



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:38 AM UTC

PDB ID : 8T6E / pdb_00008t6e
Title : Crystal structure of T33-28.3: Deep-learning sequence design of co-assembling tetrahedron protein nanoparticles
Authors : Bera, A.K.; de Haas, R.J.; Kang, A.; Sankaran, B.; King, N.P.
Deposited on : 2023-06-15
Resolution : 2.48 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

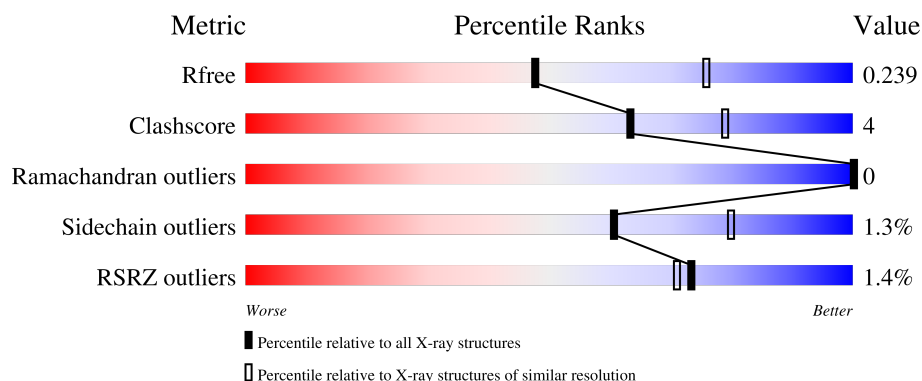
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	157	89% 10% ..
1	C	157	92% 7% .
1	E	157	84% 15% .
1	G	157	87% 13% .
1	I	157	89% 11% .

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Mol	Chain	Length	Quality of chain
1	K	157	 90% 8% ..
1	M	157	 80% 19% .
1	O	157	 87% 12% .
1	Q	157	 90% 10% .
1	S	157	 85% 13% ..
1	U	157	 89% 11% .
1	W	157	 88% 11% ..
2	B	121	 81% 11% . 7%
2	D	121	 86% 6% 8%
2	F	121	 79% 13% 7%
2	H	121	 88% . 8%
2	J	121	 78% 15% 7%
2	L	121	 82% 10% . 7%
2	N	121	 88% . 8%
2	P	121	 81% 12% 7%
2	R	121	 80% 12% 8%
2	T	121	 87% 6% 7%
2	V	121	 81% 12% 7%
2	X	121	 79% 13% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25788 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 T33-28.3: A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	C	156	Total	C	N	O	S	0	1	0
			1244	778	218	242	6			
1	E	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	G	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	I	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	K	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	M	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	O	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	Q	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	S	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	U	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			
1	W	156	Total	C	N	O	S	0	0	0
			1233	772	214	241	6			

- Molecule 2 is a protein called T33-28.3: B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			869	561	142	159	7			
2	D	111	Total	C	N	O	S	0	0	0
			861	555	141	158	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	112	Total 869	C 561	N 142	O 159	S 7	0	0	0
2	H	111	Total 861	C 555	N 141	O 158	S 7	0	0	0
2	J	112	Total 869	C 561	N 142	O 159	S 7	0	0	0
2	L	112	Total 869	C 561	N 142	O 159	S 7	0	0	0
2	N	111	Total 861	C 555	N 141	O 158	S 7	0	0	0
2	P	112	Total 869	C 561	N 142	O 159	S 7	0	0	0
2	R	111	Total 861	C 555	N 141	O 158	S 7	0	0	0
2	T	112	Total 869	C 561	N 142	O 159	S 7	0	0	0
2	V	112	Total 869	C 561	N 142	O 159	S 7	0	0	0
2	X	111	Total 861	C 555	N 141	O 158	S 7	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total 62	O 62	0	0
3	B	20	Total 20	O 20	0	0
3	C	46	Total 46	O 46	0	0
3	D	15	Total 15	O 15	0	0
3	E	30	Total 30	O 30	0	0
3	F	14	Total 14	O 14	0	0
3	G	31	Total 31	O 31	0	0
3	H	13	Total 13	O 13	0	0
3	I	29	Total 29	O 29	0	0

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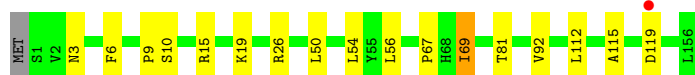
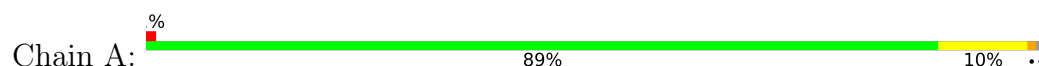
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	10	Total 10	O 10	0	0
3	K	39	Total 39	O 39	0	0
3	L	22	Total 22	O 22	0	0
3	M	47	Total 47	O 47	0	0
3	N	16	Total 16	O 16	0	0
3	O	28	Total 28	O 28	0	0
3	P	11	Total 11	O 11	0	0
3	Q	35	Total 35	O 35	0	0
3	R	17	Total 17	O 17	0	0
3	S	21	Total 21	O 21	0	0
3	T	10	Total 10	O 10	0	0
3	U	16	Total 16	O 16	0	0
3	V	17	Total 17	O 17	0	0
3	W	25	Total 25	O 25	0	0
3	X	19	Total 19	O 19	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.

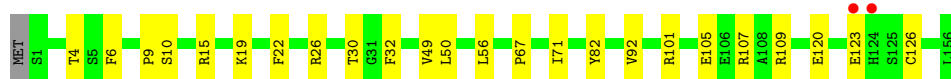
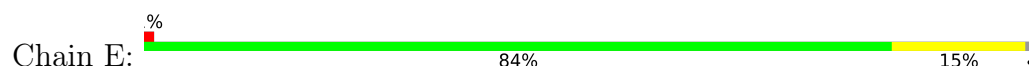
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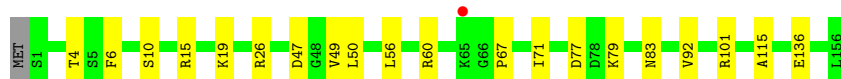
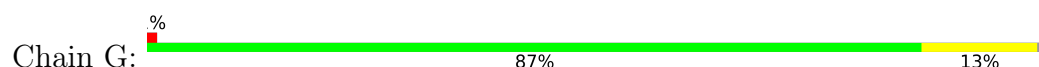
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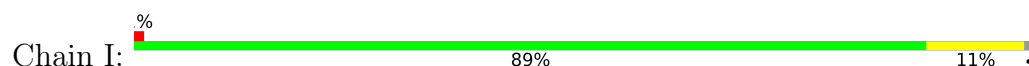
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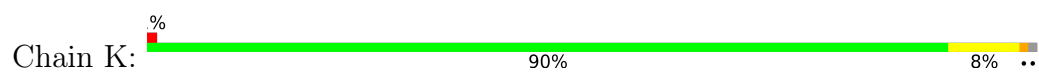
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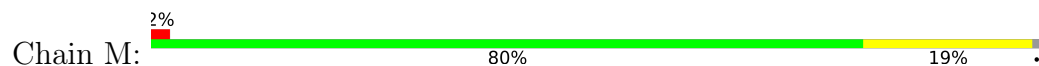
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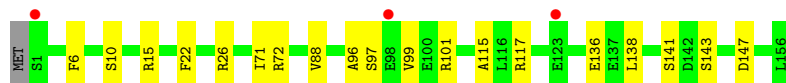
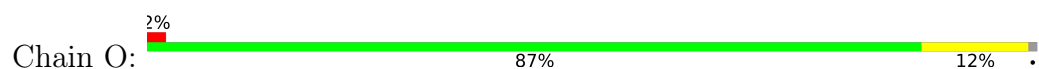
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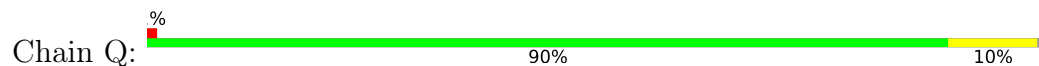
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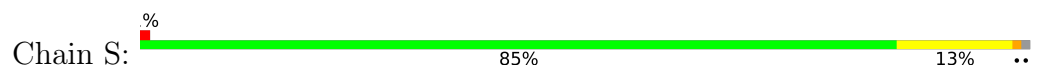
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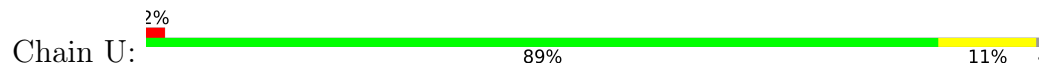
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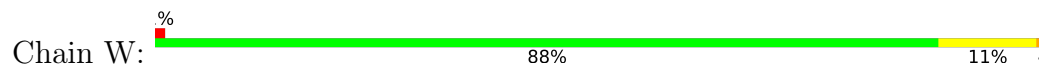
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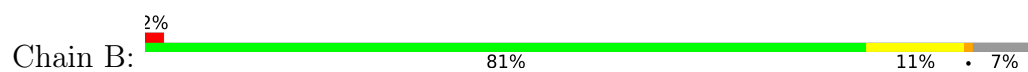
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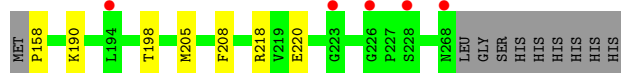
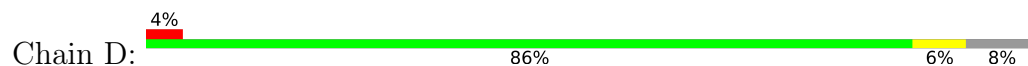
- Molecule 1: T33-28.3: A



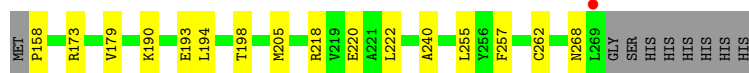
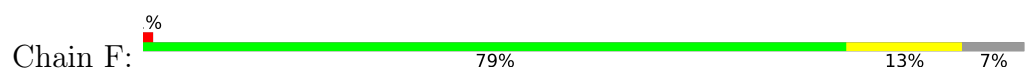
- Molecule 2: T33-28.3: B



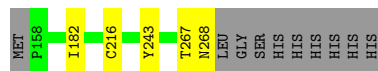
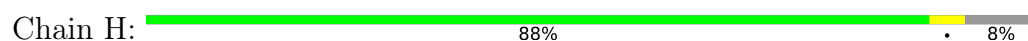
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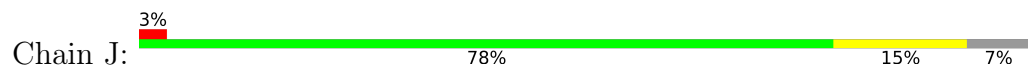
• Molecule 2: T33-28.3: B



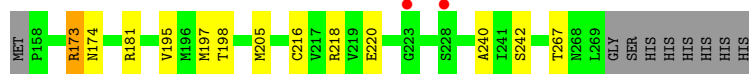
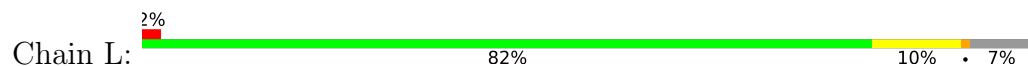
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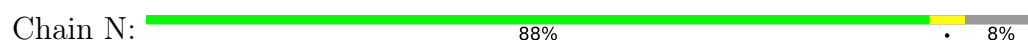
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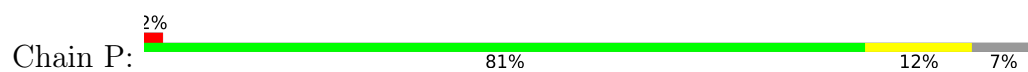
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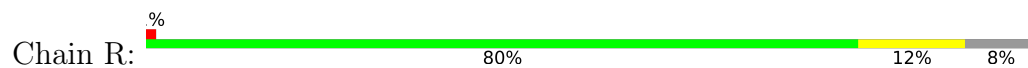
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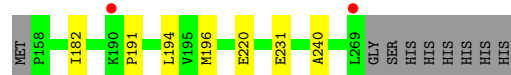
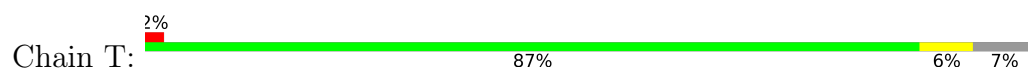
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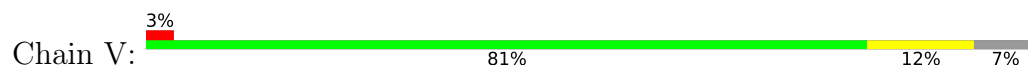
• Molecule 2: T33-28.3: B



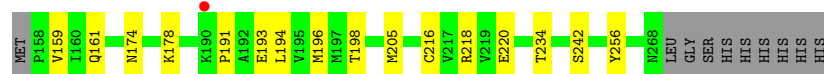
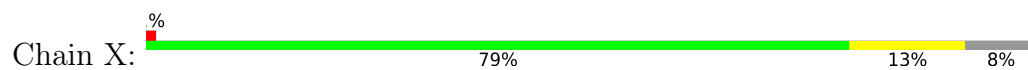
• Molecule 2: T33-28.3: B



• Molecule 2: T33-28.3: B



• Molecule 2: T33-28.3: B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.74Å 114.05Å 114.20Å 62.09° 77.86° 89.41°	Depositor
Resolution (Å)	48.47 – 2.48 48.47 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.47-2.48) 97.9 (48.47-2.48)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.205 , 0.240 0.205 , 0.239	Depositor DCC
R_{free} test set	1993 reflections (1.14%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25788	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.09	0/1255	0.26	0/1692
1	C	0.08	0/1266	0.27	0/1706
1	E	0.08	0/1255	0.28	0/1692
1	G	0.08	0/1255	0.26	0/1692
1	I	0.09	0/1255	0.26	0/1692
1	K	0.09	0/1255	0.25	0/1692
1	M	0.08	0/1255	0.25	0/1692
1	O	0.08	0/1255	0.25	0/1692
1	Q	0.09	0/1255	0.25	0/1692
1	S	0.07	0/1255	0.24	0/1692
1	U	0.07	0/1255	0.22	0/1692
1	W	0.09	0/1255	0.27	0/1692
2	B	0.10	0/892	0.23	0/1216
2	D	0.08	0/884	0.26	0/1205
2	F	0.08	0/892	0.23	0/1216
2	H	0.08	0/884	0.27	0/1205
2	J	0.09	0/892	0.23	0/1216
2	L	0.10	0/892	0.23	0/1216
2	N	0.10	0/884	0.25	0/1205
2	P	0.08	0/892	0.22	0/1216
2	R	0.09	0/884	0.25	0/1205
2	T	0.09	0/892	0.25	0/1216
2	V	0.09	0/892	0.23	0/1216
2	X	0.09	0/884	0.25	0/1205
All	All	0.08	0/25735	0.25	0/34855

There are no bond length outliers.

There are no bond angle outliers.

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	1233	0	1208	10	0
1	C	1244	0	1220	7	0
1	E	1233	0	1208	17	0
1	G	1233	0	1208	14	0
1	I	1233	0	1208	14	0
1	K	1233	0	1208	12	0
1	M	1233	0	1208	20	0
1	O	1233	0	1208	13	0
1	Q	1233	0	1208	10	0
1	S	1233	0	1208	15	0
1	U	1233	0	1208	11	0
1	W	1233	0	1208	12	0
2	B	869	0	868	10	0
2	D	861	0	857	6	0
2	F	869	0	868	10	0
2	H	861	0	857	4	0
2	J	869	0	868	13	0
2	L	869	0	868	8	0
2	N	861	0	857	4	0
2	P	869	0	868	9	0
2	R	861	0	857	10	0
2	T	869	0	868	6	0
2	V	869	0	868	11	0
2	X	861	0	857	12	0
3	A	62	0	0	0	0
3	B	20	0	0	0	0
3	C	46	0	0	0	0
3	D	15	0	0	0	0
3	E	30	0	0	1	0
3	F	14	0	0	1	0
3	G	31	0	0	1	0
3	H	13	0	0	0	0
3	I	29	0	0	1	0
3	J	10	0	0	0	0
3	K	39	0	0	1	0
3	L	22	0	0	1	0
3	M	47	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	16	0	0	0	0
3	O	28	0	0	1	0
3	P	11	0	0	0	0
3	Q	35	0	0	0	0
3	R	17	0	0	0	0
3	S	21	0	0	1	0
3	T	10	0	0	0	0
3	U	16	0	0	0	0
3	V	17	0	0	0	0
3	W	25	0	0	1	0
3	X	19	0	0	1	0
All	All	25788	0	24869	198	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 4.

All (198) 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)
2:R:177:THR:HA	2:R:197:MET:HE1	1.59	0.84
1:U:56:LEU:HD23	1:U:67:PRO:HG2	1.64	0.79
1:M:56:LEU:HD13	1:M:67:PRO:HG2	1.67	0.77
1:G:92:VAL:HG21	1:G:101:ARG:HG3	1.73	0.71
1:S:19:LYS:NZ	1:S:47:ASP:OD1	2.23	0.70
2:J:177:THR:HA	2:J:197:MET:HE1	1.76	0.66
1:Q:19:LYS:NZ	1:Q:47:ASP:OD1	2.28	0.66
2:J:220:GLU:OE1	2:P:218:ARG:NH1	2.29	0.65
1:I:99:VAL:O	1:I:103:THR:OG1	2.14	0.65
1:S:101:ARG:NE	1:S:136:GLU:OE2	2.30	0.64
1:M:109:ARG:HG3	1:M:132:MET:HE2	1.79	0.64
1:G:101:ARG:NH1	1:G:136:GLU:OE2	2.31	0.63
2:J:193:GLU:HG2	2:J:194:LEU:HD22	1.81	0.62
1:E:56:LEU:HD13	1:E:67:PRO:HG2	1.80	0.62
2:J:198:THR:HG22	2:P:205:MET:HG2	1.82	0.61
2:D:158:PRO:HD3	2:D:190:LYS:HD3	1.83	0.61
1:U:83:ASN:HD22	1:U:127:VAL:HB	1.66	0.61
2:B:198:THR:HG22	2:R:205:MET:HG2	1.82	0.60
2:R:198:THR:HG22	2:X:205:MET:HG2	1.82	0.60
1:M:67:PRO:HB3	1:M:92:VAL:HG12	1.83	0.60
2:L:173:ARG:NH2	3:L:301:HOH:O	2.34	0.59
1:C:69:ILE:HD11	1:C:112:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:GLY:HA2	2:B:268:ASN:HA	1.85	0.59
1:K:101:ARG:NH2	1:K:136:GLU:OE2	2.36	0.58
1:S:101:ARG:HD3	1:S:134:LEU:HD21	1.85	0.58
2:F:205:MET:HG2	2:P:198:THR:HG22	1.86	0.58
2:V:264:TRP:HE3	2:V:269:LEU:HD21	1.69	0.58
1:M:54:LEU:HD13	2:N:240:ALA:HA	1.86	0.58
1:A:56:LEU:HD13	1:A:67:PRO:HG2	1.85	0.57
1:A:67:PRO:HB3	1:A:92:VAL:HG12	1.87	0.56
2:D:220:GLU:OE1	2:V:218:ARG:NH2	2.38	0.56
1:Q:92:VAL:HG21	1:Q:101:ARG:HG2	1.86	0.56
1:W:56:LEU:HD13	1:W:67:PRO:HG2	1.86	0.56
1:G:56:LEU:HD13	1:G:67:PRO:HG2	1.87	0.56
1:O:138:LEU:HD23	1:O:141:SER:HB2	1.88	0.56
2:N:218:ARG:NH2	2:T:220:GLU:OE1	2.29	0.56
1:M:1:SER:N	3:M:203:HOH:O	2.37	0.56
2:R:220:GLU:OE2	2:X:218:ARG:NH2	2.31	0.55
1:I:94:THR:HA	1:I:136:GLU:HG2	1.88	0.55
1:M:49:VAL:HG13	1:M:69:ILE:HG22	1.89	0.55
1:A:19:LYS:HB3	1:A:50:LEU:HD11	1.88	0.54
1:I:94:THR:HG21	1:I:138:LEU:HD23	1.90	0.54
1:Q:119:ASP:OD1	1:Q:129:GLN:NE2	2.39	0.54
1:G:60:ARG:NH1	2:H:243:TYR:O	2.41	0.54
1:I:19:LYS:HB3	1:I:50:LEU:HD11	1.89	0.54
1:E:19:LYS:HB3	1:E:50:LEU:HD11	1.90	0.53
2:N:253:PHE:HB2	2:T:196:MET:HE1	1.89	0.53
2:F:158:PRO:HD3	2:F:190:LYS:HE3	1.89	0.53
1:W:49:VAL:HG13	1:W:69:ILE:HG22	1.88	0.53
1:K:67:PRO:HB3	1:K:92:VAL:HG12	1.90	0.53
1:E:15:ARG:HG2	1:E:22:PHE:HD2	1.72	0.53
1:G:79:LYS:HE3	1:K:143:SER:HB3	1.89	0.53
1:Q:115:ALA:HB2	2:R:182:ILE:HD11	1.92	0.52
1:A:115:ALA:HB2	2:B:182:ILE:HD11	1.91	0.52
1:O:72:ARG:NH1	1:O:147:ASP:OD1	2.36	0.52
2:F:198:THR:HG22	2:J:205:MET:HG2	1.92	0.51
1:W:67:PRO:HB3	1:W:92:VAL:HG12	1.93	0.51
2:D:205:MET:HG2	2:L:198:THR:HG22	1.93	0.51
1:O:71:ILE:HA	1:O:88:VAL:HG12	1.91	0.51
1:O:115:ALA:HB2	2:P:182:ILE:HD11	1.91	0.51
2:D:218:ARG:NH2	2:L:220:GLU:OE1	2.39	0.51
2:F:268:ASN:HB2	2:J:231:GLU:HG2	1.93	0.51
1:M:6:PHE:CZ	1:O:15:ARG:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:195:VAL:HG13	2:P:197:MET:HE2	1.91	0.51
1:A:54:LEU:HD13	2:B:240:ALA:HA	1.92	0.51
1:C:101:ARG:HD3	1:C:134:LEU:HD21	1.93	0.51
1:U:92:VAL:HG21	1:U:101:ARG:HG2	1.92	0.51
2:R:180:TYR:HB2	2:R:197:MET:HE3	1.94	0.50
1:M:150:GLU:HA	1:M:153:LYS:HD2	1.93	0.50
2:V:179:VAL:HG11	2:V:240:ALA:HB2	1.93	0.50
1:S:54:LEU:HD13	2:T:240:ALA:HA	1.92	0.50
1:I:55:TYR:HE2	1:I:107:ARG:HG2	1.75	0.50
2:D:198:THR:HG22	2:V:205:MET:HG2	1.94	0.50
2:H:268:ASN:N	2:T:231:GLU:OE2	2.44	0.50
2:B:218:ARG:NH1	2:X:220:GLU:OE1	2.43	0.50
2:F:218:ARG:NH1	2:P:220:GLU:OE1	2.45	0.50
2:F:220:GLU:HG2	2:F:257:PHE:HB2	1.93	0.49
1:G:115:ALA:HB2	2:H:182:ILE:HD11	1.94	0.49
1:A:15:ARG:HG2	1:C:6:PHE:CZ	2.47	0.49
2:F:222:LEU:HD22	2:F:262:CYS:HB3	1.92	0.49
2:R:184:THR:HA	2:R:188:LEU:HD12	1.94	0.49
1:W:42:CYS:O	1:W:46:MET:HG3	2.13	0.49
2:B:196:MET:SD	2:R:216:CYS:HB2	2.53	0.48
1:K:54:LEU:HD13	2:L:240:ALA:HA	1.94	0.48
1:G:4:THR:OG1	1:K:3:ASN:ND2	2.46	0.48
2:L:181:ARG:HG3	2:L:197:MET:HE1	1.94	0.48
2:J:179:VAL:HG11	2:J:240:ALA:HB2	1.94	0.48
1:G:6:PHE:CZ	1:K:15:ARG:HG2	2.49	0.48
2:L:205:MET:HG2	2:V:198:THR:HG22	1.95	0.48
1:Q:67:PRO:HB3	1:Q:92:VAL:HG12	1.95	0.48
1:W:94:THR:HG23	1:W:137:GLU:C	2.39	0.48
1:M:77:ASP:HB3	1:M:83:ASN:HB2	1.95	0.47
1:C:15:ARG:HG2	1:E:6:PHE:CZ	2.49	0.47
1:M:10:SER:O	1:M:26:ARG:HA	2.12	0.47
1:O:117:ARG:NH1	3:O:202:HOH:O	2.33	0.47
1:K:81:THR:HG23	1:K:83:ASN:HD21	1.79	0.47
2:V:182:ILE:O	2:V:186:THR:OG1	2.31	0.47
1:G:15:ARG:HG2	1:I:6:PHE:CZ	2.50	0.47
1:U:67:PRO:HB3	1:U:92:VAL:HG12	1.98	0.46
1:W:101:ARG:NH1	3:W:202:HOH:O	2.47	0.46
1:I:55:TYR:CE2	1:I:107:ARG:HG2	2.50	0.46
2:J:220:GLU:HG2	2:J:257:PHE:HB2	1.96	0.46
1:E:67:PRO:HB3	1:E:92:VAL:HG12	1.98	0.46
1:E:10:SER:O	1:E:26:ARG:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:92:VAL:HG23	1:U:136:GLU:HG3	1.98	0.46
1:G:15:ARG:NH1	3:G:203:HOH:O	2.49	0.46
1:I:15:ARG:HG2	1:K:6:PHE:CZ	2.51	0.46
1:I:67:PRO:HB3	1:I:92:VAL:HG12	1.97	0.46
1:K:26:ARG:O	1:K:26:ARG:HG2	2.16	0.46
1:O:6:PHE:CZ	1:Q:15:ARG:HG2	2.50	0.46
1:I:81:THR:HG23	1:I:83:ASN:HD21	1.81	0.46
1:O:97:SER:C	1:O:99:VAL:H	2.23	0.46
1:A:69:ILE:HD11	1:A:112:LEU:HD21	1.97	0.46
2:B:205:MET:HG2	2:X:198:THR:HG22	1.97	0.46
1:S:1:SER:OG	1:S:2:VAL:N	2.46	0.46
1:S:56:LEU:HD13	1:S:67:PRO:HG2	1.98	0.46
1:M:123:GLU:CD	1:M:123:GLU:H	2.24	0.46
1:Q:19:LYS:HB3	1:Q:50:LEU:HD11	1.98	0.46
1:M:15:ARG:HG2	1:Q:6:PHE:CZ	2.51	0.46
2:J:184:THR:HA	2:J:188:LEU:HB2	1.98	0.45
1:M:72:ARG:NH2	1:M:146:PRO:O	2.46	0.45
2:L:218:ARG:NH2	2:V:220:GLU:OE1	2.45	0.45
2:R:196:MET:HE3	2:R:196:MET:HB2	1.84	0.45
1:G:77:ASP:HB3	1:G:83:ASN:HB2	1.98	0.45
1:S:20:GLY:O	1:S:70:ARG:NH2	2.49	0.45
1:A:6:PHE:CZ	1:E:15:ARG:HG3	2.51	0.45
1:U:15:ARG:HG2	1:W:6:PHE:CZ	2.51	0.45
1:E:120:GLU:N	1:E:120:GLU:OE1	2.49	0.45
1:G:19:LYS:HD3	1:G:50:LEU:HD12	1.98	0.45
1:O:101:ARG:NE	1:O:136:GLU:OE2	2.49	0.45
1:I:55:TYR:O	1:I:107:ARG:NH1	2.50	0.45
1:U:94:THR:HA	1:U:136:GLU:HG2	1.98	0.45
2:B:184:THR:HG21	2:B:195:VAL:HG22	1.99	0.44
2:P:179:VAL:HG11	2:P:240:ALA:HB2	2.00	0.44
1:A:10:SER:O	1:A:26:ARG:HA	2.17	0.44
1:G:49:VAL:HG21	1:G:71:ILE:HB	2.00	0.44
1:W:101:ARG:HD2	1:W:134:LEU:HD21	1.99	0.44
1:M:29:ARG:HD3	1:M:77:ASP:OD1	2.18	0.44
1:M:79:LYS:HE3	1:O:143:SER:HB3	1.99	0.44
1:S:90:LEU:HB2	1:S:132:MET:HE2	2.00	0.44
2:V:183:VAL:HG13	2:V:187:ILE:HD12	1.98	0.44
2:H:216:CYS:HB2	2:N:196:MET:SD	2.57	0.44
1:U:26:ARG:NE	1:U:75:ASP:OD2	2.50	0.44
2:X:191:PRO:HB2	2:X:194:LEU:HD23	2.00	0.44
2:L:216:CYS:HB2	2:V:196:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:LEU:HD13	2:J:240:ALA:HA	2.00	0.43
1:W:72:ARG:NH1	1:W:147:ASP:OD1	2.49	0.43
1:M:19:LYS:HB3	1:M:50:LEU:HD11	2.00	0.43
2:T:191:PRO:HB2	2:T:194:LEU:HD23	2.00	0.43
1:U:72:ARG:NH1	1:U:147:ASP:OD1	2.49	0.43
1:C:3:ASN:ND2	1:E:4:THR:OG1	2.51	0.43
1:M:49:VAL:HG21	1:M:71:ILE:HB	2.00	0.43
1:O:10:SER:O	1:O:26:ARG:HA	2.18	0.43
1:E:105:GLU:HG2	1:E:109:ARG:NH1	2.33	0.43
1:G:10:SER:O	1:G:26:ARG:HA	2.18	0.43
1:C:72:ARG:NH2	1:C:146:PRO:O	2.39	0.43
1:M:9:PRO:HG3	1:O:22:PHE:CD1	2.54	0.43
1:M:30:THR:HB	1:M:32:PHE:CE1	2.53	0.43
1:E:30:THR:HB	1:E:32:PHE:CE1	2.54	0.43
1:W:46:MET:HG2	1:W:71:ILE:HD13	2.00	0.43
2:X:193:GLU:HG2	2:X:194:LEU:HD22	2.01	0.43
2:X:234:THR:HG1	2:X:256:TYR:HH	1.64	0.43
1:Q:30:THR:HB	1:Q:32:PHE:CE1	2.54	0.43
2:B:255:LEU:HD11	2:X:159:VAL:HG21	2.00	0.43
2:F:179:VAL:HG11	2:F:240:ALA:HB2	2.00	0.42
2:J:159:VAL:HG21	2:P:255:LEU:HD11	2.00	0.42
2:P:234:THR:O	2:P:238:THR:OG1	2.34	0.42
2:J:242:SER:OG	2:J:247:ILE:O	2.37	0.42
1:W:19:LYS:HB3	1:W:50:LEU:HD11	2.01	0.42
1:M:117:ARG:NH1	1:M:120:GLU:OE2	2.52	0.42
1:E:107:ARG:NH1	3:E:206:HOH:O	2.52	0.42
1:I:19:LYS:NZ	3:I:203:HOH:O	2.52	0.42
2:F:173:ARG:NH2	3:F:302:HOH:O	2.39	0.42
1:S:143:SER:HB3	1:U:79:LYS:HE3	2.01	0.42
2:V:196:MET:HE3	2:V:196:MET:HB2	1.84	0.42
2:F:255:LEU:HB3	2:F:257:PHE:CE2	2.55	0.42
1:S:6:PHE:CZ	1:W:15:ARG:HG2	2.55	0.42
1:K:101:ARG:NH2	3:K:202:HOH:O	2.44	0.42
1:S:71:ILE:HA	1:S:88:VAL:HG13	2.01	0.42
2:J:196:MET:HE3	2:J:196:MET:HB2	1.84	0.41
1:K:10:SER:O	1:K:26:ARG:HA	2.20	0.41
1:A:9:PRO:HG3	1:E:22:PHE:CD1	2.55	0.41
1:Q:88:VAL:HG23	1:Q:132:MET:HG3	2.03	0.41
1:C:22:PHE:CD1	1:E:9:PRO:HG3	2.56	0.41
2:R:196:MET:SD	2:X:216:CYS:HB2	2.60	0.41
1:S:115:ALA:HB2	2:T:182:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:TYR:CD2	1:E:126:CYS:HB2	2.55	0.41
1:O:96:ALA:HB3	1:O:101:ARG:CZ	2.50	0.41
2:B:216:CYS:HB2	2:X:196:MET:SD	2.60	0.41
2:D:220:GLU:CD	2:V:218:ARG:HH21	2.29	0.41
1:E:49:VAL:HG21	1:E:71:ILE:HB	2.02	0.40
1:I:22:PHE:CD1	1:K:9:PRO:HG3	2.56	0.40
1:S:15:ARG:HG2	1:U:6:PHE:CZ	2.56	0.40
1:S:15:ARG:NH1	3:S:203:HOH:O	2.54	0.40
2:X:161:GLN:NE2	3:X:303:HOH:O	2.52	0.40
2:X:174:ASN:O	2:X:178:LYS:HG3	2.22	0.40
1:S:67:PRO:HB3	1:S:92:VAL:HG12	2.03	0.40
1:E:92:VAL:HG21	1:E:101:ARG:HG2	2.03	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	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
1	C	155/157 (99%)	150 (97%)	5 (3%)	0	100	100
1	E	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
1	G	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
1	I	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
1	K	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
1	M	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
1	O	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
1	Q	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
1	S	154/157 (98%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	154/157 (98%)	148 (96%)	6 (4%)	0	100	100
1	W	154/157 (98%)	149 (97%)	5 (3%)	0	100	100
2	B	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
2	D	109/121 (90%)	107 (98%)	2 (2%)	0	100	100
2	F	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
2	H	109/121 (90%)	105 (96%)	4 (4%)	0	100	100
2	J	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
2	L	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
2	N	109/121 (90%)	106 (97%)	3 (3%)	0	100	100
2	P	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
2	R	109/121 (90%)	106 (97%)	3 (3%)	0	100	100
2	T	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
2	V	110/121 (91%)	109 (99%)	1 (1%)	0	100	100
2	X	109/121 (90%)	106 (97%)	3 (3%)	0	100	100
All	All	3164/3336 (95%)	3072 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/135 (99%)	130 (97%)	4 (3%)	36	61
1	C	135/135 (100%)	134 (99%)	1 (1%)	76	88
1	E	134/135 (99%)	133 (99%)	1 (1%)	76	88
1	G	134/135 (99%)	133 (99%)	1 (1%)	76	88
1	I	134/135 (99%)	134 (100%)	0	100	100
1	K	134/135 (99%)	131 (98%)	3 (2%)	45	70
1	M	134/135 (99%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	134/135 (99%)	134 (100%)	0	100	100
1	Q	134/135 (99%)	134 (100%)	0	100	100
1	S	134/135 (99%)	132 (98%)	2 (2%)	57	78
1	U	134/135 (99%)	132 (98%)	2 (2%)	57	78
1	W	134/135 (99%)	133 (99%)	1 (1%)	76	88
2	B	99/107 (92%)	96 (97%)	3 (3%)	36	61
2	D	98/107 (92%)	97 (99%)	1 (1%)	68	84
2	F	99/107 (92%)	97 (98%)	2 (2%)	48	72
2	H	98/107 (92%)	97 (99%)	1 (1%)	68	84
2	J	99/107 (92%)	98 (99%)	1 (1%)	68	84
2	L	99/107 (92%)	94 (95%)	5 (5%)	21	40
2	N	98/107 (92%)	97 (99%)	1 (1%)	68	84
2	P	99/107 (92%)	97 (98%)	2 (2%)	48	72
2	R	98/107 (92%)	95 (97%)	3 (3%)	35	60
2	T	99/107 (92%)	99 (100%)	0	100	100
2	V	99/107 (92%)	98 (99%)	1 (1%)	68	84
2	X	98/107 (92%)	97 (99%)	1 (1%)	68	84
All	All	2792/2904 (96%)	2756 (99%)	36 (1%)	61	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	69	ILE
1	A	81	THR
1	A	119	ASP
2	B	174	ASN
2	B	195	VAL
2	B	208	PHE
1	C	138	LEU
2	D	208	PHE
1	E	123	GLU
2	F	193	GLU
2	F	194	LEU
1	G	47	ASP
2	H	267	THR

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Mol	Chain	Res	Type
2	J	174	ASN
1	K	26	ARG
1	K	83	ASN
1	K	127	VAL
2	L	173	ARG
2	L	174	ASN
2	L	195	VAL
2	L	242	SER
2	L	267	THR
2	N	174	ASN
2	P	193	GLU
2	P	253	PHE
2	R	208	PHE
2	R	248	VAL
2	R	267	THR
1	S	81	THR
1	S	88	VAL
1	U	50	LEU
1	U	102	GLU
2	V	242	SER
1	W	46	MET
2	X	242	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	21	GLN
1	A	68	HIS
1	C	68	HIS
2	D	261	HIS
1	E	21	GLN
1	E	68	HIS
1	E	129	GLN
2	F	174	ASN
2	F	265	ASN
1	G	21	GLN
2	H	161	GLN
1	I	21	GLN
1	I	68	HIS
2	L	161	GLN
2	L	265	ASN

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Mol	Chain	Res	Type
2	L	268	ASN
1	M	68	HIS
1	M	80	HIS
1	O	21	GLN
1	O	68	HIS
1	O	80	HIS
1	Q	21	GLN
1	Q	68	HIS
1	Q	80	HIS
2	T	170	HIS
2	T	261	HIS
1	U	80	HIS
1	U	129	GLN
2	V	265	ASN
1	W	21	GLN
1	W	129	GLN
2	X	161	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 ⓘ

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	156/157 (99%)	-0.17	1 (0%) 85 83	29, 40, 60, 84	0
1	C	156/157 (99%)	-0.07	1 (0%) 85 83	19, 47, 69, 85	1 (0%)
1	E	156/157 (99%)	0.05	2 (1%) 75 72	32, 49, 80, 89	0
1	G	156/157 (99%)	-0.02	1 (0%) 85 83	34, 48, 67, 86	0
1	I	156/157 (99%)	0.22	1 (0%) 85 83	37, 56, 85, 91	0
1	K	156/157 (99%)	-0.08	1 (0%) 85 83	33, 46, 67, 87	0
1	M	156/157 (99%)	-0.03	3 (1%) 66 63	33, 47, 78, 88	0
1	O	156/157 (99%)	0.22	3 (1%) 66 63	37, 56, 85, 107	0
1	Q	156/157 (99%)	-0.07	1 (0%) 85 83	34, 49, 69, 81	0
1	S	156/157 (99%)	0.15	2 (1%) 75 72	44, 58, 78, 91	0
1	U	156/157 (99%)	0.38	3 (1%) 66 63	48, 66, 90, 107	0
1	W	156/157 (99%)	0.09	2 (1%) 75 72	41, 55, 75, 87	0
2	B	112/121 (92%)	0.00	2 (1%) 67 65	37, 49, 65, 91	0
2	D	111/121 (91%)	0.21	5 (4%) 38 34	39, 54, 80, 89	0
2	F	112/121 (92%)	0.20	1 (0%) 81 79	49, 59, 78, 89	0
2	H	111/121 (91%)	0.07	0 100 100	43, 55, 73, 81	0
2	J	112/121 (92%)	0.34	4 (3%) 46 42	49, 62, 87, 95	0
2	L	112/121 (92%)	0.19	2 (1%) 67 65	44, 52, 71, 83	0
2	N	111/121 (91%)	0.04	0 100 100	42, 54, 69, 81	0
2	P	112/121 (92%)	0.28	2 (1%) 67 65	48, 61, 80, 89	0
2	R	111/121 (91%)	-0.01	1 (0%) 81 79	42, 52, 72, 82	0
2	T	112/121 (92%)	0.15	2 (1%) 67 65	50, 59, 75, 82	0
2	V	112/121 (92%)	0.36	4 (3%) 46 42	47, 59, 78, 85	0
2	X	111/121 (91%)	0.17	1 (0%) 81 79	46, 54, 73, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3211/3336 (96%)	0.10	45 (1%) 73 71	19, 54, 78, 107	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	LEU	6.6
2	V	269	LEU	4.2
2	D	194	LEU	4.1
1	K	1	SER	4.0
2	D	223	GLY	3.6
2	F	269	LEU	3.3
1	Q	1	SER	3.3
2	J	269	LEU	3.3
2	T	269	LEU	3.3
2	V	226	GLY	3.1
2	T	190	LYS	3.0
1	O	1	SER	3.0
2	J	223	GLY	3.0
1	W	1	SER	3.0
1	M	121	ALA	2.9
2	P	269	LEU	2.9
2	D	268	ASN	2.8
2	B	268	ASN	2.8
2	L	228	SER	2.8
2	J	194	LEU	2.8
2	D	226	GLY	2.7
2	V	227	PRO	2.7
2	P	227	PRO	2.7
1	G	65	LYS	2.7
2	D	228	SER	2.7
1	O	123	GLU	2.7
1	C	1	SER	2.6
1	E	123	GLU	2.5
1	U	69	ILE	2.4
1	I	99	VAL	2.4
2	V	190	LYS	2.4
1	U	1	SER	2.4
1	O	98	GLU	2.4
1	S	106	GLU	2.3
1	E	124	HIS	2.3
1	S	1	SER	2.3
2	R	194	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	119	ASP	2.2
1	A	119	ASP	2.2
1	U	99	VAL	2.2
1	M	153	LYS	2.2
1	W	81	THR	2.1
2	L	223	GLY	2.0
2	X	190	LYS	2.0
2	J	190	LYS	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.