



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 24, 2017 – 11:02 PM EST

PDB ID : 5OLB  
Title : crystal structure of autotaxin in complex with PF-8380  
Authors : Hoerer, S.; Lammens, A.  
Deposited on : 2017-07-27  
Resolution : 1.82 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

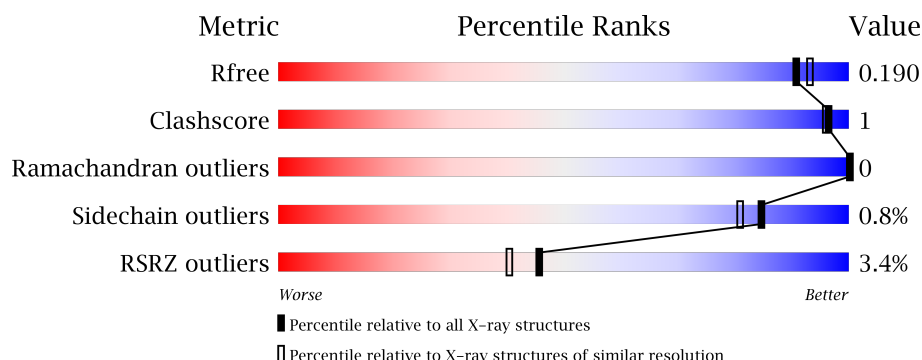
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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))
$R_{free}$	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	844	<div> <div>3%</div> <div>89%</div> <div>7%</div> </div>

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
5	MAN	A	913	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7550 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.

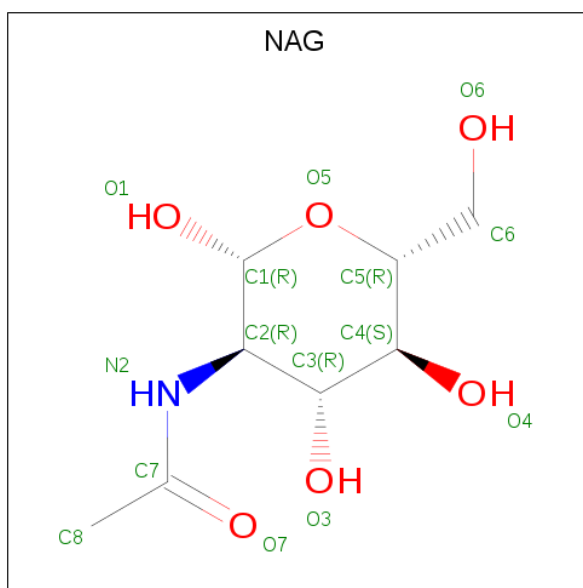
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	785	Total	C	N	O	S	86	21	0
			6520	4128	1132	1209	51			

There are 25 discrepancies between the modelled and reference sequences:

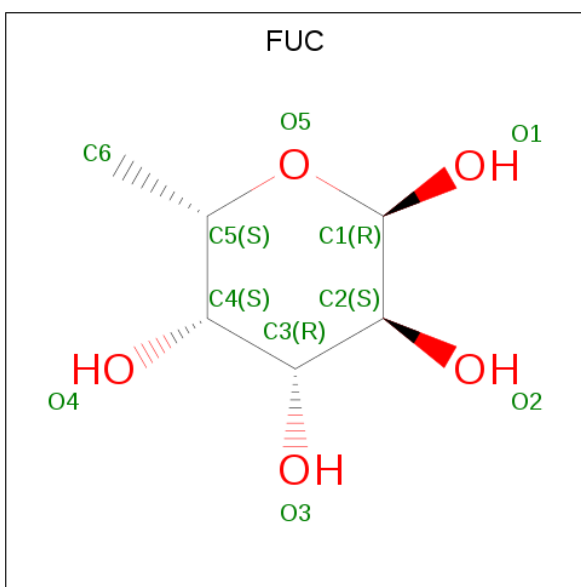
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	-	expression tag	UNP Q9R1E6
A	33	PRO	-	expression tag	UNP Q9R1E6
A	34	SER	-	expression tag	UNP Q9R1E6
A	35	MET	-	expression tag	UNP Q9R1E6
A	?	-	LYS	deletion	UNP Q9R1E6
A	?	-	VAL	deletion	UNP Q9R1E6
A	?	-	GLU	deletion	UNP Q9R1E6
A	?	-	PRO	deletion	UNP Q9R1E6
A	859	SER	-	expression tag	UNP Q9R1E6
A	860	ARG	-	expression tag	UNP Q9R1E6
A	861	GLU	-	expression tag	UNP Q9R1E6
A	862	ASN	-	expression tag	UNP Q9R1E6
A	863	LEU	-	expression tag	UNP Q9R1E6
A	864	TYR	-	expression tag	UNP Q9R1E6
A	865	PHE	-	expression tag	UNP Q9R1E6
A	866	GLN	-	expression tag	UNP Q9R1E6
A	867	GLY	-	expression tag	UNP Q9R1E6
A	868	HIS	-	expression tag	UNP Q9R1E6
A	869	HIS	-	expression tag	UNP Q9R1E6
A	870	HIS	-	expression tag	UNP Q9R1E6
A	871	HIS	-	expression tag	UNP Q9R1E6
A	872	HIS	-	expression tag	UNP Q9R1E6
A	873	HIS	-	expression tag	UNP Q9R1E6
A	874	HIS	-	expression tag	UNP Q9R1E6
A	875	HIS	-	expression tag	UNP Q9R1E6

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



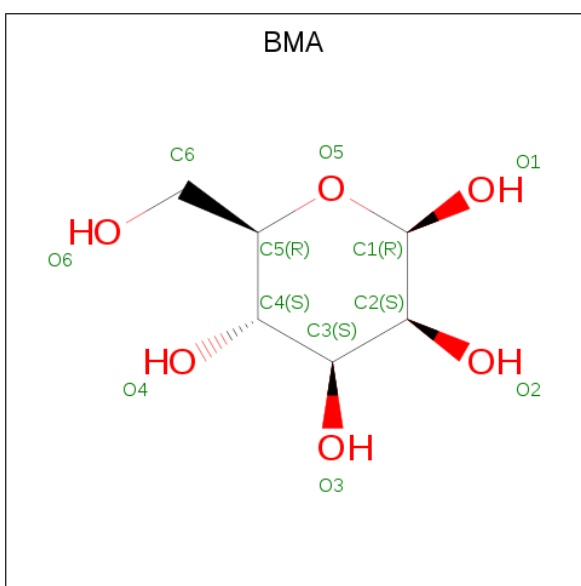
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



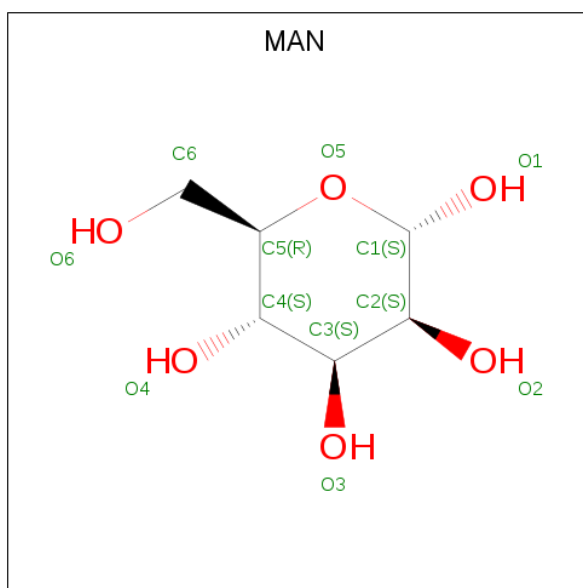
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

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

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

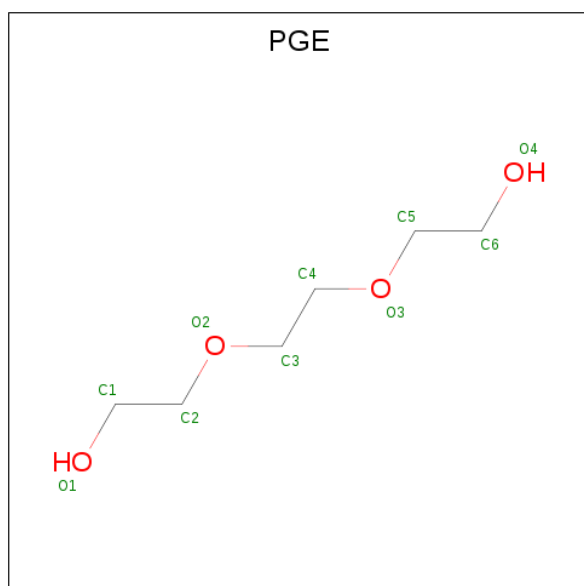
- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

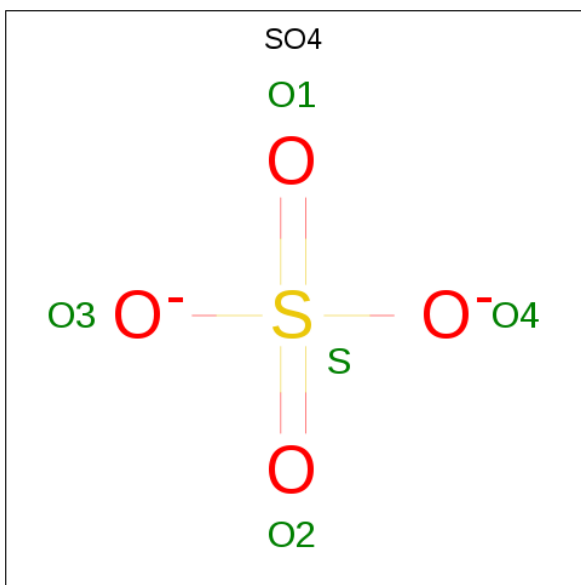
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



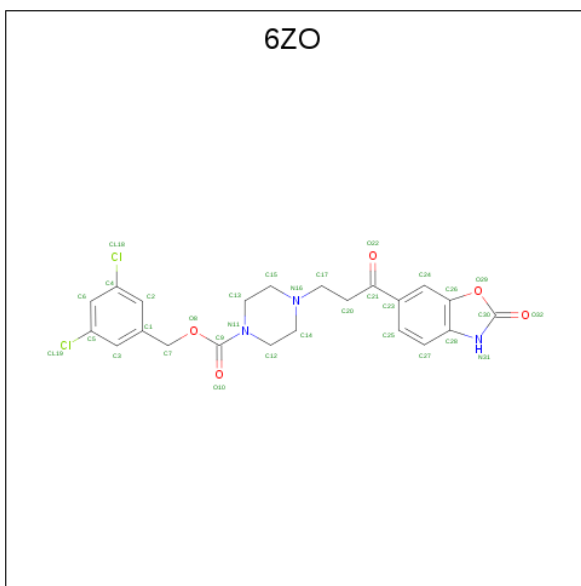
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 10 6 4	0	0

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 13 is (3,5-dichlorophenyl)methyl 4-[3-oxo-3-(2-oxo-2,3-dihydro-1,3-benzoxazol-6-yl)propyl]piperazine-1-carboxylate (three-letter code: 6ZO) (formula: C<sub>22</sub>H<sub>21</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Cl	N	O	0	0
			32	22	2	3	5		

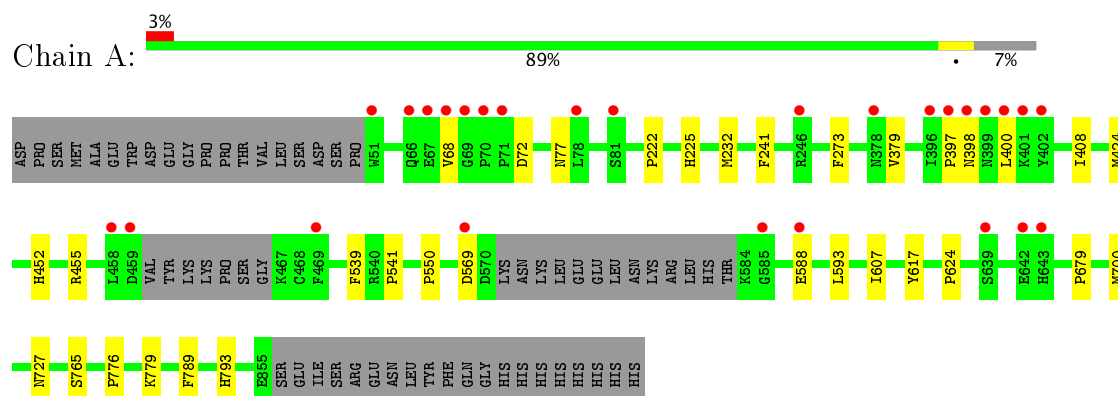
- Molecule 14 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	805	Total 805	O 805	0	0



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.73 Å   100.05 Å   78.78 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	26.65 – 1.82 26.46 – 1.82	Depositor EDS
% Data completeness (in resolution range)	95.2 (26.65-1.82) 95.2 (26.46-1.82)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.82 Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.172   ,   0.191 0.176   ,   0.190	Depositor DCC
$R_{free}$ test set	1690 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, BMA, 6ZO, NAG, CL, NA, K, PGE, FUC, CA, 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	0.42	0/6703	0.59	0/9091

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	6520	0	6249	15	0
2	A	84	0	71	0	0
3	A	20	0	20	0	0
4	A	22	0	18	0	0
5	A	44	0	38	0	0
6	A	2	0	0	0	0
7	A	2	0	0	0	0
8	A	2	0	0	0	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
11	A	10	0	14	1	0
12	A	5	0	0	0	0
13	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	805	0	0	2	0
All	All	7550	0	6410	15	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 (15) 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:222:PRO:HA	1:A:225:HIS:CE1	2.43	0.54
1:A:273:PHE:H	11:A:923:PGE:H22	1.77	0.49
1:A:679:PRO:HD2	14:A:1744:HOH:O	2.13	0.48
1:A:776:PRO:HG2	1:A:779:LYS:HB2	1.96	0.47
1:A:765:SER:HB2	1:A:789:PHE:CZ	2.50	0.47
1:A:593:LEU:HD12	1:A:727:ASN:HB2	1.99	0.44
1:A:68:VAL:CG1	1:A:72:ASP:HB2	2.48	0.44
1:A:379:VAL:HB	1:A:455:ARG:HG2	2.00	0.44
1:A:539:PHE:O	1:A:541:PRO:HD3	2.19	0.43
1:A:232[A]:MET:HG2	1:A:241:PHE:HB3	1.99	0.42
1:A:408:ILE:HD11	1:A:424:MET:SD	2.60	0.42
1:A:617:TYR:HA	1:A:624:PRO:HA	2.02	0.41
1:A:397:PRO:HA	14:A:1187:HOH:O	2.21	0.41
1:A:700:MET:HA	1:A:793:HIS:NE2	2.35	0.41
1:A:550:PRO:HB2	1:A:607:ILE:HG12	2.03	0.41

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	800/844 (95%)	776 (97%)	24 (3%)	0	<a href="#">100</a> <a href="#">100</a>

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	734/768 (96%)	728 (99%)	6 (1%)	85 81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	398	ASN
1	A	400	LEU
1	A	452	HIS
1	A	569	ASP
1	A	588	GLU

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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	$\# Z  > 2$
2	NAG	A	901	1,3,2	14,14,15	0.26	0	15,19,21	0.70	0
3	FUC	A	902	2	9,10,11	0.41	0	13,14,16	0.68	0
2	NAG	A	903	2,4	14,14,15	0.31	0	15,19,21	0.73	1 (6%)
4	BMA	A	904	2,5	11,11,12	0.32	0	13,15,17	0.77	1 (7%)
5	MAN	A	905	4	11,11,12	0.37	0	13,15,17	0.96	1 (7%)
3	FUC	A	906	2	9,10,11	0.31	0	13,14,16	0.60	0
2	NAG	A	907	1,2	14,14,15	0.29	0	15,19,21	0.77	0
2	NAG	A	908	2	14,14,15	0.30	0	15,19,21	0.49	0
2	NAG	A	909	1,2	14,14,15	0.29	0	15,19,21	1.01	1 (6%)
2	NAG	A	910	2,4	14,14,15	0.29	0	15,19,21	0.57	0
4	BMA	A	911	2,5	11,11,12	0.52	0	13,15,17	2.41	3 (23%)
5	MAN	A	912	5,4	11,11,12	0.46	0	13,15,17	1.03	1 (7%)
5	MAN	A	913	5	11,11,12	0.41	0	13,15,17	0.76	1 (7%)
5	MAN	A	914	5	11,11,12	0.41	0	13,15,17	0.88	1 (7%)
11	PGE	A	923	-	9,9,9	0.16	0	8,8,8	0.16	0
12	SO4	A	924	-	4,4,4	0.28	0	6,6,6	0.15	0
13	6ZO	A	925	6	31,35,35	2.19	1 (3%)	41,49,49	0.86	1 (2%)

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	A	901	1,3,2	-	0/6/23/26	0/1/1/1
3	FUC	A	902	2	-	0/0/17/20	0/1/1/1
2	NAG	A	903	2,4	-	0/6/23/26	0/1/1/1
4	BMA	A	904	2,5	-	0/2/19/22	0/1/1/1
5	MAN	A	905	4	-	0/2/19/22	0/1/1/1
3	FUC	A	906	2	-	0/0/17/20	0/1/1/1
2	NAG	A	907	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	908	2	-	0/6/23/26	0/1/1/1
2	NAG	A	909	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	910	2,4	-	0/6/23/26	0/1/1/1
4	BMA	A	911	2,5	-	0/2/19/22	0/1/1/1
5	MAN	A	912	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	913	5	-	0/2/19/22	0/1/1/1
5	MAN	A	914	5	-	0/2/19/22	0/1/1/1
11	PGE	A	923	-	-	0/7/7/7	0/0/0/0
12	SO4	A	924	-	-	0/0/0/0	0/0/0/0
13	6ZO	A	925	6	-	0/18/28/28	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	925	6ZO	O32-C30	11.63	1.33	1.19

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	909	NAG	O5-C1-C2	-3.00	107.30	111.47
2	A	903	NAG	O5-C1-C2	-2.16	108.47	111.47
4	A	911	BMA	C1-C2-C3	2.05	112.25	109.65
5	A	913	MAN	C1-O5-C5	2.09	115.04	112.17
4	A	911	BMA	O5-C1-C2	2.24	114.30	110.79
4	A	904	BMA	C1-O5-C5	2.42	115.50	112.17
13	A	925	6ZO	C17-N16-C15	2.64	118.02	111.26
5	A	914	MAN	C1-O5-C5	2.69	115.88	112.17
5	A	905	MAN	C1-O5-C5	2.90	116.17	112.17
5	A	912	MAN	C1-O5-C5	3.03	116.34	112.17
4	A	911	BMA	C1-O5-C5	8.06	123.28	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	923	PGE	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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, 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	785/844 (93%)	-0.12	27 (3%) 46 40	13, 20, 42, 75	30 (3%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	GLY	7.9
1	A	400	LEU	5.2
1	A	469	PHE	4.9
1	A	458	LEU	4.5
1	A	68	VAL	4.1
1	A	81	SER	4.0
1	A	398	ASN	3.9
1	A	585	GLY	3.3
1	A	399	ASN	3.2
1	A	70	PRO	3.2
1	A	51	TRP	3.0
1	A	397	PRO	3.0
1	A	67	GLU	2.7
1	A	639[A]	SER	2.7
1	A	78	LEU	2.6
1	A	71	PRO	2.6
1	A	459	ASP	2.5
1	A	588	GLU	2.4
1	A	642	GLU	2.4
1	A	401	LYS	2.3
1	A	66	GLN	2.3
1	A	569	ASP	2.3
1	A	246	ARG	2.3
1	A	378	ASN	2.2
1	A	396	ILE	2.0
1	A	402	TYR	2.0
1	A	643	HIS	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](#)

There are no carbohydrates in this entry.

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	A	913	11/12	0.53	0.28	18.19	54,55,59,59	0
5	MAN	A	905	11/12	0.75	0.19	1.90	42,47,49,49	0
8	NA	A	918	1/1	0.98	0.15	1.47	24,24,24,24	0
2	NAG	A	907	14/15	0.85	0.20	1.39	34,40,47,51	0
8	NA	A	922	1/1	0.84	0.26	1.19	37,37,37,37	1
11	PGE	A	923	10/10	0.76	0.16	0.85	41,47,48,49	0
12	SO4	A	924	5/5	0.97	0.16	0.64	34,34,36,39	5
13	6ZO	A	925	32/32	0.92	0.11	0.25	28,38,43,44	0
2	NAG	A	909	14/15	0.97	0.08	-0.48	14,16,20,20	0
2	NAG	A	901	14/15	0.95	0.08	-0.48	26,29,34,35	0
10	CL	A	921	1/1	1.00	0.06	-1.64	22,22,22,22	0
6	ZN	A	916	1/1	1.00	0.04	-1.93	19,19,19,19	0
7	CA	A	917	1/1	1.00	0.04	-2.33	16,16,16,16	0
9	K	A	919	1/1	1.00	0.05	-2.64	13,13,13,13	0
6	ZN	A	915	1/1	1.00	0.05	-3.18	18,18,18,18	0
5	MAN	A	912	11/12	0.52	0.31	-	57,60,61,61	0
2	NAG	A	903	14/15	0.87	0.16	-	29,41,45,47	0
3	FUC	A	906	10/11	0.92	0.12	-	30,33,35,36	0
2	NAG	A	908	14/15	0.81	0.33	-	56,61,63,64	0
3	FUC	A	902	10/11	0.91	0.12	-	37,38,41,41	0
5	MAN	A	914	11/12	0.63	0.24	-	46,49,51,51	0
7	CA	A	920	1/1	0.79	0.10	-	61,61,61,61	0
2	NAG	A	910	14/15	0.90	0.16	-	24,28,35,44	0
4	BMA	A	911	11/12	0.65	0.40	-	52,57,60,60	0
4	BMA	A	904	11/12	0.72	0.33	-	49,51,55,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.