



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:52 pm GMT

PDB ID : 3WKM
Title : The periplasmic PDZ tandem fragment of the RseP homologue from Aquifex
aeolicus in complex with the Fab fragment
Authors : Nogi, T.; Tabata, S.; Tamura-kawakami, K.; Takagi, J.
Deposited on : 2013-10-28
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

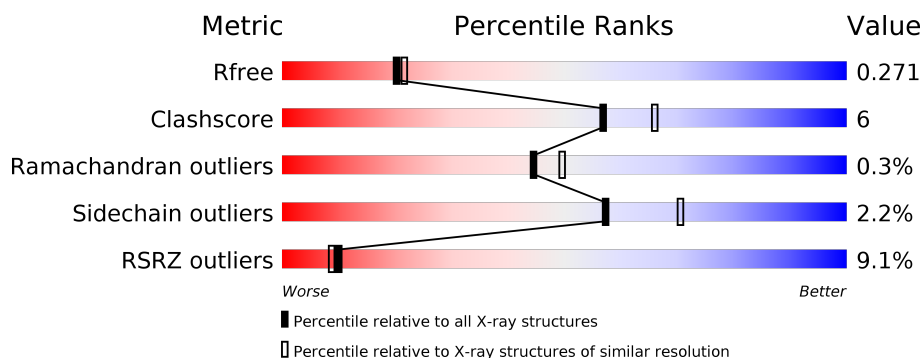
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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	180	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 77% 20% .. </div> </div>
1	B	180	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 14% .. </div> </div>
2	H	225	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 5% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 12% . </div> </div>
2	I	225	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 20% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 78% 8% 14% </div> </div>
3	L	218	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 86% 12% .. </div> </div>
3	M	218	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 21% </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 13% .. </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9781 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 Putative zinc metalloprotease aq_1964.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	6	0
			1433	928	249	255	1			
1	B	179	Total	C	N	O	S	0	3	0
			1427	922	245	259	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLY	-	EXPRESSION TAG	UNP O67776
A	114	SER	-	EXPRESSION TAG	UNP O67776
B	113	GLY	-	EXPRESSION TAG	UNP O67776
B	114	SER	-	EXPRESSION TAG	UNP O67776

- Molecule 2 is a protein called MOUSE IGG1-KAPPA FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	1	0
			1647	1042	271	327	7			
2	I	194	Total	C	N	O	S	0	3	0
			1502	947	250	299	6			

- Molecule 3 is a protein called MOUSE IGG1-KAPPA FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	3	0
			1692	1056	284	345	7			
3	M	214	Total	C	N	O	S	0	4	0
			1693	1057	283	346	7			

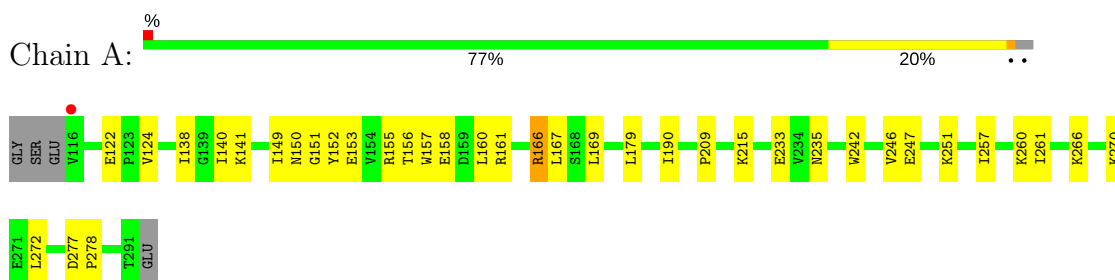
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	67	Total O 67 67	0	0
4	H	71	Total O 71 71	0	0
4	L	87	Total O 87 87	0	0
4	B	53	Total O 53 53	0	0
4	I	49	Total O 49 49	0	0
4	M	60	Total O 60 60	0	0

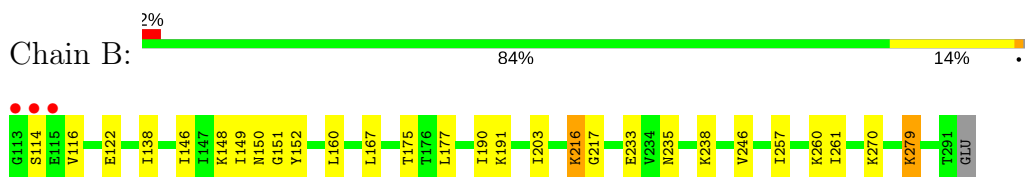
3 Residue-property plots

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

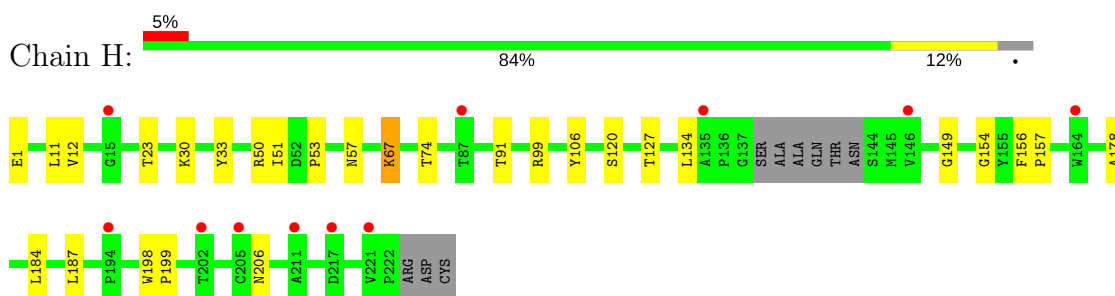
- Molecule 1: Putative zinc metalloprotease aq_1964



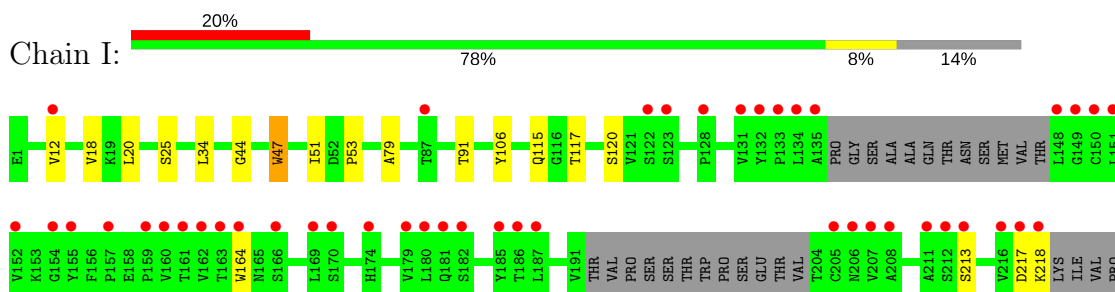
- Molecule 1: Putative zinc metalloprotease aq_1964



- Molecule 2: MOUSE IGG1-KAPPA FAB (HEAVY CHAIN)

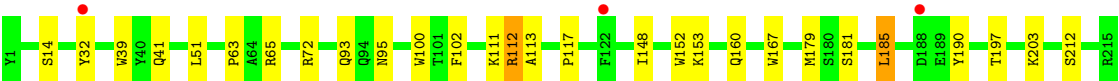
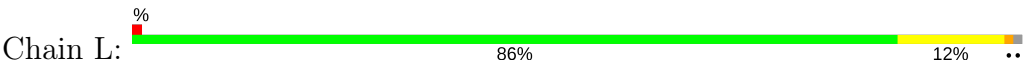


- Molecule 2: MOUSE IGG1-KAPPA FAB (HEAVY CHAIN)



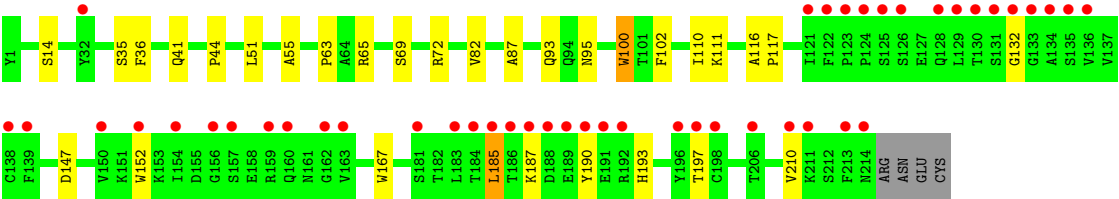
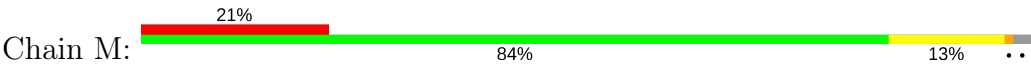
ARG
ASP
CYS

• Molecule 3: MOUSE IGG1-KAPPA FAB (LIGHT CHAIN)



ASN
GLU
CYS

• Molecule 3: MOUSE IGG1-KAPPA FAB (LIGHT CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.24Å 86.04Å 92.54Å 100.84° 96.92° 101.32°	Depositor
Resolution (Å)	47.44 – 2.20 47.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.44-2.20) 91.1 (47.44-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.272 0.224 , 0.271	Depositor DCC
R_{free} test set	3771 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9781	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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	0.45	1/1456 (0.1%)	0.58	0/1960
1	B	0.46	0/1450	0.59	0/1954
2	H	0.53	0/1690	0.59	0/2312
2	I	0.52	2/1538 (0.1%)	0.56	0/2097
3	L	0.52	3/1732 (0.2%)	0.63	0/2357
3	M	0.51	3/1733 (0.2%)	0.60	0/2358
All	All	0.50	9/9599 (0.1%)	0.59	0/13038

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	167	TRP	CD2-CE2	5.48	1.48	1.41
3	M	167	TRP	CD2-CE2	5.30	1.47	1.41
3	L	39	TRP	CD2-CE2	5.16	1.47	1.41
3	M	152	TRP	CD2-CE2	5.16	1.47	1.41
2	I	164	TRP	CD2-CE2	5.09	1.47	1.41
2	I	47	TRP	CD2-CE2	5.08	1.47	1.41
1	A	157	TRP	CD2-CE2	5.08	1.47	1.41
3	M	100	TRP	CD2-CE2	5.04	1.47	1.41
3	L	152	TRP	CD2-CE2	5.03	1.47	1.41

There are no bond angle outliers.

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	1433	0	1547	36	0
1	B	1427	0	1528	31	0
2	H	1647	0	1600	14	0
2	I	1502	0	1447	10	0
3	L	1692	0	1610	11	0
3	M	1693	0	1609	17	0
4	A	67	0	0	2	0
4	B	53	0	0	1	0
4	H	71	0	0	1	0
4	I	49	0	0	0	0
4	L	87	0	0	0	0
4	M	60	0	0	4	0
All	All	9781	0	9341	107	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 (107) 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:138[B]:ILE:CD1	1:B:138[B]:ILE:HD12	1.76	1.15
1:A:138[B]:ILE:HD12	1:B:138[B]:ILE:CD1	1.83	1.08
2:H:23:THR:HG22	4:H:316:HOH:O	1.54	1.03
1:A:138[B]:ILE:HD12	1:B:138[B]:ILE:HD12	1.37	1.03
1:A:150:ASN:CG	1:A:151:GLY:H	1.65	0.96
1:B:150:ASN:CG	1:B:151:GLY:H	1.79	0.83
1:A:138[B]:ILE:HD11	1:B:138[B]:ILE:HD12	1.60	0.80
1:A:150:ASN:CG	1:A:151:GLY:N	2.35	0.79
4:A:2006:HOH:O	1:B:191:LYS:HE3	1.82	0.78
2:I:115[A]:GLN:O	2:I:115[A]:GLN:HG3	1.81	0.78
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.68	0.75
1:B:138[A]:ILE:HG23	4:B:328:HOH:O	1.86	0.75
1:A:150:ASN:HD21	1:A:152:TYR:HD1	1.34	0.74
1:A:138[A]:ILE:HD13	1:A:190:ILE:CG2	2.19	0.72
1:B:150:ASN:CG	1:B:151:GLY:N	2.42	0.71
1:B:150:ASN:HD21	1:B:152:TYR:HD1	1.36	0.70
1:A:138[A]:ILE:HD13	1:A:190:ILE:HG22	1.78	0.66
2:I:20:LEU:HD22	2:I:117:THR:HG21	1.78	0.64
3:L:112:ARG:HD3	3:L:113:ALA:O	1.98	0.64
1:B:149:ILE:O	1:B:150:ASN:ND2	2.31	0.63
1:A:179[B]:LEU:C	1:A:179[B]:LEU:HD12	2.18	0.63
1:A:149:ILE:O	1:A:150:ASN:ND2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:HD12	1:B:177:LEU:HD21	1.82	0.62
1:B:138[A]:ILE:HD13	1:B:190:ILE:HG22	1.82	0.62
3:L:93:GLN:HG3	3:L:102:PHE:CE1	2.35	0.61
1:A:138[B]:ILE:CD1	1:B:138[B]:ILE:CD1	2.53	0.61
1:A:158:GLU:HG3	1:A:161[B]:ARG:NH2	2.16	0.59
1:A:235:ASN:HD21	1:A:257:ILE:HG22	1.66	0.59
3:M:95:ASN:HB2	3:M:100:TRP:CE2	2.38	0.59
1:A:150:ASN:OD1	1:A:151:GLY:N	2.21	0.59
1:B:122[B]:GLU:N	1:B:122[B]:GLU:OE2	2.36	0.58
1:B:138[B]:ILE:HG13	1:B:138[B]:ILE:O	2.03	0.58
3:L:63:PRO:HB2	3:L:65:ARG:HG2	1.86	0.58
3:M:111:LYS:HE2	4:M:321:HOH:O	2.03	0.58
1:B:138[A]:ILE:HD13	1:B:190:ILE:CG2	2.34	0.57
1:A:209:PRO:HA	1:A:242:TRP:HE3	1.71	0.56
1:A:138[B]:ILE:HD12	1:B:138[B]:ILE:HD11	1.85	0.54
2:H:30:LYS:HE3	2:H:74:THR:HG21	1.89	0.54
3:M:44:PRO:HA	4:M:305:HOH:O	2.06	0.54
3:M:87:ALA:HB2	3:M:110:ILE:HD12	1.89	0.54
3:L:185:LEU:HD13	3:L:190:TYR:HB2	1.89	0.53
2:H:67:LYS:NZ	2:H:67:LYS:HB2	2.21	0.53
1:A:150:ASN:ND2	1:A:167:LEU:HD21	2.24	0.53
1:B:150:ASN:OD1	1:B:151:GLY:N	2.28	0.53
1:B:233:GLU:HG2	1:B:238:LYS:HD2	1.89	0.53
4:A:2052:HOH:O	2:H:99:ARG:HD2	2.11	0.51
1:B:160:LEU:HD21	1:B:203:ILE:HD11	1.92	0.51
3:M:63:PRO:HB2	3:M:65:ARG:HG2	1.93	0.51
1:A:179[B]:LEU:O	1:A:179[B]:LEU:HD12	2.11	0.50
3:M:41:GLN:HB2	3:M:51:LEU:HD11	1.92	0.50
3:M:93:GLN:HG3	3:M:102:PHE:CE1	2.46	0.50
2:H:154:GLY:HA2	2:H:184:LEU:HB3	1.94	0.50
2:H:11:LEU:HD22	2:H:157:PRO:HD3	1.94	0.50
1:A:261:ILE:HD12	1:A:270:LYS:HG3	1.94	0.50
2:H:178:ALA:HA	2:H:187:LEU:HB3	1.93	0.50
2:I:91:THR:HG23	2:I:120:SER:HA	1.93	0.50
1:B:261:ILE:HD12	1:B:270:LYS:HG3	1.94	0.49
2:I:47:TRP:CD2	3:M:100:TRP:HB2	2.48	0.49
2:I:44:GLY:HA3	4:M:356:HOH:O	2.13	0.49
2:H:91:THR:HG23	2:H:120:SER:HA	1.94	0.48
1:A:233:GLU:HB3	1:A:260:LYS:HB2	1.95	0.48
1:A:153:GLU:OE1	1:A:155:ARG:NH2	2.47	0.47
1:A:246:VAL:HG21	2:H:106:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:117:PRO:HG3	3:L:148:ILE:HD11	1.96	0.47
3:M:185:LEU:HD13	3:M:190:TYR:HB2	1.96	0.47
1:A:150:ASN:ND2	1:A:152:TYR:CD1	2.64	0.47
1:B:279:LYS:HD2	3:M:36:PHE:CZ	2.49	0.47
1:A:166[A]:ARG:HH12	1:A:169:LEU:HB2	1.80	0.46
1:B:116:VAL:HG12	4:M:333:HOH:O	2.14	0.46
1:A:150:ASN:HD22	1:A:167:LEU:HD11	1.80	0.46
1:B:114:SER:HB3	3:M:69:SER:HA	1.97	0.46
3:M:132:GLY:HA2	3:M:187:LYS:HE3	1.98	0.46
2:I:115[A]:GLN:O	2:I:115[A]:GLN:CG	2.59	0.46
2:I:34:LEU:HD12	2:I:79:ALA:HB2	1.98	0.46
3:L:153:LYS:HB2	3:L:197:THR:HB	1.98	0.45
3:L:95:ASN:HB2	3:L:100:TRP:CE2	2.51	0.45
3:L:14:SER:HA	3:L:111:LYS:HB3	1.98	0.45
3:M:35:SER:HB2	3:M:55:ALA:HB2	1.98	0.45
3:M:14:SER:HA	3:M:111:LYS:HB3	1.99	0.45
1:A:124:VAL:HG11	1:A:160:LEU:HD22	1.98	0.44
2:H:134:LEU:HD12	2:H:149:GLY:HA3	1.99	0.44
3:M:187:LYS:HA	3:M:190:TYR:HB3	1.98	0.44
1:A:277:ASP:HA	1:A:278:PRO:HD3	1.85	0.43
2:H:33:TYR:CD2	2:H:50:ARG:HD2	2.53	0.43
1:A:247:GLU:O	1:A:251:LYS:HG3	2.19	0.43
2:H:198:TRP:HA	2:H:199:PRO:HA	1.85	0.43
1:A:122:GLU:O	1:A:156:THR:HA	2.19	0.43
1:B:235:ASN:HD21	1:B:257:ILE:HG22	1.83	0.43
1:B:216:LYS:HE2	1:B:217:GLY:N	2.34	0.43
1:B:150:ASN:HD22	1:B:167:LEU:HD11	1.85	0.42
1:B:150:ASN:ND2	1:B:167:LEU:HD11	2.34	0.42
3:M:197:THR:HG23	3:M:210:VAL:HG13	2.02	0.42
1:A:150:ASN:ND2	1:A:167:LEU:HD11	2.35	0.42
1:B:148:LYS:HE2	1:B:151:GLY:HA2	2.02	0.42
1:A:150:ASN:CG	1:A:167:LEU:HD21	2.40	0.42
1:A:215:LYS:HG3	3:L:32:TYR:CZ	2.54	0.41
1:A:138[B]:ILE:HG23	1:A:138[B]:ILE:O	2.20	0.41
2:I:12:VAL:HG11	2:I:18:VAL:HB	2.01	0.41
1:A:138[A]:ILE:HD11	1:A:140:ILE:HD11	2.02	0.41
1:B:246:VAL:HG21	2:I:106:TYR:CD1	2.55	0.41
1:A:257:ILE:HG13	1:A:272:LEU:HD23	2.03	0.41
2:I:51:ILE:O	2:I:53:PRO:HD3	2.21	0.41
3:L:179:MET:HE3	3:L:181:SER:HB2	2.03	0.40
2:H:156:PHE:HA	2:H:157:PRO:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HB3	1:B:175:THR:OG1	2.21	0.40
2:H:51:ILE:O	2:H:53:PRO:HD3	2.21	0.40
3:M:116:ALA:HA	3:M:117:PRO:HD2	1.96	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	180/180 (100%)	177 (98%)	3 (2%)	0	100	100
1	B	180/180 (100%)	174 (97%)	6 (3%)	0	100	100
2	H	213/225 (95%)	202 (95%)	11 (5%)	0	100	100
2	I	191/225 (85%)	181 (95%)	9 (5%)	1 (0%)	32	34
3	L	216/218 (99%)	209 (97%)	5 (2%)	2 (1%)	20	18
3	M	216/218 (99%)	202 (94%)	12 (6%)	2 (1%)	20	18
All	All	1196/1246 (96%)	1145 (96%)	46 (4%)	5 (0%)	44	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	203	LYS
3	L	72	ARG
2	I	213	SER
3	M	72[A]	ARG
3	M	72[B]	ARG

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	158/155 (102%)	154 (98%)	4 (2%)	53	65
1	B	157/155 (101%)	154 (98%)	3 (2%)	62	76
2	H	187/193 (97%)	181 (97%)	6 (3%)	44	56
2	I	168/193 (87%)	165 (98%)	3 (2%)	64	77
3	L	192/192 (100%)	188 (98%)	4 (2%)	59	72
3	M	192/192 (100%)	187 (97%)	5 (3%)	51	64
All	All	1054/1080 (98%)	1029 (98%)	25 (2%)	57	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	A	166[A]	ARG
1	A	166[B]	ARG
1	A	266	LYS
2	H	1	GLU
2	H	12	VAL
2	H	57	ASN
2	H	67	LYS
2	H	127	THR
2	H	206	ASN
3	L	112	ARG
3	L	160	GLN
3	L	185	LEU
3	L	212	SER
1	B	216	LYS
1	B	260	LYS
1	B	279	LYS
2	I	25	SER
2	I	217	ASP
2	I	218	LYS
3	M	82[A]	VAL
3	M	82[B]	VAL

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Mol	Chain	Res	Type
3	M	147	ASP
3	M	185	LEU
3	M	193	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	96	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

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	176/180 (97%)	-0.11	1 (0%) 89 88	20, 30, 44, 59	0
1	B	179/180 (99%)	-0.04	3 (1%) 70 68	21, 31, 53, 78	0
2	H	216/225 (96%)	0.33	11 (5%) 29 27	18, 43, 67, 75	0
2	I	194/225 (86%)	0.91	45 (23%) 1 1	20, 47, 90, 102	0
3	L	215/218 (98%)	0.14	3 (1%) 75 73	16, 32, 56, 66	0
3	M	214/218 (98%)	0.91	46 (21%) 1 1	17, 35, 100, 110	0
All	All	1194/1246 (95%)	0.38	109 (9%) 10 9	16, 34, 85, 110	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	GLY	7.4
3	M	124	PRO	6.2
3	M	121	ILE	6.0
2	I	182	SER	6.0
3	M	123	PRO	5.8
3	M	154	ILE	5.6
3	M	131	SER	5.6
3	M	213	PHE	5.6
2	I	134	LEU	5.4
2	I	207	VAL	5.3
2	I	216	VAL	5.1
3	M	192	ARG	5.1
3	M	122	PHE	5.0
3	M	198	CYS	4.9
3	M	196	TYR	4.9
3	M	152	TRP	4.8
2	I	133	PRO	4.7
3	M	191	GLU	4.6
3	M	136	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
2	I	132	TYR	4.5
3	M	132	GLY	4.4
2	I	148	LEU	4.4
2	I	160	VAL	4.3
3	M	138	CYS	4.3
2	I	166	SER	4.2
2	I	169	LEU	4.2
3	M	188	ASP	4.1
3	M	159	ARG	4.1
3	M	210	VAL	4.0
3	M	184	THR	4.0
2	I	208	ALA	3.9
2	I	151	LEU	3.9
3	M	214	ASN	3.9
2	I	154	GLY	3.9
2	H	135	ALA	3.8
3	M	130	THR	3.8
3	M	160	GLN	3.7
2	I	162	VAL	3.7
3	M	157	SER	3.6
2	I	159	PRO	3.6
2	H	202	THR	3.5
3	M	125	SER	3.4
2	H	194	PRO	3.4
2	I	150	CYS	3.4
2	I	128	PRO	3.2
3	M	133	GLY	3.2
2	I	205	CYS	3.2
2	I	135	ALA	3.2
3	M	185	LEU	3.2
3	M	183	LEU	3.1
3	M	181	SER	3.1
2	I	170	SER	3.1
3	M	211	LYS	3.0
3	M	189	GLU	3.0
3	L	32	TYR	3.0
2	I	185	TYR	3.0
3	M	128	GLN	2.9
2	H	211	ALA	2.9
2	I	206	ASN	2.9
2	I	211	ALA	2.9
2	I	157	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	114	SER	2.8
2	I	213	SER	2.8
3	M	139	PHE	2.8
2	I	179	VAL	2.8
3	M	134	ALA	2.8
2	I	164	TRP	2.8
3	M	190	TYR	2.8
2	H	146	VAL	2.8
2	I	181	GLN	2.7
2	I	87	THR	2.7
3	M	150	VAL	2.7
3	M	129	LEU	2.7
3	M	32	TYR	2.7
2	I	152	VAL	2.7
2	H	87	THR	2.7
2	H	15	GLY	2.6
3	M	186	THR	2.6
3	M	187	LYS	2.5
2	I	131	VAL	2.4
3	M	197	THR	2.4
2	I	12	VAL	2.4
2	H	221	VAL	2.4
2	I	217	ASP	2.4
2	I	163	THR	2.3
2	I	122	SER	2.3
3	M	126	SER	2.3
2	I	212	SER	2.3
2	I	161	THR	2.3
3	M	206	THR	2.3
3	M	163	VAL	2.3
2	I	123	SER	2.3
3	M	156	GLY	2.2
2	I	149	GLY	2.2
3	M	162	GLY	2.2
2	H	164	TRP	2.2
2	I	186	THR	2.2
1	A	116	VAL	2.2
3	L	122	PHE	2.2
2	H	217	ASP	2.2
1	B	115	GLU	2.1
2	I	174	HIS	2.1
3	L	188	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	155	TYR	2.1
3	M	135	SER	2.1
2	I	218	LYS	2.1
2	H	205	CYS	2.0
2	I	180	LEU	2.0
2	I	187	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 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.