



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:27 AM UTC

PDB ID : 3AMI / pdb_00003ami
Title : The crystal structure of the M16B metallopeptidase subunit from *Sphingomonas* sp. A1
Authors : Maruyama, Y.; Chuma, A.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on : 2010-08-20
Resolution : 2.40 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

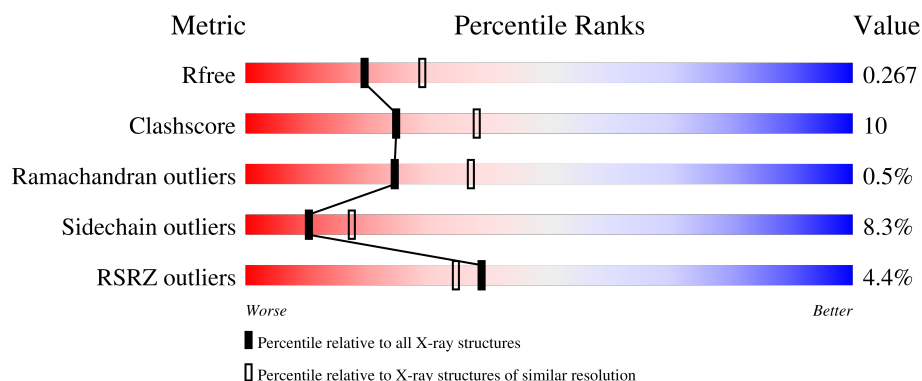
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	445	 4% 73% 19% • 5%
1	B	445	 5% 73% 20% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6799 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 zinc peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	2	0
			3291	2063	594	621	13			
1	B	422	Total	C	N	O	S	0	1	0
			3286	2063	590	620	13			

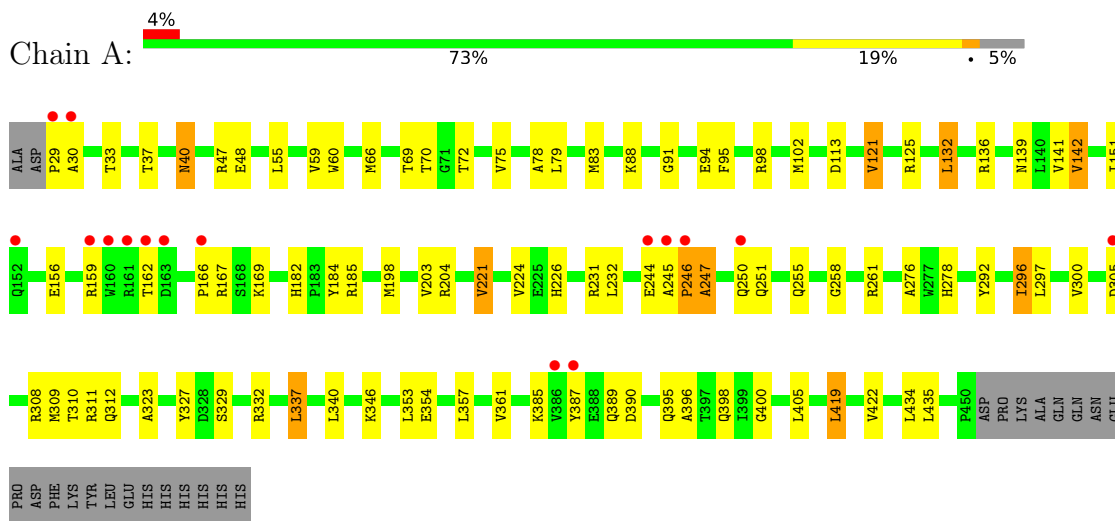
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		
2	B	114	Total	O	0	0
			114	114		

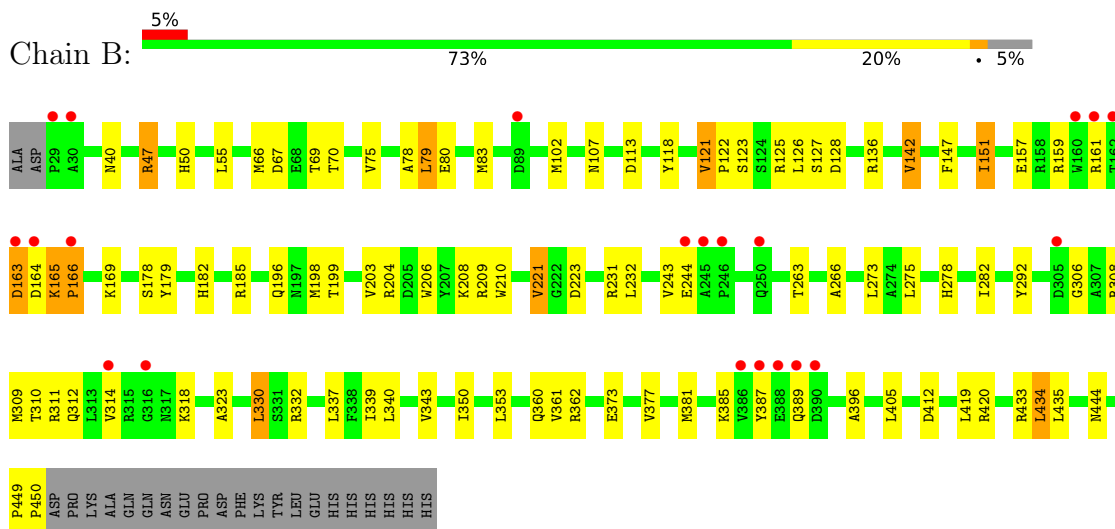
3 Residue-property plots [i](#)

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: zinc peptidase



- Molecule 1: zinc peptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.41Å 139.76Å 63.71Å 90.00° 107.91° 90.00°	Depositor
Resolution (Å)	42.78 – 2.40 42.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.78-2.40) 99.8 (42.78-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.196 , 0.266 0.199 , 0.267	Depositor DCC
R_{free} test set	1660 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6799	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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	0.42	0/3360	0.76	2/4559 (0.0%)
1	B	0.42	0/3353	0.76	2/4550 (0.0%)
All	All	0.42	0/6713	0.76	4/9109 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	LYS	CA-C-N	8.71	130.73	119.84
1	B	165	LYS	C-N-CA	8.71	130.73	119.84
1	A	91	GLY	CA-C-N	6.12	127.49	119.84
1	A	91	GLY	C-N-CA	6.12	127.49	119.84

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	3291	0	3280	56	0
1	B	3286	0	3270	75	0
2	A	108	0	0	2	0
2	B	114	0	0	5	0
All	All	6799	0	6550	128	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 10.

All (128) 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:B:164:ASP:O	1:B:165:LYS:HD2	1.48	1.13
1:B:78:ALA:HB3	1:B:198:MET:HE1	1.39	1.02
1:B:142:VAL:CG1	1:B:204:ARG:HG2	1.96	0.96
1:A:78:ALA:HB3	1:A:198:MET:HE1	1.50	0.92
1:B:78:ALA:CB	1:B:198:MET:HE1	2.04	0.87
1:A:309:MET:HE2	1:A:323:ALA:HB1	1.62	0.80
1:A:66:MET:HE1	1:A:332:ARG:HB3	1.62	0.80
1:B:66:MET:HE1	1:B:332:ARG:HB3	1.63	0.79
1:B:142:VAL:HG11	1:B:204:ARG:HG2	1.65	0.78
1:A:66:MET:HE2	1:A:113:ASP:OD2	1.85	0.76
1:A:278:HIS:HD2	2:A:526:HOH:O	1.69	0.74
1:B:199:THR:HB	2:B:523:HOH:O	1.86	0.73
1:A:244:GLU:O	1:A:244:GLU:HG3	1.89	0.72
1:B:142:VAL:HG13	1:B:204:ARG:HG2	1.70	0.72
1:A:142:VAL:CG1	1:A:204:ARG:HG2	2.20	0.72
1:B:79:LEU:HD12	1:B:206:TRP:HD1	1.55	0.71
1:A:385:LYS:O	1:A:389:GLN:HG2	1.95	0.67
1:B:308:ARG:HD3	1:B:373:GLU:OE2	1.96	0.66
1:B:309:MET:HE2	1:B:323:ALA:HB1	1.76	0.66
1:A:66:MET:CE	1:A:113:ASP:OD2	2.45	0.64
1:A:182:HIS:HD2	1:A:184:TYR:H	1.46	0.64
1:A:78:ALA:CB	1:A:198:MET:HE1	2.28	0.63
1:A:261:ARG:NH2	1:A:354:GLU:OE2	2.32	0.62
1:A:198:MET:CE	1:A:203:VAL:HG22	2.30	0.61
1:A:121:VAL:HG13	1:A:125:ARG:HB2	1.83	0.61
1:A:142:VAL:HG13	1:A:204:ARG:HG2	1.81	0.60
1:B:47:ARG:HB3	1:B:221:VAL:HB	1.83	0.60
1:A:66:MET:HE1	1:A:332:ARG:CB	2.32	0.59
1:A:182:HIS:O	1:A:185:ARG:HG2	2.01	0.59
1:B:306:GLY:O	1:B:311:ARG:NH1	2.36	0.58
1:B:198:MET:HE3	1:B:203:VAL:HG22	1.84	0.58
1:B:362:ARG:HD2	2:B:490:HOH:O	2.03	0.58
1:A:40:ASN:C	1:A:40:ASN:HD22	2.12	0.57
1:B:121:VAL:HG13	1:B:125:ARG:HB2	1.87	0.57
1:B:83:MET:CE	1:B:136:ARG:HG2	2.34	0.57
1:A:47:ARG:HE	1:A:395:GLN:HE21	1.53	0.57
1:A:142:VAL:HG13	1:A:204:ARG:CG	2.34	0.56
1:A:245:ALA:N	1:A:246:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLU:HG2	1:B:161:ARG:HD3	1.88	0.56
1:B:221:VAL:HG13	1:B:396:ALA:HB2	1.87	0.56
1:A:69:THR:HG23	1:B:69:THR:HG23	1.88	0.55
1:B:107:ASN:HB3	1:B:118:TYR:CZ	2.42	0.55
1:B:221:VAL:CG1	1:B:396:ALA:HB2	2.36	0.55
1:B:102:MET:CE	1:B:128:ASP:HB3	2.37	0.55
1:A:48:GLU:OE1	1:A:226:HIS:HD2	1.90	0.55
1:B:83:MET:O	1:B:136:ARG:HD2	2.07	0.55
1:B:67:ASP:OD2	1:B:332:ARG:NH2	2.35	0.54
1:A:142:VAL:CG1	1:A:204:ARG:CG	2.85	0.53
1:B:169:LYS:HD3	1:B:266:ALA:HB2	1.92	0.52
1:A:311:ARG:HG2	1:A:312:GLN:HG3	1.91	0.52
1:B:314:VAL:O	1:B:318:LYS:HG3	2.09	0.52
1:A:83:MET:O	1:A:136:ARG:HD2	2.10	0.51
1:A:296:ILE:HD13	1:A:422:VAL:HG21	1.93	0.51
1:B:273:LEU:HD13	1:B:350:ILE:HG23	1.91	0.51
1:A:182:HIS:CD2	1:A:184:TYR:H	2.27	0.51
1:A:292:TYR:HD1	1:A:419:LEU:HD13	1.76	0.50
1:B:66:MET:HE1	1:B:332:ARG:CB	2.36	0.50
1:B:198:MET:CE	1:B:203:VAL:HG22	2.41	0.50
1:A:88:LYS:HZ2	1:A:139:ASN:HB3	1.77	0.49
1:B:66:MET:CE	1:B:113:ASP:OD2	2.60	0.49
1:B:147:PHE:CZ	1:B:151:ILE:HG13	2.48	0.49
1:A:327:TYR:CE2	1:A:329:SER:HB3	2.48	0.49
1:B:55:LEU:HD23	1:B:123:SER:HA	1.94	0.48
1:B:102:MET:HE2	1:B:128:ASP:HB3	1.94	0.48
1:B:102:MET:HB3	1:B:125:ARG:HG3	1.95	0.48
1:B:66:MET:HE2	1:B:113:ASP:OD2	2.13	0.48
1:A:60:TRP:CE2	1:A:400:GLY:HA3	2.48	0.47
1:B:127:SER:HA	1:B:232:LEU:HD21	1.96	0.47
1:A:246:PRO:O	1:A:247:ALA:C	2.56	0.47
1:B:164:ASP:C	1:B:165:LYS:HD2	2.31	0.47
1:B:278:HIS:HD2	2:B:492:HOH:O	1.96	0.47
1:B:78:ALA:CB	1:B:198:MET:CE	2.87	0.47
1:B:55:LEU:HD21	1:B:126:LEU:HB2	1.97	0.47
1:B:178:SER:O	1:B:278:HIS:HE1	1.97	0.46
1:A:198:MET:HE2	1:A:203:VAL:CG2	2.44	0.46
1:B:67:ASP:CG	1:B:332:ARG:HH22	2.21	0.46
1:A:75:VAL:HG23	1:A:198:MET:HE3	1.98	0.46
1:A:48:GLU:HG2	1:A:224:VAL:O	2.16	0.46
1:A:72:THR:HG22	1:A:72:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PHE:HE1	1:B:198:MET:HE2	1.80	0.45
1:B:178:SER:O	1:B:278:HIS:CE1	2.69	0.45
1:B:385:LYS:HE2	1:B:389:GLN:HE21	1.82	0.45
1:A:98:ARG:O	1:A:102:MET:HG3	2.15	0.45
1:A:258:GLY:HA3	1:B:263:THR:O	2.16	0.45
1:B:292:TYR:HD1	1:B:419:LEU:HD12	1.81	0.45
1:B:309:MET:CE	1:B:323:ALA:HB1	2.42	0.45
1:A:55:LEU:C	1:A:55:LEU:HD12	2.41	0.45
1:B:361:VAL:HG11	1:B:434:LEU:HB3	1.98	0.45
1:B:444:ASN:ND2	2:B:22:HOH:O	2.37	0.45
1:B:275:LEU:O	1:B:339:ILE:HA	2.18	0.44
1:B:312:GLN:NE2	1:B:360:GLN:HE22	2.15	0.44
1:A:296:ILE:O	1:A:300:VAL:HG23	2.18	0.44
1:A:95:PHE:CE2	1:A:132:LEU:HB3	2.52	0.44
1:B:179:TYR:HB2	1:B:185:ARG:HB3	1.99	0.44
1:A:88:LYS:NZ	1:A:139:ASN:HB3	2.32	0.43
1:A:40:ASN:C	1:A:40:ASN:ND2	2.75	0.43
1:B:377:VAL:O	1:B:381:MET:HG3	2.19	0.43
1:A:66:MET:CE	1:A:332:ARG:HB3	2.42	0.43
1:B:165:LYS:HA	1:B:166:PRO:HD2	1.64	0.43
1:B:142:VAL:HG13	1:B:204:ARG:CG	2.45	0.43
1:B:208:LYS:O	1:B:243:VAL:HG11	2.19	0.43
1:A:309:MET:HE3	1:A:357:LEU:HD22	2.01	0.42
1:A:276:ALA:HB1	1:A:337:LEU:HD22	2.01	0.42
1:B:151:ILE:HD13	1:B:151:ILE:HA	1.84	0.42
1:A:33:THR:OG1	1:A:47:ARG:HD3	2.20	0.42
1:B:449:PRO:HA	1:B:450:PRO:HD3	1.82	0.42
1:B:282:ILE:HD12	1:B:330:LEU:HD13	2.02	0.42
1:A:251:GLN:HE22	1:B:70:THR:HG22	1.84	0.42
1:B:196:GLN:HE21	1:B:196:GLN:HA	1.85	0.42
1:A:309:MET:HE3	1:A:357:LEU:CD2	2.50	0.41
1:A:29:PRO:HB2	1:A:30:ALA:H	1.67	0.41
1:B:350:ILE:HG22	2:B:508:HOH:O	2.20	0.41
1:B:75:VAL:HG23	1:B:198:MET:HE3	2.03	0.41
1:B:196:GLN:HA	1:B:196:GLN:NE2	2.36	0.41
1:A:221:VAL:CG1	1:A:396:ALA:HB2	2.51	0.41
1:B:198:MET:HE3	1:B:203:VAL:CG2	2.49	0.41
1:B:50:HIS:ND1	1:B:223:ASP:OD1	2.38	0.41
1:B:147:PHE:CZ	1:B:151:ILE:CG1	3.04	0.41
1:B:244:GLU:O	1:B:244:GLU:HG3	2.21	0.41
1:B:121:VAL:HG13	1:B:122:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:O	1:A:98:ARG:HG3	2.21	0.40
1:A:346:LYS:HG3	2:A:545:HOH:O	2.21	0.40
1:A:198:MET:CE	1:A:203:VAL:CG2	2.97	0.40
1:B:159:ARG:HA	1:B:163:ASP:HB2	2.03	0.40
1:A:156:GLU:HA	1:A:159:ARG:HD3	2.04	0.40
1:B:182:HIS:O	1:B:185:ARG:HG2	2.22	0.40
1:B:433:ARG:HG2	1:B:434:LEU:HD13	2.04	0.40
1:B:209:ARG:HD3	1:B:210:TRP:NE1	2.37	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	422/445 (95%)	407 (96%)	12 (3%)	3 (1%)	18	28
1	B	421/445 (95%)	408 (97%)	12 (3%)	1 (0%)	43	58
All	All	843/890 (95%)	815 (97%)	24 (3%)	4 (0%)	24	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	PRO
1	A	246	PRO
1	A	247	ALA
1	A	166	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	341/360 (95%)	307 (90%)	34 (10%)	7	11
1	B	340/360 (94%)	318 (94%)	22 (6%)	15	27
All	All	681/720 (95%)	625 (92%)	56 (8%)	10	18

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	40	ASN
1	A	59	VAL
1	A	70	THR
1	A	79	LEU
1	A	121	VAL
1	A	132	LEU
1	A	141	VAL
1	A	142	VAL
1	A	151	ILE
1	A	162	THR
1	A	167	ARG
1	A	169	LYS
1	A	221	VAL
1	A	231	ARG
1	A	232	LEU
1	A	250	GLN
1	A	255	GLN
1	A	296	ILE
1	A	297	LEU
1	A	305	ASP
1	A	308	ARG
1	A	310	THR
1	A	337	LEU
1	A	340	LEU
1	A	353	LEU
1	A	361	VAL
1	A	387	TYR
1	A	390	ASP
1	A	398	GLN
1	A	405	LEU
1	A	419	LEU
1	A	434	LEU

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Mol	Chain	Res	Type
1	A	435	LEU
1	B	40	ASN
1	B	47	ARG
1	B	79	LEU
1	B	80	GLU
1	B	121	VAL
1	B	142	VAL
1	B	151	ILE
1	B	163	ASP
1	B	221	VAL
1	B	231	ARG
1	B	310	THR
1	B	330	LEU
1	B	337	LEU
1	B	340	LEU
1	B	343	VAL
1	B	353	LEU
1	B	387	TYR
1	B	405	LEU
1	B	412	ASP
1	B	420	ARG
1	B	434	LEU
1	B	435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	120	GLN
1	A	139	ASN
1	A	182	HIS
1	A	196	GLN
1	A	201	GLN
1	A	226	HIS
1	A	251	GLN
1	A	278	HIS
1	A	335	GLN
1	A	352	GLN
1	A	360	GLN
1	A	395	GLN
1	B	40	ASN
1	B	120	GLN

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Mol	Chain	Res	Type
1	B	139	ASN
1	B	152	GLN
1	B	193	ASN
1	B	196	GLN
1	B	197	ASN
1	B	201	GLN
1	B	226	HIS
1	B	251	GLN
1	B	278	HIS
1	B	312	GLN
1	B	335	GLN
1	B	360	GLN
1	B	395	GLN
1	B	398	GLN
1	B	417	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	422/445 (94%)	0.24	16 (3%) 44 40	23, 35, 59, 81	2 (0%)
1	B	422/445 (94%)	0.22	21 (4%) 34 30	16, 35, 57, 79	1 (0%)
All	All	844/890 (94%)	0.23	37 (4%) 39 34	16, 35, 59, 81	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	5.4
1	A	162	THR	4.4
1	B	160	TRP	4.3
1	A	387	TYR	4.3
1	A	160	TRP	4.1
1	B	162	THR	3.9
1	B	387	TYR	3.8
1	A	29	PRO	3.6
1	B	250	GLN	3.5
1	A	244	GLU	3.4
1	B	245	ALA	3.4
1	B	386	VAL	3.4
1	B	166	PRO	3.4
1	B	29	PRO	3.2
1	A	246	PRO	2.9
1	A	30	ALA	2.8
1	A	159	ARG	2.8
1	B	305	ASP	2.7
1	A	250	GLN	2.6
1	B	390	ASP	2.6
1	A	386	VAL	2.6
1	B	161	ARG	2.5
1	B	163	ASP	2.5
1	B	388	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	246	PRO	2.5
1	B	389	GLN	2.5
1	B	314	VAL	2.3
1	B	244	GLU	2.3
1	A	163	ASP	2.3
1	A	305	ASP	2.2
1	B	164	ASP	2.2
1	A	166	PRO	2.2
1	B	30	ALA	2.1
1	A	161	ARG	2.1
1	A	152	GLN	2.0
1	B	316	GLY	2.0
1	B	89	ASP	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.