



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2016 – 03:07 PM EDT

PDB ID : 5EWM
Title : CRYSTAL STRUCTURE OF AMINO TERMINAL DOMAINS OF THE
NMDA RECEPTOR SUBUNIT GLUN1 AND GLUN2B IN COMPLEX
WITH EVT-101
Authors : Pandit, J.
Deposited on : 2015-11-20
Resolution : 2.76 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.

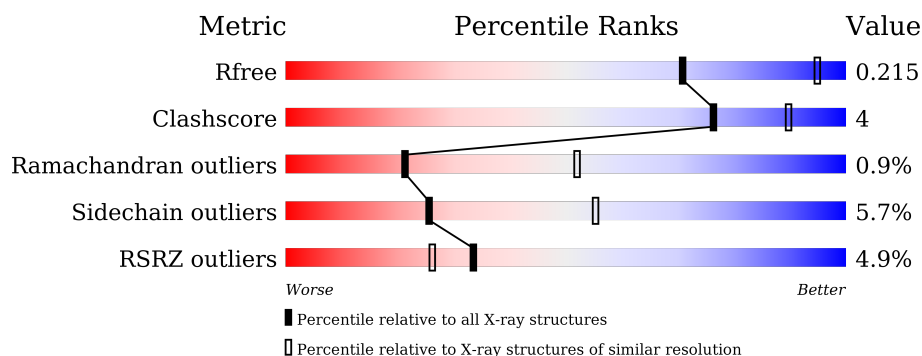
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (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 : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

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X-RAY DIFFRACTION

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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	390	<div> <div></div> <div>80%</div> <div>12%</div> <div>8%</div> </div>
1	C	390	<div> <div>7%</div> <div></div> <div>78%</div> <div>11%</div> <div>9%</div> </div>
2	B	364	<div> <div>4%</div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div>
2	D	364	<div> <div>7%</div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	501	-	-	-	X
3	NA	C	501	-	-	-	X
4	NAG	A	502	-	-	-	X
4	NAG	C	502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11534 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 NMDA glutamate receptor subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2752	1753	477	511	11			
1	C	356	Total	C	N	O	S	0	0	0
			2737	1741	479	507	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP Q91977
A	371	GLN	ASN	engineered mutation	UNP Q91977
A	409	LEU	-	expression tag	UNP Q91977
A	410	VAL	-	expression tag	UNP Q91977
A	411	PRO	-	expression tag	UNP Q91977
A	412	ARG	-	expression tag	UNP Q91977
C	61	GLN	ASN	engineered mutation	UNP Q91977
C	371	GLN	ASN	engineered mutation	UNP Q91977
C	409	LEU	-	expression tag	UNP Q91977
C	410	VAL	-	expression tag	UNP Q91977
C	411	PRO	-	expression tag	UNP Q91977
C	412	ARG	-	expression tag	UNP Q91977

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2781	1793	443	530	15			
2	D	355	Total	C	N	O	S	0	0	0
			2778	1791	436	535	16			

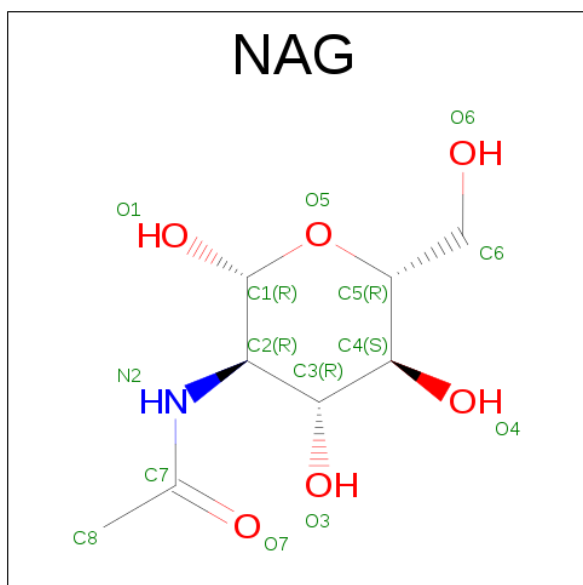
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q13224
D	348	ASP	ASN	engineered mutation	UNP Q13224

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	3	Total Na 3 3	0	0
3	C	1	Total Na 1 1	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



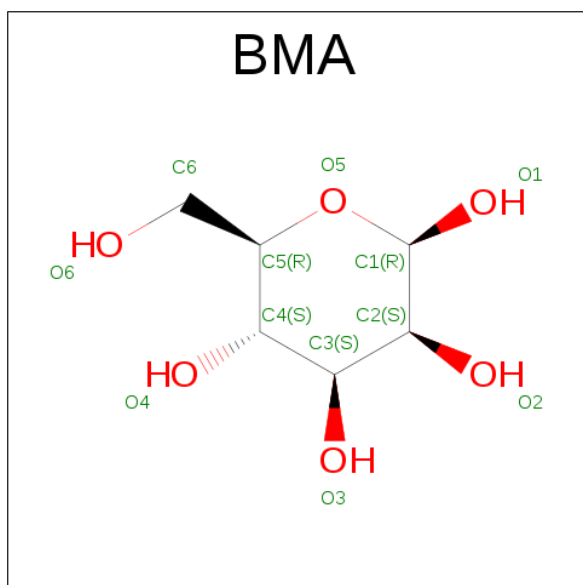
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0

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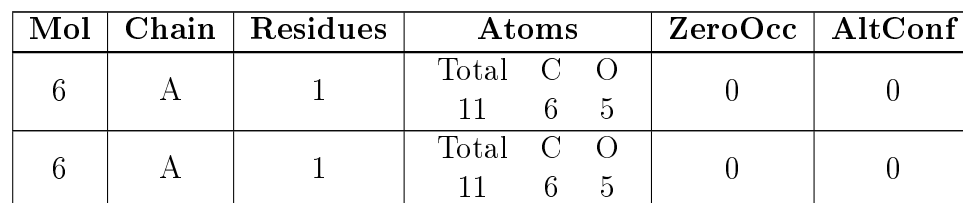
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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



- # 5SM
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- The chemical structure of 5SM is shown with atom labels. The indole ring system is labeled with N1, N2, C1, C2, C3, and C4. The pyridine ring is labeled with N3, N4, C5, C6, C7, and C8. The benzene ring is labeled with C9, C10, C11, C12, C13, and C14. The fluorine atoms are labeled F1, F2, and F3. The structure is a 5-substituted melatonin derivative.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	F	N	0	0
			23	16	3	4		



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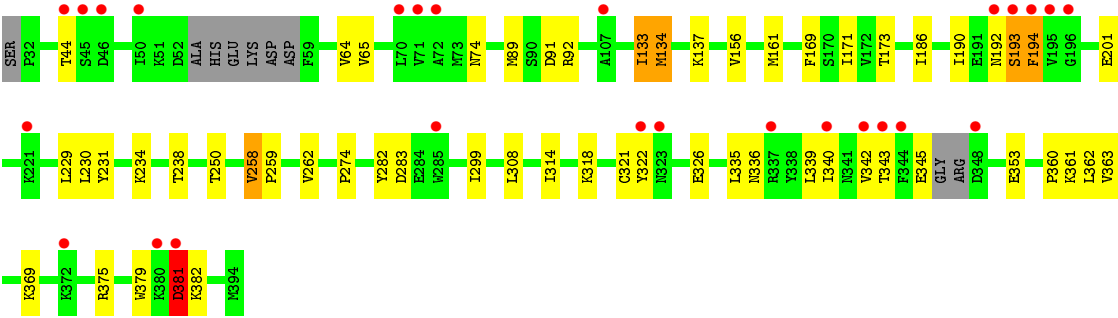
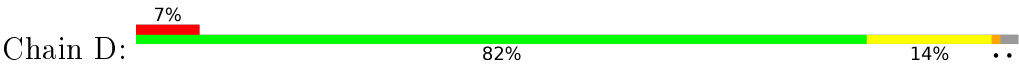
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	F	N	0	0
			23	16	3	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	115	Total	O	0	0
			115	115		
8	B	86	Total	O	0	0
			86	86		
8	C	39	Total	O	0	0
			39	39		
8	D	50	Total	O	0	0
			50	50		

MET

• Molecule 2: Glutamate receptor ionotropic, NMDA 2B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.40Å 60.61Å 144.50Å 90.00° 116.27° 90.00°	Depositor
Resolution (Å)	40.41 – 2.76 40.11 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.41-2.76) 98.2 (40.11-2.76)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.171 , 0.211 0.172 , 0.215	Depositor DCC
R_{free} test set	2608 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53264 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11534	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, 5SM, BMA, 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	0.58	0/2809	0.72	0/3819
1	C	0.47	0/2792	0.69	1/3794 (0.0%)
2	B	0.51	0/2846	0.71	1/3874 (0.0%)
2	D	0.49	0/2841	0.72	1/3864 (0.0%)
All	All	0.52	0/11288	0.71	3/15351 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	HIS	C-N-CA	5.49	135.41	121.70
2	D	381	ASP	C-N-CA	5.07	134.38	121.70
1	C	130	ASP	C-N-CA	5.05	134.33	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	2752	0	2717	20	0
1	C	2737	0	2705	25	0
2	B	2781	0	2685	21	0
2	D	2778	0	2691	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	42	0	37	0	0
4	B	28	0	26	0	0
4	C	14	0	13	1	0
4	D	28	0	26	0	0
5	A	11	0	8	0	0
6	A	22	0	20	0	0
7	B	23	0	0	1	0
7	D	23	0	0	0	0
8	A	115	0	0	1	0
8	B	86	0	0	0	0
8	C	39	0	0	1	0
8	D	50	0	0	0	0
All	All	11534	0	10928	84	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 4.

The worst 5 of 84 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:376:ASN:HD21	1:A:401:ILE:H	1.36	0.73
1:A:402:TRP:HD1	1:A:406:GLU:HA	1.60	0.65
1:A:270:VAL:HG13	1:A:274:GLU:HB2	1.81	0.62
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.82	0.62
1:C:270:VAL:HG13	1:C:274:GLU:HB2	1.84	0.60

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	351/390 (90%)	343 (98%)	7 (2%)	1 (0%)	46	77
1	C	350/390 (90%)	338 (97%)	8 (2%)	4 (1%)	17	46
2	B	352/364 (97%)	334 (95%)	17 (5%)	1 (0%)	46	77
2	D	349/364 (96%)	334 (96%)	9 (3%)	6 (2%)	11	32
All	All	1402/1508 (93%)	1349 (96%)	41 (3%)	12 (1%)	21	52

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	382	LYS
2	B	283	ASP
1	C	54	PHE
1	C	56	ARG
2	D	194	PHE

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	292/336 (87%)	281 (96%)	11 (4%)	40	73
1	C	289/336 (86%)	273 (94%)	16 (6%)	27	56
2	B	301/326 (92%)	283 (94%)	18 (6%)	24	53
2	D	305/326 (94%)	282 (92%)	23 (8%)	17	40
All	All	1187/1324 (90%)	1119 (94%)	68 (6%)	25	55

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	27	VAL
1	C	273	ARG
2	D	343	THR
1	C	44	GLU
1	C	136	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	28	ASN
1	C	53	HIS
2	D	105	GLN
2	B	311	HIS
1	C	376	ASN

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 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	$\# Z > 2$
4	NAG	A	502	1	14,14,15	0.29	0	15,19,21	1.07	1 (6%)
4	NAG	A	503	1,4	14,14,15	0.35	0	15,19,21	0.49	0
4	NAG	A	504	5,4	14,14,15	0.27	0	15,19,21	0.54	0
5	BMA	A	505	4,6	11,11,12	0.25	0	15,15,17	0.84	1 (6%)
6	MAN	A	506	5	11,11,12	0.31	0	15,15,17	0.84	1 (6%)
6	MAN	A	507	5	11,11,12	0.32	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	501	2	14,14,15	0.28	0	15,19,21	0.64	0
4	NAG	B	502	2	14,14,15	0.28	0	15,19,21	0.65	0
7	5SM	B	503	-	20,25,25	0.39	0	24,35,35	0.94	2 (8%)
4	NAG	C	502	1	14,14,15	0.40	0	15,19,21	0.57	0
4	NAG	D	501	2	14,14,15	0.35	0	15,19,21	0.39	0
4	NAG	D	502	2	14,14,15	0.31	0	15,19,21	0.53	0
7	5SM	D	503	-	20,25,25	0.36	0	24,35,35	0.76	1 (4%)

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
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	NAG	A	503	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	504	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	505	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	506	5	-	0/2/19/22	0/1/1/1
6	MAN	A	507	5	-	0/2/19/22	0/1/1/1
4	NAG	B	501	2	-	0/6/23/26	0/1/1/1
4	NAG	B	502	2	-	0/6/23/26	0/1/1/1
7	5SM	B	503	-	-	0/10/12/12	0/3/3/3
4	NAG	C	502	1	-	0/6/23/26	0/1/1/1
4	NAG	D	501	2	-	0/6/23/26	0/1/1/1
4	NAG	D	502	2	-	0/6/23/26	0/1/1/1
7	5SM	D	503	-	-	0/10/12/12	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	503	5SM	C5-C6-C7	-2.49	119.40	121.96
7	D	503	5SM	C4-N2-C2	-2.17	106.56	108.60
7	B	503	5SM	C4-N2-C2	-2.03	106.69	108.60
6	A	506	MAN	C1-C2-C3	2.20	112.21	109.55
5	A	505	BMA	C1-O5-C5	2.40	115.67	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	503	5SM	1	0
4	C	502	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	357/390 (91%)	-0.21	3 (0%) 87 83	36, 53, 85, 109	0
1	C	356/390 (91%)	0.32	28 (7%) 15 10	61, 87, 116, 145	0
2	B	356/364 (97%)	0.19	13 (3%) 45 38	44, 73, 109, 142	0
2	D	355/364 (97%)	0.27	26 (7%) 18 13	55, 80, 120, 139	0
All	All	1424/1508 (94%)	0.14	70 (4%) 33 26	36, 76, 113, 145	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	381	ASP	5.3
1	C	259	LEU	5.1
1	C	358	ARG	4.9
2	D	193	SER	4.4
1	C	369	PHE	4.4

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
3	NA	A	501	1/1	0.90	0.42	21.56	67,67,67,67	0
3	NA	C	501	1/1	0.93	0.29	4.18	80,80,80,80	0
4	NAG	A	502	14/15	0.96	0.20	2.70	56,69,75,79	0
4	NAG	C	502	14/15	0.80	0.27	2.05	98,105,107,111	0
6	MAN	A	506	11/12	0.98	0.16	0.89	55,61,69,71	0
7	5SM	D	503	23/23	0.98	0.22	0.25	66,71,72,73	0
7	5SM	B	503	23/23	0.97	0.22	0.03	42,48,57,60	0
3	NA	A	508	1/1	0.94	0.12	-0.68	45,45,45,45	0
4	NAG	A	503	14/15	0.96	0.11	-1.83	45,59,64,68	0
3	NA	B	504	1/1	0.92	0.09	-1.92	57,57,57,57	0
3	NA	A	509	1/1	0.94	0.09	-2.22	62,62,62,62	0
4	NAG	B	501	14/15	0.69	0.27	-	140,143,145,147	0
4	NAG	D	502	14/15	0.71	0.44	-	152,158,161,163	0
4	NAG	D	501	14/15	0.70	0.41	-	150,154,158,160	0
4	NAG	B	502	14/15	0.81	0.30	-	128,136,142,145	0
5	BMA	A	505	11/12	0.95	0.15	-	62,69,75,83	0
6	MAN	A	507	11/12	0.92	0.17	-	88,89,93,96	0
4	NAG	A	504	14/15	0.96	0.12	-	61,65,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.