



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:57 am BST

PDB ID : 3AMI  
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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

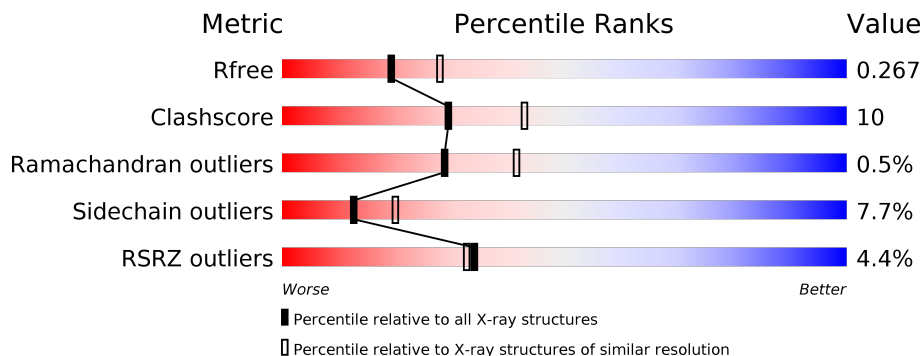
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	445	

## 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
			Total	C	N	O	S			
1	A	422	3291	2063	594	621	13	0	2	0
1	B	422	3286	2063	590	620	13	0	1	0

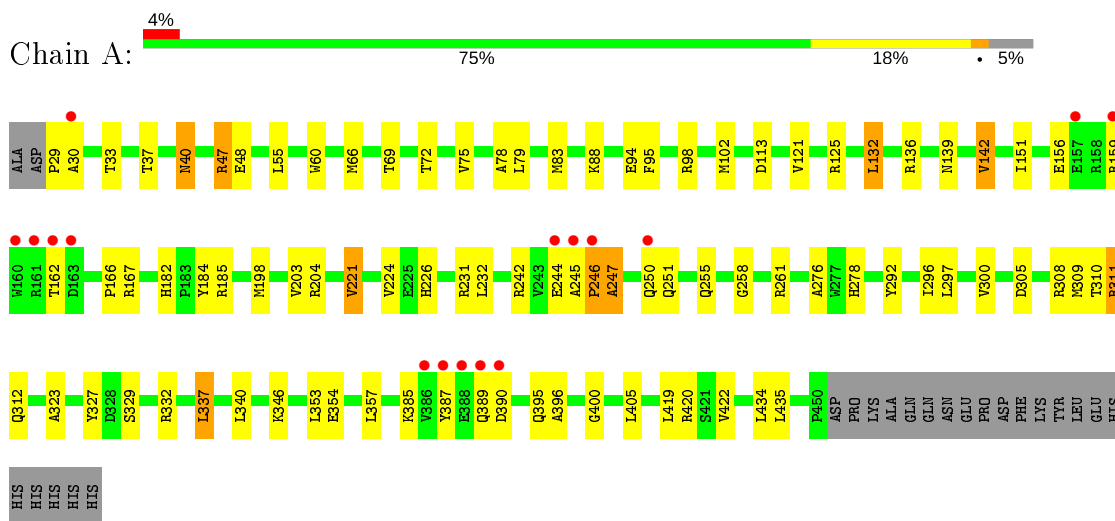
- Molecule 2 is water.

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

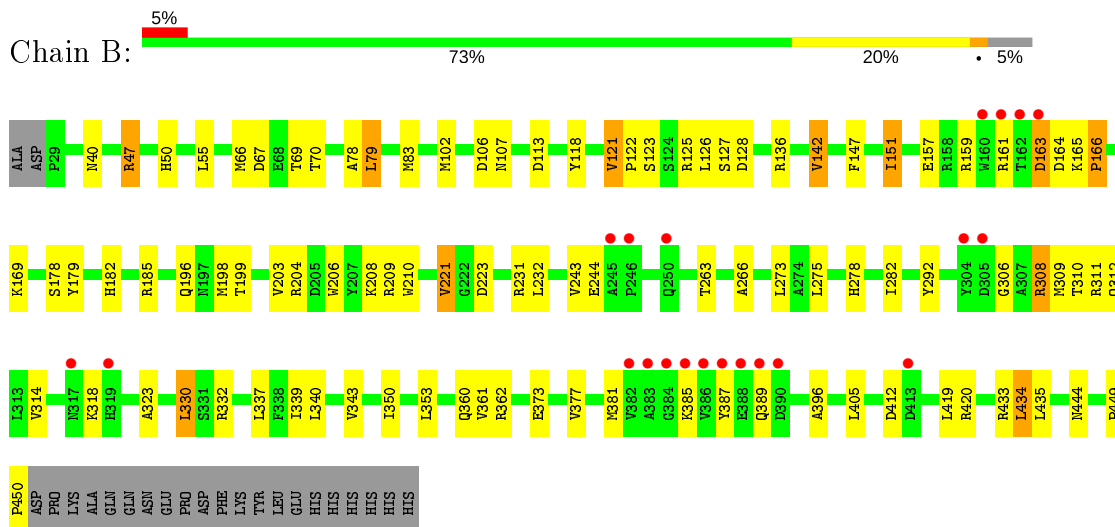
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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: 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, $\alpha$ , $\beta$ , $\gamma$	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) 99.7 (42.78-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.84 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.196 , 0.266 0.198 , 0.267	Depositor DCC
$R_{free}$ test set	1660 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtrriage
Anisotropy	0.216	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.31	0/3360	0.51	0/4559
1	B	0.32	0/3353	0.49	0/4550
All	All	0.32	0/6713	0.50	0/9109

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	3291	0	3280	55	0
1	B	3286	0	3270	73	0
2	A	108	0	0	2	0
2	B	114	0	0	5	0
All	All	6799	0	6550	125	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 (125) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:CG1	1:B:204:ARG:HG2	1.96	0.96
1:B:78:ALA:HB3	1:B:198:MET:HE1	1.64	0.79
1:B:142:VAL:HG11	1:B:204:ARG:HG2	1.65	0.78
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:HG3	1:A:244:GLU:O	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:A:66:MET:CE	1:A:113:ASP:OD2	2.45	0.65
1:A:66:MET:HE2	1:A:113:ASP:OD2	1.97	0.64
1:A:182:HIS:HD2	1:A:184:TYR:H	1.46	0.64
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:66:MET:HE1	1:B:332:ARG:HB3	1.84	0.60
1:B:47:ARG:HB3	1:B:221:VAL:HB	1.83	0.60
1:A:78:ALA:HB3	1:A:198:MET:HE1	1.83	0.59
1:A:182:HIS:O	1:A:185:ARG:HG2	2.01	0.59
1:A:309:MET:HE2	1:A:323:ALA:HB1	1.86	0.58
1:B:306:GLY:O	1:B:311:ARG:NH1	2.36	0.58
1:B:362:ARG:HD2	2:B:490:HOH:O	2.03	0.58
1:B:121:VAL:HG13	1:B:125:ARG:HB2	1.87	0.57
1:B:309:MET:HE2	1:B:323:ALA:HB1	1.86	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:B:78:ALA:HB3	1:B:198:MET:CE	2.34	0.56
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
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:A:66:MET:HE1	1:A:332:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:MET:HE3	1:B:203:VAL:HG22	1.89	0.54
1:B:67:ASP:OD2	1:B:332:ARG:NH2	2.35	0.54
1:B:198:MET:HE3	1:B:203:VAL:CG2	2.38	0.54
1:A:40:ASN:C	1:A:40:ASN:HD22	2.12	0.53
1:A:142:VAL:CG1	1:A:204:ARG:CG	2.85	0.53
1:B:78:ALA:CB	1:B:198:MET:CE	2.87	0.52
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:113:ASP:OD2	2.12	0.50
1:B:198:MET:CE	1:B:203:VAL:HG22	2.41	0.50
1:B:309:MET:CE	1:B:323:ALA:HB1	2.42	0.50
1:A:66:MET:CE	1:A:332:ARG:HB3	2.42	0.49
1:A:88:LYS:HZ2	1:A:139:ASN:HB3	1.77	0.49
1:B:147:PHE:CZ	1:B:151:ILE:HG13	2.48	0.49
1:B:66:MET:CE	1:B:113:ASP:OD2	2.60	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:HB3	1:B:125:ARG:HG3	1.95	0.48
1:A:78:ALA:HB3	1:A:198:MET:CE	2.43	0.47
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:B:278:HIS:HD2	2:B:492:HOH:O	1.96	0.47
1:A:75:VAL:HA	1:A:198:MET:HE1	1.97	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: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
1:B:178:SER:O	1:B:278:HIS:CE1	2.69	0.45
1:A:198:MET:HE3	1:A:203:VAL:HG22	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:377:VAL:O	1:B:381:MET:HG3	2.19	0.43
1:B:165:LYS:HA	1:B:166:PRO:HD2	1.64	0.43
1:A:246:PRO:O	1:A:247:ALA:C	2.56	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:B:164:ASP:C	1:B:165:LYS:HD2	2.31	0.42
1:A:276:ALA:HB1	1:A:337:LEU:HD22	2.01	0.42
1:A:309:MET:HE1	1:A:357:LEU:HD22	2.00	0.42
1:B:151:ILE:HD13	1:B:151:ILE:HA	1.84	0.42
1:A:198:MET:CE	1:A:203:VAL:CG2	2.97	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:HA	1:B:196:GLN:HE21	1.85	0.42
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:67:ASP:CG	1:B:332:ARG:HH22	2.21	0.41
1:B:196:GLN:HA	1:B:196:GLN:NE2	2.36	0.41
1:B:66:MET:CE	1:B:332:ARG:HB3	2.50	0.41
1:A:221:VAL:CG1	1:A:396:ALA:HB2	2.51	0.41
1:A:385:LYS:O	1:A:385:LYS:HG2	2.20	0.41
1:B:147:PHE:CZ	1:B:151:ILE:CG1	3.04	0.41
1:B:50:HIS:ND1	1:B:223:ASP:OD1	2.38	0.41
1:B:244:GLU:HG3	1:B:244:GLU:O	2.21	0.41
1:B:121:VAL:HG13	1:B:122:PRO:O	2.21	0.41
1:A:309:MET:CE	1:A:323:ALA:HB1	2.49	0.40
1:A:346:LYS:HG3	2:A:545:HOH:O	2.21	0.40
1:A:94:GLU:O	1:A:98:ARG:HG3	2.21	0.40
1:B:102:MET:HE1	1:B:128:ASP:HB3	2.03	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:A:55:LEU:HD12	1:A:55:LEU:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	22	32
1	B	421/445 (95%)	408 (97%)	12 (3%)	1 (0%)	47	62
All	All	843/890 (95%)	815 (97%)	24 (3%)	4 (0%)	29	41

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%)	312 (92%)	29 (8%)	10	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/360 (94%)	317 (93%)	23 (7%)	16	25
All	All	681/720 (95%)	629 (92%)	52 (8%)	13	20

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	40	ASN
1	A	47	ARG
1	A	79	LEU
1	A	132	LEU
1	A	142	VAL
1	A	151	ILE
1	A	162	THR
1	A	167	ARG
1	A	221	VAL
1	A	231	ARG
1	A	232	LEU
1	A	242	ARG
1	A	250	GLN
1	A	255	GLN
1	A	297	LEU
1	A	305	ASP
1	A	308	ARG
1	A	310	THR
1	A	311	ARG
1	A	337	LEU
1	A	340	LEU
1	A	353	LEU
1	A	387	TYR
1	A	390	ASP
1	A	405	LEU
1	A	420	ARG
1	A	434	LEU
1	A	435	LEU
1	B	40	ASN
1	B	47	ARG
1	B	79	LEU
1	B	106	ASP
1	B	121	VAL
1	B	142	VAL
1	B	151	ILE

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Mol	Chain	Res	Type
1	B	163	ASP
1	B	221	VAL
1	B	231	ARG
1	B	308	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	201	GLN
1	A	226	HIS
1	A	251	GLN
1	A	278	HIS
1	A	335	GLN
1	A	389	GLN
1	A	395	GLN
1	B	40	ASN
1	B	120	GLN
1	B	196	GLN
1	B	197	ASN
1	B	201	GLN
1	B	226	HIS
1	B	251	GLN
1	B	255	GLN
1	B	278	HIS
1	B	312	GLN
1	B	335	GLN

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Mol	Chain	Res	Type
1	B	389	GLN
1	B	395	GLN
1	B	398	GLN
1	B	417	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	422/445 (94%)	0.08	16 (3%) 40 39	24, 35, 59, 81	0
1	B	422/445 (94%)	0.11	21 (4%) 28 27	23, 35, 57, 79	0
All	All	844/890 (94%)	0.09	37 (4%) 34 33	23, 35, 59, 81	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	THR	8.6
1	A	387	TYR	6.6
1	B	387	TYR	6.0
1	A	245	ALA	5.9
1	A	160	TRP	5.7
1	B	389	GLN	4.8
1	B	162	THR	4.5
1	B	160	TRP	4.0
1	A	244	GLU	3.9
1	B	390	ASP	3.9
1	B	386	VAL	3.8
1	A	246	PRO	3.7
1	B	305	ASP	3.6
1	A	161	ARG	3.5
1	B	382	VAL	3.3
1	B	245	ALA	3.3
1	B	388	GLU	3.3
1	B	246	PRO	3.2
1	B	384	GLY	3.1
1	A	157	GLU	3.0
1	A	163	ASP	3.0
1	A	390	ASP	2.9
1	B	250	GLN	2.9
1	B	163	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	161	ARG	2.8
1	B	304	TYR	2.8
1	B	385	LYS	2.7
1	A	386	VAL	2.6
1	B	317	ASN	2.5
1	A	159	ARG	2.5
1	A	250	GLN	2.3
1	A	30	ALA	2.3
1	B	319	HIS	2.2
1	B	383	ALA	2.1
1	A	389	GLN	2.1
1	A	388	GLU	2.0
1	B	413	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 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.