



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:38 AM GMT

PDB ID : 3BL8  
Title : Crystal structure of the extracellular domain of neuroligin 2A from mouse  
Authors : Jin, X.; Koehnke, J.; Shapiro, L.  
Deposited on : 2007-12-10  
Resolution : 3.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

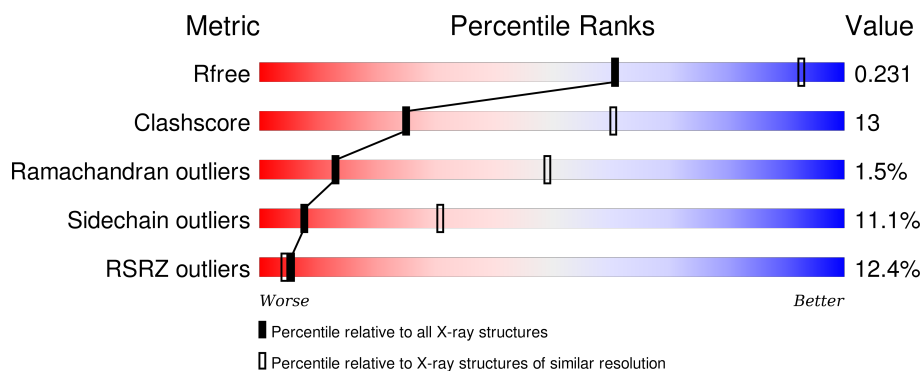
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	580	<div> <div>4%</div> <div>59%</div> <div>31%</div> <div>6%</div> <div>.</div> </div>
1	B	580	<div> <div>11%</div> <div>64%</div> <div>24%</div> <div>6%</div> <div>6%</div> </div>
1	C	580	<div> <div>8%</div> <div>66%</div> <div>25%</div> <div>.</div> <div>6%</div> </div>
1	D	580	<div> <div>23%</div> <div>65%</div> <div>24%</div> <div>.</div> <div>7%</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
2	MAN	A	703	X	-	-	-
3	NAG	A	710	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17374 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 Neuroligin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4358	2782	744	814	18			
1	B	546	Total	C	N	O	S	0	0	0
			4283	2737	731	797	18			
1	C	545	Total	C	N	O	S	0	0	0
			4282	2736	732	796	18			
1	D	541	Total	C	N	O	S	0	0	0
			4249	2714	726	791	18			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLN	-	EXPRESSION TAG	UNP Q69ZK9
A	41	LYS	-	EXPRESSION TAG	UNP Q69ZK9
A	613	HIS	-	EXPRESSION TAG	UNP Q69ZK9
A	614	HIS	-	EXPRESSION TAG	UNP Q69ZK9
A	615	HIS	-	EXPRESSION TAG	UNP Q69ZK9
A	616	HIS	-	EXPRESSION TAG	UNP Q69ZK9
A	617	HIS	-	EXPRESSION TAG	UNP Q69ZK9
A	618	HIS	-	EXPRESSION TAG	UNP Q69ZK9
A	619	HIS	-	EXPRESSION TAG	UNP Q69ZK9
B	40	GLN	-	EXPRESSION TAG	UNP Q69ZK9
B	41	LYS	-	EXPRESSION TAG	UNP Q69ZK9
B	613	HIS	-	EXPRESSION TAG	UNP Q69ZK9
B	614	HIS	-	EXPRESSION TAG	UNP Q69ZK9
B	615	HIS	-	EXPRESSION TAG	UNP Q69ZK9
B	616	HIS	-	EXPRESSION TAG	UNP Q69ZK9
B	617	HIS	-	EXPRESSION TAG	UNP Q69ZK9
B	618	HIS	-	EXPRESSION TAG	UNP Q69ZK9
B	619	HIS	-	EXPRESSION TAG	UNP Q69ZK9
C	40	GLN	-	EXPRESSION TAG	UNP Q69ZK9
C	41	LYS	-	EXPRESSION TAG	UNP Q69ZK9
C	613	HIS	-	EXPRESSION TAG	UNP Q69ZK9

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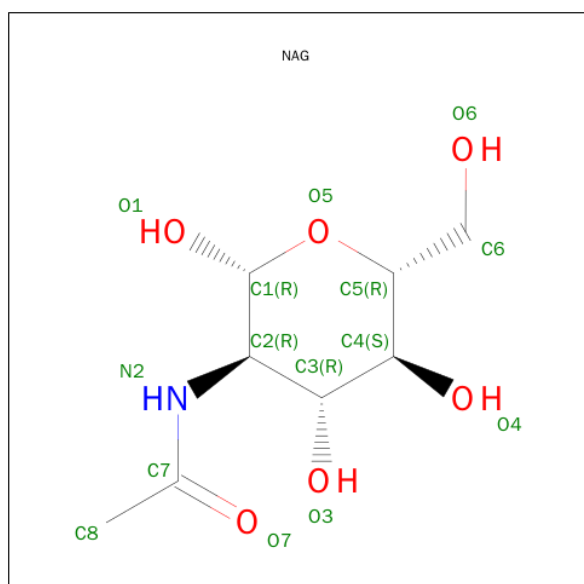
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Chain	Residue	Modelled	Actual	Comment	Reference
C	614	HIS	-	EXPRESSION TAG	UNP Q69ZK9
C	615	HIS	-	EXPRESSION TAG	UNP Q69ZK9
C	616	HIS	-	EXPRESSION TAG	UNP Q69ZK9
C	617	HIS	-	EXPRESSION TAG	UNP Q69ZK9
C	618	HIS	-	EXPRESSION TAG	UNP Q69ZK9
C	619	HIS	-	EXPRESSION TAG	UNP Q69ZK9
D	40	GLN	-	EXPRESSION TAG	UNP Q69ZK9
D	41	LYS	-	EXPRESSION TAG	UNP Q69ZK9
D	613	HIS	-	EXPRESSION TAG	UNP Q69ZK9
D	614	HIS	-	EXPRESSION TAG	UNP Q69ZK9
D	615	HIS	-	EXPRESSION TAG	UNP Q69ZK9
D	616	HIS	-	EXPRESSION TAG	UNP Q69ZK9
D	617	HIS	-	EXPRESSION TAG	UNP Q69ZK9
D	618	HIS	-	EXPRESSION TAG	UNP Q69ZK9
D	619	HIS	-	EXPRESSION TAG	UNP Q69ZK9

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is SUGAR (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	B	1	Total	C	N	O	0	0
			14	8	1	5		

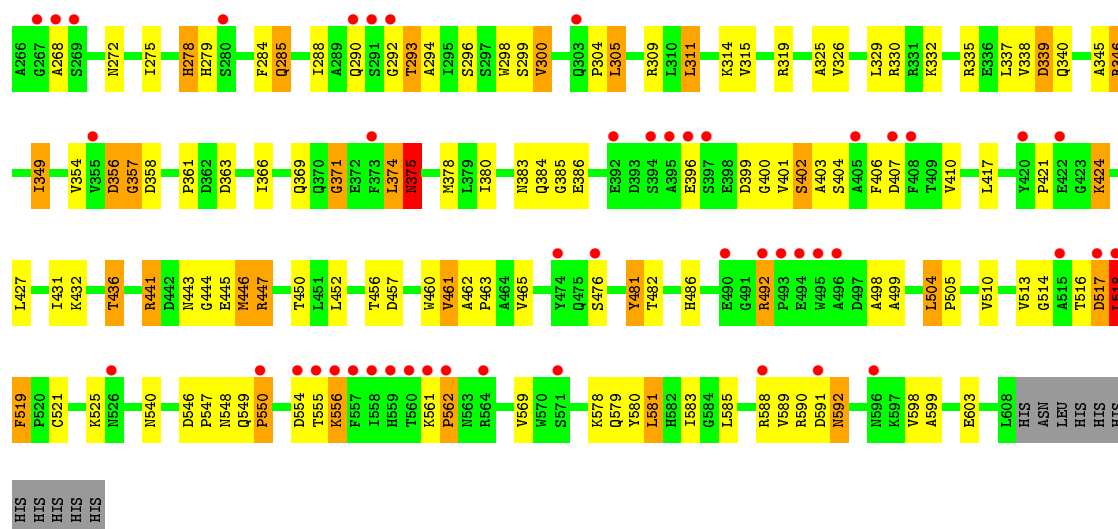
- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	7	Total	C	N	O	0	0
			83	46	2	35		

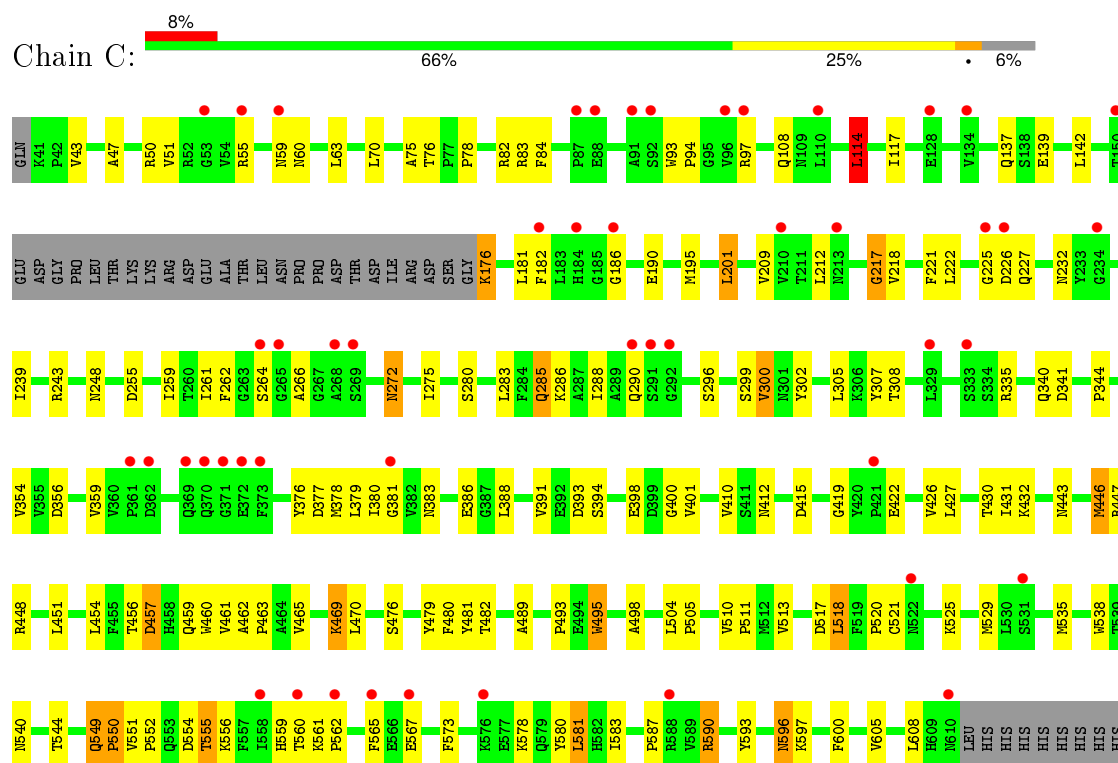
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	11	Total	O	0	0
			11	11		
5	C	5	Total	O	0	0
			5	5		
5	D	5	Total	O	0	0
			5	5		

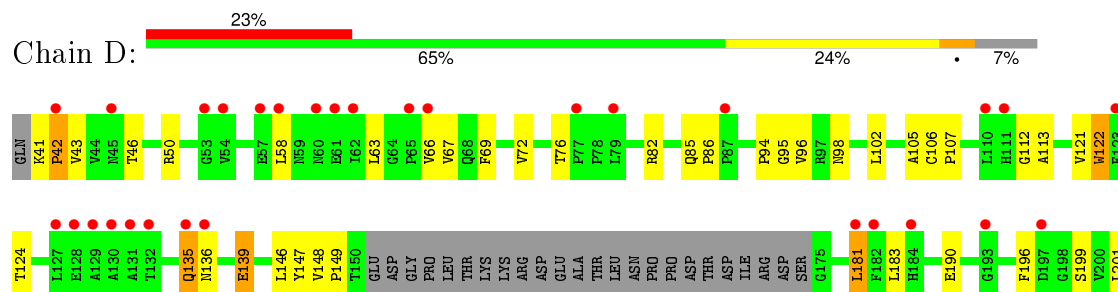




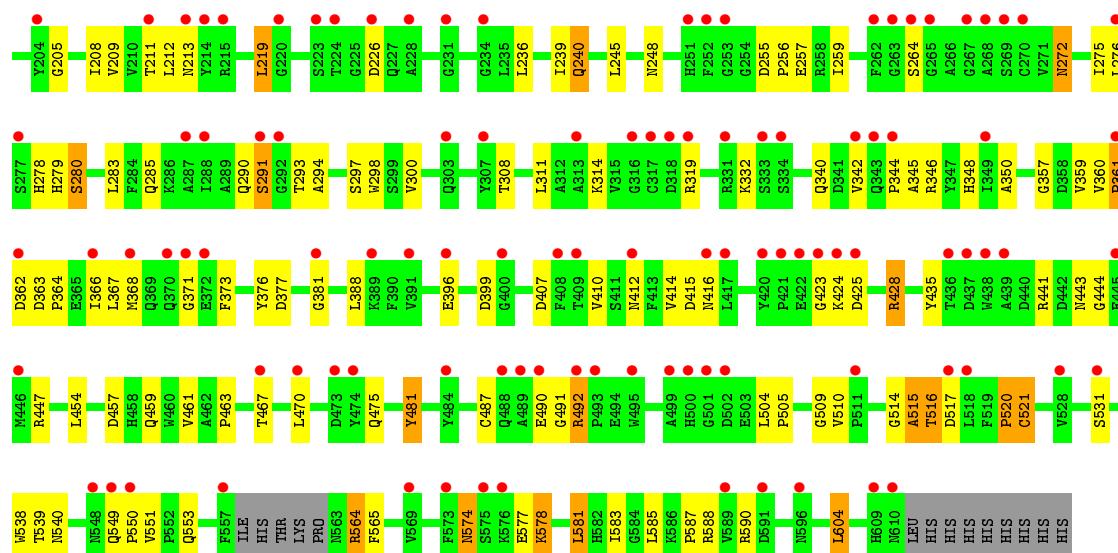
• Molecule 1: Neuroligin-2



• Molecule 1: Neuroligin-2







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.72Å 92.57Å 188.41Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.74 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-3.30) 98.5 (29.74-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.219 , 0.262 0.229 , 0.231	Depositor DCC
$R_{free}$ test set	2748 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	108.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 135.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 54385 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.44	0/4478	0.65	6/6101 (0.1%)
1	B	0.36	0/4401	0.60	5/5996 (0.1%)
1	C	0.38	0/4401	0.57	4/5998 (0.1%)
1	D	0.34	0/4365	0.61	12/5945 (0.2%)
All	All	0.38	0/17645	0.61	27/24040 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	1
1	D	0	3
2	A	1	0
All	All	1	13

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	GLU	CB-CA-C	-9.49	91.41	110.40
1	A	395	ALA	CB-CA-C	-9.02	96.57	110.10
1	D	279	HIS	N-CA-C	9.01	135.33	111.00
1	D	279	HIS	CB-CA-C	-8.34	93.72	110.40
1	D	113	ALA	N-CA-CB	8.23	121.62	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	703	MAN	C1

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	TYR	Peptide
1	A	419	GLY	Peptide
1	A	420	TYR	Peptide
1	A	494	GLU	Peptide
1	A	549	GLN	Peptide

## 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	4358	0	4194	157	0
1	B	4283	0	4129	102	0
1	C	4282	0	4123	91	0
1	D	4249	0	4091	80	0
2	A	39	0	34	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	B	83	0	70	4	0
5	A	31	0	0	0	0
5	B	11	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
All	All	17374	0	16667	433	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 13.

The worst 5 of 433 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:420:TYR:H	1:A:421:PRO:HA	1.02	1.17
1:B:561:LYS:HG3	1:B:562:PRO:HD2	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:ASN:HD21	1:C:551:VAL:HG12	1.18	1.03
1:A:420:TYR:H	1:A:421:PRO:CA	1.77	0.98
1:A:421:PRO:O	1:A:424:LYS:N	1.97	0.97

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	552/580 (95%)	490 (89%)	56 (10%)	6 (1%)	17	57
1	B	542/580 (93%)	467 (86%)	66 (12%)	9 (2%)	11	47
1	C	541/580 (93%)	469 (87%)	67 (12%)	5 (1%)	21	60
1	D	535/580 (92%)	456 (85%)	67 (12%)	12 (2%)	8	41
All	All	2170/2320 (94%)	1882 (87%)	256 (12%)	32 (2%)	13	49

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	PRO
1	B	357	GLY
1	C	550	PRO
1	D	94	PRO
1	D	550	PRO

### 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	462/488 (95%)	413 (89%)	49 (11%)	8	33
1	B	454/488 (93%)	388 (86%)	66 (14%)	4	18
1	C	454/488 (93%)	415 (91%)	39 (9%)	13	45
1	D	450/488 (92%)	402 (89%)	48 (11%)	8	32
All	All	1820/1952 (93%)	1618 (89%)	202 (11%)	8	31

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	436	THR
1	B	589	VAL
1	D	425	ASP
1	B	446	MET
1	B	510	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	459	GLN
1	C	137	GLN
1	D	416	ASN
1	B	540	ASN
1	B	592	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

10 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
2	NAG	A	701	1,2	14,14,15	0.62	0	15,19,21	1.23	2 (13%)
2	NAG	A	702	2	14,14,15	0.54	0	15,19,21	1.09	1 (6%)
2	MAN	A	703	2	11,11,12	0.67	0	14,15,17	0.80	0
4	NAG	B	801	1,4	14,14,15	1.16	1 (7%)	15,19,21	1.16	1 (6%)
4	NAG	B	802	4	14,14,15	0.50	0	15,19,21	1.49	4 (26%)
4	BMA	B	803	4	11,11,12	0.91	0	14,15,17	2.10	2 (14%)
4	MAN	B	804	4	11,11,12	0.84	0	14,15,17	2.74	4 (28%)
4	MAN	B	805	4	11,11,12	0.63	0	14,15,17	1.94	3 (21%)
4	MAN	B	806	4	11,11,12	0.67	0	14,15,17	2.92	6 (42%)
4	MAN	B	807	4	11,11,12	0.58	0	14,15,17	2.27	2 (14%)

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	701	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	702	2	-	0/6/23/26	0/1/1/1
2	MAN	A	703	2	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	B	801	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	802	4	-	0/6/23/26	0/1/1/1
4	BMA	B	803	4	-	0/2/19/22	0/1/1/1
4	MAN	B	804	4	-	0/2/19/22	0/1/1/1
4	MAN	B	805	4	-	0/2/19/22	0/1/1/1
4	MAN	B	806	4	-	0/2/19/22	0/1/1/1
4	MAN	B	807	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	NAG	O5-C1	-3.97	1.37	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	BMA	C3-C4-C5	-5.91	99.90	110.20
4	B	804	MAN	C1-C2-C3	-5.82	102.65	109.54
4	B	806	MAN	O3-C3-C2	-3.91	102.93	110.00
4	B	804	MAN	O4-C4-C3	-3.74	101.93	110.34
4	B	803	BMA	O6-C6-C5	-3.16	100.88	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	703	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	NAG	4	0
4	B	803	BMA	4	0

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
3	NAG	A	710	-	14,14,15	0.66	0	15,19,21	1.24	1 (6%)
3	NAG	B	810	1	14,14,15	0.68	0	15,19,21	1.38	2 (13%)

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	710	-	-	0/6/23/26	0/1/1/1
3	NAG	B	810	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	B	810	NAG	C3-C4-C5	2.72	114.94	110.20
3	A	710	NAG	C4-C3-C2	3.61	116.85	111.23
3	B	810	NAG	C4-C3-C2	4.03	117.50	111.23

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	556/580 (95%)	0.30	24 (4%) 39 32	37, 122, 137, 148	0
1	B	546/580 (94%)	0.69	64 (11%) 6 5	33, 127, 137, 145	0
1	C	545/580 (93%)	0.57	49 (8%) 12 9	33, 123, 134, 139	0
1	D	541/580 (93%)	1.17	135 (24%) 1 1	34, 130, 138, 153	0
All	All	2188/2320 (94%)	0.68	272 (12%) 5 4	33, 126, 137, 153	0

The worst 5 of 272 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	557	PHE	8.4
1	C	92	SER	7.3
1	C	91	ALA	7.3
1	D	437	ASP	6.9
1	D	57	GLU	6.7

### 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( $\text{\AA}^2$ )	Q<0.9
4	MAN	B	804	11/12	0.92	0.35	1.68	89,91,93,95	0
4	NAG	B	802	14/15	0.94	0.29	1.07	89,90,93,93	0
2	NAG	A	701	14/15	0.82	0.34	0.76	136,138,140,144	0
4	NAG	B	801	14/15	0.90	0.25	-0.18	95,99,101,103	0
4	BMA	B	803	11/12	0.93	0.19	-0.24	87,88,91,94	0
4	MAN	B	805	11/12	0.81	0.37	-	112,113,115,115	0
2	NAG	A	702	14/15	0.82	0.46	-	148,149,151,153	0
4	MAN	B	806	11/12	0.85	0.38	-	99,105,108,110	0
2	MAN	A	703	11/12	0.55	0.39	-	155,157,157,157	0
4	MAN	B	807	11/12	0.73	0.47	-	112,113,113,114	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	710	14/15	0.45	0.68	3.32	174,176,176,176	0
3	NAG	B	810	14/15	0.65	0.57	-	142,144,144,144	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.