



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 01:30 PM JST

PDB ID : 9IUN / pdb_00009iun
Title : Crystal structure of Trim25 Pspry
Authors : Li, Y.L.; Lin, T.W.
Deposited on : 2024-07-22
Resolution : 2.70 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

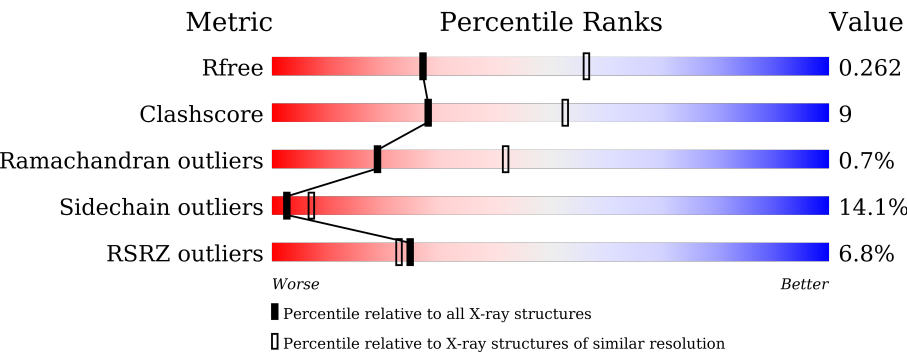
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	205	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>67%22%5%5%</div></div>
1	B	205	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>74%20%5%.</div></div>
1	C	205	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>67%25%5%.</div></div>
1	D	205	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>69%23%.5%</div></div>
1	E	205	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>69%21%.6%</div></div>
1	F	205	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>64%26%.6%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	205	<div><div></div><div>3%</div><div>73%</div><div>18%</div><div>•</div><div>6%</div></div>
1	H	205	<div><div></div><div>6%</div><div>75%</div><div>20%</div><div>•</div><div>•</div></div>
1	I	205	<div><div></div><div>13%</div><div>65%</div><div>27%</div><div>5%</div><div>•</div></div>
1	J	205	<div><div></div><div>4%</div><div>68%</div><div>21%</div><div>5%</div><div>5%</div></div>
1	K	205	<div><div></div><div>6%</div><div>67%</div><div>25%</div><div>•</div><div>5%</div></div>
1	L	205	<div><div></div><div>8%</div><div>67%</div><div>22%</div><div>•</div><div>6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19317 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	195	Total	C	N	O	S	0	0	0
			1570	1016	267	276	11			
1	B	201	Total	C	N	O	S	0	0	0
			1625	1052	276	286	11			
1	C	199	Total	C	N	O	S	0	0	0
			1614	1045	276	282	11			
1	D	194	Total	C	N	O	S	0	0	0
			1564	1013	266	274	11			
1	E	193	Total	C	N	O	S	0	0	0
			1557	1008	265	273	11			
1	F	193	Total	C	N	O	S	0	0	0
			1556	1007	265	273	11			
1	G	193	Total	C	N	O	S	0	0	0
			1556	1007	265	273	11			
1	H	201	Total	C	N	O	S	0	0	0
			1625	1052	276	286	11			
1	I	199	Total	C	N	O	S	0	0	0
			1614	1045	276	282	11			
1	J	194	Total	C	N	O	S	0	0	0
			1565	1013	267	274	11			
1	K	195	Total	C	N	O	S	0	0	0
			1570	1015	267	277	11			
1	L	193	Total	C	N	O	S	0	0	0
			1556	1007	265	273	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q14258
A	199	TYR	-	expression tag	UNP Q14258
A	200	LEU	-	expression tag	UNP Q14258
A	201	GLU	-	expression tag	UNP Q14258
A	202	HIS	-	expression tag	UNP Q14258

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Chain	Residue	Modelled	Actual	Comment	Reference
A	203	HIS	-	expression tag	UNP Q14258
A	204	HIS	-	expression tag	UNP Q14258
B	0	MET	-	initiating methionine	UNP Q14258
B	199	TYR	-	expression tag	UNP Q14258
B	200	LEU	-	expression tag	UNP Q14258
B	201	GLU	-	expression tag	UNP Q14258
B	202	HIS	-	expression tag	UNP Q14258
B	203	HIS	-	expression tag	UNP Q14258
B	204	HIS	-	expression tag	UNP Q14258
C	0	MET	-	initiating methionine	UNP Q14258
C	199	TYR	-	expression tag	UNP Q14258
C	200	LEU	-	expression tag	UNP Q14258
C	201	GLU	-	expression tag	UNP Q14258
C	202	HIS	-	expression tag	UNP Q14258
C	203	HIS	-	expression tag	UNP Q14258
C	204	HIS	-	expression tag	UNP Q14258
D	0	MET	-	initiating methionine	UNP Q14258
D	199	TYR	-	expression tag	UNP Q14258
D	200	LEU	-	expression tag	UNP Q14258
D	201	GLU	-	expression tag	UNP Q14258
D	202	HIS	-	expression tag	UNP Q14258
D	203	HIS	-	expression tag	UNP Q14258
D	204	HIS	-	expression tag	UNP Q14258
E	0	MET	-	initiating methionine	UNP Q14258
E	199	TYR	-	expression tag	UNP Q14258
E	200	LEU	-	expression tag	UNP Q14258
E	201	GLU	-	expression tag	UNP Q14258
E	202	HIS	-	expression tag	UNP Q14258
E	203	HIS	-	expression tag	UNP Q14258
E	204	HIS	-	expression tag	UNP Q14258
F	0	MET	-	initiating methionine	UNP Q14258
F	199	TYR	-	expression tag	UNP Q14258
F	200	LEU	-	expression tag	UNP Q14258
F	201	GLU	-	expression tag	UNP Q14258
F	202	HIS	-	expression tag	UNP Q14258
F	203	HIS	-	expression tag	UNP Q14258
F	204	HIS	-	expression tag	UNP Q14258
G	0	MET	-	initiating methionine	UNP Q14258
G	199	TYR	-	expression tag	UNP Q14258
G	200	LEU	-	expression tag	UNP Q14258
G	201	GLU	-	expression tag	UNP Q14258
G	202	HIS	-	expression tag	UNP Q14258

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Chain	Residue	Modelled	Actual	Comment	Reference
G	203	HIS	-	expression tag	UNP Q14258
G	204	HIS	-	expression tag	UNP Q14258
H	0	MET	-	initiating methionine	UNP Q14258
H	199	TYR	-	expression tag	UNP Q14258
H	200	LEU	-	expression tag	UNP Q14258
H	201	GLU	-	expression tag	UNP Q14258
H	202	HIS	-	expression tag	UNP Q14258
H	203	HIS	-	expression tag	UNP Q14258
H	204	HIS	-	expression tag	UNP Q14258
I	0	MET	-	initiating methionine	UNP Q14258
I	199	TYR	-	expression tag	UNP Q14258
I	200	LEU	-	expression tag	UNP Q14258
I	201	GLU	-	expression tag	UNP Q14258
I	202	HIS	-	expression tag	UNP Q14258
I	203	HIS	-	expression tag	UNP Q14258
I	204	HIS	-	expression tag	UNP Q14258
J	0	MET	-	initiating methionine	UNP Q14258
J	199	TYR	-	expression tag	UNP Q14258
J	200	LEU	-	expression tag	UNP Q14258
J	201	GLU	-	expression tag	UNP Q14258
J	202	HIS	-	expression tag	UNP Q14258
J	203	HIS	-	expression tag	UNP Q14258
J	204	HIS	-	expression tag	UNP Q14258
K	0	MET	-	initiating methionine	UNP Q14258
K	199	TYR	-	expression tag	UNP Q14258
K	200	LEU	-	expression tag	UNP Q14258
K	201	GLU	-	expression tag	UNP Q14258
K	202	HIS	-	expression tag	UNP Q14258
K	203	HIS	-	expression tag	UNP Q14258
K	204	HIS	-	expression tag	UNP Q14258
L	0	MET	-	initiating methionine	UNP Q14258
L	199	TYR	-	expression tag	UNP Q14258
L	200	LEU	-	expression tag	UNP Q14258
L	201	GLU	-	expression tag	UNP Q14258
L	202	HIS	-	expression tag	UNP Q14258
L	203	HIS	-	expression tag	UNP Q14258
L	204	HIS	-	expression tag	UNP Q14258

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0

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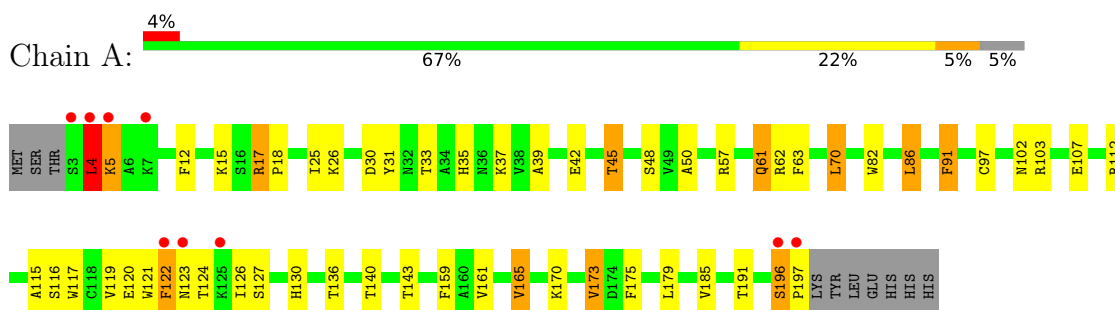
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	46	Total 46	O 46	0	0
2	C	16	Total 16	O 16	0	0
2	D	30	Total 30	O 30	0	0
2	E	19	Total 19	O 19	0	0
2	F	28	Total 28	O 28	0	0
2	G	30	Total 30	O 30	0	0
2	H	34	Total 34	O 34	0	0
2	I	22	Total 22	O 22	0	0
2	J	35	Total 35	O 35	0	0
2	K	18	Total 18	O 18	0	0
2	L	30	Total 30	O 30	0	0

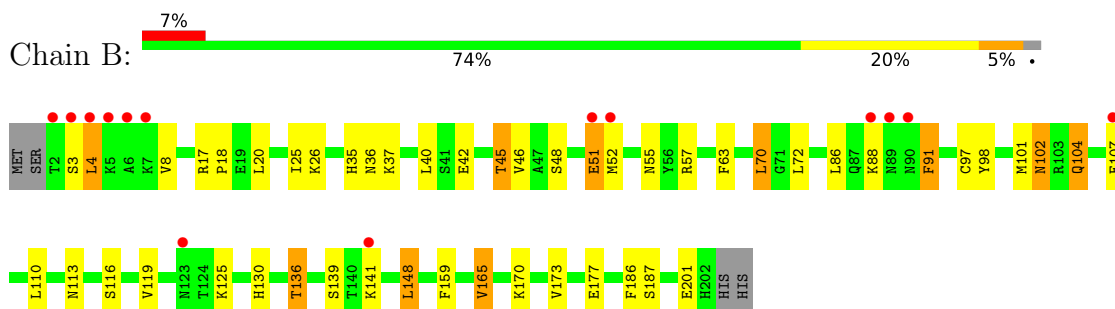
3 Residue-property plots [i](#)

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.

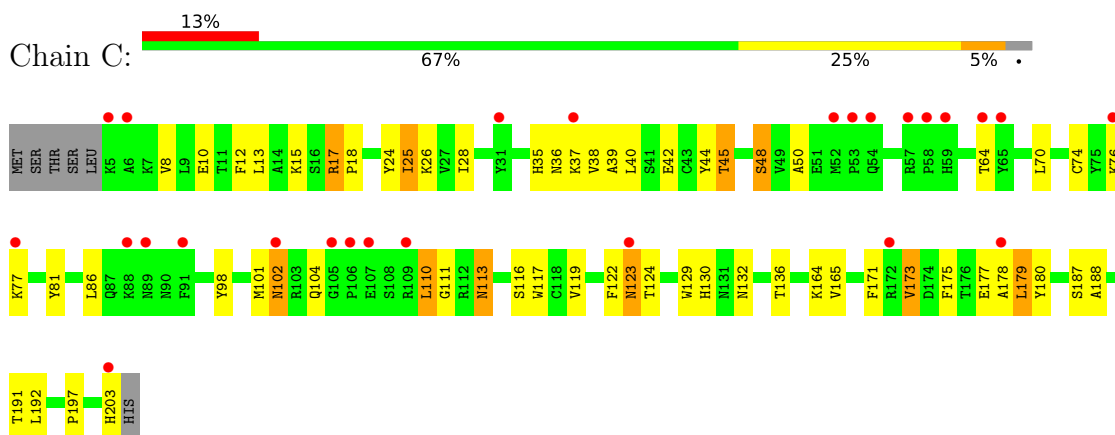
- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25



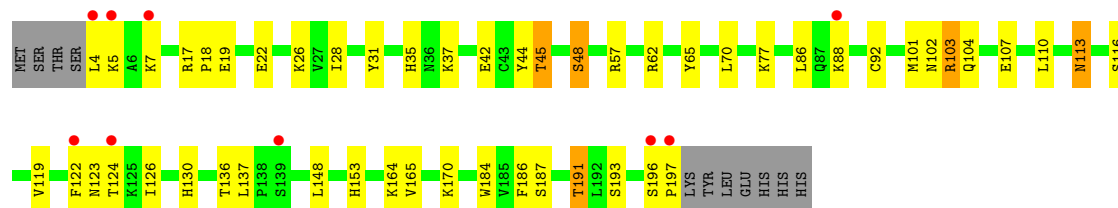
- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25



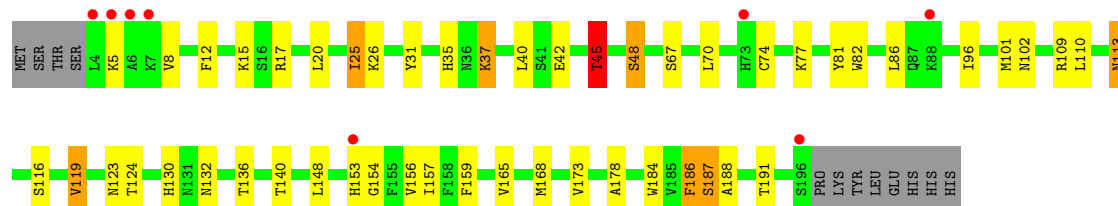
- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25



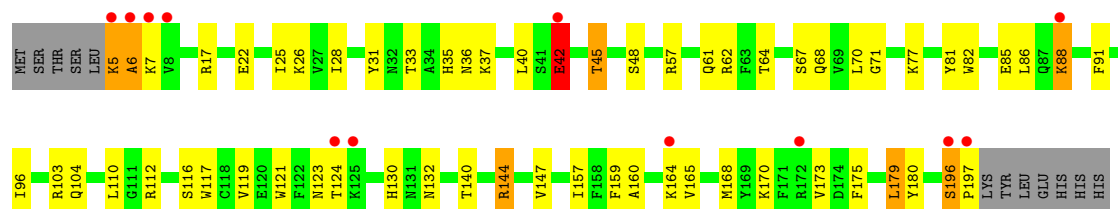
- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25



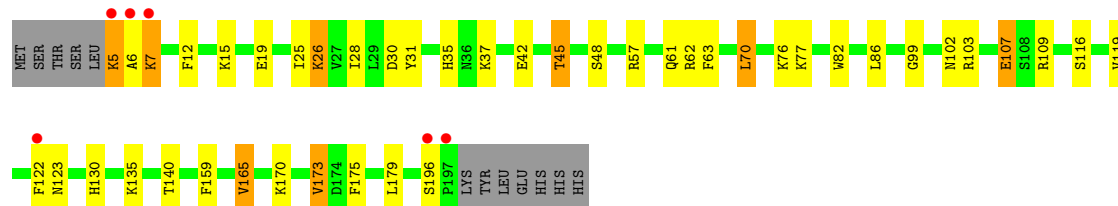
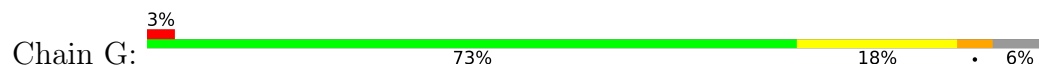
- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25



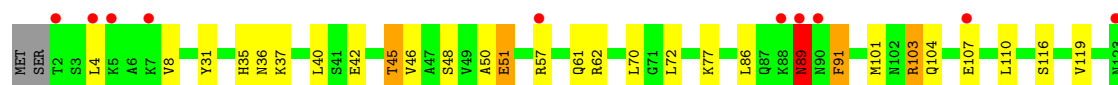
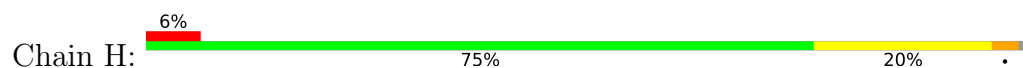
- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25

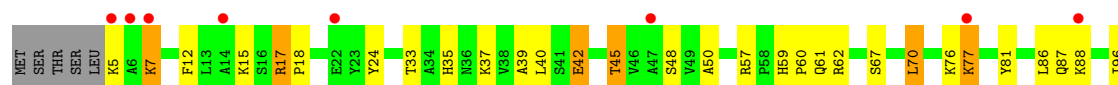


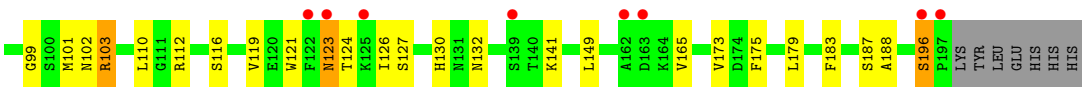
- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25



- Molecule 1: E3 ubiquitin/ISG15 ligase TRIM25







4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.01Å 182.01Å 221.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.51 – 2.70 47.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.51-2.70) 99.9 (47.51-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.265 0.214 , 0.262	Depositor DCC
R_{free} test set	5783 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19317	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8041e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.04	1/1616 (0.1%)	1.34	1/2194 (0.0%)
1	B	1.03	0/1673	1.36	3/2271 (0.1%)
1	C	1.04	0/1663	1.40	1/2257 (0.0%)
1	D	1.08	0/1610	1.36	4/2186 (0.2%)
1	E	1.03	1/1602 (0.1%)	1.41	3/2174 (0.1%)
1	F	1.08	2/1602 (0.1%)	1.37	0/2175
1	G	1.00	0/1602	1.35	0/2175
1	H	1.03	0/1673	1.40	6/2271 (0.3%)
1	I	1.04	0/1663	1.35	1/2257 (0.0%)
1	J	1.07	0/1611	1.40	4/2186 (0.2%)
1	K	1.04	0/1615	1.38	3/2192 (0.1%)
1	L	1.10	0/1602	1.38	0/2175
All	All	1.05	4/19532 (0.0%)	1.37	26/26513 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
1	L	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	LEU	N-CA	6.19	1.50	1.46
1	F	88	LYS	C-O	5.71	1.31	1.24
1	E	67	SER	C-O	5.51	1.29	1.23
1	F	42	GLU	C-O	5.29	1.30	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	45	THR	CA-CB-OG1	-8.30	97.14	109.60
1	K	45	THR	CA-CB-OG1	-7.34	98.60	109.60
1	E	186	PHE	CA-CB-CG	-6.87	106.93	113.80
1	E	45	THR	CA-CB-OG1	-6.71	99.53	109.60
1	B	136	THR	CA-CB-OG1	-6.65	99.62	109.60
1	A	136	THR	CA-CB-OG1	-6.56	99.77	109.60
1	D	191	THR	CA-CB-OG1	-6.48	99.88	109.60
1	D	186	PHE	CA-C-O	-6.10	114.85	121.20
1	E	136	THR	CA-CB-OG1	-5.95	100.67	109.60
1	K	55	ASN	CB-CA-C	-5.91	103.34	111.73
1	C	203	HIS	CA-CB-CG	5.58	119.38	113.80
1	K	136	THR	CA-CB-OG1	-5.52	101.32	109.60
1	H	135	LYS	CA-C-N	5.52	128.94	121.05
1	H	135	LYS	C-N-CA	5.52	128.94	121.05
1	J	186	PHE	CA-C-O	-5.50	116.07	121.02
1	H	89	ASN	CB-CA-C	5.42	120.44	112.09
1	I	64	THR	CB-CA-C	5.25	117.47	109.34
1	D	19	GLU	CB-CG-CD	5.20	121.43	112.60
1	J	30	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	136	THR	CB-CA-C	5.06	116.74	109.71
1	J	185	VAL	CA-C-O	-5.03	115.19	120.27
1	H	163	ASP	N-CA-C	-5.02	105.69	111.07
1	H	50	ALA	CA-C-N	5.01	126.95	120.44
1	H	50	ALA	C-N-CA	5.01	126.95	120.44
1	B	97	CYS	CA-C-N	5.00	127.97	120.87
1	B	97	CYS	C-N-CA	5.00	127.97	120.87

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	189	GLY	Peptide
1	L	87	GLN	Peptide

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	1570	0	1542	37	0
1	B	1625	0	1595	23	0
1	C	1614	0	1579	34	0
1	D	1564	0	1537	21	0
1	E	1557	0	1530	36	0
1	F	1556	0	1526	29	0
1	G	1556	0	1526	24	0
1	H	1625	0	1595	21	0
1	I	1614	0	1579	33	0
1	J	1565	0	1539	33	0
1	K	1570	0	1542	31	0
1	L	1556	0	1526	25	0
2	A	37	0	0	0	0
2	B	46	0	0	1	0
2	C	16	0	0	0	0
2	D	30	0	0	1	0
2	E	19	0	0	1	0
2	F	28	0	0	0	0
2	G	30	0	0	2	0
2	H	34	0	0	0	0
2	I	22	0	0	1	0
2	J	35	0	0	2	0
2	K	18	0	0	0	0
2	L	30	0	0	0	0
All	All	19317	0	18616	331	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 9.

All (331) 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:K:42:GLU:O	1:K:45:THR:HB	1.60	1.00
1:G:42:GLU:O	1:G:45:THR:HB	1.69	0.92
1:E:101:MET:HE3	1:E:116:SER:HB3	1.55	0.88
1:I:116:SER:O	1:I:130:HIS:HD2	1.56	0.88
1:B:42:GLU:O	1:B:45:THR:HB	1.74	0.87
1:A:35:HIS:HD2	1:A:37:LYS:H	1.24	0.85
1:F:85:GLU:OE1	1:F:144:ARG:NH1	2.11	0.83
1:F:35:HIS:HD2	1:F:37:LYS:H	1.25	0.82
1:C:42:GLU:O	1:C:45:THR:HB	1.80	0.81
1:J:42:GLU:O	1:J:45:THR:HB	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:42:GLU:HB2	1:L:45:THR:OG1	1.84	0.76
1:A:42:GLU:O	1:A:45:THR:HB	1.87	0.74
1:G:109:ARG:NH1	2:G:301:HOH:O	2.21	0.74
1:H:89:ASN:O	1:H:89:ASN:ND2	2.19	0.74
1:I:175:PHE:CD1	1:I:179:LEU:HD21	2.22	0.74
1:E:101:MET:CE	1:E:116:SER:HB3	2.16	0.74
1:L:39:ALA:HB2	1:L:50:ALA:HB2	1.69	0.74
1:I:42:GLU:O	1:I:45:THR:HB	1.88	0.72
1:E:42:GLU:O	1:E:45:THR:HB	1.91	0.71
1:G:35:HIS:HD2	1:G:37:LYS:H	1.38	0.71
1:L:35:HIS:HD2	1:L:37:LYS:H	1.38	0.70
1:H:31:TYR:O	1:H:62:ARG:NH2	2.25	0.70
1:J:57:ARG:O	1:J:62:ARG:NH1	2.24	0.70
1:I:6:ALA:HA	2:I:303:HOH:O	1.92	0.69
1:C:101:MET:HE3	1:C:116:SER:HB3	1.73	0.69
1:D:42:GLU:O	1:D:45:THR:HB	1.94	0.68
1:A:12:PHE:HA	1:A:15:LYS:HD2	1.76	0.68
1:E:25:ILE:HD13	1:E:25:ILE:H	1.59	0.67
1:J:35:HIS:CD2	1:J:37:LYS:H	2.13	0.66
1:E:12:PHE:HA	1:E:15:LYS:HD2	1.78	0.66
1:F:116:SER:O	1:F:130:HIS:HD2	1.77	0.66
1:I:31:TYR:O	1:I:62:ARG:NH2	2.29	0.65
1:B:35:HIS:HD2	1:B:37:LYS:H	1.43	0.65
1:E:101:MET:HE3	1:E:116:SER:CB	2.25	0.65
1:B:101:MET:HE3	1:B:113:ASN:HD21	1.61	0.65
1:G:122:PHE:HD2	2:G:309:HOH:O	1.80	0.65
1:F:42:GLU:HB3	1:F:45:THR:OG1	1.97	0.65
1:B:116:SER:O	1:B:130:HIS:HD2	1.80	0.64
1:F:35:HIS:HD2	1:F:37:LYS:N	1.95	0.64
1:F:160:ALA:HA	1:F:168:MET:HE3	1.79	0.64
1:A:31:TYR:CE1	1:E:31:TYR:CE1	2.85	0.64
1:H:51:GLU:H	1:H:51:GLU:CD	2.06	0.63
1:F:196:SER:H	1:F:197:PRO:CD	2.11	0.63
1:A:86:LEU:HD12	1:A:143:THR:C	2.25	0.62
1:H:101:MET:O	1:H:103:ARG:HD3	1.99	0.62
1:C:12:PHE:HA	1:C:15:LYS:HD2	1.81	0.61
1:B:51:GLU:CD	1:B:51:GLU:H	2.08	0.61
1:A:35:HIS:CD2	1:A:37:LYS:H	2.13	0.61
1:H:35:HIS:CD2	1:H:37:LYS:H	2.19	0.61
1:J:109:ARG:NH2	2:J:301:HOH:O	2.28	0.61
1:D:196:SER:HB3	1:D:197:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:HIS:CD2	1:F:37:LYS:H	2.13	0.60
1:H:57:ARG:O	1:H:62:ARG:NH1	2.34	0.60
1:J:109:ARG:HD2	1:J:184:TRP:CH2	2.35	0.60
1:C:122:PHE:O	1:E:186:PHE:CE2	2.54	0.60
1:I:113:ASN:C	1:I:113:ASN:HD22	2.10	0.60
1:C:25:ILE:HD13	1:C:25:ILE:H	1.66	0.60
1:I:13:LEU:HD13	1:I:157:ILE:HD13	1.83	0.60
1:H:135:LYS:HG2	1:H:169:TYR:CE1	2.37	0.59
1:K:25:ILE:HD13	1:K:25:ILE:H	1.65	0.59
1:D:5:LYS:HE3	1:D:153:HIS:O	2.03	0.59
1:L:96:ILE:HD12	1:L:179:LEU:HD22	1.84	0.59
1:A:57:ARG:O	1:A:62:ARG:NH1	2.36	0.58
1:G:57:ARG:O	1:G:62:ARG:NH1	2.36	0.58
1:K:25:ILE:HD13	1:K:25:ILE:N	2.19	0.57
1:H:35:HIS:HD2	1:H:37:LYS:H	1.53	0.57
1:E:101:MET:CE	1:E:116:SER:CB	2.80	0.57
1:D:35:HIS:CD2	1:D:37:LYS:H	2.22	0.57
1:E:20:LEU:CD2	1:E:148:LEU:HD13	2.35	0.57
1:E:186:PHE:O	1:E:186:PHE:CD2	2.57	0.57
1:C:122:PHE:O	1:E:186:PHE:HE2	1.87	0.57
1:A:196:SER:HB2	1:A:197:PRO:HD3	1.86	0.57
1:D:48:SER:HB3	1:D:191:THR:HG22	1.87	0.57
1:E:35:HIS:HD2	1:E:37:LYS:H	1.53	0.57
1:J:82:TRP:CZ2	1:J:147:VAL:HG11	2.39	0.57
1:A:91:PHE:N	1:A:91:PHE:HD1	2.03	0.56
1:A:91:PHE:N	1:A:91:PHE:CD1	2.74	0.56
1:A:196:SER:HB2	1:A:197:PRO:CD	2.35	0.56
1:G:5:LYS:HB2	1:G:7:LYS:HE3	1.87	0.56
1:B:35:HIS:CD2	1:B:37:LYS:H	2.23	0.56
1:D:35:HIS:HD2	1:D:37:LYS:H	1.53	0.56
1:A:35:HIS:HD2	1:A:37:LYS:N	1.98	0.56
1:B:51:GLU:CD	1:B:51:GLU:N	2.64	0.56
1:J:91:PHE:HB3	1:J:186:PHE:CE2	2.41	0.56
1:F:25:ILE:HD11	1:F:82:TRP:CE3	2.40	0.55
1:A:30:ASP:OD2	1:B:201:GLU:OE1	2.23	0.55
1:J:198:LYS:HE3	1:J:198:LYS:HA	1.88	0.55
1:B:101:MET:HE3	1:B:113:ASN:ND2	2.21	0.55
1:I:173:VAL:HG13	1:I:175:PHE:CZ	2.41	0.55
1:H:186:PHE:HE2	1:J:122:PHE:O	1.88	0.55
1:D:31:TYR:O	1:D:62:ARG:NH2	2.40	0.55
1:E:35:HIS:CD2	1:E:37:LYS:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:SER:O	1:L:130:HIS:HD2	1.90	0.55
1:L:57:ARG:O	1:L:62:ARG:NH1	2.39	0.55
1:J:35:HIS:HD2	1:J:37:LYS:H	1.56	0.54
1:J:101:MET:O	1:J:103:ARG:HD3	2.08	0.54
1:F:91:PHE:HA	1:F:121:TRP:O	2.07	0.54
1:F:57:ARG:O	1:F:62:ARG:NH1	2.41	0.54
1:F:117:TRP:CE2	1:F:130:HIS:CD2	2.96	0.54
1:I:187:SER:O	1:I:188:ALA:C	2.51	0.53
1:K:57:ARG:O	1:K:62:ARG:NH1	2.39	0.53
1:F:117:TRP:NE1	1:F:130:HIS:CD2	2.76	0.53
1:I:113:ASN:ND2	1:I:116:SER:OG	2.36	0.53
1:H:42:GLU:O	1:H:45:THR:HB	2.09	0.53
1:A:126:ILE:CD1	1:A:140:THR:HG22	2.39	0.53
1:C:113:ASN:ND2	1:C:116:SER:OG	2.42	0.52
1:J:31:TYR:O	1:J:62:ARG:NH2	2.42	0.52
1:J:197:PRO:O	1:J:198:LYS:HG2	2.09	0.52
1:G:31:TYR:O	1:G:62:ARG:NH2	2.42	0.52
1:F:31:TYR:O	1:F:62:ARG:NH2	2.42	0.52
1:I:122:PHE:O	1:K:186:PHE:CE2	2.63	0.52
1:I:175:PHE:CG	1:I:179:LEU:HD21	2.44	0.52
1:G:31:TYR:CE1	1:K:31:TYR:CE1	2.97	0.52
1:E:25:ILE:HD11	1:E:82:TRP:HE3	1.75	0.52
1:K:35:HIS:CD2	1:K:37:LYS:H	2.27	0.52
1:H:186:PHE:CE2	1:J:122:PHE:O	2.63	0.52
1:I:74:CYS:SG	1:I:178:ALA:HB1	2.50	0.52
1:J:12:PHE:HA	1:J:15:LYS:HD2	1.92	0.51
1:J:110:LEU:HD11	1:J:182:ALA:HB1	1.93	0.51
1:K:19:GLU:O	1:K:22:GLU:HB2	2.11	0.51
1:F:35:HIS:CD2	1:F:36:ASN:N	2.79	0.51
1:I:35:HIS:HD2	1:I:37:LYS:H	1.57	0.51
1:B:98:TYR:CD1	1:B:177:GLU:HG3	2.45	0.51
1:G:107:GLU:CD	1:G:107:GLU:H	2.19	0.51
1:J:116:SER:O	1:J:130:HIS:HD2	1.93	0.51
1:I:116:SER:O	1:I:130:HIS:CD2	2.48	0.51
1:C:35:HIS:CD2	1:C:37:LYS:H	2.29	0.51
1:F:196:SER:H	1:F:197:PRO:HD2	1.76	0.50
1:J:91:PHE:HA	1:J:121:TRP:O	2.11	0.50
1:L:149:LEU:HD11	1:L:179:LEU:HD13	1.92	0.50
1:E:157:ILE:HG21	1:E:159:PHE:CZ	2.47	0.50
1:E:5:LYS:O	1:E:8:VAL:HG12	2.11	0.50
1:E:119:VAL:HG11	1:E:168:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:GLU:CD	1:H:51:GLU:N	2.70	0.50
1:A:122:PHE:O	1:A:122:PHE:CG	2.65	0.50
1:J:185:VAL:HG23	1:J:185:VAL:O	2.11	0.50
1:K:45:THR:HG22	1:K:46:VAL:HG23	1.93	0.50
1:A:5:LYS:HD3	1:A:5:LYS:C	2.37	0.49
1:E:101:MET:CE	1:E:113:ASN:HD21	2.26	0.49
1:F:160:ALA:CA	1:F:168:MET:HE3	2.41	0.49
1:A:161:VAL:HG22	1:A:165:VAL:HG22	1.93	0.49
1:B:186:PHE:HE2	1:D:122:PHE:O	1.96	0.49
1:K:25:ILE:HD12	1:K:80:HIS:HB3	1.94	0.49
1:B:63:PHE:HE2	1:B:70:LEU:HD13	1.78	0.49
1:I:12:PHE:HA	1:I:15:LYS:HD2	1.93	0.49
1:K:96:ILE:HD12	1:K:179:LEU:HB3	1.94	0.49
1:F:116:SER:O	1:F:130:HIS:CD2	2.63	0.49
1:B:91:PHE:CD1	1:B:91:PHE:N	2.80	0.49
1:B:4:LEU:O	1:B:8:VAL:HG12	2.12	0.49
1:B:20:LEU:HD22	1:B:148:LEU:HD13	1.95	0.49
1:F:33:THR:HG22	1:F:61:GLN:HG3	1.94	0.49
1:F:5:LYS:O	1:F:6:ALA:HB3	2.13	0.49
1:J:15:LYS:HG2	1:J:19:GLU:HB3	1.95	0.49
1:B:55:ASN:HB2	2:B:332:HOH:O	2.11	0.49
1:I:112:ARG:O	1:I:132:ASN:HB2	2.13	0.48
1:L:112:ARG:HG3	1:L:132:ASN:HD22	1.78	0.48
1:L:175:PHE:CG	1:L:179:LEU:HD11	2.48	0.48
1:A:91:PHE:HA	1:A:121:TRP:O	2.13	0.48
1:A:97:CYS:HA	1:A:115:ALA:O	2.13	0.48
1:B:45:THR:HG22	1:B:46:VAL:HG23	1.95	0.48
1:I:185:VAL:HG13	1:I:192:LEU:HD22	1.95	0.48
1:G:116:SER:O	1:G:130:HIS:HD2	1.96	0.48
1:I:159:PHE:CD1	1:I:165:VAL:HG13	2.49	0.48
1:H:4:LEU:O	1:H:8:VAL:HG12	2.14	0.48
1:I:17:ARG:CB	1:I:18:PRO:HD3	2.43	0.48
1:J:184:TRP:CE2	1:J:186:PHE:CD1	3.02	0.48
1:L:76:LYS:H	1:L:77:LYS:CD	2.26	0.48
1:H:116:SER:O	1:H:130:HIS:HD2	1.96	0.48
1:I:17:ARG:HB2	1:I:18:PRO:HD3	1.95	0.48
1:E:25:ILE:HD13	1:E:81:TYR:O	2.13	0.48
1:C:35:HIS:HD2	1:C:37:LYS:HB2	1.78	0.48
1:C:74:CYS:HB2	1:C:178:ALA:HB1	1.95	0.48
1:G:35:HIS:CD2	1:G:37:LYS:H	2.26	0.48
1:J:70:LEU:HD12	1:J:182:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:LYS:HD2	1:L:77:LYS:N	2.29	0.47
1:D:193:SER:HB3	2:D:313:HOH:O	2.15	0.47
1:I:99:GLY:O	1:I:103:ARG:NH1	2.46	0.47
1:K:28:ILE:HG23	1:K:44:TYR:HB2	1.96	0.47
1:H:175:PHE:CG	1:H:179:LEU:HD21	2.49	0.47
1:J:113:ASN:ND2	1:J:116:SER:OG	2.47	0.47
1:B:159:PHE:CD1	1:B:165:VAL:HG13	2.49	0.47
1:B:91:PHE:N	1:B:91:PHE:HD1	2.13	0.47
1:H:91:PHE:N	1:H:91:PHE:CD1	2.82	0.47
1:C:17:ARG:CB	1:C:18:PRO:HD3	2.45	0.47
1:L:77:LYS:CD	1:L:77:LYS:N	2.78	0.47
1:C:123:ASN:HB3	1:E:186:PHE:CE2	2.50	0.47
1:F:96:ILE:HA	1:F:180:TYR:O	2.13	0.47
1:J:109:ARG:HD3	1:J:184:TRP:CZ2	2.50	0.47
1:C:123:ASN:HB3	1:E:186:PHE:CZ	2.50	0.47
1:C:187:SER:O	1:C:188:ALA:C	2.58	0.47
1:J:109:ARG:CD	1:J:184:TRP:CZ2	2.98	0.47
1:K:113:ASN:ND2	1:K:116:SER:OG	2.48	0.47
1:L:24:TYR:HA	1:L:81:TYR:O	2.15	0.47
1:A:112:ARG:NH1	1:A:120:GLU:OE1	2.45	0.46
1:E:186:PHE:O	1:E:186:PHE:CG	2.66	0.46
1:J:5:LYS:O	1:J:6:ALA:HB3	2.15	0.46
1:G:99:GLY:O	1:G:103:ARG:NH1	2.48	0.46
1:G:173:VAL:HG13	1:G:175:PHE:CE1	2.50	0.46
1:I:74:CYS:HB3	1:I:180:TYR:CD1	2.51	0.46
1:A:173:VAL:HG22	1:A:175:PHE:CD1	2.51	0.46
1:F:157:ILE:HG21	1:F:159:PHE:CZ	2.51	0.46
1:A:25:ILE:HD11	1:A:82:TRP:CE3	2.50	0.46
1:G:15:LYS:HA	1:G:19:GLU:OE2	2.16	0.46
1:A:116:SER:O	1:A:130:HIS:HD2	1.99	0.46
1:C:173:VAL:HG13	1:C:175:PHE:CZ	2.51	0.46
1:A:117:TRP:CE2	1:A:130:HIS:CD2	3.04	0.45
1:A:159:PHE:CD1	1:A:165:VAL:HG13	2.51	0.45
1:C:116:SER:O	1:C:130:HIS:HD2	1.99	0.45
1:A:63:PHE:HE2	1:A:70:LEU:HD13	1.81	0.45
1:C:101:MET:HG2	1:C:102:ASN:N	2.32	0.45
1:K:31:TYR:O	1:K:62:ARG:NH2	2.49	0.45
1:D:101:MET:O	1:D:103:ARG:HD3	2.16	0.45
1:E:101:MET:CE	1:E:116:SER:OG	2.65	0.45
1:I:97:CYS:HA	1:I:115:ALA:O	2.17	0.45
1:C:122:PHE:C	1:E:186:PHE:HE2	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:SER:HB3	1:E:191:THR:HG22	1.98	0.45
1:G:159:PHE:CD1	1:G:165:VAL:HG13	2.52	0.45
1:K:157:ILE:HG21	1:K:159:PHE:CZ	2.52	0.45
1:C:28:ILE:HG23	1:C:44:TYR:HB2	1.99	0.45
1:C:101:MET:HE1	1:C:110:LEU:HD12	1.98	0.45
1:C:175:PHE:CD1	1:C:179:LEU:HD21	2.52	0.45
1:I:67:SER:HB3	1:I:185:VAL:O	2.16	0.45
1:L:99:GLY:O	1:L:103:ARG:NH1	2.50	0.45
1:J:185:VAL:HG12	1:J:192:LEU:HG	1.99	0.44
1:I:113:ASN:C	1:I:113:ASN:ND2	2.76	0.44
1:G:63:PHE:HE2	1:G:70:LEU:HD13	1.82	0.44
1:K:119:VAL:HG11	1:K:168:MET:HE1	1.99	0.44
1:D:101:MET:SD	1:D:116:SER:HB3	2.57	0.44
1:K:25:ILE:HD11	1:K:82:TRP:HE3	1.82	0.44
1:K:119:VAL:HG12	1:K:121:TRP:CZ3	2.53	0.44
1:K:131:ASN:O	1:K:133:VAL:HG23	2.18	0.44
1:D:17:ARG:HB3	1:D:18:PRO:HD3	1.99	0.44
1:K:17:ARG:HD3	1:K:83:GLU:OE2	2.17	0.44
1:F:68:GLN:OE1	1:F:110:LEU:N	2.46	0.44
1:E:119:VAL:HG11	1:E:168:MET:HE1	1.99	0.44
1:I:17:ARG:NH1	1:I:83:GLU:OE1	2.51	0.44
1:D:57:ARG:O	1:D:62:ARG:NH1	2.51	0.43
1:E:8:VAL:HG11	1:E:153:HIS:ND1	2.32	0.43
1:F:110:LEU:HD12	1:F:110:LEU:HA	1.86	0.43
1:L:183:PHE:CD1	1:L:183:PHE:N	2.86	0.43
1:J:5:LYS:HG3	1:J:7:LYS:HB2	2.00	0.43
1:L:175:PHE:CD1	1:L:179:LEU:HD11	2.54	0.43
1:C:101:MET:HE3	1:C:116:SER:CB	2.47	0.43
1:I:39:ALA:HB2	1:I:50:ALA:HB2	2.00	0.43
1:K:20:LEU:CD2	1:K:148:LEU:HD12	2.48	0.43
1:A:61:GLN:NE2	1:A:103:ARG:NH2	2.67	0.43
1:I:122:PHE:O	1:K:186:PHE:HE2	1.98	0.43
1:G:5:LYS:CG	1:G:7:LYS:HE3	2.48	0.43
1:J:109:ARG:CD	1:J:184:TRP:CH2	2.99	0.43
1:B:102:ASN:HD22	1:B:104:GLN:H	1.65	0.43
1:L:59:HIS:ND1	1:L:60:PRO:HD2	2.34	0.43
1:C:24:TYR:CE1	1:C:197:PRO:CD	3.02	0.43
1:A:17:ARG:CB	1:A:18:PRO:HD3	2.48	0.43
1:A:33:THR:HG21	1:A:70:LEU:HB2	2.01	0.43
1:D:126:ILE:N	1:D:126:ILE:HD12	2.33	0.43
1:H:175:PHE:CD1	1:H:179:LEU:HD21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ILE:HD13	1:C:25:ILE:N	2.33	0.42
1:C:35:HIS:HD2	1:C:37:LYS:H	1.67	0.42
1:H:91:PHE:N	1:H:91:PHE:HD1	2.17	0.42
1:K:96:ILE:HD13	1:K:96:ILE:HA	1.71	0.42
1:E:96:ILE:HD11	1:E:156:VAL:HG11	1.99	0.42
1:I:129:TRP:CZ2	1:I:134:GLU:HB2	2.54	0.42
1:J:84:VAL:HA	1:J:193:SER:O	2.19	0.42
1:C:117:TRP:HD1	1:C:171:PHE:CG	2.37	0.42
1:D:92:CYS:HA	1:D:184:TRP:O	2.20	0.42
1:G:35:HIS:HD2	1:G:37:LYS:N	2.12	0.42
1:J:109:ARG:NE	2:J:301:HOH:O	2.37	0.42
1:A:117:TRP:NE1	1:A:130:HIS:CD2	2.87	0.42
1:E:74:CYS:HB2	1:E:178:ALA:HB1	2.00	0.42
1:C:38:VAL:O	1:C:38:VAL:HG12	2.20	0.42
1:E:25:ILE:HD11	1:E:82:TRP:CE3	2.54	0.42
1:E:109:ARG:HD3	1:E:184:TRP:CZ2	2.55	0.42
1:B:186:PHE:CE2	1:D:122:PHE:O	2.72	0.42
1:K:12:PHE:CE1	1:K:15:LYS:HE3	2.54	0.42
1:K:35:HIS:HD2	1:K:37:LYS:H	1.67	0.42
1:A:39:ALA:HB2	1:A:50:ALA:HB2	2.02	0.42
1:F:81:TYR:HA	1:F:147:VAL:O	2.19	0.42
1:C:111:GLY:HA3	1:C:129:TRP:HB3	2.01	0.42
1:B:125:LYS:HD2	1:D:65:TYR:CZ	2.54	0.42
1:L:17:ARG:HB3	1:L:18:PRO:HD3	2.02	0.42
1:A:4:LEU:HD13	1:A:4:LEU:N	2.35	0.41
1:C:98:TYR:HB3	1:C:177:GLU:CD	2.45	0.41
1:F:112:ARG:HG3	1:F:132:ASN:ND2	2.35	0.41
1:C:74:CYS:HB3	1:C:180:TYR:CD1	2.56	0.41
1:E:154:GLY:CA	2:E:308:HOH:O	2.68	0.41
1:K:17:ARG:CB	1:K:18:PRO:HD3	2.50	0.41
1:D:116:SER:O	1:D:130:HIS:HD2	2.04	0.41
1:F:64:THR:OG1	1:F:104:GLN:HG3	2.19	0.41
1:H:172:ARG:C	1:H:173:VAL:HG12	2.46	0.41
1:K:183:PHE:CD1	1:K:183:PHE:N	2.88	0.41
1:L:12:PHE:HA	1:L:15:LYS:HD2	2.01	0.41
1:C:101:MET:CE	1:C:116:SER:HB3	2.47	0.41
1:A:126:ILE:HD13	1:A:140:THR:HG22	2.03	0.41
1:D:113:ASN:ND2	1:D:116:SER:OG	2.54	0.41
1:G:26:LYS:HD2	1:G:28:ILE:HD11	2.02	0.41
1:I:183:PHE:CD1	1:I:183:PHE:N	2.88	0.41
1:L:101:MET:SD	1:L:116:SER:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ALA:HB2	1:C:50:ALA:HB2	2.03	0.41
1:C:48:SER:HB3	1:C:191:THR:HG22	2.02	0.41
1:E:187:SER:O	1:E:188:ALA:C	2.64	0.41
1:J:99:GLY:O	1:J:103:ARG:NH1	2.53	0.41
1:L:33:THR:HG21	1:L:70:LEU:HB2	2.02	0.41
1:A:31:TYR:O	1:A:62:ARG:NH2	2.54	0.41
1:A:63:PHE:CE2	1:A:70:LEU:HD13	2.56	0.41
1:D:126:ILE:HG22	1:D:137:LEU:HD12	2.03	0.41
1:F:175:PHE:CG	1:F:179:LEU:HD21	2.55	0.41
1:H:45:THR:HG22	1:H:46:VAL:HG23	2.02	0.41
1:I:66:CYS:SG	1:I:109:ARG:HB2	2.61	0.41
1:J:185:VAL:CG1	1:J:192:LEU:HG	2.50	0.41
1:K:24:TYR:HA	1:K:81:TYR:O	2.21	0.41
1:L:187:SER:O	1:L:188:ALA:C	2.64	0.41
1:F:28:ILE:O	1:F:71:GLY:HA2	2.20	0.41
1:G:30:ASP:OD2	1:H:201:GLU:OE2	2.40	0.41
1:G:61:GLN:NE2	1:G:103:ARG:HH21	2.19	0.41
1:K:4:LEU:O	1:K:8:VAL:HG12	2.21	0.41
1:A:196:SER:CB	1:A:197:PRO:HD3	2.51	0.40
1:C:24:TYR:HA	1:C:81:TYR:O	2.20	0.40
1:D:28:ILE:HG23	1:D:44:TYR:HB2	2.03	0.40
1:B:17:ARG:N	1:B:18:PRO:CD	2.85	0.40
1:E:113:ASN:HD22	1:E:113:ASN:C	2.28	0.40
1:K:117:TRP:CE2	1:K:130:HIS:CD2	3.09	0.40
1:L:76:LYS:H	1:L:77:LYS:HD2	1.85	0.40
1:A:185:VAL:O	1:A:185:VAL:HG23	2.22	0.40
1:K:186:PHE:O	1:K:186:PHE:CD2	2.75	0.40
1:G:12:PHE:HA	1:G:15:LYS:HD2	2.02	0.40
1:I:20:LEU:HD22	1:I:148:LEU:HD13	2.04	0.40
1:E:116:SER:O	1:E:130:HIS:HD2	2.04	0.40
1:G:25:ILE:HD11	1:G:82:TRP:CE3	2.56	0.40
1:G:61:GLN:NE2	1:G:103:ARG:NH2	2.70	0.40
1:L:7:LYS:H	1:L:7:LYS:HG2	1.82	0.40
1:L:121:TRP:CD1	1:L:126:ILE:HG12	2.57	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	193/205 (94%)	181 (94%)	10 (5%)	2 (1%)	13	33
1	B	199/205 (97%)	190 (96%)	7 (4%)	2 (1%)	13	33
1	C	197/205 (96%)	177 (90%)	19 (10%)	1 (0%)	25	49
1	D	192/205 (94%)	183 (95%)	8 (4%)	1 (0%)	25	49
1	E	191/205 (93%)	176 (92%)	14 (7%)	1 (0%)	25	49
1	F	191/205 (93%)	175 (92%)	13 (7%)	3 (2%)	8	21
1	G	191/205 (93%)	183 (96%)	7 (4%)	1 (0%)	25	49
1	H	199/205 (97%)	195 (98%)	4 (2%)	0	100	100
1	I	197/205 (96%)	185 (94%)	11 (6%)	1 (0%)	25	49
1	J	192/205 (94%)	179 (93%)	12 (6%)	1 (0%)	25	49
1	K	193/205 (94%)	178 (92%)	15 (8%)	0	100	100
1	L	191/205 (93%)	175 (92%)	13 (7%)	3 (2%)	8	21
All	All	2326/2460 (95%)	2177 (94%)	133 (6%)	16 (1%)	19	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	SER
1	C	123	ASN
1	F	196	SER
1	G	6	ALA
1	I	123	ASN
1	L	123	ASN
1	L	196	SER
1	A	123	ASN
1	B	88	LYS
1	D	123	ASN
1	F	123	ASN
1	J	123	ASN

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Mol	Chain	Res	Type
1	E	123	ASN
1	L	42	GLU
1	B	3	SER
1	F	6	ALA

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	170/180 (94%)	149 (88%)	21 (12%)	4	9
1	B	176/180 (98%)	149 (85%)	27 (15%)	2	6
1	C	174/180 (97%)	146 (84%)	28 (16%)	2	5
1	D	169/180 (94%)	146 (86%)	23 (14%)	3	7
1	E	168/180 (93%)	148 (88%)	20 (12%)	4	10
1	F	168/180 (93%)	144 (86%)	24 (14%)	2	7
1	G	168/180 (93%)	148 (88%)	20 (12%)	4	10
1	H	176/180 (98%)	149 (85%)	27 (15%)	2	6
1	I	174/180 (97%)	146 (84%)	28 (16%)	2	5
1	J	169/180 (94%)	143 (85%)	26 (15%)	2	6
1	K	170/180 (94%)	148 (87%)	22 (13%)	3	8
1	L	168/180 (93%)	145 (86%)	23 (14%)	3	7
All	All	2050/2160 (95%)	1761 (86%)	289 (14%)	3	7

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LYS
1	A	17	ARG
1	A	26	LYS
1	A	45	THR
1	A	48	SER

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Mol	Chain	Res	Type
1	A	61	GLN
1	A	70	LEU
1	A	86	LEU
1	A	91	PHE
1	A	102	ASN
1	A	107	GLU
1	A	119	VAL
1	A	122	PHE
1	A	124	THR
1	A	127	SER
1	A	165	VAL
1	A	170	LYS
1	A	173	VAL
1	A	179	LEU
1	A	191	THR
1	B	4	LEU
1	B	25	ILE
1	B	26	LYS
1	B	36	ASN
1	B	40	LEU
1	B	45	THR
1	B	48	SER
1	B	51	GLU
1	B	52	MET
1	B	57	ARG
1	B	70	LEU
1	B	72	LEU
1	B	86	LEU
1	B	91	PHE
1	B	102	ASN
1	B	104	GLN
1	B	107	GLU
1	B	110	LEU
1	B	119	VAL
1	B	136	THR
1	B	139	SER
1	B	141	LYS
1	B	148	LEU
1	B	165	VAL
1	B	170	LYS
1	B	173	VAL
1	B	187	SER

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Mol	Chain	Res	Type
1	C	8	VAL
1	C	10	GLU
1	C	13	LEU
1	C	17	ARG
1	C	25	ILE
1	C	26	LYS
1	C	36	ASN
1	C	40	LEU
1	C	45	THR
1	C	48	SER
1	C	64	THR
1	C	70	LEU
1	C	76	LYS
1	C	77	LYS
1	C	86	LEU
1	C	102	ASN
1	C	104	GLN
1	C	110	LEU
1	C	113	ASN
1	C	119	VAL
1	C	124	THR
1	C	132	ASN
1	C	136	THR
1	C	164	LYS
1	C	165	VAL
1	C	173	VAL
1	C	179	LEU
1	C	192	LEU
1	D	4	LEU
1	D	7	LYS
1	D	22	GLU
1	D	26	LYS
1	D	45	THR
1	D	48	SER
1	D	70	LEU
1	D	77	LYS
1	D	86	LEU
1	D	88	LYS
1	D	102	ASN
1	D	103	ARG
1	D	104	GLN
1	D	107	GLU

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Mol	Chain	Res	Type
1	D	110	LEU
1	D	113	ASN
1	D	119	VAL
1	D	124	THR
1	D	148	LEU
1	D	164	LYS
1	D	165	VAL
1	D	170	LYS
1	D	187	SER
1	E	17	ARG
1	E	25	ILE
1	E	26	LYS
1	E	37	LYS
1	E	40	LEU
1	E	45	THR
1	E	48	SER
1	E	70	LEU
1	E	77	LYS
1	E	86	LEU
1	E	102	ASN
1	E	110	LEU
1	E	113	ASN
1	E	119	VAL
1	E	124	THR
1	E	132	ASN
1	E	140	THR
1	E	165	VAL
1	E	173	VAL
1	E	187	SER
1	F	5	LYS
1	F	7	LYS
1	F	17	ARG
1	F	22	GLU
1	F	26	LYS
1	F	40	LEU
1	F	42	GLU
1	F	45	THR
1	F	48	SER
1	F	67	SER
1	F	70	LEU
1	F	77	LYS
1	F	86	LEU

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Mol	Chain	Res	Type
1	F	88	LYS
1	F	103	ARG
1	F	119	VAL
1	F	124	THR
1	F	140	THR
1	F	144	ARG
1	F	164	LYS
1	F	165	VAL
1	F	170	LYS
1	F	173	VAL
1	F	179	LEU
1	G	5	LYS
1	G	7	LYS
1	G	26	LYS
1	G	45	THR
1	G	48	SER
1	G	70	LEU
1	G	76	LYS
1	G	77	LYS
1	G	86	LEU
1	G	102	ASN
1	G	107	GLU
1	G	119	VAL
1	G	123	ASN
1	G	135	LYS
1	G	140	THR
1	G	165	VAL
1	G	170	LYS
1	G	173	VAL
1	G	179	LEU
1	G	196	SER
1	H	36	ASN
1	H	40	LEU
1	H	45	THR
1	H	48	SER
1	H	51	GLU
1	H	61	GLN
1	H	70	LEU
1	H	72	LEU
1	H	77	LYS
1	H	86	LEU
1	H	89	ASN

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Mol	Chain	Res	Type
1	H	91	PHE
1	H	103	ARG
1	H	104	GLN
1	H	107	GLU
1	H	110	LEU
1	H	119	VAL
1	H	124	THR
1	H	136	THR
1	H	139	SER
1	H	164	LYS
1	H	165	VAL
1	H	170	LYS
1	H	173	VAL
1	H	187	SER
1	H	191	THR
1	H	196	SER
1	I	9	LEU
1	I	13	LEU
1	I	17	ARG
1	I	25	ILE
1	I	26	LYS
1	I	36	ASN
1	I	40	LEU
1	I	45	THR
1	I	48	SER
1	I	51	GLU
1	I	64	THR
1	I	70	LEU
1	I	86	LEU
1	I	102	ASN
1	I	103	ARG
1	I	104	GLN
1	I	110	LEU
1	I	113	ASN
1	I	116	SER
1	I	119	VAL
1	I	124	THR
1	I	135	LYS
1	I	136	THR
1	I	165	VAL
1	I	170	LYS
1	I	173	VAL

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Mol	Chain	Res	Type
1	I	179	LEU
1	I	192	LEU
1	J	5	LYS
1	J	7	LYS
1	J	17	ARG
1	J	25	ILE
1	J	26	LYS
1	J	36	ASN
1	J	40	LEU
1	J	45	THR
1	J	48	SER
1	J	70	LEU
1	J	86	LEU
1	J	91	PHE
1	J	102	ASN
1	J	103	ARG
1	J	104	GLN
1	J	107	GLU
1	J	110	LEU
1	J	113	ASN
1	J	119	VAL
1	J	124	THR
1	J	127	SER
1	J	135	LYS
1	J	141	LYS
1	J	165	VAL
1	J	174	ASP
1	J	198	LYS
1	K	4	LEU
1	K	7	LYS
1	K	17	ARG
1	K	25	ILE
1	K	26	LYS
1	K	40	LEU
1	K	45	THR
1	K	70	LEU
1	K	86	LEU
1	K	96	ILE
1	K	102	ASN
1	K	104	GLN
1	K	107	GLU
1	K	110	LEU

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Mol	Chain	Res	Type
1	K	113	ASN
1	K	119	VAL
1	K	124	THR
1	K	145	VAL
1	K	164	LYS
1	K	173	VAL
1	K	187	SER
1	K	196	SER
1	L	5	LYS
1	L	7	LYS
1	L	17	ARG
1	L	40	LEU
1	L	45	THR
1	L	48	SER
1	L	61	GLN
1	L	67	SER
1	L	70	LEU
1	L	77	LYS
1	L	86	LEU
1	L	88	LYS
1	L	102	ASN
1	L	103	ARG
1	L	110	LEU
1	L	119	VAL
1	L	123	ASN
1	L	124	THR
1	L	127	SER
1	L	141	LYS
1	L	165	VAL
1	L	173	VAL
1	L	196	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	61	GLN
1	A	130	HIS
1	A	132	ASN
1	B	35	HIS
1	B	54	GLN
1	B	102	ASN

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Mol	Chain	Res	Type
1	B	104	GLN
1	B	130	HIS
1	B	132	ASN
1	C	35	HIS
1	C	59	HIS
1	C	73	HIS
1	C	113	ASN
1	C	130	HIS
1	C	132	ASN
1	C	153	HIS
1	D	35	HIS
1	D	113	ASN
1	D	130	HIS
1	D	132	ASN
1	D	153	HIS
1	E	35	HIS
1	E	89	ASN
1	E	90	ASN
1	E	102	ASN
1	E	113	ASN
1	E	123	ASN
1	E	130	HIS
1	E	132	ASN
1	F	35	HIS
1	F	61	GLN
1	F	73	HIS
1	F	130	HIS
1	F	132	ASN
1	G	35	HIS
1	G	36	ASN
1	G	61	GLN
1	G	73	HIS
1	G	89	ASN
1	G	90	ASN
1	G	123	ASN
1	G	130	HIS
1	G	132	ASN
1	G	153	HIS
1	G	166	HIS
1	H	35	HIS
1	H	73	HIS
1	H	90	ASN

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Mol	Chain	Res	Type
1	H	130	HIS
1	H	132	ASN
1	H	202	HIS
1	I	35	HIS
1	I	89	ASN
1	I	113	ASN
1	I	123	ASN
1	I	130	HIS
1	I	132	ASN
1	I	202	HIS
1	J	35	HIS
1	J	36	ASN
1	J	113	ASN
1	J	130	HIS
1	J	132	ASN
1	K	35	HIS
1	K	89	ASN
1	K	90	ASN
1	K	113	ASN
1	K	123	ASN
1	K	130	HIS
1	K	132	ASN
1	L	35	HIS
1	L	80	HIS
1	L	123	ASN
1	L	130	HIS
1	L	132	ASN
1	L	166	HIS

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	195/205 (95%)	-0.10	9 (4%) 38 36	18, 29, 62, 107	0
1	B	201/205 (98%)	0.01	14 (6%) 24 22	18, 30, 73, 133	0
1	C	199/205 (97%)	0.81	26 (13%) 8 8	24, 49, 92, 127	0
1	D	194/205 (94%)	0.11	9 (4%) 38 36	21, 33, 66, 94	0
1	E	193/205 (94%)	0.25	8 (4%) 42 40	19, 38, 69, 115	0
1	F	193/205 (94%)	0.24	12 (6%) 28 26	21, 36, 66, 120	0
1	G	193/205 (94%)	-0.19	6 (3%) 51 49	19, 29, 56, 98	0
1	H	201/205 (98%)	-0.04	12 (5%) 29 27	19, 30, 72, 87	0
1	I	199/205 (97%)	0.72	27 (13%) 8 7	25, 48, 91, 118	0
1	J	194/205 (94%)	0.15	8 (4%) 42 40	23, 33, 68, 95	0
1	K	195/205 (95%)	0.28	13 (6%) 25 23	19, 39, 73, 102	0
1	L	193/205 (94%)	0.57	16 (8%) 19 17	22, 38, 75, 116	0
All	All	2350/2460 (95%)	0.23	160 (6%) 25 23	18, 35, 77, 133	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4	LEU	9.4
1	L	197	PRO	8.9
1	A	197	PRO	8.6
1	G	197	PRO	7.5
1	B	4	LEU	7.5
1	C	5	LYS	6.5
1	F	5	LYS	6.4
1	D	197	PRO	6.4
1	F	197	PRO	6.3
1	A	122	PHE	6.2
1	I	107	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	107	GLU	5.9
1	C	52	MET	5.8
1	L	5	LYS	5.7
1	A	4	LEU	5.7
1	I	88	LYS	5.7
1	L	7	LYS	5.6
1	K	2	THR	5.5
1	L	88	LYS	5.4
1	J	6	ALA	5.3
1	L	122	PHE	5.3
1	I	53	PRO	5.2
1	G	5	LYS	4.9
1	K	5	LYS	4.8
1	C	123	ASN	4.8
1	B	3	SER	4.7
1	E	5	LYS	4.6
1	L	77	LYS	4.6
1	E	7	LYS	4.6
1	I	5	LYS	4.5
1	B	7	LYS	4.5
1	B	5	LYS	4.4
1	C	88	LYS	4.3
1	F	6	ALA	4.2
1	D	4	LEU	4.2
1	H	89	ASN	4.2
1	B	88	LYS	4.2
1	J	198	LYS	4.0
1	E	88	LYS	3.9
1	E	153	HIS	3.9
1	L	139	SER	3.9
1	C	53	PRO	3.8
1	K	4	LEU	3.8
1	C	6	ALA	3.7
1	A	123	ASN	3.7
1	K	153	HIS	3.7
1	J	8	VAL	3.7
1	B	141	LYS	3.6
1	I	109	ARG	3.6
1	H	88	LYS	3.6
1	C	58	PRO	3.6
1	J	88	LYS	3.5
1	D	7	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	5	LYS	3.5
1	K	88	LYS	3.5
1	I	6	ALA	3.4
1	C	109	ARG	3.4
1	J	5	LYS	3.4
1	I	52	MET	3.4
1	H	2	THR	3.4
1	I	60	PRO	3.3
1	I	123	ASN	3.3
1	B	2	THR	3.3
1	A	3	SER	3.2
1	J	124	THR	3.2
1	L	6	ALA	3.2
1	D	88	LYS	3.2
1	K	7	LYS	3.2
1	I	36	ASN	3.1
1	F	125	LYS	3.1
1	H	107	GLU	3.0
1	E	6	ALA	3.0
1	F	124	THR	3.0
1	D	5	LYS	3.0
1	K	184	TRP	2.9
1	I	106	PRO	2.9
1	B	6	ALA	2.9
1	C	106	PRO	2.9
1	C	37	LYS	2.9
1	I	7	LYS	2.9
1	F	7	LYS	2.8
1	C	57	ARG	2.8
1	B	52	MET	2.8
1	F	88	LYS	2.8
1	I	57	ARG	2.8
1	K	123	ASN	2.8
1	I	61	GLN	2.8
1	C	76	LYS	2.8
1	J	141	LYS	2.8
1	I	89	ASN	2.7
1	G	6	ALA	2.7
1	B	89	ASN	2.7
1	L	123	ASN	2.7
1	A	5	LYS	2.7
1	F	164	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	59	HIS	2.7
1	C	65	TYR	2.6
1	H	123	ASN	2.6
1	L	125	LYS	2.6
1	D	124	THR	2.6
1	F	196	SER	2.6
1	C	31	TYR	2.6
1	L	22	GLU	2.6
1	G	7	LYS	2.6
1	D	196	SER	2.6
1	B	51	GLU	2.6
1	B	107	GLU	2.6
1	I	37	LYS	2.6
1	K	122	PHE	2.6
1	K	6	ALA	2.6
1	F	42	GLU	2.5
1	L	14	ALA	2.5
1	A	125	LYS	2.5
1	G	196	SER	2.5
1	I	102	ASN	2.5
1	L	196	SER	2.5
1	I	203	HIS	2.4
1	I	90	ASN	2.4
1	H	57	ARG	2.4
1	K	188	ALA	2.4
1	L	162	ALA	2.4
1	I	51	GLU	2.4
1	J	123	ASN	2.4
1	C	77	LYS	2.4
1	C	203	HIS	2.4
1	C	105	GLY	2.3
1	H	4	LEU	2.3
1	A	7	LYS	2.3
1	I	64	THR	2.3
1	A	196	SER	2.3
1	H	7	LYS	2.3
1	C	89	ASN	2.3
1	H	184	TRP	2.3
1	I	72	LEU	2.3
1	B	123	ASN	2.2
1	C	102	ASN	2.2
1	E	73	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	178	ALA	2.2
1	I	58	PRO	2.2
1	B	90	ASN	2.2
1	G	122	PHE	2.2
1	D	139	SER	2.2
1	L	163	ASP	2.2
1	I	105	GLY	2.2
1	C	64	THR	2.1
1	H	90	ASN	2.1
1	F	172	ARG	2.1
1	K	3	SER	2.1
1	D	122	PHE	2.1
1	L	47	ALA	2.1
1	I	187	SER	2.1
1	F	8	VAL	2.1
1	C	91	PHE	2.1
1	I	104	GLN	2.1
1	H	141	LYS	2.0
1	I	66	CYS	2.0
1	K	124	THR	2.0
1	C	54	GLN	2.0
1	C	172	ARG	2.0
1	E	196	SER	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.