



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:32 PM BST

PDB ID : 6W35
Title : A new Autotaxin Inhibitor for the Treatment of Idiopathic Pulmonary Fibrosis:
A Clinical Candidate Discovered Using DNA-Encoded Chemistry
Authors : Cuzzo, J.W.
Deposited on : 2020-03-09
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

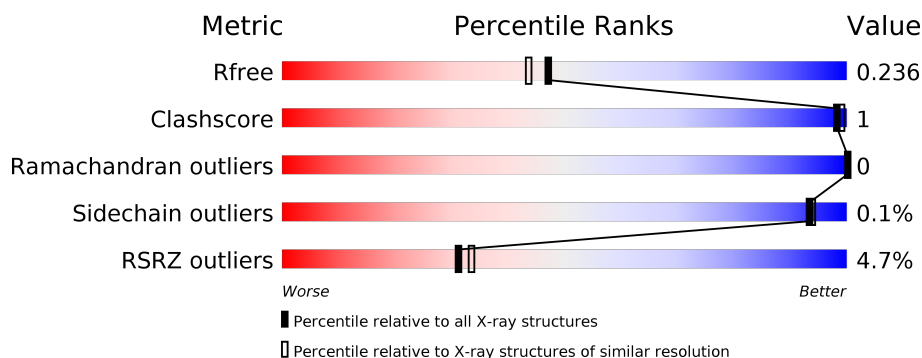
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	818	<div> <div>5%</div> <div>95%</div> <div>..</div> </div>
2	B	7	<div> <div>14%</div> <div>86%</div> </div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7099 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.

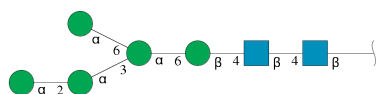
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	93	0	0
			6410	4071	1105	1186	48			

There are 16 discrepancies between the modelled and reference sequences:

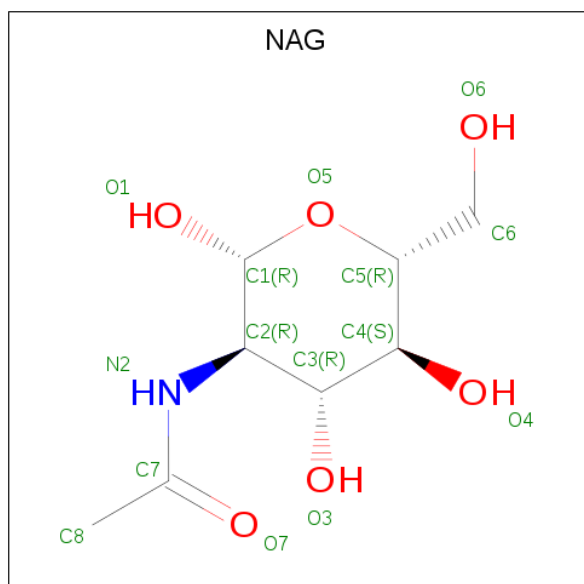
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	HIS	ASN	engineered mutation	UNP K7CID1
A	552	ASN	SER	engineered mutation	UNP K7CID1
A	620	GLU	GLN	engineered mutation	UNP K7CID1
A	641	VAL	ILE	engineered mutation	UNP K7CID1
A	860	LEU	-	expression tag	UNP K7CID1
A	861	VAL	-	expression tag	UNP K7CID1
A	862	PRO	-	expression tag	UNP K7CID1
A	863	ARG	-	expression tag	UNP K7CID1
A	864	GLY	-	expression tag	UNP K7CID1
A	865	SER	-	expression tag	UNP K7CID1
A	866	HIS	-	expression tag	UNP K7CID1
A	867	HIS	-	expression tag	UNP K7CID1
A	868	HIS	-	expression tag	UNP K7CID1
A	869	HIS	-	expression tag	UNP K7CID1
A	870	HIS	-	expression tag	UNP K7CID1
A	871	HIS	-	expression tag	UNP K7CID1

- 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.



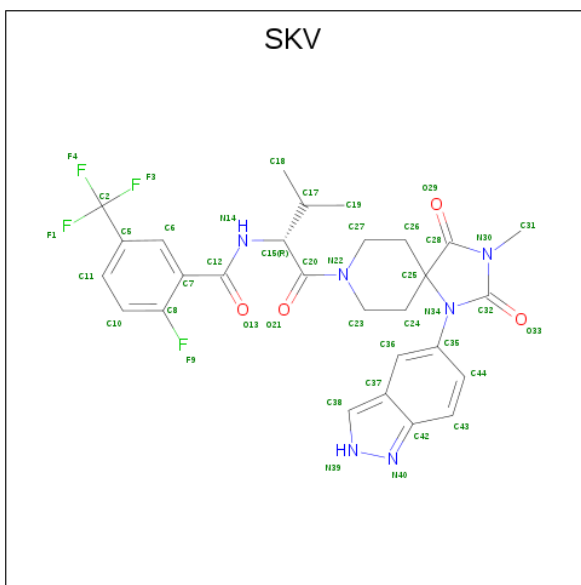
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-fluoranyl- {N}-[(2 {R})-1-[1-(2 {H}-indazol-5-yl)-3-methyl-2,4-bis(oxidanyl idene)-1,3,8-triazaspiro[4.5]decan-8-yl]-3-methyl-1-oxidanylidene-butan-2-yl]-5-(trifluorom ethyl)benzamide (three-letter code: SKV) (formula: $C_{28}H_{28}F_4N_6O_4$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			42	28	4	6	4		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

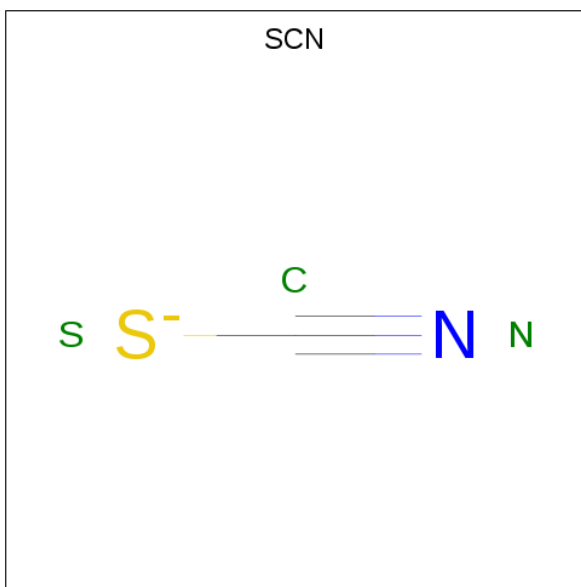
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Mg 2 2	0	0

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	12	Total	Cl	0	0
			12	12		

- Molecule 10 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	5	Total	I	0	0
			5	5		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	518	Total	O	0	0
			518	518		

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase 2



- Molecule 2: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.72Å 77.38Å 94.43Å 90.00° 112.11° 90.00°	Depositor
Resolution (Å)	87.49 – 1.98 45.62 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.8 (87.49-1.98) 95.8 (45.62-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.179 , 0.230 0.187 , 0.236	Depositor DCC
R_{free} test set	1928 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7099	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: MG, SKV, NAG, CL, CA, ZN, SCN, BMA, IOD, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	0/6591	0.77	5/8935 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	714	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	394	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	724	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	175	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	714	ARG	NE-CZ-NH2	-5.36	117.62	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	6410	0	6173	8	0
2	B	83	0	70	0	0
3	A	14	0	13	0	0
4	A	42	0	0	0	0
5	A	2	0	0	0	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
7	A	2	0	0	0	0
8	A	9	0	0	0	0
9	A	12	0	0	1	0
10	A	5	0	0	1	0
11	A	518	0	0	2	0
All	All	7099	0	6256	8	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 1.

All (8) 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:580:LYS:HD2	11:A:1172:HOH:O	2.08	0.54
1:A:223:PRO:HA	1:A:226:HIS:CE1	2.50	0.47
1:A:310:GLN:HG2	10:A:923:IOD:I	2.86	0.46
1:A:766:SER:HB2	1:A:790:PHE:CZ	2.51	0.45
1:A:451:ARG:NH1	11:A:1002:HOH:O	2.36	0.42
1:A:628:THR:O	1:A:730:ILE:HA	2.20	0.41
1:A:386:VAL:O	1:A:391:GLY:HA2	2.20	0.41
1:A:572:LYS:HG2	9:A:930:CL:CL	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	786/818 (96%)	766 (98%)	20 (2%)	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	719/742 (97%)	718 (100%)	1 (0%)	93 94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ARG

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

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](#)

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	B	1	1,2	14,14,15	0.86	0	17,19,21	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	2	2	14,14,15	0.48	0	17,19,21	1.07	1 (5%)
2	BMA	B	3	2	11,11,12	0.67	0	15,15,17	1.16	0
2	MAN	B	4	2	11,11,12	0.78	0	15,15,17	1.88	4 (26%)
2	MAN	B	5	2	11,11,12	1.15	1 (9%)	15,15,17	1.61	4 (26%)
2	MAN	B	6	2	11,11,12	0.97	1 (9%)	15,15,17	1.28	2 (13%)
2	MAN	B	7	2	11,11,12	0.57	0	15,15,17	1.20	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	MAN	B	7	2	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	MAN	O2-C2	-2.64	1.37	1.43
2	B	5	MAN	C1-C2	2.56	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	C1-O5-C5	4.37	118.11	112.19
2	B	4	MAN	O3-C3-C2	3.95	117.56	109.99
2	B	4	MAN	C1-O5-C5	3.58	117.04	112.19
2	B	6	MAN	C1-O5-C5	3.41	116.81	112.19
2	B	5	MAN	C1-O5-C5	3.00	116.26	112.19
2	B	4	MAN	O3-C3-C4	-2.78	103.92	110.35
2	B	1	NAG	C3-C4-C5	2.57	114.82	110.24
2	B	5	MAN	O5-C5-C6	2.55	111.20	107.20
2	B	5	MAN	O5-C1-C2	-2.24	107.31	110.77
2	B	2	NAG	C2-N2-C7	2.13	125.94	122.90
2	B	5	MAN	C3-C4-C5	2.07	113.92	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	MAN	C1-C2-C3	2.05	112.18	109.67
2	B	4	MAN	O5-C5-C6	2.02	110.36	107.20

There are no chirality outliers.

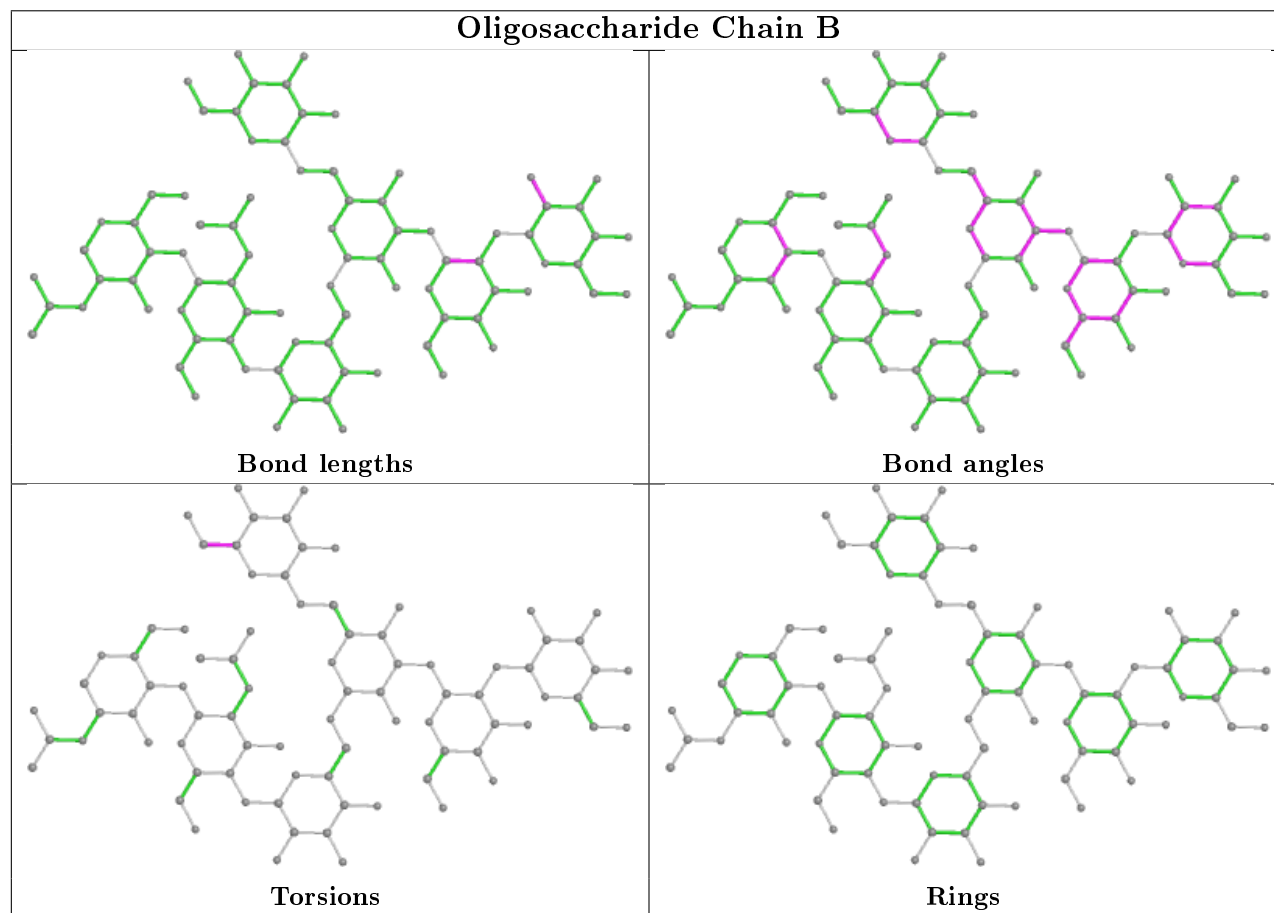
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	MAN	C4-C5-C6-O6
2	B	7	MAN	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 28 ligands modelled in this entry, 23 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
8	SCN	A	932	-	1,2,2	0.09	0	0,1,1	0.00	-
3	NAG	A	908	1	14,14,15	0.66	0	17,19,21	1.50	2 (11%)
4	SKV	A	909	-	43,46,46	1.14	3 (6%)	59,71,71	1.72	10 (16%)
8	SCN	A	931	-	1,2,2	0.33	0	0,1,1	0.00	-
8	SCN	A	916	-	1,2,2	1.11	0	0,1,1	0.00	-

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	NAG	A	908	1	-	0/6/23/26	0/1/1/1
4	SKV	A	909	-	-	0/30/66/66	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	909	SKV	C32-N34	-2.70	1.34	1.38
4	A	909	SKV	C38-C37	2.68	1.46	1.40
4	A	909	SKV	C32-N30	-2.56	1.33	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	909	SKV	C28-C25-N34	7.88	103.33	100.77
4	A	909	SKV	C24-C23-N22	-4.65	101.75	110.92
3	A	908	NAG	O5-C1-C2	-4.32	104.47	111.29
4	A	909	SKV	C10-C8-C7	-2.96	119.89	123.11
4	A	909	SKV	O33-C32-N34	-2.87	122.96	127.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	909	SKV	O21-C20-N22	-2.76	118.44	121.67
4	A	909	SKV	F3-C2-F1	2.33	114.26	105.72
4	A	909	SKV	C20-C15-N14	-2.22	102.80	108.03
3	A	908	NAG	O7-C7-C8	-2.07	118.21	122.06
4	A	909	SKV	C26-C27-N22	-2.07	106.84	110.92
4	A	909	SKV	C7-C12-N14	2.05	120.60	116.80
4	A	909	SKV	C17-C15-C20	2.00	114.78	110.73

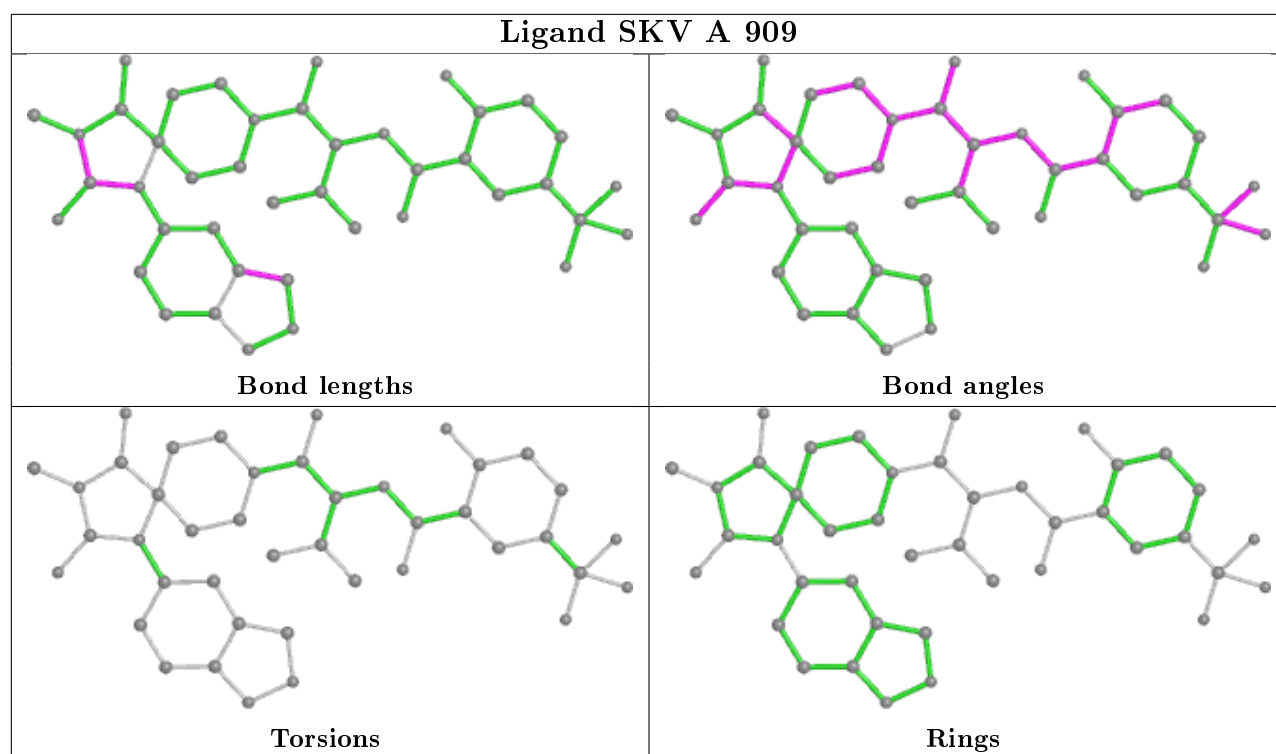
There are no chirality outliers.

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	792/818 (96%)	0.15	37 (4%) 31 33	20, 34, 69, 88	34 (4%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	LEU	5.3
1	A	108	CYS	5.2
1	A	397	PHE	5.1
1	A	109	GLY	4.9
1	A	111	VAL	4.8
1	A	664	LEU	4.6
1	A	55	ILE	4.5
1	A	104	THR	4.3
1	A	134	TYR	4.2
1	A	401	ALA	3.9
1	A	72	PRO	3.8
1	A	61	GLY	3.7
1	A	138	CYS	3.7
1	A	106	ASP	3.4
1	A	140	GLY	3.3
1	A	149	CYS	3.1
1	A	564	ASP	3.1
1	A	537	THR	2.9
1	A	120	CYS	2.9
1	A	137	VAL	2.9
1	A	130	CYS	2.8
1	A	398	SER	2.7
1	A	58	SER	2.5
1	A	54	ASN	2.4
1	A	123	ASP	2.4
1	A	56	SER	2.3
1	A	113	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	400	ASN	2.3
1	A	141	GLU	2.3
1	A	381	ASP	2.2
1	A	399	ASN	2.2
1	A	59	CYS	2.1
1	A	121	SER	2.1
1	A	402	LYS	2.1
1	A	142	SER	2.0
1	A	417	PRO	2.0
1	A	124	CYS	2.0

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

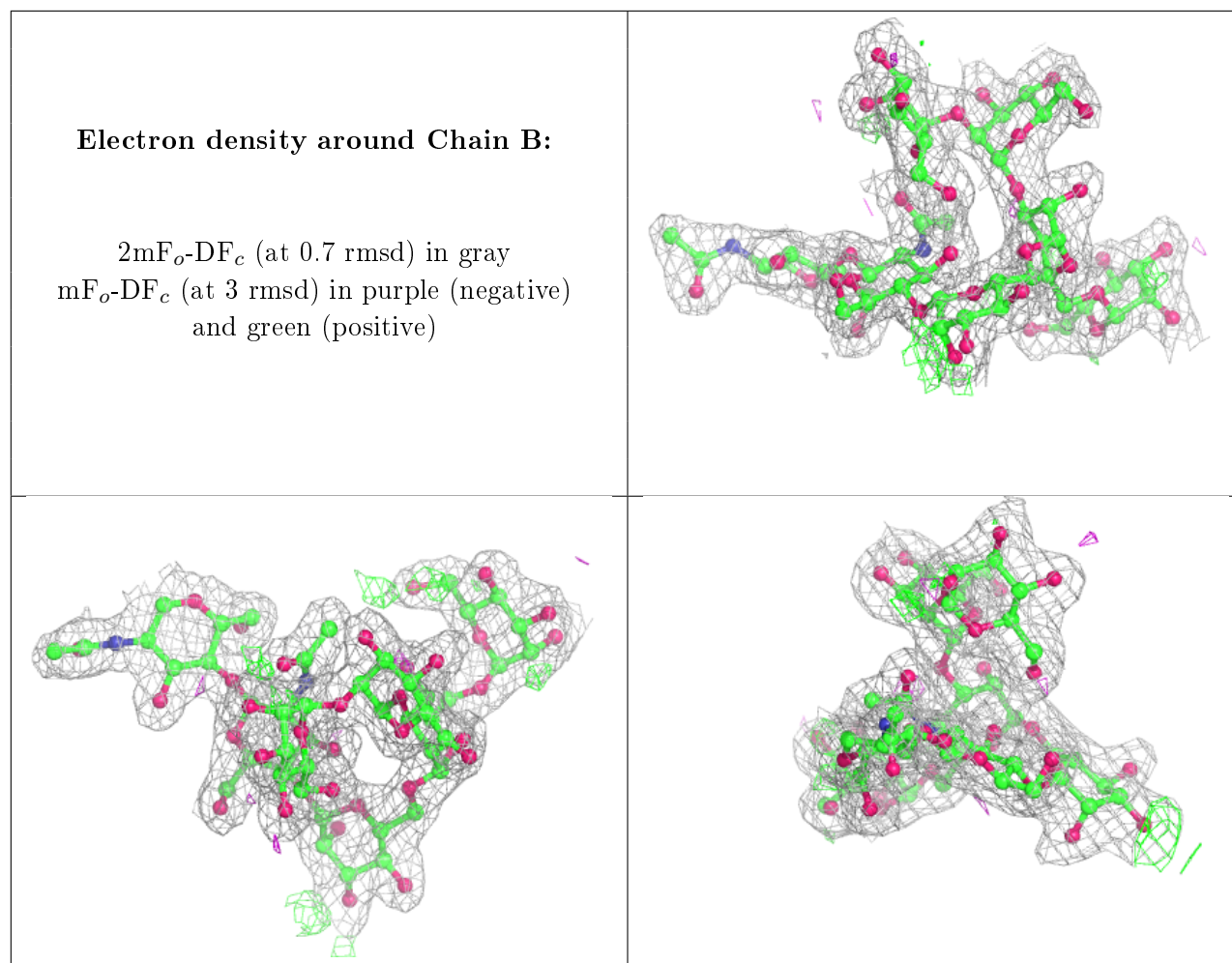
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	MAN	B	7	11/12	0.90	0.09	49,51,57,59	0
2	MAN	B	6	11/12	0.93	0.10	24,31,34,34	0
2	BMA	B	3	11/12	0.93	0.08	36,39,43,46	0
2	NAG	B	2	14/15	0.95	0.08	27,31,36,42	0
2	MAN	B	4	11/12	0.96	0.07	37,38,41,42	0
2	NAG	B	1	14/15	0.96	0.12	24,26,30,32	0
2	MAN	B	5	11/12	0.96	0.09	31,33,40,49	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.



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.

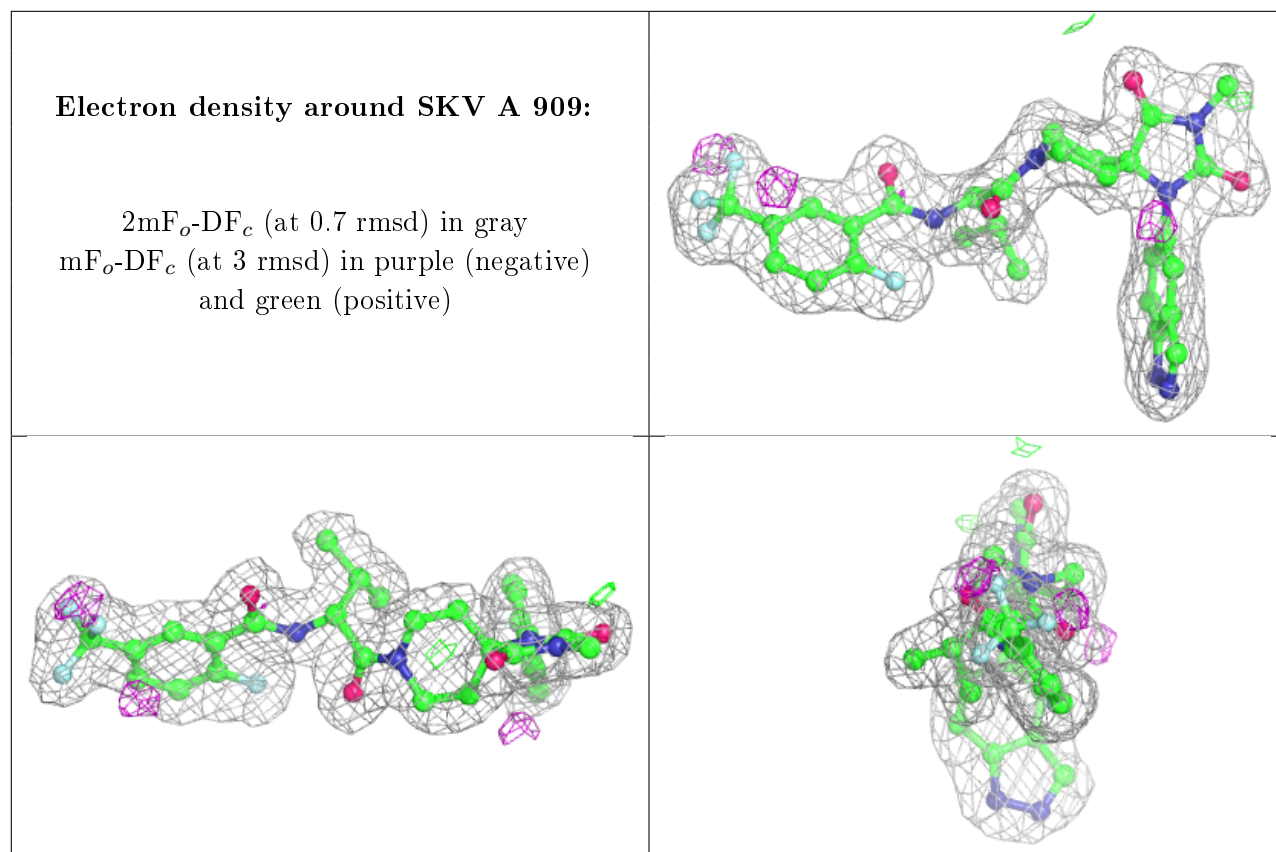
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	A	914	1/1	0.88	0.09	41,41,41,41	0
8	SCN	A	916	3/3	0.90	0.12	42,42,43,45	0
9	CL	A	928	1/1	0.90	0.12	60,60,60,60	0
9	CL	A	929	1/1	0.92	0.06	53,53,53,53	0
9	CL	A	935	1/1	0.93	0.11	40,40,40,40	0
4	SKV	A	909	42/42	0.94	0.10	21,30,40,42	0
3	NAG	A	908	14/15	0.95	0.11	46,49,56,60	0
9	CL	A	922	1/1	0.95	0.11	39,39,39,39	0
7	MG	A	915	1/1	0.95	0.16	38,38,38,38	0
9	CL	A	927	1/1	0.95	0.05	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CL	A	930	1/1	0.97	0.05	43,43,43,43	0
6	CA	A	912	1/1	0.97	0.13	44,44,44,44	0
9	CL	A	919	1/1	0.97	0.06	40,40,40,40	0
5	ZN	A	910	1/1	0.97	0.10	48,48,48,48	0
9	CL	A	918	1/1	0.97	0.12	37,37,37,37	0
10	IOD	A	926	1/1	0.97	0.04	53,53,53,53	1
8	SCN	A	932	3/3	0.98	0.11	38,38,39,52	0
8	SCN	A	931	3/3	0.98	0.13	42,42,44,46	0
9	CL	A	934	1/1	0.99	0.14	24,24,24,24	0
9	CL	A	921	1/1	0.99	0.08	44,44,44,44	0
6	CA	A	913	1/1	0.99	0.07	26,26,26,26	0
9	CL	A	920	1/1	0.99	0.05	43,43,43,43	0
9	CL	A	917	1/1	0.99	0.15	42,42,42,42	0
10	IOD	A	923	1/1	0.99	0.08	42,42,42,42	1
10	IOD	A	925	1/1	0.99	0.03	52,52,52,52	1
10	IOD	A	924	1/1	1.00	0.07	41,41,41,41	1
10	IOD	A	933	1/1	1.00	0.09	37,37,37,37	0
5	ZN	A	911	1/1	1.00	0.10	25,25,25,25	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.