Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:01 pm BST

PDB ID	:	1P3A
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	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

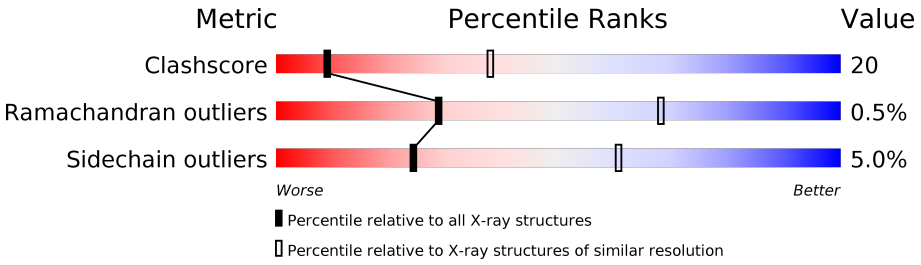
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	41% 55% .
1	J	146	36% 63% .
2	A	135	49% 21% . 27%
2	E	135	43% 24% . . 27%
3	B	102	52% 25% 23%
3	F	102	53% 23% . 21%
4	C	129	46% 34% . 17%
4	G	129	53% 26% . 19%

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Mol	Chain	Length	Quality of chain
5	D	125	42% 28% 27%
5	H	125	46% 25% 26%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12029 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
			807	509	155	140	3			
2	E	98	Total	C	N	O	S	0	0	0
			807	509	155	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	516	HIS	ARG	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	716	HIS	ARG	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	81	Total	C	N	O	S	0	0	0
			648	410	126	111	1			

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	107	Total	C	N	O	0	0	0
			825	520	161	144			
4	G	104	Total	C	N	O	0	0	0
			804	507	157	140			

There are 48 discrepancies between the modelled and reference sequences:

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

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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	91	Total	C	N	O	S	0	0	0
			709	447	125	135	2			
5	H	92	Total	C	N	O	S	0	0	0
			718	453	127	136	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	22	Total	O	0	0
			22	22		
6	J	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	5	Total O 5 5	0	0
6	C	9	Total O 9 9	0	0
6	D	7	Total O 7 7	0	0
6	E	9	Total O 9 9	0	0
6	F	7	Total O 7 7	0	0
6	G	8	Total O 8 8	0	0
6	H	2	Total O 2 2	0	0

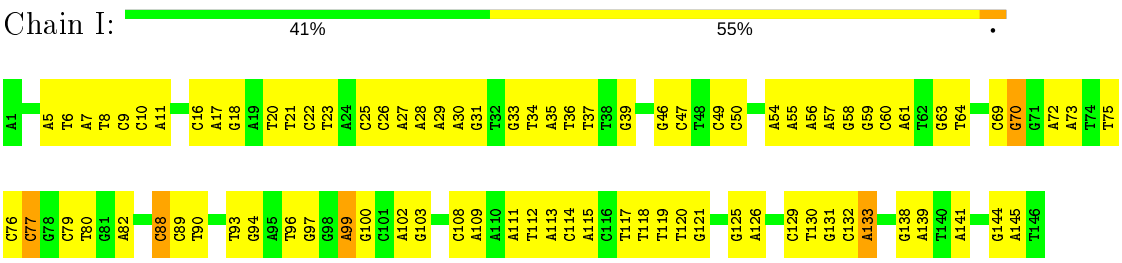
3 Residue-property plots (i)

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

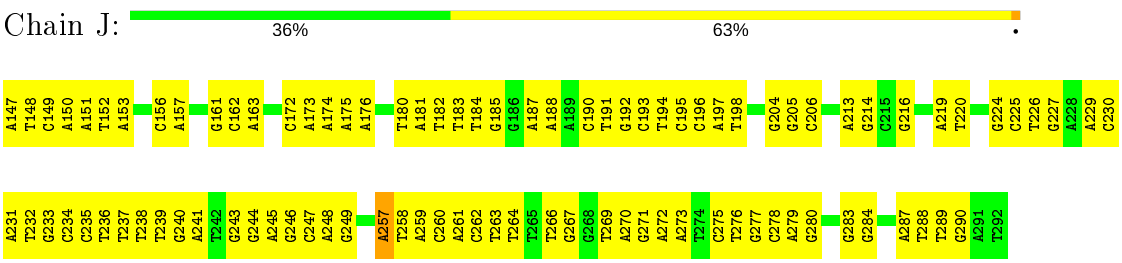
- Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment

Chain I:



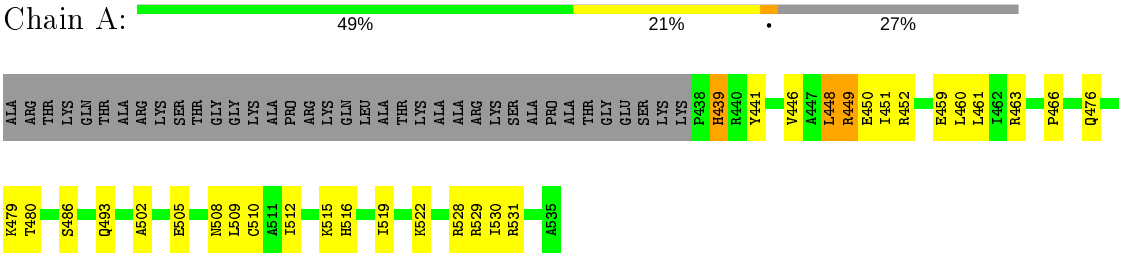
- Molecule 1: Palindromic 146bp Human Alpha-Satellite DNA fragment

Chain J:



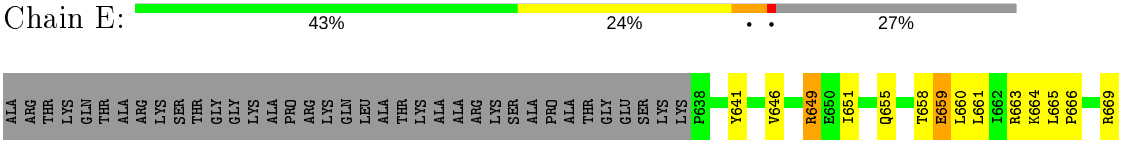
- Molecule 2: Histone H3

Chain A:



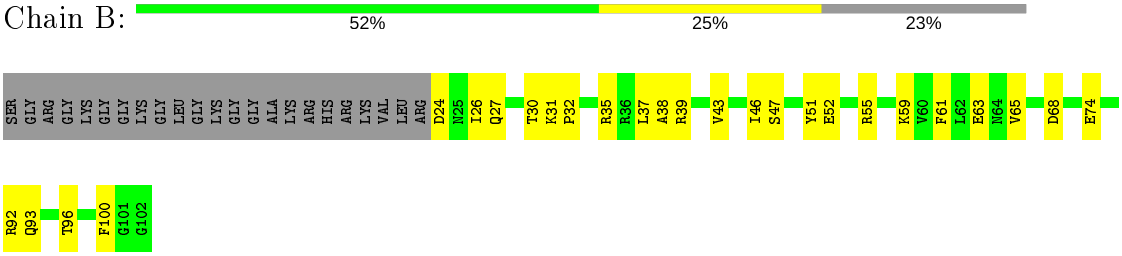
- Molecule 2: Histone H3

Chain E:



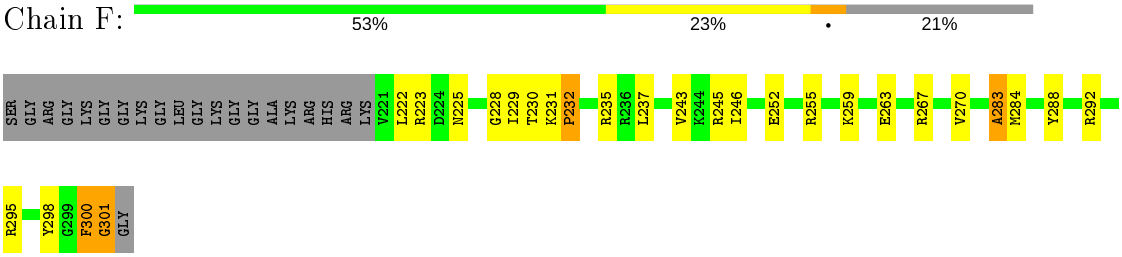
- Molecule 3: Histone H4

Chain B:



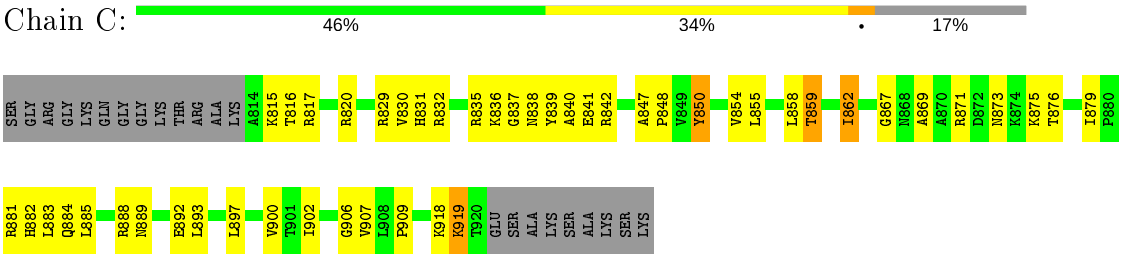
- Molecule 3: Histone H4

Chain F:



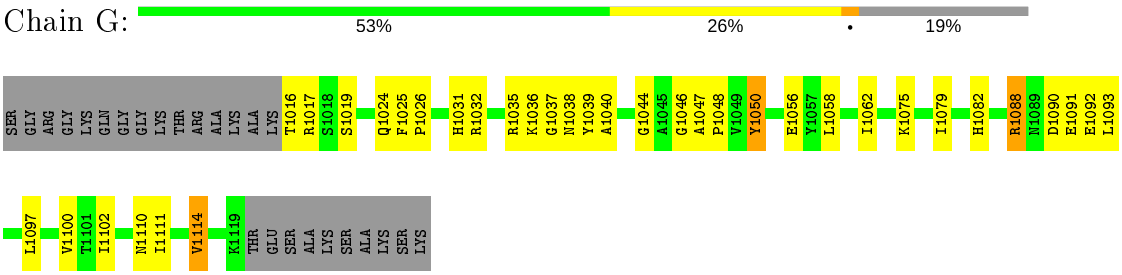
- Molecule 4: Histone H2A

Chain C:



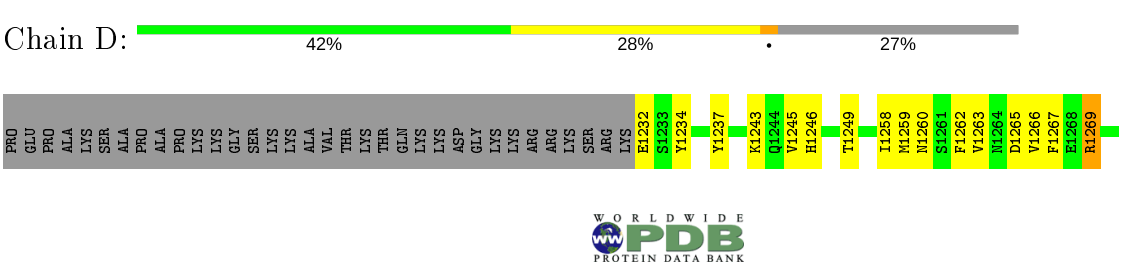
- Molecule 4: Histone H2A

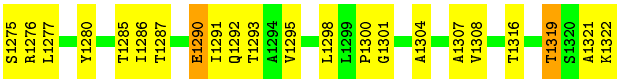
Chain G:



- Molecule 5: Histone H2B

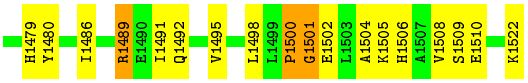
Chain D:





- Molecule 5: Histone H2B

Chain H:



4 Data and refinement statistics (i)

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	105.42Å 109.72Å 180.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	93.7 (50.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12029	wwPDB-VP
Average B, all atoms (Å^2)	75.0	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	0.54	0/3354	0.77	1/5175 (0.0%)
1	J	0.57	0/3354	0.76	0/5175
2	A	0.63	0/820	0.78	0/1100
2	E	0.98	1/820 (0.1%)	1.00	5/1100 (0.5%)
3	B	0.68	0/634	0.82	0/848
3	F	0.92	2/655 (0.3%)	1.09	4/878 (0.5%)
4	C	0.68	0/835	0.80	0/1127
4	G	0.57	0/814	0.74	0/1099
5	D	0.72	0/720	0.81	0/969
5	H	0.65	0/729	0.76	0/980
All	All	0.65	3/12735 (0.0%)	0.80	10/18451 (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	4
1	J	0	5
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	677	ASP	CB-CG	17.61	1.88	1.51
3	F	283	ALA	CA-CB	-8.49	1.34	1.52
3	F	301	GLY	CA-C	5.52	1.60	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	300	PHE	N-CA-C	9.24	135.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	734	ARG	N-CA-C	-8.88	87.02	111.00
2	E	677	ASP	CB-CG-OD1	7.62	125.15	118.30
3	F	300	PHE	CA-C-N	-7.20	101.80	116.20
2	E	677	ASP	CB-CG-OD2	6.88	124.50	118.30
2	E	677	ASP	OD1-CG-OD2	-6.86	110.28	123.30
3	F	300	PHE	C-N-CA	6.20	135.33	122.30
2	E	677	ASP	CB-CA-C	5.64	121.67	110.40
1	I	77	DC	C3'-C2'-C1'	-5.50	95.90	102.50
3	F	300	PHE	CA-C-O	5.03	130.67	120.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	133	DA	Sidechain
1	I	70	DG	Sidechain
1	I	88	DC	Sidechain
1	I	99	DA	Sidechain
1	J	192	DG	Sidechain
1	J	198	DT	Sidechain
1	J	214	DG	Sidechain
1	J	219	DA	Sidechain
1	J	257	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	102	0
1	J	2990	0	1651	110	0
2	A	807	0	840	36	0
2	E	807	0	840	52	0
3	B	627	0	663	30	0
3	F	648	0	693	31	0
4	C	825	0	884	49	0
4	G	804	0	859	37	0
5	D	709	0	727	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	718	0	740	33	0
6	A	7	0	0	4	0
6	B	5	0	0	0	0
6	C	9	0	0	1	0
6	D	7	0	0	0	0
6	E	9	0	0	3	0
6	F	7	0	0	2	0
6	G	8	0	0	3	0
6	H	2	0	0	0	0
6	I	22	0	0	1	0
6	J	28	0	0	5	0
All	All	12029	0	9548	432	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 20.

All (432) 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:677:ASP:CG	2:E:677:ASP:CB	1.88	1.42
2:A:528:ARG:HA	6:A:69:HOH:O	1.35	1.27
3:F:283:ALA:HB2	3:F:301:GLY:C	1.58	1.23
2:A:531:ARG:HB2	6:A:69:HOH:O	1.51	1.10
3:F:283:ALA:HB2	3:F:301:GLY:O	1.50	1.08
2:E:677:ASP:OD2	6:E:64:HOH:O	1.70	1.07
3:F:283:ALA:CB	3:F:301:GLY:C	2.31	0.99
3:F:295:ARG:HD3	6:F:70:HOH:O	1.63	0.96
1:I:8:DT:H1'	1:I:9:DC:H5'	1.47	0.95
4:C:892:GLU:HG2	5:D:1300:PRO:HB2	1.48	0.92
1:J:261:DA:H2"	1:J:262:DC:H5"	1.50	0.92
2:E:687:SER:HB2	3:F:301:GLY:C	1.92	0.89
5:H:1504:ALA:O	5:H:1508:VAL:HG23	1.71	0.89
2:A:529:ARG:HD3	2:A:529:ARG:O	1.72	0.88
2:E:677:ASP:OD1	6:E:64:HOH:O	1.90	0.88
4:C:842:ARG:HB2	5:D:1285:THR:HG23	1.54	0.88
5:D:1287:THR:H	5:D:1290:GLU:HG2	1.39	0.87
1:I:30:DA:OP2	4:C:832:ARG:HD3	1.76	0.85
1:J:248:DA:H5"	6:J:62:HOH:O	1.75	0.85
1:I:59:DG:H2"	1:I:60:DC:C6	2.12	0.85
1:J:246:DG:H2"	1:J:247:DC:C5	2.12	0.85
4:C:850:TYR:OH	5:D:1292:GLN:HG3	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:729:ARG:HG3	2:E:735:ALA:HA	1.58	0.83
2:E:729:ARG:O	2:E:735:ALA:HB2	1.79	0.83
1:I:20:DT:H1'	1:I:21:DT:H5'	1.61	0.82
4:C:855:LEU:O	4:C:859:THR:HG23	1.80	0.82
2:E:679:LYS:HD3	2:E:680:THR:H	1.42	0.81
2:A:463:ARG:HH12	3:B:30:THR:HG21	1.45	0.81
1:J:205:DG:H1'	1:J:206:DC:H5"	1.62	0.80
1:J:270:DA:H4'	1:J:271:DG:OP1	1.79	0.79
3:F:231:LYS:HB3	3:F:232:PRO:HD3	1.65	0.78
1:I:60:DC:H5"	2:A:463:ARG:NH1	1.98	0.77
1:J:234:DC:H2"	1:J:235:DC:C5	2.19	0.77
1:J:248:DA:H2"	1:J:249:DG:C8	2.18	0.77
2:A:476:GLN:NE2	2:A:480:THR:HG22	2.00	0.77
2:E:734:ARG:O	2:E:735:ALA:CB	2.33	0.76
3:F:235:ARG:HH11	3:F:235:ARG:HG3	1.49	0.76
1:J:280:DG:N7	6:J:92:HOH:O	2.18	0.76
5:D:1304:ALA:O	5:D:1308:VAL:HG23	1.86	0.76
5:H:1489:ARG:HH11	5:H:1489:ARG:HG2	1.50	0.76
5:H:1506:HIS:O	5:H:1510:GLU:HG2	1.87	0.75
1:J:229:DA:H2"	1:J:230:DC:H5'	1.69	0.75
2:A:439:HIS:C	2:A:439:HIS:ND1	2.40	0.75
2:A:519:ILE:HG13	2:A:519:ILE:O	1.87	0.74
3:F:259:LYS:O	3:F:263:GLU:HG3	1.87	0.74
1:I:58:DG:H2"	1:I:59:DG:OP2	1.87	0.73
4:C:919:LYS:HD3	4:C:919:LYS:N	2.03	0.73
1:J:261:DA:C2'	1:J:262:DC:H5"	2.18	0.73
1:I:57:DA:H2"	1:I:58:DG:C8	2.23	0.73
5:H:1445:VAL:HG12	5:H:1446:HIS:CD2	2.24	0.73
1:I:89:DC:H2"	1:I:90:DT:H71	1.69	0.72
1:I:56:DA:H1'	1:I:57:DA:H5'	1.70	0.72
2:A:529:ARG:HD3	2:A:529:ARG:C	2.10	0.71
4:G:1062:ILE:HG12	4:G:1093:LEU:HD13	1.72	0.71
1:J:230:DC:H2"	1:J:231:DA:C8	2.24	0.71
1:I:77:DC:H42	1:J:216:DG:H1	1.39	0.70
3:B:96:THR:HG21	4:G:1100:VAL:HG22	1.73	0.70
1:I:25:DC:H2"	1:I:26:DC:H5'	1.75	0.69
1:J:246:DG:N7	6:J:94:HOH:O	2.26	0.69
3:F:284:MET:HE3	3:F:288:TYR:CZ	2.28	0.69
1:J:261:DA:H2"	1:J:262:DC:C5'	2.23	0.69
2:E:679:LYS:HD3	2:E:680:THR:N	2.08	0.68
2:A:461:LEU:HD12	3:B:37:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1277:LEU:HD21	5:D:1293:THR:HG21	1.77	0.67
2:E:729:ARG:HG3	2:E:735:ALA:CA	2.25	0.67
4:G:1017:ARG:HH12	4:G:1031:HIS:HD2	1.43	0.67
4:C:881:ARG:NH2	4:C:907:VAL:O	2.28	0.65
1:J:193:DC:H2"	1:J:194:DT:H72	1.78	0.65
1:I:88:DC:H2"	1:I:89:DC:C6	2.32	0.65
2:A:486:SER:HB3	6:A:48:HOH:O	1.96	0.65
1:I:55:DA:H1'	1:I:56:DA:C8	2.32	0.65
1:J:151:DA:H2"	1:J:152:DT:H5"	1.79	0.65
1:I:69:DC:H2"	1:I:70:DG:C8	2.32	0.65
1:J:175:DA:H2'	1:J:176:DA:C8	2.33	0.64
1:J:262:DC:H2'	1:J:263:DT:H72	1.78	0.64
4:G:1114:VAL:O	4:G:1114:VAL:HG22	1.97	0.64
4:C:862:ILE:HD11	4:C:883:LEU:HD22	1.79	0.63
1:I:27:DA:H61	1:J:266:DT:H3	1.47	0.63
1:I:69:DC:H42	1:J:224:DG:H1	1.47	0.63
2:A:446:VAL:O	2:A:450:GLU:HG3	1.97	0.63
1:I:93:DT:H1'	1:I:94:DG:H5"	1.80	0.63
1:J:152:DT:H2"	1:J:153:DA:C8	2.34	0.63
3:B:30:THR:HB	3:B:32:PRO:HD2	1.80	0.63
4:C:918:LYS:C	4:C:919:LYS:HD3	2.19	0.63
4:C:871:ARG:HD2	6:C:31:HOH:O	1.99	0.62
2:E:734:ARG:O	2:E:735:ALA:HB3	1.99	0.62
5:H:1437:TYR:O	5:H:1441:VAL:HG23	1.98	0.62
1:I:132:DC:H2"	1:I:133:DA:N7	2.14	0.62
1:I:8:DT:H1'	1:I:9:DC:C5'	2.25	0.62
1:I:10:DC:H42	1:J:283:DG:H1	1.45	0.62
3:F:231:LYS:HE2	3:F:235:ARG:NH2	2.14	0.62
1:I:89:DC:H2"	1:I:90:DT:C7	2.30	0.62
1:J:278:DC:H2"	1:J:279:DA:N7	2.15	0.62
1:I:36:DT:H2"	1:I:37:DT:OP2	1.99	0.62
1:I:93:DT:H2"	1:I:94:DG:H5'	1.80	0.62
3:B:52:GLU:OE2	3:B:55:ARG:NH1	2.33	0.62
5:D:1277:LEU:HD21	5:D:1293:THR:CG2	2.29	0.62
1:J:266:DT:H2"	1:J:267:DG:N7	2.14	0.62
1:I:88:DC:H2"	1:I:89:DC:C5	2.35	0.61
4:C:817:ARG:HH22	4:C:831:HIS:CD2	2.17	0.61
2:E:660:LEU:HD11	2:E:690:MET:HE1	1.81	0.61
2:E:687:SER:CB	3:F:301:GLY:C	2.67	0.61
1:J:239:DT:H2"	1:J:240:DG:C8	2.36	0.61
5:D:1291:ILE:O	5:D:1295:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1489:ARG:HG2	5:H:1489:ARG:NH1	2.16	0.60
1:J:147:DA:H2'	1:J:148:DT:H72	1.84	0.60
1:I:144:DG:H2"	1:I:145:DA:OP2	2.02	0.60
4:G:1017:ARG:HH12	4:G:1031:HIS:CD2	2.20	0.60
1:I:57:DA:H2"	1:I:58:DG:N7	2.16	0.60
1:J:151:DA:H2"	1:J:152:DT:C5'	2.31	0.60
4:C:837:GLY:HA3	4:C:839:TYR:CE1	2.37	0.60
1:I:30:DA:H2"	1:I:31:DG:OP2	2.02	0.59
4:C:879:ILE:HG12	4:C:882:HIS:CE1	2.37	0.59
1:I:26:DC:H1'	1:I:27:DA:C5	2.38	0.59
1:I:59:DG:H2"	1:I:60:DC:C5	2.38	0.59
2:E:678:PHE:CE1	3:F:267:ARG:HG3	2.38	0.58
1:J:262:DC:H2'	1:J:263:DT:C7	2.32	0.58
2:E:714:ALA:O	2:E:715:LYS:HB2	2.04	0.58
1:I:111:DA:OP1	4:G:1044:GLY:HA2	2.03	0.58
1:I:5:DA:H2"	1:I:6:DT:H5'	1.85	0.58
2:A:460:LEU:HB3	2:A:493:GLN:HE21	1.68	0.58
1:J:231:DA:H2"	1:J:232:DT:OP2	2.03	0.58
4:G:1110:ASN:HA	6:G:45:HOH:O	2.04	0.58
5:D:1316:THR:O	5:D:1319:THR:HG22	2.04	0.57
1:J:283:DG:H2"	1:J:284:DG:C8	2.39	0.57
2:A:508:ASN:O	2:A:512:ILE:HG13	2.04	0.57
1:J:258:DT:H2"	1:J:259:DA:H5'	1.85	0.57
1:J:197:DA:H5'	2:E:683:ARG:NH1	2.20	0.57
2:A:463:ARG:O	2:A:466:PRO:HD2	2.04	0.57
3:B:59:LYS:O	3:B:63:GLU:HG3	2.05	0.57
4:C:906:GLY:HA3	2:E:658:THR:HG22	1.87	0.57
1:J:237:DT:H5'	2:A:463:ARG:HH21	1.70	0.56
1:J:267:DG:H5"	5:D:1237:TYR:OH	2.05	0.56
5:H:1475:SER:HA	5:H:1486:ILE:HD11	1.86	0.56
1:I:36:DT:C6	1:I:37:DT:H72	2.41	0.56
1:J:248:DA:H2"	1:J:249:DG:N7	2.20	0.56
3:B:26:ILE:O	3:B:55:ARG:HD3	2.04	0.56
4:C:906:GLY:CA	2:E:658:THR:HG22	2.36	0.56
5:H:1470:ILE:HG12	5:H:1498:LEU:HD12	1.86	0.56
1:J:151:DA:C2'	1:J:152:DT:H5"	2.35	0.56
5:H:1445:VAL:HG12	5:H:1446:HIS:HD2	1.71	0.56
1:J:257:DA:C8	1:J:258:DT:H72	2.40	0.56
3:B:35:ARG:O	3:B:39:ARG:HG3	2.06	0.56
1:I:29:DA:H2"	1:I:30:DA:O5'	2.06	0.56
1:J:227:DG:H5'	3:B:47:SER:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:DT:H2"	1:I:76:DC:C6	2.41	0.55
4:G:1037:GLY:HA3	4:G:1039:TYR:CE1	2.41	0.55
2:E:676:GLN:HA	2:E:679:LYS:O	2.05	0.55
1:I:80:DT:O4	1:J:213:DA:N1	2.40	0.55
2:E:660:LEU:HD12	2:E:664:LYS:NZ	2.22	0.55
3:F:235:ARG:NH1	3:F:235:ARG:HG3	2.14	0.55
1:J:246:DG:H2"	1:J:247:DC:H5	1.66	0.55
2:E:678:PHE:HD2	3:F:270:VAL:HG11	1.71	0.55
1:J:235:DC:H2"	1:J:236:DT:OP2	2.06	0.55
1:I:28:DA:H1'	1:I:29:DA:H5"	1.89	0.55
1:I:120:DT:H2"	1:I:121:DG:N7	2.21	0.54
1:I:55:DA:H1'	1:I:56:DA:N7	2.22	0.54
1:J:172:DC:H2"	1:J:173:DA:N7	2.22	0.54
1:J:205:DG:H2"	1:J:206:DC:H5'	1.89	0.54
3:F:228:GLY:C	3:F:229:ILE:HD13	2.28	0.54
4:C:836:LYS:O	5:H:1479:HIS:HE1	1.90	0.54
1:J:233:DG:H2"	1:J:234:DC:OP2	2.08	0.54
2:E:660:LEU:HD12	2:E:664:LYS:HZ3	1.72	0.54
4:C:831:HIS:CE1	4:C:835:ARG:NH2	2.76	0.54
4:C:881:ARG:HG3	4:C:881:ARG:O	2.08	0.54
4:G:1050:TYR:OH	5:H:1492:GLN:HG3	2.08	0.54
2:A:452:ARG:HH11	2:A:452:ARG:HG3	1.73	0.54
1:J:184:DT:H2"	1:J:185:DG:N7	2.23	0.54
1:J:258:DT:H2"	1:J:259:DA:C5'	2.38	0.54
3:B:100:PHE:CD1	3:B:100:PHE:N	2.74	0.54
2:E:677:ASP:CB	6:E:99:HOH:O	2.56	0.54
2:E:719:ILE:O	2:E:719:ILE:HG13	2.07	0.54
1:I:99:DA:H2"	1:I:100:DG:C8	2.43	0.54
1:I:112:DT:P	4:G:1035:ARG:HH22	2.31	0.53
1:I:130:DT:H2"	1:I:131:DG:N7	2.22	0.53
1:I:26:DC:H4'	1:I:27:DA:OP1	2.08	0.53
1:I:60:DC:H2"	1:I:61:DA:C8	2.43	0.53
2:A:461:LEU:HD12	3:B:37:LEU:HA	1.91	0.53
5:H:1502:GLU:OE2	5:H:1505:LYS:HD3	2.08	0.53
1:J:266:DT:H2"	1:J:267:DG:C8	2.42	0.53
1:I:59:DG:H2"	1:I:60:DC:H6	1.67	0.53
5:D:1265:ASP:O	5:D:1269:ARG:HG2	2.08	0.53
1:J:244:DG:N2	1:J:245:DA:C2	2.77	0.53
4:C:900:VAL:HG11	3:F:298:TYR:CE2	2.44	0.53
4:C:831:HIS:CD2	4:C:848:PRO:HG3	2.43	0.53
5:H:1476:ARG:HG2	5:H:1480:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:DT:H4'	1:I:120:DT:OP1	2.08	0.53
1:J:288:DT:H2"	1:J:289:DT:H5'	1.90	0.53
2:A:529:ARG:CD	2:A:529:ARG:C	2.77	0.53
1:I:121:DG:H5"	5:H:1437:TYR:OH	2.09	0.53
1:I:79:DC:H2"	1:I:80:DT:H72	1.91	0.53
1:J:269:DT:H2"	1:J:270:DA:C8	2.44	0.53
1:J:288:DT:H1'	1:J:289:DT:H5"	1.90	0.53
2:A:449:ARG:CB	2:A:449:ARG:HH11	2.22	0.52
1:J:237:DT:C5'	2:A:463:ARG:HH21	2.21	0.52
3:F:252:GLU:OE2	3:F:255:ARG:NH1	2.42	0.52
1:J:276:DT:H2"	1:J:277:DG:N7	2.24	0.52
1:I:102:DA:H2"	1:I:103:DG:OP2	2.10	0.52
1:J:226:DT:H2"	1:J:227:DG:C8	2.44	0.52
5:H:1476:ARG:HG2	5:H:1480:TYR:OH	2.09	0.52
2:A:530:ILE:HG22	2:A:530:ILE:O	2.10	0.52
2:A:449:ARG:HB2	2:A:449:ARG:HH11	1.75	0.52
2:A:463:ARG:HH12	3:B:30:THR:CG2	2.20	0.52
1:I:82:DA:H3'	2:E:646:VAL:HG21	1.92	0.52
5:H:1443:LYS:O	5:H:1447:PRO:HG3	2.09	0.52
2:E:663:ARG:NE	2:E:663:ARG:HA	2.24	0.51
2:E:678:PHE:CD2	3:F:270:VAL:HG11	2.45	0.51
5:D:1245:VAL:HG23	5:D:1246:HIS:CD2	2.45	0.51
2:E:661:LEU:HD12	3:F:237:LEU:HD23	1.91	0.51
4:C:839:TYR:HB3	5:D:1275:SER:HB2	1.92	0.51
4:C:816:THR:O	4:C:820:ARG:HG3	2.11	0.51
1:I:138:DG:H2"	1:I:139:DA:OP2	2.09	0.51
1:I:93:DT:H2"	1:I:94:DG:C5'	2.39	0.51
1:J:180:DT:H2"	1:J:181:DA:OP2	2.10	0.51
1:J:182:DT:H2"	1:J:183:DT:OP2	2.11	0.51
1:J:225:DC:H2"	1:J:226:DT:H72	1.92	0.51
1:I:5:DA:H2"	1:I:6:DT:C5'	2.40	0.51
4:C:850:TYR:O	4:C:854:VAL:HG23	2.11	0.51
3:B:30:THR:CB	3:B:32:PRO:HD2	2.41	0.51
5:H:1446:HIS:HB3	5:H:1449:THR:HB	1.93	0.51
2:E:708:ASN:HB2	3:F:243:VAL:HG22	1.93	0.50
1:J:187:DA:H2"	1:J:188:DA:H8	1.76	0.50
1:J:235:DC:C6	1:J:236:DT:H72	2.47	0.50
1:I:138:DG:H1'	1:I:139:DA:C8	2.46	0.50
2:A:448:LEU:HD13	2:A:451:ILE:HD12	1.92	0.50
2:E:701:VAL:O	2:E:705:GLU:HG3	2.10	0.50
1:J:258:DT:H2'	1:J:259:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:275:DC:H2'	1:J:276:DT:H72	1.94	0.50
1:I:8:DT:C1'	1:I:9:DC:H5'	2.29	0.50
2:E:729:ARG:CG	2:E:735:ALA:HA	2.34	0.50
4:G:1062:ILE:HG12	4:G:1093:LEU:CD1	2.40	0.50
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.94	0.50
4:G:1047:ALA:N	4:G:1048:PRO:HD2	2.27	0.49
1:J:290:DG:H5"	2:E:641:TYR:HA	1.94	0.49
2:A:502:ALA:HA	2:A:505:GLU:HG3	1.95	0.49
3:B:68:ASP:OD2	3:B:92:ARG:NH1	2.46	0.49
3:B:96:THR:CG2	4:G:1100:VAL:HG22	2.39	0.49
1:I:33:DG:H1	1:J:260:DC:H42	1.60	0.49
1:J:156:DC:H2"	1:J:157:DA:C8	2.48	0.49
3:B:31:LYS:HG3	3:B:51:TYR:CE1	2.48	0.49
4:G:1040:ALA:HB2	5:H:1486:ILE:HG13	1.95	0.49
2:E:649:ARG:HH11	2:E:649:ARG:HG3	1.78	0.49
1:I:17:DA:H2"	1:I:18:DG:C8	2.47	0.49
1:J:173:DA:H2"	1:J:174:DA:C8	2.48	0.49
1:I:8:DT:OP1	2:E:649:ARG:HD3	2.13	0.49
1:I:39:DG:N7	6:I:150:HOH:O	2.34	0.49
2:A:479:LYS:HD2	3:B:74:GLU:CG	2.43	0.49
5:D:1321:ALA:O	5:D:1322:LYS:HB2	2.11	0.49
1:J:275:DC:C6	1:J:276:DT:H72	2.48	0.49
4:C:881:ARG:HH21	4:C:906:GLY:HA3	1.78	0.48
2:E:665:LEU:HB3	2:E:666:PRO:HD3	1.94	0.48
5:H:1491:ILE:O	5:H:1495:VAL:HG23	2.13	0.48
5:D:1298:LEU:HG	5:D:1298:LEU:O	2.12	0.48
4:C:854:VAL:HG13	5:D:1307:ALA:HB1	1.95	0.48
1:I:125:DG:H1'	1:I:126:DA:H5'	1.95	0.48
1:J:263:DT:H2"	1:J:264:DT:OP2	2.13	0.48
1:I:114:DC:H4'	1:I:114:DC:OP1	2.13	0.48
1:J:195:DC:H1'	1:J:196:DC:C5	2.48	0.48
1:J:289:DT:H2"	1:J:290:DG:C8	2.49	0.48
4:G:1114:VAL:O	4:G:1114:VAL:CG2	2.62	0.48
1:I:6:DT:H2"	1:I:7:DA:C8	2.48	0.48
4:C:847:ALA:HB3	4:C:848:PRO:HD3	1.96	0.48
1:I:117:DT:C2'	1:I:118:DT:H71	2.44	0.48
5:H:1446:HIS:HB3	5:H:1449:THR:CB	2.44	0.48
1:J:269:DT:H2"	1:J:270:DA:N7	2.28	0.48
1:I:117:DT:H2"	1:I:118:DT:OP2	2.14	0.47
1:I:129:DC:C6	1:I:130:DT:H72	2.49	0.47
1:I:25:DC:N4	1:I:26:DC:N4	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:DC:H2"	1:I:23:DT:OP2	2.13	0.47
4:C:830:VAL:HG13	5:D:1267:PHE:HE1	1.79	0.47
4:C:873:ASN:O	4:C:875:LYS:HG2	2.14	0.47
1:J:175:DA:C2'	1:J:176:DA:C8	2.97	0.47
3:B:39:ARG:NH1	3:B:39:ARG:HG2	2.30	0.47
5:D:1287:THR:O	5:D:1291:ILE:HG12	2.14	0.47
2:E:718:THR:HA	3:F:245:ARG:O	2.14	0.47
4:G:1026:PRO:HD3	5:H:1437:TYR:CD2	2.49	0.47
1:I:108:DC:H2"	1:I:109:DA:N7	2.29	0.47
1:I:27:DA:H1'	1:I:28:DA:O5'	2.13	0.47
1:J:245:DA:H2"	1:J:246:DG:C8	2.50	0.47
4:G:1016:THR:O	4:G:1019:SER:OG	2.33	0.47
4:G:1025:PHE:HE1	5:H:1441:VAL:HG21	1.79	0.47
4:G:1102:ILE:HG23	5:H:1458:ILE:HD13	1.95	0.47
5:D:1245:VAL:HG23	5:D:1246:HIS:N	2.30	0.47
4:G:1090:ASP:O	4:G:1091:GLU:C	2.53	0.47
3:B:26:ILE:HG13	3:B:55:ARG:HB3	1.95	0.46
1:J:195:DC:H1'	1:J:196:DC:C6	2.50	0.46
2:A:446:VAL:O	2:A:449:ARG:HG2	2.15	0.46
4:C:858:LEU:CD1	5:D:1266:VAL:HG11	2.46	0.46
1:J:220:DT:C5'	6:J:75:HOH:O	2.63	0.46
1:J:225:DC:H2"	1:J:226:DT:C7	2.45	0.46
3:B:61:PHE:O	3:B:65:VAL:HG23	2.15	0.46
2:A:529:ARG:NH1	2:E:706:ASP:OD1	2.48	0.46
1:I:8:DT:P	2:E:649:ARG:HD3	2.55	0.46
2:E:676:GLN:HG2	2:E:676:GLN:O	2.15	0.46
1:J:237:DT:H2'	1:J:238:DT:H72	1.96	0.46
2:A:510:CYS:O	2:E:713:HIS:HE1	1.99	0.46
4:C:840:ALA:HA	4:G:1038:ASN:OD1	2.15	0.46
1:J:204:DG:H4'	1:J:205:DG:OP1	2.16	0.46
1:I:29:DA:H5'	1:I:29:DA:H8	1.80	0.46
1:J:150:DA:H2"	1:J:151:DA:OP2	2.14	0.46
4:C:876:THR:O	5:D:1249:THR:HG23	2.15	0.46
5:D:1259:MET:O	5:D:1263:VAL:HG23	2.16	0.46
3:B:38:ALA:HB3	3:B:46:ILE:HD11	1.98	0.46
4:C:858:LEU:HD12	5:D:1266:VAL:HG11	1.98	0.46
1:J:272:DA:H1'	1:J:273:DA:O5'	2.16	0.46
1:I:133:DA:C2	1:J:161:DG:N2	2.84	0.45
4:C:850:TYR:CZ	5:D:1292:GLN:HG3	2.50	0.45
1:I:46:DG:H2"	1:I:47:DC:C6	2.51	0.45
5:D:1243:LYS:HD2	5:D:1243:LYS:HA	1.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:DG:H2"	1:J:206:DC:C5'	2.45	0.45
1:I:49:DC:H1'	1:I:50:DC:C6	2.51	0.45
1:J:190:DC:H1'	1:J:191:DT:H5'	1.97	0.45
3:B:68:ASP:OD2	3:B:93:GLN:NE2	2.50	0.45
5:D:1245:VAL:CG2	5:D:1246:HIS:N	2.80	0.45
3:F:230:THR:HB	3:F:232:PRO:HD2	1.99	0.45
3:B:38:ALA:O	3:B:43:VAL:HB	2.17	0.45
5:H:1469:ARG:O	5:H:1498:LEU:HD11	2.17	0.45
5:D:1286:ILE:HA	5:D:1290:GLU:HG3	1.99	0.45
1:I:144:DG:C2	1:J:150:DA:C2	3.04	0.45
5:H:1446:HIS:HB3	5:H:1449:THR:OG1	2.17	0.45
1:I:54:DA:H61	1:J:239:DT:H3	1.65	0.45
2:A:531:ARG:CD	6:A:69:HOH:O	2.65	0.45
5:D:1262:PHE:O	5:D:1266:VAL:HG23	2.17	0.44
2:E:663:ARG:HE	2:E:663:ARG:HA	1.82	0.44
1:I:111:DA:H2"	1:I:112:DT:OP2	2.17	0.44
4:G:1032:ARG:HD2	4:G:1036:LYS:NZ	2.31	0.44
1:I:120:DT:H2"	1:I:121:DG:C5	2.52	0.44
5:D:1267:PHE:C	5:D:1267:PHE:CD2	2.91	0.44
2:A:515:LYS:O	2:A:516:HIS:HD2	2.01	0.44
2:E:694:GLU:HG3	3:F:300:PHE:CE1	2.52	0.44
1:J:152:DT:H2"	1:J:153:DA:H8	1.83	0.44
4:C:897:LEU:HD22	4:C:900:VAL:HG21	2.00	0.44
1:J:149:DC:H2"	1:J:150:DA:O5'	2.18	0.44
1:J:262:DC:H2"	1:J:263:DT:C6	2.52	0.44
1:J:271:DG:C6	1:J:272:DA:N6	2.86	0.44
5:D:1269:ARG:HB2	5:D:1298:LEU:HD22	2.00	0.44
2:E:669:ARG:HD2	3:F:225:ASN:OD1	2.18	0.44
4:G:1046:GLY:C	4:G:1048:PRO:HD2	2.38	0.44
4:G:1088:ARG:HG2	4:G:1088:ARG:H	1.47	0.44
4:G:1040:ALA:CB	5:H:1486:ILE:HG13	2.48	0.44
1:I:63:DG:H2"	1:I:64:DT:OP2	2.18	0.44
1:I:77:DC:N4	1:J:216:DG:H1	2.12	0.44
3:B:39:ARG:HH11	3:B:39:ARG:HG2	1.83	0.44
1:I:22:DC:C6	1:I:23:DT:H73	2.53	0.44
1:I:25:DC:C2'	1:I:26:DC:H5'	2.45	0.43
1:J:243:DG:H2"	1:J:244:DG:C8	2.53	0.43
3:F:300:PHE:HD2	3:F:301:GLY:H	1.66	0.43
1:I:100:DG:H5"	2:E:683:ARG:HD2	1.99	0.43
1:I:25:DC:C4	1:I:26:DC:N4	2.86	0.43
1:I:80:DT:H3'	3:F:246:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1035:ARG:NH1	4:G:1035:ARG:HG2	2.34	0.43
4:G:1024:GLN:N	4:G:1056:GLU:OE1	2.50	0.43
4:G:1058:LEU:HD23	4:G:1058:LEU:HA	1.84	0.43
1:J:187:DA:H2"	1:J:188:DA:C8	2.53	0.43
1:J:287:DA:C8	1:J:288:DT:H72	2.53	0.43
3:B:26:ILE:HG23	3:B:27:GLN:N	2.33	0.43
2:E:660:LEU:HD13	2:E:693:GLN:NE2	2.33	0.43
1:I:113:DA:C2	1:J:181:DA:C2	3.05	0.43
1:J:162:DC:H2"	1:J:163:DA:N7	2.33	0.43
1:J:224:DG:H2"	1:J:225:DC:C6	2.54	0.43
4:C:832:ARG:HH22	5:D:1232:GLU:CD	2.21	0.43
4:C:892:GLU:CG	5:D:1300:PRO:HB2	2.35	0.43
4:G:1032:ARG:HD2	4:G:1036:LYS:HZ1	1.82	0.43
1:I:96:DT:H2"	1:I:97:DG:OP2	2.19	0.43
1:J:246:DG:H2"	1:J:247:DC:C6	2.49	0.43
1:J:262:DC:C6	1:J:263:DT:H72	2.54	0.43
1:J:153:DA:H5'	2:A:441:TYR:OH	2.18	0.43
2:E:651:ILE:O	2:E:655:GLN:HG3	2.19	0.43
5:D:1234:TYR:HB2	5:D:1260:ASN:OD1	2.18	0.43
1:I:59:DG:C2'	1:I:60:DC:C5	3.01	0.43
4:C:902:ILE:CG2	5:D:1258:ILE:HD13	2.49	0.43
2:A:510:CYS:SG	2:E:730:ILE:HD11	2.59	0.43
1:I:21:DT:H2"	1:I:22:DC:O5'	2.18	0.43
1:I:79:DC:H2"	1:I:80:DT:C7	2.49	0.43
5:H:1500:PRO:O	5:H:1501:GLY:C	2.57	0.43
1:I:130:DT:C4	1:J:162:DC:N4	2.87	0.43
4:C:847:ALA:N	4:C:848:PRO:HD2	2.34	0.43
1:I:9:DC:H2"	1:I:10:DC:H5'	2.01	0.43
4:C:893:LEU:HD23	4:C:893:LEU:HA	1.85	0.42
1:I:34:DT:H2"	1:I:35:DA:O5'	2.18	0.42
4:C:884:GLN:NE2	4:C:906:GLY:O	2.52	0.42
2:E:731:ARG:NH1	2:E:733:GLU:OE2	2.53	0.42
1:I:141:DA:C2	1:J:153:DA:C2	3.07	0.42
4:C:847:ALA:HB3	4:C:848:PRO:CD	2.50	0.42
2:E:660:LEU:HB3	2:E:693:GLN:HE21	1.85	0.42
4:G:1035:ARG:HH11	4:G:1035:ARG:HG2	1.84	0.42
1:I:144:DG:N2	1:J:150:DA:C2	2.87	0.42
1:J:193:DC:H2"	1:J:194:DT:C7	2.49	0.42
1:J:235:DC:C2'	1:J:236:DT:H72	2.50	0.42
3:F:267:ARG:HD3	6:F:60:HOH:O	2.19	0.42
1:I:10:DC:C4	1:I:11:DA:N6	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:869:ALA:O	4:C:873:ASN:ND2	2.53	0.42
5:H:1466:VAL:O	5:H:1470:ILE:HG13	2.20	0.42
5:H:1509:SER:OG	5:H:1510:GLU:N	2.53	0.42
2:A:479:LYS:HD2	3:B:74:GLU:HG2	2.02	0.41
1:I:129:DC:H2"	1:I:130:DT:C6	2.56	0.41
1:I:33:DG:H1	1:J:260:DC:N4	2.18	0.41
1:J:262:DC:H2"	1:J:263:DT:H6	1.85	0.41
2:E:734:ARG:O	2:E:735:ALA:HB2	2.16	0.41
4:G:1092:GLU:OE2	5:H:1502:GLU:HB3	2.21	0.41
1:I:113:DA:H2"	1:I:114:DC:O5'	2.20	0.41
1:I:72:DA:H2"	1:I:73:DA:C8	2.56	0.41
4:C:841:GLU:OE2	4:G:1038:ASN:ND2	2.50	0.41
4:C:892:GLU:HG2	5:D:1300:PRO:CB	2.34	0.41
2:E:659:GLU:HG3	2:E:659:GLU:H	1.52	0.41
3:F:292:ARG:HH21	5:H:1498:LEU:HD23	1.86	0.41
1:I:10:DC:N4	1:J:283:DG:H1	2.13	0.41
4:C:815:LYS:HE2	4:C:815:LYS:HB3	1.96	0.41
4:G:1111:ILE:N	6:G:45:HOH:O	2.51	0.41
1:I:16:DC:H2"	1:I:17:DA:C8	2.56	0.41
3:B:26:ILE:CG2	3:B:27:GLN:N	2.84	0.41
4:G:1079:ILE:HG12	4:G:1082:HIS:CE1	2.56	0.41
5:D:1276:ARG:HG2	5:D:1280:TYR:CZ	2.56	0.41
2:E:687:SER:CB	3:F:301:GLY:O	2.69	0.41
3:F:283:ALA:CB	3:F:301:GLY:CA	2.99	0.41
1:J:278:DC:O3'	1:J:279:DA:C8	2.74	0.41
4:C:888:ARG:HD3	4:C:888:ARG:HA	1.88	0.41
3:F:229:ILE:N	3:F:229:ILE:HD13	2.35	0.41
4:G:1032:ARG:HH22	5:H:1432:GLU:CD	2.23	0.41
1:J:277:DG:H2"	1:J:278:DC:C6	2.56	0.41
3:B:38:ALA:CB	3:B:46:ILE:HD11	2.51	0.40
5:D:1277:LEU:HD12	5:D:1277:LEU:HA	1.86	0.40
2:A:509:LEU:HA	2:A:509:LEU:HD23	1.79	0.40
4:C:885:LEU:O	4:C:889:ASN:ND2	2.54	0.40
4:C:867:GLY:HA3	5:D:1246:HIS:CD2	2.56	0.40
1:I:114:DC:H2"	1:I:115:DA:O5'	2.21	0.40
1:J:220:DT:H5'	6:J:75:HOH:O	2.20	0.40
3:B:46:ILE:HD13	3:B:46:ILE:HG21	1.88	0.40
4:C:817:ARG:HH12	4:C:831:HIS:HD2	1.68	0.40
4:G:1075:LYS:HD3	6:G:16:HOH:O	2.20	0.40
4:G:1097:LEU:HD21	5:H:1462:PHE:HE1	1.87	0.40
1:J:240:DG:H2"	1:J:241:DA:OP2	2.20	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%)	89 (93%)	7 (7%)	0	100	100
2	E	96/135 (71%)	89 (93%)	6 (6%)	1 (1%)	15	53
3	B	77/102 (76%)	73 (95%)	4 (5%)	0	100	100
3	F	79/102 (78%)	75 (95%)	4 (5%)	0	100	100
4	C	105/129 (81%)	99 (94%)	6 (6%)	0	100	100
4	G	102/129 (79%)	94 (92%)	7 (7%)	1 (1%)	15	53
5	D	89/125 (71%)	80 (90%)	8 (9%)	1 (1%)	14	50
5	H	90/125 (72%)	83 (92%)	6 (7%)	1 (1%)	14	50
All	All	734/982 (75%)	682 (93%)	48 (6%)	4 (0%)	29	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	1301	GLY
5	H	1501	GLY
2	E	734	ARG
4	G	1114	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	85/111 (77%)	80 (94%)	5 (6%)	19	54
2	E	85/111 (77%)	79 (93%)	6 (7%)	14	46
3	B	64/78 (82%)	63 (98%)	1 (2%)	62	86
3	F	67/78 (86%)	64 (96%)	3 (4%)	27	64
4	C	85/100 (85%)	78 (92%)	7 (8%)	11	39
4	G	83/100 (83%)	81 (98%)	2 (2%)	49	79
5	D	77/105 (73%)	74 (96%)	3 (4%)	32	69
5	H	78/105 (74%)	74 (95%)	4 (5%)	24	60
All	All	624/788 (79%)	593 (95%)	31 (5%)	24	60

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	439	HIS
2	A	448	LEU
2	A	449	ARG
2	A	459	GLU
2	A	522	LYS
3	B	24	ASP
4	C	829	ARG
4	C	838	ASN
4	C	850	TYR
4	C	859	THR
4	C	862	ILE
4	C	909	PRO
4	C	919	LYS
5	D	1269	ARG
5	D	1290	GLU
5	D	1319	THR
2	E	649	ARG
2	E	659	GLU
2	E	676	GLN
2	E	681	ASP
2	E	687	SER
2	E	731	ARG
3	F	222	LEU
3	F	223	ARG
3	F	232	PRO
4	G	1050	TYR
4	G	1088	ARG

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Mol	Chain	Res	Type
5	H	1433	SER
5	H	1489	ARG
5	H	1500	PRO
5	H	1522	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	476	GLN
2	A	493	GLN
2	A	516	HIS
3	B	93	GLN
4	C	831	HIS
4	C	838	ASN
2	E	668	GLN
2	E	693	GLN
2	E	716	HIS
3	F	275	HIS
4	G	1031	HIS
5	H	1446	HIS
5	H	1479	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.