Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:48 PM GMT

PDB ID	:	1M4U
Title	:	Crystal structure of Bone Morphogenetic Protein-7 (BMP-7) in complex with the secreted antagonist Noggin
Authors	:	Groppe, J.; Greenwald, J.; Wiater, E.; Rodriguez-Leon, J.; Economides, A.N.; Kwiatkowski, W.; Affolter, M.; Vale, W.W.; Izpisua-Belmonte, J.C.; Choe, S.
Deposited on	:	2002-07-03
Resolution	:	2.42 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

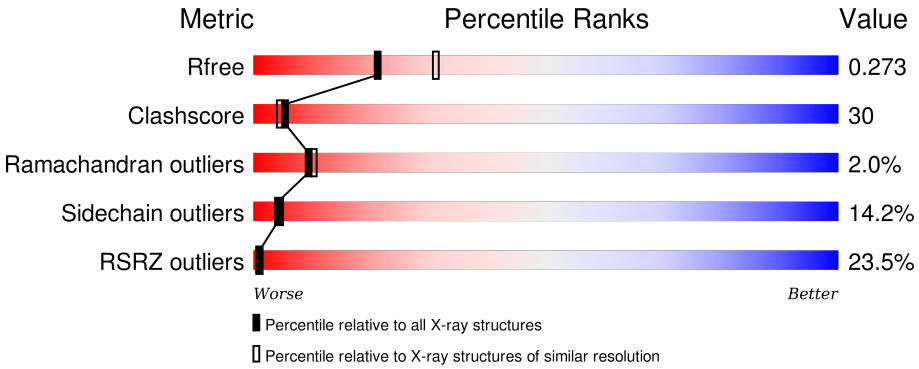
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 <=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	L	139	11% 47% 27% 6% • 19%
2	A	206	28% 49% 32% 14% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2559 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 Bone Morphogenetic Protein-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	112	Total	C	N	O	S	0	0	0
			890	563	152	166	9			

- Molecule 2 is a protein called Noggin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	199	Total	C	N	O	S	0	0	0
			1595	1012	289	280	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	INITIATING MET	UNP Q13253

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	L	2	Total	C	N	O	0	0
			28	16	2	10		

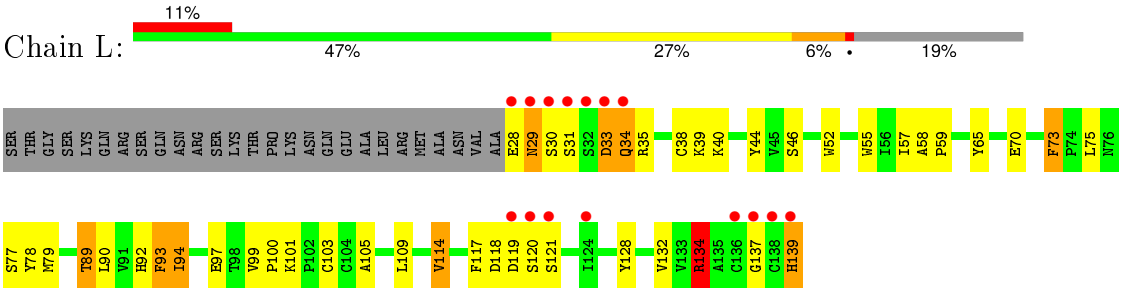
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	L	22	Total	O	0	0
			22	22		

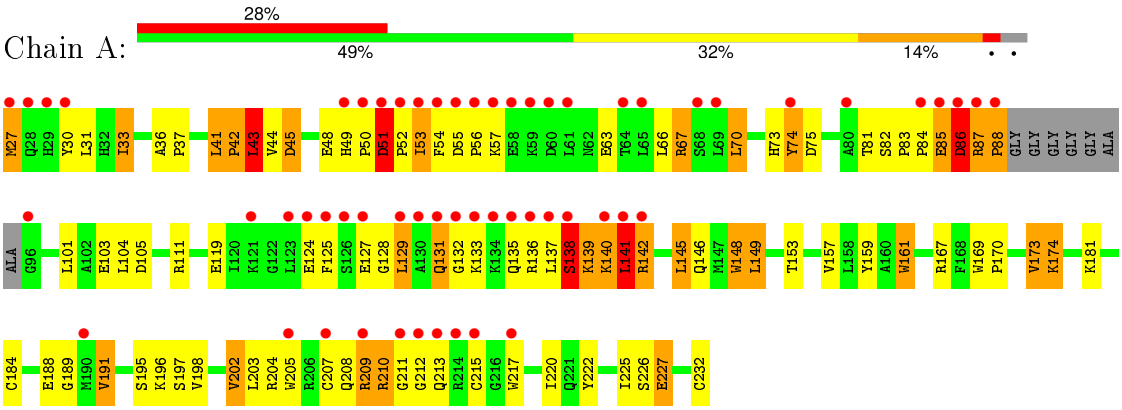
3 Residue-property plots (i)

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: Bone Morphogenetic Protein-7



- Molecule 2: Noggin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.83Å 99.83Å 150.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.05 – 2.42 60.05 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.7 (60.05-2.42) 95.7 (60.05-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.241 , 0.273 0.247 , 0.273	Depositor DCC
R_{free} test set	1441 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 28443 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2559	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	L	1.71	8/914 (0.9%)	1.38	9/1244 (0.7%)
2	A	1.54	12/1639 (0.7%)	1.57	25/2214 (1.1%)
All	All	1.60	20/2553 (0.8%)	1.51	34/3458 (1.0%)

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
2	A	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	74	TYR	CD1-CE1	-10.66	1.23	1.39
2	A	191	VAL	CB-CG2	-10.31	1.31	1.52
2	A	74	TYR	CD2-CE2	-7.94	1.27	1.39
2	A	161	TRP	CB-CG	-7.68	1.36	1.50
2	A	148	TRP	CB-CG	7.51	1.63	1.50
1	L	65	TYR	CG-CD2	-7.35	1.29	1.39
1	L	101	LYS	CB-CG	-6.85	1.34	1.52
1	L	65	TYR	CE1-CZ	-6.48	1.30	1.38
1	L	93	PHE	CD1-CE1	-6.35	1.26	1.39
2	A	119	GLU	CD-OE2	6.27	1.32	1.25
2	A	157	VAL	CB-CG2	-6.26	1.39	1.52
2	A	173	VAL	CB-CG1	-6.13	1.40	1.52
1	L	103	CYS	C-O	-5.68	1.12	1.23
1	L	78	TYR	CE2-CZ	-5.63	1.31	1.38
2	A	181	LYS	CE-NZ	5.52	1.62	1.49
1	L	40	LYS	CB-CG	-5.43	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	103	GLU	CG-CD	5.30	1.59	1.51
2	A	222	TYR	CB-CG	-5.18	1.43	1.51
2	A	36	ALA	CA-C	5.13	1.66	1.52
1	L	117	PHE	C-O	-5.06	1.13	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	86	ASP	CB-CG-OD1	-17.84	102.24	118.30
2	A	86	ASP	CB-CG-OD2	15.62	132.36	118.30
2	A	105	ASP	CB-CG-OD1	-9.40	109.84	118.30
2	A	104	LEU	CB-CG-CD1	8.68	125.75	111.00
2	A	105	ASP	CB-CG-OD2	8.32	125.79	118.30
1	L	134	ARG	NE-CZ-NH1	8.13	124.37	120.30
2	A	232	CYS	CA-C-O	-7.95	103.41	120.10
2	A	87	ARG	C-N-CD	-7.66	103.74	120.60
2	A	88	PRO	N-CA-C	7.45	131.46	112.10
2	A	55	ASP	CB-CG-OD2	6.99	124.59	118.30
2	A	141	LEU	CA-CB-CG	6.93	131.24	115.30
2	A	43	LEU	CB-CA-C	-6.88	97.13	110.20
1	L	139	HIS	CA-C-O	-6.84	105.74	120.10
2	A	51	ASP	CB-CG-OD2	6.71	124.34	118.30
2	A	86	ASP	CB-CA-C	-6.61	97.18	110.40
1	L	119	ASP	CB-CG-OD2	6.54	124.18	118.30
2	A	30	TYR	CB-CG-CD1	-6.50	117.10	121.00
2	A	145	LEU	CA-CB-CG	-6.49	100.37	115.30
1	L	73	PHE	CB-CG-CD2	-6.48	116.26	120.80
2	A	74	TYR	CB-CG-CD1	-6.37	117.18	121.00
2	A	30	TYR	CB-CG-CD2	6.17	124.70	121.00
2	A	45	ASP	CB-CG-OD1	6.15	123.83	118.30
2	A	149	LEU	CA-CB-CG	-5.95	101.61	115.30
2	A	43	LEU	N-CA-C	5.93	127.01	111.00
1	L	44	TYR	CB-CG-CD1	5.82	124.49	121.00
2	A	209	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	L	57	ILE	CG1-CB-CG2	-5.64	98.99	111.40
2	A	87	ARG	CA-C-N	5.52	132.56	117.10
2	A	87	ARG	C-N-CA	5.50	145.08	122.00
1	L	94	ILE	N-CA-C	5.24	125.16	111.00
1	L	118	ASP	CB-CG-OD1	5.13	122.92	118.30
1	L	73	PHE	CB-CG-CD1	5.12	124.38	120.80
2	A	111	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	A	188	GLU	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	86	ASP	Sidechain

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	L	890	0	840	26	1
2	A	1595	0	1587	121	2
3	L	28	0	25	2	0
4	A	24	0	0	0	0
4	L	22	0	0	1	0
All	All	2559	0	2452	149	2

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 30.

All (149) 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:A:125:PHE:CB	2:A:137:LEU:HD12	1.69	1.21
2:A:140:LYS:HG2	2:A:141:LEU:N	1.48	1.18
2:A:125:PHE:HB2	2:A:137:LEU:HD12	1.26	1.09
2:A:127:GLU:HA	2:A:132:GLY:HA2	1.26	1.07
2:A:140:LYS:CG	2:A:141:LEU:N	2.18	1.04
2:A:128:GLY:HA3	2:A:136:ARG:HD3	1.34	1.04
2:A:140:LYS:HG2	2:A:141:LEU:H	0.86	1.03
2:A:125:PHE:CZ	2:A:145:LEU:HD22	1.96	1.01
2:A:145:LEU:C	2:A:145:LEU:HD23	1.85	0.97
2:A:125:PHE:HB3	2:A:137:LEU:HD12	1.46	0.95
2:A:140:LYS:CG	2:A:141:LEU:H	1.78	0.94
2:A:145:LEU:O	2:A:145:LEU:HD23	1.70	0.92
2:A:125:PHE:CB	2:A:137:LEU:CD1	2.50	0.89
2:A:127:GLU:CA	2:A:132:GLY:HA2	2.03	0.89
1:L:34:GLN:O	1:L:70:GLU:HG3	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:ALA:HB3	1:L:139:HIS:CD2	2.12	0.84
1:L:134:ARG:HH11	1:L:134:ARG:HG2	1.40	0.84
2:A:125:PHE:HB3	2:A:137:LEU:CD1	2.05	0.83
2:A:145:LEU:HD21	2:A:149:LEU:CD1	2.09	0.83
2:A:129:LEU:HB2	2:A:133:LYS:HD2	1.58	0.83
2:A:145:LEU:HD21	2:A:149:LEU:HD11	1.60	0.83
2:A:139:LYS:C	2:A:139:LYS:HD2	2.01	0.79
2:A:48:GLU:OE2	2:A:204:ARG:NH2	2.16	0.78
1:L:114:VAL:HG13	1:L:128:TYR:CD2	2.18	0.78
2:A:128:GLY:HA3	2:A:136:ARG:CD	2.14	0.77
2:A:125:PHE:CE2	2:A:145:LEU:HD22	2.21	0.75
2:A:125:PHE:HB2	2:A:137:LEU:CD1	2.12	0.75
2:A:54:PHE:O	2:A:205:TRP:HD1	1.70	0.74
2:A:139:LYS:O	2:A:139:LYS:HD2	1.88	0.73
2:A:67:ARG:CG	2:A:67:ARG:HH11	2.02	0.73
2:A:54:PHE:O	2:A:205:TRP:CD1	2.41	0.72
2:A:139:LYS:HE3	2:A:140:LYS:HA	1.70	0.71
2:A:207:CYS:HB3	2:A:212:GLY:HA2	1.72	0.71
2:A:142:ARG:HH11	2:A:146:GLN:NE2	1.90	0.69
2:A:220:ILE:C	2:A:220:ILE:HD12	2.13	0.69
2:A:125:PHE:CD1	2:A:125:PHE:N	2.61	0.69
2:A:128:GLY:CA	2:A:136:ARG:HD3	2.19	0.68
2:A:70:LEU:HD22	2:A:73:HIS:HB2	1.76	0.68
2:A:139:LYS:CD	2:A:139:LYS:C	2.63	0.67
2:A:27:MET:O	2:A:27:MET:HG3	1.94	0.66
1:L:114:VAL:CG1	1:L:128:TYR:CD2	2.78	0.66
2:A:139:LYS:HE3	2:A:140:LYS:CA	2.27	0.65
3:L:180:NAG:O7	3:L:180:NAG:O3	2.11	0.64
1:L:109:LEU:HA	1:L:132:VAL:O	1.99	0.63
1:L:97:GLU:HA	1:L:97:GLU:OE2	1.98	0.62
2:A:148:TRP:CZ3	2:A:149:LEU:HD23	2.34	0.61
2:A:56:PRO:HG3	2:A:205:TRP:CG	2.36	0.61
2:A:43:LEU:N	2:A:43:LEU:HD23	2.15	0.61
2:A:207:CYS:CB	2:A:212:GLY:HA2	2.31	0.61
2:A:139:LYS:HE3	2:A:140:LYS:N	2.16	0.60
1:L:90:LEU:HD12	1:L:90:LEU:O	2.01	0.60
2:A:48:GLU:HG3	2:A:167:ARG:NH1	2.17	0.60
2:A:84:PRO:O	2:A:86:ASP:N	2.35	0.60
2:A:145:LEU:CD2	2:A:149:LEU:CD1	2.81	0.59
2:A:145:LEU:C	2:A:145:LEU:CD2	2.60	0.59
2:A:148:TRP:CZ3	2:A:149:LEU:CD2	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:GLU:CG	2:A:167:ARG:NH1	2.67	0.58
2:A:37:PRO:O	2:A:37:PRO:HG2	2.05	0.57
2:A:148:TRP:CE3	2:A:149:LEU:HD23	2.40	0.56
2:A:129:LEU:HG	2:A:133:LYS:NZ	2.20	0.56
2:A:84:PRO:O	2:A:85:GLU:C	2.42	0.56
2:A:125:PHE:H	2:A:125:PHE:HD1	1.50	0.56
2:A:124:GLU:HG2	2:A:142:ARG:NH2	2.20	0.56
2:A:140:LYS:O	2:A:142:ARG:N	2.39	0.56
2:A:139:LYS:O	2:A:140:LYS:C	2.45	0.55
2:A:159:TYR:HB3	2:A:174:LYS:HD3	1.87	0.55
2:A:142:ARG:HH11	2:A:146:GLN:HE22	1.53	0.55
1:L:31:SER:OG	1:L:33:ASP:OD2	2.23	0.55
2:A:67:ARG:HH11	2:A:67:ARG:HG2	1.70	0.55
1:L:29:ASN:O	1:L:30:SER:OG	2.25	0.54
2:A:66:LEU:HD13	2:A:169:TRP:CD1	2.43	0.54
2:A:169:TRP:HA	2:A:170:PRO:C	2.27	0.53
1:L:97:GLU:CA	1:L:97:GLU:OE2	2.57	0.53
2:A:50:PRO:O	2:A:52:PRO:HD3	2.08	0.53
2:A:142:ARG:NH1	2:A:146:GLN:HE22	2.07	0.53
2:A:202:VAL:CG1	2:A:203:LEU:N	2.70	0.53
2:A:142:ARG:NH1	2:A:146:GLN:NE2	2.57	0.52
1:L:92:HIS:O	1:L:93:PHE:C	2.47	0.52
2:A:141:LEU:O	2:A:141:LEU:HD12	2.10	0.52
2:A:48:GLU:CG	2:A:167:ARG:HH11	2.23	0.51
2:A:145:LEU:CD2	2:A:149:LEU:HD12	2.40	0.51
1:L:120:SER:O	1:L:121:SER:OG	2.25	0.50
1:L:137:GLY:O	1:L:139:HIS:CD2	2.65	0.50
2:A:41:LEU:CB	2:A:42:PRO:HA	2.32	0.50
1:L:38:CYS:HB3	1:L:79:MET:HE3	1.94	0.49
2:A:49:HIS:CD2	2:A:51:ASP:H	2.30	0.49
2:A:148:TRP:HZ3	2:A:149:LEU:CD2	2.25	0.49
2:A:211:GLY:C	2:A:213:GLN:NE2	2.66	0.49
1:L:52:TRP:CD2	1:L:55:TRP:HZ3	2.30	0.49
2:A:124:GLU:HG2	2:A:142:ARG:HH22	1.78	0.48
1:L:134:ARG:NH1	1:L:134:ARG:HG2	2.17	0.48
2:A:148:TRP:HZ3	2:A:149:LEU:HD21	1.78	0.48
2:A:67:ARG:HG3	2:A:67:ARG:HH11	1.79	0.48
2:A:48:GLU:HG3	2:A:167:ARG:HH11	1.79	0.48
1:L:120:SER:O	1:L:121:SER:C	2.51	0.47
2:A:149:LEU:HD23	2:A:149:LEU:HA	1.73	0.47
2:A:67:ARG:CZ	2:A:74:TYR:CE2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:180:NAG:HO3	3:L:180:NAG:C7	2.20	0.47
2:A:129:LEU:HG	2:A:133:LYS:HZ3	1.81	0.46
2:A:202:VAL:HG13	2:A:203:LEU:H	1.80	0.46
2:A:205:TRP:CZ2	2:A:215:CYS:HB2	2.51	0.46
2:A:67:ARG:NH1	2:A:67:ARG:HG3	2.29	0.46
2:A:124:GLU:CD	2:A:142:ARG:NH2	2.70	0.46
2:A:49:HIS:HD2	2:A:51:ASP:HB2	1.80	0.46
2:A:127:GLU:HB2	2:A:131:GLN:HA	1.97	0.45
2:A:142:ARG:O	2:A:146:GLN:HG3	2.17	0.45
2:A:204:ARG:O	2:A:217:TRP:HA	2.16	0.45
2:A:31:LEU:HB3	2:A:33:ILE:HG23	1.98	0.45
2:A:127:GLU:HB2	2:A:131:GLN:C	2.37	0.45
2:A:128:GLY:N	2:A:132:GLY:HA2	2.32	0.45
2:A:137:LEU:HB3	2:A:141:LEU:HG	1.98	0.45
2:A:148:TRP:CE3	2:A:149:LEU:CD2	2.99	0.45
2:A:195:SER:O	2:A:196:LYS:HG2	2.18	0.44
2:A:48:GLU:HG2	2:A:167:ARG:NH1	2.32	0.44
2:A:124:GLU:CG	2:A:142:ARG:NH2	2.80	0.44
1:L:99:VAL:HG22	1:L:100:PRO:HD2	1.99	0.44
2:A:138:SER:OG	2:A:140:LYS:NZ	2.49	0.43
2:A:226:SER:O	2:A:227:GLU:HG2	2.18	0.43
2:A:139:LYS:O	2:A:142:ARG:CB	2.67	0.43
2:A:82:SER:HA	2:A:83:PRO:HD2	1.77	0.43
2:A:140:LYS:C	2:A:142:ARG:N	2.71	0.43
2:A:128:GLY:H	2:A:132:GLY:CA	2.31	0.43
2:A:66:LEU:HA	2:A:66:LEU:HD23	1.66	0.43
1:L:73:PHE:HB2	1:L:89:THR:HG23	2.00	0.43
1:L:94:ILE:HG21	1:L:94:ILE:HD13	1.61	0.43
1:L:58:ALA:HA	1:L:59:PRO:C	2.39	0.43
2:A:148:TRP:CZ3	2:A:149:LEU:HD21	2.54	0.43
2:A:211:GLY:O	2:A:213:GLN:NE2	2.52	0.43
2:A:41:LEU:HA	2:A:42:PRO:HA	1.58	0.42
2:A:209:ARG:HB2	2:A:213:GLN:HB2	2.01	0.42
1:L:114:VAL:HG13	1:L:128:TYR:HD2	1.78	0.42
2:A:66:LEU:HD13	2:A:169:TRP:CG	2.55	0.42
2:A:153:THR:HG22	2:A:184:CYS:O	2.20	0.42
2:A:51:ASP:HB3	2:A:53:ILE:HD11	2.02	0.42
1:L:120:SER:C	1:L:121:SER:OG	2.57	0.42
2:A:42:PRO:HB3	2:A:225:ILE:HD11	2.01	0.42
1:L:33:ASP:HB3	4:L:197:HOH:O	2.19	0.42
2:A:128:GLY:HA3	2:A:136:ARG:CG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:70:LEU:HA	2:A:70:LEU:HD23	1.91	0.41
1:L:94:ILE:O	1:L:94:ILE:CG2	2.66	0.41
2:A:125:PHE:CE2	2:A:145:LEU:CD2	3.00	0.41
2:A:140:LYS:C	2:A:142:ARG:H	2.24	0.41
2:A:75:ASP:OD1	2:A:75:ASP:C	2.59	0.41
2:A:44:VAL:HG12	2:A:45:ASP:N	2.35	0.41
2:A:125:PHE:CE2	2:A:145:LEU:HD13	2.57	0.40
2:A:127:GLU:HA	2:A:132:GLY:CA	2.20	0.40
2:A:127:GLU:HB3	2:A:131:GLN:NE2	2.37	0.40
2:A:129:LEU:N	2:A:132:GLY:O	2.54	0.40
2:A:85:GLU:HB2	2:A:161:TRP:HD1	1.87	0.40

All (2) 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)
1:L:77:SER:O	2:A:88:PRO:O[6_455]	1.49	0.71
2:A:135:GLN:OE1	2:A:210:ARG:NH2[4_444]	2.00	0.20

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	L	110/139 (79%)	101 (92%)	8 (7%)	1 (1%)	21 29
2	A	195/206 (95%)	170 (87%)	20 (10%)	5 (3%)	7 6
All	All	305/345 (88%)	271 (89%)	28 (9%)	6 (2%)	9 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	ASN

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Mol	Chain	Res	Type
2	A	85	GLU
2	A	63	GLU
2	A	138	SER
2	A	141	LEU
2	A	189	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	L	98/121 (81%)	88 (90%)	10 (10%)	9 13
2	A	177/177 (100%)	148 (84%)	29 (16%)	3 3
All	All	275/298 (92%)	236 (86%)	39 (14%)	4 4

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	28	GLU
1	L	33	ASP
1	L	34	GLN
1	L	35	ARG
1	L	39	LYS
1	L	46	SER
1	L	75	LEU
1	L	89	THR
1	L	114	VAL
1	L	134	ARG
2	A	27	MET
2	A	33	ILE
2	A	41	LEU
2	A	42	PRO
2	A	43	LEU
2	A	51	ASP
2	A	53	ILE
2	A	57	LYS

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Mol	Chain	Res	Type
2	A	67	ARG
2	A	70	LEU
2	A	81	THR
2	A	87	ARG
2	A	101	LEU
2	A	129	LEU
2	A	131	GLN
2	A	138	SER
2	A	139	LYS
2	A	140	LYS
2	A	141	LEU
2	A	142	ARG
2	A	173	VAL
2	A	174	LYS
2	A	191	VAL
2	A	197	SER
2	A	198	VAL
2	A	202	VAL
2	A	208	GLN
2	A	210	ARG
2	A	227	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	GLN
2	A	32	HIS
2	A	49	HIS
2	A	131	GLN
2	A	146	GLN
2	A	213	GLN

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)

2 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	$\#\|Z\| > 2$
3	NAG	L	180	1,3	14,14,15	1.74	3 (21%)	15,19,21	3.59	6 (40%)
3	NAG	L	181	3	14,14,15	1.72	4 (28%)	15,19,21	2.70	9 (60%)

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	L	180	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	181	3	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	180	NAG	C2-N2	-4.80	1.37	1.46
3	L	180	NAG	O5-C1	-2.48	1.39	1.43
3	L	181	NAG	O3-C3	-2.33	1.37	1.43
3	L	181	NAG	C4-C5	2.50	1.58	1.53
3	L	180	NAG	C1-C2	2.61	1.56	1.52
3	L	181	NAG	O5-C1	2.96	1.48	1.43
3	L	181	NAG	C2-N2	3.03	1.51	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	180	NAG	O4-C4-C5	-6.92	90.91	109.24
3	L	180	NAG	C2-N2-C7	-6.68	114.45	123.04
3	L	181	NAG	O3-C3-C2	-4.84	99.52	109.11
3	L	180	NAG	C1-O5-C5	-4.34	106.74	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	181	NAG	C3-C4-C5	-4.23	102.82	110.20
3	L	180	NAG	C4-C3-C2	-4.05	104.93	111.23
3	L	181	NAG	C3-C2-N2	-3.21	102.88	110.56
3	L	180	NAG	C3-C2-N2	-3.12	103.08	110.56
3	L	181	NAG	O7-C7-C8	-2.43	117.61	122.06
3	L	181	NAG	O5-C5-C6	2.10	111.89	107.35
3	L	181	NAG	O3-C3-C4	2.31	115.53	110.34
3	L	181	NAG	C1-O5-C5	3.07	116.15	112.25
3	L	181	NAG	O4-C4-C5	3.26	117.87	109.24
3	L	181	NAG	C2-N2-C7	3.80	127.93	123.04
3	L	180	NAG	O4-C4-C3	6.70	125.42	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	180	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^{th} 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	L	112/139 (80%)	1.35	15 (13%)	4	4	33, 46, 105, 141	0
2	A	199/206 (96%)	1.64	58 (29%)	1	1	35, 58, 118, 130	0
All	All	311/345 (90%)	1.54	73 (23%)	1	1	33, 52, 115, 141	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	88	PRO	10.0
2	A	87	ARG	8.8
1	L	29	ASN	7.3
2	A	134	LYS	6.6
2	A	51	ASP	6.4
2	A	214	ARG	6.0
2	A	86	ASP	5.9
1	L	33	ASP	5.9
2	A	132	GLY	5.8
2	A	53	ILE	5.7
2	A	65	LEU	5.5
2	A	27	MET	5.3
2	A	130	ALA	5.3
2	A	59	LYS	5.3
2	A	28	GLN	5.0
1	L	34	GLN	4.9
1	L	30	SER	4.8
2	A	141	LEU	4.8
2	A	50	PRO	4.8
1	L	32	SER	4.7
1	L	31	SER	4.6
1	L	28	GLU	4.5
2	A	131	GLN	4.4
2	A	54	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
2	A	135	GLN	4.0
2	A	126	SER	4.0
2	A	58	GLU	4.0
2	A	215	CYS	3.8
2	A	61	LEU	3.8
2	A	213	GLN	3.7
2	A	49	HIS	3.6
2	A	124	GLU	3.6
2	A	209	ARG	3.6
2	A	138	SER	3.5
2	A	29	HIS	3.4
2	A	64	THR	3.4
2	A	127	GLU	3.4
2	A	60	ASP	3.4
2	A	56	PRO	3.3
2	A	211	GLY	3.2
2	A	96	GLY	3.1
2	A	142	ARG	3.1
2	A	68	SER	3.0
2	A	137	LEU	2.9
1	L	119	ASP	2.9
1	L	137	GLY	2.8
2	A	212	GLY	2.7
2	A	69	LEU	2.7
2	A	136	ARG	2.5
2	A	121	LYS	2.5
2	A	74	TYR	2.5
2	A	125	PHE	2.4
2	A	52	PRO	2.4
2	A	123	LEU	2.4
1	L	139	HIS	2.4
1	L	138	CYS	2.4
2	A	84	PRO	2.4
2	A	30	TYR	2.4
2	A	57	LYS	2.4
1	L	136	CYS	2.3
2	A	80	ALA	2.3
1	L	121	SER	2.3
2	A	133	LYS	2.2
2	A	140	LYS	2.2
2	A	217	TRP	2.2
2	A	55	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	207	CYS	2.1
1	L	124	ILE	2.1
1	L	120	SER	2.1
2	A	205	TRP	2.1
2	A	129	LEU	2.1
2	A	85	GLU	2.0
2	A	190	MET	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^{th} 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	L	180	14/15	0.82	0.23	-0.30	35,54,71,82	0
3	NAG	L	181	14/15	0.72	0.28	-	64,77,84,85	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.