



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:47 PM UTC

PDB ID : 1P3F / pdb_00001p3f
Title : Crystallographic Studies of Nucleosome Core Particles containing Histone 'Sin' Mutants
Authors : Muthurajan, U.M.; Bao, Y.; Forsberg, L.J.; Edayathumangalam, R.S.; Dyer, P.N.; White, C.L.; Luger, K.
Deposited on : 2003-04-17
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<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

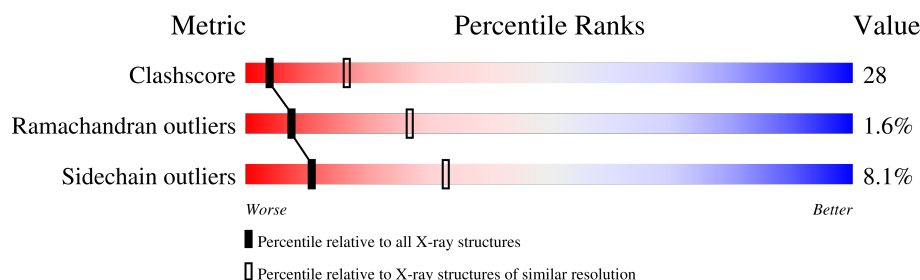
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	J	146	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	129	
4	G	129	

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Mol	Chain	Length	Quality of chain
5	D	125	33%30%8%27%
5	H	125	32%34%10%24%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12150 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called Palindromic 146bp Human Alpha-Satellite DNA fragment.

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

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	99	Total	C	N	O	S	0	0	0
			817	515	158	141	3			
2	E	99	Total	C	N	O	S	0	0	0
			817	515	158	141	3			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	80	Total	C	N	O	S	0	0	0
			633	398	122	111	2			
3	F	82	Total	C	N	O	S	0	0	0
			648	409	124	113	2			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Histone H2A.

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

There are 48 discrepancies between the modelled and reference sequences:

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

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

- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	91	Total	C	N	O	S	0	0	0
			709	447	125	135	2			
5	H	95	Total	C	N	O	S	0	0	0
			744	468	134	140	2			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is water.

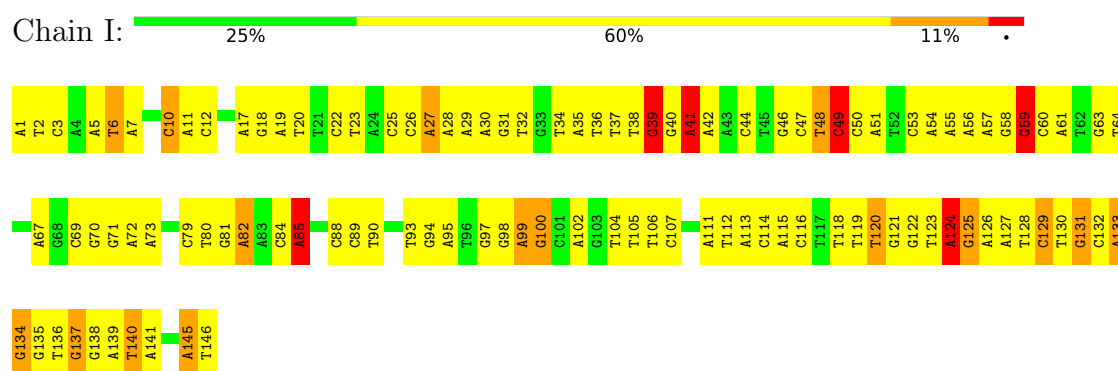
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	39	Total 39	O 39	0	0
6	J	39	Total 39	O 39	0	0
6	A	9	Total 9	O 9	0	0
6	B	8	Total 8	O 8	0	0
6	C	16	Total 16	O 16	0	0
6	D	9	Total 9	O 9	0	0
6	E	17	Total 17	O 17	0	0
6	F	16	Total 16	O 16	0	0
6	G	13	Total 13	O 13	0	0
6	H	5	Total 5	O 5	0	0

3 Residue-property plots

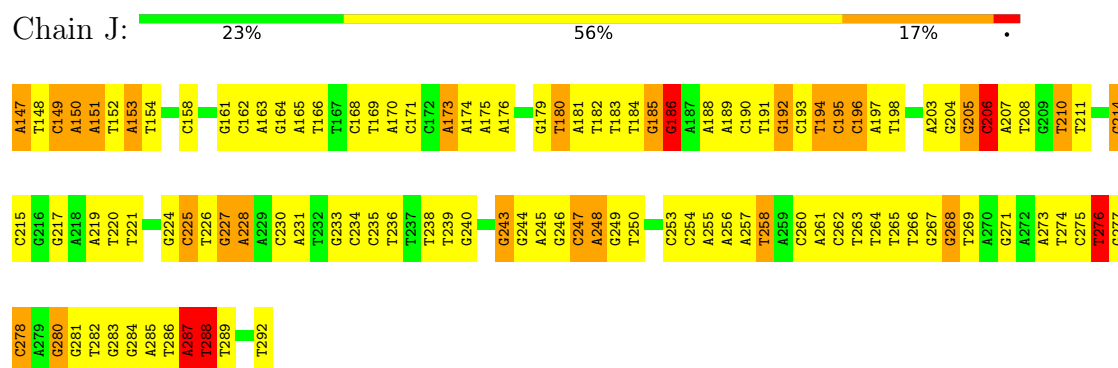
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

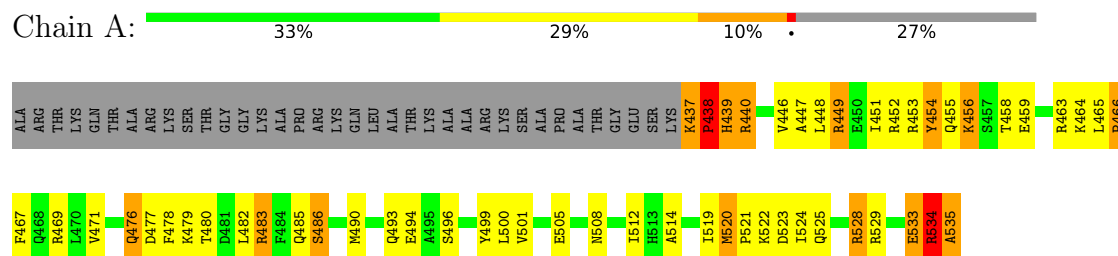
• Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment



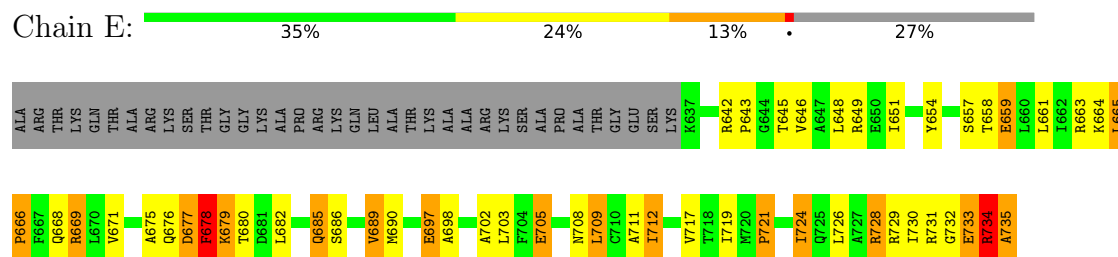
• Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment



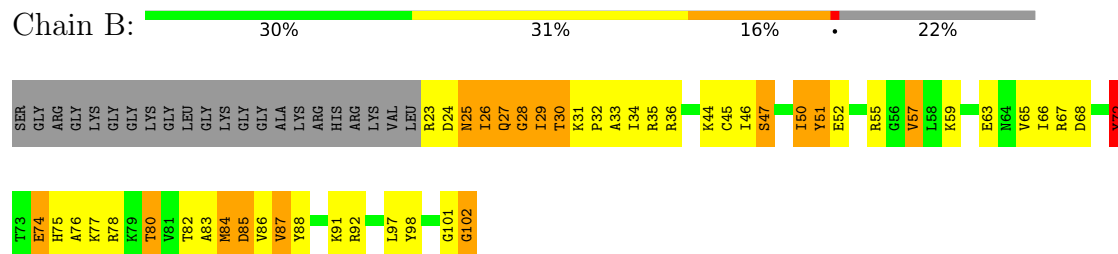
• Molecule 2: Histone H3



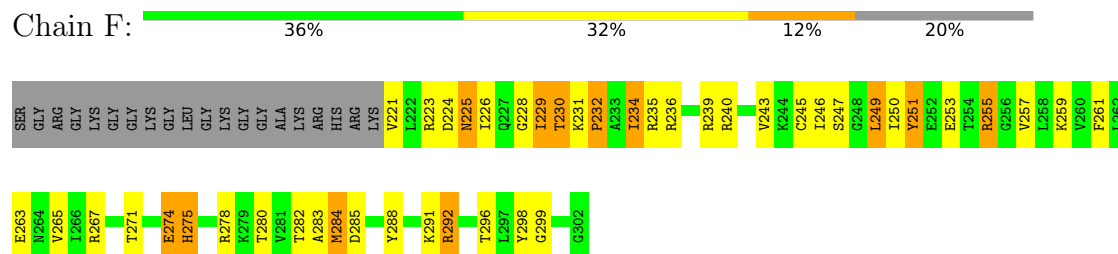
• Molecule 2: Histone H3



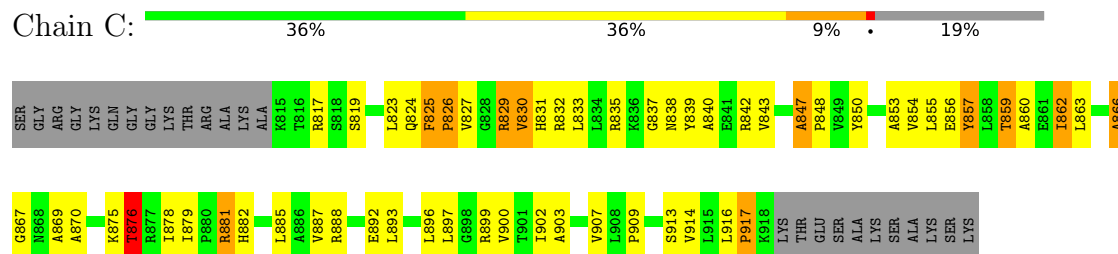
- Molecule 3: Histone H4



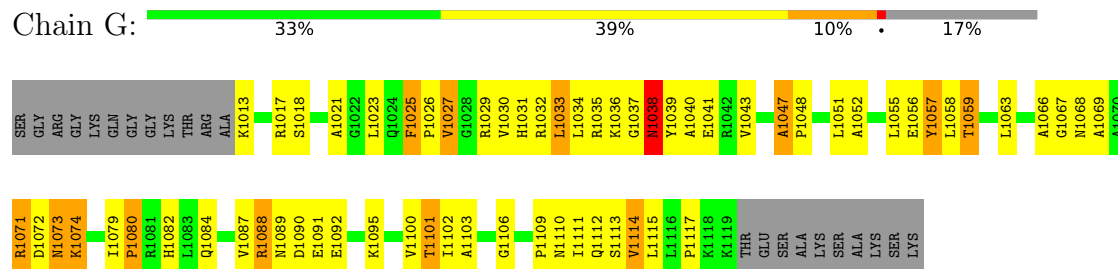
- Molecule 3: Histone H4



- Molecule 4: Histone H2A

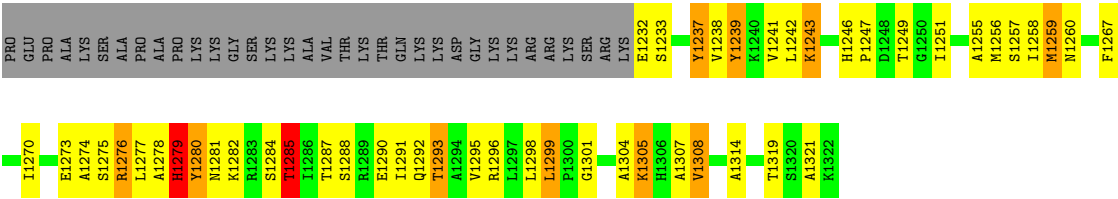


- Molecule 4: Histone H2A



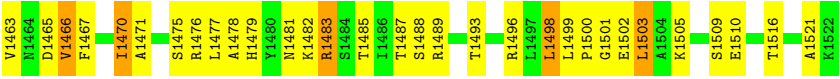
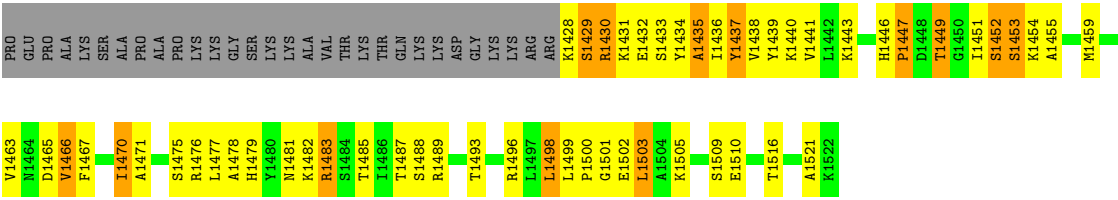
- Molecule 5: Histone H2B

Chain D: 33% 30% 8% 27%



● Molecule 5: Histone H2B

Chain H: 32% 34% 10% 24%



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	105.74Å 109.50Å 181.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	94.1 (40.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12150	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	I	0.77	0/3354	1.16	17/5175 (0.3%)
1	J	0.76	0/3354	1.15	19/5175 (0.4%)
2	A	1.87	18/829 (2.2%)	1.89	21/1111 (1.9%)
2	E	2.13	24/829 (2.9%)	1.89	24/1111 (2.2%)
3	B	1.82	9/640 (1.4%)	1.72	16/856 (1.9%)
3	F	2.03	19/655 (2.9%)	1.83	13/877 (1.5%)
4	C	1.80	13/814 (1.6%)	1.82	18/1099 (1.6%)
4	G	1.65	12/837 (1.4%)	1.64	16/1128 (1.4%)
5	D	1.77	9/720 (1.2%)	1.81	16/969 (1.7%)
5	H	1.73	11/755 (1.5%)	1.52	4/1013 (0.4%)
All	All	1.40	115/12787 (0.9%)	1.46	164/18514 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	18
1	J	0	25
2	A	0	1
2	E	0	1
3	B	0	3
3	F	0	1
4	C	0	1
4	G	0	1
5	D	0	3
All	All	0	54

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	735	ALA	C-O	14.81	1.53	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	677	ASP	CB-CG	11.71	1.81	1.52
2	E	677	ASP	CA-CB	11.65	1.68	1.52
2	E	732	GLY	C-O	-11.55	1.08	1.23
5	D	1255	ALA	CA-CB	-11.05	1.35	1.53
3	B	34	ILE	CA-CB	-10.52	1.41	1.54
3	F	251	TYR	CA-C	-9.88	1.40	1.52
4	C	870	ALA	CA-CB	-9.75	1.38	1.53
2	E	735	ALA	CA-CB	9.72	1.84	1.52
5	H	1438	VAL	CA-CB	-9.71	1.43	1.54
2	E	665	LEU	N-CA	-9.34	1.36	1.46
3	B	84	MET	SD-CE	9.21	2.02	1.79
4	G	1040	ALA	CA-CB	-9.04	1.38	1.53
2	E	735	ALA	C-OXT	8.84	1.41	1.23
3	B	87	VAL	CA-CB	-8.44	1.44	1.54
2	A	534	ARG	CA-C	8.42	1.63	1.52
2	E	678	PHE	N-CA	8.37	1.56	1.46
5	H	1466	VAL	CA-CB	-8.00	1.45	1.54
3	F	243	VAL	CA-CB	-7.64	1.45	1.54
2	E	677	ASP	CA-C	7.51	1.62	1.53
4	G	1027	VAL	CA-CB	-7.49	1.45	1.54
2	A	476	GLN	C-O	-7.43	1.14	1.24
4	C	827	VAL	CA-CB	-7.32	1.45	1.54
2	E	717	VAL	CA-CB	-7.32	1.46	1.54
2	E	733	GLU	CG-CD	7.29	1.70	1.52
3	B	65	VAL	CA-CB	-7.27	1.46	1.54
5	H	1437	TYR	CA-C	-7.24	1.42	1.52
3	B	86	VAL	CA-CB	7.20	1.63	1.54
3	F	283	ALA	CA-CB	-7.18	1.40	1.53
4	C	875	LYS	CB-CG	-7.16	1.30	1.52
3	B	97	LEU	C-O	-7.16	1.15	1.24
2	A	471	VAL	CA-CB	-7.15	1.46	1.54
5	D	1233	SER	C-O	-6.79	1.15	1.23
5	H	1478	ALA	CA-CB	-6.76	1.42	1.53
4	C	896	LEU	CA-C	-6.71	1.43	1.52
2	E	734	ARG	N-CA	-6.61	1.37	1.46
2	A	519	ILE	CA-CB	-6.56	1.47	1.54
4	C	866	ALA	CA-CB	-6.48	1.43	1.53
4	G	1052	ALA	CA-CB	-6.48	1.43	1.53
4	G	1038	ASN	C-O	-6.42	1.16	1.23
2	A	505	GLU	CA-CB	-6.39	1.43	1.53
4	C	903	ALA	CA-CB	-6.39	1.42	1.53
3	F	275	HIS	CA-C	-6.36	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	533	GLU	CG-CD	6.35	1.68	1.52
4	C	824	GLN	C-O	-6.35	1.15	1.24
2	A	446	VAL	CA-CB	-6.33	1.45	1.54
4	G	1102	ILE	CA-CB	-6.32	1.46	1.54
4	C	888	ARG	CA-C	-6.16	1.44	1.52
2	E	651	ILE	CA-CB	-6.09	1.47	1.54
2	E	671	VAL	CA-C	-6.08	1.45	1.52
3	F	275	HIS	N-CA	-6.05	1.39	1.46
2	E	669	ARG	CA-C	-6.04	1.44	1.52
5	D	1270	ILE	CA-C	-6.04	1.45	1.52
2	E	698	ALA	CA-CB	-6.04	1.42	1.53
2	A	437	LYS	CD-CE	6.02	1.70	1.52
4	G	1059	THR	CA-C	-6.01	1.45	1.52
4	C	876	THR	CA-C	-5.99	1.44	1.52
2	E	671	VAL	CA-CB	-5.99	1.47	1.54
4	C	888	ARG	C-O	-5.94	1.16	1.24
4	G	1030	VAL	CA-CB	-5.93	1.47	1.54
3	F	225	ASN	N-CA	-5.89	1.38	1.46
5	H	1496	ARG	CZ-NH1	5.86	1.41	1.32
3	F	240	ARG	C-O	-5.85	1.17	1.24
3	F	243	VAL	CB-CG2	-5.83	1.33	1.52
3	B	85	ASP	C-O	-5.81	1.16	1.24
5	H	1447	PRO	CA-C	-5.81	1.44	1.52
3	F	246	ILE	CA-CB	-5.80	1.46	1.54
5	D	1270	ILE	CA-CB	-5.79	1.47	1.54
2	E	724	ILE	CA-CB	-5.75	1.47	1.54
3	F	234	ILE	CB-CG2	5.75	1.71	1.52
3	F	271	THR	CA-CB	-5.75	1.43	1.53
4	C	847	ALA	CA-CB	-5.75	1.46	1.53
5	H	1449	THR	CA-CB	-5.72	1.44	1.53
3	F	284	MET	SD-CE	5.71	1.93	1.79
4	C	826	PRO	CA-C	-5.67	1.44	1.52
3	B	33	ALA	CA-CB	-5.59	1.44	1.53
2	A	535	ALA	CA-C	5.58	1.64	1.52
2	E	733	GLU	CA-CB	5.53	1.62	1.53
4	G	1047	ALA	N-CA	-5.53	1.42	1.46
4	G	1095	LYS	CA-C	5.51	1.59	1.52
3	F	292	ARG	C-O	-5.51	1.17	1.24
2	A	535	ALA	N-CA	5.48	1.56	1.46
4	G	1114	VAL	CA-C	5.48	1.59	1.52
2	A	456	LYS	C-O	-5.47	1.17	1.24
4	G	1030	VAL	N-CA	-5.46	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	437	LYS	CE-NZ	5.46	1.65	1.49
5	D	1260	ASN	N-CA	-5.42	1.39	1.46
3	B	47	SER	CA-C	5.40	1.59	1.52
5	H	1496	ARG	C-O	-5.39	1.18	1.24
3	F	299	GLY	C-O	-5.36	1.16	1.24
5	H	1470	ILE	CA-CB	-5.33	1.48	1.54
5	D	1257	SER	CA-CB	-5.30	1.45	1.53
5	D	1296	ARG	CA-C	-5.29	1.45	1.52
2	A	486	SER	N-CA	-5.29	1.39	1.46
2	E	709	LEU	CA-C	-5.27	1.46	1.52
2	E	702	ALA	CA-CB	-5.26	1.44	1.53
4	G	1103	ALA	CA-CB	-5.25	1.45	1.53
2	A	524	ILE	C-O	-5.24	1.17	1.24
4	C	900	VAL	CA-C	-5.23	1.46	1.52
3	F	255	ARG	C-O	-5.22	1.18	1.24
2	E	711	ALA	CA-CB	-5.19	1.45	1.53
2	A	494	GLU	N-CA	-5.17	1.39	1.46
3	F	291	LYS	CE-NZ	5.17	1.64	1.49
5	H	1487	THR	CA-CB	-5.15	1.44	1.53
3	F	253	GLU	CA-C	-5.14	1.45	1.52
2	E	712	ILE	CA-CB	-5.14	1.47	1.54
2	E	658	THR	CA-CB	5.12	1.65	1.53
3	F	291	LYS	CD-CE	5.12	1.67	1.52
2	A	533	GLU	CA-CB	5.09	1.60	1.53
5	D	1259	MET	SD-CE	-5.07	1.66	1.79
5	H	1435	ALA	CA-CB	-5.03	1.45	1.53
5	D	1314	ALA	N-CA	-5.02	1.40	1.46
3	F	239	ARG	CA-C	-5.01	1.46	1.52
2	A	449	ARG	CA-C	5.01	1.59	1.52
2	A	520	MET	C-O	-5.00	1.19	1.24

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	534	ARG	N-CA-C	24.03	145.14	113.18
1	I	39	DG	C2'-C3'-O3'	14.39	133.08	111.50
5	D	1278	ALA	CA-C-N	-12.14	102.51	122.54
5	D	1278	ALA	C-N-CA	-12.14	102.51	122.54
2	E	677	ASP	N-CA-C	-11.50	94.70	110.68
4	C	825	PHE	CA-C-N	11.15	133.78	119.84
4	C	825	PHE	C-N-CA	11.15	133.78	119.84
4	C	847	ALA	CA-C-N	-9.74	108.57	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	847	ALA	C-N-CA	-9.74	108.57	119.28
2	E	665	LEU	CA-C-N	-9.70	109.15	119.24
2	E	665	LEU	C-N-CA	-9.70	109.15	119.24
1	J	205	DG	C4'-C3'-O3'	9.59	124.38	110.00
1	J	173	DA	C2'-C3'-O3'	-9.32	97.52	111.50
5	D	1280	TYR	N-CA-C	-8.72	102.55	113.01
2	E	717	VAL	N-CA-C	-8.33	105.02	113.10
2	E	677	ASP	CB-CA-C	8.28	123.56	111.88
3	B	30	THR	N-CA-C	8.25	121.69	110.55
4	C	887	VAL	N-CA-CB	-8.00	101.90	110.62
3	F	228	GLY	N-CA-C	-7.94	104.92	115.32
1	I	85	DA	N9-C1'-C2'	-7.86	101.71	113.50
2	E	685	GLN	N-CA-C	-7.85	98.66	110.28
3	F	246	ILE	N-CA-C	7.80	119.14	107.75
4	G	1071	ARG	N-CA-C	-7.79	102.47	110.97
4	G	1087	VAL	N-CA-C	7.76	117.80	110.74
2	E	733	GLU	N-CA-C	-7.72	94.35	110.80
2	E	726	LEU	N-CA-C	-7.72	101.72	112.45
3	B	101	GLY	N-CA-C	-7.72	94.89	113.18
1	I	134	DG	C5'-C4'-C3'	-7.60	103.50	114.90
4	C	862	ILE	CG1-CB-CG2	-7.28	88.87	110.70
1	I	133	DA	C2'-C3'-O3'	-7.25	100.62	111.50
5	D	1279	HIS	N-CA-C	7.23	122.28	113.17
2	A	535	ALA	N-CA-C	7.23	131.23	111.00
1	J	268	DG	C5'-C4'-C3'	-7.22	104.07	114.90
1	J	248	DA	C5'-C4'-C3'	-7.20	104.10	114.90
5	D	1305	LYS	N-CA-C	-7.17	102.65	111.33
5	D	1293	THR	N-CA-C	-7.17	103.47	111.28
3	B	28	GLY	N-CA-C	-7.14	105.52	114.16
3	B	46	ILE	N-CA-C	7.06	119.09	107.24
1	I	49	DC	C2'-C3'-O3'	-7.05	100.92	111.50
5	D	1273	GLU	N-CA-C	-6.99	103.74	111.36
2	A	438	PRO	N-CA-C	6.88	126.64	112.47
2	A	533	GLU	CA-C-O	-6.87	112.20	120.65
4	C	819	SER	N-CA-C	-6.84	103.75	111.07
2	A	439	HIS	N-CA-C	-6.80	98.98	109.52
1	J	206	DC	C5'-C4'-C3'	-6.79	104.71	114.90
3	F	274	GLU	CA-C-N	-6.77	111.40	120.54
3	F	274	GLU	C-N-CA	-6.77	111.40	120.54
4	G	1021	ALA	N-CA-C	-6.74	105.03	113.18
1	I	6	DT	C5'-C4'-O4'	-6.71	99.34	109.40
5	D	1299	LEU	N-CA-C	6.68	119.31	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	296	THR	CB-CA-C	-6.60	101.68	109.80
1	I	100	DG	C2'-C3'-O3'	-6.59	101.61	111.50
2	A	447	ALA	N-CA-C	-6.58	104.03	111.07
3	B	87	VAL	CB-CA-C	-6.52	103.63	111.97
3	B	102	GLY	N-CA-C	-6.51	94.41	113.30
4	G	1111	ILE	N-CA-C	6.48	117.36	107.77
5	H	1498	LEU	N-CA-C	6.47	121.17	113.28
1	I	59	DG	C5'-C4'-C3'	-6.42	105.27	114.90
3	B	27	GLN	N-CA-C	-6.40	105.45	113.20
3	F	285	ASP	N-CA-C	-6.39	104.23	111.07
5	D	1308	VAL	CB-CA-C	-6.38	103.71	111.88
2	A	477	ASP	N-CA-C	-6.35	105.54	113.28
2	E	728	ARG	N-CA-C	-6.32	104.27	112.23
4	G	1074	LYS	N-CA-C	-6.28	103.27	111.74
2	A	455	GLN	N-CA-C	-6.27	105.60	113.18
4	C	913	SER	N-CA-C	6.24	118.63	111.02
4	G	1025	PHE	CA-C-N	6.23	127.63	119.84
4	G	1025	PHE	C-N-CA	6.23	127.63	119.84
4	G	1057	TYR	N-CA-C	6.18	118.81	111.33
1	J	276	DT	N1-C1'-C2'	6.18	122.76	113.50
1	I	41	DA	C2'-C3'-O3'	6.15	120.72	111.50
3	F	240	ARG	N-CA-C	-6.14	104.58	111.28
1	I	140	DT	C2'-C3'-O3'	-6.14	102.30	111.50
5	H	1485	THR	N-CA-C	6.11	118.90	109.07
3	F	230	THR	N-CA-C	6.08	119.48	110.48
2	A	524	ILE	N-CA-C	-6.05	104.40	111.00
4	G	1089	ASN	CB-CA-C	-6.05	100.33	110.56
1	J	186	DG	N9-C1'-C2'	6.05	122.57	113.50
2	E	689	VAL	CB-CA-C	-6.04	103.89	112.22
2	A	471	VAL	CB-CA-C	-6.03	104.26	111.97
2	A	483	ARG	N-CA-C	-6.02	100.19	109.52
2	E	677	ASP	OD1-CG-OD2	-6.01	108.48	122.90
3	B	72	TYR	N-CA-C	-5.97	104.68	111.07
4	C	823	LEU	N-CA-C	5.97	118.93	109.50
3	F	280	THR	N-CA-C	5.95	118.42	108.73
3	B	35	ARG	N-CA-C	-5.92	104.52	110.97
3	B	57	VAL	N-CA-C	-5.88	104.79	110.72
5	D	1298	LEU	N-CA-C	5.87	120.46	113.12
1	I	125	DG	C2'-C3'-O3'	5.85	120.27	111.50
2	E	677	ASP	CA-C-N	5.84	132.70	121.54
2	E	677	ASP	C-N-CA	5.84	132.70	121.54
3	F	221	VAL	CB-CA-C	-5.83	100.33	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	733	GLU	CA-C-O	5.82	128.84	120.51
4	C	860	ALA	CA-C-N	5.79	127.97	120.44
4	C	860	ALA	C-N-CA	5.79	127.97	120.44
2	E	645	THR	N-CA-C	-5.73	104.95	111.14
1	J	225	DC	C2'-C3'-O3'	-5.71	102.94	111.50
3	B	74	GLU	CA-C-N	-5.70	112.06	120.38
3	B	74	GLU	C-N-CA	-5.70	112.06	120.38
1	J	217	DG	N9-C1'-C2'	5.68	122.02	113.50
4	C	899	ARG	N-CA-C	-5.68	103.86	111.87
1	J	210	DT	C2'-C3'-O3'	-5.62	103.06	111.50
1	J	227	DG	C5'-C4'-C3'	-5.62	106.47	114.90
1	I	133	DA	C4'-C3'-O3'	5.61	118.42	110.00
5	D	1257	SER	CA-CB-OG	-5.60	99.89	111.10
4	C	869	ALA	CA-C-N	-5.58	112.80	120.28
4	C	869	ALA	C-N-CA	-5.58	112.80	120.28
5	D	1301	GLY	CA-C-N	-5.58	112.37	120.29
5	D	1301	GLY	C-N-CA	-5.58	112.37	120.29
1	J	266	DT	C2'-C3'-O3'	-5.57	103.14	111.50
4	G	1033	LEU	CA-C-N	-5.51	113.09	120.54
4	G	1033	LEU	C-N-CA	-5.51	113.09	120.54
2	E	697	GLU	N-CA-C	-5.50	105.36	111.36
2	A	528	ARG	CA-C-N	-5.50	112.97	120.44
2	A	528	ARG	C-N-CA	-5.50	112.97	120.44
3	B	50	ILE	CB-CA-C	-5.44	105.01	111.81
4	G	1110	ASN	N-CA-C	5.43	117.22	108.32
4	C	899	ARG	CA-C-N	-5.40	115.61	123.06
4	C	899	ARG	C-N-CA	-5.40	115.61	123.06
2	E	728	ARG	CA-C-N	-5.39	113.54	120.65
2	E	728	ARG	C-N-CA	-5.39	113.54	120.65
3	F	228	GLY	CA-C-N	-5.37	116.04	122.22
3	F	228	GLY	C-N-CA	-5.37	116.04	122.22
2	E	648	LEU	N-CA-C	-5.37	105.59	111.82
2	A	501	VAL	CB-CA-C	-5.36	104.90	112.14
2	E	733	GLU	CB-CG-CD	5.34	121.69	112.60
1	I	10	DC	C5'-C4'-C3'	-5.34	106.89	114.90
1	J	287	DA	C5'-C4'-C3'	-5.34	106.90	114.90
2	E	678	PHE	CB-CA-C	-5.33	99.81	110.42
2	A	454	TYR	N-CA-C	5.29	117.95	111.82
2	A	499	TYR	N-CA-C	-5.22	104.51	111.24
1	I	27	DA	C4'-C3'-O3'	-5.21	102.18	110.00
4	C	843	VAL	CB-CA-C	-5.19	104.25	110.99
2	E	732	GLY	CA-C-O	-5.18	111.55	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	731	ARG	NE-CZ-NH1	-5.18	116.32	121.50
4	G	1043	VAL	CB-CA-C	-5.18	104.51	110.41
3	B	25	ASN	N-CA-C	5.18	116.92	111.28
5	H	1432	GLU	N-CA-C	5.17	117.39	110.35
4	C	830	VAL	N-CA-C	-5.17	105.34	110.62
2	E	705	GLU	N-CA-C	-5.16	104.92	111.11
5	D	1285	THR	N-CA-C	5.14	117.78	109.40
5	D	1288	SER	N-CA-C	-5.14	105.86	111.82
5	H	1438	VAL	CB-CA-C	-5.14	105.30	111.88
4	G	1101	THR	CA-C-N	5.14	128.79	122.37
4	G	1101	THR	C-N-CA	5.14	128.79	122.37
2	A	466	PRO	N-CA-C	-5.12	106.41	113.53
1	J	194	DT	C4'-C3'-O3'	-5.12	102.32	110.00
4	G	1058	LEU	N-CA-C	-5.12	105.88	111.82
2	A	534	ARG	CB-CA-C	-5.11	101.24	110.23
2	A	519	ILE	N-CA-C	5.10	116.98	109.63
3	F	249	LEU	N-CA-C	5.10	119.13	113.01
3	B	65	VAL	CB-CA-C	-5.10	105.29	111.87
2	A	514	ALA	N-CA-C	-5.09	106.66	112.92
2	A	533	GLU	CB-CG-CD	5.08	121.23	112.60
1	J	258	DT	C5'-C4'-C3'	-5.07	107.30	114.90
1	J	289	DT	C5'-C4'-O4'	-5.05	101.82	109.40
1	J	288	DT	O3'-P-O5'	-5.05	96.43	104.00
1	I	124	DA	C5'-C4'-C3'	-5.04	107.34	114.90
1	I	82	DA	C4'-C3'-O3'	-5.04	102.45	110.00
5	D	1276	ARG	N-CA-C	5.03	117.15	111.11
1	I	125	DG	C4'-C3'-O3'	-5.01	102.48	110.00
1	J	195	DC	N1-C1'-C2'	5.01	121.01	113.50
1	J	164	DG	N9-C1'-C2'	5.01	121.01	113.50
3	B	29	ILE	N-CA-C	-5.01	99.92	107.73

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	478	PHE	Sidechain
3	B	51	TYR	Sidechain
3	B	72	TYR	Sidechain
3	B	98	TYR	Sidechain
4	C	857	TYR	Sidechain
5	D	1237	TYR	Sidechain
5	D	1239	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	D	1279	HIS	Sidechain
2	E	654	TYR	Sidechain
3	F	298	TYR	Sidechain
4	G	1057	TYR	Sidechain
1	I	102	DA	Sidechain
1	I	116	DC	Sidechain
1	I	120	DT	Sidechain
1	I	124	DA	Sidechain
1	I	129	DC	Sidechain
1	I	131	DG	Sidechain
1	I	137	DG	Sidechain
1	I	145	DA	Sidechain
1	I	39	DG	Sidechain
1	I	41	DA	Sidechain
1	I	44	DC	Sidechain
1	I	48	DT	Sidechain
1	I	49	DC	Sidechain
1	I	51	DA	Sidechain
1	I	59	DG	Sidechain
1	I	67	DA	Sidechain
1	I	85	DA	Sidechain
1	I	99	DA	Sidechain
1	J	147	DA	Sidechain
1	J	149	DC	Sidechain
1	J	150	DA	Sidechain
1	J	151	DA	Sidechain
1	J	153	DA	Sidechain
1	J	158	DC	Sidechain
1	J	161	DG	Sidechain
1	J	180	DT	Sidechain
1	J	185	DG	Sidechain
1	J	186	DG	Sidechain
1	J	192	DG	Sidechain
1	J	196	DC	Sidechain
1	J	206	DC	Sidechain
1	J	214	DG	Sidechain
1	J	221	DT	Sidechain
1	J	228	DA	Sidechain
1	J	238	DT	Sidechain
1	J	243	DG	Sidechain
1	J	247	DC	Sidechain
1	J	276	DT	Sidechain

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2990	0	1651	164	0
1	J	2990	0	1651	153	0
2	A	817	0	858	42	0
2	E	817	0	858	48	0
3	B	633	0	668	41	0
3	F	648	0	688	26	0
4	C	804	0	859	50	0
4	G	827	0	890	61	0
5	D	709	0	727	43	0
5	H	744	0	771	56	0
6	A	9	0	0	1	0
6	B	8	0	0	0	0
6	C	16	0	0	0	0
6	D	9	0	0	1	0
6	E	17	0	0	5	0
6	F	16	0	0	0	0
6	G	13	0	0	1	0
6	H	5	0	0	2	0
6	I	39	0	0	12	0
6	J	39	0	0	4	0
All	All	12150	0	9621	600	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 28.

All (600) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:735:ALA:CB	2:E:735:ALA:CA	1.84	1.52
2:E:677:ASP:CB	2:E:677:ASP:CG	1.81	1.51
3:B:84:MET:SD	3:B:84:MET:CE	2.02	1.46
4:C:850:TYR:OH	5:D:1292:GLN:HG3	1.45	1.16
2:E:677:ASP:OD2	6:E:97:HOH:O	1.70	1.10
3:B:87:VAL:HG11	3:B:102:GLY:HA3	1.10	1.05
4:C:838:ASN:HB3	6:H:156:HOH:O	1.55	1.05
2:A:437:LYS:HB3	2:A:438:PRO:HD3	1.38	1.04
1:I:134:DG:O6	6:I:170:HOH:O	1.78	1.01
4:C:817:ARG:HH22	4:C:831:HIS:CD2	1.78	1.00
1:I:125:DG:N2	1:J:168:DC:N3	2.11	0.98
1:I:53:DC:N4	1:J:240:DG:H1	1.62	0.97
4:C:902:ILE:HG23	5:D:1258:ILE:HD13	1.47	0.97
1:I:124:DA:H1'	1:I:125:DG:OP1	1.64	0.96
1:I:22:DC:H42	1:J:271:DG:H1	1.02	0.95
2:E:677:ASP:OD1	6:E:97:HOH:O	1.82	0.95
1:J:151:DA:H2''	1:J:152:DT:H5'	1.47	0.95
1:I:128:DT:H1'	1:I:129:DC:H5'	1.50	0.94
3:B:87:VAL:HG11	3:B:102:GLY:CA	1.97	0.94
1:I:98:DG:H1	1:J:195:DC:H42	1.01	0.91
4:C:817:ARG:HH22	4:C:831:HIS:HD2	1.12	0.90
1:J:151:DA:H2''	1:J:152:DT:C5'	2.00	0.90
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.51	0.90
1:J:206:DC:H2''	1:J:207:DA:C8	2.06	0.90
1:J:230:DC:H2''	1:J:231:DA:C8	2.06	0.89
1:I:125:DG:H1	1:J:168:DC:H42	0.92	0.88
1:I:53:DC:H42	1:J:240:DG:H1	0.91	0.88
1:I:98:DG:H1	1:J:195:DC:N4	1.70	0.88
1:J:262:DC:H2'	1:J:263:DT:H71	1.55	0.86
1:I:22:DC:H2'	1:I:23:DT:H71	1.58	0.85
4:C:826:PRO:HG3	5:D:1237:TYR:CZ	2.11	0.85
2:A:529:ARG:HA	2:A:534:ARG:HB2	1.59	0.84
2:E:663:ARG:HE	2:E:663:ARG:HA	1.43	0.84
4:G:1026:PRO:HB2	4:G:1029:ARG:HB3	1.60	0.84
1:J:176:DA:OP2	4:G:1032:ARG:HD3	1.78	0.84
1:I:97:DG:N7	6:I:159:HOH:O	2.10	0.83
1:I:125:DG:H1	1:J:168:DC:N4	1.74	0.83
1:J:267:DG:H1'	1:J:268:DG:C8	2.14	0.83
3:B:59:LYS:HE2	3:B:63:GLU:OE2	1.78	0.82
4:G:1026:PRO:HG3	5:H:1437:TYR:CE2	2.14	0.82
1:I:135:DG:H2''	1:I:136:DT:OP2	1.79	0.82
1:I:93:DT:H1'	1:I:94:DG:H5''	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:DG:H1	1:J:235:DC:H42	1.29	0.81
5:H:1489:ARG:HH11	5:H:1489:ARG:HG2	1.47	0.80
2:E:729:ARG:HG3	2:E:735:ALA:HA	1.62	0.80
1:J:249:DG:H1'	1:J:250:DT:H5'	1.62	0.79
1:I:145:DA:H5'	6:A:90:HOH:O	1.82	0.79
4:C:817:ARG:NH2	4:C:831:HIS:HD2	1.79	0.79
1:J:261:DA:H2''	1:J:262:DC:H5''	1.64	0.79
1:J:246:DG:H2''	1:J:247:DC:C5	2.18	0.78
4:G:1079:ILE:HG12	4:G:1082:HIS:CE1	2.19	0.78
1:J:147:DA:H2'	1:J:148:DT:H72	1.64	0.78
1:I:124:DA:C1'	1:I:125:DG:OP1	2.32	0.77
4:G:1026:PRO:HG3	5:H:1437:TYR:CZ	2.20	0.77
2:A:463:ARG:O	2:A:466:PRO:HD2	1.85	0.77
1:I:138:DG:H1'	1:I:139:DA:C8	2.20	0.76
2:E:678:PHE:HE2	3:F:267:ARG:HB2	1.50	0.76
5:D:1287:THR:H	5:D:1290:GLU:HG2	1.48	0.76
1:J:286:DT:H2''	1:J:287:DA:O5'	1.86	0.75
4:G:1079:ILE:HG12	4:G:1082:HIS:ND1	2.02	0.75
1:J:280:DG:O6	6:J:321:HOH:O	2.04	0.75
1:I:124:DA:OP1	5:H:1428:LYS:HD2	1.86	0.75
5:H:1483:ARG:HG2	5:H:1483:ARG:HH11	1.49	0.75
1:I:134:DG:C6	6:I:170:HOH:O	2.32	0.74
2:A:528:ARG:C	2:A:534:ARG:HG3	2.12	0.74
4:G:1051:LEU:HD12	4:G:1051:LEU:O	1.87	0.74
1:J:257:DA:C8	1:J:258:DT:H72	2.22	0.74
1:I:11:DA:H1'	6:I:173:HOH:O	1.87	0.74
4:C:855:LEU:O	4:C:859:THR:HG23	1.88	0.73
3:B:23:ARG:HH11	3:B:28:GLY:HA2	1.53	0.73
3:B:59:LYS:O	3:B:63:GLU:HG3	1.88	0.73
1:J:197:DA:H2''	1:J:198:DT:H5'	1.69	0.73
1:I:29:DA:H2''	1:I:30:DA:O5'	1.89	0.72
2:A:437:LYS:HB3	2:A:438:PRO:CD	2.15	0.72
1:I:29:DA:H5'	1:I:29:DA:H8	1.54	0.71
1:I:128:DT:H1'	1:I:129:DC:C5'	2.20	0.71
1:J:225:DC:H2''	1:J:226:DT:H72	1.73	0.71
5:D:1277:LEU:CD2	5:D:1293:THR:HB	2.21	0.71
2:E:734:ARG:O	2:E:735:ALA:HB3	1.91	0.71
1:I:22:DC:H4'	1:I:22:DC:OP1	1.90	0.71
3:F:259:LYS:O	3:F:263:GLU:HG3	1.91	0.71
1:J:227:DG:H5'	3:B:47:SER:HA	1.73	0.70
6:J:310:HOH:O	3:F:245:CYS:SG	2.49	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:151:DA:H1'	1:J:152:DT:H5''	1.74	0.70
2:E:668:GLN:HG3	2:E:689:VAL:HG11	1.73	0.70
1:I:26:DC:H1'	1:I:27:DA:C5	2.27	0.69
1:J:151:DA:C2'	1:J:152:DT:H5''	2.22	0.69
1:I:29:DA:H5'	1:I:29:DA:C8	2.28	0.69
2:A:464:LYS:HE2	2:A:490:MET:HE1	1.74	0.69
2:A:520:MET:CE	2:A:522:LYS:HE3	2.23	0.69
5:H:1483:ARG:HG2	5:H:1483:ARG:NH1	2.07	0.69
1:I:7:DA:C2	1:J:287:DA:C2	2.80	0.68
1:J:287:DA:C8	1:J:287:DA:H5''	2.28	0.68
1:I:57:DA:H2''	1:I:58:DG:C8	2.28	0.68
4:C:826:PRO:HG3	5:D:1237:TYR:CE2	2.28	0.68
1:J:174:DA:H2''	1:J:175:DA:H5''	1.75	0.68
1:J:287:DA:H5''	1:J:287:DA:H8	1.58	0.68
1:J:268:DG:H2''	1:J:269:DT:H5'	1.76	0.67
4:G:1017:ARG:HH12	4:G:1031:HIS:CD2	2.12	0.67
4:C:850:TYR:OH	5:D:1292:GLN:CG	2.33	0.67
4:G:1047:ALA:HB3	4:G:1048:PRO:HD3	1.74	0.67
2:E:663:ARG:HA	2:E:663:ARG:NE	2.10	0.67
5:D:1243:LYS:HE2	5:D:1243:LYS:HA	1.77	0.67
1:I:5:DA:H2''	1:I:6:DT:H5'	1.77	0.67
3:B:74:GLU:O	3:B:75:HIS:C	2.35	0.67
1:J:151:DA:C2'	1:J:152:DT:C5'	2.73	0.66
1:J:181:DA:H2''	1:J:182:DT:OP2	1.94	0.66
1:J:182:DT:H1'	1:J:183:DT:H5'	1.76	0.66
5:H:1498:LEU:O	5:H:1499:LEU:HD23	1.95	0.66
1:I:82:DA:H3'	2:E:646:VAL:HG21	1.77	0.66
1:J:274:DT:H2''	1:J:275:DC:OP2	1.95	0.66
5:D:1277:LEU:HD21	5:D:1293:THR:HB	1.77	0.66
1:J:225:DC:H2''	1:J:226:DT:C7	2.26	0.66
4:G:1037:GLY:HA3	4:G:1039:TYR:CE1	2.31	0.66
1:I:53:DC:H2''	1:I:54:DA:OP2	1.96	0.66
2:A:476:GLN:NE2	2:A:480:THR:HG22	2.10	0.66
1:I:58:DG:H1	1:J:235:DC:N4	1.92	0.66
1:J:168:DC:H2'	1:J:169:DT:H71	1.78	0.65
1:I:48:DT:OP1	5:H:1428:LYS:NZ	2.27	0.65
2:E:734:ARG:O	2:E:735:ALA:CB	2.44	0.65
4:G:1084:GLN:OE1	4:G:1088:ARG:HD2	1.95	0.65
4:C:850:TYR:CZ	5:D:1292:GLN:HG3	2.32	0.65
1:J:283:DG:H2''	1:J:284:DG:OP2	1.96	0.64
2:A:464:LYS:HE2	2:A:490:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:679:LYS:HB3	2:E:682:LEU:HD11	1.78	0.64
4:C:825:PHE:HZ	4:C:859:THR:HG21	1.63	0.64
2:A:534:ARG:O	2:A:535:ALA:HB3	1.95	0.64
4:C:837:GLY:HA3	4:C:839:TYR:CE1	2.33	0.64
4:C:854:VAL:HG22	5:D:1307:ALA:HB1	1.78	0.64
1:I:1:DA:H2'	1:I:2:DT:H71	1.80	0.64
1:I:22:DC:N4	1:J:271:DG:H1	1.84	0.64
4:C:867:GLY:HA3	5:D:1246:HIS:CD2	2.33	0.63
3:F:274:GLU:O	3:F:275:HIS:C	2.35	0.63
1:I:36:DT:H1'	1:I:37:DT:H5'	1.81	0.63
1:I:98:DG:H4'	1:I:99:DA:OP1	1.97	0.63
1:J:147:DA:H2'	1:J:148:DT:C7	2.28	0.63
2:E:664:LYS:HZ1	2:E:690:MET:HE1	1.63	0.63
1:J:287:DA:H2''	1:J:288:DT:O5'	1.99	0.63
1:I:5:DA:H1'	1:I:6:DT:H5''	1.81	0.63
4:C:831:HIS:CE1	4:C:835:ARG:NH2	2.67	0.62
3:F:278:ARG:NH1	3:F:282:THR:HG23	2.14	0.62
4:G:1079:ILE:HG22	5:H:1452:SER:HB3	1.81	0.62
1:I:94:DG:H5'	1:I:94:DG:H8	1.64	0.62
1:I:10:DC:O2	6:I:177:HOH:O	2.14	0.62
1:I:38:DT:H2''	1:I:39:DG:N7	2.14	0.62
4:G:1032:ARG:HE	4:G:1036:LYS:NZ	1.98	0.62
6:I:177:HOH:O	1:J:283:DG:N2	2.32	0.62
4:C:840:ALA:HA	4:G:1038:ASN:OD1	2.00	0.62
4:G:1017:ARG:HH12	4:G:1031:HIS:HD2	1.48	0.62
1:I:130:DT:H2''	1:I:131:DG:N7	2.15	0.62
4:G:1047:ALA:N	4:G:1048:PRO:HD2	2.15	0.62
2:A:451:ILE:O	2:A:452:ARG:C	2.42	0.61
2:E:677:ASP:CG	6:E:97:HOH:O	2.17	0.61
1:J:260:DC:H2''	1:J:261:DA:OP2	2.01	0.61
2:E:678:PHE:O	2:E:679:LYS:HB2	2.01	0.61
4:G:1032:ARG:HG2	4:G:1036:LYS:HE3	1.82	0.61
1:I:94:DG:H5'	1:I:94:DG:C8	2.36	0.61
1:I:114:DC:H4'	1:I:114:DC:OP1	2.00	0.61
4:G:1047:ALA:N	4:G:1048:PRO:CD	2.63	0.61
1:J:225:DC:C2'	1:J:226:DT:H72	2.31	0.61
5:H:1443:LYS:NZ	5:H:1449:THR:O	2.30	0.61
1:J:147:DA:H2''	1:J:148:DT:O5'	2.00	0.61
3:F:231:LYS:HB3	3:F:232:PRO:CD	2.28	0.61
1:I:119:DT:H2''	1:I:120:DT:H72	1.83	0.61
4:C:825:PHE:CD1	4:C:856:GLU:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:DC:H2''	1:I:115:DA:O5'	2.01	0.61
2:E:663:ARG:HB3	2:E:666:PRO:HD2	1.83	0.60
1:J:239:DT:H2''	1:J:240:DG:H8	1.67	0.60
1:J:247:DC:H2''	1:J:248:DA:OP2	2.00	0.60
1:J:267:DG:N7	6:J:296:HOH:O	2.31	0.60
4:C:825:PHE:CZ	4:C:859:THR:HG21	2.36	0.60
1:I:133:DA:H4'	1:I:134:DG:OP1	2.00	0.60
1:J:267:DG:H1'	1:J:268:DG:N7	2.16	0.60
1:J:262:DC:C2'	1:J:263:DT:H71	2.30	0.60
2:E:675:ALA:O	2:E:678:PHE:HB2	2.01	0.60
5:H:1498:LEU:C	5:H:1499:LEU:HD23	2.27	0.59
1:I:40:DG:O6	6:I:171:HOH:O	2.17	0.59
1:J:173:DA:C2	1:J:174:DA:C2	2.90	0.59
1:I:119:DT:H2''	1:I:120:DT:C7	2.33	0.59
1:J:249:DG:H5''	5:H:1428:LYS:HA	1.84	0.59
4:G:1079:ILE:HB	4:G:1080:PRO:CD	2.33	0.59
1:I:98:DG:N2	1:J:195:DC:N3	2.42	0.59
1:I:133:DA:H2'	1:I:133:DA:O5'	2.03	0.58
4:C:838:ASN:CB	6:H:156:HOH:O	2.31	0.58
1:J:249:DG:P	5:H:1429:SER:OG	2.61	0.58
5:H:1489:ARG:HG2	5:H:1489:ARG:NH1	2.15	0.58
1:J:273:DA:H2''	1:J:274:DT:OP2	2.02	0.58
1:J:277:DG:H5''	4:C:876:THR:HG21	1.84	0.58
1:J:168:DC:C2'	1:J:169:DT:H71	2.33	0.58
2:A:483:ARG:O	3:B:80:THR:HA	2.02	0.58
4:C:831:HIS:CG	4:C:848:PRO:HG3	2.37	0.58
1:I:46:DG:H2''	1:I:47:DC:C6	2.39	0.58
1:J:162:DC:H2''	1:J:163:DA:N7	2.19	0.58
1:J:244:DG:H2''	1:J:245:DA:N7	2.19	0.58
2:A:520:MET:HE3	2:A:522:LYS:HE3	1.85	0.58
1:I:80:DT:H2''	1:I:81:DG:C8	2.38	0.58
4:C:826:PRO:HB2	4:C:829:ARG:HB3	1.85	0.57
1:I:94:DG:C2'	1:I:95:DA:H8	2.17	0.57
1:J:197:DA:C2'	1:J:198:DT:H5'	2.34	0.57
1:J:234:DC:H4'	1:J:235:DC:OP1	2.03	0.57
1:J:246:DG:H2''	1:J:247:DC:C6	2.38	0.57
1:I:26:DC:H1'	1:I:27:DA:N7	2.19	0.57
4:C:881:ARG:O	4:C:881:ARG:HG3	1.96	0.57
2:E:678:PHE:CE2	3:F:267:ARG:HB2	2.38	0.57
1:I:17:DA:OP2	1:I:17:DA:C8	2.58	0.57
5:H:1437:TYR:O	5:H:1441:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1451:ILE:HG13	5:H:1455:ALA:HB3	1.86	0.57
2:A:452:ARG:O	2:A:456:LYS:HG3	2.04	0.57
1:I:40:DG:OP1	5:D:1285:THR:OG1	2.13	0.57
1:I:70:DG:H2''	6:I:153:HOH:O	2.05	0.57
1:J:264:DT:C2'	1:J:265:DT:H71	2.34	0.57
4:G:1032:ARG:HE	4:G:1036:LYS:HZ2	1.52	0.57
1:I:140:DT:H1'	1:I:141:DA:C8	2.40	0.56
3:F:292:ARG:HB3	3:F:292:ARG:NH1	2.20	0.56
5:H:1500:PRO:HD2	5:H:1503:LEU:HD23	1.87	0.56
1:I:123:DT:O4	6:I:182:HOH:O	2.18	0.56
4:G:1013:LYS:O	4:G:1013:LYS:HG3	2.04	0.56
1:I:17:DA:H2''	1:I:18:DG:C8	2.40	0.56
4:G:1066:ALA:O	4:G:1069:ALA:HB3	2.05	0.56
2:A:508:ASN:O	2:A:512:ILE:HG13	2.05	0.56
2:A:529:ARG:HH11	2:A:529:ARG:HG2	1.70	0.56
1:I:25:DC:H2''	1:I:26:DC:H5'	1.87	0.56
3:B:44:LYS:HG2	3:B:45:CYS:SG	2.45	0.56
2:E:735:ALA:CB	2:E:735:ALA:N	2.65	0.56
1:J:150:DA:H2''	1:J:151:DA:OP2	2.06	0.56
3:B:50:ILE:HG22	3:B:51:TYR:N	2.20	0.56
1:J:147:DA:H8	1:J:147:DA:HO5'	1.53	0.56
3:B:87:VAL:CG2	3:B:102:GLY:OXT	2.54	0.56
3:B:50:ILE:O	3:B:51:TYR:C	2.47	0.55
3:B:68:ASP:OD2	3:B:92:ARG:NH1	2.36	0.55
4:G:1025:PHE:CD1	4:G:1056:GLU:HG3	2.41	0.55
1:I:22:DC:H2''	1:I:23:DT:O5'	2.05	0.55
1:J:195:DC:H1'	1:J:196:DC:C6	2.41	0.55
3:F:231:LYS:HE2	3:F:235:ARG:NH2	2.21	0.55
1:J:261:DA:C2'	1:J:262:DC:H5''	2.35	0.55
2:E:735:ALA:CB	2:E:735:ALA:OXT	2.54	0.55
1:J:154:DT:OP1	2:A:449:ARG:HD2	2.07	0.55
3:B:26:ILE:O	3:B:55:ARG:HD3	2.06	0.55
2:E:663:ARG:HE	2:E:663:ARG:CA	2.15	0.55
1:I:94:DG:C2'	1:I:95:DA:C8	2.90	0.55
1:J:203:DA:H2''	1:J:204:DG:C8	2.42	0.55
1:I:31:DG:C2'	1:I:32:DT:H71	2.37	0.55
1:I:89:DC:H2''	1:I:90:DT:H72	1.88	0.54
1:I:5:DA:H2''	1:I:6:DT:C5'	2.36	0.54
1:J:195:DC:H1'	1:J:196:DC:C5	2.42	0.54
5:D:1277:LEU:HD21	5:D:1293:THR:CB	2.37	0.54
5:H:1443:LYS:O	5:H:1447:PRO:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:151:DA:C1'	1:J:152:DT:H5''	2.37	0.54
1:J:281:DG:H1'	1:J:282:DT:H5'	1.90	0.54
2:A:529:ARG:HD3	2:E:709:LEU:CD1	2.37	0.54
3:F:234:ILE:O	3:F:234:ILE:HG22	2.08	0.54
4:G:1025:PHE:HE1	5:H:1441:VAL:HG21	1.72	0.54
5:H:1475:SER:O	5:H:1479:HIS:HD2	1.91	0.54
1:I:129:DC:C6	1:I:130:DT:H72	2.42	0.54
1:J:210:DT:H2'	1:J:211:DT:H72	1.90	0.54
1:J:235:DC:H2''	1:J:236:DT:OP2	2.07	0.54
5:H:1477:LEU:HD11	5:H:1493:THR:CG2	2.38	0.54
1:I:60:DC:H2''	1:I:61:DA:C8	2.43	0.53
5:H:1465:ASP:O	5:H:1466:VAL:C	2.45	0.53
1:I:17:DA:OP2	1:I:17:DA:H8	1.92	0.53
1:J:239:DT:H2''	1:J:240:DG:C8	2.43	0.53
2:A:529:ARG:HG2	2:A:529:ARG:NH1	2.24	0.53
1:I:132:DC:H2''	1:I:133:DA:N7	2.22	0.53
1:J:276:DT:H2''	1:J:277:DG:N7	2.23	0.53
1:J:207:DA:H2''	1:J:208:DT:O5'	2.08	0.53
1:J:174:DA:C2'	1:J:175:DA:H5''	2.39	0.53
1:J:224:DG:H2''	1:J:225:DC:C5	2.44	0.53
2:A:483:ARG:HB2	3:B:80:THR:HG23	1.89	0.53
3:B:23:ARG:CG	3:B:24:ASP:N	2.71	0.53
5:D:1304:ALA:O	5:D:1308:VAL:HG23	2.08	0.53
2:E:665:LEU:O	2:E:666:PRO:C	2.47	0.53
1:I:134:DG:H2''	1:I:135:DG:H8	1.72	0.52
4:C:863:LEU:HD13	5:D:1242:LEU:HB2	1.89	0.52
4:G:1033:LEU:O	4:G:1034:LEU:C	2.50	0.52
1:J:268:DG:H2''	1:J:269:DT:C5'	2.38	0.52
2:E:719:ILE:HG13	3:F:250:ILE:CD1	2.39	0.52
4:G:1067:GLY:HA3	5:H:1446:HIS:CD2	2.44	0.52
2:A:520:MET:N	2:A:523:ASP:OD2	2.37	0.52
1:I:94:DG:H2''	1:I:95:DA:H8	1.74	0.52
3:B:87:VAL:HG22	3:B:102:GLY:OXT	2.09	0.52
5:D:1243:LYS:HA	5:D:1243:LYS:CE	2.40	0.52
1:I:70:DG:H2''	1:I:71:DG:C8	2.44	0.52
1:J:147:DA:C2'	1:J:148:DT:H72	2.37	0.52
2:A:485:GLN:HG3	3:B:82:THR:HA	1.91	0.52
2:E:663:ARG:CB	2:E:666:PRO:HD2	2.39	0.52
1:I:130:DT:C2	1:I:131:DG:C6	2.98	0.52
2:E:642:ARG:O	2:E:643:PRO:C	2.53	0.52
1:J:188:DA:H2''	1:J:189:DA:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1274:ALA:O	5:D:1275:SER:C	2.51	0.52
1:I:84:DC:H2''	1:I:85:DA:C8	2.45	0.52
1:J:193:DC:O2	1:J:194:DT:C4	2.63	0.52
5:D:1287:THR:N	5:D:1290:GLU:HG2	2.20	0.51
2:E:678:PHE:HE2	3:F:267:ARG:CB	2.22	0.51
1:I:27:DA:H2''	1:I:28:DA:C8	2.45	0.51
1:J:255:DA:H8	1:J:255:DA:OP2	1.92	0.51
1:J:249:DG:OP1	5:H:1429:SER:OG	2.29	0.51
3:B:72:TYR:HE2	5:D:1277:LEU:HD13	1.75	0.51
3:B:84:MET:HE2	3:B:88:TYR:OH	2.10	0.51
3:F:229:ILE:HD13	3:F:229:ILE:N	2.26	0.51
1:J:193:DC:C2	1:J:194:DT:C4	2.98	0.51
1:I:132:DC:C2	1:I:133:DA:C6	2.99	0.51
1:J:154:DT:P	2:A:449:ARG:HD2	2.50	0.51
1:J:215:DC:H5'	2:E:643:PRO:HG3	1.92	0.51
1:J:227:DG:C6	1:J:228:DA:N6	2.79	0.51
2:A:439:HIS:CD2	2:A:440:ARG:H	2.28	0.51
3:F:261:PHE:O	3:F:265:VAL:HG23	2.11	0.51
1:J:277:DG:H1'	1:J:278:DC:H5'	1.92	0.51
3:F:284:MET:HE2	3:F:288:TYR:OH	2.11	0.51
4:G:1063:LEU:HG	5:H:1459:MET:HE2	1.93	0.51
1:I:88:DC:N4	1:J:204:DG:C6	2.79	0.51
3:B:84:MET:HE3	3:B:88:TYR:CZ	2.46	0.51
1:I:114:DC:H2'	1:I:115:DA:C8	2.47	0.50
4:G:1056:GLU:O	4:G:1059:THR:HB	2.11	0.50
4:C:878:ILE:HA	4:C:882:HIS:ND1	2.26	0.50
4:G:1031:HIS:HB2	4:G:1048:PRO:HB3	1.93	0.50
1:I:59:DG:H4'	1:I:59:DG:OP1	2.11	0.50
1:I:99:DA:H2''	1:I:100:DG:C8	2.46	0.50
5:H:1466:VAL:O	5:H:1467:PHE:C	2.51	0.50
1:I:46:DG:H2''	1:I:47:DC:C5	2.46	0.50
1:J:268:DG:OP1	4:C:829:ARG:NH2	2.40	0.50
3:B:84:MET:CE	3:B:88:TYR:CZ	2.95	0.50
4:G:1035:ARG:NH1	4:G:1035:ARG:HG2	2.26	0.50
1:I:133:DA:O5'	1:I:133:DA:C2'	2.59	0.50
1:I:136:DT:H1'	1:I:137:DG:H5'	1.94	0.50
1:J:188:DA:H2''	1:J:189:DA:C8	2.47	0.50
2:A:522:LYS:HG3	2:A:523:ASP:N	2.27	0.50
4:G:1079:ILE:CG1	4:G:1082:HIS:ND1	2.73	0.49
1:J:149:DC:H2''	1:J:150:DA:O5'	2.12	0.49
4:G:1067:GLY:O	4:G:1068:ASN:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:DT:H1'	1:J:170:DA:H5'	1.93	0.49
1:J:287:DA:H2''	1:J:288:DT:C5'	2.41	0.49
1:I:30:DA:P	4:C:832:ARG:NH1	2.86	0.49
1:I:106:DT:H2''	1:I:107:DC:C6	2.48	0.49
3:B:78:ARG:HH22	3:B:85:ASP:CG	2.20	0.49
1:I:131:DG:H1'	1:I:132:DC:H5'	1.94	0.49
5:H:1477:LEU:CD1	5:H:1493:THR:HB	2.43	0.49
1:I:69:DC:H2''	1:I:70:DG:C8	2.47	0.49
1:J:219:DA:C8	1:J:220:DT:H71	2.46	0.49
1:I:58:DG:N2	1:J:235:DC:N3	2.54	0.49
1:J:257:DA:H2''	1:J:258:DT:OP2	2.13	0.49
1:J:206:DC:H2''	1:J:207:DA:N7	2.26	0.49
5:H:1481:ASN:O	5:H:1482:LYS:C	2.56	0.49
1:I:55:DA:H2''	1:I:56:DA:N7	2.28	0.49
1:J:179:DG:H2''	1:J:180:DT:OP2	2.13	0.49
2:A:520:MET:HB3	2:A:521:PRO:HD2	1.94	0.49
1:I:31:DG:H2'	1:I:32:DT:H71	1.95	0.48
1:J:274:DT:H1'	1:J:275:DC:H5'	1.95	0.48
3:F:234:ILE:O	3:F:234:ILE:CG2	2.61	0.48
3:F:232:PRO:O	3:F:236:ARG:HG3	2.12	0.48
3:F:223:ARG:O	3:F:225:ASN:N	2.46	0.48
5:H:1502:GLU:OE1	5:H:1505:LYS:CD	2.62	0.48
1:J:233:DG:H2''	1:J:234:DC:OP2	2.12	0.48
3:B:52:GLU:OE2	3:B:55:ARG:NH1	2.46	0.48
1:I:79:DC:C5'	6:I:162:HOH:O	2.61	0.48
2:A:463:ARG:C	2:A:466:PRO:HD2	2.38	0.48
5:D:1279:HIS:C	5:D:1281:ASN:N	2.68	0.48
4:G:1026:PRO:HB2	4:G:1029:ARG:CB	2.38	0.48
1:J:287:DA:H8	1:J:287:DA:C5'	2.25	0.48
1:J:282:DT:H2''	1:J:283:DG:OP2	2.13	0.48
3:B:82:THR:O	3:B:83:ALA:C	2.54	0.48
4:C:847:ALA:O	4:C:848:PRO:C	2.54	0.48
3:B:30:THR:OG1	3:B:32:PRO:HD2	2.13	0.47
5:H:1502:GLU:O	5:H:1503:LEU:C	2.54	0.47
1:I:19:DA:C4	1:I:20:DT:C5	3.02	0.47
1:I:72:DA:H1'	1:I:73:DA:H5'	1.96	0.47
1:J:243:DG:C2	1:J:244:DG:C2	3.02	0.47
5:D:1239:TYR:CE2	5:D:1243:LYS:HD2	2.50	0.47
1:I:1:DA:H2''	1:I:2:DT:C6	2.49	0.47
1:J:175:DA:C2'	1:J:176:DA:C8	2.98	0.47
2:E:669:ARG:NH1	6:E:35:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:DA:H2'	1:I:112:DT:H72	1.96	0.47
1:I:49:DC:C2	1:I:50:DC:C4	3.03	0.47
1:I:127:DA:C2	1:I:128:DT:C2	3.03	0.47
3:F:292:ARG:HB3	3:F:292:ARG:CZ	2.45	0.47
1:I:124:DA:OP1	5:H:1428:LYS:CD	2.60	0.47
3:F:249:LEU:HD23	3:F:249:LEU:HA	1.49	0.47
1:I:28:DA:H2''	1:I:29:DA:H5''	1.96	0.47
1:J:267:DG:C2	1:J:268:DG:C6	3.02	0.46
2:A:529:ARG:HA	2:A:534:ARG:CB	2.39	0.46
2:E:708:ASN:O	2:E:712:ILE:HG13	2.14	0.46
1:I:145:DA:H2''	1:I:146:DT:OP2	2.14	0.46
5:H:1437:TYR:N	5:H:1437:TYR:CD1	2.82	0.46
1:I:54:DA:H2''	1:I:55:DA:C8	2.51	0.46
1:I:124:DA:C4'	1:I:125:DG:OP1	2.64	0.46
2:E:663:ARG:NE	2:E:663:ARG:CA	2.75	0.46
4:G:1037:GLY:O	4:G:1038:ASN:C	2.54	0.46
5:H:1489:ARG:NH1	5:H:1489:ARG:CG	2.79	0.46
3:B:72:TYR:CE2	5:D:1277:LEU:HD13	2.49	0.46
1:I:112:DT:OP2	4:G:1035:ARG:NH2	2.48	0.46
5:H:1502:GLU:O	5:H:1505:LYS:HB3	2.15	0.46
1:I:128:DT:H2''	1:I:129:DC:O5'	2.14	0.46
2:A:520:MET:O	2:A:521:PRO:C	2.58	0.46
4:C:830:VAL:HG13	5:D:1267:PHE:HE1	1.81	0.46
4:C:857:TYR:CD1	4:C:857:TYR:O	2.69	0.46
1:J:165:DA:C2	1:J:166:DT:C2	3.03	0.46
2:E:728:ARG:O	2:E:729:ARG:C	2.59	0.46
1:J:227:DG:C5'	3:B:47:SER:HA	2.43	0.46
1:J:249:DG:OP2	5:H:1429:SER:OG	2.33	0.46
4:C:850:TYR:OH	5:D:1292:GLN:NE2	2.49	0.46
4:G:1088:ARG:H	4:G:1088:ARG:HG2	1.48	0.46
2:E:729:ARG:O	2:E:730:ILE:C	2.56	0.45
1:I:29:DA:C2'	1:I:30:DA:C8	2.99	0.45
1:J:219:DA:C8	1:J:220:DT:C7	2.99	0.45
1:J:245:DA:H2''	1:J:246:DG:C8	2.51	0.45
2:E:664:LYS:HD3	6:E:157:HOH:O	2.16	0.45
4:G:1071:ARG:O	4:G:1073:ASN:N	2.49	0.45
5:H:1459:MET:O	5:H:1463:VAL:HG23	2.16	0.45
1:I:122:DG:H4'	5:H:1430:ARG:HB3	1.97	0.45
2:A:525:GLN:O	2:A:534:ARG:HD3	2.16	0.45
4:C:825:PHE:CG	4:C:856:GLU:HB2	2.50	0.45
4:G:1090:ASP:O	4:G:1091:GLU:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:41:DA:H2''	1:I:42:DA:O5'	2.17	0.45
1:I:69:DC:H42	1:J:224:DG:H1	1.63	0.45
1:I:131:DG:H2''	1:I:132:DC:O5'	2.15	0.45
4:G:1100:VAL:CG1	4:G:1101:THR:N	2.78	0.45
1:J:255:DA:C6	1:J:256:DA:C6	3.04	0.45
5:D:1277:LEU:HD21	5:D:1293:THR:CG2	2.47	0.45
5:D:1279:HIS:ND1	6:D:107:HOH:O	2.36	0.45
4:G:1068:ASN:O	4:G:1069:ALA:C	2.59	0.45
1:I:26:DC:H4'	1:I:27:DA:OP1	2.17	0.45
1:I:136:DT:H2''	1:I:137:DG:O5'	2.16	0.45
1:J:249:DG:P	5:H:1429:SER:HG	2.39	0.45
2:E:664:LYS:NZ	2:E:690:MET:HE1	2.30	0.45
1:I:98:DG:C4'	1:I:99:DA:OP1	2.64	0.45
2:A:467:PHE:CZ	2:A:493:GLN:HA	2.52	0.45
4:C:832:ARG:NH2	5:D:1232:GLU:OE2	2.50	0.45
1:I:63:DG:H2''	1:I:64:DT:OP2	2.16	0.45
1:J:149:DC:H2''	1:J:150:DA:C8	2.52	0.45
3:B:23:ARG:HG2	3:B:24:ASP:N	2.30	0.45
1:I:97:DG:C5	1:I:98:DG:C6	3.05	0.45
1:I:111:DA:H2'	1:I:112:DT:C7	2.47	0.45
1:I:133:DA:H2''	1:I:134:DG:C8	2.52	0.45
1:I:138:DG:H2'	1:I:138:DG:O5'	2.17	0.45
1:I:28:DA:C2'	1:I:29:DA:H5''	2.46	0.45
1:J:248:DA:H2''	1:J:249:DG:C8	2.52	0.45
1:I:94:DG:H2''	1:I:95:DA:C8	2.52	0.44
1:I:118:DT:H2'	1:I:119:DT:H71	1.98	0.44
1:I:141:DA:C2	1:J:153:DA:C2	3.05	0.44
1:J:190:DC:H2''	1:J:191:DT:O5'	2.16	0.44
1:J:204:DG:H4'	1:J:205:DG:OP1	2.17	0.44
3:B:29:ILE:HG23	3:B:29:ILE:HD12	1.60	0.44
1:I:49:DC:H1'	1:I:50:DC:C6	2.53	0.44
1:I:89:DC:H2''	1:I:90:DT:C7	2.47	0.44
1:I:119:DT:C2'	1:I:120:DT:H72	2.46	0.44
1:J:149:DC:C2'	1:J:150:DA:C8	3.00	0.44
4:G:1113:SER:OG	4:G:1114:VAL:N	2.49	0.44
1:I:48:DT:H2'	1:I:49:DC:C5	2.52	0.44
4:C:879:ILE:HG12	4:C:882:HIS:CE1	2.52	0.44
5:D:1251:ILE:HG21	5:D:1256:MET:HE2	2.00	0.44
1:I:34:DT:H2''	1:I:35:DA:O5'	2.18	0.44
1:J:281:DG:H2''	1:J:282:DT:O5'	2.17	0.44
4:C:881:ARG:NH2	4:C:907:VAL:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1279:HIS:C	5:D:1281:ASN:H	2.24	0.44
5:H:1451:ILE:CG1	5:H:1455:ALA:HB3	2.48	0.44
1:I:134:DG:C5	6:I:170:HOH:O	2.64	0.44
3:B:31:LYS:N	3:B:32:PRO:CD	2.80	0.44
5:D:1281:ASN:O	5:D:1282:LYS:C	2.60	0.44
4:G:1084:GLN:O	4:G:1088:ARG:HG2	2.17	0.44
1:I:55:DA:H2''	1:I:56:DA:C8	2.53	0.44
5:H:1451:ILE:HG13	5:H:1455:ALA:CB	2.47	0.44
2:A:458:THR:HG22	4:G:1106:GLY:HA3	1.99	0.44
4:G:1026:PRO:CG	5:H:1437:TYR:CZ	2.98	0.44
5:H:1477:LEU:HD11	5:H:1493:THR:HB	1.98	0.44
1:I:28:DA:H2''	1:I:29:DA:C5'	2.48	0.44
1:J:176:DA:P	4:G:1032:ARG:HH11	2.41	0.44
1:J:286:DT:C2'	1:J:287:DA:O5'	2.62	0.44
2:E:676:GLN:C	2:E:678:PHE:H	2.25	0.44
3:F:234:ILE:HD12	3:F:251:TYR:HB3	2.00	0.44
4:G:1112:GLN:HB2	4:G:1115:LEU:HD12	2.00	0.44
1:I:27:DA:H1'	1:I:28:DA:O4'	2.17	0.44
1:I:104:DT:H2''	1:I:105:DT:C6	2.53	0.44
1:I:111:DA:C8	1:I:112:DT:H72	2.53	0.44
1:I:121:DG:OP2	1:I:121:DG:H8	2.00	0.44
1:J:147:DA:C2'	1:J:148:DT:C7	2.94	0.44
1:J:264:DT:H2''	1:J:265:DT:H71	1.99	0.44
2:A:500:LEU:HD23	2:A:500:LEU:HA	1.79	0.44
3:B:26:ILE:CG2	3:B:27:GLN:N	2.78	0.44
4:C:817:ARG:NH2	4:C:831:HIS:CD2	2.58	0.44
2:E:665:LEU:HB3	2:E:666:PRO:HD3	2.00	0.44
4:G:1031:HIS:O	4:G:1032:ARG:C	2.61	0.44
4:G:1051:LEU:HD12	4:G:1051:LEU:C	2.37	0.44
4:G:1092:GLU:HB3	5:H:1503:LEU:HD22	1.99	0.44
1:I:129:DC:C2'	1:I:130:DT:H72	2.48	0.43
2:A:454:TYR:CZ	3:B:36:ARG:HG2	2.53	0.43
1:J:189:DA:C6	1:J:190:DC:N4	2.86	0.43
1:I:38:DT:O3'	1:I:39:DG:C8	2.72	0.43
1:I:93:DT:H1'	1:I:94:DG:C5'	2.41	0.43
4:C:817:ARG:HH22	4:C:831:HIS:CG	2.32	0.43
4:C:866:ALA:O	4:C:867:GLY:C	2.61	0.43
4:C:881:ARG:O	4:C:885:LEU:HG	2.19	0.43
2:E:676:GLN:C	2:E:678:PHE:N	2.76	0.43
4:C:826:PRO:CB	4:C:829:ARG:HB3	2.47	0.43
2:E:685:GLN:O	2:E:686:SER:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:230:THR:O	3:F:231:LYS:C	2.61	0.43
4:G:1051:LEU:HD21	5:H:1467:PHE:CE1	2.54	0.43
1:I:30:DA:P	4:C:832:ARG:HH11	2.42	0.43
2:E:724:ILE:O	2:E:728:ARG:HG3	2.18	0.43
1:I:124:DA:C6	1:I:125:DG:C6	3.07	0.43
2:A:479:LYS:HD2	3:B:74:GLU:HG2	1.99	0.43
2:A:520:MET:HB3	2:A:521:PRO:CD	2.49	0.43
5:D:1299:LEU:HB2	5:D:1304:ALA:HB2	2.00	0.43
5:H:1434:TYR:O	5:H:1435:ALA:C	2.60	0.43
1:I:2:DT:H2''	1:I:3:DC:OP2	2.18	0.43
2:A:469:ARG:HD2	3:B:25:ASN:OD1	2.18	0.43
5:D:1237:TYR:O	5:D:1241:VAL:HG23	2.18	0.43
4:G:1100:VAL:HG12	4:G:1101:THR:N	2.33	0.43
5:H:1439:TYR:O	5:H:1440:LYS:C	2.61	0.43
2:E:661:LEU:H	2:E:697:GLU:CD	2.26	0.43
5:H:1453:SER:O	5:H:1454:LYS:C	2.60	0.43
5:H:1476:ARG:O	5:H:1477:LEU:C	2.61	0.43
1:I:93:DT:C1'	1:I:94:DG:H5''	2.40	0.43
1:J:150:DA:C2'	1:J:151:DA:OP2	2.66	0.43
1:J:227:DG:C2	1:J:228:DA:C6	3.07	0.43
3:B:76:ALA:O	3:B:77:LYS:HB2	2.18	0.43
4:C:853:ALA:O	4:C:854:VAL:C	2.61	0.43
2:E:734:ARG:C	2:E:735:ALA:CB	2.91	0.43
5:H:1436:ILE:O	5:H:1440:LYS:HG3	2.19	0.43
4:C:831:HIS:HA	4:C:848:PRO:HB3	2.00	0.43
4:C:833:LEU:HD23	4:C:833:LEU:HA	1.68	0.43
5:H:1475:SER:O	5:H:1476:ARG:C	2.62	0.43
1:I:114:DC:C2'	1:I:115:DA:C8	3.01	0.42
2:A:479:LYS:HB3	2:A:482:LEU:HD11	2.00	0.42
2:A:528:ARG:HB3	2:A:534:ARG:HG3	2.01	0.42
5:D:1276:ARG:HH11	5:D:1276:ARG:HD2	1.64	0.42
4:G:1035:ARG:HG2	4:G:1035:ARG:HH11	1.83	0.42
5:H:1470:ILE:O	5:H:1471:ALA:C	2.61	0.42
1:I:39:DG:H4'	4:C:842:ARG:NH1	2.34	0.42
1:J:253:DC:H4'	1:J:254:DC:OP1	2.18	0.42
1:J:190:DC:H1'	1:J:191:DT:H5'	2.02	0.42
1:J:193:DC:H2''	1:J:194:DT:H72	2.02	0.42
1:J:284:DG:H2''	1:J:285:DA:OP2	2.19	0.42
2:E:721:PRO:HG2	3:F:249:LEU:HB3	2.01	0.42
4:G:1018:SER:O	4:G:1023:LEU:N	2.38	0.42
4:G:1055:LEU:HD23	4:G:1055:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1026:PRO:O	4:G:1027:VAL:C	2.59	0.42
5:H:1499:LEU:HA	5:H:1500:PRO:HD3	1.83	0.42
1:I:124:DA:H8	1:I:124:DA:H2'	1.74	0.42
1:J:261:DA:O5'	1:J:261:DA:H2'	2.19	0.42
1:J:267:DG:O6	6:J:296:HOH:O	2.21	0.42
5:H:1429:SER:C	5:H:1430:ARG:O	2.61	0.42
1:I:11:DA:C4	1:I:12:DC:C5	3.06	0.42
1:I:17:DA:C2	1:I:18:DG:C2	3.07	0.42
1:I:119:DT:H4'	1:I:120:DT:OP1	2.20	0.42
2:A:465:LEU:O	2:A:466:PRO:C	2.59	0.42
3:B:66:ILE:O	3:B:67:ARG:C	2.62	0.42
1:I:126:DA:C6	1:I:127:DA:C6	3.08	0.42
1:J:152:DT:H2''	1:J:153:DA:C8	2.54	0.42
1:J:214:DG:H2''	1:J:215:DC:C6	2.54	0.42
3:B:51:TYR:O	3:B:52:GLU:C	2.56	0.42
5:D:1238:VAL:HG12	5:D:1256:MET:HE1	2.02	0.42
5:D:1276:ARG:HB3	5:D:1280:TYR:CZ	2.55	0.42
5:D:1319:THR:C	5:D:1321:ALA:H	2.28	0.42
1:I:1:DA:H2'	1:I:2:DT:C7	2.47	0.42
2:A:453:ARG:O	2:A:456:LYS:HB2	2.19	0.42
5:D:1246:HIS:HB3	5:D:1249:THR:OG1	2.19	0.42
5:D:1239:TYR:O	5:D:1243:LYS:HG2	2.19	0.42
2:E:669:ARG:HD2	3:F:225:ASN:OD1	2.20	0.42
4:G:1047:ALA:HB3	4:G:1048:PRO:CD	2.47	0.42
1:I:111:DA:H2''	1:I:112:DT:O5'	2.19	0.41
1:I:118:DT:C2'	1:I:119:DT:H71	2.50	0.41
3:B:30:THR:CB	3:B:32:PRO:HD2	2.50	0.41
2:E:675:ALA:O	2:E:678:PHE:CB	2.67	0.41
1:J:185:DG:C2	1:J:186:DG:C2	3.08	0.41
5:D:1290:GLU:O	5:D:1291:ILE:C	2.62	0.41
1:I:113:DA:C6	1:I:114:DC:N4	2.88	0.41
1:J:170:DA:H2''	1:J:171:DC:C5	2.55	0.41
1:I:88:DC:N4	1:J:204:DG:O6	2.54	0.41
2:A:476:GLN:HE22	2:A:480:THR:HG22	1.81	0.41
1:J:175:DA:H2''	1:J:176:DA:C8	2.56	0.41
1:J:287:DA:C8	1:J:287:DA:C5'	3.01	0.41
4:G:1068:ASN:O	4:G:1071:ARG:N	2.54	0.41
5:H:1436:ILE:HG13	5:H:1437:TYR:CE1	2.56	0.41
1:I:1:DA:C2'	1:I:2:DT:H71	2.49	0.41
1:I:19:DA:C2	1:I:20:DT:C2	3.09	0.41
1:I:89:DC:N4	1:J:203:DA:N6	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:DT:C2'	1:I:105:DT:H72	2.50	0.41
1:I:121:DG:N7	6:I:147:HOH:O	2.37	0.41
1:J:192:DG:H2''	1:J:193:DC:O5'	2.19	0.41
4:C:893:LEU:O	4:C:897:LEU:HB2	2.20	0.41
4:G:1071:ARG:C	4:G:1073:ASN:N	2.78	0.41
4:G:1073:ASN:O	4:G:1074:LYS:HB2	2.20	0.41
5:H:1488:SER:O	5:H:1489:ARG:C	2.62	0.41
5:H:1509:SER:O	5:H:1510:GLU:C	2.63	0.41
1:J:184:DT:H2''	1:J:185:DG:N7	2.36	0.40
4:C:862:ILE:CG2	5:D:1259:MET:HE1	2.51	0.40
4:C:916:LEU:HB3	4:C:917:PRO:CD	2.51	0.40
1:J:196:DC:H2''	1:J:197:DA:C8	2.56	0.40
3:F:226:ILE:HG13	3:F:255:ARG:HB3	2.03	0.40
4:G:1090:ASP:HB2	6:G:150:HOH:O	2.20	0.40
1:I:135:DG:C2'	1:I:136:DT:OP2	2.54	0.40
3:B:74:GLU:O	3:B:76:ALA:N	2.54	0.40
5:D:1304:ALA:O	5:D:1305:LYS:C	2.65	0.40
2:E:657:SER:OG	2:E:659:GLU:OE2	2.33	0.40
1:I:112:DT:P	4:G:1035:ARG:HH22	2.44	0.40
1:J:193:DC:O2	1:J:194:DT:N3	2.55	0.40
4:C:916:LEU:HB3	4:C:917:PRO:HD2	2.03	0.40
5:D:1277:LEU:HD21	5:D:1293:THR:HG21	2.03	0.40
2:E:709:LEU:HD23	2:E:709:LEU:HA	1.61	0.40
1:I:114:DC:H42	1:J:179:DG:H1	1.69	0.40
1:J:283:DG:C6	1:J:284:DG:C6	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	97/135 (72%)	91 (94%)	4 (4%)	2 (2%)	5 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	97/135 (72%)	93 (96%)	0	4 (4%)	2	9
3	B	78/102 (76%)	75 (96%)	3 (4%)	0	100	100
3	F	80/102 (78%)	76 (95%)	3 (4%)	1 (1%)	9	32
4	C	102/129 (79%)	93 (91%)	8 (8%)	1 (1%)	12	39
4	G	105/129 (81%)	97 (92%)	7 (7%)	1 (1%)	12	39
5	D	89/125 (71%)	84 (94%)	5 (6%)	0	100	100
5	H	93/125 (74%)	83 (89%)	7 (8%)	3 (3%)	3	13
All	All	741/982 (76%)	692 (93%)	37 (5%)	12 (2%)	7	27

All (12) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	86/111 (78%)	79 (92%)	7 (8%)	11	33
2	E	86/111 (78%)	78 (91%)	8 (9%)	8	27
3	B	65/78 (83%)	61 (94%)	4 (6%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	67/78 (86%)	63 (94%)	4 (6%)	17	47
4	C	83/100 (83%)	76 (92%)	7 (8%)	10	31
4	G	85/100 (85%)	78 (92%)	7 (8%)	10	32
5	D	77/105 (73%)	71 (92%)	6 (8%)	11	35
5	H	81/105 (77%)	73 (90%)	8 (10%)	7	24
All	All	630/788 (80%)	579 (92%)	51 (8%)	11	33

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	438	PRO
2	A	448	LEU
2	A	459	GLU
2	A	486	SER
2	A	496	SER
2	A	533	GLU
2	A	534	ARG
3	B	26	ILE
3	B	57	VAL
3	B	80	THR
3	B	91	LYS
4	C	829	ARG
4	C	859	THR
4	C	876	THR
4	C	881	ARG
4	C	892	GLU
4	C	909	PRO
4	C	914	VAL
5	D	1243	LYS
5	D	1247	PRO
5	D	1279	HIS
5	D	1284	SER
5	D	1285	THR
5	D	1295	VAL
2	E	649	ARG
2	E	659	GLU
2	E	666	PRO
2	E	680	THR
2	E	703	LEU
2	E	705	GLU

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Mol	Chain	Res	Type
2	E	721	PRO
2	E	734	ARG
3	F	229	ILE
3	F	232	PRO
3	F	247	SER
3	F	257	VAL
4	G	1038	ASN
4	G	1041	GLU
4	G	1073	ASN
4	G	1080	PRO
4	G	1088	ARG
4	G	1109	PRO
4	G	1117	PRO
5	H	1429	SER
5	H	1431	LYS
5	H	1433	SER
5	H	1452	SER
5	H	1453	SER
5	H	1483	ARG
5	H	1503	LEU
5	H	1516	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	439	HIS
2	A	476	GLN
2	A	485	GLN
2	A	493	GLN
3	B	27	GLN
3	B	93	GLN
4	C	831	HIS
5	D	1292	GLN
3	F	293	GLN
4	G	1024	GLN
4	G	1031	HIS
4	G	1038	ASN
5	H	1479	HIS
5	H	1492	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.