



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 09:24 am BST

PDB ID : 4CFG  
Title : Structure of the TRIM25 coiled-coil  
Authors : James, L.  
Deposited on : 2013-11-15  
Resolution : 2.80 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

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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>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

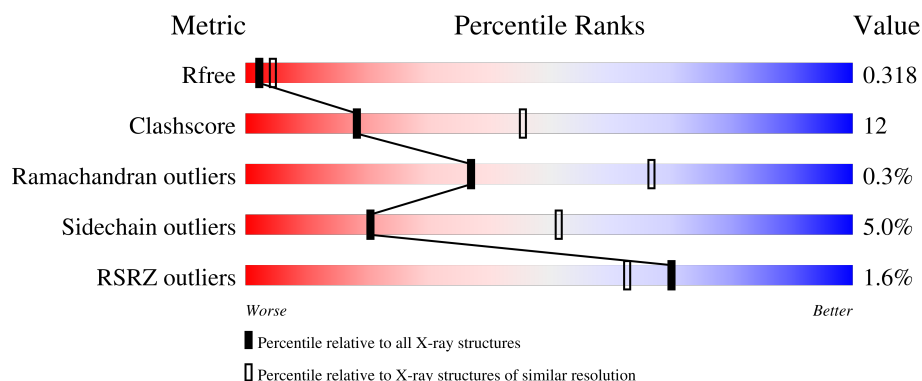
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	630	 19% 7% 74%
1	B	630	 18% 7% 74%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2669 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 E3 UBIQUITIN/ISG15 LIGASE TRIM25.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	Se	0	0	0
			1337	828	240	265	1	3			
1	B	162	Total	C	N	O	S	Se	0	0	0
			1324	821	238	261	1	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLN	LYS	engineered mutation	UNP Q14258
A	320	GLN	LYS	engineered mutation	UNP Q14258
B	273	GLN	LYS	engineered mutation	UNP Q14258
B	320	GLN	LYS	engineered mutation	UNP Q14258

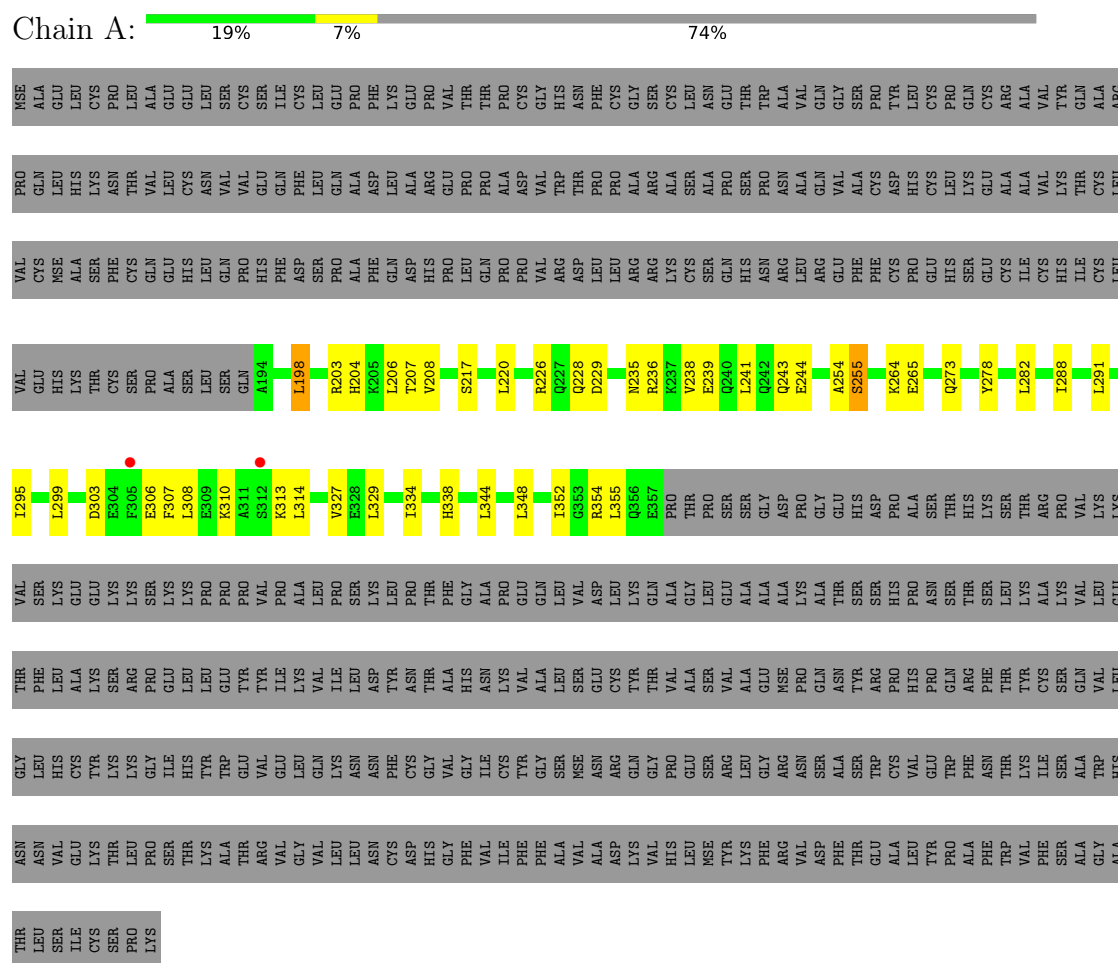
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	4	Total	O	0	0
			4	4		

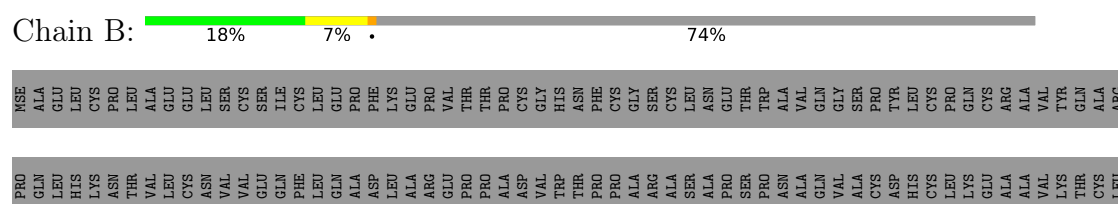
### 3 Residue-property plots

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: E3 UBIQUITIN/ISG15 LIGASE TRIM25



#### • Molecule 1: E3 UBIQUITIN/ISG15 LIGASE TRIM25



PHE	ILE	CYS	ALA	ARG	VAL	VAL
SER	SER	SER	LYS	PRO	ARG	GLU
ALA	ALA	GLN	VAL	VAL	VAL	HIS
GLY	TRP	VAL	LEU	LYS	LYS	ALA
ALA	HIS	LEU	GLU	VAL	THR	THR
THR	ASN	GLY	THR	VAL	VAL	CYS
LEU	ASN	HIS	PHE	SER	SER	SER
SER	VAL	HIS	LEU	LYS	T300	GLN
ILE	GLU	CYS	ALA	GLU	K301	GLU
CYS	LYS	TYR	LYS	GLU	SER	HIS
SER	THR	LYS	SER	LYS	E304	LEU
PRO	LEU	LYS	ARG	LYS	LYS	GLN
LYS	PRO	GLY	PRO	SER	F307	PRO
	THR	ILE	GLU	LYS	L308	HIS
	SER	HIS	LEU	LYS	E309	PHE
	THR	TYR	LEU	PRO	K310	ASP
	ALA	TRP	GLU	PRO	A311	SER
	THR	GLU	TYR	PRO	LYS	PRO
	ARG	VAL	TYR	VAL	L314	ALA
	VAL	GLU	ILE	PRO	Q320	PHE
	GLY	LEU	LYS	ALA	P321	ASP
	VAL	GLN	VAL	LEU	P322	HIS
	VAL	LYS	ILE	PRO	Y323	PRO
	LEU	ASN	LEU	SER	K205	LEU
	ASN	ASN	ASP	LYS	L206	PRO
	CYS	PHE	TYR	LEU	T207	GLN
	ASP	CYS	ASN	PRO	E326	PRO
	HIS	GLY	THR	THR	V327	PRO
	GLY	VAL	ALA	PHE	M209	VAL
	PHE	GLY	HIS	GLY	H331	ARG
	VAL	ILE	ASN	ALA	L348	ASP
	ILE	CYS	LYS	PRO	LYS	LEU
	PHE	TYR	VAL	VAL	C351	LEU
	PHE	GLY	ALA	GLN	L352	ARG
	ALA	SER	LEU	LEU	G353	ARG
	VAL	MSE	SER	VAL	R354	LYS
	ALA	ASN	GLU	ASP	L355	CYS
	ASP	ARG	GLY	LEU	Q356	SER
	LYS	GLN	TYR	LYS	GLU	GLN
	VAL	GLY	THR	GLN	K237	HIS
	HIS	PRO	VAL	ALA	PRO	ASN
	LEU	GLU	ALA	GLY	THR	ARG
	MSE	SER	SER	LEU	PRO	LEU
	TYR	ARG	VAL	GLU	SER	ARG
	LYS	LEU	ALA	ALA	SER	ARG
	PHE	GLY	GLU	ALA	GLY	GLU
	PHE	ARG	MSE	ALA	ASP	PHE
	VAL	ASN	PRO	LYS	PRO	PHE
	ASP	SER	GLN	ALA	GLY	CYS
	PHE	ALA	TYR	THR	GLU	PRO
	THR	TRP	TYR	SER	HIS	GLU
	GLU	CYS	PRO	SER	S259	HIS
	LEU	VAL	ARG	PRO	T260	GLU
	TYR	VAL	HIS	ALA	R261	CYS
	PRO	GLU	PRO	ASN	SER	GLY
	PRO	TRP	GLN	THR	HIS	ILE
	PHE	ASN	PHE	THR	E265	CYS
	TRP	LYS	ARG	LYS	F274	ILE
	VAL	THR	THR	SER	T275	CYS
						LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.88Å 68.78Å 100.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.88 – 2.80 56.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (56.88-2.80) 96.1 (56.88-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0002	Depositor
R, $R_{free}$	0.251 , 0.309 0.255 , 0.318	Depositor DCC
$R_{free}$ test set	975 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2669	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% 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	0.62	0/1345	0.85	2/1795 (0.1%)
1	B	0.66	0/1332	0.88	3/1778 (0.2%)
All	All	0.64	0/2677	0.87	5/3573 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	281	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	B	198	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	226	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	209	MSE	CA-CB-CG	-5.02	104.77	113.30

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	1337	0	1372	42	0
1	B	1324	0	1365	42	0
2	A	4	0	0	2	0
2	B	4	0	0	1	0
All	All	2669	0	2737	64	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 12.

All (64) 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:237:LYS:HD3	1:B:240:GLN:NE2	1.94	0.83
1:B:237:LYS:HD3	1:B:240:GLN:HE22	1.49	0.76
1:A:307:PHE:CE1	2:A:2002:HOH:O	2.45	0.69
1:B:281:LEU:CD2	1:B:322:VAL:HB	2.29	0.63
1:A:295:ILE:HD13	1:B:202:LEU:CD2	2.29	0.63
1:B:241:LEU:C	1:B:241:LEU:HD12	2.20	0.62
1:B:348:LEU:C	1:B:348:LEU:HD23	2.19	0.62
1:B:304:GLU:N	1:B:304:GLU:OE1	2.33	0.62
1:A:291:LEU:HD21	1:A:313:LYS:HB3	1.82	0.61
1:A:295:ILE:HD13	1:B:202:LEU:HD23	1.83	0.61
1:A:228:GLN:HG2	1:A:229:ASP:N	2.16	0.60
1:A:348:LEU:HD12	1:B:348:LEU:HD12	1.84	0.59
1:A:241:LEU:HD21	1:B:259:SER:HB3	1.86	0.58
1:A:344:LEU:HD23	1:B:248:MSE:HE1	1.87	0.57
1:A:344:LEU:HD12	1:B:351:CYS:HB3	1.87	0.56
1:A:228:GLN:CG	1:A:229:ASP:N	2.70	0.55
1:A:354:ARG:HG3	1:A:355:LEU:HD12	1.88	0.55
1:A:291:LEU:HB3	1:B:209:MSE:HE1	1.88	0.55
1:A:303:ASP:O	1:A:306:GLU:HB3	2.06	0.54
1:A:220:LEU:HD11	1:B:282:LEU:HD23	1.89	0.54
1:A:295:ILE:HG23	1:B:202:LEU:HD22	1.89	0.53
1:A:238:VAL:HG23	1:A:239:GLU:N	2.24	0.52
1:B:355:LEU:HD12	1:B:355:LEU:O	2.10	0.52
1:A:264:LYS:NZ	1:B:235:ASN:OD1	2.36	0.51
1:B:241:LEU:HD12	1:B:242:GLN:N	2.24	0.50
1:A:314:LEU:HD21	1:B:205:LYS:HB3	1.92	0.50
1:A:348:LEU:CD1	1:B:348:LEU:HD12	2.41	0.50
1:B:297:GLN:O	1:B:300:THR:HB	2.12	0.50
1:B:331:HIS:HB2	2:B:2003:HOH:O	2.12	0.50
1:A:235:ASN:O	1:A:238:VAL:HG22	2.12	0.49
1:B:323:TYR:O	1:B:323:TYR:CG	2.63	0.49
1:B:310:LYS:O	1:B:314:LEU:HG	2.14	0.48
1:A:278:TYR:CZ	1:B:220:LEU:HD22	2.49	0.47
1:B:204:HIS:O	1:B:207:THR:HB	2.15	0.47
1:A:254:ALA:O	1:A:255:SER:C	2.51	0.47
1:A:288:ILE:HG22	1:B:213:ILE:HD11	1.98	0.46
1:A:295:ILE:CG2	1:B:202:LEU:HD22	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLN:HB2	1:B:321:PRO:HD2	1.98	0.45
1:A:198:LEU:HD22	1:B:311:ALA:HB1	1.99	0.45
1:B:277:ILE:HD13	1:B:325:PRO:HD2	1.99	0.44
1:A:344:LEU:CD1	1:B:351:CYS:HB3	2.47	0.44
1:A:238:VAL:CG2	1:A:239:GLU:N	2.80	0.44
1:B:355:LEU:HD12	1:B:355:LEU:C	2.38	0.44
1:A:278:TYR:CE1	1:B:220:LEU:HD22	2.53	0.43
1:B:274:PHE:CZ	1:B:327:VAL:HG23	2.54	0.43
1:A:352:ILE:HD11	1:B:252:LEU:HD23	1.99	0.43
1:B:327:VAL:HG23	1:B:327:VAL:O	2.19	0.43
1:A:278:TYR:CE2	1:A:282:LEU:HD12	2.54	0.43
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.88	0.42
1:A:220:LEU:CD1	1:B:282:LEU:HD23	2.48	0.42
1:A:228:GLN:HG2	1:A:229:ASP:H	1.82	0.42
1:B:201:THR:O	1:B:205:LYS:HG2	2.19	0.42
1:B:323:TYR:O	1:B:323:TYR:CD2	2.72	0.42
1:B:320:GLN:HB2	1:B:321:PRO:CD	2.50	0.42
1:A:329:LEU:HD22	1:A:334:ILE:HD11	2.01	0.42
1:A:273:GLN:HB2	1:A:327:VAL:HG11	2.02	0.42
1:A:306:GLU:O	1:A:310:LYS:HG2	2.21	0.41
1:B:195:SER:OG	1:B:196:ALA:N	2.52	0.41
1:A:203:ARG:O	1:A:207:THR:HG23	2.20	0.41
1:A:243:GLN:O	1:A:244:GLU:C	2.59	0.41
1:A:299:LEU:HA	2:A:2002:HOH:O	2.20	0.41
1:A:338:HIS:ND1	1:A:338:HIS:C	2.75	0.41
1:A:299:LEU:HD23	1:A:307:PHE:CZ	2.56	0.40
1:A:204:HIS:O	1:A:208:VAL:HG23	2.20	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	162/630 (26%)	151 (93%)	11 (7%)	0	100	100
1	B	160/630 (25%)	152 (95%)	7 (4%)	1 (1%)	22	51
All	All	322/1260 (26%)	303 (94%)	18 (6%)	1 (0%)	37	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	353	GLY

### 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	151/551 (27%)	146 (97%)	5 (3%)	33	67
1	B	150/551 (27%)	140 (93%)	10 (7%)	13	38
All	All	301/1102 (27%)	286 (95%)	15 (5%)	20	51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	LEU
1	A	217	SER
1	A	255	SER
1	A	265	GLU
1	A	308	LEU
1	B	202	LEU
1	B	232	MSE
1	B	255	SER
1	B	261	ARG
1	B	265	GLU
1	B	298	SER
1	B	301	LYS
1	B	304	GLU
1	B	308	LEU
1	B	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	271	ASN
1	A	331	HIS
1	A	350	GLN
1	B	242	GLN
1	B	320	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	161/630 (25%)	0.11	2 (1%) 76 69	37, 69, 119, 142	0
1	B	159/630 (25%)	0.04	3 (1%) 66 58	34, 65, 125, 148	0
All	All	320/1260 (25%)	0.08	5 (1%) 70 63	34, 67, 123, 148	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	PHE	3.1
1	B	230	VAL	2.7
1	B	356	GLN	2.6
1	A	312	SER	2.6
1	B	307	PHE	2.2

### 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 monosaccharides 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.