Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:29 PM GMT

PDB ID	:	1KJ3
Title	:	Mhc Class I H-2Kb molecule complexed with pKB1 peptide
Authors	:	Reiser, J.-B.; Gregoire, C.; Darnault, C.; Mosser, T.; Guimezanes, A.; Schmitt-Verhulst, A.-M.; Fontecilla-Camps, J.C.; Mazza, G.; Malissen, B.; Housset, D.
Deposited on	:	2001-12-04
Resolution	:	2.30 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:

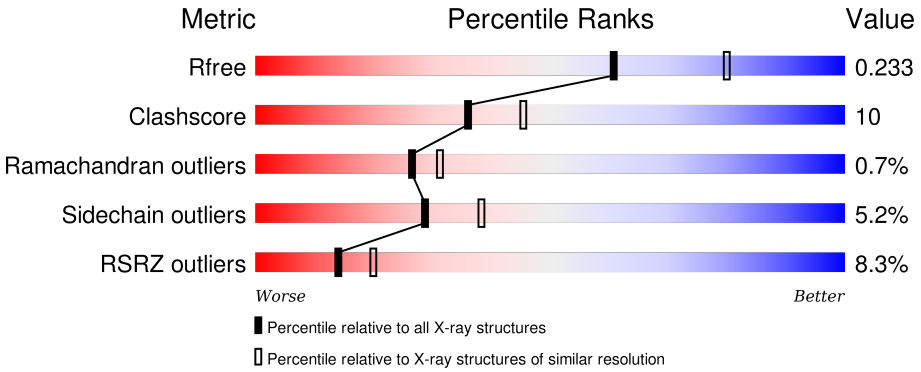
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	H	279	9% 79% 16%
1	I	279	11% 77% 21%
2	P	8	88% 13%
2	Q	8	63% 38%
3	L	99	3% 84% 14%

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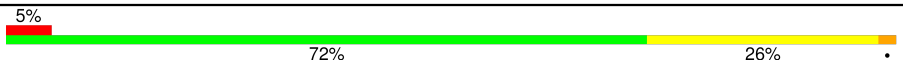
Mol	Chain	Length	Quality of chain
3	M	99	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6694 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 H-2KB MHC CLASS I MOLECULE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	279	Total	C	N	O	S	7	1	0
			2276	1437	401	428	10			
1	I	278	Total	C	N	O	S	0	1	0
			2266	1431	397	429	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	ALA	CLONING ARTIFACT	UNP P01901
I	0	MET	ALA	CLONING ARTIFACT	UNP P01901

- Molecule 2 is a protein called NATURALLY PROCESSED OCTAPEPTIDE PKB1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	0	0	0
			67	46	9	12			
2	Q	8	Total	C	N	O	0	0	0
			67	46	9	12			

- Molecule 3 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
3	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	127	Total	O	0	0
			127	127		

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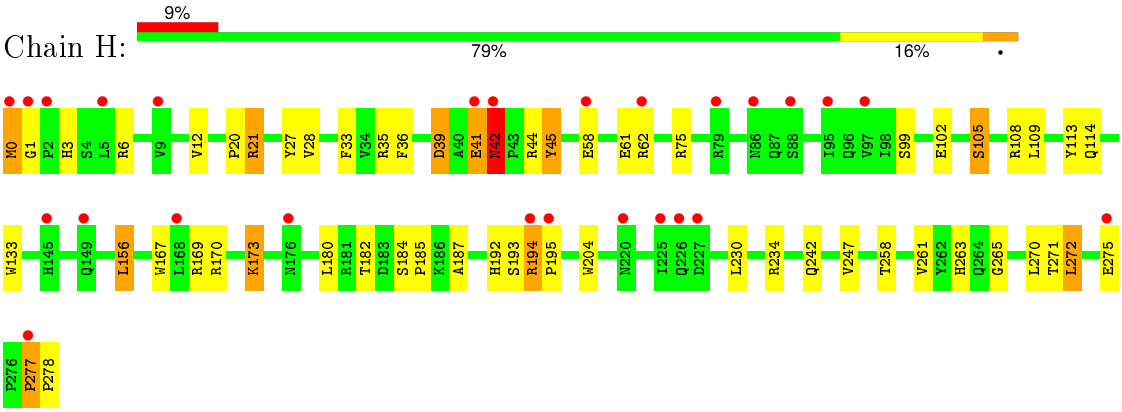
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	121	Total O 121 121	0	0
4	L	62	Total O 62 62	0	0
4	M	53	Total O 53 53	0	0
4	P	7	Total O 7 7	0	0
4	Q	6	Total O 6 6	0	0

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.

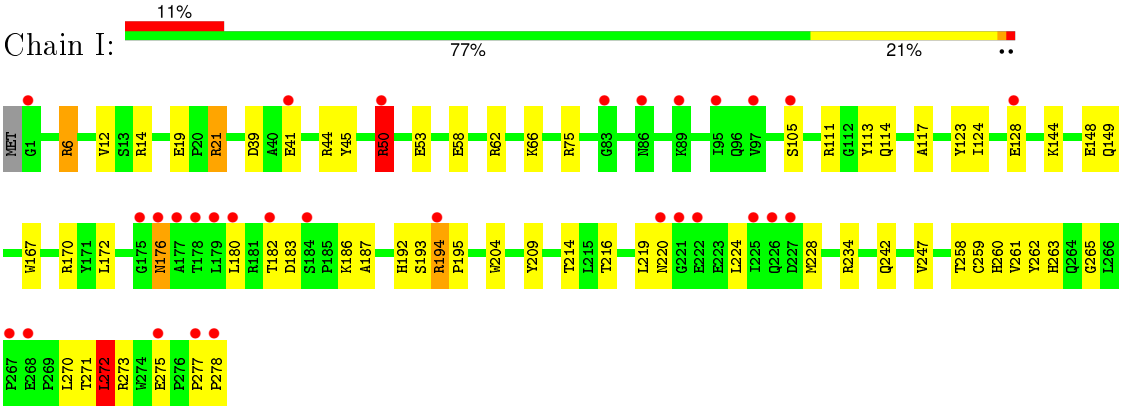
• Molecule 1: H-2KB MHC CLASS I MOLECULE ALPHA CHAIN

Chain H:



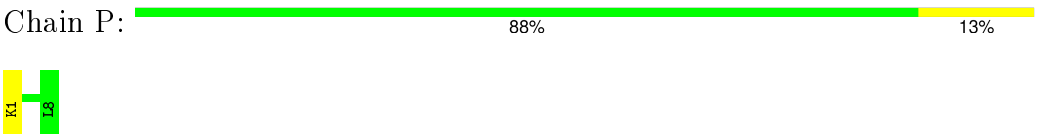
• Molecule 1: H-2KB MHC CLASS I MOLECULE ALPHA CHAIN

Chain I:



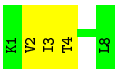
• Molecule 2: NATURALLY PROCESSED OCTAPEPTIDE PKB1

Chain P:



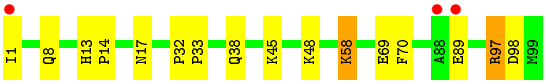
• Molecule 2: NATURALLY PROCESSED OCTAPEPTIDE PKB1

Chain Q:



• Molecule 3: BETA-2 MICROGLOBULIN

Chain L:



• Molecule 3: BETA-2 MICROGLOBULIN

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.24Å 90.63Å 89.58Å 90.00° 111.51° 90.00°	Depositor
Resolution (Å)	12.00 – 2.30 22.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.30) 98.5 (22.48-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.74 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.259 0.204 , 0.233	Depositor DCC
R_{free} test set	4328 reflections (11.21%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.2	EDS
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 43628 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6694	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.95 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.6191e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	H	0.49	0/2344	1.06	7/3185 (0.2%)
1	I	0.48	0/2334	1.06	4/3173 (0.1%)
2	P	0.51	0/67	0.82	0/88
2	Q	0.47	0/67	0.83	0/88
3	L	0.50	0/847	1.04	1/1148 (0.1%)
3	M	0.49	0/847	0.99	1/1148 (0.1%)
All	All	0.49	0/6506	1.04	13/8830 (0.1%)

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	H	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	35	ARG	NE-CZ-NH1	8.69	124.65	120.30
3	L	97	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	I	272	LEU	CA-CB-CG	6.73	130.79	115.30
1	H	35	ARG	CD-NE-CZ	6.58	132.81	123.60
1	I	6	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	H	0	MET	CA-CB-CG	-5.94	103.20	113.30
1	H	277	PRO	C-N-CD	5.35	139.64	128.40
3	M	81	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	H	278	PRO	N-CA-CB	5.28	109.63	103.30
1	I	50	ARG	CD-NE-CZ	5.22	130.91	123.60
1	H	272	LEU	CA-CB-CG	5.16	127.17	115.30
1	H	194	ARG	N-CA-C	-5.15	97.09	111.00
1	I	219	LEU	N-CA-CB	5.07	120.55	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	277	PRO	Mainchain
1	H	42	ASN	Mainchain

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	H	2276	0	2168	49	0
1	I	2266	0	2152	43	0
2	P	67	0	77	1	0
2	Q	67	0	77	2	0
3	L	821	0	796	20	0
3	M	821	0	796	20	0
4	H	127	0	0	3	0
4	I	121	0	0	8	0
4	L	62	0	0	0	0
4	M	53	0	0	0	0
4	P	7	0	0	0	0
4	Q	6	0	0	0	0
All	All	6694	0	6066	119	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 10.

All (119) 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:H:0:MET:CE	1:H:180:LEU:HD21	1.44	1.43
1:H:0:MET:SD	1:H:0:MET:N	2.11	1.18
1:H:6[A]:ARG:HH22	3:L:58:LYS:CE	1.57	1.17
1:H:6[A]:ARG:NH2	3:L:58:LYS:HE2	1.62	1.14
1:H:0:MET:HE2	1:H:180:LEU:HD21	1.26	1.08
1:H:0:MET:HE1	1:H:180:LEU:HD21	1.35	1.04
1:H:0:MET:CE	1:H:180:LEU:CD2	2.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6[A]:ARG:HH22	3:L:58:LYS:HE2	0.78	0.94
1:H:234:ARG:HH11	3:L:8:GLN:NE2	1.78	0.82
1:I:234:ARG:HE	1:I:242:GLN:HE21	1.25	0.81
1:I:6:ARG:HD3	4:I:305:HOH:O	1.86	0.76
1:H:6[A]:ARG:NH2	3:L:58:LYS:CE	2.35	0.75
3:L:17:ASN:OD1	3:L:97:ARG:NH2	2.20	0.74
1:H:1:GLY:HA2	1:H:105:SER:OG	1.88	0.73
1:I:234:ARG:HE	1:I:242:GLN:NE2	1.85	0.72
1:H:0:MET:SD	1:H:180:LEU:HD21	2.28	0.72
1:H:0:MET:HE2	1:H:180:LEU:CD2	2.12	0.72
1:H:0:MET:HE1	1:H:180:LEU:CD2	2.14	0.72
1:H:234:ARG:HE	1:H:242:GLN:HE21	1.36	0.72
1:H:263:HIS:HD2	1:H:265:GLY:H	1.39	0.71
1:H:263:HIS:CD2	1:H:265:GLY:H	2.10	0.69
3:M:17:ASN:OD1	3:M:97:ARG:NH2	2.27	0.67
1:H:169:ARG:O	1:H:173:LYS:HD2	1.94	0.67
1:I:193:SER:HB2	4:I:325:HOH:O	1.95	0.66
1:H:193:SER:HB2	4:H:394:HOH:O	1.95	0.66
1:H:6[B]:ARG:NH2	4:H:303:HOH:O	2.31	0.63
1:H:0:MET:HA	1:H:3:HIS:NE2	2.13	0.63
1:H:167:TRP:CZ3	1:H:170:ARG:HD3	2.34	0.62
1:I:21:ARG:HE	1:I:39:ASP:HB2	1.64	0.62
1:I:6:ARG:HH21	3:M:58:LYS:NZ	2.00	0.58
3:M:40:LEU:HD23	3:M:45:LYS:HA	1.85	0.58
1:I:216:THR:OG1	1:I:260:HIS:HB2	2.05	0.56
1:I:123:TYR:HD2	1:I:124:ILE:HG22	1.71	0.56
3:L:32:PRO:CB	3:L:33:PRO:HD2	2.37	0.55
1:H:234:ARG:HE	1:H:242:GLN:NE2	2.03	0.55
3:L:38:GLN:HE22	3:L:45:LYS:CE	2.20	0.54
1:H:234:ARG:HH11	3:L:8:GLN:HE22	1.56	0.53
1:H:6[B]:ARG:HG2	1:H:27:TYR:HB2	1.90	0.53
3:L:13:HIS:HB3	3:L:14:PRO:HD2	1.90	0.53
1:H:20:PRO:HB2	1:H:75:ARG:NH1	2.24	0.53
1:I:14:ARG:NH1	1:I:21:ARG:HG2	2.24	0.52
3:L:48:LYS:HZ2	3:L:69:GLU:H	1.57	0.52
1:I:111:ARG:HD3	1:I:113:TYR:CZ	2.44	0.52
1:I:66:LYS:HD2	2:Q:2:VAL:HG13	1.91	0.52
3:L:32:PRO:HB2	3:L:33:PRO:HD2	1.91	0.51
1:I:117:ALA:HB2	3:M:60:TRP:CE2	2.46	0.51
3:M:22:ILE:CD1	3:M:69:GLU:HG2	2.41	0.51
3:M:13:HIS:HB3	3:M:14:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:GLN:HG2	4:I:330:HOH:O	2.09	0.51
3:L:38:GLN:HE22	3:L:45:LYS:HE2	1.76	0.50
3:M:32:PRO:HB2	3:M:33:PRO:HD2	1.93	0.50
3:L:48:LYS:NZ	3:L:69:GLU:H	2.09	0.50
1:I:263:HIS:CD2	1:I:265:GLY:H	2.29	0.50
1:I:224:LEU:O	1:I:228:MET:HB2	2.11	0.50
1:H:44:ARG:HH12	1:H:61:GLU:CD	2.14	0.50
1:I:6:ARG:NH2	3:M:58:LYS:NZ	2.60	0.50
1:I:19:GLU:HB3	1:I:75:ARG:HH21	1.76	0.50
1:I:19:GLU:HB3	1:I:75:ARG:NH2	2.27	0.50
1:I:187:ALA:HA	1:I:204:TRP:O	2.12	0.50
1:H:41:GLU:CG	1:H:42:ASN:H	2.22	0.50
1:I:192:HIS:CE1	3:M:98:ASP:HB3	2.47	0.49
1:H:258:THR:CG2	1:H:271:THR:HG23	2.41	0.49
1:H:6[A]:ARG:NH2	3:L:58:LYS:NZ	2.60	0.48
1:H:75:ARG:NE	4:H:318:HOH:O	2.44	0.48
1:H:21:ARG:HE	1:H:39:ASP:HB2	1.78	0.48
1:H:0:MET:CA	1:H:3:HIS:NE2	2.77	0.48
1:I:172:LEU:O	1:I:176:ASN:HB3	2.13	0.48
1:I:258:THR:CG2	1:I:271:THR:HG23	2.43	0.48
1:I:261:VAL:HB	1:I:270:LEU:HB2	1.96	0.47
1:H:187:ALA:HA	1:H:204:TRP:O	2.14	0.47
1:I:193:SER:HA	4:I:322:HOH:O	2.15	0.46
3:M:32:PRO:CB	3:M:33:PRO:HD2	2.46	0.46
1:H:0:MET:SD	1:H:180:LEU:CD2	3.00	0.46
3:M:36:GLU:HB3	3:M:83:LYS:HG3	1.98	0.46
1:H:36:PHE:HB2	1:H:45:TYR:CD1	2.51	0.46
1:I:214:THR:HB	1:I:262:TYR:HB2	1.98	0.45
1:I:111:ARG:HD3	1:I:113:TYR:OH	2.16	0.45
1:I:234:ARG:HH11	3:M:8:GLN:NE2	2.14	0.45
1:H:102:GLU:O	1:H:109:LEU:HD12	2.16	0.45
1:I:58[B]:GLU:HB2	4:I:334:HOH:O	2.17	0.44
1:I:128:GLU:HG2	4:I:373:HOH:O	2.18	0.44
3:M:51:MET:HB3	3:M:51:MET:HE2	1.83	0.43
1:I:259:CYS:HB3	1:I:272:LEU:HD13	2.00	0.43
1:I:277:PRO:O	1:I:278:PRO:C	2.56	0.43
1:H:261:VAL:HB	1:H:270:LEU:HB2	2.00	0.43
1:I:167:TRP:CZ3	1:I:170:ARG:HD3	2.54	0.43
1:I:144:LYS:NZ	1:I:148:GLU:OE2	2.52	0.43
1:I:50:ARG:HA	1:I:53:GLU:OE2	2.18	0.43
3:L:48:LYS:NZ	3:L:69:GLU:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:VAL:HG23	1:H:33:PHE:CD1	2.55	0.42
3:M:2:GLN:HG2	3:M:32:PRO:HD3	2.01	0.42
1:I:258:THR:HG21	1:I:271:THR:HG23	2.01	0.42
1:I:14:ARG:HH12	1:I:21:ARG:HG2	1.83	0.42
3:M:24:ASN:HB3	3:M:65:LEU:HD11	2.02	0.42
1:H:275:GLU:HG2	1:H:275:GLU:H	1.49	0.42
1:I:44:ARG:NH2	4:I:317:HOH:O	2.53	0.41
1:I:41:GLU:H	1:I:41:GLU:CD	2.23	0.41
3:L:38:GLN:NE2	3:L:45:LYS:HD3	2.35	0.41
2:Q:3:ILE:HG12	2:Q:4:THR:H	1.86	0.41
1:I:194:ARG:HD2	1:I:194:ARG:HA	1.57	0.41
1:H:234:ARG:NH1	3:L:8:GLN:NE2	2.58	0.41
3:M:31:HIS:ND1	3:M:32:PRO:HA	2.36	0.41
1:H:192:HIS:CE1	3:L:98:ASP:HB3	2.56	0.41
3:M:6:GLN:HG2	3:M:29:GLN:HB2	2.02	0.41
3:M:38:GLN:HE21	3:M:45:LYS:HG3	1.85	0.41
3:M:37:ILE:HD12	3:M:51:MET:HE1	2.02	0.41
1:H:1:GLY:HA2	1:H:105:SER:HG	1.82	0.41
1:H:167:TRP:CE2	2:P:1:LYS:HD2	2.55	0.41
3:M:13:HIS:HB3	3:M:14:PRO:CD	2.50	0.41
1:H:184:SER:HB2	1:H:185:PRO:HD2	2.03	0.41
1:H:133:TRP:HH2	1:H:156:LEU:HD13	1.86	0.41
1:H:0:MET:HE2	1:H:180:LEU:HD11	2.03	0.40
1:H:58:GLU:O	1:H:62:ARG:HG2	2.21	0.40
1:I:180:LEU:HD23	1:I:180:LEU:HA	1.94	0.40
1:I:75:ARG:HG2	4:I:368:HOH:O	2.21	0.40
1:H:99:SER:HA	1:H:113:TYR:O	2.21	0.40
3:L:1:ILE:HA	3:L:1:ILE:HD13	1.95	0.40
1:I:183:ASP:HB2	1:I:209:TYR:HB3	2.03	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	H	278/279 (100%)	265 (95%)	11 (4%)	2 (1%)	26 31
1	I	277/279 (99%)	267 (96%)	7 (2%)	3 (1%)	17 18
2	P	6/8 (75%)	5 (83%)	1 (17%)	0	100 100
2	Q	6/8 (75%)	4 (67%)	2 (33%)	0	100 100
3	L	97/99 (98%)	94 (97%)	3 (3%)	0	100 100
3	M	97/99 (98%)	94 (97%)	3 (3%)	0	100 100
All	All	761/772 (99%)	729 (96%)	27 (4%)	5 (1%)	26 31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	41	GLU
1	H	195	PRO
1	I	195	PRO
1	I	220	ASN
1	I	176	ASN

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	H	238/237 (100%)	223 (94%)	15 (6%)	22 29
1	I	237/237 (100%)	224 (94%)	13 (6%)	27 36
2	P	8/8 (100%)	8 (100%)	0	100 100
2	Q	8/8 (100%)	8 (100%)	0	100 100
3	L	94/94 (100%)	91 (97%)	3 (3%)	46 62
3	M	94/94 (100%)	90 (96%)	4 (4%)	35 47
All	All	679/678 (100%)	644 (95%)	35 (5%)	29 38

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	VAL
1	H	21	ARG
1	H	39	ASP
1	H	42	ASN
1	H	45	TYR
1	H	105	SER
1	H	108	ARG
1	H	114	GLN
1	H	156	LEU
1	H	173	LYS
1	H	182	THR
1	H	194	ARG
1	H	230	LEU
1	H	247	VAL
1	H	272	LEU
3	L	58	LYS
3	L	70	PHE
3	L	89	GLU
1	I	12	VAL
1	I	21	ARG
1	I	45	TYR
1	I	50	ARG
1	I	105	SER
1	I	114	GLN
1	I	182	THR
1	I	186	LYS
1	I	194	ARG
1	I	247	VAL
1	I	272	LEU
1	I	273	ARG
1	I	275	GLU
3	M	48	LYS
3	M	58	LYS
3	M	89	GLU
3	M	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	114	GLN
1	H	127	ASN
1	H	242	GLN
1	H	263	HIS

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Mol	Chain	Res	Type
3	L	8	GLN
3	L	38	GLN
1	I	54	GLN
1	I	114	GLN
1	I	127	ASN
1	I	174	ASN
1	I	226	GLN
1	I	242	GLN
1	I	260	HIS
1	I	263	HIS
3	M	8	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	H	278/279 (99%)	0.56	26 (9%) 11 16	23, 38, 62, 81	15 (5%)
1	I	278/279 (99%)	0.60	30 (10%) 8 11	22, 38, 68, 87	11 (3%)
2	P	8/8 (100%)	0.28	0 100 100	30, 34, 38, 41	0
2	Q	8/8 (100%)	0.24	0 100 100	30, 33, 41, 44	0
3	L	99/99 (100%)	0.27	3 (3%) 54 63	25, 35, 50, 63	9 (9%)
3	M	99/99 (100%)	0.35	5 (5%) 32 41	26, 38, 54, 73	4 (4%)
All	All	770/772 (99%)	0.50	64 (8%) 14 20	22, 38, 62, 87	39 (5%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ILE	8.2
1	H	0	MET	7.3
1	H	277	PRO	6.9
1	H	1	GLY	6.8
1	H	176	ASN	5.3
1	I	278	PRO	5.2
1	I	176	ASN	5.2
1	I	194	ARG	5.1
1	H	194	ARG	4.8
1	H	2	PRO	4.7
1	H	225	ILE	4.7
1	I	225	ILE	4.5
1	I	180	LEU	4.5
1	I	177	ALA	4.4
1	H	226	GLN	4.3
1	I	222	GLU	4.3
1	I	220	ASN	3.8
1	I	268	GLU	3.7
3	M	89	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	178	THR	3.5
1	H	145	HIS	3.4
1	I	227	ASP	3.3
1	I	50	ARG	3.3
1	I	179	LEU	3.3
1	I	226	GLN	3.2
1	H	62	ARG	3.2
3	L	1	ILE	3.2
1	H	58	GLU	3.1
1	I	41	GLU	3.1
1	I	277	PRO	3.1
1	H	41	GLU	2.9
3	L	88	ALA	2.8
1	I	86	ASN	2.8
1	H	227	ASP	2.8
1	H	95	ILE	2.8
1	H	42	ASN	2.7
1	I	267	PRO	2.7
1	I	97	VAL	2.7
1	I	221	GLY	2.7
1	I	89	LYS	2.6
1	I	175	GLY	2.6
1	I	182	THR	2.6
3	M	48	LYS	2.5
3	L	89	GLU	2.5
1	H	275	GLU	2.5
1	I	95	ILE	2.5
1	I	83	GLY	2.4
3	M	18	GLY	2.4
1	H	220	ASN	2.4
1	I	105	SER	2.3
1	H	88	SER	2.3
1	H	168	LEU	2.2
1	I	1	GLY	2.2
1	H	149	GLN	2.1
1	H	195	PRO	2.1
1	H	86	ASN	2.1
1	H	9	VAL	2.1
3	M	19	LYS	2.1
1	I	275	GLU	2.1
1	I	184	SER	2.1
1	I	128	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	97	VAL	2.1
1	H	5	LEU	2.0
1	H	79	ARG	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.