



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2019 – 03:31 AM EST

PDB ID : 5ZO1  
Title : Crystal structure of mouse nectin-like molecule 4 (mNecl-4) full ectodomain (Ig1-Ig3), 2.2A  
Authors : Liu, X.; An, T.; Li, D.; Fan, Z.; Xiang, P.; Li, C.; Ju, W.; Li, J.; Hu, G.; Qin, B.; Yin, B.; Wojdyla, J.A.; Wang, M.; Yuan, J.; Qiang, B.; Shu, P.; Cui, S.; Peng, X.  
Deposited on : 2018-04-12  
Resolution : 2.20 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](mailto: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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
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-20031633

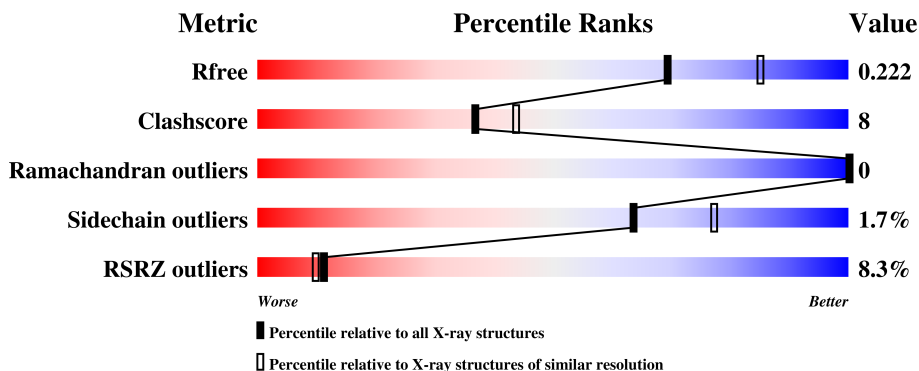
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

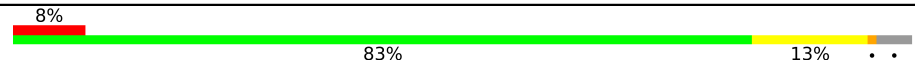
The reported resolution of this entry is 2.20 Å.

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	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	299	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4698 atoms, of which 2188 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.

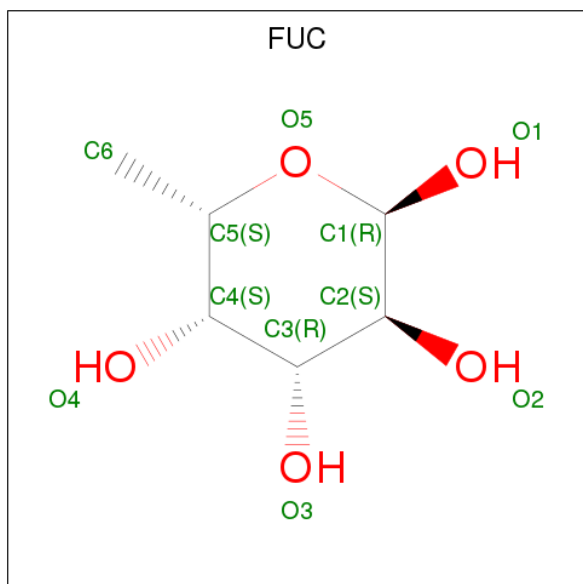
- Molecule 1 is a protein called Cell adhesion molecule 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	288	4444	1408	2172	418	439	7	0	5	0

There are 9 discrepancies between the modelled and reference sequences:

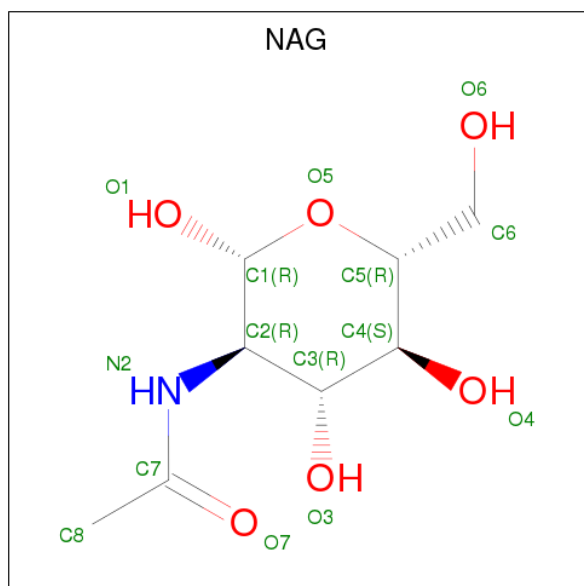
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLN	ASN	engineered mutation	UNP Q8R464
A	262	GLN	ASN	engineered mutation	UNP Q8R464
A	286	GLN	ASN	engineered mutation	UNP Q8R464
A	318	HIS	-	expression tag	UNP Q8R464
A	319	HIS	-	expression tag	UNP Q8R464
A	320	HIS	-	expression tag	UNP Q8R464
A	321	HIS	-	expression tag	UNP Q8R464
A	322	HIS	-	expression tag	UNP Q8R464
A	323	HIS	-	expression tag	UNP Q8R464

- Molecule 2 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



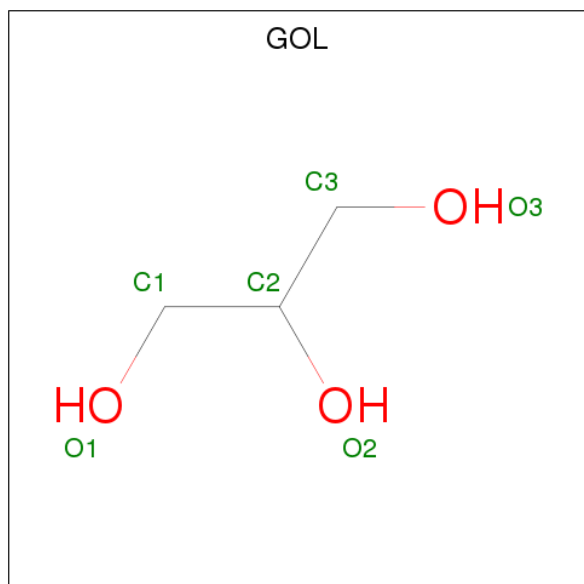
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

- 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		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

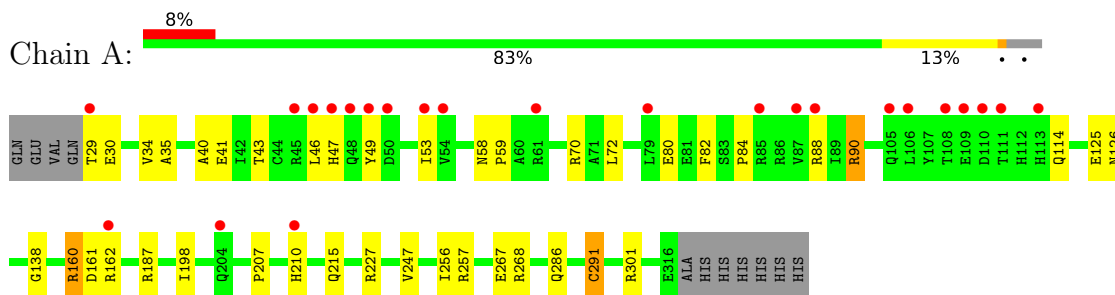
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	188	Total	O	0	0
			188	188		

### 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: Cell adhesion molecule 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.50Å 109.50Å 182.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.20 47.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.30-2.20) 99.7 (47.29-2.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.200 , 0.220 0.202 , 0.222	Depositor DCC
$R_{free}$ test set	1388 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: GOL, NAG, FUC

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	0.41	0/2327	0.60	1/3163 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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	2272	2172	2235	36	0
2	A	10	0	10	3	0
3	A	28	0	24	4	0
4	A	12	16	16	1	0
5	A	188	0	0	12	2
All	All	2510	2188	2285	39	2

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 8.



All (39) 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:34:VAL:HG21	1:A:40:ALA:HB2	1.38	1.03
1:A:34:VAL:CG2	1:A:40:ALA:HB2	2.01	0.90
1:A:126:ASN:OD1	5:A:501:HOH:O	1.91	0.89
1:A:41:GLU:OE2	1:A:90:ARG:NH1	2.22	0.73
1:A:268:ARG:NH2	5:A:506:HOH:O	2.23	0.71
1:A:30:GLU:OE1	5:A:502:HOH:O	2.09	0.71
1:A:70:ARG:NH2	5:A:505:HOH:O	2.15	0.69
1:A:80:GLU:OE2	1:A:88:ARG:NH1	2.27	0.68
2:A:401:FUC:H61	3:A:403:NAG:H5	1.77	0.65
1:A:80:GLU:OE1	1:A:90:ARG:NH1	2.32	0.63
2:A:401:FUC:H61	3:A:403:NAG:O4	2.00	0.61
1:A:34:VAL:HG12	1:A:35:ALA:O	2.01	0.60
1:A:256:ILE:HG23	1:A:291[A]:CYS:SG	2.43	0.59
1:A:29:THR:HG22	1:A:114:GLN:O	2.06	0.56
1:A:301:ARG:NH1	5:A:514:HOH:O	2.39	0.56
1:A:70:ARG:HD2	1:A:72:LEU:O	2.08	0.54
1:A:53:ILE:HG13	3:A:402:NAG:H82	1.88	0.54
1:A:47:HIS:N	5:A:503:HOH:O	2.11	0.54
1:A:46:LEU:HD11	1:A:84:PRO:O	2.09	0.53
1:A:46:LEU:HA	5:A:503:HOH:O	2.09	0.52
1:A:160:ARG:HG2	5:A:504:HOH:O	2.10	0.51
1:A:247:VAL:HG21	1:A:256:ILE:CD1	2.43	0.49
1:A:227[B]:ARG:NE	5:A:515:HOH:O	2.39	0.49
1:A:198:ILE:HD13	1:A:215:GLN:HG3	1.96	0.48
1:A:138:GLY:O	1:A:187:ARG:NH1	2.48	0.47
1:A:46:LEU:HD13	1:A:49:TYR:HB2	1.95	0.46
2:A:401:FUC:C6	3:A:403:NAG:O4	2.63	0.46
1:A:46:LEU:CD1	1:A:49:TYR:HB2	2.46	0.46
1:A:43:THR:HG22	1:A:88:ARG:HG3	1.97	0.45
1:A:286:GLN:CD	4:A:405:GOL:H12	2.38	0.44
1:A:58:ASN:HB2	1:A:59:PRO:CD	2.48	0.44
1:A:161:ASP:O	1:A:162:ARG:HB2	2.19	0.42
1:A:160:ARG:NE	5:A:504:HOH:O	2.12	0.42
1:A:125:GLU:HG2	5:A:561:HOH:O	2.19	0.41
1:A:198:ILE:CD1	1:A:215:GLN:HG3	2.51	0.41
1:A:46:LEU:HD12	1:A:46:LEU:C	2.41	0.41
1:A:43:THR:HG22	1:A:88:ARG:CG	2.50	0.41
1:A:267[A]:GLU:HG3	5:A:580:HOH:O	2.21	0.41
1:A:207:PRO:HB2	1:A:210:HIS:ND1	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:605:HOH:O	5:A:670:HOH:O[10_675]	2.09	0.11
5:A:583:HOH:O	5:A:653:HOH:O[12_465]	2.13	0.07

## 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	291/299 (97%)	281 (97%)	10 (3%)	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	246/251 (98%)	241 (98%)	5 (2%)	58 72

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

Mol	Chain	Res	Type
1	A	82	PHE
1	A	90	ARG
1	A	160	ARG
1	A	291[A]	CYS
1	A	291[B]	CYS

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](#)

5 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	FUC	A	401	3	9,10,11	1.90	3 (33%)	13,14,16	1.47	1 (7%)
3	NAG	A	402	1,3,2	14,14,15	1.05	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	A	403	3	14,14,15	0.81	1 (7%)	17,19,21	2.05	5 (29%)
4	GOL	A	404	-	5,5,5	0.29	0	5,5,5	0.44	0
4	GOL	A	405	-	5,5,5	0.86	0	5,5,5	0.84	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	FUC	A	401	3	-	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	402	1,3,2	-	0/6/23/26	0/1/1/1
3	NAG	A	403	3	-	0/6/23/26	0/1/1/1
4	GOL	A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	A	405	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FUC	O5-C1	-3.33	1.38	1.43
3	A	403	NAG	O5-C1	-2.71	1.39	1.43
3	A	402	NAG	O5-C1	2.32	1.47	1.43
2	A	401	FUC	C1-C2	2.99	1.59	1.52
2	A	401	FUC	C2-C3	3.11	1.57	1.52
3	A	402	NAG	C1-C2	3.13	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NAG	O4-C4-C5	-5.43	95.71	109.31
3	A	403	NAG	C1-O5-C5	-2.75	108.41	112.19
3	A	403	NAG	O4-C4-C3	-2.42	104.69	110.34
3	A	403	NAG	C4-C3-C2	2.59	114.81	111.02
3	A	403	NAG	C3-C4-C5	3.88	117.19	110.24
3	A	402	NAG	C1-O5-C5	4.19	117.96	112.19
2	A	401	FUC	C1-C2-C3	4.40	115.22	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FUC	3	0
3	A	402	NAG	1	0
3	A	403	NAG	3	0
4	A	405	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	288/299 (96%)	0.49	24 (8%) <b>11</b> <b>10</b>	22, 36, 83, 200	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	THR	6.3
1	A	113	HIS	5.8
1	A	47	HIS	4.8
1	A	48	GLN	4.4
1	A	162	ARG	4.2
1	A	61	ARG	3.7
1	A	108	THR	3.7
1	A	54	VAL	3.6
1	A	50	ASP	3.6
1	A	106	LEU	3.6
1	A	210	HIS	3.5
1	A	110	ASP	3.5
1	A	85	ARG	3.2
1	A	45	ARG	3.1
1	A	109	GLU	3.0
1	A	105	GLN	2.7
1	A	49	TYR	2.7
1	A	53	ILE	2.4
1	A	204	GLN	2.4
1	A	88	ARG	2.2
1	A	79	LEU	2.1
1	A	46	LEU	2.1
1	A	29	THR	2.1
1	A	87	VAL	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	A	401	10/11	0.54	0.37	251,272,282,290	0
3	NAG	A	402	14/15	0.59	0.20	64,95,131,164	0
3	NAG	A	403	14/15	0.75	0.27	96,135,143,148	0
4	GOL	A	404	6/6	0.81	0.21	44,56,72,81	0
4	GOL	A	405	6/6	0.96	0.27	28,35,45,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.