



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 09:12 PM UTC

PDB ID : 7XVM / pdb_00007xvm
Title : Crystal Structure of Nucleosome-H5 Linker Histone Assembly (sticky-169a DNA fragment)
Authors : Adhireksan, Z.; Qiuye, B.; Lee, P.L.; Sharma, D.; Padavattan, S.; Davey, C.A.
Deposited on : 2022-05-24
Resolution : 2.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

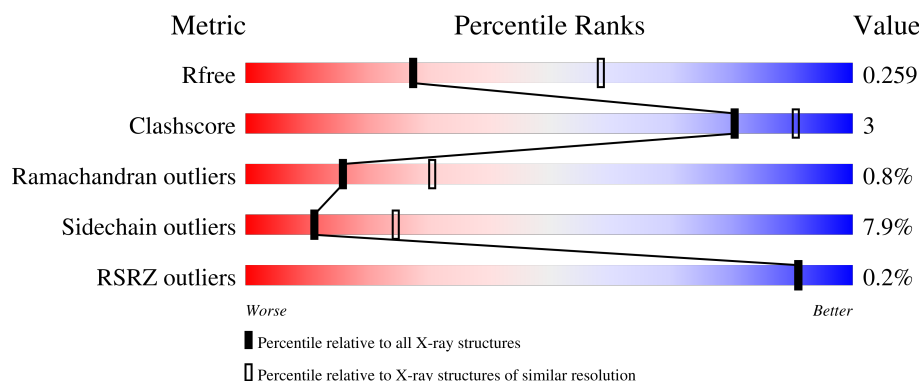
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

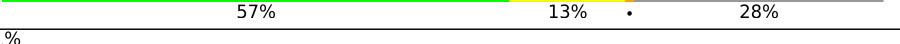
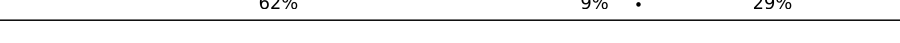
The reported resolution of this entry is 2.84 Å.

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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	138	
1	E	138	
1	K	138	
1	O	138	
2	B	105	

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Mol	Chain	Length	Quality of chain
2	F	105	 78% . . 17%
2	L	105	 70% 6% . 24%
2	P	105	 76% 10% 13%
3	C	132	 73% 8% . 17%
3	G	132	 % 71% 12% . 14%
3	M	132	 73% 10% 17%
3	Q	132	 % 73% 9% 18%
4	D	128	 67% 7% . 24%
4	H	128	 62% 12% . 23%
4	N	128	 % 65% 11% . 23%
4	R	128	 66% 9% . 24%
5	I	169	 82% 17% .
5	S	169	 90% 10%
6	J	169	 82% 18% .
6	T	169	 88% 11% .
7	U	190	 36% 8% . 55%
7	V	190	 % 34% 9% . 56%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27693 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 Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	K	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	O	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P68431
A	-1	SER	-	expression tag	UNP P68431
E	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
K	-2	GLY	-	expression tag	UNP P68431
K	-1	SER	-	expression tag	UNP P68431
O	-2	GLY	-	expression tag	UNP P68431
O	-1	SER	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			708	445	143	119	1			
2	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			
2	L	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	P	91	Total	C	N	O	S	0	0	0
			725	455	147	122	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62805
B	-1	SER	-	expression tag	UNP P62805
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
L	-2	GLY	-	expression tag	UNP P62805
L	-1	SER	-	expression tag	UNP P62805
P	-2	GLY	-	expression tag	UNP P62805
P	-1	SER	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	109	Total	C	N	O	0	0	0
			844	532	167	145			
3	G	114	Total	C	N	O	0	0	0
			886	556	176	154			
3	M	110	Total	C	N	O	0	0	0
			849	535	168	146			
3	Q	108	Total	C	N	O	0	0	0
			835	526	165	144			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04908
C	-1	SER	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
M	-2	GLY	-	expression tag	UNP P04908
M	-1	SER	-	expression tag	UNP P04908
Q	-2	GLY	-	expression tag	UNP P04908
Q	-1	SER	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			
4	H	98	Total	C	N	O	S	0	0	0
			775	486	144	143	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	98	Total	C	N	O	S	0	0	0
			775	486	144	143	2			
4	R	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
H	-2	GLY	-	expression tag	UNP P06899
H	-1	SER	-	expression tag	UNP P06899
N	-2	GLY	-	expression tag	UNP P06899
N	-1	SER	-	expression tag	UNP P06899
R	-2	GLY	-	expression tag	UNP P06899
R	-1	SER	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	169	Total	C	N	O	P	0	0	0
			3462	1646	637	1011	168			
5	S	169	Total	C	N	O	P	0	0	0
			3462	1646	637	1011	168			

- Molecule 6 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	169	Total	C	N	O	P	0	0	0
			3461	1646	634	1013	168			
6	T	169	Total	C	N	O	P	0	0	0
			3461	1646	634	1013	168			

- Molecule 7 is a protein called Histone H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	86	Total	C	N	O	S	0	0	0
			657	404	134	118	1			
7	V	84	Total	C	N	O	S	0	0	0
			640	395	129	115	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	1	SER	-	expression tag	UNP P02259
V	1	SER	-	expression tag	UNP P02259

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ca 1 1	0	0
8	I	8	Total Ca 8 8	0	0
8	J	3	Total Ca 3 3	0	0
8	S	4	Total Ca 4 4	0	0
8	T	2	Total Ca 2 2	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Cl 1 1	0	0
9	H	1	Total Cl 1 1	0	0
9	M	1	Total Cl 1 1	0	0

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	I	1	Total K 1 1	0	0
10	T	1	Total K 1 1	0	0

- Molecule 11 is water.

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

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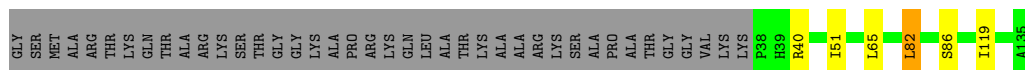
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total 1	O 1	0	0
11	D	1	Total 1	O 1	0	0
11	E	1	Total 1	O 1	0	0
11	G	1	Total 1	O 1	0	0
11	H	1	Total 1	O 1	0	0
11	I	1	Total 1	O 1	0	0
11	Q	1	Total 1	O 1	0	0

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.

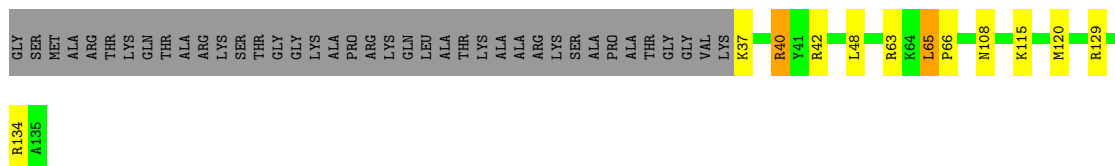
- Molecule 1: Histone H3.1

Chain A: 



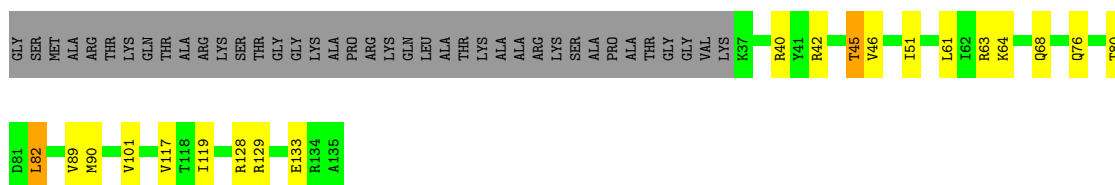
- Molecule 1: Histone H3.1

Chain E: 



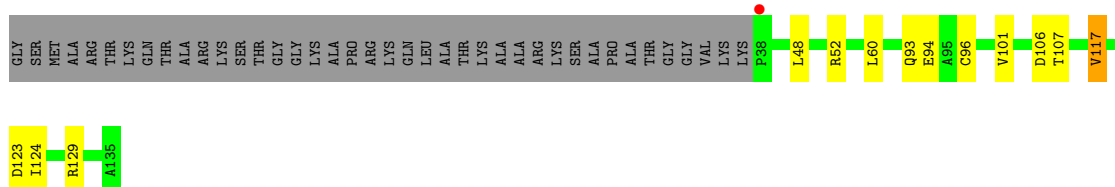
- Molecule 1: Histone H3.1

Chain K: 



- Molecule 1: Histone H3.1

Chain O: 



- Molecule 2: Histone H4



- | |
|------|
| GLY | SER | MET | SER | GLY | ARG | GLY | LYS | GLY | GLY | LYS | GLY | LEU | GLY | LYS | GLY | GLY | ALA | K16 | R19 | K20 | V21 | L22 | Q27 | R35 | G102 |
|------|

- | |
|------|
| GLY | SER | MET | SER | SER | GLY | ARG | GLY | GLY | GLY | LYS | GLY | GLY | LEU | GLY | LYS | GLY | GLY | ALA | LYS | ARG | HIS | ARG | LYS | VAL | LEU | R23 | R23 | T30 | R40 | V43 | I50 | D68 | V81 | R92 | G102 |
|------|

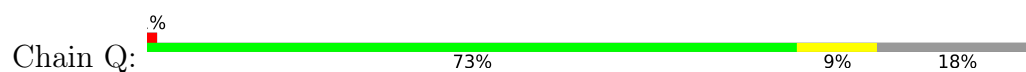
- | |
|------|
| GLY | SER | MET | SER | GLY | ARG | GLY | LYS | GLY | GLY | LYS | GLY | LEU | GLY | K12 | K16 | R17 | H18 | R19 | K20 | V21 | R45 | I46 | S47 | L62 | D68 | Q93 | G102 |
|------|

- | | | | | | | | | | | | | | | |
|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | SER | NET | SER | GLY | ARG | GLY | LYS | GLN | GLY | GLY | LYS | ALA | R11 | A12 | K13 | Q24 | R42 | R81 | E91 | E92 | I102 | P109 | L115 | K118 | K119 | THR | GLU | SER | HIS | HIS | LYS | ALA | LYS | GLY | LYS |
|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

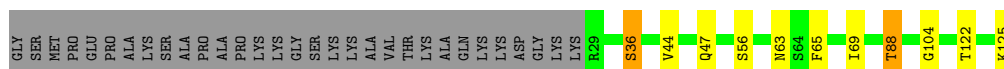
- | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|
| GLY | SER | MET | SER | GLY | ARG | GLY | GLN | GLY | LYS | ALA | R11 | A12 | K13 | A14 | K15 | R29 | V30 | H31 | P48 | N73 | P80 | R81 | L85 | I102 | L108 | P109 | N110 | I111 | P117 | K118 | K119 | T120 | E121 | S122 | H123 | H124 | LYS | ALA | LYS | GLY | LYS |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | SER | MET | SER | GLY | ARG | GLY | LYS | GLN | GLY | LYS | A10 | R11 | A14 | K15 | Q24 | K36 | L63 | I79 | P80 | R81 | Q104 | V107 | I111 | L115 | K118 | K119 | THR | GLU | SER | HIS | HIS | LYS | ALA | LYS | GLY | LYS |
|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

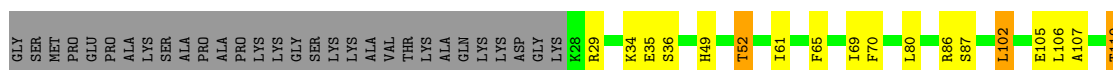
- WORLDWIDE
PDB
PROTEIN DATA BANK



- Molecule 4: Histone H2B type 1-J



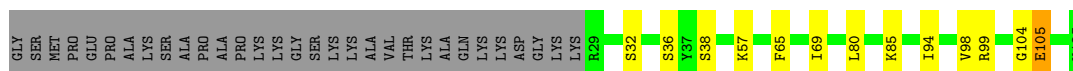
- Molecule 4: Histone H2B type 1-J



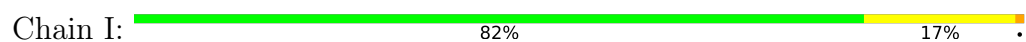
- Molecule 4: Histone H2B type 1-J



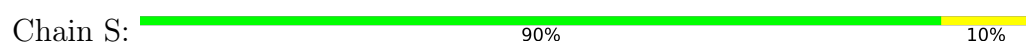
- Molecule 4: Histone H2B type 1-J

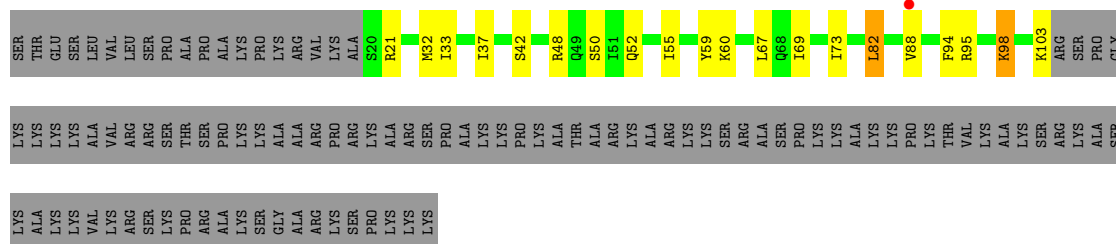


- Molecule 5: DNA (169-MER)



- Molecule 5: DNA (169-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.16Å 103.76Å 212.96Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	48.03 – 2.84 48.03 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.03-2.84) 98.8 (48.03-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.200 , 0.259 0.204 , 0.259	Depositor DCC
R_{free} test set	2096 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	98.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27693	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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: CL, CA, K

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	0.77	0/819	1.01	0/1097
1	E	0.79	0/828	1.08	0/1109
1	K	0.68	0/828	0.99	0/1109
1	O	0.74	0/819	0.95	0/1097
2	B	0.84	0/716	0.96	0/955
2	F	0.82	0/711	1.01	0/948
2	L	0.68	0/645	0.92	1/862 (0.1%)
2	P	0.79	0/733	0.99	0/976
3	C	0.76	0/854	0.93	0/1150
3	G	0.82	0/898	1.06	1/1210 (0.1%)
3	M	0.68	0/859	0.97	0/1157
3	Q	0.65	0/845	0.91	0/1139
4	D	0.76	0/777	1.05	0/1040
4	H	0.75	0/786	1.03	0/1051
4	N	0.66	0/786	0.97	0/1051
4	R	0.64	0/777	0.96	0/1040
5	I	0.39	0/3884	0.88	6/5993 (0.1%)
5	S	0.35	0/3884	0.81	3/5993 (0.1%)
6	J	0.40	0/3882	0.89	5/5990 (0.1%)
6	T	0.35	0/3882	0.80	3/5990 (0.1%)
7	U	0.74	0/664	0.93	0/881
7	V	0.78	0/647	0.96	0/859
All	All	0.58	0/29524	0.91	19/42697 (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
3	G	0	2

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	-47	DT	C2'-C3'-O3'	9.65	125.97	111.50
6	J	-63	DC	C2'-C3'-O3'	7.41	122.61	111.50
3	G	122	SER	N-CA-C	6.92	120.95	109.95
6	T	-79	DT	C4'-C3'-O3'	6.72	120.09	110.00
5	I	-76	DT	C2'-C3'-O3'	6.55	121.33	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	121	GLU	Peptide
3	G	122	SER	Peptide

5.2 Too-close contacts [i](#)

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	807	0	844	4	0
1	E	816	0	856	5	0
1	K	816	0	856	16	0
1	O	807	0	844	10	0
2	B	708	0	760	6	0
2	F	703	0	755	1	0
2	L	638	0	676	6	0
2	P	725	0	779	5	0
3	C	844	0	910	3	0
3	G	886	0	942	6	0
3	M	849	0	915	8	0
3	Q	835	0	897	4	0
4	D	766	0	797	4	0
4	H	775	0	810	8	0
4	N	775	0	810	6	0
4	R	766	0	797	3	0
5	I	3462	0	1901	19	0
5	S	3462	0	1901	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	3461	0	1902	19	0
6	T	3461	0	1902	13	0
7	U	657	0	696	9	0
7	V	640	0	678	8	0
8	C	1	0	0	0	0
8	I	8	0	0	0	0
8	J	3	0	0	0	0
8	S	4	0	0	0	0
8	T	2	0	0	0	0
9	C	1	0	0	0	0
9	H	1	0	0	0	0
9	M	1	0	0	0	0
10	I	1	0	0	0	0
10	T	1	0	0	0	0
11	A	2	0	0	0	0
11	B	2	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
11	Q	1	0	0	0	0
All	All	27693	0	22228	130	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 3.

The worst 5 of 130 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)
6:J:-46:DC:H2''	6:J:-45:DA:C8	2.15	0.82
6:J:2:DC:H4'	7:U:49:GLN:HE22	1.45	0.81
1:K:117:VAL:HG13	3:Q:115:LEU:HD22	1.79	0.65
3:M:104:GLN:NE2	1:O:94:GLU:OE2	2.27	0.64
4:H:49:HIS:HB3	4:H:52:THR:CG2	2.28	0.62

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	96/138 (70%)	95 (99%)	1 (1%)	0	100	100
1	E	97/138 (70%)	94 (97%)	3 (3%)	0	100	100
1	K	97/138 (70%)	92 (95%)	5 (5%)	0	100	100
1	O	96/138 (70%)	93 (97%)	3 (3%)	0	100	100
2	B	86/105 (82%)	80 (93%)	6 (7%)	0	100	100
2	F	85/105 (81%)	77 (91%)	7 (8%)	1 (1%)	10	22
2	L	78/105 (74%)	72 (92%)	6 (8%)	0	100	100
2	P	89/105 (85%)	79 (89%)	9 (10%)	1 (1%)	11	23
3	C	107/132 (81%)	105 (98%)	2 (2%)	0	100	100
3	G	112/132 (85%)	103 (92%)	6 (5%)	3 (3%)	4	8
3	M	108/132 (82%)	101 (94%)	6 (6%)	1 (1%)	14	27
3	Q	106/132 (80%)	101 (95%)	5 (5%)	0	100	100
4	D	95/128 (74%)	90 (95%)	4 (4%)	1 (1%)	11	23
4	H	96/128 (75%)	89 (93%)	5 (5%)	2 (2%)	5	12
4	N	96/128 (75%)	90 (94%)	5 (5%)	1 (1%)	12	24
4	R	95/128 (74%)	91 (96%)	2 (2%)	2 (2%)	5	12
7	U	84/190 (44%)	80 (95%)	3 (4%)	1 (1%)	10	22
7	V	82/190 (43%)	73 (89%)	8 (10%)	1 (1%)	10	22
All	All	1705/2392 (71%)	1605 (94%)	86 (5%)	14 (1%)	16	31

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	123	HIS
4	D	104	GLY
3	G	118	LYS
3	M	14	ALA

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Mol	Chain	Res	Type
4	R	32	SER

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	85/112 (76%)	81 (95%)	4 (5%)	23	47
1	E	86/112 (77%)	78 (91%)	8 (9%)	8	19
1	K	86/112 (77%)	83 (96%)	3 (4%)	32	57
1	O	85/112 (76%)	82 (96%)	3 (4%)	32	57
2	B	72/80 (90%)	66 (92%)	6 (8%)	10	23
2	F	72/80 (90%)	68 (94%)	4 (6%)	19	40
2	L	65/80 (81%)	65 (100%)	0	100	100
2	P	73/80 (91%)	70 (96%)	3 (4%)	27	52
3	C	86/101 (85%)	76 (88%)	10 (12%)	5	11
3	G	91/101 (90%)	82 (90%)	9 (10%)	7	16
3	M	86/101 (85%)	80 (93%)	6 (7%)	14	30
3	Q	85/101 (84%)	77 (91%)	8 (9%)	8	18
4	D	83/106 (78%)	78 (94%)	5 (6%)	17	36
4	H	84/106 (79%)	73 (87%)	11 (13%)	4	8
4	N	84/106 (79%)	75 (89%)	9 (11%)	6	13
4	R	83/106 (78%)	76 (92%)	7 (8%)	10	22
7	U	68/152 (45%)	60 (88%)	8 (12%)	5	11
7	V	66/152 (43%)	56 (85%)	10 (15%)	3	5
All	All	1440/1900 (76%)	1326 (92%)	114 (8%)	11	25

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	40	ARG

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Mol	Chain	Res	Type
7	V	88	VAL
4	N	69	ILE
7	V	82	LEU
7	U	49	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	49	GLN
7	U	64	ASN
1	K	76	GLN
4	H	47	GLN
7	U	84	GLN

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 ⓘ

Of 23 ligands modelled in this entry, 23 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	98/138 (71%)	-0.52	0 100 100	55, 70, 110, 137	0
1	E	99/138 (71%)	-0.52	0 100 100	57, 74, 115, 138	0
1	K	99/138 (71%)	-0.30	0 100 100	85, 106, 143, 168	0
1	O	98/138 (71%)	-0.28	1 (1%) 79 75	81, 102, 142, 184	0
2	B	88/105 (83%)	-0.47	0 100 100	55, 69, 172, 200	0
2	F	87/105 (82%)	-0.38	0 100 100	58, 75, 182, 200	0
2	L	80/105 (76%)	-0.33	0 100 100	83, 100, 129, 136	0
2	P	91/105 (86%)	-0.34	0 100 100	71, 100, 200, 226	0
3	C	109/132 (82%)	-0.30	0 100 100	60, 78, 119, 177	0
3	G	114/132 (86%)	-0.30	1 (0%) 81 76	53, 74, 164, 210	0
3	M	110/132 (83%)	-0.34	0 100 100	78, 98, 146, 181	0
3	Q	108/132 (81%)	-0.29	1 (0%) 81 76	90, 110, 158, 200	0
4	D	97/128 (75%)	-0.34	0 100 100	58, 79, 136, 183	0
4	H	98/128 (76%)	-0.35	0 100 100	57, 77, 136, 159	0
4	N	98/128 (76%)	-0.40	1 (1%) 79 75	78, 98, 133, 170	0
4	R	97/128 (75%)	-0.26	0 100 100	87, 108, 160, 182	0
5	I	169/169 (100%)	-0.82	0 100 100	77, 117, 190, 264	0
5	S	169/169 (100%)	-0.71	0 100 100	100, 147, 226, 309	0
6	J	169/169 (100%)	-0.83	0 100 100	77, 117, 193, 252	0
6	T	169/169 (100%)	-0.71	0 100 100	100, 147, 226, 292	0
7	U	86/190 (45%)	-0.03	0 100 100	138, 169, 207, 218	1 (1%)
7	V	84/190 (44%)	0.01	1 (1%) 76 71	117, 148, 201, 225	1 (1%)
All	All	2417/3068 (78%)	-0.45	5 (0%) 91 91	53, 105, 184, 309	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	28	LYS	3.4
1	O	38	PRO	2.9
3	G	13	LYS	2.3
3	Q	33	LEU	2.2
7	V	88	VAL	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CA	I	108	1/1	0.79	0.20	129,129,129,129	0
8	CA	J	102	1/1	0.81	0.16	139,139,139,139	0
8	CA	T	101	1/1	0.81	0.21	143,143,143,143	0
8	CA	T	102	1/1	0.81	0.14	141,141,141,141	0
10	K	T	103	1/1	0.82	0.13	126,126,126,126	0
8	CA	I	107	1/1	0.84	0.13	124,124,124,124	0
8	CA	I	103	1/1	0.85	0.12	146,146,146,146	0
8	CA	S	101	1/1	0.87	0.09	136,136,136,136	0
10	K	I	109	1/1	0.88	0.11	110,110,110,110	0
8	CA	S	104	1/1	0.90	0.23	127,127,127,127	0
8	CA	J	103	1/1	0.91	0.14	141,141,141,141	0
8	CA	I	104	1/1	0.92	0.12	136,136,136,136	0
8	CA	I	106	1/1	0.92	0.21	112,112,112,112	0
8	CA	C	201	1/1	0.92	0.08	123,123,123,123	0
8	CA	I	105	1/1	0.93	0.16	122,122,122,122	0
9	CL	H	201	1/1	0.95	0.07	92,92,92,92	0
8	CA	S	103	1/1	0.95	0.04	126,126,126,126	0
8	CA	S	102	1/1	0.95	0.05	100,100,100,100	0
9	CL	C	202	1/1	0.96	0.08	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	J	101	1/1	0.96	0.09	121,121,121,121	0
8	CA	I	102	1/1	0.97	0.10	89,89,89,89	0
8	CA	I	101	1/1	0.98	0.13	88,88,88,88	0
9	CL	M	201	1/1	0.99	0.05	92,92,92,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.