



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 AM UTC

PDB ID : 1EQZ / pdb_00001eqz
Title : X-RAY STRUCTURE OF THE NUCLEOSOME CORE PARTICLE AT 2.5
A RESOLUTION
Authors : Hanson, B.L.; Harp, J.M.; Timm, D.E.; Bunick, G.J.
Deposited on : 2000-04-06
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

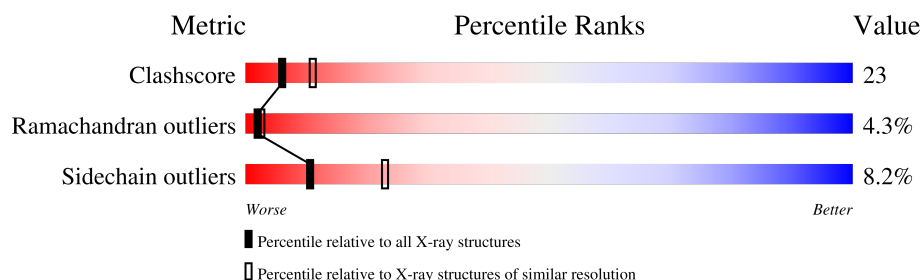
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	40% 58% .
1	J	146	33% 60% 7%
2	A	129	62% 23% 11% . .
2	E	129	57% 35% 7% .
3	B	126	54% 22% 10% 14%
3	F	126	55% 25% 6% 15%
4	C	136	51% 21% 7% . 21%
4	G	136	53% 26% 10% 12%

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Mol	Chain	Length	Quality of chain
5	D	103	
5	H	103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CAC	G	451	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13325 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 146 NUCLEOTIDES LONG DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2994	1430	541	877	146			
1	J	146	Total	C	N	O	P	0	0	0
			2994	1430	541	877	146			

- Molecule 2 is a protein called PROTEIN (HISTONE H2A).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	125	Total	C	N	O	0	0	0
			950	594	190	166			
2	E	127	Total	C	N	O	0	0	0
			968	606	194	168			

- Molecule 3 is a protein called PROTEIN (HISTONE H2B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	108	Total	C	N	O	S	0	0	0
			852	534	157	159	2			
3	F	107	Total	C	N	O	S	0	0	0
			845	529	156	158	2			

- Molecule 4 is a protein called PROTEIN (HISTONE H3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	107	Total	C	N	O	S	0	1	0
			875	550	171	151	3			
4	G	120	Total	C	N	O	S	0	3	0
			996	627	197	169	3			

- Molecule 5 is a protein called PROTEIN (HISTONE H4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	89	Total	C	N	O	S	0	1	0
			723	453	148	121	1			
5	H	95	Total	C	N	O	S	0	0	0
			750	471	152	126	1			

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	K	0	0
			1	1		
6	J	6	Total	K	0	0
			6	6		

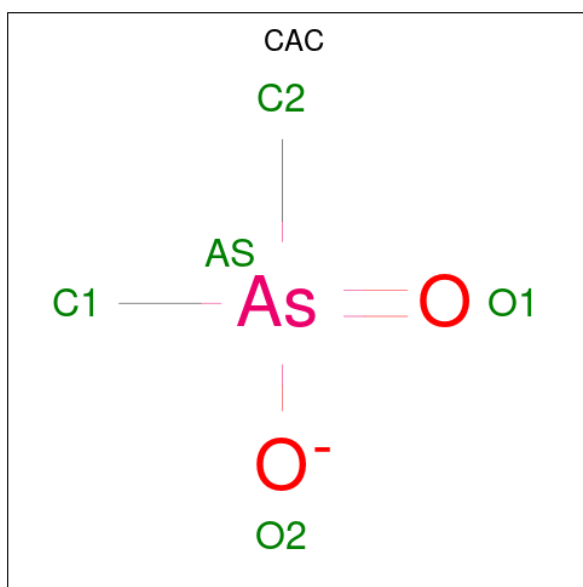
- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	9	Total	Mn	0	0
			9	9		
7	J	6	Total	Mn	0	0
			6	6		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	E	1	Total	Cl	0	0
			1	1		

- Molecule 9 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	I	45	Total	O	0	0
			45	45		
10	J	45	Total	O	0	0
			45	45		
10	A	43	Total	O	0	0
			43	43		
10	B	15	Total	O	0	0
			15	15		
10	C	39	Total	O	0	0
			39	39		
10	D	26	Total	O	0	0
			26	26		
10	E	39	Total	O	0	0
			39	39		
10	F	16	Total	O	0	0
			16	16		
10	G	48	Total	O	0	0
			48	48		
10	H	33	Total	O	0	0
			33	33		

3 Residue-property plots [i](#)

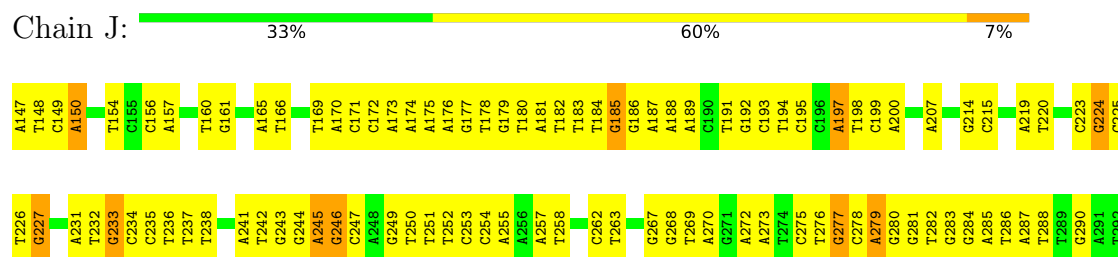
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

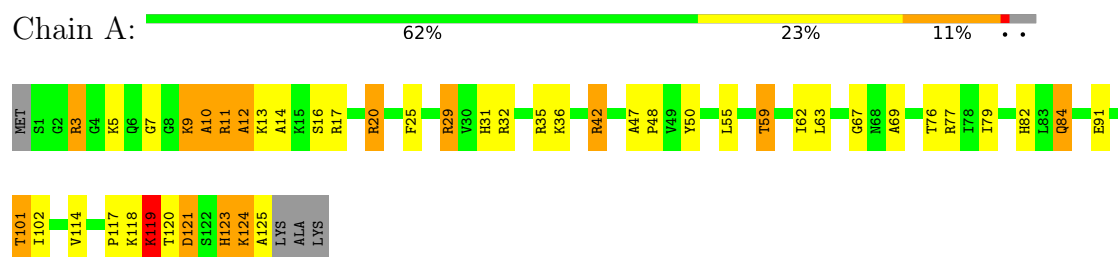
• Molecule 1: 146 NUCLEOTIDES LONG DNA



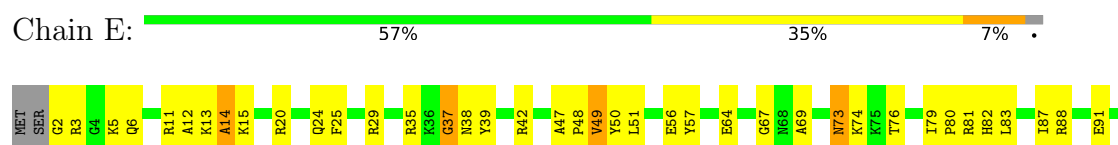
• Molecule 1: 146 NUCLEOTIDES LONG DNA



• Molecule 2: PROTEIN (HISTONE H2A)



• Molecule 2: PROTEIN (HISTONE H2A)





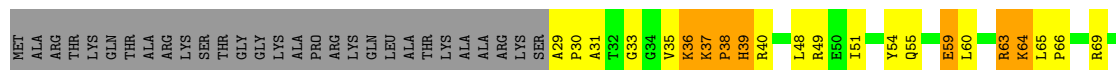
• Molecule 3: PROTEIN (HISTONE H2B)



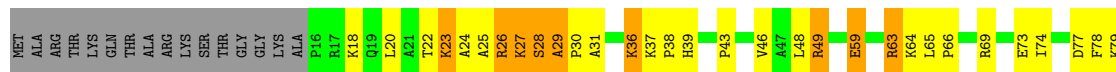
• Molecule 3: PROTEIN (HISTONE H2B)



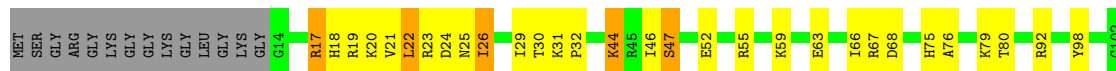
• Molecule 4: PROTEIN (HISTONE H3)



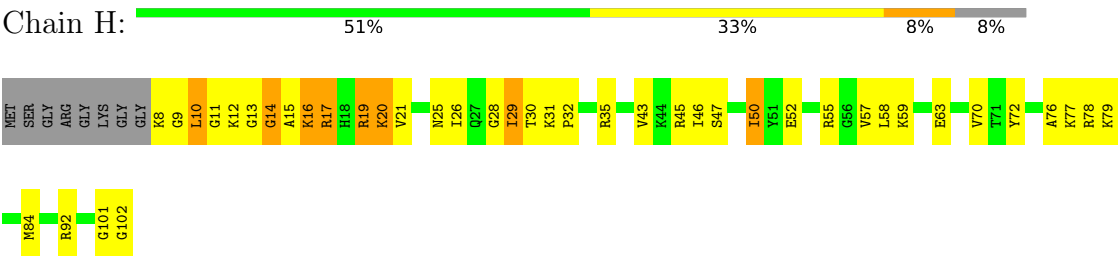
• Molecule 4: PROTEIN (HISTONE H3)



• Molecule 5: PROTEIN (HISTONE H4)



● Molecule 5: PROTEIN (HISTONE H4)



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	105.28Å 109.71Å 181.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.34 – 2.50	Depositor
% Data completeness (in resolution range)	98.6 (25.34-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13325	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	0/3358	0.84	1/5179 (0.0%)
1	J	0.44	0/3358	0.89	4/5179 (0.1%)
2	A	1.01	0/961	1.19	6/1289 (0.5%)
2	E	0.94	1/979 (0.1%)	1.15	4/1310 (0.3%)
3	B	1.02	0/863	1.22	5/1151 (0.4%)
3	F	0.95	1/856 (0.1%)	1.15	3/1141 (0.3%)
4	C	1.02	0/865	1.33	11/1159 (0.9%)
4	G	1.01	1/944 (0.1%)	1.23	8/1260 (0.6%)
5	D	0.99	0/708	1.29	8/943 (0.8%)
5	H	1.12	2/758 (0.3%)	1.23	4/1008 (0.4%)
All	All	0.78	5/13650 (0.0%)	1.05	54/19619 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	3
1	J	0	8
2	E	0	1
3	F	0	1
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	50	ILE	CA-CB	6.74	1.62	1.54
2	E	100	VAL	C-O	-5.58	1.18	1.24
5	H	84	MET	SD-CE	5.25	1.92	1.79
3	F	48	VAL	CA-CB	5.20	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	74	ILE	CA-CB	5.12	1.60	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	133	GLU	N-CA-C	-12.19	98.39	113.01
4	C	117	VAL	N-CA-C	-8.85	104.71	113.20
4	C	134	ARG	N-CA-C	8.75	129.45	110.80
3	B	101	LEU	N-CA-C	8.36	121.98	111.69
4	G	24	ALA	N-CA-C	-8.31	103.26	113.15
4	G	133	GLU	N-CA-C	-8.24	102.95	113.16
2	E	25	PHE	CA-C-N	7.85	129.65	119.84
2	E	25	PHE	C-N-CA	7.85	129.65	119.84
4	G	117	VAL	N-CA-C	-7.50	106.00	113.20
1	I	50	DC	C5'-C4'-C3'	-7.38	103.82	114.90
2	A	12	ALA	N-CA-C	7.08	121.19	111.71
3	F	101	LEU	N-CA-C	7.07	120.38	111.69
3	B	123	SER	N-CA-C	-7.02	104.84	113.19
5	H	46	ILE	N-CA-C	7.00	117.98	107.75
1	J	227	DG	C5'-C4'-C3'	-7.00	104.39	114.90
3	B	38	SER	N-CA-C	6.91	122.77	111.37
4	C	64	LYS	N-CA-C	6.89	119.43	111.02
4	G	85	GLN	N-CA-C	-6.88	100.30	110.48
1	J	277	DG	C5'-C4'-C3'	-6.36	105.36	114.90
4	C	39	HIS	N-CA-C	6.35	124.32	110.80
5	D	29	ILE	N-CA-C	-6.25	98.50	107.37
5	H	28	GLY	N-CA-C	-6.20	107.20	115.32
2	A	91	GLU	N-CA-C	6.19	118.54	111.11
5	H	29	ILE	N-CA-C	-6.13	96.45	106.32
3	B	59	MET	N-CA-C	-6.12	104.69	111.36
5	D	18	HIS	N-CA-C	6.09	120.54	109.32
2	E	37	GLY	N-CA-C	6.07	121.35	114.67
4	C	133	GLU	CA-C-N	6.02	133.03	121.54
4	C	133	GLU	C-N-CA	6.02	133.03	121.54
5	D	30	THR	N-CA-C	5.84	118.44	110.55
4	G	117	VAL	CB-CA-C	5.81	116.45	110.70
5	D	46	ILE	N-CA-C	5.71	116.22	107.77
5	H	17	ARG	N-CA-C	5.65	122.83	110.80
4	C	36	LYS	CB-CA-C	-5.63	110.10	116.63
4	G	94	GLU	N-CA-C	-5.60	105.33	111.82
1	J	246	DG	C5'-C4'-C3'	-5.54	106.59	114.90
1	J	185	DG	C5'-C4'-C3'	-5.45	106.72	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	49	VAL	N-CA-C	-5.38	105.36	110.42
5	D	76	ALA	N-CA-C	-5.38	106.49	113.16
2	A	3	ARG	N-CA-C	-5.38	105.33	111.14
4	G	81	ASP	N-CA-C	5.33	119.06	112.24
4	G	117	VAL	N-CA-CB	-5.31	104.54	112.67
2	A	84	GLN	CB-CA-C	-5.29	102.58	110.88
4	C	54	TYR	N-CA-C	5.22	119.08	112.72
2	A	42	ARG	N-CA-C	5.17	117.66	109.50
5	D	80	THR	N-CA-C	5.15	117.04	108.02
5	D	44	LYS	N-CA-C	5.13	119.62	112.90
4	C	83	ARG	N-CA-C	-5.13	102.61	110.14
2	A	69	ALA	N-CA-C	-5.12	105.88	111.82
3	B	41	VAL	N-CA-C	-5.11	105.41	110.62
3	F	38	SER	N-CA-C	5.05	117.18	111.02
3	F	60	GLY	N-CA-C	-5.04	106.31	112.77
5	D	22	LEU	N-CA-C	-5.04	100.08	110.80
4	C	94	GLU	N-CA-C	-5.03	105.70	111.14

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	57	TYR	Sidechain
3	F	40	TYR	Sidechain
1	I	41	DA	Sidechain
1	I	59	DG	Sidechain
1	I	79	DC	Sidechain
1	J	150	DA	Sidechain
1	J	197	DA	Sidechain
1	J	214	DG	Sidechain
1	J	224	DG	Sidechain
1	J	233	DG	Sidechain
1	J	245	DA	Sidechain
1	J	267	DG	Sidechain
1	J	279	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	2994	0	1650	126	0
1	J	2994	0	1650	121	0
2	A	950	0	1021	52	0
2	E	968	0	1044	50	0
3	B	852	0	900	54	0
3	F	845	0	891	39	0
4	C	875	0	920	43	0
4	G	996	0	1059	64	0
5	D	723	0	775	24	0
5	H	750	0	809	57	0
6	I	1	0	0	0	0
6	J	6	0	0	0	0
7	I	9	0	0	0	0
7	J	6	0	0	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
9	G	5	0	0	1	0
10	A	43	0	0	5	0
10	B	15	0	0	0	0
10	C	39	0	0	1	0
10	D	26	0	0	0	0
10	E	39	0	0	2	0
10	F	16	0	0	0	0
10	G	48	0	0	1	0
10	H	33	0	0	5	0
10	I	45	0	0	0	0
10	J	45	0	0	0	0
All	All	13325	0	10719	536	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 23.

All (536) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:188:DA:H2''	1:J:189:DA:H5'	1.26	1.17
2:A:17:ARG:HH22	2:A:31:HIS:CD2	1.65	1.14
1:I:124:DA:H2''	1:I:125:DG:H5''	1.33	1.09
1:J:187:DA:H2''	1:J:188:DA:H5''	1.35	1.07
1:I:103:DG:H2''	1:I:104:DT:H5'	1.34	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:30:PRO:HA	4:C:38:PRO:HA	1.37	1.05
1:I:125:DG:H2''	1:I:126:DA:H5'	1.40	1.03
2:A:17:ARG:NH2	2:A:31:HIS:HD2	1.59	1.01
1:I:2:DT:H2''	1:I:3:DC:H5'	1.41	1.00
4:C:30:PRO:HA	4:C:38:PRO:CA	1.95	0.95
5:H:10:LEU:HD22	5:H:10:LEU:H	1.31	0.94
3:F:86:ARG:HG2	3:F:86:ARG:HH11	1.33	0.94
1:I:129:DC:H4'	1:I:130:DT:OP1	1.70	0.91
1:J:187:DA:C2'	1:J:188:DA:H5''	2.01	0.91
1:I:100:DG:OP1	5:H:10:LEU:HD11	1.72	0.90
4:G:81:ASP:HB3	5:H:10:LEU:HD23	1.54	0.89
1:J:246:DG:H2''	1:J:247:DC:C5	2.06	0.89
4:G:49:ARG:HG3	4:G:49:ARG:HH11	1.36	0.89
1:J:179:DG:H4'	1:J:180:DT:OP1	1.73	0.89
2:A:119:LYS:H	2:A:119:LYS:HD2	1.37	0.89
1:J:197:DA:H2''	1:J:198:DT:H5'	1.53	0.89
5:D:19:ARG:HG2	5:D:20:LYS:H	1.33	0.88
1:J:272:DA:H2''	1:J:273:DA:H5''	1.56	0.86
2:E:42:ARG:HB2	3:F:88:THR:HB	1.56	0.86
1:J:250:DT:H2''	1:J:251:DT:H71	1.55	0.86
2:A:118:LYS:HD3	2:A:125:ALA:HB3	1.57	0.85
4:C:30:PRO:HG3	4:C:38:PRO:HB3	1.56	0.85
1:I:40:DG:OP1	3:B:88:THR:HG23	1.76	0.84
1:J:262:DC:C6	1:J:263:DT:H72	2.11	0.84
1:J:263:DT:H6	1:J:263:DT:H5'	1.42	0.84
1:J:165:DA:H2''	1:J:166:DT:H5'	1.59	0.84
3:F:19:THR:C	3:F:20:LYS:HD2	2.03	0.84
1:I:124:DA:C2'	1:I:125:DG:H5''	2.06	0.83
2:A:55:LEU:O	2:A:59:THR:HG23	1.78	0.83
1:I:61:DA:H2''	1:I:62:DT:H5'	1.61	0.82
1:J:188:DA:C2'	1:J:189:DA:H5'	2.10	0.81
1:I:52:DT:H2''	1:I:53:DC:C5'	2.11	0.81
5:D:19:ARG:HD3	5:D:20:LYS:HD3	1.63	0.81
1:J:268:DG:H4'	3:B:33:ARG:HG3	1.63	0.80
1:I:125:DG:C2'	1:I:126:DA:H5'	2.11	0.80
1:J:149:DC:H2''	1:J:150:DA:C8	2.16	0.80
1:J:231:DA:H2''	1:J:232:DT:O5'	1.81	0.80
4:G:36:LYS:HD3	4:G:37:LYS:N	1.97	0.80
4:G:36:LYS:NZ	4:G:38:PRO:HD3	1.97	0.80
5:H:20:LYS:HD3	10:H:414:HOH:O	1.80	0.80
1:J:284:DG:H2''	1:J:285:DA:C8	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:DT:H2''	1:I:53:DC:H5''	1.64	0.79
4:C:117:VAL:HG13	2:E:115:LEU:CD2	2.13	0.79
2:A:42:ARG:HB2	3:B:88:THR:HB	1.62	0.79
1:J:236:DT:OP1	5:D:21:VAL:HB	1.82	0.79
4:C:31:ALA:O	4:C:36:LYS:HD3	1.83	0.78
1:I:4:DA:H2''	1:I:5:DA:H5'	1.63	0.78
4:G:23:LYS:HD2	4:G:26:ARG:HH21	1.48	0.78
1:J:197:DA:H2''	1:J:198:DT:C5'	2.14	0.78
2:A:17:ARG:HH22	2:A:31:HIS:HD2	0.82	0.78
5:D:17:ARG:HG2	5:D:21:VAL:HG13	1.66	0.78
4:G:81:ASP:HB3	5:H:10:LEU:CD2	2.14	0.78
1:J:281:DG:H2''	1:J:282:DT:O5'	1.84	0.78
1:J:170:DA:H2''	1:J:171:DC:OP2	1.84	0.77
5:D:19:ARG:HG2	5:D:20:LYS:N	2.00	0.77
2:E:12:ALA:O	2:E:13:LYS:HG2	1.86	0.76
1:I:52:DT:C2'	1:I:53:DC:H5''	2.17	0.75
1:I:103:DG:H2''	1:I:104:DT:C5'	2.17	0.75
1:J:186:DG:OP1	3:F:88:THR:HG23	1.86	0.75
2:E:3:ARG:N	2:E:3:ARG:HD2	2.02	0.74
2:E:125:ALA:O	2:E:126:LYS:HB3	1.87	0.74
5:H:20:LYS:HA	10:H:414:HOH:O	1.87	0.74
1:I:124:DA:H2''	1:I:125:DG:C5'	2.15	0.74
1:I:26:DC:H2''	1:I:27:DA:N7	2.02	0.73
1:J:165:DA:H2''	1:J:166:DT:C5'	2.17	0.73
1:I:57:DA:H2''	1:I:58:DG:C8	2.24	0.73
4:G:29:ALA:H	4:G:30:PRO:HD3	1.53	0.73
4:G:81:ASP:OD1	5:H:10:LEU:HB2	1.88	0.73
3:B:29:ARG:HG2	3:B:29:ARG:HH11	1.53	0.73
1:I:47:DC:H5''	3:F:29:ARG:HG3	1.70	0.73
4:G:36:LYS:HZ2	4:G:38:PRO:HD3	1.51	0.73
4:C:69:ARG:HD2	5:D:25:ASN:OD1	1.89	0.72
1:I:26:DC:H2''	1:I:27:DA:C8	2.24	0.72
1:I:47:DC:H2''	1:I:48:DT:H71	1.72	0.72
4:C:37:LYS:N	4:C:37:LYS:HE2	2.05	0.72
4:C:64:LYS:HE2	4:C:90:MET:HE1	1.71	0.71
1:I:2:DT:C2'	1:I:3:DC:H5'	2.20	0.71
5:H:10:LEU:HD21	5:H:79:LYS:HE2	1.72	0.71
1:J:250:DT:OP2	3:F:30:LYS:HE3	1.91	0.71
4:G:29:ALA:N	4:G:30:PRO:HD3	2.05	0.71
5:D:17:ARG:HD3	5:D:22:LEU:HA	1.73	0.71
2:E:2:GLY:C	2:E:3:ARG:HD2	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:119:LYS:HD2	2:A:119:LYS:N	2.01	0.70
1:I:2:DT:H4'	1:I:2:DT:OP1	1.92	0.70
4:G:81:ASP:CG	5:H:10:LEU:HB2	2.16	0.70
1:J:246:DG:H5'	5:D:79:LYS:HG3	1.73	0.69
1:I:36:DT:H2''	1:I:37:DT:OP2	1.92	0.69
4:C:117:VAL:HG13	2:E:115:LEU:HD22	1.75	0.69
3:B:24:LYS:HG3	3:B:25:GLY:H	1.57	0.69
3:B:27:LYS:HD2	3:B:27:LYS:N	2.07	0.69
5:H:15:ALA:O	5:H:16:LYS:HB2	1.91	0.69
2:A:118:LYS:NZ	2:A:124:LYS:HB2	2.08	0.69
4:G:81:ASP:CB	5:H:10:LEU:HD23	2.22	0.69
4:C:132:GLY:C	4:C:134:ARG:H	1.97	0.69
4:G:26:ARG:HA	4:G:26:ARG:NE	2.08	0.69
3:B:18:VAL:HG12	3:B:19:THR:N	2.07	0.68
1:I:24:DA:H2'	1:I:25:DC:C6	2.28	0.68
2:A:17:ARG:NH2	2:A:31:HIS:CD2	2.45	0.68
5:H:20:LYS:CD	10:H:414:HOH:O	2.40	0.68
3:B:18:VAL:HG12	3:B:19:THR:H	1.58	0.68
1:I:139:DA:H4'	1:I:140:DT:OP1	1.93	0.68
4:C:37:LYS:HE2	4:C:37:LYS:H	1.59	0.68
1:J:250:DT:OP1	3:F:30:LYS:HB2	1.94	0.67
1:J:250:DT:C2'	1:J:251:DT:H71	2.23	0.67
5:H:59:LYS:O	5:H:63:GLU:HG3	1.94	0.67
1:J:199:DC:H2''	1:J:200:DA:H5'	1.75	0.67
1:J:254:DC:H2''	1:J:255:DA:N7	2.10	0.67
2:E:29:ARG:NH2	3:F:35:GLU:HG2	2.08	0.67
2:A:114:VAL:HG13	10:A:461:HOH:O	1.95	0.67
4:C:30:PRO:CG	4:C:38:PRO:HB3	2.24	0.67
1:I:17:DA:N6	1:J:275:DC:N4	2.43	0.66
1:I:65:DT:H4'	1:I:65:DT:OP1	1.96	0.66
2:A:120:THR:HG23	2:A:121:ASP:H	1.59	0.66
2:E:37:GLY:HA3	2:E:39:TYR:CE2	2.29	0.66
1:I:127:DA:H2''	1:I:128:DT:O5'	1.96	0.66
2:E:13:LYS:O	2:E:14:ALA:HB2	1.94	0.66
2:A:101:THR:HG22	10:H:251:HOH:O	1.95	0.66
1:J:187:DA:C3'	1:J:188:DA:H5''	2.25	0.66
1:I:129:DC:C6	1:I:130:DT:H72	2.30	0.66
3:F:25:GLY:C	3:F:27:LYS:H	2.04	0.66
1:J:272:DA:C2'	1:J:273:DA:H5''	2.23	0.66
2:E:14:ALA:O	2:E:15:LYS:HB2	1.96	0.65
5:H:10:LEU:H	5:H:10:LEU:CD2	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:DT:H2''	1:I:22:DC:O5'	1.95	0.65
4:C:132:GLY:C	4:C:134:ARG:N	2.50	0.65
1:J:169:DT:H2''	1:J:170:DA:O5'	1.95	0.65
3:F:84:ASN:O	3:F:86:ARG:HD3	1.97	0.65
3:B:31:LYS:HG3	3:B:32:SER:H	1.61	0.65
3:F:34:LYS:NZ	3:F:34:LYS:HB3	2.11	0.64
4:C:117:VAL:HG12	4:C:117:VAL:O	1.95	0.64
4:G:23:LYS:C	4:G:25:ALA:H	2.05	0.64
4:G:119:ILE:HD13	5:H:43:VAL:HG11	1.79	0.64
4:G:22:THR:O	4:G:23:LYS:HG3	1.97	0.64
2:A:102:ILE:HG23	3:B:61:ILE:HD13	1.78	0.64
2:A:118:LYS:NZ	2:A:124:LYS:CB	2.61	0.64
5:D:31:LYS:HB3	5:D:32:PRO:HD3	1.80	0.64
10:A:468:HOH:O	4:C:129:ARG:HG3	1.96	0.64
2:E:20:ARG:HG2	2:E:20:ARG:HH11	1.62	0.64
1:J:276:DT:H2''	1:J:277:DG:N7	2.13	0.63
1:I:20:DT:H1'	1:I:21:DT:H5'	1.80	0.63
1:I:23:DT:H2''	1:I:24:DA:O5'	1.98	0.63
5:H:31:LYS:HB3	5:H:32:PRO:HD3	1.80	0.63
1:J:193:DC:H2''	1:J:194:DT:H71	1.81	0.63
1:J:207:DA:H5''	4:G:63:ARG:CZ	2.28	0.63
1:J:241:DA:H2'	1:J:242:DT:H71	1.81	0.63
3:B:46:LYS:HA	3:B:46:LYS:HE2	1.81	0.63
1:I:48:DT:OP1	3:F:29:ARG:CZ	2.47	0.62
1:J:257:DA:C8	1:J:258:DT:H72	2.34	0.62
1:J:207:DA:OP1	4:G:63:ARG:HD3	1.98	0.62
1:J:263:DT:H5'	1:J:263:DT:C6	2.31	0.62
1:I:32:DT:H6	1:I:32:DT:H5'	1.64	0.62
4:G:49:ARG:HH11	4:G:49:ARG:CG	2.12	0.62
1:J:207:DA:H5''	4:G:63:ARG:NH1	2.14	0.62
1:J:225:DC:H2''	1:J:226:DT:H71	1.82	0.62
2:A:7:GLY:HA2	2:A:9:LYS:HE2	1.80	0.62
5:D:17:ARG:HD3	5:D:22:LEU:CA	2.30	0.62
4:C:37:LYS:HE2	4:C:37:LYS:CA	2.30	0.61
4:G:129[1]:ARG:CZ	4:G:135:ALA:O	2.48	0.61
3:F:86:ARG:HG2	3:F:86:ARG:NH1	2.10	0.61
4:G:18:LYS:H	4:G:20:LEU:HD13	1.65	0.61
1:J:237:DT:P	4:C:69:ARG:HH22	2.24	0.61
1:J:156:DC:H2''	1:J:157:DA:OP2	2.01	0.61
4:C:110:CYS:SG	4:C:126:LEU:HD23	2.41	0.61
4:G:101:VAL:O	4:G:105:GLU:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:19:THR:O	3:F:20:LYS:HD2	2.01	0.60
1:J:175:DA:H2''	1:J:176:DA:C8	2.35	0.60
3:B:18:VAL:O	3:B:19:THR:HG22	2.01	0.60
5:H:12:LYS:HD2	5:H:16:LYS:HE3	1.84	0.60
3:B:31:LYS:O	3:B:32:SER:HB2	2.00	0.60
1:I:52:DT:H2''	1:I:53:DC:H5'	1.84	0.60
1:I:82:DA:H3'	4:G:46:VAL:HG21	1.83	0.60
1:J:174:DA:H2''	1:J:175:DA:H8	1.65	0.60
3:F:29:ARG:O	3:F:30:LYS:HB2	2.02	0.60
1:J:172:DC:H2''	1:J:173:DA:N7	2.16	0.59
1:I:104:DT:H4'	3:B:28:LYS:HE2	1.83	0.59
5:H:10:LEU:HD21	5:H:79:LYS:CE	2.32	0.59
5:H:20:LYS:HD2	5:H:21:VAL:N	2.18	0.59
2:E:67:GLY:HA3	3:F:49:HIS:CD2	2.38	0.59
1:I:23:DT:H2'	1:I:23:DT:OP2	2.03	0.59
1:I:115:DA:H2''	1:I:116:DC:OP2	2.03	0.59
1:J:275:DC:H2'	1:J:276:DT:C6	2.37	0.59
1:I:53:DC:H2''	1:I:54:DA:C8	2.37	0.59
1:I:128:DT:H2''	1:I:129:DC:O5'	2.01	0.59
3:B:22:GLN:O	3:B:22:GLN:HG2	2.02	0.59
1:J:192:DG:H4'	1:J:193:DC:OP1	2.03	0.58
2:A:118:LYS:HZ3	2:A:124:LYS:HB2	1.67	0.58
5:H:11:GLY:C	5:H:12:LYS:HG3	2.29	0.58
2:E:15:LYS:NZ	2:E:20:ARG:HH12	2.01	0.58
3:B:125:LYS:HD2	3:B:125:LYS:C	2.29	0.58
4:C:30:PRO:HG3	4:C:38:PRO:CB	2.30	0.58
1:I:1:DA:H2'	1:I:2:DT:H71	1.85	0.58
4:G:26:ARG:CZ	4:G:27:LYS:H	2.17	0.58
3:B:26:ASP:C	3:B:27:LYS:HD2	2.28	0.58
4:C:64:LYS:HE2	4:C:90:MET:CE	2.33	0.58
5:H:19:ARG:O	5:H:20:LYS:HB3	2.04	0.58
2:E:76:THR:O	3:F:52:THR:HG23	2.03	0.57
2:A:124:LYS:NZ	2:A:124:LYS:HB3	2.19	0.57
5:H:35:ARG:HG3	5:H:35:ARG:HH11	1.68	0.57
1:I:16:DC:H2''	1:I:17:DA:N7	2.19	0.57
1:I:65:DT:H2'	1:I:66:DC:C6	2.40	0.57
5:H:10:LEU:HD22	5:H:10:LEU:N	2.13	0.57
1:J:181:DA:H2''	1:J:182:DT:O5'	2.05	0.57
1:J:252:DT:H2''	1:J:253:DC:C6	2.39	0.57
1:J:194:DT:H2'	1:J:195:DC:C6	2.40	0.56
1:J:246:DG:H5'	5:D:79:LYS:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:285:DA:H2''	1:J:286:DT:C6	2.41	0.56
4:G:36:LYS:HD3	4:G:37:LYS:H	1.67	0.56
1:I:29:DA:C2'	1:I:30:DA:C8	2.88	0.56
1:I:76:DC:H2''	1:I:77:DC:C5	2.40	0.56
1:I:123:DT:H2''	1:I:124:DA:H5'	1.88	0.56
2:A:118:LYS:HZ3	2:A:124:LYS:CB	2.18	0.56
3:B:96:THR:HG21	5:D:75:HIS:ND1	2.20	0.56
2:E:24:GLN:N	2:E:56:GLU:OE1	2.39	0.56
4:G:26:ARG:HG3	4:G:27:LYS:H	1.70	0.56
1:I:31:DG:H5''	2:A:16:SER:HA	1.87	0.56
1:I:103:DG:C2'	1:I:104:DT:H5'	2.23	0.56
1:I:22:DC:N4	1:J:270:DA:N6	2.54	0.56
1:I:47:DC:OP1	3:F:27:LYS:HD3	2.06	0.56
2:E:20:ARG:HG2	2:E:20:ARG:NH1	2.21	0.56
1:J:165:DA:C2'	1:J:166:DT:H5'	2.35	0.55
2:E:87:ILE:HD13	2:E:97:LEU:HD12	1.87	0.55
4:G:81:ASP:HB3	5:H:10:LEU:CG	2.35	0.55
1:I:9:DC:H2''	1:I:10:DC:C6	2.41	0.55
2:A:55:LEU:O	2:A:59:THR:CG2	2.52	0.55
5:H:29:ILE:HG13	5:H:58:LEU:HD23	1.89	0.55
4:C:117:VAL:O	4:C:117:VAL:CG1	2.55	0.55
3:B:122:THR:C	3:B:124:SER:H	2.13	0.55
5:H:17:ARG:HA	5:H:17:ARG:NE	2.22	0.55
1:J:282:DT:H4'	1:J:282:DT:OP1	2.07	0.54
5:D:52:GLU:OE2	5:D:55:ARG:NH1	2.40	0.54
4:G:26:ARG:NH1	4:G:27:LYS:H	2.05	0.54
2:E:83:LEU:O	2:E:87:ILE:HG13	2.07	0.54
5:H:11:GLY:HA2	5:H:17:ARG:HD2	1.87	0.54
1:J:250:DT:C6	1:J:251:DT:H73	2.42	0.54
3:F:86:ARG:HH11	3:F:86:ARG:CG	2.09	0.54
1:J:175:DA:C2'	1:J:176:DA:C8	2.91	0.54
2:A:20:ARG:HH11	3:B:124:SER:HB3	1.72	0.54
4:C:37:LYS:HE2	4:C:37:LYS:HA	1.90	0.54
4:C:40:ARG:NH1	10:C:145:HOH:O	2.39	0.54
5:H:101:GLY:O	5:H:102:GLY:C	2.50	0.54
1:I:76:DC:H2''	1:I:77:DC:C6	2.43	0.54
1:I:47:DC:H2''	1:I:48:DT:C7	2.37	0.54
2:E:123:HIS:O	2:E:125:ALA:N	2.41	0.54
2:A:13:LYS:HG3	2:A:14:ALA:H	1.73	0.54
5:H:8:LYS:O	5:H:10:LEU:N	2.41	0.54
1:I:30:DA:OP2	2:A:32:ARG:HD3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:29:ARG:HH11	3:B:29:ARG:CG	2.19	0.53
5:H:13:GLY:H	5:H:17:ARG:HG2	1.72	0.53
1:I:61:DA:C2'	1:I:62:DT:H5'	2.37	0.53
2:A:42:ARG:CB	3:B:88:THR:HB	2.37	0.53
3:B:31:LYS:CG	3:B:32:SER:H	2.19	0.53
1:I:107:DC:H2''	1:I:108:DC:C5	2.44	0.53
2:A:10:ALA:O	2:A:11:ARG:HB3	2.09	0.53
4:G:23:LYS:HD2	4:G:26:ARG:NH2	2.20	0.53
5:H:30:THR:HB	5:H:32:PRO:HD2	1.89	0.53
1:I:29:DA:H2'	1:I:30:DA:C8	2.44	0.53
1:I:2:DT:OP1	1:I:2:DT:C4'	2.56	0.53
1:I:55:DA:H2''	1:I:56:DA:H5'	1.89	0.53
4:G:78[2]:PHE:HD2	5:H:70:VAL:HG11	1.74	0.53
1:J:278:DC:H2''	1:J:279:DA:N7	2.24	0.53
1:I:64:DT:H2''	1:I:65:DT:O5'	2.09	0.52
1:J:175:DA:H2''	1:J:176:DA:H8	1.74	0.52
1:J:227:DG:H5'	5:D:47:SER:HA	1.90	0.52
5:H:10:LEU:CD2	5:H:79:LYS:NZ	2.72	0.52
1:J:154:DT:OP1	4:C:49:ARG:HD2	2.10	0.52
1:J:182:DT:C2'	1:J:183:DT:H71	2.40	0.52
1:J:169:DT:O4	1:J:170:DA:N6	2.43	0.52
1:J:287:DA:H1'	1:J:288:DT:H5'	1.92	0.52
5:D:19:ARG:CG	5:D:20:LYS:N	2.70	0.52
4:G:29:ALA:C	4:G:31:ALA:H	2.18	0.52
2:E:73:ASN:N	2:E:73:ASN:HD22	2.08	0.52
4:G:18:LYS:N	4:G:20:LEU:HD13	2.24	0.51
1:I:100:DG:P	5:H:10:LEU:HD11	2.50	0.51
1:I:139:DA:C4'	1:I:140:DT:OP1	2.56	0.51
2:E:126:LYS:O	2:E:127:ALA:HB2	2.10	0.51
4:G:65:LEU:HB3	4:G:66:PRO:HD3	1.91	0.51
1:I:104:DT:C2'	1:I:105:DT:H71	2.40	0.51
1:J:282:DT:H2'	1:J:283:DG:C8	2.44	0.51
1:J:173:DA:H1'	1:J:174:DA:C8	2.46	0.51
2:A:62:ILE:HD12	3:B:65:PHE:CE2	2.45	0.51
1:I:22:DC:N4	1:J:270:DA:H62	2.07	0.51
1:J:284:DG:H2''	1:J:285:DA:H8	1.70	0.51
5:H:20:LYS:HD2	5:H:21:VAL:H	1.75	0.51
1:J:223:DC:H2''	1:J:224:DG:C8	2.46	0.51
1:J:237:DT:H2'	1:J:238:DT:H71	1.93	0.51
4:C:29:ALA:HA	4:C:30:PRO:C	2.35	0.51
4:C:101:VAL:O	4:C:105:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:20:LYS:HD3	10:H:433:HOH:O	2.10	0.51
4:G:39:HIS:CD2	4:G:39:HIS:C	2.88	0.50
1:J:172:DC:H2''	1:J:173:DA:C8	2.47	0.50
4:G:26:ARG:HG3	4:G:27:LYS:HG3	1.92	0.50
5:D:44:LYS:NZ	2:E:115:LEU:O	2.42	0.50
2:E:13:LYS:O	2:E:14:ALA:CB	2.59	0.50
1:I:7:DA:C2	1:J:287:DA:C2	2.99	0.50
1:I:105:DT:OP1	3:B:28:LYS:NZ	2.41	0.50
3:B:32:SER:O	3:B:33:ARG:HB3	2.12	0.50
1:J:194:DT:C2'	1:J:195:DC:C6	2.94	0.50
1:J:254:DC:H2''	1:J:255:DA:C8	2.46	0.50
2:E:101:THR:HA	10:E:453:HOH:O	2.11	0.50
4:G:118:THR:OG1	5:H:45:ARG:HD3	2.11	0.50
3:B:22:GLN:C	3:B:24:LYS:H	2.19	0.50
1:I:131:DG:H3'	2:E:76:THR:HG22	1.94	0.50
3:B:18:VAL:CG1	3:B:19:THR:H	2.23	0.50
3:F:54:ILE:HG23	3:F:54:ILE:O	2.11	0.49
1:I:4:DA:H2''	1:I:5:DA:OP2	2.11	0.49
1:I:27:DA:C4'	1:I:28:DA:H5'	2.43	0.49
1:J:174:DA:H2''	1:J:175:DA:C8	2.46	0.49
5:D:98:TYR:CD1	3:F:64:SER:HB3	2.47	0.49
3:F:86:ARG:NH1	3:F:86:ARG:CG	2.69	0.49
2:A:77:ARG:HD2	10:A:480:HOH:O	2.11	0.49
1:J:225:DC:H2''	1:J:226:DT:C6	2.47	0.49
1:J:280:DG:H1'	1:J:281:DG:C8	2.48	0.49
2:A:120:THR:HG23	2:A:121:ASP:N	2.26	0.49
5:D:79:LYS:HB3	5:D:79:LYS:HZ3	1.78	0.49
2:E:12:ALA:O	2:E:13:LYS:CG	2.60	0.49
3:B:31:LYS:HG3	3:B:32:SER:N	2.27	0.49
1:J:185:DG:H8	1:J:185:DG:OP2	1.96	0.49
1:J:191:DT:H1'	3:B:29:ARG:HH21	1.78	0.49
2:E:79:ILE:HG12	2:E:82:HIS:CE1	2.47	0.49
3:F:119:THR:O	3:F:120:LYS:C	2.56	0.49
4:C:106:ASP:HB3	4:G:130:ILE:HD12	1.94	0.49
2:A:79:ILE:HG12	2:A:82:HIS:CE1	2.48	0.48
5:D:26:ILE:HD12	5:D:55:ARG:HB3	1.95	0.48
1:J:250:DT:OP1	3:F:30:LYS:CB	2.60	0.48
1:I:51:DA:H2''	1:I:52:DT:OP2	2.12	0.48
5:H:11:GLY:O	5:H:12:LYS:HG3	2.13	0.48
1:J:225:DC:H2''	1:J:226:DT:C7	2.43	0.48
2:A:11:ARG:HG2	2:A:11:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:184:DT:H2''	1:J:185:DG:N7	2.29	0.48
3:B:23:LYS:O	3:B:24:LYS:C	2.56	0.48
3:F:34:LYS:HB3	3:F:34:LYS:HZ2	1.79	0.48
2:A:63:LEU:HD13	3:B:45:LEU:HB2	1.96	0.48
2:E:112:GLN:HG2	10:E:455:HOH:O	2.13	0.48
1:J:286:DT:H4'	1:J:287:DA:OP1	2.13	0.48
1:I:3:DC:H4'	1:I:4:DA:OP1	2.13	0.48
4:G:29:ALA:N	4:G:30:PRO:CD	2.74	0.48
4:C:48:LEU:CD1	2:E:117:PRO:HD3	2.43	0.48
1:I:69:DC:H2''	1:I:70:DG:C8	2.49	0.47
2:A:101:THR:HA	10:A:452:HOH:O	2.14	0.47
4:C:90:MET:HA	4:C:90:MET:HE2	1.96	0.47
2:A:118:LYS:NZ	2:A:124:LYS:HB3	2.29	0.47
4:C:30:PRO:HA	4:C:38:PRO:CB	2.44	0.47
2:A:117:PRO:HD3	4:G:48:LEU:CD1	2.44	0.47
1:I:48:DT:H2'	1:I:49:DC:C6	2.49	0.47
3:B:125:LYS:HD2	3:B:125:LYS:OXT	2.14	0.47
2:E:124:LYS:CD	2:E:127:ALA:HB3	2.45	0.47
1:J:197:DA:C2'	1:J:198:DT:C5'	2.91	0.47
2:A:25:PHE:CZ	2:A:59:THR:HG21	2.50	0.47
2:A:118:LYS:O	2:A:120:THR:N	2.47	0.47
1:I:116:DC:H2''	1:I:117:DT:H71	1.96	0.47
1:J:192:DG:H5''	3:B:27:LYS:HB2	1.95	0.47
4:C:129:ARG:HA	4:C:134:ARG:HA	1.96	0.47
2:E:125:ALA:O	2:E:126:LYS:CB	2.59	0.47
2:E:51:LEU:HD12	2:E:51:LEU:O	2.15	0.47
1:I:47:DC:C5'	3:F:29:ARG:HG3	2.40	0.47
2:A:118:LYS:HZ1	2:A:124:LYS:HB2	1.79	0.47
3:B:27:LYS:C	3:B:28:LYS:HG2	2.39	0.47
5:D:19:ARG:C	5:D:21:VAL:H	2.21	0.47
3:F:25:GLY:C	3:F:27:LYS:N	2.73	0.47
5:H:76:ALA:O	5:H:77:LYS:HB2	2.15	0.47
2:A:67:GLY:HA3	3:B:49:HIS:CD2	2.50	0.47
5:D:68:ASP:OD2	5:D:92:ARG:NH1	2.49	0.46
1:J:269:DT:H4'	3:B:31:LYS:HD3	1.97	0.46
4:C:134:ARG:HG2	4:C:135:ALA:N	2.30	0.46
3:F:111:VAL:O	3:F:115:THR:HG23	2.16	0.46
5:H:13:GLY:O	5:H:14:GLY:C	2.59	0.46
1:I:46:DG:H2''	1:I:47:DC:C6	2.50	0.46
3:B:122:THR:C	3:B:124:SER:N	2.73	0.46
1:I:26:DC:C2	1:I:27:DA:C6	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:DC:P	3:F:27:LYS:HD3	2.55	0.46
1:I:52:DT:H1'	1:I:53:DC:H5''	1.97	0.46
1:J:157:DA:OP2	1:J:157:DA:H8	1.97	0.46
1:J:177:DG:C8	1:J:178:DT:H72	2.49	0.46
1:J:257:DA:H2'	1:J:258:DT:H72	1.97	0.46
1:I:50:DC:H2''	1:I:51:DA:C8	2.51	0.46
1:I:118:DT:H2''	1:I:119:DT:OP2	2.15	0.46
1:I:31:DG:H2''	1:I:32:DT:OP2	2.16	0.46
1:I:48:DT:H5''	1:I:48:DT:H6	1.80	0.46
1:J:199:DC:C2'	1:J:200:DA:H5'	2.42	0.46
3:B:70:PHE:CD1	3:B:70:PHE:C	2.93	0.46
5:H:59:LYS:NZ	5:H:63:GLU:OE2	2.47	0.46
1:J:197:DA:H1'	1:J:198:DT:H5''	1.98	0.46
1:J:225:DC:H2''	1:J:226:DT:C5	2.51	0.46
1:J:272:DA:H2''	1:J:273:DA:C5'	2.37	0.46
4:C:30:PRO:O	4:C:37:LYS:O	2.34	0.46
5:H:10:LEU:HD21	5:H:79:LYS:NZ	2.30	0.46
1:I:1:DA:H2''	1:I:2:DT:C6	2.51	0.46
4:C:60:LEU:HD12	4:C:64:LYS:HE3	1.98	0.46
2:A:120:THR:CG2	2:A:121:ASP:H	2.23	0.45
3:B:80:LEU:HD22	3:B:96:THR:OG1	2.16	0.45
5:H:16:LYS:HG3	5:H:17:ARG:H	1.81	0.45
1:I:133:DA:C2	1:J:161:DG:N2	2.84	0.45
3:B:20:LYS:O	3:B:21:THR:HG23	2.15	0.45
4:G:73:GLU:OE1	5:H:25:ASN:ND2	2.48	0.45
1:I:115:DA:H2'	1:I:115:DA:OP2	2.17	0.45
3:B:18:VAL:C	3:B:20:LYS:H	2.24	0.45
4:G:25:ALA:O	4:G:26:ARG:HB2	2.17	0.45
4:G:78[2]:PHE:CD2	5:H:70:VAL:HG11	2.52	0.45
1:I:49:DC:H1'	1:I:50:DC:C5	2.52	0.45
4:C:51:ILE:O	4:C:55:GLN:HG3	2.17	0.45
2:E:79:ILE:HB	2:E:80:PRO:CD	2.47	0.45
4:G:64[1]:LYS:HG3	4:G:90:MET:HE1	1.97	0.45
4:G:81:ASP:HB3	5:H:10:LEU:HG	1.99	0.45
4:G:119:ILE:HG13	5:H:50:ILE:HG13	1.98	0.45
2:A:29:ARG:NH2	3:B:36:SER:O	2.49	0.45
3:B:18:VAL:CG1	3:B:19:THR:N	2.75	0.45
3:B:125:LYS:C	3:B:125:LYS:CD	2.89	0.45
4:G:36:LYS:CD	4:G:38:PRO:HD3	2.47	0.45
5:H:10:LEU:HD22	5:H:79:LYS:NZ	2.31	0.45
1:I:131:DG:C3'	2:E:76:THR:HG22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:DA:C8	1:J:220:DT:C7	3.00	0.45
2:E:11:ARG:HA	2:E:11:ARG:NE	2.32	0.45
4:G:28:SER:CB	4:G:30:PRO:HD3	2.47	0.45
5:H:72:TYR:OH	5:H:92:ARG:HD2	2.17	0.45
1:J:215:DC:H5'	4:G:43:PRO:HG2	1.98	0.44
2:E:124:LYS:HE2	2:E:127:ALA:HB3	1.98	0.44
1:I:103:DG:N2	3:B:29:ARG:HH22	2.15	0.44
1:I:129:DC:H2''	1:I:130:DT:H73	1.99	0.44
1:J:237:DT:OP2	4:C:69:ARG:NH2	2.50	0.44
1:I:4:DA:C2'	1:I:5:DA:H5'	2.40	0.44
1:I:4:DA:C2	1:J:290:DG:N2	2.85	0.44
1:I:30:DA:H2''	1:I:31:DG:H8	1.82	0.44
2:A:5:LYS:C	2:A:7:GLY:H	2.25	0.44
4:C:63:ARG:O	4:C:66:PRO:HD2	2.17	0.44
5:H:17:ARG:NE	5:H:17:ARG:CA	2.81	0.44
3:B:29:ARG:CG	3:B:29:ARG:NH1	2.78	0.44
4:C:97:GLU:O	4:C:101:VAL:HG23	2.17	0.44
2:E:50:TYR:OH	3:F:95:GLN:NE2	2.47	0.44
4:G:126:LEU:O	4:G:130:ILE:HG12	2.17	0.44
1:I:22:DC:C4	1:J:270:DA:N6	2.86	0.44
1:J:175:DA:C2'	1:J:176:DA:H8	2.30	0.44
4:C:64:LYS:HE2	4:C:90:MET:SD	2.57	0.44
2:E:127:ALA:C	2:E:128:LYS:HD2	2.42	0.44
1:I:107:DC:H2''	1:I:108:DC:C6	2.53	0.44
1:J:173:DA:C2	1:J:174:DA:C2	3.06	0.44
1:J:234:DC:O2	1:J:235:DC:C2	2.71	0.44
1:J:244:DG:N2	1:J:245:DA:C2	2.86	0.44
1:I:29:DA:H2''	1:I:30:DA:C8	2.52	0.44
1:I:104:DT:H2''	1:I:105:DT:H71	1.99	0.44
1:J:187:DA:H2''	1:J:188:DA:C5'	2.26	0.44
1:J:277:DG:H2''	1:J:278:DC:C6	2.53	0.44
4:G:26:ARG:HG3	4:G:27:LYS:N	2.32	0.44
4:G:129[1]:ARG:NE	4:G:135:ALA:O	2.50	0.44
4:C:65:LEU:HB3	4:C:66:PRO:HD3	2.00	0.43
1:J:188:DA:C6	1:J:189:DA:C6	3.06	0.43
1:I:49:DC:H1'	1:I:50:DC:C6	2.53	0.43
3:B:86:ARG:NH1	3:B:86:ARG:HG2	2.33	0.43
2:A:9:LYS:O	2:A:10:ALA:HB2	2.18	0.43
4:C:59:GLU:OE1	4:C:59:GLU:C	2.62	0.43
1:I:17:DA:N6	1:J:275:DC:H42	2.15	0.43
1:J:243:DG:H2''	1:J:244:DG:O5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:101:LEU:HD23	5:H:92:ARG:NH2	2.34	0.43
1:I:120:DT:H2''	1:I:121:DG:C8	2.54	0.43
4:G:29:ALA:O	4:G:31:ALA:N	2.50	0.43
2:E:69:ALA:O	2:E:73:ASN:ND2	2.52	0.43
5:H:17:ARG:H	5:H:17:ARG:HE	1.66	0.43
1:I:75:DT:H2''	1:I:76:DC:C6	2.53	0.43
2:A:13:LYS:HD2	2:A:13:LYS:HA	1.87	0.43
2:A:35:ARG:HD2	10:A:456:HOH:O	2.18	0.43
2:A:47:ALA:HB3	2:A:48:PRO:HD3	2.01	0.43
2:A:42:ARG:O	3:B:88:THR:HA	2.18	0.43
2:A:20:ARG:HH11	2:A:20:ARG:HG2	1.83	0.42
2:A:20:ARG:HG2	2:A:20:ARG:NH1	2.34	0.42
4:G:79:LYS:HA	10:G:481:HOH:O	2.19	0.42
1:J:173:DA:H2''	1:J:174:DA:C8	2.54	0.42
4:G:27:LYS:O	4:G:28:SER:O	2.37	0.42
1:I:90:DT:OP2	4:G:69:ARG:NH2	2.53	0.42
1:I:52:DT:C1'	1:I:53:DC:H5''	2.47	0.42
3:B:125:LYS:OXT	3:B:125:LYS:NZ	2.48	0.42
2:E:37:GLY:O	2:E:38:ASN:HB2	2.19	0.42
2:E:73:ASN:O	2:E:74:LYS:HB2	2.18	0.42
1:J:175:DA:H4'	1:J:175:DA:OP1	2.18	0.42
4:G:59:GLU:H	4:G:59:GLU:HG3	1.17	0.42
1:I:32:DT:H2''	1:I:33:DG:O5'	2.20	0.42
1:I:60:DC:H2''	1:I:61:DA:N7	2.34	0.42
1:I:104:DT:H2''	1:I:105:DT:C6	2.54	0.42
2:E:49:VAL:HG11	3:F:118:VAL:HA	2.02	0.42
1:I:59:DG:C6	1:J:233:DG:O6	2.73	0.42
1:J:249:DG:P	3:F:32:SER:HB2	2.59	0.42
2:A:50:TYR:OH	3:B:95:GLN:HG3	2.19	0.42
2:E:5:LYS:HE2	2:E:5:LYS:HB3	1.82	0.42
2:E:20:ARG:NH1	3:F:124:SER:O	2.53	0.42
3:F:20:LYS:HD2	3:F:20:LYS:N	2.33	0.42
1:I:31:DG:N2	1:I:32:DT:C2	2.87	0.42
3:B:80:LEU:CD2	3:B:96:THR:OG1	2.67	0.42
2:E:47:ALA:N	2:E:48:PRO:HD2	2.35	0.42
5:H:17:ARG:HE	5:H:17:ARG:N	2.17	0.42
1:I:127:DA:C2	1:I:128:DT:C2	3.07	0.42
3:F:23:LYS:HB3	3:F:26:ASP:OD1	2.20	0.41
4:G:26:ARG:CZ	4:G:27:LYS:N	2.81	0.41
1:I:51:DA:H2''	1:I:52:DT:H5'	2.02	0.41
1:I:131:DG:H3'	2:E:76:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:11:ARG:HG3	2:A:12:ALA:N	2.35	0.41
1:I:19:DA:N6	1:J:273:DA:N6	2.68	0.41
1:I:117:DT:C6	1:I:118:DT:H72	2.55	0.41
5:D:79:LYS:HB3	5:D:79:LYS:NZ	2.34	0.41
3:F:28:LYS:O	3:F:28:LYS:HG3	2.20	0.41
4:G:18:LYS:HE3	4:G:18:LYS:HB2	1.89	0.41
1:I:116:DC:H2''	1:I:117:DT:OP2	2.20	0.41
1:I:125:DG:C1'	1:I:126:DA:H5'	2.50	0.41
1:J:176:DA:C2	1:J:177:DG:C5	3.09	0.41
1:J:249:DG:H4'	3:F:30:LYS:O	2.21	0.41
3:B:20:LYS:O	3:B:21:THR:OG1	2.32	0.41
4:C:30:PRO:CA	4:C:38:PRO:HB3	2.51	0.41
4:G:77:ASP:OD1	9:G:451:CAC:O2	2.37	0.41
1:J:160:DT:H2''	1:J:161:DG:N7	2.36	0.41
1:J:237:DT:P	4:C:69:ARG:NH2	2.92	0.41
2:A:20:ARG:HD2	3:B:124:SER:OG	2.21	0.41
4:G:23:LYS:C	4:G:25:ALA:N	2.71	0.41
1:I:80:DT:H4'	5:H:45:ARG:CZ	2.51	0.41
1:J:184:DT:O3'	1:J:185:DG:C8	2.74	0.41
1:I:31:DG:C4	1:I:32:DT:H72	2.55	0.41
1:I:140:DT:H1'	1:I:141:DA:C8	2.56	0.41
2:E:2:GLY:C	2:E:3:ARG:CD	2.91	0.41
4:G:103:LEU:CD2	5:H:57:VAL:HG11	2.51	0.41
1:I:101:DC:H5'	5:H:78:ARG:CD	2.51	0.41
1:J:285:DA:C2'	1:J:286:DT:C6	3.03	0.41
5:D:59:LYS:O	5:D:63:GLU:HG3	2.21	0.41
2:E:35:ARG:HG2	2:E:35:ARG:HH11	1.85	0.41
1:I:4:DA:H1'	1:I:5:DA:C5'	2.51	0.40
1:I:32:DT:H5'	1:I:32:DT:C6	2.49	0.40
1:I:15:DG:C5	1:I:16:DC:N4	2.89	0.40
1:I:57:DA:H2''	1:I:58:DG:H8	1.83	0.40
5:D:66:ILE:O	5:D:67:ARG:C	2.63	0.40
1:I:108:DC:H2''	1:I:109:DA:N7	2.36	0.40
1:J:147:DA:C8	1:J:148:DT:H72	2.56	0.40
3:F:102:LEU:HA	3:F:103:PRO:HD3	1.88	0.40
4:G:128:ARG:HD2	4:G:133:GLU:OE1	2.21	0.40
5:H:26:ILE:CG1	5:H:55:ARG:HB3	2.51	0.40
2:E:124:LYS:HD3	2:E:127:ALA:HB3	2.03	0.40
4:G:28:SER:OG	4:G:30:PRO:HD3	2.22	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	123/129 (95%)	108 (88%)	9 (7%)	6 (5%)	1	2
2	E	125/129 (97%)	102 (82%)	16 (13%)	7 (6%)	1	1
3	B	106/126 (84%)	94 (89%)	6 (6%)	6 (6%)	1	1
3	F	105/126 (83%)	97 (92%)	6 (6%)	2 (2%)	6	11
4	C	106/136 (78%)	93 (88%)	7 (7%)	6 (6%)	1	1
4	G	121/136 (89%)	103 (85%)	14 (12%)	4 (3%)	3	4
5	D	88/103 (85%)	81 (92%)	5 (6%)	2 (2%)	5	8
5	H	93/103 (90%)	82 (88%)	7 (8%)	4 (4%)	2	2
All	All	867/988 (88%)	760 (88%)	70 (8%)	37 (4%)	2	2

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	9	LYS
2	A	10	ALA
2	A	119	LYS
2	A	121	ASP
3	B	21	THR
3	B	24	LYS
3	B	32	SER
4	C	134	ARG
5	D	17	ARG
5	D	23	ARG
2	E	6	GLN
2	E	14	ALA
2	E	124	LYS
2	E	127	ALA
4	G	27	LYS
4	G	28	SER
5	H	16	LYS

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Mol	Chain	Res	Type
2	A	11	ARG
3	B	104	GLY
4	C	33	GLY
4	C	39	HIS
2	E	119	LYS
3	F	104	GLY
4	G	23	LYS
5	H	9	GLY
2	E	126	LYS
4	C	37	LYS
4	C	38	PRO
2	A	123	HIS
3	B	31	LYS
2	E	123	HIS
3	F	30	LYS
4	G	29	ALA
5	H	20	LYS
3	B	28	LYS
5	H	14	GLY
4	C	35	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	95/98 (97%)	84 (88%)	11 (12%)	5	11
2	E	96/98 (98%)	88 (92%)	8 (8%)	10	22
3	B	94/107 (88%)	83 (88%)	11 (12%)	5	11
3	F	93/107 (87%)	84 (90%)	9 (10%)	8	17
4	C	89/111 (80%)	85 (96%)	4 (4%)	24	49
4	G	97/111 (87%)	89 (92%)	8 (8%)	10	23
5	D	71/79 (90%)	68 (96%)	3 (4%)	26	52
5	H	75/79 (95%)	71 (95%)	4 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	710/790 (90%)	652 (92%)	58 (8%)	10	23

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	ARG
2	A	20	ARG
2	A	29	ARG
2	A	36	LYS
2	A	59	THR
2	A	76	THR
2	A	84	GLN
2	A	101	THR
2	A	119	LYS
2	A	123	HIS
2	A	124	LYS
3	B	19	THR
3	B	20	LYS
3	B	27	LYS
3	B	63	ASN
3	B	86	ARG
3	B	88	THR
3	B	96	THR
3	B	106	LEU
3	B	108	LYS
3	B	112	SER
3	B	125	LYS
4	C	59	GLU
4	C	63	ARG
4	C	121	PRO
4	C	129	ARG
5	D	24	ASP
5	D	26	ILE
5	D	47	SER
2	E	64	GLU
2	E	73	ASN
2	E	81	ARG
2	E	88	ARG
2	E	91	GLU
2	E	95	LYS
2	E	101	THR
2	E	114	VAL

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Mol	Chain	Res	Type
3	F	22	GLN
3	F	34	LYS
3	F	36	SER
3	F	48	VAL
3	F	63	ASN
3	F	86	ARG
3	F	88	THR
3	F	106	LEU
3	F	115	THR
4	G	26	ARG
4	G	36	LYS
4	G	49	ARG
4	G	59	GLU
4	G	63	ARG
4	G	80	THR
4	G	117	VAL
4	G	126	LEU
5	H	10	LEU
5	H	19	ARG
5	H	47	SER
5	H	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	HIS
3	B	63	ASN
4	C	39	HIS
5	D	27	GLN
2	E	73	ASN
3	F	95	GLN
4	G	39	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 24 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	CAC	G	451	4,3	2,4,4	6.89	2 (100%)	4,6,6	1.88	2 (50%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	451	CAC	AS-C2	-6.91	1.74	1.90
9	G	451	CAC	AS-C1	-6.87	1.74	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	451	CAC	O1-AS-C2	-2.56	108.32	111.50
9	G	451	CAC	O1-AS-C1	-2.05	108.95	111.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	451	CAC	1	0

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.