



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 PM GMT

PDB ID : 4KUD  
Title : Crystal structure of N-terminal acetylated Sir3 BAH domain D205N mutant in complex with yeast nucleosome core particle  
Authors : Yang, D.; Fang, Q.; Wang, M.; Ren, R.; Wang, H.; He, M.; Sun, Y.; Yang, N.; Xu, R.M.  
Deposited on : 2013-05-22  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

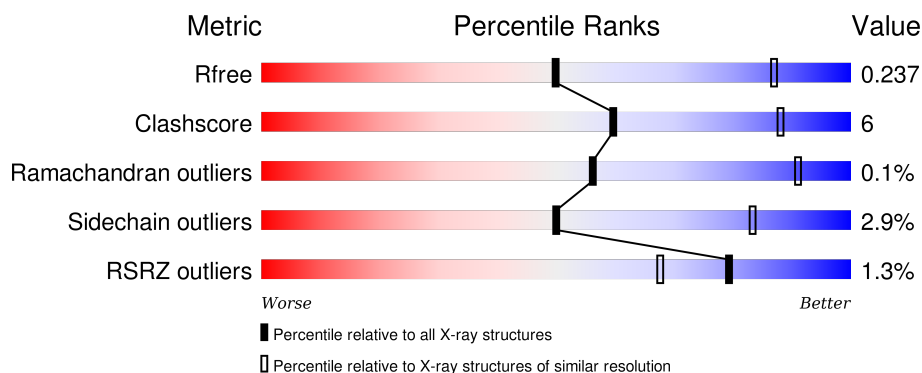
# 1 Overall quality at a glance

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.



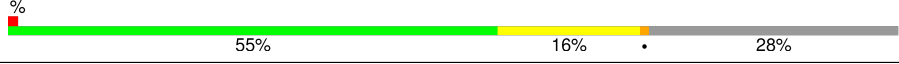
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>61%</div> <div>10%</div> <div>29%</div> </div>
1	E	136	<div> <div>62%</div> <div>10%</div> <div>28%</div> </div>
2	B	103	<div> <div>73%</div> <div>13%</div> <div>15%</div> </div>
2	F	103	<div> <div>67%</div> <div>20%</div> <div>13%</div> </div>
3	C	132	<div> <div>62%</div> <div>14%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	132	
4	D	131	
4	H	131	
5	I	146	
5	J	146	
6	K	224	
6	L	224	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15732 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	0	0	0
			790	502	151	137			
1	E	98	Total	C	N	O	0	0	0
			808	514	155	139			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	0	0	0
			709	446	142	121			
2	F	90	Total	C	N	O	0	0	0
			717	450	144	123			

- Molecule 3 is a protein called Histone H2A.2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	0	0	0
			795	499	156	140			
3	G	105	Total	C	N	O	0	0	0
			810	508	159	143			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ALA	SER	ENGINEERED MUTATION	UNP P04912
G	1	ALA	SER	ENGINEERED MUTATION	UNP P04912

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	93	Total	C	N	O	S	0	0	0
			724	455	125	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	94	Total	C	N	O	S	0	0	0
			735	461	129	144	1			

- Molecule 5 is a DNA chain called nucleosome DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			
5	J	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			

- Molecule 6 is a protein called Regulatory protein SIR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	213	Total	C	N	O	S	0	0	0
			1799	1158	303	336	2			
6	L	213	Total	C	N	O	S	0	0	0
			1799	1158	303	336	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	205	ASN	ASP	ENGINEERED MUTATION	UNP P06701
K	220	HIS	-	EXPRESSION TAG	UNP P06701
K	221	HIS	-	EXPRESSION TAG	UNP P06701
K	222	HIS	-	EXPRESSION TAG	UNP P06701
K	223	HIS	-	EXPRESSION TAG	UNP P06701
K	224	HIS	-	EXPRESSION TAG	UNP P06701
K	225	HIS	-	EXPRESSION TAG	UNP P06701
L	205	ASN	ASP	ENGINEERED MUTATION	UNP P06701
L	220	HIS	-	EXPRESSION TAG	UNP P06701
L	221	HIS	-	EXPRESSION TAG	UNP P06701
L	222	HIS	-	EXPRESSION TAG	UNP P06701
L	223	HIS	-	EXPRESSION TAG	UNP P06701
L	224	HIS	-	EXPRESSION TAG	UNP P06701
L	225	HIS	-	EXPRESSION TAG	UNP P06701

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	6	Total O 6 6	0	0

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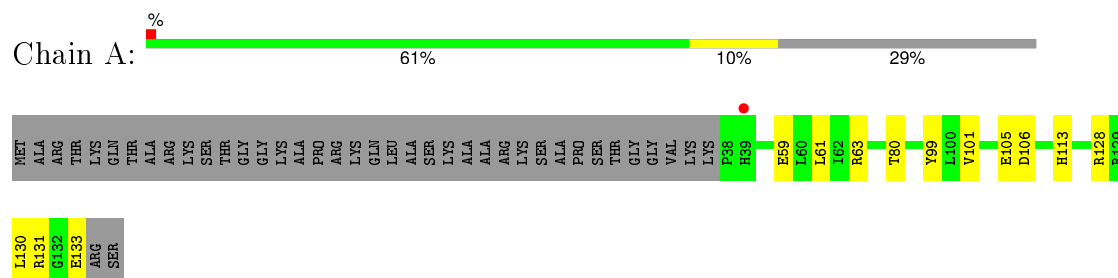
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	6	Total 6	O 6	0	0
7	C	4	Total 4	O 4	0	0
7	D	7	Total 7	O 7	0	0
7	E	4	Total 4	O 4	0	0
7	F	8	Total 8	O 8	0	0
7	G	2	Total 2	O 2	0	0
7	H	7	Total 7	O 7	0	0
7	K	14	Total 14	O 14	0	0
7	L	8	Total 8	O 8	0	0

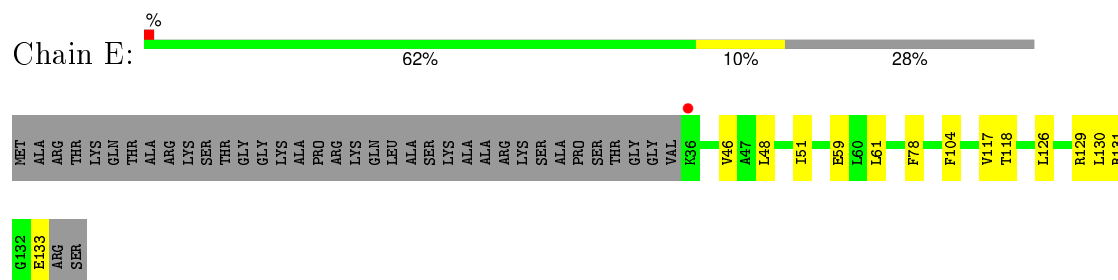
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

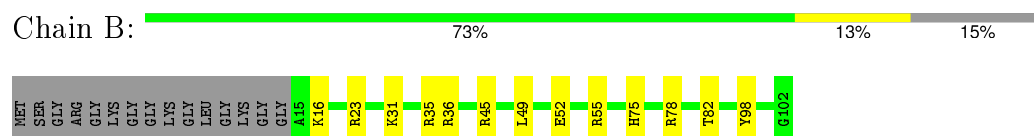
- Molecule 1: Histone H3



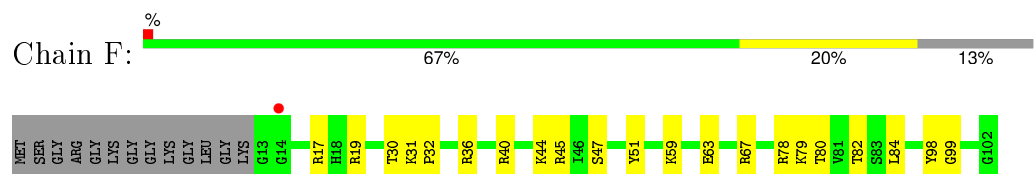
- Molecule 1: Histone H3



- Molecule 2: Histone H4



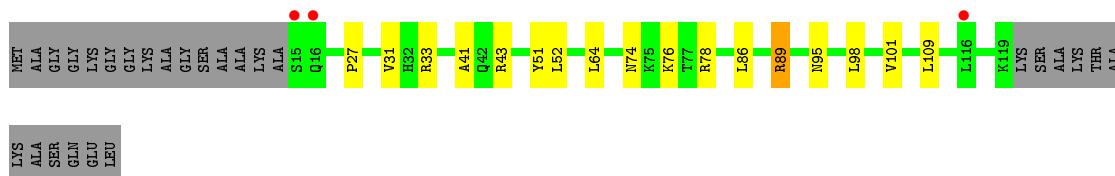
- Molecule 2: Histone H4



- Molecule 3: Histone H2A.2



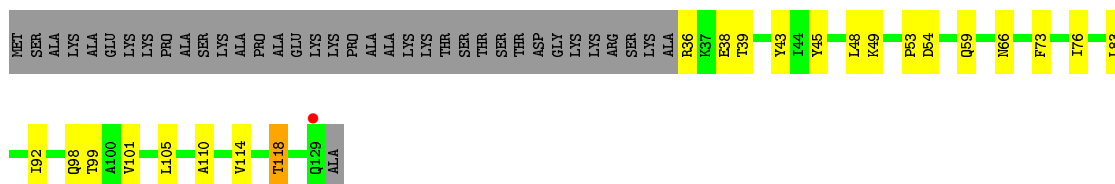
- Molecule 3: Histone H2A.2



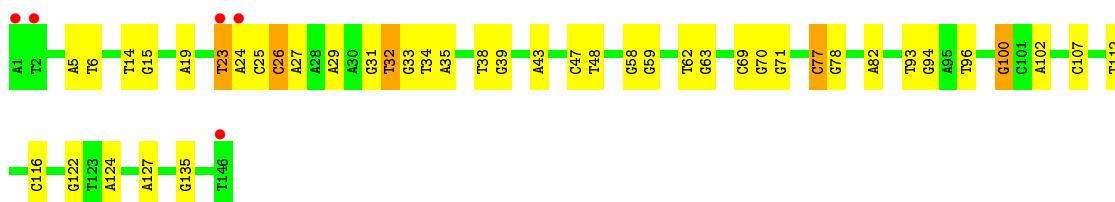
- Molecule 4: Histone H2B.1



- Molecule 4: Histone H2B.1



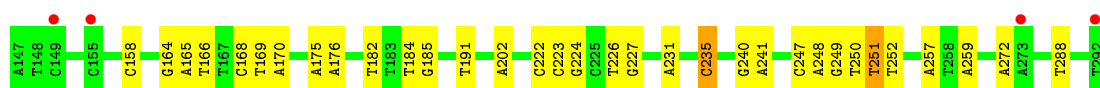
- Molecule 5: nucleosome DNA



- Molecule 5: nucleosome DNA

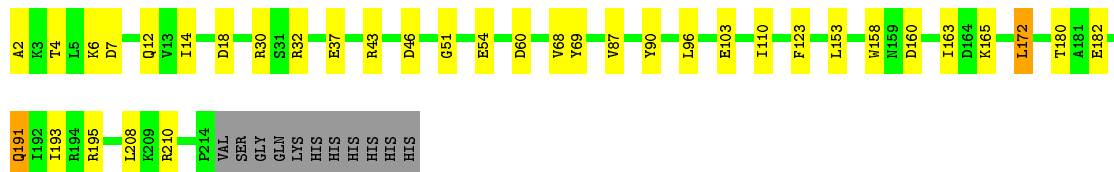






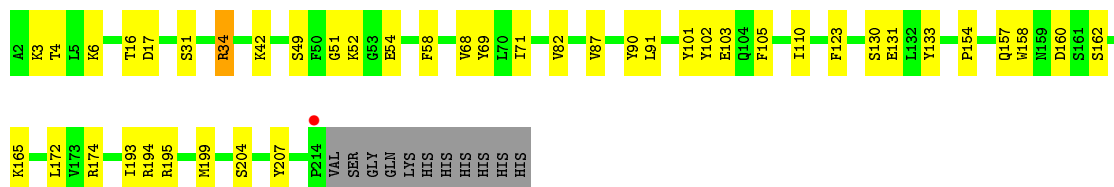
- Molecule 6: Regulatory protein SIR3

Chain K: 79% 15% 5%



- Molecule 6: Regulatory protein SIR3

Chain L: 76% 19% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.33Å 108.33Å 498.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.39 – 3.20 49.68 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.39-3.20) 99.5 (49.68-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.198 , 0.237 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	2758 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.1	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.4	EDS
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53854 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: AYA

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	0.34	0/801	0.48	0/1072
1	E	0.36	0/819	0.49	0/1095
2	B	0.38	0/717	0.52	0/956
2	F	0.35	0/725	0.49	0/966
3	C	0.32	0/806	0.50	0/1091
3	G	0.34	0/821	0.50	0/1110
4	D	0.35	0/734	0.50	0/989
4	H	0.37	0/745	0.51	0/1003
5	I	0.51	0/3354	1.20	17/5175 (0.3%)
5	J	0.53	0/3354	1.23	18/5175 (0.3%)
6	K	0.35	0/1832	0.52	0/2475
6	L	0.35	0/1832	0.53	0/2475
All	All	0.42	0/16540	0.89	35/23582 (0.1%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	170	DA	O4'-C1'-N9	9.90	114.93	108.00
5	I	23	DT	O4'-C1'-N1	8.32	113.82	108.00
5	I	116	DC	O4'-C1'-N1	7.74	113.42	108.00
5	I	23	DT	O4'-C4'-C3'	-7.58	101.45	106.00
5	J	170	DA	C1'-O4'-C4'	-7.51	102.59	110.10
5	J	202	DA	O4'-C1'-N9	6.92	112.84	108.00
5	J	231	DA	O4'-C1'-N9	6.81	112.77	108.00
5	I	29	DA	C3'-C2'-C1'	-6.51	94.69	102.50
5	J	251	DT	O4'-C4'-C3'	-6.24	102.00	104.50
5	J	288	DT	O4'-C1'-C2'	-6.23	100.92	105.90
5	I	26	DC	O4'-C1'-N1	5.90	112.13	108.00
5	J	166	DT	O4'-C1'-N1	5.90	112.13	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	226	DT	C3'-C2'-C1'	-5.86	95.47	102.50
5	J	272	DA	O4'-C1'-N9	5.81	112.07	108.00
5	J	241	DA	O4'-C1'-N9	5.81	112.07	108.00
5	I	77	DC	O4'-C1'-C2'	-5.58	101.44	105.90
5	J	226	DT	O4'-C1'-C2'	-5.51	101.49	105.90
5	I	23	DT	C1'-O4'-C4'	-5.38	104.72	110.10
5	I	26	DC	C1'-O4'-C4'	-5.35	104.75	110.10
5	I	96	DT	O4'-C1'-C2'	-5.35	101.62	105.90
5	J	235	DC	O4'-C1'-N1	5.34	111.74	108.00
5	I	102	DA	O4'-C1'-N9	5.34	111.74	108.00
5	J	191	DT	O4'-C1'-N1	5.28	111.69	108.00
5	I	27	DA	C3'-C2'-C1'	-5.23	96.23	102.50
5	I	96	DT	C3'-C2'-C1'	-5.18	96.28	102.50
5	I	77	DC	C3'-C2'-C1'	-5.12	96.36	102.50
5	J	250	DT	N3-C4-O4	5.10	122.96	119.90
5	I	96	DT	C1'-O4'-C4'	-5.09	105.01	110.10
5	J	240	DG	O4'-C1'-N9	5.09	111.56	108.00
5	I	32	DT	N3-C4-O4	5.08	122.95	119.90
5	J	202	DA	C1'-O4'-C4'	-5.05	105.05	110.10
5	I	127	DA	O4'-C1'-N9	5.04	111.53	108.00
5	J	182	DT	N3-C4-O4	5.03	122.92	119.90
5	I	100	DG	O4'-C1'-N9	5.01	111.51	108.00
5	J	170	DA	O4'-C1'-C2'	-5.01	101.89	105.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	790	0	838	8	0
1	E	808	0	863	11	0
2	B	709	0	763	9	0
2	F	717	0	769	17	0
3	C	795	0	834	17	0
3	G	810	0	852	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	724	0	743	13	0
4	H	735	0	756	18	0
5	I	2990	0	1651	27	0
5	J	2990	0	1651	21	0
6	K	1799	0	1781	20	0
6	L	1799	0	1781	27	0
7	A	6	0	0	0	0
7	B	6	0	0	0	0
7	C	4	0	0	0	0
7	D	7	0	0	0	0
7	E	4	0	0	0	0
7	F	8	0	0	0	0
7	G	2	0	0	0	0
7	H	7	0	0	0	0
7	K	14	0	0	0	0
7	L	8	0	0	0	0
All	All	15732	0	13282	157	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 6.

All (157) 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)
3:G:33:ARG:NH1	5:J:176:DA:OP1	2.17	0.77
3:C:46:SER:OG	5:J:257:DA:OP2	2.04	0.75
6:L:172:LEU:HD21	6:L:174:ARG:HD3	1.71	0.72
1:A:130:LEU:HD12	1:E:130:LEU:HD12	1.71	0.71
6:K:4:THR:HG22	6:K:6:LYS:H	1.56	0.70
1:A:131:ARG:NH1	1:A:133:GLU:OE2	2.26	0.69
1:A:61:LEU:HD13	2:B:36:ARG:HB3	1.74	0.69
4:D:51:THR:O	4:D:52:HIS:ND1	2.27	0.68
6:K:103:GLU:HA	6:K:110:ILE:HG13	1.80	0.64
1:E:131:ARG:NH1	1:E:133:GLU:OE2	2.30	0.63
4:H:36:ARG:HD2	5:I:122:DG:H4'	1.80	0.63
2:F:30:THR:HB	2:F:32:PRO:HD2	1.80	0.63
5:I:59:DG:N2	5:J:235:DC:O2	2.32	0.62
4:D:101:VAL:HG13	4:D:105:LEU:HD12	1.80	0.62
3:G:33:ARG:NH2	4:H:38:GLU:OE2	2.26	0.61
4:H:101:VAL:HG13	4:H:105:LEU:HD12	1.83	0.60
4:H:36:ARG:HH22	5:J:175:DA:H5'	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:HG23	2:F:45:ARG:HB3	1.84	0.59
3:G:89:ARG:NH2	3:G:98:LEU:O	2.33	0.59
6:L:91:LEU:HB2	6:L:133:TYR:HB2	1.85	0.59
6:L:51:GLY:H	6:L:54:GLU:HG3	1.68	0.58
5:I:25:DC:H1'	5:I:26:DC:H5'	1.84	0.58
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.37	0.57
6:L:154:PRO:HG2	6:L:157:GLN:HG3	1.86	0.57
6:K:51:GLY:H	6:K:54:GLU:HG3	1.69	0.56
6:L:71:ILE:HA	6:L:87:VAL:HG12	1.88	0.56
6:L:195:ARG:O	6:L:199:MET:HG2	2.06	0.56
3:G:78:ARG:HH11	5:J:165:DA:H5'	1.70	0.55
3:C:78:ARG:HE	5:I:19:DA:H5'	1.71	0.55
1:E:48:LEU:HD23	1:E:51:ILE:HD12	1.89	0.54
3:G:74:ASN:HB3	3:G:76:LYS:HD3	1.88	0.54
2:B:16:LYS:HE3	6:K:60:ASP:OD2	2.08	0.54
2:F:78:ARG:NH1	2:F:82:THR:HG23	2.22	0.54
2:B:98:TYR:CE2	3:G:101:VAL:HG11	2.43	0.54
6:K:69:TYR:HB3	6:K:87:VAL:HB	1.89	0.53
1:E:78:PHE:CE1	2:F:67:ARG:HD2	2.43	0.53
5:J:164:DG:H2''	5:J:165:DA:C8	2.44	0.53
6:L:68:VAL:O	6:L:90:TYR:HB2	2.08	0.53
6:L:158:TRP:CE3	6:L:165:LYS:HD2	2.43	0.53
5:I:93:DT:H2''	5:I:94:DG:H5''	1.90	0.53
5:I:33:DG:O6	5:J:259:DA:N6	2.43	0.52
6:L:16:THR:HG22	6:L:17:ASP:O	2.08	0.52
6:L:199:MET:HG3	6:L:204:SER:HB3	1.91	0.51
3:C:81:PRO:HG2	4:D:60:LYS:HD2	1.93	0.51
3:G:43:ARG:HE	5:J:185:DG:H5'	1.76	0.51
5:J:247:DC:H2''	5:J:248:DA:H5''	1.92	0.51
5:J:227:DG:H5''	5:J:227:DG:C8	2.45	0.51
5:I:71:DG:N2	5:J:222:DC:O2	2.44	0.50
4:H:39:THR:HB	4:H:66:ASN:OD1	2.11	0.50
5:I:14:DT:H2''	5:I:15:DG:C8	2.46	0.50
2:B:75:HIS:HB2	4:D:99:THR:HG21	1.93	0.49
6:L:58:PHE:HB2	6:L:69:TYR:HE2	1.75	0.49
5:I:135:DG:H1	5:J:158:DC:H42	1.59	0.49
2:F:79:LYS:NZ	5:I:100:DG:OP2	2.39	0.49
5:I:48:DT:H5''	5:I:48:DT:H6	1.77	0.49
5:I:31:DG:H2'	5:I:32:DT:H71	1.94	0.49
3:G:43:ARG:HE	5:J:185:DG:C5'	2.25	0.49
6:K:163:ILE:O	6:K:165:LYS:HE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:LEU:HD13	2:F:36:ARG:HB3	1.94	0.48
3:C:105:GLN:HG3	4:D:60:LYS:NZ	2.28	0.48
5:I:5:DA:H2"	5:I:6:DT:H5"	1.95	0.48
6:K:180:THR:OG1	6:K:182:GLU:HG3	2.12	0.48
5:I:62:DT:H2"	5:I:63:DG:C8	2.48	0.48
6:L:172:LEU:HD21	6:L:174:ARG:HH11	1.79	0.48
5:I:47:DC:H2"	5:I:48:DT:H71	1.95	0.48
6:K:12:GLN:HG3	6:K:14:ILE:HD11	1.96	0.48
6:L:34:ARG:HB3	6:L:34:ARG:HH11	1.79	0.47
6:L:31:SER:HB3	6:L:34:ARG:HG3	1.96	0.47
3:C:80:ILE:HG12	3:C:83:HIS:CE1	2.48	0.47
4:H:45:TYR:CZ	4:H:49:LYS:HE2	2.50	0.47
2:B:23:ARG:NH2	6:K:210:ARG:HA	2.30	0.47
4:H:114:VAL:O	4:H:118:THR:OG1	2.28	0.47
1:A:128:ARG:HD2	1:A:133:GLU:OE1	2.14	0.47
6:K:43:ARG:NH2	6:K:46:ASP:OD2	2.41	0.47
3:G:43:ARG:HH21	5:J:184:DT:H4'	1.80	0.46
6:L:160:ASP:OD1	6:L:162:SER:N	2.44	0.46
1:E:46:VAL:HB	5:I:82:DA:P	2.56	0.46
6:L:42:LYS:HB2	6:L:49:SER:HB3	1.98	0.46
6:L:131:GLU:OE1	6:L:174:ARG:NH1	2.49	0.46
3:C:94:LEU:HA	3:C:94:LEU:HD23	1.61	0.46
6:K:30:ARG:HH21	6:K:37:GLU:HB3	1.81	0.46
5:I:69:DC:H2"	5:I:70:DG:C8	2.50	0.46
6:L:103:GLU:HA	6:L:110:ILE:HD11	1.97	0.46
6:K:158:TRP:CE3	6:K:165:LYS:HD2	2.51	0.46
3:C:19:SER:O	3:C:24:LEU:N	2.41	0.46
6:L:195:ARG:HD2	6:L:207:TYR:CE2	2.51	0.45
1:A:99:TYR:OH	1:A:133:GLU:OE1	2.29	0.45
5:J:251:DT:H2'	5:J:252:DT:C6	2.52	0.45
4:D:71:ASP:OD2	2:F:98:TYR:OH	2.35	0.45
5:I:58:DG:H2"	5:I:59:DG:C8	2.52	0.45
4:H:49:LYS:HD2	4:H:53:PRO:HA	1.99	0.45
6:K:2:AYA:HB1	6:K:7:ASP:HB2	1.99	0.45
3:G:89:ARG:HA	3:G:95:ASN:HB2	1.99	0.44
2:F:17:ARG:HH21	2:F:19:ARG:HG2	1.82	0.44
3:C:78:ARG:HE	5:I:19:DA:C5'	2.29	0.44
2:F:78:ARG:NH1	2:F:80:THR:O	2.50	0.44
4:H:73:PHE:CD1	4:H:73:PHE:C	2.91	0.44
6:L:3:LYS:O	6:L:82:VAL:HG23	2.18	0.44
6:L:102:TYR:CE2	6:L:123:PHE:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:124:DA:H61	5:J:168:DC:H42	1.66	0.44
3:C:59:LEU:O	3:C:63:ILE:HG22	2.17	0.44
6:L:158:TRP:HA	6:L:165:LYS:HD3	1.98	0.44
4:D:65:LEU:O	4:D:69:VAL:HG23	2.18	0.44
1:A:106:ASP:HB3	1:E:130:LEU:HD22	2.00	0.43
3:G:86:LEU:HD23	3:G:109:LEU:HD23	2.00	0.43
3:G:43:ARG:NH1	5:I:112:DT:H5'	2.33	0.43
3:C:101:VAL:HG11	2:F:98:TYR:CE2	2.53	0.43
4:H:105:LEU:O	4:H:110:ALA:HB2	2.18	0.43
6:L:195:ARG:HD2	6:L:207:TYR:CZ	2.53	0.43
3:G:78:ARG:NH1	5:J:165:DA:H5'	2.33	0.43
3:G:64:LEU:HD22	4:H:48:LEU:HD13	2.00	0.43
5:I:38:DT:H2''	5:I:39:DG:C8	2.53	0.43
3:C:51:TYR:O	3:C:55:VAL:HG23	2.18	0.43
6:K:153:LEU:HD12	6:K:165:LYS:HG2	2.00	0.43
4:D:49:LYS:HD2	4:D:53:PRO:HA	2.00	0.43
2:F:59:LYS:O	2:F:63:GLU:HG3	2.19	0.43
6:K:158:TRP:CD1	6:K:172:LEU:HB2	2.54	0.43
5:I:77:DC:H2''	5:I:78:DG:C8	2.54	0.43
3:G:51:TYR:OH	4:H:98:GLN:HG3	2.19	0.42
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.54	0.42
4:H:83:LEU:HD13	4:H:99:THR:HB	2.00	0.42
3:C:104:ALA:HB3	2:F:99:GLY:HA3	2.01	0.42
6:L:101:TYR:CE1	6:L:105:PHE:HD2	2.38	0.42
3:G:27:PRO:HD3	4:H:43:TYR:CG	2.54	0.42
4:H:59:GLN:HG2	5:J:165:DA:P	2.59	0.42
3:C:31:VAL:HG13	4:D:73:PHE:HE2	1.83	0.42
2:B:31:LYS:HE3	2:B:35:ARG:HH21	1.84	0.42
1:A:101:VAL:O	1:A:105:GLU:HG3	2.19	0.42
3:G:52:LEU:HD13	4:H:76:ILE:HG21	2.02	0.42
5:I:43:DA:N6	5:J:249:DG:O6	2.53	0.42
6:K:110:ILE:HD13	6:K:110:ILE:HA	1.94	0.42
5:I:23:DT:H2''	5:I:24:DA:C8	2.55	0.42
5:J:223:DC:H2''	5:J:224:DG:C8	2.55	0.42
5:I:34:DT:H2'	5:I:35:DA:C8	2.55	0.42
2:B:78:ARG:NH1	2:B:82:THR:HG23	2.35	0.42
3:C:116:LEU:HD22	2:F:44:LYS:HB2	2.02	0.41
3:C:19:SER:HB3	3:C:24:LEU:O	2.20	0.41
1:E:59:GLU:HG3	2:F:40:ARG:HH22	1.85	0.41
6:L:52:LYS:HA	6:L:71:ILE:HG22	2.02	0.41
6:K:191:GLN:O	6:K:195:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:107:DC:H6	5:I:107:DC:H2'	1.76	0.41
2:B:23:ARG:HH22	6:K:210:ARG:HA	1.85	0.41
6:L:4:THR:HG22	6:L:6:LYS:H	1.86	0.41
4:D:119:ARG:HG2	4:D:123:LYS:HE3	2.01	0.41
3:C:64:LEU:HD23	3:C:64:LEU:HA	1.89	0.41
4:D:106:PRO:O	4:D:109:LEU:HB2	2.21	0.41
1:E:78:PHE:CZ	2:F:67:ARG:HB2	2.56	0.41
4:D:83:LEU:HD13	4:D:99:THR:HB	2.02	0.41
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.56	0.41
6:K:96:LEU:HD12	6:K:123:PHE:HZ	1.86	0.40
4:D:64:ILE:HG23	2:F:98:TYR:HB3	2.03	0.40
5:J:168:DC:C6	5:J:169:DT:H72	2.56	0.40
3:G:31:VAL:HG13	4:H:73:PHE:CE2	2.57	0.40
3:G:41:ALA:HB3	4:H:92:ILE:HG13	2.03	0.40
6:K:68:VAL:O	6:K:90:TYR:HB2	2.21	0.40
3:C:82:ARG:O	3:C:82:ARG:HG3	2.17	0.40
6:L:69:TYR:HB3	6:L:87:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	94/136 (69%)	94 (100%)	0	0	100	100
1	E	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
2	B	86/103 (84%)	84 (98%)	2 (2%)	0	100	100
2	F	88/103 (85%)	86 (98%)	2 (2%)	0	100	100
3	C	101/132 (76%)	96 (95%)	5 (5%)	0	100	100
3	G	103/132 (78%)	99 (96%)	4 (4%)	0	100	100
4	D	91/131 (70%)	87 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	92/131 (70%)	89 (97%)	3 (3%)	0	100	100
6	K	211/224 (94%)	201 (95%)	9 (4%)	1 (0%)	34	78
6	L	211/224 (94%)	200 (95%)	11 (5%)	0	100	100
All	All	1173/1452 (81%)	1131 (96%)	41 (4%)	1 (0%)	56	91

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	K	160	ASP

### 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	84/113 (74%)	81 (96%)	3 (4%)	42	79
1	E	86/113 (76%)	83 (96%)	3 (4%)	43	80
2	B	74/81 (91%)	72 (97%)	2 (3%)	52	85
2	F	74/81 (91%)	72 (97%)	2 (3%)	52	85
3	C	82/98 (84%)	77 (94%)	5 (6%)	23	64
3	G	84/98 (86%)	83 (99%)	1 (1%)	78	93
4	D	81/109 (74%)	79 (98%)	2 (2%)	55	86
4	H	82/109 (75%)	80 (98%)	2 (2%)	57	86
6	K	200/210 (95%)	194 (97%)	6 (3%)	48	82
6	L	200/210 (95%)	196 (98%)	4 (2%)	63	88
All	All	1047/1222 (86%)	1017 (97%)	30 (3%)	50	83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	63	ARG

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Mol	Chain	Res	Type
1	A	80	THR
2	B	45	ARG
2	B	49	LEU
3	C	51	TYR
3	C	78	ARG
3	C	82	ARG
3	C	86	LEU
3	C	92	ASP
4	D	99	THR
4	D	118	THR
1	E	104	PHE
1	E	117	VAL
1	E	129	ARG
2	F	47	SER
2	F	84	LEU
3	G	89	ARG
4	H	54	ASP
4	H	118	THR
6	K	18	ASP
6	K	32	ARG
6	K	172	LEU
6	K	191	GLN
6	K	193	ILE
6	K	208	LEU
6	L	34	ARG
6	L	130	SER
6	L	193	ILE
6	L	194	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	74	ASN
4	H	87	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	AYA	K	2	6	6,7,8	1.86	2 (33%)	7,8,10	1.17	0
6	AYA	L	2	6	6,7,8	1.67	2 (33%)	7,8,10	1.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AYA	K	2	6	-	0/4/6/8	0/0/0/0
6	AYA	L	2	6	-	0/4/6/8	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	2	AYA	CA-N	-3.64	1.42	1.46
6	L	2	AYA	CA-N	-2.85	1.43	1.46
6	K	2	AYA	CT-N	2.15	1.42	1.34
6	L	2	AYA	CT-N	2.38	1.43	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	AYA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	96/136 (70%)	-0.00	1 (1%) 84 75	47, 65, 107, 135	0
1	E	98/136 (72%)	-0.10	1 (1%) 84 75	48, 64, 107, 124	0
2	B	88/103 (85%)	-0.13	0 100 100	49, 61, 76, 83	0
2	F	90/103 (87%)	-0.20	1 (1%) 82 72	47, 60, 80, 92	0
3	C	103/132 (78%)	-0.14	2 (1%) 70 55	56, 68, 103, 112	0
3	G	105/132 (79%)	0.04	3 (2%) 55 41	49, 63, 98, 113	0
4	D	93/131 (70%)	-0.04	1 (1%) 82 72	49, 66, 98, 112	0
4	H	94/131 (71%)	-0.04	1 (1%) 82 72	47, 61, 86, 108	0
5	I	146/146 (100%)	0.07	5 (3%) 49 34	86, 128, 193, 202	0
5	J	146/146 (100%)	0.16	4 (2%) 58 44	86, 135, 195, 209	0
6	K	212/224 (94%)	-0.34	0 100 100	49, 62, 93, 107	1 (0%)
6	L	212/224 (94%)	-0.17	1 (0%) 91 87	47, 67, 104, 117	0
All	All	1483/1744 (85%)	-0.09	20 (1%) 79 67	47, 68, 162, 209	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	146	DT	4.1
3	G	16	GLN	4.1
3	G	15	SER	3.5
1	A	39	HIS	3.2
5	J	292	DT	3.2
5	I	24	DA	3.1
1	E	36	LYS	2.9
5	J	155	DC	2.9
5	J	273	DA	2.9
6	L	214	PRO	2.7
4	D	45	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	116	LEU	2.6
2	F	14	GLY	2.5
5	I	2	DT	2.3
5	I	1	DA	2.3
4	H	129	GLN	2.2
5	I	23	DT	2.1
5	J	149	DC	2.1
3	C	78	ARG	2.1
3	C	77	THR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	AYA	L	2	8/9	0.98	0.22	-	55,56,60,60	0
6	AYA	K	2	8/9	0.97	0.20	-	56,59,63,63	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.