



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:54 AM UTC

PDB ID : 5HQ2 / pdb_00005hq2
Title : Structural model of Set8 histone H4 Lys20 methyltransferase bound to nucleosome core particle
Authors : Tavarekere, G.; McGinty, R.K.; Tan, S.
Deposited on : 2016-01-21
Resolution : 4.50 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
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

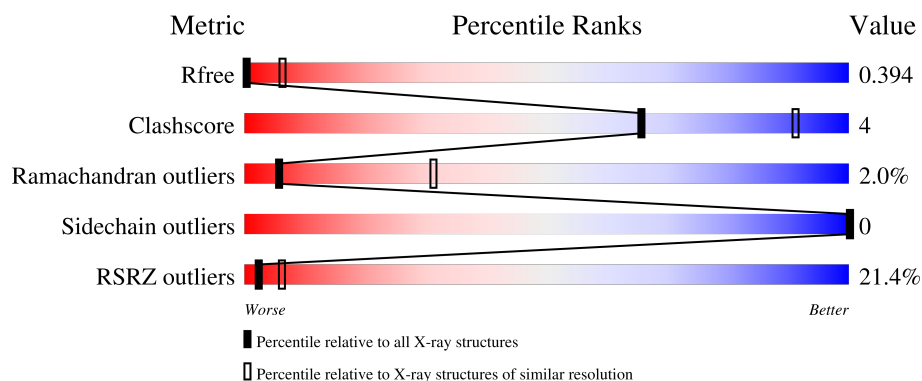
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	A	135	 7% 59% 13% • 27%
2	B	102	 9% 68% 9% 24%
3	G	129	 7% 72% 9% 19%
4	H	122	 8% 68% 10% 22%
5	I	149	 11% 48% • 51%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	J	149	
7	K	483	
8	M	202	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7738 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 H3.2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	0	0	0
			495	297	99	99			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	0	0	0
			384	228	78	78			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	105	Total	C	N	O	0	0	0
			516	306	105	105			

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	95	Total	C	N	O	0	0	0
			473	283	95	95			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called DNA (149-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	73	Total	C	N	O	P	0	0	0
			1487	707	271	436	73			

- Molecule 6 is a DNA chain called DNA (149-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	72	Total	C	N	O	P	0	0	0
			1484	704	274	434	72			

- Molecule 7 is a protein called Guanine nucleotide exchange factor SRM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	422	Total	C	N	O	0	0	0
			2112	1268	422	422			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP P21827
K	1	SER	-	expression tag	UNP P21827

- Molecule 8 is a protein called N-lysine methyltransferase SETD8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	160	Total	C	N	O	0	0	0
			787	467	160	160			

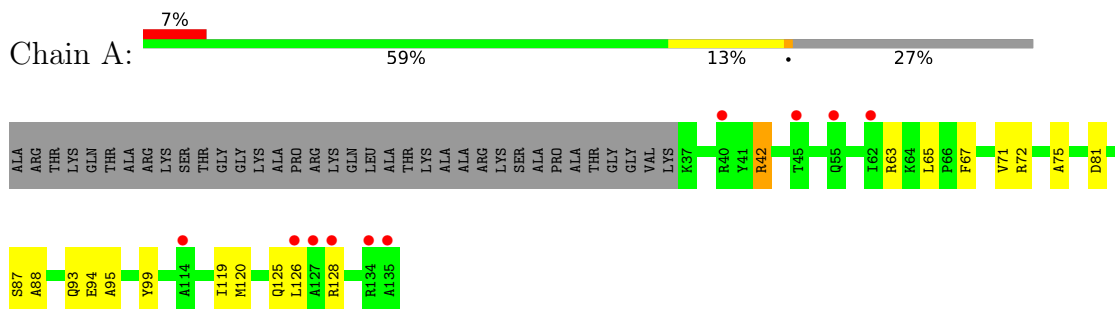
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	151	GLY	-	expression tag	UNP Q9NQR1
M	152	SER	-	expression tag	UNP Q9NQR1
M	347	PHE	HIS	conflict	UNP Q9NQR1

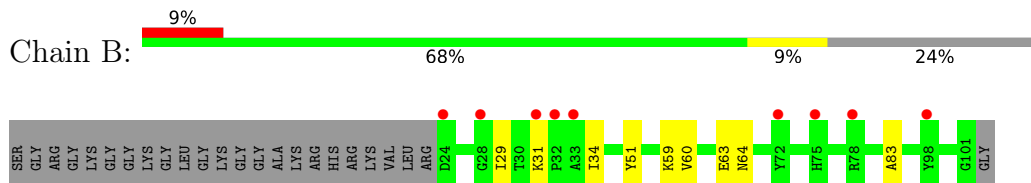
3 Residue-property plots

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.

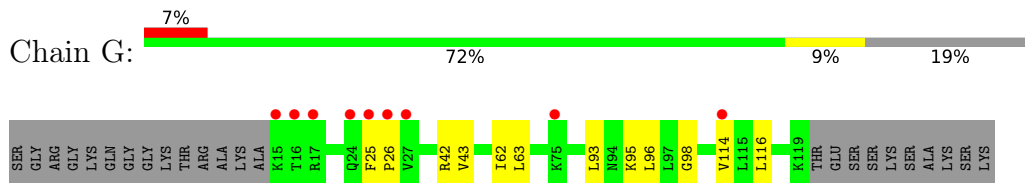
- Molecule 1: Histone H3.2



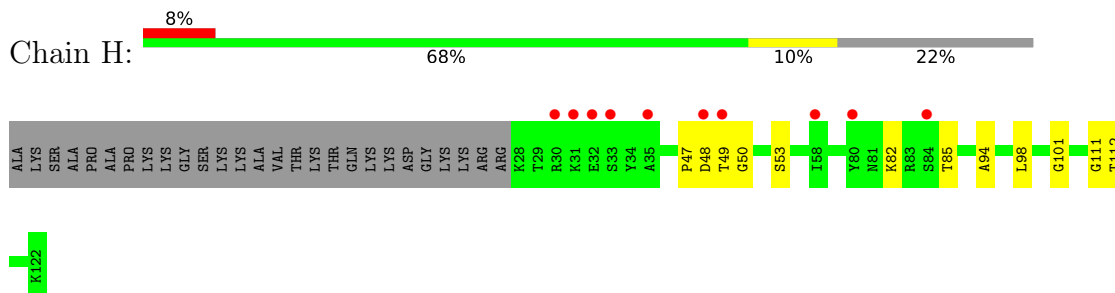
- Molecule 2: Histone H4



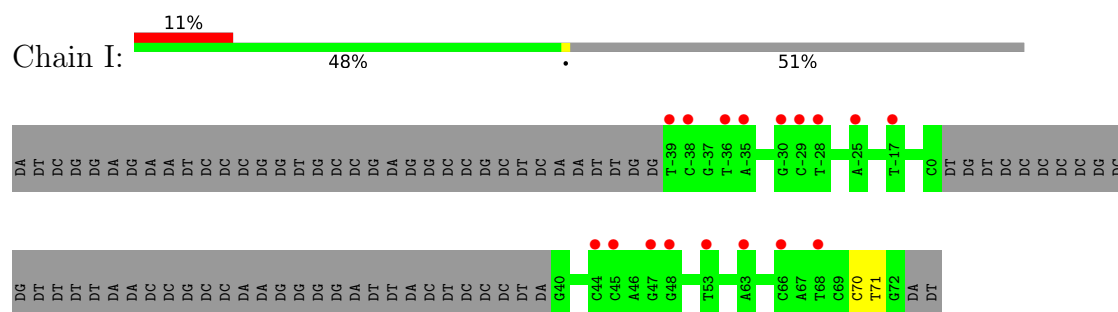
- Molecule 3: Histone H2A



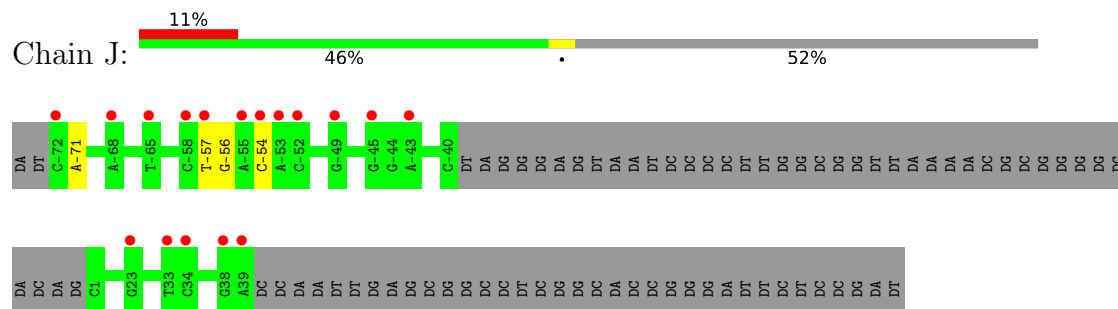
- Molecule 4: Histone H2B 1.1



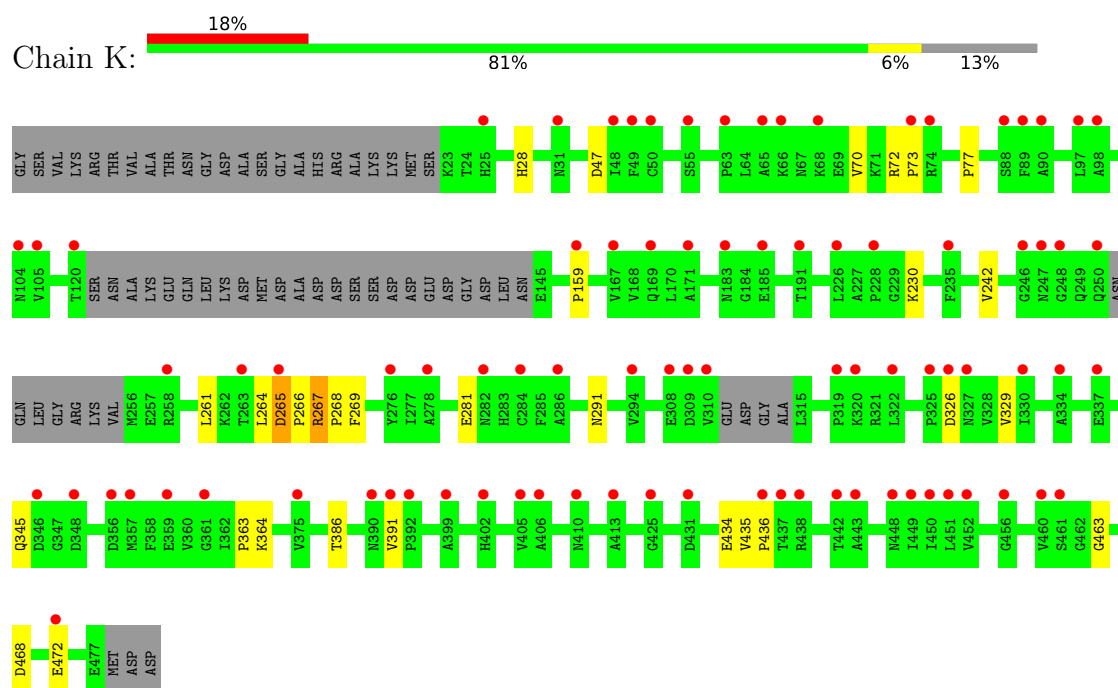
- Molecule 5: DNA (149-MER)



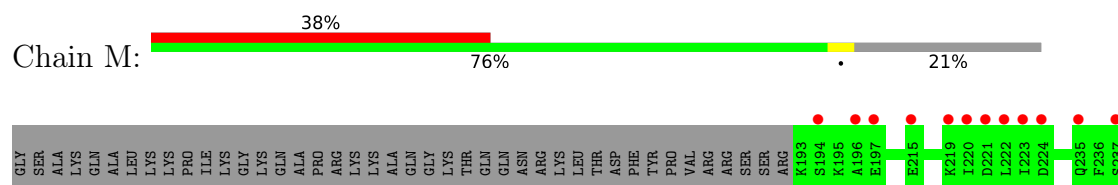
• Molecule 6: DNA (149-MER)

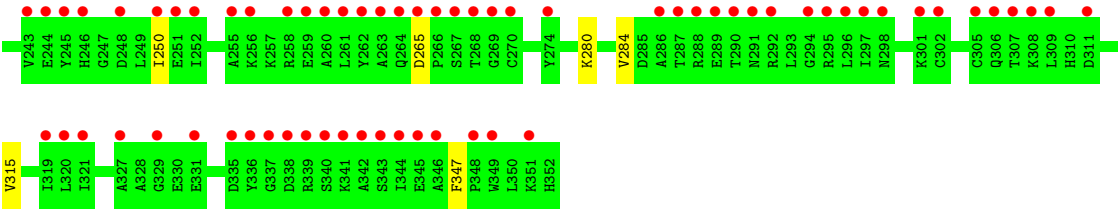


• Molecule 7: Guanine nucleotide exchange factor SRM1



• Molecule 8: N-lysine methyltransferase SETD8





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.73Å 300.75Å 182.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 4.50 46.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.00-4.50) 99.3 (46.00-4.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.339 , 0.397 0.346 , 0.394	Depositor DCC
R_{free} test set	845 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	213.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 366.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7738	wwPDB-VP
Average B, all atoms (Å ²)	221.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.78	0/495	1.27	9/691 (1.3%)
2	B	0.75	0/384	1.30	3/532 (0.6%)
3	G	0.73	0/515	1.20	4/714 (0.6%)
4	H	0.71	0/473	1.20	2/659 (0.3%)
5	I	0.31	0/1665	0.59	0/2562
6	J	0.32	0/1664	0.62	0/2566
7	K	0.64	0/2130	1.00	4/2968 (0.1%)
8	M	0.61	0/786	1.12	6/1091 (0.5%)
All	All	0.56	0/8112	0.93	28/11783 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	265	ASP	CA-C-N	10.90	130.68	119.56
8	M	265	ASP	C-N-CA	10.90	130.68	119.56
8	M	347	PHE	CA-C-N	8.74	128.97	119.87
8	M	347	PHE	C-N-CA	8.74	128.97	119.87
7	K	391	VAL	CA-C-N	7.82	127.72	120.21
7	K	391	VAL	C-N-CA	7.82	127.72	120.21
2	B	51	TYR	N-CA-C	7.20	119.80	111.02
4	H	101	GLY	N-CA-C	6.71	129.09	113.18
1	A	42	ARG	CA-C-N	6.51	127.97	119.84
1	A	42	ARG	C-N-CA	6.51	127.97	119.84
4	H	82	LYS	N-CA-C	6.42	120.23	111.17
3	G	25	PHE	CA-C-N	6.29	127.71	119.84
3	G	25	PHE	C-N-CA	6.29	127.71	119.84
7	K	261	LEU	N-CA-C	6.12	117.61	108.31
7	K	159	PRO	N-CA-C	6.10	118.14	110.70
2	B	34	ILE	N-CA-C	-6.00	103.98	110.23
1	A	119	ILE	N-CA-C	5.86	115.69	107.37
8	M	315	VAL	CA-C-N	5.63	125.39	119.76
8	M	315	VAL	C-N-CA	5.63	125.39	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	N-CA-C	5.59	117.45	110.91
1	A	63	ARG	N-CA-C	5.50	118.45	110.42
1	A	65	LEU	CA-C-N	5.41	124.59	118.97
1	A	65	LEU	C-N-CA	5.41	124.59	118.97
3	G	116	LEU	CA-C-N	5.37	126.55	119.84
3	G	116	LEU	C-N-CA	5.37	126.55	119.84
1	A	120	MET	CA-C-N	5.22	126.36	119.84
1	A	120	MET	C-N-CA	5.22	126.36	119.84
2	B	31	LYS	N-CA-C	5.13	121.16	109.81

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	A	495	0	234	10	0
2	B	384	0	186	5	0
3	G	516	0	249	5	0
4	H	473	0	227	7	0
5	I	1487	0	821	4	0
6	J	1484	0	812	3	0
7	K	2112	0	1078	17	0
8	M	787	0	362	0	0
All	All	7738	0	3969	44	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 4.

All (44) 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)
5:I:70:DC:H2"	5:I:71:DT:H71	1.52	0.89
3:G:42:ARG:CB	4:H:85:THR:CB	2.59	0.80
5:I:71:DT:O4	6:J:-71:DA:N1	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:70:DC:H2"	5:I:71:DT:C7	2.22	0.68
7:K:266:PRO:HA	7:K:267:ARG:CB	2.27	0.64
7:K:266:PRO:CA	7:K:267:ARG:CB	2.75	0.63
1:A:42:ARG:N	5:I:70:DC:OP1	2.33	0.62
7:K:266:PRO:HB3	7:K:267:ARG:CB	2.31	0.61
4:H:94:ALA:O	4:H:98:LEU:N	2.35	0.60
7:K:230:LYS:CB	7:K:281:GLU:O	2.50	0.60
3:G:93:LEU:O	3:G:96:LEU:N	2.35	0.59
1:A:88:ALA:HB2	2:B:83:ALA:HA	1.84	0.58
7:K:268:PRO:HB2	7:K:269:PHE:CB	2.33	0.58
7:K:267:ARG:CB	7:K:268:PRO:CD	2.82	0.58
4:H:49:THR:CB	4:H:50:GLY:CA	2.81	0.58
3:G:95:LYS:O	3:G:98:GLY:N	2.36	0.57
1:A:88:ALA:CB	2:B:83:ALA:HA	2.36	0.56
1:A:72:ARG:O	1:A:75:ALA:HB3	2.09	0.53
1:A:67:PHE:O	1:A:71:VAL:N	2.36	0.53
1:A:88:ALA:HB2	2:B:83:ALA:CA	2.41	0.51
1:A:93:GLN:O	1:A:94:GLU:C	2.54	0.51
1:A:95:ALA:O	1:A:99:TYR:N	2.39	0.50
3:G:95:LYS:O	3:G:96:LEU:C	2.55	0.50
7:K:72:ARG:CB	7:K:73:PRO:CD	2.90	0.49
7:K:266:PRO:CB	7:K:267:ARG:CB	2.92	0.48
7:K:72:ARG:CB	7:K:73:PRO:HD2	2.45	0.46
7:K:264:LEU:O	7:K:265:ASP:CB	2.64	0.45
2:B:63:GLU:O	2:B:64:ASN:C	2.59	0.45
4:H:48:ASP:HA	4:H:49:THR:HA	1.81	0.45
4:H:111:GLY:O	4:H:112:THR:C	2.60	0.44
7:K:47:ASP:N	7:K:463:GLY:O	2.51	0.43
7:K:435:VAL:CB	7:K:436:PRO:HD2	2.48	0.43
4:H:53:SER:N	6:J:-54:DC:OP1	2.52	0.42
7:K:363:PRO:HB3	7:K:434:GLU:CB	2.50	0.42
7:K:468:ASP:O	7:K:472:GLU:N	2.52	0.42
6:J:-57:DT:H2"	6:J:-56:DG:C8	2.54	0.42
1:A:125:GLN:O	1:A:128:ARG:N	2.53	0.42
3:G:62:ILE:O	3:G:63:LEU:C	2.63	0.42
7:K:329:VAL:O	7:K:345:GLN:N	2.53	0.41
1:A:125:GLN:O	1:A:126:LEU:C	2.62	0.41
2:B:59:LYS:O	2:B:60:VAL:C	2.63	0.41
7:K:268:PRO:HB2	7:K:269:PHE:CA	2.51	0.41
4:H:49:THR:CB	4:H:50:GLY:HA2	2.50	0.41
7:K:267:ARG:CB	7:K:268:PRO:HD2	2.51	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	A	97/135 (72%)	77 (79%)	19 (20%)	1 (1%)	12	47
2	B	76/102 (74%)	59 (78%)	16 (21%)	1 (1%)	9	41
3	G	103/129 (80%)	82 (80%)	18 (18%)	3 (3%)	3	23
4	H	93/122 (76%)	77 (83%)	15 (16%)	1 (1%)	11	45
7	K	414/483 (86%)	316 (76%)	88 (21%)	10 (2%)	4	27
8	M	158/202 (78%)	137 (87%)	18 (11%)	3 (2%)	6	32
All	All	941/1173 (80%)	748 (80%)	174 (18%)	19 (2%)	6	31

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	265	ASP
7	K	267	ARG
8	M	280	LYS
7	K	70	VAL
7	K	386	THR
3	G	26	PRO
7	K	28	HIS
7	K	326	ASP
1	A	87	SER
7	K	291	ASN
4	H	47	PRO
7	K	77	PRO
7	K	364	LYS
2	B	29	ILE
3	G	43	VAL
8	M	250	ILE
8	M	284	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	K	242	VAL
3	G	114	VAL

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	A	1/110 (1%)	1 (100%)	0	100	100
2	B	1/78 (1%)	1 (100%)	0	100	100
4	H	1/102 (1%)	1 (100%)	0	100	100
7	K	22/400 (6%)	22 (100%)	0	100	100
All	All	25/690 (4%)	25 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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](#)

There are no ligands in this entry.

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	A	99/135 (73%)	0.51	10 (10%)	12 16	42, 88, 196, 253	0
2	B	78/102 (76%)	0.56	9 (11%)	9 14	38, 86, 140, 180	0
3	G	105/129 (81%)	0.47	9 (8%)	16 20	39, 103, 172, 195	0
4	H	95/122 (77%)	0.49	10 (10%)	11 16	54, 100, 211, 276	0
5	I	73/149 (48%)	1.44	17 (23%)	2 5	136, 222, 304, 352	0
6	J	72/149 (48%)	1.39	17 (23%)	2 5	141, 216, 296, 318	0
7	K	422/483 (87%)	1.03	87 (20%)	2 6	120, 236, 335, 381	0
8	M	160/202 (79%)	2.40	77 (48%)	0 1	201, 444, 500, 500	0
All	All	1104/1471 (75%)	1.10	236 (21%)	2 6	38, 205, 488, 500	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	M	336	TYR	13.0
8	M	259	GLU	11.1
8	M	222	LEU	9.4
4	H	32	GLU	8.9
8	M	261	LEU	8.0
8	M	321	ILE	7.3
8	M	221	ASP	7.0
7	K	55	SER	7.0
2	B	32	PRO	7.0
8	M	335	ASP	6.7
8	M	270	CYS	6.7
7	K	50	CYS	6.6
8	M	337	GLY	6.5
1	A	127	ALA	6.3
7	K	356	ASP	6.1
8	M	289	GLU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	K	263	THR	5.3
8	M	287	THR	5.2
7	K	282	ASN	5.2
7	K	247	ASN	5.2
8	M	320	LEU	4.9
8	M	255	ALA	4.9
7	K	90	ALA	4.9
7	K	97	LEU	4.9
1	A	134	ARG	4.8
7	K	167	VAL	4.7
8	M	343	SER	4.7
7	K	250	GLN	4.7
6	J	-58	DC	4.6
8	M	263	ALA	4.5
8	M	291	ASN	4.5
7	K	451	LEU	4.5
7	K	406	ALA	4.5
7	K	437	THR	4.5
3	G	27	VAL	4.5
8	M	306	GLN	4.5
1	A	135	ALA	4.5
8	M	345	GLU	4.4
8	M	256	LYS	4.4
4	H	31	LYS	4.3
8	M	196	ALA	4.2
7	K	472	GLU	4.2
8	M	307	THR	4.2
7	K	89	PHE	4.1
8	M	305	CYS	4.0
3	G	75	LYS	4.0
6	J	-57	DT	4.0
7	K	319	PRO	4.0
8	M	290	THR	4.0
3	G	25	PHE	4.0
7	K	450	ILE	3.9
8	M	302	CYS	3.9
7	K	310	VAL	3.9
7	K	98	ALA	3.7
4	H	33	SER	3.7
2	B	33	ALA	3.7
7	K	286	ALA	3.7
2	B	98	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	M	339	ARG	3.7
8	M	264	GLN	3.6
8	M	246	HIS	3.6
4	H	30	ARG	3.6
8	M	220	ILE	3.6
8	M	295	ARG	3.6
7	K	322	LEU	3.6
7	K	326	ASP	3.5
8	M	338	ASP	3.5
8	M	340	SER	3.5
7	K	346	ASP	3.5
7	K	449	ILE	3.5
7	K	25	HIS	3.5
7	K	31	ASN	3.5
7	K	191	THR	3.5
2	B	28	GLY	3.5
7	K	73	PRO	3.5
8	M	351	LYS	3.4
7	K	460	VAL	3.4
5	I	45	DC	3.4
7	K	402	HIS	3.4
8	M	237	SER	3.4
8	M	262	TYR	3.3
7	K	248	GLY	3.3
7	K	327	ASN	3.3
8	M	251	GLU	3.3
8	M	298	ASN	3.3
7	K	436	PRO	3.3
8	M	346	ALA	3.3
3	G	16	THR	3.3
5	I	-35	DA	3.2
7	K	357	MET	3.2
7	K	284	CYS	3.2
7	K	442	THR	3.2
6	J	-53	DA	3.2
7	K	330	ILE	3.2
6	J	-45	DG	3.2
8	M	215	GLU	3.1
7	K	169	GLN	3.1
8	M	244	GLU	3.1
8	M	268	THR	3.1
7	K	105	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	K	413	ALA	3.1
7	K	276	TYR	3.1
8	M	342	ALA	3.1
8	M	296	LEU	3.1
5	I	-38	DC	3.1
6	J	-72	DC	3.1
3	G	26	PRO	3.0
8	M	297	ILE	3.1
8	M	269	GLY	3.0
8	M	319	ILE	3.0
8	M	294	GLY	3.0
8	M	309	LEU	3.0
5	I	53	DT	3.0
8	M	341	LYS	3.0
8	M	348	PRO	2.9
8	M	260	ALA	2.9
8	M	329	GLY	2.9
7	K	226	LEU	2.9
8	M	223	ILE	2.9
5	I	-29	DC	2.9
7	K	278	ALA	2.9
6	J	-52	DC	2.9
8	M	349	TRP	2.9
5	I	-39	DT	2.9
3	G	17	ARG	2.8
7	K	348	ASP	2.8
6	J	34	DC	2.8
7	K	410	ASN	2.8
7	K	48	ILE	2.8
7	K	399	ALA	2.8
8	M	245	TYR	2.8
1	A	40	ARG	2.7
5	I	-28	DT	2.7
8	M	258	ARG	2.7
5	I	48	DG	2.7
2	B	75	HIS	2.7
1	A	45	THR	2.7
1	A	128	ARG	2.7
7	K	375	VAL	2.7
7	K	452	VAL	2.7
8	M	308	LYS	2.6
6	J	39	DA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	K	65	ALA	2.6
3	G	24	GLN	2.6
7	K	88	SER	2.6
8	M	248	ASP	2.6
7	K	49	PHE	2.6
7	K	246	GLY	2.6
8	M	292	ARG	2.6
4	H	48	ASP	2.6
8	M	288	ARG	2.6
6	J	-55	DA	2.6
7	K	461	SER	2.5
7	K	438	ARG	2.5
7	K	171	ALA	2.5
6	J	-68	DA	2.5
8	M	311	ASP	2.5
7	K	74	ARG	2.5
8	M	243	VAL	2.5
8	M	327	ALA	2.5
7	K	159	PRO	2.5
5	I	-25	DA	2.5
1	A	55	GLN	2.5
6	J	-49	DG	2.5
6	J	23	DG	2.5
1	A	62	ILE	2.5
8	M	250	ILE	2.5
7	K	392	PRO	2.5
2	B	31	LYS	2.5
5	I	68	DT	2.4
8	M	265	ASP	2.4
7	K	104	ASN	2.4
7	K	228	PRO	2.4
7	K	120	THR	2.4
7	K	185	GLU	2.4
7	K	294	VAL	2.4
7	K	320	LYS	2.4
8	M	194	SER	2.4
2	B	24	ASP	2.4
7	K	265	ASP	2.4
8	M	252	ILE	2.4
8	M	331	GLU	2.4
8	M	344	ILE	2.4
5	I	44	DC	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	K	361	GLY	2.3
6	J	-65	DT	2.3
6	J	33	DT	2.3
7	K	337	GLU	2.3
1	A	126	LEU	2.3
8	M	197	GLU	2.3
4	H	80	TYR	2.3
7	K	448	ASN	2.2
8	M	267	SER	2.2
2	B	78	ARG	2.2
5	I	-17	DT	2.2
7	K	66	LYS	2.2
7	K	68	LYS	2.2
8	M	235	GLN	2.2
8	M	224	ASP	2.2
7	K	425	GLY	2.2
4	H	35	ALA	2.2
7	K	235	PHE	2.2
6	J	-54	DC	2.2
7	K	405	VAL	2.2
7	K	443	ALA	2.2
5	I	-36	DT	2.2
7	K	183	ASN	2.2
7	K	391	VAL	2.2
4	H	84	SER	2.1
7	K	258	ARG	2.1
8	M	286	ALA	2.1
7	K	325	PRO	2.1
8	M	301	LYS	2.1
5	I	47	DG	2.1
8	M	266	PRO	2.1
4	H	58	ILE	2.1
5	I	63	DA	2.1
7	K	431	ASP	2.1
5	I	66	DC	2.1
7	K	390	ASN	2.1
2	B	72	TYR	2.1
4	H	49	THR	2.1
7	K	359	GLU	2.1
6	J	38	DG	2.1
3	G	114	VAL	2.1
8	M	219	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	K	334	ALA	2.1
7	K	63	PRO	2.1
7	K	456	GLY	2.0
5	I	-30	DG	2.0
8	M	274	TYR	2.0
1	A	114	ALA	2.0
6	J	-43	DA	2.0
7	K	309	ASP	2.0
3	G	15	LYS	2.0
7	K	308	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.