Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:33 pm BST

PDB ID	:	5OXV
Title	:	Structure of the 4_601_157 tetranucleosome (C2 form)
Authors	:	Ekundayo, B.; Schalch, T.
Deposited on	:	2017-09-07
Resolution	:	6.72 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 ①) were used in the production of this report:

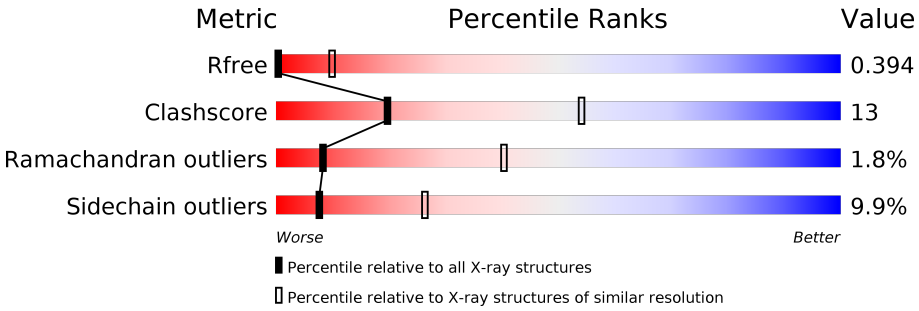
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.72 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	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)
Ramachandran outliers	138981	1000 (9.50-3.90)
Sidechain outliers	138945	1000 (9.50-3.86)

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 <=5%

Mol	Chain	Length	Quality of chain
1	J	312	44% 44% 12% •
2	D	126	43% 27% 5% • 25%
2	H	126	44% 27% • 26%
2	N	126	44% 26% 5% • 25%
2	R	126	44% 26% • 26%
3	C	130	51% 24% 5% 21%
3	G	130	48% 28% 5% 19%

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Mol	Chain	Length	Quality of chain
3	M	130	52% 23% 5% 21%
3	Q	130	46% 31% 19%
4	B	102	44% 32% 5% 19%
4	F	102	61% 14% 24%
4	L	102	44% 32% 5% 19%
4	P	102	60% 15% 24%
5	A	135	49% 19% 28%
5	E	135	52% 20% 28%
5	K	135	49% 19% 28%
5	O	135	53% 19% 28%
6	I	313	45% 42% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24648 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 DNA chain called DNA STRAND 1 (601-based sequence model).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	310	Total	C	N	O	P	0	0	0
			6394	3024	1203	1857	310			

- Molecule 2 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
2	N	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
2	H	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
2	D	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	29	THR	SER	conflict	UNP P02281
N	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281
D	29	THR	SER	conflict	UNP P02281

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	105	Total	C	N	O	0	0	0
			809	510	158	141			
3	M	103	Total	C	N	O	0	0	0
			795	501	155	139			
3	G	105	Total	C	N	O	0	0	0
			809	510	158	141			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	0	0	0
			795	501	155	139			

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
4	L	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
4	F	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
4	B	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			

- Molecule 5 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	O	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
5	K	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
5	E	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
5	A	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	102	ALA	GLY	conflict	UNP P84233
K	102	ALA	GLY	conflict	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233
A	102	ALA	GLY	conflict	UNP P84233

- Molecule 6 is a DNA chain called DNA STRAND 2 (601-based sequence model).

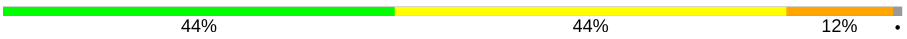
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	311	Total	C	N	O	P	0	0	0
			6336	3009	1146	1870	311			

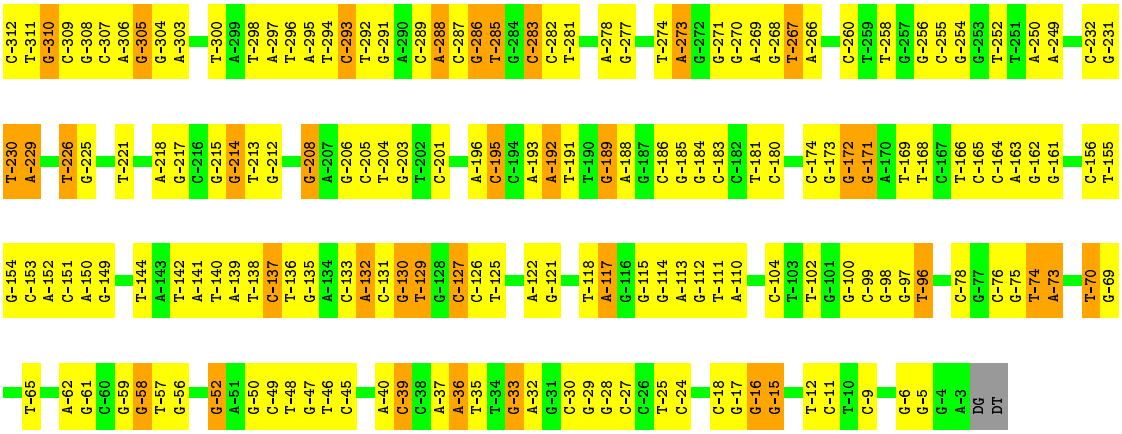
3 Residue-property plots (i)

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.

- Molecule 1: DNA STRAND 1 (601-based sequence model)

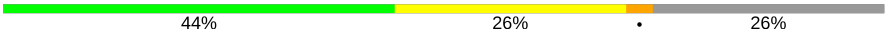
Chain J:

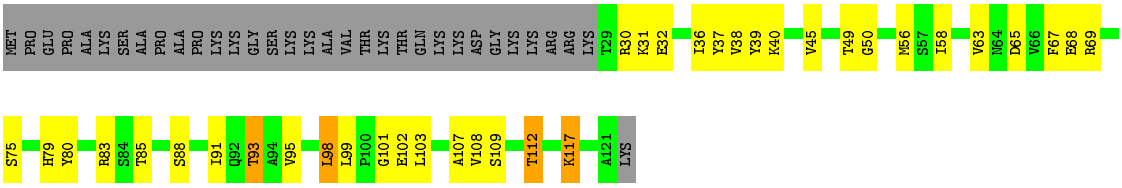




- Molecule 2: Histone H2B 1.1

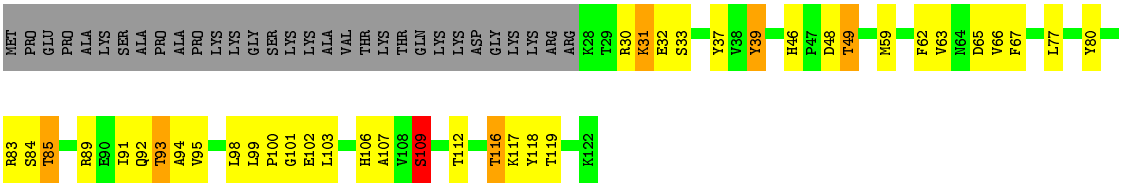
Chain R:





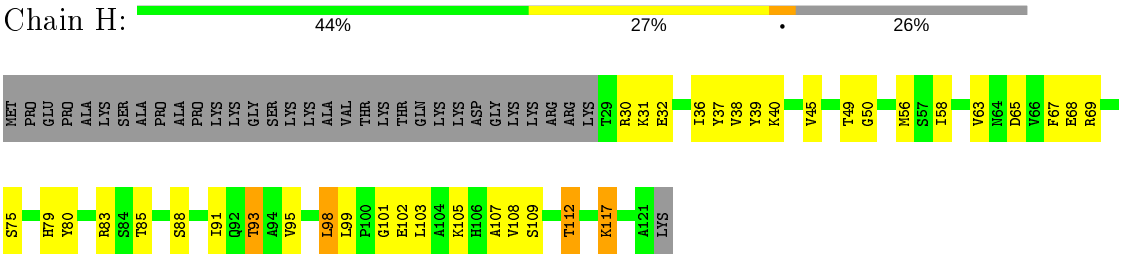
- Molecule 2: Histone H2B 1.1

Chain N:



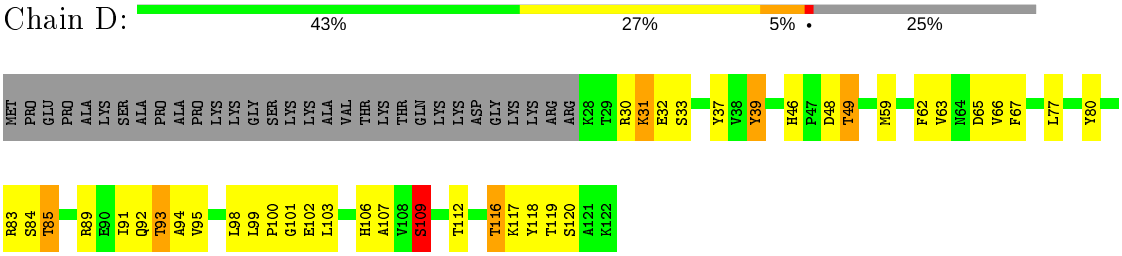
- Molecule 2: Histone H2B 1.1

Chain H:



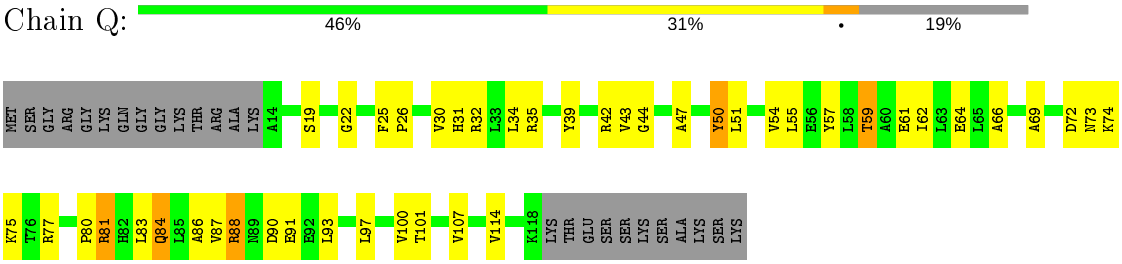
• Molecule 2: Histone H2B 1.1

Chain D:



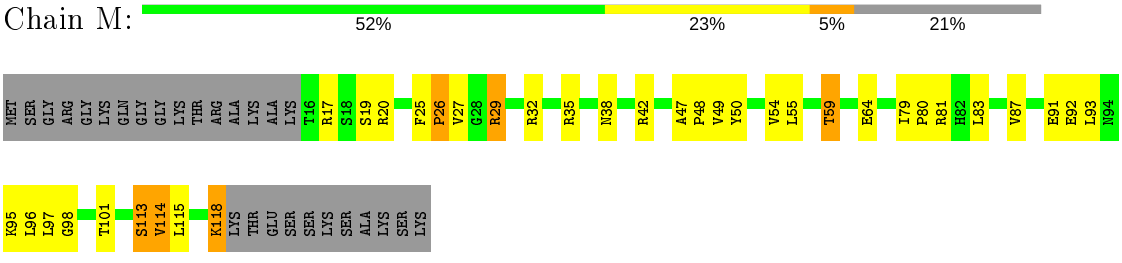
• Molecule 3: Histone H2A

Chain Q:



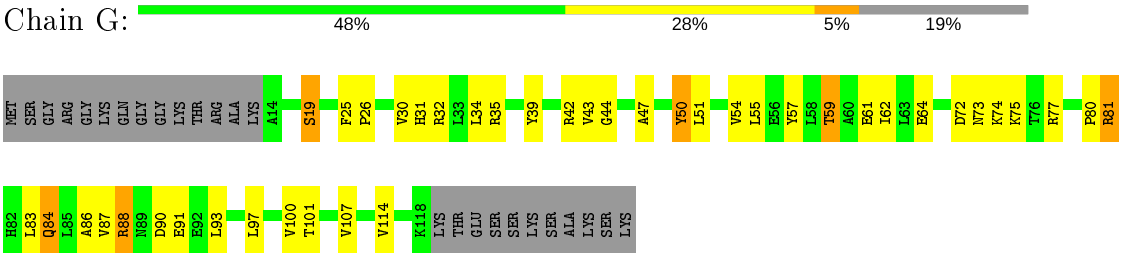
• Molecule 3: Histone H2A

Chain M:



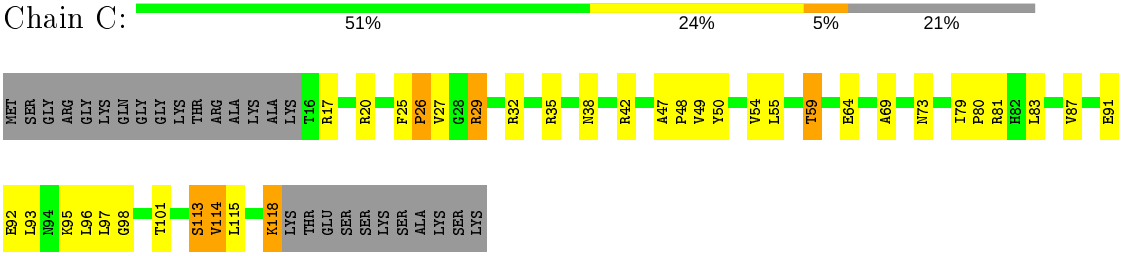
• Molecule 3: Histone H2A

Chain G:



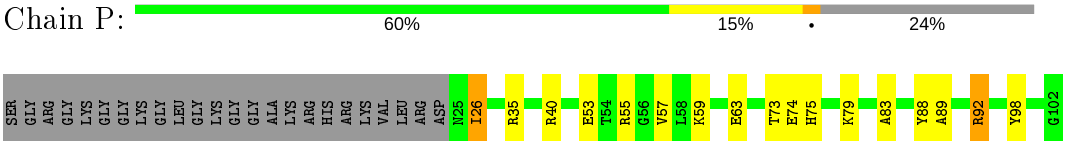
• Molecule 3: Histone H2A

Chain C:



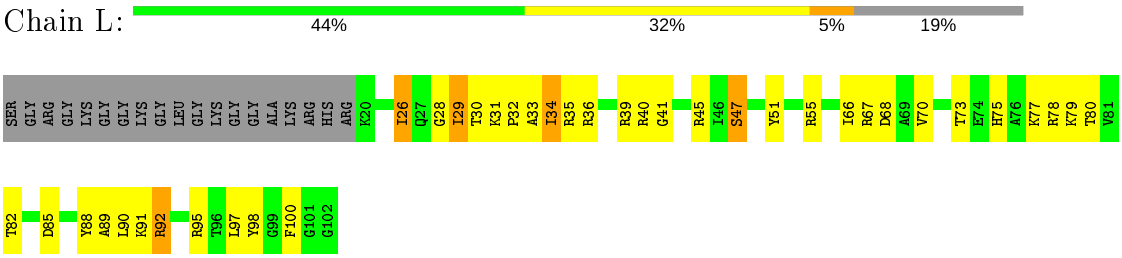
- Molecule 4: Histone H4

Chain P:



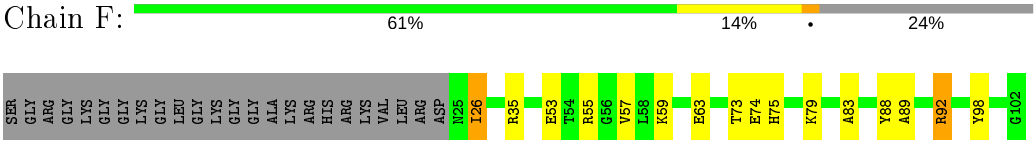
- Molecule 4: Histone H4

Chain L:



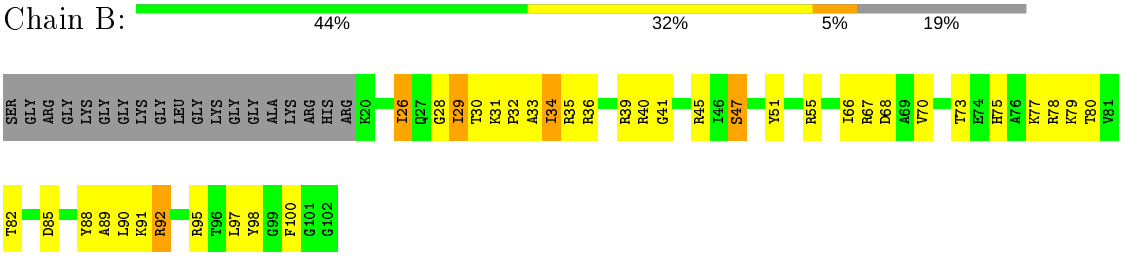
- Molecule 4: Histone H4

Chain F:



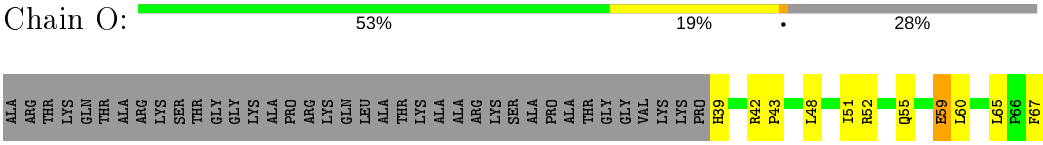
- Molecule 4: Histone H4

Chain B:



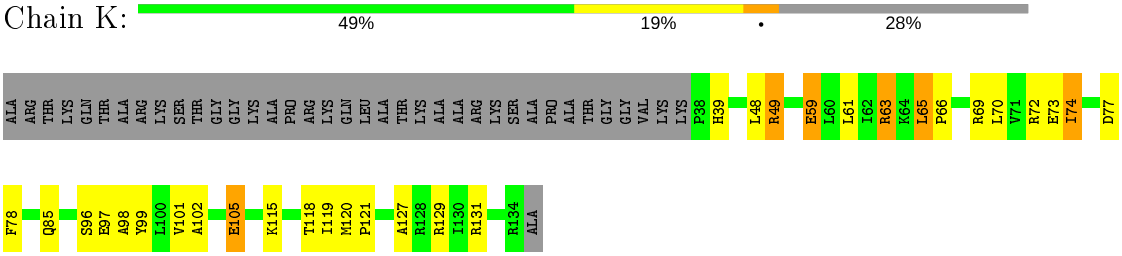
- Molecule 5: Histone H3.2

Chain O:



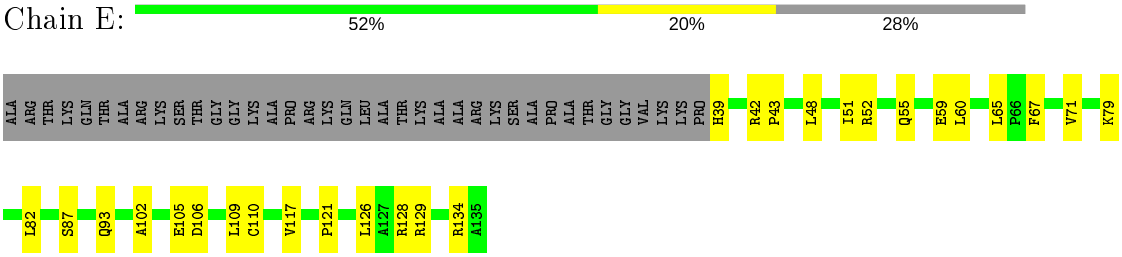
• Molecule 5: Histone H3.2

Chain K:



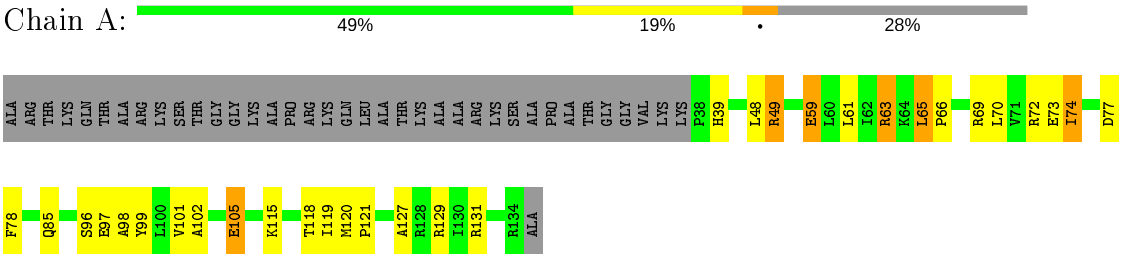
• Molecule 5: Histone H3.2

Chain E:



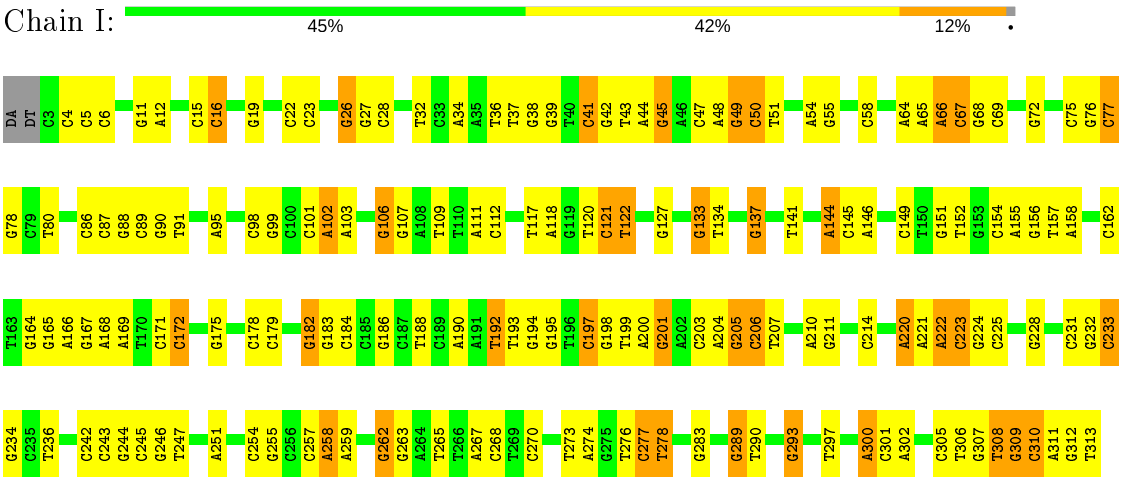
• Molecule 5: Histone H3.2

Chain A:



• Molecule 6: DNA STRAND 2 (601-based sequence model)

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	348.84Å 63.27Å 271.36Å 90.00° 124.74° 90.00°	Depositor
Resolution (Å)	71.67 – 6.72 222.99 – 6.72	Depositor EDS
% Data completeness (in resolution range)	87.8 (71.67-6.72) 82.3 (222.99-6.72)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.22 (at 6.74Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.317 , 0.352 0.358 , 0.394	Depositor DCC
R_{free} test set	1169 reflections (12.72%)	wwPDB-VP
Wilson B-factor (Å^2)	308.9	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.04 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	24648	wwPDB-VP
Average B, all atoms (Å^2)	637.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	J	0.74	2/7182 (0.0%)	1.47	96/11093 (0.9%)
2	D	0.49	0/756	0.64	0/1015
2	H	0.62	0/737	0.70	0/993
2	N	0.49	0/756	0.64	0/1015
2	R	0.62	0/737	0.70	0/993
3	C	0.42	0/805	0.61	0/1088
3	G	0.62	0/819	0.76	0/1106
3	M	0.43	0/805	0.61	0/1088
3	Q	0.63	0/819	0.76	0/1106
4	B	0.67	0/669	0.84	0/894
4	F	0.46	0/626	0.61	0/837
4	L	0.67	0/669	0.84	0/894
4	P	0.45	0/626	0.61	0/837
5	A	0.66	0/814	0.73	0/1092
5	E	0.41	0/812	0.58	0/1088
5	K	0.66	0/814	0.73	0/1092
5	O	0.41	0/812	0.58	0/1088
6	I	0.74	4/7098 (0.1%)	1.38	84/10943 (0.8%)
All	All	0.66	6/26356 (0.0%)	1.17	180/38262 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	-310	DG	C1'-N9	-6.27	1.38	1.47
6	I	310	DC	C1'-N1	5.73	1.56	1.49
1	J	-305	DG	C1'-N9	-5.53	1.39	1.47
6	I	312	DG	C1'-N9	-5.43	1.39	1.47
6	I	308	DT	C1'-N1	5.30	1.56	1.49
6	I	309	DG	C1'-N9	-5.26	1.39	1.47

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	-163	DA	O3'-P-O5'	33.99	168.59	104.00
1	J	-163	DA	P-O3'-C3'	29.81	155.47	119.70
1	J	-163	DA	OP1-P-O3'	-20.17	60.83	105.20
6	I	162	DC	O3'-P-O5'	14.02	130.63	104.00
1	J	-163	DA	OP2-P-O3'	-12.28	78.18	105.20
1	J	-59	DG	O3'-P-O5'	-11.99	81.22	104.00
1	J	-215	DG	O3'-P-O5'	-11.99	81.22	104.00
6	I	162	DC	OP1-P-O3'	-10.31	82.53	105.20
1	J	-59	DG	OP2-P-O3'	-10.03	83.14	105.20
1	J	-215	DG	OP2-P-O3'	-10.00	83.20	105.20
6	I	162	DC	P-O3'-C3'	9.12	130.64	119.70
1	J	-221	DT	O4'-C1'-N1	8.87	114.21	108.00
1	J	-65	DT	O4'-C1'-N1	8.83	114.18	108.00
1	J	-58	DG	O4'-C1'-N9	8.42	113.89	108.00
1	J	-214	DG	O4'-C1'-N9	8.41	113.89	108.00
1	J	-45	DC	P-O3'-C3'	8.03	129.34	119.70
1	J	-201	DC	P-O3'-C3'	8.00	129.30	119.70
1	J	-15	DG	P-O3'-C3'	7.90	129.18	119.70
1	J	-171	DG	P-O3'-C3'	7.88	129.15	119.70
1	J	-74	DT	O4'-C1'-N1	7.77	113.44	108.00
1	J	-230	DT	O4'-C1'-N1	7.75	113.43	108.00
6	I	188	DT	O4'-C1'-N1	7.67	113.37	108.00
6	I	32	DT	O4'-C1'-N1	7.67	113.37	108.00
6	I	182	DG	P-O3'-C3'	7.61	128.83	119.70
6	I	26	DG	P-O3'-C3'	7.50	128.71	119.70
1	J	-258	DT	O4'-C1'-N1	7.30	113.11	108.00
1	J	-102	DT	O4'-C1'-N1	7.29	113.10	108.00
6	I	214	DC	O4'-C1'-N1	7.24	113.07	108.00
6	I	58	DC	O4'-C1'-N1	7.23	113.06	108.00
1	J	-114	DG	O4'-C1'-N9	-7.22	102.94	108.00
1	J	-270	DG	O4'-C1'-N9	-7.08	103.04	108.00
1	J	-16	DG	P-O3'-C3'	7.08	128.20	119.70
1	J	-172	DG	P-O3'-C3'	7.05	128.16	119.70
6	I	204	DA	O4'-C1'-N9	7.02	112.92	108.00
6	I	48	DA	O4'-C1'-N9	6.99	112.89	108.00
1	J	-273	DA	P-O3'-C3'	6.97	128.06	119.70
1	J	-181	DT	P-O3'-C3'	6.92	128.01	119.70
1	J	-117	DA	P-O3'-C3'	6.90	127.98	119.70
1	J	-25	DT	P-O3'-C3'	6.88	127.95	119.70
6	I	278	DT	P-O3'-C3'	6.86	127.94	119.70
6	I	277	DC	P-O3'-C3'	6.84	127.91	119.70
1	J	-142	DT	O4'-C1'-N1	6.84	112.78	108.00
6	I	122	DT	P-O3'-C3'	6.84	127.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	-212	DG	O4'-C1'-N9	6.83	112.78	108.00
6	I	121	DC	P-O3'-C3'	6.82	127.88	119.70
1	J	-214	DG	P-O3'-C3'	6.80	127.86	119.70
6	I	184	DC	P-O3'-C3'	6.80	127.86	119.70
1	J	-58	DG	P-O3'-C3'	6.78	127.84	119.70
1	J	-298	DT	O4'-C1'-N1	6.76	112.73	108.00
1	J	-56	DG	O4'-C1'-N9	6.75	112.73	108.00
6	I	28	DC	P-O3'-C3'	6.74	127.79	119.70
6	I	102	DA	P-O3'-C3'	6.73	127.78	119.70
1	J	-268	DG	P-O3'-C3'	6.73	127.78	119.70
1	J	-112	DG	P-O3'-C3'	6.71	127.75	119.70
6	I	258	DA	P-O3'-C3'	6.68	127.72	119.70
6	I	67	DC	P-O3'-C3'	6.65	127.67	119.70
6	I	223	DC	P-O3'-C3'	6.63	127.66	119.70
6	I	66	DA	P-O3'-C3'	6.57	127.58	119.70
6	I	172	DC	P-O3'-C3'	6.55	127.56	119.70
6	I	16	DC	P-O3'-C3'	6.53	127.54	119.70
6	I	222	DA	P-O3'-C3'	6.53	127.54	119.70
6	I	137	DG	O4'-C1'-N9	-6.50	103.45	108.00
1	J	-100	DG	P-O3'-C3'	6.49	127.49	119.70
1	J	-256	DG	P-O3'-C3'	6.49	127.49	119.70
1	J	-37	DA	P-O3'-C3'	6.48	127.48	119.70
1	J	-193	DA	P-O3'-C3'	6.44	127.43	119.70
1	J	-49	DC	O4'-C1'-N1	6.44	112.51	108.00
6	I	293	DG	O4'-C1'-N9	-6.44	103.49	108.00
6	I	251	DA	O4'-C1'-N9	6.42	112.49	108.00
1	J	-133	DC	P-O3'-C3'	6.41	127.39	119.70
1	J	-205	DC	O4'-C1'-N1	6.39	112.47	108.00
1	J	-130	DG	P-O3'-C3'	6.38	127.36	119.70
1	J	-286	DG	P-O3'-C3'	6.38	127.36	119.70
6	I	95	DA	O4'-C1'-N9	6.35	112.45	108.00
1	J	-289	DC	P-O3'-C3'	6.34	127.31	119.70
1	J	-58	DG	O5'-P-OP2	6.34	118.30	110.70
1	J	-59	DG	P-O3'-C3'	6.29	127.24	119.70
6	I	117	DT	P-O3'-C3'	6.28	127.24	119.70
1	J	-214	DG	O5'-P-OP2	6.27	118.22	110.70
1	J	-215	DG	P-O3'-C3'	6.22	127.17	119.70
6	I	273	DT	P-O3'-C3'	6.22	127.16	119.70
1	J	-59	DG	C3'-C2'-C1'	-6.15	95.12	102.50
1	J	-215	DG	C3'-C2'-C1'	-6.09	95.19	102.50
6	I	64	DA	O4'-C1'-N9	6.07	112.25	108.00
6	I	257	DC	O4'-C1'-N1	6.05	112.24	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	49	DG	P-O3'-C3'	6.03	126.93	119.70
1	J	-70	DT	N3-C2-O2	-6.03	118.69	122.30
6	I	205	DG	P-O3'-C3'	6.02	126.93	119.70
1	J	-226	DT	N3-C2-O2	-6.02	118.69	122.30
6	I	220	DA	O4'-C1'-N9	6.01	112.21	108.00
6	I	101	DC	O4'-C1'-N1	6.00	112.20	108.00
6	I	247	DT	O4'-C1'-N1	6.00	112.20	108.00
6	I	91	DT	O4'-C1'-N1	5.98	112.19	108.00
1	J	-59	DG	OP1-P-O3'	-5.97	92.07	105.20
1	J	-215	DG	OP1-P-O3'	-5.96	92.10	105.20
6	I	206	DC	P-O3'-C3'	5.95	126.84	119.70
6	I	50	DC	P-O3'-C3'	5.95	126.83	119.70
6	I	265	DT	P-O3'-C3'	5.89	126.77	119.70
6	I	109	DT	P-O3'-C3'	5.89	126.77	119.70
6	I	276	DT	O4'-C1'-N1	5.86	112.10	108.00
1	J	-298	DT	C1'-O4'-C4'	-5.84	104.26	110.10
6	I	120	DT	O4'-C1'-N1	5.82	112.08	108.00
1	J	-104	DC	O4'-C1'-N1	5.77	112.04	108.00
1	J	-132	DA	O4'-C1'-N9	5.76	112.03	108.00
1	J	-142	DT	C1'-O4'-C4'	-5.74	104.36	110.10
6	I	192	DT	P-O3'-C3'	5.73	126.57	119.70
6	I	36	DT	P-O3'-C3'	5.71	126.56	119.70
6	I	144	DA	O4'-C1'-N9	5.71	112.00	108.00
1	J	-288	DA	O4'-C1'-N9	5.69	111.98	108.00
6	I	162	DC	O4'-C1'-N1	5.69	111.98	108.00
6	I	133	DG	P-O3'-C3'	5.68	126.52	119.70
1	J	-260	DC	O4'-C1'-N1	5.68	111.98	108.00
6	I	197	DC	P-O3'-C3'	5.68	126.52	119.70
1	J	-293	DC	P-O3'-C3'	5.66	126.49	119.70
1	J	-137	DC	P-O3'-C3'	5.66	126.49	119.70
6	I	300	DA	P-O3'-C3'	5.63	126.45	119.70
6	I	41	DC	P-O3'-C3'	5.62	126.45	119.70
6	I	289	DG	P-O3'-C3'	5.62	126.44	119.70
6	I	300	DA	O4'-C1'-N9	5.62	111.94	108.00
6	I	175	DG	O4'-C1'-N9	5.62	111.93	108.00
6	I	144	DA	P-O3'-C3'	5.60	126.42	119.70
6	I	19	DG	O4'-C1'-N9	5.58	111.91	108.00
6	I	233	DC	O4'-C1'-N1	5.54	111.88	108.00
6	I	111	DA	O4'-C1'-N9	5.51	111.86	108.00
6	I	45	DG	C3'-C2'-C1'	-5.50	95.90	102.50
6	I	201	DG	C3'-C2'-C1'	-5.49	95.91	102.50
6	I	231	DC	P-O3'-C3'	5.49	126.29	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	-195	DC	P-O3'-C3'	5.49	126.28	119.70
6	I	75	DC	P-O3'-C3'	5.48	126.28	119.70
1	J	-214	DG	C1'-O4'-C4'	-5.48	104.62	110.10
6	I	267	DA	O4'-C1'-N9	5.47	111.83	108.00
1	J	-100	DG	C1'-O4'-C4'	-5.46	104.64	110.10
1	J	-58	DG	C1'-O4'-C4'	-5.46	104.64	110.10
6	I	236	DT	O4'-C1'-N1	5.45	111.81	108.00
6	I	77	DC	O4'-C1'-N1	5.44	111.81	108.00
1	J	-39	DC	P-O3'-C3'	5.42	126.21	119.70
1	J	-256	DG	C1'-O4'-C4'	-5.41	104.69	110.10
1	J	-33	DG	O4'-C1'-N9	-5.41	104.21	108.00
1	J	-189	DG	O4'-C1'-N9	-5.38	104.23	108.00
6	I	106	DG	O4'-C1'-N9	5.36	111.75	108.00
6	I	80	DT	O4'-C1'-N1	5.36	111.75	108.00
1	J	-252	DT	P-O3'-C3'	5.34	126.11	119.70
1	J	-132	DA	P-O3'-C3'	5.33	126.10	119.70
1	J	-283	DC	O4'-C1'-N1	5.32	111.72	108.00
1	J	-127	DC	O4'-C1'-N1	5.30	111.71	108.00
1	J	-36	DA	P-O3'-C3'	5.30	126.06	119.70
1	J	-96	DT	P-O3'-C3'	5.29	126.05	119.70
1	J	-206	DG	O4'-C1'-N9	5.28	111.70	108.00
1	J	-192	DA	P-O3'-C3'	5.28	126.03	119.70
6	I	195	DG	O4'-C1'-N9	5.27	111.69	108.00
6	I	77	DC	C1'-O4'-C4'	-5.24	104.86	110.10
1	J	-288	DA	P-O3'-C3'	5.24	125.98	119.70
1	J	-208	DG	C1'-O4'-C4'	-5.24	104.86	110.10
1	J	-271	DG	P-O3'-C3'	5.23	125.97	119.70
1	J	-50	DG	O4'-C1'-N9	5.22	111.65	108.00
1	J	-52	DG	C1'-O4'-C4'	-5.21	104.89	110.10
1	J	-115	DG	P-O3'-C3'	5.19	125.93	119.70
6	I	32	DT	C1'-O4'-C4'	-5.18	104.92	110.10
6	I	233	DC	C1'-O4'-C4'	-5.18	104.92	110.10
6	I	39	DG	O4'-C1'-N9	5.18	111.62	108.00
6	I	262	DG	O4'-C1'-N9	5.17	111.62	108.00
1	J	-214	DG	OP1-P-OP2	5.17	127.35	119.60
6	I	188	DT	C1'-O4'-C4'	-5.14	104.96	110.10
6	I	203	DC	O4'-C1'-N1	5.13	111.59	108.00
6	I	95	DA	C1'-O4'-C4'	-5.13	104.97	110.10
1	J	-73	DA	C3'-C2'-C1'	-5.13	96.35	102.50
1	J	-58	DG	OP1-P-OP2	5.11	127.26	119.60
1	J	-78	DC	O4'-C1'-N1	5.10	111.57	108.00
1	J	-255	DC	O4'-C1'-N1	5.08	111.56	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	270	DC	O4'-C1'-N1	5.08	111.56	108.00
1	J	-129	DT	O4'-C1'-N1	5.08	111.55	108.00
1	J	-229	DA	C3'-C2'-C1'	-5.07	96.42	102.50
1	J	-99	DC	O4'-C1'-N1	5.06	111.54	108.00
1	J	-267	DT	O4'-C1'-N1	5.05	111.54	108.00
6	I	78	DG	P-O3'-C3'	5.05	125.76	119.70
6	I	251	DA	C1'-O4'-C4'	-5.05	105.05	110.10
1	J	-285	DT	O4'-C1'-N1	5.04	111.53	108.00
6	I	234	DG	P-O3'-C3'	5.04	125.75	119.70
6	I	47	DC	O4'-C1'-N1	5.04	111.53	108.00
6	I	186	DG	O4'-C1'-N9	5.02	111.52	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	6394	0	3474	141	2
2	D	745	0	773	37	3
2	H	726	0	747	36	2
2	N	745	0	773	36	2
2	R	726	0	747	35	2
3	C	795	0	846	25	0
3	G	809	0	864	43	1
3	M	795	0	846	26	1
3	Q	809	0	864	44	1
4	B	662	0	709	36	0
4	F	619	0	659	16	0
4	L	662	0	709	36	0
4	P	619	0	659	17	0
5	A	802	0	841	22	0
5	E	801	0	838	15	0
5	K	802	0	841	21	0
5	O	801	0	838	17	0
6	I	6336	0	3489	146	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24648	0	19517	554	8

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 13.

All (554) 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)
2:D:93:THR:HG21	4:B:75:HIS:CD2	1.58	1.37
2:N:93:THR:HG21	4:L:75:HIS:CD2	1.58	1.37
1:J:-306:DA:C2	6:I:307:DG:N2	1.97	1.32
1:J:-306:DA:H2	6:I:307:DG:C2	1.48	1.29
1:J:-306:DA:C2	6:I:307:DG:C2	2.28	1.21
2:N:93:THR:CG2	4:L:75:HIS:HD2	1.55	1.19
2:D:93:THR:CG2	4:B:75:HIS:HD2	1.55	1.19
2:R:93:THR:HG21	4:P:75:HIS:CD2	1.80	1.16
2:H:93:THR:HG21	4:F:75:HIS:CD2	1.80	1.16
1:J:-305:DG:N2	6:I:306:DT:C2	2.16	1.13
1:J:-306:DA:H2	6:I:307:DG:N2	1.42	1.00
1:J:-310:DG:C2	6:I:311:DA:C2	2.54	0.96
1:J:-310:DG:N2	6:I:311:DA:C2	2.35	0.94
1:J:-305:DG:N2	6:I:306:DT:O2	2.00	0.93
1:J:-310:DG:N2	6:I:311:DA:N3	2.18	0.91
3:C:55:LEU:O	3:C:59:THR:HG22	1.70	0.90
3:M:55:LEU:O	3:M:59:THR:HG22	1.70	0.89
2:N:93:THR:HG21	4:L:75:HIS:HD2	0.71	0.85
6:I:154:DC:C4	6:I:155:DA:N6	2.45	0.84
2:D:93:THR:HG21	4:B:75:HIS:HD2	0.71	0.82
2:R:93:THR:CG2	4:P:75:HIS:CD2	2.63	0.81
3:G:62:ILE:HG12	3:G:93:LEU:HD11	1.64	0.79
1:J:-164:DC:N4	6:I:164:DG:O6	2.13	0.79
3:Q:62:ILE:HG12	3:Q:93:LEU:HD11	1.64	0.79
2:N:95:VAL:HG13	2:N:99:LEU:HD12	1.66	0.78
2:D:93:THR:CG2	4:B:75:HIS:CD2	2.44	0.78
2:H:93:THR:CG2	4:F:75:HIS:CD2	2.63	0.78
5:E:60:LEU:HD13	5:E:93:GLN:HG2	1.66	0.77
2:D:95:VAL:HG13	2:D:99:LEU:HD12	1.66	0.77
5:O:60:LEU:HD13	5:O:93:GLN:HG2	1.66	0.77
4:F:53:GLU:HG3	5:E:121:PRO:HB3	1.66	0.77
3:G:25:PHE:HZ	3:G:59:THR:HG21	1.48	0.76
3:Q:25:PHE:HZ	3:Q:59:THR:HG21	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:26:DG:OP2	2:D:39:TYR:OH	2.02	0.76
1:J:-113:DA:OP1	2:H:85:THR:HG22	1.85	0.76
4:P:53:GLU:HG3	5:O:121:PRO:HB3	1.66	0.76
1:J:-269:DA:OP1	2:R:85:THR:HG22	1.85	0.76
2:N:93:THR:CG2	4:L:75:HIS:CD2	2.44	0.76
2:H:37:TYR:CZ	3:G:26:PRO:HG3	2.21	0.75
6:I:154:DC:N3	6:I:155:DA:C6	2.53	0.75
2:N:39:TYR:OH	6:I:182:DG:OP2	2.02	0.75
2:R:37:TYR:CZ	3:Q:26:PRO:HG3	2.21	0.75
6:I:26:DG:H2"	6:I:27:DG:OP2	1.87	0.74
1:J:-33:DG:H4'	1:J:-32:DA:OP1	1.87	0.74
6:I:182:DG:H2"	6:I:183:DG:OP2	1.87	0.74
2:N:33:SER:O	3:M:29:ARG:NH2	2.20	0.74
3:Q:62:ILE:HG12	3:Q:93:LEU:CD1	2.18	0.73
2:H:93:THR:HG21	4:F:75:HIS:HD2	1.54	0.73
3:G:62:ILE:HG12	3:G:93:LEU:CD1	2.18	0.72
6:I:155:DA:H2"	6:I:156:DG:C8	2.24	0.72
3:G:83:LEU:O	3:G:87:VAL:HG23	1.89	0.72
1:J:-189:DG:H4'	1:J:-188:DA:OP1	1.87	0.72
1:J:-5:DG:O6	6:I:4:DC:N4	2.22	0.72
3:Q:83:LEU:O	3:Q:87:VAL:HG23	1.88	0.71
3:G:25:PHE:CZ	3:G:59:THR:HG21	2.25	0.71
2:D:33:SER:O	3:C:29:ARG:NH2	2.20	0.71
3:Q:25:PHE:CZ	3:Q:59:THR:HG21	2.25	0.71
1:J:-162:DG:H2"	1:J:-161:DG:C8	2.25	0.71
5:E:67:PHE:O	5:E:71:VAL:HG23	1.91	0.70
5:O:67:PHE:O	5:O:71:VAL:HG23	1.91	0.70
1:J:-196:DA:OP2	3:M:35:ARG:NH2	2.24	0.70
2:R:108:VAL:O	2:R:112:THR:HG23	1.91	0.70
2:H:108:VAL:O	2:H:112:THR:HG23	1.91	0.70
1:J:-40:DA:OP2	3:C:35:ARG:NH2	2.24	0.70
3:Q:31:HIS:CD2	3:Q:35:ARG:HH21	2.10	0.70
3:Q:88:ARG:NH2	3:Q:97:LEU:O	2.26	0.69
3:G:31:HIS:CD2	3:G:35:ARG:HH21	2.10	0.69
3:M:50:TYR:O	3:M:54:VAL:HG23	1.93	0.69
2:R:93:THR:HG21	4:P:75:HIS:HD2	1.54	0.69
1:J:-154:DG:N2	6:I:155:DA:C2	2.61	0.69
2:R:79:HIS:CE1	3:M:38:ASN:HD22	2.11	0.68
3:G:88:ARG:NH2	3:G:97:LEU:O	2.26	0.68
6:I:301:DC:H1'	6:I:302:DA:H5'	1.74	0.68
2:R:30:ARG:HH12	6:I:283:DG:H21	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:TYR:O	3:C:54:VAL:HG23	1.93	0.68
6:I:154:DC:N3	6:I:155:DA:N1	2.41	0.68
6:I:127:DG:H21	2:H:30:ARG:HH12	1.41	0.67
6:I:305:DC:H2"	6:I:306:DT:C7	2.24	0.67
4:B:47:SER:HB3	5:A:119:ILE:O	1.95	0.67
2:R:58:ILE:CD1	3:Q:80:PRO:HG3	2.25	0.67
2:H:79:HIS:CE1	3:C:38:ASN:HD22	2.11	0.66
4:L:47:SER:HB3	5:K:119:ILE:O	1.95	0.66
6:I:149:DC:H4'	5:A:39:HIS:CE1	2.30	0.66
1:J:-12:DT:H3	6:I:12:DA:H61	1.41	0.65
2:R:50:GLY:O	3:Q:77:ARG:HA	1.96	0.65
2:H:58:ILE:CD1	3:G:80:PRO:HG3	2.25	0.65
6:I:167:DG:H2"	6:I:168:DA:H5"	1.78	0.65
1:J:-311:DT:H3	6:I:311:DA:H61	1.44	0.65
1:J:-186:DC:H4'	2:N:30:ARG:HG2	1.79	0.65
2:H:50:GLY:O	3:G:77:ARG:HA	1.96	0.65
4:B:89:ALA:O	4:B:92:ARG:HB2	1.97	0.65
3:Q:42:ARG:HG2	6:I:274:DA:H5"	1.79	0.65
6:I:118:DA:H5"	3:G:42:ARG:HG2	1.79	0.64
4:L:89:ALA:O	4:L:92:ARG:HB2	1.97	0.64
2:H:98:LEU:HB3	2:H:99:LEU:HD23	1.79	0.64
1:J:-30:DC:H4'	2:D:30:ARG:HG2	1.79	0.64
2:D:102:GLU:HB3	3:C:92:GLU:OE1	1.98	0.64
6:I:154:DC:N4	6:I:155:DA:H61	1.96	0.64
2:R:98:LEU:HB3	2:R:99:LEU:HD23	1.79	0.64
6:I:154:DC:N4	6:I:155:DA:N6	2.46	0.63
1:J:-6:DG:O6	6:I:5:DC:N4	2.32	0.63
2:N:102:GLU:HB3	3:M:92:GLU:OE1	1.98	0.63
6:I:154:DC:C4	6:I:155:DA:C6	2.86	0.63
2:H:69:ARG:HB3	2:H:98:LEU:HD21	1.81	0.62
3:C:118:LYS:HA	3:C:118:LYS:HE3	1.81	0.62
6:I:307:DG:H2"	6:I:308:DT:C6	2.33	0.62
2:R:69:ARG:HB3	2:R:98:LEU:HD21	1.82	0.62
6:I:149:DC:H4'	5:A:39:HIS:HE1	1.64	0.62
3:M:118:LYS:HE3	3:M:118:LYS:HA	1.81	0.61
6:I:106:DG:H2"	6:I:107:DG:C8	2.35	0.61
1:J:-154:DG:N2	6:I:155:DA:H2	1.96	0.61
2:R:32:GLU:OE1	3:Q:32:ARG:NH2	2.28	0.61
6:I:262:DG:H2"	6:I:263:DG:C8	2.35	0.61
1:J:-306:DA:N3	6:I:307:DG:N2	2.47	0.61
3:Q:90:ASP:O	3:Q:91:GLU:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:84:GLN:HE21	3:G:84:GLN:HA	1.66	0.61
3:Q:84:GLN:HA	3:Q:84:GLN:HE21	1.66	0.60
2:D:92:GLN:O	2:D:95:VAL:HB	2.01	0.60
6:I:289:DG:H2"	6:I:290:DT:OP2	2.00	0.60
1:J:-185:DG:H2"	1:J:-184:DG:OP2	2.01	0.60
2:N:92:GLN:O	2:N:95:VAL:HB	2.01	0.60
4:B:32:PRO:O	4:B:35:ARG:HB3	2.02	0.60
6:I:133:DG:H2"	6:I:134:DT:OP2	2.00	0.60
1:J:-16:DG:H2"	1:J:-15:DG:OP2	2.01	0.60
3:M:25:PHE:CZ	3:M:59:THR:HG21	2.37	0.60
3:C:25:PHE:CZ	3:C:59:THR:HG21	2.37	0.60
3:G:90:ASP:O	3:G:91:GLU:C	2.39	0.59
3:Q:81:ARG:NH2	3:Q:107:VAL:O	2.34	0.59
6:I:11:DG:H2"	6:I:12:DA:H5"	1.84	0.59
2:D:118:TYR:HA	3:C:20:ARG:O	2.03	0.59
1:J:-29:DG:H2"	1:J:-28:DG:OP2	2.01	0.59
2:H:32:GLU:OE1	3:G:32:ARG:NH2	2.28	0.59
1:J:-172:DG:H2"	1:J:-171:DG:OP2	2.01	0.59
2:D:89:ARG:HH22	4:B:77:LYS:HG3	1.68	0.59
2:N:89:ARG:HH22	4:L:77:LYS:HG3	1.68	0.59
3:G:81:ARG:NH2	3:G:107:VAL:O	2.34	0.58
2:N:118:TYR:HA	3:M:20:ARG:O	2.03	0.58
4:L:32:PRO:O	4:L:35:ARG:HB3	2.02	0.58
5:A:65:LEU:HB3	5:A:66:PRO:HD3	1.85	0.58
4:P:98:TYR:OH	2:N:65:ASP:OD2	2.20	0.58
6:I:34:DA:H5'	2:D:30:ARG:HH12	1.69	0.58
5:E:110:CYS:SG	5:E:126:LEU:HD23	2.44	0.58
2:H:63:VAL:HG13	3:G:55:LEU:HD22	1.86	0.58
1:J:-184:DG:H2"	1:J:-183:DC:OP2	2.04	0.57
2:R:63:VAL:HG13	3:Q:55:LEU:HD22	1.86	0.57
1:J:-305:DG:H21	6:I:306:DT:H1'	1.69	0.57
3:G:84:GLN:HE22	3:G:88:ARG:HH11	1.52	0.57
5:K:65:LEU:HB3	5:K:66:PRO:HD3	1.85	0.57
2:N:30:ARG:HH12	6:I:190:DA:H5'	1.69	0.57
5:O:110:CYS:SG	5:O:126:LEU:HD23	2.44	0.57
3:Q:84:GLN:HE22	3:Q:88:ARG:HH11	1.52	0.57
6:I:171:DC:H2"	6:I:172:DC:OP2	2.05	0.57
4:F:59:LYS:HE3	4:F:63:GLU:OE2	2.04	0.57
4:P:59:LYS:HE3	4:P:63:GLU:OE2	2.04	0.57
2:D:37:TYR:CD1	3:C:26:PRO:HD3	2.40	0.56
2:N:37:TYR:CD1	3:M:26:PRO:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-305:DG:C2	6:I:306:DT:O2	2.58	0.56
2:H:37:TYR:CE2	3:G:26:PRO:HG3	2.40	0.56
1:J:-118:DT:H2"	1:J:-117:DA:C8	2.40	0.56
4:F:98:TYR:OH	2:D:65:ASP:OD2	2.20	0.56
2:R:37:TYR:CE2	3:Q:26:PRO:HG3	2.40	0.56
2:D:106:HIS:O	2:D:109:SER:HB2	2.06	0.56
1:J:-28:DG:H2"	1:J:-27:DC:OP2	2.04	0.56
4:B:26:ILE:HG13	4:B:55:ARG:HD3	1.87	0.56
5:E:102:ALA:O	5:E:105:GLU:HB2	2.06	0.56
4:L:40:ARG:HG2	5:K:101:VAL:HG11	1.87	0.56
2:N:32:GLU:OE1	3:M:32:ARG:NH2	2.34	0.56
1:J:-274:DT:H2"	1:J:-273:DA:C8	2.40	0.56
1:J:-306:DA:C2	6:I:307:DG:N1	2.72	0.56
2:N:107:ALA:HB1	3:M:54:VAL:HG13	1.88	0.56
6:I:301:DC:H2"	6:I:302:DA:OP2	2.07	0.55
1:J:-204:DT:H2"	1:J:-203:DG:C8	2.41	0.55
5:O:102:ALA:O	5:O:105:GLU:HB2	2.06	0.55
6:I:15:DC:H2"	6:I:16:DC:OP2	2.05	0.55
2:D:63:VAL:HG13	3:C:55:LEU:HD22	1.88	0.55
6:I:305:DC:H2"	6:I:306:DT:H73	1.87	0.55
2:N:106:HIS:O	2:N:109:SER:HB2	2.06	0.55
4:B:33:ALA:C	4:B:35:ARG:N	2.60	0.55
1:J:-297:DA:H61	6:I:297:DT:H3	1.54	0.55
2:N:59:MET:O	2:N:63:VAL:HG23	2.07	0.55
3:G:50:TYR:O	3:G:54:VAL:HG23	2.07	0.55
2:H:58:ILE:HD12	3:G:80:PRO:HG3	1.88	0.55
1:J:-48:DT:H2"	1:J:-47:DG:C8	2.41	0.55
2:N:63:VAL:HG13	3:M:55:LEU:HD22	1.88	0.55
4:B:40:ARG:HG2	5:A:101:VAL:HG11	1.87	0.55
1:J:-141:DA:H61	6:I:141:DT:H3	1.54	0.55
2:R:58:ILE:HD12	3:Q:80:PRO:HG3	1.88	0.55
5:K:39:HIS:CE1	6:I:305:DC:H4'	2.42	0.55
3:Q:73:ASN:O	3:Q:75:LYS:HG3	2.07	0.54
4:L:26:ILE:HG13	4:L:55:ARG:HD3	1.87	0.54
2:D:59:MET:O	2:D:63:VAL:HG23	2.07	0.54
4:L:33:ALA:C	4:L:35:ARG:N	2.60	0.54
2:D:107:ALA:HB1	3:C:54:VAL:HG13	1.88	0.54
3:Q:50:TYR:O	3:Q:54:VAL:HG23	2.07	0.54
3:G:73:ASN:O	3:G:75:LYS:HG3	2.07	0.54
6:I:145:DC:H2"	6:I:146:DA:OP2	2.07	0.53
6:I:50:DC:H2"	6:I:51:DT:OP2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:68:DG:H2"	6:I:69:DC:OP2	2.09	0.53
6:I:224:DG:H2"	6:I:225:DC:OP2	2.09	0.53
2:N:30:ARG:NH1	6:I:190:DA:H5'	2.24	0.53
4:L:31:LYS:N	4:L:32:PRO:HD2	2.23	0.53
4:L:33:ALA:O	4:L:35:ARG:N	2.42	0.53
6:I:206:DC:H2"	6:I:207:DT:OP2	2.08	0.52
1:J:-36:DA:H2"	1:J:-35:DT:OP2	2.08	0.52
4:B:31:LYS:N	4:B:32:PRO:HD2	2.23	0.52
6:I:305:DC:H2"	6:I:306:DT:H72	1.90	0.52
2:R:67:PHE:CD1	2:R:67:PHE:C	2.82	0.52
2:H:93:THR:CG2	4:F:75:HIS:HD2	2.16	0.52
2:H:67:PHE:C	2:H:67:PHE:CD1	2.82	0.52
6:I:245:DC:H2"	6:I:246:DG:C8	2.45	0.52
6:I:306:DT:H73	6:I:306:DT:OP2	2.09	0.52
1:J:-48:DT:H2"	1:J:-47:DG:H8	1.74	0.52
6:I:89:DC:H2"	6:I:90:DG:H8	1.75	0.52
6:I:245:DC:H2"	6:I:246:DG:H8	1.75	0.52
1:J:-288:DA:H2"	1:J:-287:DC:OP2	2.10	0.52
6:I:34:DA:H5'	2:D:30:ARG:NH1	2.24	0.52
3:Q:30:VAL:O	3:Q:34:LEU:HD12	2.10	0.52
4:B:33:ALA:O	4:B:35:ARG:N	2.42	0.52
4:F:26:ILE:HD12	4:F:55:ARG:HB3	1.92	0.51
1:J:-229:DA:N6	6:I:228:DG:C6	2.78	0.51
1:J:-192:DA:H2"	1:J:-191:DT:OP2	2.08	0.51
1:J:-132:DA:H2"	1:J:-131:DC:OP2	2.10	0.51
1:J:-73:DA:N6	6:I:72:DG:C6	2.78	0.51
2:H:80:TYR:CD1	4:F:88:TYR:CZ	2.98	0.51
6:I:89:DC:H2"	6:I:90:DG:C8	2.45	0.51
3:G:30:VAL:O	3:G:34:LEU:HD12	2.10	0.51
1:J:-218:DA:H2"	1:J:-217:DG:C8	2.46	0.51
1:J:-232:DC:H2"	1:J:-231:DG:C8	2.45	0.51
1:J:-76:DC:H2"	1:J:-75:DG:C8	2.45	0.51
2:N:118:TYR:HE1	3:M:17:ARG:HG2	1.76	0.51
2:R:93:THR:CG2	4:P:75:HIS:HD2	2.16	0.51
2:D:32:GLU:OE1	3:C:32:ARG:NH2	2.35	0.51
4:P:79:LYS:HD2	6:I:262:DG:OP1	2.11	0.51
4:P:26:ILE:HD12	4:P:55:ARG:HB3	1.92	0.51
2:R:80:TYR:CD1	4:P:88:TYR:CZ	2.98	0.51
2:D:118:TYR:HE1	3:C:17:ARG:HG2	1.76	0.51
2:N:62:PHE:O	2:N:66:VAL:HG23	2.11	0.51
6:I:165:DG:H2'	6:I:166:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-62:DA:H2"	1:J:-61:DG:C8	2.46	0.50
6:I:106:DG:OP1	4:F:79:LYS:HD2	2.11	0.50
1:J:-204:DT:H2"	1:J:-203:DG:H8	1.74	0.50
4:L:28:GLY:O	4:L:30:THR:HG23	2.12	0.50
2:H:58:ILE:CD1	3:G:80:PRO:CG	2.90	0.50
1:J:-304:DG:H2"	1:J:-303:DA:C8	2.46	0.50
3:M:95:LYS:O	3:M:98:GLY:N	2.45	0.50
1:J:-310:DG:O6	6:I:309:DG:O6	2.29	0.50
5:A:70:LEU:O	5:A:74:ILE:HD12	2.12	0.50
2:D:62:PHE:O	2:D:66:VAL:HG23	2.11	0.50
1:J:-98:DG:H22	6:I:98:DC:H42	1.60	0.50
1:J:-70:DT:H2"	1:J:-69:DG:H8	1.77	0.50
6:I:300:DA:H2"	6:I:301:DC:OP2	2.12	0.49
1:J:-184:DG:H2'	1:J:-184:DG:OP2	2.12	0.49
5:K:70:LEU:O	5:K:74:ILE:HD12	2.12	0.49
4:B:28:GLY:O	4:B:30:THR:HG23	2.12	0.49
6:I:67:DC:H2"	6:I:68:DG:C8	2.47	0.49
2:N:46:HIS:HB3	2:N:49:THR:OG1	2.12	0.49
4:B:36:ARG:NH2	5:A:61:LEU:O	2.43	0.49
2:D:46:HIS:HB3	2:D:49:THR:OG1	2.12	0.49
6:I:223:DC:H2"	6:I:224:DG:C8	2.47	0.49
4:L:36:ARG:NH2	5:K:61:LEU:O	2.42	0.49
1:J:-226:DT:H2"	1:J:-225:DG:H8	1.77	0.49
3:C:95:LYS:O	3:C:98:GLY:N	2.45	0.49
6:I:167:DG:C2'	6:I:168:DA:H5"	2.42	0.49
6:I:232:DG:C5	6:I:233:DC:C4	3.01	0.49
3:M:87:VAL:HG11	3:M:97:LEU:HD12	1.94	0.49
3:Q:77:ARG:HB2	6:I:293:DG:OP1	2.13	0.49
4:B:33:ALA:C	4:B:35:ARG:H	2.16	0.49
2:H:107:ALA:HB1	3:G:54:VAL:HG13	1.95	0.49
4:L:33:ALA:C	4:L:35:ARG:H	2.16	0.49
2:N:85:THR:HG23	3:M:42:ARG:HG3	1.95	0.49
1:J:-254:DG:H22	6:I:254:DC:H42	1.60	0.49
6:I:144:DA:H2"	6:I:145:DC:OP2	2.12	0.48
1:J:-70:DT:H2"	1:J:-69:DG:C8	2.48	0.48
5:K:65:LEU:HB3	5:K:66:PRO:CD	2.43	0.48
3:Q:31:HIS:CD2	3:Q:35:ARG:NH2	2.79	0.48
3:C:87:VAL:HG11	3:C:97:LEU:HD12	1.94	0.48
3:G:31:HIS:CD2	3:G:35:ARG:NH2	2.79	0.48
6:I:76:DG:C5	6:I:77:DC:C4	3.01	0.48
1:J:-28:DG:OP2	1:J:-28:DG:H2'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-307:DC:C4	1:J:-306:DA:C6	3.02	0.48
4:P:74:GLU:OE1	5:O:79:LYS:HG3	2.14	0.48
2:R:107:ALA:HB1	3:Q:54:VAL:HG13	1.95	0.48
1:J:-174:DC:H2"	1:J:-173:DG:N7	2.29	0.48
1:J:-196:DA:H1'	1:J:-195:DC:H5'	1.96	0.48
4:B:29:ILE:O	4:B:34:ILE:HD11	2.13	0.48
4:L:45:ARG:HB3	5:K:118:THR:HA	1.96	0.48
2:R:75:SER:OG	3:Q:39:TYR:O	2.23	0.48
2:D:100:PRO:O	2:D:102:GLU:N	2.47	0.48
3:G:35:ARG:HB2	3:G:35:ARG:HH11	1.79	0.48
6:I:137:DG:OP1	3:G:77:ARG:HB2	2.13	0.48
1:J:-308:DG:N1	6:I:309:DG:N1	2.55	0.48
1:J:-5:DG:N2	6:I:6:DC:O2	2.46	0.48
1:J:-226:DT:H2"	1:J:-225:DG:C8	2.48	0.48
1:J:-306:DA:N1	6:I:307:DG:N1	2.61	0.48
3:Q:35:ARG:HB2	3:Q:35:ARG:NH1	2.29	0.48
2:R:103:LEU:HD11	3:Q:61:GLU:HG2	1.96	0.48
1:J:-144:DT:H3	6:I:144:DA:H61	1.62	0.48
2:N:31:LYS:O	2:N:31:LYS:HD2	2.13	0.48
5:A:65:LEU:HB3	5:A:66:PRO:CD	2.43	0.48
1:J:-40:DA:H1'	1:J:-39:DC:H5'	1.95	0.48
6:I:198:DG:H4'	6:I:199:DT:OP1	2.14	0.48
2:D:31:LYS:HD2	2:D:31:LYS:O	2.13	0.48
6:I:223:DC:H2"	6:I:224:DG:H8	1.79	0.48
2:R:58:ILE:CD1	3:Q:80:PRO:CG	2.90	0.48
6:I:305:DC:C2'	6:I:306:DT:H72	2.44	0.47
6:I:67:DC:H2"	6:I:68:DG:H8	1.79	0.47
4:L:29:ILE:O	4:L:34:ILE:HD11	2.13	0.47
2:N:100:PRO:O	2:N:102:GLU:N	2.47	0.47
1:J:-300:DT:H3	6:I:300:DA:H61	1.61	0.47
4:B:68:ASP:OD2	4:B:92:ARG:HD3	2.15	0.47
3:C:79:ILE:HB	3:C:80:PRO:HD2	1.97	0.47
2:D:85:THR:HG23	3:C:42:ARG:HG3	1.95	0.47
4:F:74:GLU:OE1	5:E:79:LYS:HG3	2.14	0.47
2:H:103:LEU:HD11	3:G:61:GLU:HG2	1.96	0.47
1:J:-18:DC:H2"	1:J:-17:DG:N7	2.28	0.47
1:J:-305:DG:N2	6:I:306:DT:N1	2.59	0.47
6:I:154:DC:C2	6:I:155:DA:C6	3.02	0.47
6:I:42:DG:H4'	6:I:43:DT:OP1	2.14	0.47
3:Q:35:ARG:HB2	3:Q:35:ARG:HH11	1.79	0.47
4:B:39:ARG:C	4:B:41:GLY:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:35:ARG:HB2	3:G:35:ARG:NH1	2.29	0.47
1:J:-231:DG:H2"	1:J:-230:DT:OP2	2.15	0.47
6:I:168:DA:C6	6:I:169:DA:C6	3.03	0.47
1:J:-156:DC:H2"	1:J:-155:DT:C6	2.48	0.47
3:M:79:ILE:HB	3:M:80:PRO:HD2	1.97	0.47
2:D:89:ARG:NH1	4:B:77:LYS:HE3	2.30	0.47
6:I:254:DC:H2"	6:I:255:DG:H8	1.80	0.47
1:J:-283:DC:C2	1:J:-282:DC:C5	3.03	0.47
5:O:59:GLU:HG3	5:O:59:GLU:H	1.58	0.47
4:B:45:ARG:HB3	5:A:118:THR:HA	1.96	0.46
4:B:28:GLY:O	4:B:30:THR:N	2.48	0.46
3:G:34:LEU:HD11	3:G:51:LEU:HD23	1.97	0.46
2:H:91:ILE:HD12	3:G:51:LEU:HB2	1.97	0.46
1:J:-296:DT:H2'	1:J:-295:DA:C8	2.50	0.46
2:N:67:PHE:CD1	2:N:67:PHE:C	2.88	0.46
1:J:-137:DC:H42	6:I:137:DG:H1	1.63	0.46
4:L:39:ARG:C	4:L:41:GLY:N	2.68	0.46
2:R:91:ILE:HD12	3:Q:51:LEU:HB2	1.97	0.46
3:Q:34:LEU:HD11	3:Q:51:LEU:HD23	1.97	0.46
5:E:128:ARG:NH2	5:E:134:ARG:HE	2.14	0.46
2:D:67:PHE:CD1	2:D:67:PHE:C	2.88	0.46
6:I:205:DG:H2"	6:I:206:DC:OP2	2.15	0.46
1:J:-127:DC:C2	1:J:-126:DC:C5	3.03	0.46
2:N:89:ARG:NH1	4:L:77:LYS:HE3	2.30	0.46
4:L:68:ASP:OD2	4:L:92:ARG:HD3	2.15	0.46
3:Q:42:ARG:HG2	6:I:274:DA:C5'	2.46	0.46
4:F:83:ALA:HB2	5:E:87:SER:OG	2.16	0.46
6:I:309:DG:H2"	6:I:310:DC:C6	2.51	0.46
6:I:98:DC:H2"	6:I:99:DG:H8	1.80	0.46
1:J:-293:DC:H42	6:I:293:DG:H1	1.63	0.46
1:J:-75:DG:H2"	1:J:-74:DT:OP2	2.15	0.46
5:O:128:ARG:NH2	5:O:134:ARG:HE	2.14	0.46
1:J:-140:DT:H2'	1:J:-139:DA:C8	2.50	0.46
4:P:53:GLU:O	4:P:57:VAL:HG23	2.16	0.46
2:H:91:ILE:HG13	3:G:47:ALA:HB1	1.97	0.46
1:J:-111:DT:H2"	1:J:-110:DA:C8	2.51	0.46
1:J:-165:DC:OP1	5:O:42:ARG:N	2.47	0.46
1:J:-267:DT:H2"	1:J:-266:DA:C8	2.51	0.46
4:B:45:ARG:O	5:A:118:THR:HA	2.17	0.45
2:H:80:TYR:CG	4:F:88:TYR:CE2	3.03	0.45
1:J:-295:DA:H2"	1:J:-294:DT:OP2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:91:ILE:HG13	3:Q:47:ALA:HB1	1.97	0.45
2:R:80:TYR:CG	4:P:88:TYR:CE2	3.03	0.45
6:I:102:DA:H2"	6:I:103:DA:OP2	2.17	0.45
1:J:-305:DG:C2	6:I:306:DT:C2	3.00	0.45
2:R:58:ILE:HD13	3:Q:80:PRO:HB3	1.97	0.45
4:F:53:GLU:O	4:F:57:VAL:HG23	2.16	0.45
4:F:89:ALA:O	4:F:92:ARG:HB2	2.16	0.45
6:I:49:DG:H2"	6:I:50:DC:OP2	2.15	0.45
1:J:-24:DC:OP2	1:J:-24:DC:H2'	2.17	0.45
4:P:89:ALA:O	4:P:92:ARG:HB2	2.16	0.45
2:H:58:ILE:HD13	3:G:80:PRO:HB3	1.97	0.45
4:P:83:ALA:HB2	5:O:87:SER:OG	2.16	0.45
1:J:-139:DA:H2"	1:J:-138:DT:OP2	2.17	0.45
2:N:83:ARG:NH1	2:N:83:ARG:HB3	2.32	0.45
2:H:65:ASP:OD2	4:B:98:TYR:OH	2.34	0.45
3:G:100:VAL:CG1	3:G:101:THR:N	2.80	0.45
3:Q:100:VAL:CG1	3:Q:101:THR:N	2.80	0.45
2:D:83:ARG:HB3	2:D:83:ARG:NH1	2.32	0.45
1:J:-169:DT:H2"	1:J:-168:DT:C6	2.52	0.45
4:L:45:ARG:O	5:K:118:THR:HA	2.17	0.45
6:I:54:DA:H1'	6:I:55:DG:C8	2.52	0.45
5:O:42:ARG:HA	5:O:43:PRO:HD2	1.81	0.45
2:H:45:VAL:CG1	3:G:64:GLU:OE2	2.65	0.44
6:I:41:DC:H2"	6:I:42:DG:OP2	2.16	0.44
6:I:86:DC:H2"	6:I:87:DC:C6	2.53	0.44
3:C:27:VAL:HG11	3:C:49:VAL:HG22	1.99	0.44
5:K:102:ALA:O	5:K:105:GLU:HB2	2.17	0.44
2:N:103:LEU:HD21	3:M:93:LEU:HD23	1.99	0.44
6:I:210:DA:H1'	6:I:211:DG:C8	2.52	0.44
1:J:-166:DT:H6	1:J:-166:DT:H2'	1.66	0.44
5:A:102:ALA:O	5:A:105:GLU:HB2	2.17	0.44
4:B:32:PRO:O	4:B:36:ARG:HG3	2.17	0.44
6:I:258:DA:H2"	6:I:259:DA:OP2	2.17	0.44
1:J:-153:DC:H2"	1:J:-152:DA:O4'	2.18	0.44
1:J:-180:DC:H2'	1:J:-180:DC:OP2	2.17	0.44
1:J:-62:DA:H2"	1:J:-61:DG:H8	1.83	0.44
4:L:32:PRO:O	4:L:36:ARG:HG3	2.17	0.44
4:B:31:LYS:HG3	4:B:51:TYR:CE1	2.53	0.44
2:H:107:ALA:HB2	3:G:57:TYR:CD2	2.53	0.44
6:I:242:DC:H2"	6:I:243:DC:C6	2.53	0.44
6:I:305:DC:H2"	6:I:306:DT:OP2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-278:DA:H2"	1:J:-277:DG:H8	1.83	0.44
5:A:120:MET:O	5:A:121:PRO:C	2.56	0.44
1:J:-218:DA:H2"	1:J:-217:DG:H8	1.83	0.44
5:O:79:LYS:HB3	5:O:82:LEU:HD11	1.99	0.44
1:J:-152:DA:H2	6:I:152:DT:H3	1.66	0.44
6:I:197:DC:H2"	6:I:198:DG:OP2	2.16	0.44
2:R:65:ASP:OD2	4:L:98:TYR:OH	2.34	0.44
3:G:43:VAL:HG12	3:G:44:GLY:O	2.18	0.43
1:J:-113:DA:N6	6:I:112:DC:H42	2.16	0.43
1:J:-62:DA:P	5:A:69:ARG:HH21	2.41	0.43
4:L:31:LYS:HG3	4:L:51:TYR:CE1	2.53	0.43
2:R:45:VAL:CG1	3:Q:64:GLU:OE2	2.65	0.43
6:I:107:DG:OP1	4:F:79:LYS:N	2.51	0.43
6:I:178:DC:H2"	6:I:179:DC:C5	2.53	0.43
3:M:17:ARG:NH2	6:I:192:DT:OP2	2.51	0.43
6:I:65:DA:C2	6:I:66:DA:C4	3.06	0.43
2:D:103:LEU:HD21	3:C:93:LEU:HD23	1.99	0.43
6:I:193:DT:H2"	6:I:194:DG:C8	2.54	0.43
2:R:107:ALA:HB2	3:Q:57:TYR:CD2	2.53	0.43
1:J:-122:DA:H2"	1:J:-121:DG:H8	1.83	0.43
1:J:-151:DC:N4	6:I:151:DG:H1	2.16	0.43
1:J:-310:DG:C2	6:I:311:DA:H2	2.30	0.43
3:M:27:VAL:HG11	3:M:49:VAL:HG22	1.99	0.43
1:J:-144:DT:OP1	5:A:49:ARG:HD2	2.19	0.43
1:J:-150:DA:H2"	1:J:-149:DG:C8	2.54	0.43
1:J:-269:DA:N6	6:I:268:DC:H42	2.16	0.43
2:D:80:TYR:CD1	4:B:88:TYR:CZ	3.06	0.43
5:E:79:LYS:HB3	5:E:82:LEU:HD11	1.99	0.43
6:I:37:DT:H2"	6:I:38:DG:C8	2.54	0.43
6:I:88:DG:H5'	5:E:43:PRO:HA	2.01	0.43
1:J:-305:DG:H2"	1:J:-304:DG:C8	2.54	0.43
4:L:82:THR:HG22	5:K:85:GLN:NE2	2.34	0.43
2:R:36:ILE:HD11	2:R:37:TYR:CZ	2.54	0.43
2:H:99:LEU:HD23	2:H:99:LEU:N	2.34	0.43
4:L:28:GLY:O	4:L:30:THR:N	2.48	0.43
4:L:66:ILE:HG22	4:L:70:VAL:HG23	2.01	0.43
2:N:80:TYR:CD1	4:L:88:TYR:CZ	3.06	0.43
3:Q:83:LEU:O	3:Q:86:ALA:HB3	2.19	0.43
4:B:66:ILE:HG22	4:B:70:VAL:HG23	2.01	0.43
3:C:83:LEU:O	3:C:87:VAL:HG23	2.19	0.43
2:H:75:SER:OG	3:G:39:TYR:O	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:221:DA:C2	6:I:222:DA:C4	3.06	0.43
4:P:79:LYS:N	6:I:263:DG:OP1	2.51	0.43
4:L:78:ARG:HH22	4:L:85:ASP:CG	2.23	0.43
3:M:47:ALA:N	3:M:48:PRO:HD2	2.34	0.43
2:R:38:VAL:HB	2:R:56:MET:HE1	2.01	0.43
4:B:82:THR:HG22	5:A:85:GLN:NE2	2.34	0.42
3:C:113:SER:O	3:C:115:LEU:N	2.52	0.42
5:E:42:ARG:HA	5:E:43:PRO:HD2	1.81	0.42
4:B:78:ARG:HH22	4:B:85:ASP:CG	2.23	0.42
1:J:-218:DA:P	5:K:69:ARG:HH21	2.41	0.42
3:M:83:LEU:O	3:M:87:VAL:HG23	2.19	0.42
4:B:97:LEU:HD21	4:B:100:PHE:CD2	2.54	0.42
4:L:34:ILE:H	4:L:34:ILE:HG13	1.71	0.42
2:H:36:ILE:HD11	2:H:37:TYR:CZ	2.54	0.42
6:I:22:DC:H2"	6:I:23:DC:C5	2.53	0.42
2:D:112:THR:O	2:D:116:THR:OG1	2.38	0.42
2:H:103:LEU:HD21	3:G:93:LEU:HD23	2.02	0.42
1:J:-12:DT:H2"	1:J:-11:DC:C6	2.53	0.42
1:J:-307:DC:N4	1:J:-306:DA:N6	2.68	0.42
3:Q:43:VAL:HG12	3:Q:44:GLY:O	2.18	0.42
2:R:39:TYR:O	2:R:40:LYS:C	2.58	0.42
3:Q:100:VAL:HG12	3:Q:101:THR:N	2.34	0.42
5:A:72:ARG:HG2	5:A:72:ARG:HH11	1.85	0.42
3:G:83:LEU:O	3:G:86:ALA:HB3	2.19	0.42
1:J:-282:DC:H2"	1:J:-281:DT:H71	2.01	0.42
2:R:99:LEU:N	2:R:99:LEU:HD23	2.34	0.42
4:L:97:LEU:HD21	4:L:100:PHE:CD2	2.54	0.42
2:N:112:THR:O	2:N:116:THR:OG1	2.38	0.42
5:A:59:GLU:HG3	5:A:59:GLU:H	1.51	0.42
1:J:-154:DG:H21	6:I:155:DA:H2	1.64	0.42
1:J:-155:DT:H2'	1:J:-154:DG:C8	2.55	0.42
1:J:-300:DT:OP1	5:K:49:ARG:HD2	2.19	0.42
3:C:47:ALA:N	3:C:48:PRO:HD2	2.34	0.42
6:I:145:DC:C2	6:I:146:DA:C8	3.08	0.42
5:E:51:ILE:O	5:E:55:GLN:HG3	2.20	0.41
1:J:-168:DT:H3	6:I:168:DA:H61	1.66	0.41
6:I:200:DA:H1'	6:I:201:DG:H5'	2.01	0.41
1:J:-136:DT:H2"	1:J:-135:DG:C8	2.55	0.41
6:I:118:DA:C5'	3:G:42:ARG:HG2	2.46	0.41
1:J:-310:DG:C5	1:J:-309:DC:C4	3.08	0.41
5:K:63:ARG:HB2	5:K:63:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:113:SER:O	3:M:115:LEU:N	2.52	0.41
4:B:30:THR:O	4:B:34:ILE:HG13	2.20	0.41
5:E:106:ASP:HA	5:E:109:LEU:HD12	2.03	0.41
3:G:62:ILE:HG12	3:G:93:LEU:HD13	1.98	0.41
2:H:105:LYS:HE3	2:H:105:LYS:HB2	1.93	0.41
1:J:-165:DC:O5'	5:O:42:ARG:HG3	2.20	0.41
3:G:100:VAL:HG12	3:G:101:THR:N	2.34	0.41
1:J:-126:DC:H2"	1:J:-125:DT:H71	2.01	0.41
5:K:96:SER:O	5:K:99:TYR:HB3	2.20	0.41
6:I:44:DA:H1'	6:I:45:DG:H5'	2.01	0.41
1:J:-208:DG:P	4:L:79:LYS:HD3	2.61	0.41
2:H:39:TYR:O	2:H:40:LYS:C	2.58	0.41
4:L:30:THR:O	4:L:34:ILE:HG13	2.21	0.41
5:O:43:PRO:HA	6:I:244:DG:H5'	2.01	0.41
5:A:127:ALA:O	5:A:131:ARG:HG3	2.21	0.41
5:A:63:ARG:CZ	5:A:63:ARG:HB2	2.50	0.41
5:K:120:MET:O	5:K:121:PRO:C	2.56	0.41
5:K:72:ARG:HH11	5:K:72:ARG:HG2	1.85	0.41
2:N:30:ARG:HH22	6:I:190:DA:H5"	1.86	0.41
3:Q:62:ILE:HG12	3:Q:93:LEU:HD13	1.98	0.41
1:J:-29:DG:OP1	2:D:31:LYS:HE3	2.20	0.41
5:E:48:LEU:O	5:E:52:ARG:HG3	2.20	0.41
2:H:38:VAL:HB	2:H:56:MET:HE1	2.03	0.41
6:I:121:DC:H2"	6:I:122:DT:OP2	2.21	0.41
6:I:157:DT:H2'	6:I:158:DA:C8	2.56	0.41
1:J:-174:DC:H2"	1:J:-173:DG:C8	2.55	0.41
1:J:-286:DG:H2"	1:J:-285:DT:OP2	2.21	0.41
5:K:127:ALA:O	5:K:131:ARG:HG3	2.21	0.41
4:L:90:LEU:HB3	4:L:95:ARG:O	2.21	0.41
4:B:67:ARG:HB2	5:A:78:PHE:CZ	2.56	0.41
1:J:-169:DT:H2"	1:J:-168:DT:C5	2.55	0.41
1:J:-58:DG:H2"	1:J:-57:DT:OP2	2.21	0.41
5:K:59:GLU:HG3	5:K:59:GLU:H	1.51	0.41
5:O:48:LEU:O	5:O:52:ARG:HG3	2.20	0.41
1:J:-52:DG:P	4:B:79:LYS:HD3	2.61	0.41
4:B:39:ARG:C	4:B:41:GLY:H	2.24	0.41
2:D:65:ASP:OD1	2:D:65:ASP:C	2.59	0.41
1:J:-5:DG:N2	6:I:6:DC:C2	2.89	0.41
2:N:91:ILE:O	2:N:94:ALA:HB3	2.21	0.41
5:O:51:ILE:O	5:O:55:GLN:HG3	2.20	0.41
2:R:103:LEU:HD21	3:Q:93:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:96:SER:O	5:A:99:TYR:HB3	2.20	0.40
2:D:91:ILE:O	2:D:94:ALA:HB3	2.21	0.40
6:I:220:DA:C6	6:I:221:DA:C6	3.09	0.40
1:J:-155:DT:H2"	1:J:-154:DG:O4'	2.21	0.40
1:J:-214:DG:H2"	1:J:-213:DT:OP2	2.21	0.40
5:A:97:GLU:O	5:A:98:ALA:C	2.60	0.40
4:L:67:ARG:HB2	5:K:78:PHE:CZ	2.56	0.40
6:I:277:DC:H2"	6:I:278:DT:OP2	2.21	0.40
1:J:-122:DA:H2"	1:J:-121:DG:C8	2.57	0.40
1:J:-130:DG:H2"	1:J:-129:DT:OP2	2.21	0.40
1:J:-185:DG:OP1	2:N:31:LYS:HE3	2.20	0.40
1:J:-18:DC:H2"	1:J:-17:DG:C8	2.55	0.40
1:J:-292:DT:H2"	1:J:-291:DG:C8	2.56	0.40
1:J:-47:DG:H2"	1:J:-46:DT:H71	2.03	0.40
1:J:-97:DG:H2"	1:J:-96:DT:OP2	2.21	0.40
3:M:42:ARG:HD2	6:I:200:DA:H4'	2.03	0.40
3:M:95:LYS:O	3:M:96:LEU:C	2.60	0.40
4:B:90:LEU:HB3	4:B:95:ARG:O	2.21	0.40
6:I:34:DA:H5"	2:D:30:ARG:HH22	1.86	0.40
1:J:-155:DT:H2"	1:J:-154:DG:H5'	2.03	0.40
1:J:-62:DA:C6	1:J:-61:DG:C6	3.10	0.40
5:K:97:GLU:O	5:K:98:ALA:C	2.60	0.40
4:P:40:ARG:HG2	5:O:101:VAL:HG11	2.03	0.40
3:C:69:ALA:O	3:C:73:ASN:ND2	2.53	0.40
3:C:95:LYS:O	3:C:96:LEU:C	2.60	0.40
1:J:-218:DA:C6	1:J:-217:DG:C6	3.10	0.40
1:J:-250:DA:H2"	1:J:-249:DA:H8	1.87	0.40
1:J:-9:DC:H5"	5:E:42:ARG:HG3	2.03	0.40
3:Q:66:ALA:O	3:Q:69:ALA:HB3	2.22	0.40

All (8) 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)
2:H:117:LYS:CE	2:D:117:LYS:NZ[1_545]	1.23	0.97
1:J:-312:DC:P	6:I:313:DT:O3'[2_656]	1.61	0.59
1:J:-312:DC:OP2	6:I:313:DT:O3'[2_656]	1.79	0.41
2:H:117:LYS:CE	2:D:117:LYS:CE[1_545]	1.86	0.34
2:R:117:LYS:CE	2:N:117:LYS:NZ[1_565]	1.90	0.30
3:Q:22:GLY:CA	2:N:117:LYS:CE[1_565]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:117:LYS:NZ	3:M:19:SER:O[1_565]	2.07	0.13
3:G:19:SER:OG	2:D:120:SER:OG[1_545]	2.11	0.09

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
2	D	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6 35
2	H	91/126 (72%)	79 (87%)	11 (12%)	1 (1%)	14 52
2	N	93/126 (74%)	81 (87%)	10 (11%)	2 (2%)	6 35
2	R	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14 52
3	C	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3 23
3	G	103/130 (79%)	88 (85%)	15 (15%)	0	100 100
3	M	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3 23
3	Q	103/130 (79%)	88 (85%)	15 (15%)	0	100 100
4	B	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3 24
4	F	76/102 (74%)	67 (88%)	9 (12%)	0	100 100
4	L	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3 24
4	P	76/102 (74%)	67 (88%)	9 (12%)	0	100 100
5	A	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4 26
5	E	95/135 (70%)	86 (90%)	9 (10%)	0	100 100
5	K	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4 26
5	O	95/135 (70%)	86 (90%)	9 (10%)	0	100 100
All	All	1470/1972 (74%)	1286 (88%)	158 (11%)	26 (2%)	8 40

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	101	GLY
4	L	29	ILE
5	K	73	GLU
2	D	101	GLY
4	B	29	ILE
5	A	73	GLU
2	R	101	GLY
2	N	109	SER
5	K	77	ASP
2	H	101	GLY
2	D	109	SER
5	A	77	ASP
4	L	34	ILE
4	B	34	ILE
3	M	64	GLU
3	M	113	SER
3	C	64	GLU
3	C	113	SER
4	L	26	ILE
5	K	74	ILE
4	B	26	ILE
5	A	74	ILE
3	M	114	VAL
3	C	114	VAL
3	M	26	PRO
3	C	26	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
2	D	81/106 (76%)	69 (85%)	12 (15%)	3 15
2	H	79/106 (74%)	67 (85%)	12 (15%)	3 14
2	N	81/106 (76%)	69 (85%)	12 (15%)	3 15
2	R	79/106 (74%)	67 (85%)	12 (15%)	3 14
3	C	82/102 (80%)	75 (92%)	7 (8%)	10 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	G	83/102 (81%)	74 (89%)	9 (11%)	6 23
3	M	82/102 (80%)	75 (92%)	7 (8%)	10 33
3	Q	83/102 (81%)	74 (89%)	9 (11%)	6 23
4	B	68/78 (87%)	63 (93%)	5 (7%)	13 38
4	F	63/78 (81%)	59 (94%)	4 (6%)	18 43
4	L	68/78 (87%)	63 (93%)	5 (7%)	13 38
4	P	63/78 (81%)	59 (94%)	4 (6%)	18 43
5	A	85/110 (77%)	77 (91%)	8 (9%)	8 28
5	E	84/110 (76%)	79 (94%)	5 (6%)	19 44
5	K	85/110 (77%)	77 (91%)	8 (9%)	8 28
5	O	84/110 (76%)	79 (94%)	5 (6%)	19 44
All	All	1250/1584 (79%)	1126 (90%)	124 (10%)	8 26

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	31	LYS
2	R	49	THR
2	R	68	GLU
2	R	83	ARG
2	R	88	SER
2	R	93	THR
2	R	95	VAL
2	R	98	LEU
2	R	102	GLU
2	R	109	SER
2	R	112	THR
2	R	117	LYS
3	Q	19	SER
3	Q	50	TYR
3	Q	59	THR
3	Q	72	ASP
3	Q	74	LYS
3	Q	81	ARG
3	Q	84	GLN
3	Q	88	ARG
3	Q	114	VAL
4	P	26	ILE

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Mol	Chain	Res	Type
4	P	35	ARG
4	P	73	THR
4	P	92	ARG
5	O	39	HIS
5	O	59	GLU
5	O	65	LEU
5	O	117	VAL
5	O	129	ARG
2	N	31	LYS
2	N	39	TYR
2	N	48	ASP
2	N	49	THR
2	N	77	LEU
2	N	84	SER
2	N	85	THR
2	N	93	THR
2	N	98	LEU
2	N	109	SER
2	N	116	THR
2	N	119	THR
3	M	29	ARG
3	M	59	THR
3	M	81	ARG
3	M	91	GLU
3	M	101	THR
3	M	114	VAL
3	M	118	LYS
4	L	47	SER
4	L	73	THR
4	L	80	THR
4	L	91	LYS
4	L	92	ARG
5	K	48	LEU
5	K	49	ARG
5	K	59	GLU
5	K	63	ARG
5	K	65	LEU
5	K	105	GLU
5	K	115	LYS
5	K	129	ARG
2	H	31	LYS
2	H	49	THR

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Mol	Chain	Res	Type
2	H	68	GLU
2	H	83	ARG
2	H	88	SER
2	H	93	THR
2	H	95	VAL
2	H	98	LEU
2	H	102	GLU
2	H	109	SER
2	H	112	THR
2	H	117	LYS
3	G	19	SER
3	G	50	TYR
3	G	59	THR
3	G	72	ASP
3	G	74	LYS
3	G	81	ARG
3	G	84	GLN
3	G	88	ARG
3	G	114	VAL
4	F	26	ILE
4	F	35	ARG
4	F	73	THR
4	F	92	ARG
5	E	39	HIS
5	E	59	GLU
5	E	65	LEU
5	E	117	VAL
5	E	129	ARG
2	D	31	LYS
2	D	39	TYR
2	D	48	ASP
2	D	49	THR
2	D	77	LEU
2	D	84	SER
2	D	85	THR
2	D	93	THR
2	D	98	LEU
2	D	109	SER
2	D	116	THR
2	D	119	THR
3	C	29	ARG
3	C	59	THR

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Mol	Chain	Res	Type
3	C	81	ARG
3	C	91	GLU
3	C	101	THR
3	C	114	VAL
3	C	118	LYS
4	B	47	SER
4	B	73	THR
4	B	80	THR
4	B	91	LYS
4	B	92	ARG
5	A	48	LEU
5	A	49	ARG
5	A	59	GLU
5	A	63	ARG
5	A	65	LEU
5	A	105	GLU
5	A	115	LYS
5	A	129	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	31	HIS
3	Q	84	GLN
5	O	68	GLN
3	M	38	ASN
3	M	112	GLN
4	L	75	HIS
3	G	31	HIS
3	G	84	GLN
5	E	68	GLN
3	C	38	ASN
3	C	73	ASN
3	C	112	GLN
4	B	75	HIS
5	A	39	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.