



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 PM UTC

PDB ID : 3CVH / pdb_00003cvh
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

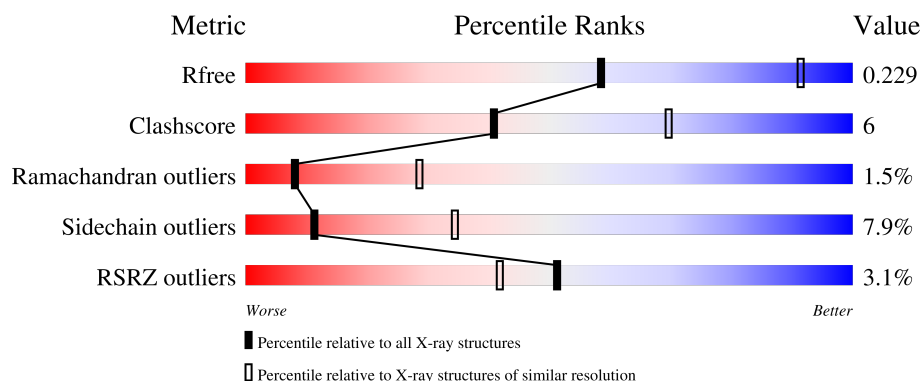
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	
1	M	274	
2	B	99	
2	N	99	
3	C	8	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	8	 75% 25%
4	H	219	 75% 18% . .
4	Q	219	 11% 80% 14% . .
5	L	209	 82% 17% .
5	R	209	 9% 71% 24% 5%

2 Entry composition

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
1	A	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			
1	M	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			

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

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

- Molecule 3 is a protein called Ovalbumin.

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

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

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

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

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

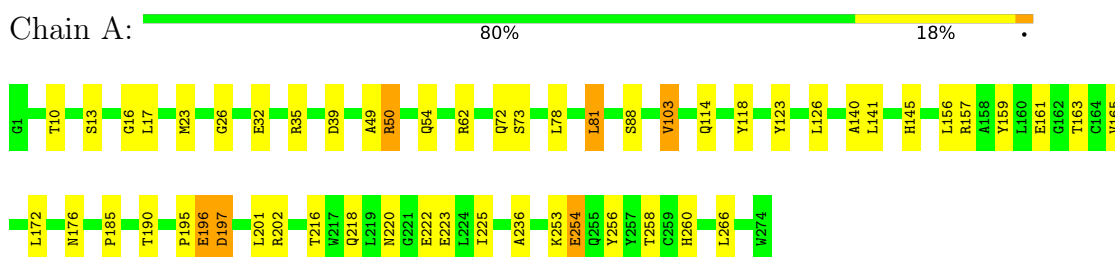
- Molecule 6 is water.

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

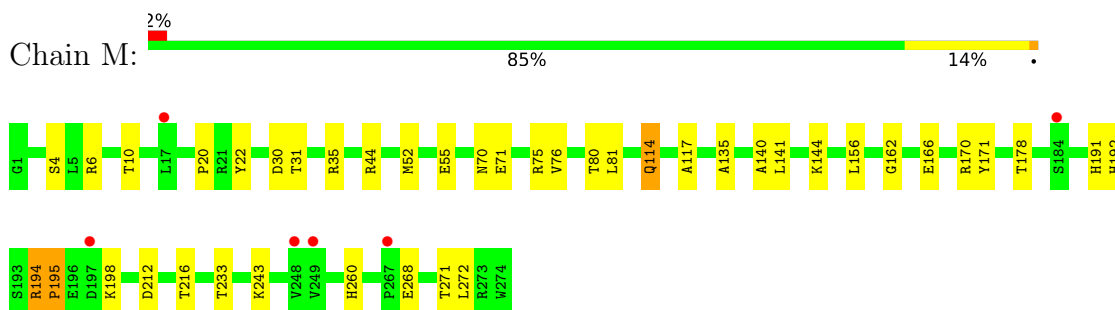
3 Residue-property plots

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.

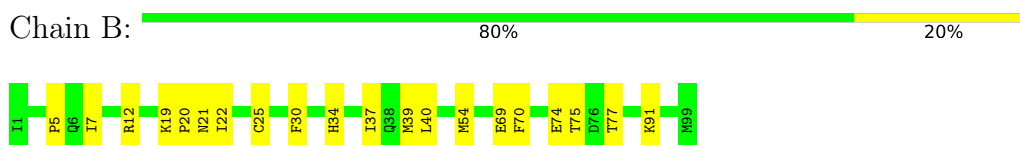
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



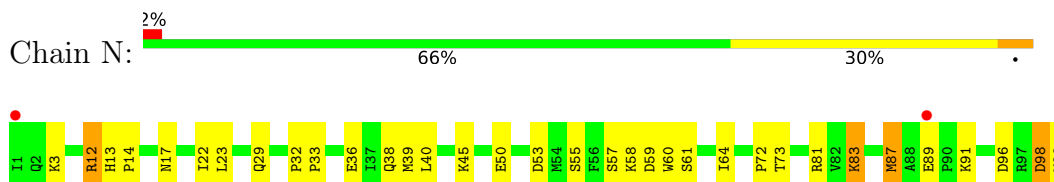
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain



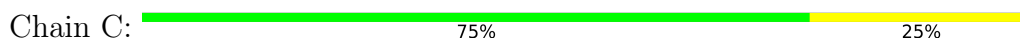
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

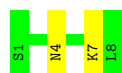
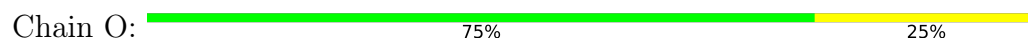


- Molecule 3: Ovalbumin

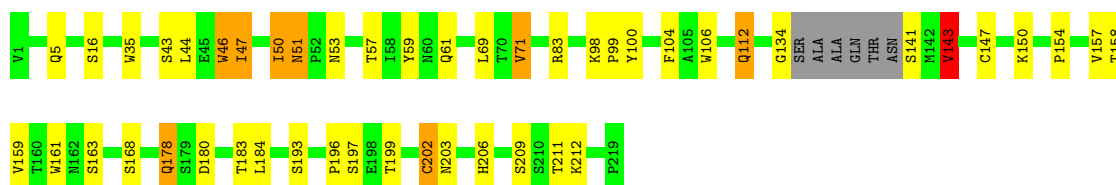
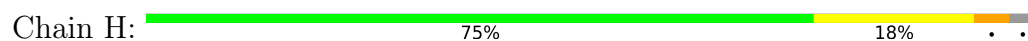




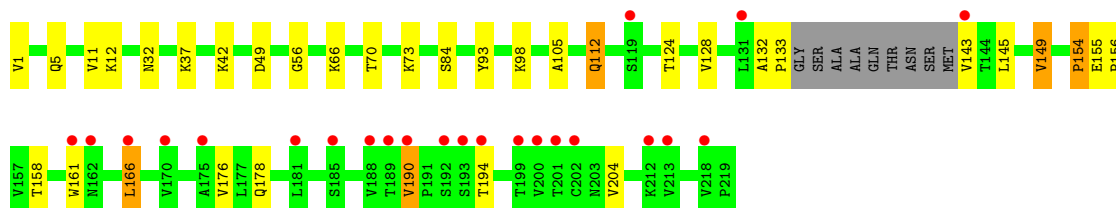
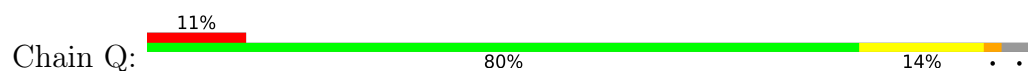
- Molecule 3: Ovalbumin



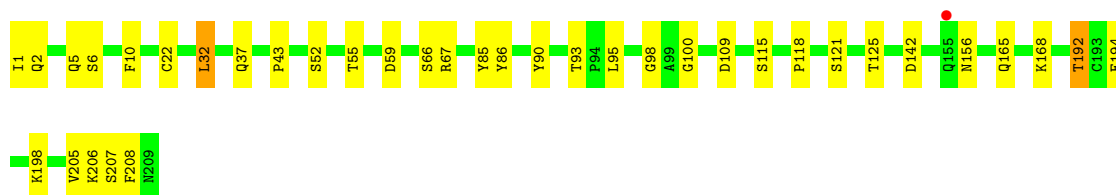
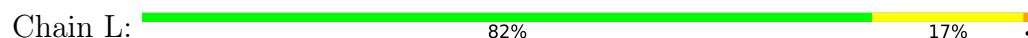
- Molecule 4: 25-D1.16 heavy chain



- Molecule 4: 25-D1.16 heavy chain

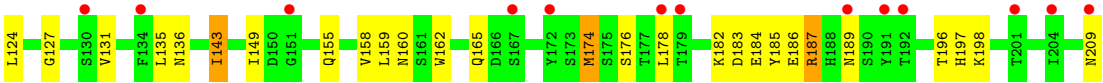


- Molecule 5: 25-D1.16 light chain



- Molecule 5: 25-D1.16 light chain





4 Data and refinement statistics

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 19.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.90) 97.7 (19.98-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.296 0.222 , 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)	0.29 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.52	0/2293	0.79	0/3113
1	M	0.46	0/2293	0.78	0/3113
2	B	0.54	0/847	0.75	0/1148
2	N	0.46	0/847	0.75	0/1148
3	C	0.51	0/68	0.87	0/88
3	O	0.54	0/68	0.88	0/88
4	H	0.58	0/1665	0.84	1/2277 (0.0%)
4	Q	0.52	0/1647	0.78	0/2254
5	L	0.54	0/1660	0.78	0/2256
5	R	0.52	0/1660	0.77	3/2256 (0.1%)
All	All	0.52	0/13048	0.79	4/17741 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	28	ILE	N-CA-C	5.21	117.12	112.17
4	H	143	VAL	N-CA-C	5.15	120.05	109.34
5	R	118	PRO	CA-C-N	5.12	126.23	119.84
5	R	118	PRO	C-N-CA	5.12	126.23	119.84

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	2232	0	2123	34	0
1	M	2232	0	2123	20	0
2	B	821	0	796	8	0
2	N	821	0	796	19	0
3	C	68	0	74	1	0
3	O	68	0	74	1	0
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	25	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	162	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 (162) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:N:99:MET:C	2:N:99:MET:SD	2.86	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
4:H:50:ILE:HG23	4:H:57:THR:HG22	1.90	0.53
5:R:174:MET:HE3	5:R:176:SER:HB2	1.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:MET:HE1	1:M:171:TYR:CE1	2.45	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
2:N:87:MET:HE1	2:N:91:LYS:HD2	1.92	0.51
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
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
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
1:A:49:ALA:O	1:A:50:ARG:C	2.56	0.48
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:A:157:ARG:HE	1:A:161:GLU:CD	2.23	0.46
4:H:184:LEU:HD12	4:H:184:LEU:C	2.40	0.46
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
2:B:25:CYS:HB2	2:B:39:MET:HE3	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:184:GLU:HA	5:R:187:ARG:HH21	1.81	0.46
1:A:32:GLU:CD	1:A:35:ARG:HH11	2.22	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
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
2:N:23:LEU:HD23	2:N:39:MET:HE2	1.99	0.45
4:H:178:GLN:HE21	4:H:183:THR:HG1	1.60	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
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
4:H:5:GLN:N	4:H:112:GLN:HE22	2.04	0.44
4:H:196:PRO:O	4:H:197:SER:C	2.61	0.43
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:13:HIS:O	2:N:14:PRO:C	2.60	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
4:H:16:SER:CB	4:H:83:ARG:HA	2.49	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
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
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%)	5 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	30	59
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%)	6	23
4	Q	206/219 (94%)	185 (90%)	19 (9%)	2 (1%)	12	39
5	L	207/209 (99%)	199 (96%)	6 (3%)	2 (1%)	12	39
5	R	207/209 (99%)	180 (87%)	19 (9%)	8 (4%)	2	10
All	All	1579/1618 (98%)	1458 (92%)	98 (6%)	23 (2%)	8	28

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 ⓘ

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%)	224 (97%)	8 (3%)	32	66
1	M	232/232 (100%)	216 (93%)	16 (7%)	14	41
2	B	94/94 (100%)	87 (93%)	7 (7%)	13	38
2	N	94/94 (100%)	84 (89%)	10 (11%)	6	22
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	15
3	O	8/8 (100%)	7 (88%)	1 (12%)	4	15
4	H	182/186 (98%)	168 (92%)	14 (8%)	12	35
4	Q	180/186 (97%)	163 (91%)	17 (9%)	8	26
5	L	186/186 (100%)	170 (91%)	16 (9%)	10	30
5	R	186/186 (100%)	165 (89%)	21 (11%)	5	19
All	All	1402/1412 (99%)	1291 (92%)	111 (8%)	11	34

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	73	SER
1	A	81	LEU
1	A	88	SER
1	A	103	VAL
1	A	141	LEU
1	A	225	ILE
1	A	254	GLU
2	B	22	ILE
2	B	37	ILE
2	B	40	LEU
2	B	69	GLU
2	B	74	GLU
2	B	75	THR
2	B	77	THR
3	C	7	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	50	ILE
4	H	51	ASN
4	H	61	GLN
4	H	71	VAL
4	H	112	GLN
4	H	147	CYS
4	H	157	VAL
4	H	158	THR
4	H	168	SER
4	H	180	ASP
4	H	193	SER
4	H	199	THR
4	H	202	CYS
4	H	212	LYS
5	L	2	GLN
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	93	THR
5	L	95	LEU
5	L	115	SER
5	L	142	ASP
5	L	156	ASN
5	L	165	GLN
5	L	168	LYS
5	L	192	THR
5	L	206	LYS
1	M	4	SER
1	M	10	THR
1	M	31	THR
1	M	80	THR
1	M	81	LEU
1	M	114	GLN
1	M	141	LEU
1	M	144	LYS
1	M	156	LEU
1	M	178	THR
1	M	191	HIS
1	M	194	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	212	ASP
1	M	268	GLU
1	M	271	THR
1	M	272	LEU
2	N	12	ARG
2	N	50	GLU
2	N	55	SER
2	N	57	SER
2	N	64	ILE
2	N	73	THR
2	N	83	LYS
2	N	87	MET
2	N	89	GLU
2	N	98	ASP
3	O	4	ASN
4	Q	1	VAL
4	Q	11	VAL
4	Q	12	LYS
4	Q	42	LYS
4	Q	49	ASP
4	Q	66	LYS
4	Q	70	THR
4	Q	73	LYS
4	Q	112	GLN
4	Q	124	THR
4	Q	145	LEU
4	Q	149	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	109	ASP
5	R	122	GLU
5	R	131	VAL
5	R	143	ILE
5	R	174	MET
5	R	183	ASP
5	R	187	ARG
5	R	189	ASN
5	R	196	THR
5	R	198	LYS
5	R	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	226	GLN
1	A	255	GLN
1	A	264	GLN
2	B	13	HIS
2	B	29	GLN
3	C	4	ASN
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	41	ASN
5	L	78	GLN
5	L	123	GLN
5	L	136	ASN
5	L	137	ASN
5	L	160	ASN
5	L	188	HIS
1	M	54	GLN
1	M	114	GLN
1	M	174	ASN
1	M	192	HIS
1	M	255	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	264	GLN
2	N	29	GLN
2	N	38	GLN
4	Q	61	GLN
4	Q	112	GLN
4	Q	178	GLN
5	R	2	GLN
5	R	78	GLN
5	R	160	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 oligosaccharides 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 ⓘ

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, 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%)	-0.18	0 100 100	24, 35, 53, 59	0
1	M	274/274 (100%)	0.13	6 (2%) 62 53	35, 46, 54, 62	0
2	B	99/99 (100%)	-0.34	0 100 100	27, 36, 43, 45	0
2	N	99/99 (100%)	-0.14	2 (2%) 65 56	34, 45, 53, 63	0
3	C	8/8 (100%)	-0.47	0 100 100	25, 26, 28, 29	0
3	O	8/8 (100%)	-0.05	0 100 100	47, 50, 51, 51	0
4	H	213/219 (97%)	-0.45	0 100 100	18, 28, 37, 43	0
4	Q	210/219 (95%)	0.71	23 (10%) 10 9	47, 56, 77, 89	0
5	L	209/209 (100%)	-0.40	1 (0%) 87 83	17, 30, 41, 51	0
5	R	209/209 (100%)	0.75	18 (8%) 16 13	51, 60, 67, 70	0
All	All	1603/1618 (99%)	0.04	50 (3%) 51 42	17, 43, 65, 89	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	119	SER	5.8
5	R	112	PRO	5.5
5	R	172	TYR	4.4
1	M	197	ASP	4.0
4	Q	213	VAL	3.9
4	Q	189	THR	3.8
5	R	189	ASN	3.7
5	R	204	ILE	3.7
5	R	192	THR	3.6
5	R	191	TYR	3.5
5	R	130	SER	3.3
5	R	209	ASN	3.2
1	M	248	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	170	VAL	2.9
4	Q	194	THR	2.9
1	M	249	VAL	2.7
5	R	119	PRO	2.7
5	R	151	GLY	2.7
4	Q	143	VAL	2.7
5	R	109	ASP	2.6
1	M	184	SER	2.6
5	R	79	THR	2.6
4	Q	192	SER	2.6
5	R	167	SER	2.6
4	Q	181	LEU	2.5
1	M	17	LEU	2.5
4	Q	162	ASN	2.5
4	Q	212	LYS	2.4
4	Q	175	ALA	2.4
5	L	155	GLN	2.4
4	Q	199	THR	2.4
4	Q	131	LEU	2.4
5	R	134	PHE	2.4
4	Q	161	TRP	2.3
4	Q	218	VAL	2.3
5	R	111	ALA	2.3
2	N	89	GLU	2.2
4	Q	190	VAL	2.2
5	R	179	THR	2.2
1	M	267	PRO	2.2
4	Q	188	VAL	2.2
4	Q	166	LEU	2.2
4	Q	200	VAL	2.2
4	Q	185	SER	2.2
5	R	178	LEU	2.1
4	Q	193	SER	2.1
2	N	1	ILE	2.1
4	Q	202	CYS	2.1
4	Q	201	THR	2.0
5	R	201	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.