



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:28 PM UTC

PDB ID : 8C3P / pdb_00008c3p
Title : Crystal structure of autotaxin gamma in complex with LPA 18:1
Authors : Eymery, M.C.; McCarthy, A.A.
Deposited on : 2022-12-28
Resolution : 2.38 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

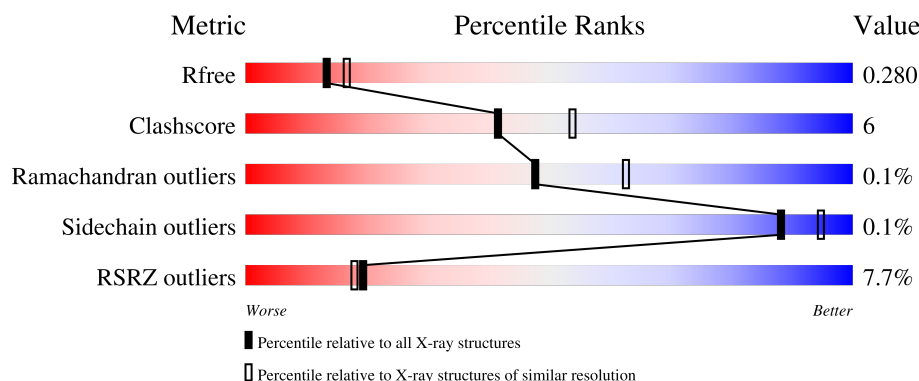
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 $\leq 5\%$. 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	888	6% 74% 14% 12%
1	B	888	7% 74% 14% 12%
2	C	3	100%
2	D	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	D	3	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13266 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.

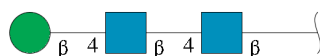
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	778	Total	C	N	O	S	3	11	0
			6264	3988	1062	1166	48			
1	B	778	Total	C	N	O	S	3	12	0
			6267	3988	1065	1166	48			

There are 4 discrepancies between the modelled and reference sequences:

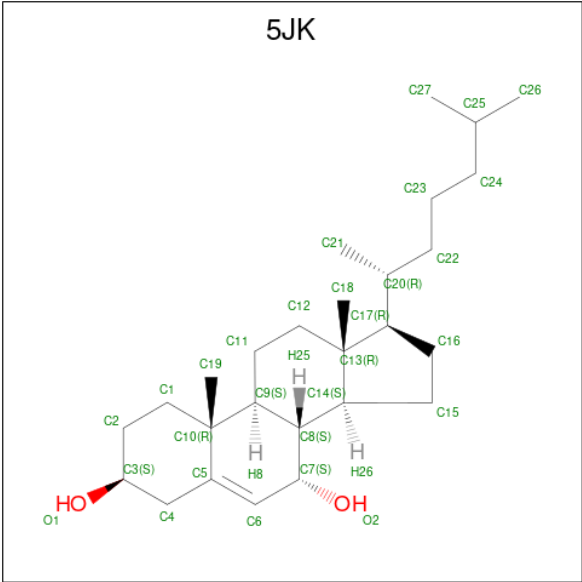
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ALA	ASN	engineered mutation	UNP Q13822
A	411	ALA	ASN	engineered mutation	UNP Q13822
B	54	ALA	ASN	engineered mutation	UNP Q13822
B	411	ALA	ASN	engineered mutation	UNP Q13822

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



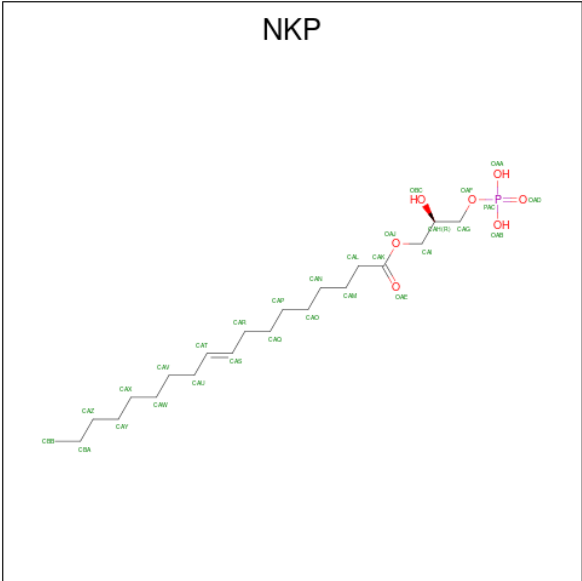
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is 7alpha-hydroxycholesterol (CCD ID: 5JK) (formula: C₂₇H₄₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			29	27	2		
3	B	1	Total	C	O	0	0
			29	27	2		

- Molecule 4 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: C₂₁H₄₁O₇P) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			29	21	7	1		

- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	I	0	0
			9	9		
5	B	8	Total	I	0	0
			8	8		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca	0	0
			2	2		
6	B	2	Total	Ca	0	0
			2	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	B	2	Total	Zn	0	0
			2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

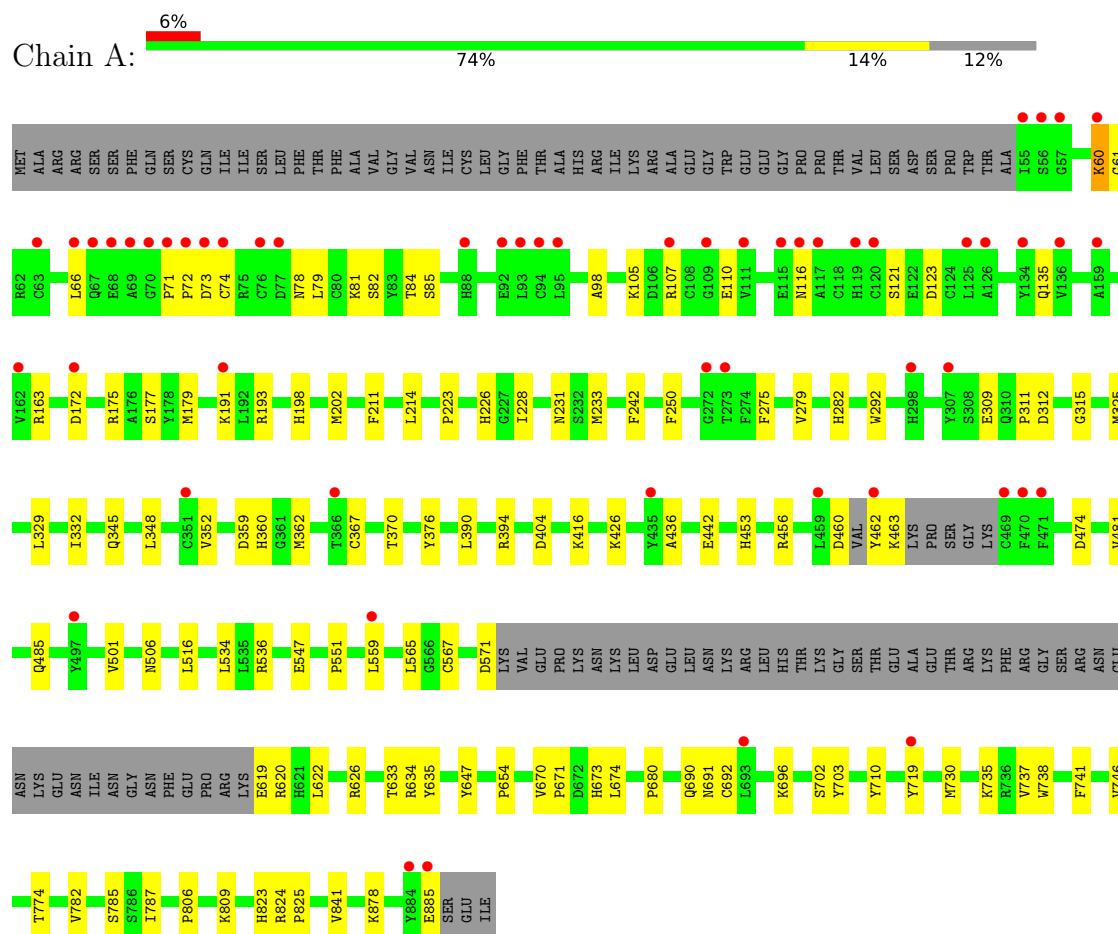
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	239	Total	O	0	0
			239	239		
9	B	271	Total	O	0	0
			271	271		

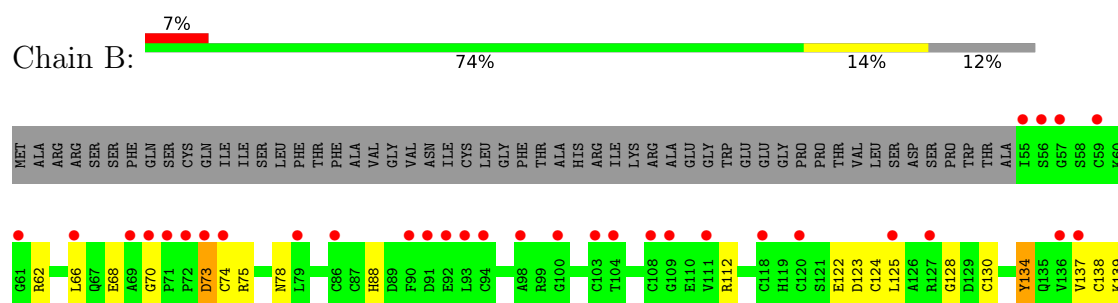
3 Residue-property plots

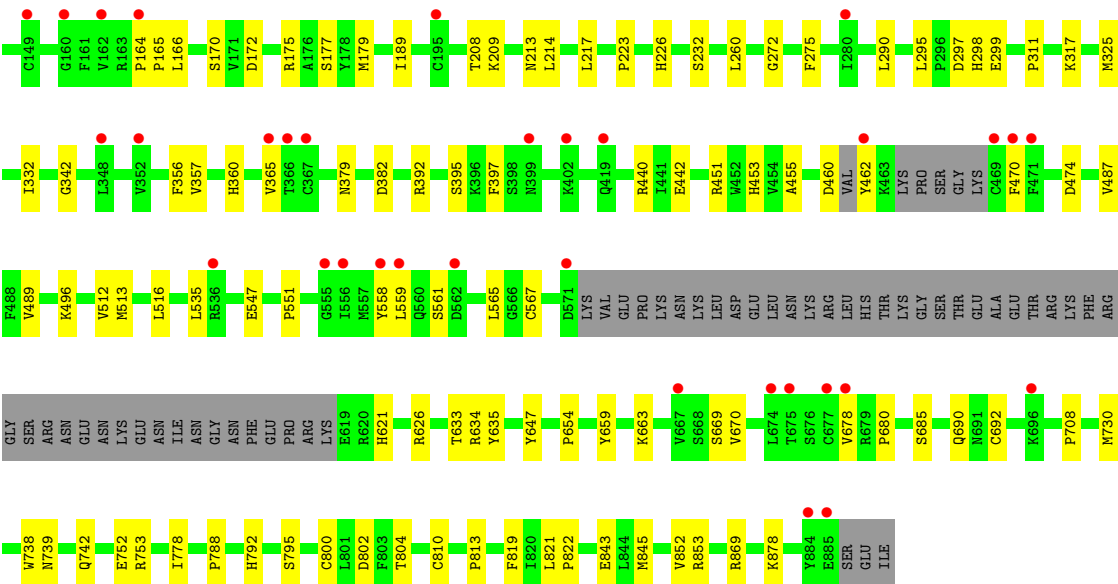
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2





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

Chain C: 100%



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

Chain D: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.94Å 57.22Å 287.93Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	53.88 – 2.38 53.88 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (53.88-2.38) 98.7 (53.88-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.222 , 0.280 0.222 , 0.280	Depositor DCC
R_{free} test set	3530 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13266	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, CA, 5JK, NKP, NAG, BMA, ZN, GOL

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	0.13	0/6474	0.32	0/8798
1	B	0.12	0/6477	0.32	0/8801
All	All	0.13	0/12951	0.32	0/17599

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	6264	0	5968	87	0
1	B	6267	0	5970	71	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	29	0	39	3	0
4	B	29	0	39	1	0
5	A	9	0	0	4	0
5	B	8	0	0	2	0
6	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	B	6	0	8	0	0
9	A	239	0	0	7	0
9	B	271	0	0	3	0
All	All	13266	0	12092	159	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 (159) 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:78:ASN:ND2	1:A:275:PHE:O	2.15	0.80
1:B:295:LEU:HD13	1:B:299:GLU:HG3	1.71	0.72
1:B:379:ASN:ND2	1:B:382:ASP:OD2	2.23	0.72
1:A:559:LEU:HD11	1:B:634:ARG:HB2	1.74	0.69
1:B:179:MET:HE3	1:B:487:VAL:HG21	1.75	0.68
1:A:671:PRO:HG2	1:A:674:LEU:HB2	1.76	0.68
1:B:567:CYS:HB3	1:B:678:VAL:HG13	1.75	0.67
1:B:70:GLY:O	1:B:73:ASP:HB2	1.95	0.67
1:A:806:PRO:HG2	1:A:809:LYS:HB2	1.77	0.67
1:B:739:ASN:ND2	9:B:1002:HOH:O	2.28	0.66
1:B:62:ARG:NH2	1:B:74:CYS:O	2.32	0.62
1:A:228:ILE:HA	1:A:233:MET:HE1	1.81	0.62
1:A:774:THR:HG22	5:A:910:IOD:I	2.70	0.61
1:B:843:GLU:OE1	1:B:843:GLU:N	2.29	0.61
1:A:367:CYS:HB2	1:A:462:TYR:HE2	1.66	0.61
1:A:481:VAL:O	1:A:485:GLN:NE2	2.29	0.61
1:B:260:LEU:HD22	1:B:513:MET:HE3	1.83	0.61
1:A:571:ASP:HB3	1:A:719:TYR:CE2	2.36	0.60
1:B:455:ALA:HB1	1:B:462:TYR:CE2	2.36	0.60
1:A:311:PRO:HB2	1:A:325:MET:HE1	1.84	0.59
1:B:122:GLU:OE2	1:B:139:LYS:NZ	2.29	0.59
1:B:311:PRO:HB2	1:B:325:MET:HE1	1.84	0.59
1:B:356:PHE:HB3	1:B:489:VAL:HB	1.85	0.59
1:B:565:LEU:HD13	1:B:690:GLN:O	2.02	0.59
1:B:214:LEU:HA	1:B:217:LEU:HD12	1.83	0.59
1:A:135:GLN:HG3	1:A:345:GLN:HG3	1.85	0.58
1:A:214:LEU:HB3	4:A:902:NKP:HAT	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:CYS:O	1:B:128:GLY:N	2.36	0.58
1:B:752:GLU:HG3	1:B:753:ARG:HG3	1.85	0.58
1:A:163:ARG:NH1	9:A:1010:HOH:O	2.38	0.57
1:A:367:CYS:HB2	1:A:462:TYR:CE2	2.39	0.57
1:A:551:PRO:HB3	1:A:635:TYR:CZ	2.39	0.57
1:B:680:PRO:HG3	5:B:915:IOD:I	2.76	0.56
1:A:680:PRO:HG3	5:A:903:IOD:I	2.76	0.55
1:B:68:GLU:HB2	1:B:75:ARG:HG2	1.87	0.55
1:A:202:MET:HE3	1:A:506:ASN:HB3	1.87	0.55
1:A:98:ALA:HB3	1:A:116:ASN:HA	1.89	0.55
1:A:619:GLU:HG3	1:A:620:ARG:H	1.72	0.54
1:A:426:LYS:HD2	1:A:436:ALA:HA	1.89	0.53
1:B:453:HIS:NE2	1:B:474:ASP:OD2	2.39	0.53
1:B:223:PRO:HA	1:B:226:HIS:CE1	2.43	0.53
1:A:60:LYS:NZ	1:A:61:GLY:H	2.06	0.53
1:B:125:LEU:HD23	1:B:130:CYS:SG	2.48	0.53
1:A:878:LYS:NZ	9:A:1013:HOH:O	2.38	0.53
1:A:547:GLU:OE2	1:A:626[B]:ARG:NH1	2.38	0.53
1:B:663:LYS:NZ	9:B:1018:HOH:O	2.42	0.53
1:A:547:GLU:OE1	1:A:626[B]:ARG:NH2	2.42	0.52
1:B:78:ASN:ND2	1:B:275:PHE:O	2.42	0.52
1:A:223:PRO:HA	1:A:226:HIS:CE1	2.45	0.52
1:A:690:GLN:HG2	1:A:787:ILE:HG12	1.91	0.52
1:A:416:LYS:NZ	9:A:1017:HOH:O	2.42	0.52
1:A:453:HIS:NE2	1:A:474:ASP:OD2	2.36	0.52
1:A:404:ASP:OD1	1:A:404:ASP:N	2.43	0.51
1:B:66:LEU:HD22	1:B:272:GLY:CA	2.40	0.51
1:B:442:GLU:OE1	1:B:442:GLU:N	2.44	0.51
1:A:175:ARG:HG2	1:A:177:SER:H	1.76	0.51
1:A:536[A]:ARG:NH2	9:A:1019:HOH:O	2.44	0.50
1:A:394:ARG:NH1	1:A:442:GLU:OE2	2.44	0.50
1:A:506:ASN:ND2	9:A:1018:HOH:O	2.42	0.50
1:B:559:LEU:C	1:B:561:SER:H	2.20	0.50
1:A:456:ARG:HH21	1:A:460:ASP:CG	2.20	0.50
1:B:621:HIS:HB3	1:B:659:TYR:HA	1.93	0.49
1:A:824:ARG:HD3	1:A:825:PRO:HD2	1.92	0.49
1:A:233:MET:HG3	1:A:242:PHE:HB3	1.94	0.49
1:A:172:ASP:OD2	4:A:902:NKP:HAIA	2.13	0.49
1:A:647:TYR:HA	1:A:654:PRO:HA	1.95	0.49
1:B:813:PRO:HA	1:B:869:ARG:HD2	1.95	0.49
1:A:60:LYS:HZ1	1:A:61:GLY:H	1.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LYS:HD3	1:A:105:LYS:H	1.79	0.48
1:B:678:VAL:HG11	1:B:692:CYS:SG	2.54	0.48
1:A:193:ARG:O	1:A:198:HIS:ND1	2.47	0.48
1:A:741:PHE:O	1:A:746:VAL:HG23	2.14	0.47
1:A:107:ARG:HA	1:A:110:GLU:HG2	1.96	0.47
1:A:702:SER:OG	1:A:703:TYR:N	2.47	0.47
1:A:565:LEU:HB3	1:A:691:ASN:HA	1.95	0.47
4:A:902:NKP:HAU	4:A:902:NKP:HAZA	1.97	0.47
1:B:821[A]:LEU:HD21	1:B:845:MET:HG2	1.96	0.47
1:A:348:LEU:HB3	1:A:352:VAL:HG23	1.97	0.47
1:B:647:TYR:HA	1:B:654:PRO:HA	1.97	0.47
1:B:669:SER:OG	1:B:670:VAL:N	2.47	0.47
1:A:71:PRO:HB2	1:A:72:PRO:HD3	1.96	0.46
1:B:558:TYR:OH	1:B:685:SER:HB2	2.15	0.46
1:A:66:LEU:HD21	1:A:292:TRP:CZ2	2.50	0.46
1:A:172:ASP:HB3	1:A:312:ASP:HB2	1.96	0.46
1:A:193:ARG:NH2	9:A:1028:HOH:O	2.49	0.46
1:A:282:HIS:NE2	1:A:309:GLU:OE2	2.49	0.46
4:B:903:NKP:HARA	4:B:903:NKP:HAUA	1.73	0.46
1:B:112:ARG:NH2	1:B:123:ASP:OD2	2.37	0.46
1:A:81:LYS:HG2	1:A:279:VAL:CG1	2.46	0.45
1:A:622:LEU:HD23	1:A:622:LEU:HA	1.82	0.45
1:B:365:VAL:HG22	1:B:451:ARG:HA	1.99	0.45
1:A:885:GLU:OE1	9:A:1001:HOH:O	2.21	0.45
1:B:496:LYS:NZ	1:B:535:LEU:O	2.41	0.45
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.70	0.45
1:A:309:GLU:H	1:A:309:GLU:CD	2.25	0.45
1:B:460:ASP:HB2	1:B:462:TYR:CE2	2.51	0.45
1:B:547:GLU:OE2	1:B:626[B]:ARG:NH2	2.47	0.45
1:B:802:ASP:OD2	1:B:804:THR:OG1	2.35	0.45
1:A:673:HIS:CE1	1:A:674:LEU:HG	2.52	0.45
1:A:696:LYS:HD3	1:A:696:LYS:HA	1.74	0.45
1:B:166:LEU:HD21	1:B:513:MET:HG2	1.98	0.45
1:A:567:CYS:SG	1:A:692:CYS:N	2.88	0.45
1:A:782:VAL:HB	1:A:785:SER:OG	2.17	0.45
1:A:390:LEU:HD21	5:A:914:IOD:I	2.88	0.44
1:B:232:SER:O	1:B:392:ARG:NH2	2.45	0.44
1:B:298:HIS:O	1:B:298:HIS:ND1	2.48	0.44
1:B:551:PRO:HB3	1:B:635:TYR:CZ	2.52	0.44
1:A:737:VAL:HG13	1:A:841:VAL:HG13	1.99	0.44
1:B:440:ARG:NH2	9:B:1035:HOH:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:SER:HB3	1:A:250:PHE:CZ	2.52	0.44
1:A:370:THR:HG23	1:A:453:HIS:HB3	1.99	0.44
1:B:297:ASP:OD1	1:B:297:ASP:N	2.51	0.44
1:A:179:MET:HG2	1:A:193:ARG:NH1	2.34	0.43
1:A:735:LYS:HB3	1:A:735:LYS:HE2	1.86	0.43
1:B:134:TYR:C	1:B:134:TYR:CD1	2.96	0.43
1:B:164:PRO:HA	1:B:165:PRO:HD3	1.90	0.43
1:B:633:THR:OG1	1:B:634:ARG:N	2.49	0.43
1:A:312:ASP:OD2	1:A:360:HIS:CE1	2.71	0.43
1:B:317:LYS:HD3	1:B:470:PHE:O	2.18	0.43
1:B:778:ILE:HG21	1:B:788:PRO:HB3	1.99	0.43
1:A:105:LYS:HD3	1:A:105:LYS:N	2.34	0.43
1:B:795:SER:HB2	1:B:819:PHE:CZ	2.53	0.43
1:A:84:THR:HA	5:A:915:IOD:I	2.89	0.42
1:B:175:ARG:NE	1:B:177:SER:OG	2.46	0.42
1:B:208:THR:HA	1:B:213:ASN:HD21	1.83	0.42
1:A:121:SER:OG	1:A:123:ASP:OD1	2.33	0.42
1:A:633:THR:OG1	1:A:634:ARG:N	2.51	0.42
1:B:66:LEU:HD22	1:B:272:GLY:HA2	2.00	0.42
1:A:462:TYR:HD1	1:A:463:LYS:HE2	1.83	0.42
1:A:501:VAL:HG11	1:A:534:LEU:HD12	2.01	0.42
1:B:730:MET:HE1	1:B:738:TRP:CE2	2.54	0.42
1:A:73:ASP:OD2	1:A:74:CYS:N	2.53	0.42
1:B:170:SER:HA	1:B:357:VAL:O	2.20	0.42
1:B:395:SER:OG	1:B:397:PHE:O	2.38	0.42
1:A:730:MET:HE1	1:A:738:TRP:CE2	2.55	0.41
1:B:792:HIS:CD2	1:B:822:PRO:HA	2.54	0.41
1:B:172:ASP:OD1	1:B:360:HIS:CE1	2.73	0.41
1:A:172:ASP:OD1	1:A:359:ASP:OD2	2.39	0.41
1:B:88:HIS:CD2	1:B:88:HIS:H	2.39	0.41
1:B:800:CYS:HB2	1:B:810:CYS:HB2	1.98	0.41
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.89	0.41
1:A:85:SER:O	1:A:85:SER:OG	2.31	0.41
1:B:137:VAL:HG13	1:B:138:CYS:SG	2.61	0.41
1:B:708:PRO:HB3	1:B:742:GLN:HB3	2.01	0.41
1:A:376:TYR:CZ	1:A:416:LYS:HD2	2.56	0.41
1:A:670:VAL:HG23	1:A:710:TYR:CE1	2.55	0.41
1:A:730:MET:HA	1:A:823:HIS:NE2	2.36	0.41
1:B:209[A]:LYS:HD2	5:B:914:IOD:I	2.90	0.41
1:B:290:LEU:HD13	1:B:342:GLY:HA3	2.02	0.41
1:B:512:VAL:O	1:B:516[A]:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:TYR:CD1	1:A:463:LYS:HG3	2.56	0.41
1:A:191:LYS:HA	1:A:191:LYS:HD3	1.75	0.40
1:B:559:LEU:C	1:B:561:SER:N	2.79	0.40
1:B:852:VAL:HB	1:B:878:LYS:HA	2.03	0.40
1:A:329:LEU:HD23	1:A:332:ILE:HD12	2.03	0.40
1:B:189:ILE:HD11	1:B:332:ILE:HG22	2.02	0.40
1:A:516[B]:LEU:HD12	1:A:516[B]:LEU:HA	1.91	0.40
1:A:211:PHE:HB2	1:A:231:ASN:OD1	2.22	0.40
1:A:315:GLY:C	1:A:362:MET:HE3	2.46	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	782/888 (88%)	752 (96%)	30 (4%)	0	100	100
1	B	782/888 (88%)	753 (96%)	27 (4%)	2 (0%)	36	48
All	All	1564/1776 (88%)	1505 (96%)	57 (4%)	2 (0%)	48	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	TYR
1	B	73	ASP

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	697/800 (87%)	696 (100%)	1 (0%)	88	95
1	B	697/800 (87%)	695 (100%)	2 (0%)	86	93
All	All	1394/1600 (87%)	1391 (100%)	3 (0%)	88	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	B	853[A]	ARG
1	B	853[B]	ARG

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	88	HIS
1	A	113	ASN
1	A	135	GLN
1	A	379	ASN
1	A	552	ASN
1	B	88	HIS
1	B	291	GLN
1	B	832	ASN

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 ⓘ

6 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	C	1	2,1	14,14,15	0.43	0	17,19,21	0.55	0
2	NAG	C	2	2	14,14,15	0.40	0	17,19,21	0.38	0
2	BMA	C	3	2	11,11,12	0.81	0	15,15,17	0.73	0
2	NAG	D	1	2,1	14,14,15	0.53	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	0.40	0
2	BMA	D	3	2	11,11,12	0.53	0	15,15,17	0.72	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	1/1/4/5	1/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	3	BMA	C1

All (1) torsion outliers are listed below:

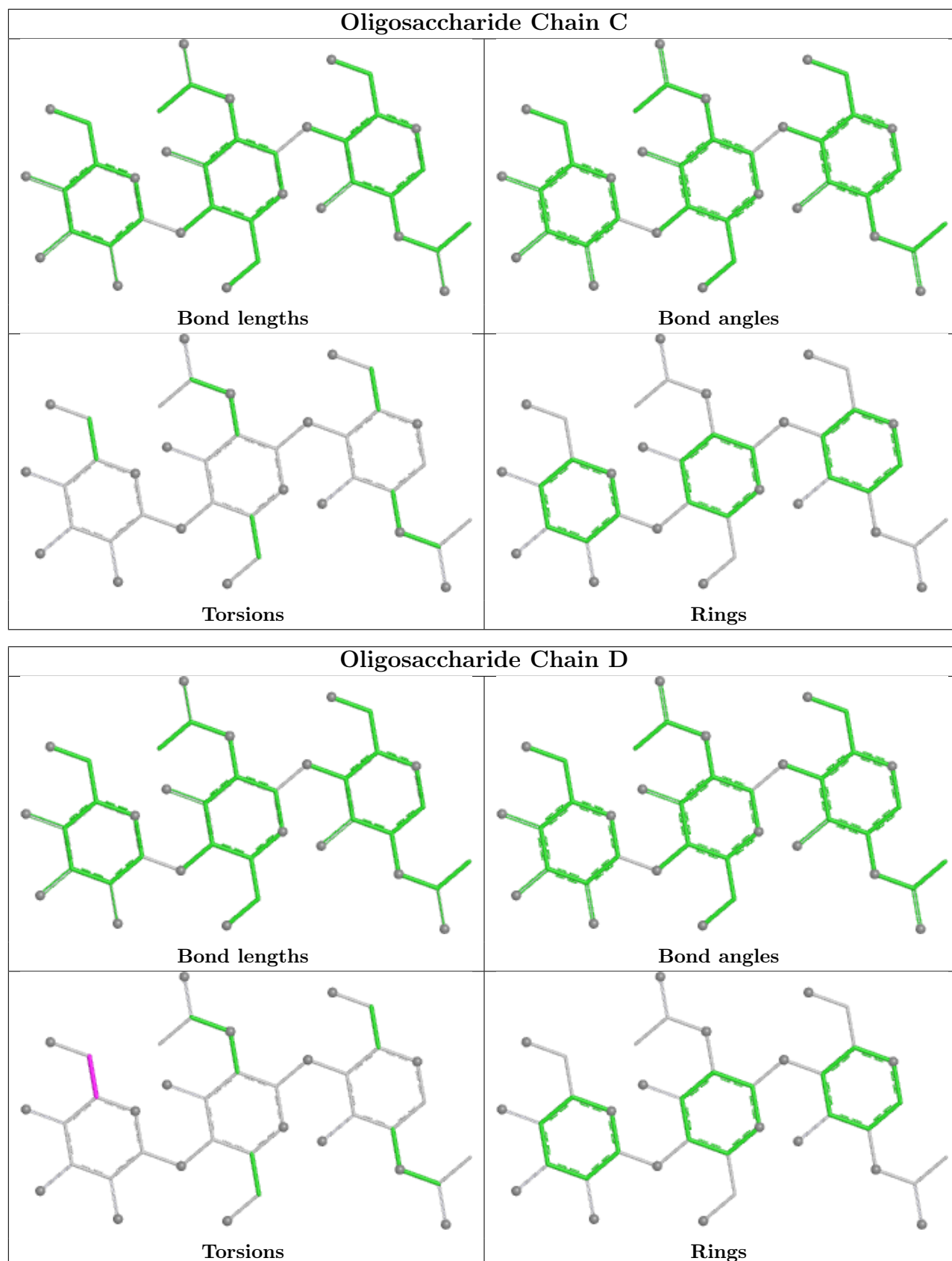
Mol	Chain	Res	Type	Atoms
2	D	3	BMA	O5-C5-C6-O6

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, 25 are monoatomic - leaving 5 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
3	5JK	A	901	-	32,32,32	4.39	14 (43%)	48,50,50	2.18	16 (33%)
4	NKP	B	903	7	28,28,28	0.88	2 (7%)	30,32,32	0.98	1 (3%)
3	5JK	B	901	-	32,32,32	4.39	14 (43%)	48,50,50	2.07	13 (27%)
8	GOL	B	902	-	5,5,5	0.93	0	5,5,5	1.05	0
4	NKP	A	902	-	28,28,28	0.89	2 (7%)	30,32,32	0.94	1 (3%)

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
3	5JK	A	901	-	-	5/10/71/71	0/4/4/4
4	NKP	B	903	7	-	15/28/28/28	-
3	5JK	B	901	-	-	2/10/71/71	0/4/4/4
8	GOL	B	902	-	-	0/4/4/4	-
4	NKP	A	902	-	-	15/28/28/28	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	5JK	C6-C5	16.16	1.58	1.33
3	A	901	5JK	C6-C5	16.12	1.58	1.33
3	A	901	5JK	C8-C7	9.46	1.63	1.53
3	B	901	5JK	C8-C7	9.25	1.63	1.53
3	A	901	5JK	C16-C15	6.49	1.71	1.54
3	B	901	5JK	C16-C15	6.43	1.71	1.54
3	B	901	5JK	C20-C17	-6.33	1.43	1.54
3	A	901	5JK	C20-C17	-6.29	1.43	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	5JK	C15-C14	5.92	1.66	1.54
3	B	901	5JK	C15-C14	5.89	1.66	1.54
3	B	901	5JK	C13-C17	5.83	1.65	1.55
3	A	901	5JK	C13-C17	5.72	1.65	1.55
3	B	901	5JK	C12-C11	4.98	1.63	1.53
3	A	901	5JK	C12-C11	4.89	1.63	1.53
3	B	901	5JK	C10-C9	3.96	1.62	1.56
3	A	901	5JK	C10-C9	3.93	1.62	1.56
3	A	901	5JK	C12-C13	-3.51	1.48	1.54
3	B	901	5JK	C12-C13	-3.42	1.48	1.54
3	B	901	5JK	O2-C7	-3.24	1.37	1.43
3	A	901	5JK	O2-C7	-3.22	1.37	1.43
3	A	901	5JK	C10-C5	-2.95	1.47	1.52
3	B	901	5JK	C10-C5	-2.93	1.47	1.52
3	A	901	5JK	C8-C9	2.85	1.59	1.53
3	B	901	5JK	C8-C9	2.76	1.59	1.53
4	B	903	NKP	OAJ-CAK	2.51	1.40	1.33
4	A	902	NKP	OAJ-CAK	2.46	1.40	1.33
3	B	901	5JK	C8-C14	-2.44	1.49	1.53
3	A	901	5JK	C8-C14	-2.33	1.49	1.53
4	A	902	NKP	OAJ-CAI	-2.22	1.40	1.45
3	B	901	5JK	C22-C20	2.16	1.59	1.54
4	B	903	NKP	OAJ-CAI	-2.12	1.40	1.45
3	A	901	5JK	C22-C20	2.07	1.59	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	5JK	C7-C6-C5	-7.87	118.03	125.18
3	B	901	5JK	C7-C6-C5	-7.45	118.41	125.18
3	B	901	5JK	C12-C13-C17	3.98	122.46	116.60
3	A	901	5JK	C12-C13-C17	3.87	122.30	116.60
3	A	901	5JK	C18-C13-C12	-3.83	104.96	110.61
3	B	901	5JK	C18-C13-C12	-3.75	105.08	110.61
3	A	901	5JK	C12-C13-C14	3.67	112.74	107.25
3	B	901	5JK	C17-C13-C14	3.62	104.25	100.10
3	A	901	5JK	C17-C13-C14	3.53	104.15	100.10
3	A	901	5JK	C18-C13-C17	-3.32	105.66	111.68
3	B	901	5JK	C18-C13-C14	-3.29	105.72	111.68
3	B	901	5JK	C12-C13-C14	3.24	112.09	107.25
3	A	901	5JK	C18-C13-C14	-3.23	105.81	111.68
3	A	901	5JK	C10-C5-C6	-3.22	116.61	122.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	5JK	C18-C13-C17	-3.11	106.03	111.68
3	B	901	5JK	C16-C17-C20	-3.03	107.59	112.18
3	A	901	5JK	C19-C10-C9	-2.96	108.34	111.66
3	B	901	5JK	C1-C10-C5	2.94	113.81	108.74
3	A	901	5JK	C1-C10-C5	2.79	113.56	108.74
3	B	901	5JK	C19-C10-C9	-2.79	108.53	111.66
3	A	901	5JK	C13-C17-C20	-2.79	115.19	119.50
4	B	903	NKP	OAJ-CAK-CAL	2.78	120.32	111.83
3	B	901	5JK	C10-C5-C6	-2.54	117.82	122.34
3	A	901	5JK	C15-C14-C8	2.49	121.77	118.36
3	A	901	5JK	C16-C17-C20	-2.46	108.46	112.18
4	A	902	NKP	OAJ-CAK-CAL	2.44	119.27	111.83
3	B	901	5JK	C13-C17-C20	-2.30	115.94	119.50
3	A	901	5JK	C21-C20-C22	-2.30	106.78	110.34
3	B	901	5JK	C8-C7-C6	2.16	114.36	111.30
3	A	901	5JK	C4-C5-C10	-2.08	113.76	116.42
3	A	901	5JK	C8-C7-C6	2.02	114.16	111.30

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	NKP	CAG-OAF-PAC-OAA
4	A	902	NKP	CAG-OAF-PAC-OAB
4	A	902	NKP	CAG-OAF-PAC-OAD
4	B	903	NKP	CAG-OAF-PAC-OAA
4	B	903	NKP	CAG-OAF-PAC-OAB
4	B	903	NKP	OAE-CAK-OAJ-CAI
4	B	903	NKP	CAL-CAK-OAJ-CAI
3	B	901	5JK	C22-C23-C24-C25
3	A	901	5JK	C22-C23-C24-C25
4	A	902	NKP	OAF-CAG-CAH-OBC
4	A	902	NKP	OAF-CAG-CAH-CAI
3	A	901	5JK	C23-C24-C25-C26
4	B	903	NKP	CAM-CAN-CAO-CAP
3	A	901	5JK	C23-C24-C25-C27
4	B	903	NKP	CAX-CAY-CAZ-CBA
4	B	903	NKP	CAO-CAP-CAQ-CAR
4	B	903	NKP	CAW-CAX-CAY-CAZ
4	A	902	NKP	CAO-CAP-CAQ-CAR
4	A	902	NKP	CAN-CAO-CAP-CAQ
4	B	903	NKP	CAT-CAU-CAV-CAW

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	902	NKP	CAX-CAY-CAZ-CBA
4	B	903	NKP	OAF-CAG-CAH-CAI
4	B	903	NKP	OAF-CAG-CAH-OBC
4	A	902	NKP	CAM-CAN-CAO-CAP
3	A	901	5JK	C20-C22-C23-C24
3	B	901	5JK	C20-C22-C23-C24
4	B	903	NKP	CAG-OAF-PAC-OAD
4	A	902	NKP	CAL-CAM-CAN-CAO
4	B	903	NKP	CAN-CAO-CAP-CAQ
4	A	902	NKP	CAV-CAW-CAX-CAY
4	B	903	NKP	CAY-CAZ-CBA-CBB
4	B	903	NKP	CAL-CAM-CAN-CAO
4	A	902	NKP	CAT-CAU-CAV-CAW
4	A	902	NKP	CAH-CAG-OAF-PAC
4	A	902	NKP	CAU-CAV-CAW-CAX
4	A	902	NKP	CAY-CAZ-CBA-CBB
3	A	901	5JK	C13-C17-C20-C21

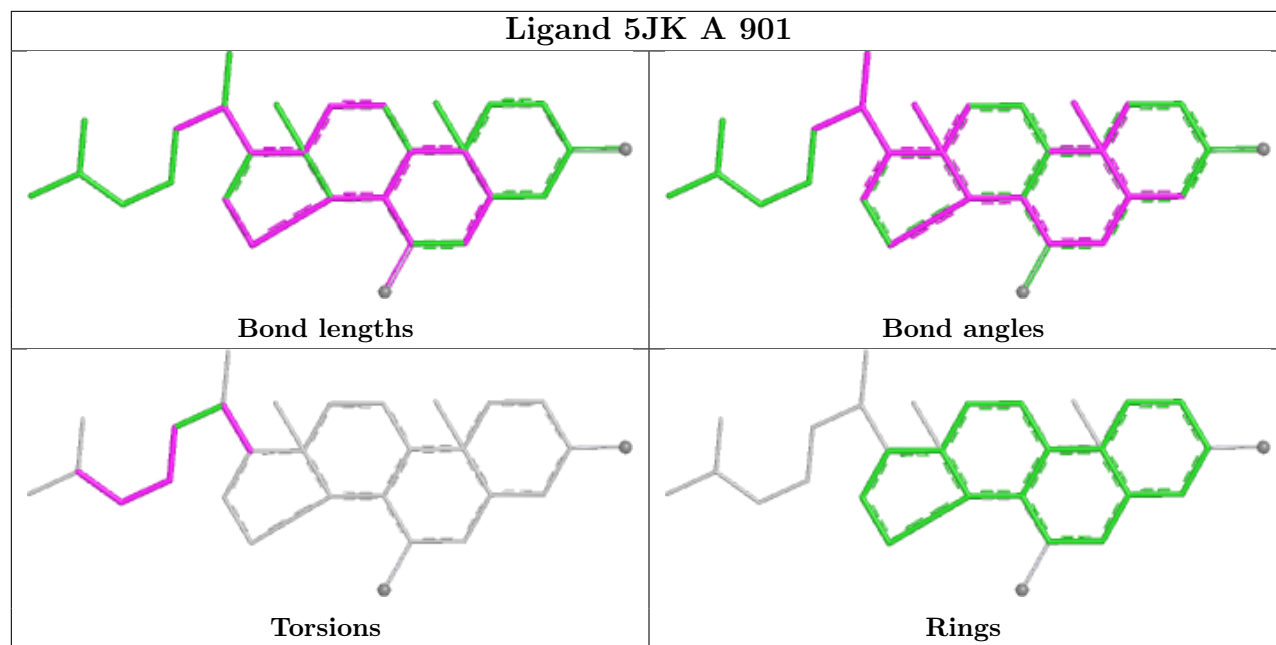
There are no ring outliers.

2 monomers are involved in 4 short contacts:

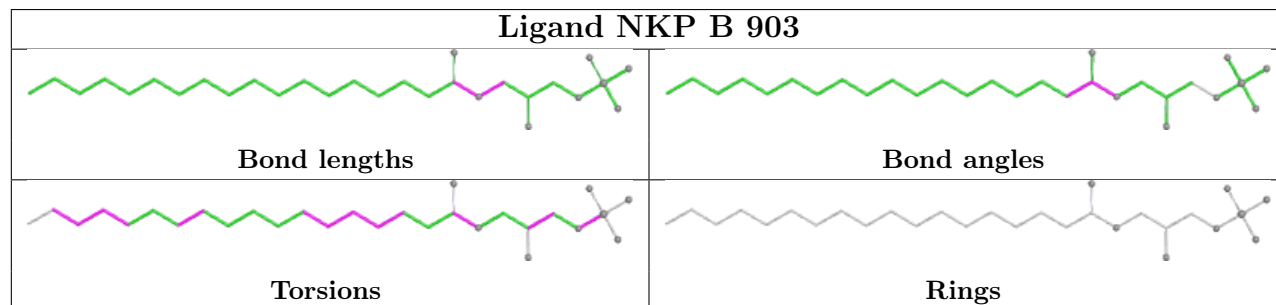
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	NKP	1	0
4	A	902	NKP	3	0

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.

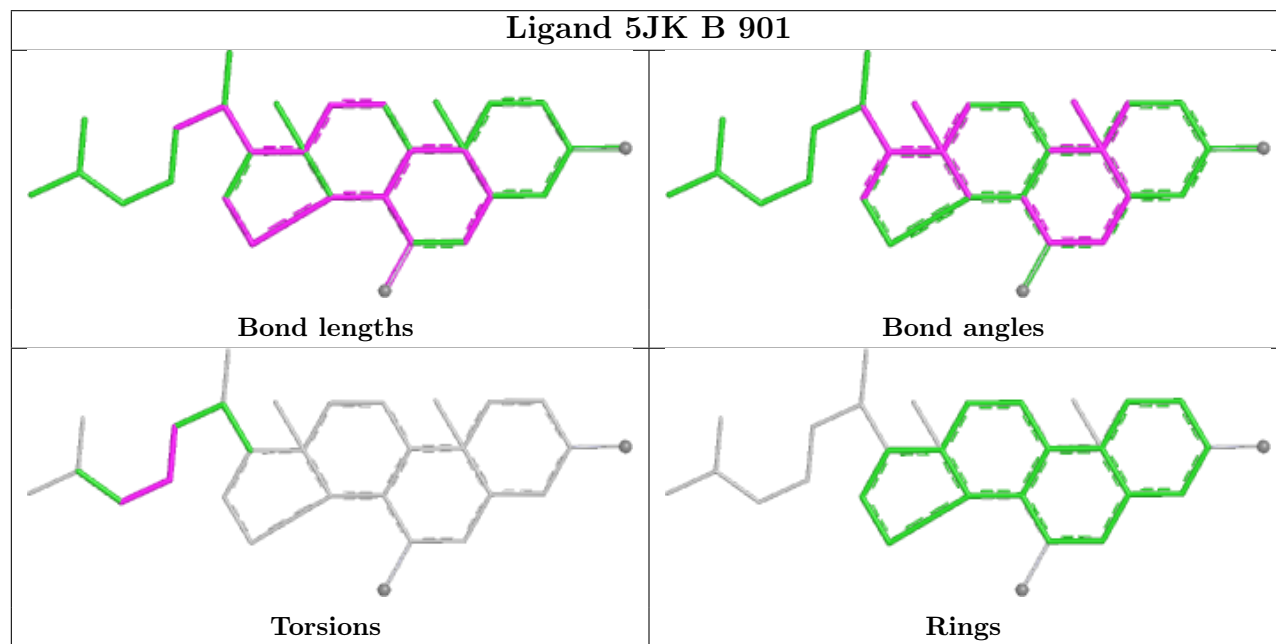
Ligand 5JK A 901

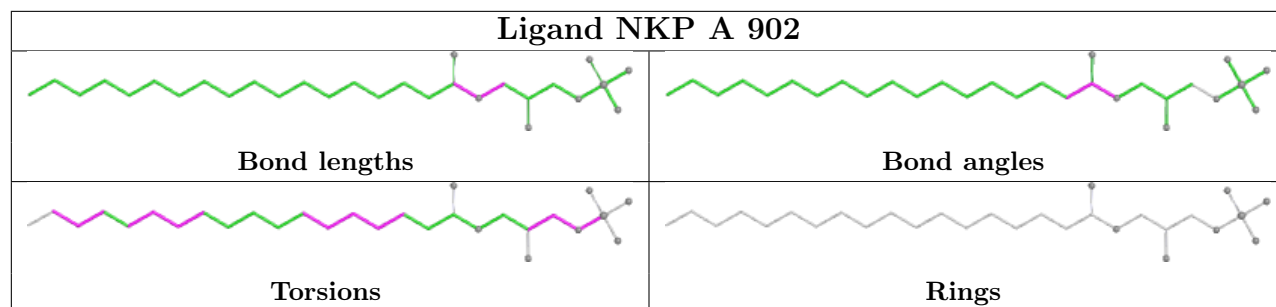


Ligand NKP B 903



Ligand 5JK B 901





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	778/888 (87%)	0.72	55 (7%)	22 20	18, 39, 72, 124	10 (1%)
1	B	778/888 (87%)	0.75	65 (8%)	17 15	17, 39, 71, 142	10 (1%)
All	All	1556/1776 (87%)	0.73	120 (7%)	19 18	17, 39, 71, 142	20 (1%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	CYS	6.6
1	B	470	PHE	6.3
1	B	71	PRO	6.1
1	A	55	ILE	5.9
1	B	462	TYR	5.5
1	A	71	PRO	5.3
1	A	469	CYS	5.2
1	B	55	ILE	5.2
1	A	462	TYR	5.0
1	B	162	VAL	4.9
1	B	57	GLY	4.8
1	B	109	GLY	4.7
1	A	72	PRO	4.6
1	B	56	SER	4.2
1	A	69	ALA	3.9
1	B	667	VAL	3.5
1	B	108	CYS	3.5
1	A	68	GLU	3.5
1	B	195	CYS	3.4
1	A	57	GLY	3.4
1	B	69	ALA	3.3
1	B	555	GLY	3.3
1	A	66	LEU	3.3
1	B	111	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	471	PHE	3.2
1	A	111	VAL	3.2
1	A	70	GLY	3.2
1	A	885	GLU	3.1
1	B	66	LEU	3.1
1	B	104	THR	3.1
1	A	76	CYS	3.1
1	A	159	ALA	3.1
1	A	93	LEU	3.0
1	A	125	LEU	3.0
1	B	419	GLN	3.0
1	B	72	PRO	3.0
1	A	95	LEU	3.0
1	A	298	HIS	2.8
1	A	73	ASP	2.8
1	A	272	GLY	2.8
1	B	558	TYR	2.8
1	B	86	CYS	2.8
1	B	93	LEU	2.8
1	B	103	CYS	2.7
1	B	559	LEU	2.7
1	A	471	PHE	2.7
1	A	63	CYS	2.7
1	B	61	GLY	2.7
1	A	117	ALA	2.6
1	A	559	LEU	2.6
1	B	885	GLU	2.6
1	B	674	LEU	2.5
1	A	351	CYS	2.5
1	B	367	CYS	2.5
1	B	70	GLY	2.5
1	B	90	PHE	2.5
1	B	571	ASP	2.5
1	A	273	THR	2.5
1	A	497	TYR	2.5
1	A	719	TYR	2.4
1	B	98	ALA	2.4
1	B	556	ILE	2.4
1	B	92	GLU	2.4
1	B	675	THR	2.4
1	B	100	GLY	2.4
1	B	120	CYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	136	VAL	2.4
1	A	56	SER	2.3
1	A	470	PHE	2.3
1	B	352	VAL	2.3
1	B	79	LEU	2.3
1	B	149	CYS	2.3
1	B	366	THR	2.3
1	A	67	GLN	2.3
1	A	94	CYS	2.2
1	A	120	CYS	2.2
1	B	94	CYS	2.2
1	B	127	ARG	2.2
1	B	118	CYS	2.2
1	A	119	HIS	2.2
1	B	884	TYR	2.2
1	B	678	VAL	2.2
1	B	91	ASP	2.2
1	A	74	CYS	2.2
1	B	74	CYS	2.2
1	A	191	LYS	2.2
1	B	402	LYS	2.2
1	B	696	LYS	2.2
1	A	307	TYR	2.2
1	B	562	ASP	2.2
1	A	88	HIS	2.2
1	B	677	CYS	2.2
1	A	435	TYR	2.1
1	B	73	ASP	2.1
1	B	365	VAL	2.1
1	B	399	ASN	2.1
1	A	115	GLU	2.1
1	A	109	GLY	2.1
1	A	60	LYS	2.1
1	A	77	ASP	2.1
1	B	536[A]	ARG	2.1
1	A	92	GLU	2.1
1	A	136	VAL	2.1
1	A	126	ALA	2.1
1	A	172	ASP	2.1
1	A	884	TYR	2.1
1	B	137	VAL	2.1
1	B	160	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	693	LEU	2.0
1	B	125	LEU	2.0
1	B	164	PRO	2.0
1	A	134	TYR	2.0
1	A	162	VAL	2.0
1	A	366	THR	2.0
1	B	59	CYS	2.0
1	A	116	ASN	2.0
1	A	459	LEU	2.0
1	B	348	LEU	2.0
1	A	107	ARG	2.0
1	B	280	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

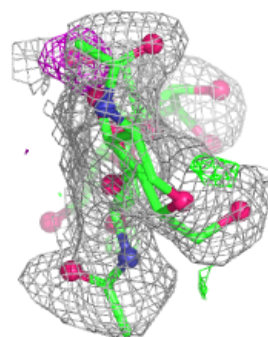
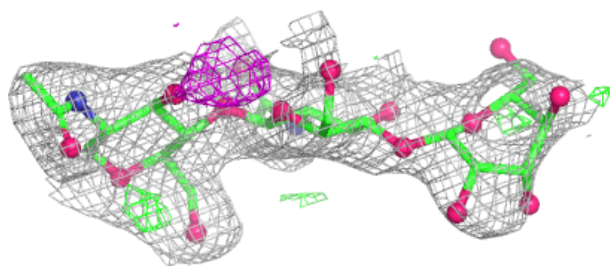
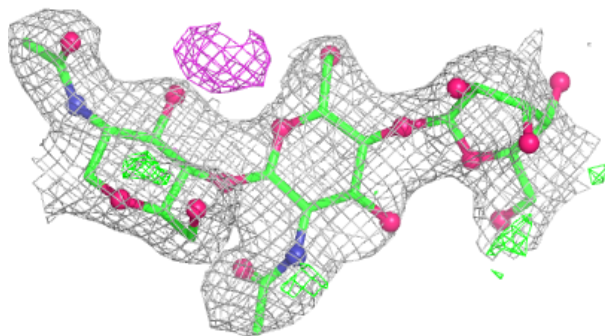
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.55	0.17	68,80,85,91	0
2	BMA	D	3	11/12	0.74	0.14	56,65,72,80	0
2	NAG	D	2	14/15	0.77	0.15	40,48,52,53	0
2	NAG	C	2	14/15	0.79	0.14	42,54,68,71	0
2	NAG	C	1	14/15	0.89	0.11	25,34,43,45	0
2	NAG	D	1	14/15	0.93	0.09	25,31,36,40	0

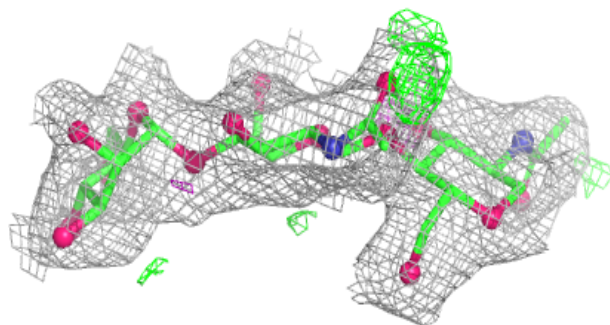
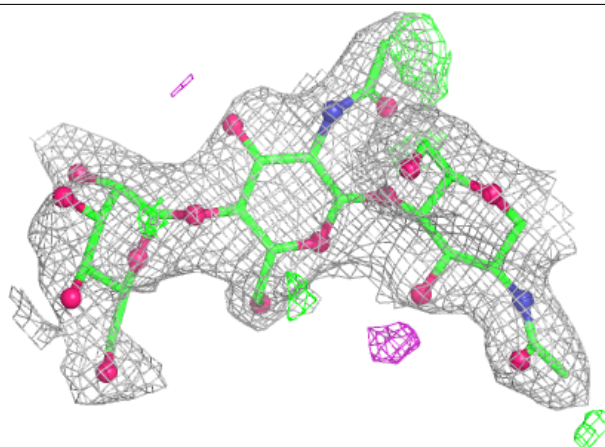
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o-DF_c$ (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 ⓘ

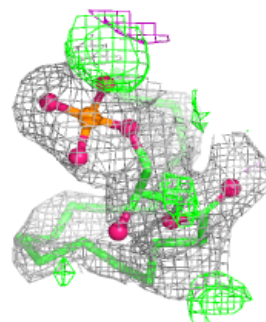
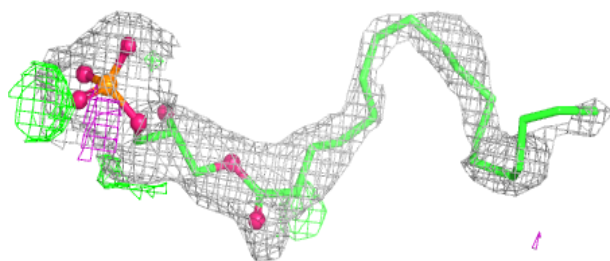
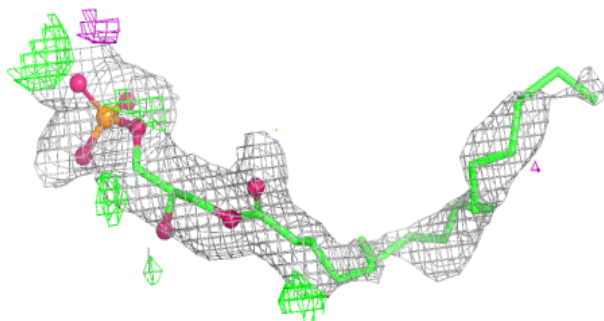
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	902	6/6	0.70	0.16	53,59,64,65	0
7	ZN	A	909	1/1	0.80	0.12	48,48,48,48	1
5	IOD	A	911	1/1	0.81	0.30	153,153,153,153	0
6	CA	A	907	1/1	0.83	0.16	60,60,60,60	0
7	ZN	B	909	1/1	0.84	0.09	34,34,34,34	1
4	NKP	A	902	29/29	0.84	0.17	35,52,63,69	0
7	ZN	A	908	1/1	0.87	0.10	36,36,36,36	1
4	NKP	B	903	29/29	0.89	0.16	31,50,58,65	0
3	5JK	A	901	29/29	0.90	0.13	22,32,54,58	0
3	5JK	B	901	29/29	0.90	0.13	23,29,49,59	0
5	IOD	A	915	1/1	0.91	0.20	119,119,119,119	0
5	IOD	A	910	1/1	0.91	0.20	115,115,115,115	0
5	IOD	B	913	1/1	0.92	0.13	130,130,130,130	0
5	IOD	B	912	1/1	0.93	0.19	101,101,101,101	0
6	CA	B	907	1/1	0.93	0.06	41,41,41,41	1
5	IOD	B	911	1/1	0.93	0.15	104,104,104,104	0
5	IOD	A	913	1/1	0.94	0.30	107,107,107,107	0
7	ZN	B	908	1/1	0.95	0.09	33,33,33,33	1
5	IOD	B	915	1/1	0.96	0.11	90,90,90,90	0
6	CA	B	906	1/1	0.96	0.05	37,37,37,37	0
5	IOD	A	912	1/1	0.97	0.05	64,64,64,64	1
5	IOD	B	910	1/1	0.97	0.24	115,115,115,115	0
5	IOD	A	903	1/1	0.98	0.05	80,80,80,80	0
5	IOD	A	905	1/1	0.99	0.10	69,69,69,69	0
6	CA	A	906	1/1	0.99	0.03	34,34,34,34	0
5	IOD	A	904	1/1	0.99	0.13	71,71,71,71	0
5	IOD	B	904	1/1	0.99	0.12	62,62,62,62	0
5	IOD	B	905	1/1	0.99	0.12	72,72,72,72	0
5	IOD	A	914	1/1	1.00	0.02	38,38,38,38	0
5	IOD	B	914	1/1	1.00	0.01	37,37,37,37	0

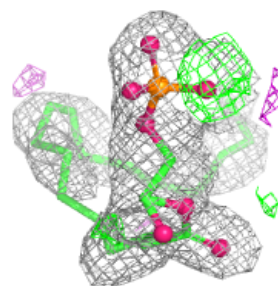
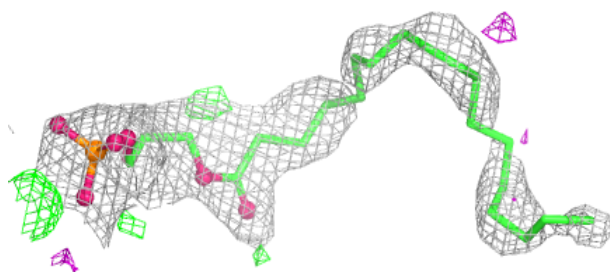
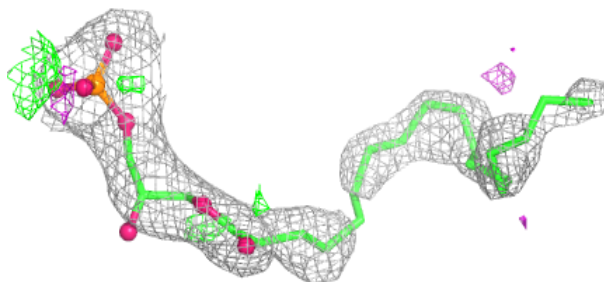
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NKP A 902:

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

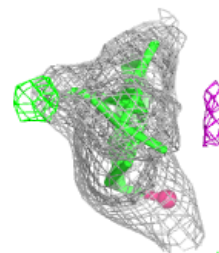
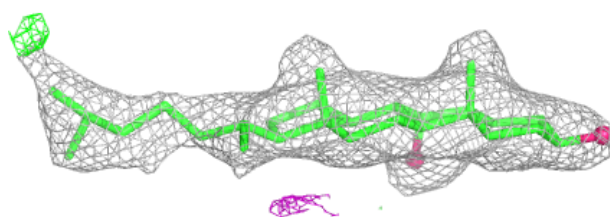
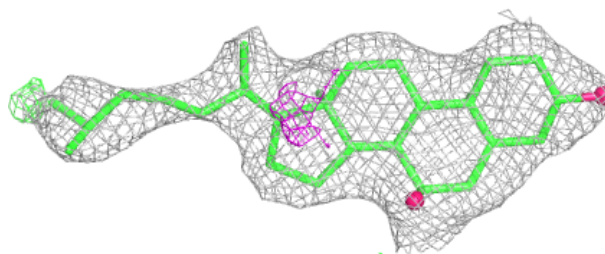
**Electron density around NKP B 903:**

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

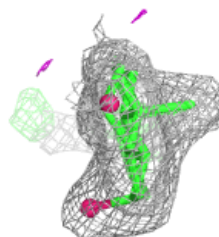
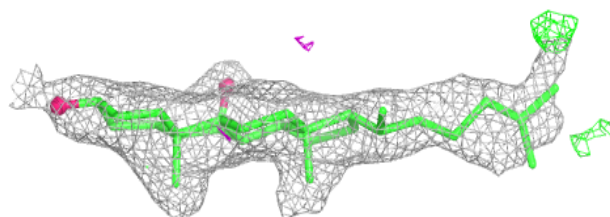
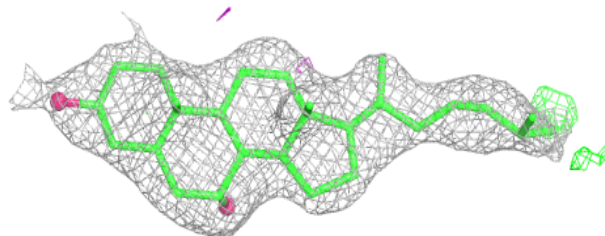


Electron density around 5JK A 901:

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

**Electron density around 5JK B 901:**

$2mF_o-DF_c$ (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.