



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2016 – 08:56 PM EDT

PDB ID : 5FI9
Title : Closed form of murine Acid Sphingomyelinase in complex with bisphosphonate inhibitor AbPA
Authors : Gorelik, A.; Illes, K.; Heinz, L.X.; Superti-Furga, G.; Nagar, B.
Deposited on : 2015-12-22
Resolution : 2.54 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939

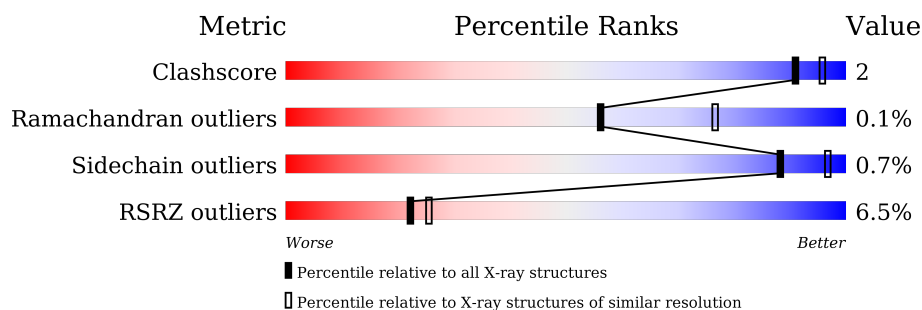
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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))
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	538	<div> <div>8%</div> <div>93%</div> <div>5%</div> </div>
1	B	538	<div> <div>4%</div> <div>94%</div> <div>5%</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	705	-	-	-	X
3	NAG	A	707	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	708	-	-	-	X
4	FUC	A	706	-	-	-	X
4	FUC	B	707	-	-	-	X
6	MAN	A	712	-	-	-	X
6	MAN	B	714	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17178 atoms, of which 8420 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 Spingomyelin phosphodiesterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	523	Total	C	H	N	O	S	0	0	0
			8121	2656	3995	709	738	23			
1	B	529	Total	C	H	N	O	S	0	0	0
			8199	2682	4031	717	746	23			

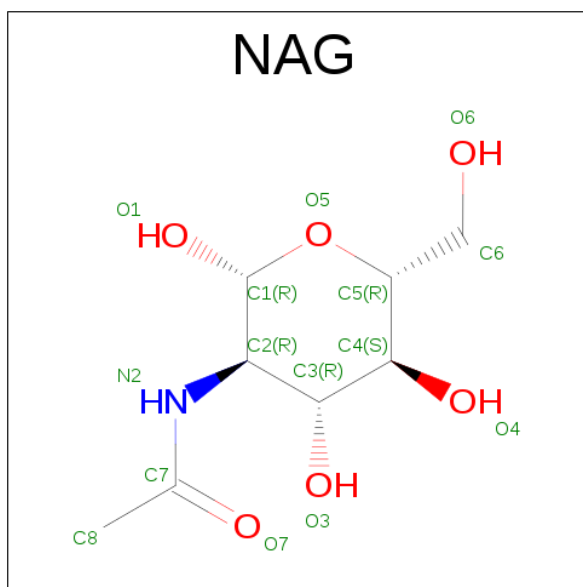
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ASP	-	expression tag	UNP Q04519
A	75	ARG	-	expression tag	UNP Q04519
A	76	HIS	-	expression tag	UNP Q04519
A	77	HIS	-	expression tag	UNP Q04519
A	78	HIS	-	expression tag	UNP Q04519
A	79	HIS	-	expression tag	UNP Q04519
A	80	HIS	-	expression tag	UNP Q04519
A	81	HIS	-	expression tag	UNP Q04519
A	82	LYS	-	expression tag	UNP Q04519
A	83	LEU	-	expression tag	UNP Q04519
B	74	ASP	-	expression tag	UNP Q04519
B	75	ARG	-	expression tag	UNP Q04519
B	76	HIS	-	expression tag	UNP Q04519
B	77	HIS	-	expression tag	UNP Q04519
B	78	HIS	-	expression tag	UNP Q04519
B	79	HIS	-	expression tag	UNP Q04519
B	80	HIS	-	expression tag	UNP Q04519
B	81	HIS	-	expression tag	UNP Q04519
B	82	LYS	-	expression tag	UNP Q04519
B	83	LEU	-	expression tag	UNP Q04519

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

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

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



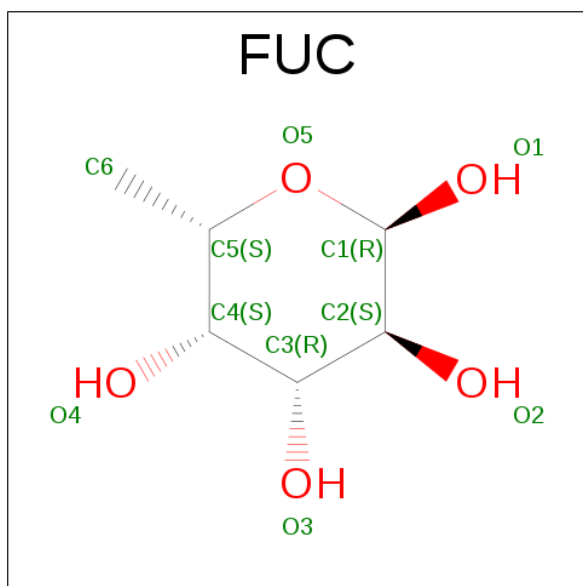
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total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

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

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



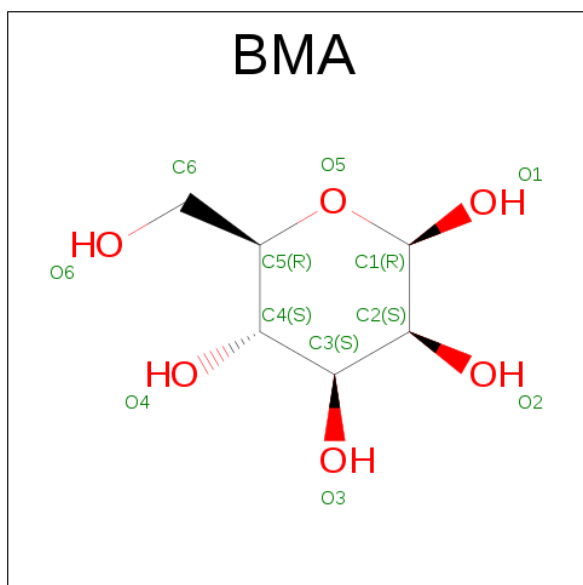
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			21	6	11	4		
4	A	1	Total	C	H	O	0	0
			21	6	11	4		
4	B	1	Total	C	H	O	0	0
			21	6	11	4		

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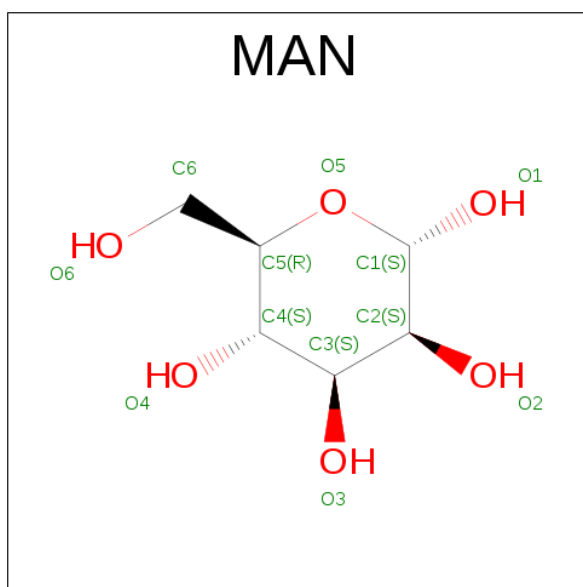
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			21	6	11	4		
4	B	1	Total	C	H	O	0	0
			21	6	11	4		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



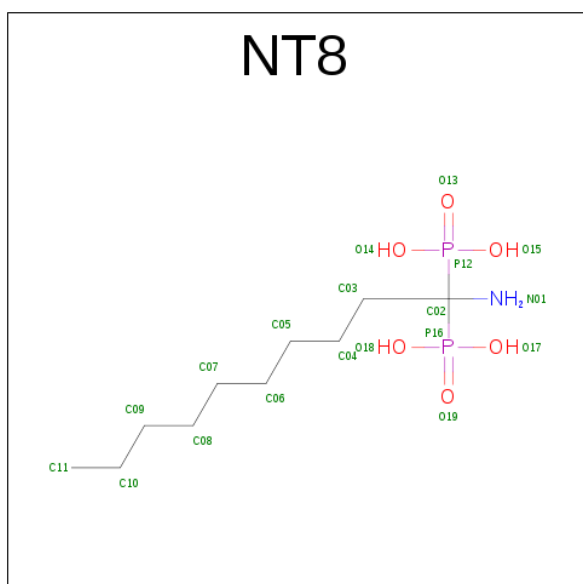
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			20	6	9	5		
5	B	1	Total	C	H	O	0	0
			22	6	11	5		
5	B	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			21	6	10	5		
6	A	1	Total	C	H	O	0	0
			22	6	11	5		
6	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 7 is (1-azanyl-1-phosphono-decyl)phosphonic acid (three-letter code: NT8) (formula: $C_{10}H_{25}NO_6P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total 40	C 10	H 21	N 1	O 6	P 2	0	0
7	B	1	Total 40	C 10	H 21	N 1	O 6	P 2	0	0

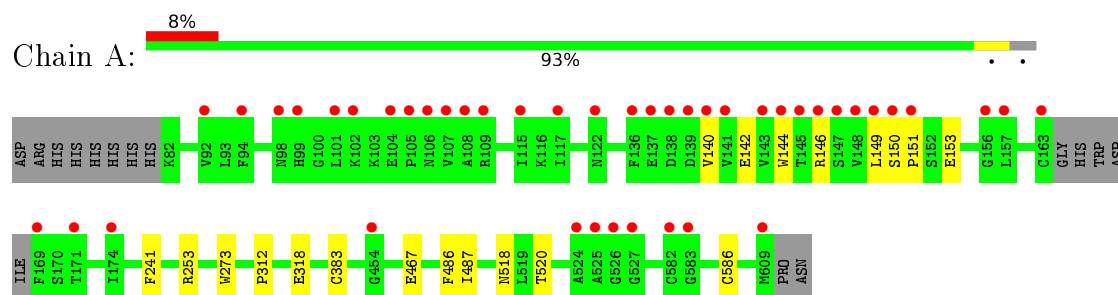
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	25	Total 25	O 25	0	0
8	B	29	Total 29	O 29	0	0

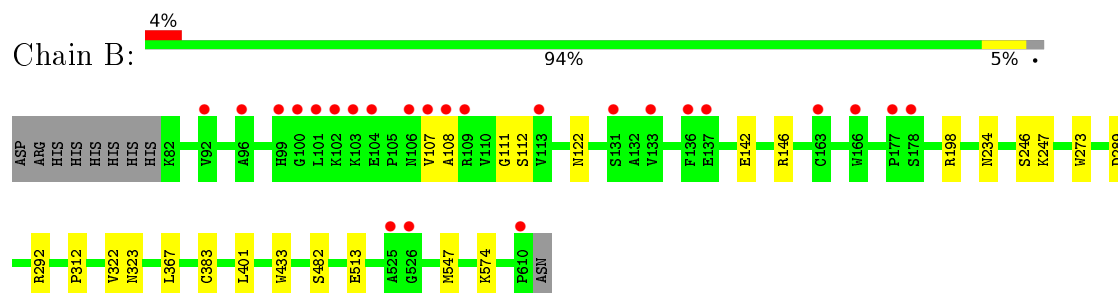
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: SpHINGOMYELIN phosphodiesterase



• Molecule 1: SpHINGOMYELIN phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.39Å 72.02Å 74.42Å 80.47° 71.52° 83.60°	Depositor
Resolution (Å)	46.65 – 2.54 44.49 – 2.54	Depositor EDS
% Data completeness (in resolution range)	92.0 (46.65-2.54) 61.6 (44.49-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.201 , 0.252 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17178	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NT8, ZN, BMA, NAG, FUC, 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	0.25	0/4265	0.42	0/5835
1	B	0.24	0/4310	0.42	0/5899
All	All	0.25	0/8575	0.42	0/11734

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 [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	4126	3995	3994	12	0
1	B	4168	4031	4030	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	140	132	122	5	0
3	B	112	103	95	8	0
4	A	20	22	20	0	0
4	B	30	33	30	2	0
5	A	11	9	8	0	0
5	B	22	21	19	1	0
6	A	22	21	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	11	11	10	0	0
7	A	19	21	0	0	0
7	B	19	21	0	0	0
8	A	25	0	0	1	0
8	B	29	0	0	0	0
All	All	8758	8420	8348	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 2.

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)
3:B:706:NAG:O7	3:B:706:NAG:O3	2.00	0.79
1:B:142:GLU:OE1	1:B:146:ARG:NH2	2.19	0.76
1:A:140:VAL:O	1:A:144:TRP:N	2.19	0.75
3:A:716:NAG:O3	3:A:717:NAG:O5	2.04	0.75
3:B:709:NAG:O7	3:B:709:NAG:O3	2.10	0.70
3:B:706:NAG:HO3	3:B:706:NAG:C7	2.02	0.66
1:B:108:ALA:O	1:B:111:GLY:N	2.28	0.65
1:A:467:GLU:OE2	8:A:801:HOH:O	2.15	0.65
1:B:198:ARG:NH2	1:B:513:GLU:OE1	2.33	0.61
1:A:518:ASN:OD1	1:A:520:THR:OG1	2.18	0.60
1:A:241:PHE:O	1:A:253:ARG:NH1	2.36	0.59
1:B:108:ALA:O	1:B:112:SER:N	2.28	0.57
1:B:122:ASN:OD1	4:B:712:FUC:O4	2.27	0.51
1:A:142:GLU:O	1:A:146:ARG:HG3	2.12	0.49
3:A:716:NAG:HO3	3:A:717:NAG:C5	2.21	0.49
1:A:150:SER:HB2	1:A:151:PRO:HD2	1.95	0.49
1:B:246:SER:OG	1:B:247:LYS:N	2.46	0.48
1:B:482:SER:O	1:B:574:LYS:NZ	2.41	0.47
1:A:273:TRP:O	1:A:312:PRO:HA	2.14	0.47
1:A:150:SER:CB	1:A:151:PRO:HD2	2.45	0.47
3:B:708:NAG:H4	3:B:709:NAG:N2	2.31	0.46
4:B:712:FUC:O5	3:B:716:NAG:H82	2.15	0.45
1:A:146:ARG:HG2	1:A:149:LEU:HD12	2.00	0.44
1:A:486:PHE:HA	1:A:487:ILE:HA	1.84	0.43
1:B:234:ASN:ND2	1:B:234:ASN:O	2.52	0.43
1:B:289:ASP:OD1	1:B:292:ARG:NH2	2.51	0.43
1:A:146:ARG:HA	1:A:149:LEU:HG	1.99	0.43
3:A:716:NAG:O3	3:A:717:NAG:C5	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TRP:O	1:B:312:PRO:HA	2.20	0.42
3:B:715:NAG:O3	3:B:716:NAG:O5	2.35	0.42
1:A:149:LEU:HD22	1:A:153:GLU:CG	2.49	0.42
3:A:703:NAG:O4	3:A:703:NAG:O6	2.34	0.42
5:B:703:BMA:O2	3:B:706:NAG:H4	2.19	0.42
1:B:401:LEU:HD21	1:B:433:TRP:NE1	2.35	0.41
3:B:715:NAG:HO3	3:B:716:NAG:C1	2.34	0.41
1:B:322:VAL:O	1:B:323:ASN:HB2	2.21	0.41
3:A:716:NAG:O3	3:A:717:NAG:C1	2.69	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	519/538 (96%)	487 (94%)	32 (6%)	0	100	100
1	B	527/538 (98%)	492 (93%)	34 (6%)	1 (0%)	52	73
All	All	1046/1076 (97%)	979 (94%)	66 (6%)	1 (0%)	56	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	VAL

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	446/460 (97%)	443 (99%)	3 (1%)	88	97
1	B	450/460 (98%)	447 (99%)	3 (1%)	88	97
All	All	896/920 (97%)	890 (99%)	6 (1%)	88	97

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

Mol	Chain	Res	Type
1	A	318	GLU
1	A	383	CYS
1	A	586	CYS
1	B	367	LEU
1	B	383	CYS
1	B	547	MET

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 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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	703	1,3	14,14,15	1.13	1 (7%)	15,19,21	1.12	1 (6%)
3	NAG	A	704	3	14,14,15	1.35	2 (14%)	15,19,21	1.39	1 (6%)
3	NAG	A	705	1,3,4	14,14,15	1.75	3 (21%)	15,19,21	1.24	2 (13%)
4	FUC	A	706	3	10,10,11	1.17	1 (10%)	13,14,16	1.83	3 (23%)
3	NAG	A	707	3	14,14,15	0.42	0	15,19,21	0.90	1 (6%)
3	NAG	A	708	1,3	14,14,15	0.48	0	15,19,21	0.45	0
3	NAG	A	709	3	14,14,15	0.22	0	15,19,21	0.42	0
5	BMA	A	710	3,6	11,11,12	0.67	0	15,15,17	1.07	0
6	MAN	A	711	5	11,11,12	0.73	0	15,15,17	0.87	1 (6%)
6	MAN	A	712	5	11,11,12	0.92	1 (9%)	15,15,17	1.55	2 (13%)
4	FUC	A	713	3	10,10,11	0.93	1 (10%)	13,14,16	1.69	2 (15%)
3	NAG	A	714	1,3,4	14,14,15	1.34	1 (7%)	15,19,21	0.62	0
3	NAG	A	715	3,5	14,14,15	0.23	0	15,19,21	0.40	0
3	NAG	A	716	1,3	14,14,15	1.50	1 (7%)	15,19,21	2.16	4 (26%)
3	NAG	A	717	3	14,14,15	0.28	0	15,19,21	0.91	0
7	NT8	A	718	2	14,18,18	0.98	0	17,26,26	1.17	1 (5%)
5	BMA	B	703	3	11,11,12	0.83	0	15,15,17	1.07	1 (6%)
3	NAG	B	704	1,3,4	14,14,15	0.26	0	15,19,21	0.54	0
4	FUC	B	705	3	10,10,11	1.30	1 (10%)	13,14,16	2.02	3 (23%)
3	NAG	B	706	3,5	14,14,15	0.23	0	15,19,21	0.66	0
4	FUC	B	707	3	10,10,11	1.62	2 (20%)	13,14,16	2.04	3 (23%)
3	NAG	B	708	1,3,4	14,14,15	0.40	0	15,19,21	0.32	0
3	NAG	B	709	3	14,14,15	0.55	0	15,19,21	0.63	1 (6%)
3	NAG	B	710	1,3	14,14,15	0.48	0	15,19,21	0.56	0
3	NAG	B	711	3	14,14,15	0.40	0	15,19,21	0.29	0
4	FUC	B	712	3	10,10,11	0.93	0	13,14,16	1.53	2 (15%)
5	BMA	B	713	3,6	11,11,12	0.55	0	15,15,17	0.82	0
6	MAN	B	714	5	11,11,12	0.64	0	15,15,17	1.10	2 (13%)
3	NAG	B	715	1,3,4	14,14,15	0.56	0	15,19,21	0.35	0
3	NAG	B	716	3,5	14,14,15	0.32	0	15,19,21	0.60	1 (6%)
7	NT8	B	717	2	14,18,18	0.96	0	17,26,26	1.11	1 (5%)

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	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	704	3	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	706	3	-	0/0/17/20	0/1/1/1
3	NAG	A	707	3	-	0/6/23/26	0/1/1/1
3	NAG	A	708	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	709	3	-	0/6/23/26	0/1/1/1
5	BMA	A	710	3,6	-	0/2/19/22	0/1/1/1
6	MAN	A	711	5	-	0/2/19/22	0/1/1/1
6	MAN	A	712	5	-	0/2/19/22	0/1/1/1
4	FUC	A	713	3	-	0/0/17/20	0/1/1/1
3	NAG	A	714	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	715	3,5	-	0/6/23/26	0/1/1/1
3	NAG	A	716	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	717	3	-	0/6/23/26	0/1/1/1
7	NT8	A	718	2	-	0/27/28/28	0/0/0/0
5	BMA	B	703	3	-	0/2/19/22	0/1/1/1
3	NAG	B	704	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	B	705	3	-	0/0/17/20	0/1/1/1
3	NAG	B	706	3,5	-	0/6/23/26	0/1/1/1
4	FUC	B	707	3	-	0/0/17/20	0/1/1/1
3	NAG	B	708	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	709	3	-	0/6/23/26	0/1/1/1
3	NAG	B	710	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	711	3	-	0/6/23/26	0/1/1/1
4	FUC	B	712	3	-	0/0/17/20	0/1/1/1
5	BMA	B	713	3,6	-	0/2/19/22	0/1/1/1
6	MAN	B	714	5	-	0/2/19/22	1/1/1/1
3	NAG	B	715	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	716	3,5	-	0/6/23/26	0/1/1/1
7	NT8	B	717	2	-	0/27/28/28	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	NAG	O5-C1	-4.87	1.35	1.43
3	A	714	NAG	O5-C1	-4.81	1.35	1.43
4	A	706	FUC	C1-C2	2.00	1.57	1.52
4	B	707	FUC	O5-C1	2.04	1.47	1.43
3	A	705	NAG	C3-C2	2.05	1.57	1.52
6	A	712	MAN	C1-C2	2.36	1.58	1.52
4	A	713	FUC	C1-C2	2.69	1.58	1.52
3	A	704	NAG	C1-C2	3.04	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	705	FUC	C4-C5	3.04	1.58	1.53
3	A	705	NAG	C1-C2	3.73	1.57	1.52
3	A	703	NAG	C1-C2	3.91	1.58	1.52
3	A	704	NAG	O5-C1	3.91	1.50	1.43
4	B	707	FUC	C1-C2	4.12	1.62	1.52
3	A	716	NAG	O5-C1	5.29	1.52	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	718	NT8	P16-C02-P12	-2.72	108.56	113.39
3	A	716	NAG	C4-C3-C2	-2.46	107.53	111.34
5	B	703	BMA	O2-C2-C3	-2.35	105.44	110.19
3	A	705	NAG	O5-C5-C4	-2.34	106.27	110.13
3	A	703	NAG	O5-C5-C4	-2.31	106.31	110.13
7	B	717	NT8	P16-C02-P12	-2.28	109.34	113.39
6	B	714	MAN	O2-C2-C3	-2.13	105.90	110.19
4	B	705	FUC	O5-C1-C2	-2.08	107.57	110.89
6	A	711	MAN	O2-C2-C3	-2.07	106.02	110.19
6	A	712	MAN	O2-C2-C3	-2.06	106.04	110.19
3	B	716	NAG	C1-O5-C5	2.07	115.18	112.14
3	B	709	NAG	C1-O5-C5	2.13	115.27	112.14
3	A	707	NAG	C3-C4-C5	2.33	114.39	110.23
3	A	716	NAG	C2-N2-C7	2.35	126.17	123.11
4	B	712	FUC	C3-C4-C5	2.38	113.22	109.66
4	A	706	FUC	O5-C5-C4	2.49	113.88	109.58
4	B	707	FUC	O5-C1-C2	2.58	115.01	110.89
3	A	716	NAG	O5-C5-C4	2.78	114.73	110.13
4	A	706	FUC	C3-C4-C5	2.89	113.97	109.66
6	B	714	MAN	C1-O5-C5	2.98	116.52	112.14
3	A	705	NAG	C4-C3-C2	3.23	116.36	111.34
4	B	707	FUC	O5-C5-C4	3.37	115.41	109.58
4	B	705	FUC	C3-C4-C5	3.64	115.10	109.66
4	A	713	FUC	C1-C2-C3	3.65	113.97	109.55
4	A	713	FUC	O5-C1-C2	3.66	116.74	110.89
4	B	712	FUC	O5-C5-C4	3.77	116.11	109.58
4	A	706	FUC	C1-C2-C3	4.03	114.44	109.55
4	B	705	FUC	O5-C5-C4	4.89	118.05	109.58
6	A	712	MAN	C1-O5-C5	4.95	119.42	112.14
3	A	704	NAG	C1-O5-C5	5.00	119.49	112.14
4	B	707	FUC	C1-C2-C3	5.21	115.86	109.55
3	A	716	NAG	C1-O5-C5	6.82	122.16	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	714	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	1	0
3	A	716	NAG	4	0
3	A	717	NAG	4	0
5	B	703	BMA	1	0
3	B	706	NAG	3	0
3	B	708	NAG	1	0
3	B	709	NAG	2	0
4	B	712	FUC	2	0
3	B	715	NAG	2	0
3	B	716	NAG	3	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	523/538 (97%)	0.43	44 (8%) 14 15	23, 40, 88, 124	0
1	B	529/538 (98%)	0.19	24 (4%) 37 43	20, 33, 69, 109	0
All	All	1052/1076 (97%)	0.31	68 (6%) 22 25	20, 36, 79, 124	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	VAL	13.4
1	A	149	LEU	10.8
1	A	146	ARG	7.3
1	A	143	VAL	7.1
1	A	147	SER	6.7
1	A	107	VAL	6.0
1	A	150	SER	5.8
1	B	107	VAL	5.6
1	A	141	VAL	5.3
1	A	139	ASP	5.2
1	A	136	PHE	5.1
1	B	106	ASN	4.9
1	B	101	LEU	4.8
1	A	144	TRP	4.8
1	A	609	MET	4.5
1	A	526	GLY	4.5
1	B	526	GLY	4.4
1	B	103	LYS	4.4
1	A	106	ASN	4.2
1	A	151	PRO	4.0
1	B	133	VAL	4.0
1	B	166	TRP	3.8
1	A	101	LEU	3.8
1	A	140	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	94	PHE	3.5
1	B	131	SER	3.5
1	B	178	SER	3.5
1	B	163	CYS	3.4
1	B	525	ALA	3.4
1	A	98	ASN	3.3
1	A	115	ILE	3.1
1	B	102	LYS	3.1
1	A	157	LEU	3.0
1	A	169	PHE	2.9
1	B	108	ALA	2.9
1	A	163	CYS	2.9
1	B	113	VAL	2.8
1	A	525	ALA	2.8
1	A	145	THR	2.8
1	A	524	ALA	2.8
1	B	109	ARG	2.8
1	A	92	VAL	2.7
1	A	583	GLY	2.6
1	B	177	PRO	2.5
1	B	136	PHE	2.5
1	A	156	GLY	2.5
1	A	582	CYS	2.5
1	A	122	ASN	2.5
1	A	527	GLY	2.5
1	A	105	PRO	2.4
1	B	92	VAL	2.4
1	B	100	GLY	2.4
1	A	108	ALA	2.4
1	A	109	ARG	2.3
1	A	137	GLU	2.3
1	A	174	ILE	2.3
1	A	454	GLY	2.3
1	A	117	ILE	2.3
1	A	171	THR	2.3
1	B	104	GLU	2.2
1	A	102	LYS	2.2
1	A	99	HIS	2.2
1	B	99	HIS	2.1
1	A	104	GLU	2.1
1	B	610	PRO	2.1
1	A	138	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	96	ALA	2.0
1	B	137	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	FUC	A	706	10/11	0.84	0.40	11.77	52,65,78,84	0
6	MAN	B	714	11/12	0.85	0.30	6.92	72,93,112,122	0
3	NAG	A	705	14/15	0.81	0.23	4.93	56,67,81,91	0
4	FUC	B	707	10/11	0.90	0.33	4.24	52,62,73,88	0
6	MAN	A	712	11/12	0.85	0.34	3.82	62,80,96,103	0
3	NAG	A	707	14/15	0.77	0.40	3.23	54,79,93,97	0
3	NAG	B	708	14/15	0.90	0.22	2.40	52,63,77,83	0
3	NAG	B	710	14/15	0.94	0.19	1.23	33,44,56,57	0
3	NAG	B	715	14/15	0.96	0.21	1.15	51,64,70,74	0
4	FUC	A	713	10/11	0.80	0.24	0.82	52,64,77,83	0
4	FUC	B	705	10/11	0.86	0.23	0.67	55,71,83,85	0
7	NT8	B	717	19/19	0.96	0.18	-0.09	24,36,47,50	0
7	NT8	A	718	19/19	0.97	0.16	-0.50	35,51,64,64	0
3	NAG	A	708	14/15	0.95	0.14	-0.92	46,58,68,72	0
3	NAG	B	716	14/15	0.95	0.13	-1.26	42,54,68,70	0
3	NAG	A	714	14/15	0.95	0.10	-1.45	41,50,57,60	0
3	NAG	A	715	14/15	0.95	0.11	-1.49	38,45,53,60	0
2	ZN	A	701	1/1	0.96	0.13	-1.59	43,43,43,43	0
2	ZN	B	701	1/1	0.97	0.12	-1.80	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	702	1/1	0.98	0.10	-3.23	47,47,47,47	0
2	ZN	B	702	1/1	0.98	0.07	-3.71	38,38,38,38	0
3	NAG	A	704	14/15	0.82	0.29	-	59,81,99,103	0
5	BMA	A	710	11/12	0.90	0.15	-	45,65,76,78	0
4	FUC	B	712	10/11	0.85	0.22	-	60,75,92,96	0
3	NAG	B	706	14/15	0.85	0.16	-	47,66,81,86	0
6	MAN	A	711	11/12	0.84	0.22	-	68,77,90,95	0
5	BMA	B	703	11/12	0.81	0.33	-	69,85,101,105	0
3	NAG	A	703	14/15	0.89	0.30	-	61,71,84,96	0
3	NAG	A	716	14/15	0.75	0.35	-	66,91,124,131	0
3	NAG	A	709	14/15	0.87	0.25	-	61,76,91,103	0
5	BMA	B	713	11/12	0.88	0.14	-	63,76,87,93	0
3	NAG	A	717	14/15	0.77	0.45	-	91,113,134,137	0
3	NAG	B	711	14/15	0.83	0.27	-	58,75,89,90	0
3	NAG	B	704	14/15	0.94	0.18	-	45,59,70,71	0
3	NAG	B	709	14/15	0.86	0.51	-	64,81,96,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.