



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2018 – 06:55 PM EDT

PDB ID : 2C4L
Title : Structure of Neuraminidase Subtype N9 Complexed with 30 MM Sialic Acid (NANA, NEU5AC), Crystal Soaked for 24 Hours at 291 K and Finally Back-soaked for 30 Min in a Cryoprotectant Solution which did not contain NEU5AC
Authors : Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.
Deposited on : 2005-10-20
Resolution : 2.15 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

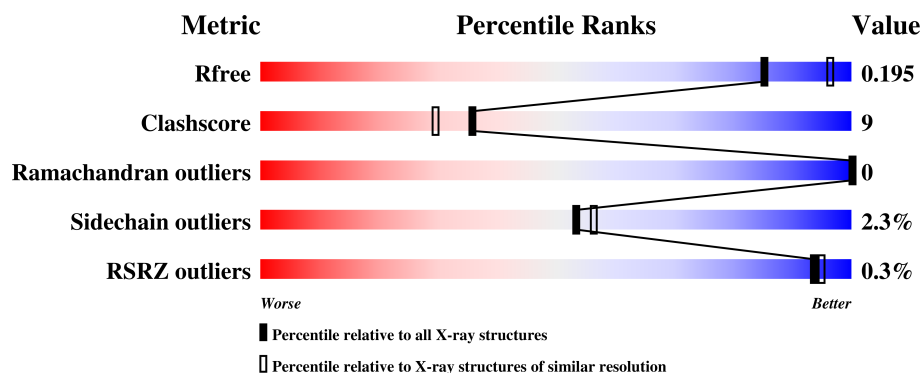
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.15 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}	111664	1287 (2.16-2.16)
Clashscore	122126	1390 (2.16-2.16)
Ramachandran outliers	120053	1368 (2.16-2.16)
Sidechain outliers	120020	1367 (2.16-2.16)
RSRZ outliers	108989	1262 (2.16-2.16)

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	388	 89% 10% .

2 Entry composition [i](#)

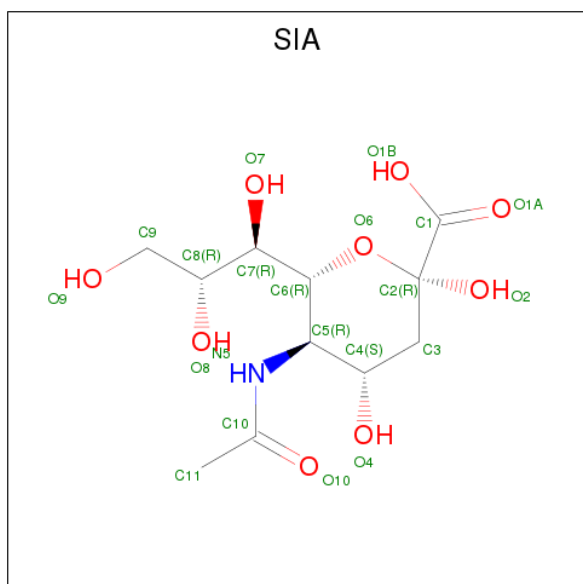
There are 7 unique types of molecules in this entry. The entry contains 3490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEURAMINIDASE SUBTYPE N9.

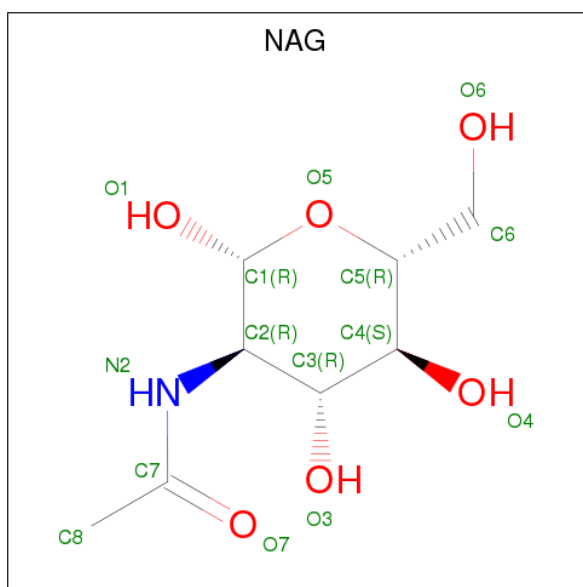
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3067	1914	538	592	23			

- Molecule 2 is O-SIALIC ACID (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



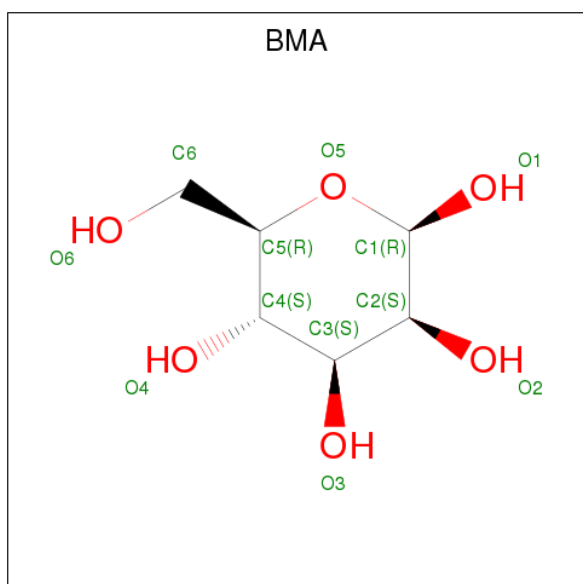
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	A	1	Total	C	N	O	0	0
			21	11	1	9		

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



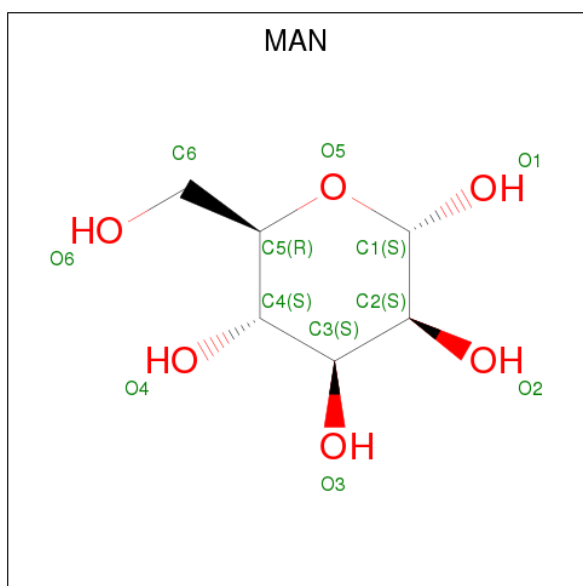
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

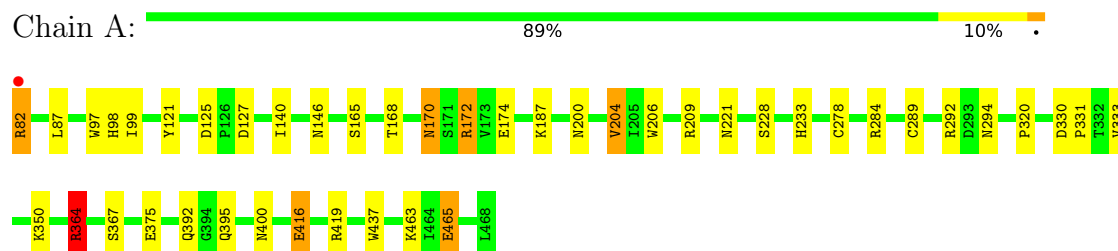
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	233	Total 233	O 233	0	0

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: NEURAMINIDASE SUBTYPE N9



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	181.18Å 181.18Å 181.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.70 – 2.15 42.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.70-2.15) 100.0 (42.70-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.59 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.155 , 0.196 0.157 , 0.195	Depositor DCC
R_{free} test set	1398 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3490	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CA, BMA, NAG, SIA

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	1.05	6/3150 (0.2%)	0.87	8/4290 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLU	CD-OE1	-27.43	0.95	1.25
1	A	333	VAL	C-N	19.11	1.67	1.33
1	A	392	GLN	C-N	15.62	1.61	1.33
1	A	463	LYS	CE-NZ	-7.21	1.31	1.49
1	A	416	GLU	CD-OE2	6.35	1.32	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	GLU	OE1-CD-OE2	21.47	149.07	123.30
1	A	416	GLU	CG-CD-OE2	-12.55	93.21	118.30
1	A	127	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	A	364	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	172	ARG	NE-CZ-NH2	-8.23	116.18	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3067	0	2895	36	0
2	A	42	0	36	0	0
3	A	70	0	63	11	0
4	A	55	0	49	8	0
5	A	22	0	19	2	0
6	A	1	0	0	0	0
7	A	233	0	0	1	0
All	All	3490	0	3062	47	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 9.

The worst 5 of 47 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:146:ASN:HD21	3:A:1475:NAG:C1	0.99	1.57
1:A:200:ASN:HD21	3:A:1471:NAG:C1	0.90	1.50
1:A:172:ARG:HD3	1:A:209:ARG:NH2	1.69	1.08
1:A:87:LEU:H	1:A:233:HIS:HD2	1.13	0.93
3:A:1473:NAG:HO4	3:A:1474:NAG:C1	1.76	0.91

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	386/388 (100%)	366 (95%)	20 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	341/341 (100%)	333 (98%)	8 (2%)	53 56

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	VAL
1	A	465	GLU
1	A	364	ARG
1	A	170	ASN
1	A	221	ASN

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	A	216	ASN
1	A	221	ASN
1	A	392	GLN
1	A	200	ASN
1	A	346	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

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
2	SIA	A	1469	-	18,21,21	1.64	2 (11%)	19,31,31	1.29	3 (15%)
2	SIA	A	1470	-	18,21,21	1.22	2 (11%)	19,31,31	1.18	2 (10%)
3	NAG	A	1471	1,3	14,14,15	0.49	0	17,19,21	1.84	5 (29%)
3	NAG	A	1472	3,4	14,14,15	0.44	0	17,19,21	1.72	5 (29%)
3	NAG	A	1473	1,3	14,14,15	0.40	0	17,19,21	1.37	2 (11%)
3	NAG	A	1474	3	14,14,15	0.71	0	17,19,21	2.45	3 (17%)
3	NAG	A	1475	1	14,14,15	0.43	0	17,19,21	1.43	2 (11%)
4	BMA	A	1476	3,5,4	11,11,12	0.30	0	15,15,17	1.47	3 (20%)
5	MAN	A	1477	5,4	11,11,12	0.47	0	15,15,17	2.27	4 (26%)
5	MAN	A	1478	5,4	11,11,12	0.52	0	15,15,17	1.54	3 (20%)
4	BMA	A	1479	5	11,11,12	0.71	0	15,15,17	1.69	2 (13%)
4	BMA	A	1480	4	11,11,12	0.40	0	15,15,17	1.76	2 (13%)
4	BMA	A	1481	4	11,11,12	0.76	0	15,15,17	1.73	4 (26%)
4	BMA	A	1482	4	11,11,12	0.56	0	15,15,17	1.83	3 (20%)

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	SIA	A	1469	-	-	0/14/38/38	0/1/1/1
2	SIA	A	1470	-	-	0/14/38/38	0/1/1/1
3	NAG	A	1471	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1472	3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	1473	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1474	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1475	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	1476	3,5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	1477	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	1478	5,4	-	0/2/19/22	0/1/1/1
4	BMA	A	1479	5	-	0/2/19/22	0/1/1/1
4	BMA	A	1480	4	-	0/2/19/22	0/1/1/1
4	BMA	A	1481	4	-	0/2/19/22	0/1/1/1
4	BMA	A	1482	4	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1470	SIA	C3-C2	2.45	1.54	1.51
2	A	1469	SIA	C3-C2	3.27	1.55	1.51
2	A	1470	SIA	O2-C2	3.87	1.44	1.39
2	A	1469	SIA	O2-C2	4.98	1.45	1.39

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1474	NAG	C4-C3-C2	-5.45	103.03	111.02
5	A	1477	MAN	O2-C2-C1	-4.85	99.39	109.17
3	A	1475	NAG	C1-C2-N2	-4.10	103.49	110.49
3	A	1474	NAG	O5-C1-C2	-3.79	106.29	111.52
3	A	1471	NAG	C4-C3-C2	-3.10	106.47	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1471	NAG	5	0
3	A	1472	NAG	3	0
3	A	1473	NAG	2	0
3	A	1474	NAG	2	0
3	A	1475	NAG	2	0
4	A	1476	BMA	3	0
5	A	1478	MAN	2	0
4	A	1479	BMA	2	0
4	A	1480	BMA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1481	BMA	2	0
4	A	1482	BMA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	333:VAL	C	335:GLY	N	1.67
1	A	392:GLN	C	394:GLY	N	1.61

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	388/388 (100%)	-0.63	1 (0%) 93 95	8, 13, 20, 41	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ARG	3.1

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. 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	B-factors(Å ²)	Q<0.9
2	SIA	A	1470	21/21	0.53	0.34	55,62,63,64	0
4	BMA	A	1481	11/12	0.54	0.23	74,76,77,77	0
3	NAG	A	1474	14/15	0.75	0.25	49,51,53,54	0
4	BMA	A	1482	11/12	0.83	0.21	41,46,47,47	0
2	SIA	A	1469	21/21	0.87	0.16	18,26,28,33	0
3	NAG	A	1475	14/15	0.88	0.21	40,42,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BMA	A	1480	11/12	0.92	0.16	30,32,34,34	0
5	MAN	A	1477	11/12	0.94	0.09	16,19,23,24	0
3	NAG	A	1473	14/15	0.95	0.15	20,24,27,28	0
3	NAG	A	1471	14/15	0.95	0.11	14,18,23,27	0
3	NAG	A	1472	14/15	0.96	0.09	14,17,19,24	0
4	BMA	A	1476	11/12	0.96	0.09	14,18,19,22	0
4	BMA	A	1479	11/12	0.96	0.09	13,15,16,16	0
5	MAN	A	1478	11/12	0.97	0.08	14,17,19,19	0
6	CA	A	1483	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.