Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2024 – 12:59 pm GMT

PDB ID	:	8Q3E
Title	:	High Resolution Structure of Nucleosome Core with Bound Foamy Virus GAG Peptide
Authors	:	De Falco, L.; Batchelor, L.K.; Dyson, P.J.; Davey, C.A.
Deposited on	:	2023-08-04
Resolution	:	2.17 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:

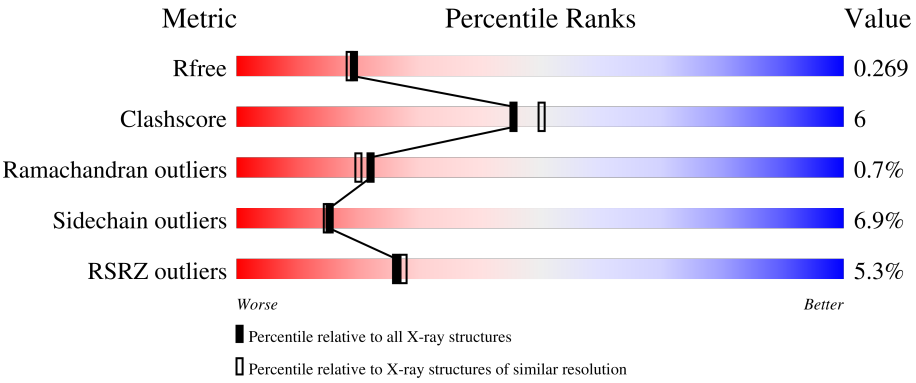
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.17 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.



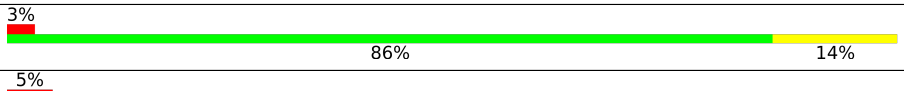
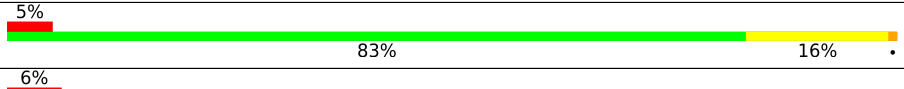
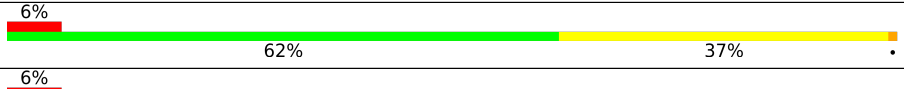
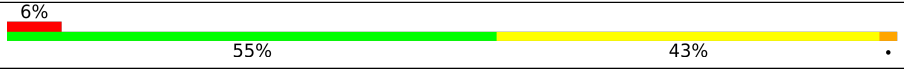
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	MMM	18	11% 72% 22% 6%
2	AAA	98	4% 87% 12% ·
2	EEE	98	5% 86% 12% ·
3	BBB	87	5% 85% 7% · 6%
3	FFF	87	7% 86% 11% ·

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12197 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 GLY-GLY-TYR-ASN-LEU-ARG-PRO-ARG-THR-TYR-GLN-PRO-GLN-ARG-TYR-GLY-GLY-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	MMM	18	Total	C	N	O	0	0	1
			141	87	30	24			

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AAA	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
2	EEE	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

- Molecule 3 is a protein called Histone H4.

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

- Molecule 4 is a protein called Histone H2A type 1-B/E.

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

- Molecule 5 is a protein called Histone H2B type 1-K.

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

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

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

- Molecule 7 is a DNA chain called DNA (145-MER).

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

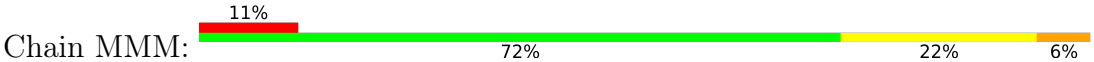
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	EEE	1	Total	Mg	0	0
			1	1		

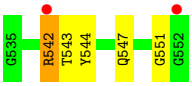
3 Residue-property plots (i)

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: GLY-GLY-TYR-ASN-LEU-ARG-PRO-ARG-THR-TYR-GLN-PRO-GLN-ARG-TYR-GLY-GLY-GLY

Chain MMM:



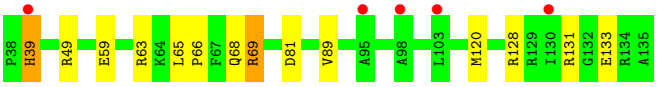


• Molecule 2: Histone H3.1

Chain AAA:

• Molecule 2: Histone H3.1

Chain EEE:



• Molecule 3: Histone H4

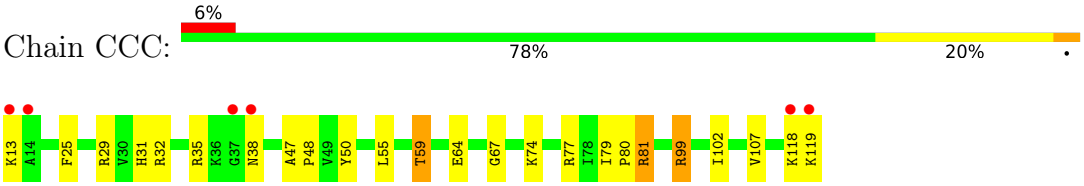
Chain BBB:

• Molecule 3: Histone H4

Chain FFF:

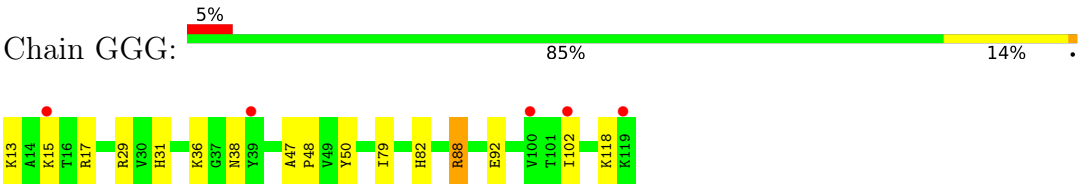
• Molecule 4: Histone H2A type 1-B/E

Chain CCC:



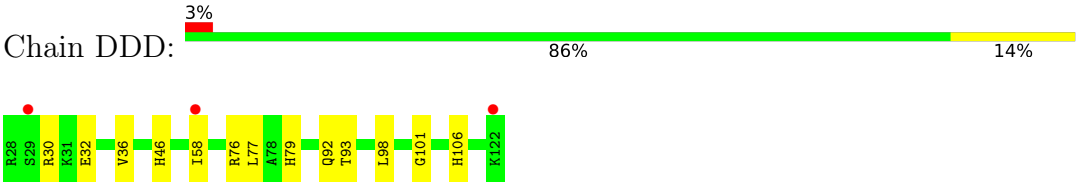
• Molecule 4: Histone H2A type 1-B/E

Chain GGG:



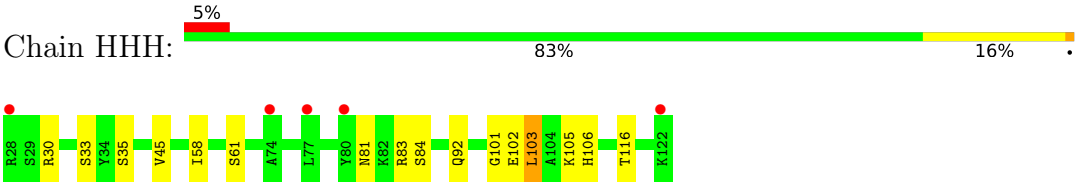
• Molecule 5: Histone H2B type 1-K

Chain DDD:



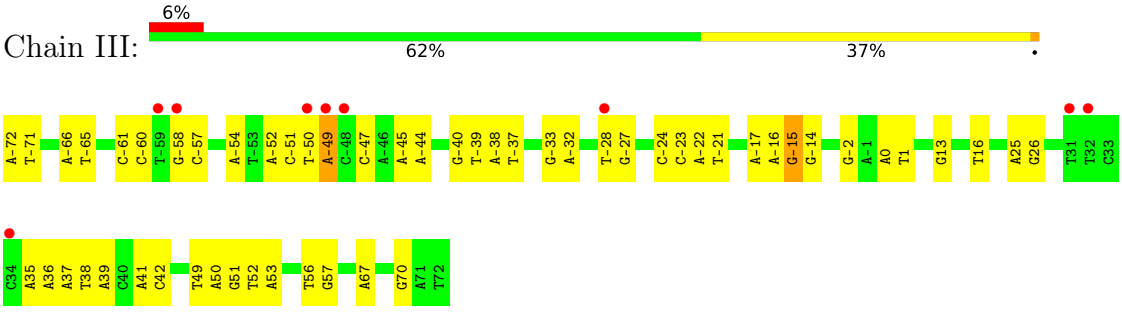
• Molecule 5: Histone H2B type 1-K

Chain HHH:



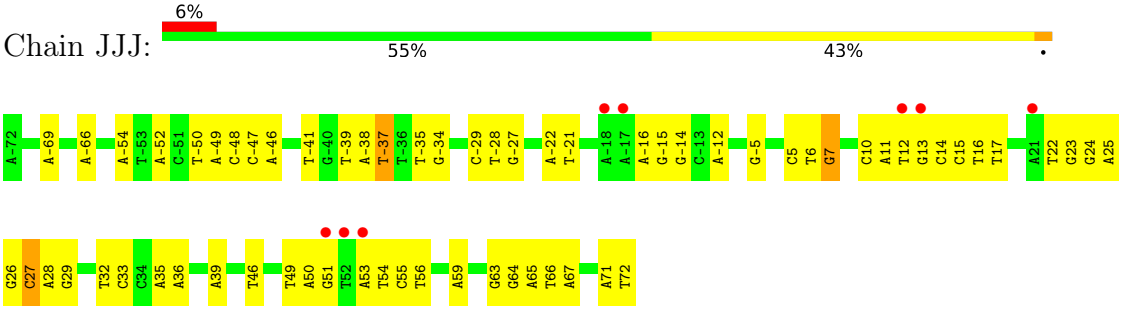
• Molecule 6: DNA (145-MER)

Chain III:



• Molecule 7: DNA (145-MER)

Chain JJJ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.17Å 109.64Å 183.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.17 48.80 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.85-2.17) 98.1 (48.80-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.270 0.239 , 0.269	Depositor DCC
R_{free} test set	2303 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12197	wwPDB-VP
Average B, all atoms (Å^2)	88.0	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.*

[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: MG

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	MMM	0.77	0/145	0.81	0/195
2	AAA	0.73	0/819	0.91	0/1097
2	EEE	0.84	0/819	1.08	2/1097 (0.2%)
3	BBB	0.74	0/660	0.91	0/883
3	FFF	0.80	1/711 (0.1%)	1.06	3/948 (0.3%)
4	CCC	0.80	1/838 (0.1%)	0.99	0/1129
4	GGG	0.73	0/838	0.90	2/1129 (0.2%)
5	DDD	0.80	0/756	0.90	1/1014 (0.1%)
5	HHH	0.81	0/756	0.89	0/1014
6	III	0.49	1/3332 (0.0%)	0.90	10/5141 (0.2%)
7	JJJ	0.50	2/3330 (0.1%)	0.85	4/5138 (0.1%)
All	All	0.65	5/13004 (0.0%)	0.91	22/18785 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	CCC	64	GLU	CD-OE2	-6.91	1.18	1.25
3	FFF	63	GLU	CD-OE1	6.06	1.32	1.25
6	III	-15	DG	O3'-P	-5.66	1.54	1.61
7	JJJ	-37	DT	O3'-P	-5.62	1.54	1.61
7	JJJ	-54	DA	O3'-P	-5.49	1.54	1.61

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	III	-49	DA	C1'-O4'-C4'	-8.92	101.18	110.10
7	JJJ	-5	DG	O5'-P-OP2	-8.74	97.83	105.70
2	EEE	128	ARG	NE-CZ-NH2	-8.65	115.97	120.30
4	GGG	88	ARG	NE-CZ-NH1	7.28	123.94	120.30
3	FFF	23	ARG	NE-CZ-NH2	-7.20	116.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	III	-49	DA	N9-C1'-C2'	6.98	125.87	112.60
6	III	-40	DG	N9-C1'-C2'	6.91	125.72	112.60
5	DDD	76	ARG	NE-CZ-NH2	-6.36	117.12	120.30
7	JJJ	7	DG	P-O5'-C5'	-6.12	111.11	120.90
6	III	-49	DA	C8-N9-C1'	5.90	138.31	127.70
6	III	-49	DA	C4-N9-C1'	-5.88	115.72	126.30
6	III	-2	DG	O5'-P-OP2	-5.59	100.67	105.70
6	III	-40	DG	C3'-C2'-C1'	-5.57	95.82	102.50
4	GGG	88	ARG	NE-CZ-NH2	-5.38	117.61	120.30
6	III	-65	DT	O5'-P-OP1	-5.29	100.94	105.70
3	FFF	92	ARG	CB-CA-C	-5.27	99.86	110.40
3	FFF	92	ARG	NE-CZ-NH1	5.18	122.89	120.30
6	III	16	DT	C4'-C3'-O3'	-5.17	96.78	109.70
7	JJJ	27	DC	O5'-P-OP2	-5.13	101.08	105.70
7	JJJ	-5	DG	O5'-P-OP1	5.07	116.78	110.70
6	III	-49	DA	C3'-C2'-C1'	-5.06	96.43	102.50
2	EEE	69	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	MMM	141	0	131	3	0
2	AAA	807	0	844	11	0
2	EEE	807	0	844	7	0
3	BBB	653	0	696	10	0
3	FFF	703	0	755	3	0
4	CCC	828	0	892	17	0
4	GGG	828	0	892	10	0
5	DDD	745	0	769	8	0
5	HHH	745	0	769	7	0
6	III	2970	0	1640	46	0
7	JJJ	2969	0	1641	60	0
8	EEE	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12197	0	9873	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (142) 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)
7:JJJ:-22:DA:H2"	7:JJJ:-21:DT:O5'	1.78	0.81
7:JJJ:-49:DA:H4'	7:JJJ:-48:DC:OP1	1.80	0.81
2:AAA:96:CYS:SG	3:BBB:58:LEU:CD1	2.70	0.80
6:III:-50:DT:C4	6:III:-49:DA:N6	2.57	0.73
4:GGG:102:ILE:HG23	5:HHH:58:ILE:HD13	1.72	0.72
7:JJJ:66:DT:H2"	7:JJJ:67:DA:OP2	1.93	0.69
2:AAA:96:CYS:SG	3:BBB:58:LEU:HD13	2.37	0.64
6:III:53:DA:C2	7:JJJ:-52:DA:C2	2.86	0.64
2:EEE:49:ARG:HH11	2:EEE:49:ARG:HG3	1.63	0.64
4:CCC:47:ALA:HB3	4:CCC:48:PRO:HD3	1.80	0.62
6:III:-58:DG:N2	7:JJJ:59:DA:C2	2.67	0.62
2:AAA:96:CYS:SG	3:BBB:58:LEU:HD11	2.40	0.61
6:III:-50:DT:C4	6:III:-49:DA:C6	2.88	0.60
2:AAA:73:GLU:OE1	3:BBB:25:ASN:HB2	2.01	0.60
7:JJJ:-15:DG:H2"	7:JJJ:-14:DG:OP2	2.02	0.60
7:JJJ:-28:DT:H3'	7:JJJ:-27:DG:H5"	1.84	0.59
6:III:49:DT:H2"	6:III:50:DA:C8	2.37	0.59
6:III:-52:DA:C2	7:JJJ:53:DA:N1	2.71	0.59
6:III:-39:DT:H2"	6:III:-38:DA:H8	1.69	0.58
2:EEE:69:ARG:HD2	3:FFF:25:ASN:OD1	2.04	0.58
7:JJJ:50:DA:H2"	7:JJJ:51:DG:OP2	2.03	0.58
6:III:-22:DA:C2	7:JJJ:23:DG:N2	2.72	0.57
4:GGG:29:ARG:NH1	5:HHH:33:SER:O	2.37	0.57
6:III:-52:DA:C2	7:JJJ:53:DA:C2	2.93	0.57
7:JJJ:24:DG:H4'	7:JJJ:25:DA:OP1	2.04	0.57
7:JJJ:13:DG:H4'	7:JJJ:14:DC:OP1	2.05	0.57
4:CCC:99:ARG:HH11	4:CCC:99:ARG:HG3	1.70	0.56
6:III:-50:DT:O4	6:III:-49:DA:N6	2.37	0.56
4:GGG:13:LYS:HD3	7:JJJ:-41:DT:OP1	2.06	0.55
4:CCC:25:PHE:CZ	4:CCC:59:THR:HG21	2.43	0.54
5:DDD:77:LEU:HD21	5:DDD:93:THR:HB	1.89	0.54
7:JJJ:54:DT:H2"	7:JJJ:55:DC:OP2	2.07	0.54
6:III:13:DG:C2	7:JJJ:-12:DA:C2	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:JJJ:-28:DT:H2'	7:JJJ:-27:DG:C8	2.42	0.54
2:AAA:76:GLN:HE21	2:AAA:80:THR:HG22	1.73	0.54
7:JJJ:5:DC:H4'	7:JJJ:6:DT:OP1	2.07	0.54
7:JJJ:-28:DT:C3'	7:JJJ:-27:DG:H5"	2.39	0.53
5:DDD:79:HIS:NE2	4:GGG:38:ASN:OD1	2.43	0.52
6:III:-28:DT:H4'	6:III:-27:DG:OP1	2.10	0.51
6:III:-24:DC:H1'	6:III:-23:DC:C6	2.45	0.51
6:III:-24:DC:H1'	6:III:-23:DC:C5	2.46	0.50
5:HHH:33:SER:HG	5:HHH:35:SER:HG	1.49	0.50
7:JJJ:35:DA:H2"	7:JJJ:36:DA:OP2	2.12	0.50
4:GGG:17:ARG:HH12	4:GGG:31:HIS:HD2	1.60	0.50
6:III:-61:DC:H2"	6:III:-60:DC:O5'	2.12	0.49
6:III:67:DA:C2	7:JJJ:-66:DA:C2	3.00	0.49
7:JJJ:-49:DA:C4'	7:JJJ:-48:DC:OP1	2.55	0.49
6:III:-22:DA:H2"	6:III:-21:DT:OP2	2.12	0.49
7:JJJ:65:DA:H2"	7:JJJ:66:DT:OP2	2.12	0.49
4:CCC:81:ARG:NH2	4:CCC:107:VAL:O	2.36	0.49
6:III:-39:DT:H2"	6:III:-38:DA:C8	2.48	0.49
7:JJJ:55:DC:C6	7:JJJ:56:DT:H72	2.48	0.48
7:JJJ:14:DC:H4'	7:JJJ:15:DC:OP1	2.13	0.48
4:CCC:47:ALA:HB3	4:CCC:48:PRO:CD	2.42	0.48
4:CCC:55:LEU:O	4:CCC:59:THR:CG2	2.61	0.48
4:GGG:17:ARG:HH12	4:GGG:31:HIS:CD2	2.32	0.48
7:JJJ:50:DA:C6	7:JJJ:51:DG:C6	3.02	0.48
2:AAA:40:ARG:HG3	7:JJJ:10:DC:H5"	1.96	0.48
7:JJJ:11:DA:H2"	7:JJJ:12:DT:O5'	2.14	0.47
4:CCC:79:ILE:HB	4:CCC:80:PRO:CD	2.44	0.47
7:JJJ:53:DA:C2	7:JJJ:54:DT:C2	3.01	0.47
1:MMM:544:TYR:CD1	1:MMM:544:TYR:N	2.82	0.47
4:GGG:79:ILE:HG12	4:GGG:82:HIS:CE1	2.50	0.47
6:III:13:DG:N2	7:JJJ:-12:DA:C2	2.83	0.47
7:JJJ:15:DC:H2"	7:JJJ:16:DT:OP2	2.13	0.47
4:CCC:32:ARG:HH22	5:DDD:32:GLU:CD	2.18	0.47
4:CCC:77:ARG:HD3	6:III:-54:DA:H5"	1.95	0.47
6:III:39:DA:C2	7:JJJ:-38:DA:C2	3.01	0.47
3:BBB:46:ILE:O	7:JJJ:7:DG:H3'	2.15	0.47
7:JJJ:22:DT:H2"	7:JJJ:23:DG:C8	2.50	0.46
7:JJJ:-34:DG:H2'	7:JJJ:-34:DG:OP2	2.16	0.46
6:III:-51:DC:H5"	6:III:-51:DC:H6	1.81	0.46
4:CCC:50:TYR:OH	5:DDD:92:GLN:NE2	2.35	0.46
7:JJJ:12:DT:H2"	7:JJJ:13:DG:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:III:-15:DG:H4'	6:III:-14:DG:OP1	2.14	0.46
6:III:70:DG:N2	7:JJJ:-69:DA:C2	2.83	0.46
4:CCC:67:GLY:HA3	5:DDD:46:HIS:CD2	2.50	0.46
6:III:25:DA:C2	6:III:26:DG:C2	3.04	0.46
6:III:41:DA:C4	6:III:42:DC:C5	3.03	0.46
4:CCC:55:LEU:O	4:CCC:59:THR:HG23	2.15	0.46
7:JJJ:-47:DC:O2	7:JJJ:-46:DA:C2	2.69	0.46
1:MMM:542:ARG:HD2	1:MMM:544:TYR:HE1	1.80	0.45
6:III:38:DT:H1'	6:III:39:DA:C8	2.52	0.45
7:JJJ:-35:DT:H2"	7:JJJ:-34:DG:C8	2.51	0.45
2:AAA:63:ARG:CZ	7:JJJ:17:DT:H4'	2.47	0.45
4:GGG:50:TYR:OH	5:HHH:92:GLN:NE2	2.35	0.45
6:III:-45:DA:H1'	6:III:-44:DA:H5'	1.98	0.44
4:CCC:32:ARG:O	4:CCC:35:ARG:HB3	2.17	0.44
2:AAA:59:GLU:OE2	3:BBB:40:ARG:NH2	2.50	0.44
4:CCC:80:PRO:HB3	5:DDD:58:ILE:CD1	2.47	0.44
6:III:-47:DC:N4	7:JJJ:46:DT:O4	2.51	0.44
4:CCC:79:ILE:HB	4:CCC:80:PRO:HD2	2.00	0.44
3:FFF:31:LYS:N	3:FFF:32:PRO:HD2	2.32	0.44
7:JJJ:-16:DA:H4'	7:JJJ:-15:DG:OP1	2.17	0.44
4:CCC:102:ILE:HG23	5:DDD:58:ILE:HD13	1.99	0.44
2:EEE:39:HIS:O	2:EEE:39:HIS:ND1	2.51	0.44
2:EEE:81:ASP:HA	3:FFF:19:ARG:HH22	1.83	0.44
5:HHH:81:ASN:O	5:HHH:83:ARG:HG2	2.17	0.44
7:JJJ:63:DG:H2"	7:JJJ:64:DG:OP2	2.18	0.44
4:GGG:92:GLU:HB3	5:HHH:103:LEU:HD22	1.99	0.43
6:III:0:DA:H2"	6:III:1:DT:OP2	2.18	0.43
6:III:51:DG:H2"	6:III:52:DT:O5'	2.19	0.43
7:JJJ:32:DT:H2"	7:JJJ:33:DC:C5	2.53	0.43
2:AAA:63:ARG:NH1	7:JJJ:17:DT:H4'	2.33	0.43
6:III:35:DA:H4'	6:III:36:DA:OP1	2.16	0.43
7:JJJ:-38:DA:H2"	7:JJJ:-37:DT:OP2	2.19	0.43
6:III:-66:DA:C2	7:JJJ:67:DA:C2	3.07	0.43
6:III:-38:DA:C2	6:III:-37:DT:C2	3.06	0.43
7:JJJ:53:DA:H4'	7:JJJ:54:DT:OP1	2.18	0.43
1:MMM:542:ARG:HD2	1:MMM:544:TYR:CE1	2.53	0.43
6:III:-50:DT:H5'	6:III:-49:DA:OP2	2.19	0.43
7:JJJ:-50:DT:C4	7:JJJ:-49:DA:N6	2.87	0.43
6:III:56:DT:H2"	6:III:57:DG:N7	2.34	0.43
7:JJJ:-22:DA:H2"	7:JJJ:-21:DT:C5'	2.48	0.43
6:III:37:DA:C5	6:III:38:DT:C4	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:III:-24:DC:C2	6:III:-23:DC:C4	3.07	0.42
3:BBB:22:LEU:HD22	3:BBB:22:LEU:C	2.39	0.42
2:EEE:131:ARG:HD3	2:EEE:133:GLU:OE2	2.19	0.42
6:III:-58:DG:N3	6:III:-57:DC:O2	2.53	0.42
6:III:-17:DA:C2	6:III:-16:DA:C5	3.08	0.42
6:III:-33:DG:N2	6:III:-32:DA:C2	2.88	0.42
7:JJJ:27:DC:C4	7:JJJ:28:DA:C6	3.07	0.42
2:AAA:83:ARG:O	3:BBB:80:THR:HA	2.20	0.41
2:AAA:63:ARG:HB2	2:AAA:66:PRO:HG2	2.02	0.41
7:JJJ:-15:DG:C2'	7:JJJ:-14:DG:OP2	2.68	0.41
7:JJJ:49:DT:H2"	7:JJJ:50:DA:C8	2.55	0.41
6:III:-47:DC:O2	6:III:-47:DC:O4'	2.37	0.41
7:JJJ:71:DA:C5	7:JJJ:72:DT:C4	3.08	0.41
7:JJJ:-39:DT:H2"	7:JJJ:-38:DA:H8	1.85	0.41
6:III:-38:DA:C2	7:JJJ:39:DA:C2	3.08	0.41
7:JJJ:28:DA:H1'	7:JJJ:29:DG:C8	2.55	0.41
6:III:-72:DA:C2	6:III:-71:DT:C2	3.09	0.41
3:BBB:47:SER:HA	7:JJJ:7:DG:H5'	2.03	0.41
4:CCC:32:ARG:NH2	5:DDD:32:GLU:OE1	2.48	0.41
2:EEE:68:GLN:HG3	2:EEE:89:VAL:HG11	2.03	0.41
6:III:35:DA:C4'	6:III:36:DA:OP1	2.68	0.41
7:JJJ:-29:DC:H2'	7:JJJ:-28:DT:C6	2.56	0.41
7:JJJ:25:DA:C5	7:JJJ:26:DG:C6	3.09	0.41
2:EEE:65:LEU:HB3	2:EEE:66:PRO:HD3	2.02	0.40
4:GGG:47:ALA:N	4:GGG:48:PRO:HD2	2.37	0.40
3:BBB:98:TYR:CD1	5:HHH:61:SER:HB3	2.56	0.40
6:III:56:DT:O3'	6:III:57:DG:C8	2.75	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	MMM	16/18 (89%)	13 (81%)	2 (12%)	1 (6%)	1 0
2	AAA	96/98 (98%)	94 (98%)	2 (2%)	0	100 100
2	EEE	96/98 (98%)	96 (100%)	0	0	100 100
3	BBB	80/87 (92%)	79 (99%)	1 (1%)	0	100 100
3	FFF	85/87 (98%)	83 (98%)	1 (1%)	1 (1%)	13 9
4	CCC	105/107 (98%)	99 (94%)	5 (5%)	1 (1%)	15 12
4	GGG	105/107 (98%)	100 (95%)	5 (5%)	0	100 100
5	DDD	93/95 (98%)	86 (92%)	6 (6%)	1 (1%)	14 11
5	HHH	93/95 (98%)	90 (97%)	2 (2%)	1 (1%)	14 11
All	All	769/792 (97%)	740 (96%)	24 (3%)	5 (1%)	22 20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	FFF	18	HIS
5	DDD	101	GLY
4	CCC	118	LYS
5	HHH	101	GLY
1	MMM	551	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	MMM	13/13 (100%)	10 (77%)	3 (23%)	1 0
2	AAA	85/85 (100%)	80 (94%)	5 (6%)	19 21
2	EEE	85/85 (100%)	81 (95%)	4 (5%)	26 30
3	BBB	67/72 (93%)	65 (97%)	2 (3%)	41 49
3	FFF	72/72 (100%)	66 (92%)	6 (8%)	11 10
4	CCC	85/85 (100%)	76 (89%)	9 (11%)	6 5
4	GGG	85/85 (100%)	81 (95%)	4 (5%)	26 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	DDD	81/81 (100%)	77 (95%)	4 (5%)	25 28
5	HHH	81/81 (100%)	73 (90%)	8 (10%)	8 6
All	All	654/659 (99%)	609 (93%)	45 (7%)	15 15

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	MMM	542	ARG
1	MMM	543	THR
1	MMM	547	GLN
2	AAA	48	LEU
2	AAA	59	GLU
2	AAA	86	SER
2	AAA	122	LYS
2	AAA	134	ARG
3	BBB	22	LEU
3	BBB	47	SER
4	CCC	13	LYS
4	CCC	29	ARG
4	CCC	31	HIS
4	CCC	38	ASN
4	CCC	59	THR
4	CCC	74	LYS
4	CCC	81	ARG
4	CCC	99	ARG
4	CCC	119	LYS
5	DDD	30	ARG
5	DDD	36	VAL
5	DDD	98	LEU
5	DDD	106	HIS
2	EEE	39	HIS
2	EEE	59	GLU
2	EEE	63	ARG
2	EEE	120	MET
3	FFF	17	ARG
3	FFF	18	HIS
3	FFF	20	LYS
3	FFF	23	ARG
3	FFF	47	SER
3	FFF	93	GLN
4	GGG	15	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	GGG	36	LYS
4	GGG	88	ARG
4	GGG	118	LYS
5	HHH	30	ARG
5	HHH	45	VAL
5	HHH	84	SER
5	HHH	102	GLU
5	HHH	103	LEU
5	HHH	105	LYS
5	HHH	106	HIS
5	HHH	116	THR

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 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, 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	MMM	18/18 (100%)	1.28	2 (11%)	5	5	57, 83, 107, 113	0
2	AAA	98/98 (100%)	0.60	4 (4%)	37	38	42, 57, 93, 139	0
2	EEE	98/98 (100%)	0.61	5 (5%)	28	29	35, 46, 71, 116	0
3	BBB	82/87 (94%)	0.57	4 (4%)	29	31	42, 56, 80, 125	0
3	FFF	87/87 (100%)	0.83	6 (6%)	16	17	36, 45, 76, 146	0
4	CCC	107/107 (100%)	0.60	6 (5%)	24	26	36, 53, 94, 150	0
4	GGG	107/107 (100%)	0.52	5 (4%)	31	32	43, 59, 104, 137	0
5	DDD	95/95 (100%)	0.60	3 (3%)	47	48	41, 57, 95, 149	0
5	HHH	95/95 (100%)	0.66	5 (5%)	26	27	43, 60, 107, 146	0
6	III	145/145 (100%)	0.39	9 (6%)	20	21	62, 114, 159, 215	0
7	JJJ	145/145 (100%)	0.37	8 (5%)	25	26	64, 113, 161, 206	0
All	All	1077/1082 (99%)	0.57	57 (5%)	26	27	35, 62, 146, 215	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	MMM	552	GLY	18.3
4	CCC	119	LYS	7.8
4	CCC	118	LYS	4.6
2	AAA	135	ALA	3.9
7	JJJ	52	DT	3.7
7	JJJ	-17	DA	3.6
7	JJJ	13	DG	3.6
4	GGG	119	LYS	3.5
5	HHH	122	LYS	3.5
7	JJJ	53	DA	3.4
5	DDD	29	SER	3.3
5	DDD	122	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	JJJ	12	DT	3.1
6	III	-58	DG	3.1
2	AAA	39	HIS	3.0
6	III	-48	DC	3.0
2	EEE	39	HIS	2.9
6	III	-50	DT	2.9
6	III	-49	DA	2.9
3	BBB	97	LEU	2.8
4	GGG	102	ILE	2.7
7	JJJ	51	DG	2.7
3	FFF	91	LYS	2.7
5	HHH	74	ALA	2.7
3	FFF	90	LEU	2.7
2	EEE	95	ALA	2.6
1	MMM	542	ARG	2.6
6	III	32	DT	2.6
4	CCC	37	GLY	2.6
5	HHH	77	LEU	2.5
4	GGG	15	LYS	2.5
3	BBB	98	TYR	2.4
3	FFF	87	VAL	2.4
5	DDD	58	ILE	2.4
6	III	34	DC	2.4
2	EEE	130	ILE	2.3
6	III	-28	DT	2.3
7	JJJ	21	DA	2.3
4	CCC	13	LYS	2.3
6	III	-59	DT	2.3
2	EEE	98	ALA	2.3
2	AAA	38	PRO	2.3
4	GGG	100	VAL	2.2
4	CCC	38	ASN	2.2
3	BBB	96	THR	2.2
3	BBB	90	LEU	2.2
3	FFF	98	TYR	2.2
4	GGG	39	TYR	2.2
4	CCC	14	ALA	2.2
2	AAA	134	ARG	2.1
3	FFF	97	LEU	2.1
3	FFF	96	THR	2.1
7	JJJ	-18	DA	2.1
5	HHH	80	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	HHH	28	ARG	2.0
6	III	31	DT	2.0
2	EEE	103	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	MG	EEE	201	1/1	0.95	0.42	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.