Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:22 PM GMT

PDB ID	:	1F66
Title	:	2.6 A CRYSTAL STRUCTURE OF A NUCLEOSOME CORE PARTICLE CONTAINING THE VARIANT HISTONE H2A.Z
Authors	:	Suto, R.K.; Clarkson, M.J.; Tremethick, D.J.; Luger, K.
Deposited on	:	2000-06-20
Resolution	:	2.60 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:

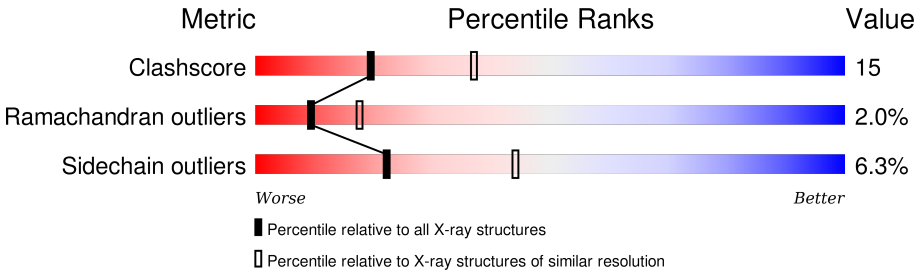
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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	40% 58% •
1	J	146	47% 48% 5%
2	A	136	59% 10% • • 26%
2	E	136	60% 13% •• 24%
3	B	103	56% 21% 22%
3	F	103	60% 19% • • 17%
4	C	128	59% 16% • • 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	128	
5	D	126	
5	H	126	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12397 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 146 BASE PAIR 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	103	Total	C	N	O	S	0	0	0
			841	530	163	145	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLU	GLY	CONFLICT	UNP Q7ZT64
A	517	VAL	ILE	CONFLICT	UNP Q7ZT64
E	634	GLU	GLY	CONFLICT	UNP Q7ZT64
E	717	VAL	ILE	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
			638	401	125	111	1			
3	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

- Molecule 4 is a protein called HISTONE H2A.Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	103	Total 781	C 490	N 152	O 139	0	0	0
4	G	107	Total 807	C 506	N 158	O 143	0	0	0

- Molecule 5 is a protein called HISTONE H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	95	Total 745	C 469	N 134	O 140	S 2	0	0	0
5	H	95	Total 745	C 469	N 134	O 140	S 2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1229	THR	SER	CONFLICT	UNP P02281
H	1429	THR	SER	CONFLICT	UNP P02281

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	Mn 1	0	0
6	J	5	Total 5	Mn 5	0	0
6	I	7	Total 7	Mn 7	0	0
6	C	1	Total 1	Mn 1	0	0
6	E	1	Total 1	Mn 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	27	Total 27	O 27	0	0
7	B	24	Total 24	O 24	0	0
7	C	31	Total 31	O 31	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	25	Total O 25 25	0	0
7	E	43	Total O 43 43	0	0
7	F	26	Total O 26 26	0	0
7	G	16	Total O 16 16	0	0
7	H	15	Total O 15 15	0	0
7	I	62	Total O 62 62	0	0
7	J	56	Total O 56 56	0	0

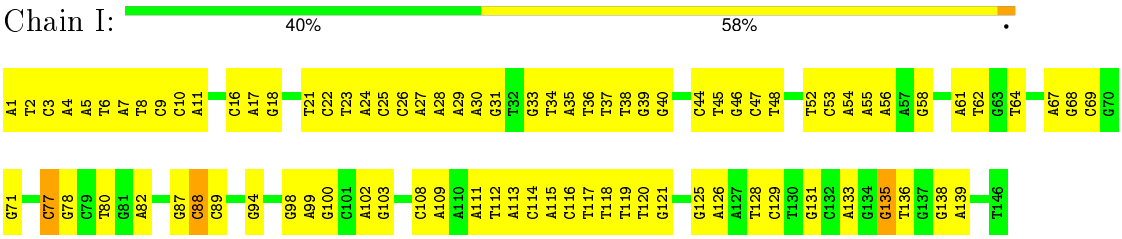
3 Residue-property plots (i)

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.

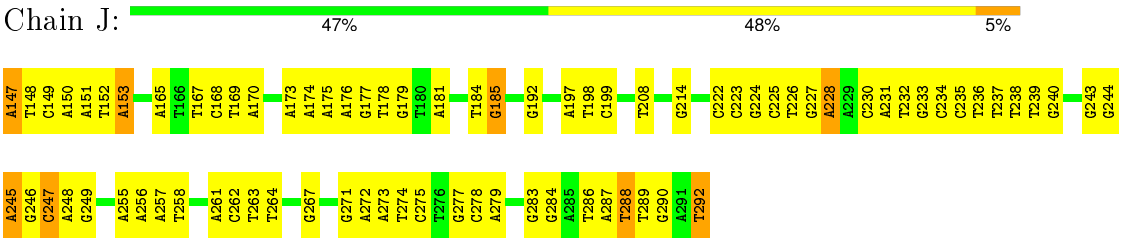
- Molecule 1: PALINDROMIC 146 BASE PAIR DNA FRAGMENT

Chain I:



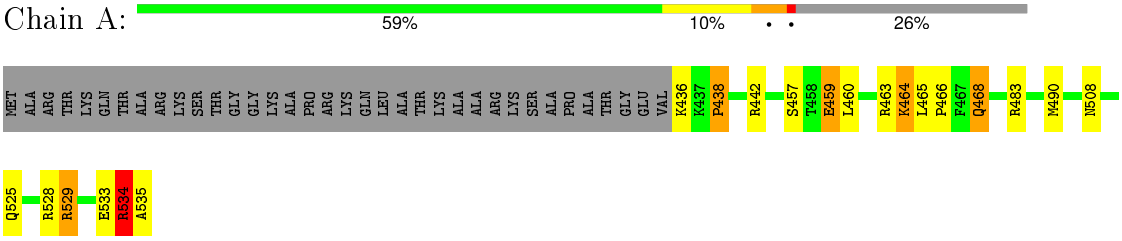
- Molecule 1: PALINDROMIC 146 BASE PAIR DNA FRAGMENT

Chain J:



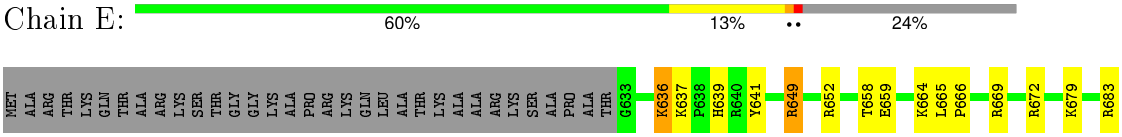
- Molecule 2: HISTONE H3

Chain A:



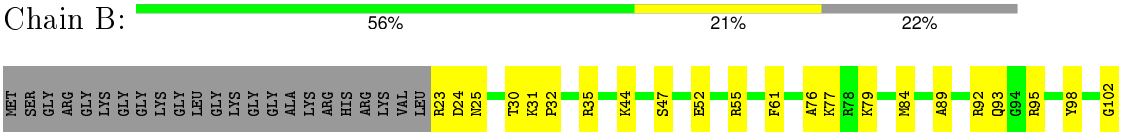
- Molecule 2: HISTONE H3

Chain E:



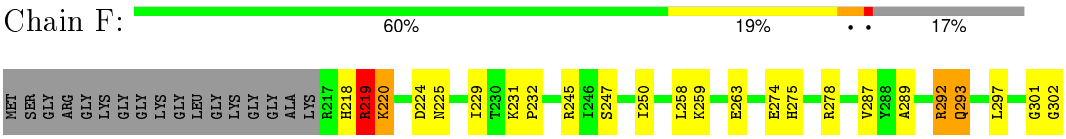
• Molecule 3: HISTONE H4

Chain B:



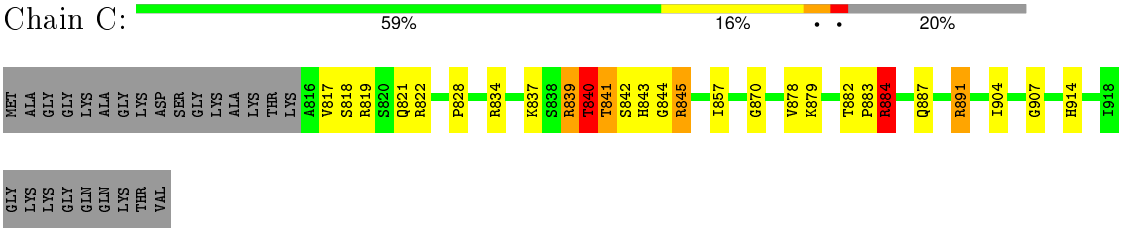
• Molecule 3: HISTONE H4

Chain F:



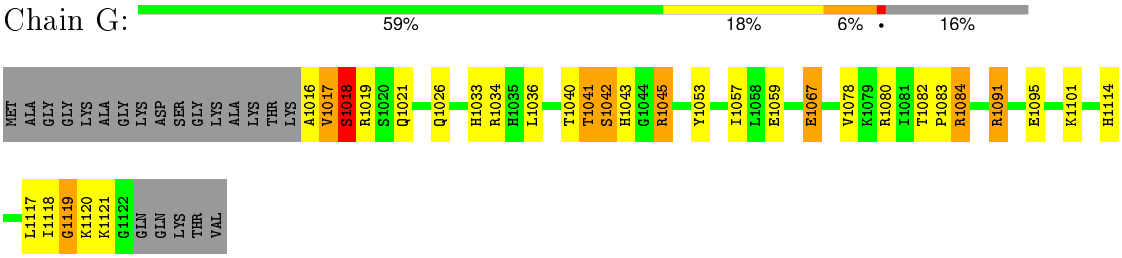
• Molecule 4: HISTONE H2A.Z

Chain C:



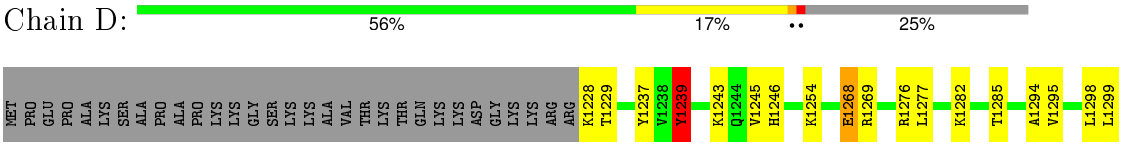
• Molecule 4: HISTONE H2A.Z

Chain G:



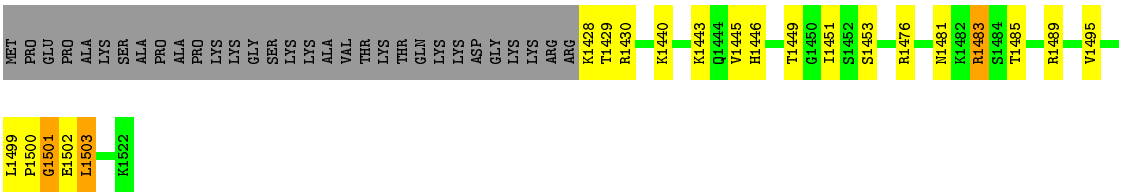
• Molecule 5: HISTONE H2B

Chain D:



• Molecule 5: HISTONE H2B

Chain H:


MET
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
K1428
T1429
R1430
K1440
K1443
Q1444
V1445
H1446
T1449
G1450
I1451
S1452
S1453
R1476
N1481
K1482
R1483
S1484
T1485
R1489
V1495
L1499
P1500
G1501
E1502
L1503
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	105.66Å 183.21Å 109.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.6 (25.00-2.60)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12397	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0/3354	0.82	1/5175 (0.0%)
1	J	0.62	0/3354	0.83	2/5175 (0.0%)
2	A	0.82	0/838	0.87	1/1122 (0.1%)
2	E	0.94	0/853	0.97	1/1142 (0.1%)
3	B	0.86	0/645	0.88	0/862
3	F	1.03	0/702	1.03	3/937 (0.3%)
4	C	0.84	0/792	0.92	2/1068 (0.2%)
4	G	0.72	0/818	0.93	3/1100 (0.3%)
5	D	0.84	0/756	0.84	0/1015
5	H	0.78	0/756	0.86	0/1015
All	All	0.74	0/12868	0.87	13/18611 (0.1%)

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	8
1	J	0	10
3	B	0	1
5	D	0	1
All	All	0	20

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	728	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	J	227	DG	C5'-C4'-C3'	-6.47	102.45	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	884	ARG	NE-CZ-NH1	6.43	123.52	120.30
4	C	884	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	J	208	DT	OP2-P-O3'	6.26	118.98	105.20
3	F	245	ARG	NE-CZ-NH1	5.92	123.26	120.30
4	G	1084	ARG	NE-CZ-NH1	5.89	123.25	120.30
4	G	1091	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	I	82	DA	OP2-P-O3'	5.83	118.03	105.20
4	G	1119	GLY	N-CA-C	5.82	127.66	113.10
3	F	278	ARG	NE-CZ-NH1	5.45	123.03	120.30
3	F	219	ARG	N-CA-C	5.18	124.99	111.00
2	A	464	LYS	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	98	TYR	Sidechain
5	D	1239	TYR	Sidechain
1	I	121	DG	Sidechain
1	I	131	DG	Sidechain
1	I	133	DA	Sidechain
1	I	135	DG	Sidechain
1	I	64	DT	Sidechain
1	I	67	DA	Sidechain
1	I	77	DC	Sidechain
1	I	88	DC	Sidechain
1	J	147	DA	Sidechain
1	J	153	DA	Sidechain
1	J	185	DG	Sidechain
1	J	214	DG	Sidechain
1	J	228	DA	Sidechain
1	J	238	DT	Sidechain
1	J	245	DA	Sidechain
1	J	247	DC	Sidechain
1	J	288	DT	Sidechain
1	J	292	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	83	0
1	J	2990	0	1651	96	0
2	A	826	0	871	22	0
2	E	841	0	884	27	0
3	B	638	0	676	18	0
3	F	694	0	742	18	0
4	C	781	0	824	41	0
4	G	807	0	856	39	0
5	D	745	0	773	30	0
5	H	745	0	773	22	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	7	0	0	0	0
6	J	5	0	0	0	0
7	A	27	0	0	0	0
7	B	24	0	0	2	0
7	C	31	0	0	0	0
7	D	25	0	0	2	0
7	E	43	0	0	1	0
7	F	26	0	0	1	0
7	G	16	0	0	1	0
7	H	15	0	0	2	0
7	I	62	0	0	5	0
7	J	56	0	0	3	0
All	All	12397	0	9701	325	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 (325) 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)
7:J:1048:HOH:O	4:G:1034:ARG:HD2	1.49	1.08
5:D:1243:LYS:HE2	5:D:1243:LYS:HA	1.40	1.03
4:C:839:ARG:HH11	4:C:839:ARG:HB2	1.26	0.98
2:E:636:LYS:HG2	2:E:637:LYS:H	1.26	0.97
4:C:822:ARG:NH2	5:D:1322:LYS:HB2	1.80	0.95
2:A:464:LYS:HE2	2:A:490:MET:HE1	1.48	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1057:ILE:HD13	5:H:1495:VAL:HG21	1.51	0.91
4:C:839:ARG:NH1	4:C:839:ARG:HB2	1.89	0.87
2:E:649:ARG:HH11	2:E:649:ARG:HG3	1.38	0.87
4:G:1053:TYR:HE1	4:G:1057:ILE:HD11	1.41	0.86
2:E:636:LYS:HG2	2:E:637:LYS:N	1.91	0.86
4:C:857:ILE:HD12	5:D:1307:ALA:HB1	1.58	0.85
5:H:1476:ARG:HD2	7:H:262:HOH:O	1.77	0.85
2:A:528:ARG:HH12	2:A:535:ALA:HB3	1.41	0.83
5:D:1254:LYS:HG2	7:D:7:HOH:O	1.77	0.83
1:J:287:DA:H2"	1:J:288:DT:H5'	1.63	0.81
1:J:257:DA:H2"	1:J:258:DT:H71	1.63	0.79
4:C:841:THR:O	4:C:841:THR:HG23	1.83	0.79
4:C:839:ARG:HH11	4:C:839:ARG:CB	1.95	0.79
3:B:95:ARG:HD3	7:B:123:HOH:O	1.81	0.78
4:G:1053:TYR:CE1	4:G:1057:ILE:HD11	2.18	0.78
1:J:197:DA:H2"	1:J:198:DT:H5'	1.66	0.78
4:G:1119:GLY:C	4:G:1121:LYS:H	1.84	0.78
4:C:840:THR:HG22	4:C:841:THR:N	1.99	0.77
5:H:1501:GLY:HA2	7:H:168:HOH:O	1.85	0.77
1:I:113:DA:H2"	1:I:114:DC:O5'	1.85	0.76
4:C:840:THR:HG22	4:C:841:THR:H	1.50	0.76
4:G:1019:ARG:HH22	4:G:1033:HIS:CD2	2.02	0.76
1:J:245:DA:H2"	1:J:246:DG:H5"	1.67	0.75
2:A:534:ARG:NE	2:A:534:ARG:HA	2.00	0.75
1:J:237:DT:H4'	2:A:463:ARG:CZ	2.18	0.74
3:F:297:LEU:O	3:F:302:GLY:HA2	1.86	0.73
1:I:125:DG:H1'	1:I:126:DA:H5'	1.70	0.73
1:J:234:DC:H4'	1:J:235:DC:OP1	1.86	0.73
4:G:1057:ILE:CD1	5:H:1495:VAL:HG21	2.18	0.73
1:I:61:DA:H2"	1:I:62:DT:H5'	1.70	0.73
1:J:149:DC:H2"	1:J:150:DA:O5'	1.89	0.72
1:J:248:DA:H2"	1:J:249:DG:C8	2.25	0.72
1:J:151:DA:H2"	1:J:152:DT:H5"	1.72	0.72
4:C:840:THR:CG2	4:C:841:THR:N	2.53	0.72
1:I:5:DA:H2"	1:I:6:DT:H5"	1.71	0.71
4:G:1057:ILE:HD13	5:H:1495:VAL:CG2	2.21	0.71
2:A:436:LYS:O	2:A:438:PRO:HD3	1.91	0.71
1:J:257:DA:C2'	1:J:258:DT:H71	2.20	0.71
1:I:27:DA:H2	1:J:267:DG:H22	1.40	0.70
1:J:246:DG:H2"	1:J:247:DC:C6	2.27	0.70
4:C:839:ARG:O	4:C:839:ARG:HG2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:857:ILE:HG13	5:D:1295:VAL:HG21	1.73	0.69
1:I:31:DG:H5"	4:C:818:SER:HA	1.74	0.69
1:I:21:DT:H2"	1:I:22:DC:O5'	1.92	0.69
4:C:828:PRO:HG3	5:D:1237:TYR:CE2	2.27	0.69
4:G:1120:LYS:HD3	4:G:1120:LYS:O	1.93	0.69
1:J:185:DG:H4'	4:G:1045:ARG:HD2	1.75	0.69
5:H:1481:ASN:O	5:H:1483:ARG:HG2	1.93	0.69
1:J:197:DA:C2'	1:J:198:DT:H5'	2.24	0.68
2:E:664:LYS:HD2	7:E:268:HOH:O	1.94	0.68
1:J:230:DC:H2"	1:J:231:DA:C8	2.29	0.67
1:J:287:DA:H2"	1:J:288:DT:C5'	2.25	0.67
3:F:287:VAL:HG11	3:F:302:GLY:H	1.59	0.67
2:A:464:LYS:CE	2:A:490:MET:HE1	2.22	0.67
4:C:834:ARG:HH11	4:C:834:ARG:HG2	1.59	0.66
4:C:840:THR:O	4:C:841:THR:HB	1.95	0.66
1:I:31:DG:H1	1:J:262:DC:H42	1.44	0.66
1:I:22:DC:N4	1:J:271:DG:H1	1.94	0.66
3:F:292:ARG:NH1	3:F:292:ARG:HB3	2.12	0.65
1:J:248:DA:H2"	1:J:249:DG:H8	1.59	0.65
4:G:1016:ALA:O	4:G:1017:VAL:HB	1.95	0.65
2:E:649:ARG:NH1	2:E:649:ARG:HG3	2.07	0.65
1:I:22:DC:H42	1:J:271:DG:H1	1.44	0.65
1:J:151:DA:H2"	1:J:152:DT:C5'	2.27	0.64
1:J:292:DT:H5'	2:E:636:LYS:HZ1	1.63	0.64
1:I:103:DG:H5"	5:D:1229:THR:CG2	2.28	0.64
5:D:1243:LYS:HE2	5:D:1243:LYS:CA	2.22	0.64
4:C:828:PRO:HG3	5:D:1237:TYR:CZ	2.32	0.64
1:I:103:DG:H5"	5:D:1229:THR:HG23	1.78	0.63
1:J:151:DA:C2'	1:J:152:DT:H5"	2.28	0.63
1:I:1:DA:H2"	1:I:2:DT:OP2	1.99	0.63
1:J:239:DT:H2"	1:J:240:DG:C8	2.34	0.63
4:C:840:THR:HG23	4:C:844:GLY:HA3	1.79	0.62
1:J:249:DG:H5"	5:H:1428:LYS:HA	1.80	0.62
2:A:528:ARG:NH1	2:A:535:ALA:OXT	2.33	0.62
1:J:246:DG:H2"	1:J:247:DC:C5	2.34	0.62
4:C:841:THR:O	4:C:841:THR:CG2	2.47	0.61
1:J:197:DA:H1'	1:J:198:DT:H5'	1.82	0.61
3:F:229:ILE:HG13	3:F:258:LEU:HD23	1.82	0.61
1:I:44:DC:H1'	1:I:45:DT:H5'	1.81	0.61
1:J:292:DT:H5'	2:E:636:LYS:NZ	2.15	0.61
4:C:822:ARG:HH22	5:D:1322:LYS:HB2	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:84:MET:HE1	3:B:102:GLY:HA3	1.84	0.60
1:J:165:DA:H4'	4:G:1080:ARG:NH2	2.16	0.60
5:D:1243:LYS:CE	5:D:1243:LYS:HA	2.25	0.60
1:I:27:DA:H2	1:J:267:DG:N2	2.00	0.59
3:F:287:VAL:CG1	3:F:302:GLY:H	2.15	0.59
5:D:1294:ALA:O	5:D:1298:LEU:HD12	2.02	0.59
1:I:71:DG:OP2	7:I:1045:HOH:O	2.17	0.59
1:I:24:DA:H1'	1:I:25:DC:H5'	1.83	0.59
1:J:184:DT:H2"	1:J:185:DG:N7	2.18	0.59
1:I:27:DA:C3'	5:D:1228:LYS:HZ1	2.15	0.58
1:I:34:DT:H5"	7:I:1023:HOH:O	2.03	0.58
1:J:149:DC:H2'	1:J:150:DA:C8	2.39	0.58
2:E:636:LYS:CG	2:E:637:LYS:H	2.10	0.58
1:J:235:DC:H2"	1:J:236:DT:OP2	2.03	0.58
1:I:111:DA:H2"	1:I:112:DT:OP2	2.03	0.58
1:I:94:DG:H1	1:J:199:DC:H42	1.51	0.58
4:G:1082:THR:HB	4:G:1083:PRO:CD	2.34	0.58
1:J:286:DT:H2"	1:J:287:DA:O5'	2.04	0.57
1:I:61:DA:C2'	1:I:62:DT:H5'	2.34	0.57
1:J:277:DG:H3'	4:C:879:LYS:HD2	1.86	0.57
3:B:31:LYS:NZ	3:B:55:ARG:HH12	2.03	0.57
3:F:275:HIS:O	5:H:1489:ARG:NH2	2.35	0.57
4:G:1119:GLY:C	4:G:1121:LYS:N	2.57	0.57
1:J:175:DA:C2'	1:J:176:DA:C8	2.88	0.57
4:C:840:THR:O	4:C:841:THR:CB	2.53	0.56
1:I:135:DG:H2"	1:I:136:DT:OP2	2.05	0.56
1:I:111:DA:H4'	4:G:1045:ARG:HE	1.69	0.56
1:I:17:DA:C2	1:I:18:DG:C2	2.93	0.56
1:I:118:DT:H2"	1:I:119:DT:H72	1.88	0.56
1:J:177:DG:H5"	4:G:1018:SER:HA	1.88	0.56
1:I:100:DG:H5"	2:E:683:ARG:HD2	1.86	0.56
1:I:111:DA:H4'	4:G:1045:ARG:NE	2.21	0.55
1:J:165:DA:H4'	4:G:1080:ARG:CZ	2.37	0.55
1:I:68:DG:OP1	2:A:442:ARG:HD3	2.06	0.55
4:C:884:ARG:O	4:C:884:ARG:HG3	2.01	0.55
1:I:55:DA:H2"	1:I:56:DA:C8	2.40	0.55
1:I:4:DA:C2	1:J:290:DG:N2	2.75	0.55
1:I:36:DT:H2"	1:I:37:DT:OP2	2.07	0.55
2:E:665:LEU:HB3	2:E:666:PRO:HD3	1.88	0.55
2:A:534:ARG:HA	2:A:534:ARG:HE	1.69	0.54
1:J:232:DT:H2"	1:J:233:DG:H8	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:228:DA:OP2	3:B:35:ARG:NH2	2.34	0.54
1:J:175:DA:H2"	1:J:176:DA:C8	2.43	0.54
4:C:834:ARG:NH1	4:C:834:ARG:HG2	2.23	0.54
1:I:22:DC:H2"	1:I:23:DT:O5'	2.08	0.54
3:F:287:VAL:HG11	3:F:302:GLY:N	2.22	0.53
1:J:192:DG:H2'	7:J:1058:HOH:O	2.08	0.53
1:J:147:DA:H2"	1:J:148:DT:C6	2.43	0.53
1:I:26:DC:C2	1:I:27:DA:C2	2.97	0.53
5:D:1276:ARG:HD2	7:D:34:HOH:O	2.07	0.53
3:B:52:GLU:OE2	3:B:55:ARG:NH1	2.41	0.53
3:B:76:ALA:O	3:B:77:LYS:HB2	2.09	0.53
4:C:837:LYS:O	4:C:840:THR:HB	2.09	0.52
1:J:277:DG:OP2	4:C:879:LYS:NZ	2.42	0.52
1:I:118:DT:C2'	1:I:119:DT:H72	2.39	0.52
1:I:2:DT:H2"	1:I:3:DC:O5'	2.09	0.52
1:I:36:DT:H1'	1:I:37:DT:H5'	1.90	0.52
1:I:58:DG:H8	7:I:1011:HOH:O	1.93	0.52
4:G:1045:ARG:HH11	4:G:1045:ARG:HG2	1.75	0.52
1:J:147:DA:H2"	1:J:148:DT:H6	1.74	0.52
1:J:169:DT:H72	1:J:170:DA:H62	1.74	0.52
4:C:840:THR:HG22	4:G:1042:SER:HA	1.92	0.52
3:F:292:ARG:HH11	3:F:292:ARG:HB3	1.74	0.52
1:J:199:DC:OP1	3:F:218:HIS:NE2	2.43	0.52
1:J:249:DG:OP1	5:H:1429:THR:HG22	2.10	0.52
1:I:119:DT:H4'	1:I:120:DT:OP1	2.09	0.52
2:A:465:LEU:N	2:A:466:PRO:CD	2.74	0.51
1:J:272:DA:H2"	1:J:273:DA:O5'	2.11	0.51
1:I:7:DA:C2	1:J:287:DA:C2	2.98	0.51
1:J:258:DT:OP1	4:C:837:LYS:NZ	2.44	0.51
4:G:1045:ARG:HD3	5:H:1485:THR:OG1	2.11	0.51
5:H:1445:VAL:HG12	5:H:1446:HIS:CD2	2.46	0.51
4:C:842:SER:C	4:C:844:GLY:H	2.14	0.51
1:I:54:DA:H61	1:J:239:DT:H3	1.59	0.51
3:B:30:THR:HB	3:B:32:PRO:HD2	1.93	0.51
1:I:46:DG:H2"	1:I:47:DC:H6	1.76	0.51
4:C:841:THR:HA	4:G:1040:THR:O	2.11	0.50
1:J:234:DC:O2	1:J:235:DC:N3	2.44	0.50
1:I:22:DC:H2'	1:I:23:DT:H72	1.94	0.50
1:I:38:DT:H2"	1:I:39:DG:N7	2.27	0.50
2:E:733:GLU:O	2:E:734:ARG:HB2	2.11	0.50
1:I:28:DA:H2"	1:I:29:DA:OP2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:882:THR:HB	4:C:883:PRO:CD	2.41	0.50
3:B:30:THR:CB	3:B:32:PRO:HD2	2.42	0.50
2:E:719:ILE:HG13	3:F:250:ILE:HG13	1.93	0.50
1:I:8:DT:H2"	1:I:9:DC:C6	2.47	0.50
1:J:292:DT:C5'	2:E:636:LYS:NZ	2.75	0.50
1:J:225:DC:H2"	1:J:226:DT:H71	1.94	0.50
1:I:61:DA:OP1	3:B:23:ARG:NH2	2.40	0.49
1:I:30:DA:H2"	1:I:31:DG:OP2	2.12	0.49
1:J:178:DT:H2"	1:J:179:DG:H8	1.78	0.49
1:I:6:DT:H2"	1:I:7:DA:C8	2.47	0.49
1:J:271:DG:H8	7:J:1045:HOH:O	1.95	0.49
2:E:734:ARG:O	2:E:735:ALA:HB2	2.13	0.49
2:A:508:ASN:HD21	4:G:1117:LEU:HD11	1.78	0.49
1:I:27:DA:H4'	5:D:1228:LYS:HZ2	1.78	0.48
1:I:27:DA:H4'	5:D:1228:LYS:NZ	2.28	0.48
2:A:468:GLN:HE21	2:A:468:GLN:HB2	1.47	0.48
4:G:1026:GLN:OE1	5:H:1440:LYS:HD3	2.13	0.48
1:J:197:DA:C1'	1:J:198:DT:H5'	2.44	0.48
1:J:234:DC:O2	1:J:235:DC:C2	2.66	0.48
1:J:178:DT:H2"	1:J:179:DG:C8	2.48	0.48
1:J:288:DT:H2"	1:J:289:DT:H5'	1.94	0.48
5:H:1443:LYS:NZ	5:H:1449:THR:O	2.44	0.48
1:I:118:DT:H2"	1:I:119:DT:C7	2.44	0.48
1:I:61:DA:H1'	1:I:62:DT:H5'	1.95	0.48
1:J:147:DA:C8	1:J:148:DT:H72	2.49	0.48
1:I:108:DC:H2"	1:I:109:DA:N7	2.29	0.47
1:I:47:DC:H2"	1:I:48:DT:H71	1.96	0.47
5:D:1243:LYS:CE	5:D:1243:LYS:CA	2.89	0.47
1:J:245:DA:C2'	1:J:246:DG:H5"	2.42	0.47
2:A:528:ARG:NH1	2:A:535:ALA:HB3	2.18	0.47
1:I:54:DA:H2"	1:I:55:DA:C8	2.50	0.47
3:F:259:LYS:HE3	3:F:263:GLU:OE2	2.15	0.47
1:I:47:DC:H2"	1:I:48:DT:C7	2.44	0.47
1:I:88:DC:H2"	1:I:89:DC:C6	2.50	0.47
2:A:457:SER:HB2	2:A:459:GLU:OE2	2.15	0.47
5:D:1245:VAL:HG23	5:D:1246:HIS:CD2	2.49	0.46
2:A:533:GLU:O	2:A:534:ARG:O	2.33	0.46
1:J:152:DT:H2"	1:J:153:DA:C8	2.50	0.46
1:I:46:DG:H2"	1:I:47:DC:C6	2.50	0.46
2:E:733:GLU:O	2:E:734:ARG:HD3	2.15	0.46
4:G:1019:ARG:NH2	4:G:1033:HIS:CD2	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1082:THR:HB	4:G:1083:PRO:HD2	1.96	0.46
3:F:219:ARG:HB2	3:F:220:LYS:H	1.26	0.46
1:J:261:DA:H2"	1:J:262:DC:H5'	1.98	0.46
5:D:1239:TYR:O	5:D:1243:LYS:HG2	2.16	0.46
1:I:40:DG:OP1	5:D:1285:THR:HB	2.15	0.46
2:E:734:ARG:HA	2:E:734:ARG:HD2	1.54	0.46
1:J:287:DA:C2'	1:J:288:DT:H5'	2.41	0.45
4:G:1045:ARG:NH1	4:G:1045:ARG:HG2	2.32	0.45
1:I:98:DG:H4'	1:I:99:DA:OP1	2.16	0.45
5:H:1489:ARG:HH11	5:H:1489:ARG:HG2	1.81	0.45
1:J:175:DA:H2"	1:J:176:DA:O5'	2.16	0.45
4:C:845:ARG:HD3	5:D:1285:THR:OG1	2.16	0.45
1:J:283:DG:H2"	1:J:284:DG:C8	2.52	0.45
4:G:1026:GLN:N	4:G:1059:GLU:OE1	2.47	0.45
5:H:1489:ARG:NH1	5:H:1489:ARG:HG2	2.32	0.45
1:J:283:DG:H2"	1:J:284:DG:OP2	2.16	0.44
4:C:817:VAL:HG13	4:C:821:GLN:HB3	1.99	0.44
5:D:1299:LEU:HD23	5:D:1299:LEU:N	2.31	0.44
4:G:1041:THR:O	4:G:1042:SER:C	2.54	0.44
4:C:882:THR:HB	4:C:883:PRO:HD2	1.98	0.44
5:H:1451:ILE:O	5:H:1451:ILE:HG23	2.16	0.44
1:I:10:DC:H1'	1:I:11:DA:C8	2.52	0.44
3:B:84:MET:CE	3:B:102:GLY:HA3	2.47	0.44
1:J:243:DG:H2"	1:J:244:DG:C8	2.52	0.44
4:G:1114:HIS:HB3	7:G:142:HOH:O	2.17	0.44
4:G:1101:LYS:HA	4:G:1101:LYS:HD3	1.64	0.44
1:I:113:DA:C2	1:J:181:DA:C2	3.05	0.44
1:I:102:DA:H2"	1:I:103:DG:OP2	2.16	0.44
3:B:89:ALA:O	3:B:93:GLN:HG3	2.16	0.44
1:I:31:DG:OP1	4:C:819:ARG:HG3	2.17	0.44
1:J:147:DA:C2'	1:J:148:DT:C7	2.96	0.44
1:I:87:DG:H4'	1:I:88:DC:OP1	2.18	0.44
4:C:914:HIS:CE1	2:E:709:LEU:HD21	2.53	0.44
5:D:1277:LEU:HD12	5:D:1277:LEU:HA	1.76	0.44
2:E:679:LYS:HG3	3:F:274:GLU:OE2	2.18	0.44
2:A:528:ARG:HH12	2:A:535:ALA:CB	2.22	0.43
3:B:31:LYS:N	3:B:32:PRO:CD	2.81	0.43
1:J:277:DG:P	4:C:879:LYS:NZ	2.92	0.43
4:G:1067:GLU:HA	5:H:1446:HIS:HE2	1.82	0.43
1:J:249:DG:P	5:H:1429:THR:HG22	2.57	0.43
1:I:80:DT:OP2	7:I:1054:HOH:O	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:DT:H2"	1:I:35:DA:O5'	2.18	0.43
1:J:274:DT:H2"	1:J:275:DC:OP2	2.17	0.43
1:I:5:DA:C2'	1:I:6:DT:H5"	2.45	0.43
1:J:278:DC:H2"	1:J:279:DA:N7	2.34	0.43
2:E:649:ARG:HH11	2:E:649:ARG:CG	2.16	0.43
1:I:52:DT:H2"	1:I:53:DC:C6	2.53	0.43
3:F:289:ALA:O	3:F:293:GLN:HG3	2.17	0.43
1:I:125:DG:H1'	1:I:126:DA:C5'	2.46	0.43
4:C:870:GLY:HA3	5:D:1246:HIS:CD2	2.54	0.43
2:E:672:ARG:HH11	2:E:672:ARG:HG2	1.83	0.43
7:I:1065:HOH:O	2:E:652:ARG:HD2	2.19	0.43
1:J:147:DA:H2'	1:J:148:DT:H72	2.01	0.42
2:A:525:GLN:O	2:A:534:ARG:NH2	2.53	0.42
1:J:247:DC:OP1	3:B:79:LYS:N	2.39	0.42
3:B:31:LYS:HZ3	3:B:55:ARG:HH12	1.67	0.42
4:C:884:ARG:HB2	2:E:658:THR:HG21	2.00	0.42
2:A:460:LEU:HD12	2:A:464:LYS:HE2	2.02	0.42
2:A:534:ARG:O	2:A:535:ALA:HB2	2.20	0.42
1:I:116:DC:H2"	1:I:117:DT:OP2	2.19	0.42
1:I:77:DC:H2"	1:I:78:DG:C8	2.55	0.42
1:I:114:DC:H2"	1:I:115:DA:C8	2.55	0.42
1:J:147:DA:H2'	1:J:148:DT:C7	2.50	0.42
4:C:891:ARG:HD3	4:C:891:ARG:HA	1.68	0.42
3:B:84:MET:CE	3:B:102:GLY:CA	2.98	0.42
1:I:94:DG:H1	1:J:199:DC:N4	2.15	0.42
3:F:231:LYS:HB3	3:F:232:PRO:HD3	2.02	0.41
1:J:167:DT:H2"	1:J:168:DC:OP2	2.19	0.41
2:A:529:ARG:HD3	2:A:529:ARG:O	2.20	0.41
2:A:465:LEU:HB3	2:A:466:PRO:HD3	2.01	0.41
1:J:272:DA:H1'	1:J:273:DA:H5'	2.01	0.41
4:C:887:GLN:HG2	4:C:907:GLY:O	2.19	0.41
1:I:69:DC:H42	1:J:224:DG:H1	1.68	0.41
4:G:1053:TYR:CE1	4:G:1057:ILE:CD1	2.98	0.41
1:I:16:DC:O2	1:I:17:DA:C2	2.73	0.41
2:E:639:HIS:HE1	2:E:641:TYR:CE2	2.37	0.41
1:I:33:DG:C2	1:J:261:DA:C2	3.08	0.41
2:E:669:ARG:HD2	3:F:225:ASN:OD1	2.20	0.41
2:E:641:TYR:CE2	2:E:649:ARG:NH2	2.88	0.41
3:B:31:LYS:NZ	7:B:109:HOH:O	2.38	0.41
3:F:259:LYS:HE2	3:F:259:LYS:HB3	1.73	0.41
1:J:175:DA:H2'	1:J:176:DA:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:734:ARG:O	2:E:735:ALA:CB	2.68	0.41
1:J:255:DA:C6	1:J:256:DA:C6	3.09	0.41
4:G:1095:GLU:HB3	5:H:1503:LEU:HD22	2.02	0.41
4:C:857:ILE:HG13	5:D:1295:VAL:CG2	2.47	0.41
1:I:31:DG:H1	1:J:262:DC:N4	2.16	0.41
1:J:225:DC:H2"	1:J:226:DT:C7	2.50	0.41
5:H:1443:LYS:HA	5:H:1443:LYS:HD3	1.66	0.41
1:I:138:DG:H2"	1:I:139:DA:OP2	2.20	0.41
3:B:24:ASP:OD1	3:B:25:ASN:N	2.54	0.41
4:G:1091:ARG:HD3	4:G:1091:ARG:HA	1.70	0.41
1:I:128:DT:H2"	1:I:129:DC:OP2	2.21	0.41
1:J:257:DA:C4	1:J:258:DT:C5	3.09	0.40
5:D:1299:LEU:HA	5:D:1300:PRO:HD3	1.89	0.40
1:J:263:DT:H2"	1:J:264:DT:OP2	2.19	0.40
4:G:1036:LEU:HD23	4:G:1036:LEU:HA	1.95	0.40
3:B:61:PHE:HE1	3:B:95:ARG:HD2	1.87	0.40
3:F:302:GLY:N	7:F:305:HOH:O	2.54	0.40
1:J:173:DA:H2"	1:J:174:DA:OP2	2.21	0.40
1:I:27:DA:C4'	5:D:1228:LYS:NZ	2.85	0.40
4:G:1017:VAL:O	4:G:1018:SER:CB	2.69	0.40
4:G:1017:VAL:O	4:G:1021:GLN:HB3	2.21	0.40
1:J:175:DA:H8	1:J:175:DA:C5'	2.33	0.40
1:I:10:DC:H2"	1:I:11:DA:H8	1.85	0.40
5:D:1268:GLU:HG2	5:D:1269:ARG:N	2.35	0.40
1:J:151:DA:H1'	1:J:152:DT:H5"	2.03	0.40
5:D:1228:LYS:HG2	5:D:1229:THR:H	1.85	0.40
2:E:733:GLU:O	2:E:734:ARG:CB	2.69	0.40
2:A:457:SER:CB	2:A:459:GLU:OE2	2.69	0.40
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.74	0.40
4:G:1017:VAL:HG12	4:G:1018:SER:N	2.37	0.40
5:H:1430:ARG:HG2	5:H:1430:ARG:HH11	1.86	0.40
1:J:222:DC:H2"	1:J:223:DC:C5	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	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	9 18
2	E	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	9 18
3	B	78/103 (76%)	78 (100%)	0	0	100 100
3	F	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	4 6
4	C	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	5 8
4	G	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	6 9
5	D	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	17 36
5	H	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	17 36
All	All	753/986 (76%)	712 (95%)	26 (4%)	15 (2%)	9 18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	534	ARG
4	C	841	THR
5	D	1301	GLY
2	E	636	LYS
4	G	1017	VAL
5	H	1501	GLY
4	C	843	HIS
4	C	840	THR
3	F	220	LYS
3	F	301	GLY
4	G	1042	SER
2	A	438	PRO
4	G	1018	SER
2	E	734	ARG
3	F	219	ARG

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	87/112 (78%)	82 (94%)	5 (6%)	25 49
2	E	88/112 (79%)	85 (97%)	3 (3%)	44 72
3	B	65/79 (82%)	62 (95%)	3 (5%)	33 61
3	F	71/79 (90%)	66 (93%)	5 (7%)	19 37
4	C	81/97 (84%)	74 (91%)	7 (9%)	13 25
4	G	83/97 (86%)	75 (90%)	8 (10%)	10 20
5	D	81/106 (76%)	76 (94%)	5 (6%)	23 45
5	H	81/106 (76%)	77 (95%)	4 (5%)	31 57
All	All	637/788 (81%)	597 (94%)	40 (6%)	22 44

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	459	GLU
2	A	468	GLN
2	A	483	ARG
2	A	529	ARG
2	A	534	ARG
3	B	44	LYS
3	B	47	SER
3	B	92	ARG
4	C	839	ARG
4	C	840	THR
4	C	845	ARG
4	C	878	VAL
4	C	884	ARG
4	C	891	ARG
4	C	904	ILE
5	D	1239	TYR
5	D	1268	GLU
5	D	1282	LYS
5	D	1309	SER
5	D	1313	LYS
2	E	649	ARG
2	E	659	GLU
2	E	734	ARG
3	F	219	ARG
3	F	224	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	247	SER
3	F	292	ARG
3	F	293	GLN
4	G	1018	SER
4	G	1041	THR
4	G	1043	HIS
4	G	1045	ARG
4	G	1067	GLU
4	G	1078	VAL
4	G	1084	ARG
4	G	1118	ILE
5	H	1453	SER
5	H	1483	ARG
5	H	1502	GLU
5	H	1503	LEU

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	508	ASN
3	B	25	ASN
3	B	75	HIS
4	C	914	HIS
5	D	1292	GLN
2	E	639	HIS
4	G	1033	HIS
4	G	1043	HIS
4	G	1114	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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.