

Full wwPDB X-ray Structure Validation 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)
resolution	·	

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	:	2.35.1
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: $X\text{-}RAY \, DIFFRACTION$

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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
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%	6.
1	KKK	98	% 95%	5%
1	000	98	92% 79	% •
2	BBB	79	96%	•



Mol	Chain	Length	Quality of chain	
2	FFF	79	95%	5%
2	LLL	79	91%	9%
2	PPP	79	99%	·
3	CCC	105	3% 91%	9%
3	MMM	105	^{2%} 91%	9%
4	DDD	96	^{2%} 85%	15%
4	NNN	96	% • 86%	12% •
5	GGG	103	.% 94%	5%•
5	QQQ	103	% 94%	5%•
6	HHH	97	2% 9 0%	8% •
6	RRR	97	4% 86%	13% •
7	III	167	2% 86 %	14%
7	SSS	167	3% 86%	14%
8	JJJ	167	% • 84%	15% •
8	TTT	167	2% 89%	11%



$8 \mathrm{QKT}$

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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1		08	Total	С	Ν	0	S	0	0	0
1	AAA	90	807	508	156	139	4	0	0	0
1	FFF	07	Total	С	Ν	0	S	0	0	0
1	בוכוכו	91	801	505	155	137	4	0	0	0
1	KKK	08	Total	С	Ν	0	S	0	0	0
1	ININ	90	807	508	156	139	4	0	0	0
1	000	07	Total	С	Ν	0	S	0	0	0
1	000	91	801	505	155	137	4	0	0	0

• Molecule 1 is a protein called Histone H3.1.

• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	BBB	70	Total	С	Ν	0	S	0	0	0
	DDD	19	627	395	121	110	1	0	0	0
0		70	Total	С	Ν	0	S	0	0	0
	ГГГ	19	627	395	121	110	1	0	0	0
0	ттт	70	Total	С	Ν	0	S	0	0	0
		19	627	395	121	110	1	0	0	0
0	DDD	70	Total	С	Ν	0	S	0	0	0
		19	627	395	121	110	1	0		U

• Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
2	CCC	105	Total	С	Ν	Ο	0	0	0
3	000	105	810	511	158	141	0	0	0
2	ммл	105	Total	С	Ν	Ο	0	0	0
3 M		105	810	511	158	141	0	0	0

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



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	מממ	06	Total	С	Ν	0	S	0	0	0
4 DDD	30	756	474	140	140	2	0	0	0	
4	NNN	06	Total	С	Ν	0	S	0	0	0
4	INININ	90	756	474	140	140	2	0	0	0

• Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
5	CCC	103	Total	С	Ν	Ο	0	0	0
9 666	105	796	502	155	139	0	0	0	
F	000	102	Total	С	Ν	0	0	0	0
5	$5 \qquad QQQ$	105	796	502	155	139	0	0	U

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	HHH	97	Total 766	C 480	N 142	0 142	${S \over 2}$	0	0	0
6	RRR	97	Total 766	C 480	N 142	0 142	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

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

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

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

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

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

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



Continued from previous page...

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.

- Chain AAA: 95% • Molecule 1: Histone H3.1 Chain EEE: 91% 8% • Molecule 1: Histone H3.1 Chain KKK: 95% 5% • Molecule 1: Histone H3.1 Chain OOO: 92% 7% • • Molecule 2: Histone H4 Chain BBB: 96% • Molecule 2: Histone H4 Chain FFF: 95% 5%
- Molecule 1: Histone H3.1



D 24 175 175 175 175 175 175 175 175 175 175		
• Molecule 2: Histone H4		
Chain LLL:	91%	9%
D24 N25 126 L37 L37 A83 A83 A83 A83 A83 A83 A83 C102		
• Molecule 2: Histone H4		
Chain PPP:	99%	•
D24 245 3102		
• Molecule 3: Histone H2A		
Chain CCC:	91%	9%
A14 H31 P48 L53 L63 L63 L63 L63 L63 L63 L63 L97 L97 L97 K118 K118		
• Molecule 3: Histone H2A		
Chain MMM:	91%	9%
114 ● R42 ● R42 ■ R42 ■ R42 ■ R47 = R77 = R77 = R77 = R7 = L97 = L97 = L97 = L97 = L97 = K118		
• Molecule 4: Histone H2B type 1-	-J	
Chain DDD:	85%	15%
R26 R30 833 833 833 833 833 833 833 844 865 861 865 861 865 861 865 861 860 861 198 810 100 810 810 810 810 810 810 810 81	1119 8120 A121	
• Molecule 4: Histone H2B type 1-	J	
Chain NNN:	86%	12% •
<u> </u>		
Molecule 5: Historya H2A	N 4	
• Molecule 5: Histone H2A		











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	108.44Å 103.72Å 185.41Å	Depositor
a, b, c, α , β , γ	90.00° 93.59° 90.00°	Depositor
Bosolution(A)	48.66 - 3.26	Depositor
Resolution (A)	48.66 - 3.26	EDS
% Data completeness	89.1 (48.66-3.26)	Depositor
(in resolution range)	89.1 (48.66-3.26)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.56 (at 3.25 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P. P.	0.269 , 0.321	Depositor
n, n_{free}	0.271 , 0.320	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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

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).

Mal	Chain	Bond	lengths	Bond angles		
MOI	Unam	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	000	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.



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
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
8	JJJ	-83	DA	C5'-C4'-C3'	5.12	123.32	114.10
7	SSS	-4	DC	C1'-O4'-C4'	-5.11	104.99	110.10
7	SSS	-83	DA	C5'-C4'-C3'	5.04	123.16	114.10

All (8) bond angle outliers are listed below:

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	000	801	0	839	2	0
2	BBB	627	0	663	0	0
2	\mathbf{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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	SSS	3421	0	1880	15	0
8	JJJ	3420	0	1881	16	0
8	TTT	3420	0	1881	15	0
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.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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
8:TTT:-70:DC:H2"	8:TTT:-69:DA:O5'	2.01	0.60
8:JJJ:-68:DC:H2"	8:JJJ:-67:DA:C8	2.35	0.60
6:HHH:46:HIS:HB3	6:HHH:49:THR:CG2	2.33	0.58
6:HHH:46:HIS:HB3	6:HHH:49:THR:HG23	1.84	0.58
3:MMM:58:LEU:O	3:MMM:62:ILE:HG22	2.03	0.57
3:MMM:87:ILE:HD13	3:MMM:97:LEU:HD12	1.87	0.56
8:JJJ:71:DA:H4'	8:JJJ:72:DA:OP1	2.06	0.55
6:RRR:46:HIS:HB3	6:RRR:49:THR:CG2	2.36	0.55
4:NNN:69:ARG:HB3	4:NNN:98:LEU:HD21	1.89	0.55
7:SSS:34:DC:H2"	7:SSS:35:DT:OP2	2.07	0.55
8:TTT:7:DC:H2'	8:TTT:8:DG:C8	2.41	0.55
7:SSS:-49:DG:H1'	7:SSS:-48:DC:C6	2.44	0.52
3:CCC:87:ILE:HD13	3:CCC:97:LEU:HD12	1.91	0.52
5:GGG:29:ARG:NH2	6:HHH:33:SER:O	2.43	0.52
1:KKK:73:GLU:OE1	2:LLL:25:ASN:HB2	2.10	0.52
7:III:49:DC:H2'	7:III:50:DG:C8	2.45	0.51
8:TTT:49:DC:H2'	8:TTT:50:DG:C8	2.46	0.51
3:MMM:62:ILE:CD1	3:MMM:87:ILE:HD11	2.41	0.51
8:TTT:-72:DT:H2"	8:TTT:-71:DT:OP1	2.10	0.50
5:GGG:102:ILE:HG23	6:HHH:58:ILE:HD13	1.91	0.50
7:III:21:DG:H2"	7:III:22:DT:OP2	2.12	0.50



A 4 amo 1	A + a == 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:SSS:70:DG:H2"	7:SSS:71:DA:OP2	2.12	0.49
8:JJJ:-69:DA:C2'	8:JJJ:-68:DC:O5'	2.59	0.49
4:DDD:104:ALA:O	4:DDD:108:VAL:HG23	2.11	0.49
1:AAA:110:CYS:SG	1:AAA:126:LEU:HD23	2.52	0.49
7:SSS:54:DT:H2"	7:SSS:55:DC:O5'	2.13	0.48
7:III:61:DC:H2"	7:III:62:DG:C8	2.48	0.48
8:JJJ:71:DA:H1'	8:JJJ:72:DA:O4'	2.13	0.48
5:QQQ:29:ARG:NH2	6:RRR:33:SER:O	2.47	0.48
7:SSS:70:DG:N2	8:TTT:-69:DA:C2	2.82	0.47
8:JJJ:-3:DG:C6	8:JJJ:-2:DG:C6	3.03	0.47
1:000:79:LYS:HB3	1:000:82:LEU:HD11	1.97	0.47
4:DDD:62:PHE:CE1	4:DDD:66:ILE:HD11	2.50	0.46
1:000:97:GLU:0	1:000:101:VAL:HG23	2.15	0.46
7:III:64:DG:H2"	7:III:65:DA:C8	2.51	0.46
7:III:-70:DC:H2"	7:III:-69:DA:C8	2.51	0.46
1:EEE:110:CYS:SG	1:EEE:126:LEU:HD23	2.55	0.46
7:SSS:68:DG:C2	8:TTT:-67:DA:C2	3.03	0.46
2:FFF:75:HIS:CD2	6:HHH:77:LEU:HD12	2.50	0.46
3:MMM:42:ARG:NH1	4:NNN:85:THR:OG1	2.48	0.46
5:QQQ:58:LEU:HD13	6:RRR:66:ILE:HD13	1.98	0.46
5:QQQ:62:ILE:HD13	5:QQQ:93:LEU:HD13	1.97	0.46
8:JJJ:63:DG:H2"	8:JJJ:64:DG:C8	2.51	0.45
3:MMM:102:ILE:HG23	4:NNN:58:ILE:HD13	1.99	0.45
3:CCC:58:LEU:O	3:CCC:62:ILE:HG22	2.16	0.45
7:III:34:DC:H2"	7:III:35:DT:OP2	2.16	0.45
7:III:-55:DG:C2	7:III:-54:DA:C2	3.04	0.45
3:MMM:62:ILE:HD12	3:MMM:87:ILE:HD11	1.99	0.45
7:SSS:-45:DA:C2	8:TTT:46:DG:N2	2.85	0.45
7:III:-49:DG:H1'	7:III:-48:DC:C6	2.52	0.44
7:III:-6:DT:H2"	7:III:-5:DA:C8	2.52	0.44
8:JJJ:-68:DC:H2"	8:JJJ:-67:DA:H8	1.80	0.44
7:SSS:-40:DG:H2"	7:SSS:-39:DT:OP2	2.16	0.44
3:MMM:77:ARG:NE	7:SSS:-54:DA:H4'	2.32	0.44
1:AAA:65:LEU:HB3	1:AAA:66:PRO:HD3	1.99	0.44
7:SSS:66:DT:H4'	7:SSS:67:DT:OP1	2.16	0.44
8:TTT:-70:DC:H2"	8:TTT:-69:DA:C5'	2.48	0.44
4:NNN:62:PHE:CE1	4:NNN:66:ILE:HD11	2.53	0.43
3:CCC:102:ILE:HG23	4:DDD:58:ILE:HD13	1.99	0.43
7:III:-72:DT:H2'	7:III:-71:DT:H72	2.00	0.43
8:JJJ:-35:DA:C5	8:JJJ:-34:DG:C6	3.06	0.43
8:TTT:-63:DC:H2"	8:TTT:-62:DC:C6	2.54	0.43



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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:GGG:85:LEU:HD23	5:GGG:108:LEU:HD23	2.01	0.43
7:III:-4:DC:H2"	7:III:-3:DG:C8	2.52	0.43
8:TTT:82:DA:H2"	8:TTT:83:DT:OP2	2.17	0.43
2:FFF:68:ASP:OD2	2:FFF:92:ARG:NH1	2.52	0.43
1:KKK:65:LEU:HB3	1:KKK:66:PRO:HD3	2.01	0.43
8:TTT:-64:DC:H2"	8:TTT:-63:DC:OP2	2.19	0.43
8:JJJ:15:DT:H2"	8:JJJ:16:DA:C8	2.53	0.43
3:CCC:63:LEU:HD11	4:DDD:38:VAL:HG13	2.01	0.42
4:DDD:33:SER:OG	4:DDD:34:TYR:N	2.52	0.42
8:JJJ:43:DA:H2"	8:JJJ:44:DT:OP2	2.20	0.42
8:JJJ:49:DC:H2'	8:JJJ:50:DG:C8	2.54	0.42
2:PPP:45:ARG:CZ	7:SSS:7:DC:H4'	2.49	0.42
6:RRR:69:ARG:HB3	6:RRR:98:LEU:HD21	2.02	0.42
7:SSS:-50:DC:H2"	7:SSS:-49:DG:C8	2.55	0.42
8:JJJ:-38:DC:H2"	8:JJJ:-37:DG:OP2	2.18	0.42
3:CCC:58:LEU:HD13	4:DDD:66:ILE:HD13	2.01	0.42
2:FFF:45:ARG:CZ	8:JJJ:-4:DC:H4'	2.50	0.42
1:AAA:56:LYS:HE3	1:AAA:56:LYS:HA	2.00	0.42
3:MMM:26:PRO:HG3	4:NNN:37:TYR:CZ	2.55	0.42
6:HHH:83:ARG:NH1	6:HHH:85:THR:O	2.53	0.42
7:SSS:-20:DC:H2"	7:SSS:-19:DG:C8	2.54	0.42
8:JJJ:65:DA:C2	8:JJJ:66:DT:C2	3.07	0.41
4:DDD:99:LEU:HB2	4:DDD:104:ALA:HB2	2.01	0.41
1:KKK:61:LEU:HD12	2:LLL:37:LEU:HD23	2.01	0.41
2:LLL:46:ILE:O	8:TTT:7:DC:H5'	2.21	0.41
2:LLL:83:ALA:O	2:LLL:87:VAL:HG23	2.21	0.41
7:SSS:28:DA:C6	7:SSS:29:DG:C6	3.09	0.41
3:CCC:31:HIS:CD2	3:CCC:48:PRO:HG3	2.57	0.40
7:III:20:DG:H4'	7:III:21:DG:OP1	2.20	0.40
8:JJJ:77:DA:C2	8:JJJ:78:DA:C4	3.09	0.40
7:SSS:71:DA:N6	8:TTT:-72:DT:O4	2.54	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.



Mol	Chain	Analysed	Favoured Allowed		Outliers	Perce	entiles
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	000	95/98~(97%)	94 (99%)	1 (1%)	0	100	100
2	BBB	77/79~(98%)	77~(100%)	0	0	100	100
2	\mathbf{FFF}	77/79~(98%)	75~(97%)	2(3%)	0	100	100
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	$9\overline{5}/97~(98\%)$	87 (92%)	7 (7%)	1 (1%)	14	46
6	RRR	95/97~(98%)	91 (96%)	2 (2%)	2(2%)	7	32
All	All	$147\overline{6/1510} \ (98\%)$	1433 (97%)	36 (2%)	7~(0%)	29	62

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

All (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	QQQ	74	LYS
4	NNN	27	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed Rotameric Outliers Per		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	000	85/85~(100%)	82~(96%)	3~(4%)	36 64
2	BBB	64/64~(100%)	61~(95%)	3~(5%)	26 57
2	\mathbf{FFF}	64/64~(100%)	64 (100%)	0	100 100
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

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

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

Mol	Chain	Res	Type
1	AAA	56	LYS
2	BBB	26	ILE
2	BBB	74	GLU
2	BBB	93	GLN
3	CCC	81	ARG
4	DDD	26	ARG
4	DDD	30	ARG
4	DDD	60	ASN
4	DDD	98	LEU
1	EEE	48	LEU
1	EEE	59	GLU
1	EEE	65	LEU
1	EEE	80	THR
1	EEE	118	THR



Mol	Chain	Res	Type
1	EEE	129	ARG
5	GGG	29	ARG
5	GGG	74	LYS
5	GGG	81	ARG
6	HHH	26	ARG
6	HHH	31	LYS
6	HHH	49	THR
6	HHH	77	LEU
1	KKK	56	LYS
2	LLL	26	ILE
2	LLL	74	GLU
3	MMM	81	ARG
4	NNN	26	ARG
4	NNN	30	ARG
4	NNN	39	TYR
4	NNN	60	ASN
4	NNN	98	LEU
1	000	48	LEU
1	000	65	LEU
1	000	129	ARG
5	QQQ	29	ARG
5	QQQ	81	ARG
6	RRR	26	ARG
6	RRR	31	LYS
6	RRR	39	TYR
6	RRR	49	THR
6	RRR	77	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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 (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, 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>	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	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	000	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	$1\overline{67/167}\ (100\%)$	-0.08	3 (1%) 68 65	60, 116, 174, 250	0
All	All	$217\overline{6/2178}$ (99%)	-0.12	29 (1%) 77 75	42, 77, 147, 250	0

All (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
8	JJJ	-83	DA	3.7
3	CCC	118	LYS	3.6
7	SSS	-83	DA	3.3
6	RRR	122	LYS	3.2
5	GGG	118	LYS	3.1
3	CCC	71	ARG	3.0
8	TTT	-81	DC	2.9
8	TTT	83	DT	2.9
8	TTT	-83	DA	2.9
4	DDD	26	ARG	2.9
3	CCC	14	ALA	2.8
7	SSS	82	DA	2.6
7	SSS	81	DG	2.6
6	RRR	27	LYS	2.5
7	III	82	DA	2.4
6	RRR	121	ALA	2.3
7	SSS	-82	DT	2.3
1	KKK	38	PRO	2.3
7	SSS	83	DT	2.3
7	III	83	DT	2.2
7	III	81	DG	2.2
3	MMM	20	ARG	2.2
4	DDD	119	THR	2.1
4	NNN	121	ALA	2.1

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,



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	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
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

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.

6.5 Other polymers (i)

There are no such residues in this entry.

