



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XOT  
Title : CRYSTAL STRUCTURE OF NEURONAL LEUCINE RICH REPEAT PROTEIN AMIGO-1  
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Deposited on : 2010-08-23  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

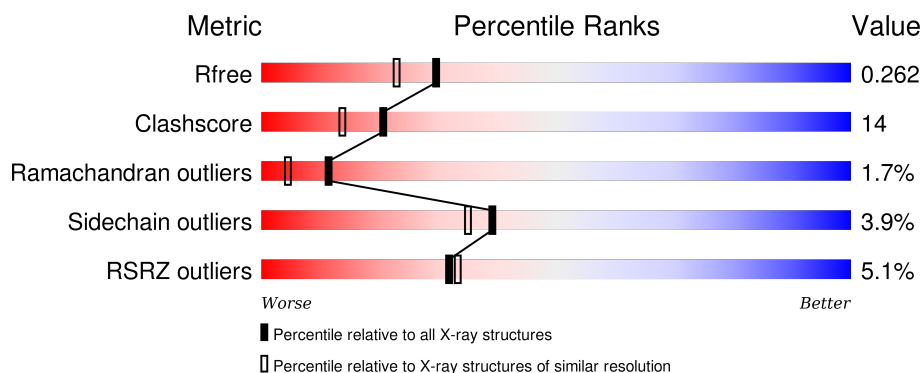
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	361	<div> <div>4%</div> <div>73% 16% • 8%</div> </div>
1	B	361	<div> <div>6%</div> <div>73% 16% • • 8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1364	-	-	-	X
2	NAG	A	1365	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5544 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 AMPHOTERIN-INDUCED PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2543	1628	424	475	16			
1	B	333	Total	C	N	O	S	0	0	0
			2535	1621	423	475	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ASP	-	EXPRESSION TAG	UNP Q80ZD8
A	24	LYS	-	EXPRESSION TAG	UNP Q80ZD8
A	25	LEU	-	EXPRESSION TAG	UNP Q80ZD8
A	26	ALA	-	EXPRESSION TAG	UNP Q80ZD8
A	27	SER	-	EXPRESSION TAG	UNP Q80ZD8
A	373	ALA	-	EXPRESSION TAG	UNP Q80ZD8
A	374	ASP	-	EXPRESSION TAG	UNP Q80ZD8
A	375	PRO	-	EXPRESSION TAG	UNP Q80ZD8
A	376	TRP	-	EXPRESSION TAG	UNP Q80ZD8
A	377	SER	-	EXPRESSION TAG	UNP Q80ZD8
A	378	HIS	-	EXPRESSION TAG	UNP Q80ZD8
A	379	PRO	-	EXPRESSION TAG	UNP Q80ZD8
A	380	GLN	-	EXPRESSION TAG	UNP Q80ZD8
A	381	PHE	-	EXPRESSION TAG	UNP Q80ZD8
A	382	GLU	-	EXPRESSION TAG	UNP Q80ZD8
A	383	LYS	-	EXPRESSION TAG	UNP Q80ZD8
B	23	ASP	-	EXPRESSION TAG	UNP Q80ZD8
B	24	LYS	-	EXPRESSION TAG	UNP Q80ZD8
B	25	LEU	-	EXPRESSION TAG	UNP Q80ZD8
B	26	ALA	-	EXPRESSION TAG	UNP Q80ZD8
B	27	SER	-	EXPRESSION TAG	UNP Q80ZD8
A	373	ALA	-	EXPRESSION TAG	UNP Q80ZD8
A	374	ASP	-	EXPRESSION TAG	UNP Q80ZD8
A	375	PRO	-	EXPRESSION TAG	UNP Q80ZD8
A	376	TRP	-	EXPRESSION TAG	UNP Q80ZD8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	377	SER	-	EXPRESSION TAG	UNP Q80ZD8
A	378	HIS	-	EXPRESSION TAG	UNP Q80ZD8
A	379	PRO	-	EXPRESSION TAG	UNP Q80ZD8
A	380	GLN	-	EXPRESSION TAG	UNP Q80ZD8
A	381	PHE	-	EXPRESSION TAG	UNP Q80ZD8
A	382	GLU	-	EXPRESSION TAG	UNP Q80ZD8
A	383	LYS	-	EXPRESSION TAG	UNP Q80ZD8

- 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		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

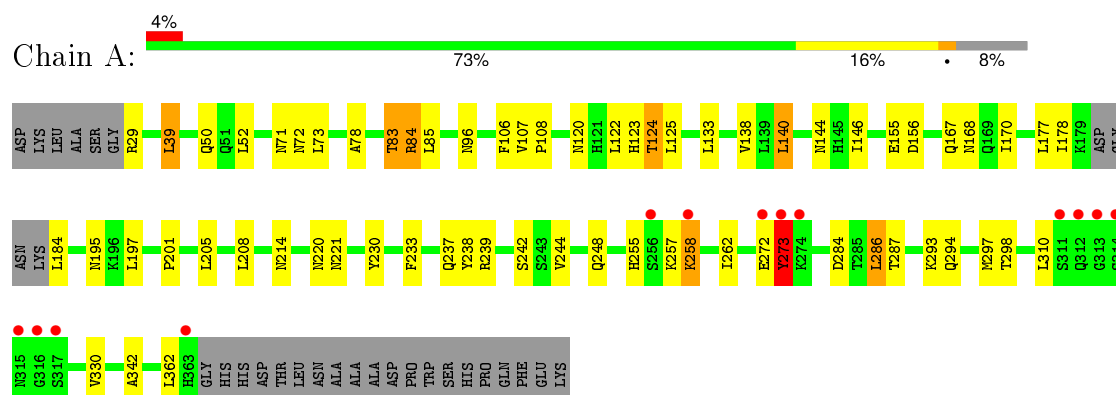
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	167	Total	O	0	0
			167	167		

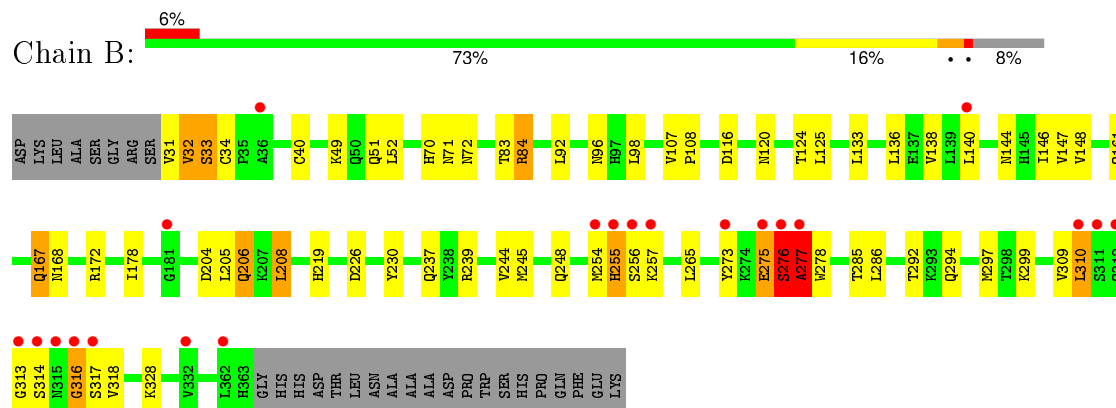
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: AMPHOTERIN-INDUCED PROTEIN 1



#### • Molecule 1: AMPHOTERIN-INDUCED PROTEIN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.44Å 74.63Å 87.27Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	29.10 – 2.00 29.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.10-2.00) 99.4 (29.10-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.255 0.215 , 0.262	Depositor DCC
$R_{free}$ test set	2624 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 52475 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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

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	0.55	0/2601	0.67	0/3551
1	B	0.58	0/2593	0.69	4/3543 (0.1%)
All	All	0.56	0/5194	0.68	4/7094 (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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	SER	N-CA-C	6.54	128.64	111.00
1	B	275	GLU	C-N-CA	5.81	136.24	121.70
1	B	32	VAL	C-N-CA	5.37	135.13	121.70
1	B	172	ARG	NE-CZ-NH1	5.23	122.91	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	THR	Peptide
1	B	276	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	B	277	ALA	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	2543	0	2377	70	0
1	B	2535	0	2350	73	0
2	A	39	0	34	4	0
2	B	39	0	34	2	0
3	A	221	0	0	5	0
3	B	167	0	0	7	0
All	All	5544	0	4795	142	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 14.

All (142) 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:72:ASN:HD21	2:A:1364:NAG:C1	0.94	1.57
1:B:72:ASN:HD21	2:B:1364:NAG:C1	1.34	1.38
1:B:277:ALA:CB	1:B:278:TRP:HA	1.70	1.20
1:B:237:GLN:HE21	1:B:248:GLN:NE2	1.58	1.01
1:B:277:ALA:HB3	1:B:278:TRP:HA	1.41	1.00
1:B:292:THR:HB	1:B:297:MET:HE1	1.40	0.99
1:B:292:THR:HB	1:B:297:MET:CE	1.92	0.99
1:B:277:ALA:HB1	1:B:278:TRP:HA	1.45	0.96
1:B:297:MET:SD	3:B:2160:HOH:O	2.24	0.94
1:A:237:GLN:HE21	1:A:248:GLN:NE2	1.67	0.91
1:A:237:GLN:HE21	1:A:248:GLN:HE21	0.98	0.91
1:B:294:GLN:O	1:B:297:MET:HE2	1.70	0.91
1:B:237:GLN:HE21	1:B:248:GLN:HE21	1.17	0.86
1:B:275:GLU:HB2	1:B:276:SER:HB3	1.58	0.85
1:A:72:ASN:HD21	2:A:1364:NAG:C2	1.89	0.84
1:B:244:VAL:HG12	1:B:245:MET:HE1	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:OG	1:B:257:LYS:N	2.10	0.82
1:A:294:GLN:HB3	1:A:297:MET:HE2	1.64	0.79
1:A:71:ASN:HB2	1:A:96:ASN:HD21	1.46	0.79
1:A:84:ARG:O	1:A:108:PRO:O	2.00	0.79
1:B:294:GLN:O	1:B:297:MET:CE	2.31	0.78
1:B:237:GLN:HA	1:B:245:MET:HE3	1.64	0.78
1:B:32:VAL:CB	1:B:34:CYS:H	1.97	0.77
1:A:237:GLN:NE2	1:A:248:GLN:HE21	1.80	0.76
1:B:277:ALA:CB	1:B:278:TRP:CA	2.54	0.76
1:B:275:GLU:CB	1:B:276:SER:HB3	2.15	0.75
1:B:316:GLY:N	1:B:317:SER:CB	2.48	0.75
1:A:123:HIS:ND1	1:A:124:THR:CG2	2.50	0.75
1:B:32:VAL:CA	1:B:34:CYS:H	2.00	0.75
1:A:123:HIS:ND1	1:A:124:THR:HG23	2.03	0.74
1:B:146:ILE:H	1:B:168:ASN:HD22	1.33	0.73
1:A:178:ILE:CD1	1:A:205:LEU:HD12	2.19	0.72
1:B:237:GLN:NE2	1:B:248:GLN:NE2	2.37	0.72
1:A:294:GLN:HB3	1:A:297:MET:CE	2.20	0.72
1:A:73:LEU:H	1:A:96:ASN:HD22	1.38	0.72
1:A:144:ASN:HB2	1:A:168:ASN:HD21	1.56	0.71
1:B:96:ASN:HB2	1:B:120:ASN:HD21	1.56	0.70
1:B:244:VAL:HG12	1:B:245:MET:CE	2.20	0.70
1:B:316:GLY:O	1:B:328:LYS:N	2.26	0.69
1:B:237:GLN:NE2	1:B:248:GLN:HE21	1.90	0.69
1:B:32:VAL:HA	1:B:34:CYS:H	1.58	0.69
1:A:72:ASN:CG	2:A:1364:NAG:C1	2.61	0.68
1:A:78:ALA:O	3:A:2045:HOH:O	2.10	0.68
1:B:147:VAL:HG12	1:B:148:VAL:HG23	1.75	0.67
1:B:178:ILE:HD12	1:B:208:LEU:HD21	1.76	0.67
1:B:316:GLY:H	1:B:317:SER:CB	2.07	0.66
1:A:120:ASN:HB2	1:A:144:ASN:HD21	1.60	0.66
1:B:277:ALA:HB3	1:B:278:TRP:CA	2.23	0.65
1:A:255:HIS:O	1:A:257:LYS:O	2.15	0.65
1:A:233:PHE:HD2	1:A:262:ILE:HD13	1.62	0.64
1:B:98:LEU:H	1:B:120:ASN:HD22	1.44	0.64
1:B:292:THR:HB	1:B:297:MET:HE3	1.77	0.64
1:A:168:ASN:HB2	1:A:195:ASN:HD21	1.62	0.64
1:B:254:MET:O	1:B:255:HIS:C	2.35	0.63
1:A:237:GLN:NE2	1:A:248:GLN:NE2	2.42	0.62
1:A:167:GLN:HG3	3:B:2006:HOH:O	2.00	0.62
1:A:29:ARG:N	3:A:2001:HOH:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:CE1	1:A:124:THR:HG23	2.36	0.61
1:A:257:LYS:O	1:A:258:LYS:CB	2.48	0.61
1:A:233:PHE:HD2	1:A:262:ILE:CD1	2.15	0.60
1:B:277:ALA:HB1	1:B:278:TRP:CA	2.25	0.60
1:A:85:LEU:HD23	1:A:85:LEU:N	2.16	0.60
1:A:272:GLU:O	1:A:273:TYR:HB3	2.02	0.59
1:A:123:HIS:ND1	1:A:124:THR:HG22	2.17	0.58
1:A:39:LEU:HD11	1:B:167:GLN:HG3	1.86	0.58
1:B:52:LEU:H	1:B:71:ASN:ND2	2.02	0.58
1:B:32:VAL:HA	1:B:34:CYS:N	2.17	0.58
1:A:170:ILE:H	1:A:195:ASN:HD22	1.50	0.58
1:A:122:LEU:H	1:A:144:ASN:HD22	1.52	0.57
1:A:71:ASN:CB	1:A:96:ASN:HD21	2.17	0.57
1:A:146:ILE:H	1:A:168:ASN:HD22	1.52	0.57
1:B:52:LEU:H	1:B:71:ASN:HD22	1.52	0.57
1:B:275:GLU:CA	1:B:276:SER:HB3	2.35	0.57
1:B:144:ASN:HB2	1:B:168:ASN:HD21	1.70	0.57
1:B:83:THR:O	1:B:84:ARG:CB	2.54	0.56
1:B:313:GLY:N	1:B:314:SER:CB	2.69	0.56
1:A:184:LEU:HD23	3:A:2143:HOH:O	2.06	0.55
1:A:50:GLN:H	1:A:71:ASN:HD21	1.53	0.55
1:B:292:THR:CB	1:B:297:MET:HE3	2.36	0.55
1:A:50:GLN:H	1:A:71:ASN:ND2	2.07	0.53
1:B:98:LEU:H	1:B:120:ASN:ND2	2.07	0.52
1:A:52:LEU:H	1:A:71:ASN:HD22	1.58	0.52
1:B:146:ILE:H	1:B:168:ASN:ND2	2.05	0.52
1:A:230:TYR:HA	1:A:262:ILE:HD11	1.90	0.52
1:A:195:ASN:HB2	1:A:221:ASN:HD21	1.75	0.50
1:A:244:VAL:O	1:A:248:GLN:HG3	2.11	0.50
1:A:273:TYR:C	1:A:273:TYR:CD1	2.84	0.50
1:B:161:GLN:NE2	3:B:2089:HOH:O	2.44	0.50
1:A:72:ASN:ND2	2:A:1364:NAG:C2	2.61	0.50
1:B:285:THR:OG1	1:B:328:LYS:O	2.21	0.50
1:A:178:ILE:CD1	1:A:205:LEU:CD1	2.88	0.49
1:A:178:ILE:HB	1:A:208:LEU:HD11	1.94	0.49
1:B:294:GLN:H	1:B:297:MET:CE	2.27	0.48
1:A:286:LEU:HD22	1:A:287:THR:N	2.28	0.48
1:B:316:GLY:H	1:B:317:SER:CA	2.26	0.48
3:A:2006:HOH:O	1:B:219:HIS:HE1	1.95	0.48
1:A:106:PHE:HB3	1:A:133:LEU:HD21	1.97	0.47
1:B:31:VAL:N	3:B:2001:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:H	1:A:297:MET:HE3	1.81	0.46
1:A:195:ASN:CB	1:A:221:ASN:HD21	2.28	0.46
1:B:294:GLN:C	1:B:297:MET:HE2	2.34	0.45
1:A:177:LEU:HD22	1:A:184:LEU:CD1	2.46	0.45
1:B:244:VAL:CG1	1:B:245:MET:CE	2.93	0.45
1:A:294:GLN:O	1:A:297:MET:HE3	2.17	0.45
1:B:72:ASN:ND2	2:B:1364:NAG:O5	2.34	0.45
1:B:40:CYS:HB3	3:B:2026:HOH:O	2.17	0.45
1:B:205:LEU:HA	1:B:208:LEU:HD22	1.99	0.45
1:A:138:VAL:HG12	1:A:140:LEU:CD1	2.47	0.45
1:A:239:ARG:O	1:A:293:LYS:HD2	2.16	0.45
1:B:316:GLY:CA	1:B:317:SER:CB	2.95	0.44
1:A:233:PHE:CD2	1:A:262:ILE:HD13	2.49	0.44
1:B:275:GLU:CB	1:B:276:SER:CB	2.92	0.44
1:A:170:ILE:H	1:A:195:ASN:ND2	2.13	0.44
1:B:275:GLU:HA	1:B:276:SER:HB3	2.00	0.43
1:A:184:LEU:N	3:A:2143:HOH:O	2.50	0.43
1:B:49:LYS:HA	1:B:70:HIS:O	2.18	0.43
1:B:230:TYR:HB2	1:B:265:LEU:HD12	2.00	0.43
1:B:239:ARG:HD3	3:B:2123:HOH:O	2.17	0.43
1:B:204:ASP:O	1:B:208:LEU:HD13	2.19	0.43
1:A:155:GLU:O	1:A:156:ASP:HB2	2.19	0.43
1:A:238:TYR:CE2	1:A:273:TYR:OH	2.70	0.42
1:B:138:VAL:HG12	1:B:140:LEU:CD1	2.49	0.42
1:A:107:VAL:N	1:A:108:PRO:CD	2.82	0.42
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.84	0.42
1:B:116:ASP:HA	1:B:140:LEU:HB2	2.00	0.42
1:A:178:ILE:HD12	1:A:205:LEU:HD12	2.00	0.42
1:B:107:VAL:N	1:B:108:PRO:CD	2.83	0.42
1:A:298:THR:O	1:A:342:ALA:HA	2.21	0.41
1:A:286:LEU:CD2	1:A:287:THR:N	2.83	0.41
1:A:197:LEU:H	1:A:221:ASN:ND2	2.19	0.41
1:B:96:ASN:CB	1:B:120:ASN:HD21	2.28	0.41
1:B:133:LEU:HB3	1:B:136:LEU:HB2	2.02	0.41
1:A:167:GLN:HE21	1:A:167:GLN:HB3	1.74	0.41
1:B:294:GLN:O	1:B:297:MET:HE3	2.18	0.41
1:A:201:PRO:O	1:A:205:LEU:HD13	2.20	0.41
1:B:309:VAL:O	1:B:310:LEU:HB2	2.20	0.41
1:A:197:LEU:H	1:A:221:ASN:HD22	1.69	0.41
1:A:195:ASN:C	1:A:221:ASN:ND2	2.75	0.41
1:B:206:GLN:CG	3:B:2067:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLY:H	1:B:317:SER:C	2.25	0.40
1:A:284:ASP:N	1:A:330:VAL:HG22	2.37	0.40
1:A:214:ASN:ND2	1:A:242:SER:H	2.19	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	327/361 (91%)	308 (94%)	16 (5%)	3 (1%)	21	13
1	B	331/361 (92%)	300 (91%)	23 (7%)	8 (2%)	7	2
All	All	658/722 (91%)	608 (92%)	39 (6%)	11 (2%)	11	4

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	LYS
1	A	273	TYR
1	B	33	SER
1	B	277	ALA
1	B	318	VAL
1	B	84	ARG
1	B	255	HIS
1	B	276	SER
1	A	84	ARG
1	B	51	GLN
1	B	316	GLY

### 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	273/333 (82%)	263 (96%)	10 (4%)	41	38
1	B	268/333 (80%)	257 (96%)	11 (4%)	37	32
All	All	541/666 (81%)	520 (96%)	21 (4%)	39	35

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	83	THR
1	A	124	THR
1	A	125	LEU
1	A	140	LEU
1	A	220	ASN
1	A	273	TYR
1	A	286	LEU
1	A	310	LEU
1	A	362	LEU
1	B	92	LEU
1	B	124	THR
1	B	125	LEU
1	B	167	GLN
1	B	206	GLN
1	B	208	LEU
1	B	226	ASP
1	B	273	TYR
1	B	286	LEU
1	B	299	LYS
1	B	310	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN

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Mol	Chain	Res	Type
1	A	72	ASN
1	A	87	ASN
1	A	96	ASN
1	A	111	ASN
1	A	144	ASN
1	A	152	ASN
1	A	159	GLN
1	A	168	ASN
1	A	195	ASN
1	A	214	ASN
1	A	219	HIS
1	A	220	ASN
1	A	221	ASN
1	A	235	HIS
1	A	248	GLN
1	A	261	ASN
1	B	71	ASN
1	B	72	ASN
1	B	111	ASN
1	B	120	ASN
1	B	143	ASN
1	B	152	ASN
1	B	168	ASN
1	B	214	ASN
1	B	219	HIS
1	B	231	GLN
1	B	248	GLN
1	B	261	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	$\# Z  > 2$
2	NAG	A	1364	1,2	14,14,15	0.69	0	15,19,21	1.67	4 (26%)
2	NAG	A	1365	2	14,14,15	0.70	1 (7%)	15,19,21	0.67	0
2	BMA	A	1366	2	11,11,12	0.71	0	14,15,17	1.05	2 (14%)
2	NAG	B	1364	1,2	14,14,15	0.61	0	15,19,21	0.93	1 (6%)
2	NAG	B	1365	2	14,14,15	0.62	0	15,19,21	0.90	0
2	BMA	B	1366	2	11,11,12	0.47	0	14,15,17	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1364	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1365	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1366	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1364	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1365	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1366	2	-	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)
2	A	1365	NAG	O5-C1	-2.06	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1364	NAG	C8-C7-N2	-2.69	110.97	116.11
2	A	1366	BMA	C1-C2-C3	2.02	111.93	109.54
2	B	1364	NAG	C3-C4-C5	2.16	113.96	110.20
2	A	1364	NAG	C3-C4-C5	2.17	113.98	110.20
2	A	1366	BMA	C1-O5-C5	2.36	115.25	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1364	NAG	C2-N2-C7	2.56	126.32	123.04
2	A	1364	NAG	O7-C7-N2	3.78	129.57	121.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1364	NAG	4	0
2	B	1364	NAG	2	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	331/361 (91%)	0.11	13 (3%) 43 45	16, 28, 46, 67	0
1	B	333/361 (92%)	0.26	21 (6%) 23 24	17, 30, 47, 67	0
All	All	664/722 (91%)	0.18	34 (5%) 32 33	16, 29, 47, 67	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	SER	11.4
1	B	313	GLY	10.1
1	A	315	ASN	7.5
1	A	314	SER	7.3
1	B	276	SER	6.4
1	A	316	GLY	6.3
1	A	313	GLY	6.3
1	A	312	GLN	6.2
1	B	316	GLY	6.0
1	A	311	SER	5.6
1	B	317	SER	5.6
1	B	315	ASN	4.6
1	B	275	GLU	4.4
1	B	36	ALA	3.7
1	A	258	LYS	3.4
1	A	274	LYS	3.4
1	B	273	TYR	3.4
1	A	273	TYR	3.4
1	B	310	LEU	3.3
1	B	255	HIS	2.9
1	B	332	VAL	2.9
1	B	312	GLN	2.8
1	B	140	LEU	2.8
1	B	181	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	256	SER	2.7
1	B	311	SER	2.5
1	A	363	HIS	2.4
1	B	362	LEU	2.3
1	B	256	SER	2.3
1	A	317	SER	2.2
1	B	277	ALA	2.1
1	B	254	MET	2.1
1	A	272	GLU	2.0
1	B	257	LYS	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](#)

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(Å <sup>2</sup> )	Q<0.9
2	NAG	A	1364	14/15	0.80	0.24	13.50	38,42,45,48	0
2	NAG	A	1365	14/15	0.87	0.29	3.88	34,44,46,47	0
2	NAG	B	1365	14/15	0.84	0.23	-	60,61,65,65	0
2	BMA	A	1366	11/12	0.78	0.29	-	45,47,50,51	0
2	BMA	B	1366	11/12	0.67	0.26	-	66,67,68,68	0
2	NAG	B	1364	14/15	0.90	0.22	-	54,56,58,59	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.