



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:27 PM GMT

PDB ID : 3IML  
Title : Crystal Structure Of S-Adenosylmethionine Synthetase From Burkholderia Pseudomallei  
Authors : Staker, B.L.  
Deposited on : 2009-08-10  
Resolution : 2.35 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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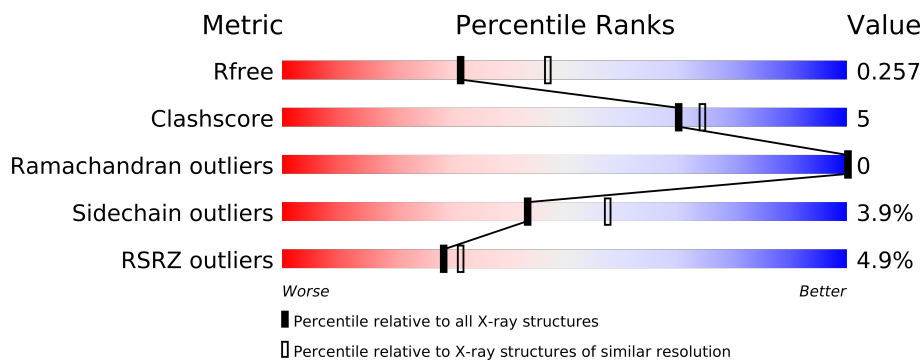
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	399	
1	B	399	
1	C	399	
1	D	399	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10507 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-adenosylmethionine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2751	1737	477	529	8			
1	B	357	Total	C	N	O	S	0	1	0
			2701	1709	471	513	8			
1	C	343	Total	C	N	O	S	0	0	0
			2583	1632	453	490	8			
1	D	311	Total	C	N	O	S	0	0	0
			2339	1488	403	441	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q63YH5
A	-2	PRO	-	EXPRESSION TAG	UNP Q63YH5
A	-1	GLY	-	EXPRESSION TAG	UNP Q63YH5
A	0	SER	-	EXPRESSION TAG	UNP Q63YH5
B	-3	GLY	-	EXPRESSION TAG	UNP Q63YH5
B	-2	PRO	-	EXPRESSION TAG	UNP Q63YH5
B	-1	GLY	-	EXPRESSION TAG	UNP Q63YH5
B	0	SER	-	EXPRESSION TAG	UNP Q63YH5
C	-3	GLY	-	EXPRESSION TAG	UNP Q63YH5
C	-2	PRO	-	EXPRESSION TAG	UNP Q63YH5
C	-1	GLY	-	EXPRESSION TAG	UNP Q63YH5
C	0	SER	-	EXPRESSION TAG	UNP Q63YH5
D	-3	GLY	-	EXPRESSION TAG	UNP Q63YH5
D	-2	PRO	-	EXPRESSION TAG	UNP Q63YH5
D	-1	GLY	-	EXPRESSION TAG	UNP Q63YH5
D	0	SER	-	EXPRESSION TAG	UNP Q63YH5

- Molecule 2 is water.

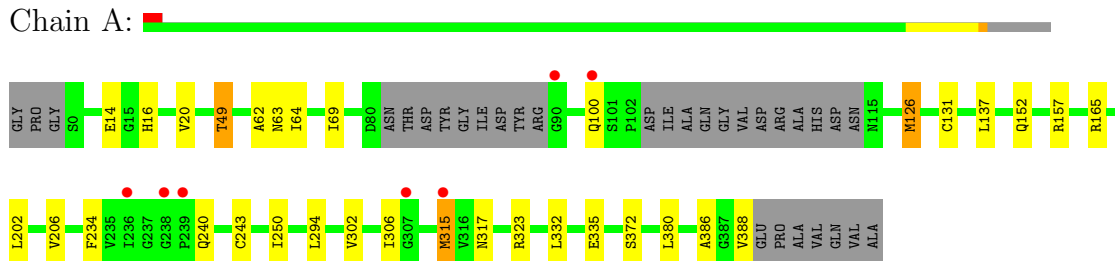
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total 44	O 44	0	0
2	B	40	Total 40	O 40	0	0
2	C	26	Total 26	O 26	0	0
2	D	23	Total 23	O 23	0	0

### 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 errors 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.

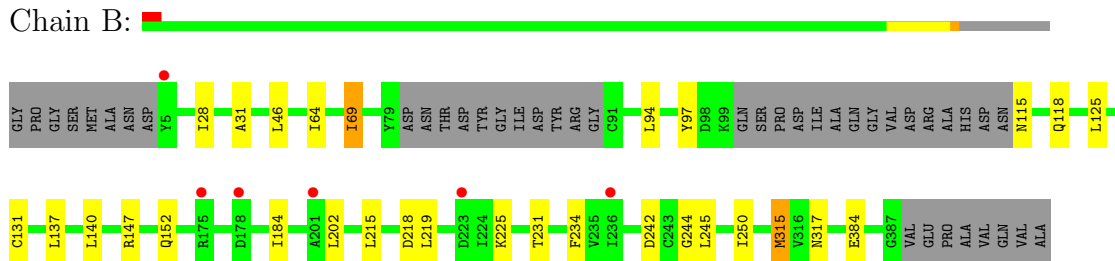
#### • Molecule 1: S-adenosylmethionine synthetase

Chain A:



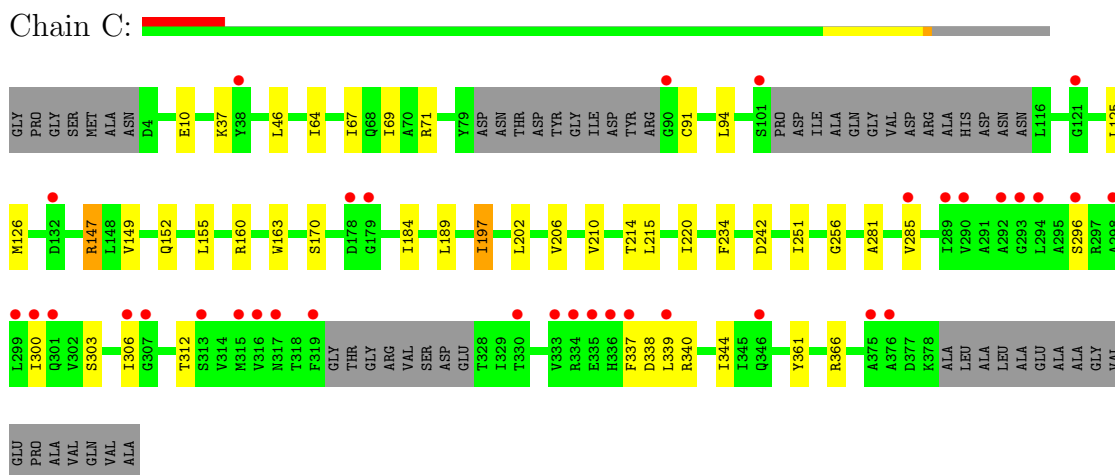
#### • Molecule 1: S-adenosylmethionine synthetase

Chain B:



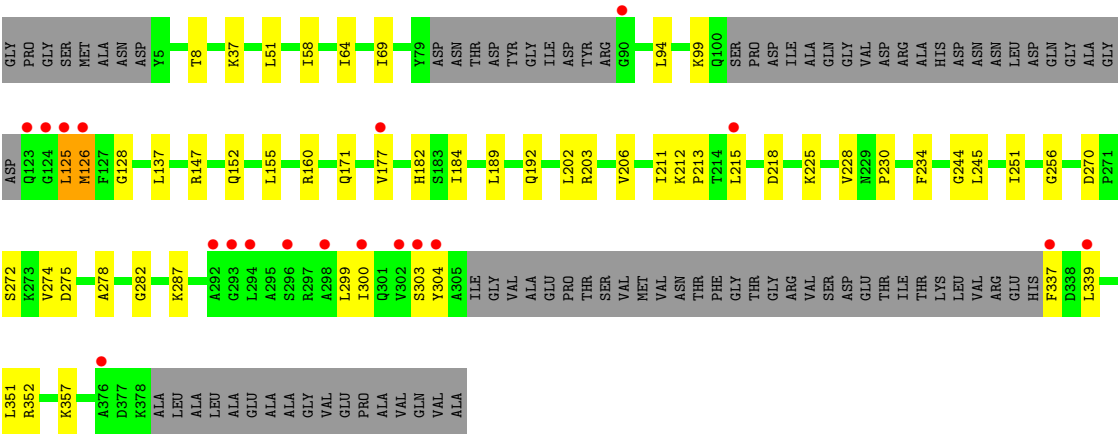
#### • Molecule 1: S-adenosylmethionine synthetase

Chain C:



#### • Molecule 1: S-adenosylmethionine synthetase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	236.30Å 119.44Å 65.35Å 90.00° 105.98° 90.00°	Depositor
Resolution (Å)	28.31 – 2.35 28.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (28.31-2.35) 97.7 (28.31-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.218 , 0.256 0.223 , 0.257	Depositor DCC
$R_{free}$ test set	3602 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , -1.4	EDS
Estimated twinning fraction	0.072 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 71116 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.55	1/2802 (0.0%)	0.67	0/3811
1	B	0.53	0/2754	0.64	0/3742
1	C	0.48	0/2631	0.62	0/3574
1	D	0.50	0/2385	0.64	0/3243
All	All	0.52	1/10572 (0.0%)	0.64	0/14370

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	CYS	CB-SG	-5.03	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2751	0	2722	21	0
1	B	2701	0	2701	14	0
1	C	2583	0	2554	33	0
1	D	2339	0	2311	35	0
2	A	44	0	0	1	0
2	B	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	26	0	0	0	0
2	D	23	0	0	0	0
All	All	10507	0	10288	94	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (94) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:177:VAL:HG12	1:D:182:HIS:HB2	1.62	0.80
1:C:285:VAL:CG2	1:C:300:ILE:HD12	2.16	0.74
1:D:37:LYS:O	1:D:351:LEU:HD22	1.92	0.70
1:D:126:MET:HE2	1:D:275:ASP:HA	1.73	0.69
1:C:285:VAL:HG21	1:C:300:ILE:HD12	1.74	0.69
1:A:388:VAL:O	1:A:388:VAL:HG12	1.94	0.67
1:D:189:LEU:HD22	1:D:206:VAL:HG11	1.78	0.66
1:D:64:ILE:CG2	1:D:69:ILE:HD12	2.27	0.64
1:C:184:ILE:HD13	1:C:215:LEU:HD22	1.82	0.62
1:A:380:LEU:HD13	2:A:404:HOH:O	2.00	0.61
1:C:94:LEU:HD21	1:D:51:LEU:HD21	1.81	0.61
1:C:64:ILE:HG23	1:C:69:ILE:CD1	2.31	0.61
1:C:197:ILE:HD13	1:C:202:LEU:HB2	1.81	0.61
1:C:163:TRP:CE2	1:C:197:ILE:HD12	2.37	0.60
1:C:306:ILE:HG23	1:D:230:PRO:HG2	1.84	0.60
1:C:64:ILE:HG23	1:C:69:ILE:HD12	1.84	0.60
1:C:125:LEU:HD13	1:D:8:THR:O	2.02	0.59
1:B:315:MET:HE1	1:B:317:ASN:HB2	1.85	0.58
1:C:285:VAL:HG23	1:C:300:ILE:HD12	1.84	0.58
1:D:64:ILE:CG2	1:D:69:ILE:CD1	2.82	0.57
1:D:202:LEU:HD23	1:D:202:LEU:C	2.26	0.57
1:C:285:VAL:HG12	1:C:337:PHE:CD1	2.40	0.56
1:D:128:GLY:O	1:D:299:LEU:HD12	2.05	0.56
1:C:10:GLU:HG2	1:D:125:LEU:HD21	1.88	0.54
1:D:137:LEU:HD12	1:D:287:LYS:HG3	1.90	0.53
1:B:184:ILE:CD1	1:B:215:LEU:HD22	2.38	0.53
1:A:64:ILE:HG23	1:A:69:ILE:HD12	1.91	0.53
1:C:64:ILE:CG2	1:C:69:ILE:HD12	2.39	0.52
1:A:250:ILE:HD11	1:B:250:ILE:HD11	1.91	0.51
1:D:339:LEU:N	1:D:339:LEU:HD12	2.26	0.51
1:A:202:LEU:O	1:A:206:VAL:HG23	2.12	0.50
1:C:339:LEU:HA	1:C:344:ILE:HD11	1.95	0.49
1:C:312:THR:HG21	1:D:171:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:215:LEU:HD13	1:C:220:ILE:HD11	1.94	0.49
1:D:184:ILE:HD13	1:D:215:LEU:HG	1.95	0.48
1:B:94:LEU:HD13	1:D:94:LEU:HB2	1.95	0.48
1:D:337:PHE:HB2	1:D:339:LEU:HD11	1.94	0.48
1:C:46:LEU:HD23	1:C:46:LEU:C	2.33	0.48
1:C:155:LEU:HD22	1:C:160:ARG:HG2	1.95	0.48
1:C:184:ILE:CD1	1:C:215:LEU:HD22	2.43	0.47
1:B:31:ALA:CB	1:B:69:ILE:HD12	2.45	0.47
1:C:155:LEU:HD12	1:C:210:VAL:HG22	1.97	0.47
1:C:303:SER:OG	1:D:8:THR:HG21	2.15	0.47
1:C:215:LEU:CD1	1:C:220:ILE:HD11	2.45	0.46
1:A:62:ALA:HB1	1:A:64:ILE:CD1	2.45	0.46
1:D:282:GLY:HA2	1:D:300:ILE:HD11	1.98	0.46
1:D:64:ILE:HG23	1:D:69:ILE:HD11	1.96	0.46
1:A:62:ALA:HB1	1:A:64:ILE:HD13	1.96	0.46
1:D:337:PHE:CB	1:D:339:LEU:HD11	2.46	0.46
1:A:315:MET:HE3	1:A:317:ASN:HB2	1.96	0.45
1:D:274:VAL:HG11	1:D:304:TYR:CD2	2.51	0.45
1:A:49:THR:HG23	1:A:240:GLN:HA	1.99	0.45
1:D:203:ARG:HG2	1:D:228:VAL:HB	1.99	0.44
1:D:189:LEU:HD22	1:D:206:VAL:CG1	2.46	0.44
1:A:126:MET:HE2	1:A:126:MET:HB2	1.72	0.44
1:B:244:GLY:C	1:B:245:LEU:HD12	2.37	0.44
1:A:294:LEU:CD2	1:A:386:ALA:CB	2.96	0.44
1:A:294:LEU:CD2	1:A:386:ALA:HB3	2.47	0.44
1:C:338:ASP:O	1:C:344:ILE:HD13	2.18	0.44
1:C:67:ILE:O	1:C:71:ARG:HG3	2.18	0.44
1:C:189:LEU:HD22	1:C:206:VAL:HG11	1.99	0.44
1:B:140:LEU:HD21	1:B:219:LEU:CD1	2.48	0.44
1:C:163:TRP:CD2	1:C:197:ILE:HD12	2.52	0.44
1:B:184:ILE:HD12	1:B:215:LEU:HD22	1.99	0.44
1:D:211:ILE:O	1:D:215:LEU:HD13	2.18	0.44
1:A:14:GLU:CD	1:A:157:ARG:HH12	2.21	0.43
1:C:149:VAL:HG13	1:C:170:SER:HB3	2.00	0.43
1:C:215:LEU:HD13	1:C:220:ILE:CD1	2.48	0.43
1:C:361:TYR:O	1:C:366:ARG:HD2	2.18	0.43
1:C:251:ILE:HG22	1:C:256:GLY:HA2	2.01	0.43
1:D:244:GLY:C	1:D:245:LEU:HD12	2.38	0.43
1:A:126:MET:CE	1:A:302:VAL:HG23	2.49	0.43
1:A:294:LEU:HD21	1:A:386:ALA:HB3	2.01	0.43
1:B:28:ILE:HD13	1:B:97:TYR:OH	2.19	0.43
1:C:281:ALA:HB2	1:C:344:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:31:ALA:HB1	1:B:64:ILE:HD12	2.00	0.42
1:A:323:ARG:NH1	1:A:388:VAL:HG13	2.34	0.42
1:D:303:SER:OG	1:D:304:TYR:N	2.51	0.42
1:B:202:LEU:HD23	1:B:202:LEU:C	2.40	0.42
1:A:131:CYS:O	1:A:137:LEU:HA	2.20	0.41
1:A:63:ASN:C	1:A:64:ILE:HD12	2.41	0.41
1:D:251:ILE:HG22	1:D:256:GLY:HA2	2.01	0.41
1:B:46:LEU:HD23	1:B:46:LEU:C	2.41	0.41
1:D:245:LEU:N	1:D:245:LEU:HD12	2.36	0.41
1:A:306:ILE:HG21	1:B:231:THR:CG2	2.51	0.41
1:D:58:ILE:O	1:D:99:LYS:HA	2.20	0.41
1:D:192:GLN:HA	1:D:234:PHE:O	2.21	0.41
1:D:126:MET:HG3	1:D:278:ALA:HB3	2.02	0.41
1:A:49:THR:HA	1:A:240:GLN:HA	2.01	0.41
1:D:270:ASP:OD1	1:D:272:SER:OG	2.31	0.40
1:B:131:CYS:O	1:B:137:LEU:HA	2.21	0.40
1:D:212:LYS:N	1:D:213:PRO:CD	2.84	0.40
1:C:147:ARG:HB3	1:C:214:THR:HG23	2.04	0.40
1:A:16:HIS:O	1:A:20:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	362/399 (91%)	345 (95%)	17 (5%)	0	100	100
1	B	352/399 (88%)	343 (97%)	9 (3%)	0	100	100
1	C	335/399 (84%)	321 (96%)	14 (4%)	0	100	100
1	D	303/399 (76%)	296 (98%)	7 (2%)	0	100	100
All	All	1352/1596 (85%)	1305 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	283/316 (90%)	273 (96%)	10 (4%)	48	63
1	B	280/316 (89%)	268 (96%)	12 (4%)	40	51
1	C	266/316 (84%)	256 (96%)	10 (4%)	44	59
1	D	239/316 (76%)	229 (96%)	10 (4%)	40	52
All	All	1068/1264 (84%)	1026 (96%)	42 (4%)	43	57

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	100	GLN
1	A	126	MET
1	A	152	GLN
1	A	165	ARG
1	A	234	PHE
1	A	315	MET
1	A	332	LEU
1	A	335	GLU
1	A	372	SER
1	B	69	ILE
1	B	115	ASN
1	B	118	GLN
1	B	125	LEU
1	B	147	ARG
1	B	152	GLN
1	B	218	ASP
1	B	225	LYS
1	B	234	PHE
1	B	242	ASP
1	B	315	MET
1	B	384	GLU
1	C	37	LYS
1	C	91	CYS
1	C	126	MET
1	C	147	ARG

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Mol	Chain	Res	Type
1	C	152	GLN
1	C	197	ILE
1	C	234	PHE
1	C	242	ASP
1	C	296	SER
1	C	340	ARG
1	D	125	LEU
1	D	126	MET
1	D	147	ARG
1	D	152	GLN
1	D	155	LEU
1	D	160	ARG
1	D	218	ASP
1	D	225	LYS
1	D	352	ARG
1	D	357	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 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	368/399 (92%)	0.44	7 (1%) 64 66	6, 15, 35, 50	0
1	B	357/399 (89%)	0.28	6 (1%) 67 70	6, 12, 24, 28	0
1	C	343/399 (85%)	0.71	35 (10%) 7 9	10, 19, 33, 44	0
1	D	311/399 (77%)	0.52	19 (6%) 21 23	9, 18, 32, 43	0
All	All	1379/1596 (86%)	0.48	67 (4%) 28 31	6, 16, 32, 50	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	VAL	7.3
1	C	337	PHE	6.5
1	C	316	VAL	5.5
1	C	90	GLY	5.2
1	C	294	LEU	4.4
1	D	302	VAL	3.9
1	D	300	ILE	3.9
1	D	303	SER	3.8
1	D	304	TYR	3.7
1	D	124	GLY	3.6
1	D	337	PHE	3.6
1	D	90	GLY	3.6
1	C	307	GLY	3.5
1	D	125	LEU	3.5
1	C	319	PHE	3.4
1	C	375	ALA	3.3
1	D	339	LEU	3.2
1	C	315	MET	3.2
1	D	292	ALA	3.1
1	D	123	GLN	3.1
1	C	339	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	376	ALA	3.1
1	D	215	LEU	3.0
1	C	330	THR	3.0
1	C	298	ALA	3.0
1	B	5	TYR	2.9
1	D	126	MET	2.9
1	D	298	ALA	2.9
1	D	294	LEU	2.8
1	C	313	SER	2.8
1	C	336	HIS	2.8
1	C	290	VAL	2.7
1	C	306	ILE	2.7
1	C	285	VAL	2.6
1	A	238	GLY	2.6
1	C	317	ASN	2.6
1	A	239	PRO	2.6
1	C	301	GLN	2.6
1	C	300	ILE	2.5
1	B	178	ASP	2.5
1	C	296	SER	2.5
1	C	293	GLY	2.4
1	D	376	ALA	2.4
1	D	177	VAL	2.4
1	C	289	ILE	2.4
1	A	315	MET	2.4
1	A	236	ILE	2.4
1	C	299	LEU	2.3
1	A	90	GLY	2.3
1	C	38	TYR	2.3
1	C	132	ASP	2.3
1	C	334	ARG	2.3
1	C	179	GLY	2.3
1	C	346	GLN	2.2
1	C	292	ALA	2.2
1	A	307	GLY	2.2
1	D	293	GLY	2.1
1	D	296	SER	2.1
1	A	100	GLN	2.1
1	B	201	ALA	2.1
1	C	178	ASP	2.1
1	C	121	GLY	2.1
1	B	175	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	236	ILE	2.1
1	B	223	ASP	2.0
1	C	101	SER	2.0
1	C	335	GLU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.