



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:17 PM GMT

PDB ID : 3WN7
Title : Crystal Structure of Keap1 in Complex with the N-terminal region of the Nrf2 transcription factor
Authors : Fukutomi, T.; Takagi, K.; Mizushima, T.; Ohuchi, N.; Yamamoto, M.
Deposited on : 2013-12-05
Resolution : 1.57 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 ⓘ symbol.

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

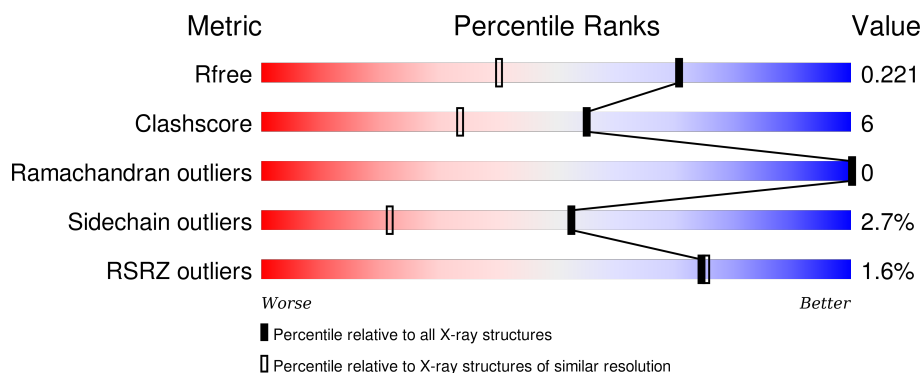
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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 $\leq 5\%$. 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	311	<div> <div>9%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>
1	L	311	<div> <div>9%</div> <div>77%</div> <div>13%</div> <div>8%</div> </div>
2	B	35	<div> <div>9%</div> <div>57%</div> <div>11%</div> <div>31%</div> </div>
2	M	35	<div> <div>9%</div> <div>57%</div> <div>11%</div> <div>31%</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
3	ACT	A	701	-	-	-	X
3	ACT	L	701	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5518 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	18	0
			2298	1436	407	437	18			
1	L	286	Total	C	N	O	S	0	14	0
			2291	1422	412	440	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	MET	-	EXPRESSION TAG	UNP Q9Z2X8
A	300	GLY	-	EXPRESSION TAG	UNP Q9Z2X8
A	301	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	302	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	303	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	304	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	305	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	306	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
A	307	ASP	-	EXPRESSION TAG	UNP Q9Z2X8
A	308	TYR	-	EXPRESSION TAG	UNP Q9Z2X8
A	309	ASP	-	EXPRESSION TAG	UNP Q9Z2X8
A	310	ILE	-	EXPRESSION TAG	UNP Q9Z2X8
A	311	PRO	-	EXPRESSION TAG	UNP Q9Z2X8
A	312	THR	-	EXPRESSION TAG	UNP Q9Z2X8
A	313	THR	-	EXPRESSION TAG	UNP Q9Z2X8
A	314	GLU	-	EXPRESSION TAG	UNP Q9Z2X8
A	315	ASN	-	EXPRESSION TAG	UNP Q9Z2X8
A	316	LEU	-	EXPRESSION TAG	UNP Q9Z2X8
A	317	TYR	-	EXPRESSION TAG	UNP Q9Z2X8
A	318	PHE	-	EXPRESSION TAG	UNP Q9Z2X8
A	319	GLN	-	EXPRESSION TAG	UNP Q9Z2X8
A	320	GLY	-	EXPRESSION TAG	UNP Q9Z2X8
L	299	MET	-	EXPRESSION TAG	UNP Q9Z2X8
L	300	GLY	-	EXPRESSION TAG	UNP Q9Z2X8
L	301	HIS	-	EXPRESSION TAG	UNP Q9Z2X8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	302	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
L	303	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
L	304	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
L	305	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
L	306	HIS	-	EXPRESSION TAG	UNP Q9Z2X8
L	307	ASP	-	EXPRESSION TAG	UNP Q9Z2X8
L	308	TYR	-	EXPRESSION TAG	UNP Q9Z2X8
L	309	ASP	-	EXPRESSION TAG	UNP Q9Z2X8
L	310	ILE	-	EXPRESSION TAG	UNP Q9Z2X8
L	311	PRO	-	EXPRESSION TAG	UNP Q9Z2X8
L	312	THR	-	EXPRESSION TAG	UNP Q9Z2X8
L	313	THR	-	EXPRESSION TAG	UNP Q9Z2X8
L	314	GLU	-	EXPRESSION TAG	UNP Q9Z2X8
L	315	ASN	-	EXPRESSION TAG	UNP Q9Z2X8
L	316	LEU	-	EXPRESSION TAG	UNP Q9Z2X8
L	317	TYR	-	EXPRESSION TAG	UNP Q9Z2X8
L	318	PHE	-	EXPRESSION TAG	UNP Q9Z2X8
L	319	GLN	-	EXPRESSION TAG	UNP Q9Z2X8
L	320	GLY	-	EXPRESSION TAG	UNP Q9Z2X8

- Molecule 2 is a protein called Peptide from Nuclear factor erythroid 2-related factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	S	0	2	0
			219	139	37	42	1			
2	M	24	Total	C	N	O	S	0	1	0
			213	136	36	40	1			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

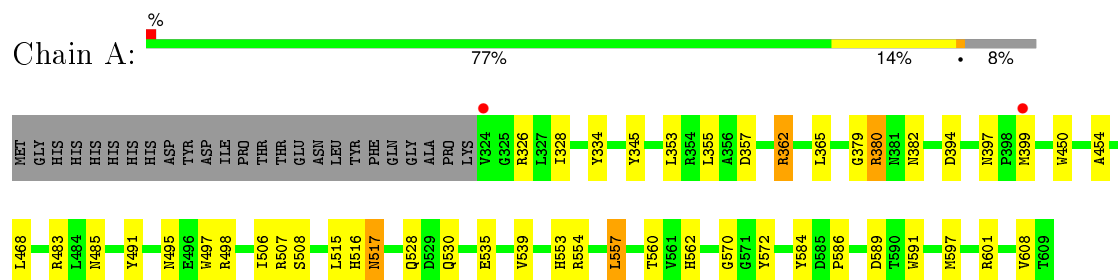
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total	O	0	0
			256	256		
4	B	13	Total	O	0	0
			13	13		
4	L	209	Total	O	0	0
			209	209		
4	M	11	Total	O	0	0
			11	11		

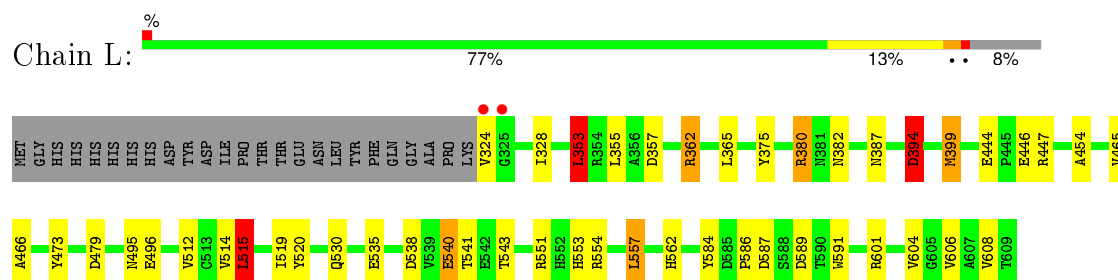
3 Residue-property plots [i](#)

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: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 2: Peptide from Nuclear factor erythroid 2-related factor 2



- Molecule 2: Peptide from Nuclear factor erythroid 2-related factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.14Å 84.39Å 69.82Å 90.00° 116.89° 90.00°	Depositor
Resolution (Å)	34.78 – 1.57 34.78 – 1.57	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.78-1.57) 98.7 (34.78-1.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.223 0.186 , 0.221	Depositor DCC
R_{free} test set	4688 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.8	EDS
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 93412 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5518	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.31	7/2387 (0.3%)	1.32	13/3248 (0.4%)
1	L	1.33	5/2354 (0.2%)	1.38	17/3203 (0.5%)
2	B	1.15	0/222	1.12	0/298
2	M	1.17	1/216 (0.5%)	1.20	0/290
All	All	1.31	13/5179 (0.3%)	1.33	30/7039 (0.4%)

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	L	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	535	GLU	CD-OE1	8.42	1.34	1.25
1	A	535	GLU	CD-OE1	6.47	1.32	1.25
1	A	483	ARG	CZ-NH1	5.91	1.40	1.33
1	A	554	ARG	CZ-NH1	5.80	1.40	1.33
1	L	380	ARG	CD-NE	-5.79	1.36	1.46
1	A	497	TRP	CD2-CE2	5.68	1.48	1.41
1	L	375	TYR	CG-CD1	5.62	1.46	1.39
1	L	591	TRP	CD2-CE2	5.45	1.47	1.41
1	A	379	GLY	N-CA	5.32	1.54	1.46
1	L	496	GLU	CD-OE2	-5.31	1.19	1.25
2	M	24	TRP	CD2-CE2	5.18	1.47	1.41
1	A	591	TRP	CG-CD1	5.10	1.43	1.36
1	A	450	TRP	CG-CD1	5.03	1.43	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	380	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	A	601	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	L	447	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	L	362	ARG	NE-CZ-NH1	-9.49	115.55	120.30
1	L	380	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	A	380	ARG	NE-CZ-NH1	-8.57	116.02	120.30
1	A	507	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	L	394	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	L	601	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	L	447	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	L	353	LEU	CA-CB-CG	7.06	131.54	115.30
1	L	589	ASP	CB-CG-OD2	6.82	124.43	118.30
1	A	584	TYR	CB-CG-CD2	-6.59	117.04	121.00
1	A	357	ASP	CB-CG-OD1	6.48	124.13	118.30
1	L	584	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	L	515	LEU	CB-CG-CD2	6.38	121.85	111.00
1	A	572	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	334	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	491	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	508[A]	SER	N-CA-CB	-5.74	101.89	110.50
1	A	508[B]	SER	N-CA-CB	-5.74	101.89	110.50
1	L	551	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	L	479	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	L	473	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	L	357	ASP	CB-CG-OD1	5.34	123.11	118.30
1	L	601	ARG	CG-CD-NE	-5.24	100.81	111.80
1	A	498	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	L	473	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	A	589	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	345	TYR	CA-CB-CG	5.03	122.96	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	394	ASP	Sidechain
1	L	554	ARG	Sidechain

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	2298	0	2222	25	0
1	L	2291	0	2176	30	0
2	B	219	0	209	5	0
2	M	213	0	205	3	0
3	A	4	0	3	0	0
3	L	4	0	3	3	0
4	A	256	0	0	7	0
4	B	13	0	0	0	0
4	L	209	0	0	4	0
4	M	11	0	0	0	0
All	All	5518	0	4818	62	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 6.

All (62) 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:399[A]:MET:HG2	4:A:1044:HOH:O	1.37	1.18
1:L:514[B]:VAL:HG12	1:L:519:ILE:HD13	1.37	1.06
1:L:514[B]:VAL:HG12	1:L:519:ILE:CD1	2.01	0.91
1:A:485:ASN:HB3	1:A:506[A]:ILE:HD13	1.53	0.89
1:L:454:ALA:H	1:L:495:ASN:HD21	1.25	0.83
1:A:454:ALA:H	1:A:495:ASN:HD21	1.23	0.83
1:A:528:GLN:NE2	4:A:1048:HOH:O	2.06	0.83
2:B:17:MET:HE1	2:B:22:ILE:HG13	1.59	0.81
1:L:380:ARG:HD3	1:L:382:ASN:OD1	1.87	0.74
2:B:17:MET:CE	2:B:22:ILE:HG13	2.17	0.73
1:A:485:ASN:HB3	1:A:506[A]:ILE:CD1	2.19	0.73
1:A:528:GLN:OE1	4:A:1009:HOH:O	2.05	0.72
1:L:514[B]:VAL:CG1	1:L:519:ILE:CD1	2.67	0.71
1:A:380:ARG:HD3	1:A:382:ASN:OD1	1.94	0.68
1:L:353:LEU:HD13	1:L:355:LEU:HD21	1.76	0.67
1:L:514[B]:VAL:CG1	1:L:519:ILE:HD13	2.20	0.66
1:L:466:ALA:HB1	1:L:514[B]:VAL:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:538:ASP:OD1	1:L:540:GLU:HG3	1.96	0.65
1:A:553:HIS:HD2	4:A:836:HOH:O	1.81	0.63
1:L:466:ALA:HB1	1:L:514[A]:VAL:HG23	1.83	0.60
1:A:362:ARG:NH1	1:A:394:ASP:OD2	2.34	0.60
1:L:365:LEU:HD23	1:L:365:LEU:H	1.68	0.58
1:L:562:HIS:HD2	4:L:837:HOH:O	1.87	0.57
1:A:562:HIS:HD2	4:A:824:HOH:O	1.87	0.57
1:A:516:HIS:HE1	4:A:975:HOH:O	1.88	0.56
1:L:466:ALA:CB	1:L:514[B]:VAL:HG13	2.34	0.55
1:A:365:LEU:H	1:A:365:LEU:HD23	1.71	0.55
1:L:514[B]:VAL:CG1	1:L:519:ILE:HD12	2.37	0.55
3:L:701:ACT:CH3	4:L:908:HOH:O	2.54	0.55
1:L:387:ASN:HD21	2:M:39:PHE:HE2	1.54	0.55
1:L:465:VAL:O	3:L:701:ACT:H1	2.11	0.51
2:B:17:MET:HE1	2:B:22:ILE:CG1	2.34	0.51
1:L:541:THR:O	1:L:543[A]:THR:HG23	2.11	0.50
1:A:553:HIS:CD2	1:A:553:HIS:H	2.29	0.50
1:L:466:ALA:HB1	1:L:514[A]:VAL:CG2	2.42	0.49
1:A:468:LEU:HD23	1:A:539:VAL:HG21	1.93	0.49
1:L:553:HIS:CD2	1:L:553:HIS:H	2.32	0.48
1:L:362:ARG:NH1	1:L:394:ASP:OD2	2.46	0.48
1:L:557:LEU:HD23	1:L:557:LEU:H	1.80	0.47
1:L:387:ASN:ND2	2:M:39:PHE:HE2	2.13	0.47
1:L:512:VAL:O	3:L:701:ACT:C	2.64	0.46
1:A:570:GLY:HA3	1:A:597[A]:MET:HE1	1.98	0.46
1:L:328:ILE:HG12	1:L:608[B]:VAL:CG1	2.45	0.45
1:A:397:ASN:OD1	1:A:399[B]:MET:HB2	2.16	0.44
1:L:512:VAL:HA	1:L:520:TYR:O	2.17	0.44
2:B:29:ASP:N	2:B:29:ASP:OD1	2.48	0.44
1:A:557:LEU:HD23	1:A:557:LEU:H	1.83	0.44
1:A:353[B]:LEU:HD23	1:A:355:LEU:HD21	1.98	0.43
1:A:560:THR:OG1	1:A:608[A]:VAL:HG23	2.19	0.43
1:L:515:LEU:HD11	1:L:586:PRO:HG3	2.00	0.43
1:A:515:LEU:HD21	1:A:586:PRO:HG3	2.01	0.42
1:L:444:GLU:HG2	1:L:446:GLU:HG2	2.01	0.42
2:M:29:ASP:N	2:M:29:ASP:OD1	2.50	0.42
2:B:17:MET:HB3	4:L:866:HOH:O	2.19	0.42
1:L:553:HIS:HD2	4:L:999:HOH:O	2.03	0.41
1:A:326:ARG:O	1:A:562:HIS:HE1	2.02	0.41
1:L:399[B]:MET:HG3	1:L:399[B]:MET:O	2.20	0.41
1:A:517[B]:ASN:O	1:A:517[B]:ASN:CG	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353[A]:LEU:HD12	1:A:355:LEU:HD21	2.02	0.40
1:A:353[A]:LEU:HD22	4:A:931:HOH:O	2.21	0.40
1:L:604:VAL:HG23	1:L:606:VAL:HG23	2.03	0.40
1:A:328:ILE:HG12	1:A:608[B]:VAL:CG1	2.51	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	301/311 (97%)	289 (96%)	12 (4%)	0	100	100
1	L	298/311 (96%)	285 (96%)	13 (4%)	0	100	100
2	B	24/35 (69%)	23 (96%)	1 (4%)	0	100	100
2	M	23/35 (66%)	22 (96%)	1 (4%)	0	100	100
All	All	646/692 (93%)	619 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	251/255 (98%)	246 (98%)	5 (2%)	63	34
1	L	247/255 (97%)	238 (96%)	9 (4%)	42	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	25/34 (74%)	24 (96%)	1 (4%)	38	10
2	M	24/34 (71%)	23 (96%)	1 (4%)	36	9
All	All	547/578 (95%)	531 (97%)	16 (3%)	52	19

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	ARG
1	A	517[A]	ASN
1	A	517[B]	ASN
1	A	530	GLN
1	A	557	LEU
2	B	35	GLU
1	L	324	VAL
1	L	353	LEU
1	L	399[A]	MET
1	L	399[B]	MET
1	L	515	LEU
1	L	530	GLN
1	L	540	GLU
1	L	557	LEU
1	L	587	ASP
2	M	17	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	387	ASN
1	A	495	ASN
1	A	516	HIS
1	A	528	GLN
1	A	530	GLN
1	A	552	HIS
1	A	553	HIS
1	A	562	HIS
1	L	359	GLN
1	L	387	ASN
1	L	424	HIS
1	L	495	ASN

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Mol	Chain	Res	Type
1	L	530	GLN
1	L	552	HIS
1	L	553	HIS
1	L	562	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	ACT	A	701	-	1,3,3	0.20	0	0,3,3	0.00	-
3	ACT	L	701	-	1,3,3	4.06	1 (100%)	0,3,3	0.00	-

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	ACT	A	701	-	-	0/0/0/0	0/0/0/0
3	ACT	L	701	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	701	ACT	CH3-C	4.06	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	701	ACT	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	286/311 (91%)	-0.11	2 (0%) 89 89	10, 15, 28, 53	0
1	L	286/311 (91%)	-0.10	2 (0%) 89 89	10, 14, 26, 52	0
2	B	24/35 (68%)	0.92	3 (12%) 5 5	14, 21, 39, 73	0
2	M	24/35 (68%)	0.94	3 (12%) 5 5	14, 21, 45, 72	0
All	All	620/692 (89%)	-0.02	10 (1%) 74 75	10, 15, 29, 73	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	324	VAL	9.9
1	A	324	VAL	8.9
2	M	40	SER	8.0
2	B	40	SER	7.3
2	M	39	PHE	7.3
2	B	39	PHE	6.9
2	M	38	ASP	3.5
2	B	38	ASP	2.5
1	L	325	GLY	2.3
1	A	399[A]	MET	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	A	701	4/4	0.86	0.15	17.33	22,29,31,33	0
3	ACT	L	701	4/4	0.81	0.18	7.52	23,29,29,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.