



## Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2024 – 10:53 PM EST

PDB ID : 7G3A  
Title : Crystal Structure of rat Autotaxin in complex with 5-tert-butyl-2-methyl-4-[(5-oxo-4-propan-2-yl-1H-1,2,4-triazol-3-yl)methoxy]benzotrile, i.e. SMILES C(C1=NNC(=O)N1C(C)C)Oc1cc(c(cc1C(C)(C)C)C#N)C with IC50=0.0371228 microM  
Authors : Stihle, M.; Benz, J.; Hunziker, D.; Richter, H.; Rudolph, M.G.  
Deposited on : 2023-06-05  
Resolution : 1.79 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.

The types of validation reports are described at

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

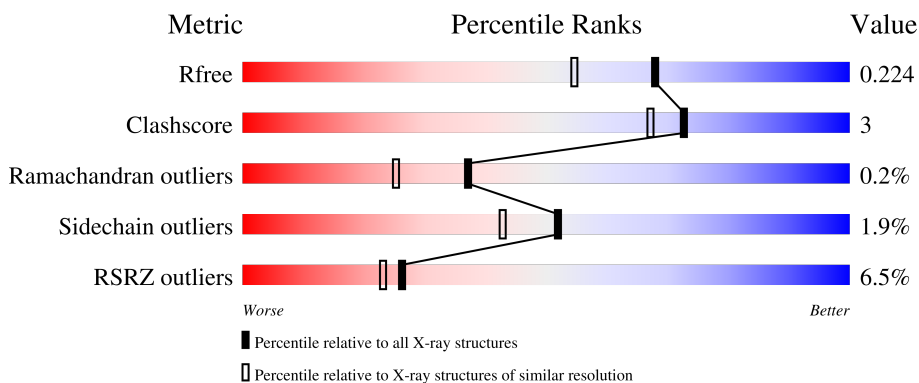
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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  $\geq 3$ , 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	846	 6% 86% 8% 5%
2	B	8	 100%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7232 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 Isoform 2 of Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	806	6601	4195	1133	1222	51	0	16	0

There are 14 discrepancies between the modelled and reference sequences:

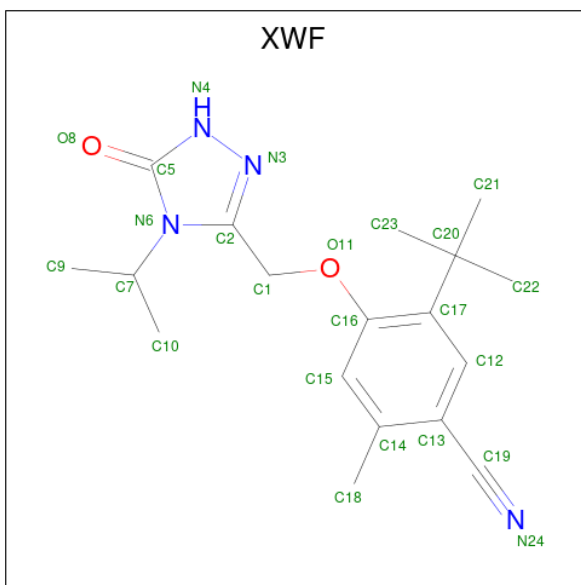
Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ALA	ASN	engineered mutation	UNP Q64610
A	410	ALA	ASN	engineered mutation	UNP Q64610
A	591	THR	ARG	engineered mutation	UNP Q64610
A	863	GLY	-	expression tag	UNP Q64610
A	864	GLY	-	expression tag	UNP Q64610
A	865	ARG	-	expression tag	UNP Q64610
A	866	HIS	-	expression tag	UNP Q64610
A	867	HIS	-	expression tag	UNP Q64610
A	868	HIS	-	expression tag	UNP Q64610
A	869	HIS	-	expression tag	UNP Q64610
A	870	HIS	-	expression tag	UNP Q64610
A	871	HIS	-	expression tag	UNP Q64610
A	872	HIS	-	expression tag	UNP Q64610
A	873	HIS	-	expression tag	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-(1-2)-alpha-D-mannopyranose-(1-3)]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	8	94	52	2	40	0	0	0

- Molecule 3 is 5-tert-butyl-2-methyl-4-[[5-oxo-4-(propan-2-yl)-4,5-dihydro-1H-1,2,4-triazol-3-yl]methoxy]benzotrile (three-letter code: XWF) (formula: C<sub>18</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	24	18	4	2	0	0

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	498	Total O 498 498	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.86Å 91.83Å 119.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.91 – 1.79 45.91 – 1.79	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.91-1.79) 95.6 (45.91-1.79)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.188 , 0.226 0.186 , 0.224	Depositor DCC
$R_{free}$ test set	4447 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: XWF, MAN, ZN, CA, BMA, NAG, NA, SO4

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	0.75	1/6835 (0.0%)	0.81	6/9262 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	GLU	CD-OE1	5.48	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	653	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	174	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	393	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	743	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	798	ARG	NE-CZ-NH2	-5.06	117.77	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	6601	0	6402	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	94	0	79	0	0
3	A	24	0	0	0	0
4	A	2	0	0	0	0
5	A	10	0	0	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	498	0	0	4	0
All	All	7232	0	6481	41	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 (41) 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:70:PRO:HB2	1:A:71:PRO:HD3	1.31	1.05
1:A:806[B]:ASN:OD1	8:A:1001:HOH:O	1.97	0.81
1:A:70:PRO:HB2	1:A:71:PRO:CD	2.12	0.79
1:A:539:PHE:O	1:A:541:PRO:HD3	1.84	0.77
1:A:70:PRO:CB	1:A:71:PRO:HD3	2.16	0.70
1:A:163:PRO:HB3	1:A:350:CYS:O	1.95	0.67
1:A:69:GLY:H	1:A:70:PRO:HD3	1.61	0.65
1:A:69:GLY:N	1:A:70:PRO:HD3	2.11	0.65
1:A:623:GLU:OE1	8:A:1002:HOH:O	2.18	0.55
1:A:550:PRO:HB2	1:A:611:ILE:HG12	1.89	0.54
1:A:69:GLY:N	1:A:70:PRO:CD	2.73	0.51
1:A:737:ILE:HB	1:A:766:HIS:HB2	1.93	0.51
1:A:580:GLU:HB3	1:A:584:ARG:HH21	1.76	0.51
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.94	0.50
1:A:594:ARG:NH2	8:A:1010:HOH:O	2.43	0.50
1:A:200:TYR:CE2	1:A:862:ILE:HG13	2.48	0.48
1:A:200:TYR:CD2	1:A:862:ILE:HG13	2.49	0.47
1:A:449:ARG:O	1:A:450[A]:ARG:HB2	2.14	0.47
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.49	0.47
1:A:216[A]:LEU:HD23	1:A:505:ASN:HB2	1.97	0.46
1:A:98:ARG:HG3	1:A:115:ASN:OD1	2.15	0.46
1:A:458:LEU:HA	1:A:461[A]:TYR:CZ	2.51	0.45
1:A:169:SER:HA	1:A:356:VAL:O	2.17	0.44
1:A:535:ARG:HG2	1:A:536:THR:HG23	1.99	0.44
1:A:74:ARG:NH2	1:A:78:LEU:HB2	2.33	0.44
1:A:109:GLU:O	1:A:120:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ARG:NH2	8:A:1003:HOH:O	2.27	0.43
1:A:821:MET:HA	1:A:821:MET:HE2	2.00	0.43
1:A:403:ASP:HA	1:A:404:PRO:HD2	1.91	0.43
1:A:310:PRO:HD3	1:A:331:ILE:CD1	2.49	0.42
1:A:621:TYR:HA	1:A:628:PRO:HA	2.02	0.42
1:A:458:LEU:HA	1:A:461[A]:TYR:CE2	2.55	0.41
1:A:414:LYS:HD3	1:A:414:LYS:HA	1.75	0.41
1:A:580:GLU:O	1:A:583:LYS:HG2	2.20	0.41
1:A:458:LEU:C	1:A:458:LEU:HD12	2.41	0.41
1:A:721[A]:LYS:HA	1:A:721[A]:LYS:HD2	1.89	0.41
1:A:673:LYS:HD3	1:A:673:LYS:HA	1.88	0.41
1:A:362:GLU:O	1:A:472:GLY:HA2	2.21	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.93	0.40
1:A:268:VAL:HG13	1:A:301:SER:HB2	2.03	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	817/846 (97%)	783 (96%)	32 (4%)	2 (0%)	44 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	71	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	746/765 (98%)	731 (98%)	15 (2%)	50 40

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	183	LYS
1	A	379	VAL
1	A	389	LEU
1	A	397	ILE
1	A	401	LYS
1	A	417	ASP
1	A	456	LYS
1	A	462	LYS
1	A	571	LYS
1	A	582	ASN
1	A	689	PRO
1	A	721[A]	LYS
1	A	721[B]	LYS
1	A	862	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	582	ASN
1	A	586	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](#)

8 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	0.66	0	17,19,21	1.51	3 (17%)
2	NAG	B	2	2	14,14,15	0.86	0	17,19,21	1.47	2 (11%)
2	BMA	B	3	2	11,11,12	0.80	0	15,15,17	1.75	3 (20%)
2	MAN	B	4	2	11,11,12	0.92	0	15,15,17	1.63	3 (20%)
2	MAN	B	5	2	11,11,12	0.84	0	15,15,17	1.14	1 (6%)
2	MAN	B	6	2	11,11,12	0.80	0	15,15,17	1.48	2 (13%)
2	MAN	B	7	2	11,11,12	0.85	0	15,15,17	2.05	4 (26%)
2	MAN	B	8	2	11,11,12	0.91	1 (9%)	15,15,17	1.10	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	-	1/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	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
2	MAN	B	8	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	MAN	C2-C3	2.26	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-O5-C5	4.74	118.54	112.19
2	B	4	MAN	C1-O5-C5	4.47	118.18	112.19
2	B	7	MAN	C1-C2-C3	4.38	116.02	109.64
2	B	2	NAG	C1-O5-C5	4.27	117.91	112.19
2	B	6	MAN	C1-O5-C5	4.18	117.78	112.19
2	B	7	MAN	C2-C3-C4	3.77	117.49	110.86
2	B	1	NAG	O5-C5-C6	3.48	114.44	107.66
2	B	8	MAN	O3-C3-C2	3.10	116.38	110.05
2	B	1	NAG	O5-C1-C2	-3.09	106.52	111.29
2	B	3	BMA	C1-C2-C3	2.96	113.96	109.64
2	B	7	MAN	C3-C4-C5	2.82	115.34	110.23
2	B	4	MAN	O3-C3-C2	2.72	115.61	110.05
2	B	2	NAG	O7-C7-C8	-2.57	117.48	122.05
2	B	6	MAN	C2-C3-C4	2.46	115.18	110.86
2	B	7	MAN	O3-C3-C4	-2.38	104.77	110.38
2	B	3	BMA	O6-C6-C5	-2.25	103.66	111.33
2	B	5	MAN	C3-C4-C5	2.18	114.19	110.23
2	B	4	MAN	O5-C5-C6	2.17	111.89	107.66
2	B	1	NAG	O4-C4-C5	-2.04	104.31	109.32

There are no chirality outliers.

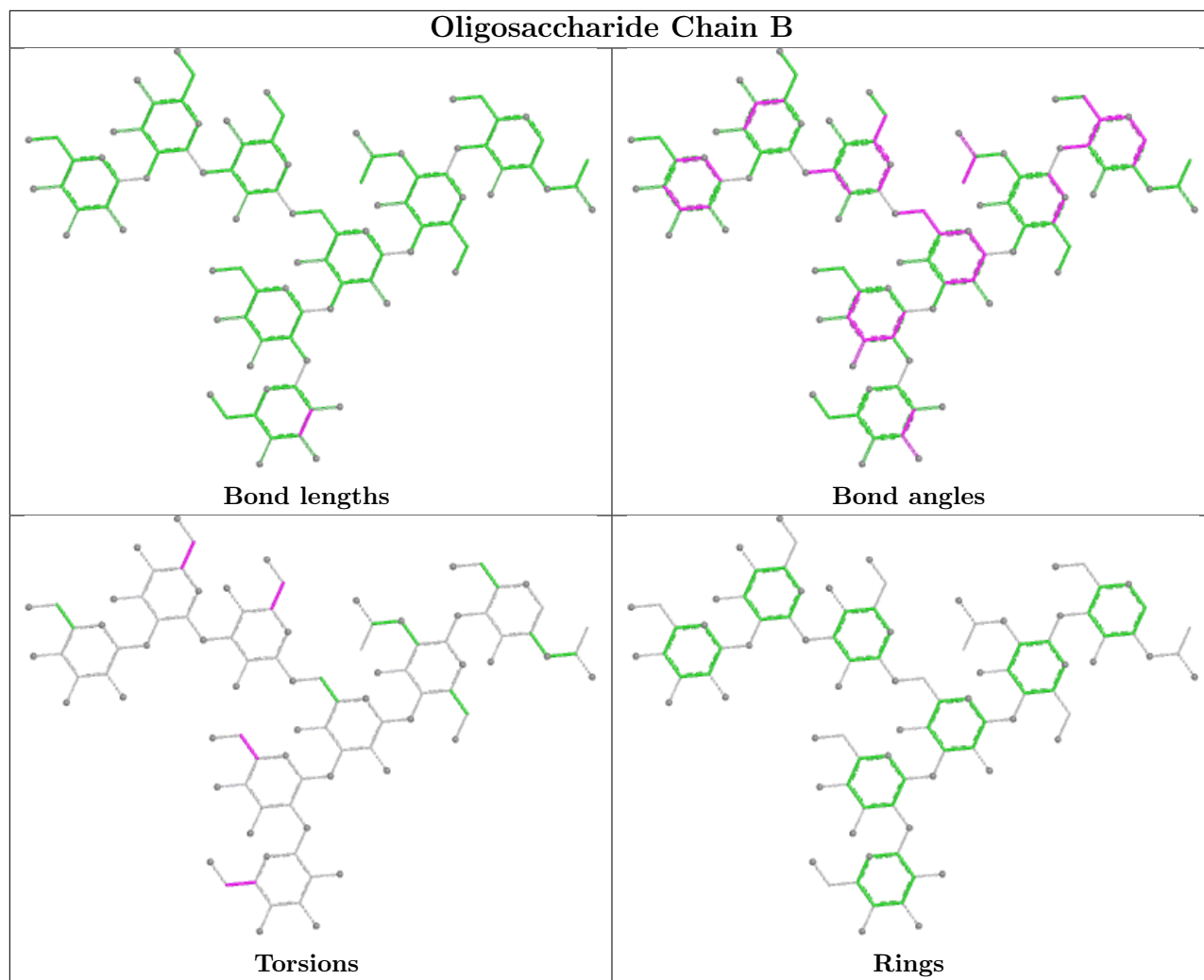
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	MAN	O5-C5-C6-O6
2	B	7	MAN	C4-C5-C6-O6
2	B	5	MAN	C4-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	8	MAN	C4-C5-C6-O6
2	B	4	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 8 ligands modelled in this entry, 5 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
5	SO4	A	904	-	4,4,4	0.60	0	6,6,6	0.53	0
3	XWF	A	901	-	25,25,25	1.89	6 (24%)	36,37,37	1.21	4 (11%)
5	SO4	A	903	-	4,4,4	0.59	0	6,6,6	0.42	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
3	XWF	A	901	-	-	0/17/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	XWF	C2-N6	5.01	1.45	1.37
3	A	901	XWF	C5-N4	4.01	1.39	1.35
3	A	901	XWF	C1-C2	3.19	1.53	1.49
3	A	901	XWF	C2-N3	3.03	1.33	1.30
3	A	901	XWF	C16-C17	2.78	1.45	1.39
3	A	901	XWF	C15-C16	2.35	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	XWF	O11-C1-C2	2.55	116.46	109.21
3	A	901	XWF	C1-C2-N6	2.55	126.27	123.32
3	A	901	XWF	O8-C5-N6	2.30	129.12	126.00
3	A	901	XWF	C12-C17-C16	-2.03	113.92	116.80

There are no chirality outliers.

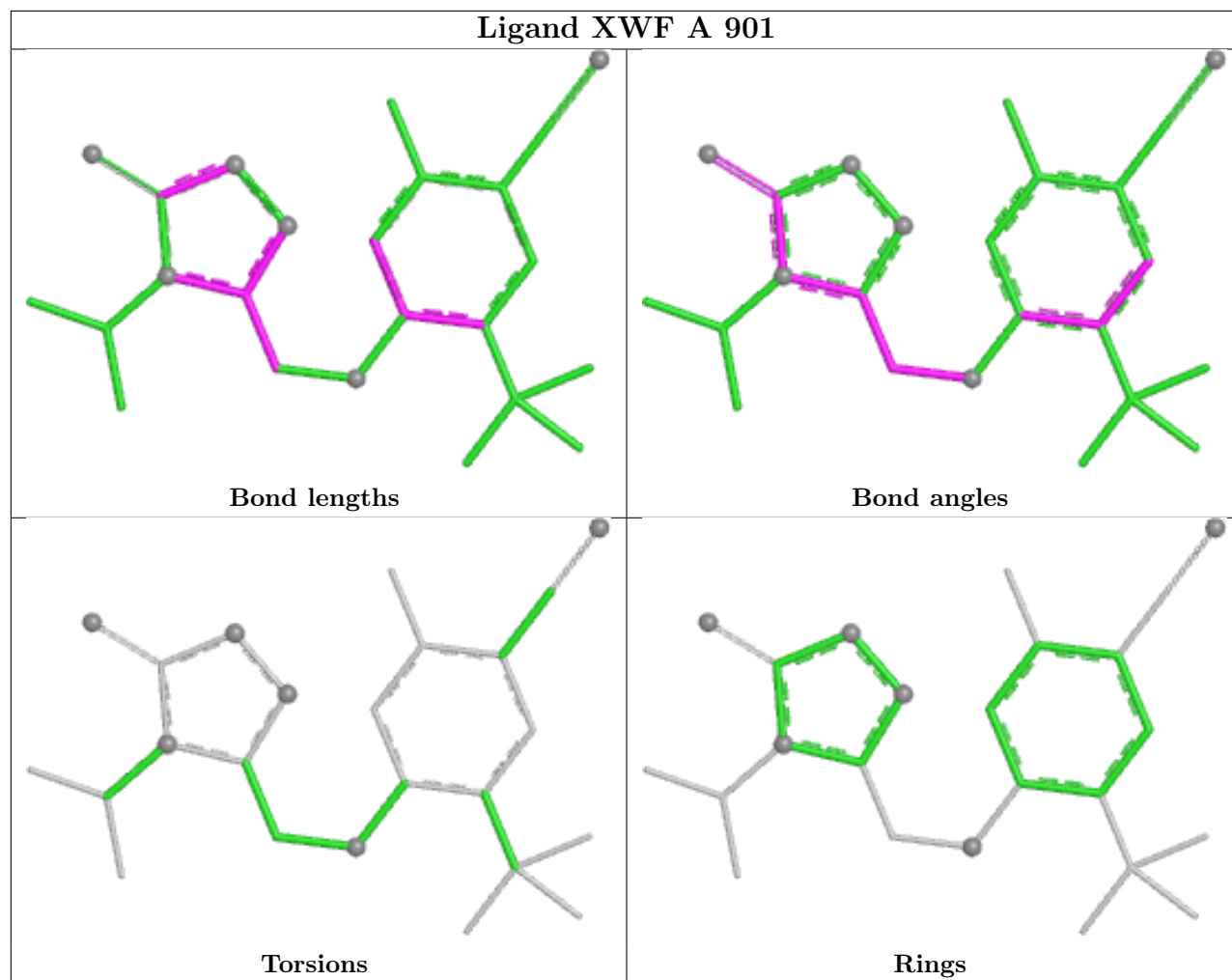
There are no torsion outliers.

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 [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	806/846 (95%)	0.09	52 (6%) <span style="border: 1px solid red; padding: 2px;">26</span> <span style="border: 1px solid red; padding: 2px;">23</span>	11, 24, 57, 80	16 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	LEU	6.9
1	A	469	PHE	6.4
1	A	51	TRP	6.3
1	A	862	ILE	6.2
1	A	70	PRO	6.2
1	A	468	CYS	6.2
1	A	572	VAL	4.9
1	A	68	VAL	4.7
1	A	581	LEU	4.4
1	A	53	ALA	4.2
1	A	71	PRO	4.0
1	A	54	THR	3.8
1	A	462	LYS	3.8
1	A	52	THR	3.6
1	A	397	ILE	3.5
1	A	55	SER	3.5
1	A	861	GLU	3.4
1	A	69	GLY	3.4
1	A	366	CYS	3.3
1	A	461[A]	TYR	3.3
1	A	573	GLU	3.2
1	A	463	LYS	3.2
1	A	243	LEU	3.0
1	A	82	TYR	2.9
1	A	585	LEU	2.8
1	A	56	GLY	2.8
1	A	72	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	576	ASN	2.7
1	A	246	ARG	2.7
1	A	237	PHE	2.7
1	A	242	HIS	2.6
1	A	577	LYS	2.5
1	A	579	GLU	2.5
1	A	81	SER	2.5
1	A	538	THR	2.4
1	A	59	LYS	2.4
1	A	378	ASN	2.3
1	A	580	GLU	2.3
1	A	346	ARG	2.3
1	A	860	SER	2.3
1	A	161	VAL	2.3
1	A	249	PHE	2.2
1	A	571	LYS	2.2
1	A	582	ASN	2.2
1	A	539	PHE	2.2
1	A	402	TYR	2.1
1	A	78	LEU	2.1
1	A	584	ARG	2.1
1	A	77	ASN	2.1
1	A	379	VAL	2.1
1	A	566	CYS	2.1
1	A	594	ARG	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.

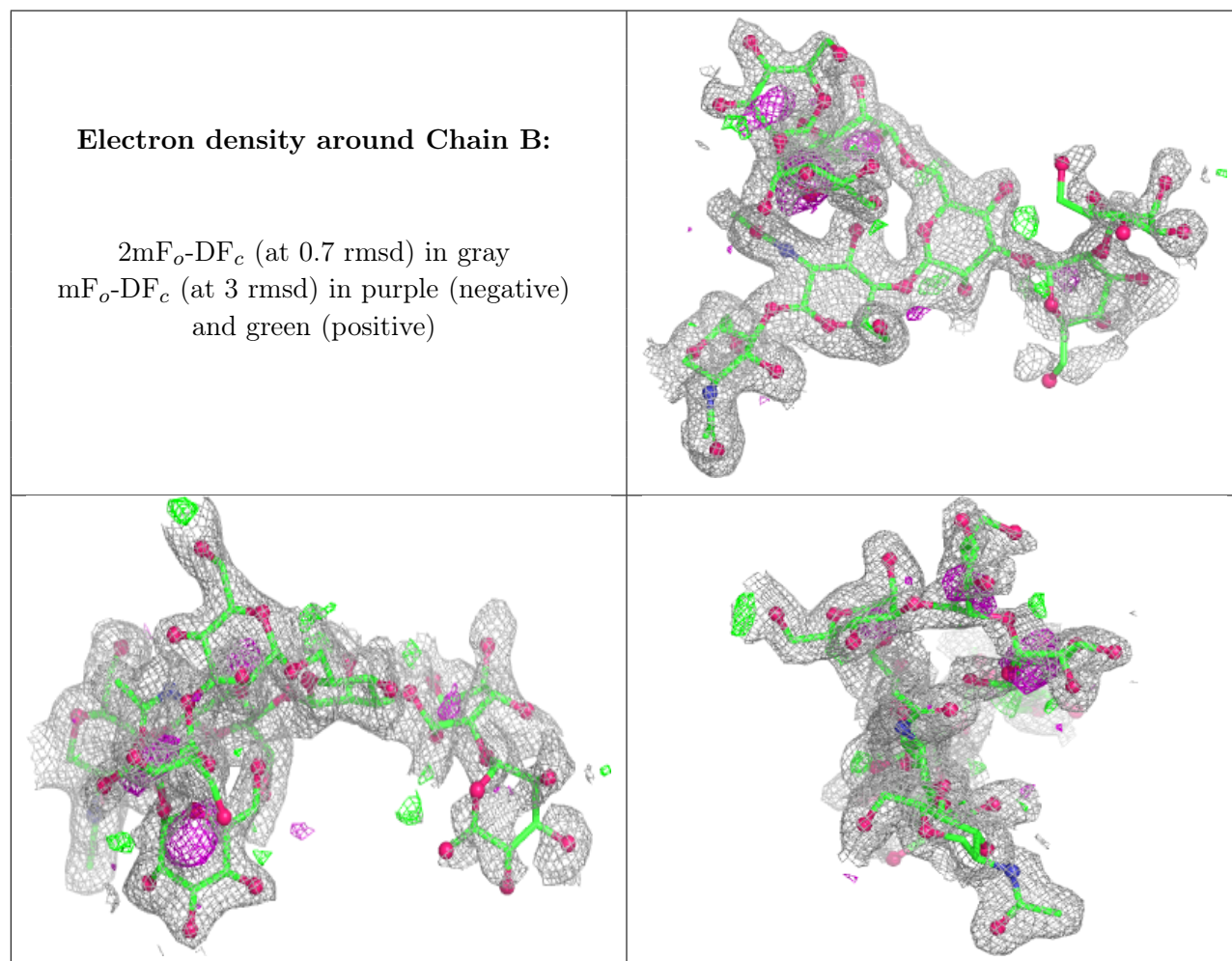
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	B	7	11/12	0.44	0.18	76,80,80,80	0
2	BMA	B	3	11/12	0.58	0.16	59,63,70,75	0
2	MAN	B	4	11/12	0.64	0.14	56,60,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	B	8	11/12	0.65	0.18	49,76,80,80	0
2	MAN	B	5	11/12	0.76	0.15	52,58,63,65	0
2	MAN	B	6	11/12	0.80	0.16	40,55,60,65	0
2	NAG	B	2	14/15	0.87	0.10	29,32,41,56	0
2	NAG	B	1	14/15	0.97	0.05	16,18,20,24	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.

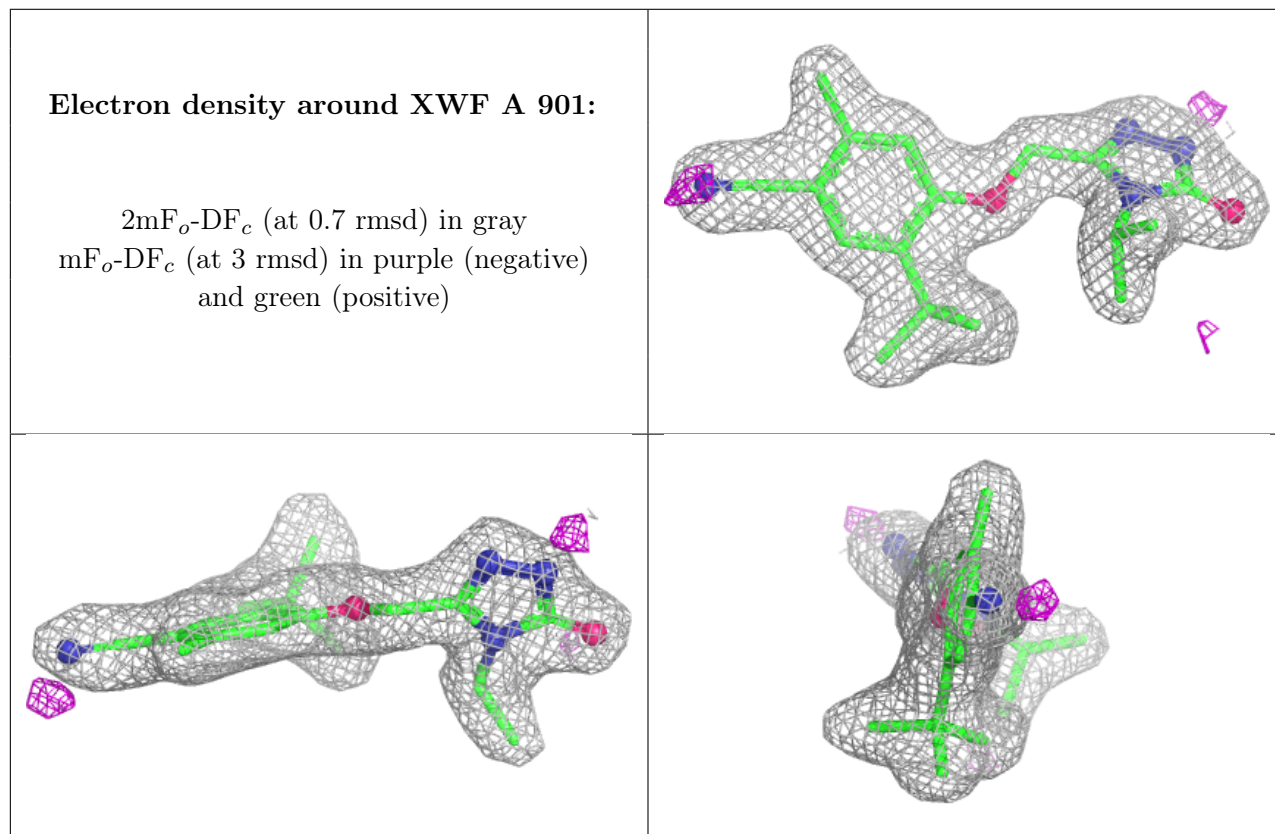


## 6.4 Ligands [i](#)

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
5	SO4	A	904	5/5	0.84	0.12	54,57,59,61	0
5	SO4	A	903	5/5	0.89	0.13	38,40,48,57	0
3	XWF	A	901	24/24	0.93	0.08	22,27,30,31	0
7	NA	A	908	1/1	0.94	0.07	29,29,29,29	0
7	NA	A	906	1/1	0.95	0.06	30,30,30,30	0
4	CA	A	902	1/1	0.99	0.03	26,26,26,26	0
4	CA	A	907	1/1	0.99	0.02	18,18,18,18	0
6	ZN	A	905	1/1	1.00	0.01	21,21,21,21	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.