



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:16 PM UTC

PDB ID : 4CFG / pdb_00004cfg
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

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

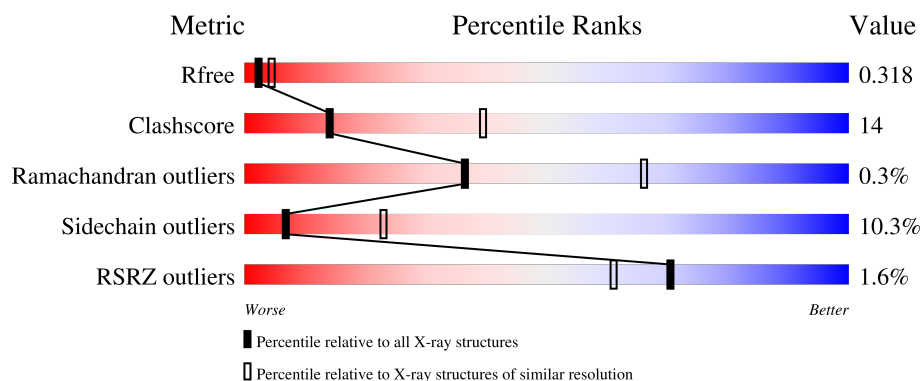
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	
1	B	630	

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

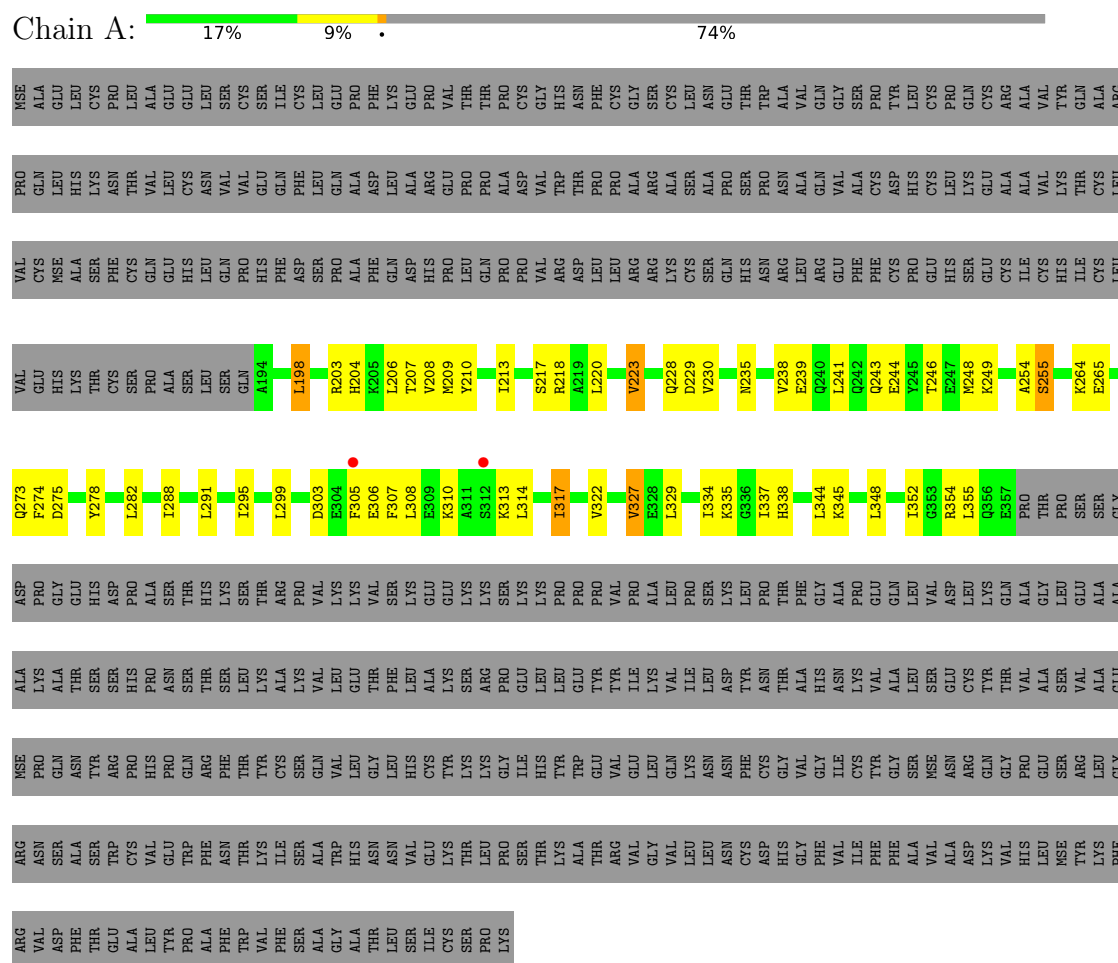
- Molecule 2 is water.

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

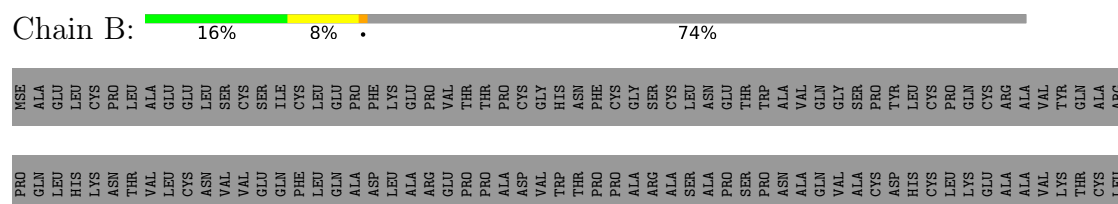
3 Residue-property plots

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



TYR	ARG	VAL	GLU	SER	E265	VAL	VAL
						GLU	HIS
LYS	LEU	ALA	ALA	SER	F274	HIS	ALA
PHE	GLY	GLU	ALA	GLY		THR	THR
ARG	ASN	MSE	LYS	PRO	I277	CYS	PHE
VAL	SER	GLN	ALA	GLY		SER	CYS
ASP	ALA	ASN	THR	GLU	L281	ALA	GLN
PHE	ALA	TYR	SER	HIS	L282	PRO	GLU
THR	SER	TRP	ARG	ASP		ALA	ALA
GLU	TRP	ARG	SER	HIS	K285	SER	HIS
ALA	CYS	VAL	HIS	PRO		LEU	LEU
LEU	VAL	HIS	PRO	ALA		SER	GLN
LEU	GLU	PRO	ASN	SER	Q289	SER	PRO
TYR	GLU	GLN	THR	THR	Q297	ALA	GLN
PRO	ALA	PHE	THR	HIS		S195	
ALA	ASN	PHE	SER	LYS	T300	ASP	
PHE	THR	THR	LEU	SER		A196	
VAL	LYS	TYR	LYS	THR	T301		
VAL	ILE	CYS	ALA	ARG	K301		
PHE	THR	SER	LYS	PRO		T201	
SER	ALA	SER	VAL	VAL	E304	ALA	
ALA	ALA	GLN	VAL	VAL		L202	
GLY	TRP	VAL	LEU	VAL		H204	
THR	HIS	LEU	GLU	LYS	F307	K205	
ALA	ASN	GLY	THR	VAL	L308	L206	
LEU	ASN	GLY	THR	VAL		T207	
LEU	VAL	LEU	PHE	SER	E309	V208	
SER	ASN	HIS	LEU	SER	K310	M209	
LEU	VAL	LEU	ALA	GLU	A311	Y210	
ILE	GLY	CYS	ALA	GLU			
ILE	LYS	TYR	LYS	GLU	L314		
CYS	THR	THR	SER	LYS			
SER	LEU	LYS	ARG	LYS	I317	T213	
PRO	PRO	GLY	PRO	SER			
LYS	ILE	ILE	GLU	LYS	Q320	L220	
	THR	HIS	LEU	LYS			
	THR	THR	LEU	PRO	P321	V230	
	ALA	TRP	GLU	PRO	V322	R231	
	ALA	GLU	TYR	PRO	Y323	M232	
	ARG	VAL	TYR	VAL	I324		
	VAL	GLU	ILE	PRO	P325	N235	
	VAL	LEU	VAL	ALA	E326	R236	
	VAL	GLN	VAL	LEU	V327	K237	
	VAL	LYS	ILE	PRO	L331		
	LEU	ASN	LEU	SER	H331	Q240	
	ASN	ASN	ASP	LYS		L241	
	CYS	PHE	TYR	LEU	I334	Q242	
	ASP	CYS	ASN	PRO	K335	Q243	
	GLY	GLY	THR	THR		E244	
	HIS	VAL	ALA	PHE	L344	V245	
	GLY	GLY	HIS	GLY	K345	T246	
	VAL	ILE	ASN	ALA		E247	
	ILE	CYS	LYS	PRO	L348	M248	
	THR	TYR	VAL	GLU			
	PHE	GLY	ALA	GLN	C351	L252	
	VAL	SER	LEU	LEU	I352	D253	
	ALA	MSE	SER	VAL	G353	A254	
	ALA	ASN	GLU	ASP	R354	S255	
	ASP	ARG	CYS	LEU	L355	E256	
	ILE	GLN	TYR	LYS	Q356	T257	
	VAL	GLY	THR	GLN	GLU	T258	
	HIS	PRO	VAL	ALA	PRO	S259	
	LEU	GLU	ALA	LEU	THR	T260	
	MSE	SER	SER	TYR		P261	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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

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	0.87	0/1345	1.09	3/1795 (0.2%)
1	B	0.96	1/1332 (0.1%)	1.12	1/1778 (0.1%)
All	All	0.92	1/2677 (0.0%)	1.10	4/3573 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LYS	N-CA	-5.09	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	GLN	N-CA-C	8.72	118.36	108.25
1	A	248	MSE	N-CA-C	-6.12	104.53	111.07
1	A	223	VAL	N-CA-CB	5.25	118.46	110.58
1	A	317	ILE	N-CA-C	5.22	115.49	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	48	0
1	B	1324	0	1365	49	0
2	A	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	1	0
All	All	2669	0	2737	77	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 14.

All (77) 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:241:LEU:C	1:B:241:LEU:HD12	2.20	0.67
1:B:348:LEU:C	1:B:348:LEU:HD23	2.19	0.67
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: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:B:355:LEU:HD12	1:B:355:LEU:O	2.10	0.52
1:A:238:VAL:HG23	1:A:239:GLU:N	2.24	0.52
1:A:254:ALA:O	1:A:255:SER:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:HD12	1:B:355:LEU:C	2.38	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: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
1:A:243:GLN:O	1:A:244:GLU:C	2.59	0.46
1:A:338:HIS:ND1	1:A:338:HIS:C	2.75	0.45
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:B:243:GLN:O	1:B:244:GLU:C	2.60	0.44
1:B:254:ALA:O	1:B:255:SER:C	2.60	0.44
1:A:238:VAL:CG2	1:A:239:GLU:N	2.80	0.44
1:A:305:PHE:O	1:A:306:GLU:C	2.61	0.44
1:A:337:ILE:O	1:A:338:HIS:C	2.61	0.44
1:A:278:TYR:CE1	1:B:220:LEU:HD22	2.53	0.43
1:B:348:LEU:C	1:B:348:LEU:CD2	2.89	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:B:344:LEU:O	1:B:345:LYS:C	2.62	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:A:334:ILE:O	1:A:335:LYS:C	2.63	0.42
1:B:320:GLN:HB2	1:B:321:PRO:CD	2.50	0.42
1:B:209:MSE:O	1:B:210:TYR:C	2.63	0.42
1:B:334:ILE:O	1:B:335:LYS:C	2.62	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:209:MSE:O	1:A:210:TYR:C	2.63	0.41
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:274:PHE:O	1:A:275:ASP:C	2.61	0.41
1:A:299:LEU:HA	2:A:2002:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:O	1:A:345:LYS:C	2.63	0.41
1:B:241:LEU:C	1:B:241:LEU:CD1	2.92	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 [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	162/630 (26%)	151 (93%)	11 (7%)	0	100	100
1	B	160/630 (25%)	152 (95%)	7 (4%)	1 (1%)	21	51
All	All	322/1260 (26%)	303 (94%)	18 (6%)	1 (0%)	36	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	353	GLY

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	151/551 (27%)	137 (91%)	14 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	150/551 (27%)	133 (89%)	17 (11%)	5	19
All	All	301/1102 (27%)	270 (90%)	31 (10%)	7	23

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	LEU
1	A	213	ILE
1	A	217	SER
1	A	218	ARG
1	A	223	VAL
1	A	230	VAL
1	A	246	THR
1	A	249	LYS
1	A	255	SER
1	A	265	GLU
1	A	308	LEU
1	A	317	ILE
1	A	322	VAL
1	A	327	VAL
1	B	202	LEU
1	B	213	ILE
1	B	230	VAL
1	B	232	MSE
1	B	241	LEU
1	B	246	THR
1	B	252	LEU
1	B	255	SER
1	B	257	THR
1	B	261	ARG
1	B	265	GLU
1	B	289	GLN
1	B	301	LYS
1	B	304	GLU
1	B	308	LEU
1	B	317	ILE
1	B	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
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, 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	161/630 (25%)	0.26	2 (1%) 76 68	37, 69, 119, 142	0
1	B	159/630 (25%)	0.19	3 (1%) 66 57	34, 65, 125, 148	0
All	All	320/1260 (25%)	0.22	5 (1%) 70 61	34, 67, 123, 148	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	PHE	3.2
1	B	230	VAL	2.8
1	B	356	GLN	2.7
1	A	312	SER	2.7
1	B	307	PHE	2.3

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.