Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 12:22 AM EST

PDB ID	:	3UT9
Title	:	Crystal Structure of Nucleosome Core Particle Assembled with a Palindromic Widom '601' Derivative (NCP-601L)
Authors	:	Chua, E.Y.D.; Vasudevan, D.; Davey, G.E.; Wu, B.; Davey, C.A.
Deposited on	:	2011-11-25
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

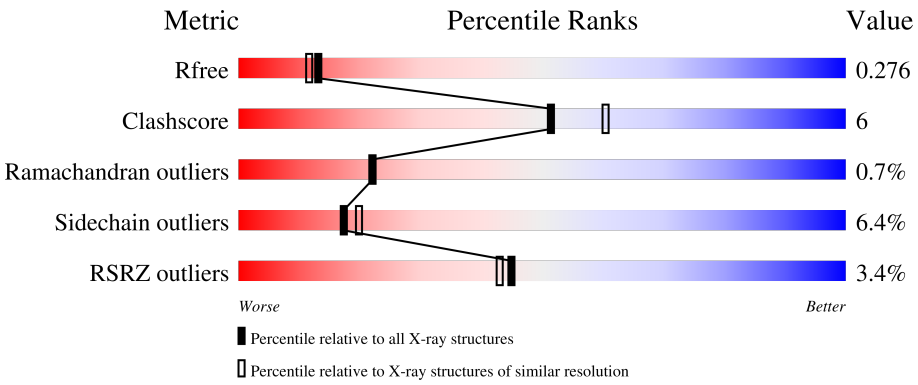
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	135	4%, 61%, 12%, 27%
1	E	135	%, 53%, 16%, •, 28%
2	B	102	%, 69%, 8%, •, 23%
2	F	102	66%, 15%, 5%, 15%
3	C	129	2%, 58%, 22%, •, 19%

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Mol	Chain	Length	Quality of chain
3	G	129	4% 70% 10% 20%
4	D	125	2% 54% 18% 5% 23%
4	H	125	9% 64% 10% • 22%
5	I	145	3% 67% 29% •
6	J	145	.% 67% 30% •

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12180 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 protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	98	808	509	156	140	3	0	0	0
1	E	97	802	506	155	138	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	SEE REMARK 999	UNP P84233
E	102	ALA	GLY	SEE REMARK 999	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	79	627	395	121	110	1	0	0	0
2	F	87	703	442	142	118	1	0	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	105	809	510	158	141	0	0	0
3	G	103	795	501	155	139	0	0	0

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	96	757	475	140	140	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	97	767	481	142	142	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	SEE REMARK 999	UNP P02281
H	29	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 5 is a DNA chain called 145-mer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	I	145	2970	1409	550	867	144	0	0	0

- Molecule 6 is a DNA chain called 145-mer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	J	145	2969	1409	547	869	144	0	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	C	1	1	1	0	0
7	G	1	1	1	0	0

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
8	E	1	1	1	0	0
8	I	14	14	14	0	0
8	J	14	14	14	0	0

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 10 is water.

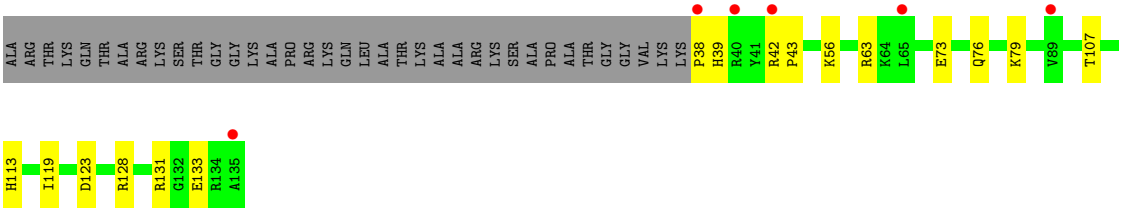
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	11	Total O 11 11	0	0
10	B	11	Total O 11 11	0	0
10	C	21	Total O 21 21	0	0
10	D	3	Total O 3 3	0	0
10	E	27	Total O 27 27	0	0
10	F	29	Total O 29 29	0	0
10	G	8	Total O 8 8	0	0
10	H	3	Total O 3 3	0	0
10	I	9	Total O 9 9	0	0
10	J	18	Total O 18 18	0	0

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 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 (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.

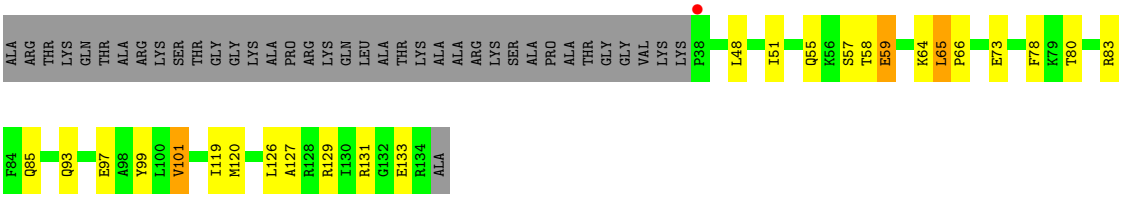
• Molecule 1: Histone H3.2

Chain A: 4% 61% 12% 27%



• Molecule 1: Histone H3.2

Chain E: % 53% 16% • 28%



• Molecule 2: Histone H4

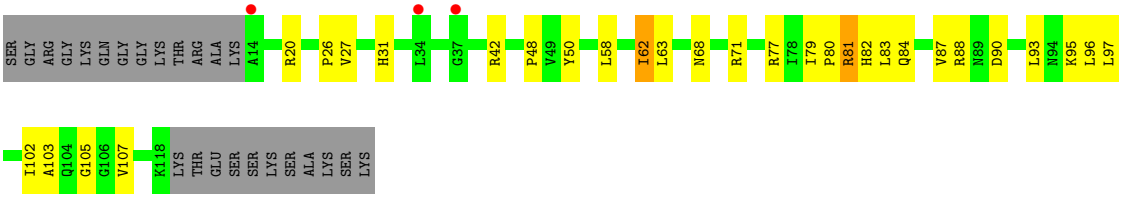
Chain B: % 69% 8% • 23%

• Molecule 2: Histone H4

Chain F: 66% 15% 5% 15%

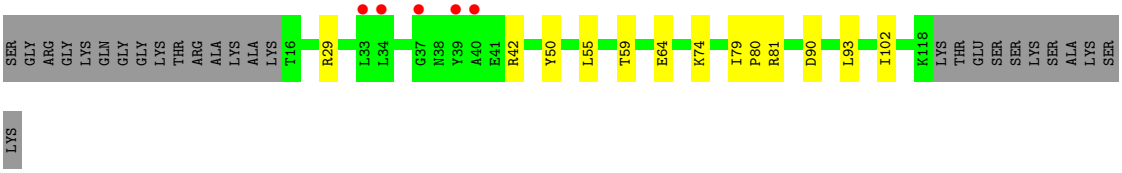
• Molecule 3: Histone H2A

Chain C: 2% 58% 22% • 19%



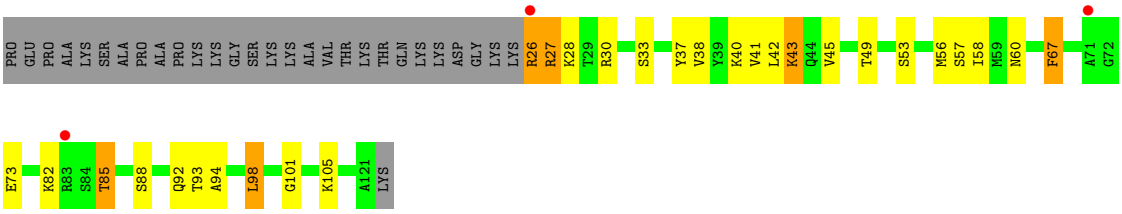
- Molecule 3: Histone H2A

Chain G:



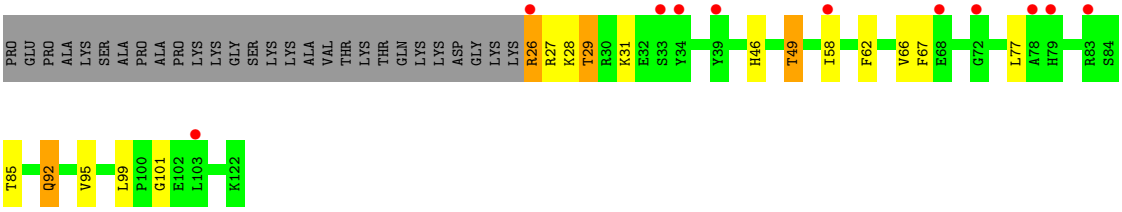
- Molecule 4: Histone H2B 1.1

Chain D:



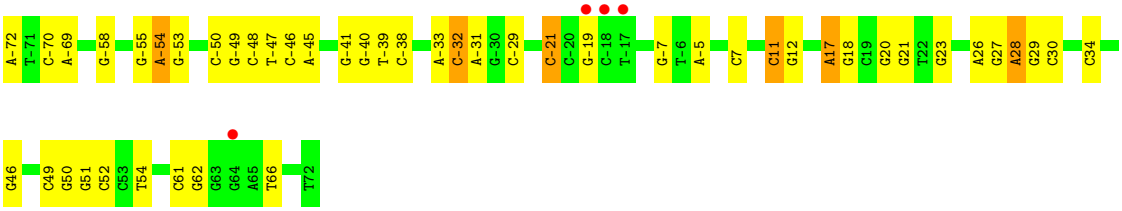
- Molecule 4: Histone H2B 1.1

Chain H:



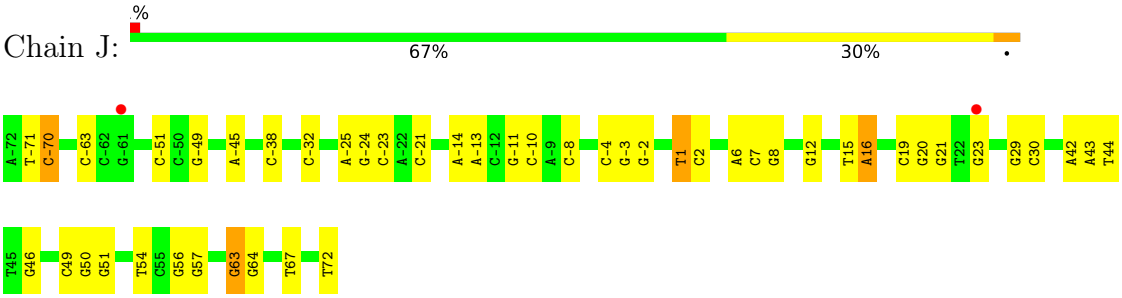
- Molecule 5: 145-mer DNA

Chain I:



- Molecule 6: 145-mer DNA

Chain J:


%
67%
30%
A-72
T-71
C-70
C-63
C-62
G-61
C-51
C-50
G-49
A-45
C-38
C-32
A-25
G-24
C-23
A-22
C-21
A-14
A-13
C-12
G-11
C-10
A-9
C-8
C-4
G-3
G-2
T1
C2
A6
C7
G8
G12
T15
A16
C19
G20
G21
T22
G23
G29
C30
A42
A43
T44
T45
G46
C49
G50
G51
T54
C55
G56
G57
G63
G64
T67
T72

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.49Å 109.53Å 174.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.55 – 2.20 42.55 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.55-2.20) 99.8 (42.55-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.289 0.247 , 0.276	Depositor DCC
R_{free} test set	2083 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12180	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	A	0.41	0/820	0.52	0/1099
1	E	0.91	2/814 (0.2%)	0.77	0/1092
2	B	0.40	0/634	0.56	0/848
2	F	0.81	0/711	0.84	0/948
3	C	0.67	0/819	0.76	2/1106 (0.2%)
3	G	0.40	0/805	0.59	0/1088
4	D	0.59	0/768	0.67	0/1032
4	H	0.47	0/778	0.62	0/1043
5	I	0.69	0/3332	1.31	23/5141 (0.4%)
6	J	0.67	0/3330	1.32	30/5138 (0.6%)
All	All	0.65	2/12811 (0.0%)	1.08	55/18535 (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
4	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	101	VAL	CB-CG2	10.59	1.75	1.52
1	E	101	VAL	CA-CB	-6.06	1.42	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	21	DG	O4'-C1'-N9	9.67	114.77	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	54	DT	P-O3'-C3'	7.97	129.26	119.70
5	I	-58	DG	P-O3'-C3'	7.55	128.76	119.70
5	I	54	DT	P-O3'-C3'	7.54	128.74	119.70
6	J	-2	DG	O4'-C1'-N9	7.46	113.22	108.00
5	I	20	DG	P-O3'-C3'	7.30	128.46	119.70
6	J	-10	DC	O4'-C1'-N1	7.12	112.98	108.00
5	I	-32	DC	O4'-C1'-N1	7.11	112.98	108.00
6	J	43	DA	P-O3'-C3'	6.86	127.93	119.70
3	C	88	ARG	NE-CZ-NH2	6.85	123.73	120.30
5	I	34	DC	P-O3'-C3'	6.84	127.91	119.70
5	I	29	DG	C3'-C2'-C1'	-6.74	94.41	102.50
5	I	-33	DA	P-O3'-C3'	6.69	127.72	119.70
6	J	42	DA	P-O3'-C3'	6.61	127.63	119.70
5	I	30	DC	O4'-C1'-N1	6.60	112.62	108.00
3	C	88	ARG	NE-CZ-NH1	-6.51	117.04	120.30
6	J	57	DG	P-O3'-C3'	6.48	127.47	119.70
6	J	23	DG	P-O3'-C3'	6.43	127.41	119.70
5	I	-38	DC	P-O3'-C3'	6.41	127.39	119.70
6	J	-38	DC	P-O3'-C3'	6.35	127.32	119.70
5	I	66	DT	O4'-C1'-N1	6.29	112.40	108.00
6	J	-32	DC	O4'-C1'-N1	6.26	112.38	108.00
6	J	16	DA	O4'-C1'-N9	6.24	112.37	108.00
6	J	-63	DC	P-O3'-C3'	6.24	127.19	119.70
5	I	-41	DG	P-O3'-C3'	6.20	127.14	119.70
6	J	-14	DA	P-O3'-C3'	6.11	127.04	119.70
5	I	11	DC	O4'-C1'-N1	6.11	112.28	108.00
6	J	-13	DA	P-O3'-C3'	6.00	126.90	119.70
6	J	30	DC	O4'-C1'-N1	5.99	112.19	108.00
5	I	-29	DC	P-O3'-C3'	5.98	126.88	119.70
5	I	-21	DC	P-O3'-C3'	5.83	126.70	119.70
5	I	18	DG	P-O3'-C3'	5.75	126.60	119.70
6	J	72	DT	O4'-C4'-C3'	-5.70	102.22	104.50
6	J	-51	DC	P-O3'-C3'	5.69	126.53	119.70
6	J	-11	DG	O4'-C1'-N9	5.68	111.98	108.00
5	I	17	DA	O4'-C1'-N9	-5.64	104.05	108.00
5	I	7	DC	O4'-C1'-N1	5.58	111.91	108.00
5	I	23	DG	P-O3'-C3'	5.51	126.32	119.70
6	J	-21	DC	O4'-C1'-N1	5.51	111.86	108.00
6	J	-70	DC	O4'-C1'-N1	5.32	111.72	108.00
6	J	-8	DC	O4'-C1'-N1	5.31	111.72	108.00
5	I	-21	DC	O4'-C1'-N1	5.26	111.68	108.00
6	J	63	DG	O4'-C1'-N9	5.20	111.64	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	28	DA	P-O3'-C3'	5.19	125.93	119.70
6	J	44	DT	O4'-C1'-N1	5.19	111.63	108.00
6	J	1	DT	P-O3'-C3'	5.17	125.90	119.70
6	J	-13	DA	O5'-P-OP2	-5.16	101.05	105.70
6	J	67	DT	P-O3'-C3'	5.15	125.88	119.70
6	J	-49	DG	O4'-C1'-N9	5.14	111.60	108.00
5	I	-54	DA	P-O3'-C3'	5.09	125.80	119.70
6	J	29	DG	O4'-C1'-N9	5.07	111.55	108.00
6	J	12	DG	O4'-C1'-N9	5.04	111.53	108.00
5	I	-53	DG	C1'-O4'-C4'	-5.03	105.07	110.10
6	J	-49	DG	O4'-C1'-C2'	-5.02	101.89	105.90
6	J	-23	DC	C1'-O4'-C4'	-5.02	105.08	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	27	ARG	Peptide

5.2 Too-close contacts (i)

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	A	808	0	846	12	0
1	E	802	0	841	21	0
2	B	627	0	663	5	0
2	F	703	0	755	13	0
3	C	809	0	864	27	0
3	G	795	0	846	7	0
4	D	757	0	786	21	0
4	H	767	0	799	12	0
5	I	2970	0	1628	24	0
6	J	2969	0	1629	17	0
7	C	1	0	0	0	0
7	G	1	0	0	0	0
8	E	1	0	0	0	0
8	I	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	14	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
10	A	11	0	0	0	0
10	B	11	0	0	0	0
10	C	21	0	0	0	0
10	D	3	0	0	0	0
10	E	27	0	0	1	0
10	F	29	0	0	0	0
10	G	8	0	0	0	0
10	H	3	0	0	0	0
10	I	9	0	0	0	0
10	J	18	0	0	0	0
All	All	12180	0	9657	122	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 6.

All (122) 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:E:101:VAL:CB	1:E:101:VAL:CG2	1.75	1.60
4:H:46:HIS:HB3	4:H:49:THR:HG23	1.45	0.97
4:H:46:HIS:HB3	4:H:49:THR:CG2	2.06	0.85
3:C:80:PRO:HB3	4:D:58:ILE:CD1	2.15	0.76
3:C:102:ILE:HG23	4:D:58:ILE:HD13	1.68	0.75
1:A:73:GLU:OE1	2:B:25:ASN:HB2	1.86	0.74
1:E:101:VAL:CG2	1:E:101:VAL:CA	2.64	0.74
1:E:101:VAL:CG2	1:E:101:VAL:CG1	2.66	0.73
3:C:63:LEU:HD13	4:D:42:LEU:HB2	1.69	0.73
4:H:26:ARG:HH11	4:H:26:ARG:CG	2.02	0.73
4:H:26:ARG:HH11	4:H:26:ARG:HG2	1.54	0.72
1:E:65:LEU:HD22	5:I:17:DA:H2'	1.71	0.70
3:C:83:LEU:O	3:C:87:VAL:HG23	1.95	0.67
5:I:11:DC:H2"	5:I:12:DG:C8	2.30	0.66
3:C:80:PRO:HB3	4:D:58:ILE:HD12	1.76	0.66
6:J:50:DG:H2"	6:J:51:DG:OP2	1.96	0.64
6:J:49:DC:H2'	6:J:50:DG:C8	2.32	0.64
3:C:97:LEU:HD23	3:C:97:LEU:N	2.14	0.64
4:H:26:ARG:HG2	4:H:26:ARG:NH1	2.10	0.63
3:G:55:LEU:O	3:G:59:THR:OG1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:61:DC:H2"	5:I:62:DG:C8	2.36	0.60
1:E:64:LYS:HE2	10:E:162:HOH:O	2.02	0.58
2:F:20:LYS:HD2	2:F:21:VAL:H	1.69	0.58
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.86	0.58
1:A:43:PRO:HG2	5:I:-5:DA:H5'	1.85	0.57
3:C:50:TYR:OH	4:D:92:GLN:NE2	2.33	0.57
4:D:43:LYS:HE2	4:D:49:THR:O	2.05	0.55
2:F:68:ASP:O	2:F:69:ALA:C	2.43	0.55
3:G:50:TYR:OH	4:H:92:GLN:NE2	2.38	0.54
2:F:89:ALA:O	2:F:92:ARG:HB2	2.08	0.54
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.42	0.54
5:I:51:DG:H1'	5:I:52:DC:H5'	1.88	0.54
5:I:-50:DC:H2"	5:I:-49:DG:C8	2.44	0.52
2:F:61:PHE:HE1	2:F:95:ARG:HD3	1.74	0.52
3:C:31:HIS:CD2	3:C:48:PRO:HG3	2.45	0.52
1:E:51:ILE:O	1:E:55:GLN:HG3	2.10	0.52
3:C:96:LEU:C	3:C:97:LEU:HD23	2.31	0.51
1:E:127:ALA:O	1:E:131:ARG:HG3	2.11	0.51
1:E:65:LEU:O	1:E:66:PRO:C	2.45	0.51
6:J:63:DG:H2"	6:J:64:DG:C8	2.45	0.51
5:I:-7:DG:C6	6:J:6:DA:N6	2.79	0.50
1:A:79:LYS:HD2	2:B:74:GLU:OE2	2.12	0.50
4:D:28:LYS:HG3	6:J:51:DG:OP1	2.12	0.50
1:E:59:GLU:O	1:E:59:GLU:HG2	2.10	0.49
1:A:76:GLN:NE2	1:A:76:GLN:HA	2.27	0.49
4:H:28:LYS:O	4:H:29:THR:HG22	2.12	0.49
1:E:120:MET:C	2:F:50:ILE:HD11	2.33	0.49
5:I:-47:DT:H2"	5:I:-46:DC:C6	2.47	0.49
3:C:42:ARG:NH1	4:D:85:THR:OG1	2.46	0.49
5:I:-40:DG:H2"	5:I:-39:DT:OP2	2.12	0.49
1:A:119:ILE:O	2:B:47:SER:HB3	2.13	0.49
1:E:83:ARG:NH2	5:I:26:DA:H4'	2.28	0.49
2:F:35:ARG:NH2	2:F:51:TYR:OH	2.45	0.49
1:E:73:GLU:OE1	2:F:25:ASN:HB2	2.14	0.48
2:F:17:ARG:HD2	2:F:18:HIS:H	1.79	0.48
1:E:65:LEU:HD22	5:I:17:DA:C2'	2.43	0.47
6:J:15:DT:H2"	6:J:16:DA:C8	2.48	0.47
3:C:62:ILE:HD11	3:C:83:LEU:HD22	1.96	0.47
5:I:-32:DC:H2"	5:I:-31:DA:OP2	2.14	0.47
4:D:94:ALA:O	4:D:98:LEU:HB2	2.14	0.47
5:I:-21:DC:H42	6:J:21:DG:H1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:67:PHE:C	4:D:67:PHE:CD2	2.88	0.47
3:C:102:ILE:O	3:C:103:ALA:C	2.53	0.46
6:J:19:DC:H2"	6:J:20:DG:C8	2.51	0.46
1:A:107:THR:HG23	1:A:123:ASP:HB2	1.97	0.46
5:I:-55:DG:N2	6:J:56:DG:N2	2.63	0.46
5:I:-19:DG:H1	6:J:19:DC:H42	1.63	0.46
2:B:92:ARG:NE	4:D:73:GLU:OE2	2.42	0.46
3:C:84:GLN:HG2	3:C:105:GLY:O	2.16	0.46
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.41	0.46
3:G:79:ILE:HB	3:G:80:PRO:CD	2.46	0.45
3:C:68:ASN:OD1	3:C:71:ARG:NH2	2.49	0.45
5:I:-72:DA:H2'	5:I:-72:DA:N3	2.32	0.45
3:C:81:ARG:NH2	3:C:107:VAL:O	2.50	0.45
4:D:67:PHE:C	4:D:67:PHE:HD2	2.20	0.45
4:H:95:VAL:HG13	4:H:99:LEU:HD12	1.99	0.45
3:C:77:ARG:NE	5:I:-54:DA:H4'	2.32	0.45
1:E:85:GLN:NE2	2:F:82:THR:HG22	2.32	0.45
1:A:42:ARG:HH21	5:I:-5:DA:P	2.39	0.45
3:C:81:ARG:HB2	1:E:58:THR:HG21	1.99	0.45
1:E:93:GLN:O	1:E:97:GLU:HG3	2.16	0.45
1:A:131:ARG:HD3	1:A:133:GLU:OE2	2.16	0.44
2:B:71:THR:HG22	4:D:93:THR:HG23	1.99	0.44
1:A:63:ARG:HD3	1:A:63:ARG:HA	1.75	0.44
3:G:79:ILE:HB	3:G:80:PRO:HD2	1.99	0.44
5:I:-70:DC:H2"	5:I:-69:DA:C8	2.53	0.44
3:G:90:ASP:OD1	3:G:93:LEU:HG	2.17	0.44
5:I:27:DG:N2	5:I:28:DA:C2	2.87	0.43
6:J:-25:DA:H1'	6:J:-24:DG:C8	2.54	0.43
4:D:45:VAL:HG12	4:D:45:VAL:O	2.18	0.43
3:C:63:LEU:HD11	4:D:38:VAL:HG13	2.00	0.43
5:I:-45:DA:C2	6:J:46:DG:N2	2.87	0.43
1:A:128:ARG:HD2	1:A:133:GLU:OE1	2.19	0.42
6:J:-71:DT:H2"	6:J:-70:DC:OP2	2.19	0.42
3:C:20:ARG:HE	3:C:20:ARG:HB2	1.53	0.42
3:C:58:LEU:O	3:C:62:ILE:HG22	2.19	0.42
4:D:26:ARG:O	4:D:27:ARG:CB	2.67	0.42
6:J:-4:DC:H2"	6:J:-3:DG:C8	2.55	0.42
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.54	0.42
4:D:40:LYS:O	4:D:41:VAL:C	2.58	0.42
6:J:7:DC:H2'	6:J:8:DG:C8	2.54	0.42
3:G:80:PRO:HB3	4:H:58:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:LYS:HE3	4:D:105:LYS:HB2	1.82	0.41
3:C:95:LYS:O	3:C:96:LEU:C	2.58	0.41
2:F:89:ALA:O	2:F:93:GLN:HG2	2.20	0.41
1:E:119:ILE:O	2:F:47:SER:HB3	2.20	0.41
5:I:46:DG:N2	6:J:-45:DA:C2	2.88	0.41
5:I:49:DC:H2'	5:I:50:DG:C8	2.56	0.41
4:H:67:PHE:CD2	4:H:67:PHE:C	2.93	0.41
4:D:33:SER:OG	4:D:60:ASN:ND2	2.54	0.41
4:D:56:MET:O	4:D:56:MET:HG3	2.20	0.41
1:A:38:PRO:HB2	1:A:39:HIS:H	1.69	0.41
1:E:78:PHE:CZ	2:F:67:ARG:HB2	2.56	0.41
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.31	0.41
3:C:27:VAL:HG13	3:C:48:PRO:HB2	2.03	0.40
6:J:1:DT:H1'	6:J:2:DC:H5'	2.03	0.40
3:C:26:PRO:HG3	4:D:37:TYR:CZ	2.56	0.40
3:C:90:ASP:HB3	3:C:93:LEU:HB2	2.02	0.40
3:C:102:ILE:O	3:C:102:ILE:HG22	2.21	0.40
4:H:62:PHE:O	4:H:66:VAL:HG23	2.21	0.40
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.89	0.40
5:I:-48:DC:C6	5:I:-47:DT:H72	2.55	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	
1	A	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
1	E	95/135 (70%)	91 (96%)	4 (4%)	0	100	100
2	B	77/102 (76%)	77 (100%)	0	0	100	100
2	F	85/102 (83%)	79 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	103/129 (80%)	96 (93%)	7 (7%)	0	100	100
3	G	101/129 (78%)	97 (96%)	4 (4%)	0	100	100
4	D	94/125 (75%)	88 (94%)	3 (3%)	3 (3%)	4	2
4	H	95/125 (76%)	88 (93%)	5 (5%)	2 (2%)	7	4
All	All	746/982 (76%)	708 (95%)	33 (4%)	5 (1%)	22	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	H	29	THR
4	D	27	ARG
4	H	101	GLY
4	D	88	SER

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	
1	A	85/110 (77%)	84 (99%)	1 (1%)	71	83
1	E	85/110 (77%)	79 (93%)	6 (7%)	14	16
2	B	64/78 (82%)	59 (92%)	5 (8%)	12	13
2	F	72/78 (92%)	65 (90%)	7 (10%)	8	7
3	C	83/101 (82%)	81 (98%)	2 (2%)	49	62
3	G	82/101 (81%)	77 (94%)	5 (6%)	18	21
4	D	82/105 (78%)	73 (89%)	9 (11%)	6	5
4	H	83/105 (79%)	77 (93%)	6 (7%)	14	15
All	All	636/788 (81%)	595 (94%)	41 (6%)	17	20

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
2	B	24	ASP
2	B	26	ILE
2	B	35	ARG
2	B	74	GLU
2	B	95	ARG
3	C	62	ILE
3	C	81	ARG
4	D	26	ARG
4	D	30	ARG
4	D	43	LYS
4	D	53	SER
4	D	57	SER
4	D	67	PHE
4	D	82	LYS
4	D	85	THR
4	D	98	LEU
1	E	48	LEU
1	E	57	SER
1	E	59	GLU
1	E	65	LEU
1	E	80	THR
1	E	129	ARG
2	F	16	LYS
2	F	17	ARG
2	F	18	HIS
2	F	21	VAL
2	F	47	SER
2	F	91	LYS
2	F	92	ARG
3	G	29	ARG
3	G	42	ARG
3	G	64	GLU
3	G	74	LYS
3	G	81	ARG
4	H	26	ARG
4	H	31	LYS
4	H	49	THR
4	H	77	LEU
4	H	85	THR
4	H	92	GLN

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

Mol	Chain	Res	Type
1	A	76	GLN
3	C	31	HIS
4	D	60	ASN
4	D	92	GLN
2	F	18	HIS
3	G	38	ASN
4	H	92	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 33 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	98/135 (72%)	0.57	6 (6%)	21	20	49, 76, 94, 107	0
1	E	97/135 (71%)	0.17	1 (1%)	82	81	28, 52, 75, 89	0
2	B	79/102 (77%)	0.63	1 (1%)	77	75	55, 68, 89, 96	0
2	F	87/102 (85%)	0.46	0	100	100	32, 50, 64, 96	0
3	C	105/129 (81%)	0.45	3 (2%)	51	49	31, 56, 78, 87	0
3	G	103/129 (79%)	0.45	5 (4%)	29	28	51, 70, 86, 92	0
4	D	96/125 (76%)	0.55	3 (3%)	49	47	45, 60, 82, 98	0
4	H	97/125 (77%)	0.71	11 (11%)	5	4	44, 70, 96, 109	0
5	I	145/145 (100%)	0.04	4 (2%)	53	51	65, 114, 140, 149	0
6	J	145/145 (100%)	0.00	2 (1%)	75	73	67, 114, 143, 164	0
All	All	1052/1272 (82%)	0.36	36 (3%)	45	43	28, 70, 128, 164	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	-19	DG	4.5
4	H	83	ARG	4.1
1	A	38	PRO	3.9
4	H	26	ARG	3.5
3	G	33	LEU	3.5
1	A	65	LEU	3.0
3	G	37	GLY	3.0
1	A	135	ALA	2.9
1	A	42	ARG	2.7
3	G	40	ALA	2.6
3	C	14	ALA	2.6
5	I	-18	DC	2.5
4	H	34	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
5	I	-17	DT	2.5
3	G	39	TYR	2.5
3	C	37	GLY	2.4
5	I	64	DG	2.4
4	H	33	SER	2.4
4	H	79	HIS	2.4
1	E	38	PRO	2.4
4	H	103	LEU	2.3
3	G	34	LEU	2.3
4	H	39	TYR	2.3
1	A	40	ARG	2.3
2	B	101	GLY	2.3
4	H	58	ILE	2.2
4	H	68	GLU	2.2
4	D	83	ARG	2.2
4	D	26	ARG	2.1
3	C	34	LEU	2.1
4	D	71	ALA	2.1
6	J	-61	DG	2.1
1	A	89	VAL	2.1
4	H	72	GLY	2.1
4	H	78	ALA	2.0
6	J	23	DG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MN	J	1026	1/1	-0.07	0.11	193,193,193,193	0
8	MN	J	1025	1/1	-0.03	0.16	169,169,169,169	0
8	MN	I	1021	1/1	0.34	0.23	154,154,154,154	0
8	MN	J	1022	1/1	0.39	0.18	157,157,157,157	0
8	MN	I	1006	1/1	0.49	0.26	148,148,148,148	0
8	MN	I	1018	1/1	0.51	0.06	135,135,135,135	0
8	MN	I	1013	1/1	0.59	0.14	149,149,149,149	0
8	MN	J	1009	1/1	0.61	0.20	146,146,146,146	0
8	MN	J	1024	1/1	0.65	0.29	194,194,194,194	0
8	MN	I	1023	1/1	0.66	0.11	167,167,167,167	0
8	MN	I	1028	1/1	0.68	0.17	199,199,199,199	0
8	MN	I	1011	1/1	0.68	0.21	128,128,128,128	0
8	MN	J	1020	1/1	0.70	0.16	145,145,145,145	0
8	MN	J	1029	1/1	0.70	0.08	126,126,126,126	0
8	MN	I	1014	1/1	0.75	0.25	150,150,150,150	0
8	MN	J	1004	1/1	0.77	0.20	104,104,104,104	0
8	MN	J	1017	1/1	0.78	0.20	127,127,127,127	0
8	MN	I	1016	1/1	0.79	0.35	141,141,141,141	0
8	MN	I	1019	1/1	0.81	0.22	160,160,160,160	0
8	MN	I	1027	1/1	0.81	0.25	150,150,150,150	0
8	MN	J	1015	1/1	0.86	0.27	142,142,142,142	0
8	MN	J	1010	1/1	0.89	0.16	114,114,114,114	0
8	MN	J	1008	1/1	0.89	0.28	110,110,110,110	0
8	MN	I	1007	1/1	0.89	0.24	106,106,106,106	0
9	K	I	1052	1/1	0.91	0.06	107,107,107,107	0
8	MN	J	1012	1/1	0.93	0.06	113,113,113,113	0
8	MN	I	1003	1/1	0.93	0.18	90,90,90,90	0
8	MN	I	1005	1/1	0.94	0.26	107,107,107,107	0
7	CL	G	1101	1/1	0.96	0.07	66,66,66,66	0
8	MN	J	1002	1/1	0.96	0.28	95,95,95,95	0
9	K	J	1051	1/1	0.96	0.10	83,83,83,83	0
7	CL	C	1102	1/1	0.98	0.06	67,67,67,67	0
8	MN	E	1001	1/1	0.98	0.13	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.