



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 07:27 pm GMT

PDB ID : 5JG8
Title : Crystal structure of human acid sphingomyelinase
Authors : Xiong, Z.J.; Prive, G.G.
Deposited on : 2016-04-19
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

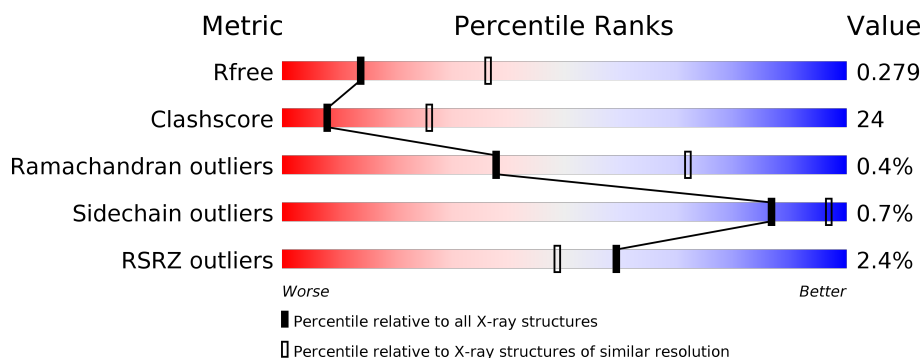
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 ≥ 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	586	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>10%</div> </div> </div>
1	B	586	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>10%</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	ACT	A	703	-	-	X	X
3	ACT	B	703	-	-	X	-
4	NAG	A	705	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8676 atoms, of which 35 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 Sphingomyelin phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4165	2686	718	738	23			
1	B	530	Total	C	N	O	S	0	0	0
			4176	2695	719	739	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	expression tag	UNP P17405
A	45	ALA	-	expression tag	UNP P17405
A	46	PRO	-	expression tag	UNP P17405
A	629	SER	CYS	engineered mutation	UNP P17405
B	44	GLY	-	expression tag	UNP P17405
B	45	ALA	-	expression tag	UNP P17405
B	46	PRO	-	expression tag	UNP P17405
B	629	SER	CYS	engineered mutation	UNP P17405

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

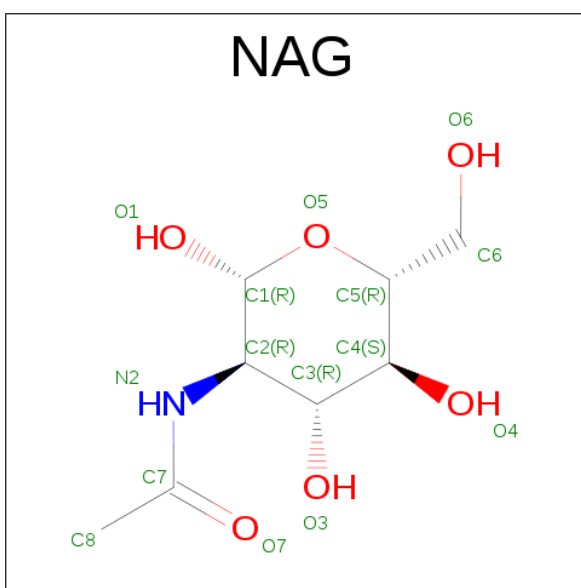
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



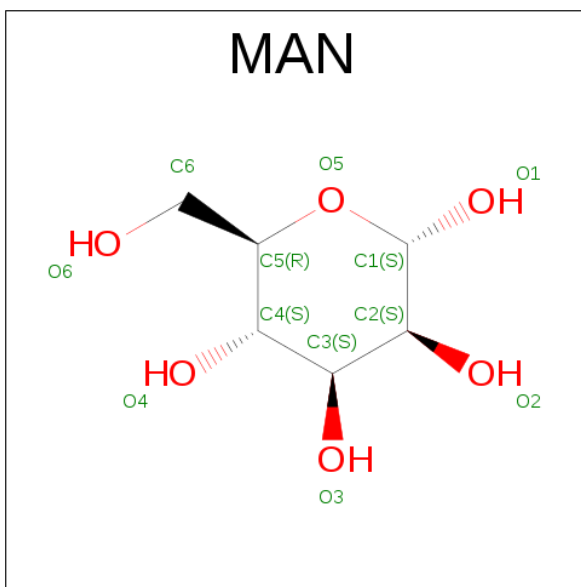
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			18	8	4	1	5		
4	A	1	Total	C	H	N	O	0	0
			18	8	4	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O			
			14	8	1	5	0	0	
4	A	1	Total	C	N	O			
			14	8	1	5	0	0	
4	A	1	Total	C	N	O			
			14	8	1	5	0	0	
4	A	1	Total	C	H	N	O		
			18	8	4	1	5	0	
4	A	1	Total	C	N	O			
			14	8	1	5	0	0	
4	A	1	Total	C	N	O			
			14	8	1	5	0	0	
4	A	1	Total	C	N	O			
			14	8	1	5	0	0	
4	B	1	Total	C	H	N	O		
			18	8	4	1	5	0	
4	B	1	Total	C	H	N	O		
			18	8	4	1	5	0	
4	B	1	Total	C	N	O			
			14	8	1	5	0	0	
4	B	1	Total	C	N	O			
			14	8	1	5	0	0	
4	B	1	Total	C	N	O			
			14	8	1	5	0	0	
4	B	1	Total	C	N	O			
			14	8	1	5	0	0	
4	B	1	Total	C	H	N	O		
			18	8	4	1	5	0	
4	B	1	Total	C	N	O			
			14	8	1	5	0	0	
4	B	1	Total	C	N	O			
			14	8	1	5	0	0	

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

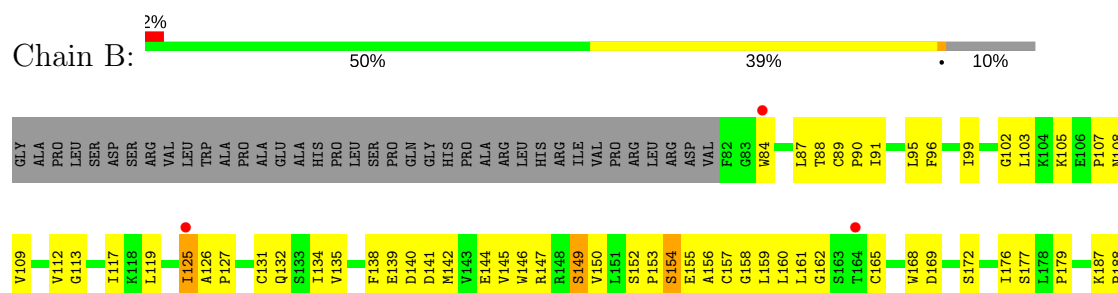
3 Residue-property plots

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

• Molecule 1: Spingomyelin phosphodiesterase



• Molecule 1: Spingomyelin phosphodiesterase



W553	W554	V557	Y558	R559	M560	F567	F570	L573	Y574	H575	K576	P580	P583	C584	G585	T586	P587	T592	L593	Q596	L597	R600	A601	D602	H611	PRO	ASP	GLY	SER	LEU	PRO	PRO	GLU	ALA	GLN	SER	LEU	TRP	PRO	PRO	ARG	PRO	LEU	PHE	SER						
G277	D278	I279	P280	A281	G282	D283	Y284	W285	A286	L287	T288	D291	R294	A295	L296	T297	T298	N301	L302	V303	L307	V310	P311	V312	Y313	P314	G317	N318	H319	E320	R416	G417	D418	K419	V420	I423	G424	H425	I426	P427	P428	L432	W435	S436	W437	M438	Y439	I442	V443	E447	
P189	G195	A196	R200	L201	L202	F203	L207	H208	W209	D210	H211	D212	T217	D218	P219	D220	C221	A222	D223	P224	L225	C226	C227	R228	R229	G230	S237	R238	Y243	W244	G245	E246	Y247	S248	K249	C250	D251	L252	P253	L254	R255	G265	P266	A267	G268	D271	M272	V273	Y274	W275	T276
L358	L361	R362	G365	F366	Y367	A368	L369	S370	P371	G374	L375	R376	L377	I378	S379	L380	N381	M382	N383	F384	C385	S386	R387	P399	L403	Q404	V407	R416	G417	D418	K419	V420	I423	G424	H425	I426	P427	P428	L432	W435	S436	W437	M438	Y439	I442	V443	E447				
M448	T449	L450	A451	A452	Q453	F454	F455	G456	H457	T458	H459	V460	D461	F466	Y467	D468	L472	L481	A482	P483	S484	A485	T486	T487	G490	L491	G494	Y495	R496	Q499	T500	S508	H509	V510	V511	L512	D513	H514	E515	L519	P531	H532	L535	L536	Y537	R538	T548				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.53Å 143.66Å 193.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.76 – 2.80 28.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (26.76-2.80) 93.8 (28.84-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.279 0.229 , 0.279	Depositor DCC
R_{free} test set	1977 reflections (4.34%)	DCC
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8676	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: ZN, ACT, NAG, 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	0.29	0/4311	0.49	1/5909 (0.0%)
1	B	0.30	0/4323	0.50	3/5925 (0.1%)
All	All	0.29	0/8634	0.50	4/11834 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	SER	O-C-N	6.43	132.99	122.70
1	A	152	SER	C-N-CD	6.34	141.72	128.40
1	B	154	SER	N-CA-C	-5.92	95.01	111.00
1	B	189	PRO	C-N-CA	-5.55	107.82	121.70

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	4165	0	4030	198	0
1	B	4176	0	4039	217	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	3	4	0
4	A	126	12	114	3	0
4	B	140	12	124	2	0
5	B	22	11	20	0	0
All	All	8641	35	8333	404	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 24.

The worst 5 of 404 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:457:HIS:CE1	3:A:703:ACT:H2	1.71	1.25
1:B:457:HIS:CE1	3:B:703:ACT:H1	1.73	1.23
1:B:117:ILE:HG12	1:B:135:VAL:HG11	1.25	1.13
1:A:117:ILE:HG12	1:A:135:VAL:HG11	1.29	1.12
1:A:125:ILE:HG12	4:B:704:NAG:H62	1.36	1.07

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	527/586 (90%)	485 (92%)	40 (8%)	2 (0%)	38	72
1	B	528/586 (90%)	490 (93%)	36 (7%)	2 (0%)	38	72
All	All	1055/1172 (90%)	975 (92%)	76 (7%)	4 (0%)	38	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	LEU
1	B	432	LEU
1	B	125	ILE
1	A	125	ILE

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	448/496 (90%)	445 (99%)	3 (1%)	87	97
1	B	449/496 (90%)	446 (99%)	3 (1%)	87	97
All	All	897/992 (90%)	891 (99%)	6 (1%)	87	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	435	TRP
1	B	435	TRP
1	B	288	THR
1	A	402	GLN
1	B	385	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	499	GLN
1	B	555	ASN
1	B	319	HIS
1	A	453	GLN
1	B	499	GLN

5.3.3 RNA ⓘ

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 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	ACT	A	703	2	1,3,3	3.98	1 (100%)	0,3,3	0.00	-
4	NAG	A	704	1	14,14,15	0.38	0	15,19,21	1.33	2 (13%)
4	NAG	A	705	1	14,14,15	0.53	0	15,19,21	1.06	1 (6%)
4	NAG	A	706	1,4	14,14,15	0.31	0	15,19,21	0.96	1 (6%)
4	NAG	A	707	4	14,14,15	0.28	0	15,19,21	0.83	0
4	NAG	A	708	1,4	14,14,15	0.31	0	15,19,21	0.95	0
4	NAG	A	709	4	14,14,15	0.29	0	15,19,21	0.81	1 (6%)
4	NAG	A	710	1,4	14,14,15	0.31	0	15,19,21	1.53	2 (13%)
4	NAG	A	711	4	14,14,15	0.34	0	15,19,21	0.79	0
4	NAG	A	712	1	14,14,15	0.28	0	15,19,21	0.69	0
3	ACT	B	703	2	1,3,3	1.82	0	0,3,3	0.00	-
4	NAG	B	704	1	14,14,15	0.37	0	15,19,21	1.38	1 (6%)
4	NAG	B	705	1	14,14,15	0.31	0	15,19,21	0.63	0
4	NAG	B	706	1,4	14,14,15	0.31	0	15,19,21	0.95	1 (6%)
4	NAG	B	707	5,4	14,14,15	0.27	0	15,19,21	0.83	0
5	MAN	B	708	4	11,11,12	0.29	0	13,15,17	0.81	1 (7%)
4	NAG	B	709	1,4	14,14,15	0.28	0	15,19,21	0.99	1 (6%)
4	NAG	B	710	5,4	14,14,15	0.34	0	15,19,21	0.94	1 (6%)
5	MAN	B	711	4	11,11,12	0.33	0	13,15,17	0.98	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	712	1,4	14,14,15	0.34	0	15,19,21	1.53	2 (13%)
4	NAG	B	713	4	14,14,15	0.47	0	15,19,21	0.90	1 (6%)
4	NAG	B	714	1,4	14,14,15	0.41	0	15,19,21	1.29	1 (6%)
4	NAG	B	715	4	14,14,15	0.30	0	15,19,21	0.76	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	ACT	A	703	2	-	0/0/0/0	0/0/0/0
4	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	706	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	707	4	-	0/6/23/26	0/1/1/1
4	NAG	A	708	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	709	4	-	0/6/23/26	0/1/1/1
4	NAG	A	710	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	711	4	-	0/6/23/26	0/1/1/1
4	NAG	A	712	1	-	0/6/23/26	0/1/1/1
3	ACT	B	703	2	-	0/0/0/0	0/0/0/0
4	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	705	1	-	0/6/23/26	0/1/1/1
4	NAG	B	706	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	707	5,4	-	0/6/23/26	0/1/1/1
5	MAN	B	708	4	-	0/2/19/22	1/1/1/1
4	NAG	B	709	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	710	5,4	-	0/6/23/26	0/1/1/1
5	MAN	B	711	4	-	0/2/19/22	0/1/1/1
4	NAG	B	712	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	713	4	-	0/6/23/26	0/1/1/1
4	NAG	B	714	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	715	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	ACT	CH3-C	3.98	1.53	1.48

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	710	NAG	C4-C3-C2	-2.83	106.86	111.02
4	B	710	NAG	O5-C1-C2	-2.60	107.85	111.47
4	B	709	NAG	O5-C1-C2	-2.44	108.08	111.47
4	A	709	NAG	O5-C1-C2	-2.06	108.61	111.47
4	B	706	NAG	C1-O5-C5	2.02	114.95	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	708	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	ACT	8	0
4	A	704	NAG	1	0
4	A	706	NAG	1	0
4	A	707	NAG	1	0
4	A	710	NAG	1	0
4	A	711	NAG	1	0
3	B	703	ACT	4	0
4	B	704	NAG	1	0
4	B	712	NAG	1	0
4	B	713	NAG	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, 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	529/586 (90%)	-0.10	12 (2%) 61 51	34, 57, 89, 125	0
1	B	530/586 (90%)	-0.08	13 (2%) 58 47	33, 58, 91, 133	0
All	All	1059/1172 (90%)	-0.09	25 (2%) 59 49	33, 57, 91, 133	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	ALA	3.3
1	A	237	SER	3.2
1	A	238	ARG	2.8
1	B	452	ALA	2.7
1	B	84	TRP	2.7

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(\AA^2)	Q<0.9
4	NAG	A	705	14/15	0.73	0.52	5.99	80,110,131,156	0
3	ACT	A	703	4/4	0.89	0.27	2.40	53,62,80,81	0
4	NAG	B	712	14/15	0.87	0.19	1.26	80,98,108,119	0
3	ACT	B	703	4/4	0.98	0.21	1.21	46,68,72,79	0
4	NAG	B	714	14/15	0.86	0.23	1.01	31,90,119,126	0
2	ZN	A	701	1/1	0.97	0.16	-0.48	55,55,55,55	0
4	NAG	B	706	14/15	0.94	0.10	-1.51	35,42,47,54	0
4	NAG	A	706	14/15	0.95	0.12	-1.80	40,62,69,71	0
2	ZN	B	701	1/1	0.91	0.09	-2.12	45,45,45,45	0
2	ZN	A	702	1/1	0.95	0.06	-2.73	90,90,90,90	0
2	ZN	B	702	1/1	0.97	0.06	-3.14	98,98,98,98	0
4	NAG	A	704	14/15	0.56	0.45	-	98,150,180,194	0
4	NAG	A	709	14/15	0.83	0.43	-	105,126,149,153	0
4	NAG	B	715	14/15	0.82	0.36	-	111,132,142,147	0
4	NAG	B	709	14/15	0.88	0.23	-	75,87,100,100	0
4	NAG	B	707	14/15	0.94	0.10	-	47,71,88,91	0
4	NAG	A	708	14/15	0.87	0.29	-	65,84,106,114	0
5	MAN	B	708	11/12	0.70	0.24	-	76,92,110,117	0
4	NAG	B	713	14/15	0.84	0.30	-	94,114,134,154	0
4	NAG	B	705	14/15	0.64	0.55	-	114,143,172,173	0
4	NAG	B	710	14/15	0.89	0.21	-	69,99,121,125	0
4	NAG	A	707	14/15	0.88	0.18	-	74,98,111,116	0
5	MAN	B	711	11/12	0.80	0.34	-	107,135,161,163	0
4	NAG	A	712	14/15	0.87	0.14	-	77,94,107,108	0
4	NAG	A	710	14/15	0.92	0.12	-	52,78,88,97	0
4	NAG	A	711	14/15	0.77	0.23	-	60,88,109,116	0
4	NAG	B	704	14/15	0.79	0.34	-	115,136,170,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.