Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:02 AM GMT

PDB ID	:	3NRO
Title	:	Crystal Structure of putative transcriptional factor Lmo1026 from Listeria monocytogenes (FRAGMENT 52-321), Northeast Structural Genomics Consortium Target LmR194
Authors	:	Kuzin, A.; Su, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Ciccosanti, C.; Lee, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-06-30
Resolution	:	2.90 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:

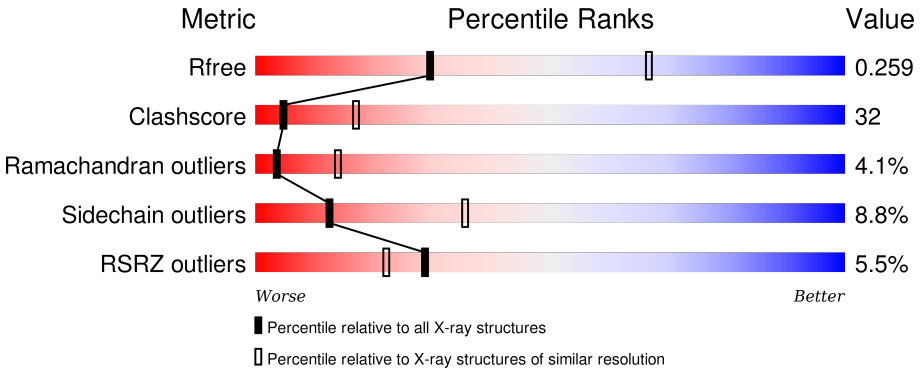
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	A	279	6% 44% 34% 5% 16%
1	B	279	3% 42% 37% 5% 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3647 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 Lmo1026 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	Se	0	0	0
			1814	1139	303	363	9			
1	B	237	Total	C	N	O	Se	0	0	0
			1833	1152	304	368	9			

There are 18 discrepancies between the modelled and reference sequences:

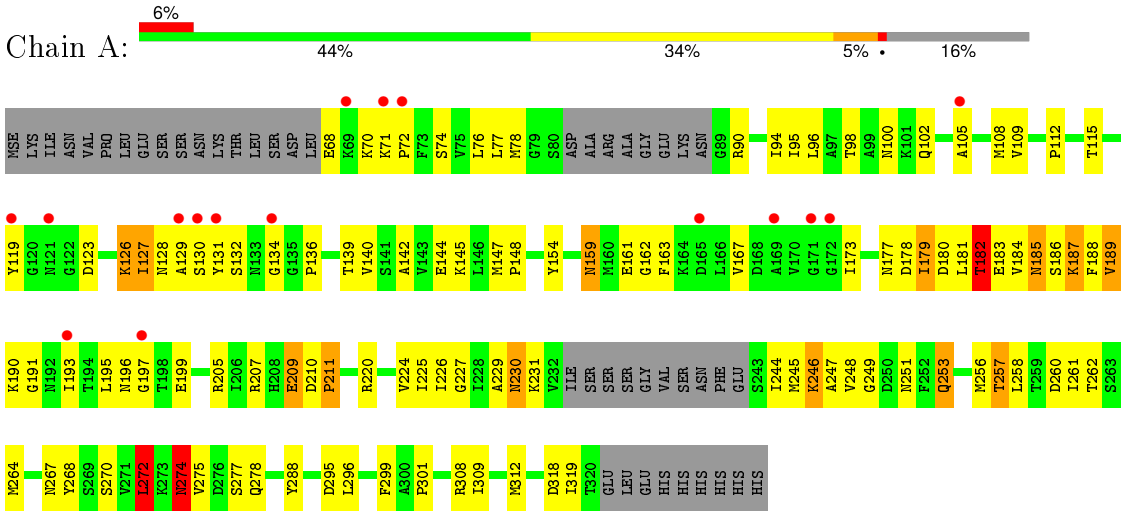
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	MSE	-	expression tag	UNP Q8Y889
A	322	LEU	-	expression tag	UNP Q8Y889
A	323	GLU	-	expression tag	UNP Q8Y889
A	324	HIS	-	expression tag	UNP Q8Y889
A	325	HIS	-	expression tag	UNP Q8Y889
A	326	HIS	-	expression tag	UNP Q8Y889
A	327	HIS	-	expression tag	UNP Q8Y889
A	328	HIS	-	expression tag	UNP Q8Y889
A	329	HIS	-	expression tag	UNP Q8Y889
B	51	MSE	-	expression tag	UNP Q8Y889
B	322	LEU	-	expression tag	UNP Q8Y889
B	323	GLU	-	expression tag	UNP Q8Y889
B	324	HIS	-	expression tag	UNP Q8Y889
B	325	HIS	-	expression tag	UNP Q8Y889
B	326	HIS	-	expression tag	UNP Q8Y889
B	327	HIS	-	expression tag	UNP Q8Y889
B	328	HIS	-	expression tag	UNP Q8Y889
B	329	HIS	-	expression tag	UNP Q8Y889

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.

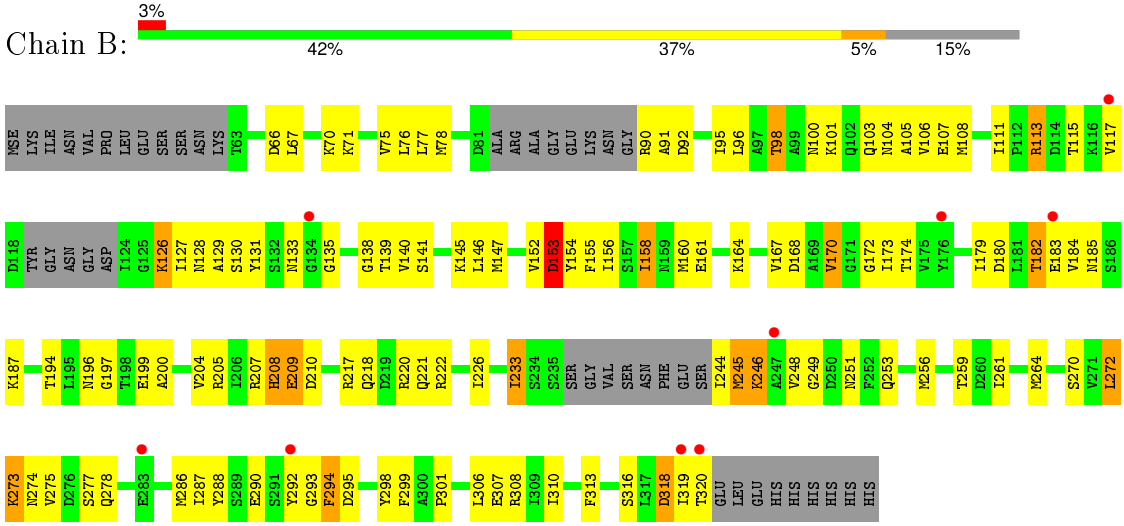
- Molecule 1: Lmo1026 protein

Chain A:



- Molecule 1: Lmo1026 protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.24Å 90.30Å 118.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 2.90 29.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.66-2.90) 99.6 (29.66-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.1_357)	Depositor
R, R_{free}	0.234 , 0.264 0.229 , 0.259	Depositor DCC
R_{free} test set	525 reflections (4.79%)	DCC
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 72.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 10964 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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

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	0.44	0/1829	0.62	1/2449 (0.0%)
1	B	0.47	0/1846	0.65	0/2472
All	All	0.45	0/3675	0.64	1/4921 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	ALA	N-CA-C	-5.12	97.19	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1814	0	1804	121	0
1	B	1833	0	1833	111	0
All	All	3647	0	3637	231	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 32.

All (231) 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:187:LYS:H	1:A:187:LYS:HD3	1.13	1.10
1:B:108:MSE:HE1	1:B:222:ARG:HG3	1.37	1.03
1:A:244:ILE:HD12	1:A:244:ILE:O	1.67	0.95
1:A:159:ASN:HD22	1:A:159:ASN:H	1.19	0.90
1:B:115:THR:HA	1:B:299:PHE:HB3	1.55	0.88
1:A:159:ASN:HD21	1:A:251:ASN:HB3	1.38	0.86
1:A:187:LYS:N	1:A:187:LYS:HD3	1.90	0.86
1:A:188:PHE:HA	1:A:193:ILE:HD13	1.61	0.82
1:A:167:VAL:HG13	1:A:173:ILE:HG12	1.62	0.82
1:A:159:ASN:HD21	1:A:162:GLY:H	1.28	0.81
1:B:273:LYS:HE2	1:B:273:LYS:HA	1.61	0.80
1:A:159:ASN:ND2	1:A:162:GLY:H	1.80	0.79
1:A:90:ARG:HD2	1:A:128:ASN:HD22	1.46	0.79
1:A:185:ASN:HD22	1:A:186:SER:H	1.32	0.77
1:A:185:ASN:H	1:A:185:ASN:ND2	1.82	0.77
1:B:160:MSE:HG3	1:B:205:ARG:HH21	1.50	0.76
1:B:113:ARG:HE	1:B:113:ARG:H	1.35	0.75
1:A:100:ASN:HD21	1:A:102:GLN:HB2	1.51	0.74
1:B:286:MSE:HG3	1:B:295:ASP:HB3	1.68	0.74
1:B:75:VAL:HG22	1:B:154:TYR:HB2	1.70	0.74
1:B:319:ILE:HG12	1:B:320:THR:H	1.52	0.73
1:A:179:ILE:HD13	1:A:180:ASP:N	2.04	0.73
1:A:105:ALA:HA	1:A:274:ASN:HB3	1.70	0.72
1:A:71:LYS:HE3	1:A:72:PRO:O	1.89	0.72
1:B:96:LEU:HD12	1:B:313:PHE:CE2	2.25	0.72
1:A:72:PRO:HG3	1:A:100:ASN:ND2	2.06	0.71
1:A:185:ASN:HD22	1:A:185:ASN:H	1.37	0.70
1:A:90:ARG:HD2	1:A:128:ASN:ND2	2.06	0.70
1:A:188:PHE:HA	1:A:193:ILE:CD1	2.20	0.70
1:B:98:THR:HG21	1:B:316:SER:HB3	1.73	0.70
1:B:208:HIS:O	1:B:210:ASP:N	2.25	0.69
1:A:126:LYS:O	1:A:130:SER:HB2	1.92	0.69
1:B:113:ARG:O	1:B:128:ASN:HB3	1.93	0.69
1:A:248:VAL:HG22	1:A:249:GLY:H	1.55	0.69
1:B:179:ILE:HD12	1:B:180:ASP:H	1.57	0.68
1:A:187:LYS:H	1:A:187:LYS:CD	2.00	0.68
1:A:167:VAL:HB	1:A:197:GLY:HA2	1.76	0.68
1:A:264:MSE:HA	1:A:268:TYR:HD2	1.58	0.68
1:A:159:ASN:ND2	1:A:251:ASN:HB3	2.07	0.68
1:B:244:ILE:HG13	1:B:245:MSE:HG3	1.77	0.67
1:B:272:LEU:HD13	1:B:273:LYS:H	1.60	0.66
1:A:257:THR:O	1:A:261:ILE:HG13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:N	1:A:246:LYS:HD2	2.11	0.66
1:B:115:THR:HG23	1:B:301:PRO:HG3	1.77	0.65
1:A:72:PRO:HG3	1:A:100:ASN:HD22	1.61	0.65
1:A:180:ASP:OD2	1:A:182:THR:HG22	1.97	0.64
1:A:132:SER:HB2	1:A:139:THR:OG1	1.97	0.64
1:A:159:ASN:HD22	1:A:159:ASN:N	1.84	0.64
1:B:179:ILE:HD12	1:B:180:ASP:N	2.12	0.64
1:A:76:LEU:HD23	1:A:140:VAL:HG22	1.79	0.64
1:A:159:ASN:ND2	1:A:159:ASN:H	1.94	0.64
1:B:130:SER:OG	1:B:139:THR:HA	1.98	0.64
1:B:104:ASN:O	1:B:274:ASN:HB2	1.98	0.63
1:A:128:ASN:CG	1:A:129:ALA:N	2.52	0.63
1:A:145:LYS:NZ	1:A:145:LYS:HB3	2.12	0.63
1:B:98:THR:HG21	1:B:316:SER:CB	2.29	0.63
1:A:109:VAL:HG11	1:A:309:ILE:HD13	1.81	0.63
1:A:112:PRO:HG2	1:A:299:PHE:CE2	2.34	0.63
1:B:272:LEU:CD1	1:B:273:LYS:H	2.12	0.62
1:B:278:GLN:NE2	1:B:308:ARG:HH22	1.97	0.62
1:A:185:ASN:ND2	1:A:185:ASN:N	2.42	0.62
1:A:179:ILE:HG23	1:A:181:LEU:HG	1.82	0.62
1:A:182:THR:C	1:A:184:VAL:H	2.01	0.62
1:A:76:LEU:HG	1:A:78:MSE:HE2	1.82	0.61
1:A:108:MSE:O	1:A:277:SER:HA	2.01	0.61
1:B:167:VAL:O	1:B:170:VAL:HG12	2.01	0.60
1:A:108:MSE:HG3	1:A:277:SER:HB2	1.82	0.60
1:A:248:VAL:HG22	1:A:249:GLY:N	2.16	0.60
1:B:167:VAL:HG13	1:B:173:ILE:HG12	1.83	0.60
1:B:287:ILE:HB	1:B:298:TYR:CD2	2.36	0.60
1:B:272:LEU:O	1:B:274:ASN:N	2.29	0.60
1:B:182:THR:C	1:B:184:VAL:H	2.04	0.60
1:B:319:ILE:HG12	1:B:320:THR:N	2.17	0.60
1:B:306:LEU:O	1:B:310:ILE:HG13	2.02	0.59
1:B:184:VAL:CG2	1:B:209:GLU:HG2	2.32	0.59
1:B:156:ILE:HG22	1:B:256:MSE:HE2	1.84	0.59
1:A:76:LEU:CD2	1:A:78:MSE:HE2	2.32	0.59
1:A:159:ASN:HD21	1:A:162:GLY:N	1.99	0.59
1:A:163:PHE:HZ	1:A:224:VAL:HG11	1.68	0.58
1:B:160:MSE:O	1:B:164:LYS:HE2	2.03	0.58
1:B:76:LEU:HD13	1:B:96:LEU:HD23	1.86	0.58
1:B:91:ALA:O	1:B:128:ASN:HB2	2.04	0.58
1:B:172:GLY:O	1:B:173:ILE:HD13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:O	1:A:187:LYS:HG2	2.04	0.57
1:A:186:SER:HB3	1:A:188:PHE:CE2	2.39	0.57
1:A:128:ASN:CG	1:A:129:ALA:H	2.08	0.57
1:A:226:ILE:HG22	1:A:230:ASN:ND2	2.20	0.56
1:A:74:SER:HA	1:A:98:THR:HA	1.86	0.56
1:A:182:THR:O	1:A:184:VAL:N	2.39	0.56
1:A:189:VAL:HG22	1:A:190:LYS:N	2.21	0.56
1:B:278:GLN:HE22	1:B:308:ARG:HH22	1.53	0.56
1:B:108:MSE:HE3	1:B:277:SER:HB2	1.87	0.56
1:A:148:PRO:HB3	1:B:290:GLU:CD	2.28	0.55
1:B:155:PHE:C	1:B:155:PHE:CD1	2.81	0.55
1:B:209:GLU:CD	1:B:209:GLU:H	2.10	0.54
1:A:145:LYS:HZ2	1:A:145:LYS:HB3	1.72	0.54
1:A:173:ILE:HD12	1:A:227:GLY:O	2.08	0.54
1:B:156:ILE:CG2	1:B:256:MSE:HE2	2.37	0.54
1:A:119:TYR:HD2	1:A:145:LYS:HE3	1.72	0.54
1:A:185:ASN:HD22	1:A:186:SER:N	2.02	0.54
1:B:158:ILE:HD13	1:B:158:ILE:H	1.73	0.53
1:A:251:ASN:N	1:A:251:ASN:HD22	2.07	0.53
1:A:190:LYS:HG2	1:A:191:GLY:N	2.24	0.53
1:A:193:ILE:O	1:A:193:ILE:HG23	2.08	0.52
1:A:173:ILE:HD12	1:A:227:GLY:C	2.30	0.52
1:B:92:ASP:O	1:B:113:ARG:HB3	2.10	0.52
1:B:248:VAL:O	1:B:251:ASN:HB2	2.09	0.52
1:B:292:TYR:HB3	1:B:294:PHE:CE2	2.45	0.52
1:A:244:ILE:CD1	1:A:244:ILE:O	2.51	0.52
1:B:105:ALA:O	1:B:270:SER:HB3	2.10	0.52
1:A:77:LEU:HD13	1:A:225:ILE:HD12	1.92	0.52
1:A:94:ILE:C	1:A:95:ILE:HD12	2.31	0.51
1:A:182:THR:C	1:A:184:VAL:N	2.64	0.51
1:B:77:LEU:HD22	1:B:156:ILE:HD11	1.92	0.51
1:A:154:TYR:CD1	1:A:256:MSE:HG2	2.45	0.51
1:A:260:ASP:C	1:A:260:ASP:OD2	2.49	0.51
1:B:77:LEU:HD23	1:B:156:ILE:HG12	1.92	0.50
1:B:196:ASN:OD1	1:B:196:ASN:C	2.50	0.50
1:B:207:ARG:HH11	1:B:207:ARG:HG3	1.77	0.50
1:A:74:SER:CB	1:A:98:THR:HG22	2.42	0.50
1:A:173:ILE:HG23	1:A:227:GLY:HA3	1.94	0.50
1:A:196:ASN:ND2	1:A:199:GLU:HG3	2.27	0.50
1:B:107:GLU:HG3	1:B:316:SER:OG	2.12	0.49
1:A:76:LEU:CG	1:A:78:MSE:HE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:NE2	1:A:312:MSE:HE1	2.28	0.49
1:A:115:THR:HA	1:A:299:PHE:HB3	1.94	0.49
1:A:159:ASN:ND2	1:A:162:GLY:N	2.54	0.48
1:A:119:TYR:O	1:A:123:ASP:HB3	2.12	0.48
1:A:195:LEU:HD22	1:A:199:GLU:HB3	1.95	0.48
1:B:204:VAL:O	1:B:204:VAL:HG12	2.13	0.48
1:A:288:TYR:HA	1:A:295:ASP:HA	1.95	0.48
1:A:177:ASN:N	1:A:191:GLY:O	2.42	0.48
1:B:160:MSE:HG3	1:B:205:ARG:NH2	2.25	0.48
1:A:127:ILE:O	1:A:131:TYR:HB2	2.11	0.48
1:B:185:ASN:HD22	1:B:187:LYS:HB3	1.78	0.48
1:A:74:SER:HB2	1:A:98:THR:HG22	1.96	0.48
1:A:173:ILE:CG2	1:A:227:GLY:HA3	2.44	0.48
1:A:96:LEU:O	1:A:108:MSE:HA	2.13	0.48
1:B:70:LYS:HD2	1:B:101:LYS:HD2	1.95	0.48
1:B:96:LEU:HD12	1:B:313:PHE:CZ	2.49	0.47
1:B:100:ASN:OD1	1:B:103:GLN:HG3	2.14	0.47
1:B:158:ILE:O	1:B:158:ILE:HD13	2.14	0.47
1:B:319:ILE:CG1	1:B:320:THR:H	2.24	0.47
1:B:106:VAL:HG23	1:B:270:SER:O	2.14	0.47
1:B:90:ARG:HB3	1:B:131:TYR:HB3	1.95	0.47
1:A:100:ASN:ND2	1:A:102:GLN:H	2.12	0.47
1:A:257:THR:O	1:A:260:ASP:OD2	2.33	0.47
1:A:131:TYR:CD1	1:A:142:ALA:HB2	2.50	0.47
1:B:155:PHE:O	1:B:155:PHE:CD1	2.67	0.46
1:A:115:THR:HG23	1:A:301:PRO:HG3	1.97	0.46
1:A:189:VAL:HG12	1:A:193:ILE:HD12	1.98	0.46
1:B:133:ASN:C	1:B:135:GLY:H	2.19	0.46
1:A:147:MSE:HE1	1:A:309:ILE:HG21	1.96	0.46
1:B:141:SER:O	1:B:145:LYS:HG3	2.16	0.46
1:B:158:ILE:N	1:B:158:ILE:HD13	2.31	0.46
1:A:253:GLN:HB2	1:A:253:GLN:HE21	1.55	0.46
1:A:159:ASN:N	1:A:159:ASN:ND2	2.57	0.46
1:A:76:LEU:HD23	1:A:78:MSE:HE2	1.98	0.46
1:B:261:ILE:O	1:B:264:MSE:HB2	2.16	0.46
1:B:182:THR:HG22	1:B:183:GLU:H	1.81	0.45
1:A:264:MSE:HA	1:A:268:TYR:CD2	2.45	0.45
1:B:307:GLU:O	1:B:308:ARG:C	2.55	0.45
1:B:155:PHE:O	1:B:155:PHE:CG	2.69	0.45
1:B:161:GLU:HB3	1:B:251:ASN:HD21	1.81	0.45
1:B:226:ILE:HD11	1:B:275:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HG13	1:A:173:ILE:CG1	2.41	0.45
1:B:168:ASP:OD1	1:B:196:ASN:HB2	2.17	0.45
1:A:180:ASP:CG	1:A:182:THR:HG22	2.37	0.45
1:B:111:ILE:HD11	1:B:147:MSE:HE1	1.98	0.45
1:A:163:PHE:O	1:A:167:VAL:HG23	2.17	0.44
1:B:182:THR:C	1:B:184:VAL:N	2.70	0.44
1:A:126:LYS:H	1:A:126:LYS:HG2	1.34	0.44
1:B:170:VAL:O	1:B:170:VAL:HG13	2.16	0.44
1:B:66:ASP:HB3	1:B:71:LYS:HD3	1.99	0.44
1:A:196:ASN:H	1:A:199:GLU:HB2	1.81	0.44
1:A:140:VAL:O	1:A:144:GLU:HG3	2.17	0.44
1:A:220:ARG:O	1:A:224:VAL:HG23	2.17	0.44
1:B:173:ILE:O	1:B:194:THR:HA	2.18	0.44
1:B:288:TYR:HE1	1:B:293:GLY:C	2.21	0.44
1:A:257:THR:H	1:A:260:ASP:CG	2.21	0.44
1:B:173:ILE:HG22	1:B:174:THR:N	2.33	0.44
1:B:275:VAL:HG13	1:B:275:VAL:O	2.17	0.44
1:B:117:VAL:HB	1:B:146:LEU:HD13	1.99	0.44
1:A:181:LEU:O	1:A:182:THR:O	2.36	0.43
1:B:146:LEU:HD23	1:B:147:MSE:HE2	2.00	0.43
1:B:182:THR:O	1:B:184:VAL:N	2.51	0.43
1:B:108:MSE:HE1	1:B:222:ARG:CG	2.27	0.43
1:A:229:ALA:C	1:A:231:LYS:H	2.22	0.43
1:B:272:LEU:C	1:B:274:ASN:H	2.19	0.43
1:A:270:SER:C	1:A:272:LEU:H	2.20	0.43
1:B:153:ASP:N	1:B:153:ASP:OD1	2.50	0.43
1:A:209:GLU:OE1	1:A:209:GLU:N	2.49	0.43
1:A:68:GLU:C	1:A:70:LYS:H	2.21	0.43
1:A:210:ASP:CB	1:A:220:ARG:HH21	2.32	0.43
1:B:126:LYS:HG3	1:B:298:TYR:CE1	2.53	0.42
1:A:270:SER:C	1:A:272:LEU:N	2.72	0.42
1:A:109:VAL:HA	1:A:278:GLN:O	2.18	0.42
1:A:181:LEU:O	1:A:188:PHE:HB2	2.20	0.42
1:B:76:LEU:HG	1:B:78:MSE:HE2	2.01	0.42
1:A:109:VAL:HG22	1:A:278:GLN:HG3	2.02	0.42
1:A:196:ASN:HD21	1:A:199:GLU:HG3	1.83	0.42
1:B:246:LYS:C	1:B:248:VAL:H	2.21	0.42
1:B:249:GLY:C	1:B:251:ASN:H	2.22	0.42
1:B:275:VAL:HG22	1:B:275:VAL:O	2.19	0.42
1:B:233:ILE:O	1:B:233:ILE:HD12	2.18	0.42
1:B:100:ASN:ND2	1:B:316:SER:O	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:C	1:A:179:ILE:HD13	2.40	0.42
1:B:287:ILE:HB	1:B:298:TYR:HD2	1.82	0.42
1:B:200:ALA:O	1:B:204:VAL:HG23	2.20	0.42
1:B:185:ASN:C	1:B:187:LYS:H	2.22	0.41
1:B:158:ILE:N	1:B:158:ILE:CD1	2.83	0.41
1:B:95:ILE:HD11	1:B:221:GLN:OE1	2.20	0.41
1:A:178:ASP:OD2	1:A:178:ASP:N	2.54	0.41
1:A:210:ASP:HA	1:A:211:PRO:HD2	1.87	0.41
1:B:139:THR:O	1:B:140:VAL:C	2.59	0.41
1:B:208:HIS:O	1:B:209:GLU:C	2.59	0.41
1:A:78:MSE:SE	1:A:136:PRO:HB3	2.71	0.41
1:B:111:ILE:CD1	1:B:147:MSE:HE1	2.51	0.41
1:B:217:ARG:HA	1:B:220:ARG:CZ	2.50	0.41
1:B:154:TYR:CD1	1:B:256:MSE:HG2	2.55	0.41
1:B:184:VAL:HG23	1:B:209:GLU:HG2	2.03	0.41
1:B:152:VAL:HG12	1:B:152:VAL:O	2.21	0.41
1:B:127:ILE:HG23	1:B:128:ASN:N	2.35	0.40
1:B:196:ASN:OD1	1:B:199:GLU:HG3	2.22	0.40
1:B:299:PHE:O	1:B:301:PRO:HD3	2.22	0.40
1:A:163:PHE:CZ	1:A:224:VAL:HG11	2.51	0.40
1:B:133:ASN:HB3	1:B:138:GLY:HA3	2.03	0.40
1:A:100:ASN:ND2	1:A:102:GLN:HB2	2.30	0.40
1:B:184:VAL:HG21	1:B:209:GLU:HG2	2.04	0.40
1:B:126:LYS:O	1:B:129:ALA:HB3	2.21	0.40
1:A:226:ILE:HD11	1:A:275:VAL:HG11	2.02	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	229/279 (82%)	181 (79%)	38 (17%)	10 (4%)	3 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	229/279 (82%)	187 (82%)	33 (14%)	9 (4%)	4 15
All	All	458/558 (82%)	368 (80%)	71 (16%)	19 (4%)	3 14

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	THR
1	A	183	GLU
1	A	272	LEU
1	B	208	HIS
1	B	209	GLU
1	B	246	LYS
1	B	153	ASP
1	B	245	MSE
1	B	273	LYS
1	A	134	GLY
1	A	274	ASN
1	A	318	ASP
1	A	319	ILE
1	A	230	ASN
1	B	197	GLY
1	B	233	ILE
1	B	318	ASP
1	A	189	VAL
1	A	211	PRO

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	201/231 (87%)	179 (89%)	22 (11%)	8 23
1	B	206/231 (89%)	192 (93%)	14 (7%)	20 49
All	All	407/462 (88%)	371 (91%)	36 (9%)	12 35

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	127	ILE
1	A	159	ASN
1	A	161	GLU
1	A	179	ILE
1	A	182	THR
1	A	185	ASN
1	A	187	LYS
1	A	205	ARG
1	A	207	ARG
1	A	209	GLU
1	A	245	MSE
1	A	246	LYS
1	A	253	GLN
1	A	257	THR
1	A	258	LEU
1	A	262	THR
1	A	267	ASN
1	A	272	LEU
1	A	274	ASN
1	A	296	LEU
1	A	308	ARG
1	B	67	LEU
1	B	98	THR
1	B	113	ARG
1	B	126	LYS
1	B	153	ASP
1	B	158	ILE
1	B	170	VAL
1	B	182	THR
1	B	218	GLN
1	B	253	GLN
1	B	259	THR
1	B	272	LEU
1	B	294	PHE
1	B	318	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	121	ASN
1	A	128	ASN

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	159	ASN
1	A	185	ASN
1	A	253	GLN
1	A	278	GLN
1	B	185	ASN
1	B	267	ASN
1	B	278	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 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	A	226/279 (81%)	0.37	16 (7%)	19	13	40, 71, 117, 151	0
1	B	228/279 (81%)	0.04	9 (3%)	43	36	27, 60, 98, 128	0
All	All	454/558 (81%)	0.20	25 (5%)	29	22	27, 66, 115, 151	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	SER	15.4
1	A	134	GLY	4.0
1	A	193	ILE	3.8
1	B	183	GLU	3.7
1	A	131	TYR	3.3
1	A	129	ALA	3.2
1	A	71	LYS	3.0
1	B	134	GLY	2.9
1	A	165	ASP	2.8
1	A	171	GLY	2.7
1	B	292	TYR	2.6
1	B	319	ILE	2.6
1	A	121	ASN	2.5
1	A	172	GLY	2.5
1	A	105	ALA	2.5
1	B	283	GLU	2.4
1	A	197	GLY	2.3
1	A	72	PRO	2.3
1	A	169	ALA	2.3
1	A	69	LYS	2.1
1	B	320	THR	2.1
1	A	119	TYR	2.1
1	B	176	TYR	2.1
1	B	247	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.