Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 05:30 PM EDT

PDB ID	:	4ZG7
Title	:	Structural basis for inhibition of human autotaxin by four novel compounds
Authors	:	Stein, A.J.; Bain, G.; Hutchinson, J.H.; Evans, J.F.
Deposited on	:	2015-04-22
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 (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:

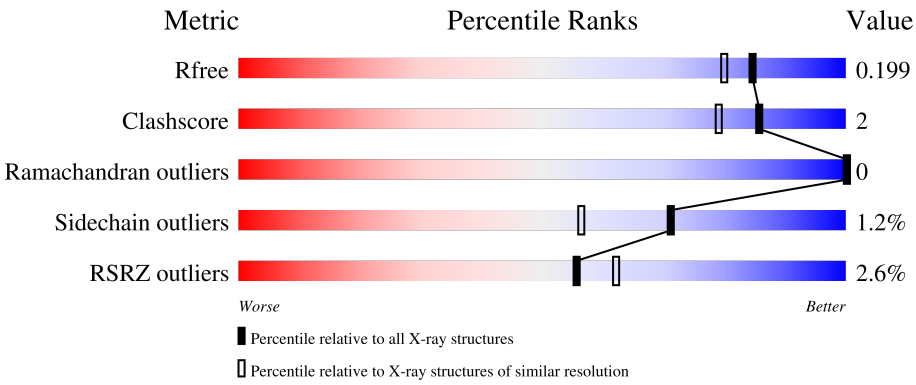
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.75 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 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	806	2% 91% 5% •
2	B	2	100%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 6888 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	776	6255	3982	1062	1163	48	0	12	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	411	ALA	ASN	conflict	UNP Q13822
A	493	PRO	SER	variant	UNP Q13822

- 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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

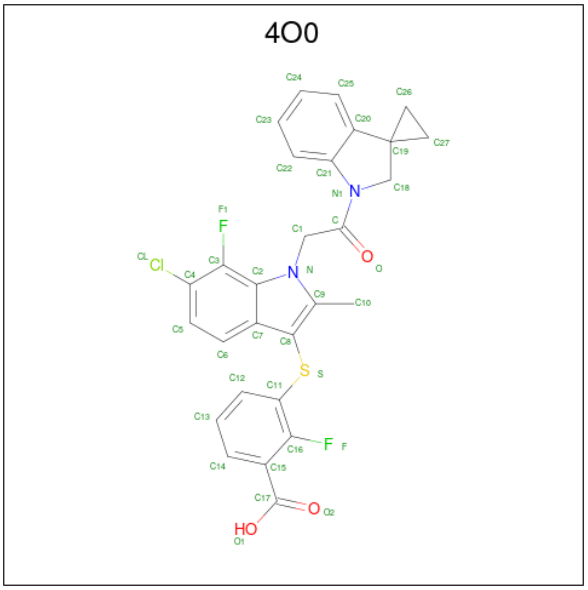
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

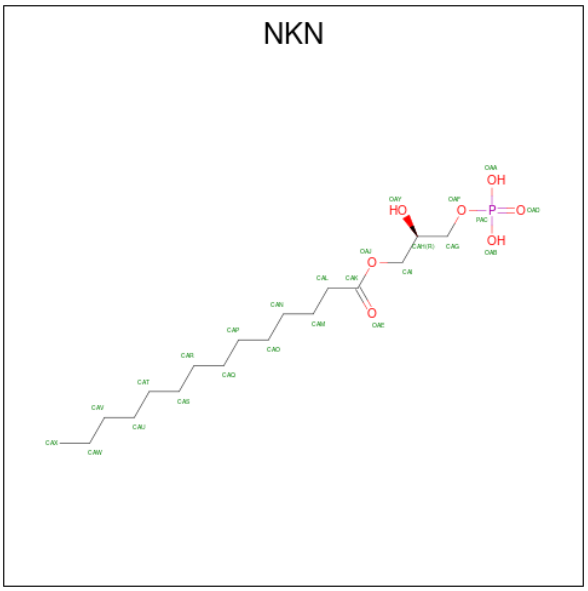
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	2	2	2	0	0

- Molecule 6 is 3-({6-chloro-7-fluoro-2-methyl-1-[2-oxo-2-(spiro[cyclopropane-1,3'-indol]-1'(2'H)-yl)ethyl]-1H-indol-3-yl}sulfanyl)-2-fluorobenzoic acid (three-letter code: 4O0) (formula: $C_{28}H_{21}ClF_2N_2O_3S$).



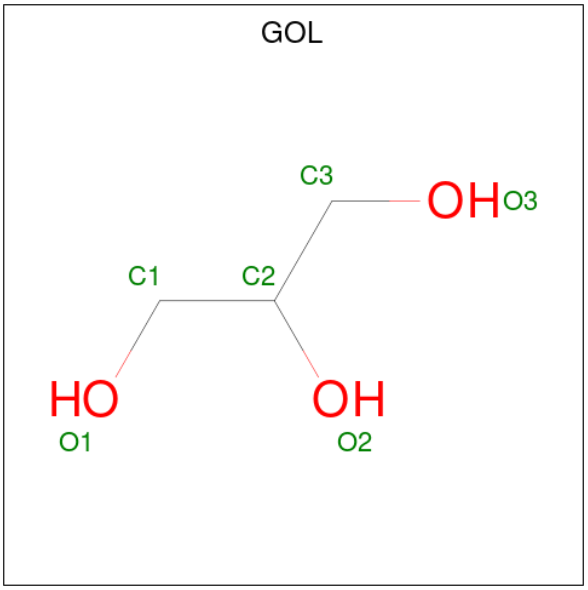
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	N	O	S		
6	A	1	37	28	1	2	2	3	1	0	0

- Molecule 7 is (2R)-2-hydroxy-3-(phosphonooxy)propyl tetradecanoate (three-letter code: NKN) (formula: $C_{17}H_{35}O_7P$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
9	A	1	1	1	0	0

- Molecule 10 is water.

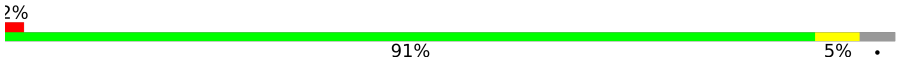
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	495	495	495	0	0

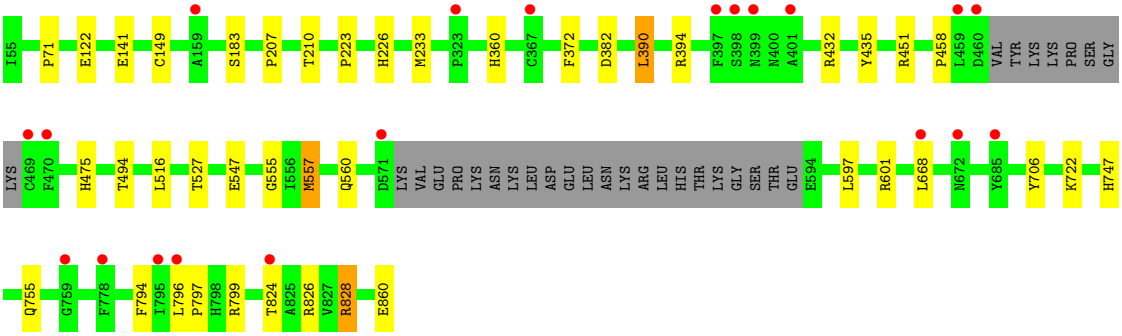
3 Residue-property plots (i)

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

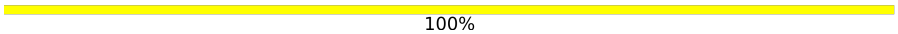
Chain A:





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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.77Å 85.82Å 83.86Å 90.00° 111.34° 90.00°	Depositor
Resolution (Å)	37.61 – 1.75 37.61 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.61-1.75) 98.5 (37.61-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.195 0.173 , 0.199	Depositor DCC
R_{free} test set	4053 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6888	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: 4O0, GOL, CL, CA, NA, NAG, ZN, NKN

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	0.52	0/6471	0.70	7/8795 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	799	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	149	CYS	CA-CB-SG	5.51	123.92	114.00
1	A	557	MET	CG-SD-CE	-5.45	91.48	100.20
1	A	799	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	826	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	394	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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	6255	0	5966	27	0
2	B	28	0	25	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
6	A	37	0	20	0	0
7	A	25	0	33	1	0
8	A	42	0	56	0	0
9	A	1	0	0	0	0
10	A	495	0	0	7	1
All	All	6888	0	6100	27	1

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 2.

All (27) 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:547:GLU:OE1	10:A:1001:HOH:O	1.85	0.93
1:A:122:GLU:CD	10:A:1008:HOH:O	2.15	0.83
1:A:794:PHE:CD1	1:A:796[B]:LEU:HD13	2.15	0.81
1:A:601[B]:ARG:HG3	1:A:601[B]:ARG:HH21	1.53	0.74
1:A:71:PRO:O	10:A:1002:HOH:O	2.06	0.72
1:A:860:GLU:OE1	10:A:1003:HOH:O	2.08	0.70
1:A:555:GLY:O	1:A:557:MET:HG2	2.01	0.60
1:A:527:THR:OG1	1:A:828[A]:ARG:HD3	2.02	0.58
1:A:747:HIS:HD2	10:A:1094:HOH:O	1.86	0.58
1:A:706:TYR:OH	1:A:755:GLN:NE2	2.34	0.58
1:A:223:PRO:HA	1:A:226:HIS:CE1	2.41	0.56
1:A:601[B]:ARG:HH21	1:A:601[B]:ARG:CG	2.16	0.54
1:A:601[B]:ARG:CG	1:A:601[B]:ARG:NH2	2.71	0.52
1:A:372:PHE:CE1	1:A:458:PRO:HA	2.48	0.48
1:A:597:LEU:HD21	1:A:601[B]:ARG:HB3	1.97	0.45
1:A:360:HIS:CE1	1:A:475:HIS:CE1	3.05	0.44
1:A:797:PRO:HB3	10:A:1448:HOH:O	2.18	0.43
1:A:390:LEU:HD12	1:A:390:LEU:O	2.18	0.43
1:A:527:THR:OG1	1:A:828[A]:ARG:CD	2.65	0.43
1:A:794:PHE:CE1	1:A:796[B]:LEU:HD22	2.53	0.42
1:A:494:THR:HG21	1:A:516[A]:LEU:HD23	2.02	0.42
1:A:597:LEU:HD21	1:A:601[B]:ARG:CB	2.49	0.42
1:A:210:THR:OG1	7:A:909:NKN:OAD	2.37	0.41
1:A:516[B]:LEU:HA	1:A:516[B]:LEU:HD12	1.82	0.41
1:A:207:PRO:HD3	1:A:435:TYR:CE1	2.56	0.41
1:A:141:GLU:OE1	10:A:1004:HOH:O	2.22	0.41
1:A:432:ARG:HD3	1:A:824:THR:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1002:HOH:O	10:A:1010:HOH:O[2_454]	1.35	0.85

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	782/806 (97%)	760 (97%)	22 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	697/730 (96%)	688 (99%)	9 (1%)	69 54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	SER
1	A	233	MET
1	A	382	ASP
1	A	390	LEU
1	A	560	GLN
1	A	668	LEU

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Mol	Chain	Res	Type
1	A	722	LYS
1	A	828[A]	ARG
1	A	828[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	291	GLN
1	A	298	HIS
1	A	472	GLN
1	A	747	HIS
1	A	755	GLN
1	A	857	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	2,1	14,14,15	0.64	0	17,19,21	1.53	3 (17%)
2	NAG	B	2	2	14,14,15	0.41	0	17,19,21	1.49	2 (11%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C1-O5-C5	-3.34	107.67	112.19
2	B	1	NAG	O5-C1-C2	-3.30	106.08	111.29
2	B	1	NAG	O5-C5-C6	3.14	112.13	107.20
2	B	2	NAG	O7-C7-C8	-2.16	118.05	122.06
2	B	1	NAG	C6-C5-C4	-2.14	108.00	113.00

There are no chirality outliers.

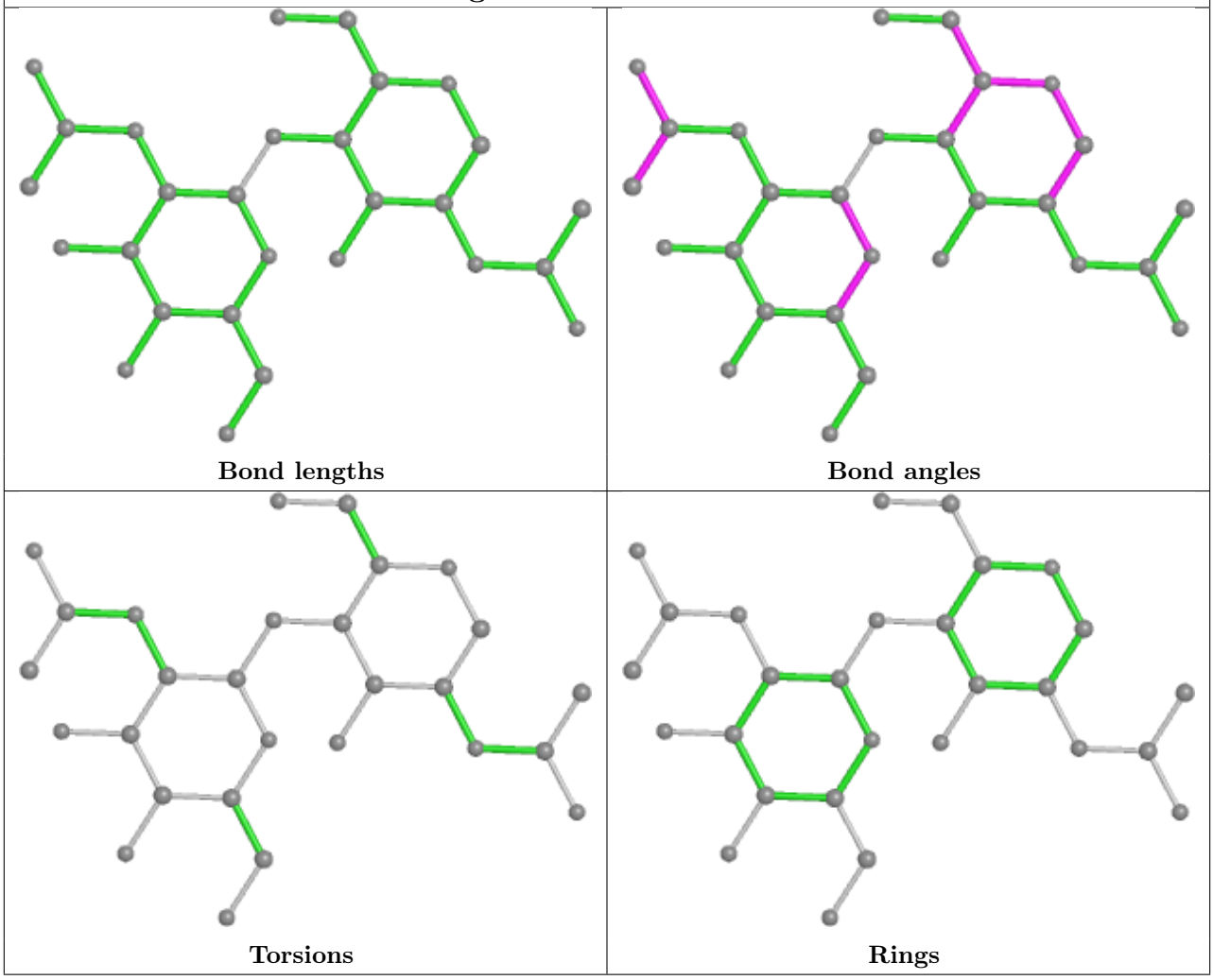
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	GOL	A	914	-	5,5,5	0.41	0	5,5,5	0.39	0
6	4O0	A	908	-	39,42,42	2.80	11 (28%)	48,65,65	2.45	15 (31%)
8	GOL	A	915	-	5,5,5	0.24	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	GOL	A	910	-	5,5,5	0.28	0	5,5,5	0.71	0
7	NKN	A	909	3	24,24,24	1.58	3 (12%)	27,28,28	1.55	6 (22%)
8	GOL	A	913	-	5,5,5	0.28	0	5,5,5	0.30	0
8	GOL	A	911	-	5,5,5	0.27	0	5,5,5	0.40	0
8	GOL	A	912	-	5,5,5	0.39	0	5,5,5	0.49	0
8	GOL	A	916	-	5,5,5	0.36	0	5,5,5	0.57	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
8	GOL	A	914	-	-	2/4/4/4	-
6	4O0	A	908	-	-	3/16/35/35	0/6/6/6
8	GOL	A	915	-	-	2/4/4/4	-
8	GOL	A	910	-	-	3/4/4/4	-
7	NKN	A	909	3	-	10/24/24/24	-
8	GOL	A	913	-	-	1/4/4/4	-
8	GOL	A	911	-	-	0/4/4/4	-
8	GOL	A	912	-	-	0/4/4/4	-
8	GOL	A	916	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	908	4O0	C4-C3	10.63	1.47	1.38
6	A	908	4O0	C11-S	-5.34	1.70	1.78
6	A	908	4O0	C9-C8	5.29	1.46	1.39
7	A	909	NKN	OAJ-CAK	5.25	1.48	1.33
6	A	908	4O0	C21-C20	5.25	1.45	1.39
6	A	908	4O0	C11-C16	5.21	1.46	1.38
7	A	909	NKN	PAC-OAD	4.31	1.64	1.50
6	A	908	4O0	C15-C16	4.18	1.46	1.38
6	A	908	4O0	C8-S	-3.32	1.73	1.78
6	A	908	4O0	C7-C2	2.89	1.46	1.41
6	A	908	4O0	C19-C20	-2.51	1.49	1.52
7	A	909	NKN	PAC-OAA	-2.50	1.45	1.54
6	A	908	4O0	C1-N	-2.35	1.44	1.49
6	A	908	4O0	C26-C19	2.13	1.53	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	908	4O0	C3-C4-CL	-6.20	117.14	119.49
6	A	908	4O0	C8-C7-C2	-5.98	100.48	114.54
6	A	908	4O0	C4-C3-C2	-5.65	115.45	121.08
6	A	908	4O0	C10-C9-C8	-5.48	126.04	129.62
6	A	908	4O0	C5-C4-C3	5.40	122.39	119.33
7	A	909	NKN	OAJ-CAK-CAL	4.52	126.10	111.91
6	A	908	4O0	C10-C9-N	4.23	128.01	122.69
6	A	908	4O0	C6-C7-C2	3.24	122.78	116.73
7	A	909	NKN	PAC-OAF-CAG	2.94	126.40	118.30
6	A	908	4O0	C15-C16-C11	-2.91	118.66	120.82
6	A	908	4O0	C-C1-N	2.78	114.07	110.76
6	A	908	4O0	C22-C21-C20	-2.76	119.00	121.76
7	A	909	NKN	OAB-PAC-OAD	-2.56	100.64	110.68
7	A	909	NKN	OAJ-CAK-OAE	-2.55	117.15	123.59
7	A	909	NKN	OAF-PAC-OAD	2.52	113.53	106.47
6	A	908	4O0	C27-C26-C19	-2.40	59.07	60.65
6	A	908	4O0	C6-C5-C4	2.37	121.84	119.63
6	A	908	4O0	C1-C-N1	-2.11	114.31	116.59
6	A	908	4O0	C12-C11-S	2.08	124.51	119.48
6	A	908	4O0	C18-C19-C20	2.07	107.74	105.73
7	A	909	NKN	OAJ-CAI-CAH	2.01	115.47	105.77

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	915	GOL	O1-C1-C2-C3
7	A	909	NKN	CAL-CAK-OAJ-CAI
7	A	909	NKN	CAT-CAU-CAV-CAW
7	A	909	NKN	OAE-CAK-OAJ-CAI
8	A	910	GOL	O1-C1-C2-C3
8	A	910	GOL	C1-C2-C3-O3
8	A	914	GOL	C1-C2-C3-O3
8	A	916	GOL	C1-C2-C3-O3
8	A	915	GOL	O1-C1-C2-O2
8	A	916	GOL	O2-C2-C3-O3
7	A	909	NKN	OAY-CAH-CAI-OAJ
7	A	909	NKN	CAG-CAH-CAI-OAJ
8	A	914	GOL	O2-C2-C3-O3
7	A	909	NKN	CAQ-CAR-CAS-CAT
7	A	909	NKN	CAH-CAG-OAF-PAC

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Mol	Chain	Res	Type	Atoms
8	A	910	GOL	O2-C2-C3-O3
7	A	909	NKN	CAR-CAS-CAT-CAU
7	A	909	NKN	CAP-CAQ-CAR-CAS
6	A	908	4O0	C12-C11-S-C8
8	A	913	GOL	O1-C1-C2-C3
6	A	908	4O0	C1-C-N1-C18
6	A	908	4O0	O-C-N1-C18
7	A	909	NKN	OAJ-CAK-CAL-CAM

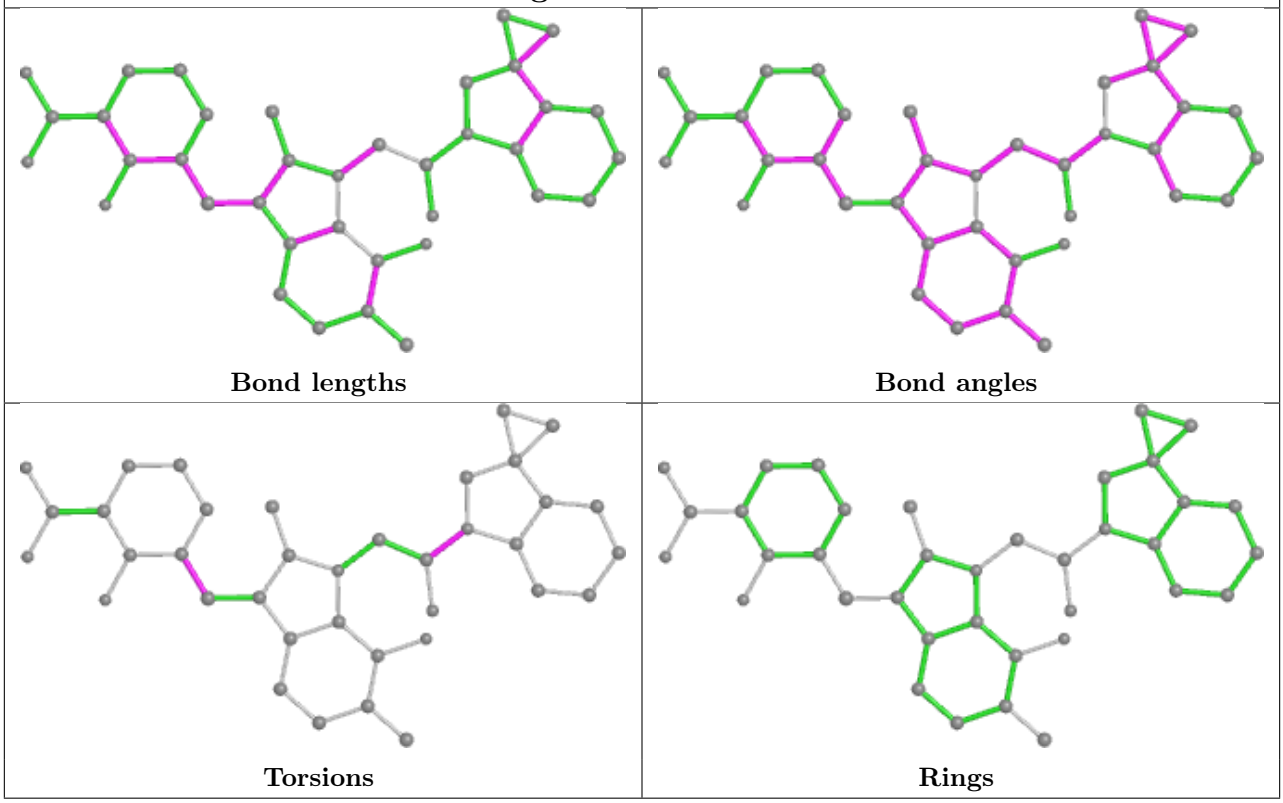
There are no ring outliers.

1 monomer is involved in 1 short contact:

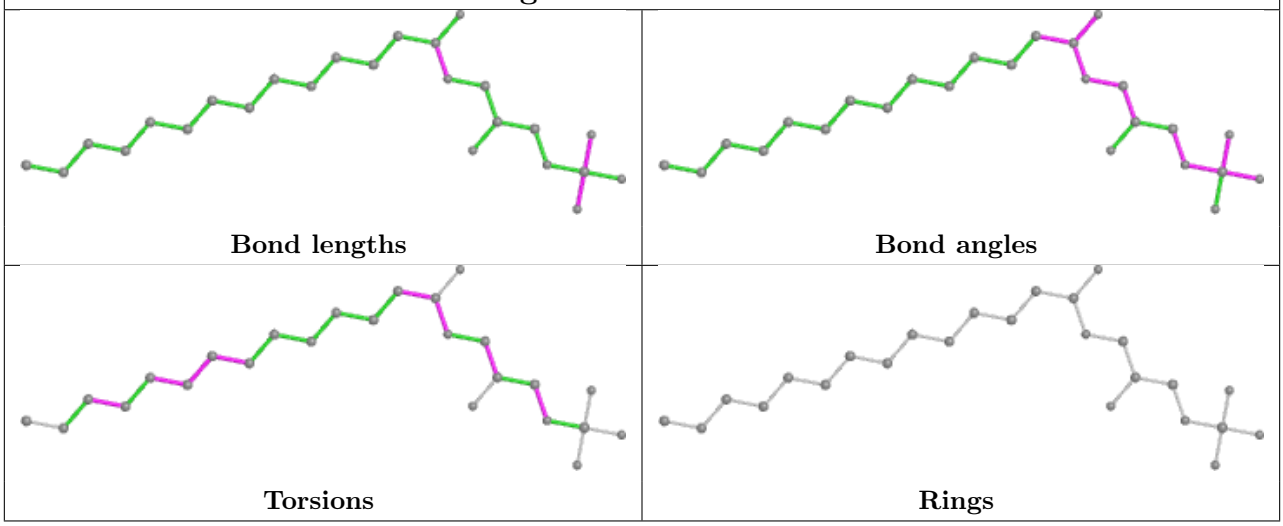
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	909	NKN	1	0

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 4O0 A 908



Ligand NKN A 909



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	776/806 (96%)	-0.09	20 (2%) 56 62	13, 21, 38, 59	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	CYS	5.2
1	A	401	ALA	4.7
1	A	685	TYR	4.2
1	A	159	ALA	3.4
1	A	459	LEU	3.2
1	A	399	ASN	3.0
1	A	672	ASN	2.9
1	A	796[A]	LEU	2.8
1	A	778	PHE	2.7
1	A	397	PHE	2.7
1	A	759	GLY	2.6
1	A	398	SER	2.6
1	A	323	PRO	2.5
1	A	470	PHE	2.4
1	A	795	ILE	2.4
1	A	367	CYS	2.3
1	A	668	LEU	2.3
1	A	824	THR	2.3
1	A	571	ASP	2.1
1	A	460	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)

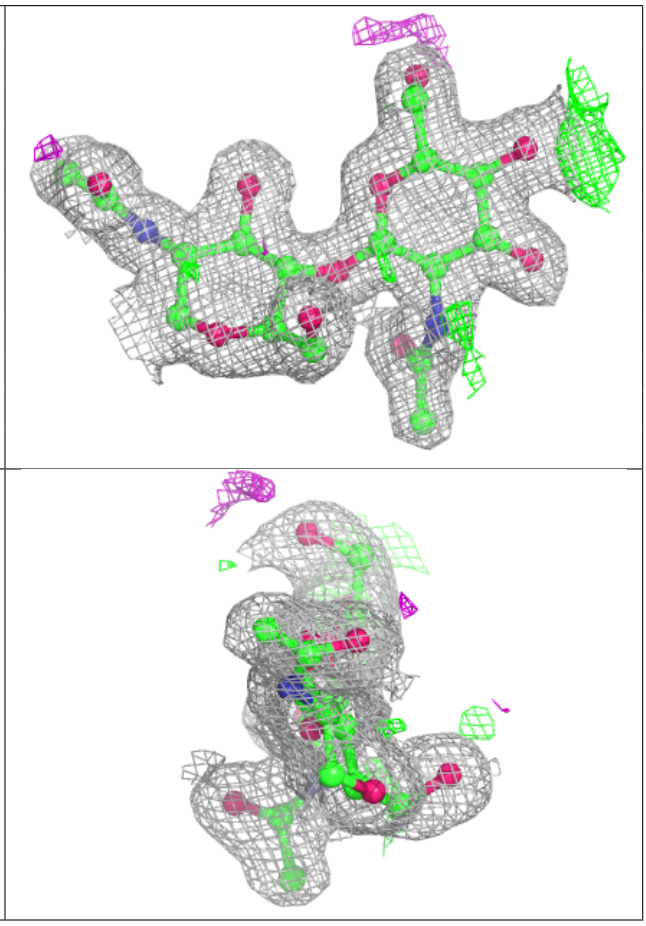
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2	14/15	0.93	0.11	23,28,32,33	0
2	NAG	B	1	14/15	0.96	0.06	16,17,20,21	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)



6.4 Ligands (i)

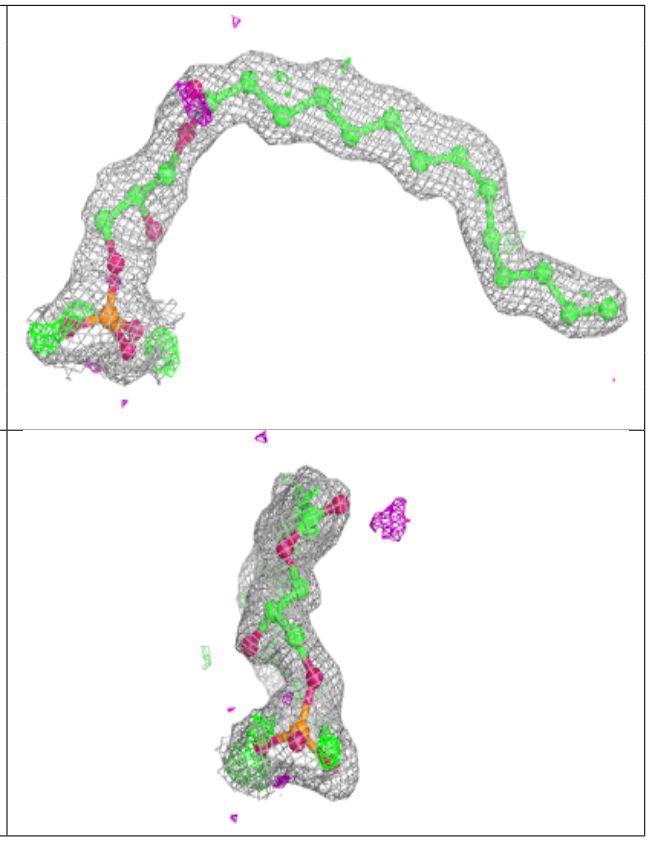
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	A	915	6/6	0.77	0.18	39,44,47,49	0
8	GOL	A	912	6/6	0.78	0.20	27,29,31,35	0
8	GOL	A	916	6/6	0.84	0.14	29,39,41,42	0
8	GOL	A	910	6/6	0.85	0.11	28,33,38,42	0
8	GOL	A	913	6/6	0.87	0.10	30,34,36,38	0
8	GOL	A	914	6/6	0.87	0.11	27,31,32,36	0
7	NKN	A	909	25/25	0.89	0.18	23,36,44,48	0
5	NA	A	906	1/1	0.91	0.09	26,26,26,26	0
8	GOL	A	911	6/6	0.93	0.12	21,26,27,27	0
6	4O0	A	908	37/37	0.98	0.06	15,18,20,21	0
5	NA	A	907	1/1	0.99	0.02	21,21,21,21	0
4	CA	A	905	1/1	0.99	0.04	16,16,16,16	0
3	ZN	A	903	1/1	1.00	0.05	16,16,16,16	0
3	ZN	A	904	1/1	1.00	0.04	20,20,20,20	0
9	CL	A	917	1/1	1.00	0.02	22,22,22,22	0

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

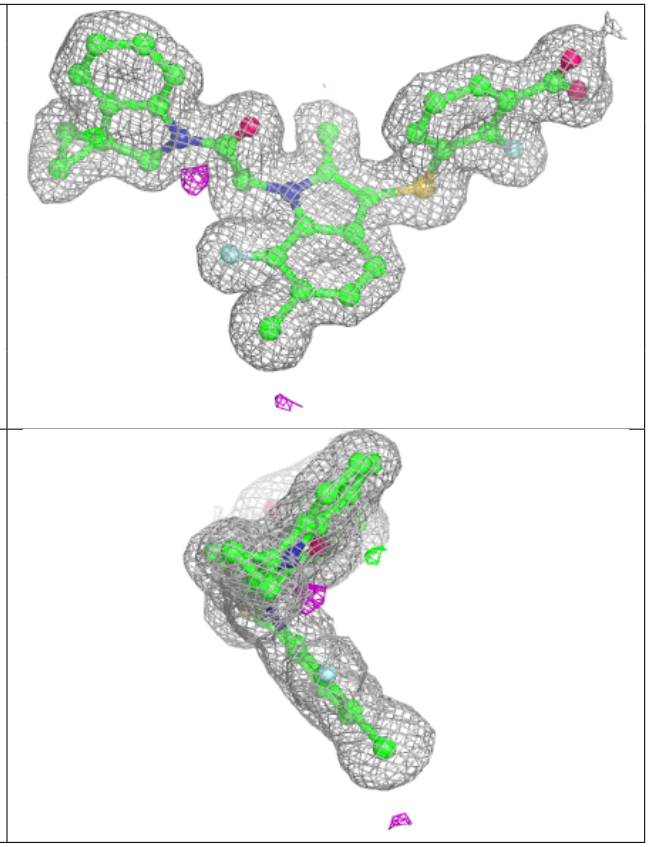
Electron density around NKN A 909:

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 4O0 A 908:

$2mF_o$-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.