



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:32 PM BST

PDB ID : 3Q41
Title : Crystal structure of the GluN1 N-terminal domain (NTD)
Authors : Farina, A.N.; Blain, K.Y.; Maruo, T.; Kwiatkowski, W.; Choe, S.; Nakagawa, T.
Deposited on : 2010-12-22
Resolution : 3.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

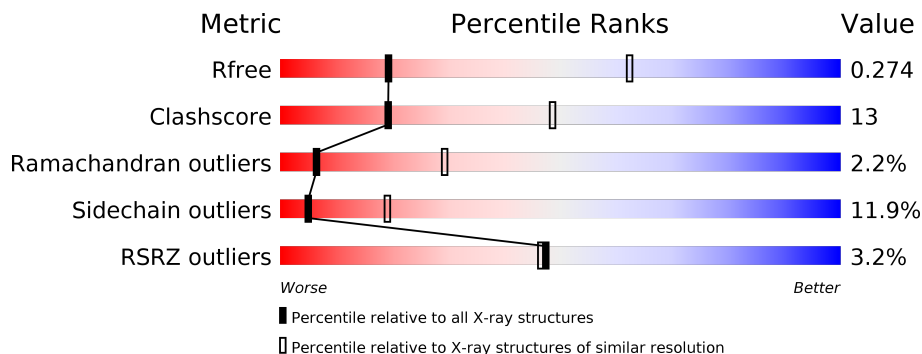
1 Overall quality at a glance i

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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 style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">66% 25% 6% .</p>
1	B	384	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">62% 27% 6% . .</p>
1	C	384	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">69% 23% . .</p>

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	CL	A	4	-	-	-	X

2 Entry composition i

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
			Total	C	N	O	S			
1	A	371	2919	1842	521	544	12	0	0	0
1	B	367	2887	1821	516	538	12	0	0	0
1	C	371	2919	1842	521	544	12	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

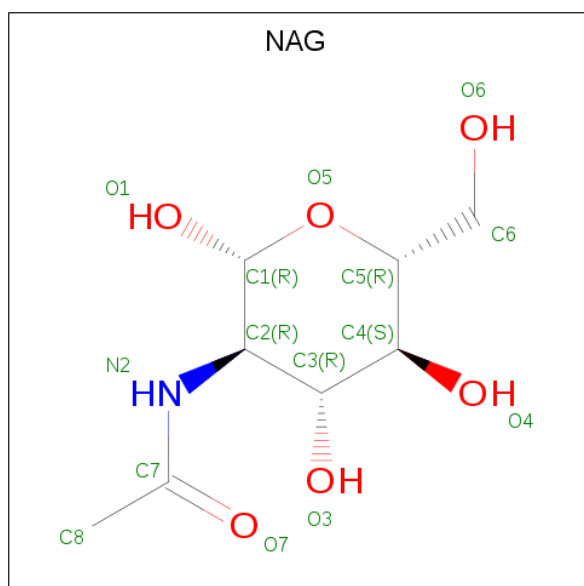
Chain	Residue	Modelled	Actual	Comment	Reference
A	394	VAL	-	expression tag	UNP P35439
A	395	ASP	-	expression tag	UNP P35439
A	396	GLY	-	expression tag	UNP P35439
A	397	GLY	-	expression tag	UNP P35439
A	398	GLY	-	expression tag	UNP P35439
A	399	GLY	-	expression tag	UNP P35439
A	400	GLY	-	expression tag	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	B	2	Total	Cl	0	0
			2	2		
3	A	4	Total	Cl	0	0
			4	4		
3	C	2	Total	Cl	0	0
			2	2		

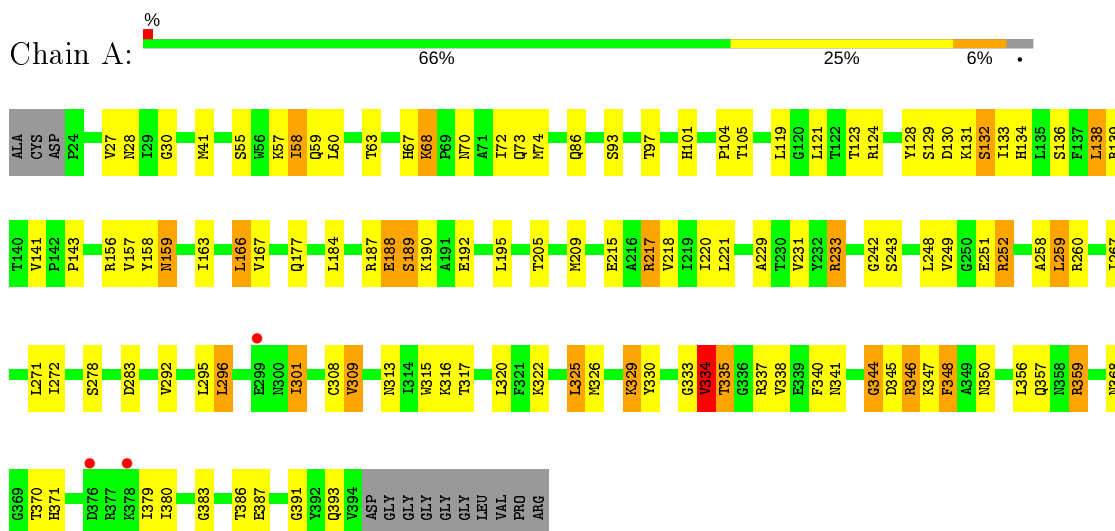
- Molecule 4 is water.

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		

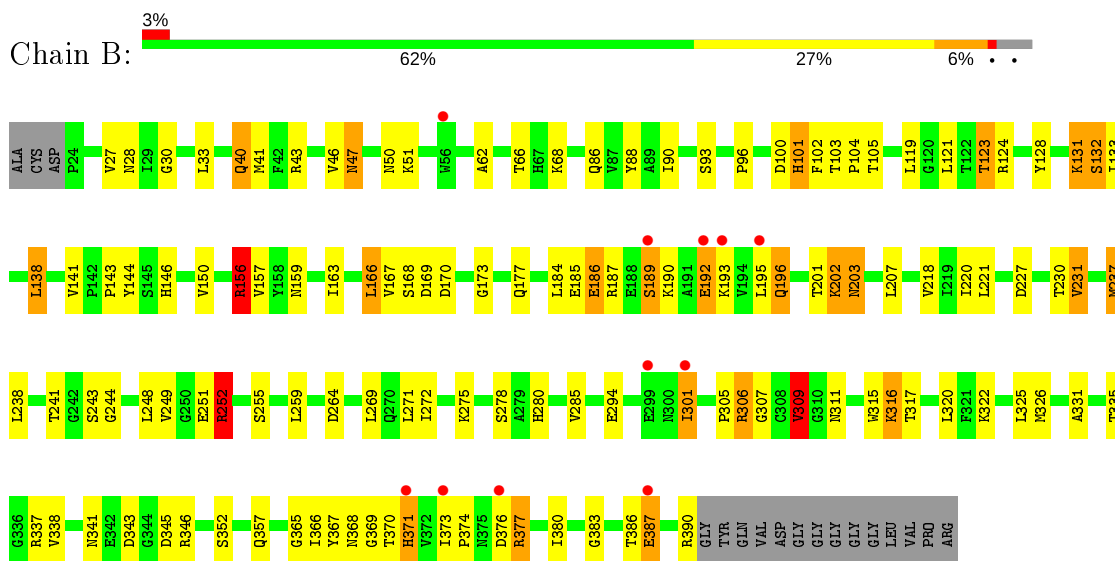
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Glutamate [NMDA] receptor subunit zeta-1

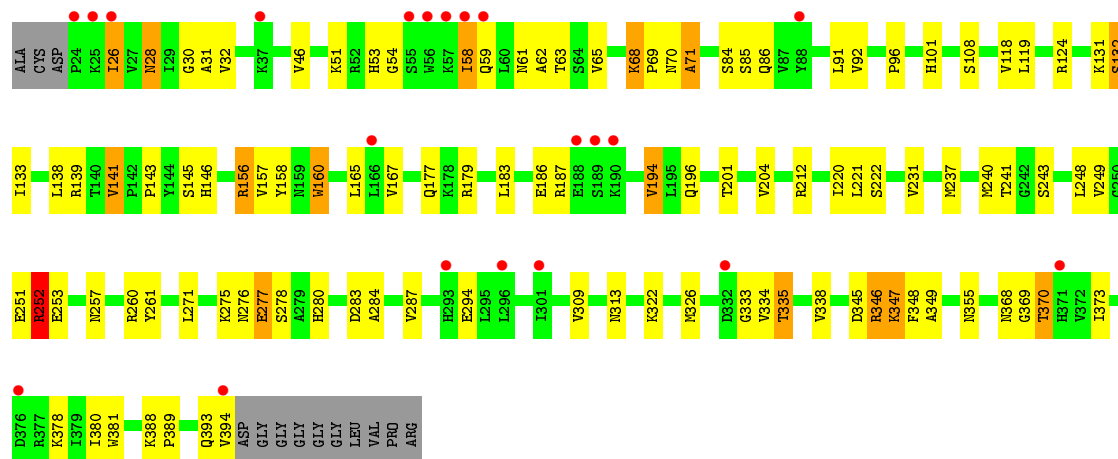


- Molecule 1: Glutamate [NMDA] receptor subunit zeta-1



- 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) 99.9 (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)	Xtrriage
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 (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL

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 [\(i\)](#)

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	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.

All (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:HH11	1:A:359:ARG:HG3	1.27	1.00
1:C:212:ARG:HB2	1:C:240:MET:HE1	1.45	0.97
1:B:46:VAL:HG11	1:B:62:ALA:HB2	1.47	0.97
1:C:346:ARG:HG3	1:C:346:ARG:HH11	1.27	0.95
1:B:377:ARG:HH11	1:B:377:ARG:HG3	1.34	0.91
1:C:334:VAL:HG21	2:C:408:NAG:H62	1.54	0.88
1:B:251:GLU:O	1:B:252:ARG:HB3	1.76	0.85
1:C:368:ASN:O	1:C:370:THR:N	2.11	0.83
1:A:97:THR:HG22	1:C:237:MET:HE1	1.60	0.82
1:C:333:GLY:O	1:C:334:VAL:CG1	2.27	0.82
1:C:346:ARG:NH1	1:C:346:ARG:HG3	1.92	0.81
1:C:124:ARG:HD2	1:C:141:VAL:CG1	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ARG:HD2	1:C:141:VAL:HG13	1.63	0.80
1:A:359:ARG:HG3	1:A:359:ARG:NH1	1.91	0.79
1:C:138:LEU:HB2	1:C:345:ASP:HB3	1.63	0.78
1:B:163:ILE:HD13	1:B:220:ILE:HD12	1.67	0.76
1:C:212:ARG:HB2	1:C:240:MET:CE	2.15	0.76
1:C:334:VAL:CG2	2:C:408:NAG:H62	2.16	0.75
1:A:308:CYS:HB3	1:B:132:SER:HB3	1.68	0.75
1:C:333:GLY:O	1:C:334:VAL:HG12	1.86	0.75
1:A:333:GLY:C	1:A:334:VAL:HG22	2.08	0.74
1:B:86:GLN:HG2	1:B:306:ARG:HB3	1.69	0.74
1:C:28:ASN:HB3	1:C:61:ASN:HB3	1.70	0.73
1:B:104:PRO:HG3	1:B:123:THR:HG21	1.68	0.73
1:B:185:GLU:O	1:B:186:GLU:HG3	1.89	0.73
1:B:221:LEU:HB3	1:B:249:VAL:HG12	1.71	0.72
1:C:138:LEU:CB	1:C:345:ASP:HB3	2.19	0.72
1:A:97:THR:HG22	1:C:237:MET:CE	2.19	0.71
1:B:377:ARG:HH11	1:B:377:ARG:CG	2.03	0.71
1:B:47:ASN:HA	1:B:50:ASN:HB2	1.72	0.70
1:A:345:ASP:O	1:A:346:ARG:HD3	1.93	0.69
1:C:143:PRO:HD3	1:C:346:ARG:HH11	1.58	0.69
1:A:129:SER:OG	1:A:346:ARG:HD2	1.93	0.68
1:C:167:VAL:HG11	1:C:177:GLN:HB2	1.74	0.68
1:C:138:LEU:HB2	1:C:345:ASP:CB	2.24	0.68
1:B:168:SER:HB2	1:B:170:ASP:OD1	1.91	0.68
1:A:243:SER:H	1:A:383:GLY:HA3	1.58	0.68
1:A:348:PHE:CD1	1:A:348:PHE:N	2.62	0.67
1:A:141:VAL:HG23	1:A:271:LEU:HD21	1.76	0.67
1:A:340:PHE:HB3	1:A:345:ASP:HB2	1.75	0.67
1:C:138:LEU:HB2	1:C:345:ASP:OD1	1.95	0.67
1:A:283:ASP:OD2	1:A:334:VAL:CG2	2.43	0.66
1:B:169:ASP:HB2	1:B:196:GLN:HB2	1.78	0.66
1:B:124:ARG:HD2	1:B:141:VAL:HG22	1.78	0.65
1:B:301:ILE:HA	1:B:317:THR:HG21	1.78	0.65
1:A:60:LEU:HD21	1:A:292:VAL:HG11	1.78	0.64
1:A:132:SER:OG	1:B:309:VAL:HA	1.98	0.64
1:B:335:THR:HB	1:B:346:ARG:HH22	1.62	0.64
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.79	0.64
1:A:221:LEU:HB3	1:A:249:VAL:HG12	1.80	0.64
1:A:138:LEU:HA	1:A:345:ASP:CG	2.19	0.63
1:A:350:ASN:HD22	1:A:368:ASN:HA	1.63	0.63
1:A:368:ASN:OD1	1:A:371:HIS:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:HG3	1:A:346:ARG:HH11	1.63	0.62
1:C:283:ASP:OD1	1:C:333:GLY:O	2.18	0.62
1:A:70:ASN:HD22	1:A:73:GLN:HG2	1.63	0.62
1:A:333:GLY:O	1:A:334:VAL:CG2	2.37	0.62
1:C:139:ARG:NE	1:C:346:ARG:HH12	1.98	0.61
1:A:258:ALA:O	1:A:259:LEU:HB3	2.01	0.61
1:B:220:ILE:HA	1:B:248:LEU:O	2.01	0.61
1:C:346:ARG:HH11	1:C:346:ARG:CG	2.08	0.61
1:B:96:PRO:HB2	1:B:275:LYS:HE2	1.83	0.61
1:A:335:THR:HB	1:A:347:LYS:NZ	2.16	0.60
1:A:348:PHE:HD1	1:A:348:PHE:N	1.97	0.60
1:C:53:HIS:HB3	1:C:58:ILE:HD12	1.83	0.60
1:C:46:VAL:HG11	1:C:62:ALA:HB2	1.83	0.60
1:C:32:VAL:HG22	1:C:92:VAL:HA	1.84	0.60
1:B:357:GLN:HG2	1:B:380:ILE:HG22	1.85	0.59
1:C:212:ARG:HD3	1:C:240:MET:CE	2.32	0.59
1:C:333:GLY:O	1:C:334:VAL:HG13	2.01	0.59
1:C:143:PRO:HD3	1:C:346:ARG:HG3	1.85	0.59
1:B:124:ARG:HD2	1:B:141:VAL:CG2	2.33	0.59
1:A:283:ASP:OD2	1:A:334:VAL:HG22	2.02	0.59
1:B:251:GLU:O	1:B:252:ARG:CB	2.47	0.58
1:B:192:GLU:HG3	1:B:193:LYS:N	2.19	0.58
1:C:280:HIS:CE1	1:C:335:THR:HG21	2.38	0.58
1:B:150:VAL:HG11	1:B:269:LEU:HD21	1.85	0.58
1:B:373:ILE:HG21	2:B:409:NAG:H82	1.85	0.57
1:C:347:LYS:HD2	1:C:349:ALA:HB2	1.87	0.57
1:C:70:ASN:O	1:C:71:ALA:HB3	2.05	0.57
1:C:46:VAL:HG11	1:C:62:ALA:CB	2.35	0.56
1:B:86:GLN:HE21	1:B:306:ARG:HD2	1.70	0.56
1:C:373:ILE:HG13	1:C:373:ILE:O	2.06	0.56
1:B:46:VAL:HG13	1:B:47:ASN:N	2.21	0.56
1:A:67:HIS:HA	1:A:74:MET:HE1	1.88	0.55
1:B:41:MET:SD	1:B:278:SER:HB2	2.46	0.55
1:C:28:ASN:H	1:C:28:ASN:ND2	2.04	0.55
1:A:139:ARG:HD2	1:A:141:VAL:O	2.08	0.54
1:C:139:ARG:HE	1:C:346:ARG:HH12	1.52	0.54
1:B:103:THR:N	1:B:104:PRO:HD2	2.22	0.54
1:A:217:ARG:HB3	1:A:391:GLY:HA2	1.88	0.54
1:B:167:VAL:HG11	1:B:177:GLN:HB2	1.89	0.54
1:B:243:SER:OG	1:B:244:GLY:N	2.41	0.54
1:C:119:LEU:HA	1:C:138:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ARG:HH11	1:A:359:ARG:CG	2.09	0.54
1:A:301:ILE:HA	1:A:317:THR:HG21	1.91	0.53
1:B:105:THR:HG23	1:B:128:TYR:OH	2.08	0.53
1:B:316:LYS:H	1:B:316:LYS:HD2	1.72	0.53
1:A:260:ARG:HD2	1:C:261:TYR:CE1	2.44	0.53
1:A:105:THR:HG23	1:A:128:TYR:OH	2.08	0.53
1:A:205:THR:O	1:A:209:MET:HG2	2.09	0.53
1:A:143:PRO:HG3	1:A:346:ARG:NH1	2.24	0.53
1:A:163:ILE:HD13	1:A:220:ILE:HD12	1.91	0.53
1:B:41:MET:SD	1:B:278:SER:CB	2.97	0.53
1:A:357:GLN:HG2	1:A:380:ILE:HG12	1.90	0.53
1:C:119:LEU:HD23	1:C:284:ALA:HB1	1.91	0.53
1:C:212:ARG:CB	1:C:240:MET:HE1	2.28	0.53
1:C:28:ASN:ND2	1:C:86:GLN:O	2.42	0.53
1:A:251:GLU:O	1:A:252:ARG:CB	2.56	0.52
1:A:242:GLY:HA3	2:A:407:NAG:H61	1.92	0.52
1:B:370:THR:O	1:B:371:HIS:HB2	2.09	0.52
1:B:202:LYS:O	1:B:203:ASN:CB	2.58	0.52
1:A:93:SER:HB2	1:A:121:LEU:HD12	1.90	0.52
1:A:138:LEU:HD11	1:A:325:LEU:HB3	1.91	0.52
1:B:377:ARG:NH1	1:B:377:ARG:CG	2.68	0.52
1:C:165:LEU:HB3	1:C:194:VAL:HG12	1.90	0.52
1:A:330:TYR:HB3	1:A:338:VAL:HB	1.91	0.52
1:B:322:LYS:O	1:B:326:MET:HG2	2.10	0.51
1:C:96:PRO:HB2	1:C:275:LYS:HE2	1.92	0.51
1:B:124:ARG:HB2	1:B:144:TYR:CE2	2.45	0.51
1:C:338:VAL:HA	1:C:347:LYS:HE3	1.91	0.51
1:A:163:ILE:HG22	1:A:218:VAL:HG13	1.92	0.51
1:C:251:GLU:O	1:C:252:ARG:HB3	2.09	0.51
1:C:30:GLY:HA2	1:C:63:THR:O	2.11	0.51
1:A:333:GLY:C	1:A:334:VAL:CG2	2.77	0.50
1:A:272:ILE:HA	2:C:407:NAG:H83	1.94	0.50
1:A:68:LYS:H	1:A:74:MET:HE2	1.77	0.50
1:C:393:GLN:HG3	1:C:394:VAL:N	2.27	0.50
1:B:124:ARG:HB2	1:B:144:TYR:CZ	2.46	0.50
1:C:146:HIS:CE1	1:C:346:ARG:HG2	2.47	0.50
1:A:301:ILE:HD13	1:A:301:ILE:H	1.77	0.49
1:C:143:PRO:HD3	1:C:346:ARG:CG	2.41	0.49
1:C:276:ASN:OD1	1:C:276:ASN:O	2.30	0.49
1:B:141:VAL:HG23	1:B:271:LEU:HD22	1.94	0.49
1:B:237:MET:HA	1:B:237:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HG11	1:A:177:GLN:HB3	1.95	0.49
1:A:335:THR:HB	1:A:347:LYS:HZ3	1.76	0.49
1:A:58:ILE:HG21	1:A:296:LEU:HD23	1.95	0.49
1:B:366:ILE:HG23	1:B:373:ILE:HG13	1.94	0.49
1:C:158:TYR:HB3	1:C:160:TRP:CH2	2.48	0.48
1:C:276:ASN:O	1:C:277:GLU:C	2.51	0.48
1:A:41:MET:SD	1:A:278:SER:HB3	2.53	0.48
1:A:28:ASN:HB2	1:A:86:GLN:O	2.13	0.48
1:B:305:PRO:HD3	1:B:315:TRP:HB3	1.95	0.48
1:A:251:GLU:O	1:A:252:ARG:HB2	2.14	0.47
1:A:133:ILE:HD12	1:A:133:ILE:HA	1.81	0.47
1:A:309:VAL:HG12	1:B:131:LYS:HB2	1.97	0.47
1:B:341:ASN:CB	1:B:345:ASP:H	2.28	0.47
1:A:104:PRO:HG2	1:A:123:THR:HG21	1.96	0.47
1:B:189:SER:O	1:B:190:LYS:HD2	2.15	0.47
1:A:267:ILE:HD11	1:A:379:ILE:HD11	1.97	0.47
1:B:156:ARG:HG3	1:B:157:VAL:N	2.30	0.47
1:B:386:THR:O	1:B:387:GLU:HB3	2.14	0.47
1:C:220:ILE:HA	1:C:248:LEU:O	2.15	0.47
1:A:141:VAL:HG23	1:A:271:LEU:CD2	2.43	0.46
1:A:70:ASN:ND2	1:A:73:GLN:HG2	2.28	0.46
1:B:243:SER:H	1:B:383:GLY:HA3	1.80	0.46
1:B:195:LEU:HB3	1:B:207:LEU:HD11	1.97	0.46
1:C:119:LEU:HD12	1:C:138:LEU:HG	1.96	0.46
1:C:156:ARG:HG3	1:C:157:VAL:N	2.29	0.46
1:A:188:GLU:HG3	1:A:188:GLU:O	2.16	0.46
1:B:104:PRO:HG3	1:B:123:THR:CG2	2.43	0.46
1:B:143:PRO:HG2	1:B:146:HIS:CD2	2.52	0.45
1:C:141:VAL:HG22	1:C:271:LEU:HD21	1.97	0.45
1:B:202:LYS:HD2	1:B:202:LYS:N	2.32	0.45
1:A:131:LYS:O	1:A:132:SER:HB2	2.16	0.45
1:A:30:GLY:HA2	1:A:63:THR:O	2.17	0.45
1:C:85:SER:O	1:C:86:GLN:C	2.54	0.45
1:A:130:ASP:HB3	1:A:133:ILE:HG22	1.98	0.45
1:B:202:LYS:HA	1:B:230:THR:HG21	1.99	0.45
1:B:227:ASP:O	1:B:231:VAL:HG13	2.16	0.45
1:B:202:LYS:HD2	1:B:202:LYS:H	1.83	0.44
1:C:108:SER:HA	1:C:118:VAL:HG21	1.99	0.44
1:B:46:VAL:CG1	1:B:47:ASN:N	2.81	0.44
1:A:344:GLY:HA3	4:A:19:HOH:O	2.17	0.44
1:C:131:LYS:O	1:C:132:SER:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG11	1:A:292:VAL:HG21	1.98	0.44
1:C:179:ARG:O	1:C:183:LEU:HG	2.18	0.43
1:C:212:ARG:CB	1:C:240:MET:CE	2.91	0.43
1:C:54:GLY:O	1:C:58:ILE:HG13	2.18	0.43
1:B:46:VAL:HA	1:B:285:VAL:HG11	1.99	0.43
1:A:220:ILE:HA	1:A:248:LEU:O	2.19	0.43
1:B:237:MET:HG3	1:B:237:MET:O	2.17	0.43
1:B:252:ARG:HA	1:B:255:SER:HB2	1.99	0.43
1:B:331:ALA:HA	1:B:337:ARG:HA	2.01	0.43
1:B:367:TYR:CZ	1:B:370:THR:HA	2.53	0.43
1:C:70:ASN:O	1:C:71:ALA:CB	2.64	0.43
1:C:222:SER:HA	1:C:253:GLU:OE2	2.18	0.43
1:A:166:LEU:HA	1:A:195:LEU:O	2.18	0.43
1:B:168:SER:H	1:B:173:GLY:HA3	1.83	0.43
1:C:322:LYS:HE3	1:C:326:MET:SD	2.59	0.43
1:B:30:GLY:O	1:B:90:ILE:HA	2.19	0.42
1:B:341:ASN:HB2	1:B:345:ASP:H	1.84	0.42
1:B:40:GLN:HG2	1:B:43:ARG:HH21	1.84	0.42
1:B:28:ASN:HB2	1:B:86:GLN:O	2.20	0.42
1:C:31:ALA:HA	1:C:91:LEU:O	2.19	0.42
1:C:355:ASN:HD21	1:C:380:ILE:H	1.67	0.42
1:B:203:ASN:OD1	2:B:406:NAG:O5	2.37	0.42
1:B:121:LEU:HB2	1:B:280:HIS:HB3	2.01	0.42
1:C:32:VAL:HA	1:C:65:VAL:O	2.20	0.42
1:A:184:LEU:HD22	1:A:189:SER:HB3	2.02	0.42
1:A:322:LYS:O	1:A:326:MET:HG3	2.19	0.42
1:A:229:ALA:O	1:A:233:ARG:HG2	2.20	0.42
1:C:156:ARG:HH22	1:C:187:ARG:HH21	1.68	0.42
1:C:68:LYS:HA	1:C:69:PRO:HD3	1.93	0.42
1:B:365:GLY:HA2	1:B:374:PRO:HA	2.02	0.41
1:A:187:ARG:HH12	1:A:188:GLU:HG3	1.85	0.41
1:B:100:ASP:O	1:B:102:PHE:N	2.53	0.41
1:C:138:LEU:HB2	1:C:345:ASP:CG	2.40	0.41
1:A:187:ARG:NH1	1:A:188:GLU:HG3	2.34	0.41
1:C:212:ARG:HD3	1:C:240:MET:HE3	1.99	0.41
1:C:284:ALA:HA	1:C:287:VAL:HG12	2.03	0.41
1:A:131:LYS:HG2	1:A:131:LYS:H	1.71	0.41
1:A:133:ILE:HG23	1:A:134:HIS:CD2	2.54	0.41
1:A:329:LYS:HB2	1:A:329:LYS:HE3	1.87	0.41
1:C:160:TRP:HH2	1:C:381:TRP:CH2	2.38	0.41
1:B:166:LEU:HA	1:B:195:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:O	1:A:159:ASN:N	2.54	0.41
1:C:204:VAL:HG21	1:C:231:VAL:HG12	2.02	0.40
1:B:33:LEU:HA	1:B:93:SER:HB3	2.03	0.40
1:C:145:SER:O	1:C:179:ARG:HD3	2.21	0.40
1:C:388:LYS:HA	1:C:389:PRO:HD3	1.95	0.40
1:A:131:LYS:O	1:A:132:SER:CB	2.69	0.40
1:A:55:SER:OG	1:A:59:GLN:NE2	2.54	0.40
1:B:272:ILE:HD11	1:B:352:SER:HB3	2.03	0.40
1:A:70:ASN:HD22	1:A:73:GLN:CG	2.32	0.40
1:B:27:VAL:HG13	1:B:88:TYR:CD2	2.57	0.40

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	369/384 (96%)	334 (90%)	29 (8%)	6 (2%)	9	34
1	B	365/384 (95%)	319 (87%)	35 (10%)	11 (3%)	4	23
1	C	369/384 (96%)	329 (89%)	33 (9%)	7 (2%)	8	31
All	All	1103/1152 (96%)	982 (89%)	97 (9%)	24 (2%)	6	29

All (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
1	A	393	GLN
1	B	156	ARG

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Mol	Chain	Res	Type
1	B	203	ASN
1	B	252	ARG
1	B	369	GLY
1	C	277	GLU
1	A	132	SER
1	B	101	HIS
1	C	201	THR
1	B	192	GLU
1	B	371	HIS
1	C	132	SER
1	B	133	ILE
1	B	387	GLU
1	C	26	ILE
1	C	71	ALA
1	A	158	TYR
1	C	252	ARG
1	B	307	GLY

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	318/325 (98%)	277 (87%)	41 (13%)	4 16
1	B	315/325 (97%)	273 (87%)	42 (13%)	4 15
1	C	318/325 (98%)	288 (91%)	30 (9%)	8 30
All	All	951/975 (98%)	838 (88%)	113 (12%)	5 19

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	58	ILE
1	A	68	LYS
1	A	72	ILE
1	A	101	HIS

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Mol	Chain	Res	Type
1	A	119	LEU
1	A	124	ARG
1	A	136	SER
1	A	138	LEU
1	A	156	ARG
1	A	166	LEU
1	A	188	GLU
1	A	189	SER
1	A	190	LYS
1	A	192	GLU
1	A	215	GLU
1	A	217	ARG
1	A	231	VAL
1	A	233	ARG
1	A	259	LEU
1	A	295	LEU
1	A	296	LEU
1	A	301	ILE
1	A	309	VAL
1	A	313	ASN
1	A	315	TRP
1	A	316	LYS
1	A	320	LEU
1	A	325	LEU
1	A	329	LYS
1	A	334	VAL
1	A	335	THR
1	A	337	ARG
1	A	341	ASN
1	A	346	ARG
1	A	348	PHE
1	A	356	LEU
1	A	359	ARG
1	A	370	THR
1	A	386	THR
1	A	387	GLU
1	B	40	GLN
1	B	47	ASN
1	B	51	LYS
1	B	66	THR
1	B	68	LYS
1	B	101	HIS

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Mol	Chain	Res	Type
1	B	119	LEU
1	B	123	THR
1	B	131	LYS
1	B	132	SER
1	B	138	LEU
1	B	156	ARG
1	B	159	ASN
1	B	166	LEU
1	B	184	LEU
1	B	186	GLU
1	B	187	ARG
1	B	189	SER
1	B	196	GLN
1	B	202	LYS
1	B	218	VAL
1	B	231	VAL
1	B	237	MET
1	B	238	LEU
1	B	241	THR
1	B	252	ARG
1	B	259	LEU
1	B	264	ASP
1	B	294	GLU
1	B	301	ILE
1	B	306	ARG
1	B	309	VAL
1	B	311	ASN
1	B	316	LYS
1	B	320	LEU
1	B	325	LEU
1	B	338	VAL
1	B	343	ASP
1	B	368	ASN
1	B	376	ASP
1	B	377	ARG
1	B	390	ARG
1	C	26	ILE
1	C	28	ASN
1	C	51	LYS
1	C	58	ILE
1	C	59	GLN
1	C	68	LYS

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Mol	Chain	Res	Type
1	C	84	SER
1	C	101	HIS
1	C	133	ILE
1	C	141	VAL
1	C	156	ARG
1	C	160	TRP
1	C	186	GLU
1	C	194	VAL
1	C	196	GLN
1	C	241	THR
1	C	243	SER
1	C	252	ARG
1	C	257	ASN
1	C	260	ARG
1	C	278	SER
1	C	294	GLU
1	C	309	VAL
1	C	313	ASN
1	C	335	THR
1	C	346	ARG
1	C	347	LYS
1	C	348	PHE
1	C	370	THR
1	C	378	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	59	GLN
1	A	70	ASN
1	A	73	GLN
1	A	270	GLN
1	A	311	ASN
1	A	313	ASN
1	A	341	ASN
1	A	350	ASN
1	A	355	ASN
1	A	371	HIS
1	B	40	GLN
1	B	47	ASN
1	B	86	GLN

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Mol	Chain	Res	Type
1	B	177	GLN
1	B	196	GLN
1	B	257	ASN
1	B	270	GLN
1	B	311	ASN
1	C	28	ASN
1	C	40	GLN
1	C	59	GLN
1	C	146	HIS
1	C	257	ASN
1	C	311	ASN
1	C	313	ASN
1	C	355	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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	405	1	14,14,15	0.48	0	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	405	1	14,14,15	0.57	0	17,19,21	0.66	0
2	NAG	C	406	1	14,14,15	0.64	0	17,19,21	1.39	2 (11%)
2	NAG	B	406	1	14,14,15	0.64	0	17,19,21	1.13	1 (5%)
2	NAG	C	409	1	14,14,15	0.49	0	17,19,21	0.77	0
2	NAG	A	409	1	14,14,15	0.58	0	17,19,21	2.47	4 (23%)
2	NAG	A	407	1	14,14,15	0.63	0	17,19,21	1.67	2 (11%)
2	NAG	A	408	1	14,14,15	0.78	0	17,19,21	1.31	1 (5%)
2	NAG	C	407	1	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
2	NAG	B	408	1	14,14,15	0.70	0	17,19,21	1.30	3 (17%)
2	NAG	C	408	1	14,14,15	0.67	1 (7%)	17,19,21	2.71	5 (29%)
2	NAG	A	406	1	14,14,15	0.88	1 (7%)	17,19,21	1.84	3 (17%)
2	NAG	B	407	1	14,14,15	0.54	0	17,19,21	1.41	2 (11%)
2	NAG	B	409	1	14,14,15	0.98	1 (7%)	17,19,21	1.57	4 (23%)
2	NAG	C	405	1	14,14,15	0.64	0	17,19,21	1.22	2 (11%)

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	405	1	-	0/6/23/26	0/1/1/1
2	NAG	B	405	1	-	0/6/23/26	0/1/1/1
2	NAG	C	406	1	-	3/6/23/26	0/1/1/1
2	NAG	B	406	1	-	2/6/23/26	0/1/1/1
2	NAG	C	409	1	-	2/6/23/26	0/1/1/1
2	NAG	A	409	1	-	2/6/23/26	0/1/1/1
2	NAG	A	407	1	-	3/6/23/26	0/1/1/1
2	NAG	A	408	1	-	0/6/23/26	0/1/1/1
2	NAG	C	407	1	-	0/6/23/26	0/1/1/1
2	NAG	B	408	1	-	2/6/23/26	0/1/1/1
2	NAG	C	408	1	-	3/6/23/26	0/1/1/1
2	NAG	A	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	B	409	1	-	4/6/23/26	0/1/1/1
2	NAG	C	405	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	406	NAG	O7-C7	2.19	1.28	1.23
2	B	409	NAG	C1-C2	2.10	1.55	1.52
2	C	408	NAG	C1-C2	2.02	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	NAG	C1-O5-C5	8.26	123.38	112.19
2	C	408	NAG	C1-O5-C5	7.80	122.75	112.19
2	C	408	NAG	C2-N2-C7	5.92	131.34	122.90
2	A	406	NAG	C1-O5-C5	5.23	119.28	112.19
2	A	407	NAG	C1-O5-C5	5.19	119.23	112.19
2	C	406	NAG	C2-N2-C7	3.95	128.53	122.90
2	C	408	NAG	C1-C2-N2	3.93	117.20	110.49
2	B	409	NAG	C4-C3-C2	3.87	116.69	111.02
2	B	407	NAG	O5-C1-C2	-3.60	105.60	111.29
2	A	408	NAG	C4-C3-C2	3.45	116.08	111.02
2	B	406	NAG	O5-C1-C2	-3.45	105.84	111.29
2	A	409	NAG	C2-N2-C7	3.26	127.55	122.90
2	A	406	NAG	O5-C1-C2	-3.04	106.49	111.29
2	B	409	NAG	O5-C5-C4	-2.98	103.58	110.83
2	A	407	NAG	O5-C1-C2	2.85	115.78	111.29
2	B	408	NAG	C1-O5-C5	2.83	116.02	112.19
2	A	406	NAG	C3-C4-C5	2.77	115.17	110.24
2	B	407	NAG	C3-C4-C5	2.61	114.90	110.24
2	C	405	NAG	C4-C3-C2	2.55	114.76	111.02
2	B	409	NAG	O5-C5-C6	2.51	111.14	107.20
2	C	405	NAG	C2-N2-C7	2.49	126.45	122.90
2	C	407	NAG	O5-C1-C2	-2.37	107.54	111.29
2	A	409	NAG	O5-C5-C4	2.33	116.51	110.83
2	C	408	NAG	C6-C5-C4	-2.23	107.78	113.00
2	B	408	NAG	C2-N2-C7	2.14	125.95	122.90
2	C	406	NAG	C1-C2-N2	2.14	114.15	110.49
2	A	409	NAG	O5-C1-C2	2.13	114.65	111.29
2	A	405	NAG	C1-O5-C5	2.12	115.07	112.19
2	B	409	NAG	C2-N2-C7	2.10	125.89	122.90
2	B	408	NAG	C4-C3-C2	2.04	114.00	111.02
2	C	408	NAG	O7-C7-N2	2.02	125.67	121.95

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	408	NAG	C3-C2-N2-C7
2	C	408	NAG	C1-C2-N2-C7
2	A	409	NAG	C3-C2-N2-C7
2	B	409	NAG	C3-C2-N2-C7
2	B	406	NAG	O5-C5-C6-O6
2	C	406	NAG	C1-C2-N2-C7
2	A	407	NAG	O5-C5-C6-O6
2	A	406	NAG	O5-C5-C6-O6
2	B	406	NAG	C4-C5-C6-O6
2	C	409	NAG	O5-C5-C6-O6
2	A	407	NAG	C4-C5-C6-O6
2	C	405	NAG	C4-C5-C6-O6
2	B	407	NAG	C4-C5-C6-O6
2	A	406	NAG	C4-C5-C6-O6
2	C	405	NAG	O5-C5-C6-O6
2	B	407	NAG	O5-C5-C6-O6
2	C	406	NAG	O5-C5-C6-O6
2	C	409	NAG	C4-C5-C6-O6
2	A	409	NAG	C4-C5-C6-O6
2	A	407	NAG	C1-C2-N2-C7
2	C	408	NAG	C4-C5-C6-O6
2	C	408	NAG	O5-C5-C6-O6
2	B	409	NAG	O5-C5-C6-O6
2	B	409	NAG	C1-C2-N2-C7
2	B	408	NAG	C1-C2-N2-C7
2	C	405	NAG	C3-C2-N2-C7
2	B	409	NAG	C4-C5-C6-O6
2	C	406	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	406	NAG	1	0
2	A	407	NAG	1	0
2	C	407	NAG	1	0
2	C	408	NAG	2	0
2	B	409	NAG	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, 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%)	0.08	3 (0%) 86 85	49, 71, 94, 109	0
1	B	367/384 (95%)	0.16	11 (2%) 50 49	52, 74, 99, 108	0
1	C	371/384 (96%)	0.22	21 (5%) 23 24	56, 75, 98, 111	0
All	All	1109/1152 (96%)	0.15	35 (3%) 47 46	49, 73, 97, 111	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	TRP	4.3
1	C	58	ILE	4.0
1	C	394	VAL	3.6
1	C	57	LYS	3.5
1	C	26	ILE	3.4
1	C	24	PRO	3.4
1	C	296	LEU	3.3
1	B	301	ILE	3.2
1	C	376	ASP	3.2
1	C	55	SER	3.1
1	B	373	ILE	3.0
1	B	371	HIS	2.9
1	B	299	GLU	2.8
1	C	25	LYS	2.7
1	C	332	ASP	2.6
1	C	301	ILE	2.6
1	A	299	GLU	2.6
1	B	189	SER	2.5
1	B	193	LYS	2.5
1	C	59	GLN	2.4
1	B	376	ASP	2.3
1	A	376	ASP	2.3
1	C	293	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	56	TRP	2.3
1	C	188	GLU	2.1
1	A	378	LYS	2.1
1	B	387	GLU	2.1
1	C	190	LYS	2.1
1	B	195	LEU	2.1
1	C	371	HIS	2.1
1	C	88	TYR	2.1
1	C	37	LYS	2.1
1	C	189	SER	2.1
1	B	192	GLU	2.0
1	C	166	LEU	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 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(Å ²)	Q<0.9
3	CL	B	6	1/1	0.53	0.32	84,84,84,84	0
3	CL	C	8	1/1	0.73	0.23	87,87,87,87	0
2	NAG	B	408	14/15	0.79	0.31	82,85,86,87	0
3	CL	B	7	1/1	0.79	0.37	95,95,95,95	0
3	CL	A	4	1/1	0.79	0.55	101,101,101,101	0
2	NAG	B	409	14/15	0.81	0.40	102,103,103,104	0
2	NAG	A	408	14/15	0.83	0.26	77,79,81,81	0
2	NAG	C	409	14/15	0.85	0.43	100,102,102,102	0
3	CL	A	3	1/1	0.86	0.37	83,83,83,83	0
2	NAG	A	407	14/15	0.86	0.27	83,86,87,87	0
2	NAG	C	405	14/15	0.86	0.32	92,93,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	408	14/15	0.87	0.23	85,88,90,90	0
2	NAG	B	407	14/15	0.88	0.24	82,84,85,85	0
2	NAG	C	407	14/15	0.88	0.23	74,75,76,76	0
2	NAG	A	409	14/15	0.90	0.41	93,93,94,94	0
2	NAG	B	405	14/15	0.91	0.18	76,79,80,80	0
3	CL	A	1	1/1	0.92	0.19	90,90,90,90	0
3	CL	A	5	1/1	0.93	0.27	88,88,88,88	0
2	NAG	A	405	14/15	0.93	0.20	77,77,78,78	0
2	NAG	B	406	14/15	0.94	0.21	80,82,83,83	0
2	NAG	A	406	14/15	0.94	0.22	69,70,72,73	0
3	CL	C	2	1/1	0.95	0.19	75,75,75,75	1
2	NAG	C	406	14/15	0.95	0.26	75,75,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.