



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2024 – 01:16 AM EST

PDB ID : 3Q41
Title : Crystal structure of the GluN1 N-terminal domain (NTD)
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Deposited on : 2010-12-22
Resolution : 3.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

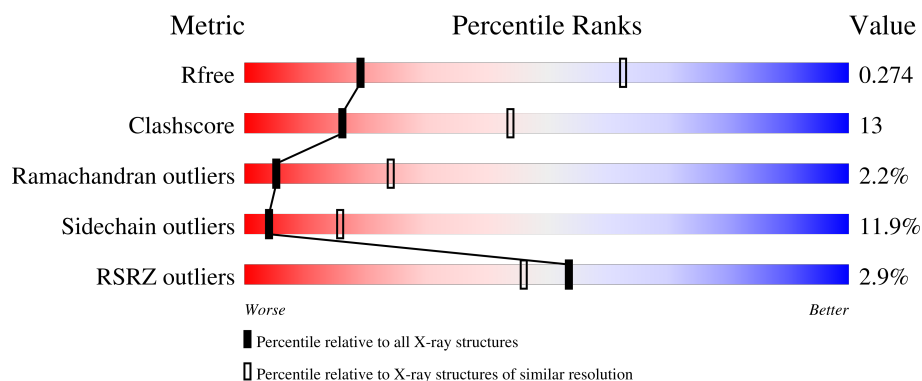
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	384	<div> <div>2%</div> <div>66%</div> <div>25%</div> <div>6%</div> <div>.</div> </div>
1	B	384	<div> <div>2%</div> <div>62%</div> <div>27%</div> <div>6%</div> <div>.</div> </div>
1	C	384	<div> <div>4%</div> <div>69%</div> <div>23%</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8968 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 Glutamate [NMDA] receptor subunit zeta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2919	1842	521	544	12			
1	B	367	Total	C	N	O	S	0	0	0
			2887	1821	516	538	12			
1	C	371	Total	C	N	O	S	0	0	0
			2919	1842	521	544	12			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	394	VAL	-	expression tag	UNP P35439
A	395	ASP	-	expression tag	UNP P35439
A	396	GLY	-	expression tag	UNP P35439
A	397	GLY	-	expression tag	UNP P35439
A	398	GLY	-	expression tag	UNP P35439
A	399	GLY	-	expression tag	UNP P35439
A	400	GLY	-	expression tag	UNP P35439
A	401	LEU	-	expression tag	UNP P35439
A	402	VAL	-	expression tag	UNP P35439
A	403	PRO	-	expression tag	UNP P35439
A	404	ARG	-	expression tag	UNP P35439
B	394	VAL	-	expression tag	UNP P35439
B	395	ASP	-	expression tag	UNP P35439
B	396	GLY	-	expression tag	UNP P35439
B	397	GLY	-	expression tag	UNP P35439
B	398	GLY	-	expression tag	UNP P35439
B	399	GLY	-	expression tag	UNP P35439
B	400	GLY	-	expression tag	UNP P35439
B	401	LEU	-	expression tag	UNP P35439
B	402	VAL	-	expression tag	UNP P35439
B	403	PRO	-	expression tag	UNP P35439
B	404	ARG	-	expression tag	UNP P35439
C	394	VAL	-	expression tag	UNP P35439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	395	ASP	-	expression tag	UNP P35439
C	396	GLY	-	expression tag	UNP P35439
C	397	GLY	-	expression tag	UNP P35439
C	398	GLY	-	expression tag	UNP P35439
C	399	GLY	-	expression tag	UNP P35439
C	400	GLY	-	expression tag	UNP P35439
C	401	LEU	-	expression tag	UNP P35439
C	402	VAL	-	expression tag	UNP P35439
C	403	PRO	-	expression tag	UNP P35439
C	404	ARG	-	expression tag	UNP P35439

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

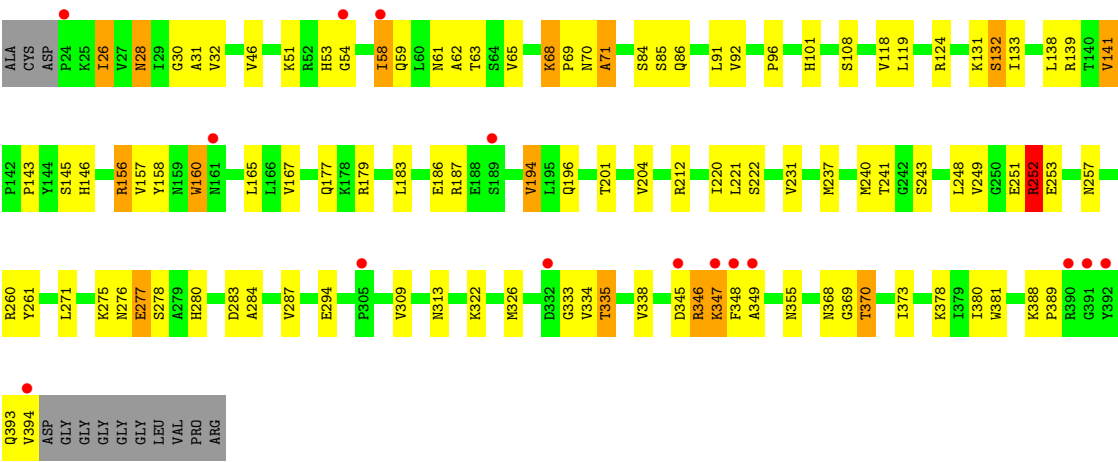
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	2	Total	Cl	0	0
			2	2		
3	C	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	10	Total	O	0	0
			10	10		
4	C	8	Total	O	0	0
			8	8		

- Molecule 1: Glutamate [NMDA] receptor subunit zeta-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.68Å 164.68Å 147.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.24 – 3.40 45.24 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.24-3.40) 99.8 (45.24-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.229 , 0.279 0.225 , 0.274	Depositor DCC
R_{free} test set	1617 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8968	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: CL, 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	0.39	0/2982	0.61	1/4046 (0.0%)
1	B	0.39	0/2949	0.62	1/4001 (0.0%)
1	C	0.41	0/2982	0.56	0/4046
All	All	0.40	0/8913	0.60	2/12093 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	GLY	N-CA-C	-6.06	97.94	113.10
1	B	138	LEU	CA-CB-CG	5.50	127.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	201	THR	Peptide

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	2919	0	2910	82	0
1	B	2887	0	2881	76	0
1	C	2919	0	2910	78	0
2	A	70	0	65	1	0
2	B	70	0	65	2	0
2	C	70	0	65	3	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	7	0	0	1	0
4	B	10	0	0	0	0
4	C	8	0	0	0	0
All	All	8968	0	8896	230	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 230 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:333:GLY:O	1:A:334:VAL:HG22	1.47	1.13
1:A:143:PRO:HD3	1:A:346:ARG:HG2	1.14	1.07
1:A:138:LEU:HA	1:A:345:ASP:OD2	1.59	1.02
1:A:359:ARG:HG3	1:A:359:ARG:HH11	1.27	1.00
1:C:212:ARG:HB2	1:C:240:MET:HE1	1.45	0.97

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	369/384 (96%)	334 (90%)	29 (8%)	6 (2%)	8	29
1	B	365/384 (95%)	319 (87%)	35 (10%)	11 (3%)	3	19
1	C	369/384 (96%)	329 (89%)	33 (9%)	7 (2%)	6	26
All	All	1103/1152 (96%)	982 (89%)	97 (9%)	24 (2%)	5	24

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	VAL
1	B	309	VAL
1	C	369	GLY
1	A	159	ASN
1	A	252	ARG

5.3.2 Protein sidechains ⓘ

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	318/325 (98%)	277 (87%)	41 (13%)	3	13
1	B	315/325 (97%)	273 (87%)	42 (13%)	3	12
1	C	318/325 (98%)	288 (91%)	30 (9%)	7	25
All	All	951/975 (98%)	838 (88%)	113 (12%)	4	16

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	187	ARG
1	C	348	PHE
1	B	306	ARG
1	C	347	LYS
1	C	243	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
1	B	270	GLN
1	C	311	ASN
1	B	257	ASN
1	B	311	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	NAG	C	406	1	14,14,15	0.64	0	17,19,21	1.45	2 (11%)
2	NAG	C	408	1	14,14,15	0.71	1 (7%)	17,19,21	2.81	5 (29%)
2	NAG	B	408	1	14,14,15	0.73	0	17,19,21	1.31	3 (17%)
2	NAG	B	409	1	14,14,15	1.02	1 (7%)	17,19,21	1.53	3 (17%)
2	NAG	A	407	1	14,14,15	0.65	0	17,19,21	1.71	2 (11%)
2	NAG	B	405	1	14,14,15	0.57	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	409	1	14,14,15	0.61	0	17,19,21	2.49	4 (23%)
2	NAG	C	407	1	14,14,15	0.70	0	17,19,21	1.05	1 (5%)
2	NAG	A	405	1	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
2	NAG	A	408	1	14,14,15	0.78	0	17,19,21	1.31	1 (5%)
2	NAG	B	406	1	14,14,15	0.63	0	17,19,21	1.15	1 (5%)
2	NAG	B	407	1	14,14,15	0.54	0	17,19,21	1.43	2 (11%)
2	NAG	C	409	1	14,14,15	0.48	0	17,19,21	0.74	0
2	NAG	C	405	1	14,14,15	0.65	0	17,19,21	1.22	2 (11%)
2	NAG	A	406	1	14,14,15	0.88	1 (7%)	17,19,21	1.87	3 (17%)

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	C	406	1	-	3/6/23/26	0/1/1/1
2	NAG	C	408	1	-	3/6/23/26	0/1/1/1
2	NAG	B	408	1	-	2/6/23/26	0/1/1/1
2	NAG	B	409	1	-	3/6/23/26	0/1/1/1
2	NAG	A	407	1	-	3/6/23/26	0/1/1/1
2	NAG	B	405	1	-	0/6/23/26	0/1/1/1
2	NAG	A	409	1	-	2/6/23/26	0/1/1/1
2	NAG	C	407	1	-	0/6/23/26	0/1/1/1
2	NAG	A	405	1	-	0/6/23/26	0/1/1/1
2	NAG	A	408	1	-	0/6/23/26	0/1/1/1
2	NAG	B	406	1	-	2/6/23/26	0/1/1/1
2	NAG	B	407	1	-	2/6/23/26	0/1/1/1
2	NAG	C	409	1	-	2/6/23/26	0/1/1/1
2	NAG	C	405	1	-	3/6/23/26	0/1/1/1
2	NAG	A	406	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	409	NAG	C1-C2	2.30	1.55	1.52
2	A	406	NAG	O7-C7	2.21	1.28	1.23
2	C	408	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	NAG	C1-O5-C5	8.36	123.38	112.19
2	C	408	NAG	C1-O5-C5	7.89	122.75	112.19
2	C	408	NAG	C2-N2-C7	6.30	131.34	122.90
2	A	406	NAG	C1-O5-C5	5.29	119.28	112.19
2	A	407	NAG	C1-O5-C5	5.26	119.23	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	407	NAG	C1-C2-N2-C7
2	A	409	NAG	C3-C2-N2-C7
2	B	408	NAG	C1-C2-N2-C7
2	B	409	NAG	C3-C2-N2-C7
2	C	406	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	408	NAG	2	0
2	B	409	NAG	1	0
2	A	407	NAG	1	0
2	C	407	NAG	1	0
2	B	406	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 [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	371/384 (96%)	0.12	9 (2%) 59 51	49, 71, 94, 109	0
1	B	367/384 (95%)	0.13	8 (2%) 62 53	52, 74, 99, 108	0
1	C	371/384 (96%)	0.25	15 (4%) 43 37	56, 75, 98, 111	0
All	All	1109/1152 (96%)	0.17	32 (2%) 54 46	49, 73, 97, 111	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	ILE	4.5
1	A	392	TYR	4.1
1	C	394	VAL	3.9
1	C	345	ASP	3.7
1	A	347	LYS	3.2

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](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	NAG	B	408	14/15	0.59	0.20	82,85,86,87	0
2	NAG	B	407	14/15	0.70	0.17	82,84,85,85	0
2	NAG	C	409	14/15	0.70	0.15	100,102,102,102	0
2	NAG	B	409	14/15	0.77	0.15	102,103,103,104	0
2	NAG	C	405	14/15	0.77	0.14	92,93,94,94	0
2	NAG	A	407	14/15	0.77	0.16	83,86,87,87	0
2	NAG	C	408	14/15	0.78	0.15	85,88,90,90	0
3	CL	A	1	1/1	0.81	0.20	90,90,90,90	0
2	NAG	A	408	14/15	0.83	0.12	77,79,81,81	0
2	NAG	C	407	14/15	0.85	0.13	74,75,76,76	0
2	NAG	A	405	14/15	0.88	0.10	77,77,78,78	0
2	NAG	A	409	14/15	0.88	0.11	93,93,94,94	0
3	CL	B	6	1/1	0.88	0.16	84,84,84,84	0
3	CL	C	8	1/1	0.89	0.07	87,87,87,87	0
3	CL	C	2	1/1	0.90	0.14	75,75,75,75	1
2	NAG	B	405	14/15	0.90	0.10	76,79,80,80	0
2	NAG	B	406	14/15	0.91	0.14	80,82,83,83	0
2	NAG	C	406	14/15	0.92	0.11	75,75,77,77	0
3	CL	B	7	1/1	0.92	0.15	95,95,95,95	0
3	CL	A	3	1/1	0.92	0.11	83,83,83,83	0
3	CL	A	5	1/1	0.92	0.14	88,88,88,88	0
3	CL	A	4	1/1	0.93	0.10	101,101,101,101	0
2	NAG	A	406	14/15	0.93	0.12	69,70,72,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.