Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 02:26 PM EDT

PDB ID	:	1ZT7
Title	:	crystal structure of class I MHC H-2Kk in complex with a nonapeptide
Authors	:	Kellenberger, C.; Roussel, A.; Malissen, B.
Deposited on	:	2005-05-26
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

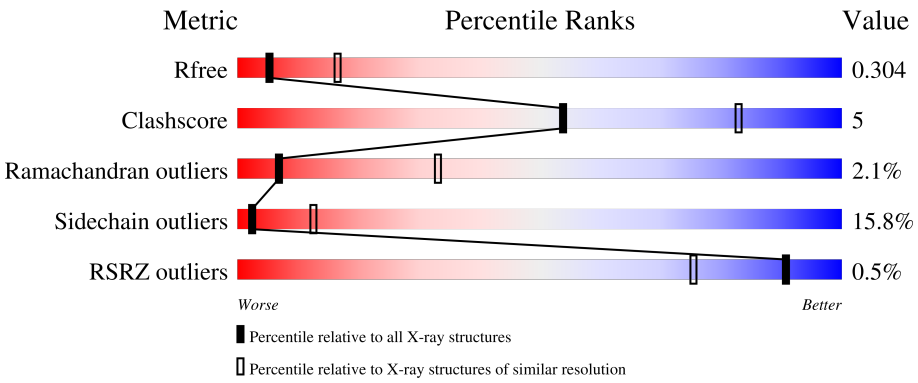
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	276	% 70% 26% •
1	C	276	% 74% 22% • •
2	B	100	73% 20% 5% • •
2	D	100	72% 23% • •
3	P	9	67% 22% 11%

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Mol	Chain	Length	Quality of chain
3	Q	9	78% 11% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6480 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-K alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2266	1432	404	421	9	0	0	0
1	C	275	2266	1432	404	421	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P04223
C	0	MET	-	initiating methionine	UNP P04223

- Molecule 2 is a protein called Beta-2-microglobulin.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P01887
D	0	MET	-	initiating methionine	UNP P01887

- Molecule 3 is a protein called SV40 epitope, SEFLLEKRI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	9	80	52	13	15	0	0	0
3	Q	9	80	52	13	15	0	0	0

- Molecule 4 is water.

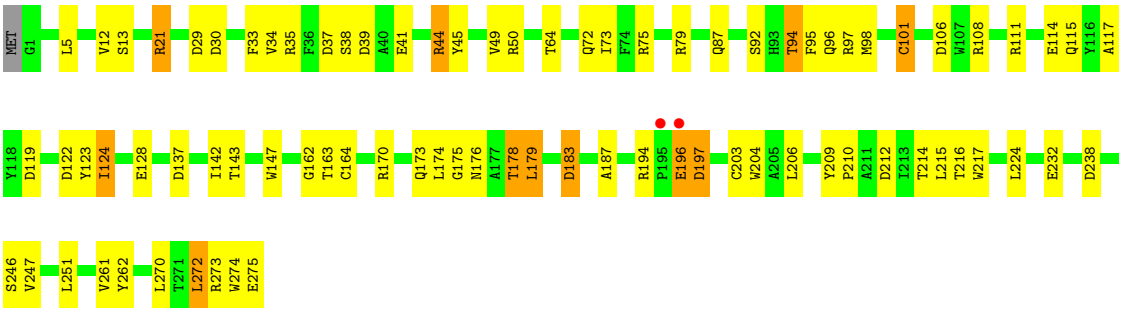
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	63	63	63	0	0
			Total	O		
4	B	9	9	9	0	0
			Total	O		
4	C	59	59	59	0	0
			Total	O		
4	D	8	8	8	0	0
			Total	O		
4	P	4	4	4	0	0
			Total	O		
4	Q	3	3	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

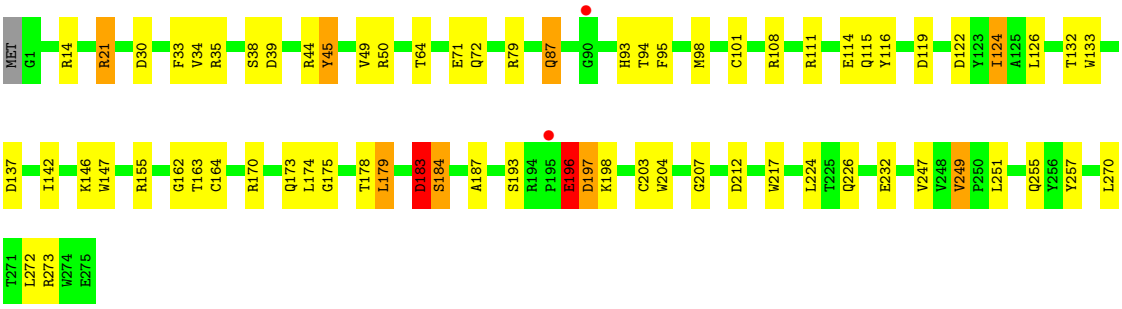
• Molecule 1: H-2 class I histocompatibility antigen, K-K alpha chain

Chain A:



• Molecule 1: H-2 class I histocompatibility antigen, K-K alpha chain

Chain C:

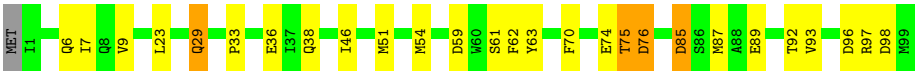


• Molecule 2: Beta-2-microglobulin

Chain B:

• Molecule 2: Beta-2-microglobulin

Chain D:



• Molecule 3: SV40 epitope, SEFLLEKRI

Chain P:

• Molecule 3: SV40 epitope, SEFLLEKRI

Chain Q:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	85.14Å 72.63Å 88.79Å 90.00° 111.24° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.7 (15.00-3.00) 89.5 (19.97-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.231 , 0.311 0.231 , 0.304	Depositor DCC
R_{free} test set	872 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6480	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 21.53 % 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 6.8845e-03. 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.50	0/2332	0.80	8/3170 (0.3%)
1	C	0.49	0/2332	0.78	5/3170 (0.2%)
2	B	0.42	0/847	0.77	5/1148 (0.4%)
2	D	0.43	0/847	0.75	3/1148 (0.3%)
3	P	0.57	0/80	0.89	1/103 (1.0%)
3	Q	0.56	0/80	0.86	0/103
All	All	0.48	0/6518	0.78	22/8842 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	ASP	CB-CG-OD2	7.30	124.87	118.30
1	C	137	ASP	CB-CG-OD2	6.56	124.20	118.30
2	B	96	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	119	ASP	CB-CG-OD2	6.19	123.87	118.30
2	D	96	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	37	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	122	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	30	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	106	ASP	CB-CG-OD2	5.57	123.31	118.30
2	B	76	ASP	CB-CG-OD2	5.51	123.26	118.30
2	D	59	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	30	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	29	ASP	CB-CG-OD2	5.41	123.17	118.30
2	B	85	ASP	CB-CG-OD2	5.39	123.15	118.30
2	B	53	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	98	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	122	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	238	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	85	ASP	CB-CG-OD2	5.05	122.85	118.30
1	C	119	ASP	CB-CG-OD2	5.04	122.83	118.30
3	P	8	ARG	NE-CZ-NH1	5.03	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ASP	CB-CG-OD2	5.00	122.80	118.30

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	2266	0	2147	31	0
1	C	2266	0	2147	24	0
2	B	821	0	796	9	0
2	D	821	0	796	6	0
3	P	80	0	87	3	0
3	Q	80	0	87	2	0
4	A	63	0	0	1	0
4	B	9	0	0	0	0
4	C	59	0	0	2	0
4	D	8	0	0	0	0
4	P	4	0	0	0	0
4	Q	3	0	0	0	0
All	All	6480	0	6060	66	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 5.

All (66) 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:C:187:ALA:HB1	1:C:272:LEU:HD11	1.50	0.93
1:A:224:LEU:HD21	1:A:247:VAL:HG21	1.64	0.79
1:C:224:LEU:HD21	1:C:247:VAL:HG21	1.65	0.78
1:C:21:ARG:HE	1:C:39:ASP:HB2	1.51	0.74
1:C:45:TYR:OH	3:Q:2:GLU:OE1	2.13	0.66
1:A:187:ALA:HB1	1:A:272:LEU:HD11	1.77	0.65
1:C:187:ALA:CB	1:C:272:LEU:HD11	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLN:NE2	4:C:312:HOH:O	2.13	0.59
1:A:12:VAL:HG12	1:A:94:THR:HB	1.85	0.58
1:A:124:ILE:HG21	1:A:147:TRP:CZ3	2.41	0.56
1:C:183:ASP:OD2	1:C:207:GLY:O	2.24	0.56
1:C:33:PHE:CD2	1:C:34:VAL:HG13	2.41	0.55
1:C:162:GLY:O	1:C:164:CYS:N	2.40	0.55
1:A:274:TRP:CE2	1:A:275:GLU:HG3	2.42	0.55
1:C:196:GLU:O	1:C:198:LYS:HG2	2.08	0.54
1:A:162:GLY:O	1:A:164:CYS:N	2.41	0.53
1:A:44:ARG:HA	1:A:64:THR:HG23	1.91	0.53
2:D:75:THR:O	2:D:76:ASP:C	2.47	0.52
2:B:75:THR:O	2:B:76:ASP:C	2.47	0.52
1:A:72:GLN:NE2	4:A:326:HOH:O	2.30	0.52
1:C:197:ASP:O	1:C:197:ASP:CG	2.48	0.51
2:B:77:THR:HG21	4:C:327:HOH:O	2.11	0.50
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.48	0.49
1:A:183:ASP:OD1	1:A:183:ASP:C	2.50	0.49
2:B:11:SER:OG	2:B:13:HIS:O	2.30	0.49
1:C:44:ARG:HA	1:C:64:THR:HG23	1.95	0.49
1:A:204:TRP:HZ2	2:B:98:ASP:O	1.95	0.49
1:A:204:TRP:HE3	1:A:206:LEU:HD21	1.78	0.48
2:D:7:ILE:HB	2:D:93:VAL:HG21	1.95	0.47
1:A:175:GLY:O	1:A:179:LEU:HD13	2.15	0.47
2:D:29:GLN:HA	2:D:61:SER:HB2	1.95	0.47
1:C:183:ASP:OD1	1:C:184:SER:N	2.48	0.46
1:A:73:ILE:HG21	3:P:5:LEU:HD23	1.98	0.46
1:A:96:GLN:NE2	2:B:60:TRP:O	2.49	0.45
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.51	0.45
1:C:183:ASP:OD1	1:C:183:ASP:C	2.55	0.45
1:A:21:ARG:NE	1:A:39:ASP:HB2	2.32	0.45
2:B:54:MET:HE1	2:B:62:PHE:CD2	2.51	0.45
1:C:124:ILE:HG21	1:C:147:TRP:CZ3	2.52	0.44
1:C:217:TRP:HB3	1:C:224:LEU:HD22	1.99	0.44
1:A:204:TRP:CE3	1:A:206:LEU:HD21	2.53	0.44
1:C:249:VAL:HB	1:C:257:TYR:CE1	2.53	0.44
1:A:187:ALA:CB	1:A:272:LEU:HD11	2.45	0.43
1:A:197:ASP:CG	1:A:197:ASP:O	2.56	0.43
1:C:175:GLY:O	1:C:179:LEU:HB2	2.18	0.43
1:C:87:GLN:NE2	1:C:93:HIS:CE1	2.87	0.43
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.49	0.43
1:A:143:THR:HG23	3:P:9:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HB	1:A:262:TYR:HB2	2.00	0.42
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.54	0.42
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.85	0.42
1:C:146:LYS:NZ	3:Q:8:ARG:HH12	2.17	0.42
1:A:5:LEU:HB3	1:A:101:CYS:SG	2.60	0.42
1:A:123:TYR:OH	1:A:143:THR:OG1	2.27	0.42
2:B:54:MET:CE	2:B:62:PHE:CD2	3.03	0.42
1:C:132:THR:HG22	1:C:133:TRP:N	2.35	0.42
1:C:204:TRP:HZ2	2:D:98:ASP:O	2.03	0.41
1:A:215:LEU:HD22	1:A:261:VAL:HG22	2.02	0.41
1:A:124:ILE:HG21	1:A:147:TRP:HZ3	1.84	0.41
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.55	0.41
2:D:9:VAL:HG12	2:D:23:LEU:HD11	2.03	0.41
2:D:33:PRO:HG3	2:D:62:PHE:CZ	2.56	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
1:A:72:GLN:OE1	1:A:75:ARG:NH2	2.55	0.40
1:A:97:ARG:NH1	3:P:5:LEU:HD13	2.36	0.40
1:C:126:LEU:HD12	1:C:132:THR: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	273/276 (99%)	243 (89%)	24 (9%)	6 (2%)	6	31
1	C	273/276 (99%)	241 (88%)	26 (10%)	6 (2%)	6	31
2	B	97/100 (97%)	83 (86%)	12 (12%)	2 (2%)	7	33
2	D	97/100 (97%)	82 (84%)	13 (13%)	2 (2%)	7	33
3	P	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	Q	7/9 (78%)	6 (86%)	1 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	754/770 (98%)	661 (88%)	77 (10%)	16 (2%)	7 33

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	THR
1	C	163	THR
2	B	76	ASP
2	D	76	ASP
1	A	196	GLU
1	C	196	GLU
1	A	38	SER
1	A	114	GLU
1	A	178	THR
2	B	54	MET
1	C	38	SER
1	C	114	GLU
2	D	54	MET
1	C	193	SER
1	A	87	GLN
1	C	87	GLN

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	235/236 (100%)	197 (84%)	38 (16%)	2 12
1	C	235/236 (100%)	199 (85%)	36 (15%)	2 13
2	B	94/95 (99%)	78 (83%)	16 (17%)	2 10
2	D	94/95 (99%)	79 (84%)	15 (16%)	2 12
3	P	9/9 (100%)	8 (89%)	1 (11%)	6 25
3	Q	9/9 (100%)	8 (89%)	1 (11%)	6 25
All	All	676/680 (99%)	569 (84%)	107 (16%)	2 12

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	21	ARG
1	A	35	ARG
1	A	41	GLU
1	A	44	ARG
1	A	45	TYR
1	A	49	VAL
1	A	50	ARG
1	A	79	ARG
1	A	92	SER
1	A	94	THR
1	A	95	PHE
1	A	98	MET
1	A	101	CYS
1	A	108	ARG
1	A	111	ARG
1	A	115	GLN
1	A	124	ILE
1	A	128	GLU
1	A	142	ILE
1	A	170	ARG
1	A	173	GLN
1	A	174	LEU
1	A	176	ASN
1	A	178	THR
1	A	179	LEU
1	A	183	ASP
1	A	194	ARG
1	A	196	GLU
1	A	197	ASP
1	A	212	ASP
1	A	216	THR
1	A	232	GLU
1	A	246	SER
1	A	251	LEU
1	A	270	LEU
1	A	272	LEU
1	A	273	ARG
2	B	6	GLN
2	B	21	ASN
2	B	29	GLN
2	B	45	LYS

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Mol	Chain	Res	Type
2	B	46	ILE
2	B	55	SER
2	B	63	TYR
2	B	70	PHE
2	B	74	GLU
2	B	75	THR
2	B	83	LYS
2	B	85	ASP
2	B	87	MET
2	B	89	GLU
2	B	92	THR
2	B	97	ARG
1	C	14	ARG
1	C	21	ARG
1	C	35	ARG
1	C	45	TYR
1	C	49	VAL
1	C	50	ARG
1	C	71	GLU
1	C	79	ARG
1	C	94	THR
1	C	95	PHE
1	C	98	MET
1	C	101	CYS
1	C	108	ARG
1	C	111	ARG
1	C	115	GLN
1	C	116	TYR
1	C	124	ILE
1	C	142	ILE
1	C	155	ARG
1	C	170	ARG
1	C	173	GLN
1	C	174	LEU
1	C	178	THR
1	C	179	LEU
1	C	183	ASP
1	C	184	SER
1	C	196	GLU
1	C	197	ASP
1	C	212	ASP
1	C	226	GLN

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Mol	Chain	Res	Type
1	C	232	GLU
1	C	249	VAL
1	C	251	LEU
1	C	255	GLN
1	C	270	LEU
1	C	273	ARG
2	D	6	GLN
2	D	29	GLN
2	D	36	GLU
2	D	38	GLN
2	D	46	ILE
2	D	51	MET
2	D	63	TYR
2	D	70	PHE
2	D	74	GLU
2	D	75	THR
2	D	85	ASP
2	D	87	MET
2	D	89	GLU
2	D	92	THR
2	D	97	ARG
3	P	8	ARG
3	Q	8	ARG

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	87	GLN
1	A	176	ASN
1	A	218	GLN
1	A	226	GLN
1	A	242	GLN
1	A	260	HIS
2	B	29	GLN
2	B	67	HIS
1	C	87	GLN
1	C	93	HIS
1	C	96	GLN
1	C	218	GLN
1	C	260	HIS
2	D	6	GLN

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 monosaccharides 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	275/276 (99%)	-0.47	2 (0%)	87	69	5, 20, 40, 71	2 (0%)
1	C	275/276 (99%)	-0.49	2 (0%)	87	69	8, 20, 40, 73	2 (0%)
2	B	99/100 (99%)	-0.14	0	100	100	24, 42, 68, 80	2 (2%)
2	D	99/100 (99%)	-0.12	0	100	100	27, 42, 67, 80	2 (2%)
3	P	9/9 (100%)	-0.90	0	100	100	12, 14, 15, 16	0
3	Q	9/9 (100%)	-0.99	0	100	100	12, 14, 16, 17	0
All	All	766/770 (99%)	-0.40	4 (0%)	91	75	5, 24, 56, 80	8 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	PRO	2.8
1	C	195	PRO	2.6
1	A	196	GLU	2.3
1	C	90	GLY	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 monosaccharides 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.