



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:53 pm GMT

PDB ID : 1KX3  
Title : X-Ray Structure of the Nucleosome Core Particle, NCP146, at 2.0 Å Resolution  
Authors : Davey, C.A.; Sargent, D.F.; Luger, K.; Maeder, A.W.; Richmond, T.J.  
Deposited on : 2002-01-31  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

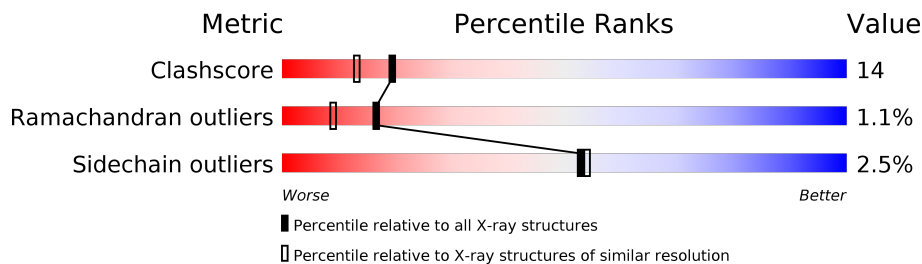
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)




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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	
1	J	146	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	128	

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Mol	Chain	Length	Quality of chain
4	G	128	
5	D	125	
5	H	125	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13023 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 DNA (5'(ATCAATATCCACCTGCAGATTCTACCAA AAGTGTATTTGGAACTGCTCCATCAAAAGGCATGTTTCAGCTGAATTCAGCTG AACATGCCTTTTGATGGAGCAGTTTCCAAATACACTTTTGGTAGAATCTGCAG GTGGATATTGAT)3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			
1	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	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
			808	509	156	140	3			
2	E	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	CONFLICT	UNP P84233
E	102	ALA	GLY	CONFLICT	UNP P84233

- Molecule 3 is a protein called histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
3	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			

- Molecule 4 is a protein called histone H2A.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	107	Total	C	N	O	0	0	0
			825	520	161	144			
4	G	106	Total	C	N	O	0	0	0
			818	516	160	142			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	VARIANT	UNP P06897
C	123	SER	ALA	CONFLICT	UNP P06897
C	?	-	ALA	DELETION	UNP P06897
G	99	ARG	GLY	VARIANT	UNP P06897
G	123	SER	ALA	CONFLICT	UNP P06897
G	?	-	ALA	DELETION	UNP P06897

- Molecule 5 is a protein called histone H2B.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			
5	H	94	Total	C	N	O	S	0	0	0
			736	463	132	139	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	VARIANT	UNP P02281
H	29	THR	SER	VARIANT	UNP P02281

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

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

- Molecule 7 is water.

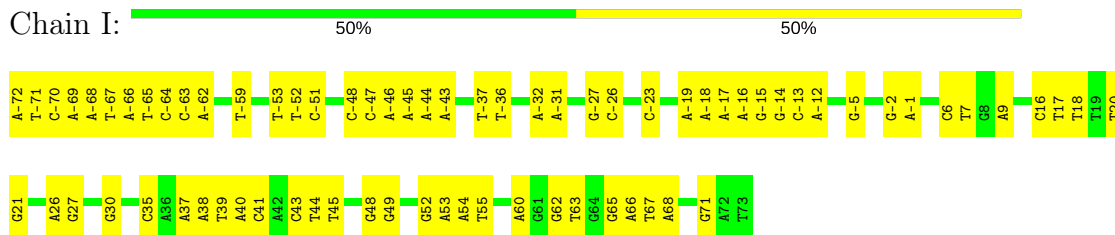
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	74	Total 74	O 74	0	0
7	B	62	Total 62	O 62	0	0
7	C	107	Total 107	O 107	0	0
7	D	77	Total 77	O 77	0	0
7	E	116	Total 116	O 116	0	0
7	F	90	Total 90	O 90	0	0
7	G	98	Total 98	O 98	0	0
7	H	45	Total 45	O 45	0	0
7	I	141	Total 141	O 141	0	0
7	J	133	Total 133	O 133	0	0

### 3 Residue-property plots

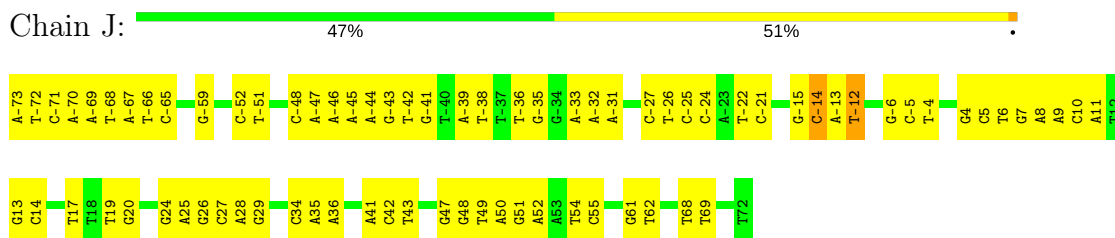
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

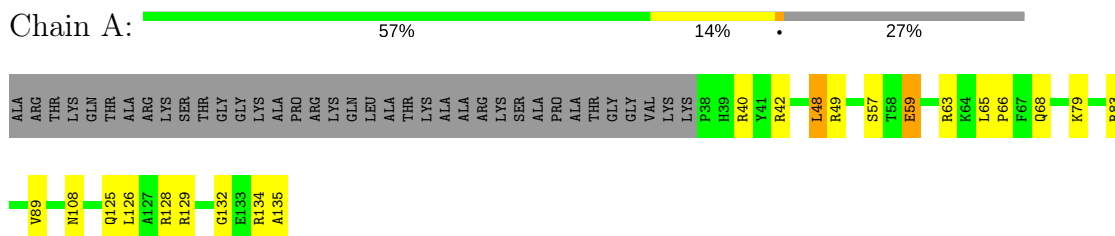
- Molecule 1: DNA (5'(ATCAATATCCACCTGCAGATTCTACCAAAGTGTATTTGGAAACTGCTCCATCAAAAGGCATGTTTCAGCTGAATTCAGCTGAACATGCCTTTTGATGGAGCAGTTTCCAAATACACTTTTGGTAGAATCTGCAGGTGGATATTGAT)3')



- Molecule 1: DNA (5'(ATCAATATCCACCTGCAGATTCTACCAAAAGTGTATTTGGAAACTGCTCCATCAAAAGGCATGTTTCAGCTGAATTCAGCTGAACATGCCTTTTGATGGAGCAGTTTCCAAATACACTTTTGGTAGAATCTGCAGGTGGATATTGAT)3')

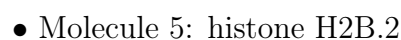
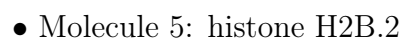
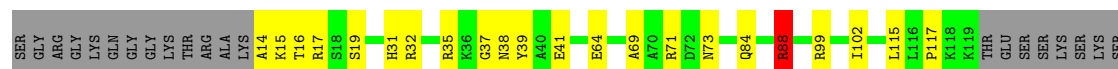
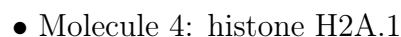
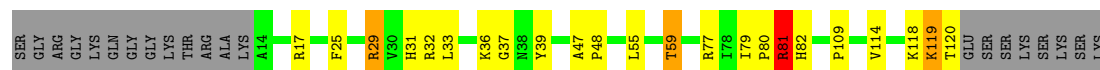
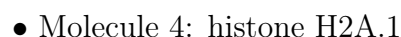
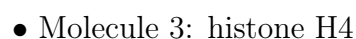
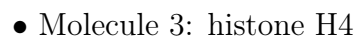


- Molecule 2: histone H3



- Molecule 2: histone H3







PRO	GLU	PRO	PRO	ALA	LYS	SER	ALA	PRO	PRO	PRO	LYS	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	THR	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	ARG	LYS	T29	R30	K31	E32	S33	I36	K43	Q44	V45	I58	R69	E73	G101	E102	L103	H106	K122
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## 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, $\alpha$ , $\beta$ , $\gamma$	105.40Å 181.54Å 109.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.9 (6.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.240 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	I	0.35	0/3354	0.70	0/5175
1	J	0.39	0/3354	0.71	1/5175 (0.0%)
2	A	0.52	0/820	0.67	0/1099
2	E	0.69	0/820	0.80	1/1099 (0.1%)
3	B	0.56	0/660	0.72	1/883 (0.1%)
3	F	0.69	0/711	0.83	1/948 (0.1%)
4	C	0.67	0/835	0.83	2/1127 (0.2%)
4	G	0.51	0/828	0.69	2/1117 (0.2%)
5	D	0.66	0/747	0.73	0/1004
5	H	0.55	0/747	0.67	0/1004
All	All	0.50	0/12876	0.72	8/18631 (0.0%)

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	J	0	2
5	D	0	1
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	81	ARG	NE-CZ-NH1	9.46	125.03	120.30
4	C	81	ARG	NE-CZ-NH2	-8.80	115.90	120.30
4	G	88	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	E	128	ARG	NE-CZ-NH2	-6.79	116.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	29	ILE	N-CA-C	-5.36	96.54	111.00
3	F	92	ARG	NE-CZ-NH1	5.25	122.92	120.30
4	G	88	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	J	-14	DC	C5'-C4'-C3'	-5.00	105.09	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	39	TYR	Sidechain
1	J	-12	DT	Sidechain
1	J	-6	DG	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	1652	75	0
1	J	2990	0	1652	92	0
2	A	808	0	846	40	0
2	E	808	0	846	41	0
3	B	653	0	696	16	0
3	F	703	0	755	25	0
4	C	825	0	884	22	0
4	G	818	0	877	25	0
5	D	736	0	760	22	0
5	H	736	0	760	15	0
6	E	1	0	0	0	0
6	I	6	0	0	0	0
6	J	6	0	0	0	0
7	A	74	0	0	3	0
7	B	62	0	0	1	0
7	C	107	0	0	3	0
7	D	77	0	0	4	0
7	E	116	0	0	6	0
7	F	90	0	0	3	0
7	G	98	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	45	0	0	3	0
7	I	141	0	0	8	0
7	J	133	0	0	5	0
All	All	13023	0	9728	312	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 14.

All (312) 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:-46:DA:H2''	1:J:-45:DA:H5''	1.27	1.17
2:E:120:MET:HE3	2:E:122:LYS:HD3	1.39	1.03
2:A:128:ARG:HD3	2:A:134:ARG:HH12	1.22	1.02
1:I:26:DA:H2''	1:I:27:DG:H5'	1.41	1.02
2:E:49:ARG:HG3	2:E:49:ARG:HH11	1.27	0.99
4:C:33:LEU:HD23	4:C:36:LYS:HD3	1.42	0.98
4:C:17:ARG:HH12	4:C:31:HIS:CD2	1.83	0.96
2:A:128:ARG:HH11	2:A:134:ARG:HH12	1.11	0.96
2:A:128:ARG:HH11	2:A:134:ARG:NH1	1.64	0.95
1:J:41:DA:H2''	1:J:42:DC:H5''	1.49	0.94
3:F:87:VAL:HG11	3:F:102:GLY:HA3	1.45	0.94
4:G:17:ARG:HH12	4:G:31:HIS:HD2	0.98	0.93
1:J:26:DG:H2''	1:J:27:DC:C5	2.03	0.93
4:G:17:ARG:HH12	4:G:31:HIS:CD2	1.88	0.90
4:C:55:LEU:O	4:C:59:THR:HG23	1.72	0.90
2:E:63:ARG:NE	7:E:1051:HOH:O	2.04	0.90
1:I:35:DC:H5'	7:I:1014:HOH:O	1.71	0.89
2:A:128:ARG:HD3	2:A:134:ARG:NH1	1.88	0.88
1:J:-46:DA:C2'	1:J:-45:DA:H5''	2.03	0.87
4:C:17:ARG:HH12	4:C:31:HIS:HD2	0.94	0.86
3:F:20:LYS:HE2	7:F:191:HOH:O	1.76	0.84
1:I:-59:DT:H2'	7:I:1097:HOH:O	1.76	0.83
4:C:17:ARG:NH1	4:C:31:HIS:HD2	1.76	0.83
2:E:120:MET:CE	2:E:122:LYS:HD3	2.08	0.82
2:A:129:ARG:HD2	2:A:135:ALA:HB2	1.62	0.82
4:G:71:ARG:HD3	7:G:205:HOH:O	1.80	0.81
2:A:128:ARG:NH1	2:A:134:ARG:NH1	2.28	0.81
1:I:71:DG:H1	1:J:-71:DC:H42	1.29	0.78
2:A:125:GLN:HG2	2:A:134:ARG:HH21	1.48	0.77
1:J:5:DC:H2''	1:J:6:DT:C7	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:DT:OP1	5:D:31:LYS:HG2	1.85	0.77
1:J:-46:DA:H2''	1:J:-45:DA:C5'	2.13	0.75
1:J:41:DA:C2'	1:J:42:DC:H5''	2.15	0.75
4:G:17:ARG:NH1	4:G:31:HIS:HD2	1.82	0.73
1:I:17:DT:OP2	2:E:69:ARG:NH2	2.20	0.73
1:I:52:DG:H2'	7:I:1085:HOH:O	1.87	0.73
1:J:17:DT:OP1	2:A:66:PRO:HG3	1.89	0.72
1:J:28:DA:H2''	1:J:29:DG:C8	2.25	0.72
5:H:73:GLU:OE1	7:H:160:HOH:O	2.08	0.72
1:I:26:DA:C2'	1:I:27:DG:H5'	2.17	0.71
2:A:128:ARG:NH1	2:A:134:ARG:HH12	1.88	0.71
1:I:17:DT:P	2:E:69:ARG:HH22	2.15	0.70
1:J:-69:DA:H2''	1:J:-68:DT:C5'	2.21	0.70
1:J:-46:DA:H4'	5:H:30:ARG:HD3	1.72	0.70
4:C:81:ARG:HD3	7:C:155:HOH:O	1.90	0.70
1:I:-45:DA:H2''	1:I:-44:DA:H5''	1.73	0.69
2:E:49:ARG:HH11	2:E:49:ARG:CG	2.03	0.69
1:J:-39:DA:H2''	1:J:-38:DT:OP2	1.92	0.69
1:J:5:DC:H2''	1:J:6:DT:H71	1.74	0.69
1:I:-48:DC:H2''	1:I:-47:DC:H5'	1.74	0.68
1:I:65:DG:H2''	1:I:66:DA:OP2	1.94	0.68
1:J:-48:DC:H1'	1:J:-47:DA:C5	2.29	0.68
2:A:83:ARG:NH1	7:A:205:HOH:O	2.26	0.67
1:I:-45:DA:C2'	1:I:-44:DA:H5''	2.25	0.66
1:J:24:DG:H2''	1:J:25:DA:N7	2.09	0.66
4:G:84:GLN:OE1	4:G:88:ARG:HD2	1.94	0.66
1:I:20:DT:H2''	1:I:21:DG:H5'	1.78	0.66
3:B:101:GLY:O	7:B:111:HOH:O	2.15	0.65
1:J:-69:DA:H2''	1:J:-68:DT:H5''	1.77	0.65
1:J:41:DA:H2''	1:J:42:DC:C5'	2.25	0.64
2:E:69:ARG:NH1	7:E:1028:HOH:O	2.30	0.64
4:G:15:LYS:HG3	4:G:19:SER:OG	1.97	0.64
2:E:76:GLN:HE22	3:F:19:ARG:NH1	1.96	0.64
2:A:129:ARG:HA	2:A:134:ARG:HB2	1.79	0.64
1:I:-13:DC:H5''	2:A:63:ARG:NH1	2.14	0.63
2:E:116:ARG:CZ	2:E:120:MET:HE2	2.28	0.63
1:J:-14:DC:H2''	1:J:-13:DA:C8	2.32	0.63
2:E:76:GLN:NE2	3:F:19:ARG:NH1	2.47	0.63
1:J:-43:DG:O3'	4:G:14:ALA:HB1	1.98	0.63
1:J:-27:DC:H2''	1:J:-26:DT:H71	1.81	0.63
1:I:-13:DC:H5''	2:A:63:ARG:CZ	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-31:DA:H3'	7:J:1072:HOH:O	1.98	0.62
1:J:10:DC:H2''	1:J:11:DA:C8	2.34	0.62
5:D:69:ARG:HD3	7:D:136:HOH:O	2.00	0.62
3:F:87:VAL:CG1	3:F:102:GLY:HA3	2.24	0.62
1:J:34:DC:H2''	1:J:35:DA:N7	2.15	0.62
1:J:54:DT:H2''	1:J:55:DC:OP2	1.98	0.62
7:A:150:HOH:O	2:E:122:LYS:HE2	2.00	0.61
1:I:-68:DA:H2''	1:I:-67:DT:H5'	1.82	0.61
1:I:-19:DA:H3'	7:I:1044:HOH:O	2.01	0.61
3:F:95:ARG:HD3	7:F:145:HOH:O	2.00	0.61
4:C:32:ARG:HH22	5:D:32:GLU:CD	2.03	0.61
2:E:134:ARG:O	2:E:135:ALA:OXT	2.18	0.60
1:J:-69:DA:C2'	1:J:-68:DT:H5''	2.31	0.60
2:A:125:GLN:HG2	2:A:134:ARG:NH2	2.16	0.59
4:C:118:LYS:C	4:C:119:LYS:HD3	2.21	0.59
1:J:-32:DA:H1'	1:J:-31:DA:O5'	2.03	0.59
2:A:134:ARG:HH11	2:A:134:ARG:HG3	1.68	0.59
2:E:132:GLY:HA2	2:E:135:ALA:HB2	1.86	0.58
1:I:-14:DG:H2''	1:I:-13:DC:C6	2.38	0.58
4:C:119:LYS:HD3	4:C:119:LYS:N	2.19	0.58
1:J:-5:DC:H5'	2:E:43:PRO:HG2	1.85	0.58
1:I:-37:DT:H2''	1:I:-36:DT:OP2	2.03	0.58
5:H:122:LYS:OXT	5:H:122:LYS:HG3	2.04	0.58
2:E:129:ARG:HG3	2:E:135:ALA:HA	1.87	0.57
1:I:-16:DA:H2''	1:I:-15:DG:C8	2.39	0.57
1:I:39:DT:OP2	4:G:35:ARG:NH2	2.31	0.57
5:D:121:ALA:O	5:D:122:LYS:HB2	2.05	0.57
4:C:29:ARG:NH2	5:D:33:SER:O	2.38	0.57
1:I:-23:DC:H1'	2:A:83:ARG:HH21	1.69	0.56
1:J:25:DA:H1'	2:A:83:ARG:NH1	2.21	0.56
4:C:114:VAL:HG11	7:E:1018:HOH:O	2.04	0.56
4:C:77:ARG:HD2	7:C:151:HOH:O	2.06	0.56
5:D:39:TYR:CZ	5:D:43:LYS:HE2	2.40	0.56
2:E:128:ARG:HE	2:E:134:ARG:HH21	1.52	0.56
2:E:52:ARG:NH2	7:E:1026:HOH:O	2.37	0.56
7:I:1092:HOH:O	3:F:79:LYS:HD3	2.05	0.56
4:G:69:ALA:O	4:G:73:ASN:ND2	2.37	0.56
1:J:68:DT:H2''	1:J:69:DT:H5'	1.87	0.56
2:E:49:ARG:HG3	2:E:49:ARG:NH1	2.06	0.56
1:I:71:DG:H1	1:J:-71:DC:N4	2.02	0.55
1:J:19:DT:H2''	1:J:20:DG:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:DT:H5''	2:E:63:ARG:HH12	1.70	0.55
1:I:-46:DA:H2	1:J:47:DG:N2	2.05	0.55
2:A:126:LEU:HD22	2:E:113:HIS:CG	2.41	0.55
1:J:-71:DC:H2''	1:J:-70:DA:O5'	2.07	0.55
2:A:57:SER:HB2	2:A:59:GLU:OE2	2.07	0.54
1:I:-45:DA:H2''	1:I:-44:DA:C5'	2.37	0.54
1:I:-63:DC:H1'	1:I:-62:DA:C8	2.41	0.54
2:E:49:ARG:NH1	2:E:49:ARG:CG	2.66	0.54
3:F:87:VAL:HG11	3:F:102:GLY:CA	2.29	0.54
3:B:31:LYS:HB3	3:B:32:PRO:HD3	1.89	0.54
1:J:-65:DC:H6	1:J:-65:DC:H5'	1.71	0.54
4:G:102:ILE:HG23	5:H:58:ILE:HD13	1.89	0.54
1:I:-65:DT:H2''	1:I:-64:DC:OP2	2.06	0.54
1:J:-42:DT:H5'	4:G:14:ALA:HB2	1.90	0.54
1:J:-69:DA:H1'	1:J:-68:DT:H5''	1.89	0.54
1:J:-44:DA:OP2	4:G:32:ARG:HD3	2.08	0.54
1:J:5:DC:H2''	1:J:6:DT:C5	2.42	0.54
1:I:-53:DT:H2''	1:I:-52:DT:OP2	2.08	0.54
1:I:41:DC:H4'	1:I:41:DC:OP1	2.08	0.54
1:I:-72:DA:H2''	1:I:-71:DT:OP2	2.07	0.53
3:B:75:HIS:CE1	5:D:77:LEU:HD21	2.44	0.53
4:G:84:GLN:CD	4:G:88:ARG:HD2	2.29	0.53
2:A:68:GLN:HE21	2:A:89:VAL:HG21	1.73	0.53
1:I:-69:DA:H2''	1:I:-68:DA:C8	2.43	0.52
1:I:54:DA:H2''	1:I:55:DT:OP2	2.09	0.52
1:I:40:DA:H2''	1:I:41:DC:O5'	2.10	0.52
3:F:102:GLY:O	7:F:152:HOH:O	2.19	0.52
1:J:29:DG:OP1	5:H:29:THR:HG22	2.09	0.52
2:E:116:ARG:CZ	2:E:120:MET:CE	2.87	0.51
4:G:99:ARG:HD3	7:G:171:HOH:O	2.11	0.51
4:G:35:ARG:HH11	4:G:35:ARG:HG2	1.76	0.51
4:C:37:GLY:HA3	4:C:39:TYR:CE1	2.45	0.51
2:E:63:ARG:CZ	7:E:1051:HOH:O	2.51	0.51
1:J:-69:DA:H2''	1:J:-68:DT:H5'	1.92	0.51
1:J:-39:DA:H2'	7:J:1086:HOH:O	2.10	0.51
5:D:113:LYS:NZ	7:D:180:HOH:O	2.33	0.51
1:I:-67:DT:H2''	1:I:-66:DA:OP2	2.11	0.51
1:J:6:DT:H2''	1:J:7:DG:C8	2.46	0.51
2:E:76:GLN:HE22	3:F:19:ARG:HH11	1.58	0.51
1:J:9:DA:N3	2:A:40:ARG:NH2	2.56	0.50
1:I:-68:DA:H1'	1:I:-67:DT:H5''	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:79:LYS:HD2	3:B:74:GLU:CG	2.41	0.50
1:I:-52:DT:H2''	1:I:-51:DC:O5'	2.11	0.50
1:I:67:DT:H2''	1:I:68:DA:OP2	2.11	0.50
3:B:84:MET:HE3	3:B:88:TYR:CZ	2.45	0.50
1:I:-45:DA:H1'	1:I:-44:DA:H5''	1.94	0.50
1:J:51:DG:H2''	1:J:52:DA:OP2	2.12	0.50
1:I:49:DG:H5'	5:H:30:ARG:NH2	2.25	0.50
1:I:-68:DA:H2''	1:I:-67:DT:C5'	2.40	0.50
4:C:25:PHE:CZ	4:C:59:THR:HG21	2.46	0.50
2:E:120:MET:HE3	2:E:122:LYS:CD	2.26	0.50
1:J:48:DG:H2''	1:J:49:DT:H5'	1.94	0.50
1:J:61:DG:H2''	1:J:62:DT:OP2	2.11	0.50
3:F:59:LYS:O	3:F:63:GLU:HG3	2.12	0.50
2:A:63:ARG:O	2:A:66:PRO:HD2	2.13	0.49
3:F:17:ARG:HB3	3:F:18:HIS:CD2	2.47	0.49
2:A:79:LYS:HD2	3:B:74:GLU:HG2	1.95	0.49
1:I:-12:DA:OP1	3:B:23:ARG:NH2	2.45	0.49
1:J:-36:DT:H2''	1:J:-35:DG:N7	2.28	0.49
2:E:128:ARG:HD2	2:E:133:GLU:OE1	2.13	0.48
2:E:65:LEU:HB3	2:E:66:PRO:HD3	1.95	0.48
2:A:65:LEU:HB3	2:A:66:PRO:HD3	1.95	0.48
5:D:64:ASN:O	5:D:68:GLU:HG3	2.13	0.48
5:D:82:LYS:NZ	7:D:184:HOH:O	2.46	0.48
1:I:41:DC:H42	1:J:-41:DG:H1	1.61	0.48
2:E:128:ARG:HH21	2:E:134:ARG:NH2	2.11	0.48
1:I:-5:DG:OP1	2:A:42:ARG:CZ	2.61	0.48
3:B:22:LEU:O	3:B:23:ARG:HB2	2.13	0.48
1:J:7:DG:H2''	1:J:8:DA:C8	2.48	0.48
2:A:57:SER:CB	2:A:59:GLU:OE2	2.62	0.48
1:I:-47:DC:H1'	1:I:-46:DA:C5	2.49	0.48
1:I:53:DA:H1'	1:I:54:DA:H5'	1.96	0.48
2:A:132:GLY:HA2	2:A:135:ALA:HB3	1.95	0.47
1:J:28:DA:H2''	1:J:29:DG:H8	1.77	0.47
1:J:-15:DG:H2''	1:J:-14:DC:O5'	2.15	0.47
1:I:-13:DC:OP1	2:A:63:ARG:HD2	2.14	0.47
4:C:80:PRO:HG3	5:D:58:ILE:HD12	1.96	0.47
1:I:48:DG:H3'	5:H:36:ILE:HD11	1.95	0.47
2:A:48:LEU:CD2	4:G:117:PRO:HD3	2.45	0.47
1:I:-44:DA:H5'	1:I:-44:DA:H8	1.80	0.47
1:J:35:DA:C6	1:J:36:DA:C6	3.03	0.47
2:E:52:ARG:NH1	7:E:980:HOH:O	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:DT:OP1	2:E:63:ARG:NH1	2.48	0.46
1:I:-46:DA:C2	1:J:47:DG:N2	2.83	0.46
1:I:-64:DC:H2''	1:I:-63:DC:O5'	2.14	0.46
3:B:30:THR:HB	3:B:32:PRO:HD2	1.95	0.46
1:J:8:DA:OP2	3:B:35:ARG:NH2	2.44	0.46
4:G:84:GLN:O	4:G:88:ARG:HG2	2.15	0.46
1:J:-27:DC:H2''	1:J:-26:DT:C7	2.45	0.46
1:J:42:DC:H2''	1:J:43:DT:O5'	2.15	0.46
5:D:39:TYR:CE2	5:D:43:LYS:HE2	2.50	0.46
2:E:128:ARG:HB2	2:E:134:ARG:HE	1.81	0.46
1:I:-51:DC:H3'	7:I:1034:HOH:O	2.16	0.46
2:E:59:GLU:H	2:E:59:GLU:HG3	1.53	0.46
3:F:59:LYS:NZ	3:F:63:GLU:OE2	2.33	0.46
2:A:129:ARG:CD	2:A:135:ALA:HB2	2.41	0.46
1:J:4:DG:H5'	7:J:1064:HOH:O	2.14	0.46
1:I:43:DC:C2'	1:I:44:DT:H72	2.46	0.46
1:J:-43:DG:H5''	4:G:16:THR:HA	1.98	0.46
5:D:79:HIS:CE1	4:G:38:ASN:OD1	2.69	0.46
3:F:30:THR:CB	3:F:32:PRO:HD2	2.45	0.46
2:A:83:ARG:HD3	7:A:168:HOH:O	2.16	0.45
1:I:-47:DC:H1'	1:I:-46:DA:C4	2.51	0.45
1:J:-72:DT:H2''	1:J:-71:DC:O5'	2.16	0.45
4:C:32:ARG:NH1	5:D:32:GLU:OE2	2.44	0.45
5:H:69:ARG:HD3	7:H:151:HOH:O	2.16	0.45
1:I:-19:DA:H2''	1:I:-18:DA:C8	2.51	0.45
2:A:79:LYS:HD2	3:B:74:GLU:CD	2.36	0.45
1:I:9:DA:N3	2:E:40:ARG:NH2	2.61	0.45
1:I:30:DG:OP1	5:D:29:THR:HG22	2.17	0.45
4:G:37:GLY:HA3	4:G:39:TYR:CE1	2.52	0.45
7:C:175:HOH:O	4:G:41:GLU:HG2	2.17	0.45
1:J:-66:DT:OP1	2:A:49:ARG:HD3	2.16	0.45
1:J:42:DC:C6	1:J:43:DT:H72	2.52	0.45
1:J:-46:DA:H4'	5:H:30:ARG:CD	2.44	0.45
5:H:29:THR:HG23	5:H:29:THR:O	2.16	0.45
1:J:-33:DA:C6	1:J:-32:DA:N6	2.84	0.45
2:A:128:ARG:CD	2:A:134:ARG:NH1	2.71	0.45
3:B:52:GLU:OE2	3:B:55:ARG:NH1	2.49	0.45
4:C:119:LYS:O	4:C:120:THR:HB	2.17	0.44
5:D:69:ARG:HD2	5:D:98:LEU:HD11	1.99	0.44
3:B:24:ASP:O	3:B:27:GLN:HB2	2.17	0.44
3:F:30:THR:OG1	3:F:32:PRO:HD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-68:DT:H2''	1:J:-67:DA:C8	2.52	0.44
5:H:102:GLU:OE1	5:H:106:HIS:CE1	2.71	0.44
4:G:35:ARG:NH1	4:G:35:ARG:HG2	2.32	0.44
1:J:-32:DA:H4'	1:J:-31:DA:OP1	2.18	0.44
1:I:39:DT:H2''	1:I:40:DA:O5'	2.17	0.44
3:F:19:ARG:NH2	3:F:22:LEU:HD11	2.33	0.44
1:I:-18:DA:H2''	1:I:-17:DA:C8	2.53	0.44
1:J:24:DG:H2''	1:J:25:DA:C8	2.53	0.44
3:B:59:LYS:O	3:B:63:GLU:HG3	2.18	0.43
7:I:997:HOH:O	2:E:49:ARG:HD2	2.17	0.43
1:I:16:DC:H2''	1:I:17:DT:H71	2.00	0.43
1:I:37:DA:H2''	1:I:38:DA:OP2	2.18	0.43
1:J:-71:DC:C2'	1:J:-70:DA:C8	3.01	0.43
1:J:-5:DC:C5'	2:E:43:PRO:HG2	2.48	0.43
2:E:79:LYS:HG3	3:F:74:GLU:OE2	2.18	0.43
1:I:-43:DA:OP2	4:C:32:ARG:HD3	2.18	0.43
4:C:47:ALA:N	4:C:48:PRO:HD2	2.33	0.43
2:A:128:ARG:CD	2:A:134:ARG:HH12	2.11	0.43
5:D:105:LYS:HB2	5:D:105:LYS:HE3	1.81	0.43
1:I:-2:DG:H1'	1:I:-1:DA:C8	2.54	0.43
4:C:79:ILE:HG12	4:C:82:HIS:CE1	2.53	0.43
5:D:102:GLU:OE2	5:D:105:LYS:HD2	2.18	0.43
1:J:-45:DA:H2''	1:J:-44:DA:C8	2.53	0.43
2:A:128:ARG:HB2	2:A:134:ARG:NH1	2.34	0.43
4:G:64:GLU:OE1	5:H:45:VAL:HG13	2.19	0.43
1:I:-18:DA:H2''	1:I:-17:DA:N7	2.34	0.43
1:J:-47:DA:H2''	1:J:-46:DA:OP2	2.19	0.42
4:C:33:LEU:HA	4:C:36:LYS:HG2	2.00	0.42
2:E:127:ALA:O	2:E:131:ARG:HG3	2.20	0.42
3:F:18:HIS:O	3:F:19:ARG:HB2	2.18	0.42
3:F:31:LYS:HE3	3:F:35:ARG:HH22	1.84	0.42
1:J:-52:DC:H2''	1:J:-51:DT:OP2	2.19	0.42
1:J:7:DG:H5'	3:B:46:ILE:O	2.19	0.42
3:F:19:ARG:HH22	3:F:22:LEU:HD11	1.83	0.42
1:I:62:DG:H2''	1:I:63:DT:OP2	2.18	0.42
1:I:-70:DC:H2''	1:I:-69:DA:OP2	2.19	0.42
5:D:79:HIS:HB3	7:D:179:HOH:O	2.19	0.42
2:A:108:ASN:HD21	4:G:115:LEU:HD11	1.85	0.42
1:J:-32:DA:C1'	1:J:-31:DA:O5'	2.66	0.42
4:C:25:PHE:HZ	4:C:59:THR:HG21	1.83	0.42
5:D:59:MET:HE2	5:D:59:MET:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:26:DG:H5'	3:B:79:LYS:HD2	2.01	0.42
1:J:-70:DA:H2''	1:J:-69:DA:OP2	2.20	0.42
5:H:102:GLU:HG3	5:H:106:HIS:CE1	2.55	0.41
1:J:-5:DC:H2''	1:J:-4:DT:H71	2.02	0.41
2:A:48:LEU:HD21	4:G:117:PRO:HD3	2.01	0.41
1:J:19:DT:H2''	1:J:20:DG:H8	1.86	0.41
3:F:31:LYS:HE3	3:F:35:ARG:NH2	2.35	0.41
5:H:73:GLU:HG3	7:H:160:HOH:O	2.19	0.41
1:J:-69:DA:C1'	1:J:-68:DT:H5''	2.49	0.41
5:D:29:THR:O	5:D:29:THR:HG23	2.18	0.41
2:E:76:GLN:NE2	3:F:19:ARG:HH11	2.17	0.41
1:I:52:DG:H8	7:I:1085:HOH:O	2.03	0.41
1:I:60:DA:C2	1:J:-59:DG:N2	2.88	0.41
1:J:-32:DA:H1'	1:J:-31:DA:C5'	2.50	0.41
1:I:30:DG:OP1	5:D:29:THR:CG2	2.69	0.41
1:I:-45:DA:C1'	1:I:-44:DA:H5''	2.49	0.41
3:F:65:VAL:HG22	3:F:93:GLN:OE1	2.20	0.41
1:J:-25:DC:H1'	1:J:-24:DC:C6	2.56	0.41
1:J:-68:DT:H2''	1:J:-67:DA:H8	1.86	0.41
2:E:76:GLN:NE2	3:F:19:ARG:HH12	2.17	0.41
2:E:79:LYS:HD3	2:E:80:THR:N	2.35	0.41
1:I:44:DT:H2''	1:I:45:DT:OP2	2.20	0.41
1:J:9:DA:H8	7:J:980:HOH:O	2.03	0.41
3:F:30:THR:HB	3:F:32:PRO:HD2	2.02	0.41
1:I:-32:DA:H2''	1:I:-31:DA:O5'	2.21	0.41
1:I:-27:DG:H2''	1:I:-26:DC:C6	2.56	0.41
1:J:-73:DA:H2'	1:J:-72:DT:H72	2.02	0.41
2:A:134:ARG:HH11	2:A:134:ARG:CG	2.34	0.41
1:J:49:DT:H1'	1:J:50:DA:C8	2.56	0.41
1:J:13:DG:H2''	1:J:14:DC:OP2	2.21	0.40
1:J:26:DG:H2''	1:J:27:DC:H5	1.76	0.40
1:I:6:DC:H2''	1:I:7:DT:C6	2.56	0.40
1:J:-12:DT:OP1	7:J:1030:HOH:O	2.22	0.40
5:H:43:LYS:HD3	5:H:43:LYS:HA	1.61	0.40
1:J:-22:DT:C4	1:J:-21:DC:N4	2.90	0.40
1:J:42:DC:H2'	1:J:43:DT:H72	2.03	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%)	96 (100%)	0	0	100	100
2	E	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
3	B	80/102 (78%)	78 (98%)	0	2 (2%)	6	2
3	F	85/102 (83%)	81 (95%)	1 (1%)	3 (4%)	4	1
4	C	105/128 (82%)	101 (96%)	4 (4%)	0	100	100
4	G	104/128 (81%)	102 (98%)	2 (2%)	0	100	100
5	D	92/125 (74%)	90 (98%)	1 (1%)	1 (1%)	17	9
5	H	92/125 (74%)	88 (96%)	2 (2%)	2 (2%)	8	3
All	All	750/980 (76%)	731 (98%)	11 (2%)	8 (1%)	17	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	19	ARG
3	B	22	LEU
5	D	101	GLY
5	H	101	GLY
3	F	20	LYS
3	B	23	ARG
3	F	18	HIS
5	H	30	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	85/110 (77%)	83 (98%)	2 (2%)	54	56
2	E	85/110 (77%)	83 (98%)	2 (2%)	54	56
3	B	67/78 (86%)	66 (98%)	1 (2%)	70	74
3	F	72/78 (92%)	71 (99%)	1 (1%)	71	76
4	C	85/101 (84%)	80 (94%)	5 (6%)	23	17
4	G	84/101 (83%)	83 (99%)	1 (1%)	75	80
5	D	80/105 (76%)	79 (99%)	1 (1%)	73	78
5	H	80/105 (76%)	77 (96%)	3 (4%)	38	35
All	All	638/788 (81%)	622 (98%)	16 (2%)	53	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	48	LEU
2	A	59	GLU
3	B	22	LEU
4	C	29	ARG
4	C	59	THR
4	C	81	ARG
4	C	109	PRO
4	C	119	LYS
5	D	33	SER
2	E	49	ARG
2	E	59	GLU
3	F	23	ARG
4	G	88	ARG
5	H	31	LYS
5	H	33	SER
5	H	103	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	68	GLN
4	C	31	HIS
4	C	38	ASN
4	C	112	GLN
5	D	79	HIS
2	E	68	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	76	GLN
3	F	18	HIS
4	G	31	HIS
5	H	79	HIS
5	H	92	GLN
5	H	106	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.