



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 07:36 PM UTC

PDB ID : 8Q3M / pdb_00008q3m
Title : Structure of Nucleosome Core with a Bound Kaposi Sarcoma Associated Herpesvirus LANA Peptide Having a Methionine to Ornithine Substitution
Authors : De Falco, L.; Batchelor, L.K.; Dyson, P.J.; Davey, C.A.
Deposited on : 2023-08-04
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

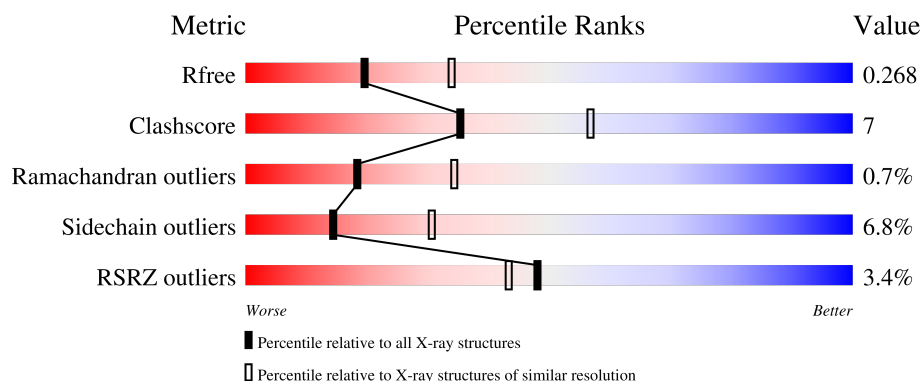
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



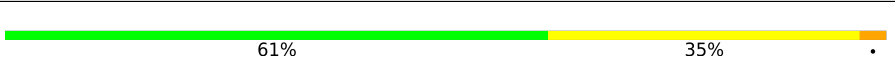
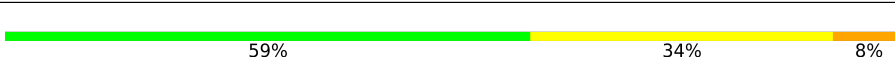
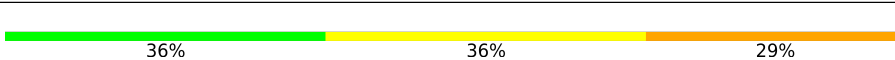
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	3% 82% 17% .
1	EEE	98	3% 88% 12%
2	BBB	87	6% 84% 9% 6% .
2	FFF	87	86% 11% ..
3	CCC	107	4% 76% 19% 6%

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Mol	Chain	Length	Quality of chain
3	GGG	107	
4	DDD	95	
4	HHH	95	
5	III	145	
6	JJJ	145	
7	MMM	14	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12155 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	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

- Molecule 2 is a protein called Histone H4.

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

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	107	Total	C	N	O	0	0	0
			828	523	162	143			
3	GGG	107	Total	C	N	O	0	0	0
			828	523	162	143			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	95	Total	C	N	O	S	0	0	0
			745	467	136	140	2			
4	HHH	95	Total	C	N	O	S	0	0	0
			745	467	136	140	2			

- Molecule 5 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	III	145	Total	C	N	O	P	0	0	0
			2970	1421	538	867	144			

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	JJJ	145	Total	C	N	O	P	0	0	0
			2969	1421	535	869	144			

- Molecule 7 is a protein called Kaposi sarcoma associated herpesvirus LANA peptide with a methionine to ornithine substitution.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	MMM	14	Total	C	N	O	0	0	0
			99	58	24	17			

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

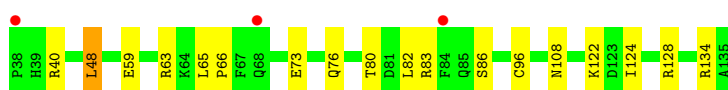
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	EEE	1	Total	Mg	0	0
			1	1		

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: 



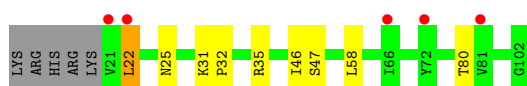
- Molecule 1: Histone H3.1

Chain EEE: 



- Molecule 2: Histone H4

Chain BBB: 



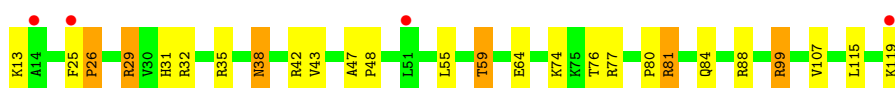
- Molecule 2: Histone H4

Chain FFF: 

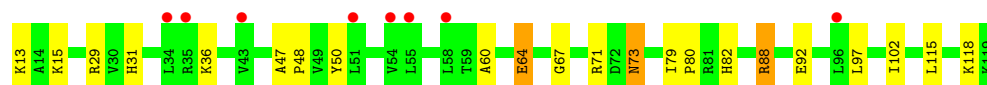
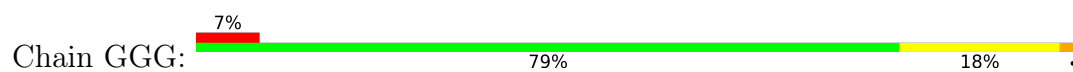


- Molecule 3: Histone H2A type 1-B/E

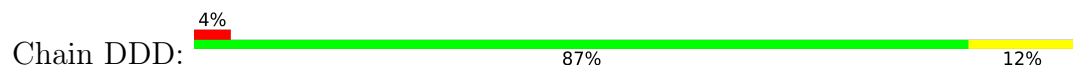
Chain CCC: 



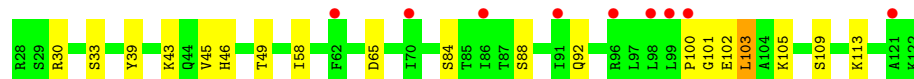
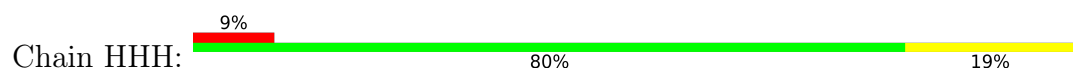
- Molecule 3: Histone H2A type 1-B/E



- Molecule 4: Histone H2B type 1-K



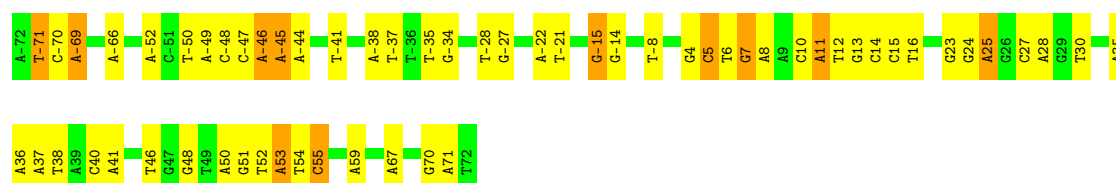
- Molecule 4: Histone H2B type 1-K



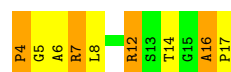
- Molecule 5: DNA (145-MER)



- Molecule 6: DNA (145-MER)



- Molecule 7: Kaposi sarcoma associated herpesvirus LANA peptide with a methionine to ornithine substitution



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.71Å 109.88Å 184.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 2.50 49.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.17-2.50) 99.8 (49.17-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.218 , 0.268 0.220 , 0.268	Depositor DCC
R_{free} test set	1513 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12155	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: MG, ORN

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	1.02	0/819	1.49	0/1097
1	EEE	1.05	1/819 (0.1%)	1.51	2/1097 (0.2%)
2	BBB	1.00	0/660	1.53	0/883
2	FFF	1.06	0/711	1.53	1/948 (0.1%)
3	CCC	1.10	1/838 (0.1%)	1.57	4/1129 (0.4%)
3	GGG	1.05	0/838	1.50	0/1129
4	DDD	1.07	0/756	1.59	0/1014
4	HHH	0.99	0/756	1.56	2/1014 (0.2%)
5	III	0.46	0/3332	1.01	20/5141 (0.4%)
6	JJJ	0.45	0/3330	0.93	15/5138 (0.3%)
7	MMM	0.95	0/91	1.43	0/118
All	All	0.80	2/12950 (0.0%)	1.26	44/18708 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	26	PRO	C-O	-6.14	1.19	1.24
1	EEE	57	SER	C-O	5.20	1.30	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	JJJ	-45	DA	C2'-C3'-O3'	-9.68	96.98	111.50
5	III	-49	DA	N9-C1'-C2'	9.53	127.79	113.50
5	III	-49	DA	C4-N9-C1'	-9.22	113.22	127.05
5	III	-49	DA	C8-N9-C1'	9.13	140.75	127.05
5	III	-40	DG	N9-C1'-C2'	9.05	127.07	113.50
5	III	-67	DT	C2'-C3'-O3'	-8.17	99.25	111.50
5	III	66	DT	C2'-C3'-O3'	8.08	123.62	111.50
5	III	-65	DT	C2'-C3'-O3'	7.04	122.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	III	-28	DT	C2'-C3'-O3'	-6.56	101.66	111.50
6	JJJ	5	DC	C4'-C3'-O3'	6.45	119.68	110.00
5	III	-69	DA	C2'-C3'-O3'	-6.23	102.16	111.50
5	III	35	DA	C4'-C3'-O3'	6.12	119.19	110.00
2	FFF	92	ARG	CB-CA-C	-5.97	100.52	110.68
5	III	-49	DA	C1'-O4'-C4'	-5.87	100.89	109.70
6	JJJ	25	DA	C2'-C3'-O3'	5.76	120.14	111.50
6	JJJ	55	DC	C2'-C3'-O3'	5.76	120.14	111.50
5	III	66	DT	C4'-C3'-O3'	-5.66	101.52	110.00
6	JJJ	53	DA	C2'-C3'-O3'	-5.58	103.13	111.50
6	JJJ	-46	DA	C2'-C3'-O3'	5.52	119.78	111.50
5	III	-26	DC	C2'-C3'-O3'	-5.52	103.22	111.50
6	JJJ	-45	DA	C4'-C3'-O3'	5.48	118.22	110.00
5	III	20	DG	C2'-C3'-O3'	5.45	119.67	111.50
6	JJJ	30	DT	C2'-C3'-O3'	-5.37	103.44	111.50
6	JJJ	-15	DG	C2'-C3'-O3'	5.36	119.54	111.50
4	HHH	100	PRO	CB-CA-C	-5.32	105.02	111.46
3	CCC	43	VAL	CA-C-N	5.29	126.21	120.44
3	CCC	43	VAL	C-N-CA	5.29	126.21	120.44
3	CCC	64	GLU	CB-CG-CD	5.29	121.58	112.60
5	III	-40	DG	C4-N9-C1'	-5.26	119.11	127.00
5	III	16	DT	C4'-C3'-O3'	-5.25	102.13	110.00
5	III	71	DA	C4'-C3'-O3'	5.19	117.78	110.00
5	III	-45	DA	C2'-C3'-O3'	5.17	119.26	111.50
3	CCC	84	GLN	CB-CA-C	5.14	119.03	110.90
5	III	44	DT	C2'-C3'-O3'	5.12	119.18	111.50
6	JJJ	-8	DT	C2'-C3'-O3'	5.11	119.17	111.50
6	JJJ	-71	DT	C4'-C3'-O3'	5.09	117.64	110.00
1	EEE	124	ILE	N-CA-C	-5.08	105.54	110.42
6	JJJ	4	DG	C2'-C3'-O3'	-5.05	103.92	111.50
1	EEE	75	ALA	N-CA-C	-5.05	105.85	111.36
6	JJJ	-69	DA	C2'-C3'-O3'	-5.05	103.92	111.50
5	III	9	DA	C2'-C3'-O3'	5.04	119.06	111.50
6	JJJ	11	DA	C2'-C3'-O3'	5.03	119.04	111.50
4	HHH	65	ASP	N-CA-C	-5.02	105.46	111.03
6	JJJ	7	DG	P-O5'-C5'	-5.01	112.48	120.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	807	0	844	15	0
1	EEE	807	0	844	5	0
2	BBB	653	0	696	9	0
2	FFF	703	0	755	7	0
3	CCC	828	0	892	18	0
3	GGG	828	0	892	17	0
4	DDD	745	0	769	10	0
4	HHH	745	0	769	9	0
5	III	2970	0	1640	44	0
6	JJJ	2969	0	1641	59	0
7	MMM	99	0	104	15	0
8	EEE	1	0	0	0	0
All	All	12155	0	9846	162	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 7.

All (162) 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)
4:HHH:45:VAL:O	7:MMM:12:ARG:NH1	2.11	0.84
6:JJJ:54:DT:H2''	6:JJJ:55:DC:OP2	1.82	0.79
6:JJJ:-49:DA:H4'	6:JJJ:-48:DC:OP1	1.85	0.76
1:AAA:96:CYS:SG	2:BBB:58:LEU:CD1	2.74	0.76
7:MMM:7:ARG:HH21	7:MMM:7:ARG:HB2	1.54	0.72
6:JJJ:-22:DA:H2''	6:JJJ:-21:DT:O5'	1.88	0.72
1:AAA:96:CYS:SG	2:BBB:58:LEU:HD13	2.31	0.70
5:III:64:DG:H1'	5:III:65:DA:C8	2.28	0.69
7:MMM:16:ALA:CB	7:MMM:17:PRO:CD	2.69	0.69
5:III:-50:DT:C4	5:III:-49:DA:N6	2.63	0.67
7:MMM:16:ALA:HB3	7:MMM:17:PRO:HD2	1.77	0.65
6:JJJ:-15:DG:H2''	6:JJJ:-14:DG:OP2	1.96	0.65
5:III:53:DA:C2	6:JJJ:-52:DA:C2	2.84	0.65
5:III:67:DA:C2	6:JJJ:-66:DA:C2	2.84	0.65
6:JJJ:24:DG:H4'	6:JJJ:25:DA:OP1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:JJJ:53:DA:C2	6:JJJ:54:DT:C2	2.87	0.62
6:JJJ:50:DA:H2''	6:JJJ:51:DG:OP2	1.99	0.62
6:JJJ:-28:DT:H3'	6:JJJ:-27:DG:H5''	1.83	0.61
2:FFF:17:ARG:O	2:FFF:18:HIS:O	2.19	0.61
5:III:-66:DA:C2	6:JJJ:67:DA:C2	2.88	0.60
4:DDD:77:LEU:HD21	4:DDD:93:THR:HB	1.82	0.60
5:III:-28:DT:H4'	5:III:-27:DG:OP1	2.01	0.60
1:EEE:49:ARG:HH11	1:EEE:49:ARG:HG3	1.66	0.60
5:III:-27:DG:H4'	5:III:-26:DC:OP1	2.03	0.59
4:DDD:28:ARG:CB	6:JJJ:50:DA:OP1	2.52	0.58
2:BBB:35:ARG:NH2	6:JJJ:8:DA:OP2	2.34	0.58
5:III:-39:DT:H2''	5:III:-38:DA:H8	1.69	0.58
6:JJJ:-28:DT:C3'	6:JJJ:-27:DG:H5''	2.34	0.58
3:GGG:64:GLU:HB2	7:MMM:8:LEU:HD23	1.86	0.57
5:III:-52:DA:C2	6:JJJ:53:DA:C2	2.92	0.57
3:GGG:102:ILE:HG23	4:HHH:58:ILE:HD13	1.85	0.57
3:CCC:55:LEU:O	3:CCC:59:THR:CG2	2.52	0.57
3:GGG:29:ARG:NH1	4:HHH:33:SER:O	2.38	0.56
7:MMM:16:ALA:HB1	7:MMM:17:PRO:HD3	1.87	0.55
5:III:-52:DA:C2	6:JJJ:53:DA:N1	2.74	0.55
6:JJJ:13:DG:H4'	6:JJJ:14:DC:OP1	2.06	0.55
1:AAA:76:GLN:NE2	1:AAA:80:THR:HG22	2.23	0.54
3:GGG:67:GLY:HA3	4:HHH:46:HIS:CD2	2.42	0.54
7:MMM:16:ALA:HB1	7:MMM:17:PRO:CD	2.38	0.54
6:JJJ:-35:DT:H2''	6:JJJ:-34:DG:C8	2.43	0.54
7:MMM:7:ARG:HB2	7:MMM:7:ARG:NH2	2.23	0.54
3:CCC:99:ARG:HH11	3:CCC:99:ARG:HG3	1.73	0.54
5:III:-61:DC:H2''	5:III:-60:DC:O5'	2.08	0.54
7:MMM:16:ALA:CB	7:MMM:17:PRO:HD2	2.37	0.53
3:CCC:25:PHE:CZ	3:CCC:59:THR:HG21	2.43	0.53
3:GGG:88:ARG:NH2	3:GGG:97:LEU:O	2.42	0.53
3:CCC:32:ARG:HH22	4:DDD:32:GLU:CD	2.15	0.53
5:III:-51:DC:H5''	5:III:-51:DC:H6	1.73	0.53
3:GGG:64:GLU:HB2	7:MMM:8:LEU:CD2	2.39	0.53
5:III:-22:DA:C2	6:JJJ:23:DG:N2	2.77	0.53
4:HHH:39:TYR:CE1	4:HHH:43:LYS:HE2	2.45	0.52
6:JJJ:53:DA:C2	6:JJJ:54:DT:O2	2.63	0.52
6:JJJ:14:DC:H4'	6:JJJ:15:DC:OP1	2.10	0.52
3:GGG:50:TYR:OH	4:HHH:92:GLN:NE2	2.36	0.52
5:III:-50:DT:C4	5:III:-49:DA:C6	2.98	0.52
1:AAA:83:ARG:O	2:BBB:80:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:III:-24:DC:H1'	5:III:-23:DC:C6	2.46	0.51
5:III:49:DT:H2''	5:III:50:DA:C8	2.46	0.51
3:CCC:55:LEU:O	3:CCC:59:THR:HG23	2.11	0.51
5:III:64:DG:C4	5:III:65:DA:N7	2.80	0.50
4:DDD:66:ILE:HG22	4:DDD:70:ILE:HD12	1.92	0.50
3:CCC:26:PRO:HG3	4:DDD:37:TYR:CE2	2.47	0.50
6:JJJ:-38:DA:H2''	6:JJJ:-37:DT:OP2	2.12	0.49
1:AAA:40:ARG:HG3	6:JJJ:10:DC:H5''	1.94	0.49
4:HHH:46:HIS:HB3	4:HHH:49:THR:HB	1.94	0.49
6:JJJ:35:DA:H2''	6:JJJ:36:DA:OP2	2.12	0.49
6:JJJ:6:DT:H4'	6:JJJ:7:DG:OP1	2.11	0.49
5:III:-58:DG:N2	6:JJJ:59:DA:C2	2.81	0.49
6:JJJ:-28:DT:H2'	6:JJJ:-27:DG:C8	2.48	0.48
6:JJJ:37:DA:H2''	6:JJJ:38:DT:OP2	2.13	0.48
1:EEE:128:ARG:HD2	1:EEE:133:GLU:OE1	2.13	0.48
5:III:-24:DC:H1'	5:III:-23:DC:C5	2.49	0.48
3:GGG:13:LYS:HD3	6:JJJ:-41:DT:OP1	2.13	0.48
3:CCC:55:LEU:O	3:CCC:59:THR:HG22	2.13	0.48
3:GGG:79:ILE:HB	3:GGG:80:PRO:HD2	1.94	0.48
5:III:-50:DT:O4	5:III:-49:DA:N6	2.47	0.48
6:JJJ:-70:DC:H2''	6:JJJ:-69:DA:OP2	2.12	0.48
1:AAA:124:ILE:O	1:AAA:128:ARG:HG3	2.14	0.47
6:JJJ:-71:DT:H2''	6:JJJ:-70:DC:O5'	2.15	0.47
5:III:-72:DA:C2	5:III:-71:DT:C2	3.02	0.47
6:JJJ:5:DC:H4'	6:JJJ:6:DT:OP1	2.13	0.47
2:BBB:22:LEU:HD22	2:BBB:22:LEU:C	2.40	0.47
5:III:-25:DT:C6	5:III:-25:DT:H5''	2.49	0.47
2:BBB:31:LYS:HB3	2:BBB:32:PRO:HD3	1.96	0.47
3:CCC:32:ARG:O	3:CCC:35:ARG:HB3	2.14	0.47
3:CCC:47:ALA:HB3	3:CCC:48:PRO:HD3	1.96	0.47
6:JJJ:53:DA:N3	6:JJJ:54:DT:C2	2.83	0.47
3:CCC:29:ARG:NH2	6:JJJ:48:DG:OP1	2.39	0.47
6:JJJ:-49:DA:C4'	6:JJJ:-48:DC:OP1	2.59	0.46
5:III:-12:DA:C2	6:JJJ:13:DG:N2	2.84	0.46
5:III:-47:DC:N4	6:JJJ:46:DT:O4	2.49	0.46
6:JJJ:15:DC:H2''	6:JJJ:16:DT:OP2	2.15	0.46
1:AAA:96:CYS:SG	2:BBB:58:LEU:HD11	2.55	0.46
6:JJJ:27:DC:C4	6:JJJ:28:DA:C6	3.04	0.46
3:CCC:77:ARG:HD3	5:III:-54:DA:H5''	1.98	0.46
2:FFF:17:ARG:C	2:FFF:18:HIS:O	2.58	0.46
6:JJJ:-47:DC:O2	6:JJJ:-46:DA:C2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:JJJ:50:DA:C6	6:JJJ:51:DG:C6	3.04	0.45
7:MMM:6:ORN:N	7:MMM:14:THR:OG1	2.48	0.45
4:DDD:28:ARG:HB2	6:JJJ:50:DA:OP1	2.15	0.45
5:III:39:DA:C2	6:JJJ:38:DA:C2	3.05	0.45
2:FFF:79:LYS:HD2	5:III:27:DC:OP1	2.16	0.45
6:JJJ:11:DA:H2''	6:JJJ:12:DT:O5'	2.16	0.44
1:AAA:63:ARG:HB2	1:AAA:66:PRO:HG2	2.00	0.44
1:AAA:73:GLU:OE1	2:BBB:25:ASN:HB2	2.17	0.44
1:EEE:69:ARG:HD2	2:FFF:25:ASN:OD1	2.18	0.44
5:III:39:DT:H2''	5:III:38:DA:C8	2.49	0.44
3:CCC:115:LEU:HD11	1:EEE:108:ASN:HD21	1.82	0.44
3:GGG:31:HIS:CD2	3:GGG:48:PRO:HG3	2.53	0.44
1:AAA:82:LEU:HD23	1:AAA:82:LEU:HA	1.86	0.44
3:GGG:73:ASN:HD22	3:GGG:73:ASN:N	2.16	0.44
3:GGG:92:GLU:HB3	4:HHH:103:LEU:HD22	1.99	0.44
5:III:38:DT:H2''	5:III:39:DA:OP2	2.17	0.44
3:CCC:88:ARG:HD3	3:CCC:88:ARG:HA	1.81	0.44
6:JJJ:47:DC:O3'	6:JJJ:46:DA:C8	2.70	0.44
5:III:47:DC:C5	5:III:46:DA:N6	2.86	0.43
6:JJJ:70:DG:H2''	6:JJJ:71:DA:OP2	2.18	0.43
3:GGG:60:ALA:HB1	7:MMM:8:LEU:HD11	1.99	0.43
1:EEE:118:THR:HA	2:FFF:45:ARG:O	2.18	0.43
5:III:72:DA:H4'	5:III:71:DT:OP1	2.19	0.43
5:III:41:DA:C4	5:III:42:DC:C5	3.07	0.43
5:III:70:DG:N2	6:JJJ:69:DA:C2	2.87	0.43
6:JJJ:24:DG:C4'	6:JJJ:25:DA:OP1	2.65	0.42
6:JJJ:55:DC:H6	6:JJJ:55:DC:O5'	2.01	0.42
2:FFF:84:MET:HE3	2:FFF:88:TYR:CZ	2.54	0.42
3:GGG:79:ILE:HG12	3:GGG:82:HIS:CE1	2.54	0.42
3:GGG:47:ALA:N	3:GGG:48:PRO:HD2	2.35	0.42
5:III:49:DA:C5	5:III:48:DC:C4	3.08	0.42
6:JJJ:51:DG:OP2	6:JJJ:51:DG:H2'	2.20	0.42
5:III:67:DT:H1'	5:III:66:DA:C8	2.54	0.42
6:JJJ:45:DA:C2	6:JJJ:44:DA:C2	3.07	0.42
2:BBB:46:ILE:O	6:JJJ:7:DG:H3'	2.19	0.42
3:CCC:81:ARG:NH2	3:CCC:107:VAL:O	2.40	0.42
4:HHH:113:LYS:NZ	7:MMM:5:GLY:O	2.25	0.42
4:DDD:30:ARG:O	4:DDD:30:ARG:HG3	2.19	0.42
2:FFF:35:ARG:HH22	5:III:8:DA:P	2.43	0.42
3:GGG:64:GLU:CB	7:MMM:8:LEU:HD23	2.50	0.42
1:AAA:65:LEU:HB3	1:AAA:66:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:III:-17:DA:C2	5:III:-16:DA:C5	3.08	0.42
5:III:51:DG:H2''	5:III:52:DT:O5'	2.19	0.42
1:AAA:65:LEU:N	1:AAA:66:PRO:HD2	2.35	0.41
6:JJJ:-45:DA:C2	6:JJJ:-44:DA:C6	3.07	0.41
6:JJJ:55:DC:O5'	6:JJJ:55:DC:C6	2.73	0.41
3:CCC:80:PRO:HG3	4:DDD:58:ILE:HD12	2.02	0.41
5:III:25:DA:H4'	5:III:26:DG:OP1	2.21	0.41
7:MMM:4:PRO:CD	7:MMM:16:ALA:HA	2.50	0.41
1:AAA:108:ASN:HD21	3:GGG:115:LEU:HD11	1.85	0.41
6:JJJ:40:DC:N3	6:JJJ:41:DA:C6	2.88	0.41
4:DDD:77:LEU:CD2	4:DDD:93:THR:HB	2.49	0.41
6:JJJ:-50:DT:C4	6:JJJ:-49:DA:N6	2.89	0.41
5:III:-50:DT:H5'	5:III:-49:DA:OP2	2.20	0.41
5:III:-72:DA:C2	5:III:-71:DT:N3	2.89	0.41
1:AAA:48:LEU:HD12	1:AAA:48:LEU:HA	1.94	0.41
5:III:-49:DA:C6	5:III:-48:DC:N3	2.89	0.41
3:CCC:32:ARG:NH2	4:DDD:32:GLU:OE1	2.49	0.40
5:III:65:DA:C2	5:III:66:DT:C2	3.09	0.40
6:JJJ:51:DG:H2''	6:JJJ:52:DT:O5'	2.22	0.40
1:AAA:76:GLN:HE21	1:AAA:80:THR:HG22	1.84	0.40
5:III:42:DC:H2''	5:III:43:DT:OP2	2.22	0.40
6:JJJ:53:DA:C5	6:JJJ:54:DT:C4	3.10	0.40
3:CCC:38:ASN:HD22	3:CCC:38:ASN:HA	1.57	0.40
3:CCC:42:ARG:NH1	6:JJJ:37:DA:H4'	2.35	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%)	91 (95%)	5 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EEE	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
2	BBB	80/87 (92%)	79 (99%)	1 (1%)	0	100	100
2	FFF	85/87 (98%)	81 (95%)	3 (4%)	1 (1%)	10	20
3	CCC	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	GGG	105/107 (98%)	100 (95%)	4 (4%)	1 (1%)	12	24
4	DDD	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	11	22
4	HHH	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	11	22
7	MMM	11/14 (79%)	10 (91%)	0	1 (9%)	0	0
All	All	764/788 (97%)	731 (96%)	28 (4%)	5 (1%)	18	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	DDD	101	GLY
2	FFF	18	HIS
7	MMM	16	ALA
4	HHH	101	GLY
3	GGG	64	GLU

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%)	80 (94%)	5 (6%)	18	37
1	EEE	85/85 (100%)	82 (96%)	3 (4%)	32	58
2	BBB	67/72 (93%)	65 (97%)	2 (3%)	36	64
2	FFF	72/72 (100%)	67 (93%)	5 (7%)	14	30
3	CCC	85/85 (100%)	75 (88%)	10 (12%)	5	11
3	GGG	85/85 (100%)	79 (93%)	6 (7%)	13	29
4	DDD	81/81 (100%)	78 (96%)	3 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	HHH	81/81 (100%)	74 (91%)	7 (9%)	10	21
7	MMM	9/9 (100%)	6 (67%)	3 (33%)	0	0
All	All	650/655 (99%)	606 (93%)	44 (7%)	14	31

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	48	LEU
1	AAA	59	GLU
1	AAA	86	SER
1	AAA	122	LYS
1	AAA	134	ARG
2	BBB	22	LEU
2	BBB	47	SER
3	CCC	13	LYS
3	CCC	29	ARG
3	CCC	31	HIS
3	CCC	38	ASN
3	CCC	59	THR
3	CCC	74	LYS
3	CCC	76	THR
3	CCC	81	ARG
3	CCC	99	ARG
3	CCC	119	LYS
4	DDD	30	ARG
4	DDD	88	SER
4	DDD	98	LEU
1	EEE	39	HIS
1	EEE	59	GLU
1	EEE	120	MET
2	FFF	16	LYS
2	FFF	17	ARG
2	FFF	18	HIS
2	FFF	23	ARG
2	FFF	26	ILE
3	GGG	15	LYS
3	GGG	36	LYS
3	GGG	71	ARG
3	GGG	73	ASN
3	GGG	88	ARG
3	GGG	118	LYS

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Mol	Chain	Res	Type
4	HHH	30	ARG
4	HHH	84	SER
4	HHH	88	SER
4	HHH	102	GLU
4	HHH	103	LEU
4	HHH	105	LYS
4	HHH	109	SER
7	MMM	4	PRO
7	MMM	7	ARG
7	MMM	12	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ORN	MMM	6	7	6,7,8	0.53	0	2,7,9	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ORN	MMM	6	7	-	1/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	MMM	6	ORN	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	MMM	6	ORN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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, 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%)	0.09	3 (3%)	51	47	58, 87, 138, 214	0
1	EEE	98/98 (100%)	0.02	3 (3%)	51	47	54, 71, 105, 149	0
2	BBB	82/87 (94%)	0.22	5 (6%)	27	23	67, 86, 111, 210	0
2	FFF	87/87 (100%)	-0.04	0	100	100	51, 71, 98, 171	0
3	CCC	107/107 (100%)	0.18	4 (3%)	45	40	57, 78, 129, 172	0
3	GGG	107/107 (100%)	0.41	8 (7%)	20	18	65, 87, 130, 194	0
4	DDD	95/95 (100%)	0.36	4 (4%)	40	36	64, 85, 132, 190	0
4	HHH	95/95 (100%)	0.51	9 (9%)	14	12	67, 91, 141, 197	0
5	III	145/145 (100%)	-0.47	0	100	100	87, 146, 191, 237	0
6	JJJ	145/145 (100%)	-0.49	0	100	100	91, 145, 191, 238	0
7	MMM	13/14 (92%)	0.12	0	100	100	94, 154, 205, 238	0
All	All	1072/1078 (99%)	0.03	36 (3%)	48	43	51, 91, 177, 238	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	38	PRO	5.1
1	AAA	84	PHE	4.7
1	EEE	38	PRO	3.9
3	GGG	55	LEU	3.9
3	GGG	51	LEU	3.8
3	GGG	43	VAL	3.8
2	BBB	22	LEU	3.6
2	BBB	21	VAL	3.5
3	CCC	51	LEU	3.3
4	DDD	88	SER	3.3
4	HHH	62	PHE	3.2
4	HHH	99	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	GGG	54	VAL	3.1
4	HHH	86	ILE	3.1
4	HHH	98	LEU	2.9
3	GGG	34	LEU	2.9
4	HHH	121	ALA	2.7
1	EEE	135	ALA	2.7
3	CCC	25	PHE	2.7
4	HHH	91	ILE	2.7
3	GGG	58	LEU	2.6
3	GGG	96	LEU	2.5
1	EEE	39	HIS	2.5
1	AAA	68	GLN	2.3
2	BBB	81	VAL	2.3
4	DDD	30	ARG	2.3
2	BBB	72	TYR	2.3
2	BBB	66	ILE	2.3
4	HHH	70	ILE	2.3
4	DDD	62	PHE	2.3
3	CCC	119	LYS	2.2
4	HHH	96	ARG	2.2
4	DDD	91	ILE	2.1
3	GGG	35	ARG	2.1
3	CCC	14	ALA	2.0
4	HHH	100	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
7	ORN	MMM	6	8/9	0.93	0.14	137,161,170,185	0

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
8	MG	EEE	201	1/1	0.83	0.30	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.