



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:47 pm GMT

PDB ID : 3POY  
Title : Crystal Structure of the alpha-Neurexin-1 ectodomain, LNS 2-6  
Authors : Miller, M.T.; Mileni, M.; Comoletti, D.; Stevens, R.C.; Harel, M.; Taylor, P.  
Deposited on : 2010-11-23  
Resolution : 3.02 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](mailto: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.

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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

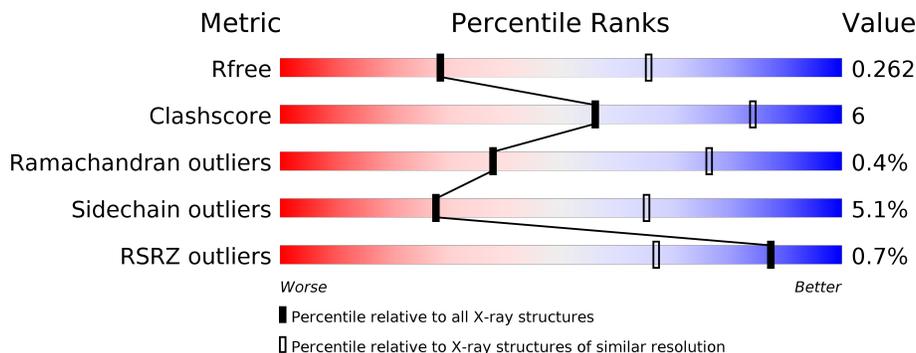
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

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  $\geq 3$ , 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	1019	 % <span style="margin-left: 100px;">82%</span> <span style="margin-left: 100px;">15%</span> ..

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	BGC	A	2000	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7878 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 Neurexin-1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1005	7795	4900	1341	1511	43	0	2	0

There are 57 discrepancies between the modelled and reference sequences:

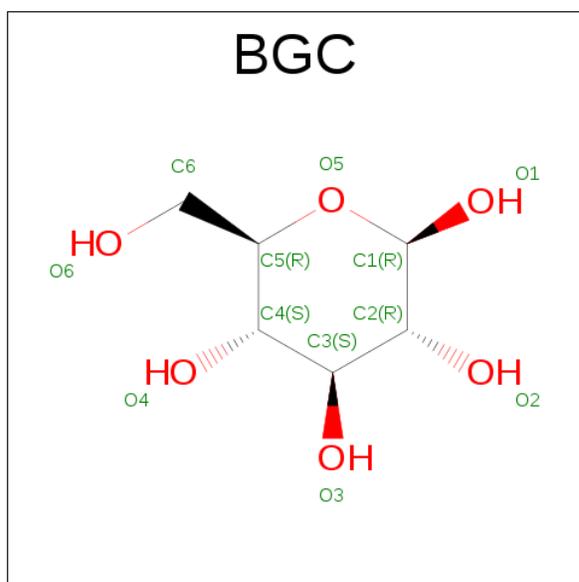
Chain	Residue	Modelled	Actual	Comment	Reference
A	292	LEU	-	EXPRESSION TAG	UNP Q28146
A	293	ALA	-	EXPRESSION TAG	UNP Q28146
A	294	ALA	-	EXPRESSION TAG	UNP Q28146
A	295	ALA	-	EXPRESSION TAG	UNP Q28146
A	?	-	THR	DELETION	UNP Q28146
A	?	-	SER	DELETION	UNP Q28146
A	?	-	GLY	DELETION	UNP Q28146
A	?	-	ILE	DELETION	UNP Q28146
A	?	-	GLY	DELETION	UNP Q28146
A	?	-	HIS	DELETION	UNP Q28146
A	?	-	ALA	DELETION	UNP Q28146
A	?	-	MET	DELETION	UNP Q28146
A	?	-	VAL	DELETION	UNP Q28146
A	?	-	ASN	DELETION	UNP Q28146
A	?	-	LYS	DELETION	UNP Q28146
A	?	-	LEU	DELETION	UNP Q28146
A	?	-	HIS	DELETION	UNP Q28146
A	?	-	CYS	DELETION	UNP Q28146
A	?	-	SER	DELETION	UNP Q28146
A	628	GLU	GLN	ENGINEERED MUTATION	UNP Q28146
A	1128	PHE	ILE	ENGINEERED MUTATION	UNP Q28146
A	?	-	GLY	DELETION	UNP Q28146
A	?	-	ASN	DELETION	UNP Q28146
A	?	-	ASN	DELETION	UNP Q28146
A	?	-	ASP	DELETION	UNP Q28146
A	?	-	ASN	DELETION	UNP Q28146
A	?	-	GLU	DELETION	UNP Q28146

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	DELETION	UNP Q28146
A	?	-	LEU	DELETION	UNP Q28146
A	?	-	ALA	DELETION	UNP Q28146
A	?	-	ILE	DELETION	UNP Q28146
A	?	-	ALA	DELETION	UNP Q28146
A	?	-	ARG	DELETION	UNP Q28146
A	?	-	GLN	DELETION	UNP Q28146
A	?	-	ARG	DELETION	UNP Q28146
A	?	-	ILE	DELETION	UNP Q28146
A	?	-	PRO	DELETION	UNP Q28146
A	?	-	TYR	DELETION	UNP Q28146
A	?	-	ARG	DELETION	UNP Q28146
A	?	-	LEU	DELETION	UNP Q28146
A	?	-	GLY	DELETION	UNP Q28146
A	?	-	ARG	DELETION	UNP Q28146
A	?	-	VAL	DELETION	UNP Q28146
A	?	-	VAL	DELETION	UNP Q28146
A	?	-	ASP	DELETION	UNP Q28146
A	?	-	GLU	DELETION	UNP Q28146
A	?	-	TRP	DELETION	UNP Q28146
A	?	-	LEU	DELETION	UNP Q28146
A	?	-	LEU	DELETION	UNP Q28146
A	?	-	ASP	DELETION	UNP Q28146
A	?	-	LYS	DELETION	UNP Q28146
A	1350	LEU	-	EXPRESSION TAG	UNP Q28146
A	1351	GLU	-	EXPRESSION TAG	UNP Q28146
A	1352	VAL	-	EXPRESSION TAG	UNP Q28146
A	1353	LEU	-	EXPRESSION TAG	UNP Q28146
A	1354	PHE	-	EXPRESSION TAG	UNP Q28146
A	1355	GLN	-	EXPRESSION TAG	UNP Q28146

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

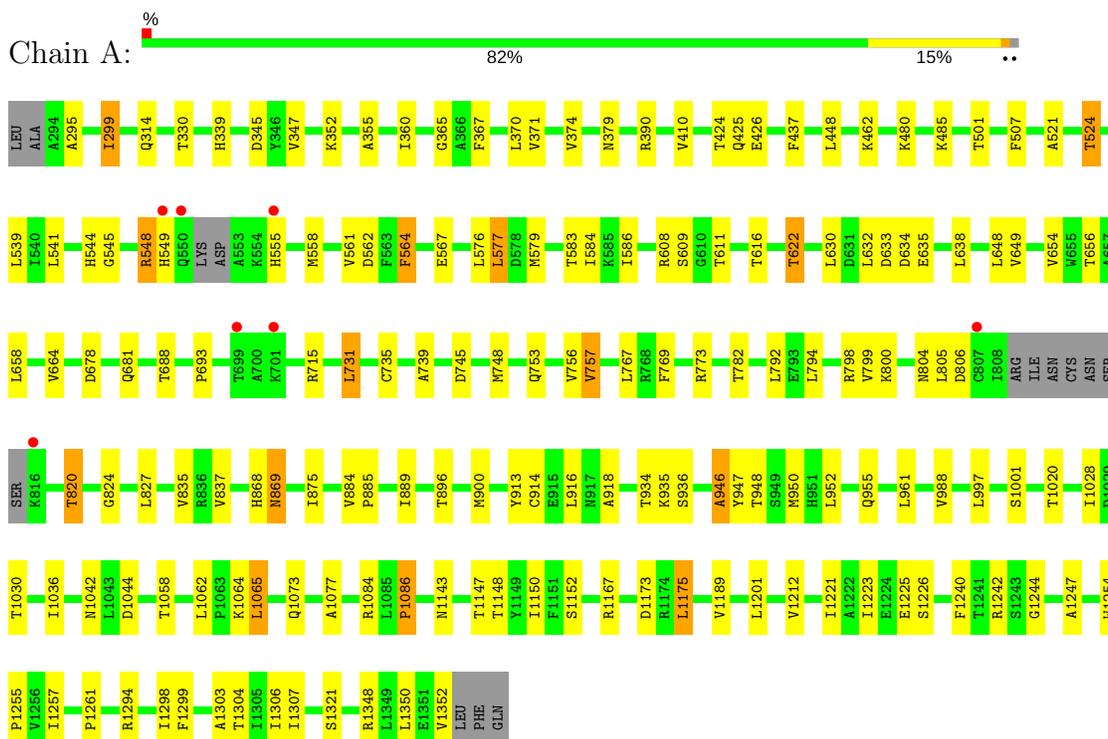
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		

### 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: Neurexin-1-alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.74Å 61.24Å 155.58Å 90.00° 121.21° 90.00°	Depositor
Resolution (Å)	38.56 – 3.02 38.56 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.56-3.02) 98.2 (38.56-3.02)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.214 , 0.269 0.216 , 0.262	Depositor DCC
$R_{free}$ test set	1586 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtrriage
Anisotropy	0.288	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7878	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: BGC, 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	0.53	0/7955	0.68	3/10769 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	CYS	CA-CB-SG	-5.49	104.13	114.00
1	A	426	GLU	N-CA-CB	5.22	120.00	110.60
1	A	1028	ILE	CB-CA-C	-5.13	101.34	111.60

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	7795	0	7628	90	0
2	A	11	0	10	0	0
3	A	39	0	34	1	0
4	A	33	0	0	0	0
All	All	7878	0	7672	90	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 6.

The worst 5 of 90 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:1148:THR:HG23	1:A:1321:SER:HB3	1.67	0.76
1:A:352:LYS:HE2	1:A:616:THR:HG23	1.71	0.73
1:A:948:THR:HG22	1:A:1020:THR:CG2	2.19	0.72
1:A:948:THR:HG22	1:A:1020:THR:HG22	1.74	0.70
1:A:579:MET:HE3	1:A:608:ARG:HA	1.74	0.70

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	1001/1019 (98%)	929 (93%)	68 (7%)	4 (0%)	38 76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	ALA
1	A	1065	LEU
1	A	693	PRO
1	A	757	VAL

### 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	859/870 (99%)	815 (95%)	44 (5%)	28 65

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	688	THR
1	A	820	THR
1	A	1294	ARG
1	A	715	ARG
1	A	756	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	891	HIS
1	A	908	ASN
1	A	1035	GLN
1	A	772	GLN
1	A	869	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](#)

3 carbohydrates 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
3	NAG	A	2001	1,3	14,14,15	0.88	0	15,19,21	0.85	0
3	NAG	A	2002	3	14,14,15	1.65	3 (21%)	15,19,21	1.17	1 (6%)
3	BMA	A	2003	3	11,11,12	1.66	3 (27%)	13,15,17	1.23	2 (15%)

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	NAG	A	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	A	2003	3	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2003	BMA	C1-C2	2.10	1.57	1.52
3	A	2002	NAG	C1-C2	2.20	1.55	1.52
3	A	2002	NAG	C8-C7	2.35	1.55	1.50
3	A	2003	BMA	O5-C5	2.49	1.48	1.43
3	A	2002	NAG	O4-C4	3.28	1.50	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	NAG	C4-C3-C2	2.06	114.03	111.02
3	A	2003	BMA	C1-C2-C3	2.13	112.35	109.65
3	A	2003	BMA	O5-C1-C2	2.50	114.70	110.79

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
3	A	2001	NAG	1	0

## 5.6 Ligand geometry [i](#)

1 ligand is 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	BGC	A	2000	1	11,11,12	1.84	3 (27%)	13,15,17	2.47	7 (53%)

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	BGC	A	2000	1	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	BGC	C6-C5	2.42	1.60	1.51
2	A	2000	BGC	O5-C5	3.06	1.49	1.43
2	A	2000	BGC	O5-C1	3.45	1.49	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	BGC	O2-C2-C3	-3.94	102.43	110.17
2	A	2000	BGC	C6-C5-C4	-3.85	103.98	113.00
2	A	2000	BGC	C1-O5-C5	2.68	115.86	112.17
2	A	2000	BGC	C1-C2-C3	2.75	113.14	109.65
2	A	2000	BGC	C3-C4-C5	2.90	115.32	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1005/1019 (98%)	-0.44	7 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">67</span>	23, 47, 71, 104	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	THR	5.2
1	A	555	HIS	3.7
1	A	816	LYS	3.3
1	A	549	HIS	2.7
1	A	550	GLN	2.2

### 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	2001	14/15	0.92	0.31	1.41	46,47,47,48	0
3	BMA	A	2003	11/12	0.82	0.49	-	48,49,49,49	0
3	NAG	A	2002	14/15	0.82	0.47	-	49,49,50,50	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BGC	A	2000	11/12	0.85	0.38	3.61	45,45,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.