



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 1P3L / pdb_00001p3l
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 : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

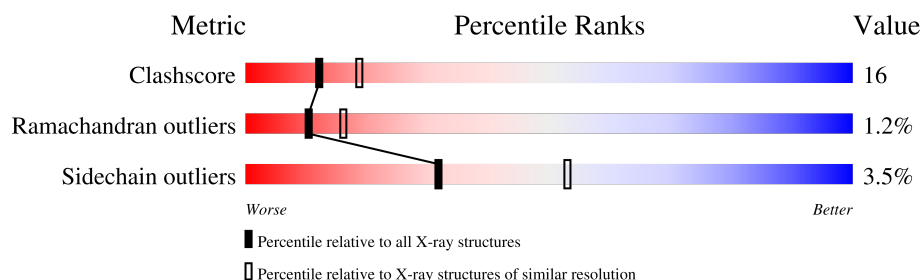
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	59% 37% .
1	J	146	55% 43% .
2	A	135	53% 16% . 27%
2	E	135	51% 19% . 27%
3	B	102	57% 18% . 23%
3	F	102	59% 18% . 19%
4	C	129	61% 17% . 18%
4	G	129	67% 14% . 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	125	60%11%26%
5	H	125	59%16%24%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12243 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
			811	511	158	139	3			
2	E	99	Total	C	N	O	S	0	0	0
			820	517	160	140	3			

There are 8 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
A	518	HIS	THR	conflict	UNP Q7ZT64
E	634	GLU	GLY	conflict	UNP Q7ZT64
E	635	SER	VAL	conflict	UNP Q7ZT64
E	702	ALA	GLY	conflict	UNP Q7ZT64
E	718	HIS	THR	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
			627	395	121	110	1			
3	F	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	106	Total	C	N	O	0	0	0
			820	517	160	143			
4	G	109	Total	C	N	O	0	0	0
			843	531	167	145			

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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	92	Total	C	N	O	S	0	0	0
			718	453	127	136	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	I	29	Total	O	0	0
			29	29		
6	J	33	Total	O	0	0
			33	33		

Continued on next page...

Continued from previous page...

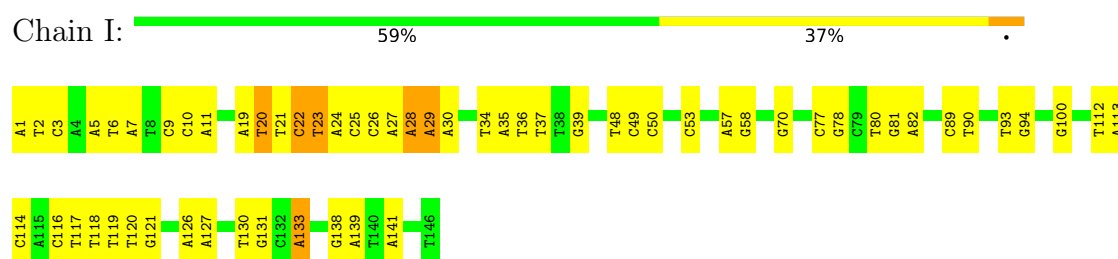
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total 20	O 20	0	0
6	B	16	Total 16	O 16	0	0
6	C	21	Total 21	O 21	0	0
6	D	17	Total 17	O 17	0	0
6	E	35	Total 35	O 35	0	0
6	F	27	Total 27	O 27	0	0
6	G	14	Total 14	O 14	0	0
6	H	6	Total 6	O 6	0	0

3 Residue-property plots

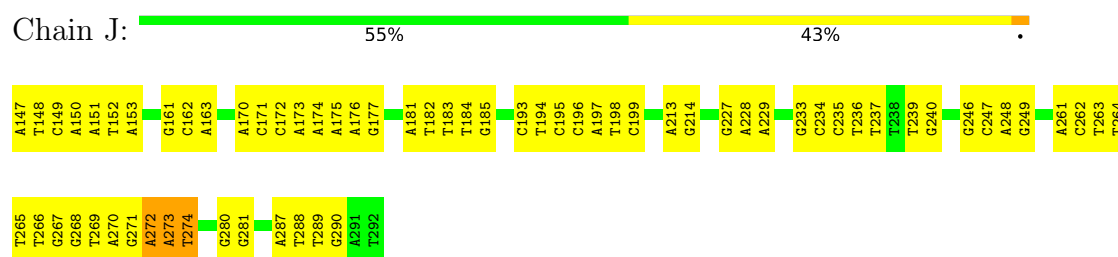
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

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



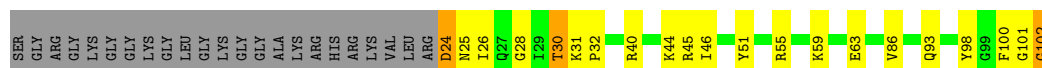
• Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment





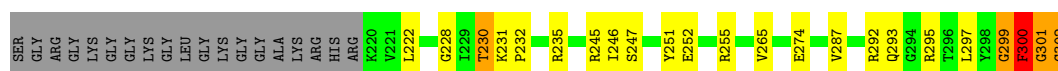
- Molecule 3: Histone H4

Chain B: 57% 18% 23%



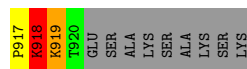
- Molecule 3: Histone H4

Chain F: 59% 18% 19%



- Molecule 4: Histone H2A

Chain C: 61% 17% 18%



- Molecule 4: Histone H2A

Chain G: 67% 14% 16%



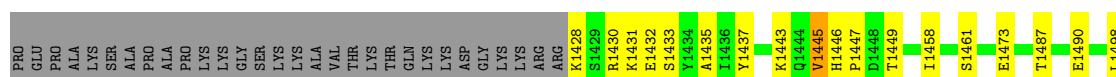
- Molecule 5: Histone H2B

Chain D: 60% 11% 26%



- Molecule 5: Histone H2B

Chain H: 59% 16% 24%



L1499	
P1500	
G1501	
	K1522

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.95Å 109.61Å 181.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.9 (50.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12243	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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	0.36	0/3354	0.76	8/5175 (0.2%)
1	J	0.35	0/3354	0.75	4/5175 (0.1%)
2	A	0.75	1/824 (0.1%)	1.10	5/1104 (0.5%)
2	E	0.82	0/833	1.14	8/1116 (0.7%)
3	B	0.80	0/634	1.24	9/848 (1.1%)
3	F	1.17	3/669 (0.4%)	1.60	11/894 (1.2%)
4	C	0.80	0/830	1.03	3/1120 (0.3%)
4	G	0.64	0/853	1.02	0/1149
5	D	0.80	0/729	1.05	4/980 (0.4%)
5	H	0.68	0/755	0.97	2/1013 (0.2%)
All	All	0.62	4/12835 (0.0%)	0.95	54/18574 (0.3%)

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
3	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	GLY	C-O	13.61	1.40	1.24
3	F	300	PHE	CB-CG	-6.09	1.36	1.50
2	A	534	ARG	CA-C	5.16	1.59	1.52
3	F	300	PHE	CA-C	-5.13	1.45	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	GLY	N-CA-C	-25.86	66.99	111.47
3	F	300	PHE	CB-CA-C	-14.68	81.21	110.42
1	I	20	DT	C2'-C3'-O3'	-9.53	97.20	111.50
3	F	302	GLY	N-CA-C	9.21	140.02	113.30
2	A	533	GLU	N-CA-C	-9.21	102.04	113.18
3	B	100	PHE	N-CA-C	-9.07	98.86	113.19
2	A	464	LYS	N-CA-C	8.38	120.03	111.07
1	J	274	DT	C2'-C3'-O3'	8.34	124.00	111.50
2	A	485	GLN	N-CA-C	-7.46	99.98	110.50
5	D	1235	ALA	N-CA-C	7.03	119.60	111.02
5	H	1435	ALA	N-CA-C	6.93	119.71	111.33
1	I	28	DA	O3'-P-O5'	-6.84	93.74	104.00
5	D	1298	LEU	N-CA-C	6.83	120.09	111.69
1	I	29	DA	C5'-C4'-C3'	-6.81	104.69	114.90
3	B	30	THR	N-CA-C	6.62	120.32	110.52
2	E	664	LYS	N-CA-C	6.56	118.22	111.14
1	J	227	DG	C5'-C4'-C3'	-6.39	105.32	114.90
3	B	102	GLY	N-CA-C	6.34	131.69	113.30
1	I	22	DC	C2'-C3'-O3'	-6.17	102.24	111.50
4	C	881	ARG	NE-CZ-NH1	-6.12	115.38	121.50
2	A	535	ALA	N-CA-C	6.11	128.12	111.00
1	I	20	DT	C3'-C2'-C1'	-6.11	92.44	101.60
3	B	46	ILE	N-CA-C	6.09	116.89	108.12
2	E	717	VAL	N-CA-C	-5.93	107.71	113.53
3	B	93	GLN	N-CA-C	-5.90	105.85	113.16
3	F	301	GLY	CA-C-O	-5.82	114.45	121.67
5	D	1321	ALA	N-CA-C	5.81	117.36	109.11
1	I	28	DA	C4'-C3'-O3'	-5.80	101.30	110.00
3	B	40	ARG	N-CA-C	-5.80	105.46	112.54
4	C	864	GLU	N-CA-C	-5.76	104.91	111.07
5	H	1445	VAL	N-CA-C	5.67	116.44	110.72
1	I	20	DT	N1-C1'-C2'	5.65	121.98	113.50
1	J	272	DA	C5'-C4'-C3'	-5.58	106.53	114.90
2	E	733	GLU	N-CA-C	-5.58	106.52	113.15
2	E	637	LYS	CA-C-N	5.54	126.76	119.84
2	E	637	LYS	C-N-CA	5.54	126.76	119.84
3	F	246	ILE	N-CA-C	5.47	115.74	107.75
1	J	273	DA	C5'-C4'-C3'	-5.43	106.75	114.90
3	F	300	PHE	CA-C-O	-5.39	112.81	120.51
3	B	24	ASP	CA-C-N	5.38	127.93	120.29
3	B	24	ASP	C-N-CA	5.38	127.93	120.29
1	I	23	DT	C5'-C4'-C3'	-5.38	106.83	114.90
5	D	1238	VAL	N-CA-C	-5.35	105.32	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	726	LEU	N-CA-C	-5.34	105.38	111.14
3	F	300	PHE	CA-C-N	-5.29	111.30	120.07
3	F	300	PHE	C-N-CA	-5.29	111.30	120.07
3	B	28	GLY	N-CA-C	-5.24	106.36	113.37
3	F	299	GLY	CA-C-N	-5.20	111.61	121.54
3	F	299	GLY	C-N-CA	-5.20	111.61	121.54
3	F	230	THR	N-CA-C	5.15	117.33	110.53
2	E	685	GLN	N-CA-C	-5.07	102.78	110.28
4	C	881	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	E	688	ALA	N-CA-C	-5.05	105.85	111.36
2	A	517	VAL	N-CA-C	-5.03	108.60	113.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	251	TYR	Sidechain
1	I	133	DA	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	88	0
1	J	2990	0	1651	85	0
2	A	811	0	846	35	0
2	E	820	0	858	35	0
3	B	627	0	663	18	0
3	F	662	0	709	50	0
4	C	820	0	879	24	0
4	G	843	0	908	32	0
5	D	718	0	740	11	0
5	H	744	0	771	18	0
6	A	20	0	0	0	0
6	B	16	0	0	0	0
6	C	21	0	0	3	0
6	D	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	35	0	0	1	0
6	F	27	0	0	2	0
6	G	14	0	0	3	0
6	H	6	0	0	2	0
6	I	29	0	0	8	0
6	J	33	0	0	4	0
All	All	12243	0	9676	336	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 16.

All (336) 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)
3:F:297:LEU:HD21	3:F:302:GLY:C	1.58	1.28
3:F:299:GLY:O	3:F:300:PHE:HB2	1.26	1.07
2:E:691:ALA:HB1	3:F:302:GLY:OXT	1.54	1.06
3:B:98:TYR:HD1	3:B:102:GLY:OXT	1.37	1.06
1:J:273:DA:H4'	1:J:274:DT:OP1	1.57	1.03
1:J:272:DA:H1'	1:J:273:DA:H5'	1.33	1.03
3:F:299:GLY:O	3:F:300:PHE:CB	2.05	1.03
3:F:297:LEU:CD2	3:F:302:GLY:C	2.32	1.02
3:F:300:PHE:HB2	3:F:302:GLY:HA2	1.39	1.02
3:F:300:PHE:HB3	3:F:302:GLY:N	1.73	1.02
3:F:297:LEU:HD21	3:F:302:GLY:OXT	1.60	1.00
1:I:21:DT:H2''	1:I:22:DC:O5'	1.61	0.99
3:F:300:PHE:CD1	3:F:302:GLY:O	2.16	0.97
1:I:3:DC:H42	1:J:290:DG:H1	1.01	0.97
1:I:3:DC:N4	1:J:290:DG:H1	1.62	0.97
1:J:213:DA:H4'	6:J:315:HOH:O	1.64	0.95
4:G:1017:ARG:HH12	4:G:1031:HIS:HD2	1.09	0.94
3:F:300:PHE:CB	3:F:302:GLY:HA2	1.98	0.94
3:B:98:TYR:CD1	3:B:102:GLY:OXT	2.21	0.93
2:E:694:GLU:HG3	3:F:300:PHE:CE1	2.03	0.93
1:J:151:DA:H2''	1:J:152:DT:H5''	1.49	0.92
1:J:272:DA:H2''	1:J:273:DA:O5'	1.68	0.92
2:E:691:ALA:CB	3:F:302:GLY:OXT	2.18	0.91
2:A:529:ARG:NE	2:A:535:ALA:HB3	1.85	0.91
4:G:1081:ARG:NH1	6:G:212:HOH:O	2.04	0.89
1:J:246:DG:H2''	1:J:247:DC:C5	2.09	0.87
2:A:529:ARG:HG3	2:A:529:ARG:HH11	1.39	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:DT:H72	1:I:24:DA:N7	1.91	0.86
2:E:729:ARG:O	2:E:735:ALA:HB2	1.74	0.86
3:F:300:PHE:HB3	3:F:301:GLY:C	1.97	0.85
1:J:237:DT:H4'	2:A:463:ARG:CZ	2.07	0.84
3:F:300:PHE:CB	3:F:302:GLY:CA	2.56	0.84
4:G:1017:ARG:HH12	4:G:1031:HIS:CD2	1.94	0.84
1:J:261:DA:H2''	1:J:262:DC:H5''	1.59	0.82
2:A:529:ARG:HA	2:A:534:ARG:HB3	1.61	0.82
4:C:902:ILE:HG23	5:D:1258:ILE:HD13	1.62	0.82
2:E:694:GLU:HG3	3:F:300:PHE:HE1	1.44	0.81
4:C:817:ARG:HH12	4:C:831:HIS:HD2	1.29	0.81
4:C:881:ARG:NH1	6:C:210:HOH:O	1.99	0.81
1:J:151:DA:C2'	1:J:152:DT:H5''	2.10	0.80
1:I:82:DA:OP1	6:I:156:HOH:O	1.97	0.80
3:F:297:LEU:HD21	3:F:302:GLY:O	1.81	0.80
3:F:300:PHE:HD1	3:F:302:GLY:O	1.65	0.79
3:F:300:PHE:HB3	3:F:302:GLY:CA	2.13	0.79
1:I:82:DA:P	6:I:156:HOH:O	2.43	0.77
6:I:156:HOH:O	2:E:646:VAL:HB	1.83	0.77
2:E:649:ARG:HG3	2:E:649:ARG:HH11	1.49	0.77
1:I:27:DA:H2''	1:I:28:DA:OP2	1.85	0.77
1:I:121:DG:N7	6:I:172:HOH:O	2.17	0.76
4:G:1081:ARG:CZ	6:G:212:HOH:O	2.33	0.76
2:A:529:ARG:CD	2:A:535:ALA:HB3	2.16	0.76
2:A:529:ARG:NH1	2:A:535:ALA:OXT	2.19	0.75
1:I:48:DT:H6	1:I:48:DT:H5'	1.52	0.74
1:I:3:DC:N3	1:J:290:DG:N2	2.35	0.74
1:I:89:DC:H2''	1:I:90:DT:H72	1.69	0.74
1:J:273:DA:C4'	1:J:274:DT:OP1	2.36	0.72
1:J:151:DA:H2''	1:J:152:DT:C5'	2.19	0.72
4:C:855:LEU:O	4:C:859:THR:HG23	1.88	0.72
1:J:193:DC:H2''	1:J:194:DT:H72	1.73	0.71
4:G:1015:LYS:HG3	4:G:1019:SER:OG	1.90	0.71
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.73	0.70
1:I:25:DC:H2''	1:I:26:DC:H5'	1.72	0.70
1:J:249:DG:H5''	5:H:1428:LYS:HA	1.72	0.70
4:C:881:ARG:NH2	6:C:210:HOH:O	2.20	0.70
5:D:1321:ALA:O	5:D:1322:LYS:HB2	1.90	0.70
3:F:295:ARG:HD3	6:F:128:HOH:O	1.91	0.70
2:E:677:ASP:OD1	6:E:113:HOH:O	2.10	0.69
1:I:22:DC:O2	1:J:272:DA:C2	2.44	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:691:ALA:CA	3:F:302:GLY:OXT	2.41	0.69
1:I:1:DA:H2''	1:I:2:DT:H71	1.73	0.68
2:E:694:GLU:HG3	3:F:300:PHE:CZ	2.29	0.68
1:J:233:DG:H2''	1:J:234:DC:OP2	1.91	0.68
3:F:300:PHE:CD1	3:F:302:GLY:C	2.71	0.68
1:J:261:DA:C2'	1:J:262:DC:H5''	2.23	0.68
3:F:300:PHE:CB	3:F:301:GLY:C	2.61	0.68
1:I:138:DG:H2''	1:I:139:DA:OP2	1.94	0.67
3:F:297:LEU:CD2	3:F:302:GLY:OXT	2.38	0.67
1:J:214:DG:H5''	6:J:302:HOH:O	1.95	0.66
2:E:725:GLN:HB3	2:E:734:ARG:NH2	2.10	0.66
1:J:246:DG:H2''	1:J:247:DC:C6	2.30	0.66
4:C:881:ARG:CZ	6:C:210:HOH:O	2.41	0.66
5:H:1445:VAL:HG12	5:H:1446:HIS:CD2	2.31	0.66
1:J:176:DA:OP2	4:G:1032:ARG:HD3	1.95	0.66
1:J:248:DA:H2''	1:J:249:DG:C8	2.31	0.65
1:J:272:DA:C1'	1:J:273:DA:H5'	2.17	0.65
4:G:1084:GLN:OE1	4:G:1088:ARG:HD2	1.95	0.65
1:J:214:DG:C5'	6:J:302:HOH:O	2.44	0.64
1:J:152:DT:H2''	1:J:153:DA:C8	2.33	0.64
1:J:271:DG:H2''	1:J:272:DA:OP2	1.97	0.63
4:G:1017:ARG:NH1	4:G:1031:HIS:HD2	1.91	0.63
1:I:20:DT:O2	1:I:21:DT:H5'	1.98	0.63
1:J:237:DT:H4'	2:A:463:ARG:NH2	2.13	0.63
3:F:287:VAL:CG2	3:F:302:GLY:N	2.62	0.62
1:I:53:DC:H42	1:J:240:DG:H1	1.48	0.62
4:C:817:ARG:HH12	4:C:831:HIS:CD2	2.15	0.62
2:A:529:ARG:HG3	2:A:529:ARG:NH1	2.07	0.62
2:A:508:ASN:HD21	4:G:1115:LEU:HD11	1.65	0.61
3:B:24:ASP:CG	3:B:25:ASN:H	2.08	0.61
3:F:292:ARG:NH2	5:H:1498:LEU:HD23	2.16	0.61
4:C:879:ILE:HG12	4:C:882:HIS:CE1	2.36	0.61
1:I:93:DT:H1'	1:I:94:DG:H5''	1.84	0.60
4:C:919:LYS:HD3	4:C:919:LYS:N	2.17	0.60
1:I:2:DT:H1'	1:I:3:DC:H5''	1.84	0.59
3:B:59:LYS:HE2	3:B:63:GLU:OE2	2.03	0.59
2:E:663:ARG:HA	2:E:663:ARG:NE	2.18	0.59
1:J:249:DG:H5''	5:H:1428:LYS:HD3	1.85	0.59
1:I:5:DA:H2''	1:I:6:DT:H5'	1.85	0.59
5:D:1277:LEU:HD21	5:D:1293:THR:HB	1.84	0.59
1:J:174:DA:H2''	1:J:175:DA:H5''	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:534:ARG:O	2:A:535:ALA:HB2	2.03	0.58
1:I:26:DC:H1'	1:I:27:DA:C5	2.39	0.58
3:F:300:PHE:CB	3:F:301:GLY:O	2.50	0.58
1:I:58:DG:H1	1:J:235:DC:H42	1.52	0.58
4:G:1084:GLN:O	4:G:1088:ARG:HG2	2.03	0.58
1:I:5:DA:H1'	1:I:6:DT:H5''	1.86	0.58
3:F:299:GLY:C	3:F:301:GLY:O	2.47	0.57
4:G:1076:THR:O	5:H:1449:THR:HG23	2.03	0.57
2:E:729:ARG:HG3	2:E:735:ALA:HA	1.85	0.57
2:E:663:ARG:HA	2:E:663:ARG:HE	1.68	0.57
1:J:261:DA:H2''	1:J:262:DC:C5'	2.32	0.57
2:A:463:ARG:HG2	2:A:463:ARG:HH11	1.69	0.57
2:E:637:LYS:HD3	2:E:637:LYS:N	2.20	0.57
1:I:20:DT:OP2	6:I:162:HOH:O	2.17	0.57
1:J:280:DG:N7	6:J:293:HOH:O	2.33	0.57
1:J:272:DA:C2'	1:J:273:DA:O5'	2.49	0.56
1:I:82:DA:C5'	6:I:156:HOH:O	2.53	0.56
1:I:100:DG:H5''	2:E:683:ARG:HD2	1.87	0.56
1:J:174:DA:C2'	1:J:175:DA:H5''	2.34	0.56
1:I:26:DC:H1'	1:I:27:DA:C4	2.41	0.56
1:I:5:DA:H2''	1:I:6:DT:C5'	2.36	0.55
1:I:126:DA:H1'	1:I:127:DA:H5'	1.88	0.55
1:I:57:DA:H2''	1:I:58:DG:C8	2.41	0.55
1:I:27:DA:C5	1:I:28:DA:C6	2.95	0.55
4:C:817:ARG:NH1	4:C:831:HIS:HD2	2.02	0.55
1:I:21:DT:C2'	1:I:22:DC:O5'	2.44	0.54
3:B:102:GLY:N	5:H:1461:SER:OG	2.37	0.54
1:I:21:DT:O2	1:J:273:DA:H2	1.91	0.54
1:J:177:DG:H5''	4:G:1016:THR:HA	1.89	0.54
2:A:492:LEU:HD13	3:B:86:VAL:HG13	1.88	0.54
1:I:93:DT:H2''	1:I:94:DG:H5'	1.90	0.54
1:J:148:DT:H2''	1:J:149:DC:O5'	2.07	0.54
1:I:6:DT:H2''	1:I:7:DA:C8	2.43	0.54
2:A:463:ARG:O	2:A:466:PRO:HD2	2.07	0.54
1:J:235:DC:H2''	1:J:236:DT:OP2	2.08	0.53
2:E:725:GLN:CB	2:E:734:ARG:NH2	2.71	0.53
4:G:1084:GLN:CD	4:G:1088:ARG:HD2	2.34	0.53
2:A:463:ARG:HG2	2:A:463:ARG:NH1	2.23	0.53
1:I:23:DT:O4	1:I:24:DA:C6	2.62	0.53
3:F:228:GLY:HA3	6:F:50:HOH:O	2.08	0.53
1:J:229:DA:N3	2:A:440:ARG:NH2	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:718:HIS:CE1	3:F:245:ARG:NH1	2.76	0.53
4:C:817:ARG:HH22	4:C:831:HIS:CD2	2.27	0.53
1:I:19:DA:N6	1:J:273:DA:N6	2.57	0.53
1:J:288:DT:H1'	1:J:289:DT:H5''	1.90	0.53
2:A:476:GLN:NE2	2:A:480:THR:HG22	2.23	0.53
1:I:20:DT:O4	1:J:273:DA:N1	2.42	0.53
4:C:902:ILE:CG2	5:D:1258:ILE:HD13	2.37	0.52
1:J:262:DC:H2'	1:J:263:DT:H71	1.91	0.52
1:J:264:DT:H2''	1:J:265:DT:OP2	2.09	0.52
3:F:300:PHE:O	3:F:302:GLY:N	2.39	0.52
2:A:492:LEU:HD13	3:B:86:VAL:CG1	2.40	0.52
1:J:147:DA:H2'	1:J:148:DT:H72	1.91	0.52
2:E:718:HIS:HE1	3:F:245:ARG:HH11	1.57	0.52
1:J:229:DA:OP1	2:A:446:VAL:HB	2.10	0.52
3:F:287:VAL:HG21	3:F:301:GLY:C	2.35	0.52
4:G:1116:LEU:HB3	4:G:1117:PRO:HD2	1.91	0.52
1:I:2:DT:H2''	1:I:3:DC:H5'	1.91	0.51
1:I:20:DT:O2	1:I:21:DT:O4'	2.28	0.51
2:E:668:GLN:HG3	2:E:689:VAL:HG11	1.92	0.51
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.92	0.51
4:C:850:TYR:OH	5:D:1292:GLN:HG3	2.09	0.51
2:E:699:TYR:OH	2:E:733:GLU:OE2	2.29	0.51
3:B:102:GLY:H	5:H:1461:SER:CB	2.23	0.51
1:J:174:DA:H1'	1:J:175:DA:H5''	1.93	0.51
1:I:23:DT:H72	1:I:24:DA:C5	2.45	0.51
1:I:70:DG:N7	6:I:147:HOH:O	2.35	0.51
1:I:48:DT:H5'	1:I:48:DT:C6	2.40	0.50
2:E:691:ALA:HA	3:F:302:GLY:OXT	2.12	0.50
1:I:21:DT:O2	1:J:273:DA:C2	2.65	0.50
1:I:49:DC:H1'	1:I:50:DC:C6	2.46	0.50
2:A:516:ARG:HD2	2:A:520:MET:HE3	1.92	0.50
4:G:1102:ILE:HG23	5:H:1458:ILE:HD13	1.94	0.50
1:J:193:DC:H2''	1:J:194:DT:C7	2.41	0.50
1:I:19:DA:C8	1:I:20:DT:H73	2.47	0.50
4:G:1079:ILE:HB	4:G:1080:PRO:CD	2.41	0.50
1:I:49:DC:H1'	1:I:50:DC:C5	2.47	0.50
3:B:24:ASP:OD1	3:B:25:ASN:N	2.44	0.50
1:I:27:DA:C6	1:I:28:DA:C6	2.99	0.49
1:I:34:DT:H2''	1:I:35:DA:O5'	2.12	0.49
1:I:7:DA:C2	1:J:287:DA:C2	3.00	0.49
1:J:182:DT:H2''	1:J:183:DT:OP2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:458:THR:HG21	4:G:1081:ARG:HG2	1.94	0.49
4:G:1035:ARG:HH11	4:G:1035:ARG:HG2	1.77	0.49
1:I:116:DC:H2''	1:I:117:DT:OP2	2.12	0.49
1:J:174:DA:H4'	5:H:1430:ARG:HD3	1.94	0.49
3:B:59:LYS:O	3:B:63:GLU:HG3	2.12	0.49
1:J:149:DC:H2''	1:J:150:DA:C8	2.47	0.49
3:B:31:LYS:HG3	3:B:51:TYR:CE1	2.47	0.49
5:D:1287:THR:H	5:D:1290:GLU:HG2	1.77	0.49
4:C:831:HIS:CE1	4:C:835:ARG:NH2	2.81	0.49
1:I:80:DT:H4'	2:E:718:HIS:CE1	2.48	0.49
2:E:679:LYS:HG3	3:F:274:GLU:OE2	2.13	0.49
4:G:1081:ARG:NH2	6:G:212:HOH:O	2.43	0.49
5:H:1473:GLU:OE2	6:H:124:HOH:O	2.19	0.48
1:J:289:DT:H5'	1:J:289:DT:H6	1.77	0.48
5:D:1239:TYR:CZ	5:D:1243:LYS:HE2	2.48	0.48
2:E:733:GLU:O	2:E:734:ARG:HB3	2.13	0.48
1:I:19:DA:C2'	1:I:20:DT:H71	2.43	0.48
1:I:23:DT:H2''	1:I:24:DA:O5'	2.13	0.48
1:J:289:DT:H2''	1:J:290:DG:C8	2.48	0.48
2:E:728:ARG:HD2	2:E:733:GLU:OE2	2.12	0.48
1:J:249:DG:C5'	5:H:1428:LYS:HD3	2.44	0.48
4:G:1081:ARG:NH2	4:G:1107:VAL:O	2.46	0.48
4:C:829:ARG:NH2	5:D:1233:SER:O	2.46	0.48
2:E:718:HIS:CE1	3:F:245:ARG:HH11	2.31	0.48
1:I:24:DA:H2''	1:I:25:DC:OP2	2.14	0.48
3:B:26:ILE:HG13	3:B:55:ARG:HD3	1.94	0.48
3:F:230:THR:HB	3:F:232:PRO:HD2	1.95	0.48
1:I:36:DT:H2''	1:I:37:DT:OP2	2.13	0.47
1:I:39:DG:H4'	4:C:842:ARG:NE	2.28	0.47
2:A:449:ARG:CB	2:A:449:ARG:HH11	2.27	0.47
1:J:270:DA:H2''	1:J:271:DG:O5'	2.13	0.47
4:G:1032:ARG:HH22	5:H:1432:GLU:CD	2.21	0.47
4:G:1114:VAL:HG22	4:G:1114:VAL:O	2.14	0.47
1:J:197:DA:H1'	1:J:198:DT:H5'	1.94	0.47
1:I:1:DA:H2''	1:I:2:DT:C7	2.43	0.47
4:C:837:GLY:HA3	4:C:839:TYR:CE1	2.49	0.47
1:I:19:DA:H2''	1:I:20:DT:H71	1.97	0.47
2:A:529:ARG:HD2	2:A:535:ALA:N	2.29	0.47
1:J:184:DT:H2''	1:J:185:DG:N7	2.29	0.47
1:J:195:DC:H1'	1:J:196:DC:C5	2.50	0.47
1:J:149:DC:C2'	1:J:150:DA:C8	2.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:529:ARG:CZ	2:A:535:ALA:OXT	2.63	0.47
3:B:101:GLY:N	6:H:21:HOH:O	2.47	0.47
5:D:1277:LEU:CD2	5:D:1293:THR:HB	2.45	0.46
1:I:81:DG:C3'	6:I:171:HOH:O	2.64	0.46
1:I:94:DG:H1	1:J:199:DC:H42	1.62	0.46
2:E:718:HIS:HE1	3:F:245:ARG:NH1	2.11	0.46
1:I:80:DT:H4'	2:E:718:HIS:HE1	1.81	0.46
2:A:529:ARG:NE	2:A:535:ALA:CB	2.68	0.46
1:I:20:DT:H1'	1:I:21:DT:H5'	1.98	0.45
1:J:170:DA:H2''	1:J:171:DC:OP2	2.15	0.45
2:A:449:ARG:HH11	2:A:449:ARG:HB3	1.80	0.45
2:E:680:THR:O	2:E:681:ASP:HB2	2.15	0.45
4:G:1031:HIS:CE1	4:G:1035:ARG:NH2	2.84	0.45
4:G:1020:ARG:HH11	4:G:1020:ARG:HG2	1.82	0.45
4:G:1079:ILE:HB	4:G:1080:PRO:HD2	1.97	0.45
2:E:659:GLU:N	2:E:659:GLU:OE1	2.49	0.45
1:I:112:DT:OP2	4:G:1035:ARG:NH2	2.50	0.45
1:I:10:DC:H1'	1:I:11:DA:C8	2.51	0.45
1:I:19:DA:C5	1:I:20:DT:H73	2.51	0.45
4:C:847:ALA:HB3	4:C:848:PRO:HD3	1.98	0.45
4:C:918:LYS:HB2	4:C:918:LYS:NZ	2.30	0.45
3:F:265:VAL:HA	3:F:293:GLN:HE22	1.82	0.45
3:F:287:VAL:HG22	3:F:302:GLY:HA3	1.98	0.45
2:A:532:GLY:C	2:A:534:ARG:N	2.74	0.45
4:G:1013:LYS:O	4:G:1014:ALA:HB2	2.17	0.45
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.88	0.45
1:J:194:DT:H2''	1:J:195:DC:C6	2.52	0.44
3:F:300:PHE:HB2	3:F:301:GLY:O	2.17	0.44
1:I:141:DA:C2	1:J:153:DA:C2	3.04	0.44
2:A:452:ARG:HG3	2:A:452:ARG:HH11	1.82	0.44
3:F:297:LEU:CD2	3:F:302:GLY:O	2.56	0.44
2:A:532:GLY:C	2:A:534:ARG:H	2.24	0.44
3:F:300:PHE:CE1	3:F:302:GLY:O	2.69	0.44
4:G:1031:HIS:CD2	4:G:1048:PRO:HG3	2.53	0.44
5:H:1487:THR:OG1	5:H:1490:GLU:OE1	2.32	0.44
1:I:9:DC:H2''	1:I:10:DC:O5'	2.16	0.43
3:B:30:THR:HB	3:B:32:PRO:HD2	2.00	0.43
3:B:102:GLY:N	5:H:1461:SER:CB	2.80	0.43
3:F:287:VAL:HG21	3:F:302:GLY:N	2.33	0.43
1:I:48:DT:C6	1:I:48:DT:C5'	3.01	0.43
1:J:174:DA:H2''	1:J:175:DA:C5'	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:299:GLY:O	3:F:301:GLY:O	2.35	0.43
1:I:130:DT:H2''	1:I:131:DG:N7	2.33	0.43
1:I:117:DT:C2'	1:I:118:DT:H71	2.48	0.43
1:J:181:DA:H2''	1:J:182:DT:OP2	2.19	0.43
1:J:247:DC:C4	1:J:248:DA:C6	3.06	0.43
1:I:114:DC:H4'	1:I:114:DC:OP1	2.18	0.43
3:F:300:PHE:CA	3:F:301:GLY:O	2.61	0.43
1:I:89:DC:H2''	1:I:90:DT:C7	2.45	0.43
4:G:1031:HIS:HE1	4:G:1035:ARG:CZ	2.32	0.43
1:I:119:DT:H4'	1:I:120:DT:OP1	2.17	0.43
1:J:162:DC:H2''	1:J:163:DA:N7	2.33	0.43
3:B:24:ASP:CG	3:B:25:ASN:N	2.72	0.43
4:C:835:ARG:HG2	4:C:835:ARG:HH11	1.84	0.43
2:A:529:ARG:HE	2:A:535:ALA:HB3	1.76	0.42
4:C:873:ASN:O	4:C:875:LYS:HG2	2.18	0.42
1:I:19:DA:C8	1:I:20:DT:C7	3.02	0.42
1:J:228:DA:H2''	1:J:229:DA:OP2	2.19	0.42
1:J:266:DT:H2''	1:J:267:DG:N7	2.34	0.42
5:D:1277:LEU:HD21	5:D:1293:THR:CB	2.49	0.42
1:I:48:DT:H6	1:I:48:DT:C5'	2.24	0.42
1:J:172:DC:O2	1:J:173:DA:C2	2.73	0.42
2:A:476:GLN:HE21	2:A:480:THR:HG22	1.84	0.42
2:A:529:ARG:CA	2:A:534:ARG:HB3	2.42	0.42
1:I:27:DA:C2'	1:I:28:DA:OP2	2.62	0.42
1:I:121:DG:H5''	5:H:1437:TYR:OH	2.19	0.42
2:A:439:HIS:ND1	2:A:439:HIS:C	2.78	0.42
2:A:510:CYS:SG	2:A:526:LEU:HD23	2.59	0.42
4:C:825:PHE:CZ	4:C:859:THR:HG21	2.54	0.42
2:E:649:ARG:HG3	2:E:649:ARG:NH1	2.25	0.42
3:F:252:GLU:OE2	3:F:255:ARG:NH1	2.53	0.42
1:I:133:DA:C2	1:J:161:DG:N2	2.88	0.42
1:J:280:DG:H1'	1:J:281:DG:C8	2.55	0.42
1:J:228:DA:H4'	2:A:443:PRO:HB3	2.01	0.41
1:J:289:DT:H5'	1:J:289:DT:C6	2.54	0.41
1:I:23:DT:H2'	1:I:23:DT:O5'	2.21	0.41
4:G:1035:ARG:HG2	4:G:1035:ARG:NH1	2.34	0.41
1:J:272:DA:H1'	1:J:273:DA:C5'	2.23	0.41
1:I:22:DC:N4	1:J:270:DA:N6	2.68	0.41
1:J:182:DT:H1'	1:J:183:DT:H5'	2.03	0.41
4:C:865:LEU:HB3	4:C:886:ALA:HB1	2.02	0.41
2:E:725:GLN:HG2	2:E:734:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:732:GLY:C	2:E:734:ARG:H	2.28	0.41
4:G:1031:HIS:HE1	4:G:1035:ARG:NH2	2.16	0.41
4:G:1031:HIS:CE1	4:G:1035:ARG:CZ	3.03	0.41
1:I:26:DC:H4'	1:I:27:DA:OP1	2.21	0.41
1:I:77:DC:H2''	1:I:78:DG:C8	2.56	0.41
1:J:149:DC:C1'	1:J:150:DA:OP1	2.68	0.41
1:I:29:DA:C2'	1:I:30:DA:C8	3.04	0.41
1:J:268:DG:H2''	1:J:269:DT:O5'	2.20	0.41
5:D:1299:LEU:HA	5:D:1300:PRO:HD3	1.91	0.41
3:F:297:LEU:HD11	3:F:302:GLY:O	2.21	0.41
5:H:1443:LYS:HD3	5:H:1443:LYS:HA	1.74	0.41
1:I:23:DT:O5'	1:I:23:DT:C2'	2.68	0.40
2:A:463:ARG:C	2:A:466:PRO:HD2	2.46	0.40
3:B:44:LYS:HG2	3:B:45:ARG:HG2	2.02	0.40
1:J:147:DA:C2'	1:J:148:DT:H72	2.52	0.40
1:J:239:DT:H2''	1:J:240:DG:C8	2.56	0.40
3:F:231:LYS:O	3:F:235:ARG:HG2	2.22	0.40
1:I:48:DT:H2'	1:I:49:DC:C6	2.56	0.40
1:I:34:DT:H2''	1:I:35:DA:H8	1.87	0.40
1:I:113:DA:H2''	1:I:114:DC:O5'	2.20	0.40
4:C:917:PRO:HD3	2:E:648:LEU:CD1	2.52	0.40
5:H:1443:LYS:O	5:H:1447:PRO:HG3	2.21	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%)	95 (99%)	1 (1%)	0	100	100
2	E	97/135 (72%)	93 (96%)	2 (2%)	2 (2%)	5	7
3	B	77/102 (76%)	75 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	81/102 (79%)	77 (95%)	3 (4%)	1 (1%)	10	16
4	C	104/129 (81%)	99 (95%)	4 (4%)	1 (1%)	12	20
4	G	107/129 (83%)	101 (94%)	3 (3%)	3 (3%)	4	3
5	D	90/125 (72%)	87 (97%)	2 (2%)	1 (1%)	11	18
5	H	93/125 (74%)	89 (96%)	3 (3%)	1 (1%)	11	18
All	All	745/982 (76%)	716 (96%)	20 (3%)	9 (1%)	10	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	734	ARG
4	G	1014	ALA
5	H	1501	GLY
5	D	1301	GLY
2	E	638	PRO
3	F	300	PHE
4	G	1013	LYS
4	C	918	LYS
4	G	1114	VAL

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	85/111 (77%)	81 (95%)	4 (5%)	23	41
2	E	86/111 (78%)	84 (98%)	2 (2%)	44	66
3	B	64/78 (82%)	64 (100%)	0	100	100
3	F	68/78 (87%)	65 (96%)	3 (4%)	25	43
4	C	85/100 (85%)	78 (92%)	7 (8%)	10	18
4	G	86/100 (86%)	84 (98%)	2 (2%)	44	66
5	D	78/105 (74%)	76 (97%)	2 (3%)	40	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	81/105 (77%)	79 (98%)	2 (2%)	42	64
All	All	633/788 (80%)	611 (96%)	22 (4%)	32	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	449	ARG
2	A	459	GLU
2	A	463	ARG
2	A	492	LEU
4	C	829	ARG
4	C	859	THR
4	C	876	THR
4	C	881	ARG
4	C	909	PRO
4	C	918	LYS
4	C	919	LYS
5	D	1233	SER
5	D	1290	GLU
2	E	637	LYS
2	E	638	PRO
3	F	222	LEU
3	F	247	SER
3	F	300	PHE
4	G	1081	ARG
4	G	1088	ARG
5	H	1431	LYS
5	H	1433	SER

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

Mol	Chain	Res	Type
2	A	476	GLN
2	A	508	ASN
2	A	518	HIS
4	C	831	HIS
4	C	838	ASN
2	E	668	GLN
2	E	718	HIS
3	F	293	GLN
4	G	1031	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	H	1506	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.