Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID	:	3QJN
Title	:	Structural flexibility of Shank PDZ domain is important for its binding to different ligands
Authors	:	Lee, J.H.; Park, H.; Park, S.J.; Kim, H.J.; Eom, S.H.
Deposited on	:	2011-01-30
Resolution	:	2.71 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 ①) were used in the production of this report:

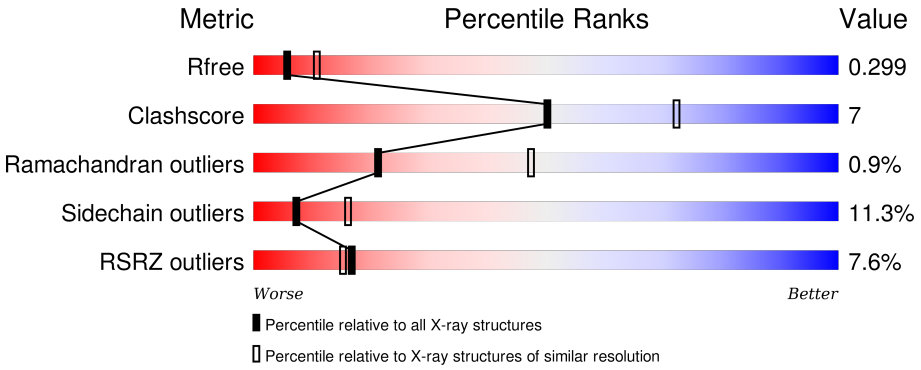
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	115	3% 60% 23% • 15%
1	B	115	7% 59% 23% • 15%
1	C	115	14% 66% 18% • 15%
1	D	115	12% 59% 24% • 15%
1	E	115	3% 63% 22% • 15%

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Mol	Chain	Length	Quality of chain
1	F	115	4% 65% 18% • 15%
1	G	115	3% 60% 22% • 15%
1	H	115	6% 67% 17% • 15%
2	I	7	57% 14% 29%
2	J	7	14% 57% 14% 29%
2	K	7	57% 14% 29%
2	L	7	14% 71% 29%
2	M	7	57% 14% 29%
2	N	7	57% 14% 29%
2	O	7	43% 29% 29%
2	P	7	71% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6545 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 SH3 and multiple ankyrin repeat domains protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			
1	B	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			
1	C	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			
1	D	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			
1	E	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			
1	F	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			
1	G	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			
1	H	98	Total	C	N	O	S	0	0	0
			762	488	134	136	4			

- Molecule 2 is a protein called Beta-PIX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	5	Total	C	N	O	0	0	0
			40	23	6	11			
2	J	5	Total	C	N	O	0	0	0
			40	23	6	11			
2	K	5	Total	C	N	O	0	0	0
			40	23	6	11			
2	L	5	Total	C	N	O	0	0	0
			40	23	6	11			
2	M	5	Total	C	N	O	0	0	0
			40	23	6	11			
2	N	5	Total	C	N	O	0	0	0
			40	23	6	11			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	O	5	Total C N O 40 23 6 11	0	0	0
2	P	5	Total C N O 40 23 6 11	0	0	0

- Molecule 3 is water.

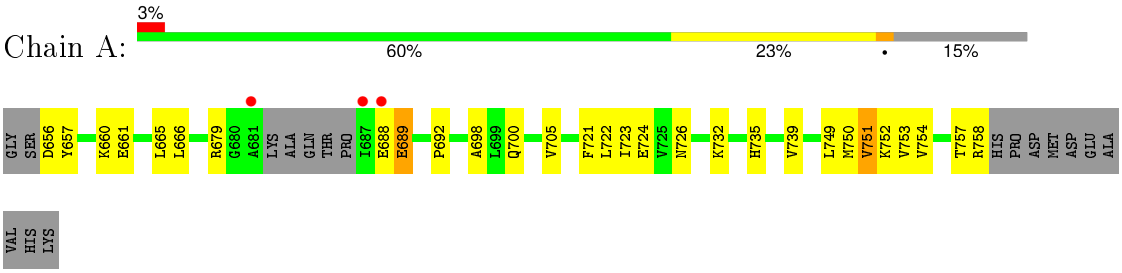
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	12	Total O 12 12	0	0
3	C	11	Total O 11 11	0	0
3	D	13	Total O 13 13	0	0
3	E	14	Total O 14 14	0	0
3	F	18	Total O 18 18	0	0
3	G	9	Total O 9 9	0	0
3	H	21	Total O 21 21	0	0
3	I	2	Total O 2 2	0	0
3	J	1	Total O 1 1	0	0
3	K	2	Total O 2 2	0	0
3	L	1	Total O 1 1	0	0
3	N	2	Total O 2 2	0	0
3	O	1	Total O 1 1	0	0
3	P	1	Total O 1 1	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.

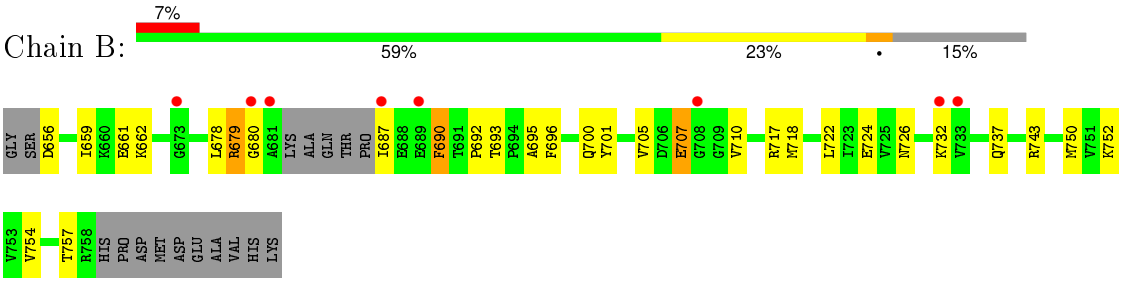
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

Chain A:



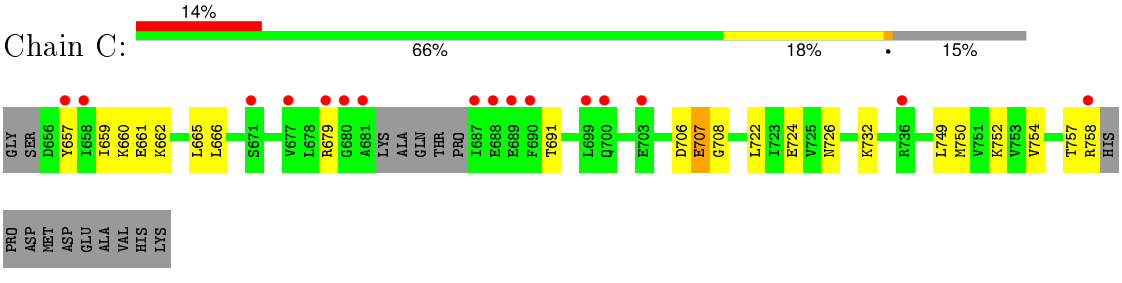
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

Chain B:



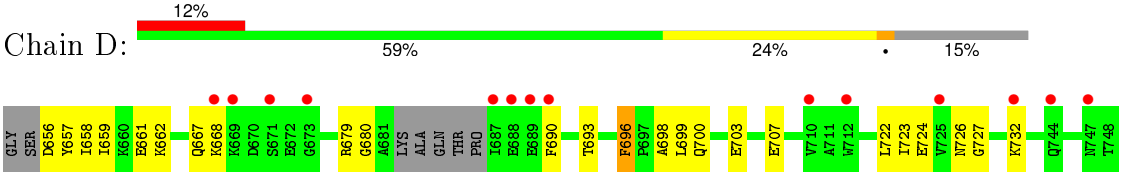
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

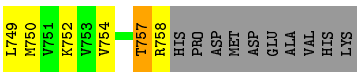
Chain C:



• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

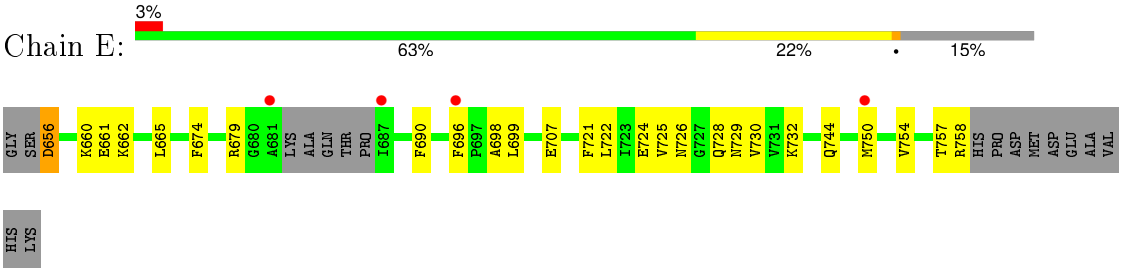
Chain D:





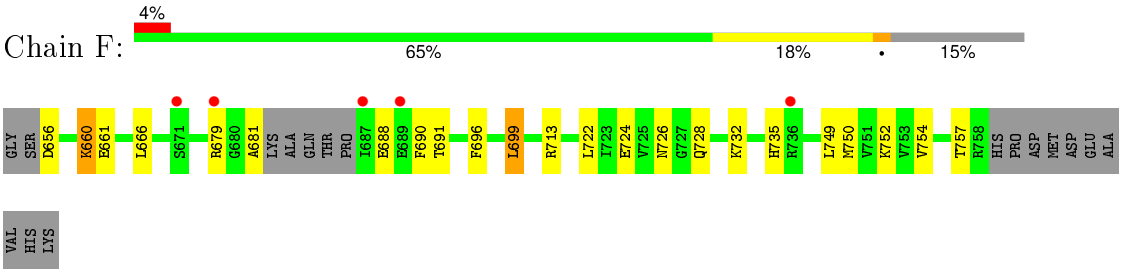
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

Chain E:



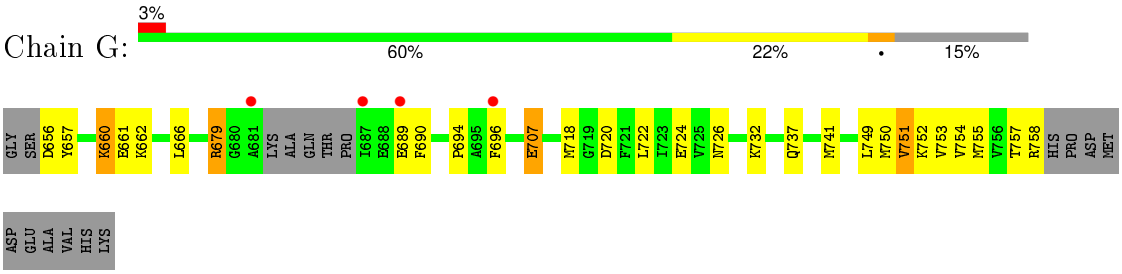
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

Chain F:



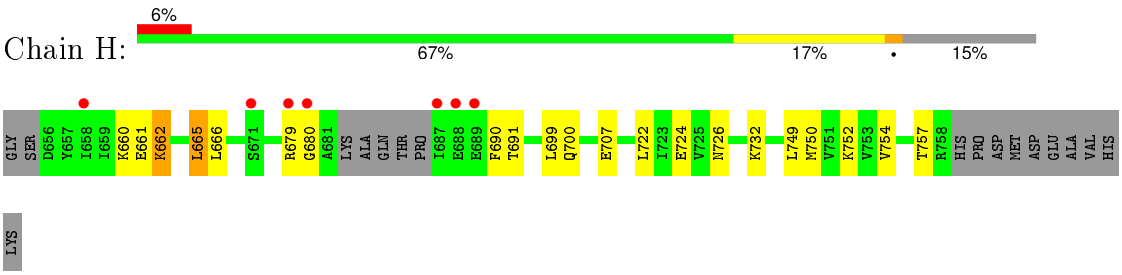
• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

Chain G:



• Molecule 1: SH3 and multiple ankyrin repeat domains protein 1

Chain H:

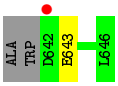


• Molecule 2: Beta-PIX

Chain I:

• Molecule 2: Beta-PIX

Chain J:



- Molecule 2: Beta-PIX

Chain K:

- Molecule 2: Beta-PIX

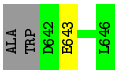
Chain L:

- Molecule 2: Beta-PIX

Chain M:

- Molecule 2: Beta-PIX

Chain N:



- Molecule 2: Beta-PIX

Chain O:

- Molecule 2: Beta-PIX

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.37Å 95.16Å 108.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.30 – 2.71 28.86 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (21.30-2.71) 93.8 (28.86-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.32 (at 2.72Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.214 , 0.272 0.232 , 0.299	Depositor DCC
R_{free} test set	1230 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	60.2	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 24372 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6545	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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	0.57	0/773	0.79	0/1040
1	B	0.51	0/773	0.77	0/1040
1	C	0.50	0/773	0.76	0/1040
1	D	0.47	0/773	0.74	1/1040 (0.1%)
1	E	0.48	0/773	0.68	0/1040
1	F	0.53	0/773	0.72	0/1040
1	G	0.51	0/773	0.79	0/1040
1	H	0.52	0/773	0.73	0/1040
2	I	0.50	0/39	0.71	0/52
2	J	0.48	0/39	0.68	0/52
2	K	0.54	0/39	0.68	0/52
2	L	0.42	0/39	0.63	0/52
2	M	0.56	0/39	0.69	0/52
2	N	0.44	0/39	0.64	0/52
2	O	0.44	0/39	0.64	0/52
2	P	0.58	0/39	0.68	0/52
All	All	0.51	0/6496	0.74	1/8736 (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	D	757	THR	C-N-CA	6.21	137.22	121.70

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	762	0	781	14	0
1	B	762	0	781	14	0
1	C	762	0	781	7	0
1	D	762	0	781	17	0
1	E	762	0	781	14	0
1	F	762	0	781	14	0
1	G	762	0	781	12	0
1	H	762	0	781	9	0
2	I	40	0	33	2	0
2	J	40	0	33	1	0
2	K	40	0	33	0	0
2	L	40	0	33	0	0
2	M	40	0	33	1	0
2	N	40	0	33	2	0
2	O	40	0	33	2	0
2	P	40	0	33	0	0
3	A	21	0	0	0	0
3	B	12	0	0	1	0
3	C	11	0	0	0	0
3	D	13	0	0	0	0
3	E	14	0	0	0	0
3	F	18	0	0	1	0
3	G	9	0	0	1	0
3	H	21	0	0	2	0
3	I	2	0	0	0	0
3	J	1	0	0	0	0
3	K	2	0	0	0	0
3	L	1	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	1	0
3	P	1	0	0	0	0
All	All	6545	0	6512	90	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 7.

All (90) 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:D:727:GLY:HA3	1:E:728:GLN:HG3	1.54	0.88
1:H:662:LYS:HD3	3:H:70:HOH:O	1.82	0.79
1:G:737:GLN:O	1:G:741:MET:HG3	1.89	0.73
1:D:727:GLY:HA3	1:E:728:GLN:CG	2.21	0.70
1:A:724:GLU:HB2	1:A:752:LYS:HB3	1.81	0.63
1:G:720:ASP:OD1	1:G:755:MET:HB3	1.99	0.61
1:G:661:GLU:HG2	1:G:754:VAL:HG12	1.83	0.61
1:E:656:ASP:O	1:E:758:ARG:HG2	2.01	0.61
1:D:667:GLN:HE21	1:E:665:LEU:HD22	1.66	0.60
1:C:661:GLU:HG2	1:C:754:VAL:HG12	1.85	0.59
1:F:679:ARG:HG3	2:N:643:GLU:HG2	1.86	0.57
1:D:726:ASN:HA	1:D:750:MET:HB3	1.87	0.56
1:H:661:GLU:HG2	1:H:754:VAL:HG12	1.88	0.56
1:H:690:PHE:HD2	1:H:732:LYS:HG2	1.72	0.55
1:B:661:GLU:HG2	1:B:754:VAL:HG12	1.89	0.55
1:E:661:GLU:HG2	1:E:754:VAL:HG12	1.88	0.55
1:D:693:THR:HG23	1:D:696:PHE:H	1.72	0.54
1:E:690:PHE:HB3	1:E:732:LYS:HE3	1.89	0.54
1:B:690:PHE:O	1:B:732:LYS:NZ	2.38	0.54
1:G:660:LYS:HG3	3:H:106:HOH:O	2.08	0.54
1:E:729:ASN:ND2	1:F:691:THR:HG21	2.23	0.53
1:A:661:GLU:HG2	1:A:754:VAL:HG12	1.90	0.53
1:A:739:VAL:HG11	2:I:644:THR:HG21	1.90	0.53
1:A:722:LEU:HD11	1:A:751:VAL:HG21	1.90	0.53
1:H:690:PHE:HB3	1:H:732:LYS:HE3	1.90	0.53
1:D:661:GLU:HG2	1:D:754:VAL:HG12	1.91	0.53
1:F:681:ALA:O	1:F:735:HIS:HB2	2.09	0.52
1:G:690:PHE:HD2	1:G:732:LYS:HG2	1.74	0.52
1:B:679:ARG:HG3	2:J:643:GLU:HG2	1.92	0.52
1:D:726:ASN:ND2	1:D:750:MET:H	2.08	0.51
1:E:724:GLU:HG2	1:E:729:ASN:HA	1.93	0.51
1:G:726:ASN:ND2	1:G:750:MET:H	2.09	0.51
1:A:698:ALA:HB2	1:A:723:ILE:HD13	1.91	0.51
1:C:657:TYR:HB2	1:D:659:ILE:HB	1.92	0.51
1:D:680:GLY:HA3	1:D:700:GLN:NE2	2.26	0.51
1:F:661:GLU:HG2	1:F:754:VAL:HG12	1.93	0.50
1:A:726:ASN:ND2	1:A:750:MET:H	2.08	0.50
1:G:724:GLU:HB2	1:G:752:LYS:HB3	1.92	0.50
1:E:656:ASP:OD1	1:F:660:LYS:HG2	2.11	0.50
1:A:660:LYS:HG2	1:B:656:ASP:OD1	2.11	0.50
1:E:726:ASN:ND2	1:E:750:MET:H	2.09	0.50
1:B:710:VAL:HG13	3:B:46:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:698:ALA:HB3	1:E:721:PHE:HB3	1.93	0.49
1:F:690:PHE:HB3	1:F:732:LYS:HE3	1.93	0.49
1:A:657:TYR:HB2	1:B:659:ILE:HB	1.94	0.49
1:A:700:GLN:NE2	1:A:735:HIS:ND1	2.61	0.48
1:B:724:GLU:HB2	1:B:752:LYS:HB3	1.95	0.48
1:G:689:GLU:HA	3:G:48:HOH:O	2.12	0.48
2:O:642:ASP:N	3:O:7:HOH:O	2.46	0.48
1:D:698:ALA:HB2	1:D:723:ILE:HD13	1.96	0.48
1:B:726:ASN:ND2	1:B:750:MET:H	2.12	0.48
1:D:757:THR:HB	1:D:758:ARG:H	1.44	0.48
1:E:690:PHE:HD2	1:E:732:LYS:HG2	1.78	0.48
1:C:726:ASN:ND2	1:C:750:MET:H	2.12	0.47
1:F:713:ARG:HG2	3:F:74:HOH:O	2.14	0.47
1:F:724:GLU:HB2	1:F:752:LYS:HB3	1.97	0.47
1:B:696:PHE:HZ	1:D:758:ARG:HG2	1.79	0.47
1:B:678:LEU:HD12	1:B:701:TYR:O	2.16	0.46
1:B:693:THR:HG22	1:B:695:ALA:H	1.80	0.46
1:G:666:LEU:HD22	1:G:749:LEU:HD23	1.97	0.46
1:F:681:ALA:HB3	1:F:699:LEU:HG	1.98	0.46
1:F:666:LEU:HD22	1:F:749:LEU:HD23	1.98	0.46
1:E:674:PHE:N	2:M:646:LEU:O	2.49	0.46
1:H:726:ASN:ND2	1:H:750:MET:H	2.13	0.45
1:C:724:GLU:HB2	1:C:752:LYS:HB3	1.96	0.45
1:A:739:VAL:CG1	2:I:644:THR:HG21	2.46	0.45
1:H:724:GLU:HB2	1:H:752:LYS:HB3	1.99	0.45
1:H:680:GLY:HA3	1:H:700:GLN:NE2	2.31	0.44
1:G:679:ARG:HG3	2:O:643:GLU:HG2	1.99	0.44
1:B:705:VAL:HG21	1:B:717:ARG:HA	2.00	0.44
1:F:750:MET:SD	1:H:665:LEU:HB2	2.58	0.44
1:H:666:LEU:HD22	1:H:749:LEU:HD23	2.00	0.43
1:A:698:ALA:HB3	1:A:721:PHE:HB3	1.99	0.43
1:F:726:ASN:ND2	1:F:750:MET:H	2.16	0.43
1:C:706:ASP:O	1:C:708:GLY:O	2.37	0.43
1:F:690:PHE:HD2	1:F:732:LYS:HG2	1.84	0.43
1:F:679:ARG:CG	2:N:643:GLU:HG2	2.47	0.43
1:A:692:PRO:HD2	1:B:692:PRO:HG2	2.00	0.43
1:D:690:PHE:HD2	1:D:732:LYS:HE3	1.83	0.42
1:D:724:GLU:HB2	1:D:752:LYS:HB3	2.00	0.42
1:A:666:LEU:HD22	1:A:749:LEU:HD23	2.01	0.42
1:E:725:VAL:HG23	1:E:730:VAL:HG21	2.01	0.42
1:G:690:PHE:HB3	1:G:732:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:ILE:HD12	1:D:758:ARG:HB3	2.02	0.42
1:B:680:GLY:HA3	1:B:700:GLN:NE2	2.35	0.42
1:A:722:LEU:HD12	1:A:753:VAL:HG12	2.02	0.41
1:C:666:LEU:HD22	1:C:749:LEU:HD23	2.01	0.41
1:C:659:ILE:HB	1:D:657:TYR:HB2	2.01	0.41
1:D:658:ILE:CD1	1:D:758:ARG:HB3	2.50	0.41
1:G:751:VAL:HG13	1:G:753:VAL:HG13	2.01	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	94/115 (82%)	89 (95%)	3 (3%)	2 (2%)	9 21
1	B	94/115 (82%)	90 (96%)	3 (3%)	1 (1%)	17 41
1	C	94/115 (82%)	91 (97%)	2 (2%)	1 (1%)	17 41
1	D	94/115 (82%)	89 (95%)	5 (5%)	0	100 100
1	E	94/115 (82%)	88 (94%)	6 (6%)	0	100 100
1	F	94/115 (82%)	89 (95%)	4 (4%)	1 (1%)	17 41
1	G	94/115 (82%)	89 (95%)	3 (3%)	2 (2%)	9 21
1	H	94/115 (82%)	89 (95%)	5 (5%)	0	100 100
2	I	3/7 (43%)	3 (100%)	0	0	100 100
2	J	3/7 (43%)	3 (100%)	0	0	100 100
2	K	3/7 (43%)	3 (100%)	0	0	100 100
2	L	3/7 (43%)	3 (100%)	0	0	100 100
2	M	3/7 (43%)	3 (100%)	0	0	100 100
2	N	3/7 (43%)	3 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	O	3/7 (43%)	3 (100%)	0	0	100 100
2	P	3/7 (43%)	3 (100%)	0	0	100 100
All	All	776/976 (80%)	738 (95%)	31 (4%)	7 (1%)	21 47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	688	GLU
1	A	688	GLU
1	B	707	GLU
1	G	694	PRO
1	A	689	GLU
1	G	707	GLU
1	C	707	GLU

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	81/96 (84%)	72 (89%)	9 (11%)	8 17
1	B	81/96 (84%)	71 (88%)	10 (12%)	6 13
1	C	81/96 (84%)	71 (88%)	10 (12%)	6 13
1	D	81/96 (84%)	71 (88%)	10 (12%)	6 13
1	E	81/96 (84%)	71 (88%)	10 (12%)	6 13
1	F	81/96 (84%)	74 (91%)	7 (9%)	13 28
1	G	81/96 (84%)	69 (85%)	12 (15%)	4 9
1	H	81/96 (84%)	72 (89%)	9 (11%)	8 17
2	I	5/6 (83%)	5 (100%)	0	100 100
2	J	5/6 (83%)	5 (100%)	0	100 100
2	K	5/6 (83%)	4 (80%)	1 (20%)	1 4
2	L	5/6 (83%)	5 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	5/6 (83%)	5 (100%)	0	100 100
2	N	5/6 (83%)	5 (100%)	0	100 100
2	O	5/6 (83%)	5 (100%)	0	100 100
2	P	5/6 (83%)	5 (100%)	0	100 100
All	All	688/816 (84%)	610 (89%)	78 (11%)	7 16

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	656	ASP
1	A	665	LEU
1	A	679	ARG
1	A	689	GLU
1	A	705	VAL
1	A	732	LYS
1	A	751	VAL
1	A	757	THR
1	A	758	ARG
1	B	662	LYS
1	B	679	ARG
1	B	687	ILE
1	B	690	PHE
1	B	707	GLU
1	B	718	MET
1	B	722	LEU
1	B	737	GLN
1	B	743	ARG
1	B	757	THR
1	C	660	LYS
1	C	662	LYS
1	C	665	LEU
1	C	679	ARG
1	C	691	THR
1	C	707	GLU
1	C	722	LEU
1	C	732	LYS
1	C	757	THR
1	C	758	ARG
1	D	656	ASP
1	D	662	LYS
1	D	668	LYS

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Mol	Chain	Res	Type
1	D	679	ARG
1	D	696	PHE
1	D	699	LEU
1	D	703	GLU
1	D	707	GLU
1	D	722	LEU
1	D	749	LEU
1	E	656	ASP
1	E	660	LYS
1	E	662	LYS
1	E	679	ARG
1	E	696	PHE
1	E	699	LEU
1	E	707	GLU
1	E	722	LEU
1	E	744	GLN
1	E	757	THR
1	F	656	ASP
1	F	660	LYS
1	F	696	PHE
1	F	699	LEU
1	F	722	LEU
1	F	728	GLN
1	F	757	THR
1	G	656	ASP
1	G	657	TYR
1	G	660	LYS
1	G	662	LYS
1	G	679	ARG
1	G	696	PHE
1	G	707	GLU
1	G	718	MET
1	G	722	LEU
1	G	751	VAL
1	G	757	THR
1	G	758	ARG
1	H	660	LYS
1	H	662	LYS
1	H	665	LEU
1	H	679	ARG
1	H	691	THR
1	H	699	LEU

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Mol	Chain	Res	Type
1	H	707	GLU
1	H	722	LEU
1	H	757	THR
2	K	642	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	700	GLN
1	A	726	ASN
1	B	700	GLN
1	B	726	ASN
1	C	700	GLN
1	C	726	ASN
1	D	667	GLN
1	D	700	GLN
1	D	726	ASN
1	E	700	GLN
1	E	726	ASN
1	E	729	ASN
1	F	700	GLN
1	F	726	ASN
1	G	700	GLN
1	G	726	ASN
1	H	700	GLN
1	H	726	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	98/115 (85%)	0.08	3 (3%) 52 53	36, 53, 85, 123	0
1	B	98/115 (85%)	0.30	8 (8%) 14 12	45, 67, 94, 108	0
1	C	98/115 (85%)	0.80	16 (16%) 2 2	43, 70, 110, 120	0
1	D	98/115 (85%)	0.96	14 (14%) 4 3	57, 83, 120, 138	0
1	E	98/115 (85%)	0.35	4 (4%) 41 41	47, 77, 108, 124	0
1	F	98/115 (85%)	0.14	5 (5%) 32 31	41, 57, 94, 110	0
1	G	98/115 (85%)	0.20	4 (4%) 41 41	38, 62, 91, 115	0
1	H	98/115 (85%)	0.25	7 (7%) 19 17	41, 60, 86, 102	0
2	I	5/7 (71%)	0.13	0 100 100	47, 69, 78, 89	0
2	J	5/7 (71%)	0.74	1 (20%) 1 1	72, 75, 86, 94	0
2	K	5/7 (71%)	1.12	0 100 100	68, 79, 89, 90	0
2	L	5/7 (71%)	1.36	1 (20%) 1 1	77, 82, 93, 94	0
2	M	5/7 (71%)	0.20	0 100 100	57, 59, 70, 77	0
2	N	5/7 (71%)	-0.61	0 100 100	53, 61, 63, 64	0
2	O	5/7 (71%)	0.14	0 100 100	56, 64, 81, 82	0
2	P	5/7 (71%)	-0.07	0 100 100	59, 63, 74, 75	0
All	All	824/976 (84%)	0.38	63 (7%) 17 15	36, 66, 104, 138	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	681	ALA	10.4
1	D	690	PHE	9.8
1	H	687	ILE	7.6
1	A	687	ILE	7.5
1	C	681	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
1	D	687	ILE	7.4
1	C	687	ILE	6.9
1	D	689	GLU	6.8
1	F	687	ILE	6.5
1	C	688	GLU	6.4
1	B	681	ALA	5.9
1	E	687	ILE	5.3
1	C	690	PHE	5.2
1	C	689	GLU	5.1
1	D	671	SER	4.9
1	C	680	GLY	4.8
1	G	687	ILE	4.7
1	C	699	LEU	4.3
1	A	688	GLU	4.3
1	E	681	ALA	4.2
1	C	679	ARG	3.9
1	D	673	GLY	3.8
1	D	668	LYS	3.6
2	L	642	ASP	3.4
1	C	658	ILE	3.4
1	H	689	GLU	3.3
1	H	688	GLU	3.2
1	D	747	ASN	3.2
1	E	696	PHE	3.2
1	F	671	SER	3.1
1	B	732	LYS	3.1
1	C	700	GLN	3.1
1	G	689	GLU	2.9
1	D	712	TRP	2.9
1	G	696	PHE	2.9
1	D	669	LYS	2.7
1	B	733	VAL	2.7
1	C	657	TYR	2.7
1	D	732	LYS	2.7
1	G	681	ALA	2.6
1	C	758	ARG	2.5
1	H	680	GLY	2.5
1	E	750	MET	2.5
1	F	689	GLU	2.5
1	C	671	SER	2.5
1	H	658	ILE	2.5
1	F	736	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	710	VAL	2.4
1	D	688	GLU	2.4
1	C	736	ARG	2.4
1	C	677	VAL	2.3
1	B	680	GLY	2.2
1	D	725	VAL	2.2
2	J	642	ASP	2.2
1	B	689	GLU	2.2
1	B	708	GLY	2.1
1	F	679	ARG	2.1
1	H	671	SER	2.1
1	B	673	GLY	2.1
1	B	687	ILE	2.1
1	D	744	GLN	2.0
1	H	679	ARG	2.0
1	C	703	GLU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.