wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 05:32 pm BST

PDB ID	:	8QKT
Title	:	Structure of a nucleosome composed of a palindromic 167-base pair blunt-ended DNA fragment
Authors	:	Ma, Z.; Davey, C.A.
Deposited on	:	2023-09-17
Resolution	:	3.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

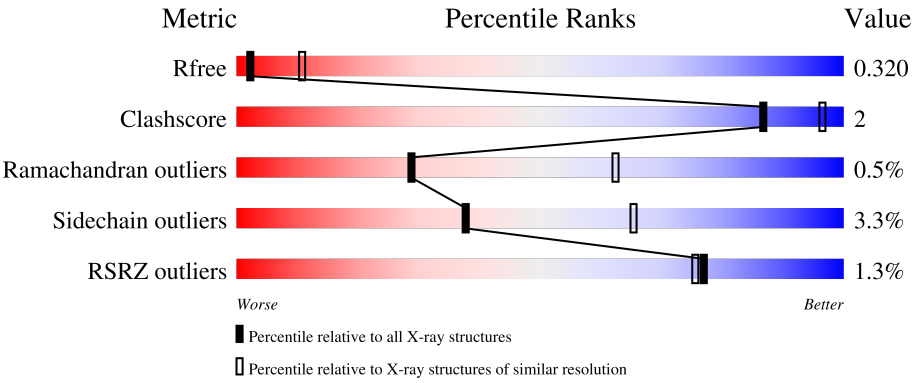
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	AAA	98	95%
1	EEE	98	91% 8%
1	KKK	98	% 95% 5%
1	OOO	98	92% 7%
2	BBB	79	96%

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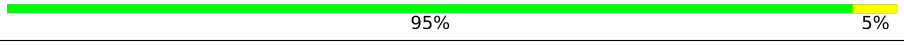
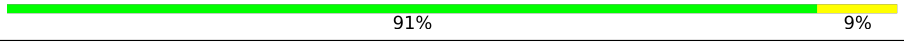
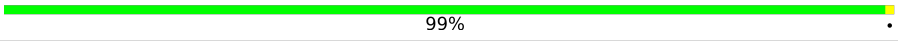
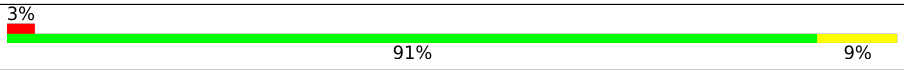
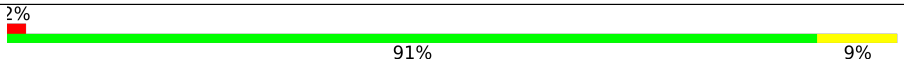
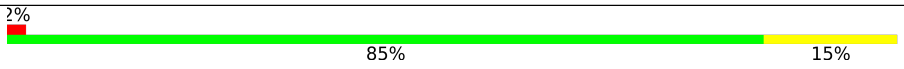
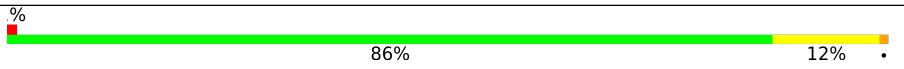
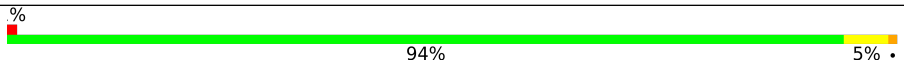
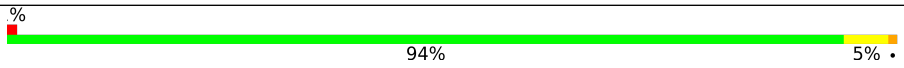
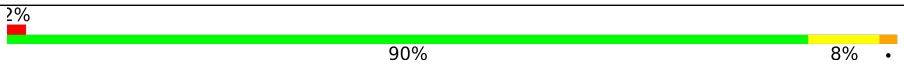
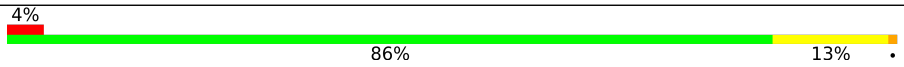
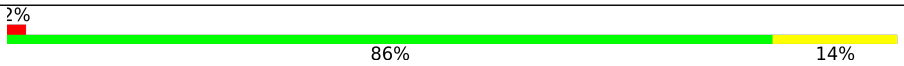
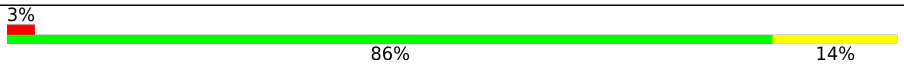
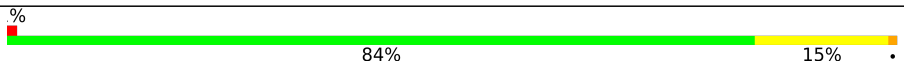
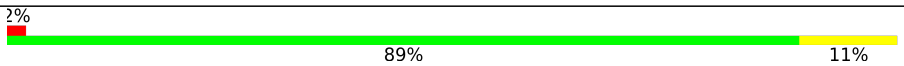
Mol	Chain	Length	Quality of chain
2	FFF	79	
2	LLL	79	
2	PPP	79	
3	CCC	105	
3	MMM	105	
4	DDD	96	
4	NNN	96	
5	GGG	103	
5	QQQ	103	
6	HHH	97	
6	RRR	97	
7	III	167	
7	SSS	167	
8	JJJ	167	
8	TTT	167	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 25695 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 H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	EEE	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	KKK	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	OOO	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	FFF	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	LLL	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	PPP	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	MMM	105	Total	C	N	O	0	0	0
			810	511	158	141			

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	96	Total	C	N	O	S	0	0	0
			756	474	140	140	2			
4	NNN	96	Total	C	N	O	S	0	0	0
			756	474	140	140	2			

- Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	GGG	103	Total	C	N	O	0	0	0
			796	502	155	139			
5	QQQ	103	Total	C	N	O	0	0	0
			796	502	155	139			

- Molecule 6 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	HHH	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			
6	RRR	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			

- Molecule 7 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	III	167	Total	C	N	O	P	0	0	0
			3421	1628	628	999	166			
7	SSS	167	Total	C	N	O	P	0	0	0
			3421	1628	628	999	166			

- Molecule 8 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	JJJ	167	Total	C	N	O	P	0	0	0
			3420	1628	625	1001	166			
8	TTT	167	Total	C	N	O	P	0	0	0
			3420	1628	625	1001	166			

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	III	11	Total	Mn	0	0
			11	11		

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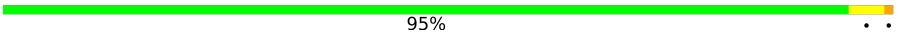
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	JJJ	8	Total Mn 8 8	0	0
9	SSS	6	Total Mn 6 6	0	0
9	TTT	8	Total Mn 8 8	0	0

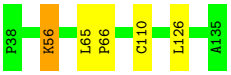
3 Residue-property plots (i)

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 H3.1

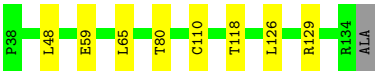
Chain AAA:





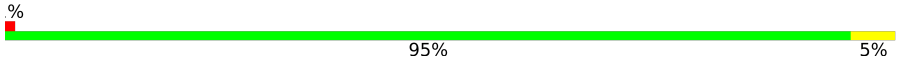
• Molecule 1: Histone H3.1

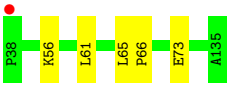
Chain EEE:



• Molecule 1: Histone H3.1

Chain KKK:



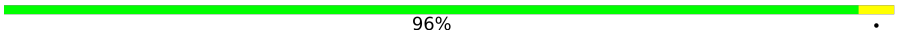


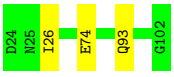
• Molecule 1: Histone H3.1

Chain OOO:

• Molecule 2: Histone H4

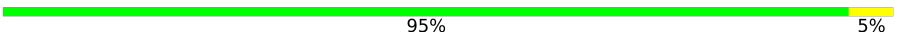
Chain BBB:





• Molecule 2: Histone H4

Chain FFF:

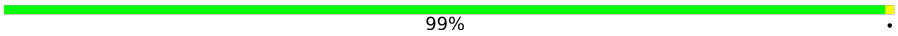


• Molecule 2: Histone H4

Chain LLL:

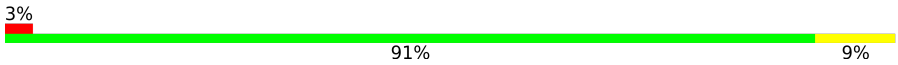
• Molecule 2: Histone H4

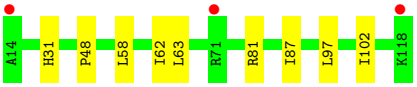
Chain PPP:



• Molecule 3: Histone H2A

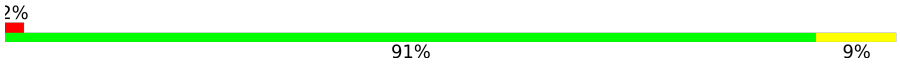
Chain CCC:

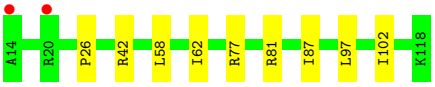




• Molecule 3: Histone H2A

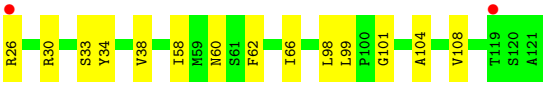
Chain MMM:





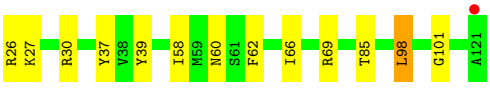
• Molecule 4: Histone H2B type 1-J

Chain DDD:



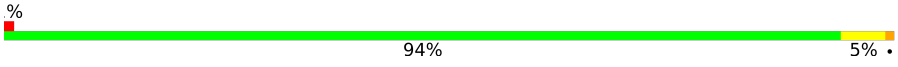
• Molecule 4: Histone H2B type 1-J

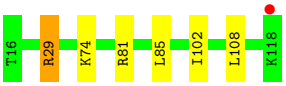
Chain NNN:



• Molecule 5: Histone H2A

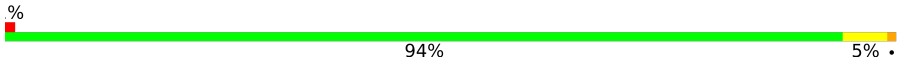
Chain GGG:





• Molecule 5: Histone H2A

Chain QQQ:

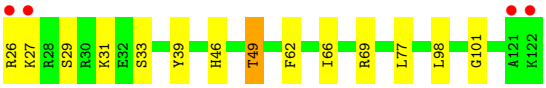


• Molecule 6: Histone H2B type 1-J

Chain HHH:

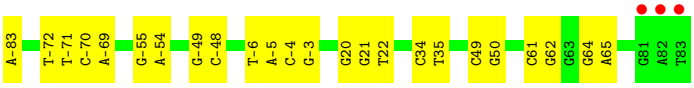
• Molecule 6: Histone H2B type 1-J

Chain RRR:



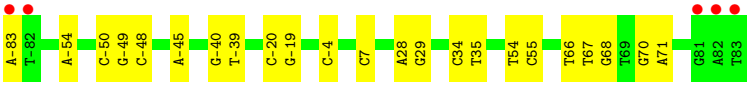
• Molecule 7: DNA (167-MER)

Chain III:



• Molecule 7: DNA (167-MER)

Chain SSS:

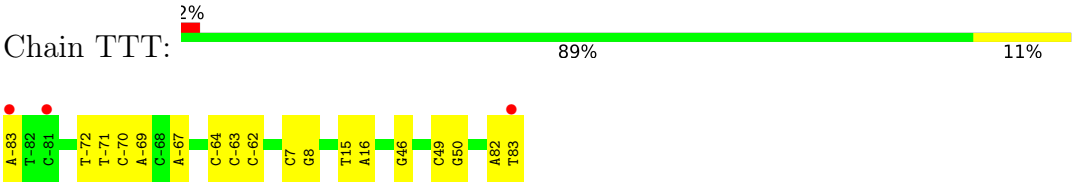


• Molecule 8: DNA (167-MER)

Chain JJJ:

• Molecule 8: DNA (167-MER)

Chain TTT:


2%
89%
11%
A-83
T-82
C-81
T-72
T-71
C-70
A-69
C-68
A-67
C-64
C-63
C-62
C7
G8
T15
A16
G46
C49
G50
A82
T83

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.44Å 103.72Å 185.41Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	48.66 – 3.26 48.66 – 3.26	Depositor EDS
% Data completeness (in resolution range)	89.1 (48.66-3.26) 89.1 (48.66-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.269 , 0.321 0.271 , 0.320	Depositor DCC
R_{free} test set	2865 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 28.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	25695	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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

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	AAA	0.31	0/819	0.55	0/1097
1	EEE	0.30	0/813	0.56	0/1090
1	KKK	0.31	0/819	0.54	0/1097
1	OOO	0.31	0/813	0.56	0/1090
2	BBB	0.31	0/634	0.61	0/848
2	FFF	0.33	0/634	0.58	0/848
2	LLL	0.33	0/634	0.61	0/848
2	PPP	0.30	0/634	0.57	0/848
3	CCC	0.29	0/820	0.52	0/1107
3	MMM	0.29	0/820	0.53	0/1107
4	DDD	0.32	0/767	0.51	0/1029
4	NNN	0.31	0/767	0.50	0/1029
5	GGG	0.29	0/806	0.52	0/1089
5	QQQ	0.28	0/806	0.53	0/1089
6	HHH	0.30	0/777	0.53	0/1040
6	RRR	0.33	0/777	0.56	0/1040
7	III	0.30	0/3838	0.78	1/5922 (0.0%)
7	SSS	0.29	0/3838	0.77	3/5922 (0.1%)
8	JJJ	0.30	0/3836	0.81	3/5919 (0.1%)
8	TTT	0.29	0/3836	0.79	1/5919 (0.0%)
All	All	0.30	0/27488	0.70	8/39978 (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
6	RRR	0	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	JJJ	71	DA	C1'-O4'-C4'	-6.60	103.50	110.10
7	SSS	-83	DA	C5'-C4'-O4'	5.31	119.39	109.30
8	JJJ	-10	DC	C1'-O4'-C4'	-5.21	104.89	110.10
8	TTT	-83	DA	C5'-C4'-C3'	5.21	123.47	114.10
7	III	-83	DA	C5'-C4'-C3'	5.14	123.35	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	RRR	27	LYS	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	AAA	807	0	844	3	0
1	EEE	801	0	839	1	0
1	KKK	807	0	844	3	0
1	OOO	801	0	839	2	0
2	BBB	627	0	663	0	0
2	FFF	627	0	663	3	0
2	LLL	627	0	663	4	0
2	PPP	627	0	663	1	0
3	CCC	810	0	866	6	0
3	MMM	810	0	866	8	0
4	DDD	756	0	784	7	0
4	NNN	756	0	784	5	0
5	GGG	796	0	848	3	0
5	QQQ	796	0	848	3	0
6	HHH	766	0	797	6	0
6	RRR	766	0	797	6	0
7	III	3421	0	1880	12	0
7	SSS	3421	0	1880	15	0
8	JJJ	3420	0	1881	16	0
8	TTT	3420	0	1881	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	III	11	0	0	0	0
9	JJJ	8	0	0	0	0
9	SSS	6	0	0	0	0
9	TTT	8	0	0	0	0
All	All	25695	0	20130	98	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 2.

The worst 5 of 98 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)
8:JJJ:-69:DA:H2"	8:JJJ:-68:DC:O5'	1.86	0.75
6:RRR:46:HIS:HB3	6:RRR:49:THR:HG23	1.74	0.68
6:RRR:62:PHE:CE1	6:RRR:66:ILE:HD11	2.34	0.63
8:TTT:15:DT:H2"	8:TTT:16:DA:C8	2.34	0.62
8:TTT:-70:DC:H2'	8:TTT:-69:DA:C8	2.36	0.61

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	AAA	96/98 (98%)	96 (100%)	0	0	100	100
1	EEE	95/98 (97%)	95 (100%)	0	0	100	100
1	KKK	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
1	OOO	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
2	BBB	77/79 (98%)	77 (100%)	0	0	100	100
2	FFF	77/79 (98%)	75 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LLL	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
2	PPP	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
3	CCC	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
3	MMM	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
4	DDD	94/96 (98%)	90 (96%)	3 (3%)	1 (1%)	14	46
4	NNN	94/96 (98%)	91 (97%)	1 (1%)	2 (2%)	7	32
5	GGG	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
5	QQQ	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	47
6	HHH	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	14	46
6	RRR	95/97 (98%)	91 (96%)	2 (2%)	2 (2%)	7	32
All	All	1476/1510 (98%)	1433 (97%)	36 (2%)	7 (0%)	29	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	HHH	29	SER
6	RRR	29	SER
4	DDD	101	GLY
4	NNN	101	GLY
6	RRR	101	GLY

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	AAA	85/85 (100%)	84 (99%)	1 (1%)	71	83
1	EEE	85/85 (100%)	79 (93%)	6 (7%)	14	42
1	KKK	85/85 (100%)	84 (99%)	1 (1%)	71	83
1	OOO	85/85 (100%)	82 (96%)	3 (4%)	36	64
2	BBB	64/64 (100%)	61 (95%)	3 (5%)	26	57
2	FFF	64/64 (100%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	LLL	64/64 (100%)	62 (97%)	2 (3%)	40 67
2	PPP	64/64 (100%)	64 (100%)	0	100 100
3	CCC	83/83 (100%)	82 (99%)	1 (1%)	71 83
3	MMM	83/83 (100%)	82 (99%)	1 (1%)	71 83
4	DDD	82/82 (100%)	78 (95%)	4 (5%)	25 55
4	NNN	82/82 (100%)	77 (94%)	5 (6%)	18 49
5	GGG	82/82 (100%)	79 (96%)	3 (4%)	34 62
5	QQQ	82/82 (100%)	80 (98%)	2 (2%)	49 72
6	HHH	83/83 (100%)	79 (95%)	4 (5%)	25 56
6	RRR	83/83 (100%)	78 (94%)	5 (6%)	19 49
All	All	1256/1256 (100%)	1215 (97%)	41 (3%)	38 65

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	NNN	39	TYR
5	QQQ	81	ARG
4	NNN	60	ASN
1	OOO	65	LEU
6	RRR	31	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	AAA	98/98 (100%)	-0.16	0	100	100	45, 63, 93, 143	0
1	EEE	97/98 (98%)	-0.14	0	100	100	49, 67, 96, 136	0
1	KKK	98/98 (100%)	-0.17	1 (1%)	82	82	47, 65, 96, 137	0
1	OOO	97/98 (98%)	-0.24	0	100	100	42, 63, 108, 140	0
2	BBB	79/79 (100%)	-0.13	0	100	100	46, 59, 78, 108	0
2	FFF	79/79 (100%)	-0.32	0	100	100	49, 64, 83, 119	0
2	LLL	79/79 (100%)	-0.23	0	100	100	47, 62, 82, 96	0
2	PPP	79/79 (100%)	-0.27	0	100	100	45, 60, 87, 101	0
3	CCC	105/105 (100%)	-0.06	3 (2%)	51	50	54, 71, 103, 118	0
3	MMM	105/105 (100%)	-0.12	2 (1%)	66	64	45, 63, 97, 138	0
4	DDD	96/96 (100%)	-0.03	2 (2%)	63	61	52, 72, 114, 168	0
4	NNN	96/96 (100%)	-0.01	1 (1%)	82	82	48, 73, 114, 141	0
5	GGG	103/103 (100%)	-0.03	1 (0%)	82	82	48, 68, 95, 111	0
5	QQQ	103/103 (100%)	-0.19	1 (0%)	82	82	58, 78, 105, 123	0
6	HHH	97/97 (100%)	0.08	2 (2%)	63	61	53, 74, 128, 165	0
6	RRR	97/97 (100%)	0.17	4 (4%)	37	34	57, 84, 136, 186	0
7	III	167/167 (100%)	-0.26	3 (1%)	68	65	60, 107, 181, 194	0
7	SSS	167/167 (100%)	-0.06	5 (2%)	50	48	53, 119, 178, 237	0
8	JJJ	167/167 (100%)	-0.22	1 (0%)	89	89	61, 110, 177, 203	0
8	TTT	167/167 (100%)	-0.08	3 (1%)	68	65	60, 116, 174, 250	0
All	All	2176/2178 (99%)	-0.12	29 (1%)	77	75	42, 77, 147, 250	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	RRR	26	ARG	7.1
3	MMM	14	ALA	5.8
6	HHH	26	ARG	5.4
6	HHH	122	LYS	4.1
5	QQQ	118	LYS	3.8

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, 95^{th} 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MN	SSS	101	1/1	0.47	0.12	114,114,114,114	0
9	MN	JJJ	102	1/1	0.70	0.08	123,123,123,123	0
9	MN	TTT	105	1/1	0.74	0.13	111,111,111,111	0
9	MN	TTT	106	1/1	0.74	0.15	102,102,102,102	0
9	MN	III	106	1/1	0.79	0.07	113,113,113,113	0
9	MN	SSS	106	1/1	0.82	0.10	129,129,129,129	0
9	MN	TTT	102	1/1	0.82	0.18	107,107,107,107	0
9	MN	JJJ	101	1/1	0.84	0.09	121,121,121,121	0
9	MN	III	103	1/1	0.85	0.05	107,107,107,107	0
9	MN	III	101	1/1	0.87	0.15	87,87,87,87	0
9	MN	TTT	107	1/1	0.87	0.12	90,90,90,90	0
9	MN	III	104	1/1	0.89	0.13	127,127,127,127	0
9	MN	JJJ	104	1/1	0.90	0.06	70,70,70,70	0
9	MN	JJJ	107	1/1	0.90	0.10	81,81,81,81	0
9	MN	SSS	103	1/1	0.91	0.08	93,93,93,93	0
9	MN	III	109	1/1	0.91	0.23	118,118,118,118	0
9	MN	III	105	1/1	0.91	0.13	93,93,93,93	0
9	MN	JJJ	108	1/1	0.92	0.12	88,88,88,88	0
9	MN	III	110	1/1	0.92	0.13	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MN	III	102	1/1	0.93	0.15	99,99,99,99	0
9	MN	JJJ	106	1/1	0.93	0.17	99,99,99,99	0
9	MN	TTT	103	1/1	0.93	0.14	95,95,95,95	0
9	MN	JJJ	105	1/1	0.94	0.12	96,96,96,96	0
9	MN	SSS	102	1/1	0.94	0.04	96,96,96,96	0
9	MN	III	108	1/1	0.94	0.05	99,99,99,99	0
9	MN	TTT	104	1/1	0.95	0.12	95,95,95,95	0
9	MN	III	107	1/1	0.95	0.19	71,71,71,71	0
9	MN	JJJ	103	1/1	0.96	0.16	79,79,79,79	0
9	MN	III	111	1/1	0.96	0.14	83,83,83,83	0
9	MN	SSS	104	1/1	0.97	0.18	85,85,85,85	0
9	MN	TTT	101	1/1	0.97	0.12	82,82,82,82	0
9	MN	SSS	105	1/1	0.98	0.24	60,60,60,60	0
9	MN	TTT	108	1/1	0.99	0.20	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.