



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:38 AM GMT

PDB ID : 3BIW
Title : Crystal structure of the Neuroligin-1/Neurexin-1beta synaptic adhesion complex
Authors : Arac, D.; Boucard, A.A.; Ozkan, E.; Strop, P.; Newell, E.; Sudhof, T.C.; Brunger, A.T.
Deposited on : 2007-12-01
Resolution : 3.50 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 (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

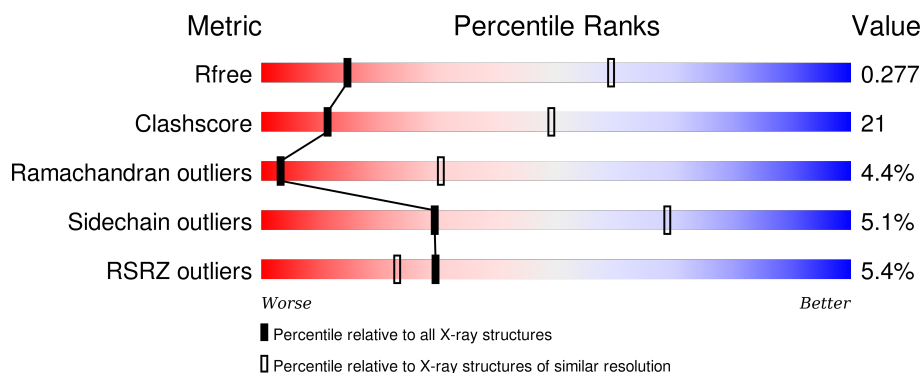
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	574	
1	B	574	
1	C	574	
1	D	574	
2	E	243	

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Mol	Chain	Length	Quality of chain
2	F	243	
2	G	243	
2	H	243	

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
3	NAG	D	702	-	-	-	X
4	NAG	E	306	-	-	X	-
4	NAG	F	306	-	-	X	-
4	NAG	G	306	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22438 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	B	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	C	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			
1	D	533	Total	C	N	O	S	0	0	0
			4186	2690	697	783	16			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	-	EXPRESSION TAG	UNP Q62765
A	44	ASP	-	EXPRESSION TAG	UNP Q62765
A	45	PRO	-	EXPRESSION TAG	UNP Q62765
A	639	HIS	-	EXPRESSION TAG	UNP Q62765
A	640	HIS	-	EXPRESSION TAG	UNP Q62765
A	641	HIS	-	EXPRESSION TAG	UNP Q62765
A	642	HIS	-	EXPRESSION TAG	UNP Q62765
A	643	HIS	-	EXPRESSION TAG	UNP Q62765
A	644	HIS	-	EXPRESSION TAG	UNP Q62765
B	43	ALA	-	EXPRESSION TAG	UNP Q62765
B	44	ASP	-	EXPRESSION TAG	UNP Q62765
B	45	PRO	-	EXPRESSION TAG	UNP Q62765
B	639	HIS	-	EXPRESSION TAG	UNP Q62765
B	640	HIS	-	EXPRESSION TAG	UNP Q62765
B	641	HIS	-	EXPRESSION TAG	UNP Q62765
B	642	HIS	-	EXPRESSION TAG	UNP Q62765
B	643	HIS	-	EXPRESSION TAG	UNP Q62765
B	644	HIS	-	EXPRESSION TAG	UNP Q62765
C	43	ALA	-	EXPRESSION TAG	UNP Q62765
C	44	ASP	-	EXPRESSION TAG	UNP Q62765
C	45	PRO	-	EXPRESSION TAG	UNP Q62765

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Chain	Residue	Modelled	Actual	Comment	Reference
C	639	HIS	-	EXPRESSION TAG	UNP Q62765
C	640	HIS	-	EXPRESSION TAG	UNP Q62765
C	641	HIS	-	EXPRESSION TAG	UNP Q62765
C	642	HIS	-	EXPRESSION TAG	UNP Q62765
C	643	HIS	-	EXPRESSION TAG	UNP Q62765
C	644	HIS	-	EXPRESSION TAG	UNP Q62765
D	43	ALA	-	EXPRESSION TAG	UNP Q62765
D	44	ASP	-	EXPRESSION TAG	UNP Q62765
D	45	PRO	-	EXPRESSION TAG	UNP Q62765
D	639	HIS	-	EXPRESSION TAG	UNP Q62765
D	640	HIS	-	EXPRESSION TAG	UNP Q62765
D	641	HIS	-	EXPRESSION TAG	UNP Q62765
D	642	HIS	-	EXPRESSION TAG	UNP Q62765
D	643	HIS	-	EXPRESSION TAG	UNP Q62765
D	644	HIS	-	EXPRESSION TAG	UNP Q62765

- Molecule 2 is a protein called Neurexin-1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	F	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	G	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			
2	H	177	Total	C	N	O	S	0	0	0
			1359	857	243	258	1			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	33	GLY	-	EXPRESSION TAG	UNP Q63373
E	34	SER	-	EXPRESSION TAG	UNP Q63373
E	35	PRO	-	EXPRESSION TAG	UNP Q63373
E	36	GLY	-	EXPRESSION TAG	UNP Q63373
E	37	ILE	-	EXPRESSION TAG	UNP Q63373
E	38	SER	-	EXPRESSION TAG	UNP Q63373
E	39	GLY	-	EXPRESSION TAG	UNP Q63373
E	40	GLY	-	EXPRESSION TAG	UNP Q63373
E	41	GLY	-	EXPRESSION TAG	UNP Q63373
E	42	GLY	-	EXPRESSION TAG	UNP Q63373
E	43	GLY	-	EXPRESSION TAG	UNP Q63373

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Chain	Residue	Modelled	Actual	Comment	Reference
E	44	ILE	-	EXPRESSION TAG	UNP Q63373
E	45	LEU	-	EXPRESSION TAG	UNP Q63373
E	46	GLU	-	EXPRESSION TAG	UNP Q63373
E	300	HIS	-	EXPRESSION TAG	UNP Q63373
E	301	HIS	-	EXPRESSION TAG	UNP Q63373
E	302	HIS	-	EXPRESSION TAG	UNP Q63373
E	303	HIS	-	EXPRESSION TAG	UNP Q63373
E	304	HIS	-	EXPRESSION TAG	UNP Q63373
E	305	HIS	-	EXPRESSION TAG	UNP Q63373
F	33	GLY	-	EXPRESSION TAG	UNP Q63373
F	34	SER	-	EXPRESSION TAG	UNP Q63373
F	35	PRO	-	EXPRESSION TAG	UNP Q63373
F	36	GLY	-	EXPRESSION TAG	UNP Q63373
F	37	ILE	-	EXPRESSION TAG	UNP Q63373
F	38	SER	-	EXPRESSION TAG	UNP Q63373
F	39	GLY	-	EXPRESSION TAG	UNP Q63373
F	40	GLY	-	EXPRESSION TAG	UNP Q63373
F	41	GLY	-	EXPRESSION TAG	UNP Q63373
F	42	GLY	-	EXPRESSION TAG	UNP Q63373
F	43	GLY	-	EXPRESSION TAG	UNP Q63373
F	44	ILE	-	EXPRESSION TAG	UNP Q63373
F	45	LEU	-	EXPRESSION TAG	UNP Q63373
F	46	GLU	-	EXPRESSION TAG	UNP Q63373
F	300	HIS	-	EXPRESSION TAG	UNP Q63373
F	301	HIS	-	EXPRESSION TAG	UNP Q63373
F	302	HIS	-	EXPRESSION TAG	UNP Q63373
F	303	HIS	-	EXPRESSION TAG	UNP Q63373
F	304	HIS	-	EXPRESSION TAG	UNP Q63373
F	305	HIS	-	EXPRESSION TAG	UNP Q63373
G	33	GLY	-	EXPRESSION TAG	UNP Q63373
G	34	SER	-	EXPRESSION TAG	UNP Q63373
G	35	PRO	-	EXPRESSION TAG	UNP Q63373
G	36	GLY	-	EXPRESSION TAG	UNP Q63373
G	37	ILE	-	EXPRESSION TAG	UNP Q63373
G	38	SER	-	EXPRESSION TAG	UNP Q63373
G	39	GLY	-	EXPRESSION TAG	UNP Q63373
G	40	GLY	-	EXPRESSION TAG	UNP Q63373
G	41	GLY	-	EXPRESSION TAG	UNP Q63373
G	42	GLY	-	EXPRESSION TAG	UNP Q63373
G	43	GLY	-	EXPRESSION TAG	UNP Q63373
G	44	ILE	-	EXPRESSION TAG	UNP Q63373
G	45	LEU	-	EXPRESSION TAG	UNP Q63373

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Chain	Residue	Modelled	Actual	Comment	Reference
G	46	GLU	-	EXPRESSION TAG	UNP Q63373
G	300	HIS	-	EXPRESSION TAG	UNP Q63373
G	301	HIS	-	EXPRESSION TAG	UNP Q63373
G	302	HIS	-	EXPRESSION TAG	UNP Q63373
G	303	HIS	-	EXPRESSION TAG	UNP Q63373
G	304	HIS	-	EXPRESSION TAG	UNP Q63373
G	305	HIS	-	EXPRESSION TAG	UNP Q63373
H	33	GLY	-	EXPRESSION TAG	UNP Q63373
H	34	SER	-	EXPRESSION TAG	UNP Q63373
H	35	PRO	-	EXPRESSION TAG	UNP Q63373
H	36	GLY	-	EXPRESSION TAG	UNP Q63373
H	37	ILE	-	EXPRESSION TAG	UNP Q63373
H	38	SER	-	EXPRESSION TAG	UNP Q63373
H	39	GLY	-	EXPRESSION TAG	UNP Q63373
H	40	GLY	-	EXPRESSION TAG	UNP Q63373
H	41	GLY	-	EXPRESSION TAG	UNP Q63373
H	42	GLY	-	EXPRESSION TAG	UNP Q63373
H	43	GLY	-	EXPRESSION TAG	UNP Q63373
H	44	ILE	-	EXPRESSION TAG	UNP Q63373
H	45	LEU	-	EXPRESSION TAG	UNP Q63373
H	46	GLU	-	EXPRESSION TAG	UNP Q63373
H	300	HIS	-	EXPRESSION TAG	UNP Q63373
H	301	HIS	-	EXPRESSION TAG	UNP Q63373
H	302	HIS	-	EXPRESSION TAG	UNP Q63373
H	303	HIS	-	EXPRESSION TAG	UNP Q63373
H	304	HIS	-	EXPRESSION TAG	UNP Q63373
H	305	HIS	-	EXPRESSION TAG	UNP Q63373

- 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	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	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		

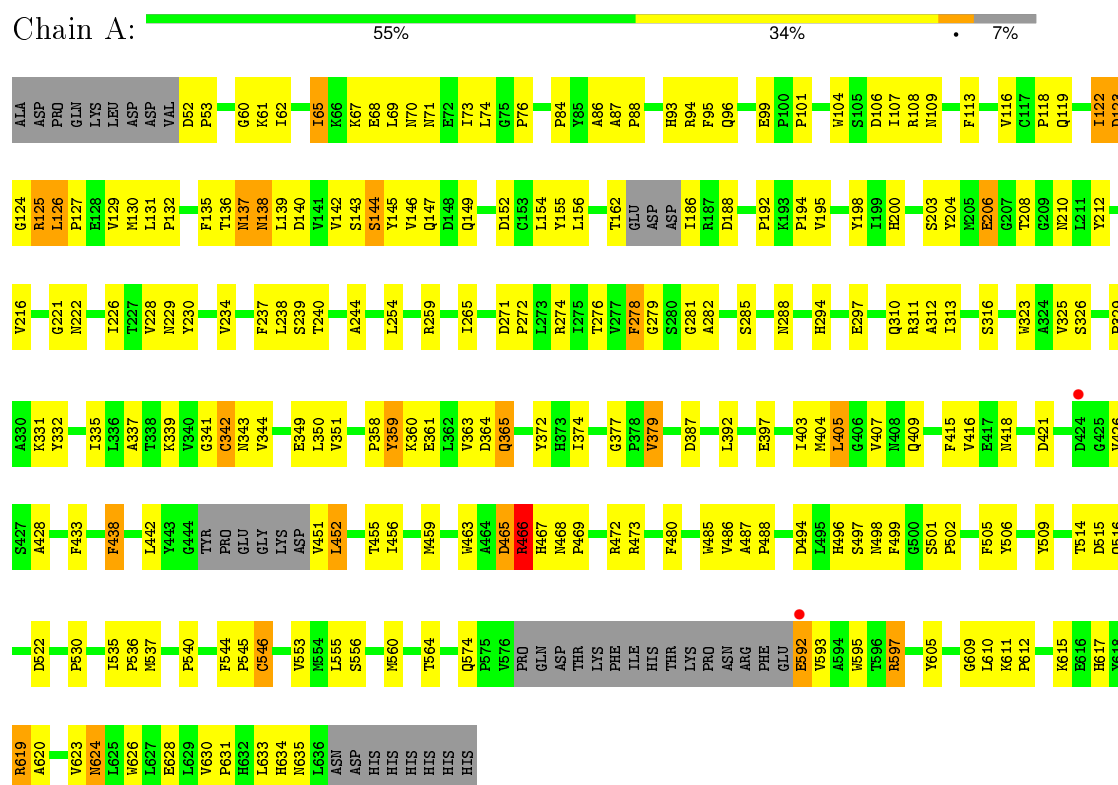
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	2	Total	Ca	0	0
			2	2		
5	F	2	Total	Ca	0	0
			2	2		
5	E	2	Total	Ca	0	0
			2	2		

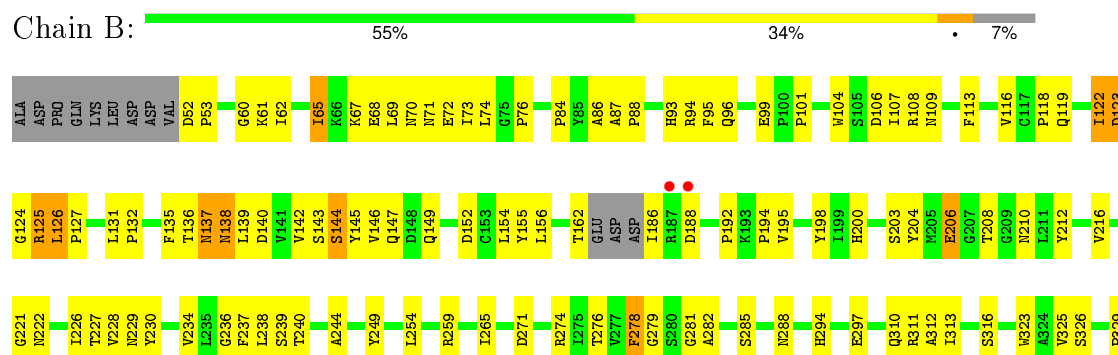
3 Residue-property plots

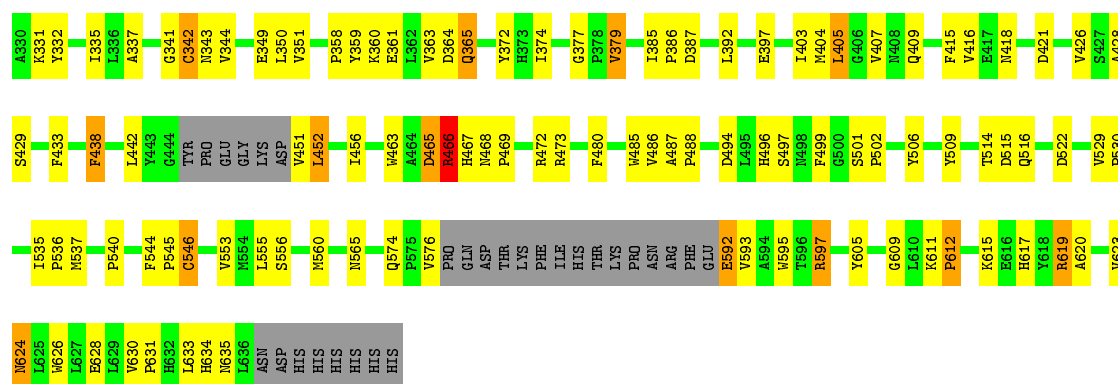
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Neuroligin-1

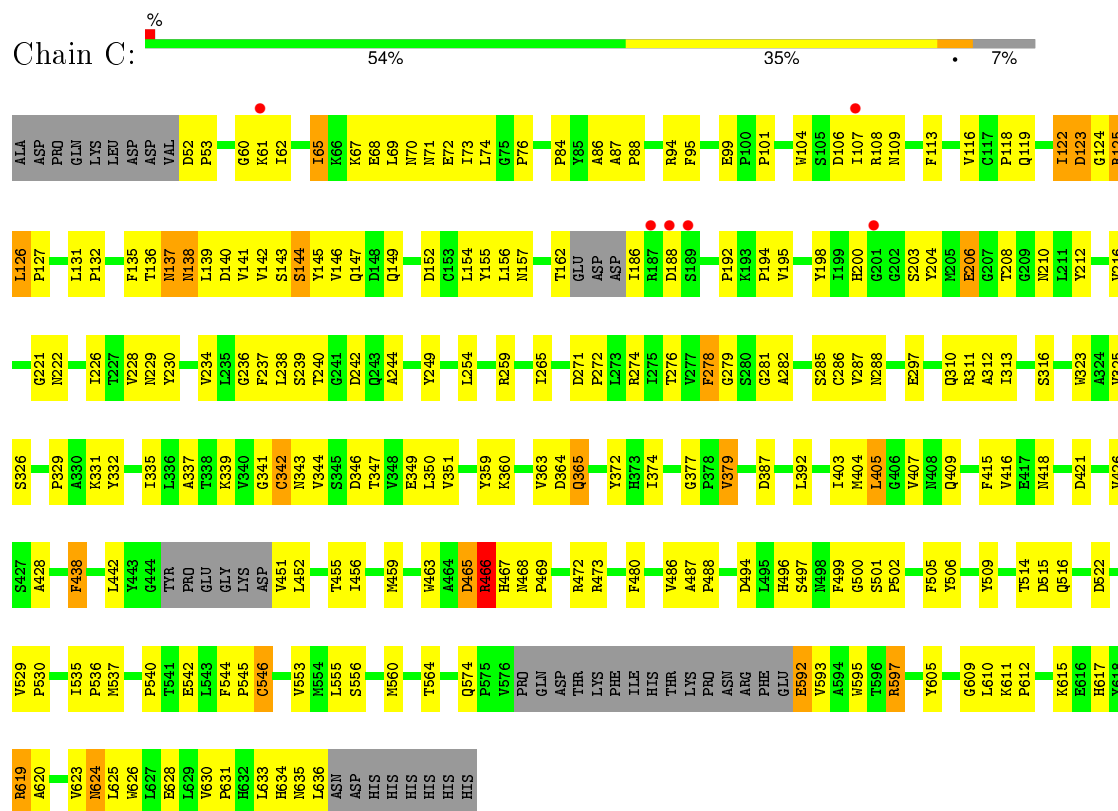


• Molecule 1: Neuroligin-1

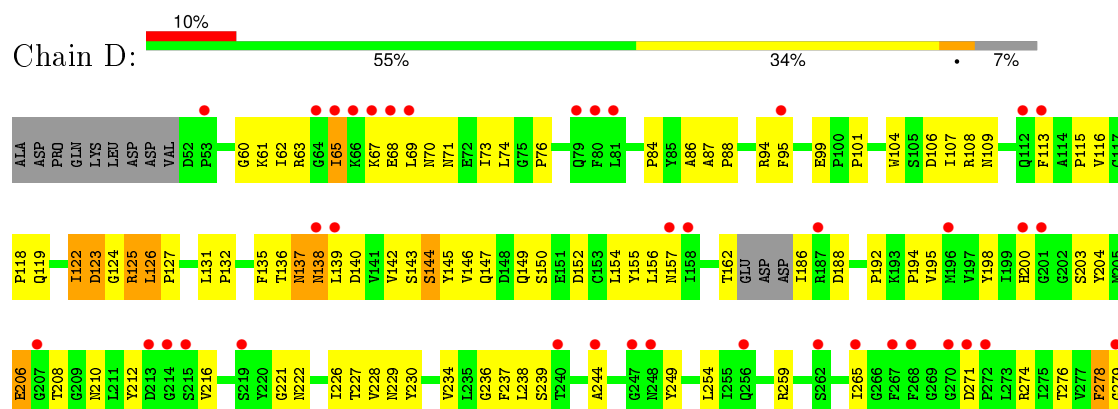




• Molecule 1: Neuroligin-1

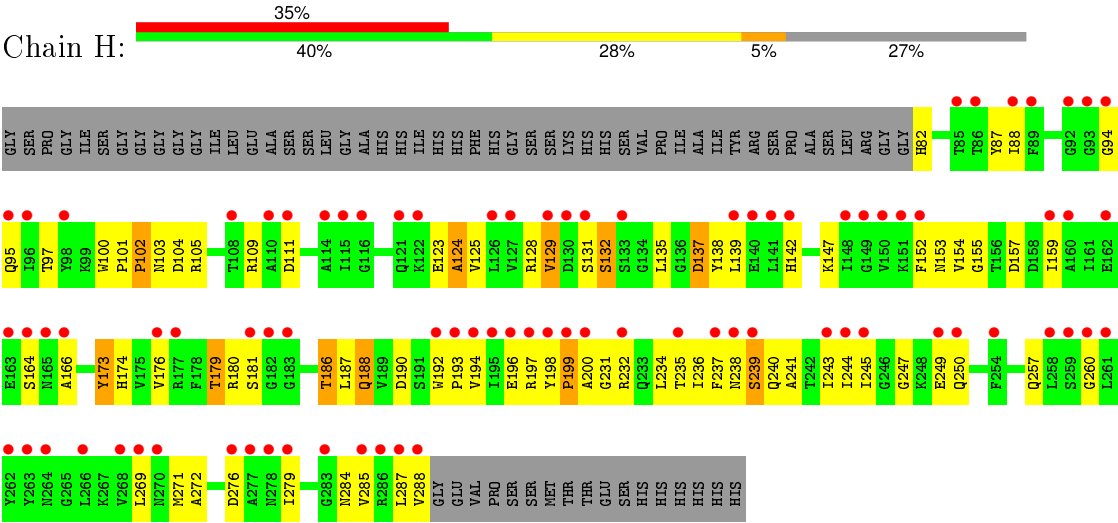


• Molecule 1: Neuroligin-1





● Molecule 2: Neurexin-1-beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.83Å 148.80Å 123.60Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	45.90 – 3.50 45.90 – 3.39	Depositor EDS
% Data completeness (in resolution range)	94.9 (45.90-3.50) 92.4 (45.90-3.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.276 0.248 , 0.277	Depositor DCC
R_{free} test set	2538 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	97.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 53460 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22438	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: CA, 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	0.45	0/4302	0.65	1/5872 (0.0%)
1	B	0.45	0/4302	0.66	1/5872 (0.0%)
1	C	0.43	0/4302	0.65	0/5872
1	D	0.36	0/4302	0.63	1/5872 (0.0%)
2	E	0.44	0/1385	0.71	0/1877
2	F	0.48	0/1385	0.71	0/1877
2	G	0.47	0/1385	0.72	0/1877
2	H	0.34	0/1385	0.67	0/1877
All	All	0.42	0/22748	0.66	3/30996 (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	D	452	LEU	N-CA-C	-5.23	96.87	111.00
1	A	452	LEU	N-CA-C	-5.09	97.24	111.00
1	B	452	LEU	N-CA-C	-5.07	97.31	111.00

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	4186	0	4046	176	0
1	B	4186	0	4046	175	0
1	C	4186	0	4046	175	0
1	D	4186	0	4045	173	0
2	E	1359	0	1345	54	1
2	F	1359	0	1345	59	0
2	G	1359	0	1345	53	0
2	H	1359	0	1347	58	0
3	A	42	0	39	3	0
3	B	42	0	39	3	0
3	C	42	0	39	3	0
3	D	42	0	39	2	0
4	E	28	0	25	7	0
4	F	28	0	25	7	0
4	G	28	0	25	7	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
All	All	22438	0	21796	916	1

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 21.

The worst 5 of 916 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)
2:G:147:LYS:HD3	2:G:164:SER:HA	1.48	0.95
2:E:147:LYS:HD3	2:E:164:SER:HA	1.47	0.93
2:F:147:LYS:HD3	2:F:164:SER:HA	1.51	0.92
2:H:147:LYS:HD3	2:H:164:SER:HA	1.50	0.90
1:D:426:VAL:HG23	1:D:473:ARG:HB2	1.62	0.80

All (1) 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)
2:E:192:TRP:NE1	2:E:192:TRP:NE1[2_556]	1.74	0.46

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	525/574 (92%)	441 (84%)	62 (12%)	22 (4%)	3	32
1	B	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	4	33
1	C	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	4	33
1	D	525/574 (92%)	441 (84%)	63 (12%)	21 (4%)	4	33
2	E	175/243 (72%)	143 (82%)	23 (13%)	9 (5%)	2	26
2	F	175/243 (72%)	143 (82%)	22 (13%)	10 (6%)	2	23
2	G	175/243 (72%)	142 (81%)	23 (13%)	10 (6%)	2	23
2	H	175/243 (72%)	143 (82%)	22 (13%)	10 (6%)	2	23
All	All	2800/3268 (86%)	2335 (83%)	341 (12%)	124 (4%)	3	30

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	A	124	GLY
1	A	138	ASN
1	A	343	ASN
1	A	465	ASP

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	455/494 (92%)	435 (96%)	20 (4%)	35	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	455/494 (92%)	435 (96%)	20 (4%)	35	73
1	C	455/494 (92%)	436 (96%)	19 (4%)	36	74
1	D	455/494 (92%)	436 (96%)	19 (4%)	36	74
2	E	143/193 (74%)	131 (92%)	12 (8%)	14	50
2	F	143/193 (74%)	132 (92%)	11 (8%)	16	54
2	G	143/193 (74%)	132 (92%)	11 (8%)	16	54
2	H	143/193 (74%)	132 (92%)	11 (8%)	16	54
All	All	2392/2748 (87%)	2269 (95%)	123 (5%)	29	69

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	592	GLU
1	D	379	VAL
2	H	102	PRO
1	C	597	ARG
1	D	206	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN
1	D	624	ASN
1	D	120	ASN
1	B	624	ASN
1	C	437	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 ⓘ

6 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$
4	NAG	E	306	2,4	14,14,15	1.19	1 (7%)	15,19,21	0.83	0
4	NAG	E	307	4	14,14,15	0.91	1 (7%)	15,19,21	0.73	0
4	NAG	F	306	2,4	14,14,15	1.22	1 (7%)	15,19,21	0.93	1 (6%)
4	NAG	F	307	4	14,14,15	0.97	1 (7%)	15,19,21	0.70	0
4	NAG	G	306	2,4	14,14,15	1.18	1 (7%)	15,19,21	0.92	0
4	NAG	G	307	4	14,14,15	1.04	1 (7%)	15,19,21	0.67	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
4	NAG	E	306	2,4	-	1/6/23/26	0/1/1/1
4	NAG	E	307	4	-	0/6/23/26	0/1/1/1
4	NAG	F	306	2,4	-	1/6/23/26	0/1/1/1
4	NAG	F	307	4	-	0/6/23/26	0/1/1/1
4	NAG	G	306	2,4	-	1/6/23/26	0/1/1/1
4	NAG	G	307	4	-	0/6/23/26	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)
4	E	307	NAG	C1-C2	2.77	1.56	1.52
4	G	306	NAG	C1-C2	3.08	1.56	1.52
4	F	307	NAG	C1-C2	3.15	1.56	1.52
4	E	306	NAG	C1-C2	3.28	1.57	1.52
4	G	307	NAG	C1-C2	3.32	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	306	NAG	O7-C7-C8	-2.02	118.36	122.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	306	NAG	O7-C7-N2-C2
4	E	306	NAG	O7-C7-N2-C2
4	F	306	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	306	NAG	7	0
4	E	307	NAG	4	0
4	F	306	NAG	7	0
4	F	307	NAG	4	0
4	G	306	NAG	7	0
4	G	307	NAG	4	0

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\# Z > 2$
3	NAG	A	701	1	14,14,15	1.00	1 (7%)	15,19,21	0.60	0
3	NAG	A	702	1	14,14,15	1.01	1 (7%)	15,19,21	0.88	1 (6%)
3	NAG	A	703	1	14,14,15	0.77	0	15,19,21	0.73	0
3	NAG	B	701	1	14,14,15	0.96	1 (7%)	15,19,21	0.62	0
3	NAG	B	702	1	14,14,15	0.88	0	15,19,21	0.93	1 (6%)
3	NAG	B	703	1	14,14,15	0.69	0	15,19,21	0.72	0
3	NAG	C	701	1	14,14,15	0.92	1 (7%)	15,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	702	1	14,14,15	0.86	1 (7%)	15,19,21	0.88	1 (6%)
3	NAG	C	703	1	14,14,15	0.75	0	15,19,21	0.75	0
3	NAG	D	701	1	14,14,15	0.72	0	15,19,21	0.52	0
3	NAG	D	702	1	14,14,15	0.76	1 (7%)	15,19,21	0.90	1 (6%)
3	NAG	D	703	1	14,14,15	0.65	0	15,19,21	0.70	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
3	NAG	A	701	1	-	0/6/23/26	0/1/1/1
3	NAG	A	702	1	-	1/6/23/26	0/1/1/1
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1	-	0/6/23/26	0/1/1/1
3	NAG	C	701	1	-	0/6/23/26	0/1/1/1
3	NAG	C	702	1	-	0/6/23/26	0/1/1/1
3	NAG	C	703	1	-	0/6/23/26	0/1/1/1
3	NAG	D	701	1	-	1/6/23/26	0/1/1/1
3	NAG	D	702	1	-	0/6/23/26	0/1/1/1
3	NAG	D	703	1	-	0/6/23/26	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	D	702	NAG	C1-C2	2.08	1.55	1.52
3	C	702	NAG	C1-C2	2.21	1.55	1.52
3	A	702	NAG	C1-C2	2.33	1.55	1.52
3	C	701	NAG	C1-C2	2.74	1.56	1.52
3	B	701	NAG	C1-C2	2.81	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAG	C2-N2-C7	-2.56	119.75	123.04
3	C	702	NAG	C2-N2-C7	-2.55	119.77	123.04
3	D	702	NAG	C2-N2-C7	-2.38	119.98	123.04
3	A	702	NAG	C2-N2-C7	-2.37	119.99	123.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NAG	O7-C7-N2-C2
3	D	701	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	NAG	1	0
3	A	702	NAG	1	0
3	A	703	NAG	1	0
3	B	701	NAG	1	0
3	B	702	NAG	1	0
3	B	703	NAG	1	0
3	C	701	NAG	1	0
3	C	702	NAG	1	0
3	C	703	NAG	1	0
3	D	701	NAG	1	0
3	D	702	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 ⓘ

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, 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	533/574 (92%)	-0.22	2 (0%) 93 90	63, 100, 139, 162	0
1	B	533/574 (92%)	-0.24	2 (0%) 93 90	61, 96, 131, 178	0
1	C	533/574 (92%)	-0.09	6 (1%) 82 73	72, 115, 153, 180	0
1	D	533/574 (92%)	0.58	56 (10%) 8 8	75, 188, 282, 506	0
2	E	177/243 (72%)	-0.14	1 (0%) 90 85	82, 120, 139, 154	0
2	F	177/243 (72%)	-0.39	0 100 100	77, 95, 110, 122	0
2	G	177/243 (72%)	-0.11	2 (1%) 82 73	78, 105, 130, 143	0
2	H	177/243 (72%)	2.21	85 (48%) 0 0	146, 268, 426, 538	0
All	All	2840/3268 (86%)	0.10	154 (5%) 29 23	61, 112, 262, 538	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	260	GLY	11.6
2	H	263	TYR	8.2
2	H	164	SER	7.7
1	D	80	PHE	6.7
2	H	127	VAL	6.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
4	NAG	F	307	14/15	0.91	0.24	-	172,174,177,178	0
4	NAG	E	307	14/15	0.86	0.17	-	146,150,151,152	0
4	NAG	G	307	14/15	0.82	0.31	-	154,158,159,159	0
4	NAG	F	306	14/15	0.69	0.23	-	122,130,133,141	0
4	NAG	E	306	14/15	0.68	0.20	-	146,152,154,157	0
4	NAG	G	306	14/15	0.69	0.28	-	127,133,136,142	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, 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(Å ²)	Q<0.9
3	NAG	D	702	14/15	0.37	0.81	3.39	205,205,205,205	0
5	CA	E	401	1/1	0.97	0.23	0.37	89,89,89,89	0
5	CA	F	401	1/1	0.95	0.20	-0.11	76,76,76,76	0
5	CA	G	401	1/1	0.99	0.16	-0.45	79,79,79,79	0
3	NAG	B	702	14/15	0.59	0.28	-	136,138,139,140	0
5	CA	E	402	1/1	0.90	0.31	-	96,96,96,96	0
5	CA	G	402	1/1	0.68	0.28	-	111,111,111,111	0
3	NAG	A	701	14/15	0.68	0.29	-	152,155,156,157	0
3	NAG	D	701	14/15	0.39	0.45	-	219,219,219,219	0
3	NAG	B	701	14/15	0.45	0.40	-	184,187,191,192	0
3	NAG	C	701	14/15	0.46	0.25	-	216,218,219,219	0
3	NAG	B	703	14/15	0.56	0.38	-	236,240,241,242	0
3	NAG	A	702	14/15	0.71	0.25	-	145,147,148,148	0
3	NAG	A	703	14/15	0.50	0.36	-	218,222,225,225	0
3	NAG	C	702	14/15	0.73	0.51	-	186,187,189,189	0
5	CA	F	402	1/1	0.86	0.27	-	96,96,96,96	0
3	NAG	D	703	14/15	0.31	0.45	-	251,251,251,251	0
3	NAG	C	703	14/15	-0.01	0.84	-	218,222,222,222	0

6.5 Other polymers [i](#)

There are no such residues in this entry.