wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 10:08 pm GMT

PDB ID	:	7Z0N
Title	:	Structure-Based Design of a Novel Class of Autotaxin Inhibitors Based on Endogenous Allosteric Modulators
Authors	:	Salgado-Polo, F.; Clark, J.M.; Macdonald, S.J.F.; Barrett, T.N.; Perrakis, A.; Jamieson, A.
Deposited on	:	2022-02-23
Resolution	:	2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

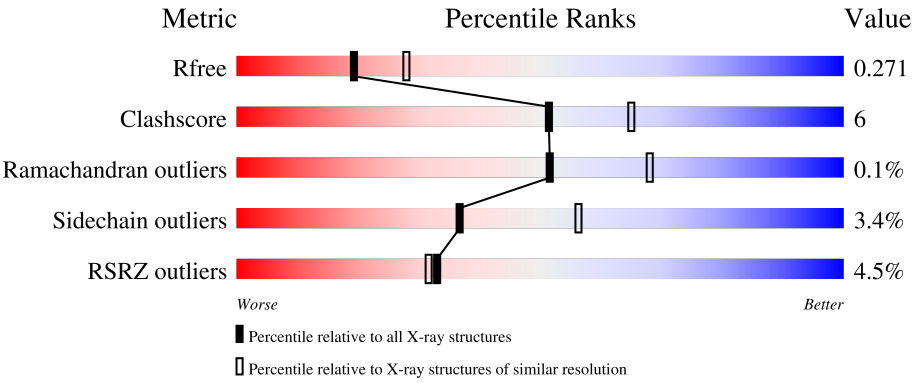
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

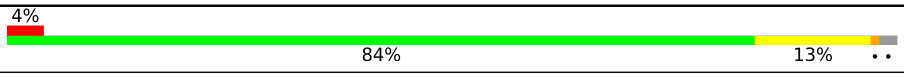
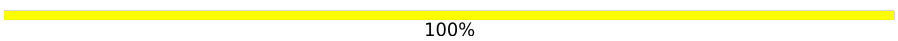
The reported resolution of this entry is 2.40 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	AAA	805	
2	AaA	7	

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
9	GOL	AAA	918	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13254 atoms, of which 6377 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.

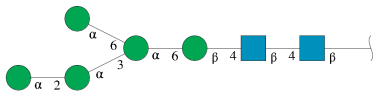
- Molecule 1 is a protein called Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	792	12608	4063	6196	1108	1192	49	204	4	1

There are 4 discrepancies between the modelled and reference sequences:

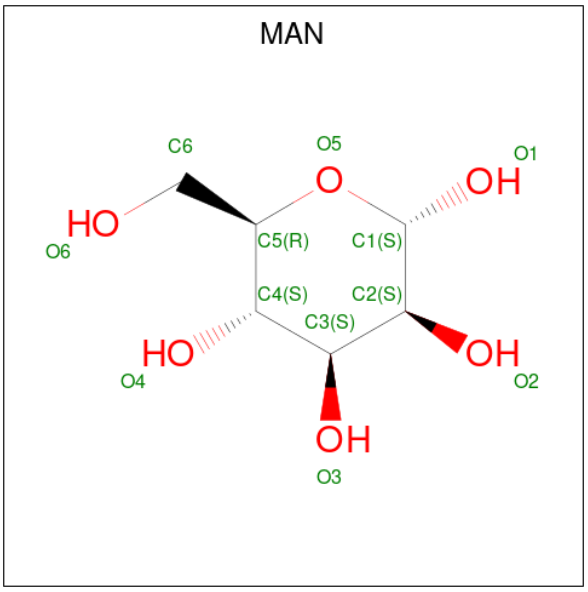
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	410	ALA	ASN	engineered mutation	UNP Q64610
AAA	580	ASP	GLU	engineered mutation	UNP Q64610
AAA	591	THR	ARG	engineered mutation	UNP Q64610
AAA	806	ALA	ASN	engineered mutation	UNP Q64610

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	AaA	7	166	46	83	2	35	21	0	0

- Molecule 3 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H O 22 6 11 5	4	0

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

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

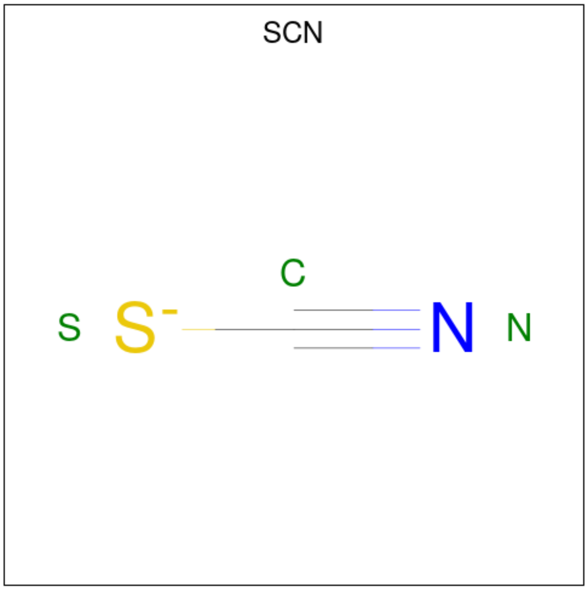
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	4	Total I 4 4	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

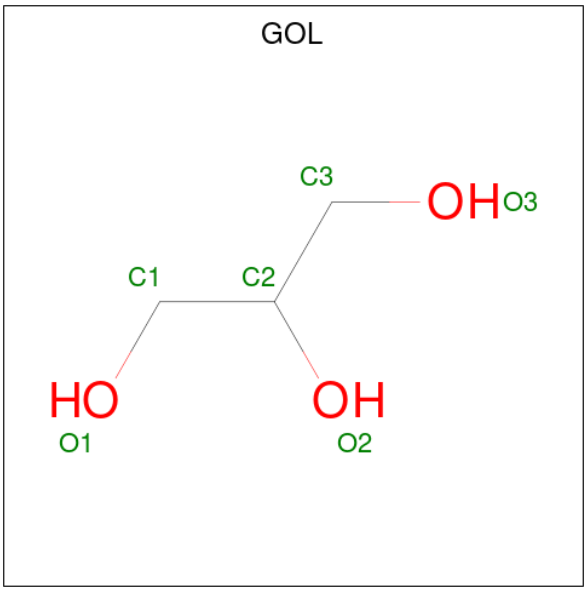


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0
7	AAA	1	Total C N S 3 1 1 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

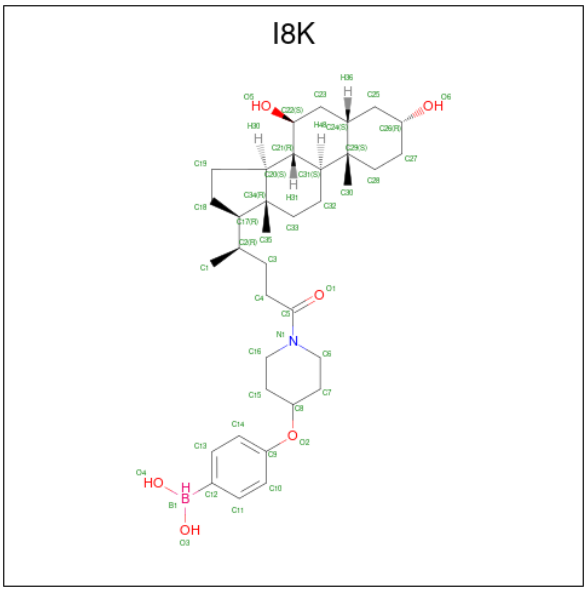
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	2	Total Na 2 2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
9	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
9	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
9	AAA	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 10 is [4-[1-[(4 {R})-4-[(3 {R},5 {S},7 {S},8 {R},9 {S},10 {S},13 {R},14 {S},17 {R }})-10,13-dimethyl-3,7-bis(oxidanyl)-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1 {H}-cyclopenta[a]phenanthren-17-yl]pentanoyl]piperidin-4-yl]oxyphenyl]-bis(oxidanyl)-$l^{4}-borane (three-letter code: I8K) (formula: $C_{35}H_{55}BNO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	AAA	1	Total	B	C	H	N	O	3	0
			98	1	35	55	1	6		

- Molecule 11 is water.

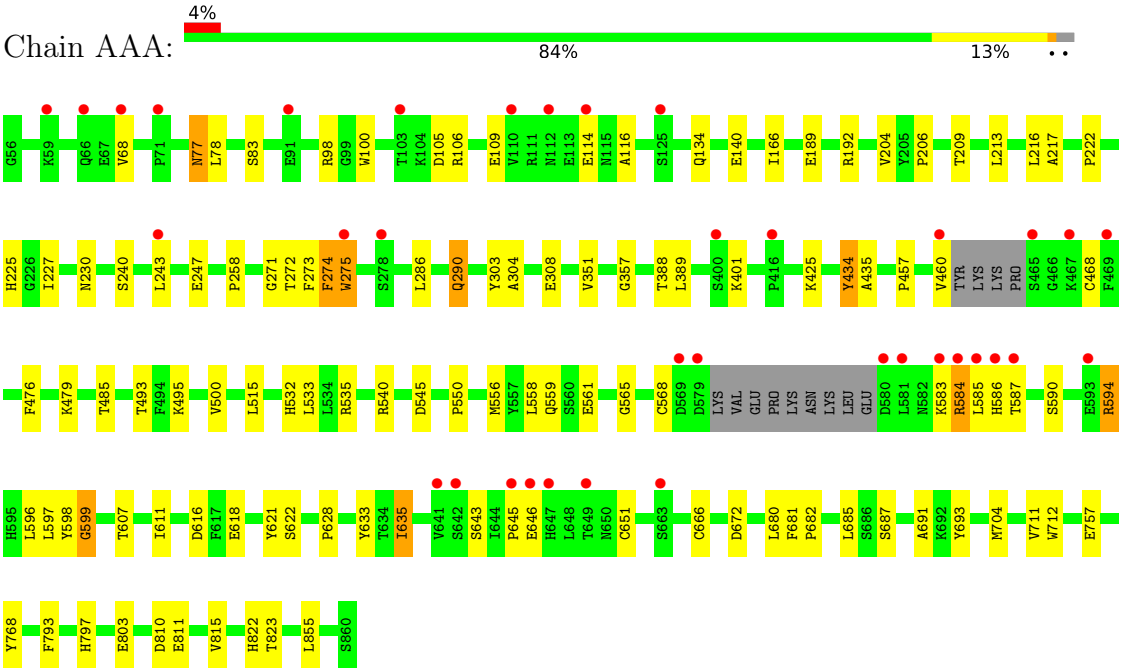
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AAA	271	Total	O	0	0
			271	271		

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: Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2

Chain AAA:



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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

Chain AaA:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.79Å 89.61Å 77.55Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	46.13 – 2.40 46.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.13-2.40) 99.9 (46.13-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.263 0.205 , 0.271	Depositor DCC
R_{free} test set	1631 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	1.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13254	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: NA, SCN, BMA, IOD, ZN, MAN, GOL, I8K, NAG, CA

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	AAA	0.71	3/6598 (0.0%)	0.80	0/8946

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	618	GLU	CG-CD	6.00	1.60	1.51
1	AAA	599	GLY	C-O	5.50	1.32	1.23
1	AAA	434	TYR	C-O	5.30	1.33	1.23

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	AAA	6412	6196	6161	71	0
2	AaA	83	83	69	0	0
3	AAA	11	11	10	0	0
4	AAA	2	0	0	0	0
5	AAA	1	0	0	0	0
6	AAA	4	0	0	0	0
7	AAA	24	0	0	1	0
8	AAA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AAA	24	32	32	2	0
10	AAA	43	55	0	1	0
11	AAA	271	0	0	1	0
All	All	6877	6377	6272	71	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.

The worst 5 of 71 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:AAA:596:LEU:HD22	1:AAA:599:GLY:O	1.94	0.68
1:AAA:500:VAL:HG21	1:AAA:533:LEU:HD21	1.79	0.65
1:AAA:425:LYS:HE2	1:AAA:435:ALA:O	1.96	0.65
1:AAA:500:VAL:HG11	1:AAA:533:LEU:HD23	1.79	0.63
1:AAA:286:LEU:O	1:AAA:290:GLN:HG2	1.99	0.63

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	AAA	790/805 (98%)	741 (94%)	48 (6%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	272	THR

5.3.2 Protein sidechains

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	AAA	719/729 (99%)	695 (97%)	24 (3%)	38 57

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	545	ASP
1	AAA	585	LEU
1	AAA	584	ARG
1	AAA	586	HIS
1	AAA	290	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

7 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	AaA	1	2,1	14,14,15	0.59	0	17,19,21	1.40	3 (17%)
2	NAG	AaA	2	2	14,14,15	0.77	0	17,19,21	1.88	3 (17%)
2	BMA	AaA	3	2	11,11,12	0.84	0	15,15,17	2.15	4 (26%)
2	MAN	AaA	4	2	11,11,12	0.71	0	15,15,17	1.59	3 (20%)
2	MAN	AaA	5	2	11,11,12	0.69	0	15,15,17	1.26	1 (6%)
2	MAN	AaA	6	2	11,11,12	0.32	0	15,15,17	1.32	2 (13%)
2	MAN	AaA	7	2	11,11,12	0.93	0	15,15,17	1.46	3 (20%)

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	AaA	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	AaA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	AaA	3	2	-	2/2/19/22	0/1/1/1
2	MAN	AaA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	5	2	-	2/2/19/22	0/1/1/1
2	MAN	AaA	6	2	-	0/2/19/22	0/1/1/1
2	MAN	AaA	7	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AaA	2	NAG	C1-C2-N2	-5.21	101.58	110.49
2	AaA	3	BMA	C1-C2-C3	4.41	115.09	109.67
2	AaA	4	MAN	O5-C5-C6	4.03	113.53	107.20
2	AaA	3	BMA	C2-C3-C4	-3.69	104.52	110.89
2	AaA	2	NAG	C8-C7-N2	3.61	122.21	116.10

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AaA	5	MAN	O5-C5-C6-O6
2	AaA	5	MAN	C4-C5-C6-O6
2	AaA	2	NAG	C8-C7-N2-C2

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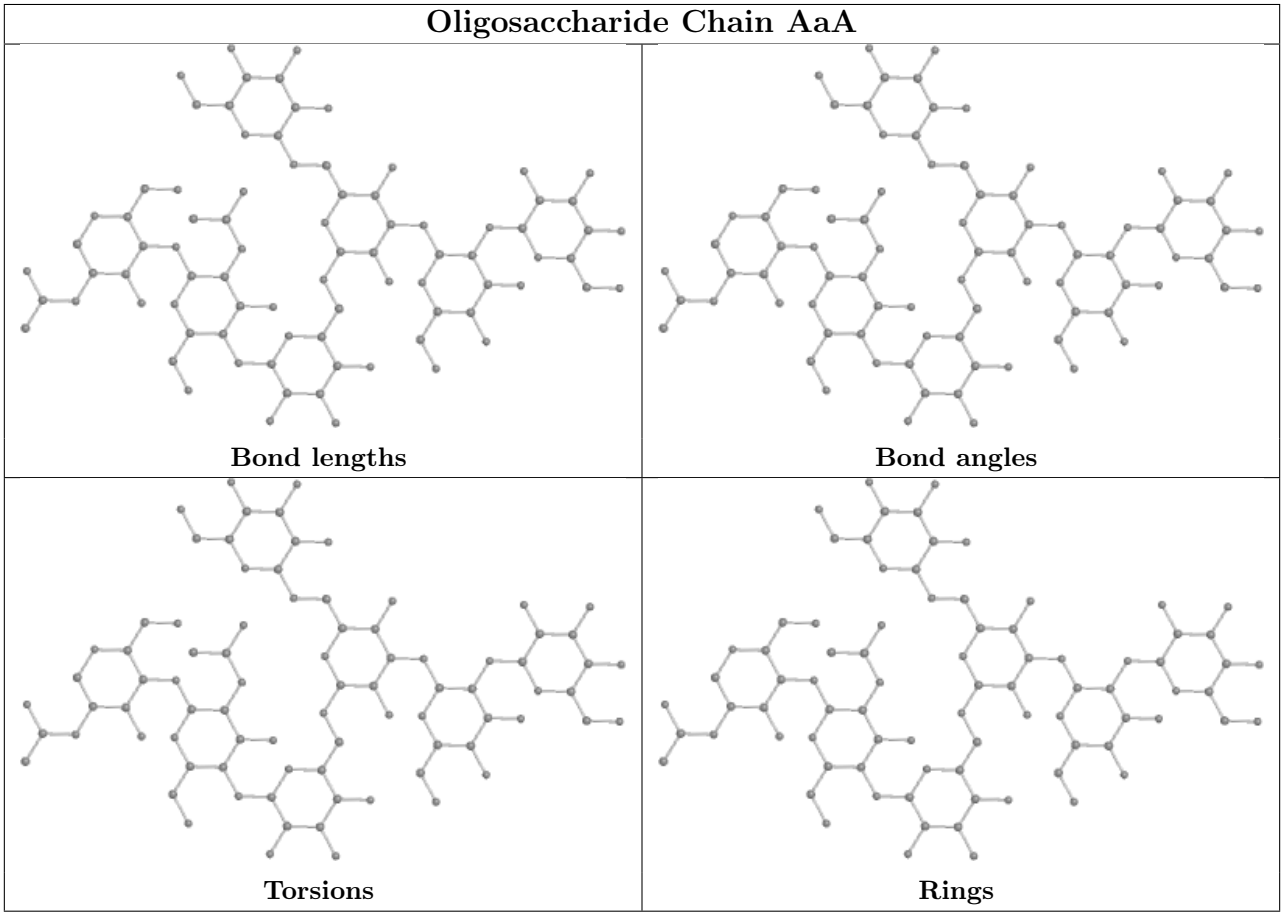
Mol	Chain	Res	Type	Atoms
2	AaA	2	NAG	O7-C7-N2-C2
2	AaA	3	BMA	C4-C5-C6-O6

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 (i)

Of 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 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	$\#\|Z\|>2$
9	GOL	AAA	922	-	5,5,5	0.10	0	5,5,5	0.33	0
7	SCN	AAA	912	-	1,2,2	1.01	0	0,1,1	-	-
7	SCN	AAA	909	-	1,2,2	0.69	0	0,1,1	-	-
7	SCN	AAA	923	-	1,2,2	1.02	0	0,1,1	-	-
7	SCN	AAA	921	-	1,2,2	3.37	1 (100%)	0,1,1	-	-
9	GOL	AAA	916	-	5,5,5	0.14	0	5,5,5	0.31	0
9	GOL	AAA	917	-	5,5,5	0.11	0	5,5,5	0.29	0
3	MAN	AAA	901	-	11,11,12	0.74	0	15,15,17	1.82	3 (20%)
7	SCN	AAA	913	-	1,2,2	0.97	0	0,1,1	-	-
9	GOL	AAA	918	-	5,5,5	0.14	0	5,5,5	0.32	0
7	SCN	AAA	911	-	1,2,2	1.60	0	0,1,1	-	-
7	SCN	AAA	910	-	1,2,2	0.57	0	0,1,1	-	-
7	SCN	AAA	919	-	1,2,2	1.41	0	0,1,1	-	-
10	I8K	AAA	920	1,4	48,48,48	1.83	3 (6%)	72,73,73	1.02	3 (4%)

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
9	GOL	AAA	922	-	-	4/4/4/4	-
9	GOL	AAA	917	-	-	4/4/4/4	-
9	GOL	AAA	916	-	-	2/4/4/4	-
9	GOL	AAA	918	-	-	2/4/4/4	-
3	MAN	AAA	901	-	-	2/2/19/22	0/1/1/1
10	I8K	AAA	920	1,4	-	5/21/92/92	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AAA	920	I8K	B1-O3	8.75	1.51	1.36
10	AAA	920	I8K	B1-O4	7.68	1.49	1.36
10	AAA	920	I8K	B1-C12	4.02	1.65	1.57
7	AAA	921	SCN	C-N	3.37	1.26	1.15

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AAA	920	I8K	O4-B1-C12	-4.55	106.36	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	901	MAN	C1-C2-C3	3.49	113.95	109.67
3	AAA	901	MAN	C1-O5-C5	-3.36	107.64	112.19
10	AAA	920	I8K	B1-C12-C13	-2.95	117.44	121.56
10	AAA	920	I8K	B1-C12-C11	2.89	125.59	121.56

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AAA	916	GOL	C1-C2-C3-O3
9	AAA	917	GOL	O1-C1-C2-O2
9	AAA	917	GOL	O1-C1-C2-C3
9	AAA	917	GOL	C1-C2-C3-O3
9	AAA	922	GOL	O1-C1-C2-C3

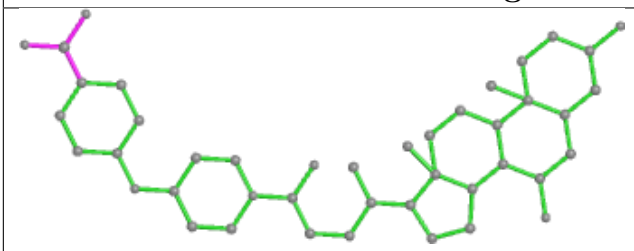
There are no ring outliers.

3 monomers are involved in 4 short contacts:

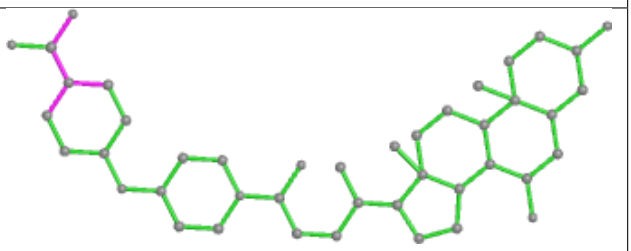
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AAA	922	GOL	2	0
7	AAA	913	SCN	1	0
10	AAA	920	I8K	1	0

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.

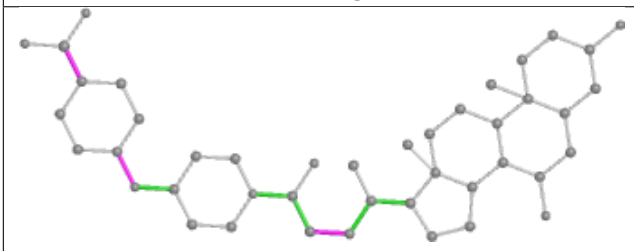
Ligand I8K AAA 920



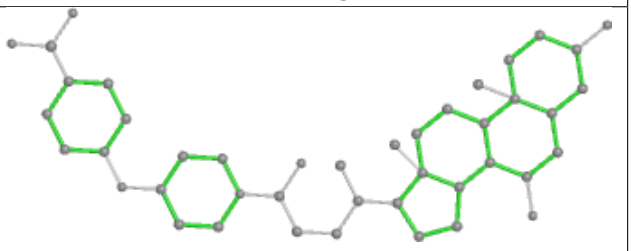
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AAA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AAA	569:ASP	C	579:ASP	N	14.58

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, 95^{th} 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	AAA	792/805 (98%)	0.29	36 (4%) 33 31	27, 46, 77, 116	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	71	PRO	4.2
1	AAA	587	THR	4.0
1	AAA	641	VAL	3.7
1	AAA	649	THR	3.6
1	AAA	416	PRO	3.5

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

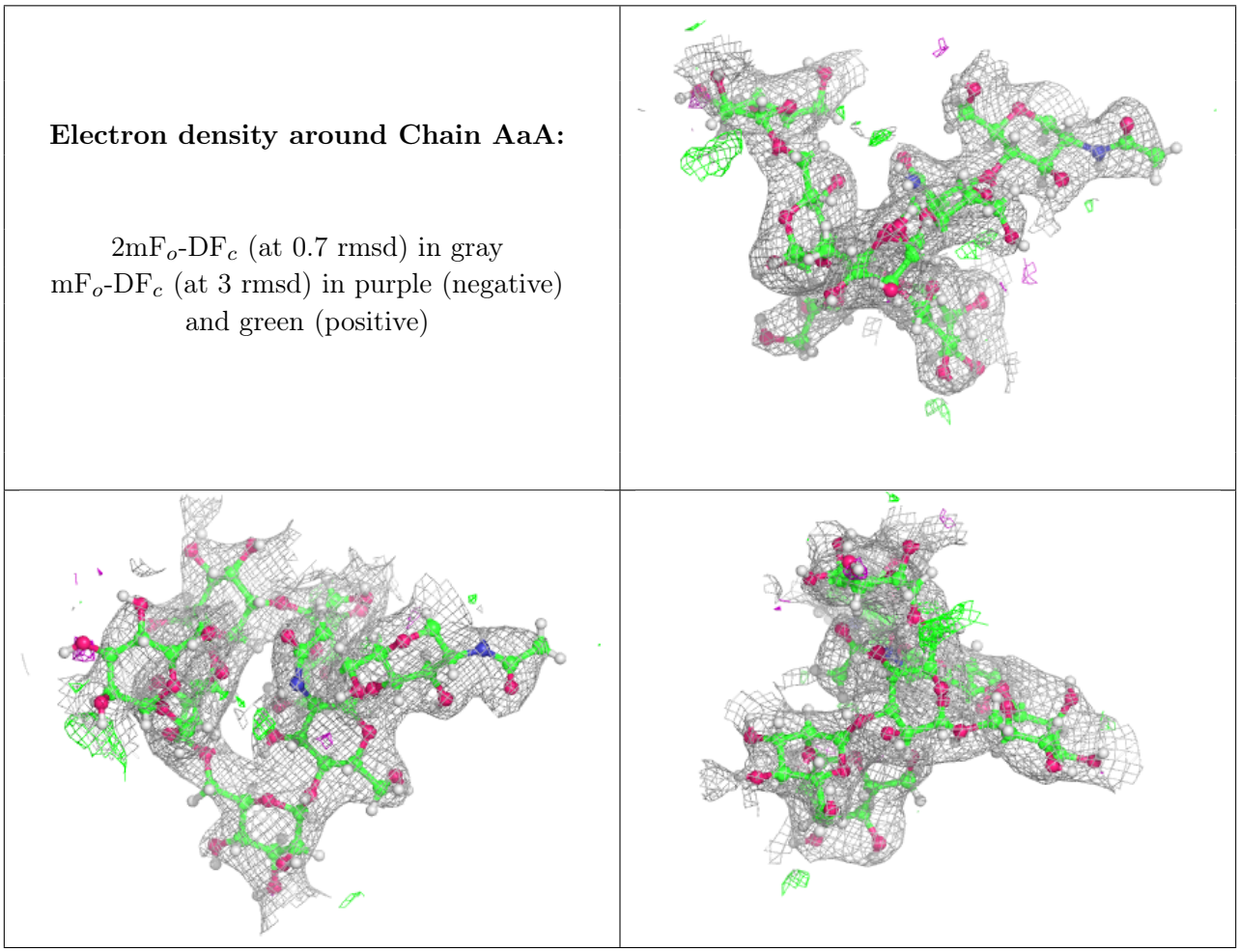
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} 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	MAN	AaA	7	11/12	0.86	0.21	30,49,55,63	4
2	BMA	AaA	3	11/12	0.92	0.16	30,51,55,57	3
2	MAN	AaA	6	11/12	0.93	0.16	30,42,48,48	4
2	MAN	AaA	5	11/12	0.95	0.14	30,49,50,53	3
2	NAG	AaA	2	14/15	0.95	0.17	30,37,42,43	2
2	MAN	AaA	4	11/12	0.95	0.12	30,46,49,52	3
2	NAG	AaA	1	14/15	0.97	0.17	27,30,33,34	2

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.



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, 95^{th} 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	NA	AAA	914	1/1	0.34	0.28	58,58,58,58	0
7	SCN	AAA	923	3/3	0.71	0.23	58,58,61,61	0
9	GOL	AAA	918	6/6	0.77	0.40	30,79,82,82	2
5	CA	AAA	904	1/1	0.79	0.17	37,37,37,37	0
9	GOL	AAA	917	6/6	0.80	0.65	30,67,69,70	2
7	SCN	AAA	921	3/3	0.81	0.54	89,89,90,91	0
7	SCN	AAA	913	3/3	0.83	0.17	68,68,70,73	0
7	SCN	AAA	911	3/3	0.83	0.23	64,64,64,66	0

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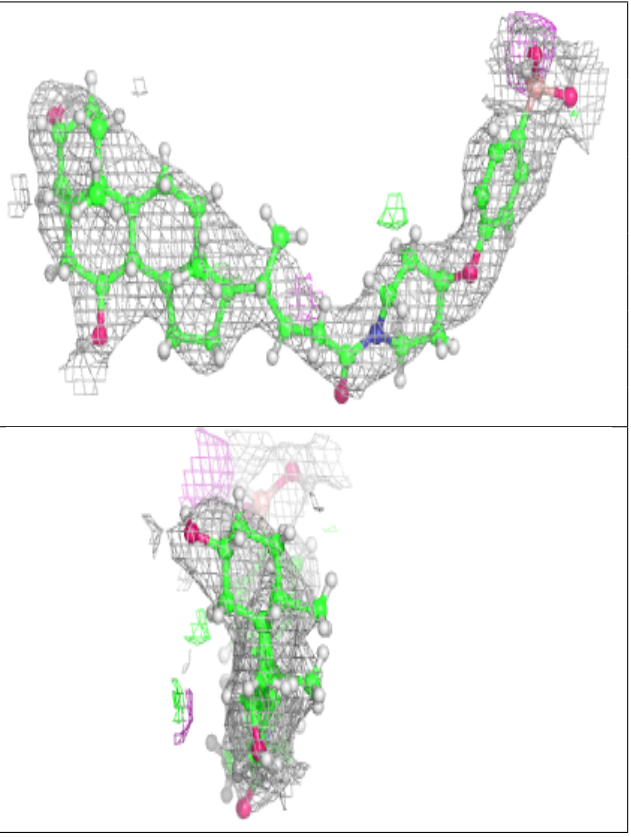
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NA	AAA	915	1/1	0.84	0.18	66,66,66,66	0
9	GOL	AAA	916	6/6	0.84	0.47	30,63,67,67	2
7	SCN	AAA	919	3/3	0.84	0.29	58,58,62,67	0
3	MAN	AAA	901	11/12	0.84	0.14	30,60,62,68	4
7	SCN	AAA	910	3/3	0.87	0.16	67,67,72,77	0
7	SCN	AAA	912	3/3	0.88	0.19	41,41,48,52	0
9	GOL	AAA	922	6/6	0.91	0.19	30,50,52,54	2
7	SCN	AAA	909	3/3	0.92	0.15	77,77,81,83	0
10	I8K	AAA	920	43/43	0.94	0.17	30,49,55,57	3
6	IOD	AAA	907	1/1	0.97	0.05	71,71,71,71	0
4	ZN	AAA	903	1/1	0.97	0.04	41,41,41,41	0
6	IOD	AAA	908	1/1	0.98	0.07	66,66,66,66	0
6	IOD	AAA	906	1/1	0.99	0.09	63,63,63,63	0
4	ZN	AAA	902	1/1	0.99	0.11	37,37,37,37	0
6	IOD	AAA	905	1/1	0.99	0.13	39,39,39,39	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 I8K AAA 920:

$2mF_o$-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.