Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:18 AM GMT

PDB ID	:	2CLV
Title	:	MHC CLASS I NATURAL MUTANT H-2KBM8 HEAVY CHAIN COMPLEXED WITH BETA-2 MICROGLOBULIN AND PBM8 PEPTIDE
Authors	:	Mazza, C.; Auphan-Anezin, N.; Guimezanes, A.; Barrett-Wilt, G.A.; Montero-Julian, F.; Roussel, A.; Hunt, D.F.; Schmitt-Verhulst, A.M.; Malissen, B.
Deposited on	:	2006-05-02
Resolution	:	1.90 Å(reported)

The following versions of software and data (see references (i)) 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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
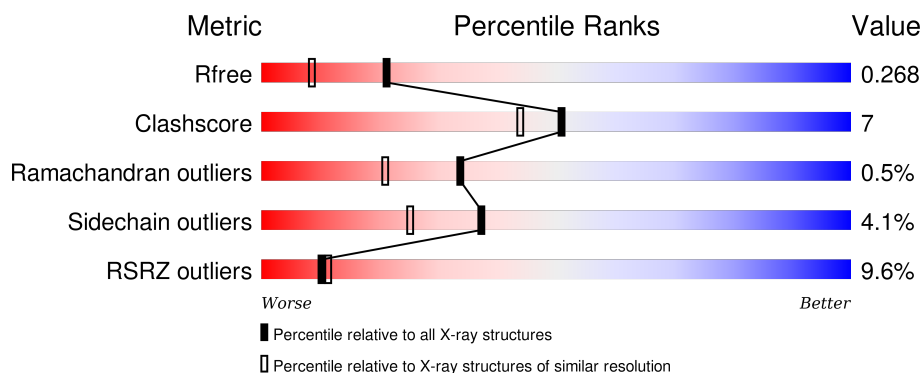
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	279	10% / 84% / 14% / ••
1	H	279	13% / 85% / 14% / •
2	B	99	6% / 92% / 8%
2	P	99	6% / 84% / 16%
3	C	8	63% / 25% / 13%

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Mol	Chain	Length	Quality of chain
3	M	8	

75% 13% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6950 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-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, K-B ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total 2258	C 1427	N 399	O 424	S 8	0	0	1
1	H	279	Total 2258	C 1427	N 399	O 424	S 8	0	0	1

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	PHE	TYR	ENGINEERED MUTATION	UNP P01901
A	23	ILE	MET	ENGINEERED MUTATION	UNP P01901
A	24	SER	GLU	ENGINEERED MUTATION	UNP P01901
A	30	ASN	ASP	ENGINEERED MUTATION	UNP P01901
H	22	PHE	TYR	ENGINEERED MUTATION	UNP P01901
H	23	ILE	MET	ENGINEERED MUTATION	UNP P01901
H	24	SER	GLU	ENGINEERED MUTATION	UNP P01901
H	30	ASN	ASP	ENGINEERED MUTATION	UNP P01901

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total 821	C 524	N 138	O 152	S 7	0	0	0
2	P	99	Total 821	C 524	N 138	O 152	S 7	0	0	0

- Molecule 3 is a protein called RBM5 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total 74	C 48	N 10	O 16	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	M	8	74	48	10	16	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total 230	O 230	0	0
4	B	108	Total 108	O 108	0	0
4	C	9	Total 9	O 9	0	0
4	H	185	Total 185	O 185	0	0
4	M	7	Total 7	O 7	0	0
4	P	105	Total 105	O 105	0	0

3 Residue-property plots ⓘ

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-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, K-B ALPHA CHAIN
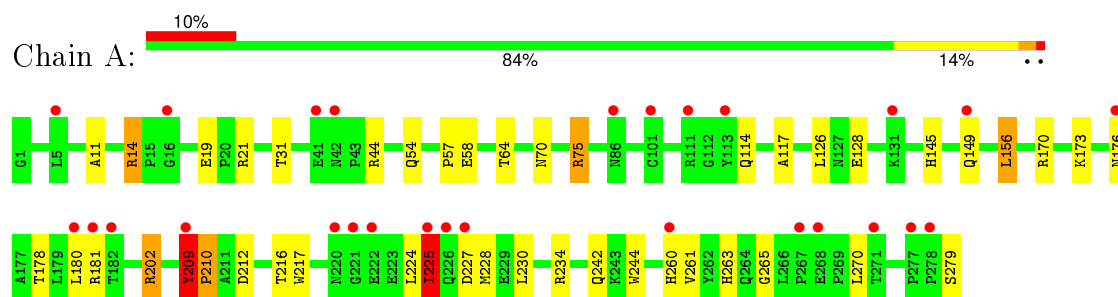
- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, K-B ALPHA CHAIN
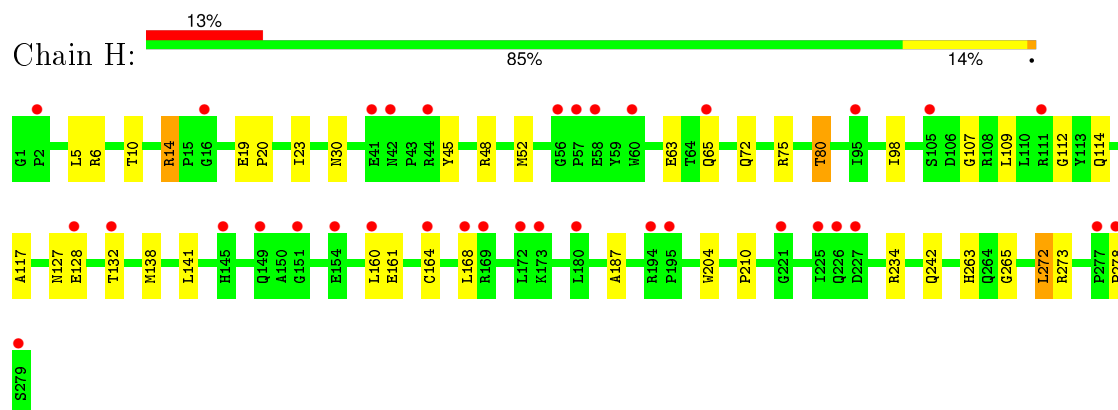
- Molecule 2: BETA-2 MICROGLOBULIN

- Molecule 2: BETA-2 MICROGLOBULIN

• Molecule 3: RBM5 PROTEIN

Chain C:

63%   25%   13%

S1 Y5 N6 S7 L8

• Molecule 3: RBM5 PROTEIN

Chain M:

75%   13%   13%

S1 N6 S7 L8

4 Data and refinement statistics (i)

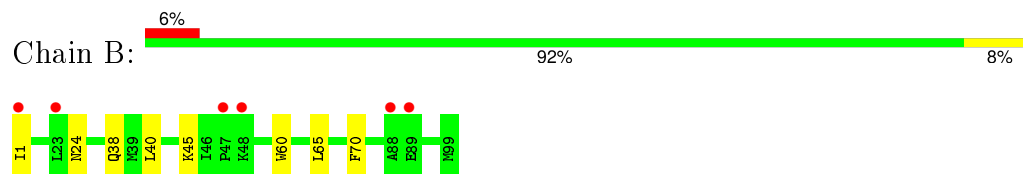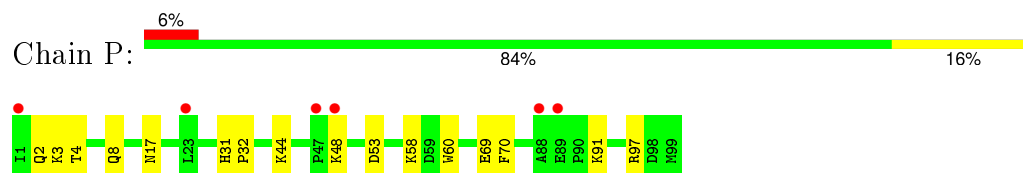| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.15Å 90.46Å 89.03Å 90.00° 111.02° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 19.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.90) 99.9 (19.96-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.73 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.251 0.226 , 0.268	Depositor DCC
R_{free} test set	3930 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.9	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	1 of 78203 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6950	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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 33.81 % 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 7.5321e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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	0.47	0/2322	0.62	1/3158 (0.0%)
1	H	0.46	0/2322	0.62	2/3158 (0.1%)
2	B	0.47	0/847	0.56	0/1148
2	P	0.49	0/847	0.57	0/1148
3	C	0.59	0/76	0.54	0/101
3	M	0.45	0/76	0.50	0/101
All	All	0.47	0/6490	0.60	3/8814 (0.0%)

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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	272	LEU	CA-CB-CG	7.97	133.63	115.30
1	A	202	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	H	272	LEU	CB-CG-CD2	-5.10	102.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	TYR	Peptide

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	2258	0	2153	40	0
1	H	2258	0	2153	35	0
2	B	821	0	796	4	0
2	P	821	0	796	9	0
3	C	74	0	64	5	0
3	M	74	0	64	3	0
4	A	230	0	0	6	0
4	B	108	0	0	0	0
4	C	9	0	0	0	0
4	H	185	0	0	5	0
4	M	7	0	0	1	0
4	P	105	0	0	1	0
All	All	6950	0	6026	85	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 (85) 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:57:PRO:HB2	1:H:138:MET:HE3	1.15	1.11
3:C:6:ASN:HD22	3:C:7:SER:H	1.06	0.94
1:A:75:ARG:HG3	1:A:75:ARG:HH11	1.34	0.90
1:A:57:PRO:HB2	1:H:138:MET:CE	2.02	0.89
3:M:6:ASN:HD22	3:M:7:SER:H	1.18	0.87
1:H:52:MET:HA	1:H:52:MET:CE	2.11	0.79
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.31	0.76
1:A:209:TYR:O	1:A:210:PRO:O	2.05	0.73
1:A:31:THR:HG22	4:A:2029:HOH:O	1.90	0.69
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.28	0.69
1:A:217:TRP:HD1	1:A:228:MET:HE2	1.58	0.68
1:A:75:ARG:CG	1:A:75:ARG:HH11	2.07	0.68
3:C:6:ASN:HD22	3:C:7:SER:N	1.87	0.68
1:H:263:HIS:CD2	1:H:265:GLY:H	2.12	0.66
2:P:17:ASN:ND2	2:P:97:ARG:HH22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HE	1:A:242:GLN:NE2	1.95	0.64
1:H:52:MET:HE1	4:H:2041:HOH:O	1.97	0.63
1:A:70:ASN:HD21	3:C:5:TYR:H	1.46	0.63
1:H:263:HIS:HD2	1:H:265:GLY:H	1.49	0.61
1:H:52:MET:HA	1:H:52:MET:HE2	1.81	0.61
1:A:217:TRP:HD1	1:A:228:MET:CE	2.13	0.60
3:M:6:ASN:HD22	3:M:7:SER:N	1.96	0.60
1:A:54:GLN:HG3	4:A:2049:HOH:O	2.02	0.59
1:H:10:THR:CG2	1:H:23:ILE:HB	2.33	0.58
1:A:126:LEU:HD22	1:A:156:LEU:HD13	1.85	0.58
1:A:260:HIS:CD2	4:A:2225:HOH:O	2.58	0.57
1:H:14:ARG:HD2	1:H:19:GLU:O	2.05	0.57
1:H:210:PRO:O	1:H:263:HIS:HE1	1.90	0.55
1:H:52:MET:HA	1:H:52:MET:HE3	1.86	0.55
1:A:209:TYR:CD2	1:A:210:PRO:HD3	2.43	0.54
1:H:138:MET:HE2	1:H:138:MET:HA	1.88	0.54
1:H:10:THR:HG22	1:H:23:ILE:HB	1.89	0.54
1:A:178:THR:O	1:A:181:ARG:HG2	2.07	0.54
1:H:72:GLN:OE1	1:H:75:ARG:NH2	2.41	0.54
1:A:209:TYR:O	1:A:210:PRO:C	2.47	0.54
1:A:202:ARG:NH1	4:A:2183:HOH:O	2.42	0.53
1:A:216:THR:OG1	1:A:260:HIS:HB2	2.08	0.52
1:H:234:ARG:HE	1:H:242:GLN:HE21	1.57	0.52
1:H:6:ARG:NH2	4:H:2003:HOH:O	2.42	0.52
1:H:80:THR:HG21	4:M:2007:HOH:O	2.08	0.52
1:H:107:GLY:HA3	4:H:2074:HOH:O	2.09	0.51
1:H:48:ARG:NH2	2:P:53:ASP:OD1	2.43	0.51
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.46	0.51
1:H:5:LEU:HB2	1:H:168:LEU:HD13	1.92	0.51
1:H:112:GLY:HA3	1:H:160:LEU:HD13	1.93	0.51
1:A:210:PRO:O	1:A:263:HIS:HE1	1.93	0.50
2:P:2:GLN:HG2	2:P:32:PRO:HD3	1.94	0.50
1:A:31:THR:CG2	4:A:2029:HOH:O	2.57	0.50
1:A:217:TRP:CD1	1:A:228:MET:CE	2.95	0.50
1:A:202:ARG:CD	1:A:244:TRP:CD2	2.95	0.50
1:H:109:LEU:HD22	1:H:161:GLU:HG2	1.94	0.49
1:H:187:ALA:HA	1:H:204:TRP:O	2.11	0.49
1:H:127:ASN:HD22	1:H:132:THR:HB	1.78	0.49
1:A:279:SER:N	4:A:2230:HOH:O	2.45	0.49
1:H:20:PRO:HG2	1:H:75:ARG:HG3	1.95	0.47
1:H:117:ALA:HB2	2:P:60:TRP:CE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:HIS:O	1:A:149:GLN:HG2	2.14	0.47
1:A:14:ARG:HD2	1:A:19:GLU:O	2.15	0.47
1:H:45:TYR:CD1	1:H:63:GLU:HB3	2.50	0.47
1:H:80:THR:HG22	4:H:2061:HOH:O	2.14	0.46
1:A:58:GLU:HG3	1:H:141:LEU:HD11	1.97	0.46
1:A:176:ASN:O	1:A:180:LEU:HB2	2.16	0.46
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.97	0.46
1:A:75:ARG:CG	1:A:75:ARG:NH1	2.72	0.46
3:C:6:ASN:ND2	3:C:7:SER:H	1.91	0.46
1:H:234:ARG:HH11	2:P:8:GLN:NE2	2.14	0.45
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.98	0.45
1:H:98:ILE:HD13	2:P:58:LYS:HD2	1.98	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.44
1:A:57:PRO:CB	1:H:138:MET:HE3	2.10	0.44
2:P:17:ASN:HD21	2:P:97:ARG:HH22	1.65	0.44
2:B:38:GLN:HG2	2:B:45:LYS:HE2	2.00	0.44
1:A:225:ILE:H	1:A:225:ILE:HG13	1.59	0.44
2:P:3:LYS:HD2	2:P:31:HIS:HB2	2.00	0.43
1:H:6:ARG:NH2	1:H:30:ASN:OD1	2.52	0.43
1:A:11:ALA:HA	1:A:21:ARG:O	2.19	0.43
1:H:160:LEU:HA	1:H:164:CYS:CB	2.49	0.43
1:H:10:THR:HG23	4:H:2012:HOH:O	2.19	0.42
1:A:70:ASN:ND2	3:C:5:TYR:H	2.16	0.42
3:M:6:ASN:ND2	3:M:7:SER:H	2.00	0.41
1:A:44:ARG:HG3	1:A:64:THR:OG1	2.21	0.41
1:A:217:TRP:HB2	1:A:228:MET:HE3	2.03	0.40
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.04	0.40
1:A:263:HIS:CD2	1:A:265:GLY:H	2.40	0.40
2:P:4:THR:HG22	4:P:2004:HOH:O	2.21	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	277/279 (99%)	269 (97%)	5 (2%)	3 (1%)	17	6
1	H	277/279 (99%)	268 (97%)	8 (3%)	1 (0%)	39	27
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	P	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	M	6/8 (75%)	6 (100%)	0	0	100	100
All	All	760/772 (98%)	739 (97%)	17 (2%)	4 (0%)	34	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	TYR
1	A	210	PRO
1	A	225	ILE
1	H	278	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/237 (100%)	224 (95%)	12 (5%)	29	17
1	H	236/237 (100%)	229 (97%)	7 (3%)	48	38
2	B	94/94 (100%)	92 (98%)	2 (2%)	61	55
2	P	94/94 (100%)	89 (95%)	5 (5%)	28	16
3	C	8/8 (100%)	7 (88%)	1 (12%)	6	2
3	M	8/8 (100%)	7 (88%)	1 (12%)	6	2
All	All	676/678 (100%)	648 (96%)	28 (4%)	37	25

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG

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Mol	Chain	Res	Type
1	A	75	ARG
1	A	114	GLN
1	A	128	GLU
1	A	156	LEU
1	A	170	ARG
1	A	173	LYS
1	A	212	ASP
1	A	224	LEU
1	A	225	ILE
1	A	227	ASP
1	A	230	LEU
2	B	1	ILE
2	B	70	PHE
3	C	6	ASN
1	H	14	ARG
1	H	65	GLN
1	H	80	THR
1	H	114	GLN
1	H	128	GLU
1	H	272	LEU
1	H	273	ARG
3	M	6	ASN
2	P	44	LYS
2	P	48	LYS
2	P	69	GLU
2	P	70	PHE
2	P	91	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	70	ASN
1	A	114	GLN
1	A	174	ASN
1	A	242	GLN
1	A	260	HIS
1	A	263	HIS
2	B	8	GLN
3	C	2	GLN
3	C	6	ASN
1	H	65	GLN

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Mol	Chain	Res	Type
1	H	70	ASN
1	H	114	GLN
1	H	127	ASN
1	H	242	GLN
1	H	263	HIS
3	M	2	GLN
3	M	6	ASN
2	P	2	GLN
2	P	8	GLN
2	P	17	ASN

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)

There are no ligands in this entry.

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	279/279 (100%)	0.60	27 (9%)	10	11	16, 25, 41, 51	0
1	H	279/279 (100%)	0.75	35 (12%)	5	5	15, 28, 40, 48	0
2	B	99/99 (100%)	0.45	6 (6%)	25	27	16, 24, 33, 42	0
2	P	99/99 (100%)	0.41	6 (6%)	25	27	15, 23, 33, 40	0
3	C	8/8 (100%)	0.26	0	100	100	20, 21, 25, 25	0
3	M	8/8 (100%)	0.64	0	100	100	27, 29, 30, 31	0
All	All	772/772 (100%)	0.61	74 (9%)	10	11	15, 25, 40, 51	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	11.7
1	A	225	ILE	10.0
2	P	1	ILE	8.7
1	H	225	ILE	6.8
1	H	278	PRO	6.7
1	A	278	PRO	5.3
1	H	42	ASN	5.2
1	H	277	PRO	5.0
1	A	226	GLN	4.4
1	H	226	GLN	4.3
1	A	227	ASP	4.0
1	H	57	PRO	4.0
1	H	279	SER	3.9
1	A	221	GLY	3.9
1	H	145	HIS	3.8
1	A	220	ASN	3.8
1	H	56	GLY	3.6
2	P	47	PRO	3.6
1	H	195	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	151	GLY	3.5
1	H	173	LYS	3.4
1	A	180	LEU	3.4
1	A	222	GLU	3.4
1	H	41	GLU	3.3
1	H	58	GLU	3.2
1	H	111	ARG	3.2
1	A	181	ARG	3.2
1	H	168	LEU	3.1
1	H	95	ILE	3.0
1	A	176	ASN	2.9
1	H	172	LEU	2.9
1	A	41	GLU	2.9
2	P	88	ALA	2.9
1	H	44	ARG	2.8
1	H	160	LEU	2.7
1	A	267	PRO	2.7
1	H	154	GLU	2.7
1	H	227	ASP	2.7
1	H	149	GLN	2.7
1	H	169	ARG	2.7
1	H	180	LEU	2.6
1	H	132	THR	2.6
1	A	149	GLN	2.6
2	B	47	PRO	2.5
2	P	89	GLU	2.5
1	A	277	PRO	2.5
2	P	23	LEU	2.5
1	H	194	ARG	2.4
1	A	209	TYR	2.4
1	A	111	ARG	2.4
1	H	60	TRP	2.4
1	H	16	GLY	2.4
1	A	268	GLU	2.4
2	B	88	ALA	2.3
1	A	271	THR	2.3
1	A	113	TYR	2.3
1	A	42	ASN	2.3
1	A	260	HIS	2.3
1	A	16	GLY	2.2
1	H	164	CYS	2.2
2	B	89	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	23	LEU	2.2
2	B	48	LYS	2.2
1	H	65	GLN	2.2
1	A	5	LEU	2.2
1	A	182	THR	2.2
1	H	221	GLY	2.1
1	A	86	ASN	2.1
1	A	131	LYS	2.1
1	A	101	CYS	2.1
2	P	48	LYS	2.1
1	H	2	PRO	2.1
1	H	105	SER	2.0
1	H	128	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.