Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2016 – 02:03 PM EDT

PDB ID	:	5HNS
Title	:	Structure of glycosylated NPC1 luminal domain C
Authors	:	Zhao, Y.; Ren, J.; Harlos, K.; Stuart, D.I.
Deposited on	:	2016-01-18
Resolution	:	2.45 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 (i) symbol.

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

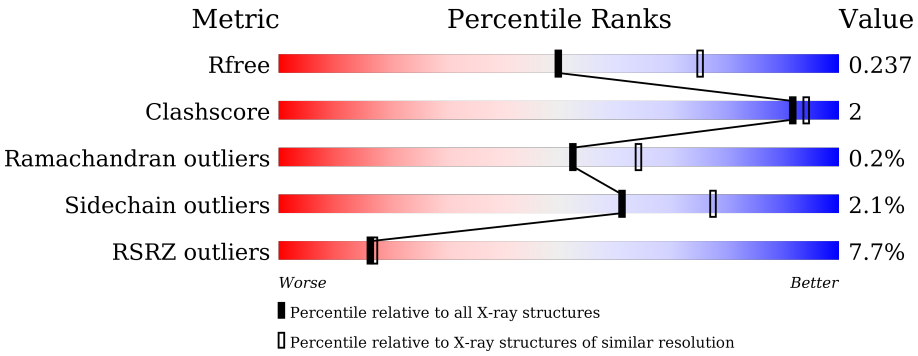
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 <=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	244	6% 82% 6% 12%
1	B	244	7% 85% · 11%

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
2	NAG	A	710	-	-	-	X
2	NAG	B	701	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3943 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.

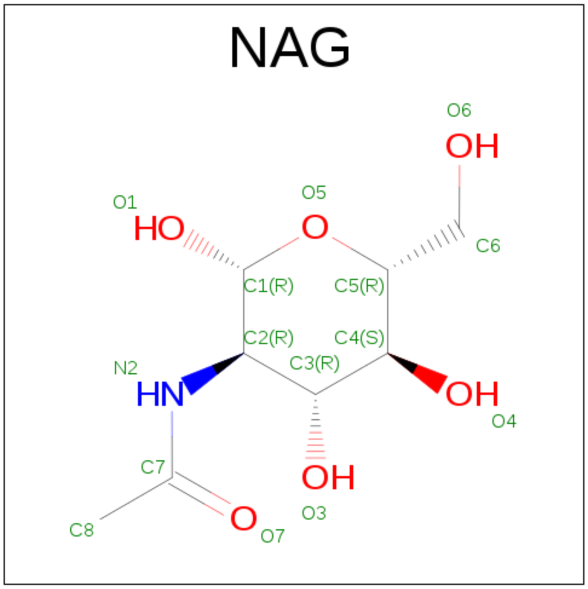
- Molecule 1 is a protein called Niemann-Pick C1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	5	0
			1787	1157	288	338	4			
1	B	216	Total	C	N	O	S	0	5	0
			1796	1162	289	341	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	384	GLU	-	expression tag	UNP O15118
A	385	THR	-	expression tag	UNP O15118
A	386	GLY	-	expression tag	UNP O15118
A	619	THR	-	expression tag	UNP O15118
A	620	GLY	-	expression tag	UNP O15118
A	621	THR	-	expression tag	UNP O15118
A	622	LEU	-	expression tag	UNP O15118
A	623	GLU	-	expression tag	UNP O15118
A	624	VAL	-	expression tag	UNP O15118
A	625	LEU	-	expression tag	UNP O15118
A	626	PHE	-	expression tag	UNP O15118
A	627	GLN	-	expression tag	UNP O15118
B	384	GLU	-	expression tag	UNP O15118
B	385	THR	-	expression tag	UNP O15118
B	386	GLY	-	expression tag	UNP O15118
B	619	THR	-	expression tag	UNP O15118
B	620	GLY	-	expression tag	UNP O15118
B	621	THR	-	expression tag	UNP O15118
B	622	LEU	-	expression tag	UNP O15118
B	623	GLU	-	expression tag	UNP O15118
B	624	VAL	-	expression tag	UNP O15118
B	625	LEU	-	expression tag	UNP O15118
B	626	PHE	-	expression tag	UNP O15118
B	627	GLN	-	expression tag	UNP O15118

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



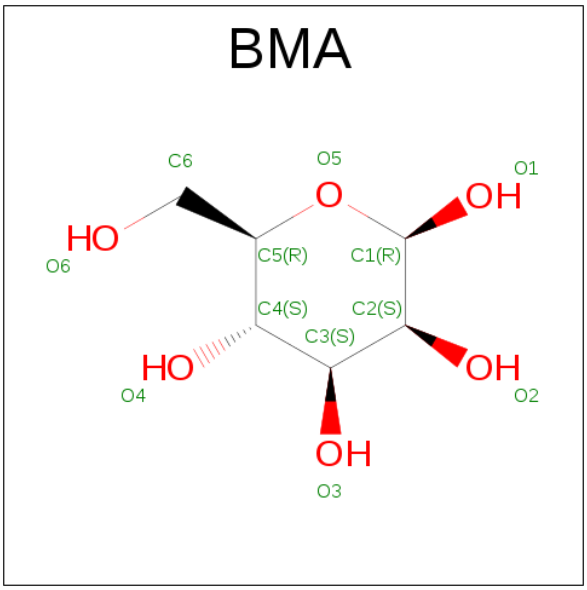
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total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

Continued on next page...

Continued from previous page...

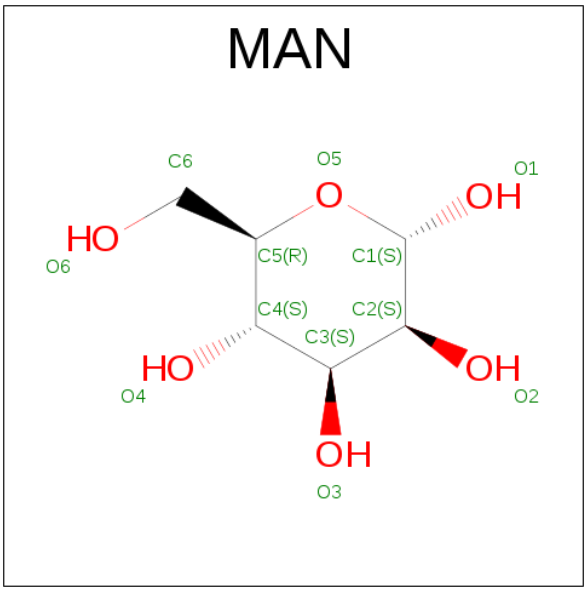
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



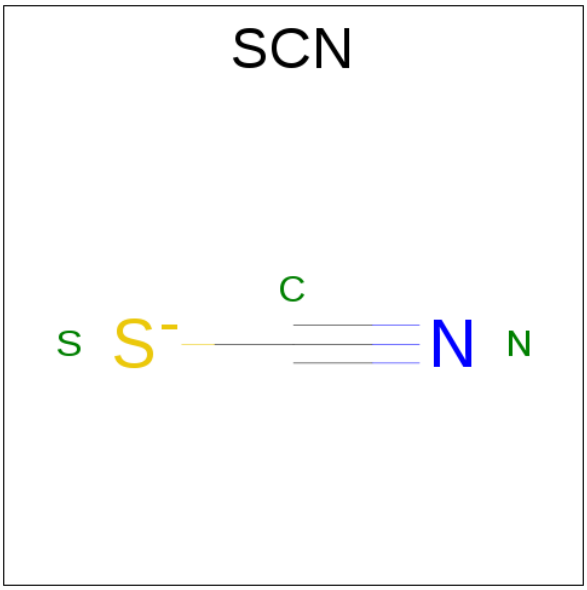
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0

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



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

- Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N S 3 1 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N S 3 1 1 1	0	0
5	B	1	Total C N S 3 1 1 1	0	0
5	B	1	Total C N S 3 1 1 1	0	0

- Molecule 6 is water.

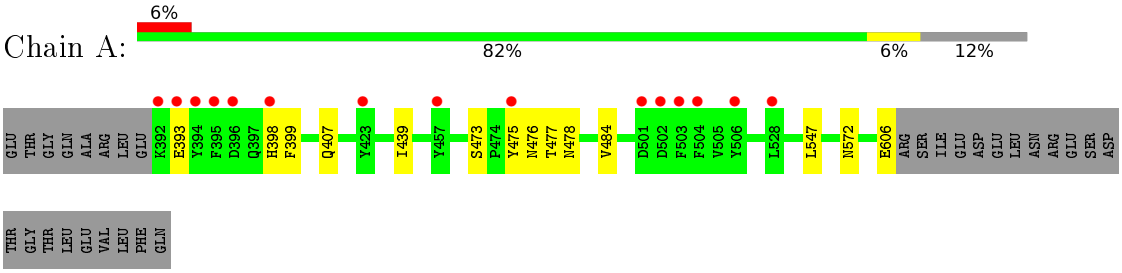
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	13	Total O 13 13	0	0
6	B	31	Total O 31 31	0	0

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 (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.

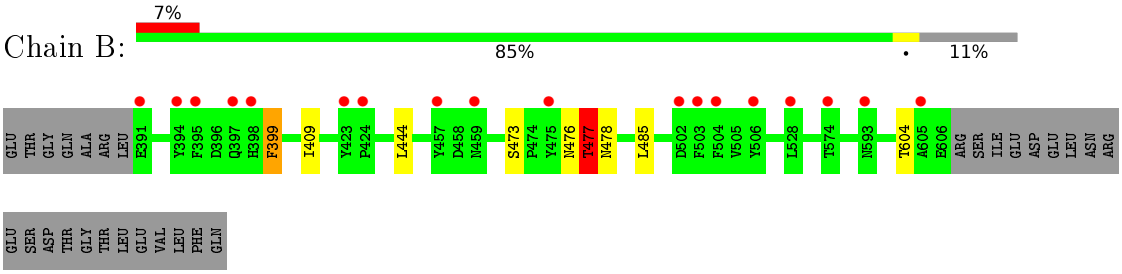
- Molecule 1: Niemann-Pick C1 protein

Chain A:



- Molecule 1: Niemann-Pick C1 protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.89Å 115.91Å 147.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.03 – 2.45 70.03 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (70.03-2.45) 100.0 (70.03-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.224 , 0.238 0.226 , 0.237	Depositor DCC
R_{free} test set	1385 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	63.4	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 28032 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3943	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, SCN, BMA, NAG

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	0/1844	0.63	0/2526
1	B	0.42	0/1853	0.62	1/2538 (0.0%)
All	All	0.42	0/3697	0.63	1/5064 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	399	PHE	CB-CG-CD2	-5.48	116.97	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	399	PHE	Peptide

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	1787	0	1677	10	0
1	B	1796	0	1685	6	0
2	A	126	0	112	0	0
2	B	112	0	98	1	0
3	A	11	0	9	0	0
3	B	22	0	18	0	0
4	A	11	0	10	0	0
4	B	22	0	20	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
6	A	13	0	0	0	0
6	B	31	0	0	0	0
All	All	3943	0	3629	16	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 (16) 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:477[A]:THR:HG22	1:A:478[A]:ASN:H	1.10	1.10
1:A:475[A]:TYR:O	1:A:476[A]:ASN:O	1.86	0.92
1:A:477[A]:THR:HG22	1:A:478[A]:ASN:N	1.87	0.88
1:B:476[A]:ASN:OD1	1:B:478[A]:ASN:N	2.13	0.75
1:A:477[A]:THR:CG2	1:A:478[A]:ASN:H	1.86	0.68
1:A:475[A]:TYR:O	1:A:476[A]:ASN:C	2.34	0.65
1:A:476[B]:ASN:OD1	1:A:478[B]:ASN:N	2.15	0.59
1:A:393:GLU:HG2	1:A:407:GLN:HE22	1.70	0.56
1:B:409:ILE:CD1	1:B:604:THR:HG22	2.39	0.52
1:A:476[B]:ASN:OD1	1:A:477[B]:THR:N	2.47	0.47
1:A:477[A]:THR:CG2	1:A:478[A]:ASN:N	2.57	0.47
1:B:476[B]:ASN:O	1:B:477[B]:THR:HB	2.14	0.47
1:A:484:VAL:HG11	1:A:547:LEU:HD21	1.98	0.46
1:B:476[A]:ASN:HD21	2:B:701:NAG:H82	1.81	0.44
1:B:476[A]:ASN:OD1	1:B:477[A]:THR:N	2.51	0.43
1:B:444:LEU:HA	1:B:485:LEU:HD13	2.02	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	218/244 (89%)	207 (95%)	11 (5%)	0	100 100
1	B	219/244 (90%)	210 (96%)	7 (3%)	2 (1%)	21 25
All	All	437/488 (90%)	417 (95%)	18 (4%)	2 (0%)	52 41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	477[A]	THR
1	B	477[B]	THR

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	198/219 (90%)	192 (97%)	6 (3%)	48 65
1	B	199/219 (91%)	196 (98%)	3 (2%)	72 84
All	All	397/438 (91%)	388 (98%)	9 (2%)	61 74

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	399	PHE
1	A	439	ILE
1	A	473	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	572	ASN
1	A	606	GLU
1	B	473	SER
1	B	477[A]	THR
1	B	477[B]	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	553	GLN
1	B	589	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	701	1,2	14,14,15	0.46	0	15,19,21	0.99	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	702	2	14,14,15	0.38	0	15,19,21	0.88	0
2	NAG	A	703	1,2	14,14,15	0.85	1 (7%)	15,19,21	2.67	2 (13%)
2	NAG	A	704	3,2	14,14,15	0.36	0	15,19,21	0.97	1 (6%)
3	BMA	A	705	2,4	11,11,12	0.42	0	15,15,17	1.08	1 (6%)
4	MAN	A	706	3	11,11,12	0.53	0	15,15,17	2.37	3 (20%)
2	NAG	A	707	1	14,14,15	0.47	0	15,19,21	0.99	0
2	NAG	A	708	1,2	14,14,15	0.33	0	15,19,21	1.46	2 (13%)
2	NAG	A	709	2	14,14,15	0.63	0	15,19,21	1.10	2 (13%)
2	NAG	A	710	1,2	14,14,15	0.33	0	15,19,21	0.59	0
2	NAG	A	711	2	14,14,15	0.29	0	15,19,21	0.91	1 (6%)
5	SCN	A	712	-	2,2,2	0.75	0	1,1,1	0.54	0
5	SCN	A	713	-	2,2,2	0.72	0	1,1,1	0.55	0
2	NAG	B	701	1,2	14,14,15	0.36	0	15,19,21	0.70	0
2	NAG	B	702	2	14,14,15	0.32	0	15,19,21	0.67	0
2	NAG	B	703	1,2	14,14,15	0.42	0	15,19,21	1.17	1 (6%)
2	NAG	B	704	2	14,14,15	0.47	0	15,19,21	0.78	0
2	NAG	B	705	1,2	14,14,15	0.22	0	15,19,21	0.72	0
2	NAG	B	706	3,2	14,14,15	0.23	0	15,19,21	0.65	0
3	BMA	B	707	2,4	11,11,12	0.47	0	15,15,17	1.47	3 (20%)
4	MAN	B	708	3	11,11,12	0.34	0	15,15,17	0.82	1 (6%)
4	MAN	B	709	3	11,11,12	0.39	0	15,15,17	0.94	1 (6%)
2	NAG	B	710	1,2	14,14,15	0.28	0	15,19,21	0.85	0
2	NAG	B	711	3,2	14,14,15	0.38	0	15,19,21	0.59	0
3	BMA	B	712	2	11,11,12	0.38	0	15,15,17	1.54	2 (13%)
5	SCN	B	713	-	2,2,2	0.70	0	1,1,1	0.32	0
5	SCN	B	714	-	2,2,2	0.69	0	1,1,1	0.32	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
2	NAG	A	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	702	2	-	0/6/23/26	0/1/1/1
2	NAG	A	703	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	704	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	705	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	706	3	-	0/2/19/22	0/1/1/1
2	NAG	A	707	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	708	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	709	2	-	0/6/23/26	0/1/1/1
2	NAG	A	710	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	711	2	-	0/6/23/26	0/1/1/1
5	SCN	A	712	-	-	0/0/0/0	0/0/0/0
5	SCN	A	713	-	-	0/0/0/0	0/0/0/0
2	NAG	B	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	702	2	-	0/6/23/26	0/1/1/1
2	NAG	B	703	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	704	2	-	0/6/23/26	0/1/1/1
2	NAG	B	705	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	706	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	707	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	708	3	-	0/2/19/22	0/1/1/1
4	MAN	B	709	3	-	0/2/19/22	0/1/1/1
2	NAG	B	710	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	711	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	712	2	-	0/2/19/22	0/1/1/1
5	SCN	B	713	-	-	0/0/0/0	0/0/0/0
5	SCN	B	714	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	703	NAG	C1-C2	2.75	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	708	NAG	O4-C4-C3	-3.37	102.75	110.36
2	B	703	NAG	O4-C4-C3	-2.94	103.72	110.36
3	A	705	BMA	O5-C1-C2	-2.75	106.50	110.89
3	B	707	BMA	O3-C3-C2	-2.29	105.81	110.01
2	A	709	NAG	O5-C5-C4	-2.01	106.81	110.13
3	B	707	BMA	C2-C3-C4	2.03	114.58	111.05
2	A	701	NAG	C1-O5-C5	2.13	115.27	112.14
3	B	712	BMA	C1-C2-C3	2.32	112.37	109.55
2	A	701	NAG	C4-C3-C2	2.33	114.96	111.34
2	A	709	NAG	C4-C3-C2	2.46	115.15	111.34
4	B	709	MAN	C1-O5-C5	2.50	115.81	112.14
2	A	704	NAG	C1-O5-C5	2.51	115.83	112.14
4	B	708	MAN	C1-O5-C5	2.57	115.92	112.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	711	NAG	C1-O5-C5	2.63	116.01	112.14
2	A	708	NAG	C1-O5-C5	3.12	116.73	112.14
4	A	706	MAN	O5-C1-C2	3.47	116.44	110.89
3	B	707	BMA	C3-C4-C5	3.52	116.50	110.23
2	A	703	NAG	O5-C5-C4	3.96	116.70	110.13
4	A	706	MAN	C1-C2-C3	4.29	114.75	109.55
3	B	712	BMA	C1-O5-C5	5.03	119.54	112.14
4	A	706	MAN	C1-O5-C5	6.93	122.33	112.14
2	A	703	NAG	C1-O5-C5	9.26	125.76	112.14

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
2	B	701	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

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^{th} 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	215/244 (88%)	0.68	15 (6%)	19	21	44, 66, 119, 189	0
1	B	216/244 (88%)	0.55	18 (8%)	14	14	44, 62, 113, 146	0
All	All	431/488 (88%)	0.61	33 (7%)	16	17	44, 63, 117, 189	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	PHE	11.8
1	A	394	TYR	9.8
1	B	503	PHE	9.3
1	A	503	PHE	6.9
1	B	605	ALA	5.9
1	A	502	ASP	5.5
1	A	392	LYS	5.3
1	A	393	GLU	5.3
1	A	423	TYR	4.9
1	B	504	PHE	4.8
1	B	397	GLN	4.7
1	B	391	GLU	4.4
1	A	504	PHE	4.3
1	B	502	ASP	3.9
1	A	396	ASP	3.9
1	B	528	LEU	3.5
1	A	475[A]	TYR	3.1
1	A	506	TYR	3.1
1	A	398	HIS	2.9
1	A	457	TYR	2.8
1	B	398	HIS	2.8
1	B	475[A]	TYR	2.7
1	B	457	TYR	2.4
1	B	506	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	424	PRO	2.3
1	B	459	ASN	2.2
1	A	501	ASP	2.2
1	B	395	PHE	2.2
1	B	394	TYR	2.1
1	B	593	ASN	2.1
1	A	528	LEU	2.1
1	B	574	THR	2.0
1	B	423	TYR	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^{th} 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
2	NAG	A	710	14/15	0.83	0.31	7.82	90,105,113,121	0
2	NAG	B	701	14/15	0.86	0.22	3.40	82,98,101,108	0
2	NAG	A	703	14/15	0.93	0.18	0.42	65,69,74,77	0
5	SCN	A	712	3/3	0.54	0.21	0.07	94,94,99,101	0
5	SCN	B	714	3/3	0.86	0.17	-0.30	102,102,105,112	0
2	NAG	B	710	14/15	0.95	0.16	-0.57	64,70,75,84	0
2	NAG	A	708	14/15	0.96	0.13	-0.83	78,83,88,100	0
2	NAG	B	705	14/15	0.95	0.14	-1.13	65,68,71,76	0
4	MAN	B	709	11/12	0.48	0.34	-	133,136,137,139	0
4	MAN	A	706	11/12	0.75	0.34	-	133,136,139,142	0
3	BMA	A	705	11/12	0.77	0.20	-	111,117,123,128	0
2	NAG	A	709	14/15	0.88	0.24	-	112,117,123,124	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	702	14/15	0.77	0.33	-	126,129,131,131	0
2	NAG	B	706	14/15	0.95	0.14	-	78,86,95,108	0
3	BMA	B	712	11/12	0.72	0.33	-	130,135,137,137	0
3	BMA	B	707	11/12	0.76	0.13	-	119,126,134,139	0
2	NAG	B	711	14/15	0.82	0.15	-	87,95,106,120	0
2	NAG	A	707	14/15	0.78	0.29	-	112,117,125,128	0
4	MAN	B	708	11/12	0.50	0.31	-	132,143,149,150	0
2	NAG	B	702	14/15	0.76	0.39	-	117,120,125,125	0
2	NAG	A	704	14/15	0.95	0.12	-	81,87,95,102	0
5	SCN	A	713	3/3	0.78	0.19	-	88,88,94,96	0
2	NAG	A	701	14/15	0.81	0.20	-	97,102,110,122	0
2	NAG	B	703	14/15	0.90	0.24	-	101,108,116,124	0
5	SCN	B	713	3/3	0.86	0.19	-	98,98,99,100	0
2	NAG	A	711	14/15	0.74	0.41	-	128,133,143,146	0
2	NAG	B	704	14/15	0.78	0.35	-	131,134,137,137	0

6.5 Other polymers (i)

There are no such residues in this entry.