Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID	:	1P3I
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	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

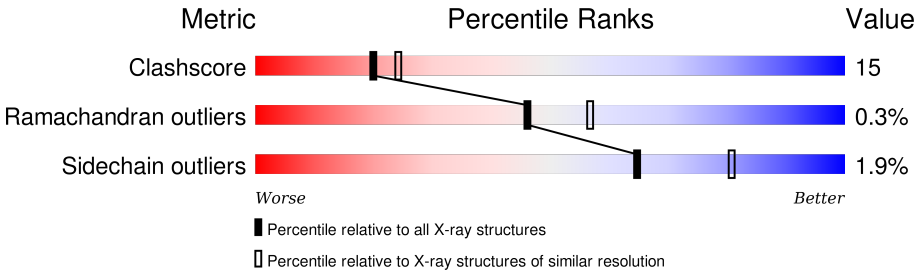
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 <=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	51% 45% •
1	J	146	56% 42% •
2	A	135	61% 10% • 27%
2	E	135	61% 15% • 23%
3	B	102	67% 10% • 23%
3	F	102	66% 11% • 23%
4	C	129	63% 16% • 20%

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Mol	Chain	Length	Quality of chain
4	G	129	65% 15% 19%
5	D	125	62% 14% 24%
5	H	125	64% 10% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12260 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	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
2	E	104	Total	C	N	O	S	0	0	0
			852	535	164	150	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	79	Total	C	N	O	S	0	0	0
			626	395	120	110	1			
3	F	79	Total	C	N	O	S	0	0	0
			626	395	120	110	1			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	G	104	Total	C	N	O	0	0	0
			804	507	157	140			

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	95	Total	C	N	O	S	0	0	0
			744	468	134	140	2			
5	H	94	Total	C	N	O	S	0	0	0
			735	462	132	139	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	27	Total O 27 27	0	0
6	B	17	Total O 17 17	0	0
6	C	30	Total O 30 30	0	0
6	D	21	Total O 21 21	0	0
6	E	41	Total O 41 41	0	0
6	F	30	Total O 30 30	0	0
6	G	27	Total O 27 27	0	0
6	H	9	Total O 9 9	0	0
6	I	41	Total O 41 41	0	0
6	J	47	Total O 47 47	0	0

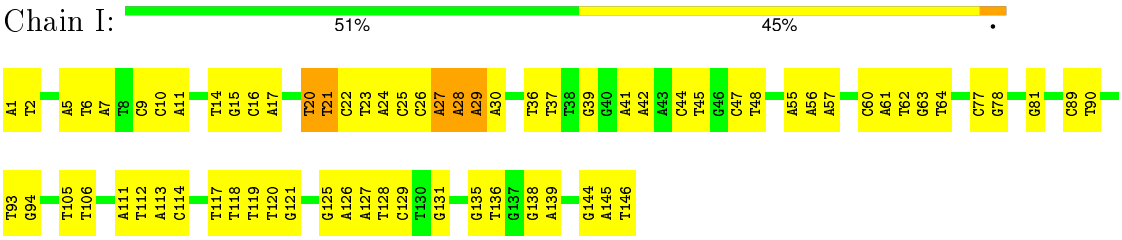
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

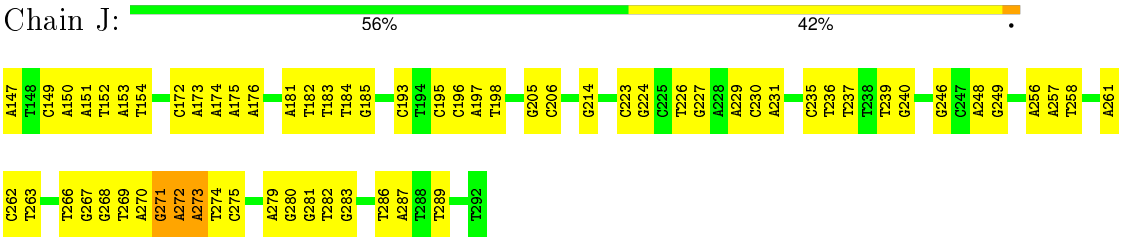
- Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment

Chain I:



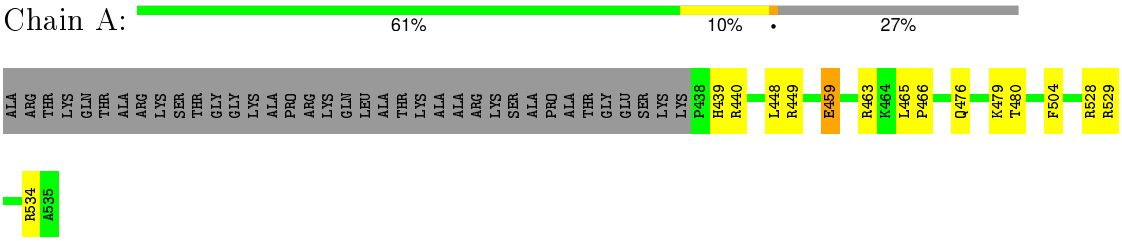
- Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment

Chain J:



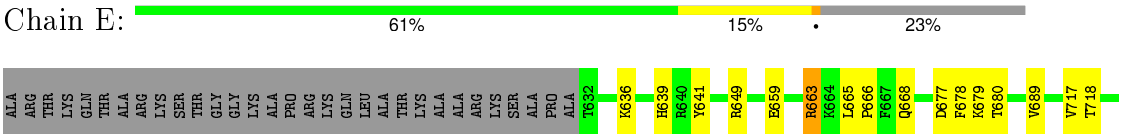
- Molecule 2: Histone H3

Chain A:



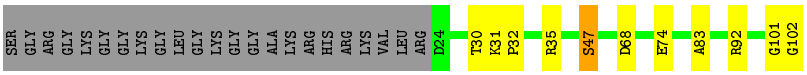
- Molecule 2: Histone H3

Chain E:



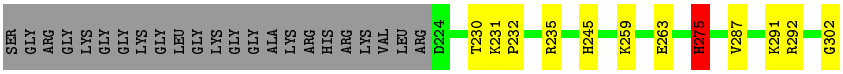
- Molecule 3: Histone H4

Chain B:



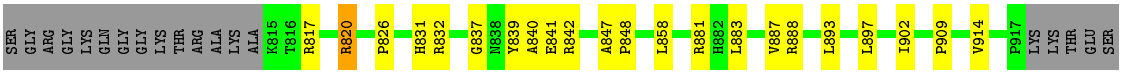
- Molecule 3: Histone H4

Chain F:



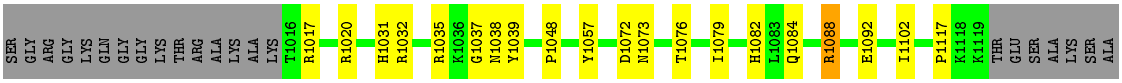
- Molecule 4: Histone H2A

Chain C:



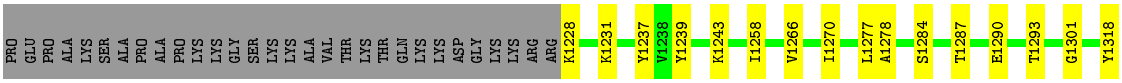
- Molecule 4: Histone H2A

Chain G:



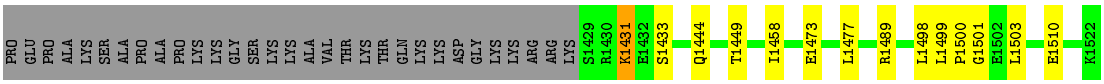
- Molecule 5: Histone H2B

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
ARG
LYS
S1429
R1430
K1431
E1432
S1433
Q1444
T1449
I1458
E1473
L1477
R1489
L1498
L1499
P1500
G1501
E1502
L1503
E1510
K1522

4 Data and refinement statistics (i)

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	106.61Å 109.75Å 182.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.0 (100.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12260	wwPDB-VP
Average B, all atoms (Å^2)	72.0	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	0.56	3/3354 (0.1%)	1.09	24/5175 (0.5%)
1	J	0.55	2/3354 (0.1%)	0.86	8/5175 (0.2%)
2	A	0.71	4/820 (0.5%)	0.72	2/1099 (0.2%)
2	E	0.68	0/864	0.73	0/1157
3	B	0.60	0/634	0.70	0/849
3	F	0.80	2/634 (0.3%)	0.97	4/849 (0.5%)
4	C	0.62	0/805	0.71	0/1088
4	G	0.52	0/814	0.64	0/1099
5	D	0.63	0/755	0.67	0/1013
5	H	0.53	0/746	0.65	0/1002
All	All	0.60	11/12780 (0.1%)	0.88	38/18506 (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	1
1	J	0	1
3	F	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	272	DA	C5-C6	-12.14	1.30	1.41
1	I	21	DT	C2-O2	-9.22	1.15	1.22
2	A	504	PHE	CD1-CE1	-6.83	1.25	1.39
1	I	21	DT	N1-C2	-6.59	1.32	1.38
2	A	504	PHE	CB-CG	5.68	1.61	1.51
2	A	504	PHE	CG-CD2	-5.48	1.30	1.38
1	J	271	DG	O3'-P	-5.45	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	275	HIS	CB-CG	5.28	1.59	1.50
2	A	504	PHE	CE1-CZ	-5.20	1.27	1.37
3	F	275	HIS	CG-CD2	5.09	1.44	1.35
1	I	20	DT	C5-C6	-5.03	1.30	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	28	DA	O5'-P-OP1	-26.42	78.99	110.70
1	J	273	DA	O5'-P-OP2	-23.07	83.01	110.70
1	I	28	DA	OP2-P-O3'	-22.68	55.30	105.20
1	I	28	DA	OP1-P-O3'	20.47	150.24	105.20
1	I	28	DA	O5'-P-OP2	-16.13	91.18	105.70
1	I	27	DA	OP2-P-O3'	-15.71	70.64	105.20
1	I	27	DA	OP1-P-O3'	-15.59	70.90	105.20
3	F	275	HIS	CB-CG-ND1	-13.19	90.21	123.20
1	J	273	DA	O5'-P-OP1	-12.31	94.62	105.70
1	I	20	DT	C3'-C2'-C1'	-11.64	88.53	102.50
1	I	20	DT	OP1-P-O3'	-9.97	83.26	105.20
3	F	275	HIS	CG-ND1-CE1	7.93	119.30	108.20
1	I	27	DA	O3'-P-O5'	7.71	118.64	104.00
1	I	20	DT	OP2-P-O3'	7.70	122.13	105.20
1	I	20	DT	C1'-O4'-C4'	-7.53	102.57	110.10
1	I	16	DC	O5'-P-OP1	-7.47	98.98	105.70
3	F	275	HIS	CB-CG-CD2	7.17	153.01	130.80
1	I	21	DT	N1-C2-N3	7.05	118.83	114.60
1	I	21	DT	N1-C2-O2	-6.75	117.70	123.10
1	J	272	DA	C5'-C4'-C3'	-6.74	101.97	114.10
1	I	28	DA	OP1-P-OP2	6.16	128.84	119.60
3	F	275	HIS	ND1-CG-CD2	-6.08	97.49	106.00
1	J	272	DA	OP2-P-O3'	5.89	118.17	105.20
1	I	20	DT	C6-N1-C1'	-5.88	111.58	120.40
1	J	271	DG	C3'-C2'-C1'	-5.70	95.67	102.50
1	J	272	DA	OP1-P-O3'	5.67	117.69	105.20
1	I	20	DT	O4'-C1'-N1	5.56	111.89	108.00
2	A	504	PHE	CB-CG-CD1	5.47	124.63	120.80
1	J	272	DA	O5'-P-OP2	5.45	117.24	110.70
1	I	27	DA	C5'-C4'-C3'	-5.43	104.32	114.10
2	A	504	PHE	CD1-CE1-CZ	5.42	126.61	120.10
1	I	21	DT	O3'-P-O5'	-5.33	93.87	104.00
1	I	20	DT	C2'-C3'-O3'	-5.32	95.03	112.60
1	I	21	DT	OP2-P-O3'	5.31	116.89	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	193	DC	C3'-C2'-C1'	-5.31	96.12	102.50
1	I	21	DT	C6-N1-C2	-5.27	118.66	121.30
1	I	29	DA	OP1-P-OP2	-5.21	111.79	119.60
1	I	20	DT	C4'-C3'-C2'	-5.11	98.50	103.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	275	HIS	Sidechain
1	I	131	DG	Sidechain
1	J	214	DG	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	111	0
1	J	2990	0	1651	93	0
2	A	808	0	846	17	0
2	E	852	0	892	24	0
3	B	626	0	657	9	0
3	F	626	0	657	16	0
4	C	795	0	846	36	0
4	G	804	0	859	26	0
5	D	744	0	771	22	0
5	H	735	0	758	15	0
6	A	27	0	0	0	0
6	B	17	0	0	1	0
6	C	30	0	0	6	0
6	D	21	0	0	1	0
6	E	41	0	0	8	0
6	F	30	0	0	1	0
6	G	27	0	0	4	0
6	H	9	0	0	3	0
6	I	41	0	0	4	0
6	J	47	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12260	0	9588	316	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 15.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:DT:O2	1:J:272:DA:N1	1.58	1.36
1:I:21:DT:H3	1:J:272:DA:N6	1.22	1.32
4:C:820:ARG:HB3	4:C:820:ARG:NH1	1.53	1.21
1:J:261:DA:H2"	1:J:262:DC:H5"	1.25	1.17
4:C:820:ARG:HH11	4:C:820:ARG:CB	1.62	1.13
2:E:678:PHE:HB3	6:E:159:HOH:O	1.51	1.09
2:E:735:ALA:HB2	6:E:58:HOH:O	1.51	1.08
4:C:887:VAL:CG1	6:C:287:HOH:O	2.02	1.07
1:I:5:DA:H2"	1:I:6:DT:H5"	1.33	1.04
4:C:887:VAL:CB	6:C:287:HOH:O	2.07	1.02
2:E:725:GLN:HG2	2:E:734:ARG:HH12	1.27	0.99
4:C:887:VAL:HB	6:C:287:HOH:O	1.62	0.99
4:C:820:ARG:NH2	5:D:1318:TYR:O	1.95	0.99
1:J:174:DA:H2"	1:J:175:DA:H5"	1.47	0.97
1:I:27:DA:H1'	1:I:28:DA:P	2.06	0.95
4:G:1017:ARG:HH12	4:G:1031:HIS:HD2	1.17	0.93
4:G:1088:ARG:NH1	6:G:286:HOH:O	2.04	0.89
1:I:27:DA:H1'	1:I:28:DA:OP1	1.72	0.89
2:E:729:ARG:HG3	6:E:142:HOH:O	1.73	0.87
4:G:1017:ARG:HH12	4:G:1031:HIS:CD2	1.91	0.87
3:F:275:HIS:HE1	5:H:1489:ARG:NH1	1.72	0.86
1:I:21:DT:O2	1:J:272:DA:C6	2.29	0.85
1:J:270:DA:OP1	5:D:1228:LYS:HD2	1.77	0.84
1:I:27:DA:C2'	1:I:28:DA:OP1	2.24	0.83
4:C:820:ARG:NH1	5:D:1318:TYR:CD1	2.47	0.83
4:C:887:VAL:HG12	6:C:287:HOH:O	1.67	0.83
1:I:61:DA:H2"	1:I:62:DT:H5'	1.60	0.82
1:J:261:DA:C2'	1:J:262:DC:H5"	2.07	0.81
4:C:902:ILE:HG23	5:D:1258:ILE:HD13	1.60	0.81
4:C:820:ARG:CB	4:C:820:ARG:NH1	2.28	0.81
1:J:229:DA:H2"	1:J:230:DC:H5'	1.60	0.81
1:I:27:DA:C1'	1:I:28:DA:P	2.69	0.81
1:I:5:DA:C2'	1:I:6:DT:H5"	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:735:ALA:CB	6:E:58:HOH:O	2.20	0.81
2:E:729:ARG:CG	6:E:142:HOH:O	2.26	0.81
4:G:1088:ARG:CZ	6:G:286:HOH:O	2.29	0.80
1:I:47:DC:H2"	1:I:48:DT:H71	1.64	0.80
2:E:663:ARG:HG3	6:F:319:HOH:O	1.81	0.79
1:I:27:DA:C1'	1:I:28:DA:OP1	2.29	0.79
4:C:820:ARG:HH11	4:C:820:ARG:HB2	1.46	0.79
4:C:887:VAL:HG11	4:C:897:LEU:HD12	1.66	0.78
1:I:9:DC:H2"	1:I:10:DC:H5'	1.66	0.77
1:I:5:DA:H2"	1:I:6:DT:C5'	2.14	0.77
1:I:89:DC:H2"	1:I:90:DT:H72	1.67	0.77
1:I:20:DT:O2	1:I:21:DT:H5'	1.85	0.76
1:I:28:DA:C2	1:I:29:DA:N3	2.54	0.75
2:E:725:GLN:HG2	2:E:734:ARG:NH1	2.00	0.75
1:I:81:DG:H5'	6:I:169:HOH:O	1.85	0.74
1:I:21:DT:N3	1:J:272:DA:N6	1.97	0.73
1:I:5:DA:C2'	6:I:170:HOH:O	2.36	0.72
3:B:31:LYS:HE2	3:B:35:ARG:HH22	1.52	0.72
1:I:21:DT:H2"	1:I:22:DC:H5'	1.72	0.71
1:I:10:DC:H42	1:J:283:DG:H1	1.39	0.71
1:J:274:DT:H1'	1:J:275:DC:H5'	1.73	0.71
2:A:529:ARG:HA	2:A:534:ARG:HB2	1.72	0.71
1:I:60:DC:H5"	2:A:463:ARG:NH1	2.05	0.70
4:C:817:ARG:HH22	4:C:831:HIS:CD2	2.09	0.70
1:I:27:DA:H2"	1:I:28:DA:OP1	1.91	0.70
1:J:267:DG:N7	6:J:322:HOH:O	2.25	0.69
1:I:21:DT:C2	1:J:272:DA:N6	2.54	0.69
1:I:28:DA:C2	1:I:29:DA:C4	2.81	0.69
5:D:1243:LYS:HE2	5:D:1243:LYS:HA	1.73	0.69
1:I:41:DA:H2"	1:I:42:DA:H5'	1.75	0.68
1:J:246:DG:N7	6:J:321:HOH:O	2.25	0.68
1:J:151:DA:H2"	1:J:152:DT:C5'	2.23	0.68
1:I:39:DG:H4'	4:C:842:ARG:HH11	1.59	0.67
1:I:21:DT:C2	1:J:272:DA:N1	2.55	0.67
3:B:31:LYS:HE2	3:B:35:ARG:NH2	2.09	0.67
5:H:1473:GLU:OE2	6:H:150:HOH:O	2.13	0.67
2:E:677:ASP:OD1	6:E:1:HOH:O	2.12	0.67
1:J:174:DA:C2'	1:J:175:DA:H5"	2.23	0.66
1:J:270:DA:H2"	1:J:271:DG:O5'	1.93	0.66
1:J:272:DA:H2"	1:J:273:DA:O5'	1.96	0.66
1:I:25:DC:H2"	1:I:26:DC:H5'	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:820:ARG:CZ	4:C:820:ARG:HB3	2.22	0.66
4:G:1088:ARG:NH2	6:G:286:HOH:O	2.28	0.65
1:J:197:DA:H2"	1:J:198:DT:H5'	1.76	0.65
1:I:128:DT:H1'	1:I:129:DC:H5'	1.78	0.65
4:C:817:ARG:HH12	4:C:831:HIS:HD2	1.46	0.64
1:J:257:DA:OP1	6:J:312:HOH:O	2.15	0.64
3:F:287:VAL:CG1	3:F:302:GLY:O	2.45	0.64
3:F:287:VAL:HG11	3:F:302:GLY:O	1.98	0.63
1:I:28:DA:N3	1:I:29:DA:C4	2.66	0.63
1:I:93:DT:H2"	1:I:94:DG:C5'	2.29	0.63
1:J:272:DA:C2'	1:J:273:DA:O5'	2.46	0.63
1:J:176:DA:OP2	4:G:1032:ARG:HD3	1.98	0.63
4:C:820:ARG:NH2	6:C:178:HOH:O	2.32	0.62
1:I:138:DG:H2"	1:I:139:DA:OP2	1.99	0.62
3:F:275:HIS:HE1	5:H:1489:ARG:HH12	1.46	0.62
1:J:271:DG:C2	1:J:272:DA:C6	2.87	0.62
4:G:1031:HIS:CD2	4:G:1048:PRO:HG3	2.35	0.62
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.82	0.62
1:I:7:DA:C2	1:J:287:DA:C2	2.87	0.61
1:I:47:DC:H2"	1:I:48:DT:C7	2.29	0.61
4:C:887:VAL:HG13	4:C:893:LEU:HB3	1.83	0.61
1:J:151:DA:H2"	1:J:152:DT:H5"	1.82	0.61
1:I:15:DG:N2	1:J:279:DA:C2	2.69	0.60
2:A:529:ARG:HH11	2:A:529:ARG:HG2	1.66	0.60
1:I:21:DT:C2	1:J:272:DA:C6	2.90	0.60
1:I:10:DC:N4	1:J:283:DG:H1	2.01	0.59
1:I:41:DA:H2"	1:I:42:DA:C5'	2.32	0.59
3:F:275:HIS:CE1	5:H:1489:ARG:NH1	2.64	0.59
1:I:118:DT:H1'	1:I:119:DT:H5'	1.84	0.59
1:J:274:DT:H2"	1:J:275:DC:OP2	2.01	0.58
1:J:266:DT:H2'	6:J:330:HOH:O	2.02	0.58
1:J:286:DT:H2"	1:J:287:DA:O5'	2.03	0.58
2:A:465:LEU:HB3	2:A:466:PRO:HD3	1.84	0.58
2:E:649:ARG:HH11	2:E:649:ARG:HG3	1.66	0.58
1:I:29:DA:H2"	1:I:30:DA:C8	2.39	0.57
2:A:529:ARG:NH1	2:A:529:ARG:HG2	2.19	0.57
3:F:275:HIS:ND1	3:F:275:HIS:C	2.50	0.57
1:I:36:DT:H2"	1:I:37:DT:OP2	2.05	0.57
1:J:267:DG:H5"	5:D:1237:TYR:OH	2.04	0.57
4:G:1076:THR:O	5:H:1449:THR:HG23	2.04	0.57
1:I:28:DA:C2	1:I:29:DA:C2	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:DT:C2'	1:I:22:DC:H5'	2.35	0.56
1:J:151:DA:C2'	1:J:152:DT:H5"	2.35	0.56
1:J:151:DA:H1'	1:J:152:DT:H5"	1.87	0.56
3:F:275:HIS:CE1	3:F:275:HIS:O	2.58	0.56
1:I:93:DT:C2'	1:I:94:DG:H5"	2.36	0.56
1:J:262:DC:C2'	1:J:263:DT:H71	2.36	0.56
4:C:817:ARG:HH22	4:C:831:HIS:HD2	1.54	0.56
1:J:239:DT:H2"	1:J:240:DG:C8	2.41	0.56
3:B:83:ALA:HB3	6:B:113:HOH:O	2.05	0.55
1:J:223:DC:H2"	1:J:224:DG:C8	2.41	0.55
1:I:93:DT:H2"	1:I:94:DG:H5"	1.89	0.55
4:C:847:ALA:N	4:C:848:PRO:HD2	2.21	0.55
4:G:1017:ARG:NH1	4:G:1031:HIS:HD2	1.97	0.55
1:I:30:DA:OP2	4:C:832:ARG:HD3	2.07	0.55
2:A:476:GLN:OE1	2:A:480:THR:HA	2.07	0.55
1:J:271:DG:N1	1:J:272:DA:N6	2.55	0.55
2:E:735:ALA:HB3	6:E:142:HOH:O	2.06	0.55
1:I:28:DA:H1'	1:I:29:DA:C8	2.42	0.55
5:D:1277:LEU:HD21	5:D:1293:THR:HB	1.88	0.55
1:J:268:DG:H2"	1:J:269:DT:C5'	2.38	0.54
1:J:235:DC:H2"	1:J:236:DT:OP2	2.06	0.54
4:G:1102:ILE:HG23	5:H:1458:ILE:HD13	1.88	0.54
1:I:22:DC:C6	1:I:23:DT:H73	2.43	0.54
2:E:636:LYS:HG3	2:E:636:LYS:O	2.06	0.54
2:E:668:GLN:HG3	2:E:689:VAL:HG11	1.89	0.54
1:J:197:DA:C2'	1:J:198:DT:H5'	2.38	0.54
1:J:271:DG:H4'	1:J:272:DA:OP1	2.08	0.54
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.89	0.54
4:G:1084:GLN:O	4:G:1088:ARG:HG2	2.08	0.54
1:I:28:DA:H1'	1:I:29:DA:C5'	2.38	0.54
1:I:146:DT:H3	1:J:147:DA:H61	1.56	0.54
3:F:275:HIS:CD2	5:H:1477:LEU:HD22	2.44	0.53
1:I:6:DT:H2"	1:I:7:DA:C8	2.44	0.53
1:I:23:DT:H72	1:I:24:DA:H62	1.73	0.53
1:I:24:DA:N6	6:J:306:HOH:O	2.40	0.53
1:I:44:DC:H1'	1:I:45:DT:H5'	1.91	0.53
2:E:679:LYS:HD3	2:E:680:THR:N	2.23	0.53
2:A:528:ARG:HH11	2:A:534:ARG:NH1	2.07	0.52
1:J:151:DA:H2"	1:J:152:DT:H5'	1.91	0.52
5:D:1287:THR:H	5:D:1290:GLU:CG	2.22	0.52
1:J:197:DA:H1'	1:J:198:DT:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:DT:H1'	1:I:21:DT:P	2.31	0.52
1:I:5:DA:H2"	6:I:170:HOH:O	2.02	0.52
2:E:663:ARG:NE	2:E:663:ARG:HA	2.25	0.52
1:I:23:DT:H72	1:I:24:DA:N6	2.25	0.52
2:E:728:ARG:HE	2:E:734:ARG:HH21	1.57	0.52
1:I:113:DA:H2"	1:I:114:DC:O5'	2.10	0.51
1:I:28:DA:N1	1:I:29:DA:C2	2.78	0.51
1:I:55:DA:H2"	1:I:56:DA:C8	2.45	0.51
2:E:665:LEU:HB3	2:E:666:PRO:HD3	1.92	0.51
1:I:22:DC:O2	1:J:272:DA:N1	2.44	0.51
1:I:39:DG:H4'	4:C:842:ARG:NH1	2.25	0.51
3:F:230:THR:HB	3:F:232:PRO:HD2	1.92	0.51
1:I:125:DG:H2"	1:I:126:DA:OP2	2.10	0.51
4:C:837:GLY:HA3	4:C:839:TYR:CE1	2.46	0.51
1:I:135:DG:H2"	1:I:136:DT:OP2	2.09	0.51
1:J:149:DC:H2"	1:J:150:DA:O5'	2.10	0.51
4:C:817:ARG:HH12	4:C:831:HIS:CD2	2.27	0.51
5:D:1239:TYR:CE2	5:D:1243:LYS:HD2	2.46	0.51
1:I:93:DT:H1'	1:I:94:DG:H5"	1.93	0.51
1:I:22:DC:H2"	1:I:23:DT:H71	1.94	0.50
4:G:1084:GLN:NE2	4:G:1088:ARG:HD2	2.26	0.50
1:I:111:DA:C2'	1:I:112:DT:H72	2.41	0.50
4:G:1084:GLN:CD	4:G:1088:ARG:HD2	2.31	0.50
1:I:89:DC:H2"	1:I:90:DT:C7	2.38	0.49
1:I:60:DC:H5"	2:A:463:ARG:CZ	2.42	0.49
5:D:1287:THR:H	5:D:1290:GLU:HG2	1.77	0.49
3:B:30:THR:HB	3:B:32:PRO:HD2	1.94	0.49
1:I:63:DG:H2"	1:I:64:DT:OP2	2.12	0.49
1:J:227:DG:H5'	3:B:47:SER:HA	1.94	0.49
5:H:1489:ARG:HH11	5:H:1489:ARG:HG2	1.77	0.49
1:J:257:DA:H2"	1:J:258:DT:OP2	2.12	0.49
1:I:23:DT:H2"	1:I:24:DA:O5'	2.11	0.49
1:I:127:DA:H1'	1:I:128:DT:H5'	1.93	0.49
1:J:280:DG:N7	6:J:310:HOH:O	2.35	0.49
1:J:184:DT:H2"	1:J:185:DG:N7	2.28	0.49
1:J:205:DG:H1'	1:J:206:DC:H5"	1.94	0.49
1:J:257:DA:P	6:J:312:HOH:O	2.70	0.49
1:J:229:DA:N3	2:A:440:ARG:NH2	2.61	0.48
2:E:663:ARG:HE	2:E:663:ARG:HA	1.78	0.48
1:I:146:DT:H3	1:J:147:DA:N6	2.11	0.48
5:H:1473:GLU:CG	6:H:150:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:DT:O5'	1:I:20:DT:H2'	2.14	0.48
1:I:26:DC:H1'	1:I:27:DA:C5	2.47	0.48
1:J:149:DC:H2'	1:J:150:DA:C8	2.49	0.48
3:F:235:ARG:HH11	3:F:235:ARG:HG3	1.79	0.48
1:J:282:DT:H2"	1:J:283:DG:C8	2.48	0.48
1:J:181:DA:H2"	1:J:182:DT:OP2	2.14	0.47
1:J:226:DT:H2"	1:J:227:DG:C8	2.48	0.47
4:C:817:ARG:NH1	4:C:831:HIS:HD2	2.10	0.47
1:J:281:DG:H1'	1:J:282:DT:H5'	1.96	0.47
4:C:883:LEU:O	4:C:887:VAL:HG23	2.14	0.47
2:A:448:LEU:HD21	4:G:1117:PRO:HD3	1.96	0.47
1:J:271:DG:C4	1:J:272:DA:N7	2.82	0.47
1:J:182:DT:H2"	1:J:183:DT:OP2	2.15	0.47
1:I:27:DA:H2'	1:I:27:DA:O5'	2.14	0.47
1:I:28:DA:C4'	1:I:29:DA:H5"	2.44	0.47
1:J:229:DA:C2'	1:J:230:DC:H5'	2.37	0.47
5:H:1473:GLU:CD	6:H:150:HOH:O	2.52	0.47
4:G:1037:GLY:HA3	4:G:1039:TYR:CE1	2.50	0.47
1:I:9:DC:C2'	1:I:10:DC:H5'	2.42	0.47
2:A:448:LEU:CD2	4:G:1117:PRO:HD3	2.46	0.46
1:I:28:DA:H1'	1:I:29:DA:H5'	1.97	0.46
1:J:237:DT:OP1	2:A:466:PRO:HG3	2.15	0.46
1:I:5:DA:H4'	2:E:639:HIS:HB2	1.96	0.46
1:I:27:DA:N6	1:I:28:DA:N6	2.63	0.46
2:E:718:THR:HA	3:F:245:HIS:HB2	1.96	0.46
1:J:268:DG:H2"	1:J:269:DT:H5'	1.97	0.46
1:J:262:DC:H2'	1:J:263:DT:H71	1.99	0.45
4:C:820:ARG:NH2	5:D:1321:ALA:O	2.49	0.45
1:I:128:DT:H2"	1:I:129:DC:OP2	2.17	0.45
1:J:149:DC:C2'	1:J:150:DA:C8	2.99	0.45
1:I:144:DG:H2"	1:I:145:DA:OP2	2.16	0.45
1:J:271:DG:H2'	1:J:271:DG:O5'	2.17	0.45
1:I:111:DA:H2"	1:I:112:DT:C7	2.47	0.45
1:J:172:DC:H1'	1:J:173:DA:C5	2.52	0.45
1:J:266:DT:H2"	1:J:267:DG:N7	2.32	0.44
1:I:61:DA:H2"	1:I:62:DT:C5'	2.38	0.44
1:J:268:DG:H2"	1:J:269:DT:O5'	2.17	0.44
1:J:230:DC:H2"	1:J:231:DA:C8	2.52	0.44
1:J:256:DA:H2"	1:J:257:DA:OP2	2.18	0.44
1:J:239:DT:H2"	1:J:240:DG:H8	1.81	0.44
4:C:888:ARG:HD3	4:C:888:ARG:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:914:VAL:HG13	6:C:52:HOH:O	2.18	0.44
2:A:479:LYS:HD2	3:B:74:GLU:HG2	1.99	0.44
5:H:1489:ARG:HG2	5:H:1489:ARG:NH1	2.33	0.44
4:G:1072:ASP:C	4:G:1073:ASN:HD22	2.22	0.44
5:D:1277:LEU:CD2	5:D:1293:THR:HB	2.48	0.43
1:I:10:DC:H1'	1:I:11:DA:C8	2.52	0.43
1:I:29:DA:H2"	1:I:30:DA:H8	1.81	0.43
1:J:281:DG:H2"	1:J:282:DT:O5'	2.18	0.43
4:G:1035:ARG:HH11	4:G:1035:ARG:HG2	1.82	0.43
3:F:259:LYS:O	3:F:263:GLU:HG3	2.18	0.43
5:D:1239:TYR:O	5:D:1243:LYS:HG2	2.18	0.43
3:F:292:ARG:HH21	5:H:1498:LEU:HD23	1.84	0.43
1:I:20:DT:H1'	1:I:21:DT:C5'	2.48	0.43
1:I:21:DT:C2	1:I:22:DC:N3	2.86	0.43
5:D:1278:ALA:HB3	6:D:240:HOH:O	2.17	0.43
1:I:1:DA:H2'	1:I:2:DT:H72	2.00	0.43
1:J:272:DA:H2"	1:J:273:DA:OP2	2.19	0.43
4:C:817:ARG:NH2	4:C:831:HIS:HD2	2.17	0.43
1:J:271:DG:C2	1:J:272:DA:C5	3.06	0.43
1:J:267:DG:C5	6:J:322:HOH:O	2.70	0.43
1:I:112:DT:P	4:G:1035:ARG:HH22	2.41	0.43
3:F:291:LYS:HB2	3:F:291:LYS:HE3	1.82	0.43
4:C:887:VAL:CG1	4:C:897:LEU:HD12	2.44	0.43
5:D:1231:LYS:HG3	5:D:1231:LYS:O	2.18	0.43
4:C:858:LEU:HD12	5:D:1266:VAL:HG11	2.00	0.43
1:J:274:DT:H1'	1:J:275:DC:C5'	2.46	0.42
1:I:120:DT:H2"	1:I:121:DG:C8	2.54	0.42
4:G:1079:ILE:HG12	4:G:1082:HIS:CE1	2.54	0.42
1:I:17:DA:N6	1:J:275:DC:H42	2.18	0.42
1:I:56:DA:H2"	1:I:57:DA:OP2	2.19	0.42
4:C:840:ALA:HA	4:G:1038:ASN:OD1	2.19	0.42
3:B:101:GLY:O	3:B:102:GLY:C	2.58	0.42
1:J:154:DT:P	2:A:449:ARG:HD2	2.60	0.42
1:J:262:DC:H2"	1:J:263:DT:H71	2.02	0.42
2:A:528:ARG:NH1	2:A:534:ARG:NH1	2.68	0.42
5:D:1266:VAL:HG12	5:D:1270:ILE:HD12	2.01	0.42
1:J:289:DT:H6	1:J:289:DT:H5'	1.84	0.42
1:I:77:DC:H2"	1:I:78:DG:C8	2.55	0.42
2:E:717:VAL:O	3:F:245:HIS:HB2	2.20	0.42
2:A:439:HIS:ND1	2:A:440:ARG:N	2.67	0.42
1:I:105:DT:H2"	1:I:106:DT:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:649:ARG:HH11	2:E:649:ARG:CG	2.32	0.42
4:G:1073:ASN:HD22	4:G:1073:ASN:N	2.17	0.42
1:J:151:DA:C1'	1:J:152:DT:H5"	2.49	0.41
1:I:117:DT:H2"	1:I:118:DT:OP2	2.19	0.41
1:J:195:DC:H1'	1:J:196:DC:C6	2.55	0.41
1:J:248:DA:H2"	1:J:249:DG:OP2	2.20	0.41
4:G:1035:ARG:NH1	4:G:1035:ARG:HG2	2.36	0.41
1:I:7:DA:H5'	2:E:641:TYR:OH	2.21	0.41
1:J:271:DG:C6	1:J:272:DA:N6	2.89	0.41
1:I:28:DA:C1'	1:I:29:DA:H5"	2.50	0.41
1:I:28:DA:C4	1:I:29:DA:C5	3.09	0.41
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.90	0.41
2:E:663:ARG:CZ	6:E:273:HOH:O	2.68	0.41
4:C:826:PRO:HD3	5:D:1237:TYR:CD2	2.56	0.41
5:D:1277:LEU:HD21	5:D:1293:THR:CG2	2.51	0.41
5:H:1431:LYS:HD2	5:H:1431:LYS:HA	1.92	0.41
4:G:1020:ARG:HH11	4:G:1020:ARG:HG2	1.85	0.41
1:J:271:DG:H1'	1:J:272:DA:C8	2.56	0.41
1:J:271:DG:C2	1:J:272:DA:N6	2.89	0.41
5:D:1277:LEU:HD21	5:D:1293:THR:CB	2.51	0.41
1:I:114:DC:OP1	1:I:114:DC:H4'	2.21	0.41
2:A:459:GLU:HG3	2:A:459:GLU:H	1.65	0.41
3:B:68:ASP:OD2	3:B:92:ARG:NH1	2.54	0.41
4:C:841:GLU:HB2	5:D:1284:SER:HB2	2.03	0.41
1:J:152:DT:H2"	1:J:153:DA:C8	2.56	0.40
1:I:113:DA:C2	1:J:181:DA:C2	3.09	0.40
1:I:21:DT:C3'	1:I:22:DC:H5'	2.47	0.40
4:C:902:ILE:CG2	5:D:1258:ILE:HD13	2.43	0.40
4:G:1092:GLU:HG3	6:G:68:HOH:O	2.20	0.40
1:I:127:DA:H2"	1:I:128:DT:OP2	2.20	0.40
1:J:182:DT:H1'	1:J:183:DT:H5'	2.03	0.40
4:G:1057:TYR:HB2	5:H:1510:GLU:HG3	2.04	0.40
1:I:20:DT:H1'	1:I:21:DT:O5'	2.21	0.40
1:I:5:DA:C3'	6:I:170:HOH:O	2.68	0.40
1:I:28:DA:N3	1:I:29:DA:N9	2.70	0.40
1:I:93:DT:H2"	1:I:94:DG:H5'	2.03	0.40
1:I:14:DT:H2"	1:I:15:DG:C8	2.56	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	96/135 (71%)	94 (98%)	2 (2%)	0	100	100
2	E	102/135 (76%)	98 (96%)	4 (4%)	0	100	100
3	B	77/102 (76%)	77 (100%)	0	0	100	100
3	F	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
4	C	101/129 (78%)	99 (98%)	2 (2%)	0	100	100
4	G	102/129 (79%)	99 (97%)	3 (3%)	0	100	100
5	D	93/125 (74%)	91 (98%)	1 (1%)	1 (1%)	17	18
5	H	92/125 (74%)	88 (96%)	3 (3%)	1 (1%)	17	18
All	All	740/982 (75%)	722 (98%)	16 (2%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	1501	GLY
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	85/111 (77%)	84 (99%)	1 (1%)	78	89
2	E	90/111 (81%)	88 (98%)	2 (2%)	60	77
3	B	64/78 (82%)	63 (98%)	1 (2%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	64/78 (82%)	64 (100%)	0	100 100
4	C	82/100 (82%)	79 (96%)	3 (4%)	41 55
4	G	83/100 (83%)	82 (99%)	1 (1%)	78 89
5	D	81/105 (77%)	81 (100%)	0	100 100
5	H	80/105 (76%)	76 (95%)	4 (5%)	30 41
All	All	629/788 (80%)	617 (98%)	12 (2%)	65 81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	459	GLU
3	B	47	SER
4	C	820	ARG
4	C	881	ARG
4	C	909	PRO
2	E	659	GLU
2	E	663	ARG
4	G	1088	ARG
5	H	1431	LYS
5	H	1433	SER
5	H	1444	GLN
5	H	1503	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	468	GLN
4	C	831	HIS
4	C	873	ASN
5	D	1279	HIS
5	D	1292	GLN
4	G	1031	HIS
4	G	1038	ASN
4	G	1073	ASN
5	H	1446	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

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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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