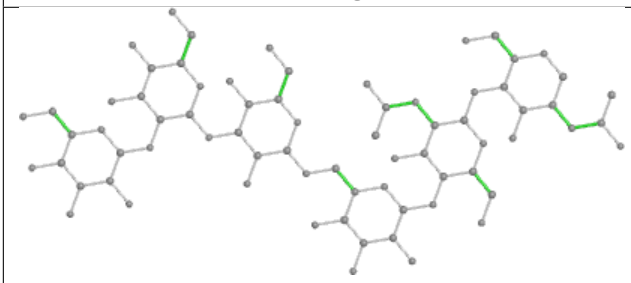
Oligosaccharide Chain C



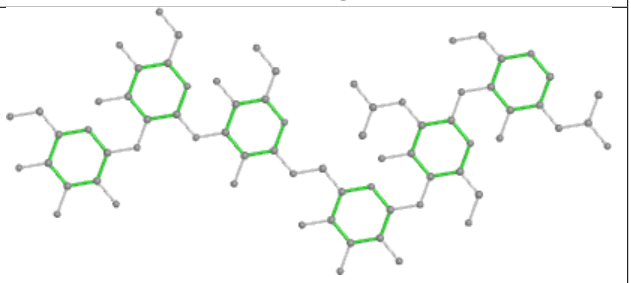
Bond lengths



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	1014	-	3,3,3	0.64	0	2,2,2	0.09	0
10	EDO	A	1025	-	3,3,3	0.46	0	2,2,2	0.35	0
10	EDO	A	1022	-	3,3,3	0.56	0	2,2,2	0.28	0
10	EDO	A	1010	-	3,3,3	0.54	0	2,2,2	0.45	0
10	EDO	A	1021	-	3,3,3	0.51	0	2,2,2	0.31	0
10	EDO	A	1030	-	3,3,3	0.50	0	2,2,2	0.28	0
9	SCN	A	1009	-	1,2,2	0.93	0	0,1,1	-	-
9	SCN	A	1008	-	1,2,2	0.92	0	0,1,1	-	-
10	EDO	A	1029	-	3,3,3	0.60	0	2,2,2	0.09	0
10	EDO	A	1024	-	3,3,3	0.51	0	2,2,2	0.22	0
10	EDO	A	1015	-	3,3,3	0.44	0	2,2,2	0.56	0
10	EDO	A	1019	-	3,3,3	0.41	0	2,2,2	0.27	0
8	NKQ	A	1007	-	7,7,28	1.89	2 (28%)	5,6,32	0.70	0
10	EDO	A	1026	-	3,3,3	0.36	0	2,2,2	0.62	0
10	EDO	A	1017	-	3,3,3	0.55	0	2,2,2	0.42	0
10	EDO	A	1011	-	3,3,3	0.70	0	2,2,2	0.30	0
8	NKQ	A	1006	4	28,28,28	1.10	2 (7%)	30,32,32	2.01	11 (36%)
10	EDO	A	1018	-	3,3,3	0.61	0	2,2,2	0.38	0
10	EDO	A	1016	-	3,3,3	0.53	0	2,2,2	0.20	0
10	EDO	A	1023	-	3,3,3	0.48	0	2,2,2	0.92	0
10	EDO	A	1013	-	3,3,3	0.55	0	2,2,2	0.34	0
10	EDO	A	1012	-	3,3,3	0.29	0	2,2,2	0.58	0
10	EDO	A	1027	-	3,3,3	0.47	0	2,2,2	0.44	0
10	EDO	A	1020	-	3,3,3	0.49	0	2,2,2	0.54	0
10	EDO	A	1028	-	3,3,3	0.56	0	2,2,2	0.31	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	1014	-	-	0/1/1/1	-
10	EDO	A	1025	-	-	0/1/1/1	-
10	EDO	A	1022	-	-	0/1/1/1	-
10	EDO	A	1010	-	-	1/1/1/1	-
10	EDO	A	1021	-	-	0/1/1/1	-
10	EDO	A	1030	-	-	0/1/1/1	-
10	EDO	A	1029	-	-	1/1/1/1	-
10	EDO	A	1024	-	-	0/1/1/1	-
10	EDO	A	1015	-	-	0/1/1/1	-
10	EDO	A	1019	-	-	0/1/1/1	-
8	NKQ	A	1007	-	-	3/5/5/28	-
10	EDO	A	1026	-	-	0/1/1/1	-
10	EDO	A	1017	-	-	1/1/1/1	-
10	EDO	A	1011	-	-	0/1/1/1	-
8	NKQ	A	1006	4	-	5/28/28/28	-
10	EDO	A	1018	-	-	0/1/1/1	-
10	EDO	A	1016	-	-	0/1/1/1	-
10	EDO	A	1023	-	-	1/1/1/1	-
10	EDO	A	1013	-	-	0/1/1/1	-
10	EDO	A	1012	-	-	0/1/1/1	-
10	EDO	A	1027	-	-	0/1/1/1	-
10	EDO	A	1020	-	-	1/1/1/1	-
10	EDO	A	1028	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1007	NKQ	CBA-CAZ	-2.93	1.37	1.51
8	A	1007	NKQ	CAU-CAV	-2.39	1.39	1.49
8	A	1006	NKQ	CBA-CAZ	-2.34	1.40	1.51
8	A	1006	NKQ	PAC-OAB	2.16	1.63	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1006	NKQ	OBC-CAH-CAI	-3.80	96.22	109.56
8	A	1006	NKQ	OAA-PAC-OAF	-3.66	96.98	106.73
8	A	1006	NKQ	CAV-CAU-CAT	-3.30	95.77	112.02
8	A	1006	NKQ	CAI-OAJ-CAK	-3.26	105.06	117.12
8	A	1006	NKQ	OAJ-CAK-CAL	3.16	121.83	111.91
8	A	1006	NKQ	CAM-CAL-CAK	-2.87	103.18	113.62
8	A	1006	NKQ	OBC-CAH-CAG	-2.78	99.81	109.56
8	A	1006	NKQ	OAB-PAC-OAF	2.62	113.70	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1006	NKQ	OAJ-CAK-OAE	-2.58	117.09	123.59
8	A	1006	NKQ	CAQ-CAR-CAS	-2.26	99.49	112.43
8	A	1006	NKQ	OAF-PAC-OAD	2.18	112.60	106.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1006	NKQ	OBC-CAH-CAI-OAJ
8	A	1006	NKQ	CAT-CAU-CAV-CAW
8	A	1007	NKQ	CAV-CAW-CAX-CAY
8	A	1007	NKQ	CAW-CAX-CAY-CAZ
8	A	1007	NKQ	CAY-CAZ-CBA-CBB
8	A	1006	NKQ	CAQ-CAR-CAS-CAT
10	A	1020	EDO	O1-C1-C2-O2
8	A	1006	NKQ	OAF-CAG-CAH-OBC
10	A	1010	EDO	O1-C1-C2-O2
10	A	1023	EDO	O1-C1-C2-O2
10	A	1029	EDO	O1-C1-C2-O2
10	A	1017	EDO	O1-C1-C2-O2
8	A	1006	NKQ	CAL-CAM-CAN-CAO

There are no ring outliers.

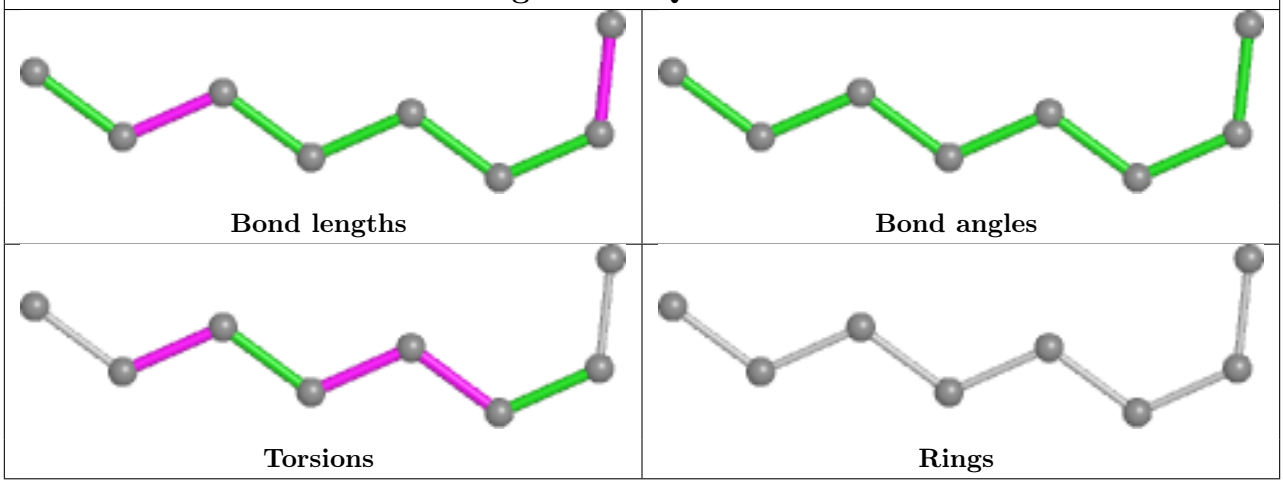
9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1025	EDO	3	0
10	A	1030	EDO	2	0
10	A	1024	EDO	5	0
10	A	1026	EDO	5	0
10	A	1011	EDO	1	0
8	A	1006	NKQ	2	0
10	A	1023	EDO	3	0
10	A	1012	EDO	3	0
10	A	1020	EDO	1	0

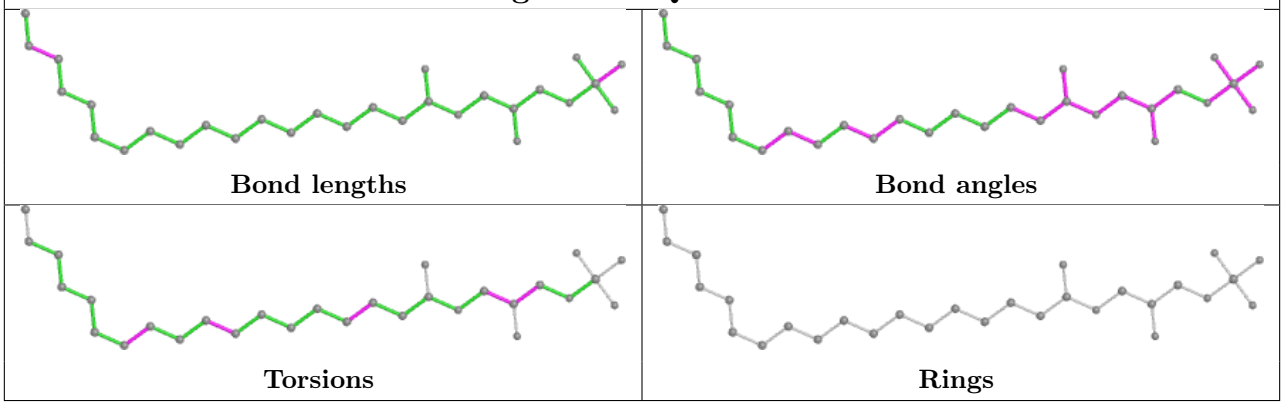
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NKQ A 1007



Ligand NKQ 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%)	0.38	69 (8%) 10 11	12, 28, 53, 68	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	7.1
1	A	83	SER	5.8
1	A	569	ASP	5.8
1	A	71	PRO	5.8
1	A	110	VAL	5.3
1	A	124	LEU	5.2
1	A	585	GLY	5.0
1	A	641	PRO	5.0
1	A	644	LEU	5.0
1	A	52	THR	4.6
1	A	637	VAL	4.5
1	A	70	PRO	4.5
1	A	556	MET	4.4
1	A	685	PRO	4.2
1	A	69	GLY	4.1
1	A	570	ASP	3.8
1	A	640	ILE	3.7
1	A	108	GLY	3.7
1	A	568	CYS	3.6
1	A	643	HIS	3.5
1	A	55	SER	3.5
1	A	469	PHE	3.4
1	A	125	SER	3.3
1	A	684	SER	3.3
1	A	136	VAL	3.3
1	A	663	LEU	3.3
1	A	634	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	3.3
1	A	243	LEU	3.3
1	A	558	LEU	3.2
1	A	562	PHE	3.2
1	A	133	TYR	3.2
1	A	73	CYS	3.1
1	A	566	CYS	3.1
1	A	135	VAL	3.1
1	A	468	CYS	2.9
1	A	158	ALA	2.9
1	A	646	ASN	2.9
1	A	72	ASP	2.9
1	A	120	SER	2.9
1	A	689	TYR	2.9
1	A	592	LEU	2.8
1	A	320	PHE	2.7
1	A	635	ALA	2.7
1	A	56	GLY	2.6
1	A	639	SER	2.6
1	A	564	LEU	2.6
1	A	587	THR	2.4
1	A	53	ASN	2.4
1	A	557	TYR	2.3
1	A	127	GLY	2.3
1	A	458	LEU	2.3
1	A	766	ILE	2.2
1	A	111	ARG	2.2
1	A	152	ARG	2.2
1	A	645	THR	2.2
1	A	113	GLU	2.2
1	A	121	GLU	2.2
1	A	126	ARG	2.1
1	A	540	ARG	2.1
1	A	103	THR	2.1
1	A	78	LEU	2.1
1	A	608	LEU	2.1
1	A	586	SER	2.1
1	A	119	CYS	2.1
1	A	112	ASN	2.1
1	A	636	GLU	2.1
1	A	81	SER	2.0
1	A	563	ASP	2.0

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

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

6.3 Carbohydrates (i)

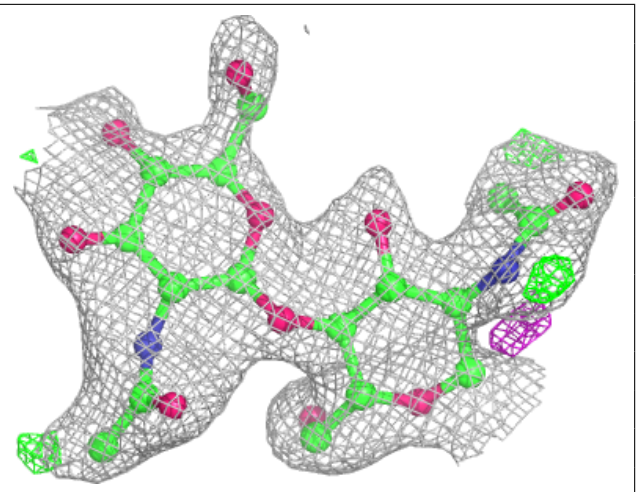
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

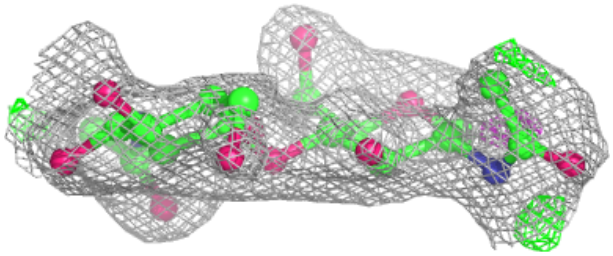
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	1	14/15	0.74	0.28	56,61,64,64	0
2	NAG	B	2	14/15	0.74	0.26	59,65,66,68	0
3	MAN	C	4	11/12	0.81	0.18	37,39,41,51	0
3	BMA	C	3	11/12	0.85	0.19	38,44,49,50	0
2	NAG	D	2	14/15	0.85	0.24	42,50,52,53	0
3	MAN	C	5	11/12	0.92	0.24	30,33,40,46	0
3	MAN	C	6	11/12	0.92	0.13	23,30,36,37	0
2	NAG	D	1	14/15	0.94	0.09	24,29,39,44	0
3	NAG	C	1	14/15	0.95	0.09	14,19,23,24	0
3	NAG	C	2	14/15	0.95	0.07	22,29,34,40	0

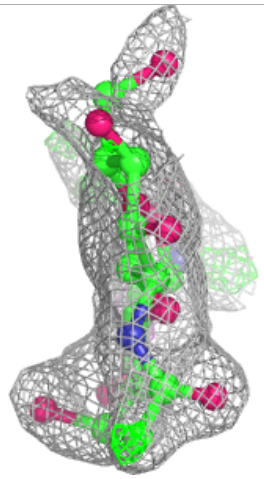
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

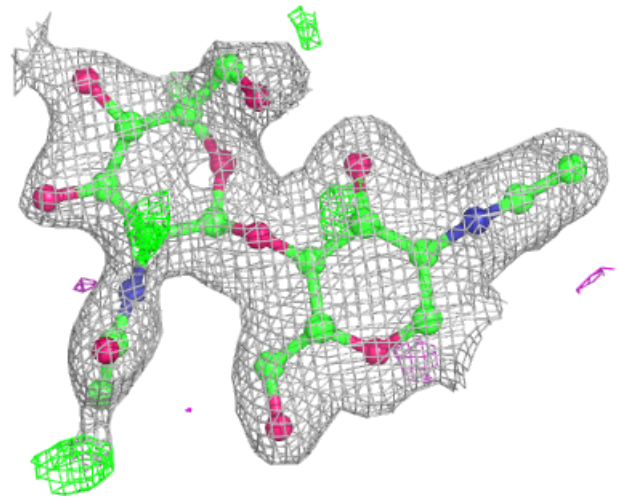


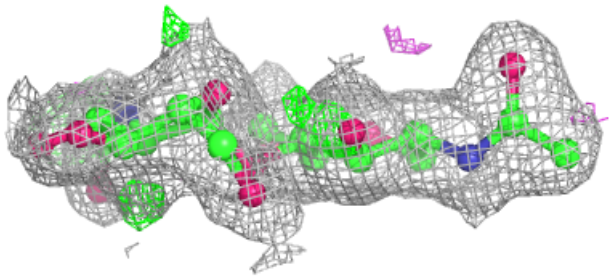


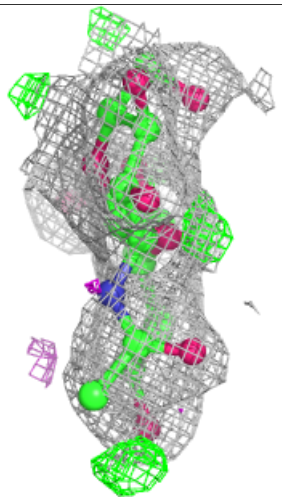


Electron density around Chain D:

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

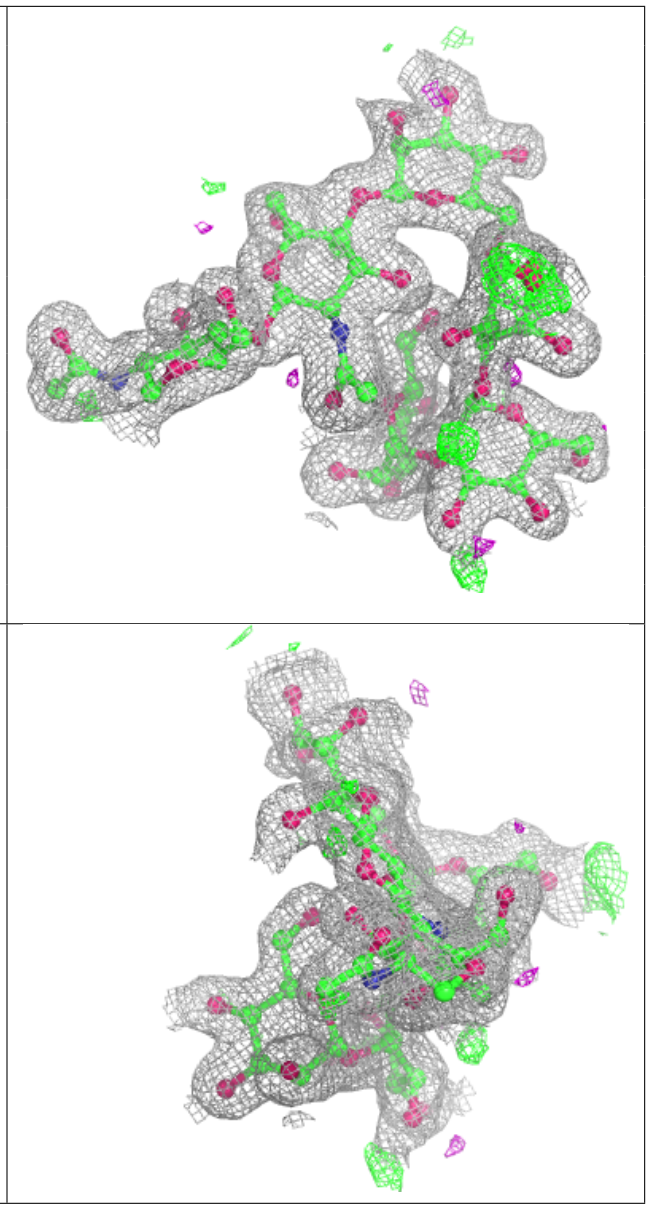






Electron density around Chain C:

$2mF_o$-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	1024	4/4	0.82	0.18	42,44,46,49	0
10	EDO	A	1011	4/4	0.84	0.17	24,28,31,34	0
10	EDO	A	1018	4/4	0.86	0.14	23,29,35,38	0
10	EDO	A	1017	4/4	0.86	0.17	36,39,40,42	0
9	SCN	A	1008	3/3	0.87	0.17	25,25,38,39	0

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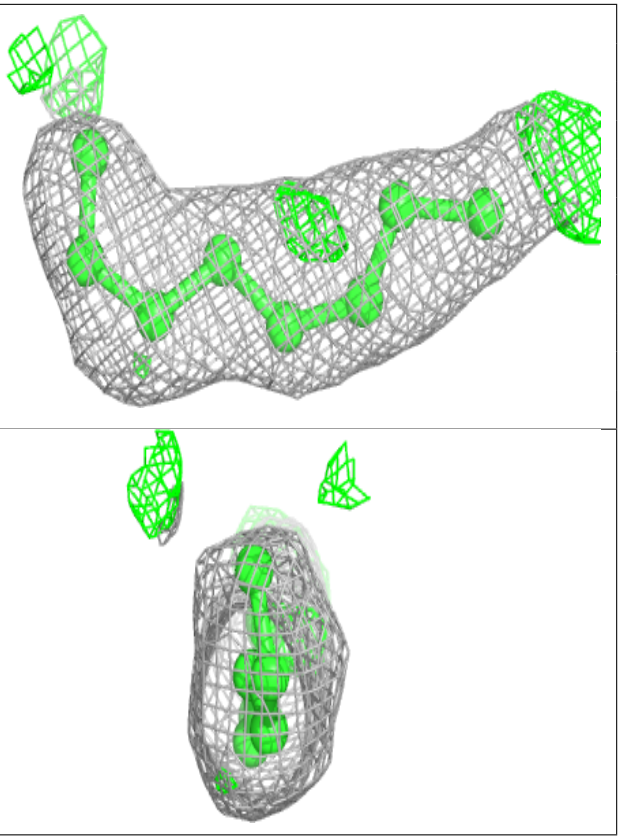
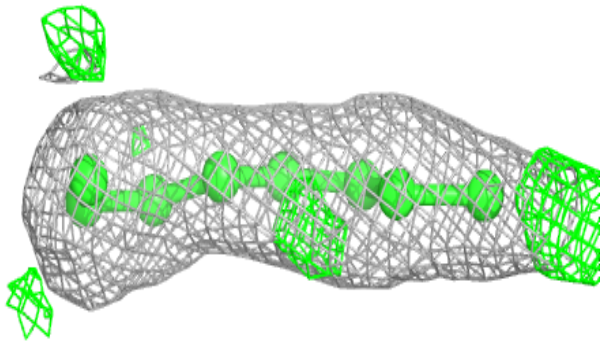
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	EDO	A	1022	4/4	0.88	0.08	38,38,40,44	0
7	K	A	1005	1/1	0.90	0.07	36,36,36,36	0
8	NKQ	A	1007	8/29	0.90	0.11	30,35,38,42	0
10	EDO	A	1014	4/4	0.92	0.14	28,28,30,32	0
10	EDO	A	1021	4/4	0.92	0.15	32,36,40,45	0
10	EDO	A	1029	4/4	0.92	0.10	26,27,30,35	0
8	NKQ	A	1006	29/29	0.93	0.13	18,33,40,45	0
10	EDO	A	1020	4/4	0.93	0.13	25,29,34,41	0
10	EDO	A	1025	4/4	0.93	0.22	32,38,39,40	0
10	EDO	A	1026	4/4	0.93	0.12	22,30,31,38	0
10	EDO	A	1013	4/4	0.93	0.12	29,30,30,31	0
10	EDO	A	1030	4/4	0.93	0.14	26,27,30,38	0
10	EDO	A	1027	4/4	0.94	0.13	29,35,40,41	0
10	EDO	A	1023	4/4	0.94	0.10	24,29,30,35	0
10	EDO	A	1012	4/4	0.94	0.13	31,31,34,35	0
10	EDO	A	1010	4/4	0.95	0.11	31,32,32,33	0
10	EDO	A	1016	4/4	0.96	0.07	26,29,30,33	0
10	EDO	A	1019	4/4	0.96	0.07	32,32,35,38	0
10	EDO	A	1015	4/4	0.96	0.08	27,27,30,31	0
10	EDO	A	1028	4/4	0.98	0.13	22,22,22,23	0
6	NA	A	1004	1/1	0.99	0.12	25,25,25,25	0
4	ZN	A	1001	1/1	0.99	0.08	19,19,19,19	0
9	SCN	A	1009	3/3	0.99	0.12	24,24,31,42	0
5	CA	A	1003	1/1	0.99	0.07	22,22,22,22	0
4	ZN	A	1002	1/1	1.00	0.08	16,16,16,16	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 NKQ A 1007:

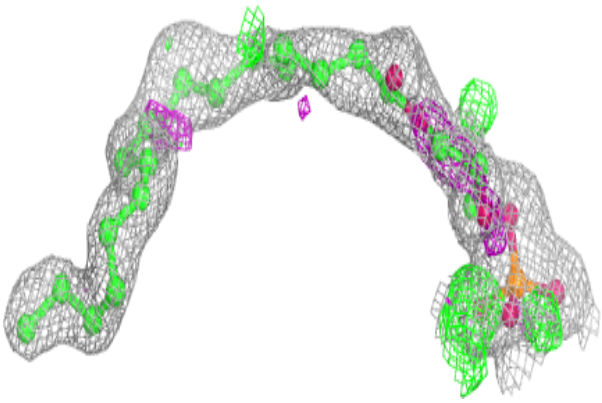
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

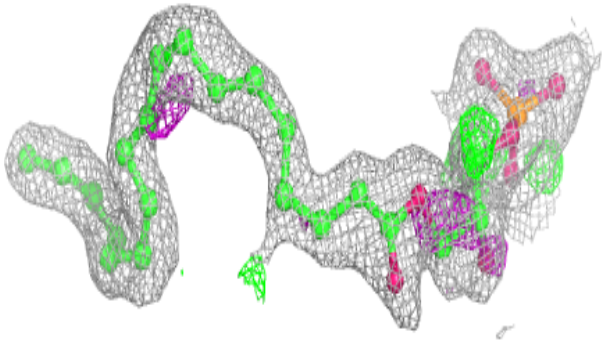


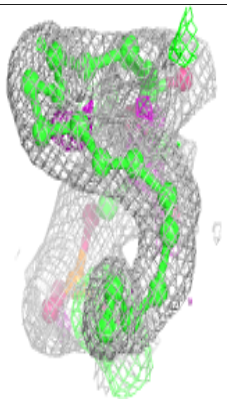


Electron density around NKQ A 1006:

$2mF_o$-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.