



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 03:52 PM EDT

PDB ID : 6OM3  
Title : Crystal structure of the Orc1 BAH domain in complex with a nucleosome core particle  
Authors : De Ioannes, P.E.; Wang, M.; Armache, K.-J.  
Deposited on : 2019-04-18  
Resolution : 3.30 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

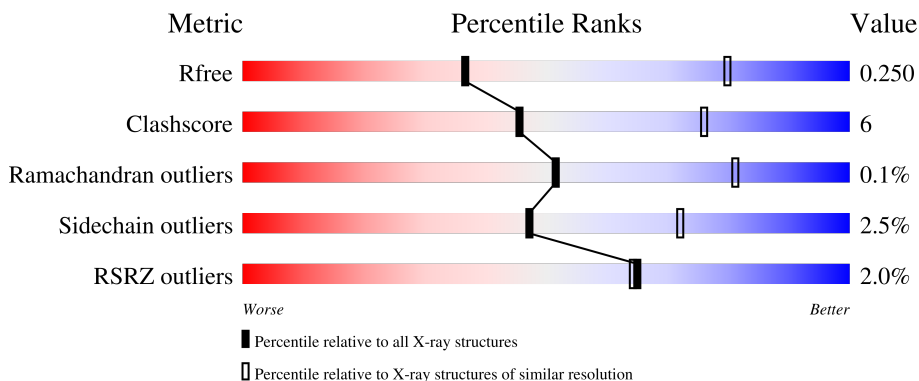
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.



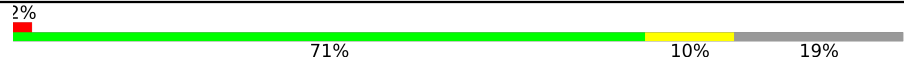

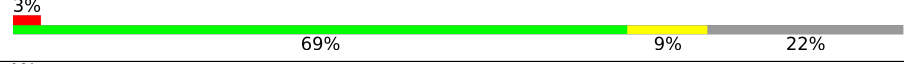

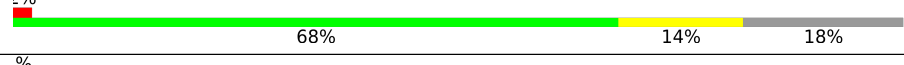
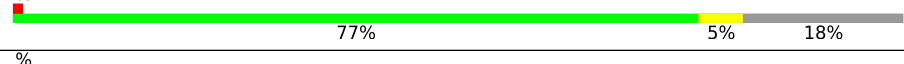
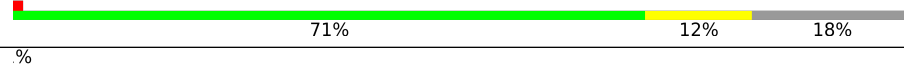

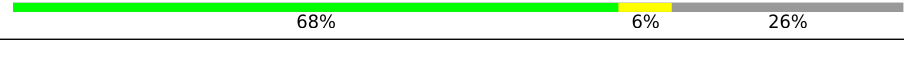



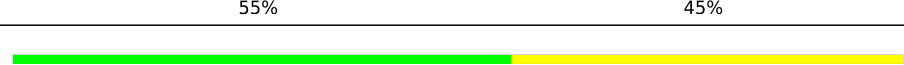
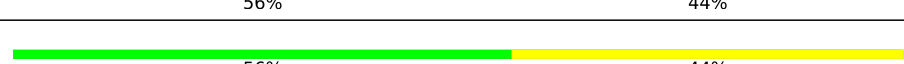

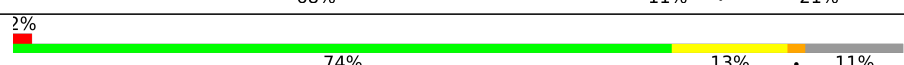
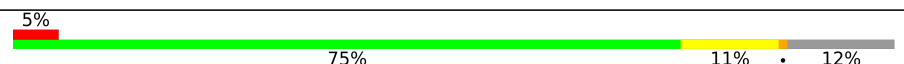


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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  $\geq 3$ , 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	135	
1	E	135	
1	M	135	
1	Q	135	
2	B	103	

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Mol	Chain	Length	Quality of chain
2	F	103	 <p>2% 71% 10% 19%</p>
2	N	103	 <p>2% 72% 10% 18%</p>
2	R	103	 <p>3% 69% 9% 22%</p>
3	C	130	 <p>2% 74% 6% 20%</p>
3	G	130	 <p>2% 68% 14% 18%</p>
3	O	130	 <p>0% 77% 5% 18%</p>
3	S	130	 <p>0% 71% 12% 18%</p>
4	D	126	 <p>0% 65% 9% 26%</p>
4	H	126	 <p>0% 68% 6% 26%</p>
4	P	126	 <p>0% 67% 6% 26%</p>
4	T	126	 <p>0% 62% 11% 26%</p>
5	I	146	 <p>0% 52% 48%</p>
5	U	146	 <p>0% 55% 45%</p>
6	J	147	 <p>0% 56% 44%</p>
6	V	147	 <p>0% 56% 44%</p>
7	K	224	 <p>2% 68% 11% 21%</p>
7	L	224	 <p>2% 74% 13% 11%</p>
7	W	224	 <p>5% 75% 11% 12%</p>
7	X	224	 <p>4% 38% 10% 51%</p>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28906 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 H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	97	788	497	150	138	3	0	0	0
1	E	95	785	495	151	136	3	0	0	0
1	M	98	798	506	154	135	3	0	0	0
1	Q	95	772	489	147	133	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	engineered mutation	UNP P84233
E	102	ALA	GLY	engineered mutation	UNP P84233
M	102	ALA	GLY	engineered mutation	UNP P84233
Q	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	84	678	428	135	114	1	0	0	0
2	F	83	649	409	126	113	1	0	0	0
2	N	84	660	417	128	114	1	0	0	0
2	R	80	635	402	122	110	1	0	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	104	782	492	150	140	0	0	0
3	G	107	797	502	154	141	0	0	0
3	O	107	810	511	159	140	0	0	0
3	S	107	808	507	158	143	0	0	0

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	93	723	454	130	137	2	0	0	0
4	H	93	714	449	128	135	2	0	0	0
4	P	93	714	448	127	137	2	0	0	0
4	T	93	718	451	128	137	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	THR	SER	engineered mutation	UNP P02281
H	32	THR	SER	engineered mutation	UNP P02281
P	32	THR	SER	engineered mutation	UNP P02281
T	32	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	I	146	2975	1414	539	876	146	0	0	0
5	U	146	2975	1414	539	876	146	0	0	0

- Molecule 6 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	J	147	3031	1436	565	883	147	0	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	V	147	3031	1436	565	883	147	0	0	0

- Molecule 7 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	K	178	1425	908	246	267	4	0	0	0
7	L	199	1484	946	250	284	4	0	0	0
7	W	196	1411	884	248	276	3	0	0	0
7	X	110	743	458	138	145	2	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP P54784
K	79	ILE	LEU	engineered mutation	UNP P54784
K	215	ALA	-	expression tag	UNP P54784
K	216	ALA	-	expression tag	UNP P54784
K	217	HIS	-	expression tag	UNP P54784
K	218	HIS	-	expression tag	UNP P54784
K	219	HIS	-	expression tag	UNP P54784
K	220	HIS	-	expression tag	UNP P54784
K	221	HIS	-	expression tag	UNP P54784
K	222	HIS	-	expression tag	UNP P54784
K	223	HIS	-	expression tag	UNP P54784
K	224	HIS	-	expression tag	UNP P54784
L	1	ACE	-	acetylation	UNP P54784
L	79	ILE	LEU	engineered mutation	UNP P54784
L	215	ALA	-	expression tag	UNP P54784
L	216	ALA	-	expression tag	UNP P54784
L	217	HIS	-	expression tag	UNP P54784
L	218	HIS	-	expression tag	UNP P54784
L	219	HIS	-	expression tag	UNP P54784
L	220	HIS	-	expression tag	UNP P54784
L	221	HIS	-	expression tag	UNP P54784
L	222	HIS	-	expression tag	UNP P54784
L	223	HIS	-	expression tag	UNP P54784
L	224	HIS	-	expression tag	UNP P54784

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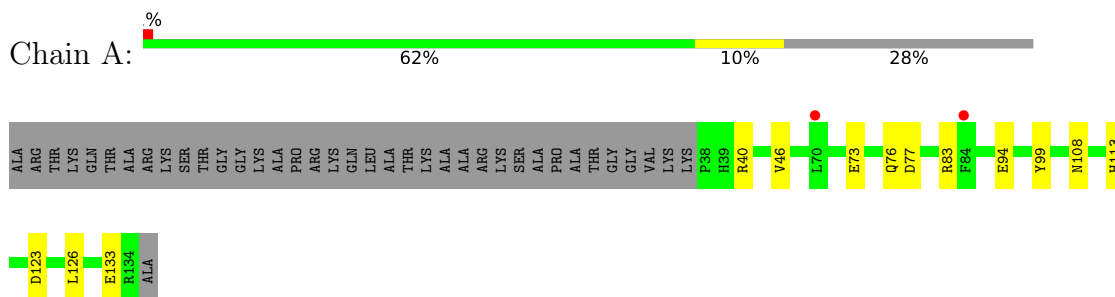
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Chain	Residue	Modelled	Actual	Comment	Reference
W	1	ACE	-	acetylation	UNP P54784
W	79	ILE	LEU	engineered mutation	UNP P54784
W	215	ALA	-	expression tag	UNP P54784
W	216	ALA	-	expression tag	UNP P54784
W	217	HIS	-	expression tag	UNP P54784
W	218	HIS	-	expression tag	UNP P54784
W	219	HIS	-	expression tag	UNP P54784
W	220	HIS	-	expression tag	UNP P54784
W	221	HIS	-	expression tag	UNP P54784
W	222	HIS	-	expression tag	UNP P54784
W	223	HIS	-	expression tag	UNP P54784
W	224	HIS	-	expression tag	UNP P54784
X	1	ACE	-	acetylation	UNP P54784
X	79	ILE	LEU	engineered mutation	UNP P54784
X	215	ALA	-	expression tag	UNP P54784
X	216	ALA	-	expression tag	UNP P54784
X	217	HIS	-	expression tag	UNP P54784
X	218	HIS	-	expression tag	UNP P54784
X	219	HIS	-	expression tag	UNP P54784
X	220	HIS	-	expression tag	UNP P54784
X	221	HIS	-	expression tag	UNP P54784
X	222	HIS	-	expression tag	UNP P54784
X	223	HIS	-	expression tag	UNP P54784
X	224	HIS	-	expression tag	UNP P54784

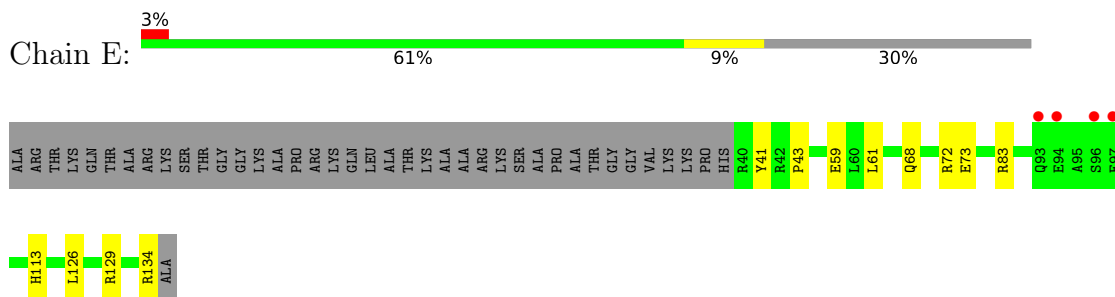
### 3 Residue-property plots [i](#)

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.

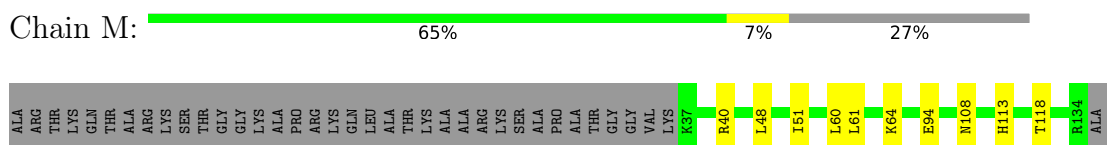
- Molecule 1: Histone H3.2



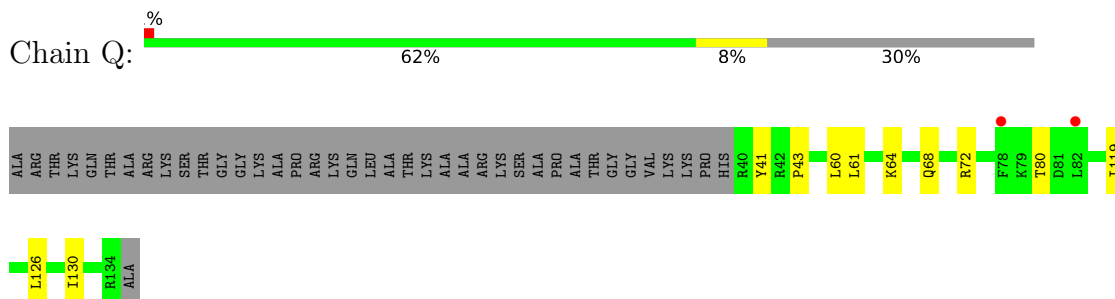
- Molecule 1: Histone H3.2



- Molecule 1: Histone H3.2

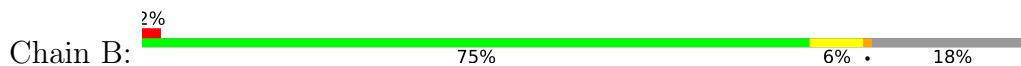


- Molecule 1: Histone H3.2





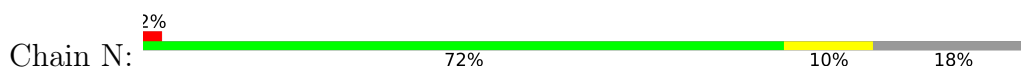
• Molecule 2: Histone H4



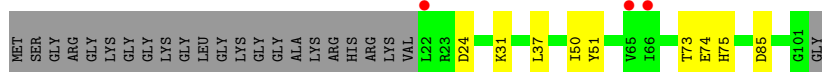
• Molecule 2: Histone H4



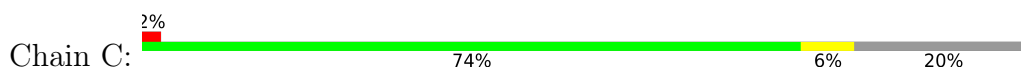
• Molecule 2: Histone H4



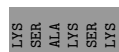
• Molecule 2: Histone H4



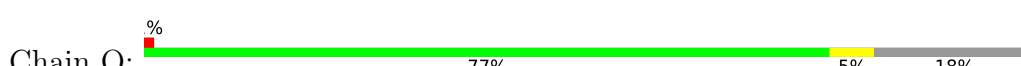
• Molecule 3: Histone H2A



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• Molecule 3: Histone H2A

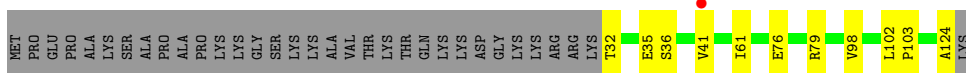




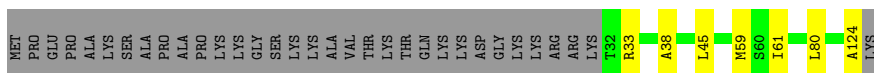
• Molecule 3: Histone H2A



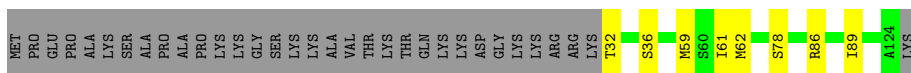
• Molecule 4: Histone H2B 1.1



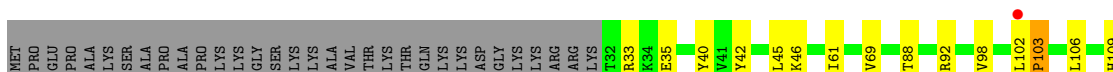
• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1



• Molecule 4: Histone H2B 1.1

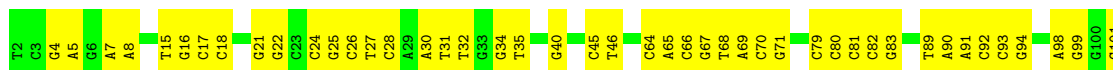


• Molecule 5: DNA (146-MER)





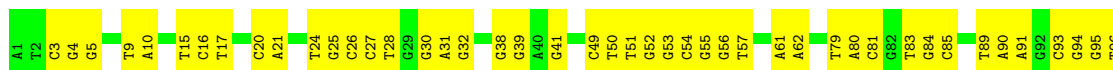
• Molecule 5: DNA (146-MER)



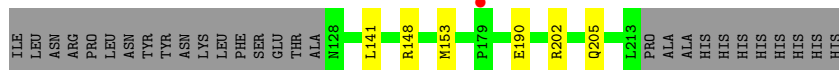
• Molecule 6: DNA (147-MER)



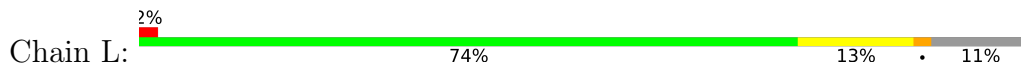
• Molecule 6: DNA (147-MER)

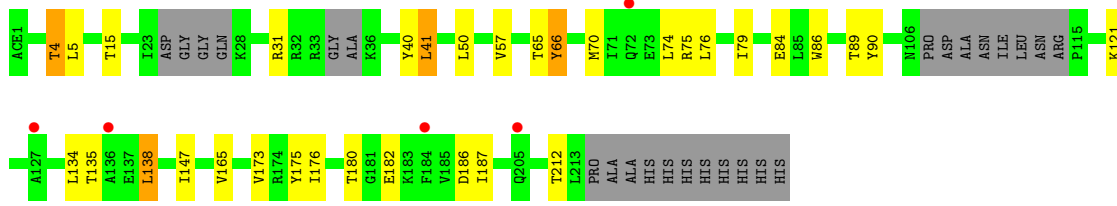


• Molecule 7: Origin recognition complex subunit 1

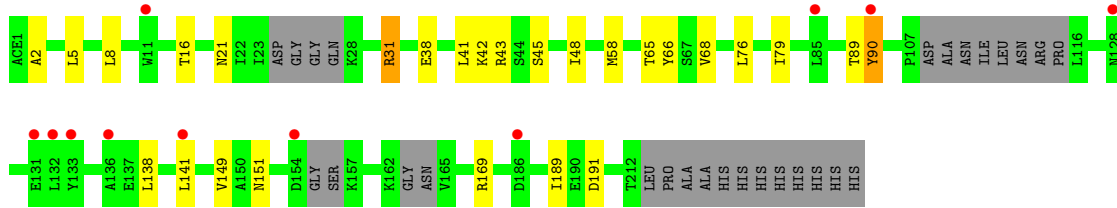
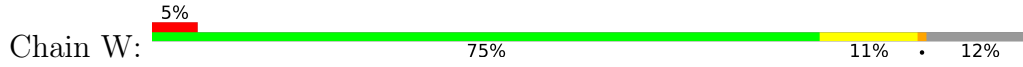


• Molecule 7: Origin recognition complex subunit 1

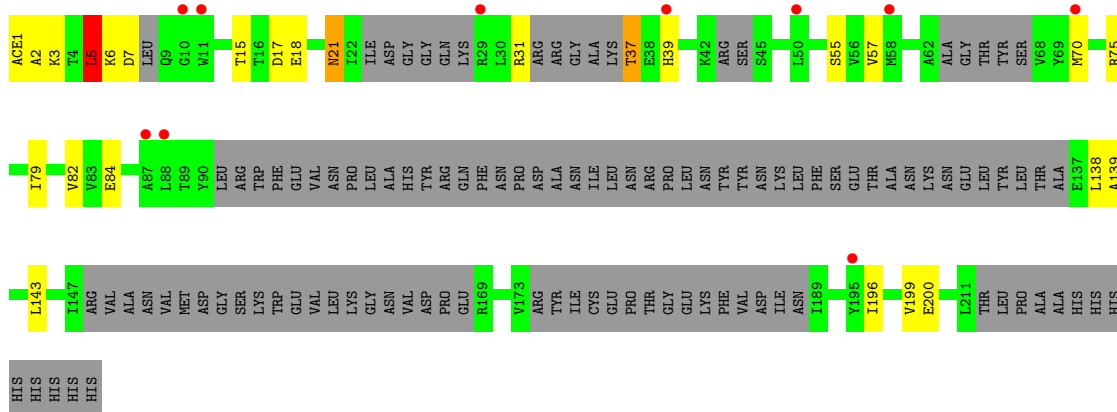
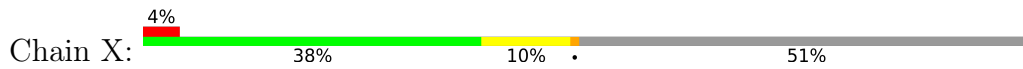




• Molecule 7: Origin recognition complex subunit 1



• Molecule 7: Origin recognition complex subunit 1



HIS  
HIS  
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HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.25Å 166.43Å 168.28Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	49.05 – 3.30 49.05 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.05-3.30) 96.4 (49.05-3.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 12-2829	Depositor
R, $R_{free}$	0.213 , 0.250 0.213 , 0.250	Depositor DCC
$R_{free}$ test set	8111 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.4	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 88.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.027 for -h,l,k 0.029 for -h,-l,-k 0.129 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	133.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 0.333 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: ACE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/800	0.39	0/1077
1	E	0.25	0/795	0.38	0/1066
1	M	0.25	0/810	0.38	0/1088
1	Q	0.25	0/782	0.40	0/1050
2	B	0.28	0/686	0.42	0/918
2	F	0.25	0/657	0.40	0/884
2	N	0.24	0/668	0.40	0/897
2	R	0.25	0/642	0.41	0/861
3	C	0.28	0/792	0.42	0/1076
3	G	0.25	0/807	0.40	0/1096
3	O	0.24	0/820	0.40	0/1110
3	S	0.24	0/818	0.40	0/1108
4	D	0.26	0/734	0.39	0/989
4	H	0.25	0/725	0.37	0/980
4	P	0.24	0/725	0.38	0/981
4	T	0.24	0/729	0.38	0/985
5	I	0.56	0/3333	0.93	0/5137
5	U	0.54	0/3333	0.92	0/5137
6	J	0.54	0/3403	0.92	0/5255
6	V	0.54	0/3403	0.92	0/5255
7	K	0.25	0/1446	0.44	0/1957
7	L	0.25	0/1508	0.44	0/2055
7	W	0.25	0/1428	0.44	0/1951
7	X	0.24	0/740	0.44	0/998
All	All	0.41	0/30584	0.70	0/43911

There are no bond length outliers.

There are no bond angle outliers.

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	788	0	808	11	0
1	E	785	0	826	12	0
1	M	798	0	836	8	0
1	Q	772	0	807	10	0
2	B	678	0	726	6	0
2	F	649	0	663	8	0
2	N	660	0	686	10	0
2	R	635	0	673	7	0
3	C	782	0	804	9	0
3	G	797	0	823	12	0
3	O	810	0	853	7	0
3	S	808	0	840	15	0
4	D	723	0	738	9	0
4	H	714	0	721	6	0
4	P	714	0	714	5	0
4	T	718	0	725	17	0
5	I	2975	0	1640	54	0
5	U	2975	0	1640	51	0
6	J	3031	0	1652	52	0
6	V	3031	0	1652	47	0
7	K	1425	0	1404	13	0
7	L	1484	0	1338	19	0
7	W	1411	0	1218	12	0
7	X	743	0	608	16	0
All	All	28906	0	23395	334	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 (334) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:123:DC:H2'	6:J:124:DG:C8	2.15	0.82
2:N:74:GLU:HB3	7:W:79:ILE:HD11	1.61	0.81
6:V:123:DC:H2'	6:V:124:DG:C8	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:24:DC:H2'	5:I:25:DG:C8	2.20	0.76
3:C:32:ARG:NH1	6:J:30:DG:OP1	2.21	0.73
2:B:19:ARG:HD3	6:J:52:DG:OP1	1.88	0.72
5:U:24:DC:H2'	5:U:25:DG:C8	2.27	0.69
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.77	0.66
1:E:129:ARG:HB2	1:E:134:ARG:HD3	1.78	0.64
3:C:16:THR:HA	6:J:31:DA:H5''	1.78	0.64
6:V:93:DC:H2''	6:V:94:DG:C8	2.33	0.64
5:I:80:DC:H2''	5:I:81:DC:C5	2.34	0.63
5:I:89:DT:H2''	5:I:90:DA:C8	2.34	0.62
3:S:92:GLU:OE1	7:X:31:ARG:NH1	2.33	0.62
6:V:105:DT:H2''	6:V:106:DG:C8	2.34	0.62
5:I:102:DG:H2''	5:I:103:DA:H5''	1.82	0.62
6:V:142:DC:H2'	6:V:143:DT:C6	2.35	0.62
7:X:17:ASP:HA	7:X:37:THR:HA	1.82	0.61
7:K:57:VAL:HG13	7:K:148:ARG:H	1.64	0.61
5:U:68:DT:H2''	5:U:69:DA:C8	2.36	0.61
3:O:32:ARG:NH1	6:V:30:DG:OP1	2.34	0.60
4:D:76:GLU:OE2	4:D:79:ARG:NH2	2.35	0.60
5:I:123:DC:H2''	5:I:124:DA:C8	2.37	0.60
5:U:79:DC:H2''	5:U:80:DC:C5	2.37	0.60
6:V:20:DC:H2''	6:V:21:DA:C8	2.35	0.60
7:X:5:LEU:HD12	7:X:6:LYS:HD2	1.83	0.60
5:I:8:DA:H2'	5:I:9:DT:C6	2.36	0.60
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.23	0.59
6:J:142:DC:H2'	6:J:143:DT:C6	2.36	0.59
5:I:129:DT:H2''	5:I:130:DC:C5	2.36	0.59
7:K:14:ILE:HD13	7:K:42:LYS:HB3	1.84	0.59
5:I:144:DC:H2''	5:I:145:DG:C8	2.37	0.59
5:I:4:DG:H2''	5:I:5:DA:C8	2.38	0.59
3:G:90:ASP:OD2	7:L:31:ARG:NH2	2.36	0.59
5:U:98:DA:H1'	5:U:99:DG:H5'	1.85	0.59
1:Q:61:LEU:HD12	2:R:37:LEU:HD23	1.85	0.58
5:U:102:DG:H2''	5:U:103:DA:H5''	1.85	0.58
6:V:111:DC:H2''	6:V:112:DG:C8	2.37	0.58
3:C:29:ARG:NH1	4:D:36:SER:O	2.37	0.58
6:J:20:DC:H2''	6:J:21:DA:C8	2.39	0.58
3:G:20:ARG:HH11	4:H:124:ALA:HB1	1.69	0.57
7:L:176:ILE:HD13	7:L:187:ILE:HG22	1.86	0.57
3:S:32:ARG:NH2	4:T:35:GLU:OE2	2.37	0.57
3:G:14:ALA:HA	5:I:32:DT:H5''	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:16:THR:HA	6:V:31:DA:H5''	1.86	0.57
5:U:144:DC:H2''	5:U:145:DG:C8	2.40	0.57
6:J:93:DC:H2''	6:J:94:DG:C8	2.40	0.57
7:X:75:ARG:HB2	7:X:84:GLU:HB2	1.86	0.57
1:E:129:ARG:HA	1:E:134:ARG:HB3	1.87	0.57
4:H:33:ARG:HE	6:J:123:DC:H1'	1.70	0.57
6:J:50:DT:H2'	6:J:51:DT:H71	1.86	0.57
6:V:4:DG:H2''	6:V:5:DG:C8	2.40	0.57
1:M:60:LEU:HD12	1:M:64:LYS:HE2	1.86	0.56
5:I:68:DT:H2''	5:I:69:DA:C8	2.40	0.56
6:J:105:DT:H2''	6:J:106:DG:C8	2.41	0.56
7:L:175:TYR:HA	7:L:186:ASP:HA	1.87	0.56
6:V:3:DC:H2''	6:V:4:DG:C8	2.41	0.56
6:V:89:DT:H2''	6:V:90:DA:C8	2.41	0.56
5:U:80:DC:H2''	5:U:81:DC:C5	2.41	0.55
5:U:17:DC:H2''	5:U:18:DC:C5	2.41	0.55
1:A:77:ASP:OD1	7:K:205:GLN:NE2	2.38	0.55
7:W:43:ARG:HD3	7:W:45:SER:HB2	1.88	0.55
3:S:90:ASP:OD2	7:X:31:ARG:NH2	2.40	0.55
2:B:92:ARG:HG3	4:D:79:ARG:HH22	1.72	0.55
5:I:17:DC:H2''	5:I:18:DC:C5	2.42	0.55
1:M:108:ASN:ND2	2:N:42:GLY:O	2.40	0.55
5:I:27:DT:H2''	5:I:28:DC:C6	2.42	0.54
7:X:1:ACE:H2	7:X:143:LEU:HG	1.88	0.54
5:U:123:DC:H2''	5:U:124:DA:C8	2.42	0.54
6:V:93:DC:H2''	6:V:94:DG:H8	1.72	0.53
7:L:121:LYS:HE2	5:U:35:DT:H5''	1.91	0.53
4:P:86:ARG:NH1	6:V:41:DG:OP2	2.41	0.53
3:C:32:ARG:NH2	4:D:35:GLU:OE2	2.42	0.53
5:U:89:DT:H2''	5:U:90:DA:C8	2.43	0.53
3:O:102:ILE:HG23	4:P:61:ILE:HD13	1.89	0.53
1:M:40:ARG:NH2	5:U:83:DG:N3	2.57	0.53
7:X:2:ALA:HB1	7:X:7:ASP:HB3	1.91	0.53
3:S:102:ILE:HG23	4:T:61:ILE:HD13	1.89	0.53
6:V:83:DT:H2''	6:V:84:DG:C8	2.43	0.53
7:X:21:ASN:OD1	7:X:21:ASN:N	2.42	0.52
7:L:90:TYR:HE1	7:L:173:VAL:HG21	1.74	0.52
5:U:119:DC:H2''	5:U:120:DA:N7	2.24	0.52
2:N:26:ILE:HD13	2:N:59:LYS:HG3	1.91	0.52
5:I:79:DC:H2''	5:I:80:DC:C5	2.45	0.52
6:J:1:DA:C8	6:J:2:DT:H72	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:42:ARG:HG3	4:T:88:THR:HB	1.92	0.52
4:T:33:ARG:HH21	6:V:122:DG:H21	1.57	0.52
6:J:38:DG:H2''	6:J:39:DG:C8	2.44	0.52
7:W:16:THR:HG23	7:W:38:GLU:HB3	1.93	0.51
5:I:127:DT:H2''	5:I:128:DG:C8	2.45	0.51
6:J:93:DC:H2''	6:J:94:DG:H8	1.75	0.51
6:J:34:DC:H2'	6:J:35:DT:C6	2.45	0.51
5:I:145:DG:H2''	5:I:146:DA:C8	2.45	0.51
7:L:65:THR:OG1	7:L:66:TYR:N	2.40	0.51
6:V:38:DG:H2''	6:V:39:DG:N7	2.25	0.51
4:P:59:MET:HE3	4:P:62:MET:HB3	1.93	0.51
1:Q:60:LEU:HD12	1:Q:64:LYS:HE2	1.93	0.50
3:S:32:ARG:NH1	5:U:30:DA:OP1	2.43	0.50
7:W:43:ARG:HG2	7:W:45:SER:H	1.77	0.50
6:J:83:DT:H2''	6:J:84:DG:C8	2.46	0.50
1:M:118:THR:OG1	2:N:45:ARG:NH1	2.41	0.50
5:I:7:DA:H2''	5:I:8:DA:C8	2.46	0.50
3:O:79:ILE:HG12	3:O:82:HIS:CE1	2.47	0.50
4:T:42:TYR:O	4:T:46:LYS:HG2	2.10	0.50
7:W:58:MET:HG3	7:W:141:LEU:HD13	1.93	0.50
7:L:89:THR:OG1	7:L:135:THR:OG1	2.21	0.50
1:Q:68:GLN:HE21	1:Q:72:ARG:HH21	1.60	0.50
3:S:58:LEU:HD12	4:T:69:VAL:HG11	1.93	0.50
6:J:109:DT:H2''	6:J:110:DA:C8	2.47	0.50
6:J:3:DC:H2''	6:J:4:DG:C8	2.46	0.49
5:U:70:DC:H2''	5:U:71:DG:C8	2.47	0.49
6:V:9:DT:H2''	6:V:10:DA:C8	2.47	0.49
5:U:4:DG:H2''	5:U:5:DA:C8	2.46	0.49
4:T:109:HIS:CE1	7:X:31:ARG:HG2	2.47	0.49
5:U:7:DA:H2''	5:U:8:DA:C8	2.48	0.49
5:I:36:DC:H2''	5:I:37:DG:C8	2.48	0.49
6:J:126:DC:H2''	6:J:127:DC:O5'	2.12	0.49
6:V:38:DG:H2''	6:V:39:DG:C8	2.47	0.49
5:I:119:DC:H2''	5:I:120:DA:N7	2.27	0.49
4:T:33:ARG:NH2	6:V:122:DG:H21	2.10	0.49
6:J:144:DC:H2''	6:J:145:DG:C8	2.48	0.49
6:J:9:DT:H2''	6:J:10:DA:C8	2.48	0.48
6:J:38:DG:H2''	6:J:39:DG:N7	2.28	0.48
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.35	0.48
1:E:41:TYR:HA	5:I:144:DC:H5''	1.95	0.48
5:I:68:DT:H2''	5:I:69:DA:N7	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:65:THR:OG1	7:W:66:TYR:N	2.45	0.48
5:I:21:DG:H2''	5:I:22:DG:C8	2.48	0.48
3:S:44:GLY:HA2	6:V:112:DG:H5''	1.94	0.48
5:U:127:DT:H2''	5:U:128:DG:C8	2.49	0.48
3:G:73:ASN:HB3	3:G:75:LYS:HE3	1.95	0.48
4:T:92:ARG:NH1	7:X:79:ILE:O	2.46	0.48
6:V:109:DT:H2''	6:V:110:DA:C8	2.48	0.48
5:U:27:DT:H2''	5:U:28:DC:C6	2.49	0.48
5:I:26:DC:H2''	5:I:27:DT:H71	1.96	0.48
1:M:61:LEU:HD12	2:N:37:LEU:HD23	1.94	0.48
3:S:93:LEU:HD23	4:T:106:LEU:HD11	1.95	0.48
5:U:26:DC:H2''	5:U:27:DT:C7	2.44	0.48
5:I:26:DC:H2''	5:I:27:DT:C7	2.42	0.48
5:I:70:DC:H2''	5:I:71:DG:C8	2.49	0.47
5:U:17:DC:H2''	5:U:18:DC:C6	2.48	0.47
6:V:119:DT:H2''	6:V:120:DG:C8	2.49	0.47
2:F:75:HIS:CD2	4:H:80:LEU:HD22	2.49	0.47
5:I:28:DC:H2''	5:I:29:DA:N7	2.28	0.47
6:J:22:DC:H2''	6:J:23:DG:H8	1.80	0.47
2:R:73:THR:OG1	2:R:85:ASP:OD2	2.27	0.47
3:C:61:GLU:OE2	7:K:31:ARG:N	2.45	0.47
7:K:73:GLU:OE2	7:K:202:ARG:NH2	2.46	0.47
1:Q:41:TYR:HA	5:U:144:DC:H5''	1.94	0.47
1:Q:80:THR:HG21	7:X:139:ALA:HA	1.96	0.47
3:C:20:ARG:NH1	4:D:124:ALA:O	2.45	0.47
5:U:93:DC:H2''	5:U:94:DG:C8	2.49	0.47
5:I:3:DC:H2''	5:I:4:DG:C8	2.50	0.47
6:J:119:DT:H2''	6:J:120:DG:C8	2.50	0.47
4:T:98:VAL:HG13	4:T:102:LEU:HD12	1.96	0.47
6:V:61:DA:H2''	6:V:62:DA:H8	1.79	0.47
2:F:78:ARG:NH2	2:F:85:ASP:OD2	2.48	0.47
6:V:26:DC:H2''	6:V:27:DC:C5	2.50	0.47
6:V:95:DG:H2'	6:V:96:DT:C6	2.49	0.47
3:C:102:ILE:HG23	4:D:61:ILE:HD13	1.96	0.47
6:J:15:DT:H2''	6:J:16:DC:O5'	2.14	0.47
2:N:79:LYS:HE2	5:U:101:DG:OP1	2.14	0.47
6:J:65:DC:H2''	6:J:66:DG:C8	2.51	0.46
6:J:94:DG:H2''	6:J:95:DG:O5'	2.15	0.46
7:L:4:THR:OG1	7:L:5:LEU:N	2.47	0.46
2:N:79:LYS:CE	5:U:101:DG:OP1	2.63	0.46
6:V:98:DC:H2''	6:V:99:DT:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:90:DA:H1'	5:I:91:DA:C8	2.51	0.46
6:J:51:DT:C2	6:J:52:DG:C8	3.03	0.46
6:J:111:DC:H2''	6:J:112:DG:C8	2.51	0.46
7:K:65:THR:OG1	7:K:66:TYR:N	2.48	0.46
3:O:29:ARG:NH1	4:P:36:SER:O	2.48	0.46
6:J:70:DG:H2''	6:J:71:DA:C8	2.51	0.46
6:J:79:DT:H2''	6:J:80:DA:C8	2.50	0.46
5:U:129:DT:H2''	5:U:130:DC:C5	2.50	0.46
6:J:31:DA:H2''	6:J:32:DG:H8	1.81	0.46
6:J:79:DT:H2''	6:J:80:DA:N7	2.31	0.46
5:U:138:DT:H2''	5:U:139:DA:C8	2.50	0.46
7:K:75:ARG:HB2	7:K:84:GLU:HB2	1.98	0.46
7:X:3:LYS:O	7:X:82:VAL:N	2.48	0.46
5:U:45:DC:C6	5:U:46:DT:H72	2.51	0.45
6:V:31:DA:H2''	6:V:32:DG:H8	1.81	0.45
7:X:199:VAL:HG22	7:X:200:GLU:H	1.82	0.45
3:G:92:GLU:OE1	7:L:31:ARG:NH1	2.48	0.45
7:K:85:LEU:HD23	7:K:141:LEU:HB2	1.97	0.45
6:V:56:DG:H1'	6:V:57:DT:H5'	1.99	0.45
2:F:74:GLU:HB2	7:L:79:ILE:HD11	1.98	0.45
7:L:180:THR:HG23	7:L:182:GLU:HG2	1.98	0.45
6:J:55:DG:H2''	6:J:56:DG:C8	2.52	0.45
6:J:95:DG:H2'	6:J:96:DT:C6	2.51	0.45
7:W:2:ALA:HB3	7:W:8:LEU:HG	1.99	0.45
6:J:22:DC:H2''	6:J:23:DG:C8	2.51	0.45
7:L:134:LEU:HB2	7:L:176:ILE:HG13	1.97	0.45
6:V:55:DG:H2''	6:V:56:DG:C8	2.52	0.45
6:V:126:DC:H2''	6:V:127:DC:O5'	2.15	0.45
3:G:63:LEU:HD13	4:H:45:LEU:HB2	1.98	0.45
6:V:51:DT:C2	6:V:52:DG:C8	3.05	0.45
5:I:72:DG:H2''	5:I:73:DA:H8	1.82	0.45
6:J:4:DG:H2''	6:J:5:DG:C8	2.51	0.45
7:L:41:LEU:HD23	7:L:74:LEU:HD11	1.99	0.45
2:N:31:LYS:HG3	2:N:51:TYR:CE1	2.52	0.45
6:V:49:DC:H2''	6:V:50:DT:H72	1.98	0.45
1:A:40:ARG:NH2	6:J:66:DG:H21	2.13	0.45
5:I:82:DC:H2''	5:I:83:DG:C8	2.52	0.45
7:K:43:ARG:HD3	7:K:45:SER:HB2	1.98	0.45
5:I:31:DT:H2'	5:I:32:DT:H71	1.98	0.45
5:I:38:DT:H2''	5:I:39:DA:N7	2.32	0.45
5:I:69:DA:H1'	5:I:70:DC:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:28:DT:H2''	6:J:29:DG:C8	2.52	0.45
6:J:89:DT:H2''	6:J:90:DA:C8	2.51	0.45
6:J:98:DC:H2''	6:J:99:DT:C6	2.52	0.45
1:Q:41:TYR:N	6:V:84:DG:OP1	2.47	0.45
5:U:90:DA:H1'	5:U:91:DA:N7	2.32	0.45
1:A:46:VAL:HG21	5:I:83:DG:H3'	1.99	0.44
5:I:77:DT:H2''	5:I:78:DC:C5	2.52	0.44
4:P:78:SER:HA	4:P:89:ILE:HD11	1.99	0.44
7:X:15:THR:HG22	7:X:39:HIS:CD2	2.51	0.44
3:O:29:ARG:HG3	3:O:32:ARG:HH12	1.83	0.44
6:V:112:DG:H2''	6:V:113:DA:C8	2.53	0.44
5:U:108:DT:H2''	5:U:109:DC:C6	2.52	0.44
7:X:55:SER:HA	7:X:70:MET:HA	1.99	0.44
3:S:32:ARG:HD3	5:U:30:DA:OP2	2.17	0.44
5:U:34:DG:H2'	5:U:35:DT:C6	2.52	0.44
5:U:82:DC:H2''	5:U:83:DG:C8	2.53	0.44
6:V:27:DC:H2''	6:V:28:DT:C5	2.53	0.44
6:V:31:DA:H2''	6:V:32:DG:C8	2.53	0.44
2:R:74:GLU:HB3	7:X:79:ILE:HD11	2.00	0.44
6:V:90:DA:H1'	6:V:91:DA:C8	2.53	0.44
5:I:2:DT:H2''	5:I:3:DC:H5	1.84	0.43
2:R:75:HIS:CE1	4:T:92:ARG:HG2	2.52	0.43
5:U:31:DT:H2'	5:U:32:DT:H71	2.00	0.43
6:V:15:DT:H2''	6:V:16:DC:O5'	2.18	0.43
7:W:151:ASN:HB3	7:W:169:ARG:O	2.18	0.43
1:M:94:GLU:OE2	3:S:104:GLN:NE2	2.50	0.43
2:N:71:THR:HG23	7:W:79:ILE:HD13	2.00	0.43
1:Q:43:PRO:HG2	5:U:69:DA:H5'	2.01	0.43
1:Q:119:ILE:HG13	2:R:50:ILE:HG13	2.00	0.43
6:V:24:DT:H2''	6:V:25:DG:C8	2.53	0.43
1:E:68:GLN:HG2	1:E:72:ARG:HE	1.84	0.43
5:U:66:DC:H2''	5:U:67:DG:C8	2.53	0.43
5:U:90:DA:H1'	5:U:91:DA:C8	2.54	0.43
3:C:63:LEU:HD11	4:D:41:VAL:HG13	1.99	0.43
5:I:72:DG:H2''	5:I:73:DA:C8	2.53	0.43
5:U:119:DC:H2''	5:U:120:DA:C8	2.54	0.43
1:Q:126:LEU:O	1:Q:130:ILE:HG12	2.19	0.42
6:J:80:DA:H2''	6:J:81:DC:C6	2.54	0.42
3:G:51:LEU:O	3:G:55:LEU:HG	2.18	0.42
3:G:102:ILE:HG23	4:H:61:ILE:HD13	2.00	0.42
7:K:21:ASN:OD1	7:K:21:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:57:VAL:HG13	7:L:147:ILE:HB	2.01	0.42
5:I:130:DC:H2''	5:I:131:DA:N7	2.34	0.42
2:N:79:LYS:NZ	5:U:101:DG:OP1	2.50	0.42
4:T:102:LEU:HA	4:T:103:PRO:HD3	1.93	0.42
3:G:32:ARG:HA	3:G:35:ARG:HG2	2.01	0.42
5:I:90:DA:H1'	5:I:91:DA:N7	2.35	0.42
7:L:75:ARG:HB2	7:L:84:GLU:HB2	2.02	0.42
5:U:64:DC:H2''	5:U:65:DA:C8	2.54	0.42
7:W:42:LYS:HA	7:W:48:ILE:O	2.20	0.42
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.54	0.42
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.53	0.42
5:I:78:DC:H2''	5:I:79:DC:C6	2.55	0.42
7:K:190:GLU:H	7:K:190:GLU:HG2	1.66	0.42
1:A:99:TYR:OH	1:A:133:GLU:OE1	2.31	0.42
7:K:43:ARG:O	7:K:47:GLY:N	2.53	0.42
7:L:40:TYR:HB2	7:L:50:LEU:O	2.20	0.42
1:M:113:HIS:CG	1:Q:126:LEU:HD22	2.55	0.42
5:I:93:DC:H2''	5:I:94:DG:C8	2.55	0.42
4:T:88:THR:HG22	5:U:40:DG:OP1	2.20	0.42
4:D:98:VAL:HG13	4:D:102:LEU:HD12	2.02	0.41
2:F:19:ARG:HA	2:F:19:ARG:HD2	1.93	0.41
5:I:21:DG:H2''	5:I:22:DG:H8	1.84	0.41
5:I:128:DG:H2''	5:I:129:DT:C6	2.55	0.41
3:O:90:ASP:CG	7:W:31:ARG:HH22	2.24	0.41
6:V:52:DG:C4	6:V:53:DG:N7	2.88	0.41
1:A:108:ASN:HB2	2:B:43:VAL:HG22	2.01	0.41
5:I:54:DC:H2'	5:I:55:DG:C8	2.55	0.41
7:L:86:TRP:HE3	7:L:138:LEU:HD22	1.86	0.41
5:U:92:DC:H2''	5:U:93:DC:C6	2.55	0.41
5:U:104:DT:C5	5:U:105:DT:H73	2.55	0.41
1:E:83:ARG:NH1	6:J:101:DG:OP1	2.53	0.41
4:H:38:ALA:HA	4:H:59:MET:HE1	2.01	0.41
5:I:85:DG:C8	5:I:86:DT:H72	2.55	0.41
5:I:132:DG:H2''	5:I:133:DA:C8	2.55	0.41
6:J:82:DG:H2'	6:J:83:DT:H71	2.02	0.41
6:V:54:DC:H2''	6:V:55:DG:C8	2.55	0.41
1:E:43:PRO:HG2	5:I:69:DA:H5'	2.03	0.41
6:J:33:DA:C5	6:J:34:DC:C4	3.09	0.41
6:J:123:DC:H2'	6:J:124:DG:H8	1.76	0.41
5:U:27:DT:H5''	5:U:27:DT:H6	1.84	0.41
5:I:111:DC:O2	6:J:38:DG:N2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:137:DA:H2'	5:I:138:DT:H71	2.03	0.41
3:S:63:LEU:HD13	4:T:45:LEU:HB2	2.01	0.41
6:V:84:DG:H2''	6:V:85:DC:C6	2.56	0.41
3:G:62:ILE:HD13	3:G:93:LEU:HD13	2.03	0.41
5:I:108:DT:H2''	5:I:109:DC:C6	2.55	0.41
6:J:119:DT:H2''	6:J:120:DG:N7	2.35	0.41
7:K:76:LEU:HD12	7:K:83:VAL:HG22	2.03	0.41
5:U:21:DG:H2''	5:U:22:DG:C8	2.56	0.41
5:U:103:DA:C8	5:U:104:DT:H72	2.56	0.41
6:V:16:DC:H2''	6:V:17:DT:C6	2.56	0.41
2:B:19:ARG:CD	6:J:52:DG:OP1	2.64	0.41
7:L:70:MET:HB2	7:L:90:TYR:CE2	2.56	0.41
6:V:132:DC:H2''	6:V:133:DA:C8	2.55	0.41
1:E:61:LEU:HD13	2:F:36:ARG:HB3	2.03	0.41
3:S:26:PRO:HD3	4:T:40:TYR:CD1	2.56	0.41
5:U:112:DT:H2''	5:U:113:DA:C8	2.56	0.41
1:A:83:ARG:HH21	6:J:50:DT:H1'	1.86	0.41
2:B:20:LYS:HE3	2:B:20:LYS:HB2	1.88	0.41
2:F:19:ARG:NH1	5:I:53:DC:OP2	2.53	0.41
6:J:54:DC:H2''	6:J:55:DG:C8	2.56	0.41
6:J:125:DG:H5'	6:J:125:DG:H8	1.85	0.41
1:M:48:LEU:HD23	1:M:51:ILE:HD12	2.02	0.41
2:R:31:LYS:HG3	2:R:51:TYR:CE1	2.55	0.41
5:U:15:DT:H2''	5:U:16:DG:C8	2.56	0.41
1:A:94:GLU:OE2	3:G:104:GLN:NE2	2.54	0.40
4:D:102:LEU:HA	4:D:103:PRO:HD3	1.93	0.40
3:G:65:LEU:HB2	3:G:86:ALA:HB1	2.04	0.40
2:R:75:HIS:HE1	4:T:92:ARG:HG2	1.86	0.40
5:U:98:DA:C6	5:U:99:DG:C6	3.09	0.40
6:V:79:DT:H2''	6:V:80:DA:C8	2.55	0.40
5:I:45:DC:C6	5:I:46:DT:H72	2.56	0.40
3:S:29:ARG:O	3:S:33:LEU:HG	2.22	0.40
5:U:111:DC:H2''	5:U:112:DT:C6	2.56	0.40
1:A:73:GLU:O	1:A:76:GLN:HG2	2.20	0.40
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.56	0.40
3:C:32:ARG:HD3	6:J:30:DG:OP2	2.21	0.40
5:I:24:DC:H2'	5:I:25:DG:H8	1.81	0.40
5:I:111:DC:H2''	5:I:112:DT:C6	2.56	0.40
7:L:90:TYR:CE1	7:L:173:VAL:HG21	2.56	0.40
3:S:79:ILE:HG12	3:S:82:HIS:CE1	2.56	0.40
5:U:24:DC:H2'	5:U:25:DG:H8	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:80:DA:H2''	6:V:81:DC:C6	2.57	0.40
6:V:79:DT:H2''	6:V:80:DA:N7	2.36	0.40
7:W:68:VAL:O	7:W:90:TYR:HB2	2.22	0.40

There are no symmetry-related clashes.

## 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	Percentiles	
1	A	95/135 (70%)	95 (100%)	0	0	100	100
1	E	93/135 (69%)	91 (98%)	2 (2%)	0	100	100
1	M	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
1	Q	93/135 (69%)	93 (100%)	0	0	100	100
2	B	82/103 (80%)	80 (98%)	2 (2%)	0	100	100
2	F	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
2	N	82/103 (80%)	78 (95%)	4 (5%)	0	100	100
2	R	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
3	C	102/130 (78%)	100 (98%)	2 (2%)	0	100	100
3	G	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
3	O	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
3	S	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
4	D	91/126 (72%)	87 (96%)	4 (4%)	0	100	100
4	H	91/126 (72%)	86 (94%)	5 (6%)	0	100	100
4	P	91/126 (72%)	87 (96%)	4 (4%)	0	100	100
4	T	91/126 (72%)	88 (97%)	2 (2%)	1 (1%)	14	45
7	K	172/224 (77%)	151 (88%)	20 (12%)	1 (1%)	25	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	L	191/224 (85%)	178 (93%)	13 (7%)	0	100	100
7	W	186/224 (83%)	167 (90%)	19 (10%)	0	100	100
7	X	92/224 (41%)	80 (87%)	11 (12%)	1 (1%)	14	45
All	All	2122/2872 (74%)	2019 (95%)	100 (5%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	17	ASP
7	X	5	LEU
4	T	103	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	82/110 (74%)	82 (100%)	0	100	100
1	E	83/110 (76%)	82 (99%)	1 (1%)	71	83
1	M	83/110 (76%)	83 (100%)	0	100	100
1	Q	80/110 (73%)	80 (100%)	0	100	100
2	B	70/79 (89%)	68 (97%)	2 (3%)	42	69
2	F	64/79 (81%)	62 (97%)	2 (3%)	40	67
2	N	66/79 (84%)	66 (100%)	0	100	100
2	R	65/79 (82%)	64 (98%)	1 (2%)	65	81
3	C	78/102 (76%)	77 (99%)	1 (1%)	69	82
3	G	78/102 (76%)	77 (99%)	1 (1%)	69	82
3	O	80/102 (78%)	80 (100%)	0	100	100
3	S	80/102 (78%)	80 (100%)	0	100	100
4	D	78/106 (74%)	77 (99%)	1 (1%)	69	82
4	H	76/106 (72%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P	76/106 (72%)	75 (99%)	1 (1%)	69	82
4	T	77/106 (73%)	77 (100%)	0	100	100
7	K	149/196 (76%)	143 (96%)	6 (4%)	31	61
7	L	139/196 (71%)	131 (94%)	8 (6%)	20	50
7	W	123/196 (63%)	112 (91%)	11 (9%)	9	32
7	X	56/196 (29%)	49 (88%)	7 (12%)	4	19
All	All	1683/2372 (71%)	1641 (98%)	42 (2%)	47	72

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	19	ARG
2	B	23	ARG
3	C	115	LEU
4	D	32	THR
1	E	59	GLU
2	F	18	HIS
2	F	22	LEU
3	G	110	ASN
7	K	19	GLN
7	K	28	LYS
7	K	41	LEU
7	K	42	LYS
7	K	57	VAL
7	K	153	MET
7	L	4	THR
7	L	15	THR
7	L	41	LEU
7	L	66	TYR
7	L	76	LEU
7	L	138	LEU
7	L	165	VAL
7	L	212	THR
4	P	32	THR
2	R	24	ASP
7	W	5	LEU
7	W	21	ASN
7	W	31	ARG
7	W	41	LEU
7	W	76	LEU

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Mol	Chain	Res	Type
7	W	89	THR
7	W	90	TYR
7	W	138	LEU
7	W	149	VAL
7	W	189	ILE
7	W	191	ASP
7	X	5	LEU
7	X	18	GLU
7	X	21	ASN
7	X	37	THR
7	X	57	VAL
7	X	138	LEU
7	X	196	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	67	ASN
7	K	77	ASN
7	K	142	GLN
1	Q	68	GLN
7	W	39	HIS

### 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](#)

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 [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<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	97/135 (71%)	0.19	2 (2%) 63 62	72, 101, 127, 152	0
1	E	95/135 (70%)	0.23	4 (4%) 36 34	70, 108, 148, 166	0
1	M	98/135 (72%)	0.24	0 100 100	61, 89, 122, 187	0
1	Q	95/135 (70%)	0.16	2 (2%) 63 62	62, 89, 136, 148	0
2	B	84/103 (81%)	0.22	2 (2%) 59 56	62, 92, 132, 153	0
2	F	83/103 (80%)	0.37	2 (2%) 59 56	72, 106, 161, 186	0
2	N	84/103 (81%)	0.23	2 (2%) 59 56	56, 82, 154, 198	0
2	R	80/103 (77%)	0.32	3 (3%) 40 37	65, 87, 128, 156	0
3	C	104/130 (80%)	0.24	2 (1%) 66 65	73, 107, 153, 168	0
3	G	107/130 (82%)	0.34	3 (2%) 53 51	67, 100, 167, 251	0
3	O	107/130 (82%)	0.21	1 (0%) 84 84	59, 93, 132, 173	0
3	S	107/130 (82%)	0.19	1 (0%) 84 84	66, 95, 142, 157	0
4	D	93/126 (73%)	0.11	1 (1%) 80 81	68, 98, 141, 173	0
4	H	93/126 (73%)	-0.03	0 100 100	72, 103, 141, 179	0
4	P	93/126 (73%)	0.06	0 100 100	58, 84, 127, 148	0
4	T	93/126 (73%)	0.16	1 (1%) 80 81	68, 97, 138, 164	0
5	I	146/146 (100%)	-0.71	0 100 100	110, 177, 240, 295	0
5	U	146/146 (100%)	-0.60	0 100 100	101, 141, 191, 259	0
6	J	147/147 (100%)	-0.62	0 100 100	112, 172, 218, 247	0
6	V	147/147 (100%)	-0.60	0 100 100	97, 143, 190, 230	0
7	K	177/224 (79%)	0.23	4 (2%) 60 59	76, 117, 173, 200	0
7	L	198/224 (88%)	0.25	5 (2%) 57 54	94, 155, 205, 222	0
7	W	195/224 (87%)	0.33	11 (5%) 24 23	85, 161, 217, 324	0
7	X	109/224 (48%)	0.45	10 (9%) 9 9	108, 174, 212, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2778/3458 (80%)	0.05	56 (2%) 65 64	56, 116, 198, 324	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	W	186	ASP	4.9
7	L	136	ALA	4.8
7	W	136	ALA	4.1
2	N	18	HIS	3.7
7	W	11	TRP	3.2
7	W	85	LEU	3.1
7	L	205	GLN	3.1
7	W	90	TYR	3.0
7	L	127	ALA	3.0
1	E	93	GLN	2.9
1	E	96	SER	2.8
1	Q	78	PHE	2.8
7	L	184	PHE	2.8
7	X	58	MET	2.8
7	W	131	GLU	2.7
2	N	21	VAL	2.7
4	D	41	VAL	2.6
7	X	70	MET	2.5
1	A	70	LEU	2.5
4	T	102	LEU	2.4
2	F	27	GLN	2.4
7	X	88	LEU	2.4
7	L	72	GLN	2.4
7	K	50	LEU	2.4
2	R	66	ILE	2.4
7	W	141	LEU	2.4
2	B	82	THR	2.4
1	E	94	GLU	2.3
3	G	23	LEU	2.3
7	K	33	ARG	2.3
7	W	128	ASN	2.3
7	X	50	LEU	2.3
7	X	11	TRP	2.3
2	F	97	LEU	2.2
2	R	65	VAL	2.2
3	O	23	LEU	2.2
7	W	154	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	43	VAL	2.2
2	B	62	LEU	2.2
7	X	195	TYR	2.2
7	X	87	ALA	2.1
1	Q	82	LEU	2.1
7	X	29	ARG	2.1
7	X	39	HIS	2.1
3	G	25	PHE	2.1
7	X	10	GLY	2.1
1	A	84	PHE	2.1
3	C	102	ILE	2.1
2	R	22	LEU	2.1
3	S	93	LEU	2.1
7	K	179	PRO	2.1
1	E	97	GLU	2.0
7	W	133	TYR	2.0
3	C	115	LEU	2.0
7	K	41	LEU	2.0
7	W	132	LEU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.