



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:00 AM UTC

PDB ID : 8QKT / pdb_00008qkt
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

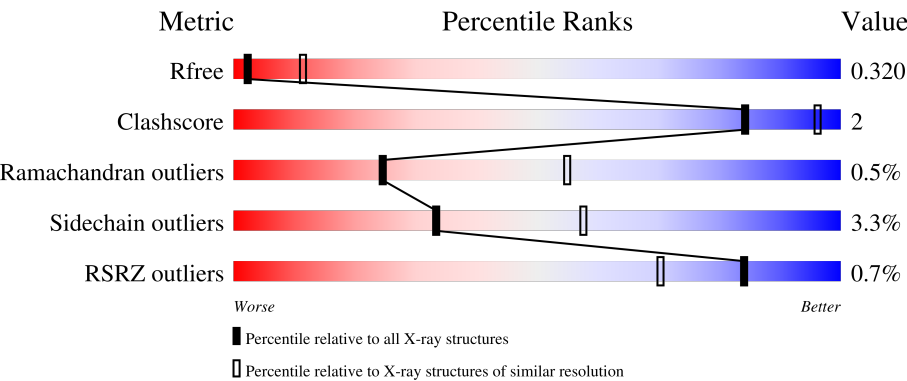
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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.



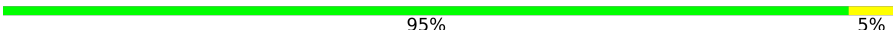
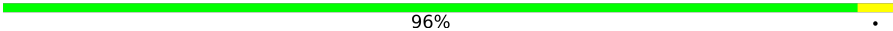
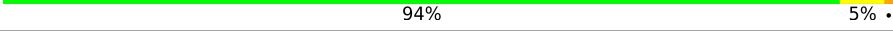
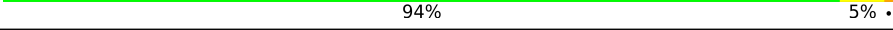
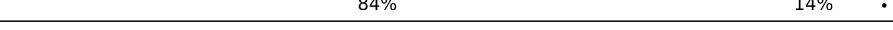
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	AAA	98	95%
1	EEE	98	2% 89% 10%
1	KKK	98	% 95% 5%
1	OOO	98	% 90% 9%
2	BBB	79	% 96%

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Mol	Chain	Length	Quality of chain
2	FFF	79	 95% 5%
2	LLL	79	 91% 9%
2	PPP	79	 96% .
3	CCC	105	 % 91% 9%
3	MMM	105	 % 91% 9%
4	DDD	96	 84% 16%
4	NNN	96	 % 85% 12% .
5	GGG	103	 % 94% 5% .
5	QQQ	103	 % 94% 5% .
6	HHH	97	 % 90% 8% .
6	RRR	97	 2% 86% 11% .
7	III	167	 % 83% 15% .
7	SSS	167	 % 85% 14% .
8	JJJ	167	 84% 14% .
8	TTT	167	 86% 14%

2 Entry composition

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	S	0	0	0
			796	502	155	139				
5	QQQ	103	Total	C	N	O	S	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 (CCD ID: MN) (formula: Mn).

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

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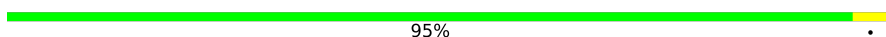
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	JJJ	8	Total 8	Mn 8	0	0
9	SSS	6	Total 6	Mn 6	0	0
9	TTT	8	Total 8	Mn 8	0	0

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:  95% ..

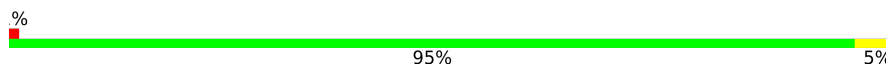


- Molecule 1: Histone H3.1

Chain EEE:  89% 10% .

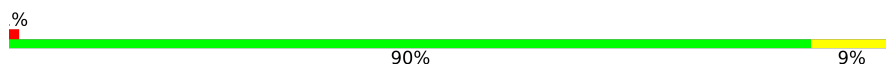


- Molecule 1: Histone H3.1

Chain KKK:  95% 5%

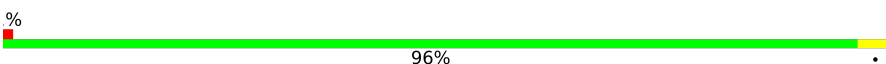


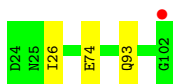
- Molecule 1: Histone H3.1

Chain OOO:  90% 9% .

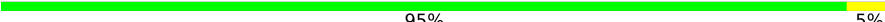


- Molecule 2: Histone H4

Chain BBB:  96% .



- Molecule 2: Histone H4

Chain FFF:  95% 5%

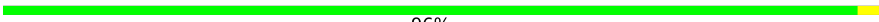


- Molecule 2: Histone H4

Chain LLL:  91% 9%



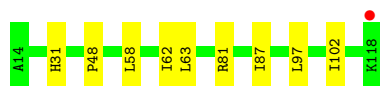
- Molecule 2: Histone H4

Chain PPP:  96% .



- Molecule 3: Histone H2A

Chain CCC:  % 91% 9%



- Molecule 3: Histone H2A

Chain MMM:  % 91% 9%



- Molecule 4: Histone H2B type 1-J

Chain DDD:  84% 16%

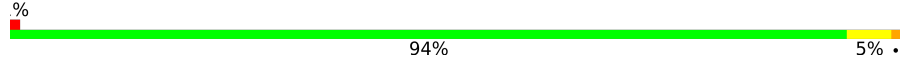


- Molecule 4: Histone H2B type 1-J

Chain NNN:  % 85% 12% .

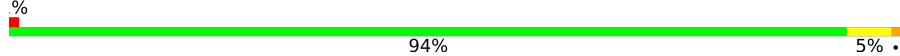


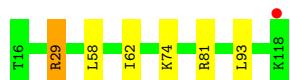
- Molecule 5: Histone H2A

Chain GGG:  94% 5% .

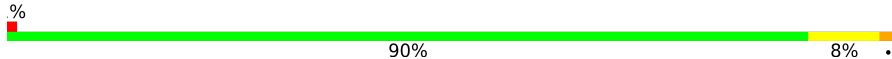


- Molecule 5: Histone H2A

Chain QQQ:  94% 5% .



- Molecule 6: Histone H2B type 1-J

Chain HHH:  90% 8% .



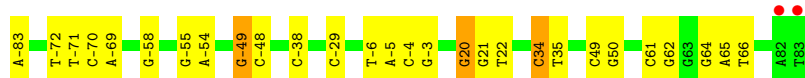
- Molecule 6: Histone H2B type 1-J

Chain RRR:  86% 11% .



- Molecule 7: DNA (167-MER)

Chain III:  83% 15% .



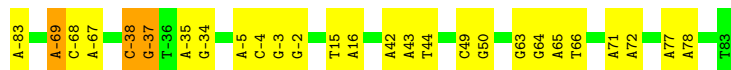
- Molecule 7: DNA (167-MER)

Chain SSS:  85% 14% .



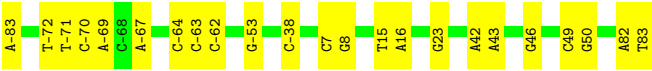
- Molecule 8: DNA (167-MER)

Chain JJJ:  84% 14% .



● Molecule 8: DNA (167-MER)

Chain TTT: 86% 14%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.25 , 18.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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.

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	0.45	0/819	0.76	0/1097
1	EEE	0.43	0/813	0.75	0/1090
1	KKK	0.43	0/819	0.76	0/1097
1	OOO	0.43	0/813	0.75	0/1090
2	BBB	0.45	0/634	0.77	0/848
2	FFF	0.47	0/634	0.78	0/848
2	LLL	0.49	0/634	0.75	0/848
2	PPP	0.45	0/634	0.75	0/848
3	CCC	0.43	0/820	0.74	0/1107
3	MMM	0.43	0/820	0.74	0/1107
4	DDD	0.45	0/767	0.80	0/1029
4	NNN	0.47	0/767	0.78	0/1029
5	GGG	0.43	0/806	0.74	0/1089
5	QQQ	0.41	0/806	0.76	0/1089
6	HHH	0.44	0/777	0.78	0/1040
6	RRR	0.48	0/777	0.84	1/1040 (0.1%)
7	III	0.32	0/3838	0.72	9/5922 (0.2%)
7	SSS	0.32	0/3838	0.71	6/5922 (0.1%)
8	JJJ	0.32	0/3836	0.74	7/5919 (0.1%)
8	TTT	0.32	0/3836	0.72	6/5919 (0.1%)
All	All	0.38	0/27488	0.74	29/39978 (0.1%)

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.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	III	20	DG	C4'-C3'-O3'	7.07	120.61	110.00
7	SSS	-83	DA	C5'-C4'-O4'	6.66	119.39	109.40
8	TTT	-38	DC	C2'-C3'-O3'	6.48	121.22	111.50
7	SSS	34	DC	C2'-C3'-O3'	6.44	121.17	111.50
7	III	34	DC	C2'-C3'-O3'	6.39	121.09	111.50
8	JJJ	-69	DA	C2'-C3'-O3'	6.29	120.93	111.50
8	TTT	42	DA	C2'-C3'-O3'	6.24	120.87	111.50
7	SSS	20	DG	C4'-C3'-O3'	6.13	119.20	110.00
7	III	-83	DA	C5'-C4'-O4'	6.10	118.55	109.40
8	TTT	-83	DA	C5'-C4'-O4'	6.09	118.54	109.40
7	III	66	DT	C2'-C3'-O3'	-6.05	102.42	111.50
8	JJJ	-38	DC	C2'-C3'-O3'	6.02	120.53	111.50
8	JJJ	-5	DA	C2'-C3'-O3'	-5.96	102.56	111.50
8	JJJ	42	DA	C2'-C3'-O3'	5.91	120.37	111.50
7	III	-58	DG	C2'-C3'-O3'	5.82	120.23	111.50
8	TTT	-83	DA	C5'-C4'-C3'	5.71	123.47	114.90
8	JJJ	-83	DA	C5'-C4'-O4'	5.65	117.88	109.40
7	III	-83	DA	C5'-C4'-C3'	5.64	123.35	114.90
7	III	-29	DC	C2'-C3'-O3'	5.61	119.92	111.50
8	JJJ	-83	DA	C5'-C4'-C3'	5.61	123.32	114.90
7	SSS	-33	DA	C2'-C3'-O3'	5.53	119.79	111.50
6	RRR	27	LYS	N-CA-C	5.52	118.10	107.44
7	SSS	-83	DA	C5'-C4'-C3'	5.51	123.16	114.90
8	JJJ	-37	DG	C2'-C3'-O3'	-5.49	103.26	111.50
8	TTT	43	DA	C2'-C3'-O3'	5.46	119.69	111.50
8	TTT	23	DG	C2'-C3'-O3'	5.40	119.61	111.50
7	SSS	-38	DC	C2'-C3'-O3'	5.20	119.30	111.50
7	III	-49	DG	C2'-C3'-O3'	-5.08	103.88	111.50
7	III	-38	DC	C2'-C3'-O3'	5.03	119.04	111.50

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	2	0
1	KKK	807	0	844	3	0
1	OOO	801	0	839	3	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	2	0
3	CCC	810	0	866	6	0
3	MMM	810	0	866	8	0
4	DDD	756	0	784	8	0
4	NNN	756	0	784	6	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	7	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	16	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	104	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 (104) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OOO:79:LYS:HB3	1:OOO:82:LEU:HD11	1.97	0.47
4:DDD:62:PHE:CE1	4:DDD:66:ILE:HD11	2.50	0.46
1:OOO:97:GLU:O	1:OOO: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:RRR:39:TYR:OH	8:TTT:-53:DG:OP2	2.32	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
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
2:PPP:84:MET:HE1	2:PPP:102:GLY:CA	2.48	0.43
1:OOO:120:MET:O	1:OOO:121:PRO:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:PHE:CD2	4:DDD:67:PHE:C	2.98	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
1:EEE:60:LEU:HD13	1:EEE:93:GLN:CD	2.46	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
4:NNN:100:PRO:O	4:NNN:101:GLY:C	2.64	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.

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
2	LLL	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
2	PPP	77/79 (98%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	11	38
4	NNN	94/96 (98%)	91 (97%)	1 (1%)	2 (2%)	5	25
5	GGG	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
5	QQQ	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	12	40
6	HHH	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	38
6	RRR	95/97 (98%)	91 (96%)	2 (2%)	2 (2%)	5	25
All	All	1476/1510 (98%)	1433 (97%)	36 (2%)	7 (0%)	24	55

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 ⓘ

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%)	63	74
1	EEE	85/85 (100%)	79 (93%)	6 (7%)	13	39
1	KKK	85/85 (100%)	84 (99%)	1 (1%)	63	74
1	OOO	85/85 (100%)	82 (96%)	3 (4%)	32	56
2	BBB	64/64 (100%)	61 (95%)	3 (5%)	23	51
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%)	35	59
2	PPP	64/64 (100%)	64 (100%)	0	100	100
3	CCC	83/83 (100%)	82 (99%)	1 (1%)	63	74
3	MMM	83/83 (100%)	82 (99%)	1 (1%)	63	74
4	DDD	82/82 (100%)	78 (95%)	4 (5%)	22	50
4	NNN	82/82 (100%)	77 (94%)	5 (6%)	17	44
5	GGG	82/82 (100%)	79 (96%)	3 (4%)	30	55
5	QQQ	82/82 (100%)	80 (98%)	2 (2%)	43	64
6	HHH	83/83 (100%)	79 (95%)	4 (5%)	23	50
6	RRR	83/83 (100%)	78 (94%)	5 (6%)	17	44
All	All	1256/1256 (100%)	1215 (97%)	41 (3%)	33	57

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
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

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Mol	Chain	Res	Type
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	OOO	48	LEU
1	OOO	65	LEU
1	OOO	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 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 oligosaccharides 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

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 [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	AAA	98/98 (100%)	0.07	0 100 100	45, 63, 93, 143	0
1	EEE	97/98 (98%)	0.08	2 (2%) 63 44	49, 67, 96, 136	0
1	KKK	98/98 (100%)	0.02	1 (1%) 79 62	47, 65, 96, 137	0
1	OOO	97/98 (98%)	-0.03	1 (1%) 79 62	42, 63, 108, 140	0
2	BBB	79/79 (100%)	0.04	1 (1%) 75 56	46, 59, 78, 108	0
2	FFF	79/79 (100%)	-0.02	0 100 100	49, 64, 83, 119	0
2	LLL	79/79 (100%)	-0.01	0 100 100	47, 62, 82, 96	0
2	PPP	79/79 (100%)	-0.12	0 100 100	45, 60, 87, 101	0
3	CCC	105/105 (100%)	0.19	1 (0%) 79 62	54, 71, 103, 118	0
3	MMM	105/105 (100%)	0.08	1 (0%) 79 62	45, 63, 97, 138	0
4	DDD	96/96 (100%)	0.20	0 100 100	52, 72, 114, 168	0
4	NNN	96/96 (100%)	0.28	1 (1%) 79 62	48, 73, 114, 141	0
5	GGG	103/103 (100%)	0.10	1 (0%) 79 62	48, 68, 95, 111	0
5	QQQ	103/103 (100%)	0.26	1 (0%) 79 62	58, 78, 105, 123	0
6	HHH	97/97 (100%)	0.26	1 (1%) 79 62	53, 74, 128, 165	0
6	RRR	97/97 (100%)	0.47	2 (2%) 63 44	57, 84, 136, 186	0
7	III	167/167 (100%)	0.32	2 (1%) 76 58	60, 107, 181, 194	0
7	SSS	167/167 (100%)	0.39	1 (0%) 85 73	53, 119, 178, 237	0
8	JJJ	167/167 (100%)	0.30	0 100 100	61, 110, 177, 203	0
8	TTT	167/167 (100%)	0.40	0 100 100	60, 116, 174, 250	0
All	All	2176/2178 (99%)	0.19	16 (0%) 84 70	42, 77, 147, 250	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CCC	118	LYS	3.8
5	QQQ	118	LYS	3.7
6	RRR	27	LYS	3.3
2	BBB	102	GLY	3.1
1	EEE	38	PRO	2.6
4	NNN	31	LYS	2.6
7	III	82	DA	2.5
6	RRR	26	ARG	2.4
7	III	83	DT	2.3
6	HHH	68	GLU	2.2
1	OOO	38	PRO	2.2
3	MMM	118	LYS	2.1
1	EEE	134	ARG	2.1
1	KKK	135	ALA	2.1
7	SSS	-83	DA	2.0
5	GGG	114	VAL	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 oligosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MN	JJJ	101	1/1	0.75	0.12	121,121,121,121	0
9	MN	III	106	1/1	0.76	0.07	113,113,113,113	0
9	MN	SSS	106	1/1	0.79	0.09	129,129,129,129	0
9	MN	JJJ	106	1/1	0.82	0.09	99,99,99,99	0
9	MN	III	101	1/1	0.82	0.10	87,87,87,87	0
9	MN	III	102	1/1	0.83	0.09	99,99,99,99	0
9	MN	III	105	1/1	0.84	0.08	93,93,93,93	0
9	MN	III	104	1/1	0.86	0.08	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MN	TTT	102	1/1	0.86	0.09	107,107,107,107	0
9	MN	JJJ	102	1/1	0.87	0.05	123,123,123,123	0
9	MN	SSS	101	1/1	0.87	0.08	114,114,114,114	0
9	MN	III	103	1/1	0.88	0.07	107,107,107,107	0
9	MN	TTT	107	1/1	0.88	0.06	90,90,90,90	0
9	MN	JJJ	105	1/1	0.89	0.08	96,96,96,96	0
9	MN	III	111	1/1	0.89	0.05	83,83,83,83	0
9	MN	TTT	106	1/1	0.91	0.06	102,102,102,102	0
9	MN	III	108	1/1	0.91	0.06	99,99,99,99	0
9	MN	III	109	1/1	0.92	0.12	118,118,118,118	0
9	MN	SSS	104	1/1	0.92	0.06	85,85,85,85	0
9	MN	JJJ	108	1/1	0.92	0.07	88,88,88,88	0
9	MN	TTT	104	1/1	0.93	0.06	95,95,95,95	0
9	MN	TTT	105	1/1	0.93	0.06	111,111,111,111	0
9	MN	TTT	101	1/1	0.93	0.05	82,82,82,82	0
9	MN	JJJ	107	1/1	0.93	0.07	81,81,81,81	0
9	MN	SSS	105	1/1	0.94	0.11	60,60,60,60	0
9	MN	III	110	1/1	0.94	0.06	85,85,85,85	0
9	MN	SSS	103	1/1	0.94	0.04	93,93,93,93	0
9	MN	JJJ	103	1/1	0.94	0.07	79,79,79,79	0
9	MN	JJJ	104	1/1	0.96	0.04	70,70,70,70	0
9	MN	TTT	103	1/1	0.96	0.05	95,95,95,95	0
9	MN	TTT	108	1/1	0.96	0.06	47,47,47,47	0
9	MN	SSS	102	1/1	0.97	0.04	96,96,96,96	0
9	MN	III	107	1/1	0.98	0.09	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.