



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:27 PM BST

PDB ID : 3NKP
Title : Crystal structure of mouse autotaxin in complex with 18:1-LPA
Authors : Nishimasu, H.; Ishitani, R.; Mihara, E.; Takagi, J.; Aoki, J.; Nureki, O.
Deposited on : 2010-06-20
Resolution : 1.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

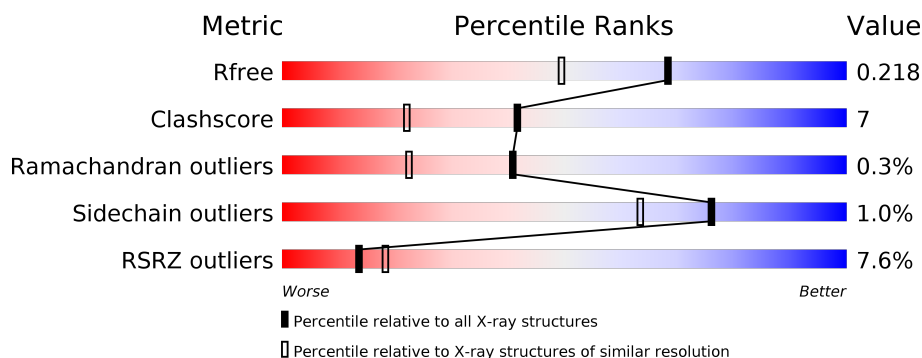
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	831	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>100%</div> </div>
3	C	6	<div> <div>33%</div> <div>67%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	EDO	A	1012	-	-	X	-
10	EDO	A	1024	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7182 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.

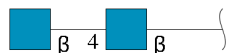
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	788	Total	C	N	O	S	0	4	0
			6312	4007	1078	1177	50			

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

- 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
3	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

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

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

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

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

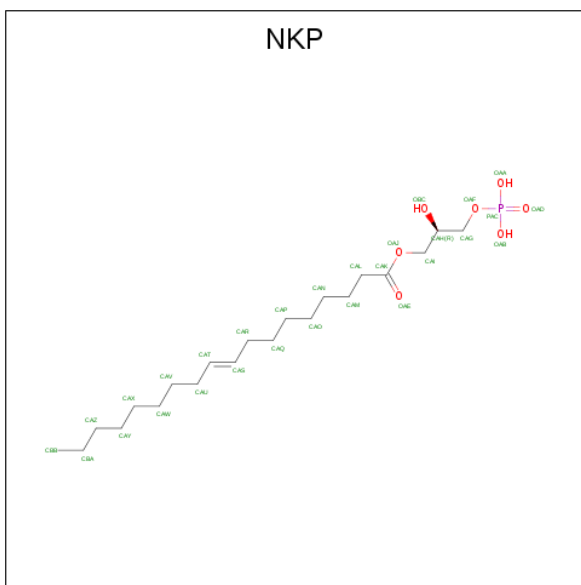
- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

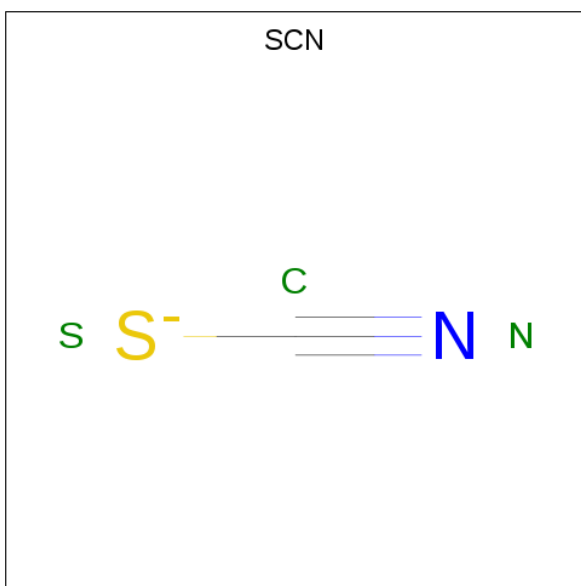
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		

- Molecule 8 is (2R)-2-hydroxy-3-(phosphonoxy)propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: C₂₁H₄₁O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 29	C 21	O 7	P 1	0	0
8	A	1	Total 6		C 6			

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



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

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

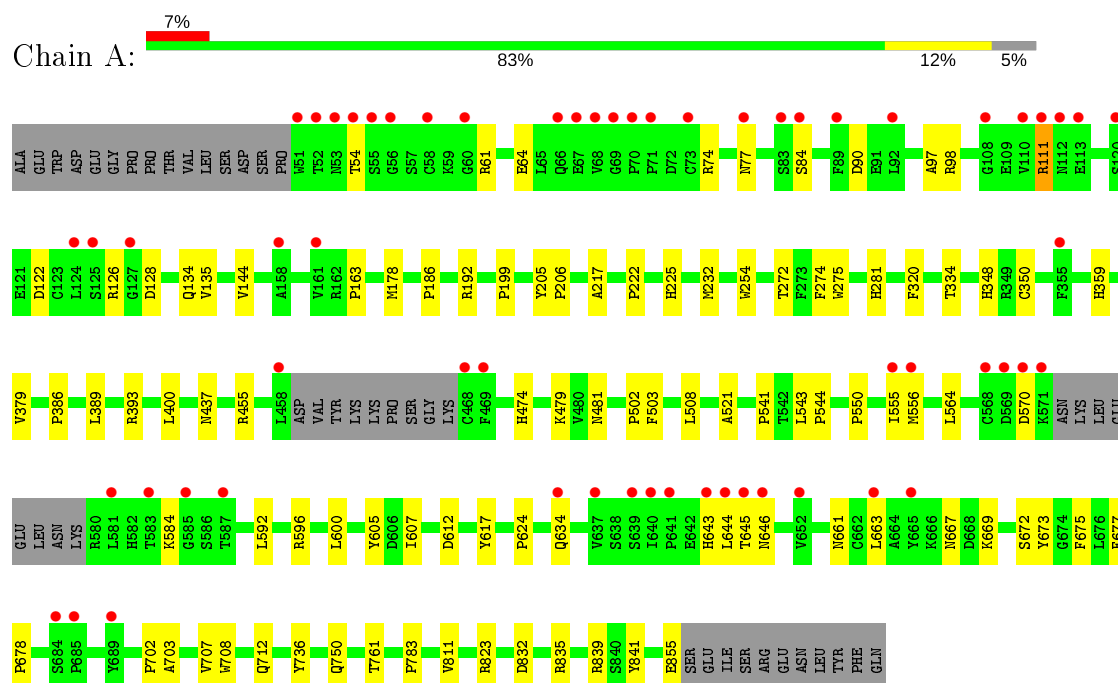
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	612	Total 612	O 612	0	0

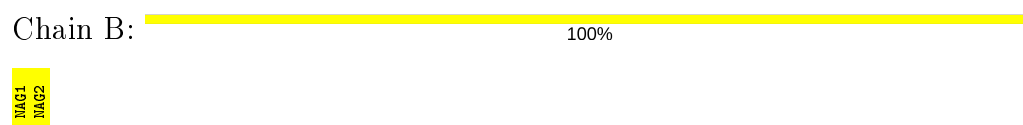
3 Residue-property plots

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.

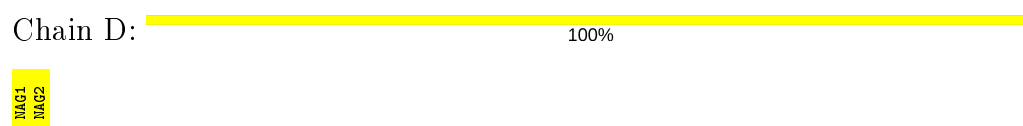
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



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




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



- 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-acetamido-2-deoxy-beta-D-glucopyranose

ido-2-deoxy-beta-D-glucopyranose

Chain C:  33% 67%

MAG 1	MAG 2	EMA 3	MAN 4	MAN 5	MAN 6
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.52Å 94.52Å 75.50Å 90.00° 94.55° 90.00°	Depositor
Resolution (Å)	26.53 – 1.75 49.51 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (26.53-1.75) 97.6 (49.51-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.6 _289	Depositor
R, R_{free}	0.189 , 0.222 0.184 , 0.218	Depositor DCC
R_{free} test set	4242 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7182	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 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, NA, K, EDO, NKP, SCN, CA, MAN

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	0.37	0/6506	0.53	0/8844

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

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	6312	0	5991	85	0
2	B	28	0	25	0	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	35	0	50	12	0
9	A	6	0	0	0	0
10	A	84	0	126	25	0
11	A	612	0	0	6	0
All	All	7182	0	6278	90	0

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

All (90) 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:77:ASN:HD21	1:A:272:THR:HG21	1.12	1.11
1:A:77:ASN:ND2	1:A:272:THR:HG21	1.66	1.09
8:A:1006:NKP:HAT	8:A:1006:NKP:CAO	1.84	1.07
1:A:675:PHE:H	10:A:1012:EDO:H11	0.98	1.07
8:A:1006:NKP:HAOA	8:A:1006:NKP:HAT	1.40	1.03
1:A:835:ARG:HE	10:A:1024:EDO:H22	1.18	1.03
1:A:77:ASN:HD21	1:A:272:THR:CG2	1.77	0.97
1:A:503:PHE:HE2	1:A:508:LEU:HD21	1.28	0.97
1:A:675:PHE:N	10:A:1012:EDO:H11	1.82	0.94
8:A:1006:NKP:CAT	8:A:1006:NKP:CAO	2.54	0.85
1:A:334:THR:OG1	10:A:1023:EDO:H22	1.76	0.85
1:A:281:HIS:ND1	10:A:1023:EDO:H21	1.91	0.84
8:A:1006:NKP:HAO	8:A:1006:NKP:CAT	2.10	0.81
1:A:275:TRP:H	8:A:1006:NKP:CAQ	1.95	0.80
1:A:503:PHE:CE2	1:A:508:LEU:HD21	2.18	0.78
1:A:111:ARG:CZ	1:A:126:ARG:HD3	2.16	0.76
1:A:503:PHE:HE2	1:A:508:LEU:CD2	2.00	0.74
1:A:275:TRP:H	8:A:1006:NKP:HAQA	1.52	0.73
1:A:77:ASN:HD21	1:A:272:THR:CB	2.02	0.72
1:A:111:ARG:NH1	1:A:122:ASP:OD1	2.23	0.71
1:A:702:PRO:HB2	10:A:1025:EDO:H22	1.72	0.69
1:A:570:ASP:HB2	1:A:643:HIS:HD2	1.58	0.67
1:A:178:MET:HE2	1:A:192:ARG:HD3	1.76	0.66
1:A:835:ARG:NE	10:A:1024:EDO:H22	2.01	0.65
1:A:634:GLN:HG3	11:A:1392:HOH:O	1.97	0.63
1:A:543:LEU:HD12	1:A:544:PRO:HD2	1.82	0.62
1:A:678:PRO:HB3	1:A:712:GLN:HB3	1.82	0.61
1:A:835:ARG:HH21	10:A:1024:EDO:H11	1.65	0.60
1:A:281:HIS:ND1	10:A:1023:EDO:C2	2.64	0.60
1:A:600:LEU:HD11	1:A:832:ASP:HB2	1.82	0.60
1:A:275:TRP:N	8:A:1006:NKP:HAR	2.19	0.57
1:A:550:PRO:HB2	1:A:607:ILE:HG12	1.86	0.56
1:A:275:TRP:H	8:A:1006:NKP:CAR	2.19	0.55
1:A:199:PRO:HG2	1:A:502:PRO:HG3	1.89	0.55
1:A:111:ARG:NH2	1:A:126:ARG:HD3	2.22	0.54
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.42	0.54
1:A:74:ARG:HD3	1:A:84:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:PRO:HB3	1:A:605:TYR:CE1	2.44	0.53
1:A:111:ARG:NH2	1:A:128:ASP:OD1	2.41	0.53
1:A:708:TRP:CD1	10:A:1012:EDO:H12	2.43	0.53
10:A:1030:EDO:H21	11:A:24:HOH:O	2.08	0.53
1:A:570:ASP:HB2	1:A:643:HIS:CD2	2.42	0.53
1:A:592:LEU:HD21	1:A:596:ARG:HB3	1.91	0.53
1:A:835:ARG:HE	10:A:1024:EDO:C2	2.06	0.53
1:A:275:TRP:H	8:A:1006:NKP:HAR	1.74	0.52
1:A:541:PRO:HG2	1:A:841:TYR:CD2	2.44	0.52
1:A:393:ARG:HA	10:A:1017:EDO:H21	1.92	0.51
1:A:134:GLN:NE2	11:A:1431:HOH:O	2.42	0.51
1:A:643:HIS:CD2	1:A:644:LEU:HG	2.45	0.51
1:A:661:ASN:OD1	1:A:663:LEU:HB3	2.11	0.51
1:A:61:ARG:HD2	1:A:64:GLU:OE1	2.10	0.50
1:A:783:PRO:HB3	10:A:1026:EDO:H21	1.92	0.50
1:A:437:ASN:HD21	10:A:1030:EDO:H22	1.76	0.50
1:A:555:ILE:O	1:A:556:MET:HG3	2.13	0.49
1:A:274:PHE:HA	8:A:1006:NKP:HAQ	1.95	0.49
1:A:703:ALA:HB2	10:A:1025:EDO:H21	1.95	0.49
1:A:379:VAL:HB	1:A:455:ARG:HG2	1.96	0.48
1:A:612:ASP:HB3	1:A:677:PHE:CZ	2.49	0.48
1:A:437:ASN:HD21	10:A:1030:EDO:C2	2.27	0.48
1:A:675:PHE:H	10:A:1012:EDO:C1	1.93	0.47
1:A:144:VAL:HG21	1:A:186:PRO:HB2	1.97	0.47
1:A:521:ALA:O	10:A:1018:EDO:H22	2.15	0.47
1:A:761:THR:HA	10:A:1015:EDO:H12	1.97	0.47
1:A:217:ALA:HA	8:A:1006:NKP:HBBB	1.97	0.47
1:A:672:SER:OG	1:A:673:TYR:N	2.47	0.47
1:A:479:LYS:O	1:A:855:GLU:HG3	2.15	0.46
1:A:272:THR:O	1:A:272:THR:HG23	2.14	0.46
1:A:564:LEU:O	1:A:661:ASN:HB2	2.16	0.46
1:A:205:TYR:CD2	1:A:206:PRO:HA	2.51	0.46
1:A:320:PHE:HE2	11:A:1464:HOH:O	1.99	0.46
1:A:359:HIS:CE1	1:A:474:HIS:CE1	3.04	0.45
1:A:541:PRO:HG2	1:A:841:TYR:HD2	1.81	0.45
1:A:839:ARG:HE	10:A:1026:EDO:H22	1.82	0.45
1:A:163:PRO:HB3	1:A:350:CYS:O	2.17	0.44
1:A:839:ARG:NE	10:A:1026:EDO:H22	2.32	0.44
1:A:90:ASP:HB3	11:A:1477:HOH:O	2.19	0.43
1:A:645:THR:HG22	1:A:646:ASN:ND2	2.35	0.42
1:A:707:VAL:HG13	1:A:811:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:PHE:HB2	10:A:1012:EDO:H21	2.01	0.42
1:A:736:TYR:OH	1:A:750:GLN:HB3	2.18	0.42
1:A:348:HIS:CD2	1:A:348:HIS:H	2.38	0.42
1:A:570:ASP:OD1	1:A:643:HIS:NE2	2.52	0.42
1:A:135:VAL:HG23	11:A:1308:HOH:O	2.19	0.42
1:A:97:ALA:O	1:A:98:ARG:HB2	2.20	0.41
1:A:254:TRP:HB2	8:A:1007:NKP:HAYA	2.01	0.41
1:A:823:ARG:CZ	10:A:1010:EDO:H22	2.50	0.41
1:A:617:TYR:HA	1:A:624:PRO:HA	2.02	0.41
1:A:272:THR:O	1:A:272:THR:CG2	2.69	0.41
1:A:675:PHE:HB2	10:A:1012:EDO:C2	2.51	0.40
1:A:206:PRO:HB3	1:A:389:LEU:HD13	2.04	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	786/831 (95%)	762 (97%)	22 (3%)	2 (0%)	41	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	584	LYS
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	703/756 (93%)	696 (99%)	7 (1%)	76	63

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	111	ARG
1	A	232	MET
1	A	400	LEU
1	A	481	ASN
1	A	667	ASN
1	A	669	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	77	ASN
1	A	118	HIS
1	A	134	GLN
1	A	337	GLN
1	A	348	HIS
1	A	374	ASN
1	A	398	ASN
1	A	643	HIS
1	A	646	ASN
1	A	667	ASN
1	A	827	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	0.45	0	17,19,21	1.46	2 (11%)
2	NAG	B	2	2	14,14,15	0.55	0	17,19,21	1.02	2 (11%)
3	NAG	C	1	1,3	14,14,15	0.62	0	17,19,21	1.42	2 (11%)
3	NAG	C	2	3	14,14,15	0.56	0	17,19,21	0.89	0
3	BMA	C	3	3	11,11,12	0.72	0	15,15,17	0.79	1 (6%)
3	MAN	C	4	3	11,11,12	0.56	0	15,15,17	0.83	1 (6%)
3	MAN	C	5	3	11,11,12	0.62	0	15,15,17	1.04	1 (6%)
3	MAN	C	6	3	11,11,12	0.68	0	15,15,17	0.92	0
2	NAG	D	1	1,2	14,14,15	0.71	0	17,19,21	1.14	2 (11%)
2	NAG	D	2	2	14,14,15	0.65	0	17,19,21	0.73	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	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	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	4.92	118.86	112.19
3	C	1	NAG	O5-C1-C2	-2.74	106.96	111.29
3	C	5	MAN	O5-C5-C6	2.63	111.33	107.20
2	B	2	NAG	O5-C5-C6	2.40	110.96	107.20
2	D	1	NAG	O4-C4-C5	-2.26	103.69	109.30
3	C	3	BMA	O5-C1-C2	-2.24	107.31	110.77
3	C	4	MAN	O5-C5-C6	2.16	110.59	107.20
2	D	1	NAG	O5-C1-C2	-2.11	107.96	111.29
2	D	2	NAG	C1-O5-C5	2.07	115.00	112.19
2	B	1	NAG	C6-C5-C4	-2.07	108.15	113.00
3	C	1	NAG	C2-N2-C7	2.03	125.79	122.90
2	B	2	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

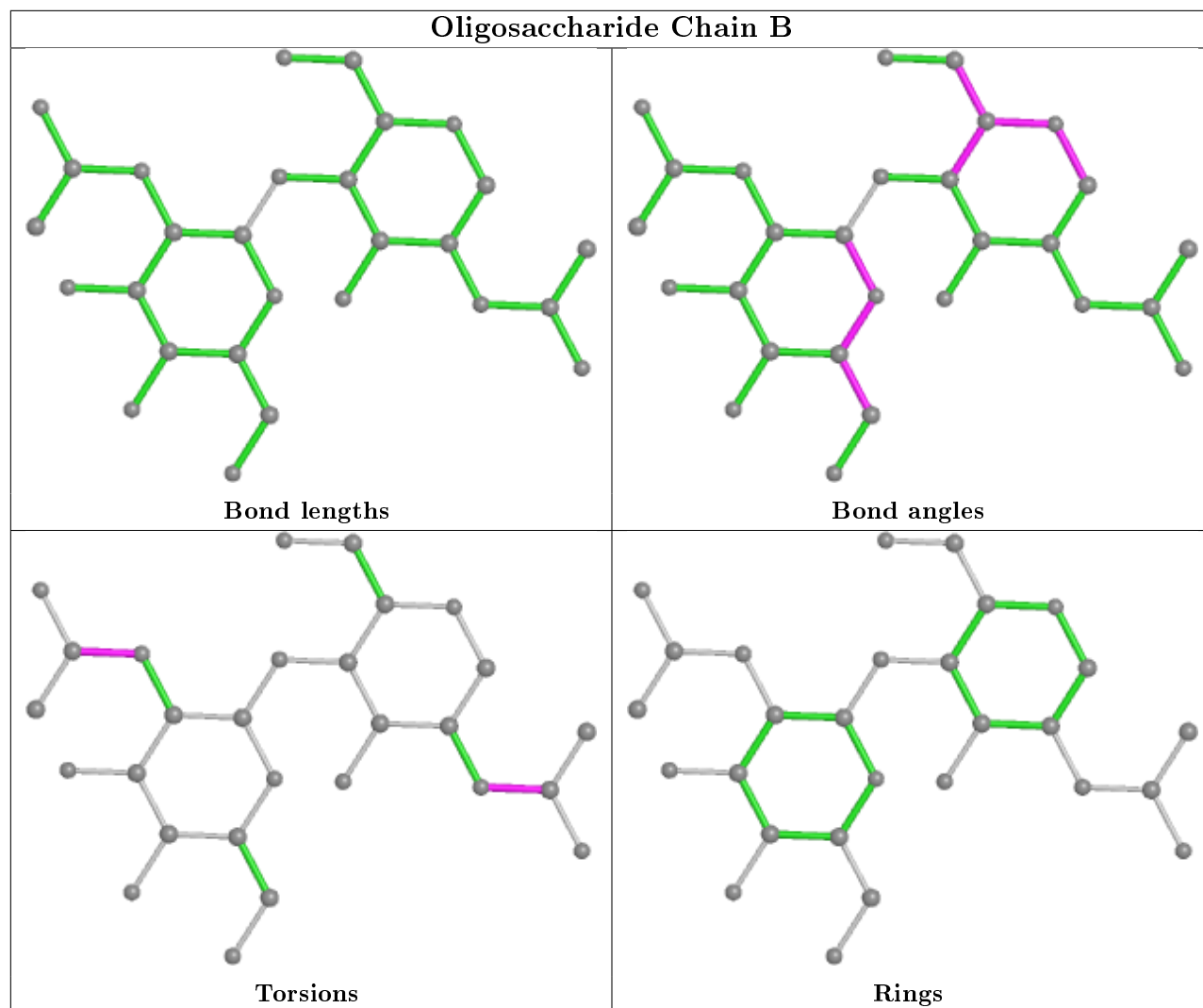
All (6) torsion outliers are listed below:

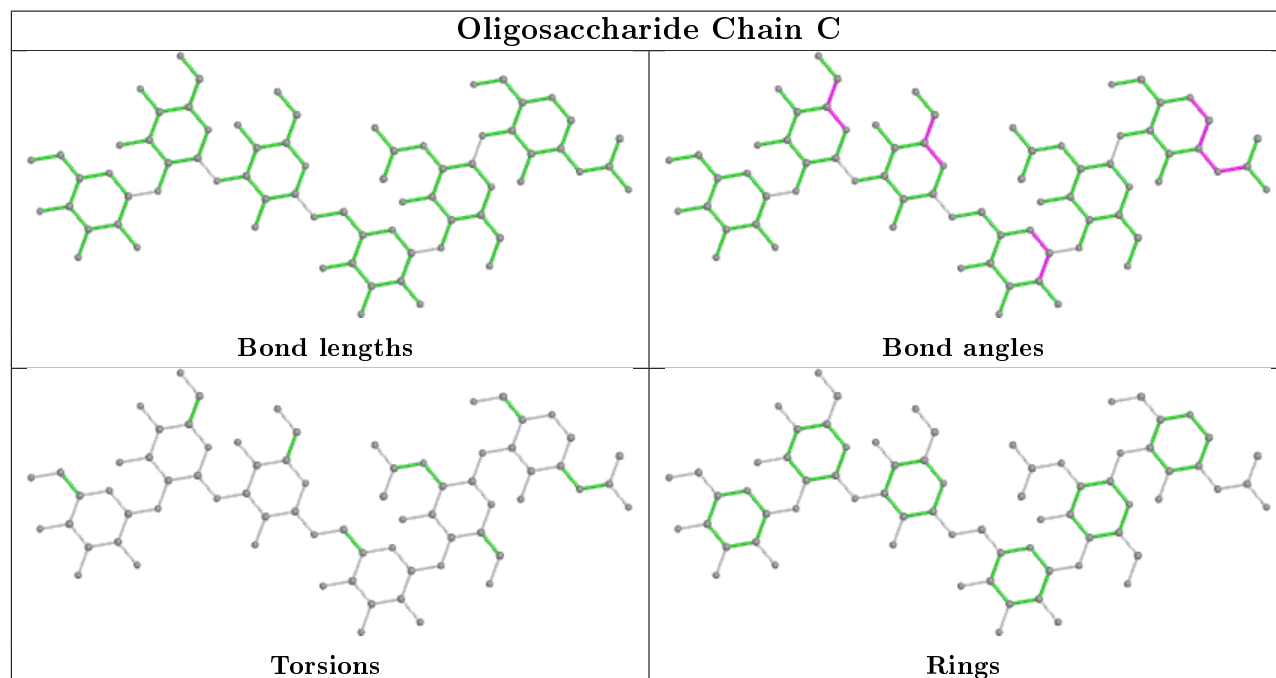
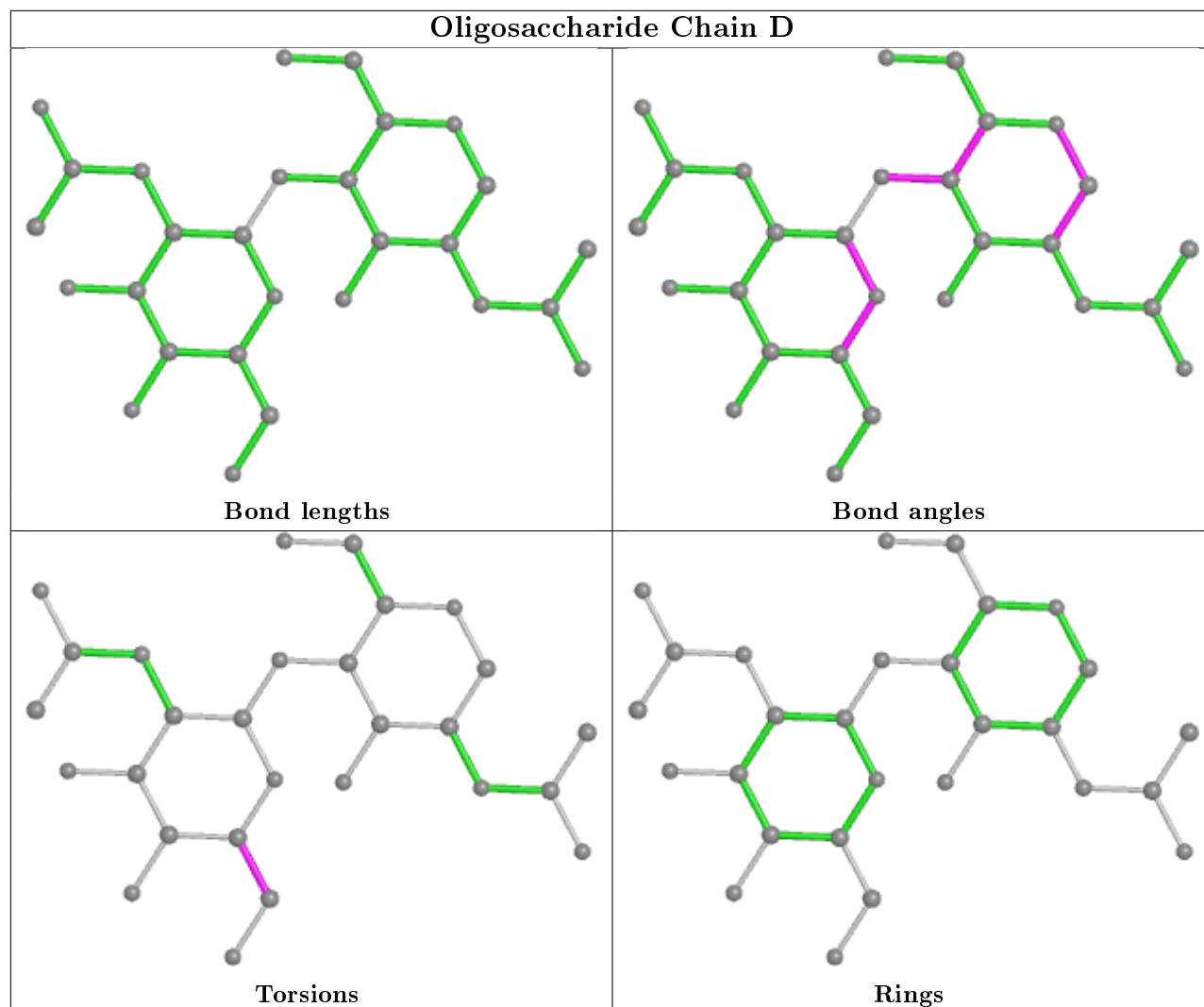
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry

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	1030	-	3,3,3	0.51	0	2,2,2	0.07	0
10	EDO	A	1015	-	3,3,3	0.47	0	2,2,2	0.26	0
10	EDO	A	1014	-	3,3,3	0.52	0	2,2,2	0.07	0
10	EDO	A	1011	-	3,3,3	0.65	0	2,2,2	0.08	0
10	EDO	A	1010	-	3,3,3	0.49	0	2,2,2	0.51	0
10	EDO	A	1024	-	3,3,3	0.50	0	2,2,2	0.27	0
10	EDO	A	1020	-	3,3,3	0.45	0	2,2,2	0.46	0
10	EDO	A	1022	-	3,3,3	0.48	0	2,2,2	0.31	0
10	EDO	A	1023	-	3,3,3	0.50	0	2,2,2	0.25	0
10	EDO	A	1029	-	3,3,3	0.54	0	2,2,2	0.31	0
10	EDO	A	1016	-	3,3,3	0.52	0	2,2,2	0.30	0
10	EDO	A	1017	-	3,3,3	0.48	0	2,2,2	0.28	0
9	SCN	A	1008	-	1,2,2	1.08	0	0,1,1	0.00	-
9	SCN	A	1009	-	1,2,2	0.92	0	0,1,1	0.00	-
10	EDO	A	1021	-	3,3,3	0.48	0	2,2,2	0.31	0
10	EDO	A	1019	-	3,3,3	0.43	0	2,2,2	0.30	0
10	EDO	A	1012	-	3,3,3	0.31	0	2,2,2	0.63	0
10	EDO	A	1018	-	3,3,3	0.54	0	2,2,2	0.19	0
10	EDO	A	1027	-	3,3,3	0.51	0	2,2,2	0.29	0
10	EDO	A	1025	-	3,3,3	0.47	0	2,2,2	0.29	0
8	NKP	A	1007	-	5,5,28	0.28	0	4,4,32	0.57	0
10	EDO	A	1013	-	3,3,3	0.50	0	2,2,2	0.30	0
10	EDO	A	1028	-	3,3,3	0.50	0	2,2,2	0.36	0
8	NKP	A	1006	4	28,28,28	0.70	1 (3%)	31,32,32	1.67	12 (38%)
10	EDO	A	1026	-	3,3,3	0.42	0	2,2,2	0.35	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	1030	-	-	0/1/1/1	-
10	EDO	A	1015	-	-	0/1/1/1	-
10	EDO	A	1014	-	-	0/1/1/1	-
10	EDO	A	1011	-	-	0/1/1/1	-
10	EDO	A	1010	-	-	1/1/1/1	-
10	EDO	A	1024	-	-	0/1/1/1	-
10	EDO	A	1020	-	-	1/1/1/1	-
10	EDO	A	1022	-	-	0/1/1/1	-
10	EDO	A	1023	-	-	1/1/1/1	-
10	EDO	A	1029	-	-	1/1/1/1	-
10	EDO	A	1016	-	-	0/1/1/1	-
10	EDO	A	1017	-	-	0/1/1/1	-
10	EDO	A	1021	-	-	0/1/1/1	-
10	EDO	A	1019	-	-	0/1/1/1	-
10	EDO	A	1012	-	-	0/1/1/1	-
10	EDO	A	1018	-	-	0/1/1/1	-
10	EDO	A	1027	-	-	0/1/1/1	-
10	EDO	A	1025	-	-	0/1/1/1	-
8	NKP	A	1007	-	-	0/3/3/28	-
10	EDO	A	1013	-	-	0/1/1/1	-
10	EDO	A	1028	-	-	0/1/1/1	-
8	NKP	A	1006	4	-	5/28/28/28	-
10	EDO	A	1026	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1006	NKP	CAR-CAS	-2.02	1.38	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1006	NKP	PAC-OAF-CAG	3.78	128.71	118.30
8	A	1006	NKP	OBC-CAH-CAG	3.30	121.13	109.56
8	A	1006	NKP	CAI-OAJ-CAK	-2.67	107.22	117.12
8	A	1006	NKP	OAA-PAC-OAF	-2.53	99.99	106.73
8	A	1006	NKP	CAP-CAQ-CAR	2.42	124.35	113.79
8	A	1006	NKP	OAJ-CAK-CAL	2.32	119.20	111.91
8	A	1006	NKP	CBA-CAZ-CAY	-2.13	95.49	115.30
8	A	1006	NKP	OAJ-CAK-OAE	-2.11	118.26	123.59
8	A	1006	NKP	CAW-CAV-CAU	-2.07	104.76	113.79
8	A	1006	NKP	CAI-CAH-CAG	-2.05	106.77	112.79
8	A	1006	NKP	CAN-CAM-CAL	-2.03	105.90	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1006	NKP	OAF-PAC-OAD	2.01	112.11	106.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1006	NKP	CAG-OAF-PAC-OAA
8	A	1006	NKP	CAG-OAF-PAC-OAB
8	A	1006	NKP	CAH-CAG-OAF-PAC
8	A	1006	NKP	CAG-OAF-PAC-OAD
10	A	1029	EDO	O1-C1-C2-O2
8	A	1006	NKP	CAS-CAT-CAU-CAV
10	A	1010	EDO	O1-C1-C2-O2
10	A	1020	EDO	O1-C1-C2-O2
10	A	1023	EDO	O1-C1-C2-O2

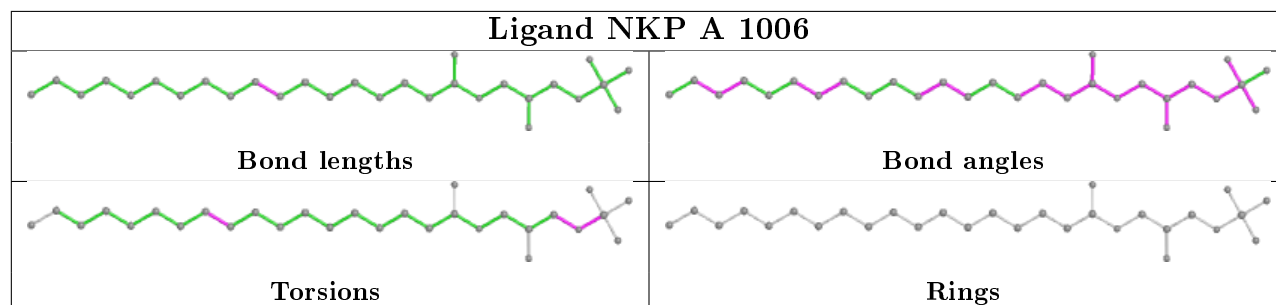
There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1030	EDO	3	0
10	A	1015	EDO	1	0
10	A	1010	EDO	1	0
10	A	1024	EDO	4	0
10	A	1023	EDO	3	0
10	A	1017	EDO	1	0
10	A	1012	EDO	6	0
10	A	1018	EDO	1	0
10	A	1025	EDO	2	0
8	A	1007	NKP	1	0
8	A	1006	NKP	11	0
10	A	1026	EDO	3	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 than 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	788/831 (94%)	0.40	60 (7%) 13 18	14, 30, 56, 73	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	7.2
1	A	110	VAL	7.1
1	A	83	SER	6.3
1	A	585	GLY	5.1
1	A	569	ASP	4.6
1	A	583	THR	4.3
1	A	52	THR	4.2
1	A	637	VAL	4.0
1	A	124	LEU	4.0
1	A	73	CYS	4.0
1	A	581	LEU	3.9
1	A	71	PRO	3.9
1	A	69	GLY	3.8
1	A	55	SER	3.7
1	A	68	VAL	3.6
1	A	640	ILE	3.6
1	A	641	PRO	3.5
1	A	644	LEU	3.5
1	A	70	PRO	3.4
1	A	469	PHE	3.4
1	A	645	THR	3.3
1	A	571	LYS	3.3
1	A	92	LEU	3.2
1	A	685	PRO	3.2
1	A	66	GLN	3.2
1	A	125	SER	3.0
1	A	458	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	56	GLY	2.9
1	A	108	GLY	2.9
1	A	684	SER	2.8
1	A	67	GLU	2.8
1	A	556	MET	2.7
1	A	58	CYS	2.7
1	A	639	SER	2.7
1	A	53	ASN	2.7
1	A	643	HIS	2.6
1	A	587	THR	2.6
1	A	111	ARG	2.6
1	A	665	TYR	2.6
1	A	158	ALA	2.5
1	A	120	SER	2.5
1	A	54	THR	2.5
1	A	161	VAL	2.5
1	A	646	ASN	2.4
1	A	570	ASP	2.4
1	A	634	GLN	2.4
1	A	77	ASN	2.4
1	A	652	VAL	2.3
1	A	112	ASN	2.3
1	A	568	CYS	2.3
1	A	84	SER	2.3
1	A	663	LEU	2.2
1	A	113	GLU	2.2
1	A	468	CYS	2.2
1	A	127	GLY	2.2
1	A	555	ILE	2.2
1	A	60	GLY	2.2
1	A	89	PHE	2.1
1	A	689	TYR	2.0
1	A	355	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

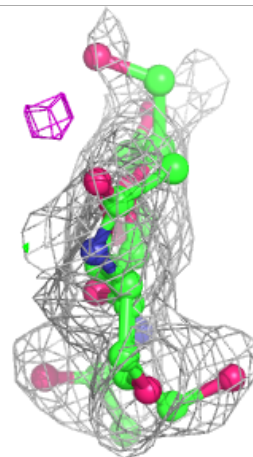
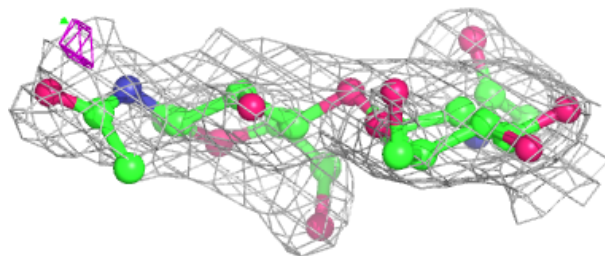
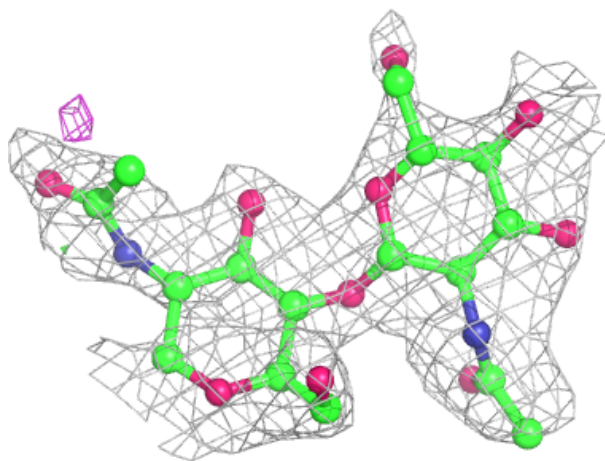
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.77	0.27	66,68,71,72	0
3	MAN	C	4	11/12	0.80	0.13	39,41,46,47	0
2	NAG	D	2	14/15	0.82	0.22	50,56,58,58	0
2	NAG	B	2	14/15	0.83	0.21	65,72,77,77	0
3	BMA	C	3	11/12	0.85	0.13	40,43,51,51	0
2	NAG	D	1	14/15	0.93	0.11	26,31,39,47	0
3	MAN	C	6	11/12	0.94	0.10	25,31,37,38	0
3	MAN	C	5	11/12	0.94	0.18	32,35,41,51	0
3	NAG	C	2	14/15	0.95	0.08	23,31,39,42	0
3	NAG	C	1	14/15	0.96	0.09	16,20,22,23	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.

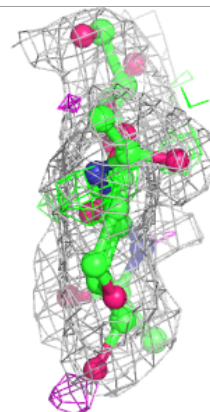
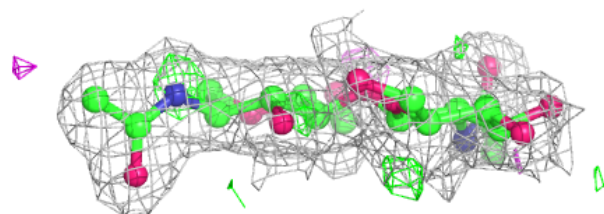
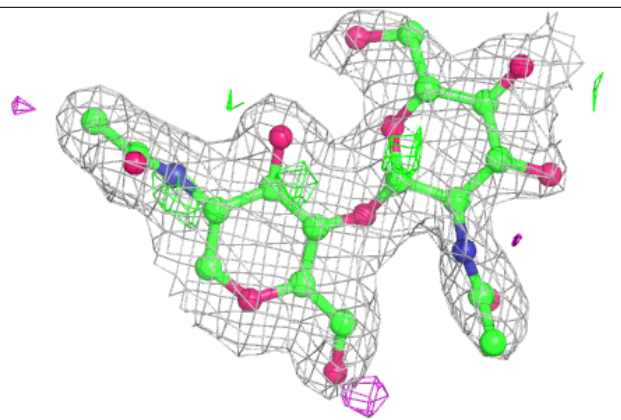
Electron density around Chain B:

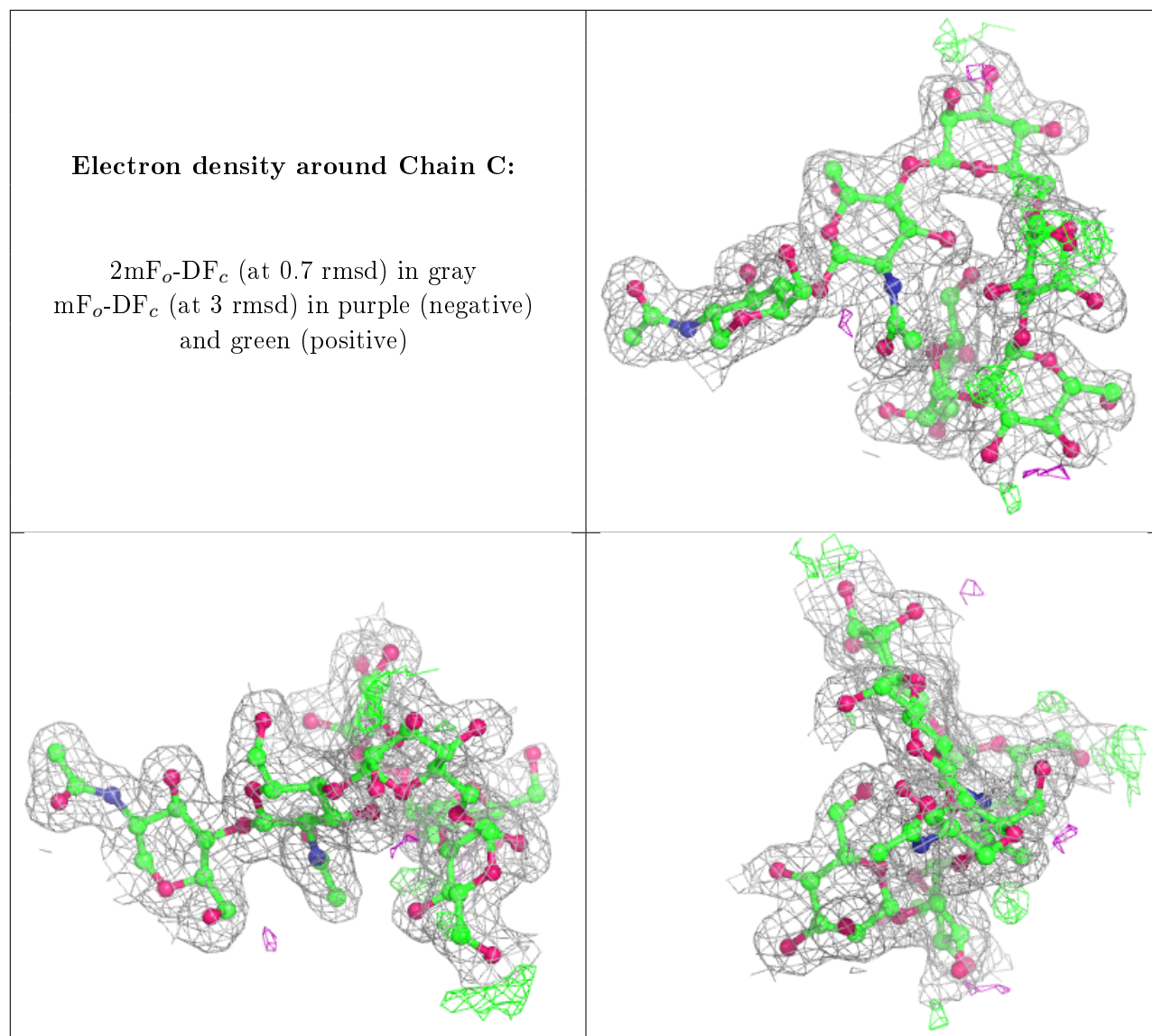
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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	0.72	0.19	46,47,49,50	0
9	SCN	A	1008	3/3	0.81	0.16	24,24,36,41	0
10	EDO	A	1018	4/4	0.83	0.18	25,31,32,40	0
10	EDO	A	1011	4/4	0.86	0.14	26,30,32,34	0
10	EDO	A	1022	4/4	0.88	0.11	34,35,38,46	0
10	EDO	A	1030	4/4	0.92	0.18	18,27,33,37	0

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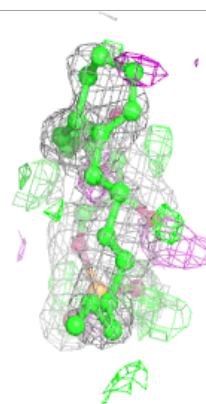
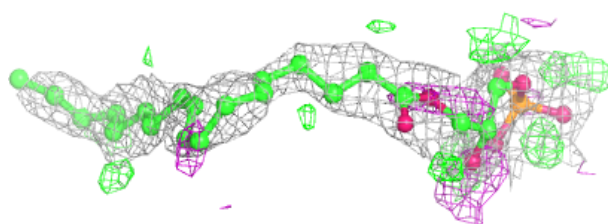
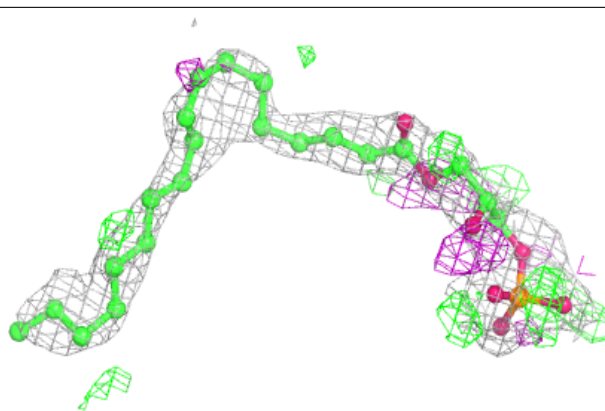
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	A	1010	4/4	0.92	0.14	33,33,35,36	0
8	NKP	A	1007	6/29	0.92	0.16	34,37,38,40	0
10	EDO	A	1026	4/4	0.92	0.16	21,28,34,39	0
10	EDO	A	1027	4/4	0.93	0.12	31,33,41,43	0
7	K	A	1005	1/1	0.93	0.09	38,38,38,38	0
10	EDO	A	1013	4/4	0.93	0.16	33,33,33,33	0
8	NKP	A	1006	29/29	0.93	0.19	21,37,46,51	0
10	EDO	A	1014	4/4	0.93	0.10	28,29,29,33	0
10	EDO	A	1016	4/4	0.94	0.12	27,29,30,31	0
10	EDO	A	1021	4/4	0.94	0.18	34,37,39,43	0
10	EDO	A	1012	4/4	0.94	0.11	30,33,33,35	0
10	EDO	A	1029	4/4	0.95	0.09	25,26,32,34	0
10	EDO	A	1015	4/4	0.95	0.09	28,30,32,35	0
10	EDO	A	1019	4/4	0.95	0.08	32,32,36,42	0
10	EDO	A	1017	4/4	0.95	0.16	22,25,29,29	0
10	EDO	A	1023	4/4	0.95	0.14	25,30,32,35	0
10	EDO	A	1020	4/4	0.96	0.10	25,27,33,37	0
10	EDO	A	1025	4/4	0.96	0.29	37,39,41,44	0
10	EDO	A	1028	4/4	0.97	0.09	19,21,23,24	0
9	SCN	A	1009	3/3	0.98	0.12	26,26,36,50	0
6	NA	A	1004	1/1	0.98	0.07	25,25,25,25	0
4	ZN	A	1001	1/1	0.99	0.10	21,21,21,21	0
4	ZN	A	1002	1/1	1.00	0.11	18,18,18,18	0
5	CA	A	1003	1/1	1.00	0.09	23,23,23,23	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 NKP 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.