



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 30, 2017 – 06:14 AM EDT

PDB ID : 5MRI
Title : Crystal structure of the Vps10p domain of human sortilin/NTS3 in complex with Triazolone 18
Authors : Andersen, J.L.; Strandbygaard, D.; Thirup, S.
Deposited on : unknown
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

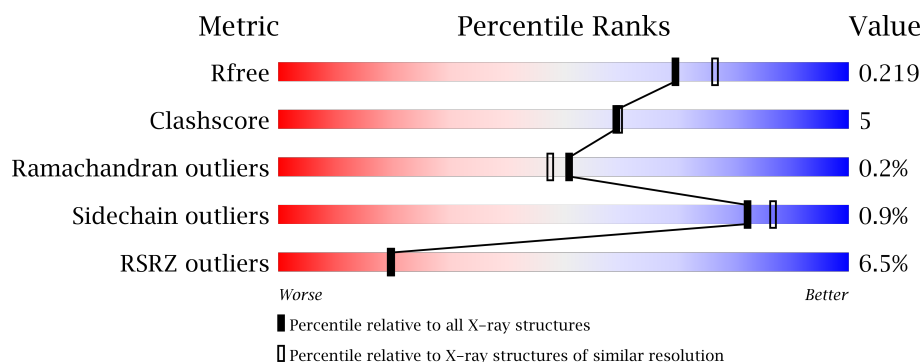
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	696	<div> <div>6%</div> <div>83%</div> <div>12%</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
2	NAG	A	806	-	-	-	X
4	Q9Y	A	807	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5686 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.

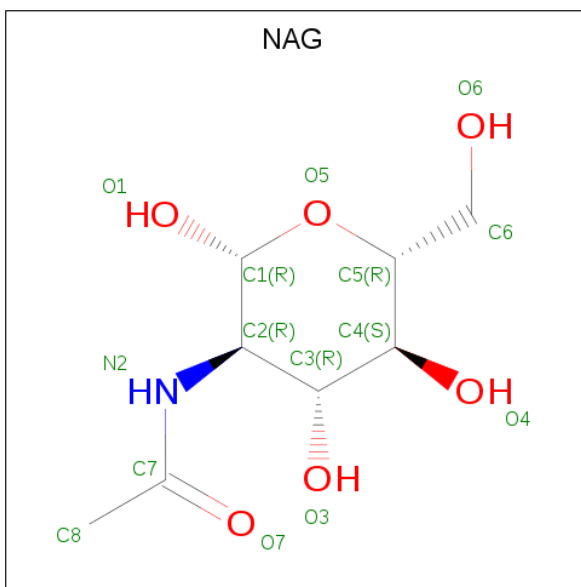
- Molecule 1 is a protein called Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	662	5243	3321	875	1017	30	0	7	0

There are 18 discrepancies between the modelled and reference sequences:

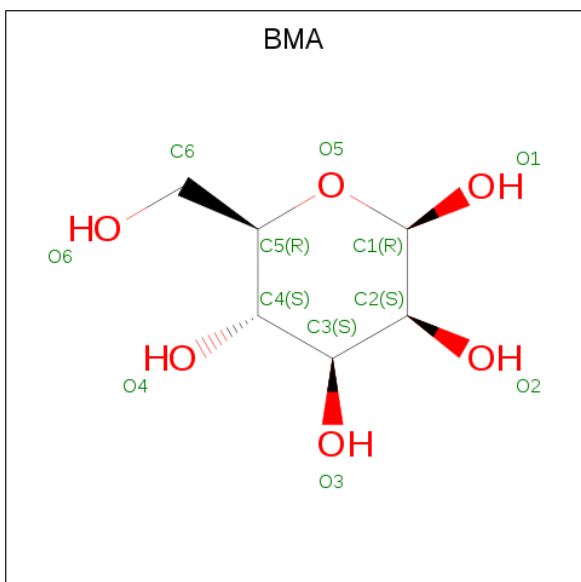
Chain	Residue	Modelled	Actual	Comment	Reference
A	617	MET	VAL	conflict	UNP Q99523
A	724	GLY	-	expression tag	UNP Q99523
A	725	SER	-	expression tag	UNP Q99523
A	726	ALA	-	expression tag	UNP Q99523
A	727	MET	-	expression tag	UNP Q99523
A	728	ILE	-	expression tag	UNP Q99523
A	729	GLU	-	expression tag	UNP Q99523
A	730	GLY	-	expression tag	UNP Q99523
A	731	ARG	-	expression tag	UNP Q99523
A	732	GLY	-	expression tag	UNP Q99523
A	733	VAL	-	expression tag	UNP Q99523
A	734	GLY	-	expression tag	UNP Q99523
A	735	HIS	-	expression tag	UNP Q99523
A	736	HIS	-	expression tag	UNP Q99523
A	737	HIS	-	expression tag	UNP Q99523
A	738	HIS	-	expression tag	UNP Q99523
A	739	HIS	-	expression tag	UNP Q99523
A	740	HIS	-	expression tag	UNP Q99523

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



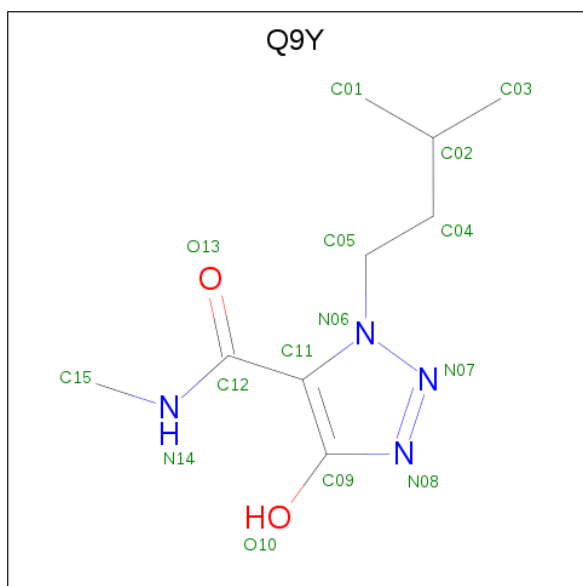
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	0	0
			11	6	5		

- Molecule 4 is {N}-methyl-3-(3-methylbutyl)-5-oxidanyl-1,2,3-triazole-4-carboxamide (three-letter code: Q9Y) (formula: C₉H₁₆N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	9	4	2		

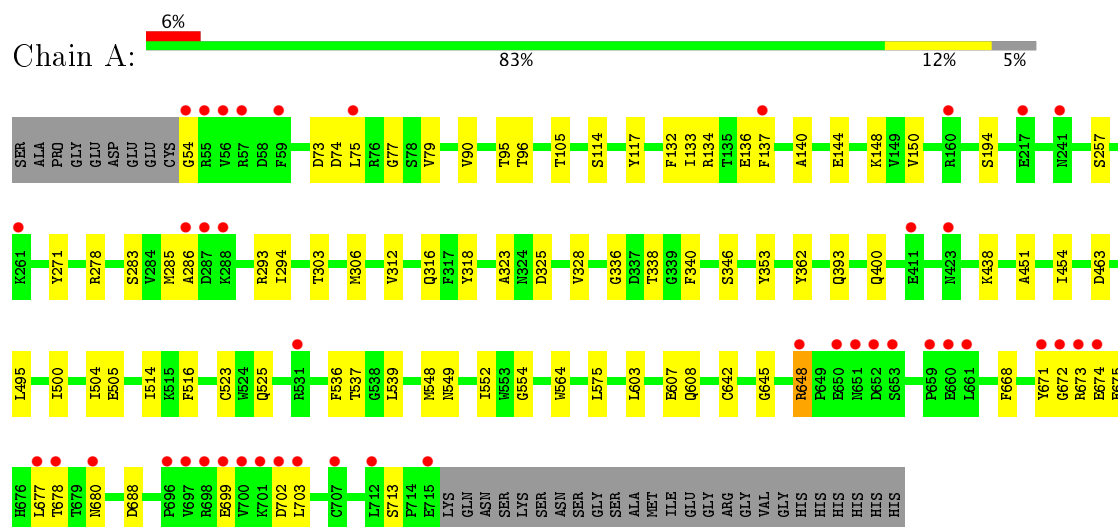
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	347	Total	O	0	0
			347	347		

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 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: Sortilin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.30 Å 81.06 Å 105.69 Å 90.00° 131.10° 90.00°	Depositor
Resolution (Å)	43.91 – 2.00 64.32 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.91-2.00) 98.4 (64.32-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.00 Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.195 , 0.219 0.194 , 0.219	Depositor DCC
R_{free} test set	2010 reflections (3.00%)	DCC
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5686	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, Q9Y, 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	0.26	0/5388	0.52	2/7301 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	278	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	648	ARG	C-N-CD	-5.06	109.46	120.60

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	5243	0	5061	56	0
2	A	70	0	62	3	0
3	A	11	0	10	0	0
4	A	15	0	0	1	0
5	A	347	0	0	13	0
All	All	5686	0	5133	57	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 5.

All (57) 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:607:GLU:OE2	5:A:901:HOH:O	2.03	0.74
1:A:713:SER:OG	5:A:902:HOH:O	2.06	0.74
1:A:438:LYS:NZ	5:A:911:HOH:O	2.23	0.71
1:A:514:ILE:HD12	1:A:552:ILE:HD11	1.73	0.69
1:A:303:THR:HB	1:A:673:ARG:HH12	1.58	0.69
1:A:285:MET:HG2	1:A:286:ALA:N	2.09	0.68
1:A:523:CYS:SG	5:A:1227:HOH:O	2.53	0.67
1:A:336:GLY:O	5:A:905:HOH:O	2.13	0.65
1:A:608:GLN:NE2	5:A:904:HOH:O	2.12	0.64
1:A:54:GLY:HA3	1:A:525:GLN:HG3	1.81	0.62
1:A:504:ILE:HG13	1:A:539:LEU:HD21	1.80	0.62
1:A:134:ARG:HD2	1:A:137:PHE:HE2	1.64	0.61
1:A:73:ASP:OD1	1:A:74:ASP:N	2.33	0.61
1:A:645:GLY:HA3	1:A:703:LEU:HD13	1.83	0.61
1:A:642:CYS:SG	1:A:648:ARG:HG3	2.42	0.59
1:A:675:GLU:N	1:A:675:GLU:OE2	2.24	0.59
1:A:680:ASN:N	5:A:903:HOH:O	2.07	0.58
1:A:318:TYR:O	4:A:807:Q9Y:N14	2.37	0.57
1:A:495:LEU:HB2	1:A:500[A]:ILE:HG23	1.90	0.54
1:A:54:GLY:N	1:A:523:CYS:HB3	2.22	0.54
1:A:505:GLU:OE2	5:A:906:HOH:O	2.18	0.54
1:A:148:LYS:NZ	1:A:194:SER:OG	2.41	0.52
1:A:306:MET:HE1	1:A:671:TYR:HB2	1.92	0.52
1:A:136:GLU:O	5:A:907:HOH:O	2.19	0.52
1:A:323:ALA:HB2	1:A:328:VAL:HG23	1.91	0.52
2:A:806:NAG:O6	5:A:908:HOH:O	2.19	0.50
1:A:140:ALA:HB3	1:A:150:VAL:HB	1.93	0.50
1:A:346:SER:HB3	1:A:353:TYR:CE2	2.47	0.49
1:A:75:LEU:HD23	1:A:564:TRP:CD1	2.47	0.49
1:A:500[A]:ILE:HD11	1:A:516:PHE:HB2	1.95	0.49
1:A:312:VAL:HB	1:A:316:GLN:HB2	1.94	0.48
1:A:105:THR:O	1:A:105:THR:HG22	2.15	0.47
1:A:463:ASP:OD2	5:A:909:HOH:O	2.20	0.46
1:A:96:THR:HB	1:A:132:PHE:CE1	2.51	0.46
1:A:294:ILE:HD11	1:A:318:TYR:CD2	2.51	0.45
1:A:271:TYR:HB3	1:A:283:SER:OG	2.16	0.45
1:A:548:MET:N	2:A:804:NAG:H82	2.32	0.45
1:A:293:ARG:NE	5:A:910:HOH:O	2.21	0.45
1:A:674:GLU:H	1:A:674:GLU:CD	2.21	0.45
1:A:96:THR:HG21	1:A:133:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PHE:HZ	1:A:539:LEU:HG	1.82	0.45
1:A:90:VAL:HA	1:A:114:SER:O	2.17	0.44
1:A:338:THR:HB	1:A:340:PHE:CE2	2.52	0.44
1:A:537:THR:HG23	1:A:554:GLY:HA2	1.99	0.44
1:A:678:THR:HG22	1:A:702:ASP:HA	2.00	0.43
1:A:668:PHE:O	1:A:672:GLY:N	2.46	0.43
1:A:117:TYR:CG	1:A:549:ASN:OD1	2.72	0.43
1:A:674:GLU:HA	1:A:677:LEU:HD12	2.01	0.43
1:A:75:LEU:HA	1:A:95:THR:HG21	2.02	0.42
1:A:285:MET:HG2	1:A:286:ALA:H	1.84	0.42
1:A:451:ALA:HB1	1:A:454[B]:ILE:HD12	2.02	0.42
1:A:500[B]:ILE:HG13	1:A:575:LEU:HD11	2.00	0.42
1:A:548:MET:HB2	2:A:804:NAG:H82	2.01	0.41
1:A:77:GLY:O	1:A:79:VAL:HG23	2.19	0.41
1:A:603:LEU:O	1:A:688:ASP:HA	2.20	0.41
1:A:75:LEU:HD23	1:A:564:TRP:CG	2.56	0.40
1:A:400:GLN:HG3	5:A:956:HOH:O	2.21	0.40

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	667/696 (96%)	649 (97%)	17 (2%)	1 (0%)	55 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLU

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	585/605 (97%)	580 (99%)	5 (1%)	82 87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	SER
1	A	325	ASP
1	A	362	TYR
1	A	393	GLN
1	A	699	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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	801	1,2	14,14,15	0.32	0	15,19,21	0.53	0
2	NAG	A	802	3,2	14,14,15	0.31	0	15,19,21	0.49	0
3	BMA	A	803	2	11,11,12	0.52	0	13,15,17	0.89	0
2	NAG	A	804	1,2	14,14,15	0.55	0	15,19,21	0.86	1 (6%)
2	NAG	A	805	2	14,14,15	0.24	0	15,19,21	0.61	0
2	NAG	A	806	1	14,14,15	0.32	0	15,19,21	0.59	0
4	Q9Y	A	807	-	14,15,15	3.24	3 (21%)	8,20,20	2.40	3 (37%)

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	801	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	802	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	803	2	-	0/2/19/22	0/1/1/1
2	NAG	A	804	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	805	2	-	0/6/23/26	0/1/1/1
2	NAG	A	806	1	-	0/6/23/26	0/1/1/1
4	Q9Y	A	807	-	-	0/7/11/11	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	807	Q9Y	C05-N06	-4.03	1.40	1.47
4	A	807	Q9Y	O10-C09	2.32	1.39	1.28
4	A	807	Q9Y	C12-N14	10.86	1.45	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	807	Q9Y	C11-N06-N07	-5.17	108.06	112.56
4	A	807	Q9Y	C15-N14-C12	-3.14	118.20	121.84
4	A	807	Q9Y	O13-C12-N14	-2.37	118.75	122.49
2	A	804	NAG	C1-O5-C5	2.17	115.16	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	NAG	2	0
2	A	806	NAG	1	0
4	A	807	Q9Y	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, 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	662/696 (95%)	0.24	43 (6%) 20 20	27, 46, 84, 136	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	697	VAL	9.6
1	A	701	LYS	6.3
1	A	54	GLY	6.2
1	A	55	ARG	6.2
1	A	286	ALA	6.0
1	A	699	GLU	5.6
1	A	700	VAL	5.0
1	A	287	ASP	4.9
1	A	651	ASN	4.7
1	A	652	ASP	4.5
1	A	698	ARG	4.2
1	A	653	SER	4.0
1	A	650	GLU	3.7
1	A	288	LYS	3.5
1	A	531	ARG	3.4
1	A	160	ARG	3.4
1	A	241	ASN	3.2
1	A	57	ARG	3.1
1	A	56	VAL	3.1
1	A	707	CYS	3.0
1	A	702	ASP	2.9
1	A	678	THR	2.7
1	A	673	ARG	2.7
1	A	659	PRO	2.6
1	A	661	LEU	2.6
1	A	703	LEU	2.6
1	A	137	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	261	LYS	2.4
1	A	75	LEU	2.4
1	A	423	ASN	2.4
1	A	715	GLU	2.4
1	A	680	ASN	2.3
1	A	648	ARG	2.3
1	A	217	GLU	2.3
1	A	677	LEU	2.2
1	A	674	GLU	2.2
1	A	660	GLU	2.2
1	A	672	GLY	2.1
1	A	411	GLU	2.1
1	A	696	PRO	2.1
1	A	671	TYR	2.1
1	A	59	PHE	2.0
1	A	712	LEU	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
2	NAG	A	806	14/15	0.88	0.20	5.45	59,69,73,74	0
4	Q9Y	A	807	15/15	0.93	0.17	2.27	34,37,64,65	0
2	NAG	A	804	14/15	0.91	0.14	0.78	33,40,42,43	0
2	NAG	A	801	14/15	0.96	0.12	-0.93	27,32,36,40	0
2	NAG	A	805	14/15	0.79	0.27	-	56,67,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BMA	A	803	11/12	0.63	0.28	-	87,94,97,99	0
2	NAG	A	802	14/15	0.90	0.12	-	41,56,66,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.