Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 06:29 AM EDT

PDB ID	:	1P3P
Title	:	Crystallographic Studies of Nucleosome Core Particles containing Histone 'Sin' Mutants
Authors	:	Muthurajan, U.M.; Bao, Y.; Forsberg, L.J.; Edayathumangalam, R.S.; Dyer, P.N.; White, C.L.; Luger, K.
Deposited on	:	2003-04-17
Resolution	:	2.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

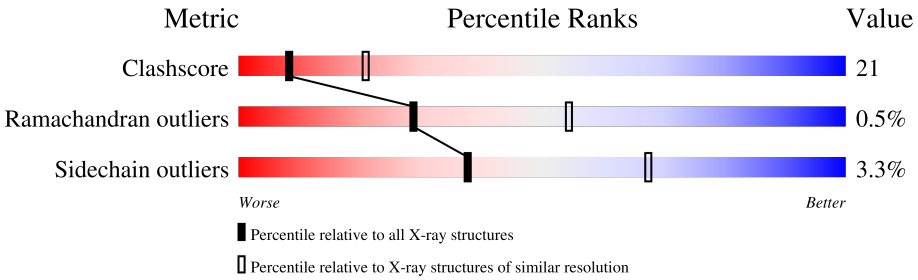
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	35% 60% 5%
1	J	146	38% 57% 5%
2	A	135	53% 16% • 26%
2	E	135	53% 19% • 26%
3	B	102	62% 17% • 21%
3	F	102	59% 22% 20%
4	C	129	64% 15% • 17%
4	G	129	66% 16% • 16%

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Mol	Chain	Length	Quality of chain
5	D	125	57% 14% 26%
5	H	125	58% 18% 23%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12360 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 Palindromic 146bp Human Alpha-Satellite DNA fragment.

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

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	100	Total	C	N	O	S	0	0	0
			826	521	160	142	3			
2	E	100	Total	C	N	O	S	0	0	0
			826	521	160	142	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLU	GLY	conflict	UNP Q7ZT64
A	435	SER	VAL	conflict	UNP Q7ZT64
A	502	ALA	GLY	conflict	UNP Q7ZT64
E	634	GLU	GLY	conflict	UNP Q7ZT64
E	635	SER	VAL	conflict	UNP Q7ZT64
E	702	ALA	GLY	conflict	UNP Q7ZT64

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	81	Total	C	N	O	S	0	0	0
			647	408	126	112	1			
3	F	82	Total	C	N	O	S	0	0	0
			654	413	127	113	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	ILE	VAL	conflict	UNP P62799
F	243	ILE	VAL	conflict	UNP P62799

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	107	Total 825	C 520	N 161	O 144	0	0	0
4	G	108	Total 832	C 525	N 163	O 144	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	814	ALA	SER	conflict	UNP Q7ZT66
C	867	GLY	TRP	conflict	UNP Q7ZT66
C	868	ASN	GLU	conflict	UNP Q7ZT66
C	869	ALA	ARG	conflict	UNP Q7ZT66
C	870	ALA	LEU	conflict	UNP Q7ZT66
C	871	ARG	PRO	conflict	UNP Q7ZT66
C	872	ASP	GLU	conflict	UNP Q7ZT66
C	873	ASN	ILE	conflict	UNP Q7ZT66
C	874	LYS	TRP	conflict	UNP Q7ZT66
C	876	THR	ARG	conflict	UNP Q7ZT66
C	877	ARG	PRO	conflict	UNP Q7ZT66
C	878	ILE	VAL	conflict	UNP Q7ZT66
C	879	ILE	LEU	conflict	UNP Q7ZT66
C	880	PRO	SER	conflict	UNP Q7ZT66
C	881	ARG	PRO	conflict	UNP Q7ZT66
C	882	HIS	GLY	conflict	UNP Q7ZT66
C	883	LEU	TRP	conflict	UNP Q7ZT66
C	884	GLN	CYS	conflict	UNP Q7ZT66
C	885	LEU	ASN	conflict	UNP Q7ZT66
C	886	ALA	SER	conflict	UNP Q7ZT66
C	887	VAL	LEU	conflict	UNP Q7ZT66
C	888	ARG	CYS	conflict	UNP Q7ZT66
C	923	ALA	SER	conflict	UNP Q7ZT66
C	926	ALA	THR	conflict	UNP Q7ZT66
G	1014	ALA	SER	conflict	UNP Q7ZT66
G	1067	GLY	TRP	conflict	UNP Q7ZT66
G	1068	ASN	GLU	conflict	UNP Q7ZT66
G	1069	ALA	ARG	conflict	UNP Q7ZT66
G	1070	ALA	LEU	conflict	UNP Q7ZT66

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1071	ARG	PRO	conflict	UNP Q7ZT66
G	1072	ASP	GLU	conflict	UNP Q7ZT66
G	1073	ASN	ILE	conflict	UNP Q7ZT66
G	1074	LYS	TRP	conflict	UNP Q7ZT66
G	1076	THR	ARG	conflict	UNP Q7ZT66
G	1077	ARG	PRO	conflict	UNP Q7ZT66
G	1078	ILE	VAL	conflict	UNP Q7ZT66
G	1079	ILE	LEU	conflict	UNP Q7ZT66
G	1080	PRO	SER	conflict	UNP Q7ZT66
G	1081	ARG	PRO	conflict	UNP Q7ZT66
G	1082	HIS	GLY	conflict	UNP Q7ZT66
G	1083	LEU	TRP	conflict	UNP Q7ZT66
G	1084	GLN	CYS	conflict	UNP Q7ZT66
G	1085	LEU	ASN	conflict	UNP Q7ZT66
G	1086	ALA	SER	conflict	UNP Q7ZT66
G	1087	VAL	LEU	conflict	UNP Q7ZT66
G	1088	ARG	CYS	conflict	UNP Q7ZT66
G	1123	ALA	SER	conflict	UNP Q7ZT66
G	1126	ALA	THR	conflict	UNP Q7ZT66

- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	93	Total	C	N	O	S	0	0	0
			729	459	131	137	2			
5	H	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1219	GLN	PRO	conflict	UNP P02281
D	1242	LEU	MET	conflict	UNP P02281
D	1257	SER	GLY	conflict	UNP P02281
D	1266	VAL	ILE	conflict	UNP P02281
H	1419	GLN	PRO	conflict	UNP P02281
H	1442	LEU	MET	conflict	UNP P02281
H	1457	SER	GLY	conflict	UNP P02281
H	1466	VAL	ILE	conflict	UNP P02281

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	33	Total O 33 33	0	0
6	J	36	Total O 36 36	0	0
6	A	29	Total O 29 29	0	0
6	B	22	Total O 22 22	0	0
6	C	32	Total O 32 32	0	0
6	D	22	Total O 22 22	0	0
6	E	43	Total O 43 43	0	0
6	F	40	Total O 40 40	0	0
6	G	19	Total O 19 19	0	0
6	H	10	Total O 10 10	0	0

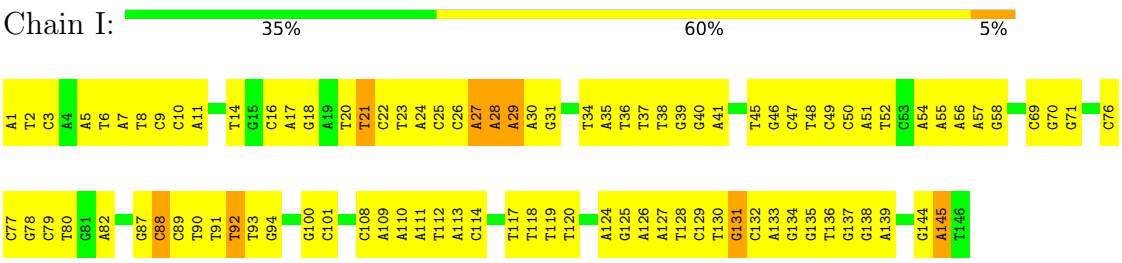
3 Residue-property plots (i)

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

Note EDS was not executed.

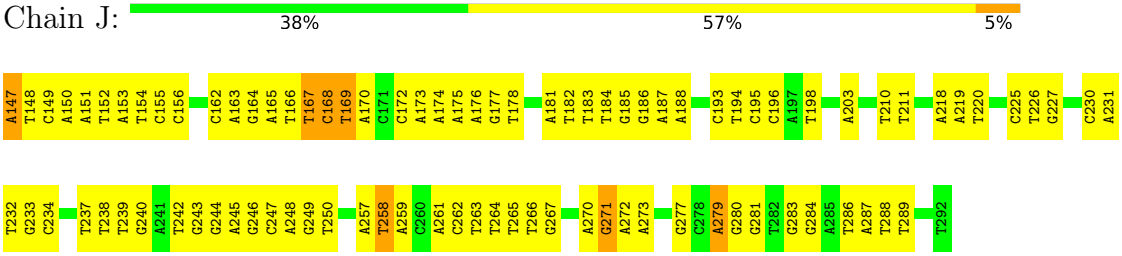
• Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment

Chain I:



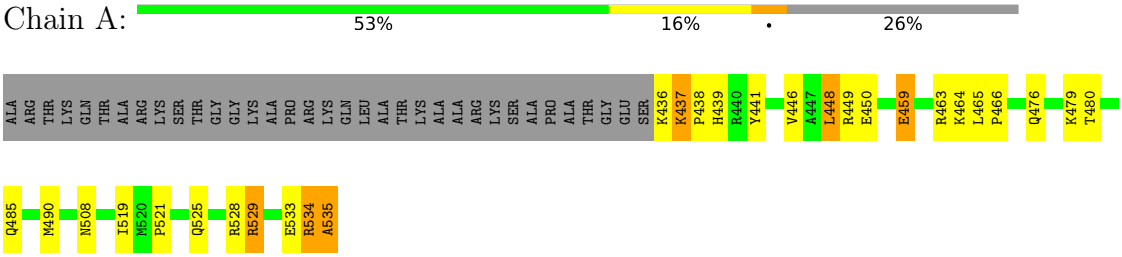
• Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment

Chain J:



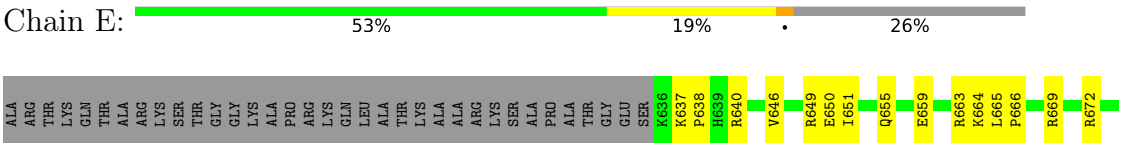
• Molecule 2: Histone H3

Chain A:



• Molecule 2: Histone H3

Chain E:



• Molecule 3: Histone H4

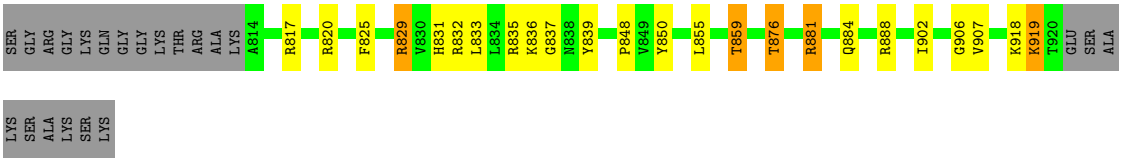
Chain B:

• Molecule 3: Histone H4

Chain F:

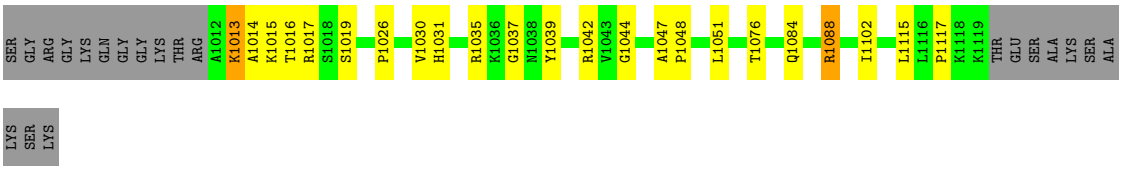
• Molecule 4: Histone H2A

Chain C:



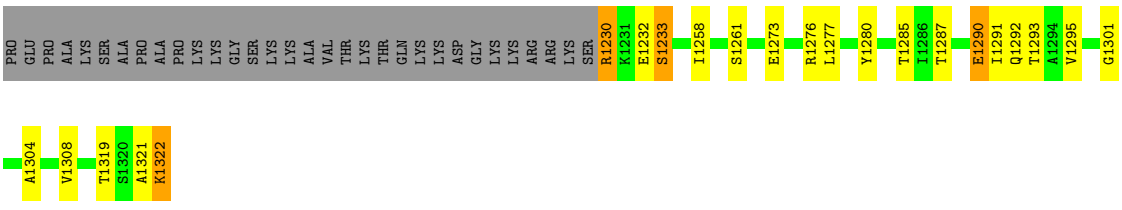
• Molecule 4: Histone H2A

Chain G:



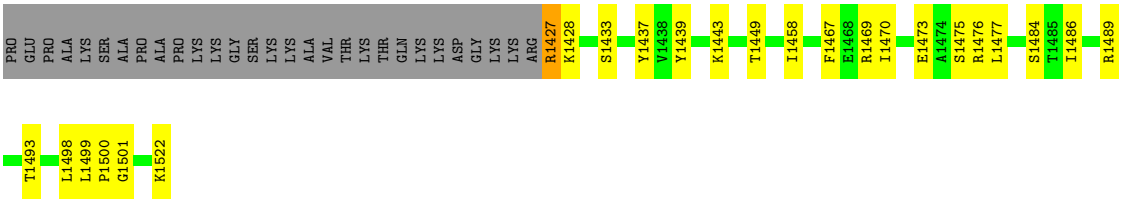
• Molecule 5: Histone H2B

Chain D:



• Molecule 5: Histone H2B

Chain H:


PRO GLU PRO ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS THR GLN LYS LYS ASP GLY LYS LYS ARG R1427 K1428 S1433 Y1437 V1438 Y1439 K1443 T1449 I1458 F1467 E1468 R1469 I1470 E1473 A1474 S1475 R1476 L1477 S1484 T1485 I1486 R1489
T1493 L1498 L1499 P1500 G1501 K1522

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.81Å 109.59Å 181.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.3 (35.00-2.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

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	I	0.62	1/3354 (0.0%)	0.89	7/5175 (0.1%)
1	J	0.61	0/3354	1.02	12/5175 (0.2%)
2	A	1.46	12/838 (1.4%)	1.35	12/1122 (1.1%)
2	E	0.71	1/838 (0.1%)	0.83	1/1122 (0.1%)
3	B	0.58	0/654	0.77	0/874
3	F	0.67	0/661	0.85	0/884
4	C	0.62	0/835	0.78	0/1127
4	G	0.54	0/842	0.70	0/1135
5	D	0.78	2/740 (0.3%)	0.78	1/994 (0.1%)
5	H	0.59	0/766	0.70	0/1027
All	All	0.71	16/12882 (0.1%)	0.92	33/18635 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	6
1	J	0	2
All	All	0	8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	534	ARG	N-CA	18.24	1.82	1.46
2	A	534	ARG	CA-C	17.83	1.99	1.52
2	A	535	ALA	N-CA	16.01	1.78	1.46
2	A	535	ALA	C-OXT	13.27	1.48	1.23
2	A	535	ALA	C-O	8.49	1.39	1.23
2	A	534	ARG	CA-CB	7.42	1.70	1.53
2	A	535	ALA	CA-CB	7.00	1.67	1.52
2	A	533	GLU	C-N	6.85	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1322	LYS	C-O	6.62	1.35	1.23
2	A	533	GLU	CB-CG	6.48	1.64	1.52
2	E	677	ASP	CB-CG	6.10	1.64	1.51
2	A	533	GLU	CA-C	5.80	1.68	1.52
1	I	28	DA	C3'-O3'	-5.79	1.36	1.44
2	A	533	GLU	CG-CD	5.61	1.60	1.51
2	A	534	ARG	C-N	5.54	1.46	1.34
5	D	1322	LYS	N-CA	-5.22	1.35	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	168	DC	OP2-P-O3'	24.39	158.87	105.20
1	J	168	DC	OP1-P-O3'	-23.19	54.17	105.20
2	A	535	ALA	CB-CA-C	-20.48	79.38	110.10
2	A	535	ALA	N-CA-CB	14.74	130.74	110.10
1	I	91	DT	OP2-P-O3'	-14.31	73.72	105.20
2	A	534	ARG	N-CA-C	13.08	146.31	111.00
1	I	91	DT	OP1-P-O3'	13.08	133.97	105.20
1	J	279	DA	OP2-P-O3'	-10.91	81.19	105.20
1	J	167	DT	OP2-P-O3'	-10.19	82.78	105.20
2	A	533	GLU	C-N-CA	9.98	146.64	121.70
1	J	167	DT	O3'-P-O5'	9.93	122.86	104.00
2	A	535	ALA	N-CA-C	9.78	137.40	111.00
2	A	534	ARG	N-CA-CB	-9.76	93.04	110.60
1	J	168	DC	O5'-P-OP2	-9.56	97.10	105.70
1	I	92	DT	O5'-P-OP2	-9.12	97.49	105.70
2	A	534	ARG	CA-C-N	8.63	136.19	117.20
2	A	534	ARG	CA-CB-CG	8.25	131.54	113.40
2	A	534	ARG	CG-CD-NE	8.25	129.12	111.80
5	D	1322	LYS	N-CA-C	-8.12	89.08	111.00
1	J	169	DT	OP1-P-OP2	-7.57	108.24	119.60
1	I	91	DT	C4'-C3'-O3'	7.17	127.64	109.70
1	J	279	DA	O3'-P-O5'	6.63	116.60	104.00
1	I	27	DA	C3'-C2'-C1'	-6.40	94.82	102.50
2	A	534	ARG	O-C-N	-6.36	112.52	122.70
1	I	91	DT	P-O3'-C3'	6.29	127.25	119.70
2	A	535	ALA	CA-C-O	-6.08	107.33	120.10
2	E	677	ASP	CB-CG-OD1	6.08	123.77	118.30
2	A	437	LYS	N-CA-C	-5.96	94.89	111.00
1	I	27	DA	O4'-C4'-C3'	-5.79	102.18	104.50
1	J	169	DT	O5'-P-OP2	-5.52	100.73	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	279	DA	OP1-P-O3'	5.18	116.59	105.20
1	J	258	DT	OP2-P-O3'	5.12	116.47	105.20
1	J	271	DG	C5'-C4'-C3'	-5.09	104.94	114.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	131	DG	Sidechain
1	I	145	DA	Sidechain
1	I	21	DT	Sidechain
1	I	29	DA	Sidechain
1	I	41	DA	Sidechain
1	I	88	DC	Sidechain
1	J	147	DA	Sidechain
1	J	198	DT	Sidechain

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	I	2990	0	1651	123	0
1	J	2990	0	1651	152	0
2	A	826	0	871	66	0
2	E	826	0	871	32	0
3	B	647	0	689	14	0
3	F	654	0	698	22	0
4	C	825	0	884	29	0
4	G	832	0	895	27	0
5	D	729	0	753	27	0
5	H	755	0	784	27	0
6	A	29	0	0	1	0
6	B	22	0	0	1	0
6	C	32	0	0	0	0
6	D	22	0	0	3	0
6	E	43	0	0	6	0
6	F	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	19	0	0	1	0
6	H	10	0	0	3	0
6	I	33	0	0	2	0
6	J	36	0	0	3	0
All	All	12360	0	9747	456	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (456) 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:A:535:ALA:N	2:A:535:ALA:CA	1.78	1.40
2:A:534:ARG:N	2:A:534:ARG:CA	1.82	1.40
1:I:27:DA:N6	1:J:266:DT:H3	1.25	1.33
2:A:534:ARG:CA	2:A:534:ARG:C	1.99	1.31
2:A:529:ARG:HE	2:A:535:ALA:CA	1.43	1.29
2:A:529:ARG:NE	2:A:535:ALA:CA	2.00	1.22
2:A:529:ARG:HE	2:A:535:ALA:C	1.45	1.19
2:A:535:ALA:N	2:A:535:ALA:HA	1.54	1.18
2:A:529:ARG:CG	2:A:535:ALA:H	1.56	1.18
1:J:166:DT:H2"	1:J:167:DT:H71	1.30	1.13
1:J:246:DG:H2"	1:J:247:DC:C5	1.87	1.10
2:A:534:ARG:C	2:A:534:ARG:HA	1.72	1.08
1:J:193:DC:H2"	1:J:194:DT:H71	1.34	1.07
2:A:529:ARG:NE	2:A:535:ALA:N	2.04	1.06
2:A:535:ALA:OXT	2:E:709:LEU:HD11	1.54	1.05
2:A:529:ARG:CD	2:A:535:ALA:H	1.68	1.05
1:I:89:DC:H2"	1:I:90:DT:H71	1.36	1.05
4:G:1017:ARG:HH12	4:G:1031:HIS:HD2	1.12	0.98
1:J:261:DA:H2"	1:J:262:DC:H5"	1.44	0.97
2:A:529:ARG:CG	2:A:535:ALA:N	2.28	0.94
2:A:529:ARG:HA	2:A:534:ARG:HB2	1.51	0.93
1:J:237:DT:H4'	2:A:463:ARG:CZ	1.99	0.92
1:J:245:DA:H2"	1:J:246:DG:C8	2.04	0.91
2:E:719:ILE:HD13	3:F:243:ILE:HD13	1.51	0.91
1:J:166:DT:C2'	1:J:167:DT:H71	2.01	0.90
2:A:529:ARG:NE	2:A:535:ALA:C	2.19	0.90
1:J:225:DC:H2"	1:J:226:DT:H71	1.51	0.90
1:J:246:DG:H2"	1:J:247:DC:C6	2.07	0.90
2:E:677:ASP:OD1	6:E:1:HOH:O	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:DC:H2"	1:I:26:DC:H5'	1.54	0.89
2:A:519:ILE:HD13	3:B:43:ILE:HD13	1.53	0.89
2:A:529:ARG:CZ	2:A:535:ALA:CA	2.51	0.88
1:J:168:DC:C6	1:J:169:DT:H72	2.09	0.87
1:J:280:DG:N7	6:J:293:HOH:O	2.07	0.87
1:I:89:DC:H2"	1:I:90:DT:C7	2.03	0.86
4:C:902:ILE:HG23	5:D:1258:ILE:HD13	1.57	0.86
1:J:174:DA:H2"	1:J:175:DA:H5"	1.58	0.85
3:F:221:VAL:O	6:F:310:HOH:O	1.95	0.84
1:J:225:DC:H2"	1:J:226:DT:C7	2.07	0.84
1:I:38:DT:H2"	1:I:39:DG:N7	1.91	0.84
1:I:14:DT:H3	1:J:279:DA:H61	1.22	0.83
2:A:529:ARG:HH21	2:A:535:ALA:C	1.81	0.83
5:D:1230:ARG:HG3	5:D:1230:ARG:O	1.77	0.82
1:J:249:DG:O3'	5:H:1427:ARG:HG3	1.80	0.82
4:G:1017:ARG:HH12	4:G:1031:HIS:CD2	1.97	0.82
1:I:27:DA:H4'	1:I:28:DA:OP1	1.78	0.81
1:J:248:DA:H2"	1:J:249:DG:C8	2.16	0.81
1:I:22:DC:H4'	1:I:22:DC:OP1	1.79	0.81
3:B:59:LYS:O	3:B:63:GLU:HG3	1.80	0.81
1:I:27:DA:N6	1:J:266:DT:N3	2.09	0.81
2:E:637:LYS:HB2	2:E:638:PRO:HD3	1.62	0.80
1:J:246:DG:H2"	1:J:247:DC:H5	1.45	0.80
1:J:258:DT:H2"	1:J:259:DA:O5'	1.83	0.79
2:E:649:ARG:HG3	2:E:649:ARG:HH11	1.47	0.78
1:I:27:DA:H1'	1:I:28:DA:C8	2.19	0.77
1:I:88:DC:H2"	1:I:89:DC:C5	2.19	0.77
1:I:22:DC:H42	1:J:271:DG:H1	1.33	0.77
1:J:261:DA:C2'	1:J:262:DC:H5"	2.14	0.77
2:E:677:ASP:HB2	6:E:14:HOH:O	1.84	0.77
1:J:175:DA:H2"	1:J:176:DA:C8	2.20	0.76
1:J:230:DC:H2"	1:J:231:DA:C8	2.21	0.76
4:C:850:TYR:OH	5:D:1292:GLN:HG3	1.85	0.76
5:H:1473:GLU:CD	6:H:285:HOH:O	2.24	0.76
1:I:22:DC:C6	1:I:23:DT:H72	2.20	0.76
2:E:725:GLN:HG2	2:E:734:ARG:HH12	1.51	0.75
2:A:529:ARG:HG3	2:A:535:ALA:H	1.47	0.75
1:J:166:DT:H2"	1:J:167:DT:C7	2.14	0.75
1:J:147:DA:H2'	1:J:148:DT:H72	1.69	0.73
1:J:155:DC:H5'	1:J:155:DC:H6	1.54	0.73
1:J:193:DC:H2"	1:J:194:DT:C7	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:535:ALA:HB3	6:A:219:HOH:O	1.88	0.73
2:A:529:ARG:NH2	2:A:535:ALA:C	2.42	0.73
3:F:230:THR:HB	3:F:232:PRO:HD2	1.70	0.72
1:J:258:DT:H2'	1:J:259:DA:C8	2.25	0.72
2:A:529:ARG:HG2	2:A:535:ALA:N	2.03	0.72
1:I:26:DC:H4'	1:I:27:DA:OP1	1.89	0.72
1:I:23:DT:H1'	1:I:24:DA:O5'	1.90	0.72
1:J:175:DA:C2'	1:J:176:DA:C8	2.72	0.72
1:J:246:DG:C2'	1:J:247:DC:C5	2.70	0.72
4:C:820:ARG:NH1	5:D:1322:LYS:OXT	2.23	0.72
2:A:529:ARG:CZ	2:A:535:ALA:HA	2.20	0.71
1:I:70:DG:N7	6:I:148:HOH:O	2.21	0.71
1:I:45:DT:H2"	1:I:46:DG:OP2	1.91	0.71
2:A:529:ARG:NH2	2:A:535:ALA:CA	2.53	0.71
1:I:130:DT:H2"	1:I:131:DG:N7	2.06	0.71
2:E:725:GLN:HG2	2:E:734:ARG:NH1	2.07	0.70
1:I:108:DC:H2"	1:I:109:DA:N7	2.07	0.69
2:A:534:ARG:N	2:A:534:ARG:CB	2.56	0.69
2:A:529:ARG:HA	2:A:534:ARG:CB	2.23	0.69
1:J:226:DT:H2"	1:J:227:DG:C8	2.28	0.69
1:I:27:DA:H61	1:J:266:DT:H3	0.71	0.68
4:C:817:ARG:HH22	4:C:831:HIS:CD2	2.12	0.67
1:J:257:DA:C2'	1:J:258:DT:H71	2.24	0.67
1:J:261:DA:H2"	1:J:262:DC:C5'	2.22	0.67
1:J:267:DG:N7	6:J:295:HOH:O	2.28	0.67
2:A:464:LYS:HE2	2:A:490:MET:HE1	1.76	0.67
1:I:77:DC:H2"	1:I:78:DG:C8	2.30	0.67
1:I:88:DC:H2"	1:I:89:DC:C6	2.31	0.66
1:J:184:DT:H2"	1:J:185:DG:N7	2.10	0.66
1:J:227:DG:N7	6:J:301:HOH:O	2.28	0.66
5:D:1321:ALA:O	5:D:1322:LYS:O	2.13	0.66
1:J:168:DC:C2'	1:J:169:DT:H72	2.26	0.65
1:I:132:DC:H2"	1:I:133:DA:N7	2.10	0.65
2:A:529:ARG:CZ	2:A:535:ALA:C	2.64	0.65
1:J:258:DT:H2'	1:J:259:DA:H8	1.60	0.65
1:I:22:DC:H2'	1:I:23:DT:H72	1.77	0.64
1:I:36:DT:H2"	1:I:37:DT:OP2	1.97	0.64
2:A:529:ARG:CA	2:A:534:ARG:HB2	2.25	0.64
1:J:247:DC:H2"	1:J:248:DA:C8	2.32	0.64
3:F:259:LYS:O	3:F:263:GLU:HG3	1.97	0.64
5:H:1469:ARG:HD3	6:H:286:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:248:DA:H2"	1:J:249:DG:N7	2.12	0.64
2:E:729:ARG:HG3	2:E:735:ALA:HA	1.80	0.64
1:J:177:DG:H5"	4:G:1016:THR:HA	1.80	0.64
1:I:16:DC:H2"	1:I:17:DA:C8	2.33	0.64
1:I:47:DC:C2'	1:I:48:DT:H72	2.27	0.64
1:J:225:DC:H2"	1:J:226:DT:C5	2.33	0.63
1:I:39:DG:H2"	1:I:40:DG:C8	2.33	0.63
1:J:175:DA:H2"	1:J:176:DA:H8	1.61	0.63
1:J:257:DA:H2"	1:J:258:DT:H71	1.80	0.63
1:J:162:DC:H2"	1:J:163:DA:N7	2.13	0.63
1:J:238:DT:C6	1:J:239:DT:H72	2.33	0.63
4:G:1084:GLN:OE1	4:G:1088:ARG:HD2	1.98	0.63
2:A:534:ARG:HA	2:A:534:ARG:O	1.99	0.63
1:I:47:DC:H42	1:J:246:DG:H1	1.45	0.63
2:A:521:PRO:O	2:A:525:GLN:HG3	1.98	0.63
4:C:855:LEU:O	4:C:859:THR:HG23	1.99	0.63
1:I:22:DC:N4	1:J:271:DG:H1	1.96	0.62
1:J:277:DG:H5"	4:C:876:THR:HG21	1.82	0.62
1:I:7:DA:C2'	1:I:8:DT:H71	2.30	0.62
1:I:26:DC:H1'	1:I:27:DA:N7	2.15	0.61
1:I:128:DT:H1'	1:I:129:DC:H5'	1.81	0.61
2:E:716:ARG:CZ	2:E:720:MET:HE3	2.30	0.61
1:I:5:DA:H2"	1:I:6:DT:C5'	2.30	0.61
2:A:529:ARG:HH21	2:A:535:ALA:CA	2.13	0.61
3:B:59:LYS:HE2	3:B:63:GLU:OE2	2.01	0.61
5:D:1322:LYS:OXT	5:D:1322:LYS:HD2	2.01	0.61
1:I:49:DC:H1'	1:I:50:DC:C6	2.35	0.60
1:J:168:DC:H2"	1:J:169:DT:C7	2.30	0.60
1:J:286:DT:H2"	1:J:287:DA:O5'	2.01	0.60
2:A:508:ASN:HD21	4:G:1115:LEU:HD11	1.67	0.60
5:D:1304:ALA:O	5:D:1308:VAL:HG23	2.01	0.60
4:G:1102:ILE:HG23	5:H:1458:ILE:HD13	1.82	0.60
1:I:100:DG:H2"	1:I:101:DC:C5	2.36	0.60
1:J:167:DT:C2	1:J:168:DC:C5	2.90	0.60
1:I:10:DC:H1'	1:I:11:DA:C8	2.36	0.60
2:A:529:ARG:CZ	2:A:535:ALA:N	2.64	0.60
4:C:919:LYS:HD3	4:C:919:LYS:N	2.17	0.60
2:E:649:ARG:HG3	2:E:649:ARG:NH1	2.17	0.59
1:J:147:DA:H2'	1:J:148:DT:C7	2.31	0.59
3:F:302:GLY:HA2	6:F:308:HOH:O	2.01	0.59
5:D:1273:GLU:HA	5:D:1276:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:DA:H2"	1:I:56:DA:C8	2.37	0.59
1:J:266:DT:H2"	1:J:267:DG:N7	2.16	0.59
4:G:1013:LYS:HE2	4:G:1013:LYS:HA	1.84	0.59
1:I:47:DC:H2"	1:I:48:DT:C7	2.31	0.59
5:D:1322:LYS:O	6:D:64:HOH:O	2.17	0.59
4:C:902:ILE:CG2	5:D:1258:ILE:HD13	2.31	0.59
1:J:178:DT:OP1	4:G:1014:ALA:HA	2.03	0.59
1:I:69:DC:H2"	1:I:70:DG:C8	2.38	0.58
1:J:271:DG:H2'	1:J:271:DG:O5'	2.03	0.58
5:H:1489:ARG:HH11	5:H:1489:ARG:HG2	1.68	0.58
2:A:476:GLN:HE21	2:A:480:THR:HG22	1.69	0.58
2:A:529:ARG:NH2	2:A:535:ALA:HA	2.19	0.58
1:J:151:DA:H2"	1:J:152:DT:C5'	2.33	0.58
1:J:239:DT:H2"	1:J:240:DG:C8	2.39	0.58
1:I:92:DT:C6	1:I:93:DT:H73	2.39	0.58
2:E:678:PHE:HZ	3:F:267:ARG:NH2	2.01	0.57
1:J:175:DA:C2'	1:J:176:DA:H8	2.17	0.57
1:I:49:DC:H1'	1:I:50:DC:C5	2.39	0.57
1:I:26:DC:H1'	1:I:27:DA:C5	2.38	0.57
1:I:138:DG:H2"	1:I:139:DA:OP2	2.04	0.57
1:J:173:DA:H2"	1:J:174:DA:C8	2.40	0.57
1:I:16:DC:H2"	1:I:17:DA:N7	2.20	0.56
1:J:155:DC:H5'	1:J:155:DC:C6	2.37	0.56
1:J:238:DT:C7	2:A:465:LEU:HD22	2.35	0.56
2:A:529:ARG:HG2	2:A:534:ARG:C	2.24	0.56
1:I:25:DC:C2'	1:I:26:DC:H5'	2.32	0.56
5:D:1322:LYS:OXT	5:D:1322:LYS:CD	2.53	0.56
1:J:163:DA:H2"	1:J:164:DG:C8	2.41	0.56
1:J:271:DG:H2"	1:J:272:DA:OP2	2.06	0.56
3:B:61:PHE:O	3:B:65:VAL:HG23	2.05	0.56
1:I:29:DA:C2'	1:I:30:DA:C8	2.88	0.56
1:I:34:DT:H2"	1:I:35:DA:O5'	2.05	0.56
1:J:262:DC:H2"	1:J:263:DT:O5'	2.04	0.56
2:A:437:LYS:O	2:A:439:HIS:N	2.39	0.56
4:G:1031:HIS:CD2	4:G:1048:PRO:HG3	2.41	0.55
1:I:1:DA:C2'	1:I:2:DT:H72	2.36	0.55
1:J:210:DT:C6	1:J:211:DT:H72	2.42	0.55
2:A:528:ARG:HH11	2:A:534:ARG:HH12	1.55	0.55
1:I:22:DC:H2'	1:I:23:DT:C7	2.36	0.55
1:I:5:DA:H2"	1:I:6:DT:H5'	1.89	0.55
1:J:165:DA:C4	1:J:166:DT:C5	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:231:LYS:HE2	3:F:235:ARG:HH21	1.71	0.55
1:I:17:DA:C2	1:I:18:DG:C2	2.94	0.55
1:I:29:DA:H2"	1:I:30:DA:C8	2.41	0.55
2:A:463:ARG:O	2:A:466:PRO:HD2	2.07	0.54
2:A:529:ARG:HG3	2:A:534:ARG:HB3	1.88	0.54
2:E:719:ILE:HD13	3:F:243:ILE:CD1	2.32	0.54
1:J:151:DA:H1'	1:J:152:DT:H5"	1.90	0.54
2:A:528:ARG:NH1	2:A:534:ARG:HH12	2.06	0.54
1:J:210:DT:H2'	1:J:211:DT:H72	1.89	0.54
1:J:280:DG:H1'	1:J:281:DG:C8	2.43	0.54
1:I:111:DA:OP1	4:G:1044:GLY:HA2	2.08	0.54
4:C:881:ARG:NH2	4:C:907:VAL:O	2.35	0.53
1:I:134:DG:H2"	1:I:135:DG:H8	1.73	0.53
5:D:1277:LEU:HD21	5:D:1293:THR:HB	1.90	0.53
2:E:663:ARG:HA	2:E:663:ARG:NE	2.23	0.53
1:J:237:DT:H4'	2:A:463:ARG:NE	2.23	0.53
2:A:529:ARG:HG3	2:A:535:ALA:N	2.15	0.53
1:I:40:DG:OP1	5:D:1285:THR:HB	2.09	0.53
1:I:47:DC:H2"	1:I:48:DT:H72	1.89	0.53
1:J:166:DT:C2'	1:J:167:DT:C7	2.81	0.53
1:J:266:DT:H2"	1:J:267:DG:C5	2.43	0.53
4:G:1015:LYS:HG3	4:G:1019:SER:OG	2.08	0.53
1:I:38:DT:O3'	1:I:39:DG:C8	2.62	0.53
1:I:48:DT:H2'	1:I:49:DC:C5	2.44	0.52
1:J:147:DA:H2"	1:J:148:DT:O5'	2.08	0.52
1:J:226:DT:H2"	1:J:227:DG:N7	2.24	0.52
2:E:665:LEU:HB3	2:E:666:PRO:HD3	1.91	0.52
1:I:133:DA:H2"	1:I:134:DG:C8	2.43	0.52
1:I:57:DA:H2"	1:I:58:DG:C8	2.44	0.52
1:J:270:DA:H1'	1:J:271:DG:H5'	1.91	0.52
2:A:529:ARG:CD	2:A:535:ALA:N	2.43	0.52
1:J:249:DG:H5"	5:H:1427:ARG:O	2.09	0.52
1:J:272:DA:C6	1:J:273:DA:C6	2.98	0.52
4:G:1026:PRO:HD3	5:H:1437:TYR:CD2	2.45	0.52
1:I:54:DA:H2"	1:I:55:DA:C8	2.45	0.52
5:D:1287:THR:H	5:D:1290:GLU:HG2	1.75	0.52
1:I:78:DG:H2"	1:I:79:DC:C5	2.45	0.51
1:J:227:DG:H5'	3:B:47:SER:HA	1.93	0.51
4:C:820:ARG:CZ	5:D:1322:LYS:OXT	2.58	0.51
5:D:1321:ALA:C	5:D:1322:LYS:O	2.48	0.51
1:I:21:DT:H2"	1:I:22:DC:O5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:DA:C2'	1:J:166:DT:H71	2.40	0.51
1:J:172:DC:H2"	1:J:173:DA:N7	2.26	0.51
1:I:125:DG:H2"	1:I:126:DA:OP2	2.11	0.51
1:J:166:DT:C2	1:J:167:DT:C4	2.98	0.51
1:I:20:DT:C5	1:I:21:DT:H73	2.45	0.51
1:J:226:DT:H4'	1:J:227:DG:OP1	2.11	0.51
1:J:283:DG:H2"	1:J:284:DG:C8	2.45	0.51
4:G:1037:GLY:HA3	4:G:1039:TYR:CE1	2.47	0.50
1:I:114:DC:H4'	1:I:114:DC:OP1	2.11	0.50
1:J:169:DT:C2	1:J:170:DA:C5	3.00	0.50
2:A:479:LYS:HD2	3:B:74:GLU:HG2	1.93	0.50
2:E:640:ARG:HD3	6:E:110:HOH:O	2.11	0.50
1:I:23:DT:C1'	1:I:24:DA:O5'	2.57	0.50
4:C:831:HIS:HA	4:C:848:PRO:HB3	1.94	0.50
1:J:149:DC:H2"	1:J:150:DA:C8	2.46	0.50
1:J:264:DT:C6	1:J:265:DT:H72	2.46	0.50
5:D:1261:SER:HB3	3:F:302:GLY:O	2.11	0.50
1:I:30:DA:OP2	4:C:832:ARG:HD3	2.12	0.50
1:J:174:DA:C2'	1:J:175:DA:H5"	2.35	0.50
2:A:459:GLU:OE2	3:B:40:ARG:NH2	2.40	0.50
1:I:1:DA:H2'	1:I:2:DT:H72	1.92	0.50
1:I:26:DC:H1'	1:I:27:DA:C8	2.47	0.50
1:J:151:DA:C2'	1:J:152:DT:H5"	2.40	0.50
1:J:168:DC:H2"	1:J:169:DT:H72	1.89	0.50
1:I:5:DA:C2'	1:I:6:DT:H5"	2.42	0.49
2:A:436:LYS:HD2	2:A:436:LYS:C	2.31	0.49
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.94	0.49
1:J:175:DA:H2'	1:J:176:DA:C8	2.47	0.49
5:D:1276:ARG:HB3	5:D:1280:TYR:CZ	2.48	0.49
2:A:448:LEU:HD21	4:G:1117:PRO:HD3	1.94	0.49
4:G:1017:ARG:NH1	4:G:1031:HIS:HD2	1.94	0.49
1:J:230:DC:H2"	1:J:231:DA:N7	2.26	0.49
1:I:7:DA:H2"	1:I:8:DT:H71	1.93	0.49
3:F:231:LYS:HE2	3:F:235:ARG:NH2	2.28	0.49
1:I:6:DT:H2"	1:I:7:DA:C8	2.47	0.49
2:A:529:ARG:NH2	2:A:535:ALA:O	2.33	0.49
2:E:646:VAL:O	2:E:650:GLU:HG3	2.12	0.49
2:A:476:GLN:NE2	2:A:480:THR:HG22	2.27	0.49
1:J:287:DA:H2'	1:J:288:DT:C7	2.42	0.49
4:C:817:ARG:HH22	4:C:831:HIS:HD2	1.57	0.49
4:C:831:HIS:CG	4:C:848:PRO:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1277:LEU:CD2	5:D:1293:THR:HB	2.42	0.49
5:H:1473:GLU:HA	5:H:1473:GLU:OE1	2.13	0.49
2:E:669:ARG:NH1	6:E:124:HOH:O	2.46	0.48
1:I:130:DT:C2	1:I:131:DG:C6	3.01	0.48
1:J:248:DA:C2	1:J:249:DG:C6	3.02	0.48
1:J:225:DC:C2'	1:J:226:DT:H71	2.34	0.48
1:J:249:DG:O3'	5:H:1427:ARG:CG	2.56	0.48
1:J:249:DG:O3'	5:H:1427:ARG:HB2	2.13	0.48
2:A:529:ARG:NE	2:A:535:ALA:HA	2.13	0.48
1:I:111:DA:C8	1:I:112:DT:H72	2.48	0.48
1:I:135:DG:H2"	1:I:136:DT:OP2	2.12	0.48
2:A:448:LEU:CD2	4:G:1117:PRO:HD3	2.44	0.48
2:A:528:ARG:NH1	2:A:534:ARG:NH1	2.62	0.48
5:H:1470:ILE:HA	5:H:1498:LEU:CD1	2.43	0.48
1:I:27:DA:C4	1:I:28:DA:C5	3.02	0.48
1:J:169:DT:H1'	1:J:170:DA:C8	2.49	0.48
4:C:884:GLN:NE2	4:C:906:GLY:O	2.45	0.48
4:C:918:LYS:HB3	4:C:919:LYS:H	1.50	0.48
1:I:5:DA:H1'	1:I:6:DT:H5"	1.95	0.48
5:H:1473:GLU:HA	5:H:1476:ARG:HH11	1.79	0.48
1:I:82:DA:H3'	2:E:646:VAL:HG21	1.94	0.47
1:I:134:DG:N7	6:I:149:HOH:O	2.35	0.47
1:J:164:DG:C2	1:J:165:DA:C5	3.02	0.47
1:J:210:DT:C2'	1:J:211:DT:H72	2.44	0.47
1:J:151:DA:H2"	1:J:152:DT:H5"	1.96	0.47
2:A:529:ARG:CG	2:A:534:ARG:C	2.83	0.47
1:J:287:DA:C8	1:J:288:DT:H72	2.48	0.47
2:A:446:VAL:O	2:A:450:GLU:HG3	2.14	0.47
1:I:70:DG:H2"	1:I:71:DG:C8	2.49	0.47
1:I:79:DC:H2"	1:I:80:DT:C5	2.49	0.47
1:J:258:DT:C2'	1:J:259:DA:C8	2.94	0.47
1:I:5:DA:H2"	1:I:6:DT:H5"	1.96	0.47
1:I:48:DT:C2'	1:I:49:DC:C6	2.96	0.47
4:G:1035:ARG:HH11	4:G:1035:ARG:HG2	1.80	0.47
1:I:27:DA:C5	1:I:28:DA:C6	3.03	0.47
1:J:155:DC:H2"	1:J:156:DC:C6	2.49	0.47
3:B:26:ILE:HG13	3:B:55:ARG:HB3	1.96	0.47
1:I:136:DT:H1'	1:I:137:DG:H5'	1.96	0.47
1:J:187:DA:H2"	1:J:188:DA:C8	2.50	0.47
1:J:272:DA:H2"	1:J:273:DA:O5'	2.14	0.47
1:I:48:DT:H2"	1:I:49:DC:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:168:DC:C6	1:J:169:DT:C7	2.92	0.47
1:J:151:DA:H2"	1:J:152:DT:H5'	1.94	0.46
2:E:729:ARG:O	2:E:735:ALA:HB2	2.16	0.46
3:F:284:MET:HE3	3:F:288:TYR:CZ	2.50	0.46
3:B:87:VAL:HG13	6:B:105:HOH:O	2.15	0.46
5:H:1439:TYR:CZ	5:H:1443:LYS:HE3	2.51	0.46
1:J:186:DG:C2	1:J:187:DA:C6	3.04	0.46
3:B:22:LEU:O	3:B:22:LEU:HG	2.16	0.46
1:I:100:DG:H2"	1:I:101:DC:H5	1.80	0.46
2:E:716:ARG:CZ	2:E:720:MET:CE	2.94	0.46
1:J:182:DT:H2"	1:J:183:DT:OP2	2.15	0.45
1:J:195:DC:H1'	1:J:196:DC:C6	2.51	0.45
2:A:465:LEU:N	2:A:466:PRO:CD	2.79	0.45
3:B:68:ASP:OD2	3:B:93:GLN:NE2	2.49	0.45
1:I:17:DA:H2"	1:I:18:DG:C8	2.51	0.45
1:J:150:DA:H2"	1:J:151:DA:OP2	2.16	0.45
2:E:678:PHE:CZ	3:F:267:ARG:NH2	2.81	0.45
2:E:718:THR:HA	3:F:245:ARG:O	2.16	0.45
1:I:20:DT:C6	1:I:21:DT:C7	2.99	0.45
4:G:1042:ARG:HD3	6:G:214:HOH:O	2.16	0.45
1:I:134:DG:H2"	1:I:135:DG:C8	2.51	0.45
1:J:148:DT:H2"	1:J:149:DC:O5'	2.16	0.45
4:C:820:ARG:NH1	5:D:1322:LYS:HB3	2.32	0.45
1:I:87:DG:H2"	1:I:88:DC:C5	2.51	0.45
1:J:152:DT:H2"	1:J:153:DA:C8	2.52	0.45
1:I:93:DT:H1'	1:I:94:DG:H5'	1.99	0.45
2:E:677:ASP:OD2	6:E:1:HOH:O	2.21	0.45
4:G:1084:GLN:CD	4:G:1088:ARG:HD2	2.37	0.45
4:C:825:PHE:CZ	4:C:859:THR:HG21	2.52	0.45
4:G:1076:THR:O	5:H:1449:THR:HG23	2.17	0.45
5:H:1477:LEU:HD11	5:H:1493:THR:CG2	2.47	0.45
1:I:113:DA:H2"	1:I:114:DC:O5'	2.17	0.44
2:A:485:GLN:HG3	3:B:82:THR:HA	1.99	0.44
2:E:679:LYS:HG3	3:F:274:GLU:OE2	2.17	0.44
1:J:182:DT:H1'	1:J:183:DT:H5'	1.99	0.44
1:J:271:DG:O5'	1:J:271:DG:C2'	2.62	0.44
4:C:918:LYS:C	4:C:919:LYS:HD3	2.37	0.44
4:C:829:ARG:HD2	5:D:1232:GLU:OE1	2.16	0.44
1:I:87:DG:H1'	1:I:88:DC:C5	2.52	0.44
1:I:124:DA:OP1	5:H:1428:LYS:HG2	2.16	0.44
2:E:651:ILE:O	2:E:655:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:DT:H2'	1:I:49:DC:C6	2.52	0.44
1:I:76:DC:H2"	1:I:77:DC:C5	2.52	0.44
1:J:164:DG:C2	1:J:165:DA:C6	3.05	0.44
4:C:829:ARG:NH2	5:D:1233:SER:O	2.50	0.44
1:J:237:DT:H4'	2:A:463:ARG:NH2	2.30	0.44
3:B:68:ASP:OD2	3:B:92:ARG:NH1	2.50	0.44
4:C:832:ARG:HH22	5:D:1232:GLU:CD	2.21	0.44
5:H:1522:LYS:O	5:H:1522:LYS:HG3	2.18	0.44
1:I:31:DG:OP1	4:C:817:ARG:HG3	2.18	0.43
1:I:47:DC:H2'	1:I:48:DT:H72	1.99	0.43
1:I:113:DA:C2	1:J:181:DA:C2	3.06	0.43
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.99	0.43
3:F:265:VAL:HA	3:F:293:GLN:HE22	1.83	0.43
1:J:195:DC:H1'	1:J:196:DC:C5	2.53	0.43
4:G:1088:ARG:H	4:G:1088:ARG:HG2	1.46	0.43
5:H:1473:GLU:HA	5:H:1476:ARG:NH1	2.33	0.43
1:J:154:DT:P	2:A:449:ARG:HD2	2.58	0.43
4:C:831:HIS:NE2	4:C:835:ARG:NH2	2.67	0.43
5:H:1470:ILE:HA	5:H:1498:LEU:HD12	2.01	0.43
1:J:219:DA:C2'	1:J:220:DT:H71	2.48	0.43
1:J:238:DT:C2'	1:J:239:DT:H72	2.48	0.43
1:J:270:DA:H2"	1:J:271:DG:OP2	2.18	0.43
2:E:664:LYS:HD3	6:E:284:HOH:O	2.18	0.43
1:I:49:DC:C1'	1:I:50:DC:C5	3.01	0.43
2:E:678:PHE:HZ	3:F:267:ARG:HH21	1.67	0.43
1:J:181:DA:H2"	1:J:182:DT:OP2	2.18	0.43
1:J:279:DA:H2"	1:J:280:DG:C8	2.53	0.43
1:J:288:DT:H1'	1:J:289:DT:H5"	2.00	0.43
1:I:22:DC:C2'	1:I:23:DT:H72	2.48	0.43
1:I:80:DT:H4'	3:F:245:ARG:CZ	2.49	0.43
1:J:242:DT:H2"	1:J:243:DG:OP2	2.19	0.43
4:C:837:GLY:HA3	4:C:839:TYR:CE1	2.53	0.43
5:D:1276:ARG:HD2	6:D:144:HOH:O	2.19	0.43
2:E:716:ARG:HD2	2:E:720:MET:HE2	2.00	0.43
4:G:1013:LYS:HE2	4:G:1013:LYS:CA	2.48	0.43
1:I:111:DA:C2'	1:I:112:DT:C7	2.97	0.42
1:I:119:DT:H2"	1:I:120:DT:O5'	2.19	0.42
4:G:1035:ARG:HG2	4:G:1035:ARG:NH1	2.33	0.42
5:H:1473:GLU:CD	6:H:272:HOH:O	2.57	0.42
2:E:716:ARG:CD	2:E:720:MET:CE	2.98	0.42
5:H:1475:SER:HA	5:H:1486:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:DA:H2"	1:I:56:DA:N7	2.34	0.42
5:D:1291:ILE:O	5:D:1295:VAL:HG23	2.19	0.42
3:F:287:VAL:HG11	3:F:302:GLY:HA3	2.01	0.42
1:J:163:DA:H2"	1:J:164:DG:H8	1.84	0.42
1:J:165:DA:C2	1:J:166:DT:C2	3.08	0.42
1:J:246:DG:C2'	1:J:247:DC:H5	2.21	0.42
1:J:149:DC:C2'	1:J:150:DA:C8	3.03	0.42
1:J:249:DG:H4'	5:H:1427:ARG:CG	2.49	0.42
4:C:835:ARG:HG2	4:C:835:ARG:HH11	1.85	0.42
5:H:1477:LEU:HD11	5:H:1493:THR:HG22	2.01	0.42
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.88	0.42
1:I:89:DC:C4	1:J:203:DA:N6	2.88	0.42
1:I:118:DT:C2'	1:I:119:DT:H72	2.50	0.42
6:D:226:HOH:O	3:F:291:LYS:HE2	2.19	0.42
2:E:672:ARG:O	2:E:676:GLN:HB2	2.20	0.42
4:C:888:ARG:HA	4:C:888:ARG:HD3	1.84	0.42
3:F:252:GLU:OE2	3:F:255:ARG:NH1	2.53	0.42
4:G:1030:VAL:HG13	5:H:1467:PHE:HE1	1.85	0.42
5:D:1230:ARG:HE	5:D:1230:ARG:HB2	1.52	0.42
1:I:22:DC:H2"	1:I:23:DT:C6	2.55	0.42
1:I:117:DT:H1'	1:I:118:DT:H5'	2.01	0.42
1:I:144:DG:H2"	1:I:145:DA:OP2	2.19	0.42
1:J:153:DA:H5'	2:A:441:TYR:OH	2.20	0.42
1:J:233:DG:H2"	1:J:234:DC:OP2	2.20	0.42
1:I:110:DA:C4	1:I:111:DA:N7	2.88	0.41
1:J:194:DT:H2"	1:J:195:DC:C6	2.55	0.41
1:J:225:DC:C2'	1:J:226:DT:C7	2.90	0.41
2:A:436:LYS:HE3	2:A:437:LYS:HG2	2.02	0.41
5:H:1489:ARG:HG2	5:H:1489:ARG:NH1	2.34	0.41
1:I:127:DA:H1'	1:I:128:DT:H5'	2.02	0.41
1:J:287:DA:H2"	1:J:288:DT:O5'	2.20	0.41
1:J:250:DT:OP1	5:H:1427:ARG:HB2	2.21	0.41
1:I:9:DC:H42	1:J:284:DG:H1	1.68	0.41
1:J:263:DT:H2"	1:J:264:DT:OP2	2.21	0.41
4:G:1051:LEU:HD12	4:G:1051:LEU:O	2.20	0.41
1:J:247:DC:H2"	1:J:248:DA:H8	1.82	0.41
4:C:825:PHE:HZ	4:C:859:THR:HG21	1.86	0.41
1:I:20:DT:C6	1:I:21:DT:H73	2.55	0.41
1:I:129:DC:C2'	1:I:130:DT:H71	2.50	0.41
1:J:176:DA:C2	1:J:177:DG:C5	3.08	0.41
1:I:2:DT:H1'	1:I:3:DC:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:DA:C8	1:I:52:DT:C7	3.04	0.41
5:D:1273:GLU:HA	5:D:1276:ARG:HH12	1.82	0.41
2:E:719:ILE:HG13	3:F:250:ILE:HG13	2.03	0.41
4:G:1047:ALA:N	4:G:1048:PRO:HD2	2.36	0.41
1:J:176:DA:C4	1:J:177:DG:N7	2.89	0.40
2:A:529:ARG:O	2:A:529:ARG:NH1	2.55	0.40
1:I:26:DC:H6	1:I:26:DC:H2'	1.70	0.40
1:I:111:DA:H2"	1:I:112:DT:C7	2.51	0.40
1:J:244:DG:H2"	1:J:245:DA:N7	2.36	0.40
4:C:833:LEU:HD23	4:C:836:LYS:HD3	2.03	0.40
1:I:111:DA:C2'	1:I:112:DT:H72	2.51	0.40
1:J:245:DA:C2'	1:J:246:DG:C8	2.91	0.40
2:A:528:ARG:HD3	2:A:534:ARG:HH12	1.85	0.40
1:J:218:DA:H1'	1:J:219:DA:C8	2.56	0.40
1:J:231:DA:C2'	1:J:232:DT:H71	2.51	0.40
1:J:181:DA:H1'	1:J:182:DT:H5'	2.04	0.40
4:G:1031:HIS:CE1	4:G:1035:ARG:NH2	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	98/135 (73%)	94 (96%)	3 (3%)	1 (1%)	15	37
2	E	98/135 (73%)	96 (98%)	1 (1%)	1 (1%)	15	37
3	B	79/102 (78%)	78 (99%)	1 (1%)	0	100	100
3	F	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
4	C	105/129 (81%)	98 (93%)	7 (7%)	0	100	100
4	G	106/129 (82%)	103 (97%)	3 (3%)	0	100	100
5	D	91/125 (73%)	88 (97%)	2 (2%)	1 (1%)	14	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	H	94/125 (75%)	89 (95%)	4 (4%)	1 (1%)	14 34
All	All	751/982 (76%)	724 (96%)	23 (3%)	4 (0%)	29 54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	734	ARG
5	H	1501	GLY
2	A	438	PRO
5	D	1301	GLY

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	A	87/111 (78%)	84 (97%)	3 (3%)	37 66
2	E	87/111 (78%)	85 (98%)	2 (2%)	50 78
3	B	66/78 (85%)	65 (98%)	1 (2%)	65 86
3	F	67/78 (86%)	66 (98%)	1 (2%)	65 86
4	C	85/100 (85%)	80 (94%)	5 (6%)	19 43
4	G	85/100 (85%)	83 (98%)	2 (2%)	49 77
5	D	79/105 (75%)	75 (95%)	4 (5%)	24 50
5	H	82/105 (78%)	79 (96%)	3 (4%)	34 63
All	All	638/788 (81%)	617 (97%)	21 (3%)	38 67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	448	LEU
2	A	459	GLU
2	A	529	ARG
3	B	47	SER

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Mol	Chain	Res	Type
4	C	829	ARG
4	C	859	THR
4	C	876	THR
4	C	881	ARG
4	C	919	LYS
5	D	1230	ARG
5	D	1233	SER
5	D	1290	GLU
5	D	1319	THR
2	E	659	GLU
2	E	678	PHE
3	F	247	SER
4	G	1013	LYS
4	G	1088	ARG
5	H	1427	ARG
5	H	1433	SER
5	H	1484	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	476	GLN
2	A	508	ASN
3	B	93	GLN
4	C	831	HIS
5	D	1279	HIS
2	E	668	GLN
3	F	293	GLN
4	G	1031	HIS
5	H	1492	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.