

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6LAB
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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 <=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 cha	ain		
1	А	136	% 58%	14%		28%
1	Е	136	60%	12%		28%
1	K	136	57%	14%	•	28%
1	О	136	% 59%	12%	•	28%
2	В	103	70%		8%	22%
2	F	103	^{2%} 67%		14%	• 18%



Mol	Chain	Length		Quality of	of chain	
2	L	103		60%	20%	19%
2	Р	103	3%	67%	16%	• 17%
3	С	130		71%	8% •	19%
3	G	130	.% <mark>-</mark>	66%	12% •	21%
3	М	130		64%	17% •	18%
3	Q	130		70%	8% •	21%
4	D	126		62%	14%	24%
4	Н	126	<u>2</u> %	59%	17% •	24%
4	Ν	126		64%	11% •	24%
4	R	126	.% •	58%	16% ·	24%
5	Ι	169	5%	75%		25%
5	S	169	2%	80%		20%
6	J	169	6%	79%		20%
6	Т	169	.% <mark>-</mark>	80%		18%
7	U	194	30%	16%	60%	
7	V	194	9%	13% 5% •	57%	



2 Entry composition (i)

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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	08	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	90	807	508	156	139	4	0	0	0
1	F	08	Total	С	Ν	0	S	0	0	0
	E	98	807	508	156	139	4	0	0	0
1	K	08	Total	С	Ν	0	S	0	0	0
	Γ	90	807	508	156	139	4	0	0	0
1	0	08	Total	С	Ν	0	S	0	0	0
	1 O	98	807	508	156	139	4			U

• Molecule 1 is a protein called Histone H3.1.

• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	Р	80	Total	С	Ν	0	S	0	0	0
	D	80	638	401	125	111	1	0	0	0
0	Б	81	Total	С	Ν	0	S	0	0	0
	Г	04	673	424	133	115	1	0	0	0
0	т	\$3	Total	С	Ν	0	S	0	0	0
		00	662	418	129	114	1	0	0	0
0	D	86	Total	С	Ν	0	S	0	0	0
	1	80	694	436	140	117	1	0	0	0

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

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
2	С	105	Total	С	Ν	Ο	0	0	0
5	U	105	810	511	158	141	0	0	0
2	С	102	Total	С	Ν	Ο	0	0	0
5	G	103	796	502	155	139	0	0	0
2	М	106	Total	С	Ν	Ο	0	0	0
5	IVI	100	819	517	160	142	0	0	0
2	0	102	Total	С	Ν	Ο	0	0	0
3 Q	103	796	502	155	139	0	0	0	





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	л	06	Total	С	Ν	0	\mathbf{S}	0	0	0
4	D	90	755	474	138	141	2	0	0	0
4	Ц	06	Total	С	Ν	0	S	0	0	0
4	11	90	755	474	138	141	2	0	0	0
4	N	06	Total	С	Ν	0	S	0	0	0
4	IN	90	755	474	138	141	2	0	0	0
4	D	06	Total	С	Ν	0	S	0	0	0
4	n	90	755	474	138	141	2		0	U

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

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

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
5	Ι	169	Total 3462	C 1646	N 637	O 1011	Р 168	0	0	0
5	S	169	Total 3462	C 1646	N 637	O 1011	Р 168	0	0	0

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

Mol	Chain	Residues		А	toms			ZeroOcc	AltConf	Trace
6	J	169	Total 3461	C 1646	N 634	O 1013	Р 168	0	0	0
6	Т	169	Total 3461	C 1646	N 634	O 1013	Р 168	0	0	0

• Molecule 7 is a protein called Histone H1.0.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	II	78	Total	С	Ν	0	S	0	0	0
1	U	10	596	370	112	113	1	0	0	0
7	V	81	Total	С	Ν	0	S	0	0	0
	v	04	647	402	121	123	1			0

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	С	1	Total Ca 1 1	0	0
8	Ι	6	Total Ca 6 6	0	0



Continued from previous page...

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

• Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	С	1	Total K 1 1	0	0
9	М	1	Total K 1 1	0	0

• Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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





• Molecule 2: Histone H4

Chain B:	70%	8%	22%
MET SER GLY GLY GLY CLY CLY CLY CLY CLY CLY	LYS GLY GLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	K91 R92 G102	
• Molecule 2: Hi	istone H4		
Chain F:	67%	14% •	18%
MET SER GLY GLY ARG ARG CLY GLY GLY CLY CLY CLY CLY	LYS GLY GLY GLY GLY ALA HIS ALA ALA ALA CL2 ALA CL2 CL2 CL2 CL2 CL2 CL2 CL2 CL2 CL2 CL2	E53 F61 V65 D68 D68 T80 R92 R93 G93 G93	
• Molecule 2: Hi	istone H4		
Chain L:	60%	20%	19%
MET SER GLY GLY CLY CLY CLY CLY CLY CLY CLY	LYS GLY GLY GLY CLYS ALA ALA ALA CL22 ALS CL22 L22 L22 L37 L22 L37 L37 CL37 CL37 CL37 CL37 CL37 CL37 C	150 154 154 162 162 163 163 163 163 168 168 171	172 188 192 101 101 102
• Molecule 2: Hi	istone H4		
Chain P:	67%	16% •	17%
MET SER GLY GLY GLY ARG ARG CLY GLY GLY GLY GLY GLY	LYS GLY GLY ALA ALA ALA ALA ALA ALS ALS ALS ALS ALS	N64 V65 D68 V80 V80 V80 R92 R92 G102	
• Molecule 3: Hi	istone H2A type $1-B/E$		
Chain C:	71%	8% •	19%
MET SER GLY GLY CLN CLN CLN CLN CLN CLN ARC	ALA LYS AI4 N54 N54 N77 N77 N77 N77 N77 N79 N81 N81 N81 N81 N81 N81 N10 N110 N110	L116 P117 L17 L18 L18 L18 R18 R18 H18 L18 L18 L18 CL1 L18 L18	
• Molecule 3: Hi	istone H2A type $1-B/E$		
Chain G:	66%	12% •	21%
MET SER GLY ARG GLY GLN GLN GLN CLY ALA ARG	LALA LALA ALA ALA ALA LYS C28 R29 R29 R29 R28 R28 R28 R28 R28 R28 R28 R28 R28 R28	R81 E91 E91 1102 A102 Q104 Q104 V107 V114 L115 L115	K118 LYS THR GLU GLU HIS HIS LYS ALA ALA ALA CLY CLY
• Molecule 3: Hi	istone H2A type $1-B/E$		
Chain M:	64%	17% •	18%



MET SER SER SER SER ARG CLY CLY CLY CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	Q24 R22 R32 R32 R32 R32 P44 V49 V49 V49 V49 V50 V50 V53 R53 R53 R53 R53 R53 R53 R53 R53 R53 R	E64 I78 P80 R81 H82 H82 R88 R88	q104 L108 P109 L115 L115 LYS LYS GLU SER
HIS HIS LIYS LIYS CLYS LIYS			
• Molecule 3: Histone H2A	type $1-B/E$		
Chain Q:	70%	8% •	21%
MET SER GLY ARG CLY CLYS CLN CLYS ALA ALA ALA ALA LYS LYS TIG TIG TIG TIG	R29 H31 K74 K75 F80 P80 P80 P80 F81 R81 R81 R81 R81 R81 R81 R81 R81 R81 R	V107 K118 LYS THR GLU GLU SER HIS HIS LYS	LYS LYS ALA
• Molecule 4: Histone H2B	type 1-J		
Chain D:	62%	14%	24%
MET PRO GRU PRO PRO PRO PRO PRO CLYS SER LYS CLYS GLY SER LYS GLY VAL VAL	LYS ALA GLN CLYS LYS ASP ASP CLYS CLYS CLYS CLYS CLYS CK36 K34 K34 K34 K34 K34	T52 458 458 458 63 675 675 677 877	R70 R86 S87 S87 S87 S87 P103 C104 C104 C104 C106
K125			
• Molecule 4: Histone H2B	type 1-J		
Chain H:	59%	17% •	24%
MET PRO GLU PRO ALA PRO ALA ALA ALA ALA ALA ALA CVS CVS CVS CVS CVS CVS CVS CVS CVS CVS	LYS ALA GLN CYS CYS ASP ASP CYS CYS CYS CYS A31 AS2 A31 A22 A31 A22 A31 A23 A31 A23 A31 A24 A2 A2 A2 A2 A2 A2 A2 A2 A3 A3 A3 A3 A3 A3 A3 A3 A3 A3 A3 A3 A3	152 152 154 154 161 161 161	L80 L80 R86 1387 T88 194 C96 C98
L102 P103 V111 V111 V111 V111 V111 V125			
• Molecule 4: Histone H2B	type 1-J		
Chain N:	64%	11% •	24%
MET PRO GUU PRO ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	LYS ALA GLA CLYS CLYS LYS LYS CLYS CLYS CLYS CLYS C	S56 F65 169 L80 Y83	R86 887 188 196 102 102 103 6104 6105 6105
• Molecule 4: Histone H2B	type 1-J		
Chain R:	58%	16% •	24%
MET PRO GLU ALA ALA ALA ALA PRO PRO CLYS SER CLYS SER ALA ALA ALA THR	LYS GLY LYS LYS LYS LYS CLY CLYS CLYS CLYS CL	142 142 144 149 149 149 152	161 161 180 180 188 188 188 1102
20 			











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	104.80Å 102.76Å 218.05Å	Depositor
a, b, c, α , β , γ	90.00° 97.40° 90.00°	Depositor
Bosolution(Å)	39.89 - 3.20	Depositor
Resolution (A)	39.86 - 3.20	EDS
% Data completeness	99.2 (39.89-3.20)	Depositor
(in resolution range)	99.3 (39.86-3.20)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.57 (at 3.18 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D	0.201 , 0.262	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.206 , 0.262	DCC
R_{free} test set	1469 reflections (1.94%)	wwPDB-VP
Wilson B-factor $(Å^2)$	90.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 80.0	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, K, CA

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.63	0/819	0.79	0/1097	
1	Е	0.64	0/819	0.84	0/1097	
1	Κ	0.69	0/819	0.89	0/1097	
1	0	0.67	0/819	0.90	0/1097	
2	В	0.67	0/645	0.85	0/862	
2	F	0.69	0/680	0.84	0/908	
2	L	0.70	0/669	0.91	0/894	
2	Р	0.70	0/702	0.92	0/937	
3	С	0.67	0/820	0.79	0/1107	
3	G	0.67	0/806	0.80	0/1089	
3	М	0.70	0/829	0.87	0/1118	
3	Q	0.69	0/806	0.87	0/1089	
4	D	0.65	0/766	0.76	0/1026	
4	Н	0.70	0/766	0.83	0/1026	
4	Ν	0.69	0/766	0.86	0/1026	
4	R	0.68	0/766	0.90	0/1026	
5	Ι	0.36	0/3884	0.77	0/5993	
5	S	0.48	0/3884	0.83	1/5993~(0.0%)	
6	J	0.36	0/3882	0.79	1/5990~(0.0%)	
6	Т	0.51	$2/\overline{3882}~(0.1\%)$	0.85	4/5990~(0.1%)	
7	U	0.77	0/602	0.85	0/802	
7	V	0.70	0/654	0.93	0/870	
All	All	0.56	2/29085~(0.0%)	0.83	$6/4\overline{2134}\ (0.0\%)$	

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
7	V	0	2



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Т	-34	DG	O3'-P	-5.70	1.54	1.61
6	Т	-62	DC	O3'-P	-5.13	1.54	1.61

All (2) bond length outliers are listed below:

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	Т	-53	DG	C1'-O4'-C4'	-6.24	103.86	110.10
6	J	-53	DG	C1'-O4'-C4'	-5.75	104.35	110.10
6	Т	56	DG	O5'-P-OP2	-5.72	100.55	105.70
6	Т	15	DT	O5'-P-OP2	-5.59	100.67	105.70
6	Т	29	DG	C1'-O4'-C4'	-5.46	104.64	110.10
5	S	81	DG	C1'-O4'-C4'	-5.28	104.82	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
7	V	56	SER	Peptide
7	V	57	HIS	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	А	807	0	844	10	1
1	Е	807	0	844	12	0
1	K	807	0	844	12	0
1	0	807	0	844	14	0
2	В	638	0	676	4	0
2	F	673	0	722	15	1
2	L	662	0	709	11	0
2	Р	694	0	742	15	0
3	С	810	0	866	8	0
3	G	796	0	848	11	0
3	М	819	0	879	15	0
3	Q	796	0	848	5	0



6LA	В
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	755	0	784	6	0
4	Н	755	0	784	13	0
4	Ν	755	0	784	10	0
4	R	755	0	784	17	0
5	Ι	3462	0	1901	30	0
5	S	3462	0	1901	23	0
6	J	3461	0	1902	21	0
6	Т	3461	0	1902	19	0
7	U	596	0	627	37	0
7	V	647	0	683	27	0
8	С	1	0	0	0	0
8	Ι	6	0	0	0	0
8	J	2	0	0	0	0
8	М	1	0	0	0	0
8	S	6	0	0	0	0
8	Т	4	0	0	0	0
9	С	1	0	0	0	0
9	М	1	0	0	0	0
10	М	1	0	0	0	0
10	Q	1	0	0	0	0
All	All	27249	0	21718	273	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 (273) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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



	,	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
1:0:83:ARG:0	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
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
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
1:0:73: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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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
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
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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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
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
1:K:48:LEU:HD23	1:K:51:ILE:HD12	1.93	0.49
4:R:70:PHE:CD1	4:R:70:PHE:C	2.86	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
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
2:L:101:GLY:O	2:L:102:GLY:C	2.51	0.47
5:S:23:DG:C4	5:S:24:DC:C5	3.03	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
1:0:131: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
3:C:77:ARG:CZ	5:I:-54:DA:H4'	2.46	0.46
7:U:54:ILE:HD12	7:U:54:ILE:C	2.36	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
3:C:90:ASP:C	3:C:90:ASP:OD1	2.55	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: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
4:D:77:ALA:O	4:D:78:SER:C	2.55	0.44
5:I:-25:DA:H1'	5:I:-24:DG:C8	2.53	0.44



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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
5:I:57:DG:H2"	5:I:58:DC:C6	2.52	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
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
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
5:I:-82:DG:H2"	5:I:-81:DC:OP2	2.19	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
2:L:62:LEU:O	2:L:63:GLU:C	2.57	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
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



	lous pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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
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
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
1:O:90:MET:HA	1:O:90:MET:CE	2.50	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
1:K:46:VAL:O	1:K:47:ALA:C	2.58	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
4:R:103:PRO:O	4:R:104:GLY:C	2.58	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
4:R:119:THR:O	4:R:122:THR:OG1	2.36	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: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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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
1:A:75:ALA:O	1:A:76:GLN:C	2.60	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 (i)

5.3.1 Protein backbone (i)

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	Perce	entiles
1	А	96/136~(71%)	90 (94%)	6 (6%)	0	100	100
1	Ε	96/136~(71%)	90 (94%)	3(3%)	3~(3%)	4	26
1	Κ	96/136~(71%)	86 (90%)	10 (10%)	0	100	100
1	Ο	96/136~(71%)	91~(95%)	5 (5%)	0	100	100
2	В	78/103~(76%)	69 (88%)	9 (12%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	F	82/103~(80%)	73~(89%)	9 (11%)	0	100	100
2	L	81/103~(79%)	67 (83%)	14 (17%)	0	100	100
2	Р	84/103 (82%)	79 (94%)	4(5%)	1 (1%)	13	49
3	С	103/130~(79%)	96~(93%)	7 (7%)	0	100	100
3	G	101/130~(78%)	92 (91%)	6 (6%)	3(3%)	4	28
3	М	104/130~(80%)	93~(89%)	9~(9%)	2(2%)	8	39
3	Q	101/130~(78%)	94 (93%)	7 (7%)	0	100	100
4	D	94/126~(75%)	86 (92%)	6~(6%)	2(2%)	7	37
4	Н	94/126~(75%)	88 (94%)	4 (4%)	2(2%)	7	37
4	Ν	94/126~(75%)	88 (94%)	5 (5%)	1 (1%)	14	51
4	R	94/126~(75%)	87 (93%)	4 (4%)	3(3%)	4	26
7	U	76/194~(39%)	67~(88%)	4(5%)	5(7%)	1	9
7	V	82/194~(42%)	65 (79%)	13 (16%)	4 (5%)	2	17
All	All	1652/2368~(70%)	1501 (91%)	125 (8%)	26 (2%)	9	43

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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	Ν	104	GLY
4	R	33	ARG
7	U	41	ASN
7	V	45	SER
7	V	87	VAL
3	М	14	ALA
4	D	103	PRO
2	Р	19	ARG
4	R	32	SER
1	Е	39	HIS
3	G	117	PRO
3	М	109	PRO
7	U	58	TYR
7	U	92	SER



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Mol	Chain	Res	Type
4	Н	31	ARG
4	Н	103	PRO
7	U	42	ARG
7	V	26	PRO
1	Е	51	ILE
4	R	104	GLY
1	Е	43	PRO

5.3.2 Protein sidechains (i)

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	85/111 (77%)	82 (96%)	3 (4%)	36	69
1	Е	85/111 (77%)	81 (95%)	4 (5%)	26	62
1	Κ	85/111 (77%)	80 (94%)	5 (6%)	19	54
1	Ο	85/111 (77%)	82 (96%)	3(4%)	36	69
2	В	65/79~(82%)	62 (95%)	3(5%)	27	63
2	F	69/79~(87%)	68 (99%)	1 (1%)	67	86
2	L	68/79~(86%)	65 (96%)	3 (4%)	28	64
2	Р	71/79~(90%)	69 (97%)	2 (3%)	43	74
3	С	83/100 (83%)	79 (95%)	4 (5%)	25	61
3	G	82/100~(82%)	77 (94%)	5 (6%)	18	54
3	М	84/100 (84%)	80 (95%)	4 (5%)	25	61
3	Q	82/100~(82%)	75 (92%)	7 (8%)	10	38
4	D	82/105~(78%)	75 (92%)	7 (8%)	10	38
4	Н	82/105~(78%)	74 (90%)	8 (10%)	8	31
4	Ν	82/105~(78%)	77 (94%)	5 (6%)	18	54
4	R	82/105~(78%)	74 (90%)	8 (10%)	8	31
7	U	65/158~(41%)	50 (77%)	15 (23%)	1	3
7	V	71/158~(45%)	55 (78%)	16 (22%)	1	4



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1408/1896~(74%)	1305 (93%)	103 (7%)	14 46

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	40	ARG
1	А	45	THR
1	А	49	ARG
2	В	23	ARG
2	В	35	ARG
2	В	91	LYS
3	С	81	ARG
3	С	90	ASP
3	С	110	ASN
3	С	118	LYS
4	D	34	LYS
4	D	46	LYS
4	D	63	ASN
4	D	86	ARG
4	D	87	SER
4	D	106	LEU
4	D	125	LYS
1	Е	40	ARG
1	Е	56	LYS
1	Е	129	ARG
1	Е	134	ARG
2	F	22	LEU
3	G	29	ARG
3	G	73	ASN
3	G	74	LYS
3	G	80	PRO
3	G	81	ARG
4	Н	30	LYS
4	Н	31	ARG
4	Н	42	TYR
4	Н	64	SER
4	Н	80	LEU
4	Н	86	ARG
4	Н	119	THR
4	Н	125	LYS
1	K	58	THR
1	K	63	ARG



Mol	Chain	Res	Type
1	K	118	THR
1	K	129	ARG
1	K	134	ARG
2	L	22	LEU
2	L	59	LYS
2	L	95	ARG
3	М	24	GLN
3	М	77	ARG
3	М	80	PRO
3	М	81	ARG
4	Ν	32	SER
4	Ν	36	SER
4	N	56	SER
4	N	86	ARG
4	Ν	105	GLU
1	0	48	LEU
1	0	129	ARG
1	0	134	ARG
2	Р	20	LYS
2	Р	27	GLN
3	Q	19	SER
3	Q	29	ARG
3	Q	73	ASN
3	Q	75	LYS
3	Q	80	PRO
3	Q	81	ARG
3	Q	118	LYS
4	R	31	ARG
4	R	36	SER
4	R	42	TYR
4	R	52	THR
4	R	57	LYS
4	R	80	LEU
4	R	88	THR
4	R	125	LYS
7	U	21	LYS
7	U	32	ILE
7	U	37	GLN
7	U	47	ARG
7	U	48	GLN
7	U	51	GLN
7	U	53	TYR



	3	1	1 0
\mathbf{Mol}	Chain	Res	Type
7	U	57	HIS
7	U	62	GLU
7	U	66	SER
7	U	67	GLN
7	U	83	GLN
7	U	87	VAL
7	U	93	PHE
7	U	94	ARG
7	V	20	LYS
7	V	25	HIS
7	V	27	LYS
7	V	32	ILE
7	V	37	GLN
7	V	47	ARG
7	V	52	LYS
7	V	56	SER
7	V	67	GLN
7	V	71	SER
7	V	80	VAL
7	V	83	GLN
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	76	GLN
3	С	24	GLN
3	С	31	HIS
3	С	110	ASN
3	С	112	GLN
4	D	47	GLN
4	D	84	ASN
4	D	95	GLN
1	Е	76	GLN
3	G	73	ASN
4	Н	47	GLN
4	Н	95	GLN
1	Κ	68	GLN
3	М	24	GLN



Mol	Chain	Res	Type
3	М	31	HIS
4	N	95	GLN
1	0	108	ASN
2	Р	27	GLN
2	Р	64	ASN
4	R	47	GLN
4	R	95	GLN
7	U	67	GLN
7	U	83	GLN
7	V	25	HIS
7	V	37	GLN
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 monosaccharides 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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	98/136~(72%)	0.07	2 (2%) 65 51	92,113,159,183	0
1	Е	98/136~(72%)	-0.05	0 100 100	80, 102, 140, 164	0
1	Κ	98/136~(72%)	-0.19	0 100 100	44, 66, 108, 139	0
1	Ο	98/136~(72%)	-0.10	1 (1%) 82 72	46, 67, 111, 144	0
2	В	80/103~(77%)	-0.06	0 100 100	84, 109, 141, 160	0
2	F	84/103~(81%)	0.02	2 (2%) 59 44	80, 95, 141, 171	0
2	L	83/103~(80%)	-0.07	0 100 100	43, 65, 129, 163	0
2	Р	86/103~(83%)	0.11	3 (3%) 44 28	45,66,142,180	0
3	С	105/130~(80%)	-0.12	0 100 100	80, 101, 133, 146	0
3	G	103/130~(79%)	0.10	1 (0%) 82 72	79, 111, 146, 162	0
3	М	106/130 (81%)	-0.17	0 100 100	53, 72, 107, 137	0
3	Q	103/130~(79%)	-0.14	0 100 100	48, 71, 103, 113	0
4	D	96/126~(76%)	-0.01	0 100 100	77, 105, 149, 169	0
4	Н	96/126~(76%)	-0.05	2 (2%) 63 49	82, 110, 156, 177	0
4	Ν	96/126~(76%)	-0.13	0 100 100	48, 75, 119, 153	0
4	R	96/126~(76%)	-0.10	1 (1%) 82 72	50, 73, 121, 172	0
5	Ι	169/169~(100%)	0.05	8 (4%) 31 19	106, 167, 249, 280	0
5	S	169/169~(100%)	-0.37	3 (1%) 68 55	71, 114, 226, 264	0
6	J	169/169~(100%)	0.09	10 (5%) 22 13	117, 168, 235, 294	0
6	Т	169/169~(100%)	-0.33	2 (1%) 79 67	74, 113, 211, 278	0
7	U	78/194~(40%)	4.07	59~(75%) 0 0	150, 196, 246, 259	1 (1%)
7	V	$\overline{84/194~(43\%)}$	0.90	17 (20%) 1 1	109, 164, 197, 213	1 (1%)
All	All	2364/3044~(77%)	0.09	111 (4%) 31 19	43, 105, 202, 294	2(0%)

All (111) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
7	U	90	SER	14.4
7	U	94	ARG	11.7
7	U	25	HIS	9.6
7	U	41	ASN	8.6
7	U	31	MET	8.5
7	V	43	ALA	8.4
7	U	36	ILE	8.3
7	U	92	SER	8.2
7	U	44	GLY	8.1
7	U	48	GLN	7.1
7	U	93	PHE	7.1
7	U	66	SER	7.0
7	U	38	ALA	7.0
7	U	43	ALA	6.9
7	U	26	PRO	6.6
7	U	91	GLY	6.5
7	U	32	ILE	6.5
7	U	39	GLU	6.1
7	U	89	ALA	6.1
7	U	37	GLN	5.9
7	U	84	THR	5.8
7	U	67	GLN	5.7
7	U	54	ILE	5.6
7	U	21	LYS	5.2
7	U	40	LYS	5.1
7	V	93	PHE	4.8
7	U	82	LYS	4.7
7	U	81	LEU	4.6
7	U	69	LYS	4.5
7	U	49	SER	4.5
4	R	125	LYS	4.5
1	А	38	PRO	4.5
7	U	35	ALA	4.4
7	U	45	SER	4.3
7	U	72	ILE	4.3
7	U	22	SER	4.3
7	U	47	ARG	4.2
7	U	95	LEU	4.1
6	J	-75	DT	4.1
7	U	33	VAL	4.1
7	V	89	ALA	4.0
7	U	74	ARG	4.0
7	V	40	LYS	3.9
		1		



Mol	Chain	Res	Type	RSRZ
2	Р	19	ARG	3.8
7	U	85	LYS	3.7
7	U	30	ASP	3.7
6	J	-70	DC	3.7
7	V	99	ASP	3.7
7	U	76	VAL	3.6
7	U	57	HIS	3.6
7	V	39	GLU	3.5
7	V	101	PRO	3.5
7	U	88	GLY	3.5
7	U	75	LEU	3.5
5	Ι	79	DA	3.4
5	Ι	42	DA	3.3
7	U	34	ALA	3.3
7	U	53	TYR	3.2
7	U	83	GLN	3.2
5	S	84	DG	3.1
7	V	103	LYS	3.0
7	V	42	ARG	3.0
1	А	40	ARG	2.9
7	V	23	THR	2.9
5	Ι	78	DA	2.9
7	U	42	ARG	2.9
7	U	55	LYS	2.8
6	Т	80	DA	2.8
7	U	24	ASP	2.7
2	Р	18	HIS	2.7
7	U	87	VAL	2.7
7	V	85	LYS	2.7
7	U	56	SER	2.6
6	J	82	DC	2.6
5	S	83	DT	2.6
7	U	79	GLY	2.5
7	U	28	TYR	2.5
7	U	98	SER	2.5
2	F	19	ARG	2.5
7	U	68	ILE	2.5
6	Т	81	DG	2.5
7	V	100	GLU	2.5
6	J	-77	DT	2.5
7	V	74	ARG	2.5
7	V	102	LYS	2.5



Mol	Chain	\mathbf{Res}	Type	RSRZ
2	Р	20	LYS	2.4
5	S	81	DG	2.4
6	J	-76	DT	2.4
3	G	74	LYS	2.4
7	V	21	LYS	2.4
5	Ι	83	DT	2.4
7	U	97	LYS	2.4
4	Н	54	ILE	2.4
7	V	65	ASP	2.3
6	J	-38	DC	2.3
5	Ι	86	DA	2.3
2	F	21	VAL	2.3
6	J	83	DT	2.3
6	J	-74	DT	2.2
7	U	86	GLY	2.2
7	U	27	LYS	2.2
7	U	46	SER	2.2
5	Ι	67	DT	2.2
7	V	22	SER	2.1
1	0	38	PRO	2.1
5	Ι	82	DC	2.1
5	Ι	-68	DC	2.1
6	J	73	DA	2.0
6	J	-39	DT	2.0
7	U	50	ILE	2.0
4	Н	51	ASP	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 monosaccharides 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, 95^{th} 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	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(A^2)$	Q < 0.9
8	CA	Ι	103	1/1	0.41	0.18	124,124,124,124	0
8	CA	S	104	1/1	0.56	0.18	119,119,119,119	0
8	CA	Ι	104	1/1	0.63	0.12	130,130,130,130	0
8	CA	J	102	1/1	0.72	0.15	128,128,128,128	0
8	CA	J	101	1/1	0.72	0.33	131,131,131,131	0
8	CA	С	201	1/1	0.76	0.10	122,122,122,122	0
8	CA	Т	101	1/1	0.76	0.27	108,108,108,108	0
8	CA	Ι	102	1/1	0.80	0.15	120,120,120,120	0
8	CA	S	102	1/1	0.80	0.22	76,76,76,76	0
8	CA	S	105	1/1	0.84	0.19	106,106,106,106	0
8	CA	S	103	1/1	0.84	0.18	121,121,121,121	0
8	CA	Ι	105	1/1	0.86	0.13	$125,\!125,\!125,\!125$	0
8	CA	S	101	1/1	0.88	0.23	86,86,86,86	0
8	CA	Т	103	1/1	0.89	0.11	113,113,113,113	0
10	CL	М	203	1/1	0.89	0.19	74,74,74,74	0
8	CA	Ι	106	1/1	0.90	0.13	127,127,127,127	0
8	CA	М	201	1/1	0.90	0.19	116,116,116,116	0
8	CA	Т	102	1/1	0.92	0.29	113,113,113,113	0
8	CA	Ι	101	1/1	0.93	0.10	104,104,104,104	0
8	CA	Т	104	1/1	0.95	0.22	101,101,101,101	0
9	K	С	202	1/1	0.97	0.55	115,115,115,115	0
8	CA	S	106	1/1	0.97	0.25	102,102,102,102	0
10	CL	Q	201	1/1	0.97	0.11	69,69,69,69	0
9	K	Μ	202	1/1	0.98	0.40	$103,\!103,\!103,\!\overline{103}$	0

6.5 Other polymers (i)

There are no such residues in this entry.

