



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 12:49 PM BST

PDB ID : 5M7M  
Title : Novel Imidazo[1,2-a]pyridine Derivatives with Potent Autotaxin/ENPP2 Inhibitor Activity  
Authors : Wolhkonig, A.; Fleury, D.; Leonard, P.; Triballeau, N.; Mollat, P.; Vercheval, L.  
Deposited on : 2016-10-28  
Resolution : 2.70 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](mailto: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.

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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

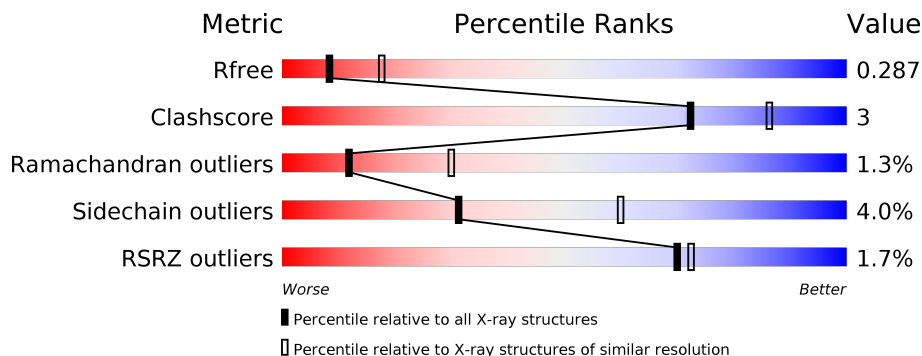
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	871	 76% 10% 13%
2	B	6	 100%

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 5999 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	759	5811	3699	996	1068	48	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

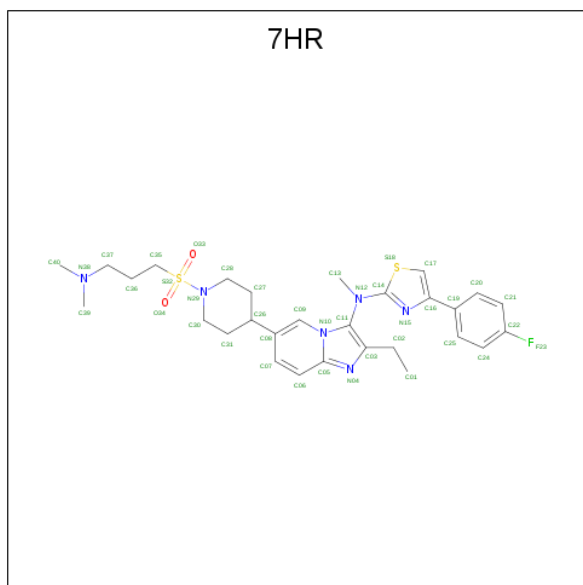
Chain	Residue	Modelled	Actual	Comment	Reference
A	493	PRO	SER	engineered mutation	UNP Q13822
A	?	-	LYS	deletion	UNP Q13822
A	?	-	VAL	deletion	UNP Q13822
A	?	-	GLU	deletion	UNP Q13822
A	?	-	PRO	deletion	UNP Q13822
A	864	LEU	-	expression tag	UNP Q13822
A	865	VAL	-	expression tag	UNP Q13822
A	866	PRO	-	expression tag	UNP Q13822
A	867	ARG	-	expression tag	UNP Q13822
A	868	GLY	-	expression tag	UNP Q13822
A	869	SER	-	expression tag	UNP Q13822
A	870	HIS	-	expression tag	UNP Q13822
A	871	HIS	-	expression tag	UNP Q13822
A	872	HIS	-	expression tag	UNP Q13822
A	873	HIS	-	expression tag	UNP Q13822
A	874	HIS	-	expression tag	UNP Q13822
A	875	HIS	-	expression tag	UNP Q13822

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	72	40	2	30	0	0	0

- Molecule 3 is {N}-[6-[1-[3-(dimethylamino)propylsulfonyl]piperidin-4-yl]-2-ethyl-imidazo[1,2-a]pyridin-3-yl]-4-(4-fluorophenyl)- {N}-methyl-1,3-thiazol-2-amine (three-letter code: 7HR) (formula: C<sub>29</sub>H<sub>37</sub>FN<sub>6</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	40	29	1	6	2	2	0	0

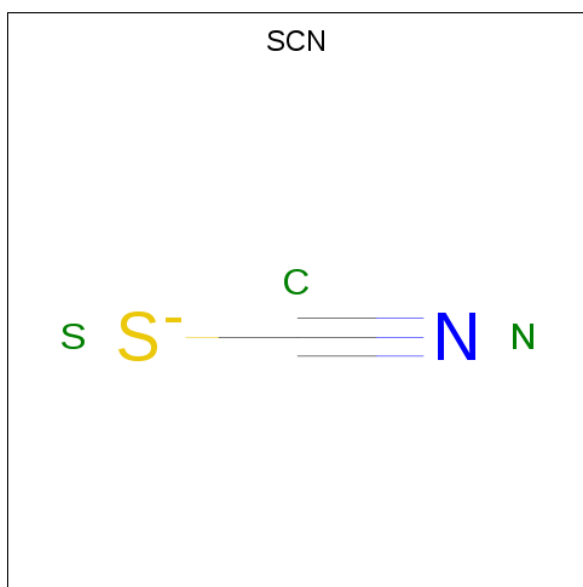
- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

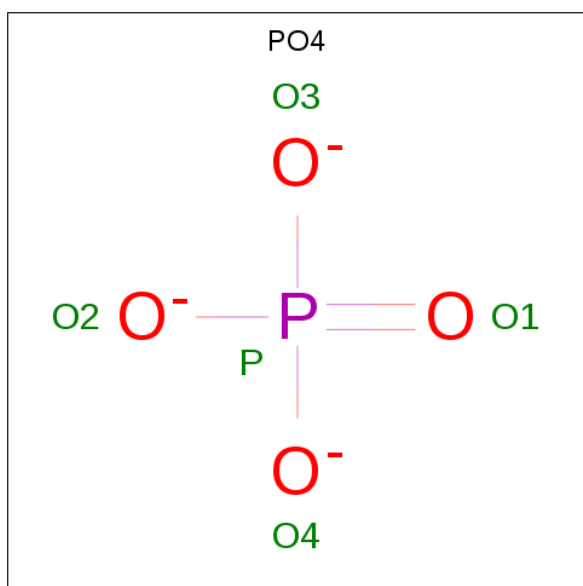


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
6	A	1	3	1	1	1	0	0

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
7	A	7	7	7	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O P 5 4 1	0	0

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

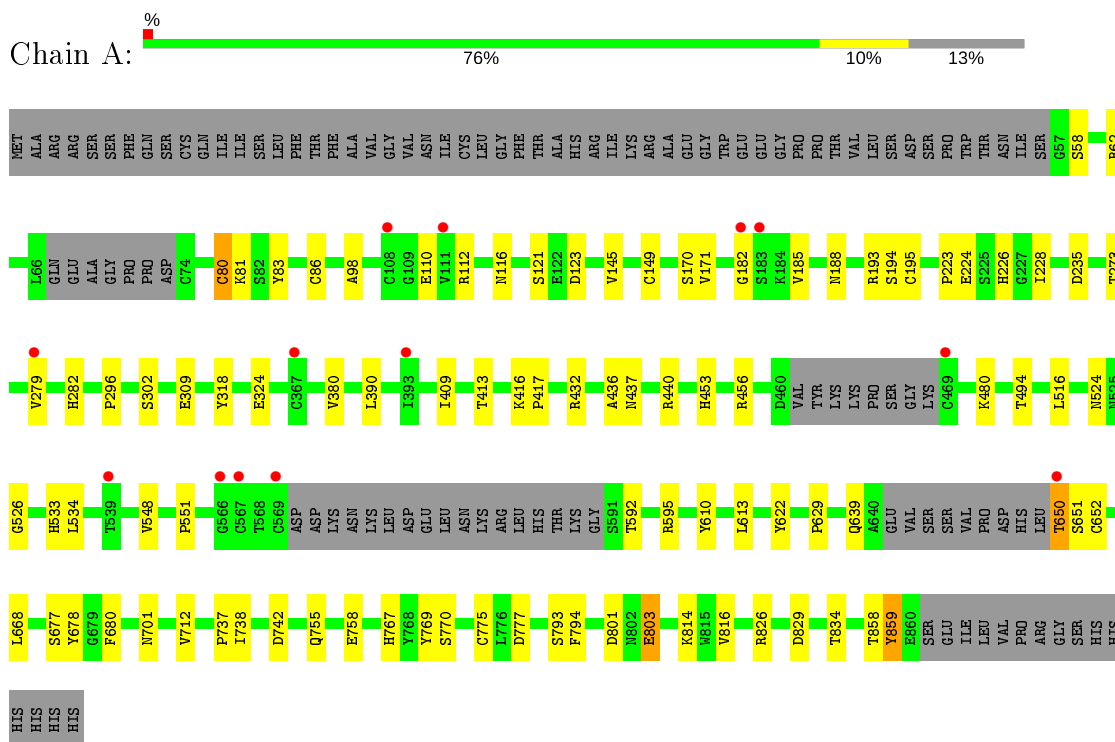
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	53	Total O 53 53	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 

Chain B: 

MANG1  
MANG2  
MANG3  
MANG4  
MANG5  
MANG6

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.45Å 78.89Å 78.57Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	78.53 – 2.70 77.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.9 (78.53-2.70) 92.9 (77.41-2.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.229 , 0.284 0.233 , 0.287	Depositor DCC
$R_{free}$ test set	1278 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for -h,-l,-k 0.026 for -h,l,k 0.022 for k,h,-l 0.029 for -k,-h,-l 0.019 for l,k,-h 0.022 for l,h,k 0.022 for k,l,h 0.022 for k,-l,-h 0.022 for -l,-h,k 0.065 for h,-k,-l 0.033 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: NI, ZN, BMA, NAG, CL, K, SCN, 7HR, IOD, PO4, 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	0.54	0/5978	0.70	1/8153 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	ASP	CB-CG-OD1	5.33	123.09	118.30

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	5811	0	5318	37	0
2	B	72	0	61	0	0
3	A	40	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	3	0	0	0	0
7	A	7	0	0	0	0
8	A	5	0	0	0	0
9	A	1	0	0	0	0
10	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	53	0	0	0	0
All	All	5999	0	5379	37	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 3.

All (37) 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:770:SER:HB2	1:A:794:PHE:CZ	2.24	0.72
1:A:58:SER:O	1:A:62:ARG:NH1	2.23	0.72
1:A:149:CYS:CB	1:A:195:CYS:HG	2.13	0.61
1:A:149:CYS:CB	1:A:195:CYS:SG	2.90	0.60
1:A:224:GLU:OE1	1:A:436:ALA:O	2.19	0.60
1:A:677:SER:OG	1:A:678:TYR:N	2.35	0.59
1:A:712:VAL:HG13	1:A:816:VAL:HG13	1.86	0.57
1:A:145:VAL:HB	1:A:188:ASN:OD1	2.06	0.56
1:A:235:ASP:OD2	1:A:440:ARG:HD2	2.06	0.55
1:A:533:HIS:CD2	1:A:534:LEU:HD12	2.42	0.55
1:A:524:ASN:HD22	1:A:526:GLY:H	1.52	0.54
1:A:680:PHE:HB3	1:A:701:ASN:ND2	2.22	0.54
1:A:801:ASP:OD2	1:A:803:GLU:HB2	2.08	0.53
1:A:769:TYR:CE2	1:A:834:THR:HG21	2.44	0.53
1:A:380:VAL:HG12	1:A:456:ARG:HD2	1.92	0.51
1:A:409:ILE:O	1:A:413:THR:OG1	2.26	0.50
1:A:551:PRO:HB3	1:A:610:TYR:CZ	2.46	0.50
1:A:98:ALA:HB3	1:A:116:ASN:HA	1.92	0.50
1:A:223:PRO:HA	1:A:226:HIS:CE1	2.49	0.48
1:A:182:GLY:HA2	1:A:185:VAL:HB	1.97	0.47
1:A:650:THR:C	1:A:652:CYS:H	2.18	0.46
1:A:80:CYS:SG	1:A:81:LYS:N	2.89	0.45
1:A:309:GLU:N	1:A:309:GLU:OE1	2.48	0.45
1:A:650:THR:C	1:A:652:CYS:N	2.71	0.44
1:A:121:SER:OG	1:A:123:ASP:OD1	2.16	0.44
1:A:279:VAL:O	1:A:279:VAL:HG22	2.18	0.43
1:A:738:ILE:HB	1:A:767:HIS:HB2	2.00	0.43
1:A:318:TYR:CD2	1:A:324:GLU:HB2	2.53	0.43
1:A:826:ARG:O	1:A:829:ASP:HB2	2.19	0.43
1:A:149:CYS:SG	1:A:149:CYS:O	2.78	0.42
1:A:494:THR:HG21	1:A:516:LEU:HD23	2.00	0.42
1:A:858:THR:O	1:A:859:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ARG:NH1	1:A:480:LYS:HE3	2.35	0.42
1:A:650:THR:O	1:A:652:CYS:N	2.54	0.41
1:A:223:PRO:O	1:A:224:GLU:C	2.59	0.41
1:A:622:TYR:HA	1:A:629:PRO:HA	2.03	0.40
1:A:416:LYS:HB2	1:A:417:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	749/871 (86%)	686 (92%)	53 (7%)	10 (1%)	12 30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLU
1	A	83	TYR
1	A	437	ASN
1	A	651	SER
1	A	758	GLU
1	A	777	ASP
1	A	296	PRO
1	A	859	TYR
1	A	228	ILE
1	A	737	PRO

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	604/787 (77%)	580 (96%)	24 (4%)	31 60

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	CYS
1	A	86	CYS
1	A	112	ARG
1	A	170	SER
1	A	171	VAL
1	A	193	ARG
1	A	194	SER
1	A	273	THR
1	A	282	HIS
1	A	302	SER
1	A	390	LEU
1	A	453	HIS
1	A	548	VAL
1	A	592	THR
1	A	595	ARG
1	A	613	LEU
1	A	639	GLN
1	A	650	THR
1	A	668	LEU
1	A	755	GLN
1	A	775	CYS
1	A	793	SER
1	A	803	GLU
1	A	814	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	GLN
1	A	524	ASN
1	A	533	HIS
1	A	538	ASN
1	A	639	GLN

### 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](#)

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	B	1	1,2	14,14,15	0.96	1 (7%)	17,19,21	1.49	3 (17%)
2	NAG	B	2	2	14,14,15	0.78	1 (7%)	17,19,21	0.93	0
2	BMA	B	3	2	11,11,12	0.58	0	15,15,17	1.57	1 (6%)
2	MAN	B	4	2	11,11,12	0.92	0	15,15,17	2.34	5 (33%)
2	MAN	B	5	2	11,11,12	0.75	0	15,15,17	1.95	4 (26%)
2	MAN	B	6	2	11,11,12	0.74	0	15,15,17	2.00	4 (26%)

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	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
2	MAN	B	6	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	1	NAG	O5-C1	-2.38	1.39	1.43
2	B	2	NAG	O5-C1	-2.04	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	MAN	C1-C2-C3	5.20	116.06	109.67
2	B	4	MAN	C1-C2-C3	5.17	116.02	109.67
2	B	3	BMA	C1-O5-C5	4.71	118.58	112.19
2	B	5	MAN	C1-O5-C5	4.33	118.06	112.19
2	B	4	MAN	C3-C4-C5	4.14	117.63	110.24
2	B	4	MAN	O5-C1-C2	-3.71	105.04	110.77
2	B	1	NAG	O4-C4-C3	-3.20	102.95	110.35
2	B	6	MAN	C3-C4-C5	3.19	115.92	110.24
2	B	4	MAN	C1-O5-C5	3.03	116.30	112.19
2	B	1	NAG	O5-C1-C2	-2.93	106.66	111.29
2	B	5	MAN	O5-C1-C2	-2.72	106.58	110.77
2	B	6	MAN	C2-C3-C4	2.53	115.27	110.89
2	B	5	MAN	O2-C2-C3	-2.45	105.23	110.14
2	B	6	MAN	O3-C3-C4	-2.36	104.89	110.35
2	B	5	MAN	O5-C5-C4	2.31	116.44	110.83
2	B	1	NAG	C4-C3-C2	-2.17	107.83	111.02
2	B	4	MAN	O6-C6-C5	2.13	118.59	111.29

There are no chirality outliers.

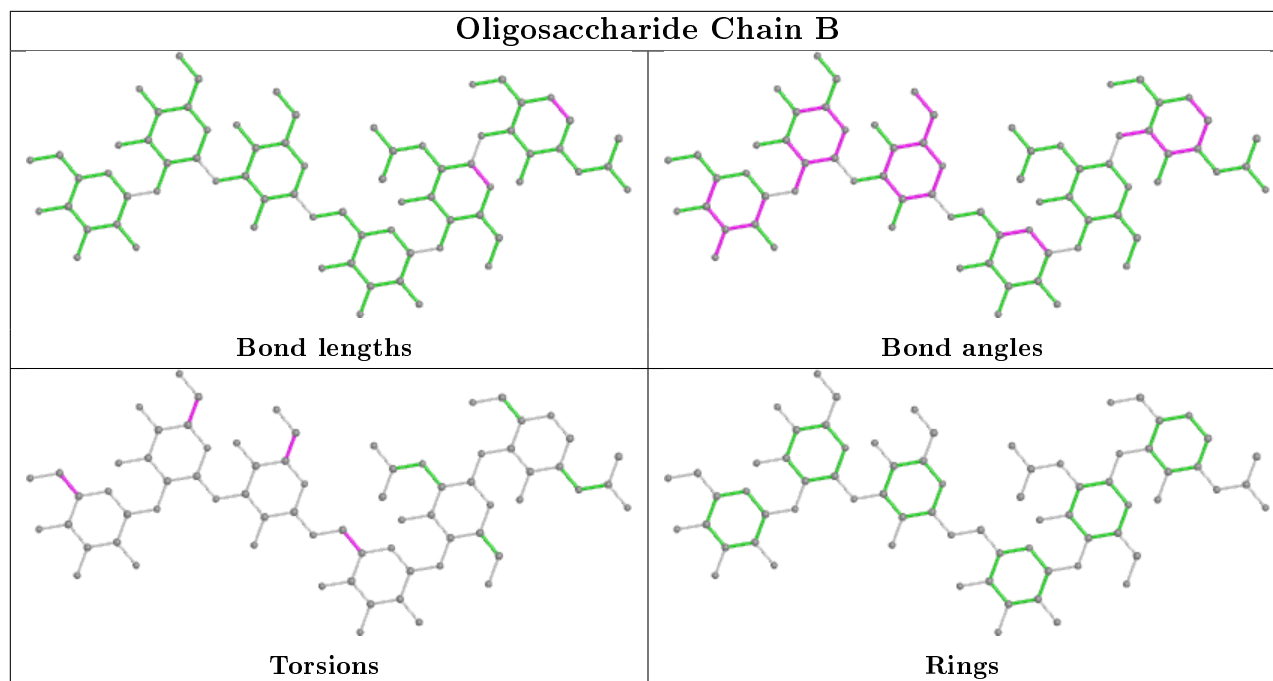
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	6	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 [i](#)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	$\# Z  > 2$
6	SCN	A	910	-	1,2,2	0.60	0	0,1,1	0.00	-
8	PO4	A	912	-	4,4,4	0.73	0	6,6,6	0.74	0
3	7HR	A	907	-	37,44,44	<b>3.81</b>	<b>12 (32%)</b>	45,64,64	<b>2.65</b>	<b>17 (37%)</b>

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	7HR	A	907	-	-	<b>8/22/41/41</b>	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	907	7HR	S32-N29	11.36	1.78	1.63
3	A	907	7HR	C19-C16	-9.69	1.33	1.48
3	A	907	7HR	O33-S32	8.87	1.53	1.43
3	A	907	7HR	O34-S32	7.87	1.52	1.43
3	A	907	7HR	C17-S18	-7.02	1.59	1.70
3	A	907	7HR	C06-C05	-5.35	1.33	1.40
3	A	907	7HR	C35-S32	5.02	1.83	1.78
3	A	907	7HR	C08-C26	-4.33	1.43	1.52
3	A	907	7HR	C11-C03	-3.46	1.35	1.42
3	A	907	7HR	C31-C30	2.46	1.59	1.52
3	A	907	7HR	C09-N10	2.14	1.40	1.36
3	A	907	7HR	C11-N12	-2.10	1.34	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	907	7HR	O34-S32-O33	-10.00	108.72	118.98
3	A	907	7HR	C27-C28-N29	-7.12	99.73	109.43
3	A	907	7HR	C17-C16-C19	-5.37	121.97	129.44
3	A	907	7HR	C16-C17-S18	-4.48	106.29	111.79
3	A	907	7HR	C28-N29-S32	-4.38	110.37	118.61
3	A	907	7HR	C28-C27-C26	-3.62	106.76	111.04
3	A	907	7HR	C01-C02-C03	-2.91	107.71	114.88
3	A	907	7HR	O34-S32-N29	2.84	109.63	107.23
3	A	907	7HR	C36-C35-S32	-2.44	104.72	114.23
3	A	907	7HR	C35-S32-N29	2.34	112.22	105.80
3	A	907	7HR	C39-N38-C37	-2.27	101.75	110.74
3	A	907	7HR	C40-N38-C39	2.24	115.52	109.73
3	A	907	7HR	C37-C36-C35	-2.23	105.35	113.14
3	A	907	7HR	C19-C16-N15	2.10	124.31	120.78
3	A	907	7HR	C24-C22-C21	-2.07	120.08	122.83
3	A	907	7HR	C40-N38-C37	-2.06	102.56	110.74
3	A	907	7HR	C20-C21-C22	2.01	120.44	118.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	907	7HR	C28-N29-S32-C35
3	A	907	7HR	C28-N29-S32-O34
3	A	907	7HR	C30-N29-S32-O34
3	A	907	7HR	C28-N29-S32-O33

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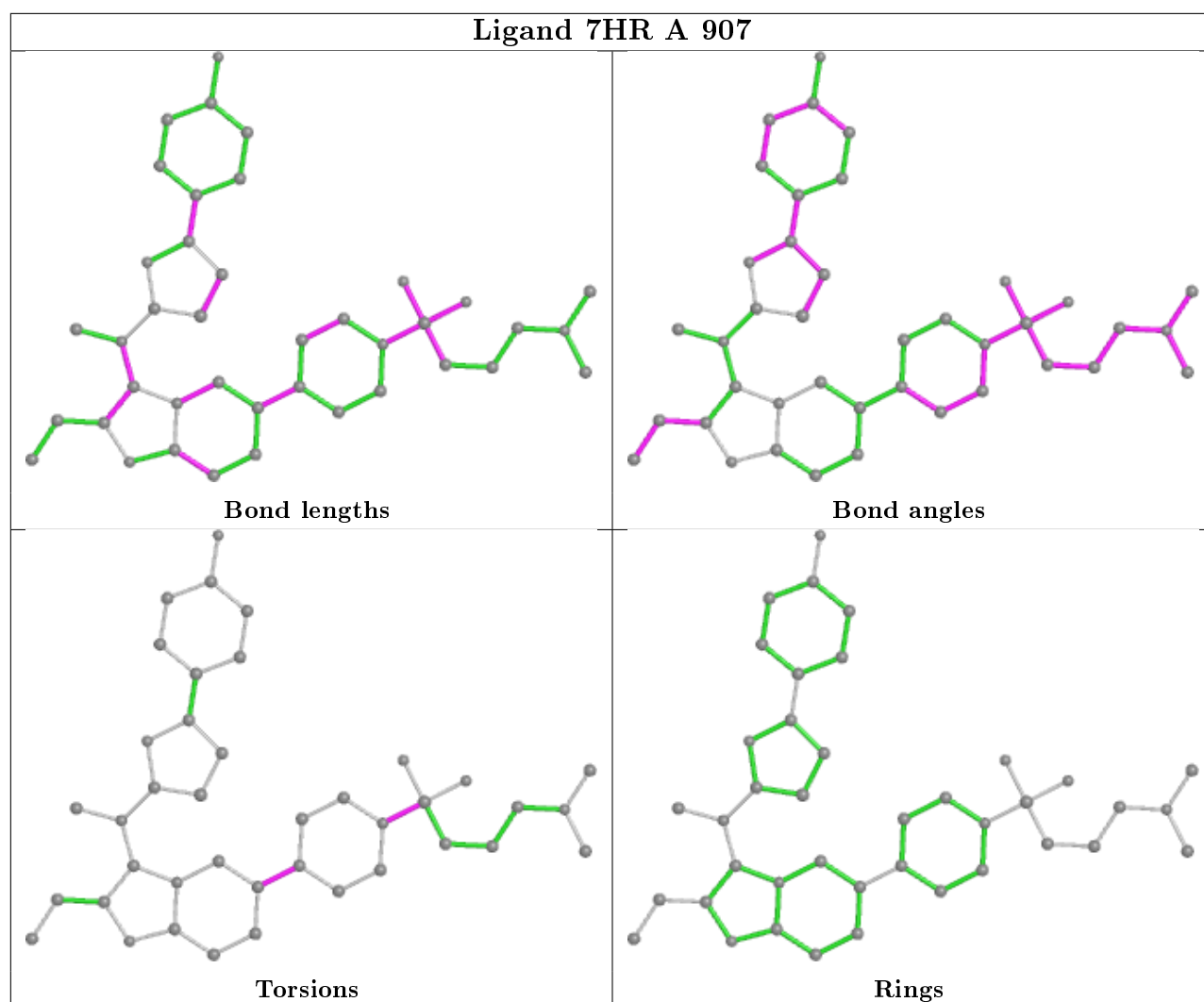
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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
3	A	907	7HR	C30-N29-S32-O33
3	A	907	7HR	C09-C08-C26-C27
3	A	907	7HR	C30-N29-S32-C35
3	A	907	7HR	C07-C08-C26-C27

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	759/871 (87%)	0.22	13 (1%) 70 72	9, 24, 54, 74	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	650	THR	4.2
1	A	569	CYS	3.3
1	A	539	THR	3.0
1	A	183	SER	2.9
1	A	279	VAL	2.6
1	A	567	CYS	2.6
1	A	367	CYS	2.6
1	A	566	GLY	2.4
1	A	182	GLY	2.4
1	A	111	VAL	2.3
1	A	393	ILE	2.1
1	A	108	CYS	2.0
1	A	469	CYS	2.0

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

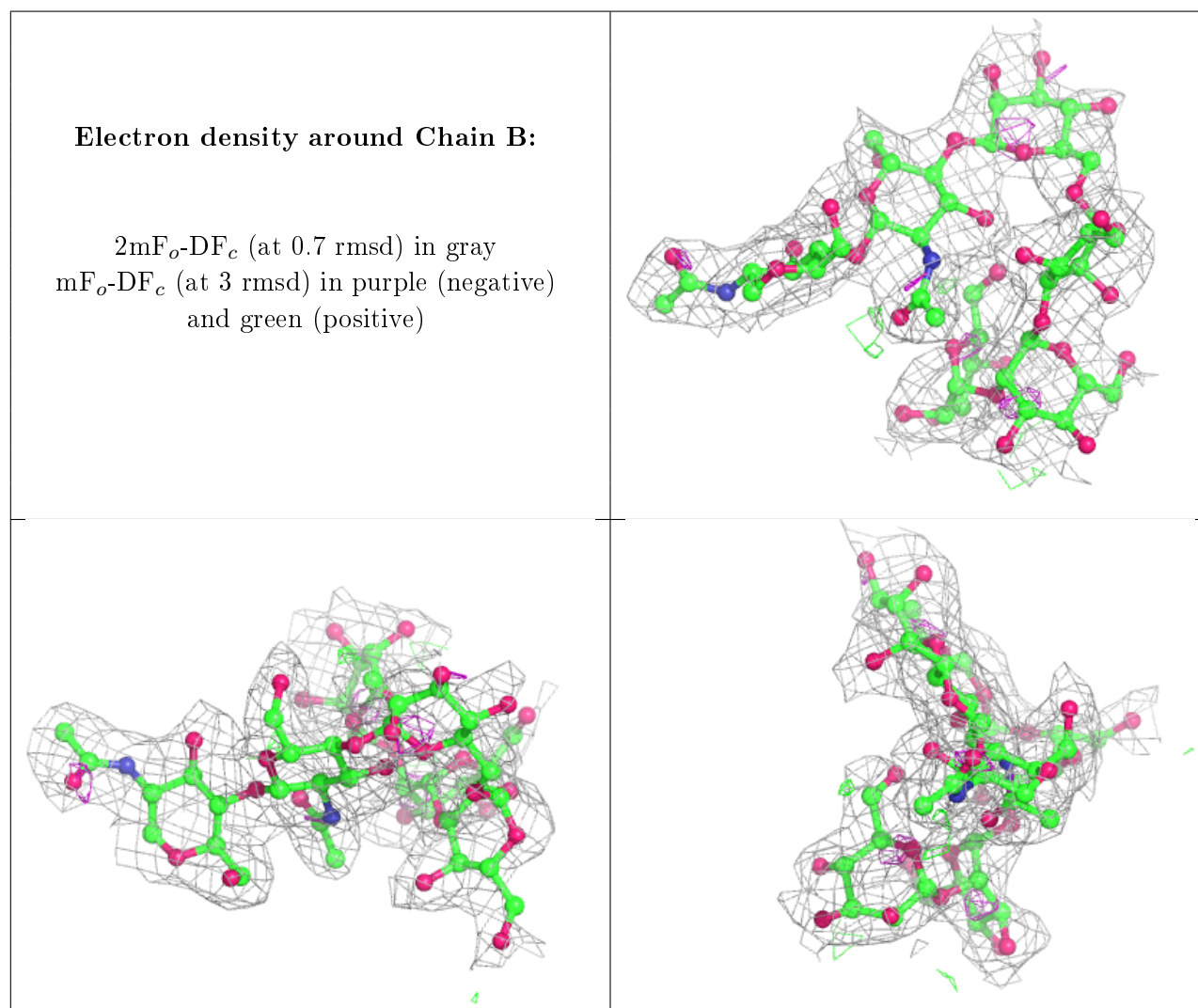
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	BMA	B	3	11/12	0.79	0.23	36,38,42,44	0
2	MAN	B	4	11/12	0.80	0.26	35,38,39,40	0
2	MAN	B	6	11/12	0.84	0.27	36,38,42,42	0
2	MAN	B	5	11/12	0.91	0.29	40,43,48,49	0
2	NAG	B	2	14/15	0.94	0.16	23,26,29,34	0
2	NAG	B	1	14/15	0.94	0.17	14,16,17,20	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.

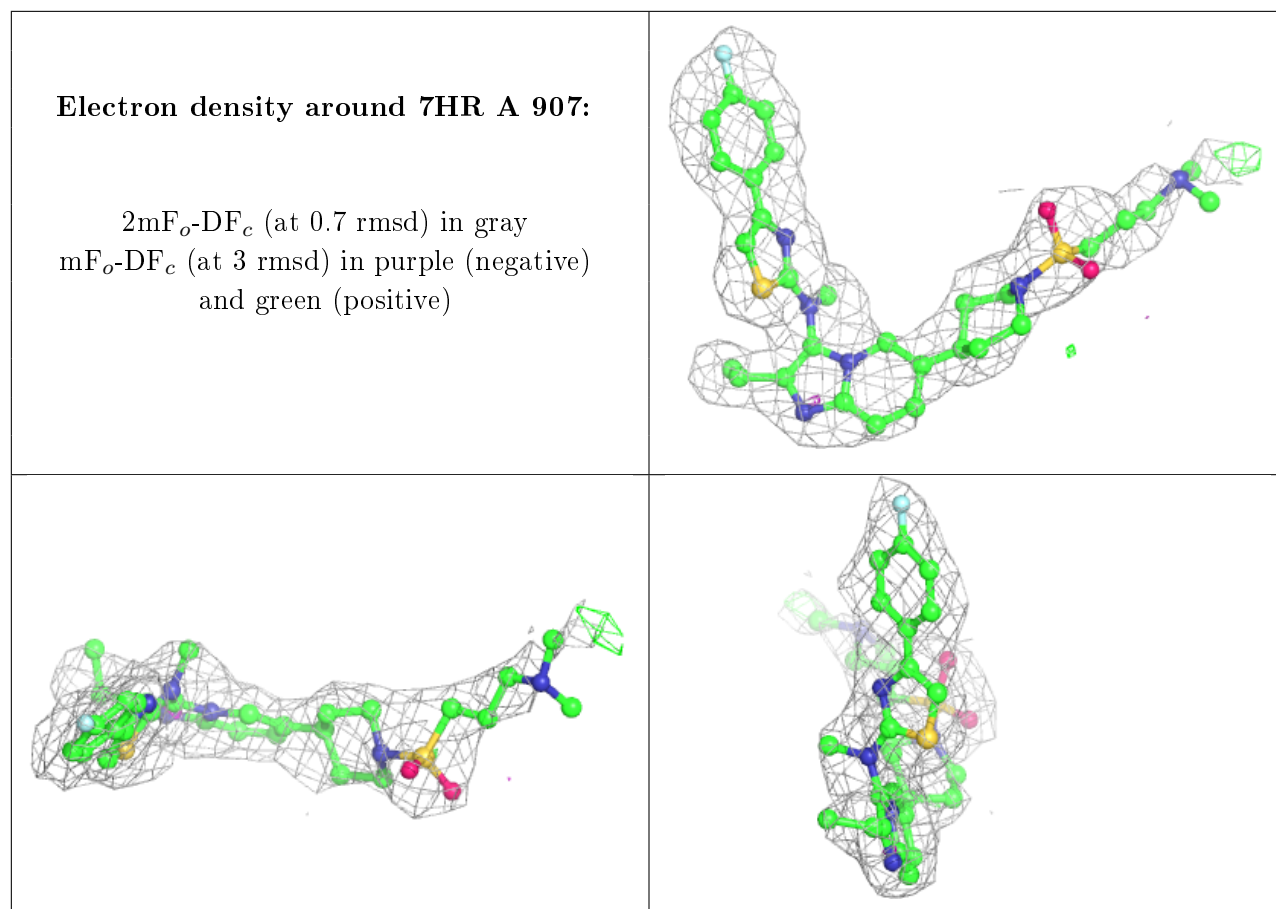


## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	PO4	A	912	5/5	0.79	0.25	66,69,69,72	0
6	SCN	A	910	3/3	0.87	0.15	30,30,33,35	0
7	NI	A	911	1/1	0.87	0.10	66,66,66,66	0
7	NI	A	922	1/1	0.88	0.09	66,66,66,66	0
5	CL	A	913	1/1	0.90	0.10	29,29,29,29	0
3	7HR	A	907	40/40	0.92	0.20	28,37,64,68	0
7	NI	A	919	1/1	0.95	0.10	53,53,53,53	0
5	CL	A	909	1/1	0.97	0.19	24,24,24,24	0
7	NI	A	924	1/1	0.97	0.06	58,58,58,58	0
10	ZN	A	916	1/1	0.98	0.06	28,28,28,28	0
9	K	A	914	1/1	0.98	0.12	51,51,51,51	0
7	NI	A	923	1/1	0.99	0.09	40,40,40,40	0
4	IOD	A	908	1/1	0.99	0.08	36,36,36,36	0
10	ZN	A	918	1/1	0.99	0.06	33,33,33,33	0
7	NI	A	920	1/1	0.99	0.08	37,37,37,37	0
10	ZN	A	915	1/1	0.99	0.11	20,20,20,20	0
10	ZN	A	917	1/1	0.99	0.06	46,46,46,46	0
7	NI	A	921	1/1	0.99	0.09	27,27,27,27	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.