



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:12 AM UTC

PDB ID : 6LAB / pdb_00006lab
Title : 169 bp nucleosome, harboring cohesive DNA termini, assembled with linker histone H1.0
Authors : Adhireksan, Z.; Sharma, D.; Bao, Q.; Lee, P.L.; Padavattan, S.; Davey, C.A.
Deposited on : 2019-11-12
Resolution : 3.20 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

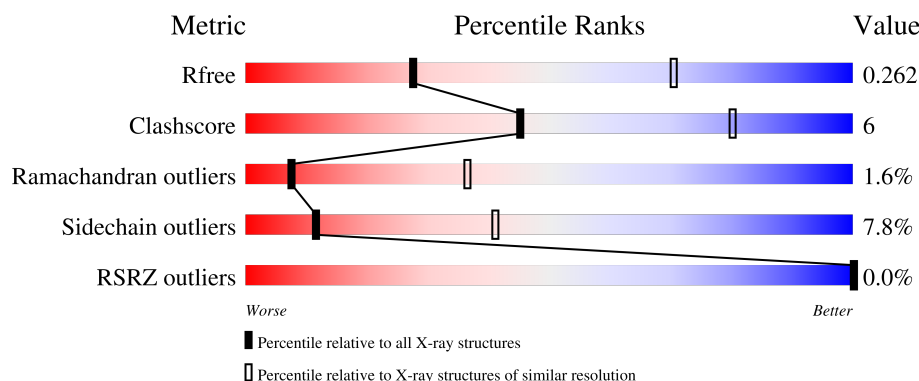
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



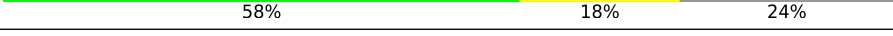
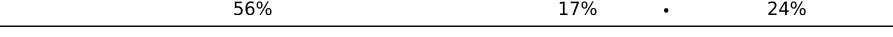
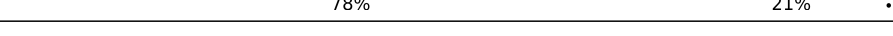
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	136	
1	E	136	
1	K	136	
1	O	136	
2	B	103	

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Mol	Chain	Length	Quality of chain
2	F	103	
2	L	103	
2	P	103	
3	C	130	
3	G	130	
3	M	130	
3	Q	130	
4	D	126	
4	H	126	
4	N	126	
4	R	126	
5	I	169	
5	S	169	
6	J	169	
6	T	169	
7	U	194	
7	V	194	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 27249 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	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	K	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	O	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	F	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			
2	L	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
2	P	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	G	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	M	106	Total	C	N	O	0	0	0
			819	517	160	142			
3	Q	103	Total	C	N	O	0	0	0
			796	502	155	139			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	H	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	N	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	R	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

- 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 H1.0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	78	Total	C	N	O	S	0	0	0
			596	370	112	113	1			
7	V	84	Total	C	N	O	S	0	0	0
			647	402	121	123	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		
8	I	6	Total	Ca	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total 2	Ca 2	0	0
8	M	1	Total 1	Ca 1	0	0
8	S	6	Total 6	Ca 6	0	0
8	T	4	Total 4	Ca 4	0	0

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

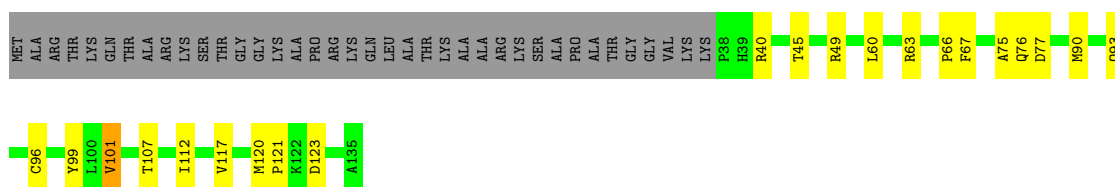
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total 1	Cl 1	0	0
10	Q	1	Total 1	Cl 1	0	0

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.

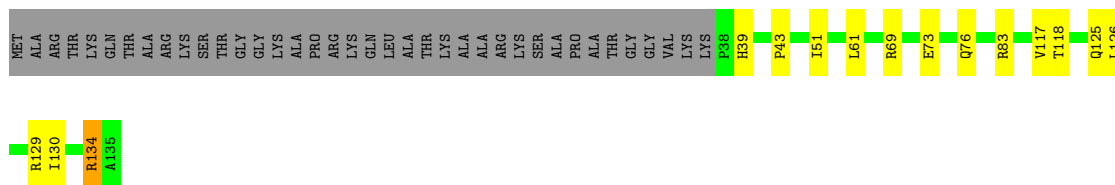
• Molecule 1: Histone H3.1

Chain A: 



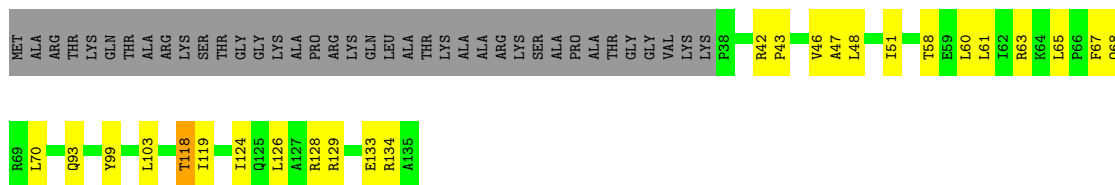
• Molecule 1: Histone H3.1

Chain E: 



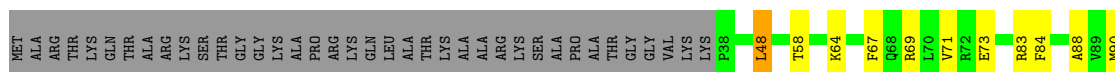
• Molecule 1: Histone H3.1

Chain K: 



• Molecule 1: Histone H3.1

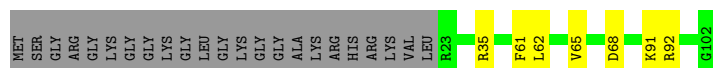
Chain O: 





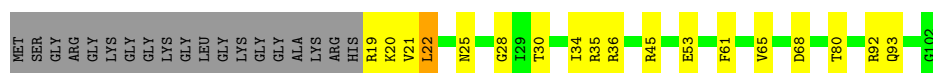
- Molecule 2: Histone H4

Chain B: 71% 7% 22%



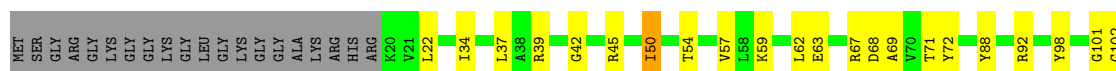
- Molecule 2: Histone H4

Chain F: 64% 17% 18%



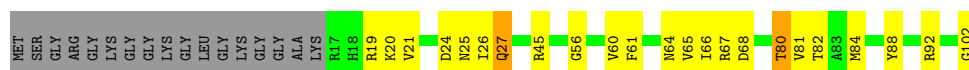
- Molecule 2: Histone H4

Chain L: 59% 20% 19%



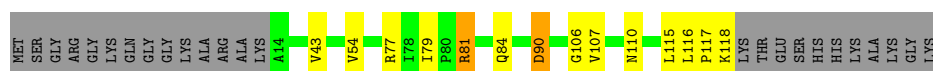
- Molecule 2: Histone H4

Chain P: 61% 20% 17%



- Molecule 3: Histone H2A type 1-B/E

Chain C: 70% 9% 19%



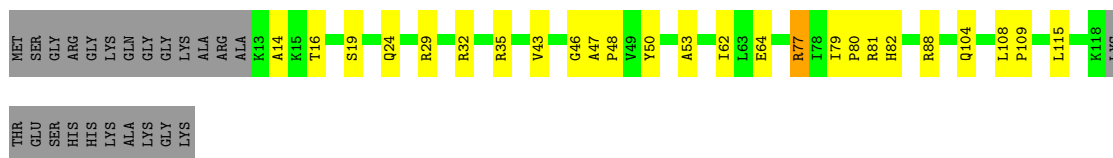
- Molecule 3: Histone H2A type 1-B/E

Chain G: 65% 12% 21%



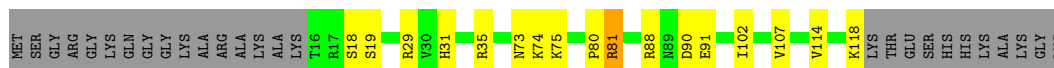
- Molecule 3: Histone H2A type 1-B/E

Chain M: 



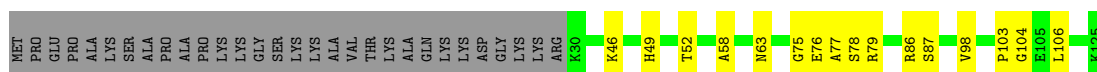
- Molecule 3: Histone H2A type 1-B/E

Chain Q: 



- Molecule 4: Histone H2B type 1-J

Chain D: 



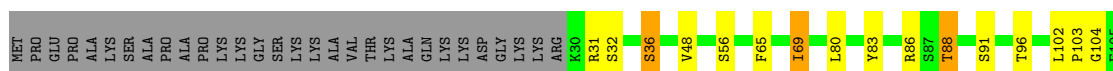
- Molecule 4: Histone H2B type 1-J

Chain H: 



- Molecule 4: Histone H2B type 1-J

Chain N: 



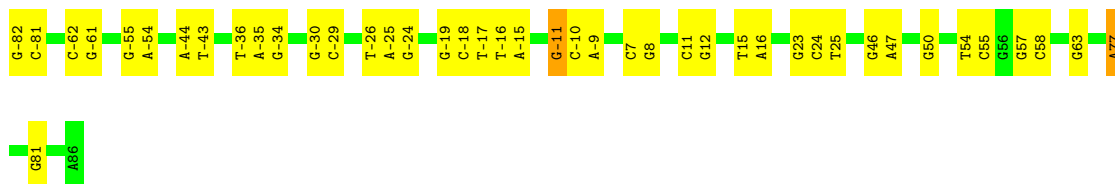
- Molecule 4: Histone H2B type 1-J

Chain R: 

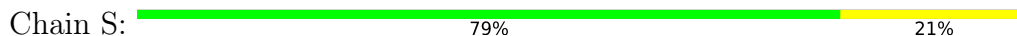




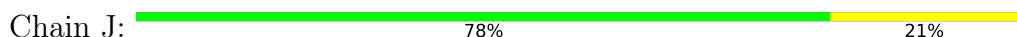
- Molecule 5: DNA (169-MER)



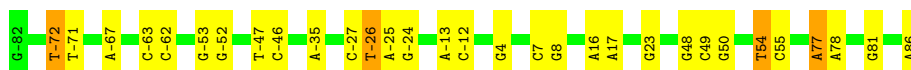
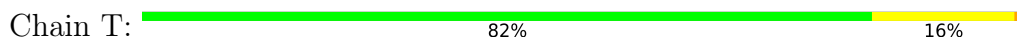
- Molecule 5: DNA (169-MER)



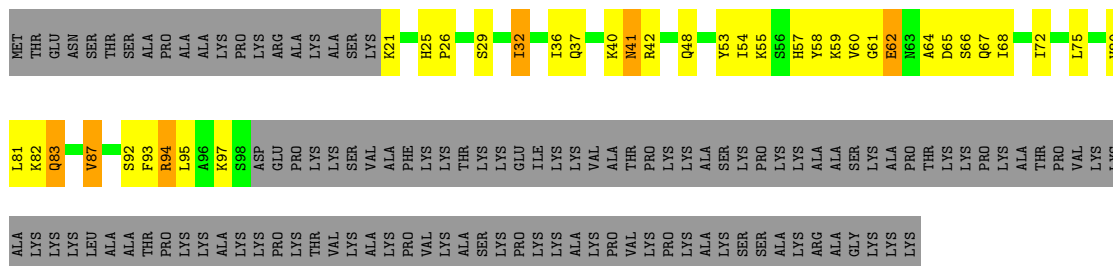
- Molecule 6: DNA (169-MER)



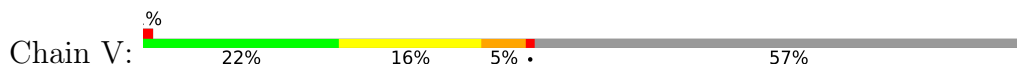
- Molecule 6: DNA (169-MER)

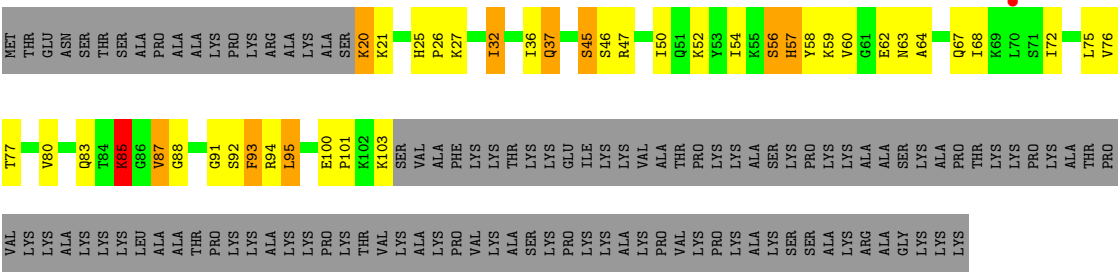


- Molecule 7: Histone H1.0



- Molecule 7: Histone H1.0





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.80Å 102.76Å 218.05Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	39.89 – 3.20 39.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.89-3.20) 99.2 (39.89-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.201 , 0.262 0.206 , 0.262	Depositor DCC
R_{free} test set	1469 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	90.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27249	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.93% 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	0.97	0/819	1.46	1/1097 (0.1%)
1	E	0.97	0/819	1.47	1/1097 (0.1%)
1	K	1.00	0/819	1.51	0/1097
1	O	0.97	0/819	1.52	4/1097 (0.4%)
2	B	0.99	0/645	1.54	0/862
2	F	1.02	0/680	1.57	0/908
2	L	1.01	0/669	1.44	0/894
2	P	1.03	1/702 (0.1%)	1.54	0/937
3	C	1.00	0/820	1.51	2/1107 (0.2%)
3	G	1.00	0/806	1.43	0/1089
3	M	1.03	0/829	1.46	2/1118 (0.2%)
3	Q	1.03	0/806	1.49	0/1089
4	D	0.96	0/766	1.52	0/1026
4	H	1.04	0/766	1.53	0/1026
4	N	1.00	0/766	1.58	1/1026 (0.1%)
4	R	1.00	0/766	1.58	3/1026 (0.3%)
5	I	0.36	0/3884	0.74	3/5993 (0.1%)
5	S	0.43	0/3884	0.86	3/5993 (0.1%)
6	J	0.36	0/3882	0.76	4/5990 (0.1%)
6	T	0.46	0/3882	0.86	6/5990 (0.1%)
7	U	1.17	0/602	1.60	2/802 (0.2%)
7	V	1.04	0/654	1.66	3/870 (0.3%)
All	All	0.75	1/29085 (0.0%)	1.17	35/42134 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	V	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	80	THR	C-O	5.22	1.30	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	54	DT	C4'-C3'-O3'	6.85	120.27	110.00
3	M	43	VAL	CA-C-N	6.76	126.52	120.10
3	M	43	VAL	C-N-CA	6.76	126.52	120.10
4	R	111	VAL	CA-C-N	6.50	129.28	120.38
4	R	111	VAL	C-N-CA	6.50	129.28	120.38
3	C	43	VAL	CA-C-N	6.35	126.14	120.10
3	C	43	VAL	C-N-CA	6.35	126.14	120.10
1	O	97	GLU	N-CA-C	-6.15	104.58	111.28
7	V	57	HIS	CA-C-N	6.13	131.85	122.23
7	V	57	HIS	C-N-CA	6.13	131.85	122.23
5	S	77	DA	C2'-C3'-O3'	6.03	120.54	111.50
6	T	4	DG	C2'-C3'-O3'	5.92	120.38	111.50
6	T	-26	DT	C4'-C3'-O3'	-5.82	101.27	110.00
6	T	-72	DT	C4'-C3'-O3'	5.81	118.72	110.00
5	S	-45	DA	C2'-C3'-O3'	-5.77	102.84	111.50
6	J	77	DA	C2'-C3'-O3'	5.64	119.97	111.50
1	O	71	VAL	N-CA-C	-5.49	105.15	110.42
1	O	103	LEU	N-CA-C	-5.49	105.38	111.36
5	I	77	DA	C2'-C3'-O3'	5.47	119.71	111.50
4	R	111	VAL	O-C-N	5.47	127.80	121.94
7	V	58	TYR	N-CA-C	-5.41	106.60	114.12
6	J	-34	DG	C2'-C3'-O3'	-5.35	103.48	111.50
1	O	133	GLU	N-CA-C	-5.31	106.81	113.28
1	E	134	ARG	CB-CA-C	5.27	118.57	110.14
7	U	40	LYS	CA-C-N	5.26	131.59	121.54
7	U	40	LYS	C-N-CA	5.26	131.59	121.54
5	I	-55	DG	C2'-C3'-O3'	-5.25	103.62	111.50
6	J	-62	DC	C2'-C3'-O3'	5.23	119.35	111.50
6	T	-35	DA	C4'-C3'-O3'	-5.23	102.16	110.00
5	I	-11	DG	C2'-C3'-O3'	5.22	119.33	111.50
4	N	91	SER	N-CA-C	-5.10	105.91	111.82
1	A	101	VAL	N-CA-C	-5.08	105.55	110.42
6	J	29	DG	C2'-C3'-O3'	-5.03	103.96	111.50
5	S	-2	DG	C2'-C3'-O3'	-5.01	103.99	111.50
6	T	77	DA	C2'-C3'-O3'	5.01	119.01	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	V	56	SER	Peptide
7	V	57	HIS	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	807	0	844	11	1
1	E	807	0	844	12	0
1	K	807	0	844	14	0
1	O	807	0	844	16	0
2	B	638	0	676	4	0
2	F	673	0	722	16	1
2	L	662	0	709	12	0
2	P	694	0	742	18	0
3	C	810	0	866	8	0
3	G	796	0	848	12	0
3	M	819	0	879	16	0
3	Q	796	0	848	6	0
4	D	755	0	784	6	0
4	H	755	0	784	13	0
4	N	755	0	784	10	0
4	R	755	0	784	18	0
5	I	3462	0	1901	30	0
5	S	3462	0	1901	23	0
6	J	3461	0	1902	21	0
6	T	3461	0	1902	19	0
7	U	596	0	627	38	0
7	V	647	0	683	29	0
8	C	1	0	0	0	0
8	I	6	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
8	S	6	0	0	0	0
8	T	4	0	0	0	0
9	C	1	0	0	0	0
9	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	1	0	0	0	0
10	Q	1	0	0	0	0
All	All	27249	0	21718	288	1

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 6.

All (288) 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:E:76:GLN:OE1	2:F:20:LYS:HG2	1.69	0.93
7:U:55:LYS:HG3	7:U:59:LYS:HD3	1.51	0.93
4:R:49:HIS:HB3	4:R:52:THR:CG2	1.98	0.93
7:U:65:ASP:HA	7:U:68:ILE:HD12	1.48	0.93
7:U:32:ILE:HD11	7:U:68:ILE:HG23	1.56	0.87
7:U:64:ALA:O	7:U:67:GLN:HG2	1.74	0.86
7:U:54:ILE:CD1	7:U:59:LYS:HE3	2.05	0.86
4:R:49:HIS:HB3	4:R:52:THR:HG23	1.60	0.81
5:I:-9:DA:OP1	7:U:61:GLY:HA3	1.81	0.81
7:V:54:ILE:HD11	7:V:68:ILE:CD1	2.11	0.81
7:U:81:LEU:CD1	7:U:95:LEU:HD23	2.13	0.78
4:H:49:HIS:HB3	4:H:52:THR:CG2	2.16	0.75
7:V:54:ILE:HD11	7:V:68:ILE:HD11	1.69	0.75
7:U:80:VAL:HG13	7:U:81:LEU:HD13	1.68	0.74
1:E:76:GLN:NE2	2:F:20:LYS:HE2	2.03	0.74
7:V:100:GLU:HG2	7:V:101:PRO:HD2	1.68	0.74
7:U:65:ASP:CA	7:U:68:ILE:HD12	2.19	0.72
7:U:60:VAL:HB	7:U:64:ALA:HB2	1.72	0.72
6:J:-46:DC:H2''	6:J:-45:DA:C8	2.24	0.71
3:M:62:ILE:HD11	4:N:65:PHE:CZ	2.27	0.70
6:T:7:DC:H2'	6:T:8:DG:C8	2.26	0.70
7:U:65:ASP:HA	7:U:68:ILE:CD1	2.22	0.69
7:V:94:ARG:HG2	7:V:95:LEU:N	2.08	0.68
2:L:39:ARG:O	2:L:42:GLY:N	2.25	0.67
7:V:72:ILE:HD13	7:V:93:PHE:CZ	2.28	0.67
1:O:83:ARG:O	2:P:80:THR:HA	1.95	0.67
1:E:83:ARG:HB3	2:F:80:THR:HG23	1.75	0.66
4:R:114:GLY:O	4:R:118:VAL:HG23	1.95	0.66
5:S:-47:DT:H2''	5:S:-46:DC:C6	2.30	0.66
7:U:26:PRO:HB2	7:U:29:SER:HB3	1.79	0.65
3:Q:102:ILE:HG23	4:R:61:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:32:ILE:HD11	7:V:68:ILE:HG23	1.79	0.64
3:G:50:TYR:OH	4:H:95:GLN:NE2	2.30	0.64
7:V:45:SER:OG	7:V:93:PHE:O	2.11	0.64
3:C:81:ARG:NH2	3:C:107:VAL:O	2.32	0.63
1:E:69:ARG:HB3	2:F:25:ASN:OD1	1.99	0.63
7:V:37:GLN:HB3	7:V:95:LEU:HD11	1.81	0.63
1:O:90:MET:HE2	1:O:90:MET:HA	1.80	0.63
7:U:81:LEU:HD11	7:U:95:LEU:HD23	1.81	0.62
1:E:76:GLN:HE22	2:F:20:LYS:HE2	1.64	0.62
1:K:119:ILE:HD12	2:L:50:ILE:HD13	1.82	0.62
4:H:95:GLN:NE2	4:H:111:VAL:HG13	2.14	0.62
7:U:81:LEU:HD12	7:U:95:LEU:HD23	1.80	0.62
6:T:54:DT:H2''	6:T:55:DC:C6	2.36	0.61
2:L:67:ARG:O	2:L:71:THR:OG1	2.18	0.60
7:U:54:ILE:HD11	7:U:59:LYS:HE3	1.81	0.60
7:U:54:ILE:HD12	7:U:59:LYS:HE3	1.82	0.60
4:R:49:HIS:CB	4:R:52:THR:HG23	2.31	0.60
2:P:26:ILE:HG23	2:P:27:GLN:NE2	2.17	0.59
3:C:115:LEU:HD22	1:E:117:VAL:HG13	1.85	0.59
1:O:73:GLU:OE1	2:P:25:ASN:ND2	2.34	0.59
3:M:50:TYR:O	3:M:53:ALA:HB3	2.02	0.58
7:U:32:ILE:O	7:U:36:ILE:HG12	2.04	0.58
7:U:65:ASP:O	7:U:68:ILE:HB	2.03	0.58
7:V:32:ILE:HD11	7:V:68:ILE:CG2	2.32	0.58
5:I:82:DG:O5'	6:T:86:DA:H2''	2.04	0.58
7:U:55:LYS:HG3	7:U:59:LYS:CD	2.30	0.58
2:F:22:LEU:N	2:F:22:LEU:HD23	2.19	0.57
4:H:49:HIS:HB3	4:H:52:THR:HG22	1.87	0.57
1:E:125:GLN:NE2	2:F:53:GLU:OE2	2.36	0.56
7:U:36:ILE:CG2	7:U:95:LEU:HG	2.35	0.56
3:M:47:ALA:N	3:M:48:PRO:HD2	2.19	0.56
4:H:49:HIS:HB3	4:H:52:THR:HG23	1.88	0.56
1:O:69:ARG:NH2	5:S:17:DA:OP2	2.39	0.56
7:V:54:ILE:HD11	7:V:68:ILE:HD13	1.88	0.56
6:T:-72:DT:H4'	6:T:-71:DT:OP1	2.06	0.56
6:T:7:DC:C2'	6:T:8:DG:C8	2.89	0.56
1:A:60:LEU:CD1	1:A:90:MET:HE1	2.35	0.55
3:M:79:ILE:HG12	3:M:82:HIS:CE1	2.41	0.55
5:I:54:DT:H4'	5:I:55:DC:OP1	2.07	0.55
1:E:126:LEU:HD11	1:E:130:ILE:HD11	1.89	0.55
7:U:36:ILE:HG21	7:U:95:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:HB3	1:A:121:PRO:CD	2.38	0.54
2:F:68:ASP:OD2	2:F:92:ARG:NH1	2.40	0.54
4:D:49:HIS:HB3	4:D:52:THR:OG1	2.08	0.54
2:L:88:TYR:CE1	4:N:83:TYR:CE1	2.96	0.54
4:R:70:PHE:CD1	4:R:70:PHE:C	2.86	0.54
3:M:77:ARG:HD3	5:S:-53:DG:OP1	2.07	0.53
6:T:49:DC:H2'	6:T:50:DG:C8	2.44	0.53
2:P:61:PHE:O	2:P:65:VAL:HG23	2.09	0.53
5:S:-80:DT:O2	6:T:81:DG:N2	2.42	0.53
6:J:49:DC:H2'	6:J:50:DG:C8	2.44	0.53
6:T:-13:DA:C5	6:T:-12:DC:C4	2.96	0.53
2:P:26:ILE:HG23	2:P:27:GLN:HE22	1.74	0.53
7:U:75:LEU:HB3	7:U:81:LEU:HD22	1.91	0.53
6:J:-63:DC:H2'	6:J:-62:DC:C6	2.44	0.52
5:S:-22:DA:C2	6:T:23:DG:C2	2.97	0.52
2:L:101:GLY:O	2:L:102:GLY:C	2.51	0.52
5:I:-9:DA:P	7:U:61:GLY:HA3	2.49	0.52
6:J:-53:DG:C6	6:J:-52:DG:C6	2.98	0.52
6:J:38:DG:H2''	6:J:39:DA:OP2	2.09	0.52
2:L:68:ASP:OD2	2:L:92:ARG:NH1	2.43	0.52
3:Q:31:HIS:CE1	3:Q:35:ARG:NH2	2.78	0.52
4:D:76:GLU:OE2	4:D:79:ARG:NH1	2.42	0.51
5:I:-62:DC:H2'	5:I:-61:DG:C8	2.44	0.51
5:I:15:DT:H2''	5:I:16:DA:C8	2.46	0.51
1:K:118:THR:HA	2:L:45:ARG:O	2.11	0.51
6:T:-63:DC:H2'	6:T:-62:DC:C6	2.45	0.51
3:M:115:LEU:HD11	1:O:108:ASN:HD21	1.75	0.51
7:U:54:ILE:HD12	7:U:54:ILE:C	2.36	0.51
3:M:64:GLU:HA	4:N:48:VAL:HG11	1.92	0.50
2:P:88:TYR:CD1	4:R:83:TYR:CZ	3.00	0.50
7:U:82:LYS:HE3	7:U:83:GLN:O	2.11	0.50
1:E:61:LEU:HD13	2:F:36:ARG:HB3	1.94	0.50
6:T:-27:DC:H2''	6:T:-26:DT:H71	1.93	0.50
7:V:47:ARG:NH1	7:V:88:GLY:O	2.44	0.50
1:A:99:TYR:CD2	2:B:61:PHE:CD2	3.00	0.50
3:C:90:ASP:C	3:C:90:ASP:OD1	2.55	0.50
6:J:23:DG:H2''	6:J:24:DC:OP2	2.12	0.50
4:N:65:PHE:CE1	4:N:69:ILE:CD1	2.95	0.50
5:I:81:DG:N2	6:J:-80:DT:O2	2.45	0.49
3:M:32:ARG:O	3:M:35:ARG:N	2.45	0.49
4:H:94:ILE:O	4:H:98:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:54:DT:H4'	6:J:55:DC:OP1	2.12	0.49
3:M:47:ALA:N	3:M:48:PRO:CD	2.75	0.49
4:D:77:ALA:O	4:D:78:SER:C	2.55	0.49
1:K:48:LEU:HD23	1:K:51:ILE:HD12	1.93	0.49
2:P:88:TYR:CE1	4:R:83:TYR:CE1	3.01	0.49
3:C:116:LEU:HB3	3:C:117:PRO:HD2	1.95	0.48
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.46	0.48
1:O:126:LEU:HD11	1:O:130:ILE:HD11	1.95	0.48
5:S:69:DT:H1'	5:S:70:DG:C5'	2.43	0.48
3:M:104:GLN:NE2	1:O:58:THR:O	2.46	0.48
1:A:101:VAL:HG11	3:G:107:VAL:HG11	1.95	0.48
6:J:62:DG:H2''	6:J:63:DG:OP2	2.14	0.48
5:S:-33:DA:C5	5:S:-32:DC:C4	3.02	0.48
7:U:29:SER:OG	7:U:75:LEU:HD21	2.14	0.47
7:U:65:ASP:HA	7:U:68:ILE:CG1	2.44	0.47
7:U:97:LYS:H	7:U:97:LYS:HD2	1.79	0.47
1:K:103:LEU:HD11	1:K:128:ARG:HG2	1.96	0.47
2:L:62:LEU:O	2:L:63:GLU:C	2.57	0.47
7:V:60:VAL:HG12	7:V:63:ASN:H	1.80	0.47
3:M:88:ARG:HB2	3:M:108:LEU:HD21	1.95	0.47
3:G:62:ILE:HD11	4:H:65:PHE:CZ	2.50	0.47
7:V:32:ILE:CD1	7:V:72:ILE:HG12	2.44	0.47
1:A:63:ARG:HB2	1:A:66:PRO:HG2	1.96	0.47
3:C:79:ILE:HA	4:D:58:ALA:HB2	1.96	0.47
2:F:61:PHE:CE1	2:F:65:VAL:HG21	2.50	0.47
5:I:46:DG:C2	5:I:47:DA:C2	3.03	0.47
1:K:61:LEU:HD12	2:L:37:LEU:HD23	1.96	0.47
2:L:69:ALA:O	2:L:72:TYR:HB2	2.15	0.47
5:S:23:DG:C4	5:S:24:DC:C5	3.03	0.47
7:V:83:GLN:CB	7:V:93:PHE:HB3	2.45	0.47
5:I:24:DC:H2''	5:I:25:DT:OP2	2.14	0.47
3:G:77:ARG:HA	4:H:53:GLY:O	2.15	0.47
7:V:32:ILE:CD1	7:V:72:ILE:CG1	2.92	0.47
7:U:82:LYS:HG3	7:U:83:GLN:N	2.28	0.46
7:U:26:PRO:CB	7:U:29:SER:HB3	2.44	0.46
7:V:100:GLU:HG2	7:V:101:PRO:CD	2.40	0.46
1:K:99:TYR:OH	1:K:133:GLU:OE1	2.28	0.46
1:O:131:ARG:HD3	1:O:133:GLU:OE2	2.15	0.46
6:T:77:DA:C2	6:T:78:DA:C2	3.03	0.46
2:B:61:PHE:O	2:B:65:VAL:HG23	2.16	0.46
1:K:46:VAL:O	1:K:47:ALA:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:103:PRO:O	4:R:104:GLY:C	2.58	0.46
3:C:77:ARG:CZ	5:I:-54:DA:H4'	2.46	0.46
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.47	0.46
1:K:124:ILE:O	1:K:128:ARG:HG3	2.16	0.46
5:S:64:DG:H2''	5:S:65:DA:OP2	2.16	0.46
5:I:77:DA:N6	6:J:-78:DT:O4	2.49	0.46
5:S:7:DC:H2'	5:S:8:DG:C8	2.51	0.46
6:T:-47:DT:H2''	6:T:-46:DC:C5	2.51	0.46
1:E:76:GLN:OE1	2:F:20:LYS:CG	2.54	0.45
3:M:16:THR:O	3:M:19:SER:OG	2.30	0.45
5:S:54:DT:H2''	5:S:55:DC:C6	2.52	0.45
5:S:54:DT:H4'	5:S:55:DC:OP1	2.16	0.45
5:I:-35:DA:C5	5:I:-34:DG:C6	3.04	0.45
2:P:56:GLY:O	2:P:60:VAL:HG23	2.15	0.45
5:S:69:DT:H1'	5:S:70:DG:H5'	1.97	0.45
7:U:32:ILE:HD12	7:U:72:ILE:HG13	1.97	0.45
7:V:20:LYS:HD3	7:V:20:LYS:N	2.31	0.45
7:V:36:ILE:HB	7:V:95:LEU:HD21	1.97	0.45
1:A:67:PHE:CZ	1:A:93:GLN:HA	2.52	0.45
3:C:84:GLN:HG2	3:C:106:GLY:O	2.17	0.45
5:I:46:DG:N2	5:I:47:DA:C2	2.85	0.45
7:V:83:GLN:HB2	7:V:92:SER:O	2.17	0.45
1:A:75:ALA:O	1:A:76:GLN:C	2.60	0.45
1:O:118:THR:HA	2:P:45:ARG:O	2.16	0.45
1:O:131:ARG:NH1	1:O:133:GLU:OE2	2.47	0.45
5:S:-62:DC:H2'	5:S:-61:DG:C8	2.52	0.45
4:R:102:LEU:N	4:R:102:LEU:HD23	2.32	0.45
5:I:63:DG:N2	6:J:-62:DC:O2	2.50	0.45
5:I:-25:DA:H1'	5:I:-24:DG:C8	2.53	0.44
5:S:46:DG:C2	5:S:47:DA:C2	3.05	0.44
1:K:48:LEU:HA	1:K:51:ILE:HD12	1.99	0.44
2:P:66:ILE:O	2:P:67:ARG:C	2.61	0.44
5:S:-13:DA:H2''	5:S:-12:DC:O5'	2.17	0.44
5:S:-16:DT:H2''	5:S:-15:DA:C8	2.53	0.44
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.43	0.44
3:Q:81:ARG:NH2	3:Q:107:VAL:O	2.50	0.44
7:U:32:ILE:CD1	7:U:72:ILE:HG13	2.48	0.44
5:I:-10:DC:OP1	7:U:62:GLU:HG2	2.18	0.44
6:J:85:DC:H2''	6:J:86:DA:C8	2.53	0.44
6:J:-31:DA:H2''	6:J:-30:DG:OP2	2.18	0.44
6:J:7:DC:H2''	6:J:8:DG:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:90:ASP:O	3:Q:91:GLU:C	2.61	0.44
5:I:57:DG:H2"	5:I:58:DC:C6	2.52	0.43
2:L:98:TYR:OH	4:R:68:ASP:OD2	2.33	0.43
3:G:80:PRO:HB2	3:G:104:GLN:O	2.18	0.43
5:I:7:DC:H2"	5:I:8:DG:C8	2.52	0.43
3:Q:88:ARG:HA	3:Q:88:ARG:HD3	1.88	0.43
7:V:62:GLU:H	7:V:62:GLU:CD	2.26	0.43
2:F:34:ILE:O	2:F:35:ARG:C	2.61	0.43
6:J:-9:DA:C5	6:J:-8:DC:C4	3.06	0.43
3:M:29:ARG:NH1	4:N:36:SER:O	2.51	0.43
1:O:105:GLU:O	1:O:106:ASP:C	2.61	0.43
3:G:102:ILE:HG23	4:H:61:ILE:HD13	1.99	0.43
5:I:50:DG:N2	6:J:-49:DG:C2	2.87	0.43
6:J:64:DG:H2"	6:J:65:DA:OP2	2.17	0.43
7:U:32:ILE:HD13	7:U:72:ILE:HD11	2.01	0.43
3:G:90:ASP:O	3:G:91:GLU:C	2.62	0.43
5:I:-82:DG:H2"	5:I:-81:DC:OP2	2.19	0.43
3:M:46:GLY:C	3:M:48:PRO:HD2	2.44	0.43
7:U:65:ASP:CB	7:U:68:ILE:HD12	2.48	0.43
3:M:62:ILE:HD11	4:N:65:PHE:CE1	2.52	0.43
4:R:49:HIS:HB3	4:R:52:THR:HG22	1.89	0.43
5:S:-50:DC:H2"	5:S:-49:DG:C8	2.53	0.43
5:S:-26:DT:C4	5:S:-25:DA:C6	3.07	0.43
7:V:46:SER:OG	7:V:91:GLY:O	2.25	0.43
1:A:117:VAL:HG13	3:G:115:LEU:HD22	2.00	0.43
5:I:-26:DT:C4	5:I:-25:DA:C6	3.07	0.43
6:J:77:DA:C2	6:J:78:DA:C2	3.07	0.42
4:N:88:THR:OG1	5:S:-34:DG:OP1	2.31	0.42
7:V:68:ILE:O	7:V:72:ILE:HG13	2.19	0.42
5:I:-11:DG:C5	5:I:-10:DC:C4	3.07	0.42
2:P:84:MET:HE1	2:P:102:GLY:HA3	2.02	0.42
3:Q:81:ARG:O	3:Q:81:ARG:HG3	2.19	0.42
2:P:24:ASP:OD1	2:P:26:ILE:HG22	2.18	0.42
2:P:68:ASP:OD2	2:P:92:ARG:NH1	2.50	0.42
4:R:31:ARG:HB2	5:S:51:DG:OP1	2.20	0.42
6:T:-25:DA:C2	6:T:-24:DG:C6	3.07	0.42
1:A:112:ILE:HG21	3:G:114:VAL:HG21	2.01	0.42
3:G:62:ILE:HD11	4:H:65:PHE:CE1	2.55	0.42
7:V:46:SER:O	7:V:50:ILE:HG13	2.20	0.42
3:C:54:VAL:HG21	4:D:98:VAL:HG21	2.02	0.42
4:H:102:LEU:HB2	4:H:107:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:23:DG:C4	5:I:24:DC:C5	3.08	0.42
6:J:10:DG:C2	6:J:11:DC:C2	3.08	0.42
1:K:60:LEU:HD13	1:K:93:GLN:CD	2.44	0.42
1:K:42:ARG:O	1:K:43:PRO:C	2.62	0.42
6:T:54:DT:H4'	6:T:55:DC:OP1	2.20	0.42
7:V:85:LYS:HA	7:V:85:LYS:HD3	1.85	0.42
4:N:80:LEU:HD13	4:N:96:THR:HB	2.02	0.42
4:R:119:THR:O	4:R:122:THR:OG1	2.36	0.42
5:I:-30:DG:C5	5:I:-29:DC:C4	3.08	0.41
1:K:126:LEU:HD22	1:O:113:HIS:CG	2.55	0.41
7:V:94:ARG:HG2	7:V:95:LEU:H	1.85	0.41
1:O:48:LEU:HD13	1:O:48:LEU:HA	1.93	0.41
6:T:48:DG:H1'	6:T:49:DC:C6	2.54	0.41
5:I:-19:DG:OP2	5:I:-19:DG:H2'	2.21	0.41
5:I:-16:DT:H2''	5:I:-15:DA:C8	2.55	0.41
6:J:63:DG:H2''	6:J:64:DG:OP2	2.19	0.41
3:M:62:ILE:CD1	4:N:65:PHE:CZ	3.01	0.41
2:P:60:VAL:O	2:P:64:ASN:ND2	2.53	0.41
4:R:49:HIS:CB	4:R:52:THR:CG2	2.84	0.41
2:P:88:TYR:CZ	4:R:83:TYR:CD1	3.08	0.41
3:G:42:ARG:O	4:H:88:THR:HA	2.20	0.41
5:I:-44:DA:C2	5:I:-43:DT:C2	3.09	0.41
4:R:44:VAL:HA	4:R:47:GLN:HE21	1.85	0.41
7:V:103:LYS:HD2	7:V:103:LYS:HA	1.95	0.41
1:A:96:CYS:SG	2:B:62:LEU:HD21	2.61	0.41
1:E:118:THR:HA	2:F:45:ARG:O	2.21	0.41
1:K:67:PHE:O	1:K:70:LEU:HB3	2.21	0.41
1:O:67:PHE:CZ	1:O:93:GLN:HA	2.55	0.41
4:D:75:GLY:O	4:D:78:SER:HB3	2.21	0.41
2:F:28:GLY:O	2:F:30:THR:HG23	2.21	0.41
4:N:102:LEU:HA	4:N:103:PRO:HD2	1.89	0.41
1:O:88:ALA:HB2	2:P:82:THR:C	2.45	0.41
6:T:16:DA:C2	6:T:17:DA:C6	3.09	0.41
7:U:75:LEU:CB	7:U:81:LEU:HD22	2.50	0.41
5:I:-36:DT:H2''	5:I:-35:DA:N7	2.36	0.41
7:U:41:ASN:CG	7:U:41:ASN:O	2.64	0.41
7:V:32:ILE:O	7:V:36:ILE:HG12	2.21	0.41
1:K:68:GLN:HE21	1:K:68:GLN:HB2	1.56	0.40
5:S:-16:DT:H4'	5:S:-16:DT:OP1	2.21	0.40
3:G:80:PRO:HD3	4:H:58:ALA:HB2	2.02	0.40
5:I:-18:DC:H2''	5:I:-17:DT:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:-53:DG:C6	6:T:-52:DG:C6	3.10	0.40
5:S:68:DG:N2	6:T:-67:DA:C2	2.89	0.40
5:I:11:DC:H2'	5:I:12:DG:C8	2.55	0.40
2:P:88:TYR:CG	4:R:83:TYR:CE2	3.10	0.40
7:V:72:ILE:O	7:V:75:LEU:N	2.54	0.40
1:A:107:THR:HG23	1:A:123:ASP:HB3	2.04	0.40
6:J:-25:DA:H1'	6:J:-24:DG:C8	2.56	0.40
2:L:34:ILE:HG23	2:L:54:THR:HG21	2.04	0.40
1:O:84:PHE:CD1	2:P:81:VAL:HB	2.56	0.40
7:U:36:ILE:HG23	7:U:94:ARG:HA	2.02	0.40
7:V:59:LYS:NZ	7:V:64:ALA:HB1	2.36	0.40

All (1) 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:77:ASP:OD2	2:F:19:ARG:NH2[2_746]	1.73	0.47

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	96/136 (71%)	90 (94%)	6 (6%)	0	100	100
1	E	96/136 (71%)	90 (94%)	3 (3%)	3 (3%)	3	22
1	K	96/136 (71%)	86 (90%)	10 (10%)	0	100	100
1	O	96/136 (71%)	91 (95%)	5 (5%)	0	100	100
2	B	78/103 (76%)	69 (88%)	9 (12%)	0	100	100
2	F	82/103 (80%)	73 (89%)	9 (11%)	0	100	100
2	L	81/103 (79%)	67 (83%)	14 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	84/103 (82%)	79 (94%)	4 (5%)	1 (1%)	10	42
3	C	103/130 (79%)	96 (93%)	7 (7%)	0	100	100
3	G	101/130 (78%)	92 (91%)	6 (6%)	3 (3%)	3	23
3	M	104/130 (80%)	93 (89%)	9 (9%)	2 (2%)	6	33
3	Q	101/130 (78%)	94 (93%)	7 (7%)	0	100	100
4	D	94/126 (75%)	86 (92%)	6 (6%)	2 (2%)	5	31
4	H	94/126 (75%)	88 (94%)	4 (4%)	2 (2%)	5	31
4	N	94/126 (75%)	88 (94%)	5 (5%)	1 (1%)	11	43
4	R	94/126 (75%)	87 (93%)	4 (4%)	3 (3%)	3	21
7	U	76/194 (39%)	67 (88%)	4 (5%)	5 (7%)	1	7
7	V	82/194 (42%)	65 (79%)	13 (16%)	4 (5%)	1	13
All	All	1652/2368 (70%)	1501 (91%)	125 (8%)	26 (2%)	7	36

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	91	GLU
7	U	87	VAL
7	V	85	LYS
4	D	104	GLY
3	G	27	VAL
4	N	104	GLY
4	R	33	ARG
7	U	41	ASN
7	V	45	SER
7	V	87	VAL
3	M	14	ALA
4	D	103	PRO
2	P	19	ARG
4	R	32	SER
1	E	39	HIS
3	G	117	PRO
3	M	109	PRO
7	U	58	TYR
7	U	92	SER
4	H	31	ARG
4	H	103	PRO
7	U	42	ARG

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Mol	Chain	Res	Type
7	V	26	PRO
1	E	51	ILE
4	R	104	GLY
1	E	43	PRO

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	85/111 (77%)	82 (96%)	3 (4%)	32	64
1	E	85/111 (77%)	83 (98%)	2 (2%)	43	70
1	K	85/111 (77%)	79 (93%)	6 (7%)	13	44
1	O	85/111 (77%)	81 (95%)	4 (5%)	23	57
2	B	65/79 (82%)	63 (97%)	2 (3%)	35	66
2	F	69/79 (87%)	67 (97%)	2 (3%)	37	67
2	L	68/79 (86%)	64 (94%)	4 (6%)	18	50
2	P	71/79 (90%)	68 (96%)	3 (4%)	26	60
3	C	83/100 (83%)	79 (95%)	4 (5%)	23	56
3	G	82/100 (82%)	75 (92%)	7 (8%)	10	37
3	M	84/100 (84%)	80 (95%)	4 (5%)	23	56
3	Q	82/100 (82%)	72 (88%)	10 (12%)	5	22
4	D	82/105 (78%)	77 (94%)	5 (6%)	17	49
4	H	82/105 (78%)	74 (90%)	8 (10%)	7	31
4	N	82/105 (78%)	74 (90%)	8 (10%)	7	31
4	R	82/105 (78%)	73 (89%)	9 (11%)	6	26
7	U	65/158 (41%)	52 (80%)	13 (20%)	1	7
7	V	71/158 (45%)	55 (78%)	16 (22%)	1	5
All	All	1408/1896 (74%)	1298 (92%)	110 (8%)	11	41

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	45	THR
1	A	49	ARG
2	B	35	ARG
2	B	91	LYS
3	C	81	ARG
3	C	90	ASP
3	C	110	ASN
3	C	118	LYS
4	D	46	LYS
4	D	63	ASN
4	D	86	ARG
4	D	87	SER
4	D	106	LEU
1	E	129	ARG
1	E	134	ARG
2	F	21	VAL
2	F	22	LEU
3	G	29	ARG
3	G	30	VAL
3	G	73	ASN
3	G	74	LYS
3	G	80	PRO
3	G	81	ARG
3	G	107	VAL
4	H	30	LYS
4	H	48	VAL
4	H	64	SER
4	H	69	ILE
4	H	80	LEU
4	H	86	ARG
4	H	119	THR
4	H	125	LYS
1	K	58	THR
1	K	63	ARG
1	K	65	LEU
1	K	118	THR
1	K	129	ARG
1	K	134	ARG
2	L	22	LEU
2	L	50	ILE
2	L	57	VAL
2	L	59	LYS

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Mol	Chain	Res	Type
3	M	24	GLN
3	M	77	ARG
3	M	80	PRO
3	M	81	ARG
4	N	31	ARG
4	N	32	SER
4	N	36	SER
4	N	56	SER
4	N	69	ILE
4	N	86	ARG
4	N	88	THR
4	N	106	LEU
1	O	48	LEU
1	O	64	LYS
1	O	129	ARG
1	O	134	ARG
2	P	20	LYS
2	P	21	VAL
2	P	27	GLN
3	Q	18	SER
3	Q	19	SER
3	Q	29	ARG
3	Q	73	ASN
3	Q	74	LYS
3	Q	75	LYS
3	Q	80	PRO
3	Q	81	ARG
3	Q	114	VAL
3	Q	118	LYS
4	R	30	LYS
4	R	31	ARG
4	R	36	SER
4	R	52	THR
4	R	57	LYS
4	R	80	LEU
4	R	88	THR
4	R	102	LEU
4	R	125	LYS
7	U	21	LYS
7	U	25	HIS
7	U	32	ILE
7	U	37	GLN

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Mol	Chain	Res	Type
7	U	48	GLN
7	U	53	TYR
7	U	57	HIS
7	U	62	GLU
7	U	66	SER
7	U	83	GLN
7	U	87	VAL
7	U	93	PHE
7	U	94	ARG
7	V	20	LYS
7	V	21	LYS
7	V	25	HIS
7	V	27	LYS
7	V	32	ILE
7	V	37	GLN
7	V	52	LYS
7	V	56	SER
7	V	67	GLN
7	V	76	VAL
7	V	77	THR
7	V	80	VAL
7	V	85	LYS
7	V	87	VAL
7	V	93	PHE
7	V	95	LEU

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

Mol	Chain	Res	Type
3	C	24	GLN
3	C	31	HIS
3	C	104	GLN
3	C	110	ASN
3	C	112	GLN
4	D	47	GLN
4	D	84	ASN
4	D	95	GLN
1	E	76	GLN
1	E	93	GLN
3	G	31	HIS
3	G	73	ASN
4	H	47	GLN

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Mol	Chain	Res	Type
4	H	95	GLN
1	K	68	GLN
1	K	93	GLN
3	M	24	GLN
3	M	31	HIS
4	N	47	GLN
4	N	67	ASN
4	N	95	GLN
1	O	76	GLN
1	O	108	ASN
2	P	27	GLN
2	P	64	ASN
4	R	47	GLN
4	R	95	GLN
7	U	37	GLN
7	U	41	ASN
7	U	67	GLN
7	U	83	GLN
7	V	25	HIS
7	V	67	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](#)

Of 24 ligands modelled in this entry, 24 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

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	98/136 (72%)	-0.41	0	100	100	92, 113, 159, 183	0
1	E	98/136 (72%)	-0.43	0	100	100	80, 102, 140, 164	0
1	K	98/136 (72%)	-0.58	0	100	100	44, 66, 108, 139	0
1	O	98/136 (72%)	-0.64	0	100	100	46, 67, 111, 144	0
2	B	80/103 (77%)	-0.48	0	100	100	84, 109, 141, 160	0
2	F	84/103 (81%)	-0.56	0	100	100	80, 95, 141, 171	0
2	L	83/103 (80%)	-0.71	0	100	100	43, 65, 129, 163	0
2	P	86/103 (83%)	-0.60	0	100	100	45, 66, 142, 180	0
3	C	105/130 (80%)	-0.58	0	100	100	80, 101, 133, 146	0
3	G	103/130 (79%)	-0.40	0	100	100	79, 111, 146, 162	0
3	M	106/130 (81%)	-0.66	0	100	100	53, 72, 107, 137	0
3	Q	103/130 (79%)	-0.66	0	100	100	48, 71, 103, 113	0
4	D	96/126 (76%)	-0.51	0	100	100	77, 105, 149, 169	0
4	H	96/126 (76%)	-0.50	0	100	100	82, 110, 156, 177	0
4	N	96/126 (76%)	-0.63	0	100	100	48, 75, 119, 153	0
4	R	96/126 (76%)	-0.61	0	100	100	50, 73, 121, 172	0
5	I	169/169 (100%)	-0.53	0	100	100	106, 167, 249, 280	0
5	S	169/169 (100%)	-0.77	0	100	100	71, 114, 226, 264	0
6	J	169/169 (100%)	-0.58	0	100	100	117, 168, 235, 294	0
6	T	169/169 (100%)	-0.76	0	100	100	74, 113, 211, 278	0
7	U	78/194 (40%)	-0.01	0	100	100	150, 196, 246, 259	1 (1%)
7	V	84/194 (43%)	-0.00	1 (1%)	76	58	109, 161, 197, 213	1 (1%)
All	All	2364/3044 (77%)	-0.55	1 (0%)	100	100	43, 105, 202, 294	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	V	70	LEU	2.3

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	S	105	1/1	0.84	0.08	106,106,106,106	0
8	CA	S	104	1/1	0.86	0.09	119,119,119,119	0
8	CA	I	103	1/1	0.87	0.09	124,124,124,124	0
8	CA	I	102	1/1	0.89	0.05	120,120,120,120	0
8	CA	I	106	1/1	0.90	0.06	127,127,127,127	0
8	CA	I	104	1/1	0.91	0.14	130,130,130,130	0
8	CA	J	101	1/1	0.91	0.07	131,131,131,131	0
8	CA	T	101	1/1	0.91	0.13	108,108,108,108	0
8	CA	T	102	1/1	0.91	0.10	113,113,113,113	0
8	CA	I	105	1/1	0.92	0.04	125,125,125,125	0
8	CA	S	103	1/1	0.92	0.08	121,121,121,121	0
8	CA	T	103	1/1	0.92	0.05	113,113,113,113	0
8	CA	C	201	1/1	0.93	0.05	122,122,122,122	0
8	CA	J	102	1/1	0.93	0.12	128,128,128,128	0
8	CA	M	201	1/1	0.94	0.06	116,116,116,116	0
8	CA	S	102	1/1	0.94	0.08	76,76,76,76	0
8	CA	T	104	1/1	0.94	0.15	101,101,101,101	0
9	K	C	202	1/1	0.94	0.11	115,115,115,115	0
8	CA	S	106	1/1	0.95	0.07	102,102,102,102	0
8	CA	I	101	1/1	0.96	0.03	104,104,104,104	0
9	K	M	202	1/1	0.96	0.05	103,103,103,103	0
10	CL	M	203	1/1	0.96	0.07	74,74,74,74	0
8	CA	S	101	1/1	0.97	0.09	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	CL	Q	201	1/1	0.97	0.06	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.