



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:30 am BST

PDB ID : 5OY7
Title : Structure of the 4_601_157 tetranucleosome (P1 form)
Authors : Ekundayo, B.; Richmond, T.J.; Schalch, T.
Deposited on : 2017-09-07
Resolution : 5.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

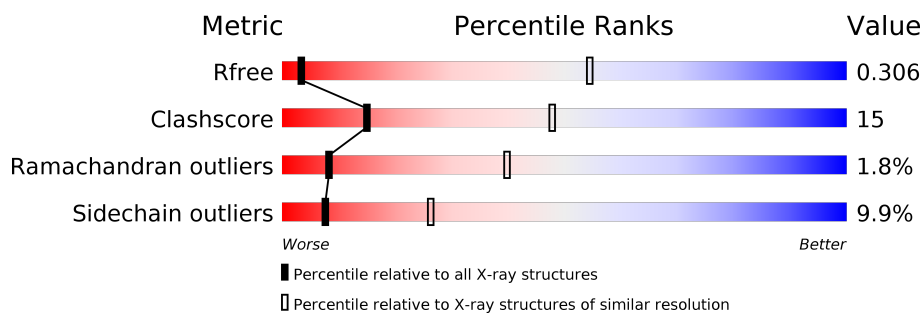
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.77 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	1008 (7.70-3.86)
Clashscore	141614	1034 (7.66-3.90)
Ramachandran outliers	138981	1003 (7.70-3.86)
Sidechain outliers	138945	1005 (7.70-3.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	D	126	<div> <div>48%</div> <div>23%</div> <div>• •</div> <div>25%</div> </div>
1	H	126	<div> <div>45%</div> <div>26%</div> <div>•</div> <div>26%</div> </div>
1	L	126	<div> <div>44%</div> <div>26%</div> <div>5% •</div> <div>25%</div> </div>
1	P	126	<div> <div>46%</div> <div>25%</div> <div>•</div> <div>26%</div> </div>
1	T	126	<div> <div>45%</div> <div>25%</div> <div>5% •</div> <div>25%</div> </div>
1	X	126	<div> <div>45%</div> <div>26%</div> <div>•</div> <div>26%</div> </div>
1	b	126	<div> <div>65%</div> <div>9%</div> <div>•</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
1	f	126	
2	A	135	
2	E	135	
2	I	135	
2	M	135	
2	Q	135	
2	U	135	
2	Y	135	
2	c	135	
3	B	102	
3	F	102	
3	J	102	
3	N	102	
3	R	102	
3	V	102	
3	Z	102	
3	d	102	
4	C	130	
4	G	130	
4	K	130	
4	O	130	
4	S	130	
4	W	130	
4	a	130	
4	e	130	

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Mol	Chain	Length	Quality of chain
5	g	634	<div><div></div><div>73%</div><div>25%</div><div></div></div>
6	h	628	<div><div></div><div>74%</div><div>24%</div><div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49215 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 H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	P	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
1	D	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	H	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
1	T	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	X	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
1	b	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	f	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	29	THR	SER	conflict	UNP P02281
P	29	THR	SER	conflict	UNP P02281
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281
T	29	THR	SER	conflict	UNP P02281
X	29	THR	SER	conflict	UNP P02281
b	29	THR	SER	conflict	UNP P02281
f	29	THR	SER	conflict	UNP P02281

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
2	Q	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	I	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	A	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	E	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
2	U	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
2	Y	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	c	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	102	ALA	GLY	conflict	UNP Q92133
M	111	ALA	GLY	conflict	UNP Q92133
Q	102	ALA	GLY	conflict	UNP Q92133
Q	111	ALA	GLY	conflict	UNP Q92133
I	102	ALA	GLY	conflict	UNP Q92133
I	111	ALA	GLY	conflict	UNP Q92133
A	102	ALA	GLY	conflict	UNP Q92133
A	111	ALA	GLY	conflict	UNP Q92133
E	102	ALA	GLY	conflict	UNP Q92133
E	111	ALA	GLY	conflict	UNP Q92133
U	102	ALA	GLY	conflict	UNP Q92133
U	111	ALA	GLY	conflict	UNP Q92133
Y	102	ALA	GLY	conflict	UNP Q92133
Y	111	ALA	GLY	conflict	UNP Q92133
c	102	ALA	GLY	conflict	UNP Q92133
c	111	ALA	GLY	conflict	UNP Q92133

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	82	Total	C	N	O	S	0	0	0
			654	412	128	113	1			
3	J	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
3	B	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
3	F	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
3	V	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
3	Z	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
3	d	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	O	105	Total	C	N	O	0	0	0
			809	510	158	141			
4	C	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	G	105	Total	C	N	O	0	0	0
			809	510	158	141			
4	K	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	S	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	W	105	Total	C	N	O	0	0	0
			809	510	158	141			
4	a	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	e	105	Total	C	N	O	0	0	0
			809	510	158	141			

- Molecule 5 is a DNA chain called DNA (619-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	g	619	Total	C	N	O	P	0	0	0
			12605	5987	2278	3721	619			

- Molecule 6 is a DNA chain called DNA (619-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	h	619	Total	C	N	O	P	0	0	0
			12774	6041	2407	3707	619			

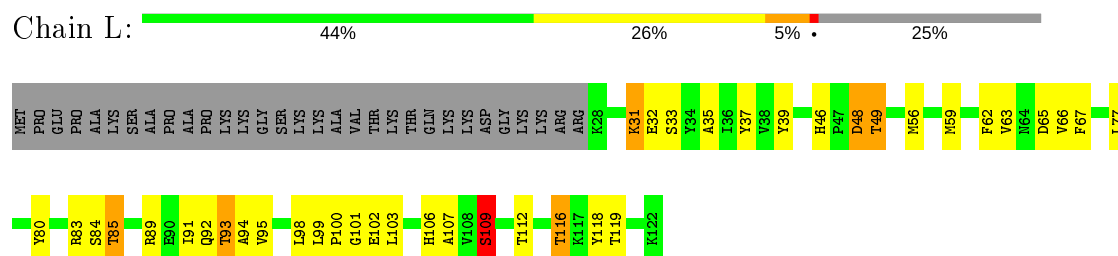
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Cl	1	0
			1	1		
7	K	1	Total	Cl	1	0
			1	1		
7	e	1	Total	Cl	1	0
			1	1		
7	C	1	Total	Cl	1	0
			1	1		
7	W	1	Total	Cl	1	0
			1	1		
7	a	1	Total	Cl	1	0
			1	1		
7	O	1	Total	Cl	1	0
			1	1		
7	S	1	Total	Cl	1	0
			1	1		

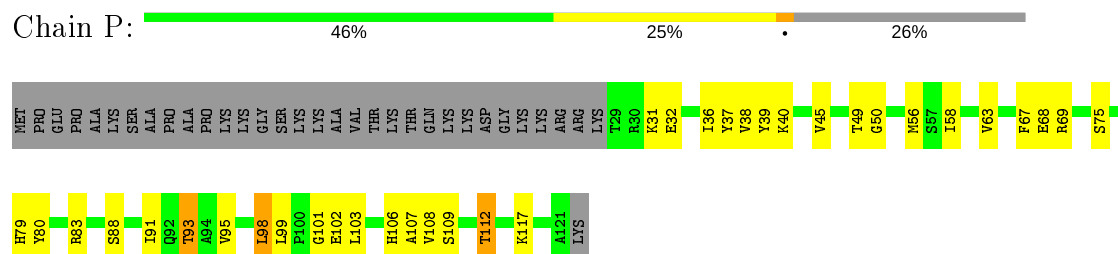
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

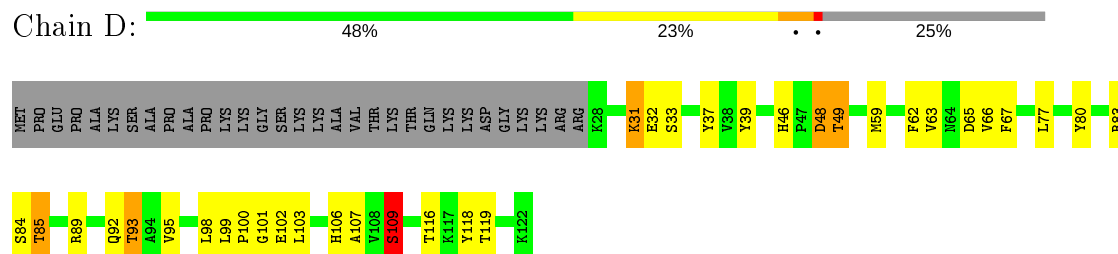
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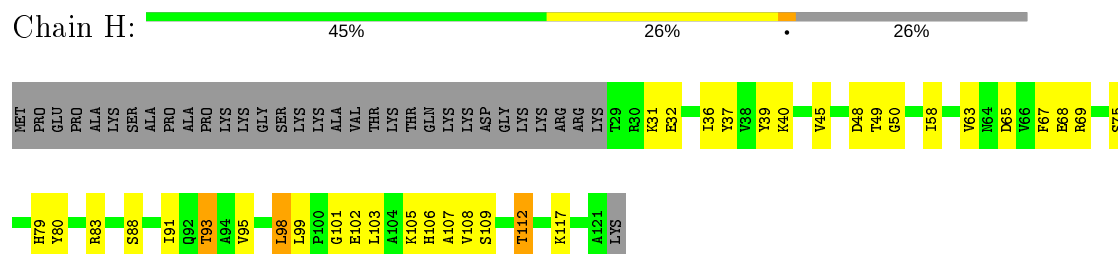
• Molecule 1: Histone H2B 1.1



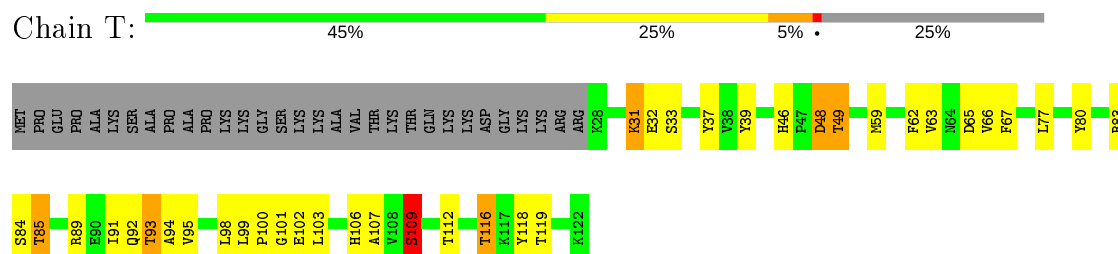
• Molecule 1: Histone H2B 1.1



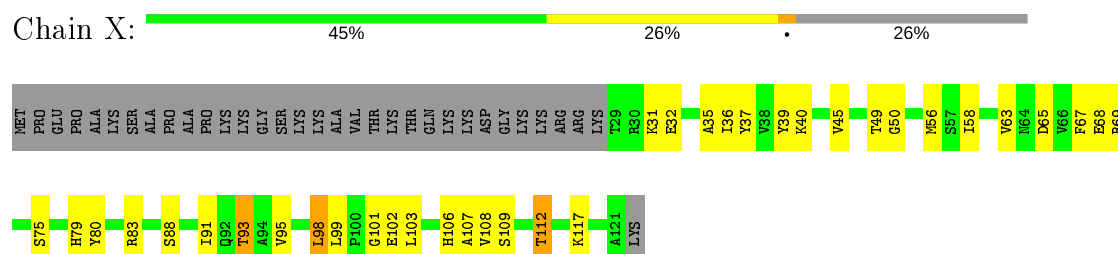
• Molecule 1: Histone H2B 1.1



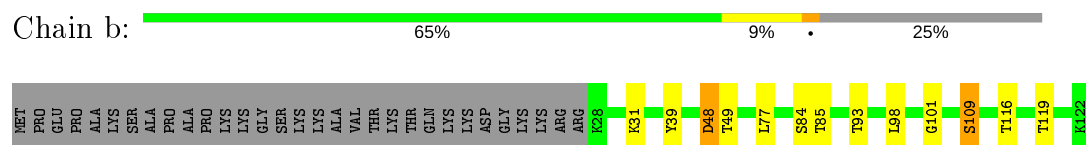
- Molecule 1: Histone H2B 1.1



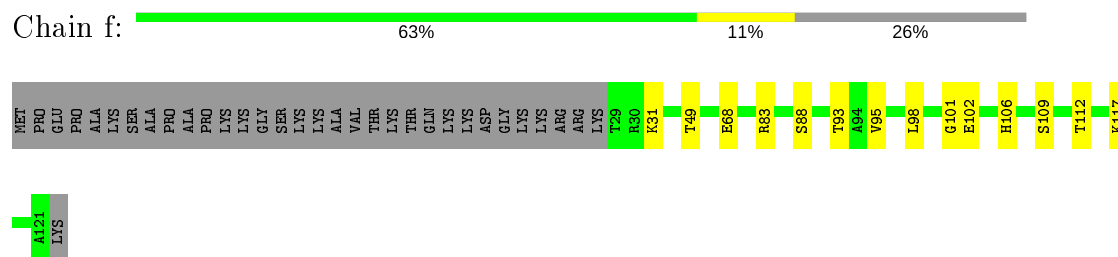
- Molecule 1: Histone H2B 1.1



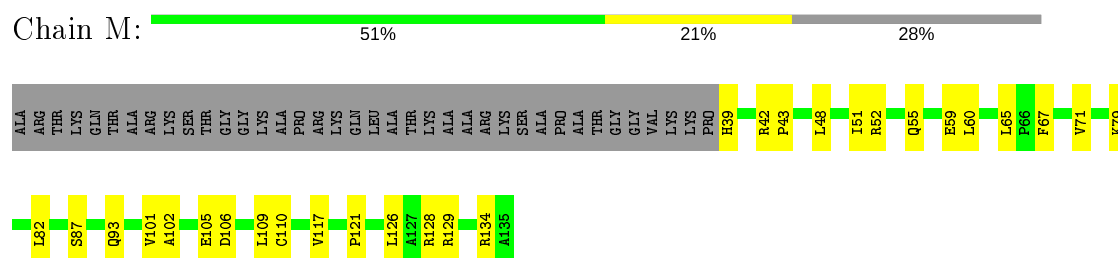
- Molecule 1: Histone H2B 1.1



- Molecule 1: Histone H2B 1.1

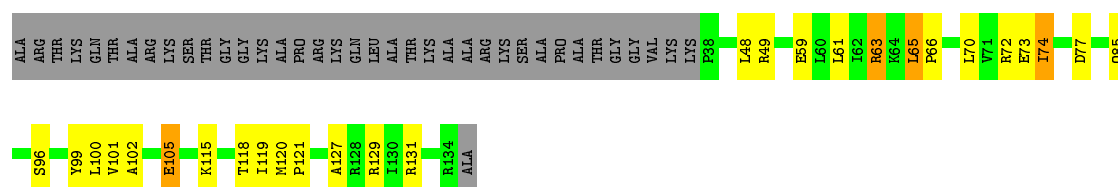


- Molecule 2: Histone H3

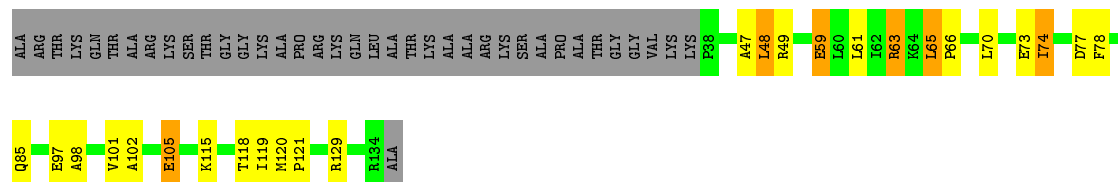


- Molecule 2: Histone H3

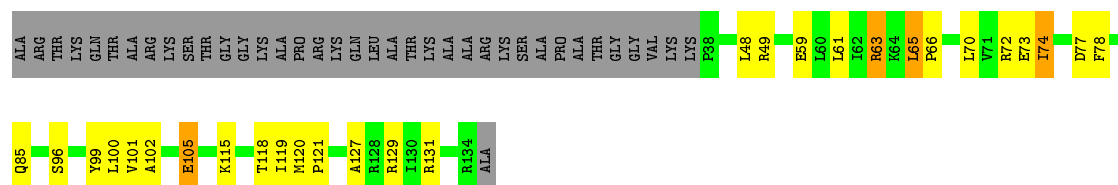




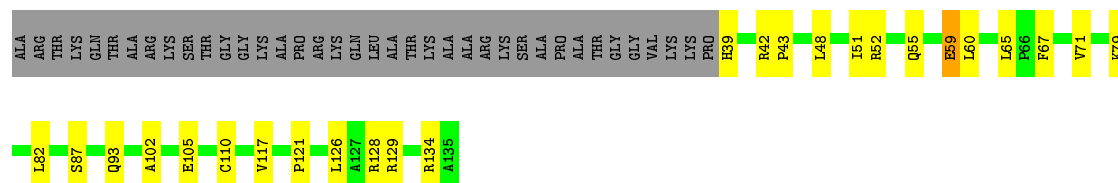
- Molecule 2: Histone H3



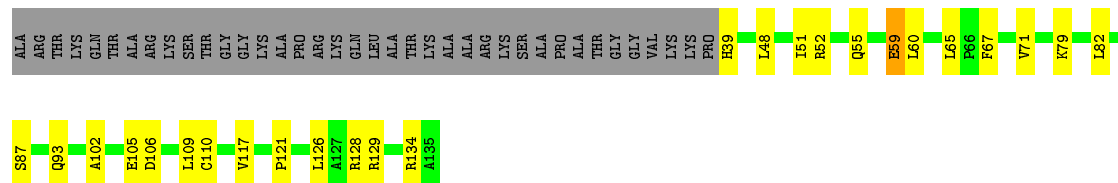
- Molecule 2: Histone H3



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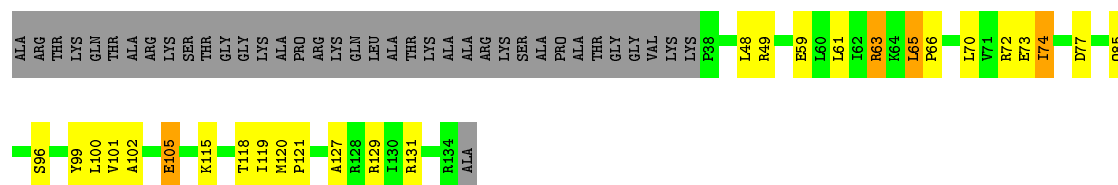


- Molecule 2: Histone H3



- Molecule 2: Histone H3





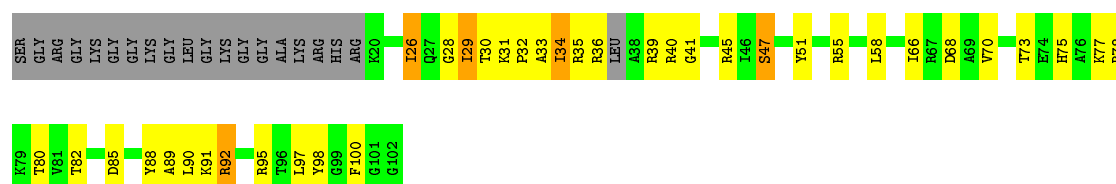
- Molecule 2: Histone H3



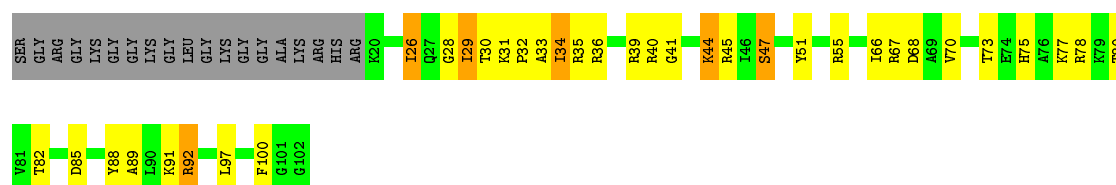
- Molecule 3: Histone H4



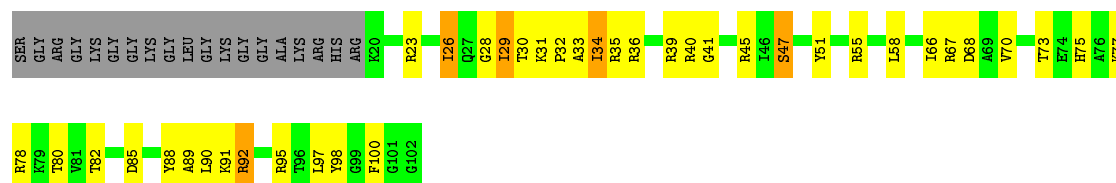
- Molecule 3: Histone H4



- Molecule 3: Histone H4

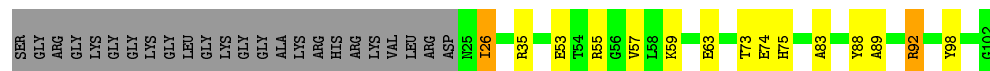


- Molecule 3: Histone H4



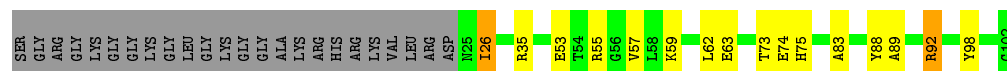
- Molecule 3: Histone H4

Chain F: 



- Molecule 3: Histone H4

Chain V: 



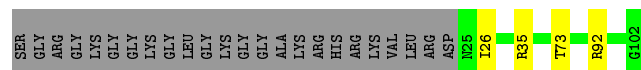
- Molecule 3: Histone H4

Chain Z: 



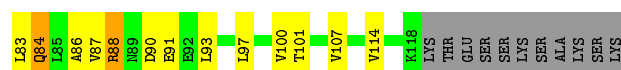
- Molecule 3: Histone H4

Chain d: 



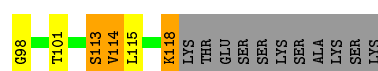
- Molecule 4: Histone H2A

Chain O: 

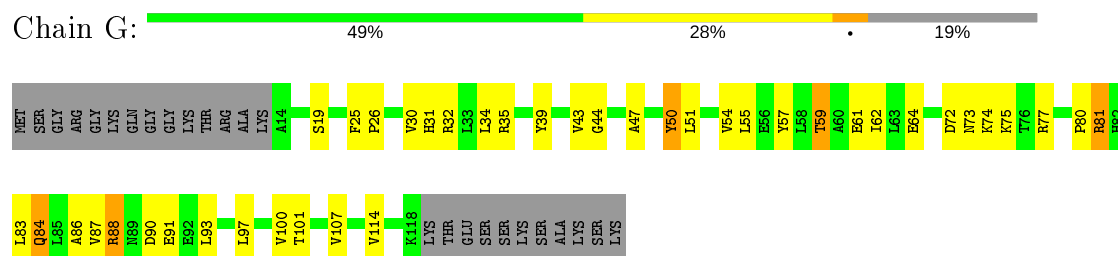


- Molecule 4: Histone H2A

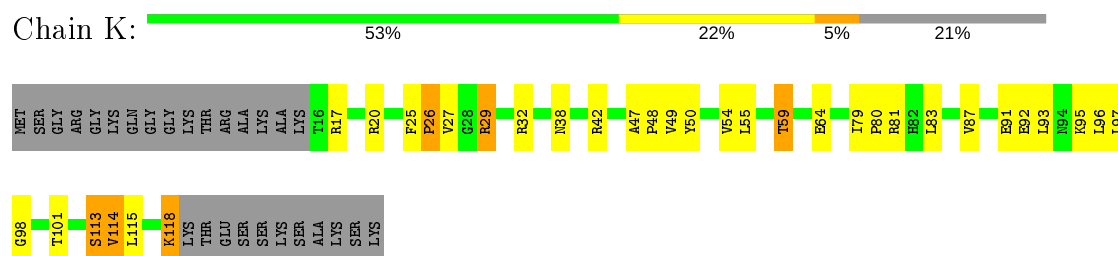
Chain C: 



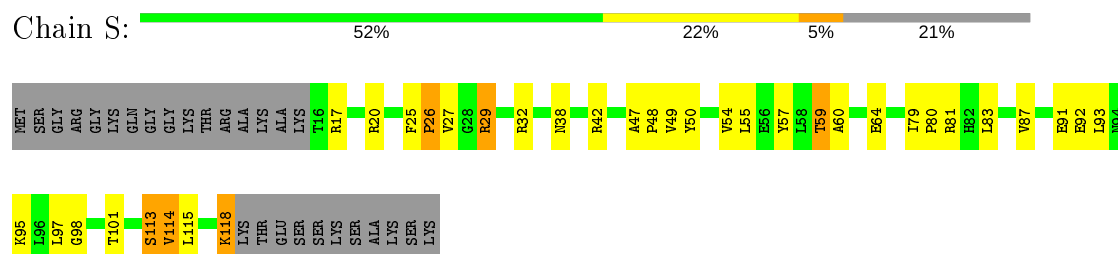
- Molecule 4: Histone H2A



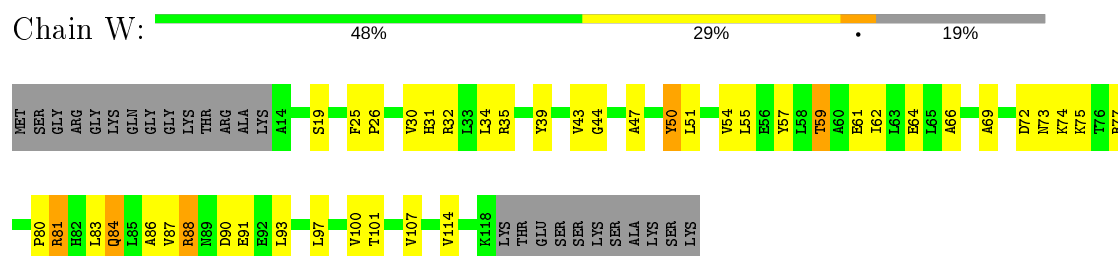
- Molecule 4: Histone H2A



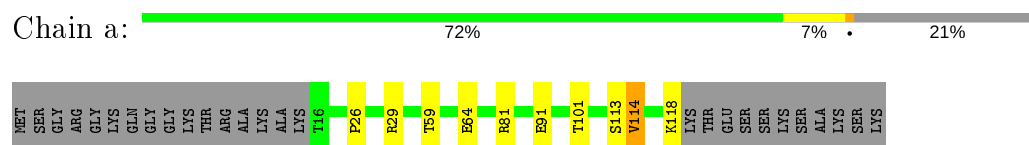
- Molecule 4: Histone H2A



- Molecule 4: Histone H2A

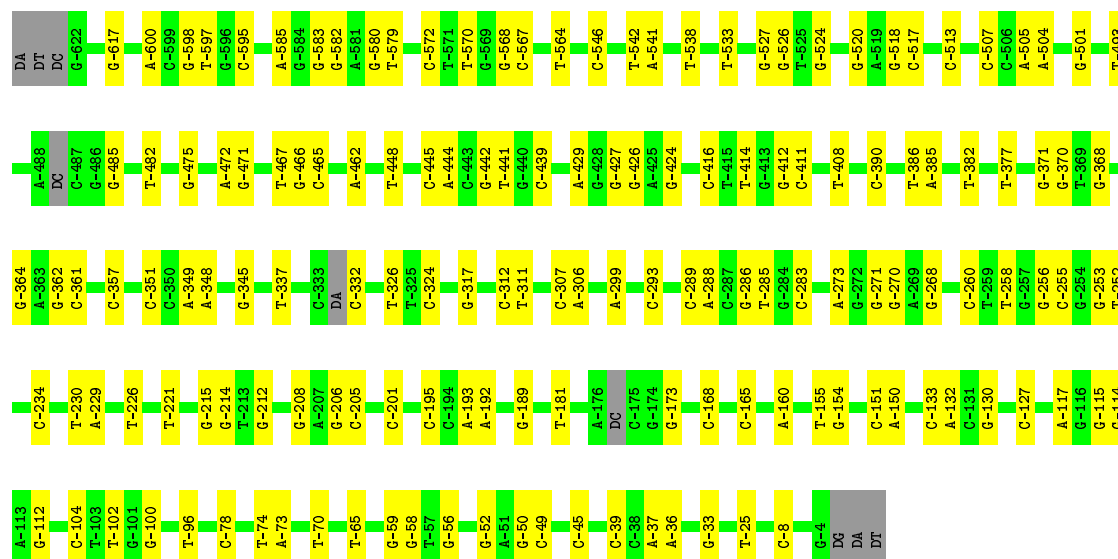


- Molecule 4: Histone H2A



- Molecule 4: Histone H2A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.62Å 161.47Å 227.91Å 78.94° 83.86° 83.74°	Depositor
Resolution (Å)	111.41 – 5.77 141.52 – 5.77	Depositor EDS
% Data completeness (in resolution range)	93.8 (111.41-5.77) 93.8 (141.52-5.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 5.77Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.219 , 0.238 0.289 , 0.306	Depositor DCC
R_{free} test set	1226 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	222.9	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 230.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	49215	wwPDB-VP
Average B, all atoms (Å ²)	246.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	D	0.49	0/756	0.64	0/1015
1	H	0.62	0/737	0.70	0/993
1	L	0.49	0/756	0.64	0/1015
1	P	0.62	0/737	0.70	0/993
1	T	0.49	0/756	0.64	0/1015
1	X	0.62	0/737	0.70	0/993
1	b	0.49	0/756	0.64	0/1015
1	f	0.62	0/737	0.70	0/993
2	A	0.66	0/814	0.73	0/1092
2	E	0.41	0/812	0.57	0/1088
2	I	0.66	0/814	0.73	0/1092
2	M	0.41	0/812	0.58	0/1088
2	Q	0.66	0/814	0.73	0/1092
2	U	0.41	0/812	0.57	0/1088
2	Y	0.66	0/814	0.73	0/1092
2	c	0.41	0/812	0.58	0/1088
3	B	0.67	0/669	0.84	0/894
3	F	0.45	0/626	0.61	0/837
3	J	0.67	0/669	0.89	1/894 (0.1%)
3	N	0.46	0/626	0.62	0/837
3	R	0.67	0/660	0.83	0/880
3	V	0.45	0/626	0.61	0/837
3	Z	0.67	0/669	0.83	0/894
3	d	0.46	0/626	0.61	0/837
4	C	0.42	0/805	0.61	0/1088
4	G	0.63	0/819	0.75	0/1106
4	K	0.43	0/805	0.61	0/1088
4	O	0.63	0/819	0.76	0/1106
4	S	0.42	0/805	0.61	0/1088
4	W	0.63	0/819	0.76	0/1106
4	a	0.43	0/805	0.61	0/1088
4	e	0.63	0/819	0.76	0/1106

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	g	0.80	28/14121 (0.2%)	1.34	144/21771 (0.7%)
6	h	0.82	29/14351 (0.2%)	1.36	165/22170 (0.7%)
All	All	0.70	57/52615 (0.1%)	1.12	310/76379 (0.4%)

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	-448	DT	O3'-P	26.30	1.92	1.61
6	h	-475	DG	C1'-N9	-8.79	1.34	1.47
5	g	622	DC	C1'-N1	7.52	1.59	1.49
5	g	151	DG	C1'-N9	-7.18	1.37	1.47
5	g	157	DT	C3'-O3'	7.08	1.53	1.44
5	g	315	DC	C1'-N1	6.62	1.57	1.49
6	h	-485	DG	C1'-N9	-6.58	1.38	1.47
6	h	-617	DG	C1'-N9	-6.58	1.38	1.47
5	g	467	DA	C1'-N9	-6.41	1.38	1.47
5	g	307	DG	C1'-N9	-6.33	1.38	1.47
6	h	-471	DG	C1'-N9	-6.32	1.38	1.47
5	g	474	DC	C1'-N1	6.27	1.57	1.49
6	h	-154	DG	C1'-N9	-6.25	1.38	1.47
5	g	449	DG	C1'-N9	-6.18	1.38	1.47
6	h	-324	DC	C1'-N1	6.18	1.57	1.49
6	h	-173	DG	C1'-N9	-6.16	1.38	1.47
5	g	313	DT	C1'-N1	6.14	1.57	1.49
6	h	-462	DA	C1'-N9	-6.12	1.38	1.47
6	h	-306	DA	C1'-N9	-6.06	1.38	1.47
5	g	620	DT	C1'-N1	6.02	1.57	1.49
5	g	480	DG	C1'-N9	-6.01	1.38	1.47
5	g	162	DC	C1'-N1	5.91	1.56	1.49
5	g	319	DC	C1'-N1	5.82	1.56	1.49
6	h	-472	DA	C1'-N9	-5.75	1.39	1.47
6	h	-8	DC	C1'-N1	5.74	1.56	1.49
6	h	-168	DC	C1'-N1	5.71	1.56	1.49
6	h	-299	DA	C1'-N9	-5.70	1.39	1.47
5	g	618	DT	C1'-N1	5.67	1.56	1.49
5	g	154	DC	C1'-N1	5.67	1.56	1.49
6	h	-165	DC	C1'-N1	5.62	1.56	1.49
5	g	312	DG	C1'-N9	-5.60	1.39	1.47
6	h	-466	DG	C1'-N9	-5.59	1.39	1.47
5	g	152	DT	C1'-N1	5.55	1.56	1.49
5	g	487	DG	C1'-N9	-5.55	1.39	1.47
5	g	465	DG	C1'-N9	-5.53	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	g	321	DG	C1'-N9	-5.52	1.39	1.47
6	h	-312	DC	C1'-N1	5.49	1.56	1.49
5	g	155	DA	C1'-N9	-5.34	1.39	1.47
6	h	-326	DT	C1'-N1	5.32	1.56	1.49
6	h	-311	DT	C1'-N1	5.28	1.56	1.49
5	g	159	DC	C1'-N1	5.28	1.56	1.49
6	h	-467	DT	C1'-N1	5.24	1.56	1.49
5	g	326	DA	C1'-N9	-5.23	1.40	1.47
6	h	-155	DT	C1'-N1	5.22	1.56	1.49
5	g	330	DC	C1'-N1	5.22	1.56	1.49
5	g	8	DG	C1'-N9	-5.21	1.40	1.47
6	h	-332	DC	C1'-N1	5.21	1.56	1.49
6	h	-160	DA	C1'-N9	-5.19	1.40	1.47
6	h	-317	DG	C1'-N9	-5.17	1.40	1.47
6	h	-465	DC	C1'-N1	5.13	1.55	1.49
6	h	-307	DC	C1'-N1	5.10	1.55	1.49
6	h	-482	DT	C1'-N1	5.09	1.55	1.49
5	g	170	DA	C1'-N9	-5.08	1.40	1.47
6	h	-150	DA	C1'-N9	-5.07	1.40	1.47
5	g	472	DT	C1'-N1	5.07	1.55	1.49
6	h	-151	DC	C1'-N1	5.06	1.55	1.49
5	g	165	DG	C1'-N9	-5.05	1.40	1.47

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	-448	DT	P-O3'-C3'	29.45	155.04	119.70
5	g	158	DA	OP1-P-OP2	17.27	145.50	119.60
5	g	157	DT	OP1-P-O3'	-14.16	74.04	105.20
5	g	157	DT	OP2-P-O3'	-13.26	76.02	105.20
6	h	-448	DT	O3'-P-O5'	12.06	126.92	104.00
6	h	-371	DG	O3'-P-O5'	-12.03	81.14	104.00
6	h	-215	DG	O3'-P-O5'	-11.97	81.25	104.00
6	h	-59	DG	O3'-P-O5'	-11.95	81.29	104.00
6	h	-527	DG	O3'-P-O5'	-11.95	81.30	104.00
6	h	-215	DG	OP2-P-O3'	-10.03	83.13	105.20
6	h	-59	DG	OP2-P-O3'	-10.02	83.15	105.20
6	h	-371	DG	OP2-P-O3'	-9.98	83.24	105.20
6	h	-527	DG	OP2-P-O3'	-9.97	83.25	105.20
6	h	-65	DT	O4'-C1'-N1	8.82	114.17	108.00
6	h	-377	DT	O4'-C1'-N1	8.79	114.15	108.00
6	h	-533	DT	O4'-C1'-N1	8.75	114.13	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	-221	DT	O4'-C1'-N1	8.68	114.08	108.00
6	h	-370	DG	O4'-C1'-N9	8.49	113.95	108.00
6	h	-526	DG	O4'-C1'-N9	8.45	113.92	108.00
6	h	-58	DG	O4'-C1'-N9	8.45	113.91	108.00
6	h	-214	DG	O4'-C1'-N9	8.41	113.89	108.00
6	h	-513	DC	P-O3'-C3'	8.03	129.34	119.70
6	h	-201	DC	P-O3'-C3'	7.99	129.29	119.70
6	h	-45	DC	P-O3'-C3'	7.97	129.26	119.70
6	h	-357	DC	P-O3'-C3'	7.96	129.25	119.70
6	h	-230	DT	O4'-C1'-N1	7.80	113.46	108.00
6	h	-74	DT	O4'-C1'-N1	7.77	113.44	108.00
6	h	-542	DT	O4'-C1'-N1	7.75	113.42	108.00
5	g	188	DT	O4'-C1'-N1	7.75	113.42	108.00
5	g	32	DT	O4'-C1'-N1	7.74	113.42	108.00
6	h	-386	DT	O4'-C1'-N1	7.68	113.38	108.00
5	g	158	DA	O5'-P-OP1	-7.62	98.84	105.70
5	g	494	DG	P-O3'-C3'	7.62	128.84	119.70
5	g	26	DG	P-O3'-C3'	7.61	128.83	119.70
5	g	344	DT	O4'-C1'-N1	7.61	113.33	108.00
5	g	500	DT	O4'-C1'-N1	7.57	113.30	108.00
5	g	182	DG	P-O3'-C3'	7.54	128.75	119.70
5	g	338	DG	P-O3'-C3'	7.51	128.71	119.70
6	h	-102	DT	O4'-C1'-N1	7.33	113.13	108.00
6	h	-570	DT	O4'-C1'-N1	7.27	113.09	108.00
6	h	-258	DT	O4'-C1'-N1	7.24	113.07	108.00
5	g	370	DC	O4'-C1'-N1	7.23	113.06	108.00
5	g	214	DC	O4'-C1'-N1	7.22	113.05	108.00
5	g	360	DA	O4'-C1'-N9	7.22	113.05	108.00
5	g	58	DC	O4'-C1'-N1	7.21	113.05	108.00
6	h	-414	DT	O4'-C1'-N1	7.21	113.04	108.00
5	g	204	DA	O4'-C1'-N9	7.18	113.03	108.00
5	g	516	DA	O4'-C1'-N9	7.12	112.99	108.00
6	h	-582	DG	O4'-C1'-N9	-7.10	103.03	108.00
5	g	48	DA	O4'-C1'-N9	7.09	112.96	108.00
6	h	-114	DG	O4'-C1'-N9	-7.08	103.05	108.00
5	g	526	DC	O4'-C1'-N1	7.07	112.95	108.00
6	h	-270	DG	O4'-C1'-N9	-7.06	103.06	108.00
6	h	-273	DA	P-O3'-C3'	7.01	128.11	119.70
6	h	-426	DG	O4'-C1'-N9	-7.00	103.10	108.00
6	h	-493	DT	P-O3'-C3'	7.00	128.09	119.70
6	h	-25	DT	P-O3'-C3'	6.96	128.05	119.70
6	h	-429	DA	P-O3'-C3'	6.95	128.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	-585	DA	P-O3'-C3'	6.95	128.04	119.70
6	h	-181	DT	P-O3'-C3'	6.95	128.04	119.70
6	h	-117	DA	P-O3'-C3'	6.89	127.97	119.70
6	h	-337	DT	P-O3'-C3'	6.89	127.97	119.70
5	g	590	DT	P-O3'-C3'	6.87	127.94	119.70
5	g	121	DC	P-O3'-C3'	6.87	127.94	119.70
6	h	-368	DG	O4'-C1'-N9	6.86	112.80	108.00
5	g	589	DC	P-O3'-C3'	6.86	127.93	119.70
5	g	434	DT	P-O3'-C3'	6.84	127.91	119.70
5	g	278	DT	P-O3'-C3'	6.84	127.91	119.70
5	g	277	DC	P-O3'-C3'	6.83	127.90	119.70
6	h	-526	DG	P-O3'-C3'	6.83	127.90	119.70
5	g	102	DA	P-O3'-C3'	6.83	127.90	119.70
5	g	122	DT	P-O3'-C3'	6.83	127.89	119.70
5	g	433	DC	P-O3'-C3'	6.82	127.89	119.70
5	g	496	DC	P-O3'-C3'	6.81	127.87	119.70
5	g	340	DC	P-O3'-C3'	6.79	127.84	119.70
6	h	-214	DG	P-O3'-C3'	6.78	127.84	119.70
6	h	-212	DG	O4'-C1'-N9	6.78	112.74	108.00
6	h	-370	DG	P-O3'-C3'	6.77	127.83	119.70
6	h	-580	DG	P-O3'-C3'	6.76	127.81	119.70
5	g	570	DA	P-O3'-C3'	6.76	127.81	119.70
5	g	28	DC	P-O3'-C3'	6.74	127.79	119.70
5	g	258	DA	P-O3'-C3'	6.74	127.78	119.70
5	g	414	DA	P-O3'-C3'	6.73	127.78	119.70
5	g	184	DC	P-O3'-C3'	6.72	127.76	119.70
6	h	-112	DG	P-O3'-C3'	6.71	127.76	119.70
6	h	-58	DG	P-O3'-C3'	6.71	127.76	119.70
6	h	-268	DG	P-O3'-C3'	6.71	127.75	119.70
6	h	-56	DG	O4'-C1'-N9	6.70	112.69	108.00
6	h	-524	DG	O4'-C1'-N9	6.69	112.69	108.00
6	h	-424	DG	P-O3'-C3'	6.69	127.72	119.70
5	g	223	DC	P-O3'-C3'	6.66	127.69	119.70
6	h	-361	DC	O4'-C1'-N1	6.64	112.65	108.00
5	g	535	DC	P-O3'-C3'	6.63	127.66	119.70
5	g	67	DC	P-O3'-C3'	6.62	127.64	119.70
6	h	-412	DG	P-O3'-C3'	6.58	127.60	119.70
6	h	-568	DG	P-O3'-C3'	6.57	127.59	119.70
6	h	-100	DG	P-O3'-C3'	6.57	127.59	119.70
5	g	534	DA	P-O3'-C3'	6.56	127.57	119.70
5	g	379	DC	P-O3'-C3'	6.55	127.56	119.70
5	g	222	DA	P-O3'-C3'	6.55	127.56	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	378	DA	P-O3'-C3'	6.55	127.56	119.70
5	g	66	DA	P-O3'-C3'	6.52	127.52	119.70
6	h	-37	DA	P-O3'-C3'	6.51	127.52	119.70
6	h	-205	DC	O4'-C1'-N1	6.49	112.55	108.00
6	h	-256	DG	P-O3'-C3'	6.49	127.49	119.70
6	h	-349	DA	P-O3'-C3'	6.45	127.44	119.70
5	g	95	DA	O4'-C1'-N9	6.45	112.51	108.00
5	g	251	DA	O4'-C1'-N9	6.45	112.51	108.00
6	h	-49	DC	O4'-C1'-N1	6.44	112.51	108.00
6	h	-442	DG	P-O3'-C3'	6.44	127.42	119.70
6	h	-193	DA	P-O3'-C3'	6.42	127.41	119.70
6	h	-286	DG	P-O3'-C3'	6.42	127.41	119.70
6	h	-505	DA	P-O3'-C3'	6.42	127.40	119.70
6	h	-289	DC	P-O3'-C3'	6.42	127.40	119.70
5	g	293	DG	O4'-C1'-N9	-6.42	103.51	108.00
6	h	-130	DG	P-O3'-C3'	6.41	127.40	119.70
5	g	407	DA	O4'-C1'-N9	6.39	112.47	108.00
6	h	-598	DG	P-O3'-C3'	6.39	127.36	119.70
6	h	-526	DG	O5'-P-OP2	6.38	118.36	110.70
6	h	-445	DC	P-O3'-C3'	6.38	127.35	119.70
5	g	563	DA	O4'-C1'-N9	6.37	112.46	108.00
6	h	-133	DC	P-O3'-C3'	6.34	127.31	119.70
6	h	-600	DA	OP2-P-O3'	6.33	119.12	105.20
6	h	-527	DG	P-O3'-C3'	6.32	127.29	119.70
5	g	585	DT	P-O3'-C3'	6.32	127.28	119.70
6	h	-517	DC	O4'-C1'-N1	6.31	112.42	108.00
6	h	-370	DG	O5'-P-OP2	6.30	118.26	110.70
6	h	-58	DG	O5'-P-OP2	6.29	118.25	110.70
5	g	273	DT	P-O3'-C3'	6.26	127.22	119.70
6	h	-59	DG	P-O3'-C3'	6.26	127.21	119.70
5	g	429	DT	P-O3'-C3'	6.26	127.21	119.70
6	h	-226	DT	N3-C2-O2	-6.26	118.55	122.30
5	g	117	DT	P-O3'-C3'	6.24	127.19	119.70
6	h	-214	DG	O5'-P-OP2	6.24	118.19	110.70
6	h	-215	DG	P-O3'-C3'	6.23	127.17	119.70
6	h	-371	DG	P-O3'-C3'	6.21	127.15	119.70
5	g	257	DC	O4'-C1'-N1	6.14	112.30	108.00
6	h	-371	DG	C3'-C2'-C1'	-6.14	95.13	102.50
6	h	-215	DG	C3'-C2'-C1'	-6.13	95.14	102.50
5	g	403	DT	O4'-C1'-N1	6.12	112.28	108.00
5	g	101	DC	O4'-C1'-N1	6.08	112.26	108.00
6	h	-59	DG	C3'-C2'-C1'	-6.08	95.21	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	569	DC	O4'-C1'-N1	6.07	112.25	108.00
6	h	-527	DG	C3'-C2'-C1'	-6.04	95.25	102.50
5	g	362	DC	P-O3'-C3'	6.03	126.93	119.70
5	g	64	DA	O4'-C1'-N9	6.02	112.21	108.00
5	g	376	DA	O4'-C1'-N9	6.02	112.21	108.00
5	g	413	DC	O4'-C1'-N1	6.00	112.20	108.00
5	g	559	DT	O4'-C1'-N1	6.00	112.20	108.00
6	h	-538	DT	N3-C2-O2	-6.00	118.70	122.30
6	h	-527	DG	OP1-P-O3'	-5.99	92.03	105.20
6	h	-59	DG	OP1-P-O3'	-5.98	92.04	105.20
5	g	532	DA	O4'-C1'-N9	5.98	112.19	108.00
5	g	361	DG	P-O3'-C3'	5.96	126.86	119.70
5	g	49	DG	P-O3'-C3'	5.96	126.85	119.70
6	h	-70	DT	N3-C2-O2	-5.96	118.72	122.30
5	g	517	DG	P-O3'-C3'	5.96	126.85	119.70
5	g	205	DG	P-O3'-C3'	5.95	126.84	119.70
5	g	206	DC	P-O3'-C3'	5.95	126.83	119.70
5	g	91	DT	O4'-C1'-N1	5.94	112.16	108.00
5	g	50	DC	P-O3'-C3'	5.93	126.82	119.70
5	g	220	DA	O4'-C1'-N9	5.93	112.16	108.00
6	h	-215	DG	OP1-P-O3'	-5.93	92.16	105.20
5	g	247	DT	O4'-C1'-N1	5.93	112.15	108.00
5	g	109	DT	P-O3'-C3'	5.91	126.80	119.70
6	h	-371	DG	OP1-P-O3'	-5.91	92.19	105.20
5	g	276	DT	O4'-C1'-N1	5.90	112.13	108.00
5	g	120	DT	O4'-C1'-N1	5.89	112.12	108.00
6	h	-382	DT	N3-C2-O2	-5.88	118.77	122.30
5	g	577	DT	P-O3'-C3'	5.88	126.76	119.70
5	g	588	DT	O4'-C1'-N1	5.88	112.12	108.00
5	g	421	DT	P-O3'-C3'	5.86	126.73	119.70
5	g	265	DT	P-O3'-C3'	5.85	126.72	119.70
5	g	518	DC	P-O3'-C3'	5.83	126.69	119.70
5	g	432	DT	O4'-C1'-N1	5.78	112.05	108.00
5	g	504	DT	P-O3'-C3'	5.76	126.62	119.70
5	g	348	DT	P-O3'-C3'	5.76	126.61	119.70
5	g	36	DT	P-O3'-C3'	5.75	126.60	119.70
6	h	-288	DA	O4'-C1'-N9	5.74	112.02	108.00
6	h	-260	DC	O4'-C1'-N1	5.73	112.01	108.00
5	g	133	DG	P-O3'-C3'	5.72	126.56	119.70
5	g	289	DG	P-O3'-C3'	5.72	126.56	119.70
5	g	197	DC	P-O3'-C3'	5.72	126.56	119.70
5	g	445	DG	P-O3'-C3'	5.72	126.56	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	111	DA	O4'-C1'-N9	5.70	111.99	108.00
5	g	192	DT	P-O3'-C3'	5.68	126.52	119.70
5	g	509	DC	P-O3'-C3'	5.68	126.51	119.70
6	h	-132	DA	O4'-C1'-N9	5.67	111.97	108.00
5	g	41	DC	P-O3'-C3'	5.65	126.48	119.70
5	g	353	DC	P-O3'-C3'	5.61	126.44	119.70
6	h	-293	DC	P-O3'-C3'	5.61	126.43	119.70
6	h	-104	DC	O4'-C1'-N1	5.58	111.91	108.00
6	h	-444	DA	O4'-C1'-N9	5.58	111.90	108.00
6	h	-416	DC	O4'-C1'-N1	5.57	111.90	108.00
6	h	-572	DC	O4'-C1'-N1	5.56	111.89	108.00
5	g	389	DC	O4'-C1'-N1	5.55	111.89	108.00
5	g	231	DC	P-O3'-C3'	5.55	126.36	119.70
5	g	77	DC	O4'-C1'-N1	5.54	111.88	108.00
5	g	267	DA	O4'-C1'-N9	5.54	111.88	108.00
5	g	236	DT	O4'-C1'-N1	5.52	111.86	108.00
5	g	543	DC	P-O3'-C3'	5.52	126.32	119.70
6	h	-189	DG	O4'-C1'-N9	-5.49	104.16	108.00
6	h	-100	DG	C1'-O4'-C4'	-5.49	104.61	110.10
6	h	-58	DG	C1'-O4'-C4'	-5.49	104.61	110.10
5	g	423	DA	O4'-C1'-N9	5.48	111.84	108.00
6	h	-351	DC	P-O3'-C3'	5.48	126.27	119.70
6	h	-526	DG	C1'-O4'-C4'	-5.47	104.63	110.10
6	h	-214	DG	C1'-O4'-C4'	-5.47	104.62	110.10
6	h	-370	DG	C1'-O4'-C4'	-5.47	104.63	110.10
5	g	579	DA	O4'-C1'-N9	5.47	111.83	108.00
6	h	-568	DG	C1'-O4'-C4'	-5.47	104.63	110.10
5	g	80	DT	O4'-C1'-N1	5.46	111.82	108.00
5	g	507	DG	O4'-C1'-N9	5.46	111.82	108.00
5	g	233	DC	O4'-C1'-N1	5.45	111.81	108.00
5	g	45	DG	C3'-C2'-C1'	-5.44	95.97	102.50
5	g	75	DC	P-O3'-C3'	5.43	126.22	119.70
5	g	357	DG	C3'-C2'-C1'	-5.43	95.98	102.50
6	h	-33	DG	O4'-C1'-N9	-5.43	104.20	108.00
5	g	513	DG	C3'-C2'-C1'	-5.43	95.98	102.50
5	g	545	DC	O4'-C1'-N1	5.43	111.80	108.00
6	h	-507	DC	P-O3'-C3'	5.43	126.21	119.70
6	h	-412	DG	C1'-O4'-C4'	-5.41	104.69	110.10
5	g	392	DT	O4'-C1'-N1	5.41	111.78	108.00
6	h	-195	DC	P-O3'-C3'	5.40	126.19	119.70
5	g	201	DG	C3'-C2'-C1'	-5.40	96.02	102.50
6	h	-39	DC	P-O3'-C3'	5.39	126.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	-501	DG	O4'-C1'-N9	-5.38	104.23	108.00
6	h	-564	DT	P-O3'-C3'	5.38	126.15	119.70
5	g	387	DC	P-O3'-C3'	5.38	126.15	119.70
6	h	-448	DT	OP2-P-O3'	-5.38	93.37	105.20
6	h	-595	DC	O4'-C1'-N1	5.36	111.75	108.00
6	h	-206	DG	O4'-C1'-N9	5.36	111.75	108.00
6	h	-256	DG	C1'-O4'-C4'	-5.36	104.74	110.10
6	h	-444	DA	P-O3'-C3'	5.35	126.12	119.70
6	h	-345	DG	O4'-C1'-N9	-5.35	104.26	108.00
6	h	-348	DA	P-O3'-C3'	5.34	126.11	119.70
6	h	-518	DG	O4'-C1'-N9	5.34	111.74	108.00
6	h	-36	DA	P-O3'-C3'	5.34	126.11	119.70
5	g	418	DG	O4'-C1'-N9	5.34	111.74	108.00
6	h	-192	DA	P-O3'-C3'	5.33	126.10	119.70
6	h	-288	DA	P-O3'-C3'	5.32	126.09	119.70
6	h	-504	DA	P-O3'-C3'	5.31	126.08	119.70
5	g	548	DT	O4'-C1'-N1	5.31	111.71	108.00
6	h	-127	DC	O4'-C1'-N1	5.29	111.70	108.00
6	h	-362	DG	O4'-C1'-N9	5.29	111.70	108.00
6	h	-132	DA	P-O3'-C3'	5.28	126.03	119.70
6	h	-364	DG	C1'-O4'-C4'	-5.27	104.83	110.10
6	h	-439	DC	O4'-C1'-N1	5.26	111.68	108.00
6	h	-408	DT	P-O3'-C3'	5.25	126.00	119.70
6	h	-520	DG	C1'-O4'-C4'	-5.25	104.85	110.10
5	g	262	DG	O4'-C1'-N9	5.25	111.67	108.00
5	g	351	DG	O4'-C1'-N9	5.25	111.67	108.00
6	h	-115	DG	P-O3'-C3'	5.25	125.99	119.70
5	g	39	DG	O4'-C1'-N9	5.24	111.67	108.00
6	h	-252	DT	P-O3'-C3'	5.24	125.99	119.70
6	h	-283	DC	O4'-C1'-N1	5.24	111.67	108.00
5	g	545	DC	C1'-O4'-C4'	-5.23	104.87	110.10
5	g	203	DC	O4'-C1'-N1	5.21	111.65	108.00
5	g	195	DG	O4'-C1'-N9	5.21	111.64	108.00
5	g	233	DC	C1'-O4'-C4'	-5.21	104.89	110.10
5	g	574	DG	O4'-C1'-N9	5.21	111.64	108.00
5	g	344	DT	C1'-O4'-C4'	-5.20	104.90	110.10
6	h	-96	DT	P-O3'-C3'	5.20	125.94	119.70
6	h	-52	DG	C1'-O4'-C4'	-5.20	104.90	110.10
5	g	500	DT	C1'-O4'-C4'	-5.20	104.90	110.10
5	g	389	DC	C1'-O4'-C4'	-5.19	104.91	110.10
6	h	-50	DG	O4'-C1'-N9	5.19	111.64	108.00
5	g	106	DG	O4'-C1'-N9	5.19	111.64	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	-583	DG	P-O3'-C3'	5.19	125.93	119.70
6	h	-271	DG	P-O3'-C3'	5.18	125.92	119.70
6	h	-255	DC	O4'-C1'-N1	5.18	111.63	108.00
6	h	-370	DG	OP1-P-OP2	5.18	127.36	119.60
5	g	186	DG	O4'-C1'-N9	5.17	111.62	108.00
6	h	-427	DG	P-O3'-C3'	5.17	125.91	119.70
3	J	44	LYS	CB-CA-C	-5.17	100.06	110.40
6	h	-234	DC	O4'-C1'-N1	5.17	111.62	108.00
5	g	32	DT	C1'-O4'-C4'	-5.16	104.94	110.10
6	h	-214	DG	OP1-P-OP2	5.15	127.32	119.60
6	h	-58	DG	OP1-P-OP2	5.14	127.32	119.60
6	h	-597	DT	O4'-C1'-N1	5.14	111.60	108.00
5	g	47	DC	O4'-C1'-N1	5.13	111.59	108.00
5	g	78	DG	P-O3'-C3'	5.12	125.85	119.70
5	g	188	DT	C1'-O4'-C4'	-5.12	104.98	110.10
6	h	-208	DG	C1'-O4'-C4'	-5.12	104.98	110.10
5	g	342	DG	O4'-C1'-N9	5.11	111.58	108.00
6	h	-526	DG	OP1-P-OP2	5.11	127.27	119.60
6	h	-78	DC	O4'-C1'-N1	5.11	111.58	108.00
5	g	563	DA	C1'-O4'-C4'	-5.11	104.99	110.10
6	h	-541	DA	C3'-C2'-C1'	-5.11	96.37	102.50
6	h	-385	DA	C3'-C2'-C1'	-5.11	96.37	102.50
5	g	251	DA	C1'-O4'-C4'	-5.10	105.00	110.10
6	h	-229	DA	C3'-C2'-C1'	-5.10	96.38	102.50
5	g	77	DC	C1'-O4'-C4'	-5.10	105.00	110.10
5	g	95	DA	C1'-O4'-C4'	-5.09	105.01	110.10
5	g	234	DG	P-O3'-C3'	5.09	125.81	119.70
6	h	-390	DC	O4'-C1'-N1	5.08	111.56	108.00
5	g	426	DC	O4'-C1'-N1	5.08	111.56	108.00
5	g	359	DC	O4'-C1'-N1	5.07	111.55	108.00
6	h	-285	DT	O4'-C1'-N1	5.07	111.55	108.00
6	h	-411	DC	O4'-C1'-N1	5.05	111.54	108.00
6	h	-73	DA	C3'-C2'-C1'	-5.05	96.43	102.50
6	h	-546	DC	O4'-C1'-N1	5.05	111.54	108.00
6	h	-441	DT	O4'-C1'-N1	5.05	111.54	108.00
6	h	-567	DC	O4'-C1'-N1	5.05	111.53	108.00
5	g	390	DG	P-O3'-C3'	5.05	125.75	119.70
6	h	-579	DT	O4'-C1'-N1	5.05	111.53	108.00
5	g	239	DC	P-O3'-C3'	5.03	125.73	119.70
5	g	515	DC	O4'-C1'-N1	5.02	111.52	108.00
5	g	582	DC	O4'-C1'-N1	5.02	111.51	108.00
5	g	30	DG	O4'-C1'-N9	5.01	111.50	108.00

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	D	745	0	773	29	5
1	H	726	0	747	33	5
1	L	745	0	773	33	5
1	P	726	0	747	32	5
1	T	745	0	773	30	5
1	X	726	0	747	33	5
1	b	745	0	773	0	4
1	f	726	0	747	0	4
2	A	802	0	841	17	0
2	E	801	0	838	13	0
2	I	802	0	841	23	0
2	M	801	0	838	14	0
2	Q	802	0	841	16	0
2	U	801	0	838	13	0
2	Y	802	0	841	17	0
2	c	801	0	838	0	0
3	B	662	0	709	37	1
3	F	619	0	659	14	0
3	J	662	0	709	44	0
3	N	619	0	659	16	0
3	R	654	0	697	34	0
3	V	619	0	659	15	0
3	Z	662	0	709	29	0
3	d	619	0	659	0	0
4	C	795	0	846	23	0
4	G	809	0	864	40	0
4	K	795	0	846	23	0
4	O	809	0	864	41	0
4	S	795	0	846	23	0
4	W	809	0	864	41	0
4	a	795	0	846	0	0
4	e	809	0	864	0	0
5	g	12605	0	6944	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	h	12774	0	6940	0	1
7	C	1	0	0	0	0
7	G	1	0	0	0	0
7	K	1	0	0	0	0
7	O	1	0	0	0	0
7	S	1	0	0	0	0
7	W	1	0	0	0	0
7	a	1	0	0	0	0
7	e	1	0	0	0	0
All	All	49215	0	38980	507	20

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 15.

All (507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:THR:HG21	3:J:75:HIS:CD2	1.58	1.37
3:B:75:HIS:CD2	1:D:93:THR:HG21	1.58	1.37
3:R:75:HIS:CD2	1:T:93:THR:HG21	1.58	1.36
3:B:75:HIS:HD2	1:D:93:THR:CG2	1.55	1.20
1:L:93:THR:CG2	3:J:75:HIS:HD2	1.55	1.19
3:R:75:HIS:HD2	1:T:93:THR:CG2	1.55	1.18
3:V:75:HIS:CD2	1:X:93:THR:HG21	1.80	1.16
3:F:75:HIS:CD2	1:H:93:THR:HG21	1.80	1.15
2:I:47:ALA:CB	3:J:44:LYS:HG3	1.77	1.15
3:N:75:HIS:CD2	1:P:93:THR:HG21	1.81	1.14
2:I:47:ALA:HB1	3:J:44:LYS:HG3	1.26	1.11
2:I:48:LEU:HD13	3:J:44:LYS:HD3	1.33	1.06
4:S:55:LEU:O	4:S:59:THR:HG22	1.70	0.91
4:C:55:LEU:O	4:C:59:THR:HG22	1.70	0.89
4:K:55:LEU:O	4:K:59:THR:HG22	1.70	0.89
3:R:75:HIS:HD2	1:T:93:THR:HG21	0.71	0.87
3:B:75:HIS:HD2	1:D:93:THR:HG21	0.71	0.84
1:L:93:THR:HG21	3:J:75:HIS:HD2	0.71	0.83
3:J:39:ARG:NH1	3:J:44:LYS:HA	1.96	0.80
3:N:75:HIS:CD2	1:P:93:THR:CG2	2.63	0.80
3:V:75:HIS:CD2	1:X:93:THR:CG2	2.63	0.79
3:F:75:HIS:CD2	1:H:93:THR:CG2	2.63	0.79
4:W:25:PHE:HZ	4:W:59:THR:HG21	1.48	0.79
1:D:95:VAL:HG13	1:D:99:LEU:HD12	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:62:ILE:HG12	4:G:93:LEU:HD11	1.64	0.78
1:T:95:VAL:HG13	1:T:99:LEU:HD12	1.66	0.78
1:L:93:THR:CG2	3:J:75:HIS:CD2	2.44	0.78
4:G:25:PHE:HZ	4:G:59:THR:HG21	1.48	0.77
4:O:62:ILE:HG12	4:O:93:LEU:HD11	1.64	0.77
4:W:62:ILE:HG12	4:W:93:LEU:HD11	1.64	0.77
2:M:60:LEU:HD13	2:M:93:GLN:HG2	1.66	0.77
1:L:95:VAL:HG13	1:L:99:LEU:HD12	1.66	0.77
2:E:60:LEU:HD13	2:E:93:GLN:HG2	1.66	0.77
2:U:121:PRO:HB3	3:V:53:GLU:HG3	1.66	0.77
4:G:26:PRO:HG3	1:H:37:TYR:CZ	2.21	0.76
2:I:47:ALA:HB3	3:J:44:LYS:HG3	1.66	0.76
4:O:25:PHE:HZ	4:O:59:THR:HG21	1.48	0.76
4:W:26:PRO:HG3	1:X:37:TYR:CZ	2.21	0.76
2:U:60:LEU:HD13	2:U:93:GLN:HG2	1.66	0.76
4:O:26:PRO:HG3	1:P:37:TYR:CZ	2.21	0.76
2:E:121:PRO:HB3	3:F:53:GLU:HG3	1.66	0.75
2:M:121:PRO:HB3	3:N:53:GLU:HG3	1.67	0.75
4:O:62:ILE:HG12	4:O:93:LEU:CD1	2.18	0.74
4:G:83:LEU:O	4:G:87:VAL:HG23	1.88	0.73
4:C:29:ARG:NH2	1:D:33:SER:O	2.20	0.73
4:W:62:ILE:HG12	4:W:93:LEU:CD1	2.18	0.73
3:B:75:HIS:CD2	1:D:93:THR:CG2	2.44	0.73
4:S:29:ARG:NH2	1:T:33:SER:O	2.20	0.73
4:O:83:LEU:O	4:O:87:VAL:HG23	1.89	0.72
4:G:62:ILE:HG12	4:G:93:LEU:CD1	2.18	0.72
4:W:83:LEU:O	4:W:87:VAL:HG23	1.89	0.72
4:G:25:PHE:CZ	4:G:59:THR:HG21	2.25	0.72
4:O:25:PHE:CZ	4:O:59:THR:HG21	2.25	0.72
1:L:33:SER:O	4:K:29:ARG:NH2	2.21	0.71
4:W:25:PHE:CZ	4:W:59:THR:HG21	2.25	0.71
1:X:108:VAL:O	1:X:112:THR:HG23	1.91	0.71
3:F:75:HIS:HD2	1:H:93:THR:HG21	1.53	0.70
2:E:67:PHE:O	2:E:71:VAL:HG23	1.91	0.70
2:M:67:PHE:O	2:M:71:VAL:HG23	1.91	0.70
1:P:108:VAL:O	1:P:112:THR:HG23	1.91	0.70
2:U:67:PHE:O	2:U:71:VAL:HG23	1.91	0.70
4:O:31:HIS:CD2	4:O:35:ARG:HH21	2.10	0.69
2:I:47:ALA:CB	3:J:44:LYS:CG	2.64	0.69
4:C:50:TYR:O	4:C:54:VAL:HG23	1.93	0.69
4:G:88:ARG:NH2	4:G:97:LEU:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:VAL:O	1:H:112:THR:HG23	1.91	0.69
1:P:79:HIS:CE1	4:K:38:ASN:HD22	2.11	0.69
4:S:38:ASN:HD22	1:X:79:HIS:CE1	2.11	0.68
3:R:75:HIS:CD2	1:T:93:THR:CG2	2.44	0.68
4:G:31:HIS:CD2	4:G:35:ARG:HH21	2.11	0.68
4:S:50:TYR:O	4:S:54:VAL:HG23	1.93	0.68
4:O:88:ARG:NH2	4:O:97:LEU:O	2.25	0.68
4:W:88:ARG:NH2	4:W:97:LEU:O	2.26	0.68
4:K:50:TYR:O	4:K:54:VAL:HG23	1.93	0.68
4:C:38:ASN:HD22	1:H:79:HIS:CE1	2.11	0.68
4:W:31:HIS:CD2	4:W:35:ARG:HH21	2.10	0.68
2:A:119:ILE:O	3:B:47:SER:HB3	1.95	0.67
4:W:80:PRO:HG3	1:X:58:ILE:CD1	2.26	0.66
2:Y:119:ILE:O	3:Z:47:SER:HB3	1.95	0.66
2:Q:119:ILE:O	3:R:47:SER:HB3	1.95	0.66
4:G:80:PRO:HG3	1:H:58:ILE:CD1	2.25	0.66
4:O:80:PRO:HG3	1:P:58:ILE:CD1	2.25	0.66
4:O:77:ARG:HA	1:P:50:GLY:O	1.96	0.65
4:W:77:ARG:HA	1:X:50:GLY:O	1.96	0.65
3:J:89:ALA:O	3:J:92:ARG:HB2	1.97	0.65
4:G:77:ARG:HA	1:H:50:GLY:O	1.96	0.65
3:Z:89:ALA:O	3:Z:92:ARG:HB2	1.97	0.65
2:I:119:ILE:O	3:J:47:SER:HB3	1.95	0.65
3:V:75:HIS:HD2	1:X:93:THR:HG21	1.54	0.65
3:B:89:ALA:O	3:B:92:ARG:HB2	1.97	0.64
1:X:98:LEU:HB3	1:X:99:LEU:HD23	1.79	0.64
3:R:89:ALA:O	3:R:92:ARG:HB2	1.97	0.64
3:N:75:HIS:HD2	1:P:93:THR:HG21	1.54	0.63
4:S:118:LYS:HA	4:S:118:LYS:HE3	1.81	0.63
1:L:102:GLU:HB3	4:K:92:GLU:OE1	1.98	0.63
2:I:48:LEU:CD1	3:J:44:LYS:HD3	2.21	0.63
4:C:92:GLU:OE1	1:D:102:GLU:HB3	1.99	0.63
1:H:98:LEU:HB3	1:H:99:LEU:HD23	1.79	0.63
4:C:118:LYS:HE3	4:C:118:LYS:HA	1.81	0.62
1:P:69:ARG:HB3	1:P:98:LEU:HD21	1.82	0.62
4:S:92:GLU:OE1	1:T:102:GLU:HB3	1.98	0.62
1:P:98:LEU:HB3	1:P:99:LEU:HD23	1.79	0.62
1:H:69:ARG:HB3	1:H:98:LEU:HD21	1.82	0.62
4:K:118:LYS:HE3	4:K:118:LYS:HA	1.81	0.61
4:G:81:ARG:NH2	4:G:107:VAL:O	2.34	0.61
1:L:92:GLN:O	1:L:95:VAL:HB	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:GLN:O	1:D:95:VAL:HB	2.01	0.61
2:I:48:LEU:HD13	3:J:44:LYS:CD	2.20	0.61
1:X:69:ARG:HB3	1:X:98:LEU:HD21	1.81	0.61
3:B:32:PRO:O	3:B:35:ARG:HB3	2.02	0.60
4:O:81:ARG:NH2	4:O:107:VAL:O	2.34	0.60
3:R:32:PRO:O	3:R:35:ARG:HB3	2.02	0.60
1:T:92:GLN:O	1:T:95:VAL:HB	2.01	0.60
4:W:84:GLN:HE21	4:W:84:GLN:HA	1.66	0.60
3:Z:32:PRO:O	3:Z:35:ARG:HB3	2.02	0.60
4:W:81:ARG:NH2	4:W:107:VAL:O	2.34	0.60
4:C:25:PHE:CZ	4:C:59:THR:HG21	2.37	0.59
2:I:47:ALA:HB3	3:J:44:LYS:CG	2.31	0.59
3:J:32:PRO:O	3:J:35:ARG:HB3	2.02	0.59
4:K:25:PHE:CZ	4:K:59:THR:HG21	2.37	0.59
4:O:90:ASP:O	4:O:91:GLU:C	2.39	0.59
4:C:20:ARG:O	1:D:118:TYR:HA	2.03	0.59
1:L:65:ASP:OD2	3:N:98:TYR:OH	2.20	0.59
2:Q:65:LEU:HB3	2:Q:66:PRO:HD3	1.85	0.59
4:S:25:PHE:CZ	4:S:59:THR:HG21	2.37	0.59
4:G:84:GLN:HA	4:G:84:GLN:HE21	1.66	0.59
1:T:65:ASP:OD2	3:V:98:TYR:OH	2.20	0.59
2:A:65:LEU:HB3	2:A:66:PRO:HD3	1.85	0.58
4:O:84:GLN:HE21	4:O:84:GLN:HA	1.66	0.58
4:G:32:ARG:NH2	1:H:32:GLU:OE1	2.28	0.58
2:I:65:LEU:HB3	2:I:66:PRO:HD3	1.85	0.58
4:S:20:ARG:O	1:T:118:TYR:HA	2.03	0.58
4:W:84:GLN:HE22	4:W:88:ARG:HH11	1.52	0.58
3:B:77:LYS:HG3	1:D:89:ARG:HH22	1.68	0.58
1:L:89:ARG:HH22	3:J:77:LYS:HG3	1.68	0.58
4:W:90:ASP:O	4:W:91:GLU:C	2.39	0.58
2:E:110:CYS:SG	2:E:126:LEU:HD23	2.44	0.58
1:D:65:ASP:OD2	3:F:98:TYR:OH	2.20	0.58
4:G:90:ASP:O	4:G:91:GLU:C	2.39	0.58
1:L:118:TYR:HA	4:K:20:ARG:O	2.03	0.58
3:R:77:LYS:HG3	1:T:89:ARG:HH22	1.68	0.58
3:F:59:LYS:HE3	3:F:63:GLU:OE2	2.04	0.57
4:O:84:GLN:HE22	4:O:88:ARG:HH11	1.52	0.57
4:O:32:ARG:NH2	1:P:32:GLU:OE1	2.29	0.57
3:V:59:LYS:HE3	3:V:63:GLU:OE2	2.04	0.57
2:Y:65:LEU:HB3	2:Y:66:PRO:HD3	1.85	0.57
2:I:101:VAL:HG11	3:J:40:ARG:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:TYR:CD1	4:K:26:PRO:HD3	2.40	0.57
2:U:110:CYS:SG	2:U:126:LEU:HD23	2.44	0.57
4:C:26:PRO:HD3	1:D:37:TYR:CD1	2.40	0.57
3:J:26:ILE:HG13	3:J:55:ARG:HD3	1.87	0.57
3:R:26:ILE:HG13	3:R:55:ARG:HD3	1.87	0.57
3:N:59:LYS:HE3	3:N:63:GLU:OE2	2.05	0.56
3:B:26:ILE:HG13	3:B:55:ARG:HD3	1.87	0.56
4:S:26:PRO:HD3	1:T:37:TYR:CD1	2.40	0.56
4:G:84:GLN:HE22	4:G:88:ARG:HH11	1.52	0.56
4:G:26:PRO:HG3	1:H:37:TYR:CE2	2.40	0.56
4:G:55:LEU:HD22	1:H:63:VAL:HG13	1.86	0.56
2:Q:101:VAL:HG11	3:R:40:ARG:HG2	1.87	0.56
4:W:55:LEU:HD22	1:X:63:VAL:HG13	1.86	0.56
4:W:26:PRO:HG3	1:X:37:TYR:CE2	2.40	0.56
4:O:55:LEU:HD22	1:P:63:VAL:HG13	1.86	0.56
3:Z:26:ILE:HG13	3:Z:55:ARG:HD3	1.87	0.56
4:G:80:PRO:HG3	1:H:58:ILE:HD12	1.88	0.56
2:M:110:CYS:SG	2:M:126:LEU:HD23	2.44	0.56
1:T:106:HIS:O	1:T:109:SER:HB2	2.06	0.56
2:U:102:ALA:O	2:U:105:GLU:HB2	2.06	0.56
4:S:55:LEU:HD22	1:T:63:VAL:HG13	1.88	0.56
2:E:102:ALA:O	2:E:105:GLU:HB2	2.06	0.56
2:M:102:ALA:O	2:M:105:GLU:HB2	2.06	0.56
2:A:101:VAL:HG11	3:B:40:ARG:HG2	1.87	0.55
1:T:59:MET:O	1:T:63:VAL:HG23	2.07	0.55
1:D:59:MET:O	1:D:63:VAL:HG23	2.07	0.55
1:L:107:ALA:HB1	4:K:54:VAL:HG13	1.88	0.55
4:O:26:PRO:HG3	1:P:37:TYR:CE2	2.40	0.55
2:Y:101:VAL:HG11	3:Z:40:ARG:HG2	1.87	0.55
4:O:80:PRO:HG3	1:P:58:ILE:HD12	1.88	0.55
3:R:33:ALA:C	3:R:35:ARG:N	2.60	0.55
1:L:106:HIS:O	1:L:109:SER:HB2	2.06	0.55
4:S:54:VAL:HG13	1:T:107:ALA:HB1	1.88	0.55
4:W:80:PRO:HG3	1:X:58:ILE:HD12	1.88	0.55
4:C:55:LEU:HD22	1:D:63:VAL:HG13	1.88	0.54
4:C:54:VAL:HG13	1:D:107:ALA:HB1	1.88	0.54
3:Z:33:ALA:C	3:Z:35:ARG:N	2.60	0.54
1:D:106:HIS:O	1:D:109:SER:HB2	2.06	0.54
4:G:50:TYR:O	4:G:54:VAL:HG23	2.07	0.54
1:L:59:MET:O	1:L:63:VAL:HG23	2.07	0.54
4:W:50:TYR:O	4:W:54:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:73:ASN:O	4:W:75:LYS:HG3	2.08	0.54
4:G:73:ASN:O	4:G:75:LYS:HG3	2.08	0.54
4:O:73:ASN:O	4:O:75:LYS:HG3	2.08	0.54
3:B:33:ALA:C	3:B:35:ARG:N	2.60	0.54
3:B:31:LYS:N	3:B:32:PRO:HD2	2.23	0.54
4:O:50:TYR:O	4:O:54:VAL:HG23	2.07	0.54
3:R:31:LYS:N	3:R:32:PRO:HD2	2.23	0.54
1:L:63:VAL:HG13	4:K:55:LEU:HD22	1.88	0.53
3:J:31:LYS:N	3:J:32:PRO:HD2	2.23	0.53
3:Z:31:LYS:N	3:Z:32:PRO:HD2	2.23	0.53
1:P:67:PHE:C	1:P:67:PHE:CD1	2.82	0.53
3:J:33:ALA:C	3:J:35:ARG:N	2.60	0.53
3:J:33:ALA:O	3:J:35:ARG:N	2.42	0.53
4:C:32:ARG:NH2	1:D:32:GLU:OE1	2.35	0.53
3:R:33:ALA:O	3:R:35:ARG:N	2.42	0.52
4:G:30:VAL:O	4:G:34:LEU:HD12	2.10	0.52
3:B:33:ALA:O	3:B:35:ARG:N	2.42	0.52
3:Z:33:ALA:O	3:Z:35:ARG:N	2.42	0.52
1:H:67:PHE:C	1:H:67:PHE:CD1	2.82	0.52
3:V:26:ILE:HD12	3:V:55:ARG:HB3	1.92	0.52
2:Y:61:LEU:O	3:Z:36:ARG:NH2	2.43	0.52
3:F:88:TYR:CZ	1:H:80:TYR:CD1	2.98	0.52
1:X:67:PHE:C	1:X:67:PHE:CD1	2.82	0.52
4:W:32:ARG:NH2	1:X:32:GLU:OE1	2.28	0.52
4:W:30:VAL:O	4:W:34:LEU:HD12	2.10	0.51
3:V:88:TYR:CZ	1:X:80:TYR:CD1	2.98	0.51
4:C:17:ARG:HG2	1:D:118:TYR:HE1	1.76	0.51
2:I:61:LEU:O	3:J:36:ARG:NH2	2.42	0.51
3:N:26:ILE:HD12	3:N:55:ARG:HB3	1.92	0.51
3:F:75:HIS:HD2	1:H:93:THR:CG2	2.16	0.51
4:O:30:VAL:O	4:O:34:LEU:HD12	2.10	0.51
4:S:17:ARG:HG2	1:T:118:TYR:HE1	1.76	0.51
1:L:118:TYR:HE1	4:K:17:ARG:HG2	1.76	0.51
1:L:32:GLU:OE1	4:K:32:ARG:NH2	2.34	0.51
4:S:32:ARG:NH2	1:T:32:GLU:OE1	2.34	0.51
1:D:62:PHE:O	1:D:66:VAL:HG23	2.11	0.51
3:F:26:ILE:HD12	3:F:55:ARG:HB3	1.92	0.51
3:N:88:TYR:CZ	1:P:80:TYR:CD1	2.98	0.51
2:Q:61:LEU:O	3:R:36:ARG:NH2	2.42	0.51
1:L:62:PHE:O	1:L:66:VAL:HG23	2.11	0.51
1:T:62:PHE:O	1:T:66:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:75:HIS:HD2	1:P:93:THR:CG2	2.16	0.50
4:O:31:HIS:CD2	4:O:35:ARG:NH2	2.79	0.50
3:R:28:GLY:O	3:R:30:THR:HG23	2.12	0.50
4:W:31:HIS:CD2	4:W:35:ARG:NH2	2.79	0.50
3:B:28:GLY:O	3:B:30:THR:HG23	2.11	0.50
4:W:80:PRO:CG	1:X:58:ILE:CD1	2.90	0.50
1:D:46:HIS:HB3	1:D:49:THR:OG1	2.12	0.50
4:G:31:HIS:CD2	4:G:35:ARG:NH2	2.79	0.49
2:I:70:LEU:O	2:I:74:ILE:HD12	2.12	0.49
3:J:28:GLY:O	3:J:30:THR:HG23	2.12	0.49
1:L:46:HIS:HB3	1:L:49:THR:OG1	2.12	0.49
1:T:46:HIS:HB3	1:T:49:THR:OG1	2.12	0.49
2:A:70:LEU:O	2:A:74:ILE:HD12	2.12	0.49
2:Y:70:LEU:O	2:Y:74:ILE:HD12	2.12	0.49
3:Z:28:GLY:O	3:Z:30:THR:HG23	2.12	0.49
4:C:95:LYS:O	4:C:98:GLY:N	2.45	0.49
2:Q:70:LEU:O	2:Q:74:ILE:HD12	2.12	0.49
3:J:33:ALA:C	3:J:35:ARG:H	2.16	0.49
4:K:87:VAL:HG11	4:K:97:LEU:HD12	1.94	0.49
4:O:80:PRO:CG	1:P:58:ILE:CD1	2.90	0.49
3:Z:33:ALA:C	3:Z:35:ARG:H	2.16	0.49
3:J:29:ILE:O	3:J:34:ILE:HD11	2.13	0.49
4:C:87:VAL:HG11	4:C:97:LEU:HD12	1.94	0.49
4:O:54:VAL:HG13	1:P:107:ALA:HB1	1.95	0.49
3:R:29:ILE:O	3:R:34:ILE:HD11	2.13	0.49
3:B:31:LYS:O	3:B:31:LYS:HD2	5.08	0.48
4:G:80:PRO:CG	1:H:58:ILE:CD1	2.90	0.48
2:A:61:LEU:O	3:B:36:ARG:NH2	2.43	0.48
2:I:65:LEU:HB3	2:I:66:PRO:CD	2.43	0.48
2:Y:65:LEU:HB3	2:Y:66:PRO:CD	2.43	0.48
4:S:95:LYS:O	4:S:98:GLY:N	2.45	0.48
4:S:87:VAL:HG11	4:S:97:LEU:HD12	1.94	0.48
4:G:35:ARG:HB2	4:G:35:ARG:NH1	2.29	0.48
4:W:39:TYR:O	1:X:75:SER:OG	2.23	0.48
3:B:29:ILE:O	3:B:34:ILE:HD11	2.13	0.48
4:G:61:GLU:HG2	1:H:103:LEU:HD11	1.96	0.48
2:M:79:LYS:HG3	3:N:74:GLU:OE1	2.13	0.48
3:R:33:ALA:C	3:R:35:ARG:H	2.16	0.48
4:S:42:ARG:HG3	1:T:85:THR:HG23	1.95	0.48
3:V:75:HIS:HD2	1:X:93:THR:CG2	2.16	0.48
4:W:35:ARG:HB2	4:W:35:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:LEU:HB3	2:A:66:PRO:CD	2.43	0.48
1:L:31:LYS:HD2	1:L:31:LYS:O	2.13	0.48
1:D:100:PRO:O	1:D:102:GLU:N	2.47	0.48
4:O:39:TYR:O	1:P:75:SER:OG	2.23	0.48
1:T:31:LYS:O	1:T:31:LYS:HD2	2.13	0.48
4:C:42:ARG:HG3	1:D:85:THR:HG23	1.95	0.48
4:G:35:ARG:HB2	4:G:35:ARG:HH11	1.79	0.48
4:G:54:VAL:HG13	1:H:107:ALA:HB1	1.95	0.48
4:O:61:GLU:HG2	1:P:103:LEU:HD11	1.96	0.48
1:T:100:PRO:O	1:T:102:GLU:N	2.47	0.48
4:W:61:GLU:HG2	1:X:103:LEU:HD11	1.96	0.48
2:Q:118:THR:HA	3:R:45:ARG:HB3	1.96	0.47
4:W:54:VAL:HG13	1:X:107:ALA:HB1	1.95	0.47
4:O:35:ARG:HH11	4:O:35:ARG:HB2	1.79	0.47
2:U:79:LYS:HG3	3:V:74:GLU:OE1	2.14	0.47
4:W:35:ARG:HB2	4:W:35:ARG:HH11	1.79	0.47
4:K:95:LYS:O	4:K:98:GLY:N	2.45	0.47
2:Q:65:LEU:HB3	2:Q:66:PRO:CD	2.43	0.47
3:Z:29:ILE:O	3:Z:34:ILE:HD11	2.13	0.47
3:Z:68:ASP:OD2	3:Z:92:ARG:HD3	2.15	0.47
1:L:85:THR:HG23	4:K:42:ARG:HG3	1.95	0.47
1:L:100:PRO:O	1:L:102:GLU:N	2.47	0.47
4:O:47:ALA:HB1	1:P:91:ILE:HG13	1.97	0.47
1:X:35:ALA:HA	1:X:56:MET:HE1	1.95	0.47
1:D:31:LYS:HD2	1:D:31:LYS:O	2.13	0.47
1:D:67:PHE:C	1:D:67:PHE:CD1	2.88	0.47
4:G:47:ALA:HB1	1:H:91:ILE:HG13	1.97	0.47
1:L:67:PHE:CD1	1:L:67:PHE:C	2.88	0.47
4:O:51:LEU:HB2	1:P:91:ILE:HD12	1.97	0.47
3:B:77:LYS:HE3	1:D:89:ARG:NH1	2.30	0.47
3:B:68:ASP:OD2	3:B:92:ARG:HD3	2.15	0.47
4:W:47:ALA:HB1	1:X:91:ILE:HG13	1.97	0.47
2:A:118:THR:HA	3:B:45:ARG:HB3	1.96	0.47
3:B:33:ALA:C	3:B:35:ARG:H	2.16	0.47
2:E:79:LYS:HG3	3:F:74:GLU:OE1	2.13	0.47
4:O:35:ARG:NH1	4:O:35:ARG:HB2	2.29	0.47
2:I:118:THR:HA	3:J:45:ARG:HB3	1.96	0.47
2:M:128:ARG:NH2	2:M:134:ARG:HE	2.13	0.47
4:W:34:LEU:HD11	4:W:51:LEU:HD23	1.97	0.47
4:W:80:PRO:HB3	1:X:58:ILE:HD13	1.97	0.46
2:Y:118:THR:HA	3:Z:45:ARG:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:39:TYR:O	1:H:75:SER:OG	2.23	0.46
3:F:88:TYR:CE2	1:H:80:TYR:CG	3.04	0.46
1:L:89:ARG:NH1	3:J:77:LYS:HE3	2.30	0.46
4:O:80:PRO:HB3	1:P:58:ILE:HD13	1.97	0.46
3:R:68:ASP:OD2	3:R:92:ARG:HD3	2.15	0.46
4:S:79:ILE:HB	4:S:80:PRO:HD2	1.97	0.46
3:Z:39:ARG:C	3:Z:41:GLY:N	2.68	0.46
4:G:80:PRO:HB3	1:H:58:ILE:HD13	1.97	0.46
3:J:68:ASP:OD2	3:J:92:ARG:HD3	2.15	0.46
1:T:67:PHE:CD1	1:T:67:PHE:C	2.88	0.46
3:N:88:TYR:CE2	1:P:80:TYR:CG	3.03	0.46
2:E:128:ARG:NH2	2:E:134:ARG:HE	2.14	0.46
4:G:34:LEU:HD11	4:G:51:LEU:HD23	1.97	0.46
4:G:51:LEU:HB2	1:H:91:ILE:HD12	1.97	0.46
3:B:39:ARG:C	3:B:41:GLY:N	2.68	0.46
4:C:79:ILE:HB	4:C:80:PRO:HD2	1.97	0.46
4:O:34:LEU:HD11	4:O:51:LEU:HD23	1.97	0.46
3:V:88:TYR:CE2	1:X:80:TYR:CG	3.04	0.46
4:K:79:ILE:HB	4:K:80:PRO:HD2	1.97	0.46
2:I:118:THR:HA	3:J:45:ARG:O	2.16	0.46
2:M:87:SER:OG	3:N:83:ALA:HB2	2.16	0.46
2:U:128:ARG:NH2	2:U:134:ARG:HE	2.13	0.46
3:F:89:ALA:O	3:F:92:ARG:HB2	2.16	0.46
3:R:77:LYS:HE3	1:T:89:ARG:NH1	2.30	0.45
3:V:89:ALA:O	3:V:92:ARG:HB2	2.16	0.45
1:L:103:LEU:HD21	4:K:93:LEU:HD23	1.99	0.45
3:V:53:GLU:O	3:V:57:VAL:HG23	2.16	0.45
1:D:83:ARG:HB3	1:D:83:ARG:NH1	2.32	0.45
2:E:87:SER:OG	3:F:83:ALA:HB2	2.16	0.45
2:I:102:ALA:O	2:I:105:GLU:HB2	2.17	0.45
2:M:79:LYS:HB3	2:M:82:LEU:HD11	1.99	0.45
3:N:53:GLU:O	3:N:57:VAL:HG23	2.16	0.45
2:U:87:SER:OG	3:V:83:ALA:HB2	2.16	0.45
3:J:39:ARG:HH12	3:J:44:LYS:HA	1.76	0.45
3:B:28:GLY:O	3:B:30:THR:N	2.48	0.45
4:C:93:LEU:HD23	1:D:103:LEU:HD21	1.99	0.45
4:G:100:VAL:CG1	4:G:101:THR:N	2.80	0.45
3:J:28:GLY:O	3:J:30:THR:N	2.48	0.45
3:R:39:ARG:C	3:R:41:GLY:N	2.68	0.45
4:W:100:VAL:CG1	4:W:101:THR:N	2.80	0.45
2:Y:118:THR:HA	3:Z:45:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:ALA:O	2:A:105:GLU:HB2	2.17	0.45
3:F:53:GLU:O	3:F:57:VAL:HG23	2.16	0.45
3:N:89:ALA:O	3:N:92:ARG:HB2	2.16	0.45
4:G:64:GLU:OE2	1:H:45:VAL:CG1	2.65	0.45
3:J:39:ARG:C	3:J:41:GLY:N	2.68	0.45
4:O:100:VAL:CG1	4:O:101:THR:N	2.80	0.45
4:W:51:LEU:HB2	1:X:91:ILE:HD12	1.97	0.45
2:Y:102:ALA:O	2:Y:105:GLU:HB2	2.17	0.45
3:R:32:PRO:O	3:R:36:ARG:HG3	2.18	0.44
2:Q:102:ALA:O	2:Q:105:GLU:HB2	2.17	0.44
2:Q:118:THR:HA	3:R:45:ARG:O	2.17	0.44
4:S:93:LEU:HD23	1:T:103:LEU:HD21	1.99	0.44
2:A:118:THR:HA	3:B:45:ARG:O	2.17	0.44
3:Z:32:PRO:O	3:Z:36:ARG:HG3	2.17	0.44
3:J:32:PRO:O	3:J:36:ARG:HG3	2.17	0.44
4:S:27:VAL:HG11	4:S:49:VAL:HG22	1.99	0.44
4:W:64:GLU:OE2	1:X:45:VAL:CG1	2.65	0.44
4:G:57:TYR:CD2	1:H:107:ALA:HB2	2.53	0.44
1:L:99:LEU:HA	1:L:100:PRO:HD3	1.75	0.44
1:L:83:ARG:HB3	1:L:83:ARG:NH1	2.32	0.44
4:O:64:GLU:OE2	1:P:45:VAL:CG1	2.65	0.44
2:E:79:LYS:HB3	2:E:82:LEU:HD11	1.99	0.44
3:R:31:LYS:HG3	3:R:51:TYR:CE1	2.53	0.44
3:B:98:TYR:OH	1:H:65:ASP:OD2	2.34	0.44
3:B:31:LYS:HG3	3:B:51:TYR:CE1	2.53	0.44
2:M:42:ARG:HA	2:M:43:PRO:HD2	1.81	0.44
3:B:32:PRO:O	3:B:36:ARG:HG3	2.17	0.43
4:C:27:VAL:HG11	4:C:49:VAL:HG22	1.99	0.43
3:J:31:LYS:HG3	3:J:51:TYR:CE1	2.53	0.43
2:U:79:LYS:HB3	2:U:82:LEU:HD11	1.99	0.43
4:G:43:VAL:HG12	4:G:44:GLY:O	2.18	0.43
3:R:88:TYR:CZ	1:T:80:TYR:CD1	3.06	0.43
1:L:80:TYR:CD1	3:J:88:TYR:CZ	3.07	0.43
4:O:43:VAL:HG12	4:O:44:GLY:O	2.18	0.43
4:W:83:LEU:O	4:W:86:ALA:HB3	2.19	0.43
4:O:83:LEU:O	4:O:86:ALA:HB3	2.19	0.43
4:O:57:TYR:CD2	1:P:107:ALA:HB2	2.53	0.43
3:Z:28:GLY:O	3:Z:30:THR:N	2.48	0.43
1:T:83:ARG:NH1	1:T:83:ARG:HB3	2.32	0.43
3:R:28:GLY:O	3:R:30:THR:N	2.48	0.43
3:B:88:TYR:CZ	1:D:80:TYR:CD1	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:47:ALA:N	4:C:48:PRO:HD2	2.34	0.43
2:I:85:GLN:NE2	3:J:82:THR:HG22	2.34	0.43
4:K:113:SER:O	4:K:115:LEU:N	2.52	0.43
4:K:27:VAL:HG11	4:K:49:VAL:HG22	1.99	0.43
1:P:36:ILE:HD11	1:P:37:TYR:CZ	2.54	0.43
3:Z:31:LYS:HG3	3:Z:51:TYR:CE1	2.53	0.43
2:Q:120:MET:O	2:Q:121:PRO:C	2.56	0.43
3:R:66:ILE:HG22	3:R:70:VAL:HG23	2.01	0.43
4:G:83:LEU:O	4:G:86:ALA:HB3	2.18	0.43
1:H:36:ILE:HD11	1:H:37:TYR:CZ	2.54	0.43
2:Y:85:GLN:NE2	3:Z:82:THR:HG22	2.34	0.43
3:Z:97:LEU:HD21	3:Z:100:PHE:CD2	2.54	0.43
4:S:113:SER:O	4:S:115:LEU:N	2.52	0.42
2:A:85:GLN:NE2	3:B:82:THR:HG22	2.34	0.42
1:P:99:LEU:HD23	1:P:99:LEU:N	2.34	0.42
2:Q:85:GLN:NE2	3:R:82:THR:HG22	2.34	0.42
4:W:57:TYR:CD2	1:X:107:ALA:HB2	2.53	0.42
2:E:59:GLU:HG3	2:E:59:GLU:H	1.58	0.42
4:K:47:ALA:N	4:K:48:PRO:HD2	2.34	0.42
4:S:47:ALA:N	4:S:48:PRO:HD2	2.34	0.42
3:Z:34:ILE:HG13	3:Z:34:ILE:H	1.71	0.42
3:B:78:ARG:HH22	3:B:85:ASP:CG	2.23	0.42
3:B:97:LEU:HD21	3:B:100:PHE:CD2	2.54	0.42
4:C:83:LEU:O	4:C:87:VAL:HG23	2.19	0.42
2:E:51:ILE:O	2:E:55:GLN:HG3	2.20	0.42
4:W:100:VAL:HG12	4:W:101:THR:N	2.34	0.42
1:X:36:ILE:HD11	1:X:37:TYR:CZ	2.54	0.42
2:M:51:ILE:O	2:M:55:GLN:HG3	2.20	0.42
3:R:78:ARG:HH22	3:R:85:ASP:CG	2.22	0.42
3:B:66:ILE:HG22	3:B:70:VAL:HG23	2.01	0.42
4:C:113:SER:O	4:C:115:LEU:N	2.52	0.42
4:G:100:VAL:HG12	4:G:101:THR:N	2.34	0.42
4:S:83:LEU:O	4:S:87:VAL:HG23	2.19	0.42
4:W:43:VAL:HG12	4:W:44:GLY:O	2.18	0.42
1:X:39:TYR:O	1:X:40:LYS:C	2.58	0.42
1:H:39:TYR:O	1:H:40:LYS:C	2.58	0.42
1:P:38:VAL:HB	1:P:56:MET:HE1	2.01	0.42
1:X:99:LEU:HD23	1:X:99:LEU:N	2.34	0.42
2:A:72:ARG:HH11	2:A:72:ARG:HG2	1.85	0.42
3:J:39:ARG:HH11	3:J:44:LYS:HA	1.80	0.42
2:Q:72:ARG:HH11	2:Q:72:ARG:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:72:ARG:HG2	2:Y:72:ARG:HH11	1.85	0.42
2:A:120:MET:O	2:A:121:PRO:C	2.56	0.42
3:Z:66:ILE:HG22	3:Z:70:VAL:HG23	2.01	0.42
3:J:97:LEU:HD21	3:J:100:PHE:CD2	2.54	0.42
4:K:83:LEU:O	4:K:87:VAL:HG23	2.19	0.42
2:U:51:ILE:O	2:U:55:GLN:HG3	2.19	0.42
2:U:48:LEU:O	2:U:52:ARG:HG3	2.20	0.41
3:Z:30:THR:O	3:Z:34:ILE:HG13	2.20	0.41
2:E:42:ARG:HA	2:E:43:PRO:HD2	1.81	0.41
1:L:112:THR:O	1:L:116:THR:OG1	2.38	0.41
2:I:120:MET:O	2:I:121:PRO:C	2.56	0.41
3:J:66:ILE:HG22	3:J:70:VAL:HG23	2.01	0.41
2:Q:96:SER:O	2:Q:99:TYR:HB3	2.21	0.41
2:A:63:ARG:CZ	2:A:63:ARG:HB2	2.50	0.41
1:H:105:LYS:HE3	1:H:105:LYS:HB2	1.94	0.41
1:H:99:LEU:N	1:H:99:LEU:HD23	2.34	0.41
2:M:48:LEU:O	2:M:52:ARG:HG3	2.20	0.41
4:W:80:PRO:O	4:W:81:ARG:C	2.59	0.41
3:R:97:LEU:HD21	3:R:100:PHE:CD2	2.54	0.41
1:T:112:THR:O	1:T:116:THR:OG1	2.38	0.41
2:U:106:ASP:HA	2:U:109:LEU:HD12	2.02	0.41
2:Y:96:SER:O	2:Y:99:TYR:HB3	2.20	0.41
2:A:127:ALA:O	2:A:131:ARG:HG3	2.21	0.41
2:A:96:SER:O	2:A:99:TYR:HB3	2.20	0.41
3:Z:78:ARG:HH22	3:Z:85:ASP:CG	2.23	0.41
3:B:34:ILE:H	3:B:34:ILE:HG13	1.71	0.41
3:J:30:THR:O	3:J:34:ILE:HG13	2.20	0.41
2:Q:63:ARG:CZ	2:Q:63:ARG:HB2	2.51	0.41
2:Y:120:MET:O	2:Y:121:PRO:C	2.56	0.41
3:Z:90:LEU:HB3	3:Z:95:ARG:O	2.21	0.41
4:G:93:LEU:HD23	1:H:103:LEU:HD21	2.02	0.41
3:J:78:ARG:HH22	3:J:85:ASP:CG	2.23	0.41
3:R:39:ARG:C	3:R:41:GLY:H	2.24	0.41
4:W:93:LEU:HD23	1:X:103:LEU:HD21	2.02	0.41
2:Y:100:LEU:HD11	3:Z:58:LEU:HD13	2.03	0.41
2:I:63:ARG:HB2	2:I:63:ARG:CZ	2.50	0.41
2:I:78:PHE:CZ	3:J:67:ARG:HB2	2.56	0.41
2:Q:127:ALA:O	2:Q:131:ARG:HG3	2.21	0.41
3:R:90:LEU:HB3	3:R:95:ARG:O	2.21	0.41
2:Y:63:ARG:CZ	2:Y:63:ARG:HB2	2.50	0.41
2:E:48:LEU:O	2:E:52:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:98:TYR:OH	1:X:65:ASP:OD2	2.34	0.41
3:Z:39:ARG:C	3:Z:41:GLY:H	2.24	0.41
3:B:30:THR:O	3:B:34:ILE:HG13	2.21	0.41
4:C:95:LYS:O	4:C:96:LEU:C	2.60	0.41
1:D:65:ASP:OD1	1:D:65:ASP:C	2.60	0.41
1:L:35:ALA:HA	1:L:56:MET:HE1	2.03	0.41
1:L:91:ILE:O	1:L:94:ALA:HB3	2.21	0.41
4:O:93:LEU:HD23	1:P:103:LEU:HD21	2.02	0.41
1:P:39:TYR:O	1:P:40:LYS:C	2.58	0.41
2:Y:127:ALA:O	2:Y:131:ARG:HG3	2.21	0.41
2:I:59:GLU:HG3	2:I:59:GLU:H	1.51	0.40
2:I:97:GLU:O	2:I:98:ALA:C	2.60	0.40
3:N:62:LEU:O	3:N:63:GLU:C	2.60	0.40
4:O:100:VAL:HG12	4:O:101:THR:N	2.34	0.40
1:T:91:ILE:O	1:T:94:ALA:HB3	2.21	0.40
3:J:39:ARG:C	3:J:41:GLY:H	2.24	0.40
4:K:95:LYS:O	4:K:96:LEU:C	2.60	0.40
1:L:65:ASP:C	1:L:65:ASP:OD1	2.60	0.40
2:A:78:PHE:CZ	3:B:67:ARG:HB2	2.56	0.40
4:G:62:ILE:HG12	4:G:93:LEU:HD13	1.98	0.40
2:M:106:ASP:HA	2:M:109:LEU:HD12	2.02	0.40
2:M:101:VAL:HG11	3:N:40:ARG:HG2	2.03	0.40
4:O:62:ILE:HG12	4:O:93:LEU:HD13	1.98	0.40
2:U:59:GLU:HG3	2:U:59:GLU:H	1.58	0.40
2:A:100:LEU:HD11	3:B:58:LEU:HD13	2.03	0.40
4:W:66:ALA:O	4:W:69:ALA:HB3	2.22	0.40
3:B:90:LEU:HB3	3:B:95:ARG:O	2.21	0.40
4:O:80:PRO:O	4:O:81:ARG:C	2.59	0.40
2:Q:100:LEU:HD11	3:R:58:LEU:HD13	2.03	0.40
4:S:57:TYR:O	4:S:60:ALA:HB3	2.22	0.40
3:V:62:LEU:O	3:V:63:GLU:C	2.60	0.40
2:Y:63:ARG:HH22	3:Z:30:THR:CG2	2.35	0.40

All (20) 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:D:48:ASP:OD2	1:H:106:HIS:ND1[1_455]	0.19	2.01
1:L:48:ASP:OD2	1:P:106:HIS:ND1[1_655]	0.47	1.73
1:T:48:ASP:OD2	1:X:106:HIS:ND1[1_655]	0.66	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:48:ASP:OD2	1:f:106:HIS:ND1[1_455]	0.75	1.45
1:D:48:ASP:OD2	1:H:106:HIS:CE1[1_455]	1.30	0.90
1:T:48:ASP:OD2	1:X:106:HIS:CE1[1_655]	1.33	0.87
1:L:48:ASP:OD2	1:P:106:HIS:CE1[1_655]	1.33	0.87
1:D:48:ASP:CG	1:H:106:HIS:ND1[1_455]	1.40	0.80
1:L:48:ASP:CG	1:P:106:HIS:ND1[1_655]	1.47	0.73
1:T:48:ASP:CG	1:X:106:HIS:ND1[1_655]	1.49	0.71
1:D:48:ASP:OD2	1:H:106:HIS:CG[1_455]	1.54	0.66
1:b:48:ASP:OD2	1:f:106:HIS:CE1[1_455]	1.77	0.43
1:L:48:ASP:OD2	1:P:106:HIS:CG[1_655]	1.78	0.42
1:b:48:ASP:CG	1:f:106:HIS:ND1[1_455]	1.83	0.37
1:T:48:ASP:OD2	1:X:106:HIS:CG[1_655]	1.91	0.29
1:b:48:ASP:OD2	1:f:106:HIS:CG[1_455]	1.93	0.27
1:D:106:HIS:CD2	1:H:48:ASP:OD1[1_455]	2.07	0.13
1:T:48:ASP:OD1	1:X:106:HIS:ND1[1_655]	2.08	0.12
3:B:23:ARG:NH1	6:h:-253:DG:OP1[1_545]	2.08	0.12
1:L:48:ASP:OD1	1:P:106:HIS:ND1[1_655]	2.18	0.02

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	D	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6	35
1	H	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14	51
1	L	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6	35
1	P	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14	51
1	T	93/126 (74%)	81 (87%)	10 (11%)	2 (2%)	6	35
1	X	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14	51
1	b	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6	35
1	f	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4	26
2	E	95/135 (70%)	86 (90%)	9 (10%)	0	100	100
2	I	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4	26
2	M	95/135 (70%)	86 (90%)	9 (10%)	0	100	100
2	Q	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4	26
2	U	95/135 (70%)	86 (90%)	9 (10%)	0	100	100
2	Y	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4	26
2	c	95/135 (70%)	86 (90%)	9 (10%)	0	100	100
3	B	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3	24
3	F	76/102 (74%)	67 (88%)	9 (12%)	0	100	100
3	J	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3	24
3	N	76/102 (74%)	67 (88%)	9 (12%)	0	100	100
3	R	78/102 (76%)	68 (87%)	7 (9%)	3 (4%)	3	24
3	V	76/102 (74%)	67 (88%)	9 (12%)	0	100	100
3	Z	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3	24
3	d	76/102 (74%)	67 (88%)	9 (12%)	0	100	100
4	C	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3	23
4	G	103/130 (79%)	88 (85%)	15 (15%)	0	100	100
4	K	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3	23
4	O	103/130 (79%)	87 (84%)	16 (16%)	0	100	100
4	S	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3	23
4	W	103/130 (79%)	88 (85%)	15 (15%)	0	100	100
4	a	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3	23
4	e	103/130 (79%)	88 (85%)	15 (15%)	0	100	100
All	All	2937/3944 (74%)	2572 (88%)	313 (11%)	52 (2%)	8	40

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	101	GLY
2	Q	73	GLU
3	R	29	ILE
2	I	73	GLU
3	J	29	ILE

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Mol	Chain	Res	Type
2	A	73	GLU
3	B	29	ILE
1	D	101	GLY
1	T	101	GLY
2	Y	73	GLU
3	Z	29	ILE
1	b	101	GLY
1	L	109	SER
1	P	101	GLY
2	Q	77	ASP
2	I	77	ASP
2	A	77	ASP
1	D	109	SER
1	H	101	GLY
1	T	109	SER
1	X	101	GLY
2	Y	77	ASP
1	b	109	SER
1	f	101	GLY
3	R	34	ILE
3	J	34	ILE
3	B	34	ILE
3	Z	34	ILE
4	C	64	GLU
4	C	113	SER
4	K	64	GLU
4	K	113	SER
4	S	64	GLU
4	S	113	SER
4	a	64	GLU
4	a	113	SER
2	Q	74	ILE
3	R	26	ILE
2	I	74	ILE
3	J	26	ILE
2	A	74	ILE
3	B	26	ILE
2	Y	74	ILE
3	Z	26	ILE
4	a	114	VAL
4	C	114	VAL
4	K	114	VAL

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Mol	Chain	Res	Type
4	S	114	VAL
4	C	26	PRO
4	K	26	PRO
4	S	26	PRO
4	a	26	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	81/106 (76%)	69 (85%)	12 (15%)	3	15
1	H	79/106 (74%)	67 (85%)	12 (15%)	3	14
1	L	81/106 (76%)	69 (85%)	12 (15%)	3	15
1	P	79/106 (74%)	67 (85%)	12 (15%)	3	14
1	T	81/106 (76%)	69 (85%)	12 (15%)	3	15
1	X	79/106 (74%)	67 (85%)	12 (15%)	3	14
1	b	81/106 (76%)	69 (85%)	12 (15%)	3	15
1	f	79/106 (74%)	67 (85%)	12 (15%)	3	14
2	A	85/110 (77%)	77 (91%)	8 (9%)	8	28
2	E	84/110 (76%)	79 (94%)	5 (6%)	19	44
2	I	85/110 (77%)	77 (91%)	8 (9%)	8	28
2	M	84/110 (76%)	79 (94%)	5 (6%)	19	44
2	Q	85/110 (77%)	77 (91%)	8 (9%)	8	28
2	U	84/110 (76%)	79 (94%)	5 (6%)	19	44
2	Y	85/110 (77%)	77 (91%)	8 (9%)	8	28
2	c	84/110 (76%)	79 (94%)	5 (6%)	19	44
3	B	68/78 (87%)	63 (93%)	5 (7%)	13	38
3	F	63/78 (81%)	59 (94%)	4 (6%)	18	42
3	J	68/78 (87%)	63 (93%)	5 (7%)	13	38
3	N	63/78 (81%)	59 (94%)	4 (6%)	18	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	R	67/78 (86%)	62 (92%)	5 (8%)	13	37
3	V	63/78 (81%)	59 (94%)	4 (6%)	18	42
3	Z	68/78 (87%)	63 (93%)	5 (7%)	13	38
3	d	63/78 (81%)	59 (94%)	4 (6%)	18	42
4	C	82/102 (80%)	75 (92%)	7 (8%)	10	33
4	G	83/102 (81%)	74 (89%)	9 (11%)	6	23
4	K	82/102 (80%)	75 (92%)	7 (8%)	10	33
4	O	83/102 (81%)	74 (89%)	9 (11%)	6	23
4	S	82/102 (80%)	75 (92%)	7 (8%)	10	33
4	W	83/102 (81%)	74 (89%)	9 (11%)	6	23
4	a	82/102 (80%)	75 (92%)	7 (8%)	10	33
4	e	83/102 (81%)	74 (89%)	9 (11%)	6	23
All	All	2499/3168 (79%)	2251 (90%)	248 (10%)	8	26

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	31	LYS
1	L	39	TYR
1	L	48	ASP
1	L	49	THR
1	L	77	LEU
1	L	84	SER
1	L	85	THR
1	L	93	THR
1	L	98	LEU
1	L	109	SER
1	L	116	THR
1	L	119	THR
2	M	39	HIS
2	M	59	GLU
2	M	65	LEU
2	M	117	VAL
2	M	129	ARG
3	N	26	ILE
3	N	35	ARG
3	N	73	THR
3	N	92	ARG

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Mol	Chain	Res	Type
4	O	19	SER
4	O	50	TYR
4	O	59	THR
4	O	72	ASP
4	O	74	LYS
4	O	81	ARG
4	O	84	GLN
4	O	88	ARG
4	O	114	VAL
1	P	31	LYS
1	P	49	THR
1	P	68	GLU
1	P	83	ARG
1	P	88	SER
1	P	93	THR
1	P	95	VAL
1	P	98	LEU
1	P	102	GLU
1	P	109	SER
1	P	112	THR
1	P	117	LYS
2	Q	48	LEU
2	Q	49	ARG
2	Q	59	GLU
2	Q	63	ARG
2	Q	65	LEU
2	Q	105	GLU
2	Q	115	LYS
2	Q	129	ARG
3	R	47	SER
3	R	73	THR
3	R	80	THR
3	R	91	LYS
3	R	92	ARG
2	I	48	LEU
2	I	49	ARG
2	I	59	GLU
2	I	63	ARG
2	I	65	LEU
2	I	105	GLU
2	I	115	LYS
2	I	129	ARG

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Mol	Chain	Res	Type
3	J	47	SER
3	J	73	THR
3	J	80	THR
3	J	91	LYS
3	J	92	ARG
2	A	48	LEU
2	A	49	ARG
2	A	59	GLU
2	A	63	ARG
2	A	65	LEU
2	A	105	GLU
2	A	115	LYS
2	A	129	ARG
3	B	47	SER
3	B	73	THR
3	B	80	THR
3	B	91	LYS
3	B	92	ARG
4	C	29	ARG
4	C	59	THR
4	C	81	ARG
4	C	91	GLU
4	C	101	THR
4	C	114	VAL
4	C	118	LYS
1	D	31	LYS
1	D	39	TYR
1	D	48	ASP
1	D	49	THR
1	D	77	LEU
1	D	84	SER
1	D	85	THR
1	D	93	THR
1	D	98	LEU
1	D	109	SER
1	D	116	THR
1	D	119	THR
2	E	39	HIS
2	E	59	GLU
2	E	65	LEU
2	E	117	VAL
2	E	129	ARG

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Mol	Chain	Res	Type
3	F	26	ILE
3	F	35	ARG
3	F	73	THR
3	F	92	ARG
4	G	19	SER
4	G	50	TYR
4	G	59	THR
4	G	72	ASP
4	G	74	LYS
4	G	81	ARG
4	G	84	GLN
4	G	88	ARG
4	G	114	VAL
1	H	31	LYS
1	H	49	THR
1	H	68	GLU
1	H	83	ARG
1	H	88	SER
1	H	93	THR
1	H	95	VAL
1	H	98	LEU
1	H	102	GLU
1	H	109	SER
1	H	112	THR
1	H	117	LYS
4	K	29	ARG
4	K	59	THR
4	K	81	ARG
4	K	91	GLU
4	K	101	THR
4	K	114	VAL
4	K	118	LYS
4	S	29	ARG
4	S	59	THR
4	S	81	ARG
4	S	91	GLU
4	S	101	THR
4	S	114	VAL
4	S	118	LYS
1	T	31	LYS
1	T	39	TYR
1	T	48	ASP

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Mol	Chain	Res	Type
1	T	49	THR
1	T	77	LEU
1	T	84	SER
1	T	85	THR
1	T	93	THR
1	T	98	LEU
1	T	109	SER
1	T	116	THR
1	T	119	THR
2	U	39	HIS
2	U	59	GLU
2	U	65	LEU
2	U	117	VAL
2	U	129	ARG
3	V	26	ILE
3	V	35	ARG
3	V	73	THR
3	V	92	ARG
4	W	19	SER
4	W	50	TYR
4	W	59	THR
4	W	72	ASP
4	W	74	LYS
4	W	81	ARG
4	W	84	GLN
4	W	88	ARG
4	W	114	VAL
1	X	31	LYS
1	X	49	THR
1	X	68	GLU
1	X	83	ARG
1	X	88	SER
1	X	93	THR
1	X	95	VAL
1	X	98	LEU
1	X	102	GLU
1	X	109	SER
1	X	112	THR
1	X	117	LYS
2	Y	48	LEU
2	Y	49	ARG
2	Y	59	GLU

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Mol	Chain	Res	Type
2	Y	63	ARG
2	Y	65	LEU
2	Y	105	GLU
2	Y	115	LYS
2	Y	129	ARG
3	Z	47	SER
3	Z	73	THR
3	Z	80	THR
3	Z	91	LYS
3	Z	92	ARG
4	a	29	ARG
4	a	59	THR
4	a	81	ARG
4	a	91	GLU
4	a	101	THR
4	a	114	VAL
4	a	118	LYS
1	b	31	LYS
1	b	39	TYR
1	b	48	ASP
1	b	49	THR
1	b	77	LEU
1	b	84	SER
1	b	85	THR
1	b	93	THR
1	b	98	LEU
1	b	109	SER
1	b	116	THR
1	b	119	THR
2	c	39	HIS
2	c	59	GLU
2	c	65	LEU
2	c	117	VAL
2	c	129	ARG
3	d	26	ILE
3	d	35	ARG
3	d	73	THR
3	d	92	ARG
4	e	19	SER
4	e	50	TYR
4	e	59	THR
4	e	72	ASP

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Mol	Chain	Res	Type
4	e	74	LYS
4	e	81	ARG
4	e	84	GLN
4	e	88	ARG
4	e	114	VAL
1	f	31	LYS
1	f	49	THR
1	f	68	GLU
1	f	83	ARG
1	f	88	SER
1	f	93	THR
1	f	95	VAL
1	f	98	LEU
1	f	102	GLU
1	f	109	SER
1	f	112	THR
1	f	117	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	68	GLN
4	O	31	HIS
4	O	84	GLN
3	R	75	HIS
3	J	75	HIS
3	B	75	HIS
4	C	38	ASN
4	C	112	GLN
2	E	68	GLN
4	G	31	HIS
4	G	84	GLN
4	K	38	ASN
4	K	112	GLN
4	S	38	ASN
4	S	112	GLN
2	U	68	GLN
4	W	31	HIS
4	W	84	GLN
3	Z	75	HIS
4	a	38	ASN
4	a	112	GLN

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Mol	Chain	Res	Type
2	c	68	GLN
4	e	31	HIS
4	e	84	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	h	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h	-448:DT	O3'	-447:DG	P	1.92

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.