



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:41 AM UTC

PDB ID : 3WKM / pdb_00003wkm
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

<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

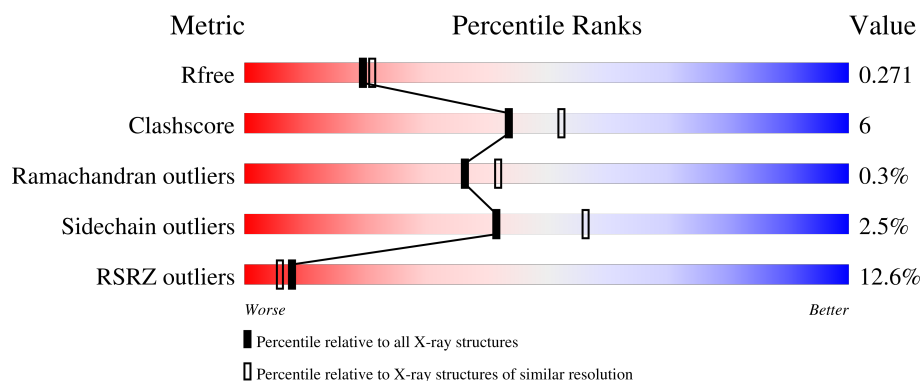
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	180	2% 77% 20% ..
1	B	180	4% 83% 15% ..
2	H	225	10% 82% 13% .
2	I	225	25% 78% 8% 14%
3	L	218	3% 87% 11% ..

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Mol	Chain	Length	Quality of chain
3	M	218	24% 84% 14%

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			

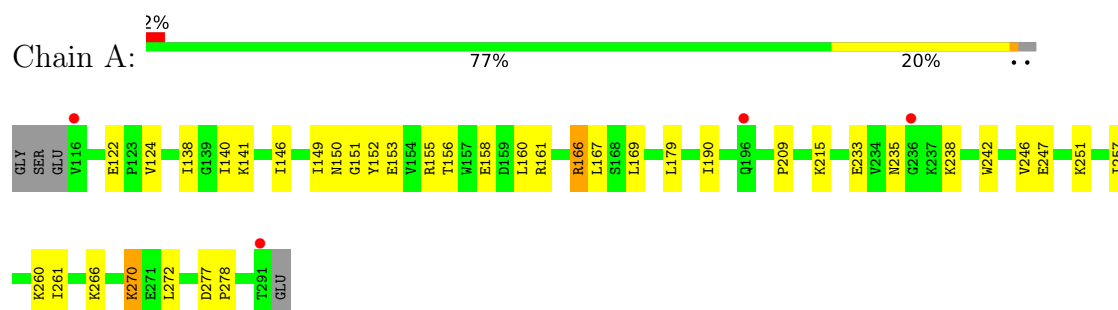
- Molecule 4 is water.

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

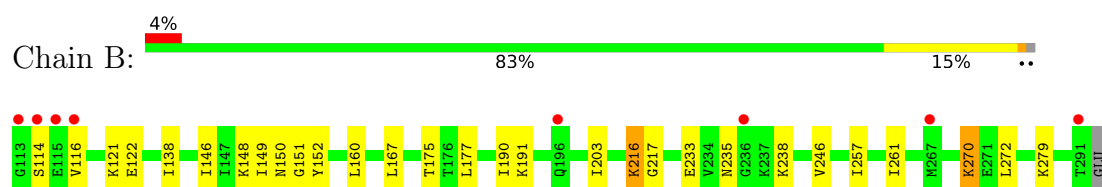
3 Residue-property plots

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.

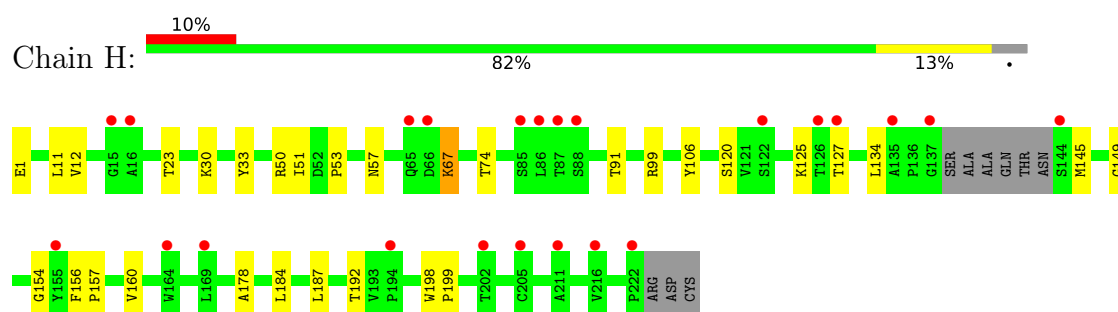
- Molecule 1: Putative zinc metalloprotease aq_1964



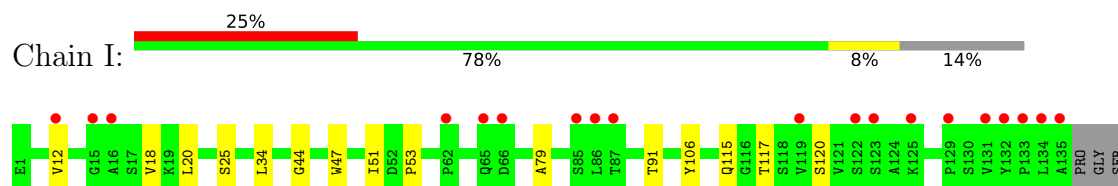
- Molecule 1: Putative zinc metalloprotease aq_1964

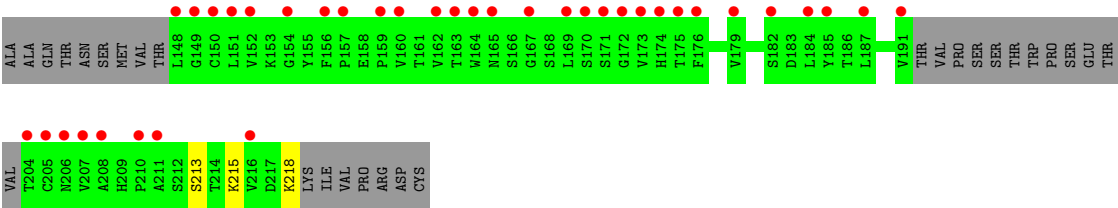


- Molecule 2: MOUSE IGG1-KAPPA FAB (HEAVY CHAIN)

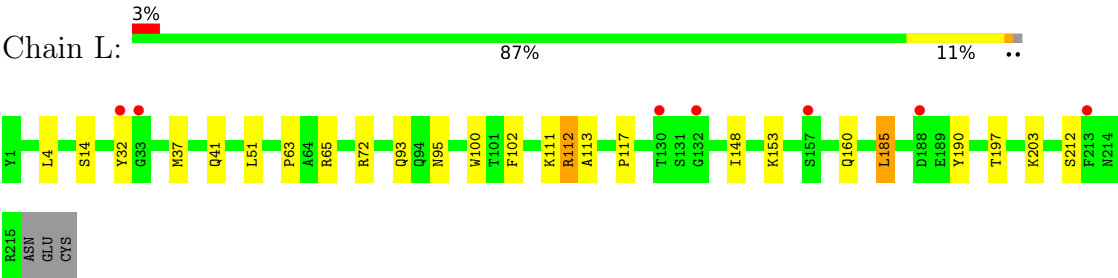


- Molecule 2: MOUSE IGG1-KAPPA FAB (HEAVY CHAIN)

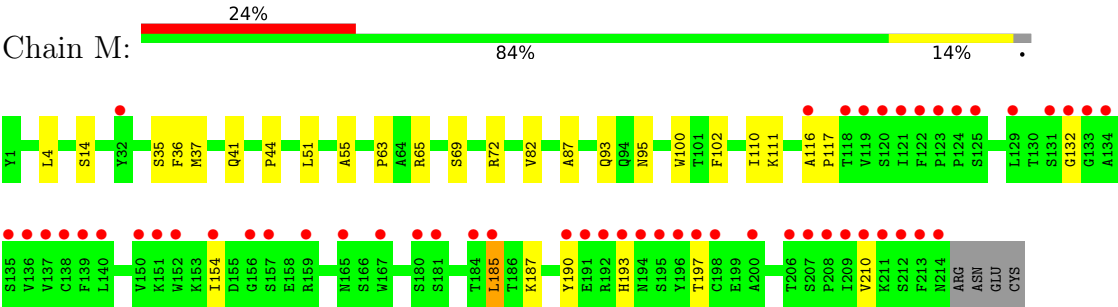




● Molecule 3: MOUSE IGG1-KAPPA FAB (LIGHT CHAIN)



● 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) 98.2 (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 (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.5	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 [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	0.57	0/1456	0.77	0/1960
1	B	0.59	0/1450	0.80	0/1954
2	H	0.64	0/1690	0.75	0/2312
2	I	0.65	0/1538	0.73	0/2097
3	L	0.61	0/1732	0.79	0/2357
3	M	0.60	0/1733	0.79	0/2358
All	All	0.61	0/9599	0.77	0/13038

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	1433	0	1547	37	0
1	B	1427	0	1528	33	0
2	H	1647	0	1600	15	0
2	I	1502	0	1447	10	0
3	L	1692	0	1610	11	0
3	M	1693	0	1609	20	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	87	0	0	0	0
4	M	60	0	0	4	0
All	All	9781	0	9341	114	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 (114) 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	1.01
1:B:150:ASN:CG	1:B:151:GLY:H	1.79	0.88
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
1:B:150:ASN:CG	1:B:151:GLY:N	2.42	0.76
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
2:H:145:MET:HE3	2:H:192:THR:HG22	1.71	0.72
1:A:138[A]:ILE:HD13	1:A:190:ILE:CG2	2.19	0.72
1:B:150:ASN:HD21	1:B:152:TYR:HD1	1.36	0.70
1:A:179[B]:LEU:C	1:A:179[B]:LEU:HD12	2.18	0.68
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:149:ILE:O	1:A:150:ASN:ND2	2.31	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122[B]:GLU:N	1:B:122[B]:GLU:OE2	2.36	0.58
3:L:63:PRO:HB2	3:L:65:ARG:HG2	1.86	0.58
1:B:138[B]:ILE:O	1:B:138[B]:ILE:HG13	2.03	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:HB2	2:H:67:LYS:NZ	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
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
1:A:179[B]:LEU:HD12	1:A:179[B]:LEU:O	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:132:GLY:HA2	3:M:187:LYS:HE3	1.98	0.46
1:A:150:ASN:CG	1:A:167:LEU:HD21	2.40	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:37[B]:MET:HE2	3:M:37[B]:MET:HB2	1.76	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:A:179[B]:LEU:C	1:A:179[B]:LEU:CD1	2.90	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:ND2	1:B:167:LEU:HD11	2.34	0.42
1:B:150:ASN:HD22	1:B:167:LEU:HD11	1.85	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:B:121:LYS:C	1:B:122[B]:GLU:OE2	2.62	0.42
3:L:4:LEU:HD22	3:L:37[A]:MET:HE1	2.03	0.41
3:M:4:LEU:HD22	3:M:37[A]:MET:HE1	2.02	0.41
1:A:215:LYS:HG3	3:L:32:TYR:CZ	2.54	0.41
1:B:272:LEU:C	1:B:272:LEU:HD12	2.45	0.41
1:A:138[B]:ILE:O	1:A:138[B]:ILE:HG23	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:M:37[B]:MET:C	3:M:37[B]:MET:SD	3.04	0.41
2:H:156:PHE:HA	2:H:157:PRO:HA	1.79	0.40
2:H:51:ILE:O	2:H:53:PRO:HD3	2.21	0.40
1:B:150:ASN:HB3	1:B:175:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	27
3	L	216/218 (99%)	209 (97%)	5 (2%)	2 (1%)	14	14
3	M	216/218 (99%)	202 (94%)	12 (6%)	2 (1%)	14	14
All	All	1196/1246 (96%)	1145 (96%)	46 (4%)	5 (0%)	36	34

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 [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	158/155 (102%)	151 (96%)	7 (4%)	25	34
1	B	157/155 (101%)	155 (99%)	2 (1%)	61	76
2	H	187/193 (97%)	180 (96%)	7 (4%)	30	41
2	I	168/193 (87%)	165 (98%)	3 (2%)	51	68
3	L	192/192 (100%)	188 (98%)	4 (2%)	47	63
3	M	192/192 (100%)	187 (97%)	5 (3%)	40	55
All	All	1054/1080 (98%)	1026 (97%)	28 (3%)	42	53

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

Mol	Chain	Res	Type
1	A	141	LYS
1	A	146	ILE
1	A	166[A]	ARG
1	A	166[B]	ARG
1	A	238	LYS
1	A	266	LYS
1	A	270	LYS
2	H	1	GLU
2	H	12	VAL
2	H	57	ASN
2	H	67	LYS
2	H	125	LYS
2	H	127	THR
2	H	160	VAL
3	L	112	ARG
3	L	160	GLN
3	L	185	LEU
3	L	212	SER
1	B	216	LYS
1	B	270	LYS
2	I	25	SER
2	I	215	LYS
2	I	218	LYS
3	M	82[A]	VAL
3	M	82[B]	VAL
3	M	154	ILE
3	M	185	LEU

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Mol	Chain	Res	Type
3	M	193	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	150	ASN
1	A	194	ASN
1	A	240	ASN
3	L	57	ASN
3	L	165	ASN
1	B	150	ASN
2	I	65	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 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	176/180 (97%)	0.12	4 (2%) 61 58	10, 30, 44, 59	6 (3%)
1	B	179/180 (99%)	0.17	8 (4%) 38 35	11, 31, 53, 78	3 (1%)
2	H	216/225 (96%)	0.79	23 (10%) 11 8	10, 43, 67, 75	1 (0%)
2	I	194/225 (86%)	1.36	56 (28%) 1 1	11, 47, 90, 102	3 (1%)
3	L	215/218 (98%)	0.22	7 (3%) 49 46	10, 32, 56, 66	3 (1%)
3	M	214/218 (98%)	0.95	53 (24%) 2 1	11, 35, 100, 110	4 (1%)
All	All	1194/1246 (95%)	0.62	151 (12%) 8 6	10, 34, 85, 110	20 (1%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	134	LEU	6.1
2	I	135	ALA	6.1
2	I	148	LEU	5.1
3	M	152	TRP	4.9
2	I	216	VAL	4.8
2	I	169	LEU	4.7
3	M	198	CYS	4.7
2	I	160	VAL	4.6
3	M	124	PRO	4.5
2	I	191	VAL	4.5
2	H	15	GLY	4.4
2	I	208	ALA	4.3
3	M	121	ILE	4.2
3	M	138	CYS	4.1
3	M	209	ILE	4.1
3	M	184	THR	4.0
3	M	123	PRO	4.0
2	I	133	PRO	3.9
2	I	207	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
3	M	136	VAL	3.8
1	A	116	VAL	3.8
3	M	213	PHE	3.7
1	B	113	GLY	3.7
1	A	291	THR	3.7
3	M	156	GLY	3.7
3	M	122	PHE	3.6
3	M	154	ILE	3.6
2	I	150	CYS	3.6
2	I	164	TRP	3.6
3	M	208	PRO	3.5
2	I	162	VAL	3.4
2	I	154	GLY	3.4
3	M	133	GLY	3.4
2	I	131	VAL	3.4
2	I	187	LEU	3.4
2	H	87	THR	3.4
2	H	205	CYS	3.4
1	B	267	MET	3.3
1	B	114	SER	3.3
3	M	134	ALA	3.3
3	M	195	SER	3.3
2	I	151	LEU	3.3
3	M	211	LYS	3.2
2	I	204	THR	3.2
2	H	135	ALA	3.2
3	M	119	VAL	3.2
2	I	167	GLY	3.2
2	I	159	PRO	3.2
3	M	214	ASN	3.2
2	I	152	VAL	3.1
3	M	181	SER	3.1
3	M	116	ALA	3.1
2	I	86	LEU	3.1
3	M	185	LEU	3.1
1	B	291	THR	3.0
2	I	174	HIS	3.0
3	M	137	VAL	3.0
3	M	190	TYR	3.0
3	M	118	THR	3.0
3	M	206	THR	3.0
2	H	137	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	I	129	PRO	3.0
3	M	150	VAL	2.9
3	M	167	TRP	2.9
2	I	12	VAL	2.9
2	H	16	ALA	2.8
3	M	139	PHE	2.8
2	I	210	PRO	2.8
3	M	196	TYR	2.8
3	L	32	TYR	2.8
3	M	32	TYR	2.8
2	I	16	ALA	2.8
3	M	151	LYS	2.8
3	L	188	ASP	2.8
3	L	157	SER	2.8
3	M	129	LEU	2.8
2	I	182	SER	2.7
3	M	135	SER	2.7
2	I	176	PHE	2.7
2	I	206	ASN	2.7
1	B	236	GLY	2.7
3	M	210	VAL	2.7
2	I	125	LYS	2.6
2	I	185	TYR	2.6
3	M	197	THR	2.6
2	H	222	PRO	2.6
2	H	86	LEU	2.6
2	I	211	ALA	2.6
1	B	116	VAL	2.6
2	H	127	THR	2.6
2	I	170	SER	2.6
2	H	169	LEU	2.6
2	I	205	CYS	2.6
2	I	173	VAL	2.5
1	A	196	GLN	2.5
2	I	149	GLY	2.5
2	H	202	THR	2.5
2	H	85	SER	2.5
3	M	131	SER	2.5
3	M	207	SER	2.5
2	H	194	PRO	2.5
2	H	164	TRP	2.4
2	I	132	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
3	M	157	SER	2.4
2	I	87	THR	2.4
2	I	85	SER	2.4
3	M	193	HIS	2.4
2	I	123	SER	2.4
2	I	62	PRO	2.3
1	A	236	GLY	2.3
2	I	172	GLY	2.3
2	H	144	SER	2.3
2	I	156	PHE	2.3
2	I	171	SER	2.3
3	M	180	SER	2.3
3	M	192	ARG	2.3
2	I	157	PRO	2.3
2	I	175	THR	2.3
3	M	191	GLU	2.3
2	I	184	LEU	2.2
2	I	179	VAL	2.2
2	I	165	ASN	2.2
2	I	65	GLN	2.2
2	I	119	VAL	2.1
1	B	196	GLN	2.1
2	H	65	GLN	2.1
2	I	15	GLY	2.1
3	L	33	GLY	2.1
3	M	132	GLY	2.1
2	H	155	TYR	2.1
3	M	140	LEU	2.1
1	B	115	GLU	2.1
2	H	66	ASP	2.1
3	M	194	ASN	2.1
2	H	126	THR	2.1
2	I	163	THR	2.1
3	M	159	ARG	2.1
2	H	216	VAL	2.1
2	H	88	SER	2.1
2	H	211	ALA	2.1
2	I	66	ASP	2.1
3	L	132	GLY	2.1
3	L	213	PHE	2.1
2	H	122	SER	2.0
3	L	130	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	M	125	SER	2.0
3	M	212	SER	2.0
2	I	122	SER	2.0
3	M	120	SER	2.0
3	M	200	ALA	2.0
3	M	165	ASN	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 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.