



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P3F
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 : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

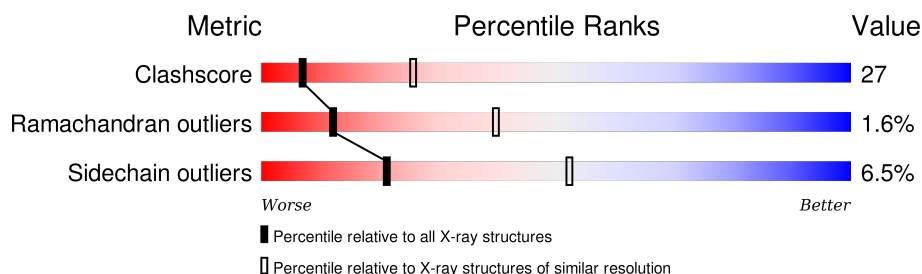
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)




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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	
1	J	146	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	129	

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Mol	Chain	Length	Quality of chain
4	G	129	 43% 36% 17%
5	D	125	 45% 24% 27%
5	H	125	 41% 32% 24%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12150 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	99	Total	C	N	O	S	0	0	0
			817	515	158	141	3			
2	E	99	Total	C	N	O	S	0	0	0
			817	515	158	141	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	80	Total	C	N	O	S	0	0	0
			633	398	122	111	2			
3	F	82	Total	C	N	O	S	0	0	0
			648	409	124	113	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	ARG	CONFLICT	UNP P62799
F	245	CYS	ARG	CONFLICT	UNP P62799

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	104	Total	C	N	O	0	0	0
			804	507	157	140			
4	G	107	Total	C	N	O	0	0	0
			827	522	162	143			

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	91	Total	C	N	O	S	0	0	0
			709	447	125	135	2			
5	H	95	Total	C	N	O	S	0	0	0
			744	468	134	140	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.

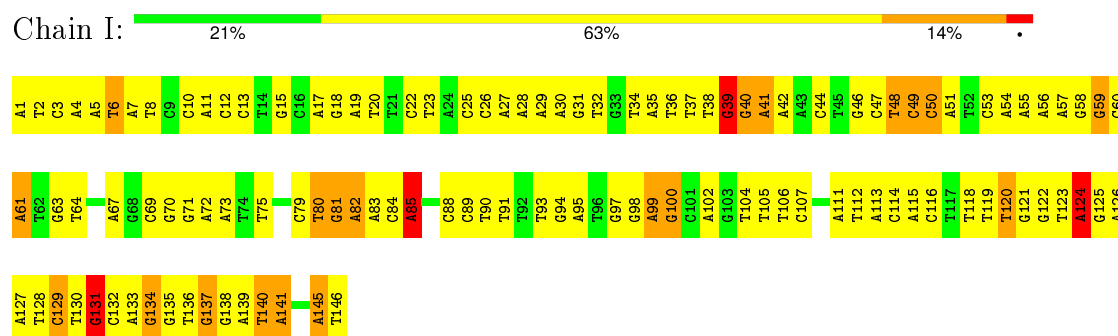
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total O 9 9	0	0
6	B	8	Total O 8 8	0	0
6	C	16	Total O 16 16	0	0
6	D	9	Total O 9 9	0	0
6	E	17	Total O 17 17	0	0
6	F	16	Total O 16 16	0	0
6	G	13	Total O 13 13	0	0
6	H	5	Total O 5 5	0	0
6	I	39	Total O 39 39	0	0
6	J	39	Total O 39 39	0	0

3 Residue-property plots

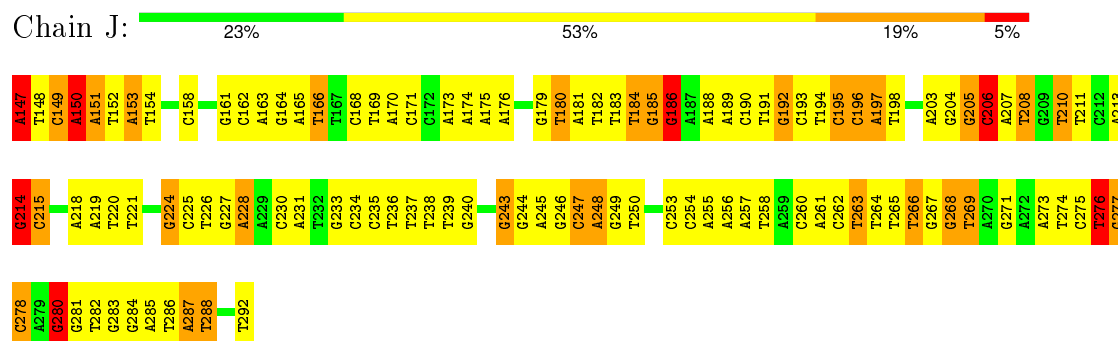
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

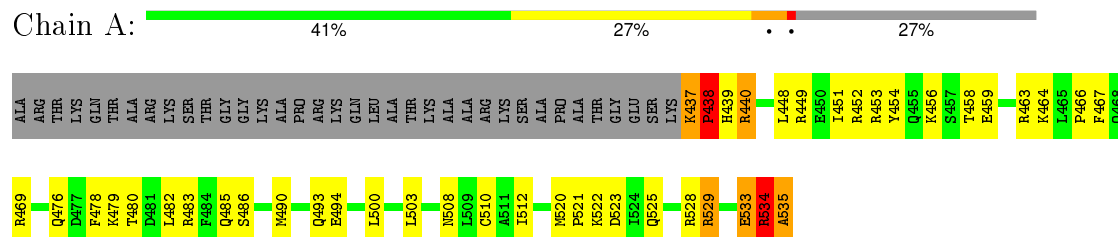
- Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment



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

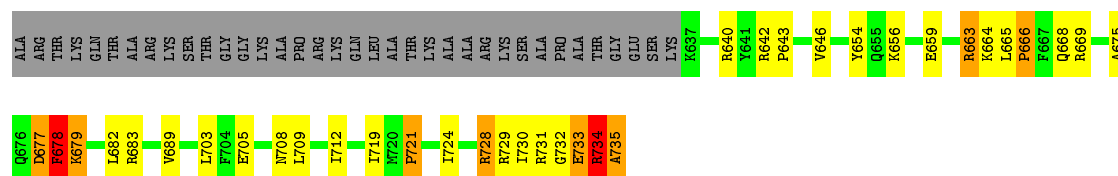


- Molecule 2: Histone H3



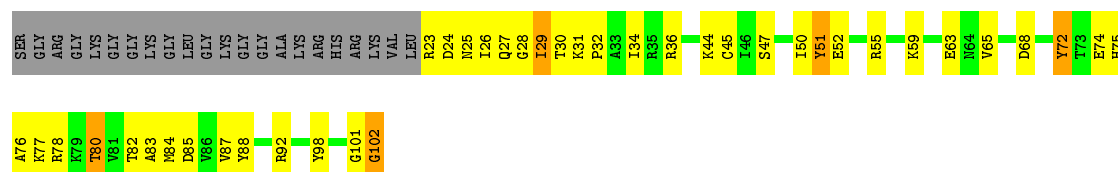
- Molecule 2: Histone H3

Chain E:  47% 19% 6% 27%



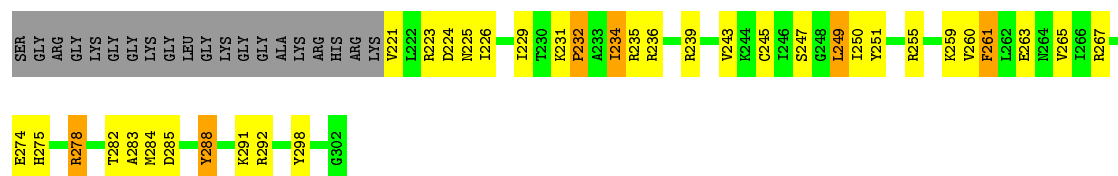
- Molecule 3: Histone H4

Chain B:  39% 34% 5% 22%



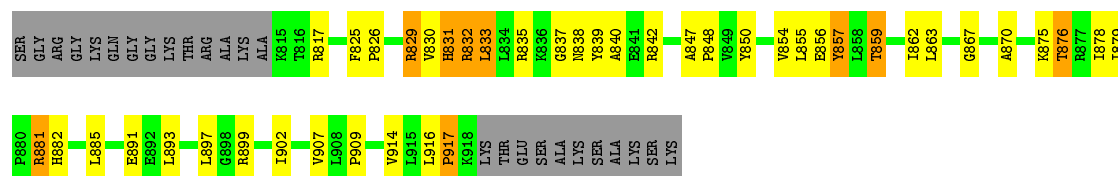
- Molecule 3: Histone H4

Chain F: 45% 29% 6% 20%



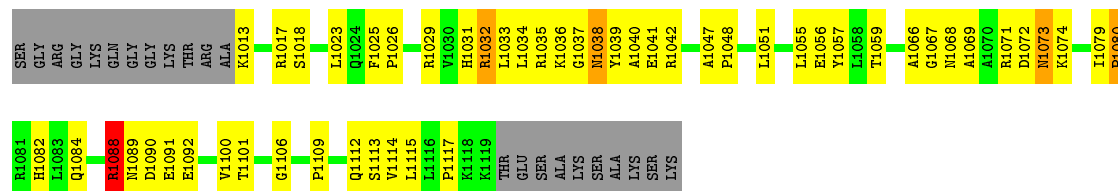
- Molecule 4: Histone H2A

Chain C: 47% 26% 7% 19%



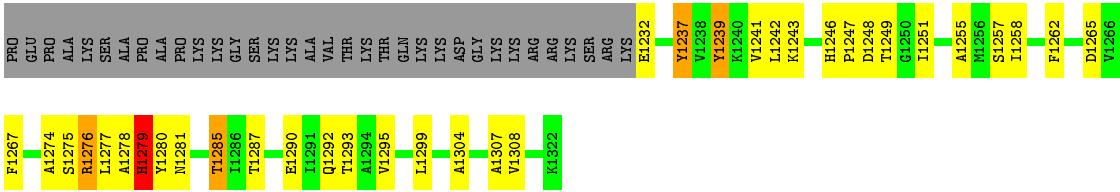
- Molecule 4: Histone H2A

Chain G:  43% 36% •• 17%

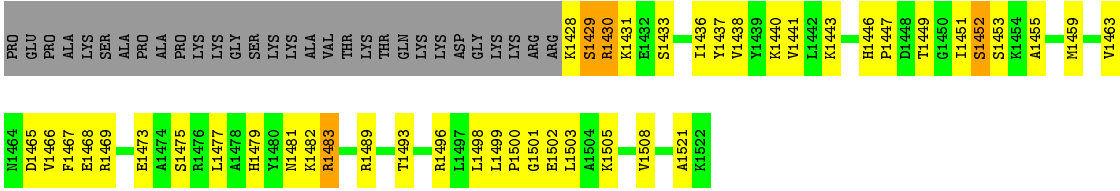


- Molecule 5: Histone H2B

Chain D:  45% 24% 2% 29%



• Molecule 5: Histone H2B



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.74Å 109.50Å 181.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	94.1 (40.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12150	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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	1.40	11/3354 (0.3%)	1.22	17/5175 (0.3%)
1	J	1.37	14/3354 (0.4%)	1.25	19/5175 (0.4%)
2	A	1.52	7/829 (0.8%)	1.42	5/1111 (0.5%)
2	E	1.82	10/829 (1.2%)	1.57	19/1111 (1.7%)
3	B	1.46	2/640 (0.3%)	1.31	3/856 (0.4%)
3	F	1.70	8/655 (1.2%)	1.51	9/877 (1.0%)
4	C	1.37	3/814 (0.4%)	1.36	5/1099 (0.5%)
4	G	1.22	1/837 (0.1%)	1.25	5/1128 (0.4%)
5	D	1.40	3/720 (0.4%)	1.37	6/969 (0.6%)
5	H	1.43	6/755 (0.8%)	1.22	3/1013 (0.3%)
All	All	1.44	65/12787 (0.5%)	1.30	91/18514 (0.5%)

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	18
1	J	0	25
2	A	0	1
2	E	0	1
3	B	0	3
3	F	0	1
4	C	0	1
4	G	0	1
5	D	0	3
All	All	0	54

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	735	ALA	C-O	15.70	1.53	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	735	ALA	CA-CB	15.32	1.84	1.52
2	E	677	ASP	CB-CG	14.08	1.81	1.51
2	E	733	GLU	CG-CD	12.22	1.70	1.51
2	A	533	GLU	CG-CD	10.66	1.68	1.51
2	E	732	GLY	C-O	-9.57	1.08	1.23
2	E	735	ALA	C-OXT	9.41	1.41	1.23
3	F	243	VAL	CB-CG2	-9.31	1.33	1.52
4	C	875	LYS	CB-CG	-8.00	1.30	1.52
5	D	1255	ALA	CA-CB	-7.89	1.35	1.52
2	A	437	LYS	CD-CE	7.70	1.70	1.51
1	I	140	DT	N1-C2	7.44	1.44	1.38
1	I	134	DG	C5-C6	-7.42	1.34	1.42
1	J	263	DT	N1-C2	7.32	1.44	1.38
2	A	533	GLU	CB-CG	7.00	1.65	1.52
1	J	218	DA	C5-C6	-6.86	1.34	1.41
4	C	870	ALA	CA-CB	-6.84	1.38	1.52
1	I	80	DT	C4-O4	6.78	1.29	1.23
1	I	40	DG	C5-C6	6.73	1.49	1.42
2	A	437	LYS	CE-NZ	6.67	1.65	1.49
5	H	1468	GLU	CG-CD	6.66	1.61	1.51
4	G	1040	ALA	CA-CB	-6.65	1.38	1.52
3	F	288	TYR	CD2-CE2	-6.62	1.29	1.39
3	F	291	LYS	CD-CE	6.62	1.67	1.51
1	I	15	DG	N1-C2	6.62	1.43	1.37
1	I	40	DG	C6-O6	6.51	1.30	1.24
2	E	677	ASP	CA-CB	6.40	1.68	1.53
3	F	291	LYS	CE-NZ	6.33	1.64	1.49
1	J	237	DT	N1-C2	6.24	1.43	1.38
5	H	1473	GLU	CD-OE2	6.20	1.32	1.25
5	H	1496	ARG	CZ-NH1	6.08	1.41	1.33
3	F	234	ILE	CB-CG2	6.03	1.71	1.52
3	F	260	VAL	CB-CG2	-6.03	1.40	1.52
5	H	1438	VAL	CB-CG2	-5.99	1.40	1.52
1	J	268	DG	N9-C4	-5.89	1.33	1.38
3	B	34	ILE	CA-CB	-5.88	1.41	1.54
1	J	266	DT	C4-C5	5.87	1.50	1.45
1	I	91	DT	N1-C2	5.85	1.42	1.38
3	B	65	VAL	CB-CG2	-5.78	1.40	1.52
1	J	268	DG	C3'-O3'	-5.76	1.36	1.44
2	E	733	GLU	CD-OE1	5.67	1.31	1.25
1	I	75	DT	N1-C2	5.63	1.42	1.38
1	J	214	DG	C6-N1	-5.62	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	733	GLU	CB-CG	5.57	1.62	1.52
1	J	197	DA	C2'-C1'	-5.57	1.46	1.52
1	I	134	DG	C5-C4	5.53	1.42	1.38
3	F	283	ALA	CA-CB	-5.51	1.40	1.52
1	J	184	DT	C4-C5	5.42	1.49	1.45
2	E	678	PHE	N-CA	5.32	1.56	1.46
2	A	494	GLU	CB-CG	-5.31	1.42	1.52
5	H	1438	VAL	CA-CB	-5.30	1.43	1.54
1	I	83	DA	N3-C4	-5.26	1.31	1.34
1	J	210	DT	N3-C4	-5.26	1.34	1.38
5	D	1257	SER	CA-CB	-5.21	1.45	1.52
3	F	261	PHE	CG-CD2	5.20	1.46	1.38
1	J	186	DG	C6-O6	5.19	1.28	1.24
1	J	224	DG	C6-N1	5.18	1.43	1.39
4	C	891	GLU	CB-CG	-5.18	1.42	1.52
1	J	206	DC	C4-N4	5.16	1.38	1.33
2	A	535	ALA	N-CA	5.16	1.56	1.46
5	H	1508	VAL	CB-CG1	-5.15	1.42	1.52
1	I	15	DG	C2-N2	5.11	1.39	1.34
1	J	280	DG	N1-C2	5.08	1.41	1.37
5	D	1262	PHE	CD1-CE1	5.03	1.49	1.39
2	A	510	CYS	CB-SG	-5.00	1.73	1.81

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	534	ARG	N-CA-C	12.64	145.14	111.00
1	J	206	DC	O5'-P-OP2	-12.29	94.64	105.70
2	E	677	ASP	CB-CG-OD1	11.81	128.93	118.30
3	F	278	ARG	NE-CZ-NH2	-10.47	115.06	120.30
4	C	862	ILE	CG1-CB-CG2	-10.24	88.87	111.40
2	E	728	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	I	82	DA	O5'-P-OP2	-9.84	96.85	105.70
1	I	81	DG	O5'-P-OP1	-8.37	98.16	105.70
3	F	239	ARG	NE-CZ-NH2	-8.16	116.22	120.30
2	E	731	ARG	NE-CZ-NH1	-7.96	116.32	120.30
2	E	677	ASP	OD1-CG-OD2	-7.80	108.48	123.30
5	D	1278	ALA	C-N-CA	-7.68	102.51	121.70
3	F	278	ARG	NE-CZ-NH1	7.59	124.10	120.30
2	A	535	ALA	N-CA-C	7.49	131.23	111.00
3	B	102	GLY	N-CA-C	-7.48	94.41	113.10
1	I	91	DT	O5'-P-OP2	-7.35	99.09	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1088	ARG	NE-CZ-NH2	-7.30	116.65	120.30
3	B	101	GLY	N-CA-C	-7.28	94.89	113.10
3	F	239	ARG	NE-CZ-NH1	7.03	123.81	120.30
3	F	291	LYS	CD-CE-NZ	7.00	127.79	111.70
2	E	733	GLU	CA-C-N	-6.94	101.93	117.20
5	D	1248	ASP	CB-CG-OD2	-6.92	112.07	118.30
5	D	1276	ARG	NE-CZ-NH1	-6.83	116.89	120.30
5	D	1248	ASP	CB-CG-OD1	6.76	124.39	118.30
4	G	1042	ARG	NE-CZ-NH1	-6.72	116.94	120.30
5	H	1496	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	J	276	DT	O5'-P-OP2	-6.62	99.75	105.70
2	E	677	ASP	CB-CA-C	6.58	123.56	110.40
4	C	832	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	J	215	DC	O5'-P-OP2	-6.49	99.86	105.70
1	J	164	DG	C1'-O4'-C4'	-6.48	103.62	110.10
2	E	733	GLU	OE1-CD-OE2	-6.33	115.71	123.30
1	I	4	DA	O5'-P-OP2	6.27	118.22	110.70
1	I	39	DG	C2'-C3'-O3'	6.21	133.08	112.60
2	E	733	GLU	N-CA-C	-6.17	94.35	111.00
4	G	1032	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	E	677	ASP	N-CA-C	-6.04	94.70	111.00
1	I	13	DC	O5'-P-OP1	-6.03	100.28	105.70
3	F	285	ASP	CB-CG-OD2	6.01	123.71	118.30
1	I	124	DA	O5'-P-OP2	-5.99	100.31	105.70
1	I	100	DG	O4'-C1'-C2'	-5.96	101.13	105.90
2	E	640	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	I	134	DG	C5'-C4'-C3'	-5.89	103.50	114.10
1	J	205	DG	C4'-C3'-O3'	5.87	124.38	109.70
1	J	208	DT	O5'-P-OP2	-5.85	100.43	105.70
3	F	221	VAL	CB-CA-C	-5.83	100.33	111.40
2	E	732	GLY	CA-C-N	5.78	129.91	117.20
1	I	85	DA	N9-C1'-C2'	-5.73	101.71	112.60
1	J	166	DT	O5'-P-OP2	5.72	117.56	110.70
4	C	833	LEU	CB-CG-CD1	5.71	120.72	111.00
2	E	735	ALA	CA-C-O	-5.70	108.13	120.10
2	E	733	GLU	CG-CD-OE1	5.69	129.69	118.30
2	E	656	LYS	CD-CE-NZ	5.67	124.75	111.70
1	I	141	DA	O5'-P-OP2	-5.67	100.60	105.70
2	A	438	PRO	N-CA-C	5.59	126.64	112.10
1	J	268	DG	C5'-C4'-C3'	-5.57	104.07	114.10
1	J	248	DA	C5'-C4'-C3'	-5.55	104.10	114.10
1	I	61	DA	O4'-C1'-N9	-5.50	104.15	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1469	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	A	529	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	E	640	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	J	269	DT	O5'-P-OP2	-5.43	100.81	105.70
1	J	147	DA	OP1-P-O3'	5.42	117.12	105.20
1	I	39	DG	C4'-C3'-C2'	5.40	107.96	103.10
4	G	1088	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	J	206	DC	O5'-P-OP1	5.38	117.15	110.70
1	J	276	DT	N1-C1'-C2'	5.35	122.76	112.60
1	J	277	DG	OP2-P-O3'	5.30	116.85	105.20
2	E	678	PHE	CB-CA-C	-5.29	99.81	110.40
1	J	150	DA	O5'-P-OP2	-5.26	100.97	105.70
1	J	186	DG	N9-C1'-C2'	5.25	122.57	112.60
1	I	6	DT	C5'-C4'-O4'	-5.24	99.34	109.30
3	B	29	ILE	CG1-CB-CG2	-5.23	99.89	111.40
2	A	503	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	I	8	DT	O5'-P-OP2	5.23	116.97	110.70
1	J	206	DC	C5'-C4'-C3'	-5.22	104.71	114.10
5	H	1469	ARG	NE-CZ-NH1	5.21	122.90	120.30
4	C	833	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	I	131	DG	O4'-C1'-N9	-5.18	104.37	108.00
4	C	899	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	J	195	DC	C3'-C2'-C1'	-5.17	96.30	102.50
5	D	1251	ILE	CG1-CB-CG2	5.13	122.69	111.40
3	F	249	LEU	CA-CB-CG	-5.13	103.50	115.30
1	I	50	DC	O5'-P-OP2	5.08	116.79	110.70
2	E	735	ALA	CB-CA-C	5.05	117.67	110.10
1	J	213	DA	C3'-C2'-C1'	-5.04	96.46	102.50
4	G	1089	ASN	CB-CA-C	-5.03	100.33	110.40
2	E	683	ARG	NE-CZ-NH1	-5.03	117.78	120.30
2	E	732	GLY	CA-C-O	-5.03	111.55	120.60
5	D	1265	ASP	CB-CG-OD1	-5.02	113.78	118.30
3	F	221	VAL	CG1-CB-CG2	-5.02	102.87	110.90

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	478	PHE	Sidechain
3	B	51	TYR	Sidechain
3	B	72	TYR	Sidechain
3	B	98	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	C	857	TYR	Sidechain
5	D	1237	TYR	Sidechain
5	D	1239	TYR	Sidechain
5	D	1279	HIS	Sidechain
2	E	654	TYR	Sidechain
3	F	298	TYR	Sidechain
4	G	1057	TYR	Sidechain
1	I	102	DA	Sidechain
1	I	116	DC	Sidechain
1	I	120	DT	Sidechain
1	I	124	DA	Sidechain
1	I	129	DC	Sidechain
1	I	131	DG	Sidechain
1	I	137	DG	Sidechain
1	I	145	DA	Sidechain
1	I	39	DG	Sidechain
1	I	41	DA	Sidechain
1	I	44	DC	Sidechain
1	I	48	DT	Sidechain
1	I	49	DC	Sidechain
1	I	51	DA	Sidechain
1	I	59	DG	Sidechain
1	I	67	DA	Sidechain
1	I	85	DA	Sidechain
1	I	99	DA	Sidechain
1	J	147	DA	Sidechain
1	J	149	DC	Sidechain
1	J	150	DA	Sidechain
1	J	151	DA	Sidechain
1	J	153	DA	Sidechain
1	J	158	DC	Sidechain
1	J	161	DG	Sidechain
1	J	180	DT	Sidechain
1	J	185	DG	Sidechain
1	J	186	DG	Sidechain
1	J	192	DG	Sidechain
1	J	196	DC	Sidechain
1	J	206	DC	Sidechain
1	J	214	DG	Sidechain
1	J	221	DT	Sidechain
1	J	228	DA	Sidechain
1	J	238	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	J	243	DG	Sidechain
1	J	247	DC	Sidechain
1	J	276	DT	Sidechain
1	J	278	DC	Sidechain
1	J	280	DG	Sidechain
1	J	287	DA	Sidechain
1	J	288	DT	Sidechain
1	J	292	DT	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2990	0	1651	166	0
1	J	2990	0	1651	154	0
2	A	817	0	858	41	0
2	E	817	0	858	39	0
3	B	633	0	668	39	0
3	F	648	0	688	25	0
4	C	804	0	859	48	0
4	G	827	0	890	56	0
5	D	709	0	727	36	0
5	H	744	0	771	46	0
6	A	9	0	0	1	0
6	B	8	0	0	0	0
6	C	16	0	0	0	0
6	D	9	0	0	1	0
6	E	17	0	0	4	0
6	F	16	0	0	0	0
6	G	13	0	0	1	0
6	H	5	0	0	2	0
6	I	39	0	0	12	0
6	J	39	0	0	5	0
All	All	12150	0	9621	567	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 27.

All (567) 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:E:735:ALA:CA	2:E:735:ALA:CB	1.84	1.52
3:B:84:MET:CE	3:B:84:MET:SD	2.02	1.46
2:E:677:ASP:CG	2:E:677:ASP:CB	1.81	1.46
4:C:850:TYR:OH	5:D:1292:GLN:HG3	1.45	1.16
2:E:677:ASP:OD2	6:E:97:HOH:O	1.70	1.10
4:C:838:ASN:HB3	6:H:156:HOH:O	1.55	1.05
3:B:87:VAL:HG11	3:B:102:GLY:HA3	1.10	1.05
2:A:437:LYS:HB3	2:A:438:PRO:HD3	1.38	1.04
1:I:134:DG:O6	6:I:170:HOH:O	1.78	1.01
4:C:817:ARG:HH22	4:C:831:HIS:CD2	1.78	1.00
1:I:125:DG:N2	1:J:168:DC:N3	2.11	0.98
4:C:902:ILE:HG23	5:D:1258:ILE:HD13	1.47	0.97
1:I:53:DC:N4	1:J:240:DG:H1	1.62	0.97
1:I:124:DA:H1'	1:I:125:DG:OP1	1.64	0.96
2:E:677:ASP:OD1	6:E:97:HOH:O	1.82	0.95
1:I:22:DC:H42	1:J:271:DG:H1	1.02	0.95
4:C:850:TYR:HH	5:D:1292:GLN:HG3	1.22	0.95
1:J:151:DA:H2''	1:J:152:DT:H5'	1.47	0.95
3:B:87:VAL:HG11	3:B:102:GLY:CA	1.97	0.94
1:I:128:DT:H1'	1:I:129:DC:H5'	1.50	0.94
1:I:98:DG:H1	1:J:195:DC:H42	1.01	0.91
4:C:817:ARG:HH22	4:C:831:HIS:HD2	1.12	0.90
1:J:151:DA:H2''	1:J:152:DT:C5'	2.00	0.90
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.51	0.90
1:J:206:DC:H2''	1:J:207:DA:C8	2.06	0.90
1:J:230:DC:H2''	1:J:231:DA:C8	2.06	0.89
1:I:125:DG:H1	1:J:168:DC:H42	0.92	0.88
1:I:53:DC:H42	1:J:240:DG:H1	0.91	0.88
1:I:98:DG:H1	1:J:195:DC:N4	1.70	0.88
4:C:826:PRO:HG3	5:D:1237:TYR:CZ	2.11	0.85
2:A:529:ARG:HA	2:A:534:ARG:HB2	1.59	0.84
2:E:663:ARG:HE	2:E:663:ARG:HA	1.43	0.84
4:G:1026:PRO:HB2	4:G:1029:ARG:HB3	1.60	0.84
1:J:176:DA:OP2	4:G:1032:ARG:HD3	1.78	0.84
1:I:97:DG:N7	6:I:159:HOH:O	2.10	0.83
1:I:125:DG:H1	1:J:168:DC:N4	1.74	0.83
1:J:267:DG:H1'	1:J:268:DG:C8	2.14	0.83
3:B:59:LYS:HE2	3:B:63:GLU:OE2	1.78	0.82
4:G:1026:PRO:HG3	5:H:1437:TYR:CE2	2.14	0.82
1:I:135:DG:H2''	1:I:136:DT:OP2	1.79	0.82
1:I:93:DT:H1'	1:I:94:DG:H5''	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:DG:H1	1:J:235:DC:H42	1.29	0.81
5:H:1489:ARG:HH11	5:H:1489:ARG:HG2	1.47	0.80
2:E:729:ARG:HG3	2:E:735:ALA:HA	1.62	0.80
1:J:249:DG:H1'	1:J:250:DT:H5'	1.62	0.79
1:I:145:DA:H5'	6:A:90:HOH:O	1.82	0.79
4:C:817:ARG:NH2	4:C:831:HIS:HD2	1.79	0.79
1:J:261:DA:H2''	1:J:262:DC:H5''	1.64	0.79
1:J:246:DG:H2''	1:J:247:DC:C5	2.18	0.78
4:G:1079:ILE:HG12	4:G:1082:HIS:CE1	2.19	0.78
1:J:147:DA:H2'	1:J:148:DT:H72	1.64	0.78
1:I:124:DA:C1'	1:I:125:DG:OP1	2.32	0.77
2:A:464:LYS:HE2	2:A:490:MET:HE1	1.65	0.77
4:G:1026:PRO:HG3	5:H:1437:TYR:CZ	2.20	0.77
2:A:463:ARG:O	2:A:466:PRO:HD2	1.85	0.77
1:I:138:DG:H1'	1:I:139:DA:C8	2.20	0.76
2:E:678:PHE:HE2	3:F:267:ARG:HB2	1.50	0.76
5:D:1287:THR:H	5:D:1290:GLU:HG2	1.48	0.76
1:J:286:DT:H2''	1:J:287:DA:O5'	1.86	0.75
4:G:1079:ILE:HG12	4:G:1082:HIS:ND1	2.02	0.75
1:J:280:DG:O6	6:J:321:HOH:O	2.04	0.75
1:I:124:DA:OP1	5:H:1428:LYS:HD2	1.86	0.75
5:H:1483:ARG:HH11	5:H:1483:ARG:HG2	1.49	0.75
1:I:134:DG:C6	6:I:170:HOH:O	2.32	0.74
4:G:1051:LEU:O	4:G:1051:LEU:HD12	1.87	0.74
3:B:84:MET:HE3	3:B:88:TYR:CZ	2.22	0.74
1:J:257:DA:C8	1:J:258:DT:H72	2.22	0.74
1:I:11:DA:H1'	6:I:173:HOH:O	1.87	0.74
4:C:855:LEU:O	4:C:859:THR:HG23	1.88	0.73
3:B:59:LYS:O	3:B:63:GLU:HG3	1.88	0.73
3:B:23:ARG:HH11	3:B:28:GLY:HA2	1.53	0.73
1:J:197:DA:H2''	1:J:198:DT:H5'	1.69	0.73
2:A:437:LYS:HB3	2:A:438:PRO:CD	2.15	0.72
1:I:29:DA:H2''	1:I:30:DA:O5'	1.89	0.72
1:I:128:DT:H1'	1:I:129:DC:C5'	2.20	0.71
1:I:29:DA:H8	1:I:29:DA:H5'	1.54	0.71
1:J:225:DC:H2''	1:J:226:DT:H72	1.73	0.71
5:D:1277:LEU:CD2	5:D:1293:THR:HB	2.21	0.71
2:E:734:ARG:O	2:E:735:ALA:HB3	1.91	0.71
1:I:22:DC:H4'	1:I:22:DC:OP1	1.90	0.71
3:F:259:LYS:O	3:F:263:GLU:HG3	1.91	0.71
1:J:227:DG:H5'	3:B:47:SER:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:310:HOH:O	3:F:245:CYS:SG	2.49	0.70
2:A:528:ARG:C	2:A:534:ARG:HG3	2.12	0.70
1:J:151:DA:H1'	1:J:152:DT:H5''	1.74	0.70
2:E:668:GLN:HG3	2:E:689:VAL:HG11	1.73	0.70
1:J:151:DA:C2'	1:J:152:DT:H5''	2.22	0.69
1:I:26:DC:H1'	1:I:27:DA:C5	2.27	0.69
1:I:29:DA:H5'	1:I:29:DA:C8	2.28	0.69
2:A:520:MET:CE	2:A:522:LYS:HE3	2.23	0.69
5:H:1483:ARG:HG2	5:H:1483:ARG:NH1	2.07	0.69
1:I:7:DA:C2	1:J:287:DA:C2	2.80	0.68
1:J:287:DA:C8	1:J:287:DA:H5''	2.28	0.68
4:C:826:PRO:HG3	5:D:1237:TYR:CE2	2.28	0.68
1:I:57:DA:H2''	1:I:58:DG:C8	2.28	0.68
1:J:174:DA:H2''	1:J:175:DA:H5''	1.75	0.68
1:J:287:DA:H5''	1:J:287:DA:H8	1.58	0.68
1:J:268:DG:H2''	1:J:269:DT:H5'	1.76	0.67
4:G:1017:ARG:HH12	4:G:1031:HIS:CD2	2.12	0.67
4:C:850:TYR:OH	5:D:1292:GLN:CG	2.33	0.67
4:G:1047:ALA:HB3	4:G:1048:PRO:HD3	1.74	0.67
2:E:663:ARG:NE	2:E:663:ARG:HA	2.10	0.67
5:D:1243:LYS:HE2	5:D:1243:LYS:HA	1.77	0.67
1:I:5:DA:H2''	1:I:6:DT:H5'	1.77	0.67
1:J:151:DA:C2'	1:J:152:DT:C5'	2.73	0.66
1:J:181:DA:H2''	1:J:182:DT:OP2	1.94	0.66
1:J:182:DT:H1'	1:J:183:DT:H5'	1.76	0.66
5:H:1498:LEU:O	5:H:1499:LEU:HD23	1.95	0.66
5:D:1277:LEU:HD21	5:D:1293:THR:HB	1.77	0.66
1:J:274:DT:H2''	1:J:275:DC:OP2	1.95	0.66
1:I:82:DA:H3'	2:E:646:VAL:HG21	1.77	0.66
1:J:225:DC:H2''	1:J:226:DT:C7	2.26	0.66
4:G:1037:GLY:HA3	4:G:1039:TYR:CE1	2.31	0.66
1:I:53:DC:H2''	1:I:54:DA:OP2	1.96	0.66
2:A:476:GLN:NE2	2:A:480:THR:HG22	2.10	0.66
1:I:58:DG:H1	1:J:235:DC:N4	1.92	0.66
2:A:534:ARG:O	2:A:535:ALA:HB3	1.95	0.65
1:J:168:DC:H2'	1:J:169:DT:H71	1.78	0.65
2:E:734:ARG:O	2:E:735:ALA:CB	2.44	0.65
1:I:48:DT:OP1	5:H:1428:LYS:NZ	2.27	0.65
4:G:1084:GLN:OE1	4:G:1088:ARG:HD2	1.95	0.65
4:C:850:TYR:CZ	5:D:1292:GLN:HG3	2.32	0.65
2:A:464:LYS:HE2	2:A:490:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:283:DG:H2''	1:J:284:DG:OP2	1.96	0.64
2:E:679:LYS:HB3	2:E:682:LEU:HD11	1.78	0.64
4:C:825:PHE:HZ	4:C:859:THR:HG21	1.63	0.64
4:C:837:GLY:HA3	4:C:839:TYR:CE1	2.33	0.64
4:C:854:VAL:HG22	5:D:1307:ALA:HB1	1.78	0.64
1:I:1:DA:H2'	1:I:2:DT:H71	1.80	0.64
1:I:22:DC:N4	1:J:271:DG:H1	1.84	0.64
4:C:867:GLY:HA3	5:D:1246:HIS:CD2	2.33	0.63
1:I:98:DG:H4'	1:I:99:DA:OP1	1.97	0.63
1:J:147:DA:H2'	1:J:148:DT:C7	2.28	0.63
1:I:36:DT:H1'	1:I:37:DT:H5'	1.81	0.63
1:J:287:DA:H2''	1:J:288:DT:O5'	1.99	0.63
1:I:5:DA:H1'	1:I:6:DT:H5''	1.81	0.63
4:C:831:HIS:CE1	4:C:835:ARG:NH2	2.67	0.62
3:F:278:ARG:NH1	3:F:282:THR:HG23	2.14	0.62
4:G:1079:ILE:HG22	5:H:1452:SER:HB3	1.81	0.62
1:I:94:DG:H5'	1:I:94:DG:H8	1.64	0.62
1:I:10:DC:O2	6:I:177:HOH:O	2.14	0.62
1:I:38:DT:H2''	1:I:39:DG:N7	2.14	0.62
4:G:1032:ARG:HE	4:G:1036:LYS:NZ	1.98	0.62
3:B:74:GLU:O	3:B:75:HIS:C	2.35	0.62
4:G:1017:ARG:HH12	4:G:1031:HIS:HD2	1.48	0.62
4:C:840:ALA:HA	4:G:1038:ASN:OD1	2.00	0.62
6:I:177:HOH:O	1:J:283:DG:N2	2.32	0.62
1:I:130:DT:H2''	1:I:131:DG:N7	2.15	0.62
4:G:1047:ALA:N	4:G:1048:PRO:HD2	2.15	0.62
4:G:1032:ARG:HG2	4:G:1036:LYS:HE3	1.82	0.61
1:J:260:DC:H2''	1:J:261:DA:OP2	2.01	0.61
2:E:678:PHE:O	2:E:679:LYS:HB2	2.01	0.61
1:I:94:DG:H5'	1:I:94:DG:C8	2.36	0.61
4:G:1047:ALA:N	4:G:1048:PRO:CD	2.63	0.61
1:I:114:DC:H4'	1:I:114:DC:OP1	2.00	0.61
1:J:225:DC:C2'	1:J:226:DT:H72	2.31	0.61
5:H:1443:LYS:NZ	5:H:1449:THR:O	2.30	0.61
1:J:147:DA:H2''	1:J:148:DT:O5'	2.00	0.61
3:F:231:LYS:HB3	3:F:232:PRO:CD	2.28	0.61
4:C:825:PHE:CD1	4:C:856:GLU:HB2	2.35	0.61
1:I:119:DT:H2''	1:I:120:DT:H72	1.83	0.61
1:I:114:DC:H2''	1:I:115:DA:O5'	2.01	0.61
2:E:663:ARG:HB3	2:E:666:PRO:HD2	1.83	0.60
1:J:247:DC:H2''	1:J:248:DA:OP2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:DT:H2''	1:J:240:DG:H8	1.67	0.60
1:J:267:DG:N7	6:J:296:HOH:O	2.31	0.60
4:C:825:PHE:CZ	4:C:859:THR:HG21	2.36	0.60
1:I:133:DA:H4'	1:I:134:DG:OP1	2.00	0.60
1:J:267:DG:H1'	1:J:268:DG:N7	2.16	0.60
2:E:675:ALA:O	2:E:678:PHE:HB2	2.01	0.60
1:I:40:DG:O6	6:I:171:HOH:O	2.17	0.59
1:J:173:DA:C2	1:J:174:DA:C2	2.90	0.59
1:J:249:DG:H5''	5:H:1428:LYS:HA	1.84	0.59
1:I:119:DT:H2''	1:I:120:DT:C7	2.33	0.59
4:G:1079:ILE:HB	4:G:1080:PRO:CD	2.33	0.59
1:I:98:DG:N2	1:J:195:DC:N3	2.42	0.59
4:C:838:ASN:CB	6:H:156:HOH:O	2.31	0.58
1:I:133:DA:O5'	1:I:133:DA:H2'	2.03	0.58
4:C:881:ARG:O	4:C:881:ARG:HG3	1.96	0.58
3:F:274:GLU:O	3:F:275:HIS:C	2.35	0.58
1:J:249:DG:P	5:H:1429:SER:OG	2.61	0.58
5:H:1489:ARG:HG2	5:H:1489:ARG:NH1	2.15	0.58
1:J:273:DA:H2''	1:J:274:DT:OP2	2.02	0.58
1:J:277:DG:H5''	4:C:876:THR:HG21	1.84	0.58
4:C:831:HIS:CG	4:C:848:PRO:HG3	2.37	0.58
1:J:168:DC:C2'	1:J:169:DT:H71	2.33	0.58
2:A:483:ARG:O	3:B:80:THR:HA	2.02	0.58
1:J:162:DC:H2''	1:J:163:DA:N7	2.19	0.58
1:I:46:DG:H2''	1:I:47:DC:C6	2.39	0.58
1:J:244:DG:H2''	1:J:245:DA:N7	2.19	0.58
1:I:80:DT:H2''	1:I:81:DG:C8	2.38	0.58
4:C:826:PRO:HB2	4:C:829:ARG:HB3	1.85	0.57
1:J:197:DA:C2'	1:J:198:DT:H5'	2.34	0.57
1:I:94:DG:C2'	1:I:95:DA:H8	2.17	0.57
1:J:234:DC:H4'	1:J:235:DC:OP1	2.03	0.57
1:J:246:DG:H2''	1:J:247:DC:C6	2.38	0.57
2:E:678:PHE:CE2	3:F:267:ARG:HB2	2.38	0.57
1:I:26:DC:H1'	1:I:27:DA:N7	2.19	0.57
1:I:22:DC:H2'	1:I:23:DT:H72	1.86	0.57
5:H:1437:TYR:O	5:H:1441:VAL:HG23	2.04	0.57
5:H:1451:ILE:HG13	5:H:1455:ALA:HB3	1.86	0.57
1:I:17:DA:C8	1:I:17:DA:OP2	2.58	0.57
2:A:452:ARG:O	2:A:456:LYS:HG3	2.04	0.57
4:G:1032:ARG:HE	4:G:1036:LYS:HZ2	1.52	0.57
1:I:70:DG:H2''	6:I:153:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:DG:OP1	5:D:1285:THR:OG1	2.13	0.57
2:A:451:ILE:O	2:A:452:ARG:C	2.42	0.57
1:J:264:DT:C2'	1:J:265:DT:H71	2.34	0.57
1:J:262:DC:C6	1:J:263:DT:H72	2.40	0.57
1:I:140:DT:H1'	1:I:141:DA:C8	2.40	0.56
3:F:292:ARG:NH1	3:F:292:ARG:HB3	2.20	0.56
5:H:1500:PRO:HD2	5:H:1503:LEU:HD23	1.87	0.56
4:G:1013:LYS:O	4:G:1013:LYS:HG3	2.04	0.56
1:I:123:DT:O4	6:I:182:HOH:O	2.18	0.56
1:I:17:DA:H2''	1:I:18:DG:C8	2.40	0.56
4:G:1066:ALA:O	4:G:1069:ALA:HB3	2.05	0.56
2:A:529:ARG:HH11	2:A:529:ARG:HG2	1.70	0.56
2:A:508:ASN:O	2:A:512:ILE:HG13	2.05	0.56
2:E:735:ALA:CB	2:E:735:ALA:N	2.65	0.56
1:I:25:DC:H2''	1:I:26:DC:H5'	1.87	0.56
3:B:44:LYS:HG2	3:B:45:CYS:SG	2.45	0.56
1:J:150:DA:H2''	1:J:151:DA:OP2	2.06	0.56
3:B:50:ILE:HG22	3:B:51:TYR:N	2.20	0.56
1:J:147:DA:HO5'	1:J:147:DA:H8	1.53	0.56
3:B:87:VAL:CG2	3:B:102:GLY:OXT	2.54	0.56
4:G:1025:PHE:CD1	4:G:1056:GLU:HG3	2.41	0.55
3:B:68:ASP:OD2	3:B:92:ARG:NH1	2.36	0.55
1:I:22:DC:H2''	1:I:23:DT:O5'	2.05	0.55
1:J:195:DC:H1'	1:J:196:DC:C6	2.41	0.55
3:F:231:LYS:HE2	3:F:235:ARG:NH2	2.21	0.55
1:J:261:DA:C2'	1:J:262:DC:H5''	2.35	0.55
2:E:735:ALA:CB	2:E:735:ALA:OXT	2.54	0.55
5:H:1498:LEU:C	5:H:1499:LEU:HD23	2.27	0.55
1:J:154:DT:OP1	2:A:449:ARG:HD2	2.07	0.55
2:E:663:ARG:HE	2:E:663:ARG:CA	2.15	0.55
3:B:26:ILE:O	3:B:55:ARG:HD3	2.06	0.55
1:I:94:DG:C2'	1:I:95:DA:C8	2.90	0.55
1:J:203:DA:H2''	1:J:204:DG:C8	2.42	0.55
1:I:31:DG:C2'	1:I:32:DT:H71	2.37	0.55
1:I:89:DC:H2''	1:I:90:DT:H72	1.88	0.54
1:I:5:DA:H2''	1:I:6:DT:C5'	2.36	0.54
1:J:195:DC:H1'	1:J:196:DC:C5	2.42	0.54
5:D:1277:LEU:HD21	5:D:1293:THR:CB	2.37	0.54
5:H:1443:LYS:O	5:H:1447:PRO:HG3	2.07	0.54
1:J:266:DT:H73	6:J:298:HOH:O	2.08	0.54
1:J:151:DA:C1'	1:J:152:DT:H5''	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:529:ARG:HD3	2:E:709:LEU:CD1	2.37	0.54
1:J:281:DG:H1'	1:J:282:DT:H5'	1.90	0.54
3:F:234:ILE:HG22	3:F:234:ILE:O	2.08	0.54
4:G:1025:PHE:HE1	5:H:1441:VAL:HG21	1.72	0.54
5:H:1475:SER:O	5:H:1479:HIS:HD2	1.91	0.54
1:I:129:DC:C6	1:I:130:DT:H72	2.42	0.54
1:J:235:DC:H2''	1:J:236:DT:OP2	2.07	0.54
1:J:210:DT:H2'	1:J:211:DT:H72	1.90	0.54
5:H:1477:LEU:HD11	5:H:1493:THR:CG2	2.38	0.54
1:I:60:DC:H2''	1:I:61:DA:C8	2.43	0.53
1:J:239:DT:H2''	1:J:240:DG:C8	2.43	0.53
2:A:529:ARG:NH1	2:A:529:ARG:HG2	2.24	0.53
1:I:17:DA:OP2	1:I:17:DA:H8	1.92	0.53
1:I:132:DC:H2''	1:I:133:DA:N7	2.22	0.53
1:J:276:DT:H2''	1:J:277:DG:N7	2.23	0.53
1:J:207:DA:H2''	1:J:208:DT:O5'	2.08	0.53
1:J:174:DA:C2'	1:J:175:DA:H5''	2.39	0.53
1:J:224:DG:H2''	1:J:225:DC:C5	2.44	0.53
2:A:520:MET:HE3	2:A:522:LYS:HE3	1.89	0.53
3:B:23:ARG:CG	3:B:24:ASP:N	2.71	0.53
2:A:483:ARG:HB2	3:B:80:THR:HG23	1.89	0.53
5:D:1304:ALA:O	5:D:1308:VAL:HG23	2.08	0.53
1:I:134:DG:H2''	1:I:135:DG:H8	1.72	0.52
4:C:863:LEU:HD13	5:D:1242:LEU:HB2	1.89	0.52
1:J:268:DG:H2''	1:J:269:DT:C5'	2.38	0.52
4:G:1067:GLY:HA3	5:H:1446:HIS:CD2	2.44	0.52
2:E:719:ILE:HG13	3:F:250:ILE:CD1	2.39	0.52
2:A:520:MET:N	2:A:523:ASP:OD2	2.37	0.52
3:B:87:VAL:HG22	3:B:102:GLY:OXT	2.09	0.52
1:I:94:DG:H2''	1:I:95:DA:H8	1.74	0.52
5:D:1243:LYS:CE	5:D:1243:LYS:HA	2.40	0.52
2:E:663:ARG:CB	2:E:666:PRO:HD2	2.39	0.52
1:J:147:DA:C2'	1:J:148:DT:H72	2.37	0.52
1:I:70:DG:H2''	1:I:71:DG:C8	2.44	0.52
2:A:485:GLN:HG3	3:B:82:THR:HA	1.91	0.52
1:I:130:DT:C2	1:I:131:DG:C6	2.98	0.52
1:J:188:DA:H2''	1:J:189:DA:H8	1.75	0.52
1:J:193:DC:O2	1:J:194:DT:C4	2.63	0.52
1:I:84:DC:H2''	1:I:85:DA:C8	2.45	0.52
2:E:678:PHE:HE2	3:F:267:ARG:CB	2.22	0.51
5:D:1287:THR:N	5:D:1290:GLU:HG2	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:DA:H2''	1:I:28:DA:C8	2.45	0.51
3:B:50:ILE:O	3:B:51:TYR:C	2.47	0.51
1:J:255:DA:H8	1:J:255:DA:OP2	1.92	0.51
1:J:249:DG:OP1	5:H:1429:SER:OG	2.29	0.51
3:B:72:TYR:HE2	5:D:1277:LEU:HD13	1.75	0.51
3:F:229:ILE:N	3:F:229:ILE:HD13	2.26	0.51
1:J:193:DC:C2	1:J:194:DT:C4	2.98	0.51
1:I:132:DC:C2	1:I:133:DA:C6	2.99	0.51
1:J:154:DT:P	2:A:449:ARG:HD2	2.50	0.51
5:H:1465:ASP:O	5:H:1466:VAL:C	2.45	0.51
1:J:227:DG:C6	1:J:228:DA:N6	2.79	0.51
3:F:261:PHE:O	3:F:265:VAL:HG23	2.11	0.51
2:A:439:HIS:CD2	2:A:440:ARG:H	2.28	0.51
1:J:215:DC:H5'	2:E:643:PRO:HG3	1.92	0.51
1:J:277:DG:H1'	1:J:278:DC:H5'	1.92	0.51
1:I:88:DC:N4	1:J:204:DG:C6	2.79	0.51
4:G:1056:GLU:O	4:G:1059:THR:HB	2.11	0.50
1:I:114:DC:H2'	1:I:115:DA:C8	2.47	0.50
4:G:1031:HIS:HB2	4:G:1048:PRO:HB3	1.93	0.50
4:C:878:ILE:HA	4:C:882:HIS:ND1	2.26	0.50
1:I:59:DG:OP1	1:I:59:DG:H4'	2.11	0.50
1:I:99:DA:H2''	1:I:100:DG:C8	2.46	0.50
1:J:268:DG:OP1	4:C:829:ARG:NH2	2.40	0.50
1:I:46:DG:H2''	1:I:47:DC:C5	2.46	0.50
4:G:1035:ARG:NH1	4:G:1035:ARG:HG2	2.26	0.50
1:I:133:DA:C2'	1:I:133:DA:O5'	2.59	0.50
1:I:136:DT:H1'	1:I:137:DG:H5'	1.94	0.50
2:A:522:LYS:HG3	2:A:523:ASP:N	2.27	0.50
1:J:188:DA:H2''	1:J:189:DA:C8	2.47	0.50
4:G:1079:ILE:CG1	4:G:1082:HIS:ND1	2.73	0.49
1:J:149:DC:H2''	1:J:150:DA:O5'	2.12	0.49
1:J:169:DT:H1'	1:J:170:DA:H5'	1.93	0.49
1:J:287:DA:H2''	1:J:288:DT:C5'	2.41	0.49
1:I:30:DA:P	4:C:832:ARG:NH1	2.86	0.49
1:I:106:DT:H2''	1:I:107:DC:C6	2.48	0.49
1:I:131:DG:H1'	1:I:132:DC:H5'	1.94	0.49
5:H:1477:LEU:CD1	5:H:1493:THR:HB	2.43	0.49
3:B:84:MET:CE	3:B:88:TYR:CZ	2.95	0.49
1:I:69:DC:H2''	1:I:70:DG:C8	2.47	0.49
1:J:219:DA:C8	1:J:220:DT:H71	2.46	0.49
1:I:58:DG:N2	1:J:235:DC:N3	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:257:DA:H2''	1:J:258:DT:OP2	2.13	0.49
1:J:206:DC:H2''	1:J:207:DA:N7	2.26	0.49
1:I:55:DA:H2''	1:I:56:DA:N7	2.28	0.49
2:A:520:MET:HB3	2:A:521:PRO:HD2	1.94	0.49
1:J:179:DG:H2''	1:J:180:DT:OP2	2.13	0.49
1:I:31:DG:H2'	1:I:32:DT:H71	1.95	0.48
1:J:274:DT:H1'	1:J:275:DC:H5'	1.95	0.48
3:F:234:ILE:CG2	3:F:234:ILE:O	2.61	0.48
1:I:22:DC:H2'	1:I:23:DT:C7	2.44	0.48
3:F:232:PRO:O	3:F:236:ARG:HG3	2.12	0.48
2:E:665:LEU:O	2:E:666:PRO:C	2.47	0.48
5:H:1502:GLU:OE1	5:H:1505:LYS:CD	2.62	0.48
3:F:223:ARG:O	3:F:225:ASN:N	2.46	0.48
1:J:233:DG:H2''	1:J:234:DC:OP2	2.12	0.48
3:B:52:GLU:OE2	3:B:55:ARG:NH1	2.46	0.48
4:G:1033:LEU:O	4:G:1034:LEU:C	2.50	0.48
4:G:1026:PRO:HB2	4:G:1029:ARG:CB	2.38	0.48
1:I:79:DC:C5'	6:I:162:HOH:O	2.61	0.48
1:J:287:DA:C5'	1:J:287:DA:H8	2.25	0.48
1:J:282:DT:H2''	1:J:283:DG:OP2	2.13	0.48
3:B:30:THR:OG1	3:B:32:PRO:HD2	2.13	0.47
1:J:243:DG:C2	1:J:244:DG:C2	3.02	0.47
1:I:19:DA:C4	1:I:20:DT:C5	3.02	0.47
1:I:72:DA:H1'	1:I:73:DA:H5'	1.96	0.47
5:D:1239:TYR:CE2	5:D:1243:LYS:HD2	2.50	0.47
1:J:175:DA:C2'	1:J:176:DA:C8	2.98	0.47
1:I:1:DA:H2''	1:I:2:DT:C6	2.49	0.47
2:E:669:ARG:NH1	6:E:35:HOH:O	2.48	0.47
2:E:642:ARG:O	2:E:643:PRO:C	2.53	0.47
1:I:111:DA:H2'	1:I:112:DT:H72	1.96	0.47
5:D:1274:ALA:O	5:D:1275:SER:C	2.51	0.47
1:I:127:DA:C2	1:I:128:DT:C2	3.03	0.47
1:I:49:DC:C2	1:I:50:DC:C4	3.03	0.47
3:F:292:ARG:CZ	3:F:292:ARG:HB3	2.45	0.47
1:I:124:DA:OP1	5:H:1428:LYS:CD	2.60	0.47
3:F:249:LEU:HA	3:F:249:LEU:HD23	1.49	0.47
5:H:1466:VAL:O	5:H:1467:PHE:C	2.51	0.47
1:I:28:DA:H2''	1:I:29:DA:H5''	1.96	0.47
1:J:267:DG:C2	1:J:268:DG:C6	3.02	0.46
2:A:529:ARG:HA	2:A:534:ARG:CB	2.39	0.46
2:E:708:ASN:O	2:E:712:ILE:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1437:TYR:N	5:H:1437:TYR:CD1	2.82	0.46
1:I:145:DA:H2"	1:I:146:DT:OP2	2.14	0.46
1:I:124:DA:C4'	1:I:125:DG:OP1	2.64	0.46
1:I:54:DA:H2"	1:I:55:DA:C8	2.51	0.46
2:E:663:ARG:NE	2:E:663:ARG:CA	2.75	0.46
5:H:1489:ARG:CG	5:H:1489:ARG:NH1	2.79	0.46
3:B:72:TYR:CE2	5:D:1277:LEU:HD13	2.49	0.46
5:H:1502:GLU:O	5:H:1505:LYS:HB3	2.15	0.46
1:I:112:DT:OP2	4:G:1035:ARG:NH2	2.48	0.46
1:I:128:DT:H2"	1:I:129:DC:O5'	2.14	0.46
4:C:857:TYR:O	4:C:857:TYR:CD1	2.69	0.46
4:C:830:VAL:HG13	5:D:1267:PHE:HE1	1.81	0.46
1:J:165:DA:C2	1:J:166:DT:C2	3.03	0.46
5:D:1279:HIS:C	5:D:1281:ASN:N	2.68	0.46
4:C:850:TYR:OH	5:D:1292:GLN:NE2	2.49	0.46
1:J:249:DG:OP2	5:H:1429:SER:OG	2.33	0.46
1:J:227:DG:C5'	3:B:47:SER:HA	2.43	0.46
4:G:1088:ARG:HG2	4:G:1088:ARG:H	1.48	0.46
1:J:245:DA:H2"	1:J:246:DG:C8	2.51	0.45
1:I:29:DA:C2'	1:I:30:DA:C8	2.99	0.45
4:G:1071:ARG:O	4:G:1073:ASN:N	2.49	0.45
1:J:219:DA:C8	1:J:220:DT:C7	2.99	0.45
5:H:1459:MET:O	5:H:1463:VAL:HG23	2.16	0.45
2:E:664:LYS:HD3	6:E:157:HOH:O	2.16	0.45
2:A:525:GLN:O	2:A:534:ARG:HD3	2.16	0.45
4:C:825:PHE:CG	4:C:856:GLU:HB2	2.50	0.45
1:I:122:DG:H4'	5:H:1430:ARG:HB3	1.97	0.45
1:I:131:DG:H2"	1:I:132:DC:O5'	2.15	0.45
1:I:69:DC:H42	1:J:224:DG:H1	1.63	0.45
4:G:1100:VAL:CG1	4:G:1101:THR:N	2.78	0.45
1:I:41:DA:H2"	1:I:42:DA:O5'	2.17	0.45
5:D:1277:LEU:HD21	5:D:1293:THR:CG2	2.47	0.45
1:J:255:DA:C6	1:J:256:DA:C6	3.04	0.45
5:D:1279:HIS:ND1	6:D:107:HOH:O	2.36	0.45
1:I:136:DT:H2"	1:I:137:DG:O5'	2.16	0.45
1:J:249:DG:P	5:H:1429:SER:HG	2.39	0.45
1:I:26:DC:H4'	1:I:27:DA:OP1	2.17	0.45
1:I:98:DG:C4'	1:I:99:DA:OP1	2.64	0.45
4:C:832:ARG:NH2	5:D:1232:GLU:OE2	2.50	0.45
3:B:26:ILE:HG23	3:B:27:GLN:N	2.32	0.45
2:A:467:PHE:CZ	2:A:493:GLN:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:149:DC:H2''	1:J:150:DA:C8	2.52	0.45
1:I:63:DG:H2''	1:I:64:DT:OP2	2.16	0.45
3:B:23:ARG:HG2	3:B:24:ASP:N	2.30	0.45
4:G:1067:GLY:O	4:G:1068:ASN:C	2.55	0.45
1:I:133:DA:H2''	1:I:134:DG:C8	2.52	0.45
1:I:97:DG:C5	1:I:98:DG:C6	3.05	0.45
1:I:138:DG:H2'	1:I:138:DG:O5'	2.17	0.45
1:I:111:DA:H2'	1:I:112:DT:C7	2.47	0.45
1:J:248:DA:H2''	1:J:249:DG:C8	2.52	0.45
1:I:28:DA:C2'	1:I:29:DA:H5''	2.46	0.45
1:I:141:DA:C2	1:J:153:DA:C2	3.05	0.44
1:I:94:DG:H2''	1:I:95:DA:C8	2.52	0.44
1:I:118:DT:H2'	1:I:119:DT:H71	1.98	0.44
1:J:204:DG:H4'	1:J:205:DG:OP1	2.17	0.44
1:J:190:DC:H2''	1:J:191:DT:O5'	2.16	0.44
3:B:29:ILE:HG23	3:B:29:ILE:HD12	1.60	0.44
3:B:78:ARG:HH22	3:B:85:ASP:CG	2.20	0.44
1:I:49:DC:H1'	1:I:50:DC:C6	2.53	0.44
1:J:149:DC:C2'	1:J:150:DA:C8	3.00	0.44
1:I:119:DT:C2'	1:I:120:DT:H72	2.46	0.44
1:I:89:DC:H2''	1:I:90:DT:C7	2.47	0.44
4:G:1113:SER:OG	4:G:1114:VAL:N	2.49	0.44
1:I:48:DT:H2'	1:I:49:DC:C5	2.52	0.44
4:C:879:ILE:HG12	4:C:882:HIS:CE1	2.52	0.44
1:J:281:DG:H2''	1:J:282:DT:O5'	2.17	0.44
4:C:881:ARG:NH2	4:C:907:VAL:O	2.43	0.44
5:H:1451:ILE:CG1	5:H:1455:ALA:HB3	2.48	0.44
1:I:34:DT:H2''	1:I:35:DA:O5'	2.18	0.44
1:I:134:DG:C5	6:I:170:HOH:O	2.64	0.44
4:G:1084:GLN:O	4:G:1088:ARG:HG2	2.17	0.44
3:B:31:LYS:N	3:B:32:PRO:CD	2.80	0.44
5:H:1481:ASN:O	5:H:1482:LYS:C	2.56	0.44
1:I:55:DA:H2''	1:I:56:DA:C8	2.53	0.44
5:H:1451:ILE:HG13	5:H:1455:ALA:CB	2.47	0.44
4:G:1026:PRO:CG	5:H:1437:TYR:CZ	2.98	0.44
5:H:1477:LEU:HD11	5:H:1493:THR:HB	1.98	0.44
2:A:458:THR:HG22	4:G:1106:GLY:HA3	1.99	0.44
1:J:176:DA:P	4:G:1032:ARG:HH11	2.41	0.44
1:J:286:DT:C2'	1:J:287:DA:O5'	2.62	0.44
1:I:28:DA:H2''	1:I:29:DA:C5'	2.48	0.44
3:F:234:ILE:HD12	3:F:251:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1112:GLN:HB2	4:G:1115:LEU:HD12	2.00	0.44
4:C:817:ARG:NH2	4:C:831:HIS:CD2	2.58	0.44
2:E:665:LEU:HB3	2:E:666:PRO:HD3	2.00	0.44
1:J:147:DA:C2'	1:J:148:DT:C7	2.94	0.44
1:I:27:DA:H1'	1:I:28:DA:O4'	2.17	0.44
4:G:1092:GLU:HB3	5:H:1503:LEU:HD22	1.99	0.44
1:J:264:DT:H2''	1:J:265:DT:H71	1.99	0.44
3:B:26:ILE:CG2	3:B:27:GLN:N	2.78	0.44
1:I:111:DA:C8	1:I:112:DT:H72	2.53	0.44
2:A:500:LEU:HD23	2:A:500:LEU:HA	1.79	0.44
1:I:104:DT:H2''	1:I:105:DT:C6	2.53	0.44
1:I:121:DG:OP2	1:I:121:DG:H8	2.00	0.44
1:I:129:DC:C2'	1:I:130:DT:H72	2.48	0.43
4:C:847:ALA:O	4:C:848:PRO:C	2.54	0.43
1:I:22:DC:C6	1:I:23:DT:H72	2.53	0.43
2:A:454:TYR:CZ	3:B:36:ARG:HG2	2.53	0.43
1:J:189:DA:C6	1:J:190:DC:N4	2.86	0.43
4:C:817:ARG:HH22	4:C:831:HIS:CG	2.32	0.43
1:I:93:DT:H1'	1:I:94:DG:C5'	2.41	0.43
1:I:38:DT:O3'	1:I:39:DG:C8	2.72	0.43
4:C:881:ARG:O	4:C:885:LEU:HG	2.19	0.43
4:C:826:PRO:CB	4:C:829:ARG:HB3	2.47	0.43
4:G:1051:LEU:HD21	5:H:1467:PHE:CE1	2.54	0.43
2:E:724:ILE:O	2:E:728:ARG:HG3	2.18	0.43
2:A:463:ARG:C	2:A:466:PRO:HD2	2.38	0.43
1:I:30:DA:P	4:C:832:ARG:HH11	2.42	0.43
1:I:124:DA:C6	1:I:125:DG:C6	3.07	0.43
2:A:520:MET:HB3	2:A:521:PRO:CD	2.49	0.43
2:A:479:LYS:HD2	3:B:74:GLU:HG2	1.99	0.43
5:D:1299:LEU:HB2	5:D:1304:ALA:HB2	2.00	0.43
5:D:1237:TYR:O	5:D:1241:VAL:HG23	2.18	0.43
1:I:2:DT:H2''	1:I:3:DC:OP2	2.18	0.43
3:B:82:THR:O	3:B:83:ALA:C	2.54	0.43
4:G:1100:VAL:HG12	4:G:1101:THR:N	2.33	0.43
2:A:469:ARG:HD2	3:B:25:ASN:OD1	2.18	0.43
5:H:1502:GLU:O	5:H:1503:LEU:C	2.54	0.43
1:J:150:DA:C2'	1:J:151:DA:OP2	2.66	0.43
5:H:1436:ILE:O	5:H:1440:LYS:HG3	2.19	0.43
1:I:93:DT:C1'	1:I:94:DG:H5''	2.40	0.43
1:J:227:DG:C2	1:J:228:DA:C6	3.07	0.43
3:B:76:ALA:O	3:B:77:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:831:HIS:HA	4:C:848:PRO:HB3	2.00	0.43
4:C:833:LEU:HA	4:C:833:LEU:HD23	1.68	0.43
2:A:528:ARG:HB3	2:A:534:ARG:HG3	2.01	0.42
2:A:479:LYS:HB3	2:A:482:LEU:HD11	2.00	0.42
1:I:114:DC:C2'	1:I:115:DA:C8	3.01	0.42
4:G:1035:ARG:HH11	4:G:1035:ARG:HG2	1.83	0.42
5:D:1276:ARG:HH11	5:D:1276:ARG:HD2	1.64	0.42
1:I:39:DG:H4'	4:C:842:ARG:NH1	2.34	0.42
1:J:253:DC:H4'	1:J:254:DC:OP1	2.18	0.42
4:G:1090:ASP:O	4:G:1091:GLU:C	2.57	0.42
1:J:284:DG:H2''	1:J:285:DA:OP2	2.19	0.42
1:J:190:DC:H1'	1:J:191:DT:H5'	2.02	0.42
1:J:193:DC:H2''	1:J:194:DT:H72	2.02	0.42
2:E:721:PRO:HG2	3:F:249:LEU:HB3	2.01	0.42
4:G:1018:SER:O	4:G:1023:LEU:N	2.38	0.42
4:G:1055:LEU:HA	4:G:1055:LEU:HD23	1.79	0.42
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.83	0.42
1:I:124:DA:H8	1:I:124:DA:H2'	1.74	0.42
1:J:267:DG:O6	6:J:296:HOH:O	2.21	0.42
1:J:261:DA:H2'	1:J:261:DA:O5'	2.19	0.42
1:I:11:DA:C4	1:I:12:DC:C5	3.06	0.42
1:I:119:DT:H4'	1:I:120:DT:OP1	2.20	0.42
1:I:17:DA:C2	1:I:18:DG:C2	3.07	0.42
1:I:126:DA:C6	1:I:127:DA:C6	3.08	0.42
1:J:152:DT:H2''	1:J:153:DA:C8	2.54	0.42
1:J:214:DG:H2''	1:J:215:DC:C6	2.54	0.42
5:D:1276:ARG:HB3	5:D:1280:TYR:CZ	2.55	0.42
1:I:1:DA:H2'	1:I:2:DT:C7	2.47	0.42
5:D:1246:HIS:HB3	5:D:1249:THR:OG1	2.19	0.42
2:A:453:ARG:O	2:A:456:LYS:HB2	2.19	0.42
4:G:1047:ALA:HB3	4:G:1048:PRO:CD	2.47	0.42
5:D:1239:TYR:O	5:D:1243:LYS:HG2	2.19	0.42
2:E:669:ARG:HD2	3:F:225:ASN:OD1	2.20	0.42
2:E:675:ALA:O	2:E:678:PHE:CB	2.67	0.41
1:I:118:DT:C2'	1:I:119:DT:H71	2.50	0.41
1:I:111:DA:H2''	1:I:112:DT:O5'	2.19	0.41
3:B:30:THR:CB	3:B:32:PRO:HD2	2.50	0.41
1:J:185:DG:C2	1:J:186:DG:C2	3.08	0.41
4:G:1037:GLY:O	4:G:1038:ASN:C	2.54	0.41
1:J:170:DA:H2''	1:J:171:DC:C5	2.55	0.41
1:I:113:DA:C6	1:I:114:DC:N4	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:476:GLN:HE22	2:A:480:THR:HG22	1.81	0.41
1:I:88:DC:N4	1:J:204:DG:O6	2.54	0.41
2:A:520:MET:O	2:A:521:PRO:C	2.58	0.41
2:E:728:ARG:O	2:E:729:ARG:C	2.59	0.41
1:J:175:DA:H2''	1:J:176:DA:C8	2.56	0.41
1:J:287:DA:C8	1:J:287:DA:C5'	3.01	0.41
2:E:729:ARG:O	2:E:730:ILE:C	2.56	0.41
5:H:1436:ILE:HG13	5:H:1437:TYR:CE1	2.56	0.41
4:G:1068:ASN:O	4:G:1071:ARG:N	2.54	0.41
1:I:1:DA:C2'	1:I:2:DT:H71	2.49	0.41
4:G:1073:ASN:O	4:G:1074:LYS:HB2	2.20	0.41
1:I:89:DC:N4	1:J:203:DA:N6	2.68	0.41
1:J:192:DG:H2''	1:J:193:DC:O5'	2.19	0.41
1:I:19:DA:C2	1:I:20:DT:C2	3.09	0.41
1:I:104:DT:C2'	1:I:105:DT:H72	2.50	0.41
1:I:121:DG:N7	6:I:147:HOH:O	2.37	0.41
4:C:893:LEU:O	4:C:897:LEU:HB2	2.20	0.41
3:F:284:MET:HE3	3:F:288:TYR:CZ	2.56	0.41
4:G:1068:ASN:O	4:G:1069:ALA:C	2.59	0.40
1:J:184:DT:H2''	1:J:185:DG:N7	2.36	0.40
4:C:916:LEU:HB3	4:C:917:PRO:CD	2.51	0.40
1:J:196:DC:H2''	1:J:197:DA:C8	2.56	0.40
4:G:1090:ASP:HB2	6:G:150:HOH:O	2.20	0.40
3:F:226:ILE:HG13	3:F:255:ARG:HB3	2.03	0.40
1:I:135:DG:C2'	1:I:136:DT:OP2	2.54	0.40
1:J:262:DC:H2'	1:J:263:DT:C7	2.51	0.40
3:B:74:GLU:O	3:B:76:ALA:N	2.54	0.40
2:E:709:LEU:HD23	2:E:709:LEU:HA	1.61	0.40
5:D:1277:LEU:HD21	5:D:1293:THR:HG21	2.03	0.40
1:J:193:DC:O2	1:J:194:DT:N3	2.55	0.40
1:I:112:DT:P	4:G:1035:ARG:HH22	2.44	0.40
4:C:916:LEU:HB3	4:C:917:PRO:HD2	2.03	0.40
1:J:283:DG:C6	1:J:284:DG:C6	3.10	0.40
1:I:114:DC:H42	1:J:179:DG:H1	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	97/135 (72%)	91 (94%)	4 (4%)	2 (2%)	9	32
2	E	97/135 (72%)	93 (96%)	0	4 (4%)	3	14
3	B	78/102 (76%)	75 (96%)	3 (4%)	0	100	100
3	F	80/102 (78%)	76 (95%)	3 (4%)	1 (1%)	15	46
4	C	102/129 (79%)	93 (91%)	8 (8%)	1 (1%)	19	54
4	G	105/129 (81%)	97 (92%)	7 (7%)	1 (1%)	19	54
5	D	89/125 (71%)	84 (94%)	5 (6%)	0	100	100
5	H	93/125 (74%)	83 (89%)	7 (8%)	3 (3%)	5	20
All	All	741/982 (76%)	692 (93%)	37 (5%)	12 (2%)	12	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	224	ASP
2	E	678	PHE
2	E	733	GLU
5	H	1430	ARG
5	H	1501	GLY
2	E	734	ARG
4	G	1072	ASP
2	A	438	PRO
2	A	440	ARG
2	E	679	LYS
5	H	1521	ALA
4	C	917	PRO

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	86/111 (78%)	80 (93%)	6 (7%)	19	47
2	E	86/111 (78%)	78 (91%)	8 (9%)	11	32
3	B	65/78 (83%)	64 (98%)	1 (2%)	72	92
3	F	67/78 (86%)	65 (97%)	2 (3%)	48	83
4	C	83/100 (83%)	76 (92%)	7 (8%)	14	37
4	G	85/100 (85%)	78 (92%)	7 (8%)	14	39
5	D	77/105 (73%)	73 (95%)	4 (5%)	29	64
5	H	81/105 (77%)	75 (93%)	6 (7%)	17	44
All	All	630/788 (80%)	589 (94%)	41 (6%)	21	52

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	438	PRO
2	A	448	LEU
2	A	459	GLU
2	A	486	SER
2	A	533	GLU
2	A	534	ARG
3	B	80	THR
4	C	829	ARG
4	C	831	HIS
4	C	859	THR
4	C	876	THR
4	C	881	ARG
4	C	909	PRO
4	C	914	VAL
5	D	1247	PRO
5	D	1279	HIS
5	D	1285	THR
5	D	1295	VAL
2	E	659	GLU
2	E	663	ARG
2	E	666	PRO
2	E	678	PHE
2	E	703	LEU

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Mol	Chain	Res	Type
2	E	705	GLU
2	E	721	PRO
2	E	734	ARG
3	F	232	PRO
3	F	247	SER
4	G	1038	ASN
4	G	1041	GLU
4	G	1073	ASN
4	G	1080	PRO
4	G	1088	ARG
4	G	1109	PRO
4	G	1117	PRO
5	H	1429	SER
5	H	1431	LYS
5	H	1433	SER
5	H	1452	SER
5	H	1453	SER
5	H	1483	ARG

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

Mol	Chain	Res	Type
2	A	439	HIS
2	A	476	GLN
4	C	831	HIS
5	D	1292	GLN
3	F	293	GLN
4	G	1031	HIS
4	G	1038	ASN
5	H	1479	HIS
5	H	1492	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.