



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:27 PM UTC

PDB ID : 6G6C / pdb_00006g6c
Title : Crystal structure of a parallel six-helix coiled coil CC-Type2-LL-L17E
Authors : Rhys, G.G.; Brady, R.L.; Woolfson, D.N.
Deposited on : 2018-04-01
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

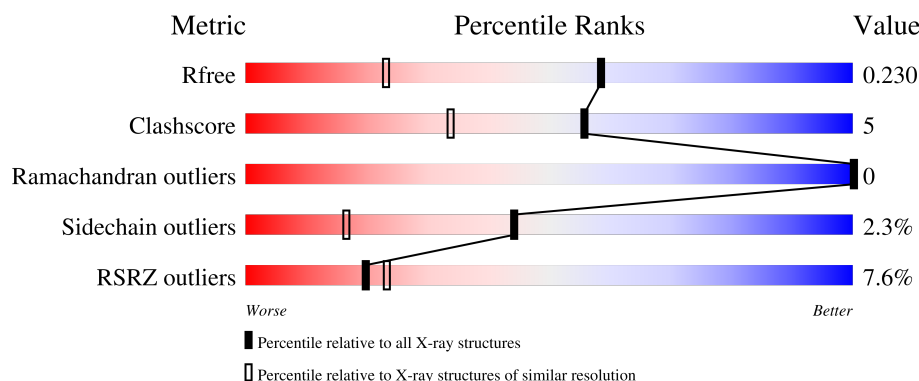
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

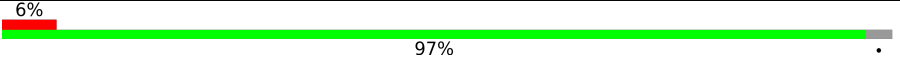
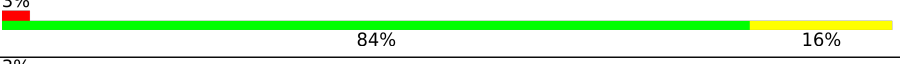
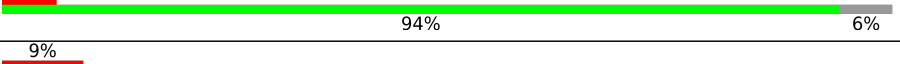
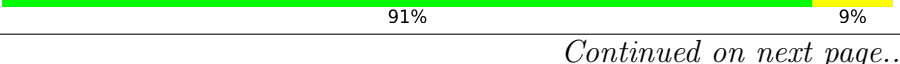
The reported resolution of this entry is 1.55 Å.

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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	32	
1	B	32	
1	C	32	
1	D	32	
1	E	32	

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Mol	Chain	Length	Quality of chain
1	F	32	
1	G	32	
1	H	32	
1	I	32	
1	J	32	
1	K	32	
1	L	32	
1	M	32	
1	N	32	
1	O	32	
1	P	32	
1	Q	32	
1	R	32	
1	S	32	
1	T	32	
1	U	32	
1	V	32	
1	W	32	
1	X	32	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6029 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 CC-Type2-LL-L17E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	31	Total	C	N	O	19	1	0
			235	152	39	44			
1	B	32	Total	C	N	O	7	3	1
			248	162	41	45			
1	C	31	Total	C	N	O	0	3	0
			245	159	40	46			
1	D	30	Total	C	N	O	10	1	0
			230	148	39	43			
1	E	32	Total	C	N	O	9	3	1
			250	163	41	46			
1	F	31	Total	C	N	O	13	1	1
			239	154	39	46			
1	G	29	Total	C	N	O	20	0	0
			222	144	37	41			
1	H	31	Total	C	N	O	10	3	0
			250	164	41	45			
1	I	31	Total	C	N	O	19	0	0
			229	148	38	43			
1	J	30	Total	C	N	O	8	2	0
			237	154	37	46			
1	K	30	Total	C	N	O	15	2	0
			237	155	38	44			
1	L	30	Total	C	N	O	7	1	0
			231	151	38	42			
1	M	31	Total	C	N	O	15	0	0
			229	148	38	43			
1	N	31	Total	C	N	O	1	2	1
			238	155	39	44			
1	O	31	Total	C	N	O	5	0	0
			229	148	38	43			
1	P	30	Total	C	N	O	7	3	0
			242	157	40	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	31	Total	C	N	O	17	3	0
			252	166	39	47			
1	R	32	Total	C	N	O	3	2	1
			248	162	41	45			
1	S	30	Total	C	N	O	10	1	0
			232	150	38	44			
1	T	30	Total	C	N	O	16	2	0
			243	158	37	48			
1	U	30	Total	C	N	O	34	0	0
			226	146	38	42			
1	V	31	Total	C	N	O	20	1	0
			235	152	38	45			
1	W	31	Total	C	N	O	19	3	1
			250	164	40	46			
1	X	31	Total	C	N	O	18	2	0
			246	162	40	44			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	27	Total	O	0	0
			27	27		
2	C	15	Total	O	0	0
			15	15		
2	D	13	Total	O	0	0
			13	13		
2	E	9	Total	O	0	0
			9	9		
2	F	15	Total	O	0	0
			15	15		
2	G	7	Total	O	0	0
			7	7		
2	H	6	Total	O	0	0
			6	6		
2	I	7	Total	O	0	0
			7	7		
2	J	10	Total	O	0	0
			10	10		
2	K	16	Total	O	0	0
			16	16		

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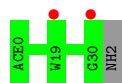
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	15	Total 15	O 15	0	0
2	M	16	Total 16	O 16	0	0
2	N	20	Total 20	O 20	0	0
2	O	16	Total 16	O 16	0	0
2	P	18	Total 18	O 18	0	0
2	Q	11	Total 11	O 11	0	0
2	R	10	Total 10	O 10	0	0
2	S	14	Total 14	O 14	0	0
2	T	6	Total 6	O 6	0	0
2	U	6	Total 6	O 6	0	0
2	V	14	Total 14	O 14	0	0
2	W	6	Total 6	O 6	0	0
2	X	8	Total 8	O 8	0	0

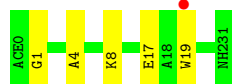
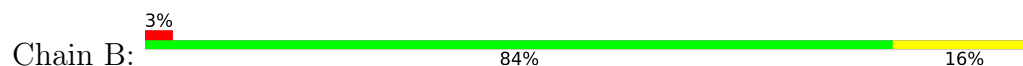
3 Residue-property plots [i](#)

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.

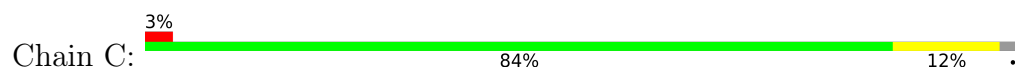
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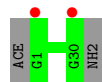
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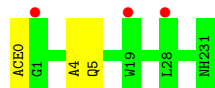
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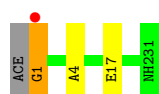
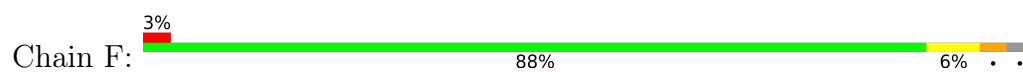
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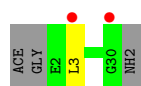
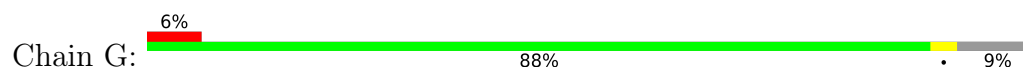
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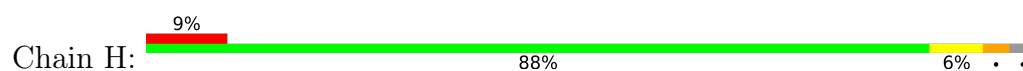
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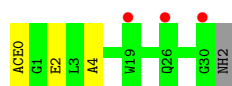
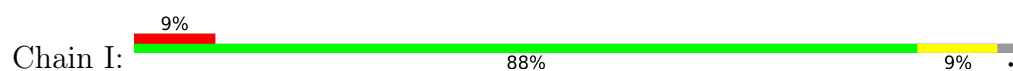
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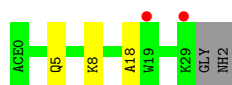
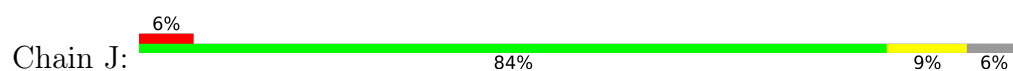
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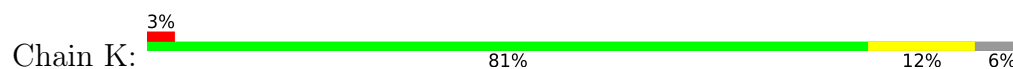
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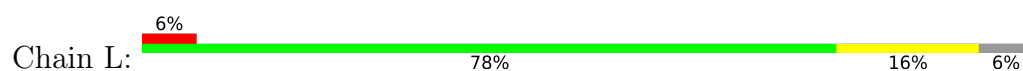
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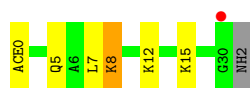
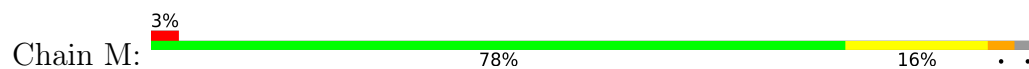
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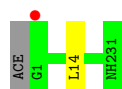
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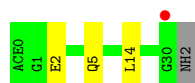
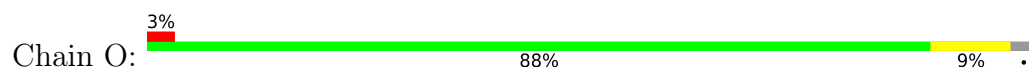
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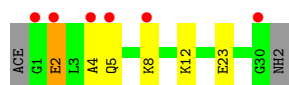
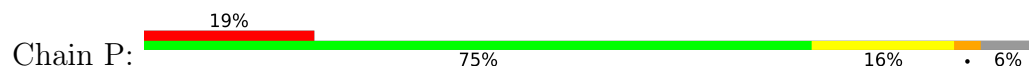
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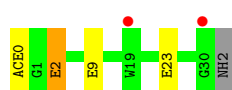
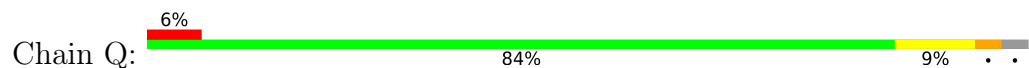
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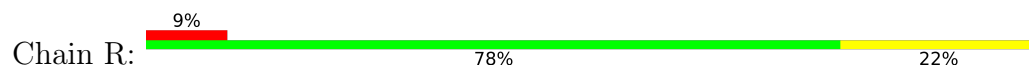
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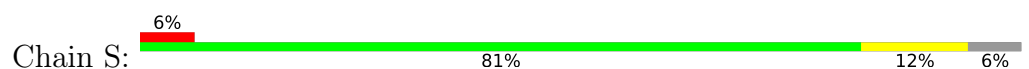
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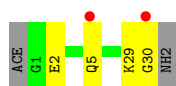


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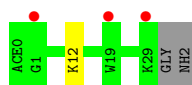
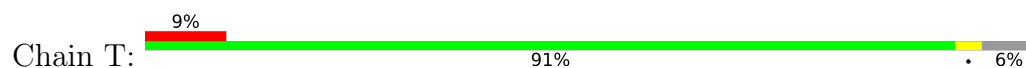


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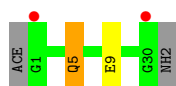
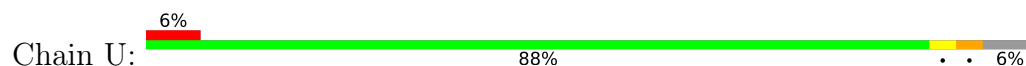




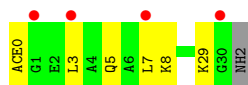
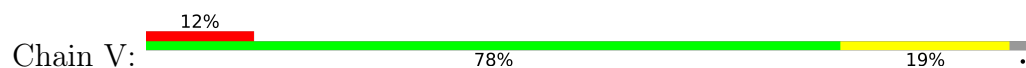
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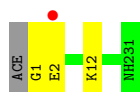
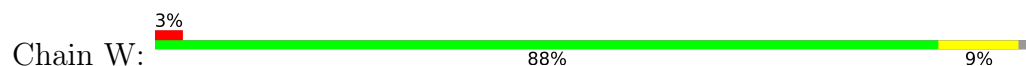
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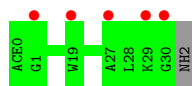
- Molecule 1: CC-Type2-LL-L17E



- Molecule 1: CC-Type2-LL-L17E



- Molecule 1: CC-Type2-LL-L17E



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.32Å 117.94Å 59.24Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	58.97 – 1.55 58.97 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.97-1.55) 100.0 (58.97-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.229 0.189 , 0.230	Depositor DCC
R_{free} test set	4475 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6029	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.77% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

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	0.93	0/237	0.84	0/316
1	B	1.02	0/255	0.89	0/338
1	C	1.09	0/249	0.94	1/329 (0.3%)
1	D	0.90	0/230	0.95	0/304
1	E	1.04	0/254	0.89	0/338
1	F	1.23	0/245	0.82	0/326
1	G	0.76	0/223	0.88	0/297
1	H	0.87	0/256	0.73	0/341
1	I	0.88	0/228	0.89	0/304
1	J	0.85	1/242 (0.4%)	0.79	0/323
1	K	1.05	0/242	1.11	1/322 (0.3%)
1	L	1.02	0/233	0.86	0/310
1	M	1.00	0/228	0.86	0/304
1	N	1.00	0/244	1.02	0/325
1	O	1.12	0/228	1.01	0/304
1	P	0.80	0/248	1.01	1/327 (0.3%)
1	Q	0.91	0/262	0.94	0/351
1	R	0.98	0/255	0.84	0/338
1	S	0.89	0/236	0.97	0/314
1	T	0.83	0/251	0.85	0/335
1	U	0.82	0/227	0.77	0/302
1	V	0.76	0/237	0.72	0/316
1	W	0.91	0/261	0.79	0/349
1	X	0.83	0/253	0.73	0/339
All	All	0.95	1/5824 (0.0%)	0.88	3/7752 (0.0%)

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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	18	ALA	CA-CB	5.02	1.61	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	LYS	N-CA-C	-6.16	104.49	111.14
1	P	2	GLU	N-CA-C	-5.68	106.30	113.18
1	K	26	GLN	N-CA-C	-5.46	105.35	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	1	GLY	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	235	0	255	0	0
1	B	248	0	279	4	0
1	C	245	0	267	3	0
1	D	230	0	247	0	0
1	E	250	0	277	1	0
1	F	239	0	258	2	0
1	G	222	0	240	0	0
1	H	250	0	268	3	0
1	I	229	0	247	3	0
1	J	237	0	256	1	0
1	K	237	0	263	3	0
1	L	231	0	257	5	0
1	M	229	0	247	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	238	0	263	2	0
1	O	229	0	247	4	0
1	P	242	0	268	8	0
1	Q	252	0	269	4	0
1	R	248	0	279	8	0
1	S	232	0	252	2	0
1	T	243	0	262	1	0
1	U	226	0	246	1	0
1	V	235	0	253	2	0
1	W	250	0	268	1	0
1	X	246	0	265	0	0
2	A	21	0	0	0	0
2	B	27	0	0	2	0
2	C	15	0	0	0	0
2	D	13	0	0	0	0
2	E	9	0	0	0	0
2	F	15	0	0	0	0
2	G	7	0	0	0	0
2	H	6	0	0	1	0
2	I	7	0	0	1	0
2	J	10	0	0	0	0
2	K	16	0	0	0	0
2	L	15	0	0	1	0
2	M	16	0	0	1	0
2	N	20	0	0	0	0
2	O	16	0	0	2	0
2	P	18	0	0	3	0
2	Q	11	0	0	4	0
2	R	10	0	0	3	0
2	S	14	0	0	1	0
2	T	6	0	0	0	0
2	U	6	0	0	0	0
2	V	14	0	0	0	0
2	W	6	0	0	1	0
2	X	8	0	0	0	0
All	All	6029	0	6233	52	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 5.

All (52) 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:Q:9[B]:GLU:OE2	2:Q:101:HOH:O	1.80	1.00
1:R:0:ACE:H1	1:R:4:ALA:H	1.28	0.97
1:P:5:GLN:HA	1:P:8:LYS:HE2	1.56	0.87
1:I:0:ACE:H1	1:I:4:ALA:H	1.37	0.85
1:Q:23[A]:GLU:OE2	2:Q:102:HOH:O	2.01	0.79
1:E:0:ACE:H2	1:E:4:ALA:H	1.54	0.73
1:P:12[A]:LYS:NZ	2:P:102:HOH:O	2.23	0.71
1:R:2:GLU:OE1	2:R:102:HOH:O	2.10	0.70
1:O:5:GLN:NE2	2:O:101:HOH:O	2.24	0.66
1:P:12[A]:LYS:NZ	2:P:103:HOH:O	2.30	0.65
1:H:2:GLU:H	1:H:2:GLU:CD	2.09	0.60
1:M:7:LEU:HD22	1:R:2:GLU:HG2	1.87	0.57
1:M:15:LYS:NZ	2:M:102:HOH:O	2.33	0.57
1:P:23:GLU:OE1	2:P:101:HOH:O	2.18	0.56
1:Q:2:GLU:HG2	2:Q:109:HOH:O	2.04	0.56
1:I:2:GLU:HG3	2:I:106:HOH:O	2.06	0.55
1:H:2:GLU:OE2	2:H:101:HOH:O	2.18	0.55
1:V:3:LEU:O	1:V:7:LEU:HD13	2.06	0.54
2:B:112:HOH:O	1:C:22[A]:LYS:HE3	2.08	0.53
1:J:5:GLN:HA	1:J:8:LYS:HE2	1.90	0.52
1:P:2:GLU:HG2	1:Q:0:ACE:H2	1.92	0.51
1:P:4:ALA:O	1:P:8:LYS:HG3	2.11	0.50
1:V:0:ACE:O	1:V:5:GLN:NE2	2.45	0.49
1:R:16:GLU:HG3	2:R:108:HOH:O	2.13	0.49
1:N:14[B]:LEU:HD21	1:O:14:LEU:HD13	1.95	0.49
1:M:0:ACE:H2	1:M:5:GLN:HG3	1.95	0.49
1:S:2:GLU:HA	1:S:5:GLN:OE1	2.13	0.48
1:I:0:ACE:H1	1:I:4:ALA:N	2.18	0.47
1:K:9:GLU:OE1	1:L:8[B]:LYS:HG2	2.14	0.47
1:L:12:LYS:HE3	1:L:12:LYS:HB2	1.56	0.47
1:N:14[B]:LEU:CD2	1:O:14:LEU:HD13	2.44	0.47
1:R:23[B]:GLU:OE2	2:R:103:HOH:O	2.21	0.47
1:B:4:ALA:O	1:B:8[B]:LYS:HG2	2.14	0.47
1:R:0:ACE:H1	1:R:4:ALA:N	2.11	0.47
1:R:19:TRP:CG	1:T:12:LYS:HE2	2.50	0.47
1:K:23:GLU:OE1	1:L:22:LYS:HG3	2.15	0.46
1:L:26:GLN:HG2	2:L:102:HOH:O	2.16	0.46
1:O:2:GLU:HG3	2:O:111:HOH:O	2.16	0.45
1:B:17[A]:GLU:OE2	1:F:17[A]:GLU:OE2	2.34	0.45
1:C:24:LEU:O	1:C:28:LEU:HG	2.17	0.45
1:P:2:GLU:HG3	1:P:5:GLN:HE22	1.81	0.45
1:M:8:LYS:O	1:M:12:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:30:GLY:HA2	2:S:114:HOH:O	2.17	0.43
1:B:1:GLY:N	2:B:101:HOH:O	2.09	0.43
1:F:1:GLY:N	1:F:4:ALA:H	2.16	0.43
1:B:19:TRP:HD1	1:C:22[A]:LYS:CE	2.32	0.42
2:Q:101:HOH:O	1:R:12[B]:LYS:HG3	2.18	0.42
1:P:2:GLU:O	1:P:5:GLN:OE1	2.36	0.42
1:H:5[B]:GLN:HG2	1:H:9:GLU:OE2	2.18	0.42
1:K:17[B]:GLU:OE1	1:L:17:GLU:OE1	2.38	0.42
1:U:5:GLN:O	1:U:9:GLU:HG3	2.19	0.42
1:W:1:GLY:N	2:W:101:HOH:O	2.52	0.42

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	30/32 (94%)	30 (100%)	0	0	100	100
1	B	33/32 (103%)	33 (100%)	0	0	100	100
1	C	31/32 (97%)	31 (100%)	0	0	100	100
1	D	28/32 (88%)	28 (100%)	0	0	100	100
1	E	33/32 (103%)	33 (100%)	0	0	100	100
1	F	31/32 (97%)	31 (100%)	0	0	100	100
1	G	27/32 (84%)	27 (100%)	0	0	100	100
1	H	31/32 (97%)	31 (100%)	0	0	100	100
1	I	29/32 (91%)	29 (100%)	0	0	100	100
1	J	30/32 (94%)	30 (100%)	0	0	100	100
1	K	30/32 (94%)	30 (100%)	0	0	100	100
1	L	29/32 (91%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	29/32 (91%)	29 (100%)	0	0	100	100
1	N	31/32 (97%)	31 (100%)	0	0	100	100
1	O	29/32 (91%)	29 (100%)	0	0	100	100
1	P	30/32 (94%)	30 (100%)	0	0	100	100
1	Q	32/32 (100%)	32 (100%)	0	0	100	100
1	R	33/32 (103%)	33 (100%)	0	0	100	100
1	S	29/32 (91%)	29 (100%)	0	0	100	100
1	T	31/32 (97%)	31 (100%)	0	0	100	100
1	U	28/32 (88%)	28 (100%)	0	0	100	100
1	V	30/32 (94%)	30 (100%)	0	0	100	100
1	W	32/32 (100%)	32 (100%)	0	0	100	100
1	X	31/32 (97%)	31 (100%)	0	0	100	100
All	All	727/768 (95%)	727 (100%)	0	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	21/20 (105%)	21 (100%)	0	100	100
1	B	23/20 (115%)	23 (100%)	0	100	100
1	C	22/20 (110%)	22 (100%)	0	100	100
1	D	20/20 (100%)	20 (100%)	0	100	100
1	E	23/20 (115%)	22 (96%)	1 (4%)	26	4
1	F	22/20 (110%)	22 (100%)	0	100	100
1	G	20/20 (100%)	19 (95%)	1 (5%)	22	2
1	H	22/20 (110%)	20 (91%)	2 (9%)	9	0
1	I	20/20 (100%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	22/20 (110%)	22 (100%)	0	100	100
1	K	22/20 (110%)	22 (100%)	0	100	100
1	L	21/20 (105%)	21 (100%)	0	100	100
1	M	20/20 (100%)	19 (95%)	1 (5%)	22	2
1	N	22/20 (110%)	22 (100%)	0	100	100
1	O	20/20 (100%)	20 (100%)	0	100	100
1	P	22/20 (110%)	22 (100%)	0	100	100
1	Q	23/20 (115%)	22 (96%)	1 (4%)	26	4
1	R	23/20 (115%)	23 (100%)	0	100	100
1	S	21/20 (105%)	20 (95%)	1 (5%)	23	3
1	T	23/20 (115%)	23 (100%)	0	100	100
1	U	20/20 (100%)	19 (95%)	1 (5%)	22	2
1	V	21/20 (105%)	19 (90%)	2 (10%)	8	0
1	W	23/20 (115%)	21 (91%)	2 (9%)	9	0
1	X	22/20 (110%)	22 (100%)	0	100	100
All	All	518/480 (108%)	506 (98%)	12 (2%)	44	16

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	GLN
1	G	3	LEU
1	H	5[A]	GLN
1	H	5[B]	GLN
1	M	8	LYS
1	Q	2	GLU
1	S	29	LYS
1	U	5	GLN
1	V	8	LYS
1	V	29	LYS
1	W	2	GLU
1	W	12	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	5	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	29:LYS	C	30[B]:GLY	N	4.22
1	D	29:LYS	C	30[B]:GLY	N	3.78

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	30/32 (93%)	0.10	2 (6%) 24 28	11, 21, 33, 46	7 (23%)
1	B	30/32 (93%)	-0.32	1 (3%) 49 57	10, 18, 27, 33	5 (16%)
1	C	30/32 (93%)	0.05	1 (3%) 49 57	9, 20, 32, 49	3 (10%)
1	D	30/32 (93%)	0.32	2 (6%) 24 28	15, 26, 45, 53	5 (16%)
1	E	30/32 (93%)	0.48	3 (10%) 12 14	12, 23, 50, 59	6 (20%)
1	F	30/32 (93%)	-0.06	1 (3%) 49 57	7, 20, 36, 43	7 (23%)
1	G	29/32 (90%)	0.68	2 (6%) 23 26	11, 27, 47, 55	5 (17%)
1	H	30/32 (93%)	0.74	3 (10%) 12 14	17, 25, 43, 52	6 (20%)
1	I	30/32 (93%)	0.49	3 (10%) 12 14	12, 25, 48, 54	6 (20%)
1	J	29/32 (90%)	0.36	2 (6%) 23 26	12, 25, 52, 59	5 (17%)
1	K	29/32 (90%)	0.12	1 (3%) 48 56	10, 19, 34, 55	6 (20%)
1	L	29/32 (90%)	0.03	2 (6%) 23 26	14, 20, 37, 48	4 (13%)
1	M	30/32 (93%)	0.30	1 (3%) 49 57	16, 23, 38, 65	5 (16%)
1	N	30/32 (93%)	0.02	1 (3%) 49 57	10, 22, 36, 42	3 (10%)
1	O	30/32 (93%)	0.06	1 (3%) 49 57	12, 21, 42, 66	2 (6%)
1	P	30/32 (93%)	0.65	6 (20%) 3 3	13, 25, 51, 65	6 (20%)
1	Q	30/32 (93%)	0.32	2 (6%) 24 28	14, 20, 44, 56	9 (30%)
1	R	30/32 (93%)	0.42	3 (10%) 12 14	10, 22, 42, 52	3 (10%)
1	S	30/32 (93%)	0.21	2 (6%) 24 28	15, 23, 40, 58	5 (16%)
1	T	29/32 (90%)	0.50	3 (10%) 12 13	9, 24, 41, 56	7 (24%)
1	U	30/32 (93%)	0.41	2 (6%) 24 28	13, 24, 34, 38	12 (40%)
1	V	30/32 (93%)	0.85	4 (13%) 7 8	13, 28, 52, 58	7 (23%)
1	W	30/32 (93%)	0.39	1 (3%) 49 57	15, 24, 39, 47	8 (26%)
1	X	30/32 (93%)	0.80	5 (16%) 4 5	17, 26, 45, 68	9 (30%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	715/768 (93%)	0.33	54 (7%) 20 23	7, 23, 47, 68	141 (19%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	19	TRP	6.1
1	H	19[A]	TRP	5.7
1	P	30[A]	GLY	5.0
1	X	30	GLY	5.0
1	G	3	LEU	4.5
1	Q	30	GLY	4.5
1	U	1	GLY	4.5
1	C	30[A]	GLY	4.3
1	Q	19[A]	TRP	4.1
1	J	19	TRP	3.9
1	V	3	LEU	3.9
1	X	19[A]	TRP	3.9
1	M	30	GLY	3.5
1	V	7	LEU	3.4
1	P	1	GLY	3.4
1	E	19	TRP	3.4
1	F	1	GLY	3.4
1	I	30	GLY	3.3
1	S	5	GLN	3.3
1	O	30	GLY	3.2
1	E	28[A]	LEU	3.2
1	A	19	TRP	3.0
1	P	5	GLN	3.0
1	H	30[A]	GLY	3.0
1	D	30[A]	GLY	2.8
1	X	1	GLY	2.8
1	R	19	TRP	2.8
1	R	27	ALA	2.7
1	K	1	GLY	2.7
1	V	1	GLY	2.6
1	R	30	GLY	2.6
1	D	1	GLY	2.5
1	E	1	GLY	2.5
1	N	1	GLY	2.5
1	P	8	LYS	2.5
1	G	30	GLY	2.4
1	J	29	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	26	GLN	2.3
1	I	19	TRP	2.3
1	P	2	GLU	2.3
1	T	29	LYS	2.2
1	L	1	GLY	2.2
1	X	27	ALA	2.2
1	X	29	LYS	2.2
1	W	2	GLU	2.2
1	U	30	GLY	2.1
1	V	30	GLY	2.1
1	L	29	LYS	2.1
1	H	5[A]	GLN	2.1
1	S	30	GLY	2.1
1	T	1	GLY	2.1
1	B	19	TRP	2.1
1	P	4	ALA	2.0
1	A	30	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.