Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 07:09 PM EDT

PDB ID	:	3CVH
Title	:	How TCR-like antibody recognizes MHC-bound peptide
Authors	:	Mareeva, T.; Martinez-Hackert, E.; Sykulev, Y.
Deposited on	:	2008-04-18
Resolution	:	2.90 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:

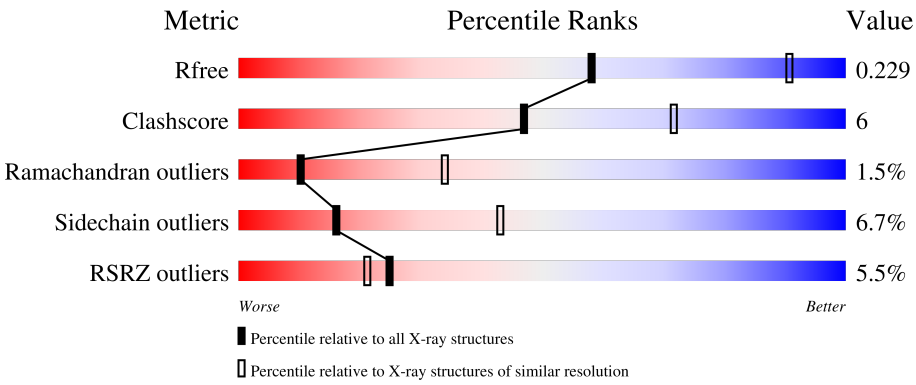
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	274	.% 80% 18% •
1	M	274	2% 86% 13% •
2	B	99	84% 15% •
2	N	99	2% 72% 26% •
3	C	8	75% 25%

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Mol	Chain	Length	Quality of chain
3	O	8	75% 25%
4	H	219	77% 16%
4	Q	219	11% 81% 13%
5	L	209	83% 16%
5	R	209	24% 73% 22% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12886 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
			Total	C	N	O	S			
1	A	274	2232	1408	393	422	9	0	0	0
1	M	274	2232	1408	393	422	9	0	0	0

- 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	N	99	821	524	138	152	7	0	0	0

- Molecule 3 is a protein called Ovalbumin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	68	45	10	13	0	0	0
3	O	8	68	45	10	13	0	0	0

- Molecule 4 is a protein called 25-D1.16 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	213	1618	1038	260	313	7	0	0	0
4	Q	210	1600	1028	257	309	6	0	0	0

- Molecule 5 is a protein called 25-D1.16 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	209	1625	1014	272	334	5	0	0	0
5	R	209	1625	1014	272	334	5	0	0	0

- Molecule 6 is water.

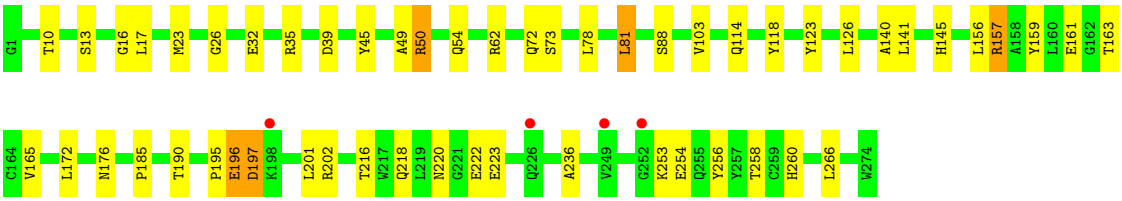
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	42	42	42	0	0
6	B	14	14	14	0	0
6	C	2	2	2	0	0
6	H	39	39	39	0	0
6	L	36	36	36	0	0
6	M	19	19	19	0	0
6	N	8	8	8	0	0
6	Q	8	8	8	0	0
6	R	8	8	8	0	0

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.

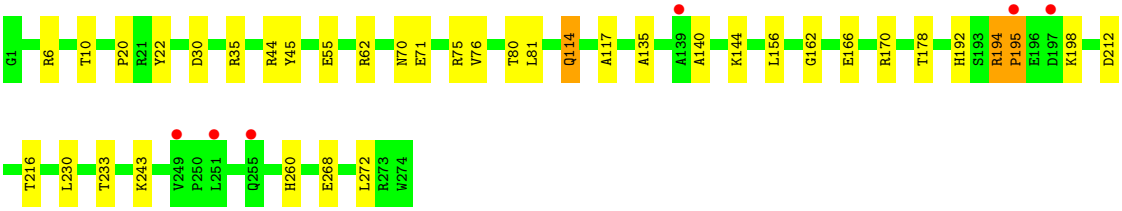
• Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain A:



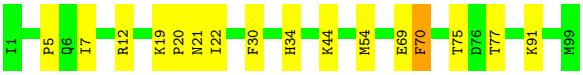
• Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain M:



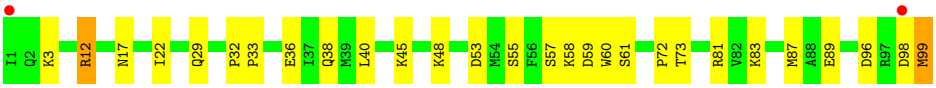
• Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin

Chain N:



• Molecule 3: Ovalbumin

Chain C: 75% 25%

S1 K7 L8

• Molecule 3: Ovalbumin

Chain O: 75% 25%

S1 N4 K7 L8

• Molecule 4: 25-D1.16 heavy chain

Chain H: 77% 16%

V1 Q5 S16 W35 S43 L44 E45 W46 I47 I50 N51 P52 N53 T57 I58 Y59 L69 T70 V71 R83 K98 P99 Y100 F104 A105 W106 Q112 G134 SER ALA ALA GLN THR ASN S141 M142 V143 C147 K150 P154 T158 V159 T160 W161

N162 S163 S168 Q178 S179 D180 T183 L184 S192 S193 C202 N203 H206 S209 S210 T211 K212 P219

• Molecule 4: 25-D1.16 heavy chain

Chain Q: 11% 81% 13%

V1 Q5 L10 V11 K12 N32 K37 K42 D49 G56 Y59 K66 T70 S84 Y93 K98 A105 Q112 S119 A120 A121 K122 T123 T124 V128 Y129 P130 L131 A132 P133 GLY SER ALA ALA GLN THR ASN SER MET V143 T144 L145

V149 F153 P154 E155 P156 V157 T158 W161 L166 A175 V176 L177 Q178 T189 V190 T194 S197 E198 T199 V204 S210 T211 K216 I217 V218 P219

• Molecule 5: 25-D1.16 light chain

Chain L: 83% 16%

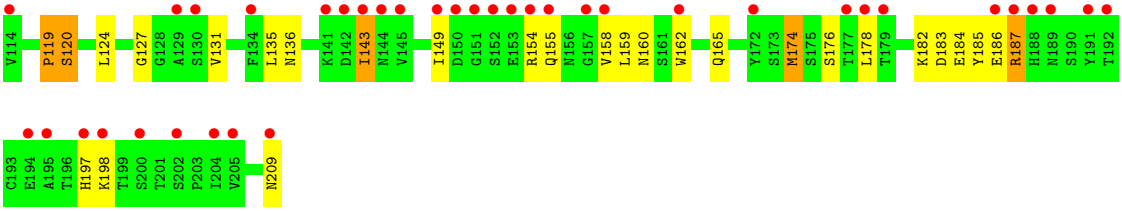
I1 Q2 Q5 S6 F10 C22 L32 Q37 P43 S52 T55 D59 S66 R67 Y85 Y86 Y90 L95 G98 A99 G100 D109 S115 P118 S121 T125 D142 Q165 K168 T192 C193 E194 K198 V205 K206

S207 F208 N209

• Molecule 5: 25-D1.16 light chain

Chain R: 24% 73% 22% 5%

I1 Q2 Q5 S6 S7 S8 S9 F10 S11 V12 S13 D16 R17 V18 T19 I20 L32 L45 L46 I47 L53 E54 T55 G56 V57 R60 R67 T71 L72 I73 I74 T75 S76 L77 Q78 D81 T84 Y85 Y86 C87 K102 L103 E104 L105 D109 P112 T113


V114
P119
S120
L124
G127
G128
A129
S130
V131
F134
L135
N136
K141
D142
I143
N144
V145
I149
D150
G151
S152
E153
R154
Q155
N156
G157
V158
L159
N160
S161
W162
Q165
Y172
S173
M174
S175
S176
T177
L178
T179
K182
D183
E184
Y185
E186
R187
H188
N189
S190
Y191
T192

C193
E194
A195
T196
H197
K198
T199
S200
T201
S202
P203
I204
V205
N209

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.57Å 111.34Å 219.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.90 49.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.90) 98.0 (49.63-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.296 0.221 , 0.229	Depositor DCC
R_{free} test set	2196 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12886	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, 0.333 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	0.44	0/2293	0.58	0/3113
1	M	0.39	0/2293	0.52	0/3113
2	B	0.43	0/847	0.52	0/1148
2	N	0.39	0/847	0.53	0/1148
3	C	0.47	0/68	0.74	0/88
3	O	0.44	0/68	0.59	0/88
4	H	0.46	0/1665	0.59	0/2277
4	Q	0.39	0/1647	0.53	0/2254
5	L	0.45	0/1660	0.57	0/2256
5	R	0.38	0/1660	0.52	0/2256
All	All	0.42	0/13048	0.55	0/17741

There are no bond length outliers.

There are no bond angle outliers.

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	2232	0	2123	34	0
1	M	2232	0	2123	19	0
2	B	821	0	796	7	0
2	N	821	0	796	16	0
3	C	68	0	74	1	0
3	O	68	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1618	0	1587	39	0
4	Q	1600	0	1570	16	0
5	L	1625	0	1569	12	0
5	R	1625	0	1569	24	0
6	A	42	0	0	5	0
6	B	14	0	0	1	0
6	C	2	0	0	0	0
6	H	39	0	0	7	0
6	L	36	0	0	0	0
6	M	19	0	0	1	0
6	N	8	0	0	0	0
6	Q	8	0	0	0	0
6	R	8	0	0	1	0
All	All	12886	0	12281	156	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 (156) 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)
4:H:112:GLN:H	4:H:112:GLN:HE21	1.05	0.95
1:A:126:LEU:HD22	1:A:156:LEU:HD23	1.57	0.85
4:H:141:SER:HB3	6:H:222:HOH:O	1.75	0.84
4:H:5:GLN:H	4:H:112:GLN:HE22	1.26	0.81
4:H:134:GLY:HA2	6:H:233:HOH:O	1.79	0.81
1:A:72:GLN:HE22	4:H:59:TYR:H	1.28	0.78
4:H:163:SER:H	4:H:203:ASN:HD21	1.30	0.78
1:M:20:PRO:HG2	1:M:75:ARG:HG2	1.67	0.77
4:H:112:GLN:HE21	4:H:112:GLN:N	1.83	0.75
1:A:72:GLN:NE2	4:H:59:TYR:H	1.85	0.74
1:A:62:ARG:HD3	6:A:297:HOH:O	1.89	0.72
1:A:176:ASN:HB2	6:A:308:HOH:O	1.92	0.69
5:L:121:SER:O	5:L:125:THR:HG23	1.93	0.69
4:H:50:ILE:HG12	4:H:69:LEU:HD23	1.76	0.67
4:H:35:TRP:O	4:H:46:TRP:O	2.12	0.67
5:L:192:THR:HB	5:L:207:SER:OG	1.93	0.66
4:H:5:GLN:H	4:H:112:GLN:NE2	1.93	0.65
2:B:34:HIS:HB2	6:B:104:HOH:O	1.97	0.65
5:R:119:PRO:O	5:R:120:SER:HB2	1.98	0.64
1:A:81:LEU:HD13	3:C:8:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:186:GLU:HB3	6:R:214:HOH:O	1.99	0.62
1:M:35:ARG:NH1	2:N:53:ASP:HB3	2.15	0.61
5:R:155:GLN:HB2	5:R:158:VAL:HG21	1.83	0.61
4:Q:5:GLN:HB2	4:Q:112:GLN:HE22	1.66	0.61
1:A:35:ARG:NH2	2:B:54:MET:O	2.34	0.60
1:M:44:ARG:HD3	6:M:277:HOH:O	2.01	0.59
6:A:316:HOH:O	5:L:1:ILE:N	2.34	0.59
2:N:12:ARG:NH2	2:N:22:ILE:HD13	2.18	0.59
5:L:194:GLU:HG2	5:L:205:VAL:HG22	1.85	0.59
4:Q:161:TRP:H	4:Q:166:LEU:HD21	1.68	0.58
5:L:5:GLN:HE21	5:L:98:GLY:HA3	1.68	0.56
4:H:16:SER:HB3	4:H:83:ARG:HA	1.86	0.56
5:R:60:ARG:HD3	5:R:76:SER:O	2.05	0.56
1:A:114:GLN:HG2	1:A:156:LEU:HD21	1.86	0.56
1:A:10:THR:HG23	1:A:23:MET:HB2	1.87	0.56
1:A:114:GLN:CG	1:A:156:LEU:HD21	2.36	0.56
1:A:236:ALA:HB1	2:B:12:ARG:HG3	1.88	0.56
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.41	0.56
1:M:162:GLY:O	1:M:166:GLU:HG3	2.06	0.55
2:N:17:ASN:HA	2:N:72:PRO:O	2.07	0.55
4:H:154:PRO:O	4:H:206:HIS:HE1	1.90	0.54
4:Q:128:VAL:HG21	4:Q:204:VAL:HG21	1.89	0.54
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.43	0.54
5:R:16:ASP:H	5:R:77:LEU:H	1.57	0.54
5:R:135:LEU:HD12	5:R:174:MET:HG2	1.88	0.53
2:N:99:MET:C	2:N:99:MET:SD	2.86	0.53
4:H:50:ILE:HG23	4:H:57:THR:HG22	1.90	0.53
1:A:103:VAL:HG11	1:A:165:VAL:HG22	1.91	0.53
4:H:99:PRO:HG3	4:H:106:TRP:CE2	2.44	0.52
1:M:194:ARG:HB2	1:M:198:LYS:O	2.10	0.52
1:A:172:LEU:O	1:A:176:ASN:HB3	2.10	0.52
4:H:51:ASN:ND2	4:H:53:ASN:H	2.06	0.52
4:H:134:GLY:CA	6:H:224:HOH:O	2.57	0.52
1:M:6:ARG:HH12	2:N:58:LYS:HE2	1.75	0.52
4:Q:166:LEU:HD22	4:Q:166:LEU:H	1.75	0.52
1:M:117:ALA:HB2	2:N:60:TRP:CE2	2.45	0.52
1:M:194:ARG:HG2	1:M:195:PRO:HD2	1.91	0.52
4:Q:143:VAL:HG13	4:Q:190:VAL:HG23	1.92	0.52
5:R:143:ILE:HG23	5:R:197:HIS:ND1	2.25	0.51
1:M:233:THR:HG23	1:M:243:LYS:HB2	1.91	0.51
1:A:145:HIS:HB3	6:A:279:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:60:ARG:NE	5:R:78:GLN:HG3	2.25	0.51
4:H:161:TRP:CZ3	4:H:202:CYS:HB2	2.46	0.51
1:M:194:ARG:CB	1:M:198:LYS:O	2.59	0.51
4:H:134:GLY:CA	6:H:233:HOH:O	2.48	0.51
5:R:127:GLY:HA2	5:R:182:LYS:HB2	1.93	0.51
4:H:141:SER:N	4:H:192:SER:HG	2.09	0.50
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.94	0.50
4:H:141:SER:N	6:H:222:HOH:O	2.44	0.50
5:R:124:LEU:O	5:R:182:LYS:HD2	2.12	0.50
4:H:46:TRP:O	4:H:47:ILE:HB	2.13	0.49
1:M:192:HIS:CE1	2:N:98:ASP:HB3	2.48	0.49
4:H:112:GLN:H	4:H:112:GLN:NE2	1.89	0.49
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.12	0.49
4:H:134:GLY:HA3	6:H:224:HOH:O	2.13	0.48
5:R:53:LEU:HD11	5:R:57:VAL:O	2.12	0.48
4:Q:98:LYS:HD3	4:Q:105:ALA:HB3	1.94	0.48
4:Q:161:TRP:HB2	4:Q:166:LEU:HD11	1.95	0.48
4:Q:178:GLN:HB3	5:R:159:LEU:HD11	1.96	0.48
5:L:37:GLN:NE2	5:L:43:PRO:HD3	2.29	0.48
4:H:43:SER:OG	4:H:44:LEU:N	2.47	0.48
1:A:114:GLN:CB	1:A:156:LEU:HD21	2.43	0.47
1:A:190:THR:HG22	1:A:202:ARG:HB3	1.96	0.47
5:L:5:GLN:HE22	5:L:86:TYR:HA	1.80	0.47
5:R:5:GLN:HE21	5:R:5:GLN:HA	1.79	0.47
1:M:30:ASP:N	1:M:30:ASP:OD1	2.48	0.46
5:R:5:GLN:NE2	5:R:87:CYS:SG	2.82	0.46
1:M:135:ALA:HB1	1:M:140:ALA:HB3	1.95	0.46
4:Q:5:GLN:CB	4:Q:112:GLN:HE22	2.29	0.46
1:A:185:PRO:HD2	1:A:266:LEU:HG	1.97	0.46
1:M:71:GLU:O	1:M:75:ARG:HG3	2.16	0.46
5:R:184:GLU:HA	5:R:187:ARG:HH21	1.81	0.46
1:M:55:GLU:OE1	1:M:170:ARG:NH2	2.49	0.46
1:A:201:LEU:HD21	1:A:254:GLU:HB2	1.98	0.46
4:H:143:VAL:HG13	4:H:143:VAL:O	2.16	0.46
1:A:218:GLN:HG3	1:A:258:THR:OG1	2.16	0.46
5:L:85:TYR:O	5:L:100:GLY:HA2	2.16	0.46
2:N:3:LYS:HE3	2:N:29:GLN:HE21	1.80	0.46
4:H:50:ILE:HG21	4:H:71:VAL:HG22	1.98	0.46
2:N:99:MET:SD	2:N:99:MET:O	2.74	0.46
1:A:253:LYS:HB3	1:A:256:TYR:CD1	2.50	0.45
5:R:160:ASN:HD22	5:R:176:SER:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:32:PRO:HB2	2:N:33:PRO:HD2	1.98	0.45
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.98	0.45
4:H:46:TRP:O	4:H:47:ILE:CB	2.64	0.45
5:L:22:CYS:SG	5:L:32:LEU:HD11	2.57	0.45
1:M:216:THR:OG1	1:M:260:HIS:HB2	2.16	0.45
5:R:84:THR:HA	5:R:102:LYS:HA	1.99	0.45
5:R:162:TRP:NE1	5:R:174:MET:SD	2.90	0.45
4:Q:128:VAL:HG22	4:Q:149:VAL:HG13	1.98	0.44
5:R:11:SER:HA	5:R:104:GLU:O	2.18	0.44
4:H:178:GLN:HE21	4:H:183:THR:HG1	1.61	0.44
1:A:222:GLU:HA	6:A:313:HOH:O	2.17	0.44
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.99	0.44
4:H:150:LYS:HG3	4:H:178:GLN:NE2	2.32	0.44
1:A:26:GLY:O	1:A:32:GLU:HA	2.18	0.44
1:A:49:ALA:O	1:A:50:ARG:C	2.56	0.44
4:H:5:GLN:N	4:H:112:GLN:HE22	2.04	0.44
4:H:98:LYS:HB2	4:H:100:TYR:O	2.17	0.43
1:A:216:THR:OG1	1:A:260:HIS:HB2	2.18	0.43
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.54	0.43
2:N:38:GLN:HE22	2:N:45:LYS:HE2	1.83	0.43
4:Q:155:GLU:HB3	4:Q:156:PRO:HA	2.01	0.43
4:H:141:SER:CB	6:H:222:HOH:O	2.49	0.43
5:R:45:LEU:CD2	5:R:54:GLU:HG3	2.49	0.43
1:A:196:GLU:HB2	1:A:197:ASP:H	1.73	0.43
2:N:29:GLN:HA	2:N:61:SER:HB2	2.01	0.43
5:L:109:ASP:OD2	5:L:198:LYS:HE3	2.19	0.42
4:H:209:SER:O	4:H:211:THR:HG23	2.19	0.42
4:H:104:PHE:HB3	5:L:90:TYR:O	2.19	0.42
2:N:59:ASP:O	2:N:60:TRP:HB2	2.19	0.42
1:M:76:VAL:HG13	4:Q:56:GLY:HA3	2.01	0.42
1:A:159:TYR:CD1	1:A:163:THR:HB	2.55	0.42
5:R:2:GLN:HE21	5:R:2:GLN:HB3	1.68	0.42
1:A:157:ARG:HE	1:A:161:GLU:CD	2.23	0.42
4:H:16:SER:CB	4:H:83:ARG:HA	2.49	0.42
4:H:184:LEU:HD12	4:H:184:LEU:C	2.40	0.42
3:O:7:LYS:HE2	4:Q:32:ASN:ND2	2.34	0.42
5:R:149:ILE:HD11	5:R:178:LEU:HD21	2.02	0.41
1:A:32:GLU:CD	1:A:35:ARG:HH11	2.22	0.41
2:N:36:GLU:HB3	2:N:83:LYS:HB2	2.03	0.41
4:H:163:SER:H	4:H:203:ASN:ND2	2.09	0.41
1:M:22:TYR:OH	1:M:70:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLY:O	1:A:17:LEU:HD23	2.21	0.41
2:B:19:LYS:HA	2:B:20:PRO:HD3	1.97	0.41
2:N:40:LEU:HD11	2:N:81:ARG:HD3	2.02	0.41
4:Q:154:PRO:HB2	4:Q:155:GLU:H	1.72	0.41
4:H:159:VAL:HA	4:H:203:ASN:O	2.20	0.41
2:N:96:ASP:O	2:N:99:MET:OXT	2.38	0.41
1:M:114:GLN:HA	1:M:114:GLN:HE21	1.86	0.41
5:R:105:LEU:HD12	5:R:165:GLN:HG2	2.03	0.40
5:L:118:PRO:HB3	5:L:208:PHE:CE1	2.56	0.40
1:A:218:GLN:HA	1:A:223:GLU:HA	2.02	0.40
4:Q:37:LYS:HG3	4:Q:93:TYR:CE1	2.56	0.40
5:R:5:GLN:OE1	5:R:86:TYR:HA	2.21	0.40
4:Q:132:ALA:HA	4:Q:133:PRO:HD3	1.98	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	272/274 (99%)	251 (92%)	15 (6%)	6 (2%)	6	24
1	M	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	34	66
2	B	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	N	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	O	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
4	H	209/219 (95%)	191 (91%)	14 (7%)	4 (2%)	8	28
4	Q	206/219 (94%)	185 (90%)	19 (9%)	2 (1%)	15	45
5	L	207/209 (99%)	199 (96%)	6 (3%)	2 (1%)	15	45
5	R	207/209 (99%)	180 (87%)	19 (9%)	8 (4%)	3	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1579/1618 (98%)	1458 (92%)	98 (6%)	23 (2%)	10 34

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	47	ILE
4	H	143	VAL
4	H	178	GLN
5	R	120	SER
5	R	136	ASN
1	A	50	ARG
5	R	81	ASP
5	R	119	PRO
5	L	6	SER
5	L	67	ARG
4	Q	84	SER
5	R	6	SER
1	A	54	GLN
1	A	220	ASN
5	R	67	ARG
1	A	195	PRO
1	A	196	GLU
1	A	197	ASP
4	H	46	TRP
5	R	7	SER
5	R	185	TYR
1	M	195	PRO
4	Q	154	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	232/232 (100%)	225 (97%)	7 (3%)	41 75
1	M	232/232 (100%)	218 (94%)	14 (6%)	19 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	94/94 (100%)	88 (94%)	6 (6%)	17	45
2	N	94/94 (100%)	86 (92%)	8 (8%)	10	31
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	14
3	O	8/8 (100%)	7 (88%)	1 (12%)	4	14
4	H	182/186 (98%)	171 (94%)	11 (6%)	19	49
4	Q	180/186 (97%)	167 (93%)	13 (7%)	14	39
5	L	186/186 (100%)	172 (92%)	14 (8%)	13	37
5	R	186/186 (100%)	167 (90%)	19 (10%)	7	22
All	All	1402/1412 (99%)	1308 (93%)	94 (7%)	16	43

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	45	TYR
1	A	73	SER
1	A	81	LEU
1	A	88	SER
1	A	141	LEU
1	A	157	ARG
2	B	22	ILE
2	B	44	LYS
2	B	69	GLU
2	B	70	PHE
2	B	75	THR
2	B	77	THR
3	C	7	LYS
4	H	50	ILE
4	H	51	ASN
4	H	71	VAL
4	H	112	GLN
4	H	147	CYS
4	H	158	THR
4	H	168	SER
4	H	180	ASP
4	H	193	SER
4	H	202	CYS
4	H	212	LYS
5	L	2	GLN

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Mol	Chain	Res	Type
5	L	10	PHE
5	L	32	LEU
5	L	52	SER
5	L	55	THR
5	L	59	ASP
5	L	66	SER
5	L	95	LEU
5	L	115	SER
5	L	142	ASP
5	L	165	GLN
5	L	168	LYS
5	L	192	THR
5	L	206	LYS
1	M	10	THR
1	M	45	TYR
1	M	62	ARG
1	M	80	THR
1	M	81	LEU
1	M	114	GLN
1	M	144	LYS
1	M	156	LEU
1	M	178	THR
1	M	194	ARG
1	M	212	ASP
1	M	230	LEU
1	M	268	GLU
1	M	272	LEU
2	N	12	ARG
2	N	48	LYS
2	N	55	SER
2	N	57	SER
2	N	73	THR
2	N	87	MET
2	N	89	GLU
2	N	99	MET
3	O	4	ASN
4	Q	12	LYS
4	Q	42	LYS
4	Q	49	ASP
4	Q	66	LYS
4	Q	70	THR
4	Q	112	GLN

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Mol	Chain	Res	Type
4	Q	124	THR
4	Q	145	LEU
4	Q	158	THR
4	Q	166	LEU
4	Q	176	VAL
4	Q	190	VAL
4	Q	194	THR
5	R	2	GLN
5	R	5	GLN
5	R	12	VAL
5	R	32	LEU
5	R	47	ILE
5	R	55	THR
5	R	71	THR
5	R	77	LEU
5	R	78	GLN
5	R	104	GLU
5	R	109	ASP
5	R	131	VAL
5	R	143	ILE
5	R	154	ARG
5	R	174	MET
5	R	183	ASP
5	R	187	ARG
5	R	198	LYS
5	R	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	226	GLN
1	A	255	GLN
4	H	38	GLN
4	H	51	ASN
4	H	112	GLN
4	H	203	ASN
4	H	206	HIS
5	L	2	GLN
5	L	5	GLN
5	L	37	GLN
5	L	78	GLN

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Mol	Chain	Res	Type
5	L	123	GLN
5	L	137	ASN
5	L	160	ASN
1	M	87	GLN
1	M	114	GLN
1	M	174	ASN
2	N	38	GLN
4	Q	61	GLN
4	Q	112	GLN
5	R	2	GLN
5	R	36	GLN
5	R	78	GLN
5	R	160	ASN
5	R	189	ASN
5	R	209	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 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	274/274 (100%)	0.13	4 (1%)	73	73	24, 35, 53, 59	0
1	M	274/274 (100%)	0.22	6 (2%)	62	59	35, 46, 54, 62	0
2	B	99/99 (100%)	-0.15	0	100	100	27, 36, 43, 45	0
2	N	99/99 (100%)	0.19	2 (2%)	65	63	34, 45, 53, 63	0
3	C	8/8 (100%)	-0.01	0	100	100	25, 26, 28, 29	0
3	O	8/8 (100%)	0.20	0	100	100	47, 50, 51, 51	0
4	H	213/219 (97%)	-0.05	0	100	100	18, 28, 37, 43	0
4	Q	210/219 (95%)	0.78	25 (11%)	4	3	47, 56, 77, 89	0
5	L	209/209 (100%)	-0.03	0	100	100	17, 30, 41, 51	0
5	R	209/209 (100%)	1.29	51 (24%)	0	0	51, 60, 67, 70	0
All	All	1603/1618 (99%)	0.32	88 (5%)	25	21	17, 43, 65, 89	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	112	PRO	7.3
5	R	179	THR	6.6
5	R	191	TYR	6.4
5	R	209	ASN	6.0
4	Q	119	SER	5.9
5	R	178	LEU	5.8
1	M	197	ASP	5.3
5	R	172	TYR	5.2
5	R	204	ILE	5.1
5	R	144	ASN	5.0
4	Q	143	VAL	4.8
2	N	1	ILE	4.4
4	Q	216	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	226	GLN	4.2
5	R	151	GLY	4.0
5	R	130	SER	4.0
4	Q	189	THR	3.9
5	R	192	THR	3.8
5	R	194	GLU	3.8
5	R	188	HIS	3.7
5	R	162	TRP	3.7
1	A	198	LYS	3.7
4	Q	218	VAL	3.5
5	R	187	ARG	3.5
5	R	205	VAL	3.4
4	Q	199	THR	3.4
5	R	189	ASN	3.4
5	R	202	SER	3.4
4	Q	211	THR	3.3
5	R	154	ARG	3.3
5	R	195	ALA	3.3
4	Q	129	TYR	3.3
5	R	105	LEU	3.3
5	R	134	PHE	3.1
4	Q	120	ALA	3.1
1	M	195	PRO	3.0
5	R	149	ILE	3.0
5	R	177	THR	3.0
5	R	7	SER	3.0
2	N	98	ASP	3.0
5	R	114	VAL	3.0
1	M	251	LEU	2.9
4	Q	131	LEU	2.9
5	R	150	ASP	2.8
5	R	152	SER	2.8
1	M	249	VAL	2.8
5	R	74	ILE	2.7
5	R	200	SER	2.7
5	R	142	ASP	2.7
5	R	86	TYR	2.7
5	R	155	GLN	2.6
4	Q	121	ALA	2.6
4	Q	210	SER	2.6
4	Q	154	PRO	2.6
5	R	153	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
5	R	198	LYS	2.6
4	Q	197	SER	2.6
5	R	145	VAL	2.6
5	R	157	GLY	2.5
5	R	143	ILE	2.5
5	R	109	ASP	2.4
5	R	197	HIS	2.4
5	R	20	ILE	2.4
1	A	252	GLY	2.3
4	Q	59	TYR	2.3
4	Q	122	LYS	2.3
5	R	9	SER	2.3
5	R	141	LYS	2.3
5	R	73	ILE	2.3
5	R	186	GLU	2.3
4	Q	198	GLU	2.3
5	R	10	PHE	2.3
4	Q	145	LEU	2.3
4	Q	190	VAL	2.2
5	R	13	SER	2.2
4	Q	177	LEU	2.2
4	Q	175	ALA	2.2
1	A	249	VAL	2.2
4	Q	153	PHE	2.2
1	M	255	GLN	2.2
5	R	158	VAL	2.2
5	R	77	LEU	2.1
1	M	139	ALA	2.1
4	Q	130	PRO	2.1
5	R	18	VAL	2.1
5	R	129	ALA	2.0
4	Q	144	THR	2.0
4	Q	10	LEU	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.