



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 10:38 AM EDT

PDB ID : 5FCB  
Title : Murine SMPDL3A in complex with AMP  
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Deposited on : 2015-12-15  
Resolution : 1.55 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

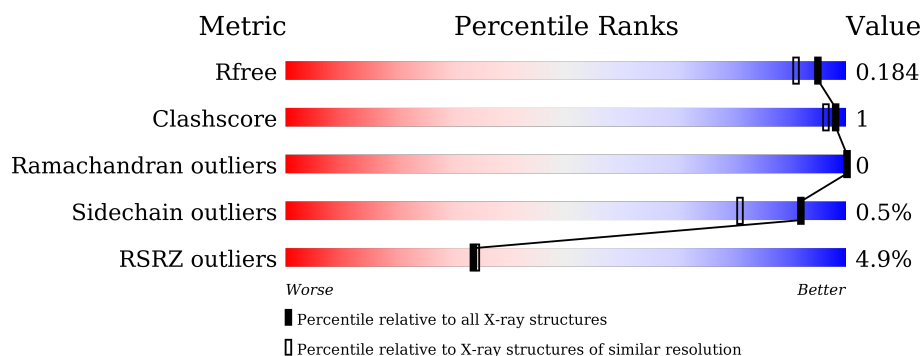
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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))
$R_{free}$	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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	433	<div> <div>5%</div> <div>96%</div> <div>...</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
3	NAG	A	503	-	-	-	X
3	NAG	A	515	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	A	507	-	-	-	X
4	FUC	A	514	-	-	-	X
8	GOL	A	520	-	-	-	X
8	GOL	A	521	-	-	-	X
8	GOL	A	522	-	-	-	X
8	GOL	A	523	-	-	-	X
8	GOL	A	524	-	-	-	X
8	GOL	A	525	-	-	-	X
8	GOL	A	526	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7809 atoms, of which 3611 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 Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	H	N	O	S	0	12	0
			6805	2221	3365	559	645	15			

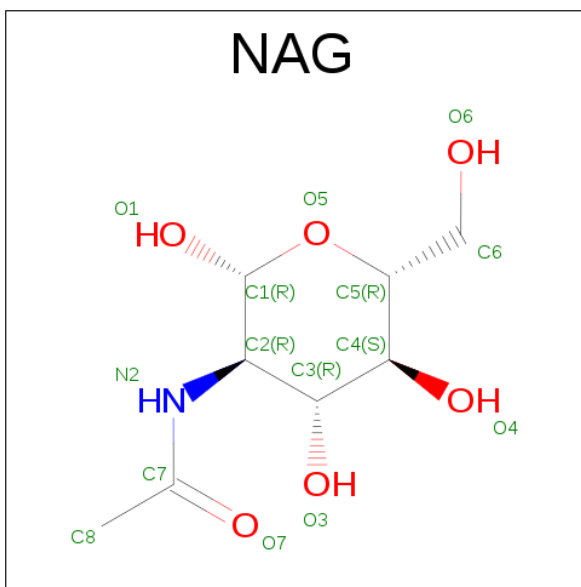
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	-	expression tag	UNP P70158
A	14	ARG	-	expression tag	UNP P70158
A	15	HIS	-	expression tag	UNP P70158
A	16	HIS	-	expression tag	UNP P70158
A	17	HIS	-	expression tag	UNP P70158
A	18	HIS	-	expression tag	UNP P70158
A	19	HIS	-	expression tag	UNP P70158
A	20	HIS	-	expression tag	UNP P70158
A	21	LYS	-	expression tag	UNP P70158
A	22	LEU	-	expression tag	UNP P70158

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

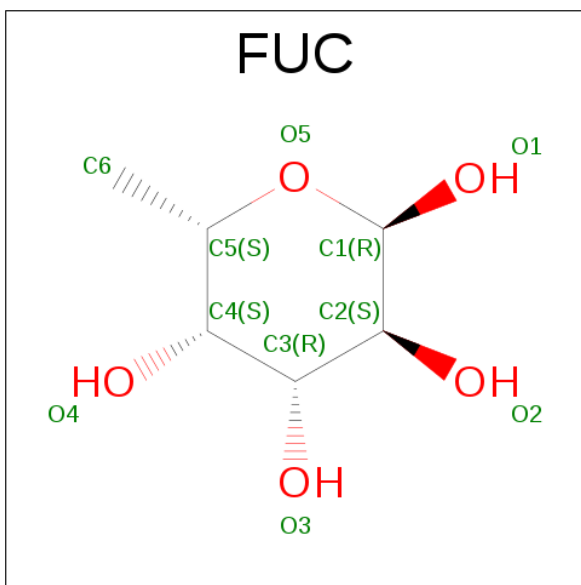
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



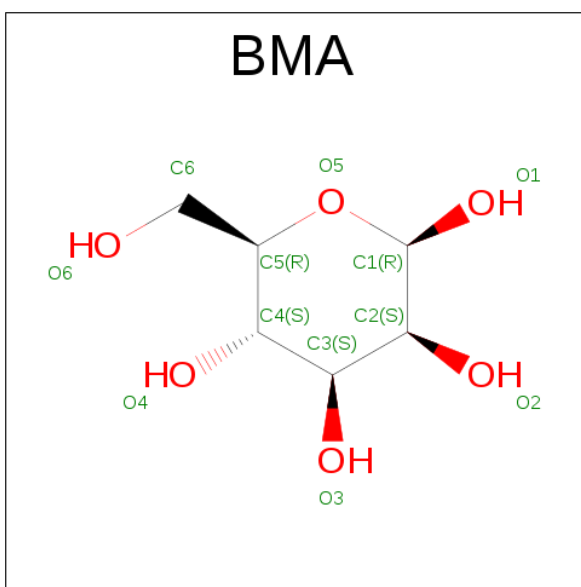
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



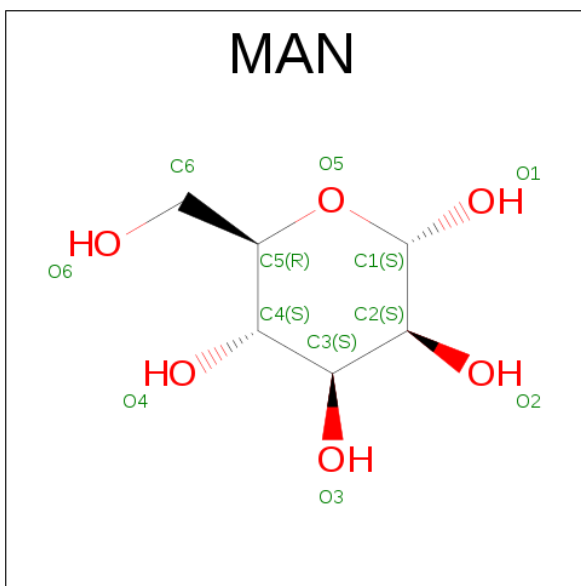
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			21	6	11	4		
4	A	1	Total	C	H	O	0	0
			21	6	11	4		
4	A	1	Total	C	H	O	0	0
			21	6	11	4		

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



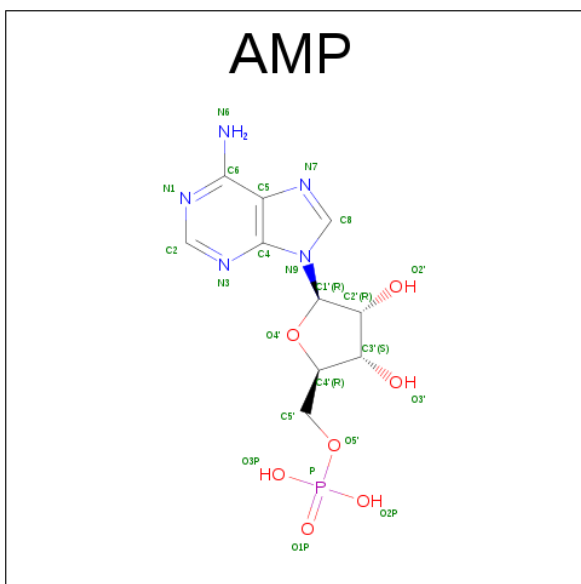
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			20	6	9	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



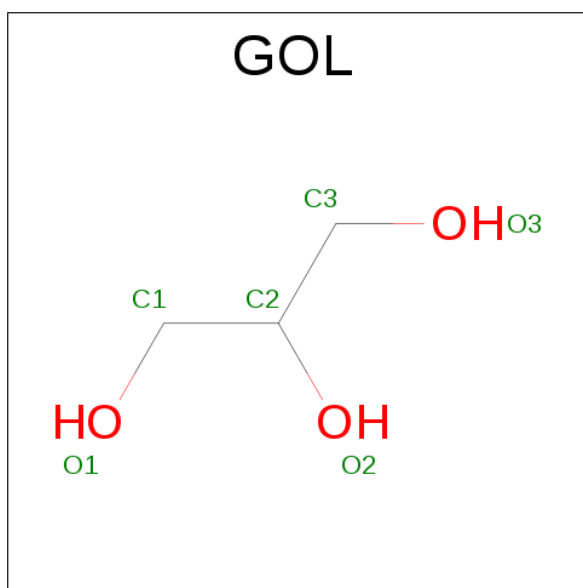
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			22	6	11	5		
6	A	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			35	10	12	5	7		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			13	3	7	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

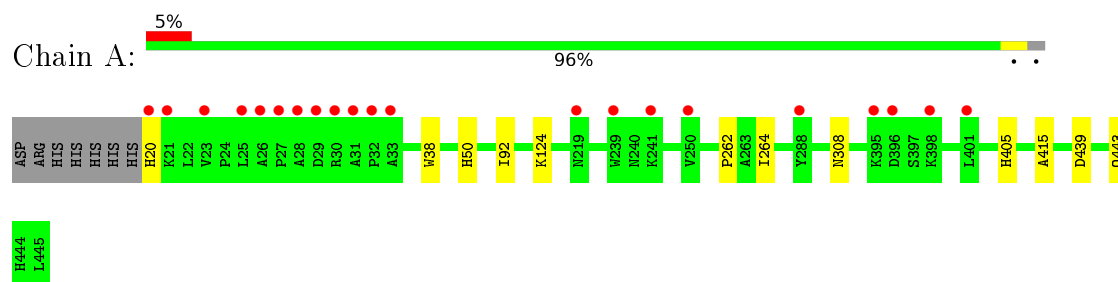
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	512	Total	O	0	0
			512	512		



**i**

- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.03 Å   132.38 Å   79.74 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	41.57 – 1.55 41.57 – 1.55	Depositor EDS
% Data completeness (in resolution range)	93.5 (41.57-1.55) 85.1 (41.57-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 1.55 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.160   ,   0.186 0.157   ,   0.184	Depositor DCC
$R_{free}$ test set	4045 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 89174 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ZN, BMA, NAG, FUC, AMP, 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	0.35	0/3574	0.55	0/4880

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	3440	3365	3386	7	0
2	A	2	0	0	0	0
3	A	98	91	84	0	0
4	A	30	33	30	1	0
5	A	11	9	8	0	0
6	A	22	22	20	0	0
7	A	23	12	12	0	0
8	A	60	79	80	1	0
9	A	512	0	0	2	0
All	All	4198	3611	3620	7	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 (7) 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:439[B]:ASP:OD2	1:A:443:GLN:NE2	2.43	0.51
1:A:415:ALA:O	8:A:523:GOL:O1	2.22	0.51
1:A:20:HIS:N	9:A:612:HOH:O	2.49	0.45
1:A:262:PRO:HB2	1:A:264:ILE:O	2.17	0.44
1:A:405:HIS:HE1	9:A:938:HOH:O	2.01	0.44
1:A:124:LYS:HE2	4:A:507:FUC:H4	2.00	0.43
1:A:38:TRP:CE2	1:A:92:ILE:HG23	2.55	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	436/433 (101%)	418 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/384 (101%)	387 (100%)	2 (0%)	92	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	308	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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$
3	NAG	A	503	1,3,4	14,14,15	0.68	1 (7%)	15,19,21	0.50	0
4	FUC	A	504	3	10,10,11	1.21	1 (10%)	13,14,16	1.91	3 (23%)
3	NAG	A	505	3	14,14,15	0.63	1 (7%)	15,19,21	0.86	1 (6%)
3	NAG	A	506	1,3,4	14,14,15	0.79	1 (7%)	15,19,21	0.63	0
4	FUC	A	507	3	10,10,11	1.54	2 (20%)	13,14,16	1.86	3 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	508	3	14,14,15	0.71	0	15,19,21	1.28	3 (20%)
5	BMA	A	509	3,6	11,11,12	0.67	0	15,15,17	1.03	1 (6%)
6	MAN	A	510	5	11,11,12	1.02	0	15,15,17	1.32	1 (6%)
6	MAN	A	511	5	11,11,12	1.06	1 (9%)	15,15,17	2.10	4 (26%)
3	NAG	A	512	1,3	14,14,15	0.34	0	15,19,21	0.44	0
3	NAG	A	513	3,5	14,14,15	0.34	0	15,19,21	0.55	0
4	FUC	A	514	3	10,10,11	1.06	0	13,14,16	1.39	2 (15%)
3	NAG	A	515	1,4	14,14,15	0.99	2 (14%)	15,19,21	0.69	0
7	AMP	A	516	2	22,25,25	1.00	1 (4%)	22,38,38	1.89	4 (18%)
8	GOL	A	517	-	5,5,5	0.29	0	5,5,5	0.31	0
8	GOL	A	518	-	5,5,5	0.32	0	5,5,5	0.33	0
8	GOL	A	519	-	5,5,5	0.32	0	5,5,5	0.27	0
8	GOL	A	520	-	5,5,5	0.37	0	5,5,5	0.20	0
8	GOL	A	521	-	5,5,5	0.34	0	5,5,5	0.23	0
8	GOL	A	522	-	5,5,5	0.29	0	5,5,5	0.28	0
8	GOL	A	523	-	5,5,5	0.34	0	5,5,5	0.35	0
8	GOL	A	524	-	5,5,5	0.29	0	5,5,5	0.78	0
8	GOL	A	525	-	5,5,5	0.37	0	5,5,5	0.17	0
8	GOL	A	526	-	5,5,5	0.37	0	5,5,5	0.18	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	NAG	A	503	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	504	3	-	0/0/17/20	0/1/1/1
3	NAG	A	505	3	-	0/6/23/26	0/1/1/1
3	NAG	A	506	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	507	3	-	0/0/17/20	0/1/1/1
3	NAG	A	508	3	-	0/6/23/26	0/1/1/1
5	BMA	A	509	3,6	-	0/2/19/22	0/1/1/1
6	MAN	A	510	5	-	0/2/19/22	0/1/1/1
6	MAN	A	511	5	-	0/2/19/22	0/1/1/1
3	NAG	A	512	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	513	3,5	-	0/6/23/26	0/1/1/1
4	FUC	A	514	3	-	0/0/17/20	0/1/1/1
3	NAG	A	515	1,4	-	0/6/23/26	0/1/1/1
7	AMP	A	516	2	-	0/6/26/26	0/3/3/3
8	GOL	A	517	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	518	-	-	0/4/4/4	0/0/0/0
8	GOL	A	519	-	-	0/4/4/4	0/0/0/0
8	GOL	A	520	-	-	0/4/4/4	0/0/0/0
8	GOL	A	521	-	-	0/4/4/4	0/0/0/0
8	GOL	A	522	-	-	0/4/4/4	0/0/0/0
8	GOL	A	523	-	-	0/4/4/4	0/0/0/0
8	GOL	A	524	-	-	0/4/4/4	0/0/0/0
8	GOL	A	525	-	-	0/4/4/4	0/0/0/0
8	GOL	A	526	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	515	NAG	O5-C1	-2.69	1.39	1.43
3	A	503	NAG	O5-C1	-2.40	1.39	1.43
3	A	506	NAG	O5-C1	-2.35	1.39	1.43
3	A	505	NAG	O5-C1	-2.14	1.40	1.43
3	A	515	NAG	C1-C2	2.22	1.55	1.52
6	A	511	MAN	C1-C2	2.54	1.58	1.52
4	A	507	FUC	O5-C1	2.95	1.48	1.43
4	A	507	FUC	C1-C2	2.96	1.59	1.52
7	A	516	AMP	C5-C4	3.11	1.47	1.40
4	A	504	FUC	C1-C2	3.16	1.59	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	516	AMP	N3-C2-N1	-7.03	123.35	128.87
7	A	516	AMP	O5'-P-O1P	-2.38	101.10	107.08
6	A	511	MAN	O2-C2-C3	-2.32	105.51	110.19
7	A	516	AMP	O3P-P-O2P	2.01	114.82	107.44
3	A	508	NAG	C3-C4-C5	2.12	114.00	110.23
4	A	507	FUC	O5-C1-C2	2.16	114.35	110.89
5	A	509	BMA	C3-C4-C5	2.17	114.10	110.23
4	A	514	FUC	O5-C5-C6	2.22	110.27	106.28
3	A	508	NAG	C1-O5-C5	2.25	115.45	112.14
3	A	505	NAG	C1-O5-C5	2.51	115.83	112.14
4	A	504	FUC	O5-C1-C2	2.61	115.06	110.89
6	A	511	MAN	C1-C2-C3	2.76	112.89	109.55
3	A	508	NAG	O5-C5-C4	2.80	114.77	110.13
7	A	516	AMP	N6-C6-N1	2.84	123.28	118.52
4	A	514	FUC	C1-C2-C3	2.91	113.08	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	510	MAN	C1-O5-C5	3.28	116.97	112.14
4	A	504	FUC	O5-C5-C4	3.52	115.68	109.58
4	A	507	FUC	O5-C5-C4	3.55	115.73	109.58
6	A	511	MAN	O5-C1-C2	3.79	116.95	110.89
4	A	507	FUC	C1-C2-C3	4.48	114.98	109.55
4	A	504	FUC	C1-C2-C3	4.51	115.02	109.55
6	A	511	MAN	C1-O5-C5	5.70	120.53	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507	FUC	1	0
8	A	523	GOL	1	0

## 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	426/433 (98%)	0.02	21 (4%) 33 34	17, 26, 46, 111	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	ASP	11.1
1	A	28	ALA	10.3
1	A	20	HIS	8.8
1	A	31	ALA	7.9
1	A	26	ALA	7.6
1	A	30	ARG	7.4
1	A	23	VAL	6.1
1	A	27	PRO	5.7
1	A	33	ALA	5.5
1	A	32	PRO	5.3
1	A	25	LEU	4.6
1	A	239	TRP	4.4
1	A	21	LYS	3.2
1	A	219	ASN	2.9
1	A	396	ASP	2.6
1	A	395	LYS	2.4
1	A	241	LYS	2.3
1	A	288	TYR	2.2
1	A	401	LEU	2.1
1	A	398	LYS	2.1
1	A	250	VAL	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
8	GOL	A	524	6/6	0.66	0.35	25.84	40,55,66,69	0
8	GOL	A	521	6/6	0.78	0.26	8.38	58,71,79,85	0
4	FUC	A	514	10/11	0.69	0.41	6.79	72,100,122,129	0
8	GOL	A	523	6/6	0.78	0.37	6.29	41,56,72,84	0
4	FUC	A	507	10/11	0.15	0.56	6.02	72,88,108,112	0
8	GOL	A	526	6/6	0.57	0.31	5.80	58,70,80,80	0
8	GOL	A	522	6/6	0.80	0.16	5.59	60,72,79,87	0
3	NAG	A	515	14/15	0.61	0.33	5.38	67,83,100,106	0
8	GOL	A	525	6/6	0.71	0.32	3.82	42,59,70,84	0
3	NAG	A	503	14/15	0.86	0.18	2.47	34,55,81,87	0
8	GOL	A	520	6/6	0.86	0.24	2.18	52,62,74,78	0
3	NAG	A	506	14/15	0.94	0.09	1.85	37,53,70,76	0
3	NAG	A	512	14/15	0.94	0.10	1.67	29,36,43,51	0
8	GOL	A	518	6/6	0.89	0.12	1.55	31,53,60,72	0
7	AMP	A	516	23/23	0.93	0.14	1.52	27,71,105,109	0
8	GOL	A	517	6/6	0.92	0.11	1.52	33,44,61,63	0
8	GOL	A	519	6/6	0.90	0.12	1.22	31,58,72,74	0
2	ZN	A	501	1/1	1.00	0.08	-1.85	22,22,22,22	0
2	ZN	A	502	1/1	1.00	0.02	-4.85	26,26,26,26	0
3	NAG	A	508	14/15	0.66	0.35	-	54,99,124,133	0
3	NAG	A	505	14/15	0.63	0.42	-	73,93,113,118	0
6	MAN	A	510	11/12	0.65	0.47	-	67,99,121,125	0
5	BMA	A	509	11/12	0.67	0.33	-	64,87,104,105	0
6	MAN	A	511	11/12	0.33	0.63	-	81,110,132,135	0
4	FUC	A	504	10/11	0.76	0.44	-	85,101,118,122	0
3	NAG	A	513	14/15	0.88	0.15	-	38,56,72,86	0

## 6.5 Other polymers

There are no such residues in this entry.