



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 04:06 PM EDT

PDB ID : 8Q36 / pdb_00008q36
Title : Structure of Nucleosome Core with a Bound Metallopeptide Conjugate (Foamy Virus GAG Peptide-Au[I] Compound)
Authors : De Falco, L.; Batchelor, L.K.; Dyson, P.J.; Davey, C.A.
Deposited on : 2023-08-03
Resolution : 2.60 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

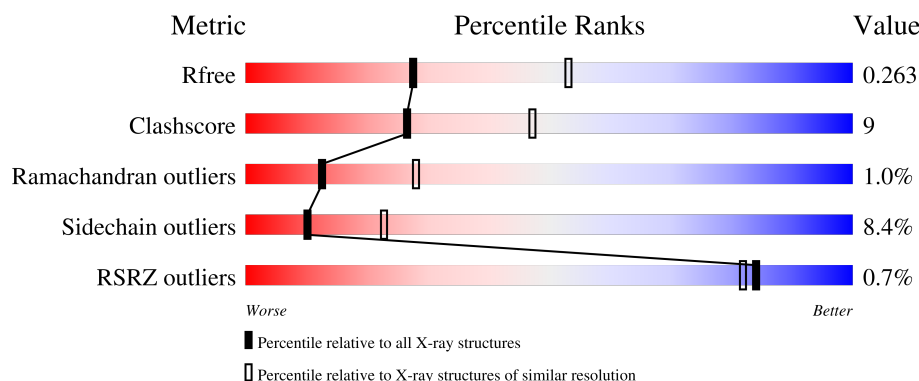
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



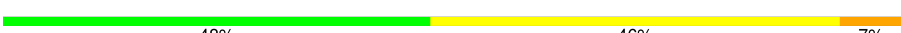
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	MMM	18	6% 67% 22% 11%
2	AAA	98	3% 72% 24% .
2	EEE	98	% 84% 13% .
3	BBB	87	% 82% 13% 6%
3	FFF	87	% 74% 24% ..

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Mol	Chain	Length	Quality of chain
4	CCC	107	 77% 19% • •
4	GGG	107	 79% 18% •
5	DDD	95	 79% 20% •
5	HHH	95	 68% 31% •
6	III	145	 49% 45% 6%
7	JJJ	145	 48% 46% 7%

2 Entry composition

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 GAG structural protein.

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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

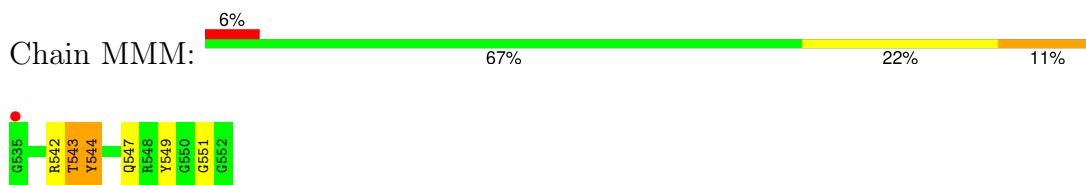
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

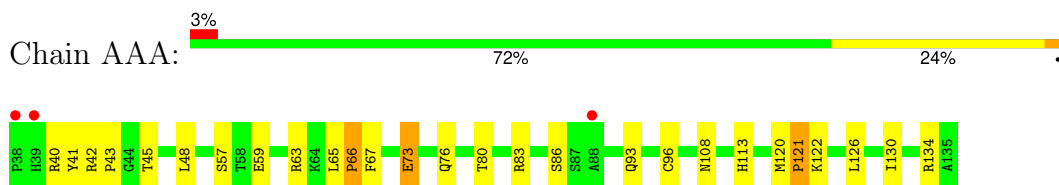
3 Residue-property plots [i](#)

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.

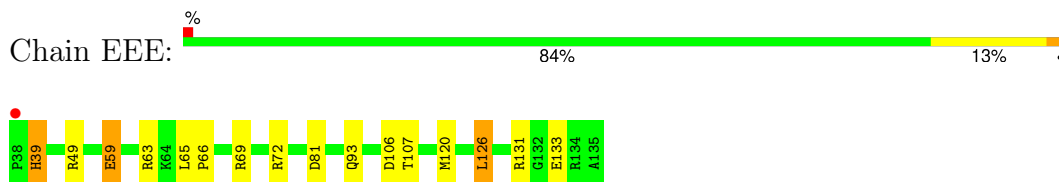
- Molecule 1: GAG structural protein



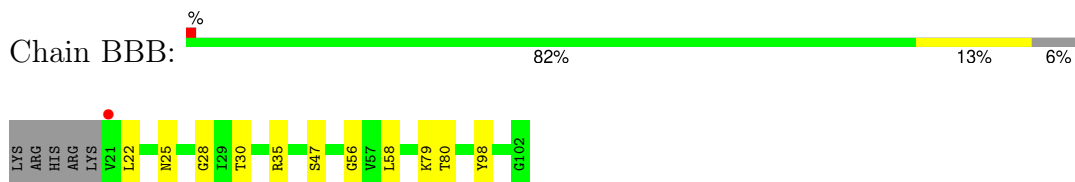
- Molecule 2: Histone H3.1



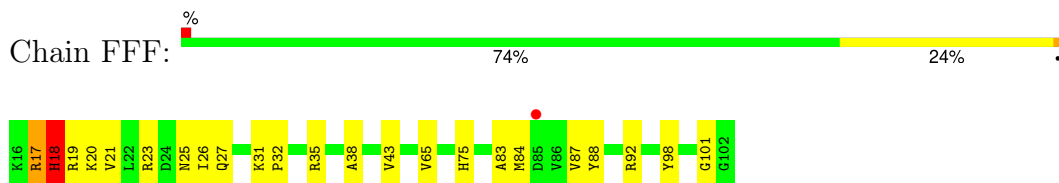
- Molecule 2: Histone H3.1



- Molecule 3: Histone H4



- Molecule 3: Histone H4



- Molecule 4: Histone H2A type 1-B/E

Chain CCC:  77% 19%



- Molecule 4: Histone H2A type 1-B/E

Chain GGG:  79% 18%



- Molecule 5: Histone H2B type 1-K

Chain DDD:  79% 20%



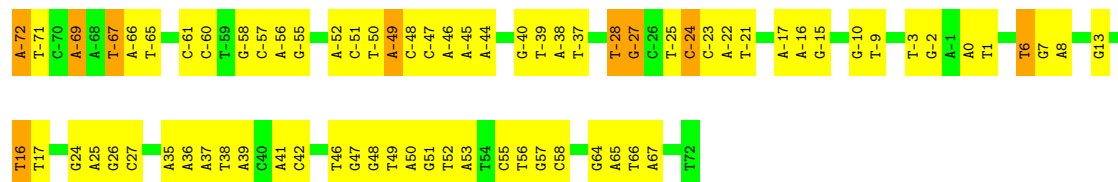
- Molecule 5: Histone H2B type 1-K

Chain HHH:  68% 31%



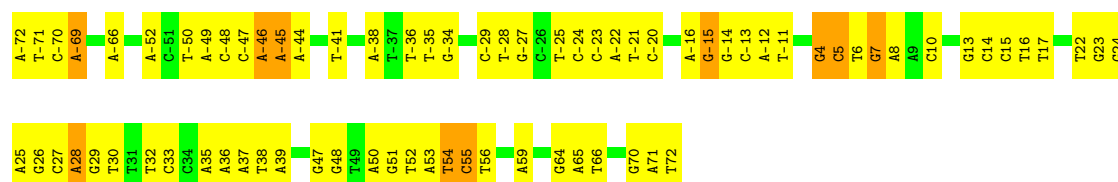
- Molecule 6: DNA (145-MER)

Chain III:  49% 45% 6%



- Molecule 7: DNA (145-MER)

Chain JJJ:  48% 46% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.19Å 109.56Å 183.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.60 48.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.6 (48.83-2.60) 93.6 (48.83-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.213 , 0.262 0.215 , 0.263	Depositor DCC
R_{free} test set	1262 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12197	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

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	0.99	0/145	1.54	2/195 (1.0%)
2	AAA	1.04	0/819	1.53	3/1097 (0.3%)
2	EEE	1.11	1/819 (0.1%)	1.60	4/1097 (0.4%)
3	BBB	1.09	0/660	1.64	3/883 (0.3%)
3	FFF	1.10	0/711	1.57	6/948 (0.6%)
4	CCC	1.06	0/838	1.57	3/1129 (0.3%)
4	GGG	1.14	1/838 (0.1%)	1.55	2/1129 (0.2%)
5	DDD	1.09	0/756	1.59	3/1014 (0.3%)
5	HHH	1.12	0/756	1.66	2/1014 (0.2%)
6	III	0.47	0/3332	1.02	15/5141 (0.3%)
7	JJJ	0.48	0/3330	1.00	14/5138 (0.3%)
All	All	0.83	2/13004 (0.0%)	1.30	57/18785 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EEE	93	GLN	C-O	5.46	1.30	1.24
4	GGG	50	TYR	C-O	5.39	1.30	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	III	6	DT	C2'-C3'-O3'	-9.60	97.10	111.50
7	JJJ	-45	DA	C2'-C3'-O3'	-9.27	97.60	111.50
6	III	-67	DT	C2'-C3'-O3'	-9.00	98.00	111.50
6	III	66	DT	C2'-C3'-O3'	8.48	124.21	111.50
6	III	16	DT	C4'-C3'-O3'	-8.22	97.67	110.00
6	III	-49	DA	N9-C1'-C2'	7.98	125.46	113.50
6	III	-40	DG	N9-C1'-C2'	7.87	125.30	113.50
5	HHH	116	THR	CB-CA-C	7.70	122.81	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	JJJ	-45	DA	C4'-C3'-O3'	7.19	120.79	110.00
6	III	-49	DA	C4-N9-C1'	-7.07	116.45	127.05
6	III	-49	DA	C8-N9-C1'	7.03	137.60	127.05
7	JJJ	4	DG	C2'-C3'-O3'	-7.03	100.96	111.50
6	III	-28	DT	C2'-C3'-O3'	-6.93	101.11	111.50
6	III	-69	DA	C2'-C3'-O3'	-6.47	101.80	111.50
7	JJJ	-25	DT	C2'-C3'-O3'	-6.21	102.18	111.50
7	JJJ	-46	DA	C2'-C3'-O3'	6.10	120.65	111.50
1	MMM	543	THR	CA-CB-OG1	-6.06	100.52	109.60
5	DDD	67	PHE	CA-C-O	-6.04	113.96	121.02
6	III	-49	DA	C1'-O4'-C4'	-5.93	100.80	109.70
7	JJJ	-69	DA	C2'-C3'-O3'	-5.85	102.73	111.50
7	JJJ	55	DC	C2'-C3'-O3'	5.81	120.22	111.50
7	JJJ	30	DT	C2'-C3'-O3'	-5.77	102.84	111.50
7	JJJ	5	DC	C4'-C3'-O3'	5.77	118.66	110.00
5	DDD	75	SER	CA-C-N	5.67	128.16	120.44
5	DDD	75	SER	C-N-CA	5.67	128.16	120.44
7	JJJ	-15	DG	C2'-C3'-O3'	5.64	119.97	111.50
6	III	-24	DC	C2'-C3'-O3'	-5.63	103.06	111.50
7	JJJ	47	DG	C2'-C3'-O3'	-5.61	103.09	111.50
4	CCC	72	ASP	CA-CB-CG	5.60	118.20	112.60
2	EEE	106	ASP	N-CA-C	-5.59	105.19	111.28
7	JJJ	54	DT	C4'-C3'-O3'	-5.55	101.67	110.00
2	EEE	126	LEU	N-CA-C	-5.47	105.40	111.36
6	III	-27	DG	C2'-C3'-O3'	-5.40	103.40	111.50
3	FFF	92	ARG	CB-CA-C	-5.37	101.55	110.68
2	AAA	66	PRO	CA-C-N	5.33	127.69	120.44
2	AAA	66	PRO	C-N-CA	5.33	127.69	120.44
2	AAA	45	THR	CA-CB-OG1	-5.30	101.65	109.60
4	CCC	81	ARG	N-CA-C	-5.25	105.56	111.28
3	BBB	56	GLY	CA-C-N	5.20	127.11	120.56
3	BBB	56	GLY	C-N-CA	5.20	127.11	120.56
1	MMM	549	TYR	CA-C-O	-5.17	115.03	120.92
7	JJJ	7	DG	P-O5'-C5'	-5.15	112.28	120.00
5	HHH	112	THR	CA-CB-OG1	-5.14	101.89	109.60
4	GGG	97	LEU	CA-C-N	5.14	125.79	120.03
4	GGG	97	LEU	C-N-CA	5.14	125.79	120.03
3	FFF	21	VAL	CA-C-N	5.14	129.25	122.42
3	FFF	21	VAL	C-N-CA	5.14	129.25	122.42
3	FFF	27	GLN	N-CA-C	-5.12	107.00	113.20
2	EEE	107	THR	CA-C-N	5.09	127.10	120.28
2	EEE	107	THR	C-N-CA	5.09	127.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	III	46	DT	C2'-C3'-O3'	-5.08	103.87	111.50
6	III	-72	DA	C4'-C3'-O3'	5.08	117.62	110.00
7	JJJ	28	DA	C2'-C3'-O3'	-5.06	103.91	111.50
3	FFF	101	GLY	CA-C-O	-5.06	117.25	122.26
3	FFF	65	VAL	N-CA-C	-5.05	105.78	110.53
4	CCC	76	THR	CA-CB-OG1	-5.03	102.06	109.60
3	BBB	79	LYS	N-CA-C	-5.02	105.86	112.94

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	MMM	141	0	131	1	0
2	AAA	807	0	844	18	0
2	EEE	807	0	844	12	0
3	BBB	653	0	696	8	0
3	FFF	703	0	755	14	0
4	CCC	828	0	892	18	0
4	GGG	828	0	892	16	0
5	DDD	745	0	769	14	0
5	HHH	745	0	769	12	0
6	III	2970	0	1640	68	0
7	JJJ	2969	0	1641	73	0
8	EEE	1	0	0	0	0
All	All	12197	0	9873	205	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 9.

All (205) 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:GGG:50:TYR:OH	5:HHH:92:GLN:NE2	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CCC:50:TYR:OH	5:DDD:92:GLN:NE2	2.07	0.85
7:JJJ:-49:DA:H4'	7:JJJ:-48:DC:OP1	1.73	0.85
4:GGG:102:ILE:HG23	5:HHH:58:ILE:HD13	1.59	0.83
7:JJJ:-22:DA:H2''	7:JJJ:-21:DT:O5'	1.80	0.80
6:III:-50:DT:C4	6:III:-49:DA:N6	2.55	0.75
5:DDD:79:HIS:NE2	4:GGG:38:ASN:OD1	2.22	0.73
2:AAA:96:CYS:SG	3:BBB:58:LEU:CD1	2.77	0.73
6:III:53:DA:C2	7:JJJ:-52:DA:C2	2.80	0.70
7:JJJ:53:DA:H4'	7:JJJ:54:DT:OP1	1.90	0.70
7:JJJ:-28:DT:H3'	7:JJJ:-27:DG:H5''	1.75	0.68
2:AAA:76:GLN:HE21	2:AAA:80:THR:HG22	1.59	0.67
4:CCC:32:ARG:HH22	5:DDD:32:GLU:CD	2.02	0.67
4:CCC:26:PRO:HG3	5:DDD:37:TYR:CZ	2.30	0.67
2:EEE:69:ARG:HD2	3:FFF:25:ASN:OD1	1.94	0.67
6:III:-52:DA:C2	7:JJJ:53:DA:N1	2.63	0.66
6:III:-52:DA:C2	7:JJJ:53:DA:C2	2.84	0.66
6:III:-58:DG:N2	7:JJJ:59:DA:C2	2.64	0.65
4:GGG:29:ARG:NH1	5:HHH:33:SER:O	2.30	0.65
7:JJJ:13:DG:H4'	7:JJJ:14:DC:OP1	1.97	0.64
2:AAA:73:GLU:OE1	3:BBB:25:ASN:HB2	1.98	0.64
4:CCC:26:PRO:HG3	5:DDD:37:TYR:CE2	2.33	0.64
4:CCC:99:ARG:HG3	4:CCC:99:ARG:HH11	1.63	0.63
5:DDD:77:LEU:HD21	5:DDD:93:THR:HB	1.80	0.63
6:III:-56:DA:H2''	6:III:-55:DG:OP2	1.98	0.63
7:JJJ:24:DG:H4'	7:JJJ:25:DA:OP1	1.99	0.62
7:JJJ:-28:DT:C3'	7:JJJ:-27:DG:H5''	2.30	0.62
7:JJJ:50:DA:H2''	7:JJJ:51:DG:OP2	2.00	0.62
2:AAA:96:CYS:SG	3:BBB:58:LEU:HD13	2.40	0.62
4:CCC:25:PHE:CZ	4:CCC:59:THR:HG21	2.35	0.61
2:AAA:41:TYR:HB2	7:JJJ:10:DC:OP1	2.01	0.61
6:III:13:DG:N2	7:JJJ:-12:DA:C2	2.70	0.60
6:III:41:DA:C4	6:III:42:DC:C5	2.89	0.59
3:FFF:35:ARG:HH22	6:III:8:DA:P	2.26	0.59
7:JJJ:5:DC:H4'	7:JJJ:6:DT:OP1	2.02	0.59
2:EEE:81:ASP:HA	3:FFF:19:ARG:HH22	1.67	0.58
6:III:-50:DT:C4	6:III:-49:DA:C6	2.91	0.58
6:III:49:DT:H2''	6:III:50:DA:C8	2.38	0.58
2:EEE:49:ARG:HG3	2:EEE:49:ARG:HH11	1.69	0.57
6:III:13:DG:C2	7:JJJ:-12:DA:C2	2.92	0.57
7:JJJ:-15:DG:H2''	7:JJJ:-14:DG:OP2	2.04	0.57
2:AAA:63:ARG:CZ	7:JJJ:17:DT:H4'	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:FFF:31:LYS:N	3:FFF:32:PRO:HD2	2.19	0.57
7:JJJ:28:DA:H4'	7:JJJ:29:DG:OP1	2.04	0.57
7:JJJ:-49:DA:C4'	7:JJJ:-48:DC:OP1	2.49	0.56
3:BBB:98:TYR:CD1	5:HHH:61:SER:HB3	2.40	0.56
6:III:-28:DT:H4'	6:III:-27:DG:OP1	2.06	0.55
4:CCC:81:ARG:O	4:CCC:81:ARG:HG3	2.07	0.54
6:III:-24:DC:C2	6:III:-23:DC:C4	2.95	0.54
7:JJJ:14:DC:H4'	7:JJJ:15:DC:OP1	2.07	0.54
2:EEE:81:ASP:HA	3:FFF:19:ARG:NH2	2.23	0.54
6:III:-39:DT:H2''	6:III:-38:DA:H8	1.73	0.53
2:AAA:83:ARG:O	3:BBB:80:THR:HA	2.07	0.53
5:DDD:30:ARG:O	5:DDD:30:ARG:HG3	2.07	0.53
4:GGG:102:ILE:CG2	5:HHH:58:ILE:HD13	2.34	0.53
4:CCC:47:ALA:HB3	4:CCC:48:PRO:HD3	1.90	0.53
6:III:-50:DT:O4	6:III:-49:DA:N6	2.40	0.53
2:AAA:96:CYS:SG	3:BBB:58:LEU:HD11	2.49	0.52
1:MMM:544:TYR:CD1	1:MMM:544:TYR:N	2.78	0.52
5:DDD:65:ASP:O	5:DDD:69:ARG:HG3	2.10	0.52
6:III:51:DG:N2	7:JJJ:-50:DT:O2	2.43	0.51
6:III:-24:DC:H1'	6:III:-23:DC:C6	2.45	0.51
6:III:-22:DA:C2	7:JJJ:23:DG:N2	2.79	0.51
2:AAA:63:ARG:HB2	2:AAA:66:PRO:HG2	1.91	0.51
6:III:-58:DG:N3	6:III:-57:DC:O2	2.44	0.51
6:III:-61:DC:H2''	6:III:-60:DC:O5'	2.11	0.50
3:BBB:28:GLY:O	3:BBB:30:THR:HG23	2.11	0.50
6:III:-24:DC:H1'	6:III:-23:DC:C5	2.46	0.50
6:III:24:DG:H2''	6:III:25:DA:OP2	2.11	0.50
4:CCC:99:ARG:HH11	4:CCC:99:ARG:CG	2.24	0.50
6:III:-22:DA:H2''	6:III:-21:DT:OP2	2.11	0.50
6:III:67:DA:C2	7:JJJ:-66:DA:C2	3.00	0.50
7:JJJ:-16:DA:H4'	7:JJJ:-15:DG:OP1	2.11	0.50
7:JJJ:55:DC:C6	7:JJJ:56:DT:H72	2.47	0.50
6:III:0:DA:H1'	6:III:1:DT:H5'	1.93	0.50
7:JJJ:51:DG:OP2	7:JJJ:51:DG:H2'	2.12	0.49
6:III:-69:DA:C2	7:JJJ:70:DG:N2	2.81	0.49
6:III:-45:DA:H1'	6:III:-44:DA:H5'	1.93	0.49
6:III:38:DT:H1'	6:III:39:DA:C8	2.48	0.49
4:GGG:76:THR:O	5:HHH:49:THR:HG23	2.11	0.49
6:III:-38:DA:C2	7:JJJ:39:DA:C2	3.00	0.49
7:JJJ:35:DA:H2''	7:JJJ:36:DA:OP2	2.12	0.49
7:JJJ:-28:DT:H2'	7:JJJ:-27:DG:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DDD:30:ARG:O	5:DDD:30:ARG:CG	2.61	0.48
7:JJJ:53:DA:C2	7:JJJ:54:DT:C2	3.01	0.48
6:III:-66:DA:C2	6:III:-65:DT:C2	3.01	0.48
2:AAA:40:ARG:HG3	7:JJJ:10:DC:H5''	1.96	0.48
7:JJJ:50:DA:C6	7:JJJ:51:DG:C6	3.02	0.48
4:GGG:13:LYS:HD3	7:JJJ:-41:DT:OP1	2.14	0.47
4:GGG:59:THR:HG22	4:GGG:63:LEU:HD12	1.96	0.47
6:III:-51:DC:H5''	6:III:-51:DC:H6	1.78	0.47
6:III:-10:DG:H2''	6:III:-9:DT:OP2	2.14	0.47
2:AAA:120:MET:O	2:AAA:121:PRO:C	2.57	0.47
7:JJJ:-13:DC:H2''	7:JJJ:-12:DA:OP2	2.14	0.47
3:FFF:17:ARG:O	3:FFF:18:HIS:O	2.31	0.47
5:HHH:39:TYR:CE1	5:HHH:43:LYS:HE2	2.49	0.47
7:JJJ:-70:DC:H2''	7:JJJ:-69:DA:OP2	2.14	0.47
2:EEE:39:HIS:O	2:EEE:39:HIS:ND1	2.48	0.47
5:HHH:46:HIS:HB3	5:HHH:49:THR:OG1	2.15	0.47
6:III:25:DA:C2	6:III:26:DG:C2	3.03	0.46
7:JJJ:25:DA:C5	7:JJJ:26:DG:C6	3.02	0.46
6:III:57:DG:C5	6:III:58:DC:C4	3.03	0.46
5:DDD:79:HIS:CE1	4:GGG:38:ASN:OD1	2.69	0.46
6:III:-39:DT:H2''	6:III:-38:DA:C8	2.51	0.46
6:III:35:DA:H4'	6:III:36:DA:OP1	2.14	0.46
7:JJJ:65:DA:H2''	7:JJJ:66:DT:OP2	2.15	0.46
4:CCC:55:LEU:O	4:CCC:59:THR:CG2	2.64	0.46
7:JJJ:-34:DG:H2'	7:JJJ:-34:DG:OP2	2.16	0.46
6:III:-25:DT:C2'	6:III:-24:DC:C6	2.98	0.46
7:JJJ:-21:DT:C4	7:JJJ:-20:DC:N4	2.83	0.46
4:GGG:31:HIS:CD2	4:GGG:48:PRO:HG3	2.51	0.46
6:III:-67:DT:H1'	6:III:-66:DA:C8	2.52	0.45
5:DDD:39:TYR:O	5:DDD:40:LYS:C	2.59	0.45
6:III:-72:DA:C2	6:III:-71:DT:C2	3.05	0.45
7:JJJ:27:DC:C4	7:JJJ:28:DA:C6	3.04	0.45
2:AAA:65:LEU:O	2:AAA:66:PRO:C	2.60	0.45
4:CCC:29:ARG:NH2	7:JJJ:48:DG:OP1	2.44	0.45
6:III:35:DA:C4'	6:III:36:DA:OP1	2.64	0.45
6:III:55:DC:C2'	6:III:56:DT:H71	2.46	0.45
3:FFF:75:HIS:CD2	3:FFF:75:HIS:O	2.70	0.45
4:GGG:88:ARG:NH2	4:GGG:97:LEU:O	2.49	0.45
6:III:39:DA:C2	7:JJJ:-38:DA:C2	3.04	0.45
6:III:51:DG:H2''	6:III:52:DT:O5'	2.16	0.45
7:JJJ:71:DA:C5	7:JJJ:72:DT:C4	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:III:38:DT:H2''	6:III:39:DA:OP2	2.17	0.45
2:AAA:63:ARG:NH1	7:JJJ:17:DT:H4'	2.31	0.45
7:JJJ:-47:DC:O3'	7:JJJ:-46:DA:C8	2.70	0.45
7:JJJ:15:DC:H2''	7:JJJ:16:DT:OP2	2.17	0.45
7:JJJ:52:DT:H2''	7:JJJ:53:DA:OP2	2.17	0.45
7:JJJ:37:DA:H2''	7:JJJ:38:DT:OP2	2.16	0.44
3:FFF:83:ALA:O	3:FFF:87:VAL:HG23	2.18	0.44
7:JJJ:28:DA:H1'	7:JJJ:29:DG:C8	2.52	0.44
4:CCC:32:ARG:O	4:CCC:35:ARG:HB3	2.17	0.44
6:III:26:DG:H1'	6:III:27:DC:H5'	1.98	0.44
6:III:64:DG:H1'	6:III:65:DA:C8	2.52	0.44
4:CCC:55:LEU:O	4:CCC:59:THR:HG22	2.18	0.44
3:FFF:84:MET:HE3	3:FFF:88:TYR:CZ	2.52	0.44
6:III:41:DA:C5	6:III:42:DC:C4	3.05	0.44
6:III:37:DA:C5	6:III:38:DT:C4	3.06	0.44
3:BBB:35:ARG:NH2	7:JJJ:8:DA:OP2	2.36	0.44
5:DDD:77:LEU:CD2	5:DDD:93:THR:HB	2.47	0.44
4:CCC:29:ARG:NH2	5:DDD:33:SER:O	2.50	0.44
4:CCC:100:VAL:HG11	3:FFF:98:TYR:CE2	2.53	0.44
5:HHH:99:LEU:HA	5:HHH:100:PRO:HD3	1.89	0.44
6:III:-17:DA:C2	6:III:-16:DA:C5	3.06	0.44
6:III:-47:DC:H4'	6:III:-46:DA:OP1	2.18	0.43
6:III:-47:DC:O2	6:III:-47:DC:O4'	2.34	0.43
6:III:-17:DA:C2	6:III:-16:DA:C4	3.06	0.43
7:JJJ:-71:DT:H2''	7:JJJ:-70:DC:O5'	2.18	0.43
2:AAA:108:ASN:HD21	4:GGG:115:LEU:HD11	1.83	0.43
7:JJJ:4:DG:H4'	7:JJJ:5:DC:OP1	2.17	0.43
7:JJJ:-24:DC:H2''	7:JJJ:-23:DC:OP2	2.19	0.43
6:III:-16:DA:H2''	6:III:-15:DG:C8	2.54	0.43
2:EEE:69:ARG:HB3	3:FFF:25:ASN:OD1	2.19	0.43
2:EEE:72:ARG:HH11	2:EEE:72:ARG:HG2	1.83	0.43
3:FFF:38:ALA:HB1	3:FFF:43:VAL:HB	2.00	0.43
6:III:-50:DT:H3'	6:III:-49:DA:O4'	2.19	0.43
7:JJJ:22:DT:H2''	7:JJJ:23:DG:C8	2.54	0.43
2:AAA:126:LEU:HD11	2:AAA:130:ILE:HD11	2.01	0.43
7:JJJ:-50:DT:C4	7:JJJ:-49:DA:N6	2.87	0.43
6:III:-3:DT:C4	6:III:-2:DG:C6	3.07	0.42
7:JJJ:37:DA:C2	7:JJJ:38:DT:C2	3.07	0.42
7:JJJ:32:DT:H2''	7:JJJ:33:DC:C5	2.55	0.42
4:CCC:62:ILE:HD12	5:DDD:62:PHE:CE2	2.53	0.42
5:HHH:35:SER:HA	5:HHH:56:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:JJJ:-47:DC:O2	7:JJJ:-46:DA:C2	2.73	0.42
7:JJJ:-29:DC:H2'	7:JJJ:-28:DT:C6	2.55	0.42
6:III:56:DT:H2''	6:III:57:DG:N7	2.35	0.42
7:JJJ:24:DG:C4'	7:JJJ:25:DA:OP1	2.67	0.42
4:CCC:81:ARG:NH2	4:CCC:107:VAL:O	2.41	0.42
4:GGG:14:ALA:O	4:GGG:15:LYS:HD2	2.19	0.42
4:GGG:32:ARG:NH2	5:HHH:32:GLU:OE2	2.38	0.42
3:FFF:31:LYS:N	3:FFF:32:PRO:CD	2.82	0.41
2:EEE:131:ARG:HD3	2:EEE:133:GLU:OE2	2.20	0.41
7:JJJ:-72:DA:H3'	7:JJJ:-71:DT:H71	2.01	0.41
7:JJJ:-13:DC:C2'	7:JJJ:-12:DA:OP2	2.68	0.41
2:EEE:69:ARG:HB3	3:FFF:25:ASN:CG	2.45	0.41
6:III:-25:DT:H2''	6:III:-24:DC:C6	2.54	0.41
6:III:13:DG:N2	7:JJJ:-12:DA:N3	2.69	0.41
6:III:50:DA:H2''	6:III:51:DG:O4'	2.20	0.41
2:EEE:59:GLU:H	2:EEE:59:GLU:HG3	1.61	0.41
5:HHH:77:LEU:HD11	5:HHH:93:THR:HG22	2.03	0.41
7:JJJ:27:DC:C5	7:JJJ:28:DA:N6	2.88	0.41
6:III:16:DT:H2''	6:III:17:DT:H72	2.03	0.41
7:JJJ:-45:DA:C2	7:JJJ:-44:DA:C6	3.08	0.41
7:JJJ:6:DT:H4'	7:JJJ:7:DG:OP1	2.21	0.41
2:AAA:113:HIS:CG	2:EEE:126:LEU:HD22	2.56	0.41
4:GGG:81:ARG:HD2	4:GGG:81:ARG:O	2.20	0.41
6:III:-56:DA:C2'	6:III:-55:DG:OP2	2.66	0.41
6:III:-50:DT:C3'	6:III:-49:DA:O4'	2.68	0.41
6:III:6:DT:H2''	6:III:7:DG:C8	2.55	0.41
7:JJJ:-36:DT:C6	7:JJJ:-35:DT:H72	2.56	0.41
7:JJJ:-12:DA:H1'	7:JJJ:-11:DT:H5'	2.03	0.41
4:GGG:35:ARG:C	4:GGG:37:GLY:H	2.29	0.41
6:III:47:DG:C2	6:III:48:DG:C2	3.09	0.40
7:JJJ:64:DG:H1'	7:JJJ:65:DA:C8	2.56	0.40
2:AAA:67:PHE:CZ	2:AAA:93:GLN:HA	2.57	0.40
6:III:-48:DC:H1'	6:III:-47:DC:C2	2.56	0.40
7:JJJ:25:DA:C6	7:JJJ:26:DG:N1	2.89	0.40
7:JJJ:51:DG:C5	7:JJJ:52:DT:C4	3.09	0.40
4:CCC:88:ARG:HA	4:CCC:88:ARG:HD3	1.89	0.40
6:III:26:DG:H2''	6:III:27:DC:OP2	2.20	0.40
2:EEE:65:LEU:HB3	2:EEE:66:PRO:HD3	2.02	0.40
6:III:-38:DA:C2	6:III:-37:DT:C2	3.09	0.40
2:AAA:42:ARG:O	2:AAA:43:PRO:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	14 (88%)	1 (6%)	1 (6%)	1	1
2	AAA	96/98 (98%)	86 (90%)	9 (9%)	1 (1%)	12	28
2	EEE	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
3	BBB	80/87 (92%)	76 (95%)	4 (5%)	0	100	100
3	FFF	85/87 (98%)	83 (98%)	1 (1%)	1 (1%)	10	23
4	CCC	105/107 (98%)	99 (94%)	4 (4%)	2 (2%)	6	13
4	GGG	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
5	DDD	93/95 (98%)	79 (85%)	13 (14%)	1 (1%)	11	25
5	HHH	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	5	10
All	All	769/792 (97%)	713 (93%)	48 (6%)	8 (1%)	12	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	FFF	18	HIS
4	CCC	118	LYS
5	DDD	101	GLY
5	HHH	51	ILE
5	HHH	101	GLY
2	AAA	73	GLU
4	CCC	18	SER
1	MMM	551	GLY

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	MMM	13/13 (100%)	9 (69%)	4 (31%)	0	0
2	AAA	85/85 (100%)	78 (92%)	7 (8%)	10	24
2	EEE	85/85 (100%)	81 (95%)	4 (5%)	23	48
3	BBB	67/72 (93%)	65 (97%)	2 (3%)	36	64
3	FFF	72/72 (100%)	67 (93%)	5 (7%)	14	32
4	CCC	85/85 (100%)	75 (88%)	10 (12%)	5	10
4	GGG	85/85 (100%)	79 (93%)	6 (7%)	13	31
5	DDD	81/81 (100%)	76 (94%)	5 (6%)	16	36
5	HHH	81/81 (100%)	69 (85%)	12 (15%)	3	6
All	All	654/659 (99%)	599 (92%)	55 (8%)	10	23

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	MMM	542	ARG
1	MMM	543	THR
1	MMM	544	TYR
1	MMM	547	GLN
2	AAA	48	LEU
2	AAA	57	SER
2	AAA	59	GLU
2	AAA	86	SER
2	AAA	121	PRO
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	36	LYS
4	CCC	59	THR
4	CCC	74	LYS
4	CCC	76	THR
4	CCC	81	ARG
4	CCC	99	ARG
4	CCC	119	LYS
5	DDD	30	ARG

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Mol	Chain	Res	Type
5	DDD	36	VAL
5	DDD	53	SER
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	26	ILE
4	GGG	15	LYS
4	GGG	36	LYS
4	GGG	75	LYS
4	GGG	80	PRO
4	GGG	88	ARG
4	GGG	118	LYS
5	HHH	30	ARG
5	HHH	33	SER
5	HHH	44	GLN
5	HHH	45	VAL
5	HHH	84	SER
5	HHH	85	THR
5	HHH	88	SER
5	HHH	102	GLU
5	HHH	103	LEU
5	HHH	105	LYS
5	HHH	106	HIS
5	HHH	109	SER

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 ⓘ

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 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	MMM	18/18 (100%)	0.34	1 (5%) 30 24	70, 98, 134, 162	0
2	AAA	98/98 (100%)	-0.13	3 (3%) 51 45	50, 69, 113, 157	0
2	EEE	98/98 (100%)	-0.39	1 (1%) 79 76	39, 55, 92, 136	0
3	BBB	82/87 (94%)	-0.20	1 (1%) 76 73	48, 68, 93, 170	0
3	FFF	87/87 (100%)	-0.21	1 (1%) 78 74	43, 56, 94, 155	0
4	CCC	107/107 (100%)	-0.33	0 100 100	45, 62, 109, 168	0
4	GGG	107/107 (100%)	-0.14	0 100 100	51, 74, 125, 159	0
5	DDD	95/95 (100%)	-0.27	0 100 100	50, 68, 120, 162	0
5	HHH	95/95 (100%)	0.09	1 (1%) 78 74	51, 78, 125, 164	0
6	III	145/145 (100%)	-0.34	0 100 100	71, 137, 185, 240	0
7	JJJ	145/145 (100%)	-0.36	0 100 100	79, 133, 184, 216	0
All	All	1077/1082 (99%)	-0.23	8 (0%) 84 82	39, 77, 168, 240	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AAA	38	PRO	5.4
2	AAA	39	HIS	2.8
2	EEE	38	PRO	2.7
5	HHH	77	LEU	2.7
1	MMM	535	GLY	2.6
2	AAA	88	ALA	2.5
3	FFF	85	ASP	2.3
3	BBB	21	VAL	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 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	0.96	0.20	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.