Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:43 AM GMT

PDB ID	:	3MWT
Title	:	Crystal structure of Lassa fever virus nucleoprotein in complex with Mn2+
Authors	:	Qi, X.; Lan, S.; Wang, W.; Schelde, L.M.; Dong, H.; Wallat, G.; Liang, Y.; Ly, H.; Dong, C.; Scottish Structural Proteomics Facility (SSPF)
Deposited on	:	2010-05-06
Resolution	:	1.98 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:

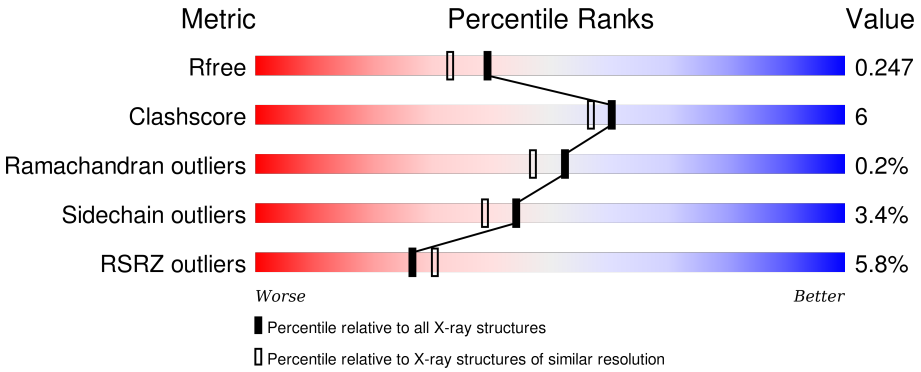
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	577	3% 78% 10% • 11%
1	B	577	3% 74% 14% • 11%
1	C	577	9% 73% 13% • 13%

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	MN	A	680	-	-	-	X
2	MN	B	680	-	-	-	X
3	ZN	A	690	-	-	-	X
3	ZN	B	690	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12279 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			4012	2521	697	767	27			
1	B	512	Total	C	N	O	S	0	0	0
			4001	2510	696	768	27			
1	C	500	Total	C	N	O	S	0	0	0
			3918	2463	681	747	27			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P13699
A	-6	ALA	-	EXPRESSION TAG	UNP P13699
A	-5	MET	-	EXPRESSION TAG	UNP P13699
A	-4	ASP	-	EXPRESSION TAG	UNP P13699
A	-3	HIS	-	EXPRESSION TAG	UNP P13699
A	-2	VAL	-	EXPRESSION TAG	UNP P13699
A	-1	GLU	-	EXPRESSION TAG	UNP P13699
A	0	PHE	-	EXPRESSION TAG	UNP P13699
B	-7	GLY	-	EXPRESSION TAG	UNP P13699
B	-6	ALA	-	EXPRESSION TAG	UNP P13699
B	-5	MET	-	EXPRESSION TAG	UNP P13699
B	-4	ASP	-	EXPRESSION TAG	UNP P13699
B	-3	HIS	-	EXPRESSION TAG	UNP P13699
B	-2	VAL	-	EXPRESSION TAG	UNP P13699
B	-1	GLU	-	EXPRESSION TAG	UNP P13699
B	0	PHE	-	EXPRESSION TAG	UNP P13699
C	-7	GLY	-	EXPRESSION TAG	UNP P13699
C	-6	ALA	-	EXPRESSION TAG	UNP P13699
C	-5	MET	-	EXPRESSION TAG	UNP P13699
C	-4	ASP	-	EXPRESSION TAG	UNP P13699
C	-3	HIS	-	EXPRESSION TAG	UNP P13699
C	-2	VAL	-	EXPRESSION TAG	UNP P13699
C	-1	GLU	-	EXPRESSION TAG	UNP P13699

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	PHE	-	EXPRESSION TAG	UNP P13699

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is water.

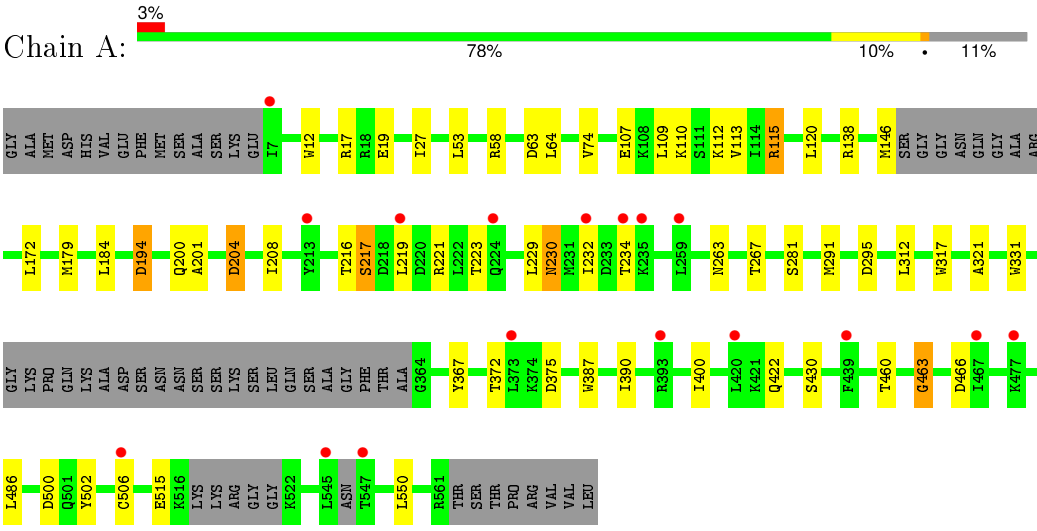
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	135	Total O 135 135	0	0
4	B	158	Total O 158 158	0	0
4	C	49	Total O 49 49	0	0

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.

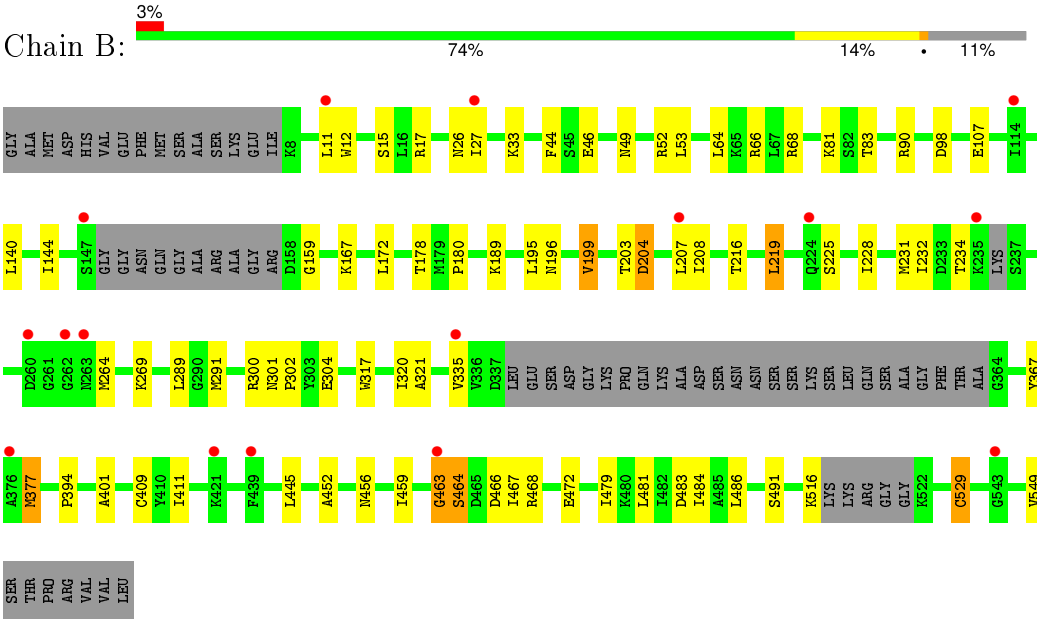
- Molecule 1: Nucleoprotein

Chain A:



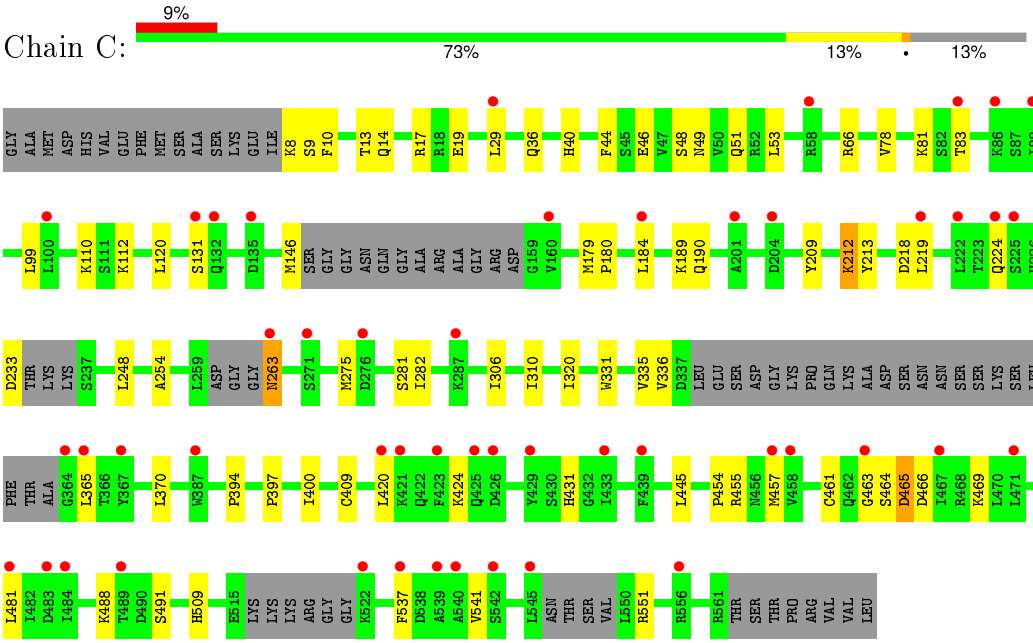
- Molecule 1: Nucleoprotein

Chain B:



- Molecule 1: Nucleoprotein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	176.88Å 176.88Å 56.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	153.18 – 1.98 47.59 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.5 (153.18-1.98) 99.8 (47.59-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, R_{free}	0.181 , 0.218 0.208 , 0.247	Depositor DCC
R_{free} test set	6834 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.7	EDS
Estimated twinning fraction	0.553 for H, K, L 0.447 for K, H, -L 0.000 for -h,-k,l 0.069 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.553 for H, K, L 0.447 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Outliers	0 of 136770 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12279	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: ZN, MN

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	0.78	2/4068 (0.0%)	0.82	4/5491 (0.1%)
1	B	0.93	3/4057 (0.1%)	0.92	7/5477 (0.1%)
1	C	0.74	0/3972	0.77	2/5360 (0.0%)
All	All	0.82	5/12097 (0.0%)	0.84	13/16328 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	CYS	CB-SG	-7.78	1.69	1.82
1	B	529	CYS	CB-SG	6.84	1.93	1.82
1	A	506	CYS	CB-SG	6.52	1.93	1.82
1	B	204	ASP	CB-CG	6.06	1.64	1.51
1	A	204	ASP	CB-CG	5.82	1.64	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	377	MET	CG-SD-CE	-10.55	83.32	100.20
1	A	115	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	68	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	A	204	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	52	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	A	115	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	B	68	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	204	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	204	ASP	CB-CA-C	5.85	122.09	110.40
1	C	370	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	98	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	98	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	184	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4012	0	4084	44	0
1	B	4001	0	4060	52	0
1	C	3918	0	3980	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	135	0	0	4	0
4	B	158	0	0	3	2
4	C	49	0	0	2	0
All	All	12279	0	12124	135	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 6.

All (135) 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:B:464:SER:HB3	1:B:483:ASP:OD2	1.85	0.77
1:A:502:TYR:CE1	1:A:550:LEU:HD13	2.21	0.75
1:B:459:ILE:HD12	1:B:479:ILE:HG21	1.69	0.75
1:A:216:THR:OG1	1:A:234:THR:CG2	2.40	0.69
1:C:46:GLU:OE2	1:C:66:ARG:HD2	1.94	0.68
1:B:463:GLY:O	1:B:467:ILE:HG12	1.95	0.66
1:A:500:ASP:OD2	4:A:572:HOH:O	2.14	0.65
1:C:51:GLN:HE22	1:C:190:GLN:HE22	1.43	0.65
1:C:397:PRO:HB2	1:C:400:ILE:HD11	1.80	0.64
1:A:208:ILE:HD11	1:B:208:ILE:HD13	1.81	0.63
1:C:120:LEU:HD23	1:C:146:MET:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:OG1	1:A:234:THR:HG23	1.99	0.61
1:C:219:LEU:HD22	1:C:248:LEU:HD13	1.82	0.61
1:A:115:ARG:HD2	1:A:375:ASP:OD2	2.00	0.61
1:C:454:PRO:O	1:C:457:MET:HG3	2.00	0.60
1:B:81:LYS:HA	1:B:321:ALA:HB1	1.83	0.60
1:A:58:ARG:NH2	4:A:669:HOH:O	2.35	0.60
1:B:367:TYR:CZ	1:B:371:MET:SD	2.96	0.58
1:A:208:ILE:CD1	1:B:208:ILE:HD13	2.34	0.58
1:A:317:TRP:HB2	1:A:321:ALA:HB2	1.86	0.58
1:A:19:GLU:HG3	1:A:281:SER:HB3	1.87	0.56
1:C:282:ILE:HD11	1:C:310:ILE:CD1	2.35	0.56
1:B:196:ASN:HA	1:B:199:VAL:HG13	1.88	0.56
1:C:99:LEU:HD22	1:C:336:VAL:HG13	1.87	0.56
1:C:431:HIS:O	1:C:509:HIS:ND1	2.35	0.56
1:B:216:THR:HG22	1:B:234:THR:HB	1.88	0.55
1:C:365:LEU:H	1:C:365:LEU:HD12	1.72	0.55
1:C:537:PHE:O	1:C:541:VAL:HG23	2.06	0.55
1:C:44:PHE:CD2	1:C:189:LYS:HG2	2.43	0.54
1:A:17:ARG:HG2	1:A:263:ASN:O	2.07	0.54
1:B:300:ARG:CZ	4:B:657:HOH:O	2.56	0.54
1:B:107:GLU:HG2	4:B:580:HOH:O	2.08	0.54
1:A:120:LEU:HD23	1:A:146:MET:SD	2.49	0.53
1:C:36:GLN:O	1:C:40:HIS:ND1	2.41	0.53
1:B:269:LYS:HD2	1:B:317:TRP:CE2	2.44	0.52
1:B:180:PRO:HB3	1:B:254:ALA:HA	1.90	0.52
1:B:232:ILE:HD13	1:B:251:ALA:CB	2.39	0.52
1:C:36:GLN:HG2	4:C:595:HOH:O	2.09	0.52
1:A:223:THR:HG21	1:A:230:ASN:HB3	1.91	0.52
1:C:461:CYS:SG	1:C:464:SER:HA	2.49	0.52
1:C:179:MET:HG3	1:C:320:ILE:O	2.10	0.52
1:C:120:LEU:HD23	1:C:146:MET:CG	2.40	0.52
1:A:216:THR:OG1	1:A:234:THR:HG21	2.09	0.52
1:B:463:GLY:O	1:B:466:ASP:OD1	2.28	0.52
1:C:110:LYS:HG3	1:C:331:TRP:CE2	2.45	0.52
1:B:301:ASN:OD1	1:B:304:GLU:HG3	2.10	0.52
1:A:390:ILE:HG22	1:A:400:ILE:HD12	1.92	0.51
1:A:390:ILE:HG22	1:A:400:ILE:CD1	2.40	0.51
1:C:209:TYR:HA	1:C:212:LYS:O	2.10	0.51
1:A:194:ASP:OD1	1:A:194:ASP:N	2.44	0.51
1:C:365:LEU:HD12	1:C:365:LEU:N	2.26	0.51
1:B:204:ASP:HA	1:B:207:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:PRO:HG3	1:C:466:ASP:HB2	1.94	0.49
1:A:74:VAL:HG11	1:A:179:MET:HE2	1.93	0.49
1:B:367:TYR:O	1:B:371:MET:HG2	2.13	0.49
1:A:200:GLN:HG2	1:B:225:SER:HB3	1.94	0.49
1:A:109:LEU:O	1:A:113:VAL:HG23	2.12	0.49
1:B:216:THR:HG22	1:B:234:THR:CB	2.43	0.49
1:B:377:MET:CE	1:B:452:ALA:HB3	2.42	0.49
1:B:140:LEU:O	1:B:144:ILE:HG12	2.13	0.49
1:C:409:CYS:HA	1:C:551:ARG:O	2.13	0.48
1:A:312:LEU:HD22	4:A:684:HOH:O	2.13	0.48
1:A:216:THR:HG23	1:A:234:THR:HG21	1.96	0.48
1:A:64:LEU:HD13	1:A:172:LEU:HD23	1.95	0.48
1:C:480:LYS:HE3	1:C:481:LEU:O	2.14	0.48
1:A:53:LEU:HD22	1:A:63:ASP:OD1	2.13	0.48
1:A:158:ASP:N	4:A:696:HOH:O	2.46	0.47
1:C:10:PHE:CE2	1:C:14:GLN:HG3	2.49	0.47
1:C:19:GLU:HG3	1:C:281:SER:HB3	1.96	0.47
1:B:459:ILE:HD12	1:B:479:ILE:CG2	2.42	0.47
1:A:463:GLY:O	1:A:466:ASP:OD1	2.32	0.47
1:B:15:SER:OG	1:B:289:LEU:HD11	2.15	0.47
1:A:484:ILE:HG22	1:A:486:LEU:HG	1.97	0.47
1:A:208:ILE:CD1	1:B:208:ILE:CD1	2.93	0.47
1:C:78:VAL:O	1:C:81:LYS:HE3	2.14	0.47
1:A:27:ILE:HD11	1:A:267:THR:HG22	1.97	0.47
1:C:13:THR:O	1:C:17:ARG:HG3	2.15	0.47
1:B:178:THR:HG21	1:B:250:ALA:HB2	1.97	0.46
1:A:208:ILE:HD13	1:B:208:ILE:CD1	2.46	0.46
1:B:126:MET:N	1:B:159:GLY:O	2.36	0.46
1:B:12:TRP:CZ2	1:B:291:MET:HA	2.52	0.45
1:B:317:TRP:HB3	1:B:320:ILE:HG13	1.98	0.45
1:C:212:LYS:NZ	1:C:218:ASP:OD2	2.50	0.45
1:C:488:LYS:O	1:C:491:SER:OG	2.29	0.45
1:B:375:ASP:HB3	4:B:586:HOH:O	2.16	0.45
1:C:263:ASN:N	4:C:603:HOH:O	2.49	0.45
1:C:179:MET:HB2	1:C:179:MET:HE2	1.83	0.45
1:A:387:TRP:CH2	1:A:484:ILE:HG13	2.52	0.45
1:B:203:THR:O	1:B:207:LEU:HG	2.17	0.44
1:B:445:LEU:HA	1:B:445:LEU:HD23	1.77	0.44
1:A:219:LEU:HD21	1:A:232:ILE:HB	1.98	0.44
1:B:46:GLU:OE2	1:B:66:ARG:HD2	2.17	0.44
1:B:401:ALA:HA	1:B:411:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TRP:CZ2	1:A:291:MET:HA	2.53	0.44
1:C:465:ASP:O	1:C:469:LYS:HD3	2.17	0.44
1:C:120:LEU:CD2	1:C:146:MET:HG3	2.47	0.44
1:C:488:LYS:N	1:C:488:LYS:HD2	2.33	0.44
1:C:48:SER:HA	1:C:51:GLN:NE2	2.32	0.44
1:B:228:ILE:O	1:B:231:MET:HG3	2.18	0.44
1:C:365:LEU:HD21	1:C:445:LEU:HD23	1.99	0.43
1:B:468:ARG:HB2	1:B:481:LEU:CD1	2.49	0.43
1:A:115:ARG:HD3	1:A:372:THR:HA	2.00	0.43
1:C:282:ILE:CD1	1:C:310:ILE:CD1	2.96	0.43
1:A:208:ILE:HD13	1:B:208:ILE:HD12	2.01	0.43
1:B:468:ARG:O	1:B:472:GLU:HG3	2.19	0.43
1:B:44:PHE:CG	1:B:189:LYS:HG2	2.54	0.43
1:C:488:LYS:HA	1:C:488:LYS:HE3	2.01	0.43
1:A:295:ASP:OD2	1:A:367:TYR:OH	2.37	0.42
1:B:195:LEU:O	1:B:199:VAL:HG12	2.19	0.42
1:A:221:ARG:HB3	1:B:207:LEU:CD2	2.49	0.42
1:C:19:GLU:CG	1:C:281:SER:HB3	2.49	0.42
1:C:49:ASN:O	1:C:53:LEU:HG	2.20	0.42
1:A:201:ALA:HB1	1:A:229:LEU:HD11	2.01	0.42
1:B:486:LEU:HD13	1:B:491:SER:HA	2.02	0.42
1:B:49:ASN:O	1:B:53:LEU:HG	2.20	0.42
1:A:204:ASP:OD2	1:B:204:ASP:OD2	2.38	0.42
1:A:110:LYS:HA	1:A:331:TRP:CZ3	2.55	0.42
1:A:502:TYR:CZ	1:A:550:LEU:HD13	2.55	0.42
1:C:306:ILE:HG12	1:C:310:ILE:HD12	2.02	0.41
1:B:219:LEU:HD22	1:B:234:THR:HG23	2.02	0.41
1:C:420:LEU:O	1:C:424:LYS:HG2	2.21	0.41
1:C:227:PRO:O	1:C:230:ASN:ND2	2.53	0.41
1:A:387:TRP:HA	1:A:460:THR:O	2.20	0.41
1:C:457:MET:HB2	1:C:479:ILE:HG12	2.03	0.41
1:C:180:PRO:HB3	1:C:254:ALA:HA	2.02	0.41
1:A:217:SER:OG	1:A:221:ARG:NH1	2.54	0.41
1:B:126:MET:SD	1:B:137:ARG:HB3	2.61	0.41
1:B:17:ARG:HD3	1:B:264:MET:HE2	2.03	0.41
1:C:48:SER:HA	1:C:51:GLN:HE21	1.85	0.40
1:C:212:LYS:HG2	1:C:213:TYR:N	2.36	0.40
1:B:64:LEU:HD13	1:B:172:LEU:HD23	2.02	0.40
1:B:394:PRO:HB3	1:B:466:ASP:O	2.21	0.40
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.68	0.40
1:B:46:GLU:OE1	1:B:66:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ASP:OD1	1:A:466:ASP:N	2.54	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)
4:B:573:HOH:O	4:B:727:HOH:O[2_455]	1.78	0.42
4:B:623:HOH:O	4:B:679:HOH:O[3_445]	2.18	0.02

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	503/577 (87%)	494 (98%)	8 (2%)	1 (0%)	52	47
1	B	502/577 (87%)	490 (98%)	11 (2%)	1 (0%)	52	47
1	C	486/577 (84%)	478 (98%)	7 (1%)	1 (0%)	52	47
All	All	1491/1731 (86%)	1462 (98%)	26 (2%)	3 (0%)	52	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	GLY
1	C	463	GLY
1	A	463	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	450/498 (90%)	439 (98%)	11 (2%)	57	55
1	B	449/498 (90%)	430 (96%)	19 (4%)	36	29
1	C	439/498 (88%)	423 (96%)	16 (4%)	42	36
All	All	1338/1494 (90%)	1292 (97%)	46 (3%)	44	39

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	112	LYS
1	A	138	ARG
1	A	184	LEU
1	A	194	ASP
1	A	217	SER
1	A	230	ASN
1	A	338	LEU
1	A	422	GLN
1	A	430	SER
1	A	515	GLU
1	B	11	LEU
1	B	26	ASN
1	B	27	ILE
1	B	33	LYS
1	B	83	THR
1	B	90	ARG
1	B	167	LYS
1	B	199	VAL
1	B	219	LEU
1	B	302	PRO
1	B	335	VAL
1	B	371	MET
1	B	456	ASN
1	B	464	SER
1	B	484	ILE
1	B	516	LYS
1	B	529	CYS
1	B	549	VAL
1	B	550	LEU
1	C	8	LYS

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Mol	Chain	Res	Type
1	C	9	SER
1	C	29	LEU
1	C	83	THR
1	C	112	LYS
1	C	131	SER
1	C	212	LYS
1	C	224	GLN
1	C	230	ASN
1	C	233	ASP
1	C	263	ASN
1	C	275	MET
1	C	335	VAL
1	C	455	ARG
1	C	465	ASP
1	C	480	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	B	36	GLN
1	B	200	GLN
1	C	14	GLN
1	C	51	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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	513/577 (88%)	0.58	20 (3%) 43 47	28, 40, 58, 83	1 (0%)
1	B	512/577 (88%)	0.61	16 (3%) 52 56	24, 34, 51, 79	0
1	C	500/577 (86%)	0.70	52 (10%) 8 10	32, 44, 64, 76	0
All	All	1525/1731 (88%)	0.63	88 (5%) 26 30	24, 40, 59, 83	1 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	THR	5.1
1	A	484	ILE	4.9
1	B	207	LEU	4.8
1	C	91	VAL	4.6
1	C	222	LEU	4.5
1	C	367	TYR	4.4
1	C	439	PHE	4.1
1	C	132	GLN	4.1
1	C	135	ASP	4.0
1	C	429	TYR	4.0
1	A	158	ASP	4.0
1	A	477	LYS	3.9
1	A	213	TYR	3.9
1	C	458	VAL	3.9
1	A	420	LEU	3.5
1	C	481	LEU	3.3
1	C	88	ILE	3.3
1	C	365	LEU	3.2
1	C	483	ASP	3.2
1	C	219	LEU	3.2
1	B	421	LYS	3.1
1	B	11	LEU	3.1
1	C	131	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	439	PHE	3.0
1	C	425	GLN	3.0
1	B	262	GLY	3.0
1	A	545	LEU	3.0
1	A	393	ARG	3.0
1	A	7	ILE	2.9
1	B	27	ILE	2.9
1	C	545	LEU	2.9
1	C	364	GLY	2.8
1	B	147	SER	2.8
1	C	540	ALA	2.6
1	C	421	LYS	2.6
1	C	423	PHE	2.6
1	C	484	ILE	2.6
1	C	457	MET	2.6
1	C	387	TRP	2.5
1	A	480	LYS	2.5
1	C	86	LYS	2.5
1	A	547	THR	2.5
1	A	232	ILE	2.5
1	B	376	ALA	2.5
1	A	219	LEU	2.5
1	C	477	LYS	2.4
1	B	260	ASP	2.4
1	C	276	ASP	2.4
1	C	160	VAL	2.4
1	C	83	THR	2.4
1	C	287	LYS	2.4
1	C	522	LYS	2.4
1	C	537	PHE	2.4
1	C	426	ASP	2.3
1	C	204	ASP	2.3
1	B	335	VAL	2.3
1	A	224	GLN	2.3
1	C	467	ILE	2.3
1	B	224	GLN	2.2
1	B	439	PHE	2.2
1	C	29	LEU	2.2
1	C	94	LEU	2.2
1	C	471	LEU	2.2
1	B	114	ILE	2.2
1	B	463	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	201	ALA	2.2
1	A	259	LEU	2.2
1	C	184	LEU	2.2
1	C	433	ILE	2.2
1	C	420	LEU	2.2
1	C	489	THR	2.2
1	B	263	ASN	2.1
1	C	263	ASN	2.1
1	A	373	LEU	2.1
1	C	463	GLY	2.1
1	C	100	LEU	2.1
1	C	542	SER	2.1
1	A	506	CYS	2.1
1	A	235	LYS	2.1
1	C	58	ARG	2.1
1	B	543	GLY	2.1
1	B	235	LYS	2.0
1	C	556	ARG	2.0
1	C	271	SER	2.0
1	C	224	GLN	2.0
1	C	225	SER	2.0
1	C	539	ALA	2.0
1	A	467	ILE	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 carbohydrates 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. 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
2	MN	A	680	1/1	0.88	0.21	4.86	76,76,76,76	0
3	ZN	A	690	1/1	0.93	0.21	3.52	57,57,57,57	0
3	ZN	B	690	1/1	0.96	0.20	2.56	46,46,46,46	0
2	MN	B	680	1/1	0.94	0.15	2.29	54,54,54,54	0
3	ZN	C	690	1/1	0.93	0.12	0.23	61,61,61,61	0
2	MN	C	680	1/1	0.95	0.12	-0.40	87,87,87,87	0

6.5 Other polymers

There are no such residues in this entry.