



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:24 AM UTC

PDB ID : 6Y31 / pdb_00006y31
Title : NG domain of human SRP54 T117 deletion mutant
Authors : Juaiire, K.D.; Lapouge, K.; Becker, M.M.M.; Kotova, I.; Haas, M.; Carapito, R.; Wild, K.; Bahram, S.; Sinning, I.
Deposited on : 2020-02-17
Resolution : 4.00 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
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

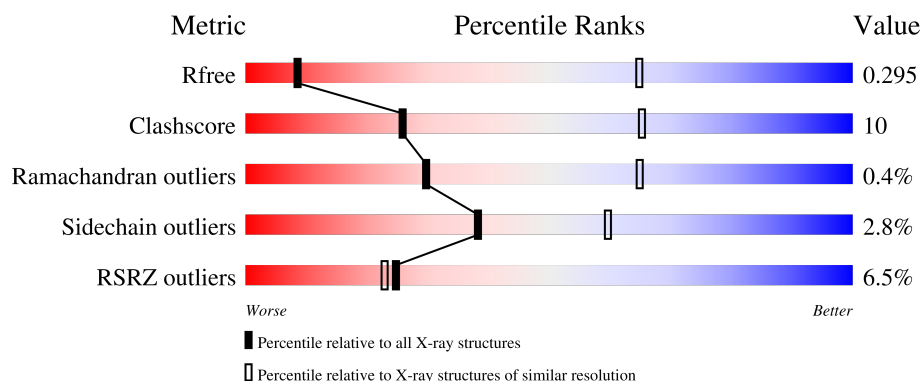
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	303	8% 72% 20% . .
1	B	303	5% 83% 13% . .
1	C	303	6% 82% 13% . .
1	D	303	6% 80% 17% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9043 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 Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2236	1424	378	421	13			
1	B	295	Total	C	N	O	S	0	0	0
			2269	1445	383	428	13			
1	C	295	Total	C	N	O	S	0	0	0
			2269	1445	383	428	13			
1	D	295	Total	C	N	O	S	0	0	0
			2269	1445	383	428	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P61011
A	-6	GLY	-	expression tag	UNP P61011
A	-5	HIS	-	expression tag	UNP P61011
A	-4	HIS	-	expression tag	UNP P61011
A	-3	HIS	-	expression tag	UNP P61011
A	-2	HIS	-	expression tag	UNP P61011
A	-1	HIS	-	expression tag	UNP P61011
A	0	HIS	-	expression tag	UNP P61011
A	?	-	THR	deletion	UNP P61011
B	-7	MET	-	initiating methionine	UNP P61011
B	-6	GLY	-	expression tag	UNP P61011
B	-5	HIS	-	expression tag	UNP P61011
B	-4	HIS	-	expression tag	UNP P61011
B	-3	HIS	-	expression tag	UNP P61011
B	-2	HIS	-	expression tag	UNP P61011
B	-1	HIS	-	expression tag	UNP P61011
B	0	HIS	-	expression tag	UNP P61011
B	?	-	THR	deletion	UNP P61011
C	-7	MET	-	initiating methionine	UNP P61011
C	-6	GLY	-	expression tag	UNP P61011
C	-5	HIS	-	expression tag	UNP P61011

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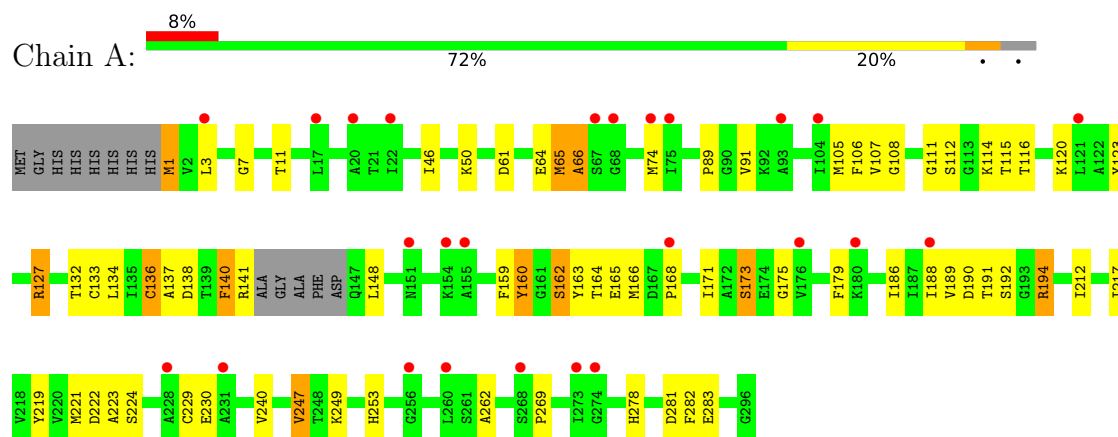
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P61011
C	-3	HIS	-	expression tag	UNP P61011
C	-2	HIS	-	expression tag	UNP P61011
C	-1	HIS	-	expression tag	UNP P61011
C	0	HIS	-	expression tag	UNP P61011
C	?	-	THR	deletion	UNP P61011
D	-7	MET	-	initiating methionine	UNP P61011
D	-6	GLY	-	expression tag	UNP P61011
D	-5	HIS	-	expression tag	UNP P61011
D	-4	HIS	-	expression tag	UNP P61011
D	-3	HIS	-	expression tag	UNP P61011
D	-2	HIS	-	expression tag	UNP P61011
D	-1	HIS	-	expression tag	UNP P61011
D	0	HIS	-	expression tag	UNP P61011
D	?	-	THR	deletion	UNP P61011

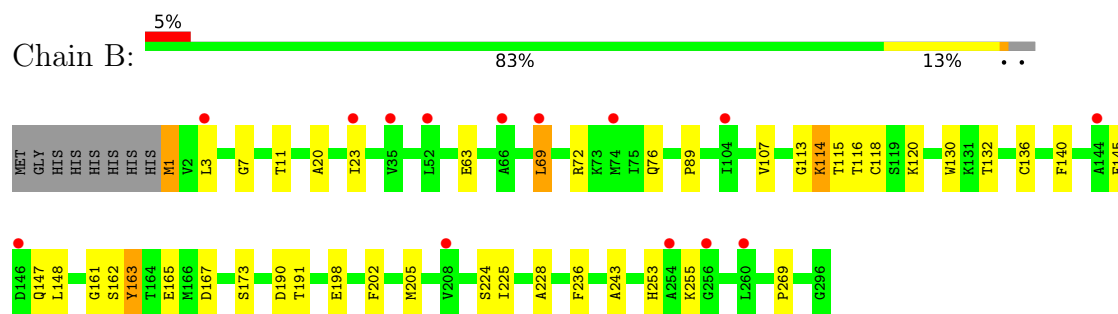
3 Residue-property plots [i](#)

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.

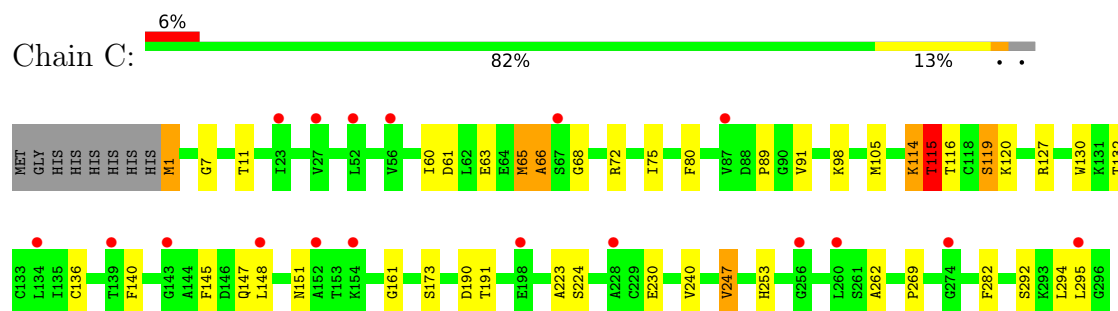
- Molecule 1: Signal recognition particle 54 kDa protein



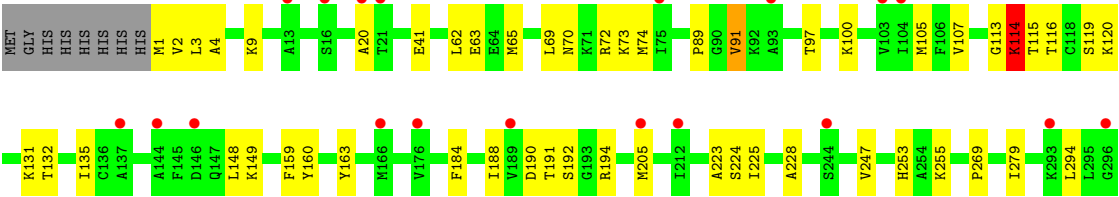
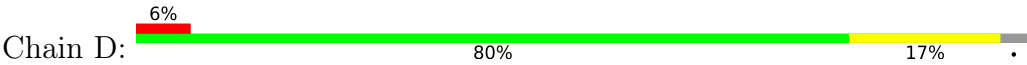
- Molecule 1: Signal recognition particle 54 kDa protein



- Molecule 1: Signal recognition particle 54 kDa protein



- Molecule 1: Signal recognition particle 54 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.36Å 50.61Å 181.63Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	45.72 – 4.00 45.72 – 4.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (45.72-4.00) 99.2 (45.72-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.311 , 0.331 0.311 , 0.295	Depositor DCC
R_{free} test set	488 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	104.3	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 108.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	9043	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.55% 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	0.32	0/2268	0.86	9/3054 (0.3%)
1	B	0.26	0/2303	0.66	2/3103 (0.1%)
1	C	0.21	0/2303	0.58	3/3103 (0.1%)
1	D	0.24	0/2303	0.68	2/3103 (0.1%)
All	All	0.26	0/9177	0.70	16/12363 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	CYS	N-CA-C	9.00	122.91	108.41
1	C	115	THR	N-CA-C	-7.83	94.11	110.80
1	A	164	THR	N-CA-C	7.63	120.49	111.71
1	B	69	LEU	CA-CB-CG	7.32	141.92	116.30
1	A	64	GLU	N-CA-C	-7.00	95.60	107.99
1	A	162	SER	CA-C-N	-6.79	109.83	122.60
1	A	162	SER	C-N-CA	-6.79	109.83	122.60
1	C	114	LYS	CA-C-N	6.75	134.44	121.54
1	C	114	LYS	C-N-CA	6.75	134.44	121.54
1	A	160	TYR	CA-C-N	-6.13	112.47	121.30
1	A	160	TYR	C-N-CA	-6.13	112.47	121.30
1	A	163	TYR	N-CA-C	6.11	120.81	112.68
1	D	114	LYS	CA-C-N	5.84	128.59	120.29
1	D	114	LYS	C-N-CA	5.84	128.59	120.29
1	A	140	PHE	CA-CB-CG	5.24	119.04	113.80
1	B	163	TYR	CA-CB-CG	-5.04	104.83	113.90

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	2236	0	2308	61	2
1	B	2269	0	2335	43	0
1	C	2269	0	2335	29	2
1	D	2269	0	2335	42	0
All	All	9043	0	9313	175	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (175) 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:A:115:THR:HG21	1:A:148:LEU:HD13	1.33	1.09
1:C:115:THR:OG1	1:C:147:GLN:NE2	1.93	1.01
1:A:111:GLY:O	1:A:249:LYS:NZ	1.98	0.96
1:A:140:PHE:HB3	1:A:162:SER:HB3	1.44	0.95
1:B:114:LYS:NZ	1:B:191:THR:OG1	2.00	0.94
1:C:115:THR:HG21	1:C:151:ASN:HD22	1.40	0.86
1:A:112:SER:HA	1:A:222:ASP:HB2	1.60	0.84
1:D:1:MET:HG3	1:D:3:LEU:H	1.42	0.83
1:D:113:GLY:C	1:D:115:THR:H	1.84	0.82
1:B:113:GLY:C	1:B:115:THR:H	1.88	0.81
1:C:114:LYS:HA	1:C:116:THR:HG23	1.63	0.79
1:C:61:ASP:HB2	1:C:65:MET:HE2	1.63	0.79
1:C:115:THR:HG21	1:C:151:ASN:ND2	1.99	0.78
1:A:115:THR:HG21	1:A:148:LEU:CD1	2.12	0.76
1:C:114:LYS:NZ	1:C:190:ASP:OD1	2.21	0.74
1:B:20:ALA:O	1:B:72:ARG:NH2	2.21	0.74
1:D:20:ALA:O	1:D:72:ARG:NH2	2.17	0.71
1:A:136:CYS:HB2	1:A:159:PHE:CZ	2.25	0.71
1:B:113:GLY:O	1:B:115:THR:N	2.24	0.70
1:B:225:ILE:HG22	1:B:228:ALA:HB3	1.74	0.70
1:D:149:LYS:NZ	1:D:163:TYR:OH	2.23	0.70
1:C:115:THR:CG2	1:C:151:ASN:HD22	2.03	0.69
1:B:162:SER:C	1:B:163:TYR:HD2	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HG3	1:B:3:LEU:H	1.59	0.67
1:A:107:VAL:HA	1:A:191:THR:OG1	1.95	0.67
1:D:114:LYS:NZ	1:D:192:SER:O	2.27	0.67
1:D:224:SER:HA	1:D:253:HIS:NE2	2.11	0.66
1:B:145:PHE:CE2	1:B:163:TYR:HE2	2.14	0.65
1:A:136:CYS:HB2	1:A:159:PHE:CE1	2.31	0.65
1:C:140:PHE:HA	1:C:145:PHE:CG	2.31	0.65
1:A:140:PHE:HD2	1:A:162:SER:HG	1.45	0.65
1:D:135:ILE:HG12	1:D:160:TYR:HB3	1.78	0.65
1:D:192:SER:OG	1:D:194:ARG:HG2	1.97	0.64
1:D:1:MET:HE3	1:D:294:LEU:HA	1.80	0.64
1:A:89:PRO:HG3	1:A:269:PRO:HA	1.79	0.63
1:A:140:PHE:CD1	1:A:141:ARG:HG3	2.34	0.62
1:B:145:PHE:CE2	1:B:163:TYR:CE2	2.87	0.62
1:D:91:VAL:HG12	1:D:269:PRO:HG3	1.82	0.61
1:B:145:PHE:CE2	1:B:161:GLY:HA3	2.36	0.61
1:C:89:PRO:HG3	1:C:269:PRO:HA	1.81	0.61
1:D:69:LEU:HB2	1:D:74:MET:SD	2.39	0.61
1:D:89:PRO:HG2	1:D:269:PRO:HA	1.82	0.61
1:D:114:LYS:HD3	1:D:190:ASP:OD1	2.02	0.59
1:D:113:GLY:O	1:D:115:THR:N	2.36	0.59
1:B:145:PHE:CD2	1:B:163:TYR:HE2	2.19	0.59
1:B:162:SER:O	1:B:163:TYR:HD2	1.86	0.59
1:D:253:HIS:CD2	1:D:255:LYS:HB2	2.38	0.58
1:C:145:PHE:HE1	1:C:161:GLY:HA3	1.68	0.58
1:D:107:VAL:HG11	1:D:205:MET:HE2	1.85	0.58
1:A:120:LYS:HD3	1:A:282:PHE:HB2	1.84	0.58
1:B:140:PHE:HB3	1:B:163:TYR:CD2	2.38	0.58
1:B:198:GLU:HB3	1:B:202:PHE:CE2	2.38	0.57
1:A:114:LYS:HG2	1:A:115:THR:N	2.19	0.57
1:B:89:PRO:HG2	1:B:269:PRO:HA	1.87	0.57
1:C:136:CYS:HB2	1:C:148:LEU:HD23	1.86	0.57
1:C:61:ASP:O	1:C:65:MET:HG2	2.05	0.57
1:D:120:LYS:HG2	1:D:279:ILE:HA	1.85	0.57
1:D:225:ILE:HG22	1:D:228:ALA:HB3	1.87	0.57
1:B:114:LYS:HD3	1:B:190:ASP:OD1	2.05	0.57
1:A:106:PHE:O	1:A:191:THR:OG1	2.21	0.55
1:A:140:PHE:HB3	1:A:162:SER:CB	2.28	0.55
1:B:116:THR:HA	1:B:120:LYS:HB2	1.88	0.55
1:A:140:PHE:CZ	1:A:166:MET:HE2	2.41	0.55
1:C:120:LYS:HD3	1:C:282:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:LYS:HZ2	1:D:192:SER:C	2.14	0.54
1:D:1:MET:HG2	1:D:294:LEU:CD1	2.39	0.53
1:D:1:MET:HG3	1:D:3:LEU:N	2.20	0.53
1:A:115:THR:CG2	1:A:148:LEU:HD13	2.22	0.53
1:C:105:MET:HE3	1:C:191:THR:HG21	1.90	0.53
1:A:65:MET:O	1:A:66:ALA:C	2.52	0.53
1:A:160:TYR:CZ	1:A:175:GLY:HA2	2.45	0.52
1:B:23:ILE:HG12	1:B:72:ARG:NH1	2.24	0.52
1:C:230:GLU:HB2	1:C:262:ALA:HB1	1.91	0.52
1:B:107:VAL:HG11	1:B:205:MET:HE2	1.90	0.52
1:B:145:PHE:CZ	1:B:163:TYR:CE2	2.97	0.52
1:C:115:THR:HG22	1:C:119:SER:OG	2.09	0.52
1:D:105:MET:HE3	1:D:191:THR:HG21	1.92	0.52
1:D:114:LYS:NZ	1:D:191:THR:OG1	2.42	0.52
1:A:108:GLY:HA2	1:A:219:TYR:CE1	2.45	0.52
1:A:137:ALA:CB	1:A:190:ASP:O	2.57	0.52
1:A:140:PHE:HD2	1:A:162:SER:OG	1.92	0.52
1:D:1:MET:HG2	1:D:294:LEU:HD13	1.92	0.52
1:B:140:PHE:HB2	1:B:163:TYR:CE2	2.45	0.51
1:D:9:LYS:NZ	1:D:41:GLU:OE2	2.41	0.51
1:A:192:SER:HB2	1:A:194:ARG:NH2	2.26	0.51
1:A:133:CYS:HB2	1:A:179:PHE:CE2	2.46	0.51
1:A:123:TYR:CZ	1:A:127:ARG:HD3	2.46	0.51
1:B:115:THR:OG1	1:B:147:GLN:OE1	2.18	0.51
1:A:108:GLY:HA2	1:A:219:TYR:HE1	1.75	0.50
1:A:165:GLU:O	1:A:171:ILE:HD11	2.11	0.50
1:A:192:SER:OG	1:A:194:ARG:HB2	2.12	0.50
1:B:253:HIS:CD2	1:B:255:LYS:HB2	2.47	0.50
1:A:140:PHE:CG	1:A:162:SER:O	2.65	0.50
1:D:131:LYS:HG2	1:D:184:PHE:CD1	2.47	0.50
1:A:173:SER:HA	1:A:212:ILE:HG22	1.95	0.49
1:B:136:CYS:HB2	1:B:148:LEU:HD23	1.94	0.49
1:B:165:GLU:HG3	1:B:167:ASP:H	1.78	0.49
1:A:114:LYS:HG2	1:A:115:THR:H	1.77	0.49
1:A:107:VAL:HG23	1:A:219:TYR:CD1	2.47	0.49
1:D:148:LEU:HD23	1:D:159:PHE:HE2	1.78	0.49
1:A:46:ILE:HD11	1:A:50:LYS:HE3	1.94	0.48
1:A:166:MET:O	1:A:168:PRO:HD3	2.13	0.48
1:D:70:ASN:O	1:D:73:LYS:N	2.46	0.48
1:C:60:ILE:HD13	1:C:75:ILE:HG12	1.95	0.48
1:A:140:PHE:HE1	1:A:141:ARG:NE	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ALA:HB2	1:C:247:VAL:HG13	1.96	0.48
1:C:145:PHE:CE1	1:C:161:GLY:HA3	2.48	0.48
1:D:135:ILE:HG23	1:D:160:TYR:HD2	1.79	0.48
1:C:1:MET:HE2	1:C:1:MET:HB3	1.82	0.48
1:C:115:THR:HG22	1:C:119:SER:HG	1.79	0.47
1:D:91:VAL:CG1	1:D:269:PRO:HG3	2.45	0.47
1:A:224:SER:HA	1:A:253:HIS:NE2	2.29	0.47
1:D:62:LEU:HA	1:D:65:MET:HE2	1.97	0.47
1:A:120:LYS:HE2	1:A:278:HIS:O	2.15	0.47
1:C:80:PHE:HE1	1:C:292:SER:HA	1.79	0.46
1:B:140:PHE:CB	1:B:163:TYR:CD2	2.98	0.46
1:B:224:SER:HA	1:B:253:HIS:NE2	2.30	0.46
1:A:222:ASP:HB2	1:A:249:LYS:HZ1	1.81	0.46
1:B:163:TYR:CD2	1:B:163:TYR:N	2.83	0.46
1:A:160:TYR:CE2	1:A:179:PHE:CE2	3.04	0.46
1:B:140:PHE:CB	1:B:163:TYR:CE2	2.99	0.46
1:A:137:ALA:HB3	1:A:190:ASP:O	2.15	0.45
1:D:1:MET:O	1:D:4:ALA:HB2	2.17	0.45
1:B:163:TYR:HD2	1:B:163:TYR:N	2.14	0.45
1:A:230:GLU:HB2	1:A:262:ALA:HB1	1.98	0.45
1:B:116:THR:O	1:B:118:CYS:C	2.57	0.45
1:A:189:VAL:HG21	1:A:212:ILE:HD12	1.99	0.45
1:B:236:PHE:CE2	1:B:243:ALA:HB1	2.52	0.45
1:D:1:MET:HE3	1:D:294:LEU:CA	2.46	0.45
1:A:107:VAL:HA	1:A:191:THR:HG1	1.80	0.45
1:D:223:ALA:HB2	1:D:247:VAL:CG1	2.47	0.44
1:D:253:HIS:HD2	1:D:255:LYS:HB2	1.79	0.44
1:A:140:PHE:CE1	1:A:141:ARG:HG3	2.52	0.44
1:B:113:GLY:C	1:B:115:THR:N	2.58	0.44
1:A:134:LEU:HB3	1:A:159:PHE:HD2	1.82	0.44
1:A:7:GLY:O	1:A:11:THR:HG23	2.18	0.44
1:A:134:LEU:HB3	1:A:159:PHE:CD2	2.54	0.43
1:A:223:ALA:HB2	1:A:247:VAL:HG13	1.99	0.43
1:A:186:ILE:HG22	1:A:188:ILE:HG13	2.00	0.43
1:B:145:PHE:CD1	1:B:145:PHE:C	2.96	0.43
1:D:97:THR:HG21	1:D:100:LYS:HD2	1.99	0.43
1:A:221:MET:HE1	1:A:229:CYS:HB3	2.01	0.43
1:C:7:GLY:O	1:C:11:THR:HG23	2.18	0.43
1:D:1:MET:HG3	1:D:2:VAL:N	2.34	0.43
1:A:105:MET:O	1:A:217:ILE:HA	2.19	0.42
1:B:107:VAL:HG21	1:B:205:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:HA	1:C:253:HIS:NE2	2.34	0.42
1:A:114:LYS:O	1:A:116:THR:N	2.52	0.42
1:A:140:PHE:CB	1:A:162:SER:O	2.67	0.42
1:B:114:LYS:CD	1:B:190:ASP:OD1	2.67	0.42
1:B:1:MET:HG3	1:B:3:LEU:N	2.32	0.42
1:A:65:MET:HE3	1:A:74:MET:HE1	2.02	0.42
1:D:70:ASN:HB3	1:D:73:LYS:HD2	2.02	0.42
1:A:138:ASP:HA	1:A:194:ARG:NH1	2.35	0.42
1:B:23:ILE:HG12	1:B:72:ARG:CZ	2.50	0.42
1:D:113:GLY:C	1:D:115:THR:N	2.57	0.42
1:A:1:MET:HE2	1:A:1:MET:HB3	1.83	0.41
1:B:72:ARG:O	1:B:76:GLN:HG3	2.20	0.41
1:D:97:THR:CG2	1:D:100:LYS:HD2	2.50	0.41
1:C:65:MET:O	1:C:66:ALA:C	2.63	0.41
1:A:1:MET:HE2	1:A:3:LEU:H	1.86	0.41
1:D:113:GLY:O	1:D:116:THR:HG23	2.20	0.41
1:A:107:VAL:HG23	1:A:219:TYR:HD1	1.85	0.41
1:B:7:GLY:O	1:B:11:THR:HG23	2.21	0.41
1:C:80:PHE:HD1	1:C:295:LEU:HD12	1.86	0.41
1:C:1:MET:HE2	1:C:294:LEU:HD13	2.02	0.41
1:D:135:ILE:N	1:D:188:ILE:O	2.46	0.41
1:A:136:CYS:H	1:A:160:TYR:HB2	1.86	0.41
1:B:1:MET:HE2	1:B:1:MET:HB2	1.68	0.41
1:B:130:TRP:O	1:B:132:THR:HG23	2.20	0.41
1:C:224:SER:HA	1:C:253:HIS:CE1	2.56	0.41
1:A:61:ASP:O	1:A:65:MET:HE2	2.21	0.40
1:B:145:PHE:CZ	1:B:161:GLY:HA3	2.56	0.40
1:C:98:LYS:HG2	1:C:130:TRP:CH2	2.57	0.40
1:A:105:MET:HE3	1:A:191:THR:HG21	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLU:OE2	1:C:68:GLY:N[2_646]	2.03	0.17
1:A:281:ASP:OD2	1:C:72:ARG:NH2[2_646]	2.17	0.03

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	286/303 (94%)	278 (97%)	7 (2%)	1 (0%)	36	70
1	B	293/303 (97%)	286 (98%)	6 (2%)	1 (0%)	36	70
1	C	293/303 (97%)	287 (98%)	4 (1%)	2 (1%)	18	54
1	D	293/303 (97%)	285 (97%)	7 (2%)	1 (0%)	36	70
All	All	1165/1212 (96%)	1136 (98%)	24 (2%)	5 (0%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	115	THR
1	A	66	ALA
1	B	114	LYS
1	C	66	ALA
1	D	114	LYS

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	243/252 (96%)	234 (96%)	9 (4%)	30	52
1	B	245/252 (97%)	241 (98%)	4 (2%)	55	70
1	C	245/252 (97%)	235 (96%)	10 (4%)	27	49
1	D	245/252 (97%)	241 (98%)	4 (2%)	55	70
All	All	978/1008 (97%)	951 (97%)	27 (3%)	38	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	65	MET
1	A	91	VAL
1	A	127	ARG
1	A	132	THR
1	A	173	SER
1	A	194	ARG
1	A	240	VAL
1	A	247	VAL
1	B	1	MET
1	B	63	GLU
1	B	69	LEU
1	B	173	SER
1	C	1	MET
1	C	63	GLU
1	C	65	MET
1	C	91	VAL
1	C	119	SER
1	C	127	ARG
1	C	132	THR
1	C	173	SER
1	C	240	VAL
1	C	247	VAL
1	D	63	GLU
1	D	91	VAL
1	D	119	SER
1	D	132	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	232	GLN
1	B	51	GLN
1	B	110	GLN
1	B	183	ASN
1	B	207	GLN
1	C	51	GLN
1	C	147	GLN
1	C	151	ASN
1	C	232	GLN

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Mol	Chain	Res	Type
1	D	147	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 ⓘ

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	290/303 (95%)	0.78	25 (8%)	16 17	90, 135, 214, 244	0
1	B	295/303 (97%)	0.65	14 (4%)	36 29	78, 135, 188, 206	0
1	C	295/303 (97%)	0.59	18 (6%)	27 24	80, 127, 211, 247	0
1	D	295/303 (97%)	0.74	19 (6%)	25 23	74, 129, 224, 247	0
All	All	1175/1212 (96%)	0.69	76 (6%)	25 23	74, 132, 215, 247	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	GLY	5.4
1	B	146	ASP	4.9
1	A	256	GLY	4.9
1	A	75	ILE	4.6
1	A	17	LEU	4.5
1	D	212	ILE	4.3
1	D	93	ALA	4.1
1	A	20	ALA	3.8
1	D	104	ILE	3.8
1	A	93	ALA	3.8
1	A	176	VAL	3.7
1	C	256	GLY	3.6
1	D	16	SER	3.5
1	C	52	LEU	3.5
1	A	154	LYS	3.4
1	A	68	GLY	3.3
1	C	260	LEU	3.2
1	A	168	PRO	3.2
1	B	66	ALA	3.2
1	D	176	VAL	3.1
1	D	137	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	27	VAL	3.0
1	B	260	LEU	3.0
1	A	273	ILE	2.9
1	D	75	ILE	2.9
1	C	56	VAL	2.9
1	A	228	ALA	2.8
1	D	166	MET	2.7
1	B	256	GLY	2.7
1	C	198	GLU	2.7
1	B	52	LEU	2.7
1	D	205	MET	2.7
1	C	274	GLY	2.7
1	B	208	VAL	2.7
1	C	148	LEU	2.7
1	A	67	SER	2.7
1	D	244	SER	2.6
1	D	144	ALA	2.6
1	A	188	ILE	2.5
1	C	134	LEU	2.5
1	A	22	ILE	2.5
1	B	104	ILE	2.5
1	C	67	SER	2.5
1	B	23	ILE	2.4
1	B	35	VAL	2.4
1	D	20	ALA	2.4
1	A	104	ILE	2.4
1	C	23	ILE	2.3
1	A	121	LEU	2.3
1	A	268	SER	2.3
1	C	87	VAL	2.3
1	A	3	LEU	2.3
1	B	144	ALA	2.3
1	C	228	ALA	2.2
1	B	74	MET	2.2
1	D	146	ASP	2.2
1	C	154	LYS	2.2
1	C	295	LEU	2.2
1	D	296	GLY	2.1
1	C	139	THR	2.1
1	D	21	THR	2.1
1	D	189	VAL	2.1
1	A	74	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	231	ALA	2.1
1	A	260	LEU	2.1
1	A	151	ASN	2.1
1	B	3	LEU	2.1
1	B	69	LEU	2.1
1	D	293	LYS	2.1
1	A	155	ALA	2.1
1	B	254	ALA	2.1
1	A	180	LYS	2.0
1	D	13	ALA	2.0
1	C	152	ALA	2.0
1	D	103	VAL	2.0
1	C	143	GLY	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.