



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:13 PM UTC

PDB ID : 3X1V / pdb_00003x1v
Title : Crystal structure of nucleosome core particle in the presence of histone variant involved in reprogramming
Authors : Sivaraman, P.; Kumarevel, T.S.
Deposited on : 2014-11-28
Resolution : 2.92 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

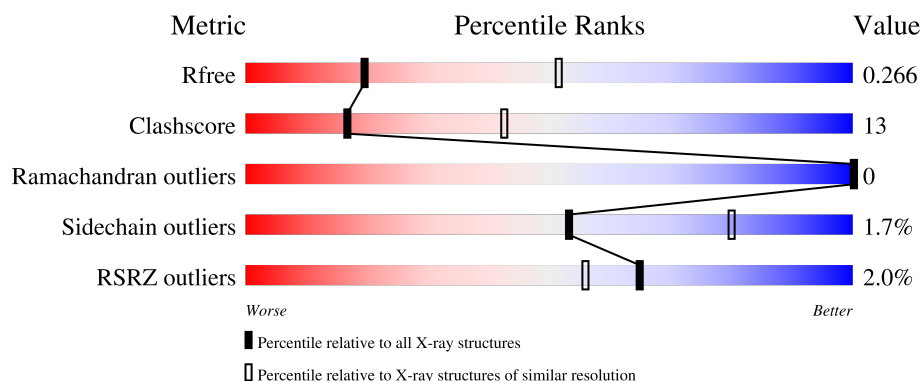
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	I	146	3% 47% 53%
1	J	146	4% 42% 57% .
2	A	135	% 53% 18% . 27%
2	E	135	% 56% 16% . 27%
3	B	102	63% 13% . 23%

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Mol	Chain	Length	Quality of chain
3	F	102	
4	C	129	
4	G	129	
5	D	126	
5	H	126	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CL	D	202	-	-	X	-

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 DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			
1	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
2	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
3	F	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	C	106	Total	C	N	O	0	0	0
			819	517	160	142			
4	G	109	Total	C	N	O	0	0	0
			844	532	167	145			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	99	Total	C	N	O	S	0	1	0
			797	499	149	146	3			
5	H	94	Total	C	N	O	S	0	1	0
			746	469	133	141	3			

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	11	Total	Mn	0	0
			11	11		
6	J	6	Total	Mn	0	0
			6	6		
6	D	1	Total	Mn	0	0
			1	1		
6	G	1	Total	Mn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	2	Total	Cl	0	0
			2	2		
7	J	2	Total	Cl	0	0
			2	2		
7	B	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

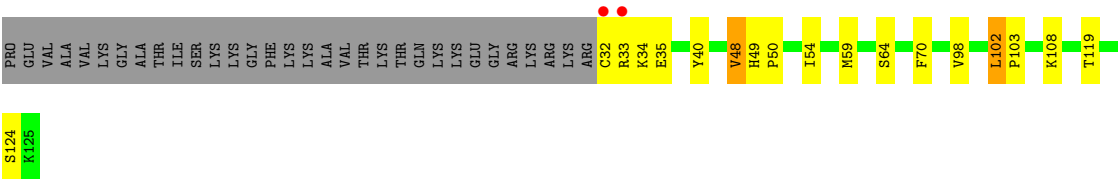
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	12	Total	O	0	0
			12	12		
8	J	5	Total	O	0	0
			5	5		
8	A	3	Total	O	0	0
			3	3		
8	C	2	Total	O	0	0
			2	2		
8	D	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	4	Total 4	O 4	0	0
8	F	4	Total 4	O 4	0	0
8	G	1	Total 1	O 1	0	0





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.33Å 108.47Å 168.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.92 39.81 – 2.92	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.81-2.92) 93.9 (39.81-2.92)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.90Å)	Xtriage
Refinement program	REFMAC, PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.191 , 0.259 0.203 , 0.266	Depositor DCC
R_{free} test set	1940 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12197	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	I	0.44	0/3354	0.66	0/5175
1	J	0.49	0/3354	0.69	1/5175 (0.0%)
2	A	0.78	1/819 (0.1%)	1.16	5/1097 (0.5%)
2	E	0.83	0/828	1.09	3/1109 (0.3%)
3	B	0.74	1/634 (0.2%)	1.01	2/848 (0.2%)
3	F	0.92	1/711 (0.1%)	1.16	2/948 (0.2%)
4	C	0.76	0/829	1.00	3/1118 (0.3%)
4	G	0.69	0/854	0.98	0/1150
5	D	0.79	0/813	1.17	7/1087 (0.6%)
5	H	0.75	0/762	0.97	4/1023 (0.4%)
All	All	0.64	3/12958 (0.0%)	0.88	27/18730 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	95	ARG	C-O	-7.78	1.14	1.23
2	A	78	PHE	CA-C	5.38	1.58	1.52
3	B	95	ARG	C-O	-5.05	1.17	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	106	LEU	N-CA-C	-10.41	100.43	113.55
5	D	27	ARG	CB-CA-C	-10.19	90.73	110.10
2	A	77	ASP	N-CA-C	-8.88	102.43	113.18
2	E	129	ARG	N-CA-C	7.83	119.89	111.36
5	D	28	LYS	N-CA-C	-7.78	96.31	108.14
5	D	29	ARG	N-CA-C	7.78	121.57	109.52
3	F	31	LYS	CA-C-N	-6.75	111.85	119.28
3	F	31	LYS	C-N-CA	-6.75	111.85	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	271	DG	O5'-P-OP1	-6.46	89.62	109.00
5	H	102	LEU	CA-C-N	6.10	126.11	119.89
5	H	102	LEU	C-N-CA	6.10	126.11	119.89
3	B	102	GLY	N-CA-C	6.07	130.91	113.30
2	A	117	VAL	N-CA-C	-6.04	107.37	113.47
2	A	103	LEU	N-CA-C	-5.86	104.97	111.36
4	C	38	ASN	N-CA-C	5.79	119.56	111.74
2	A	82	LEU	N-CA-C	-5.73	101.21	110.32
3	B	101	GLY	N-CA-C	5.68	122.52	114.85
4	C	47	ALA	CA-C-N	-5.57	113.29	119.19
4	C	47	ALA	C-N-CA	-5.57	113.29	119.19
5	D	29	ARG	N-CA-CB	-5.52	101.95	111.55
5	H	124	SER	N-CA-C	-5.50	101.76	109.96
5	H	50	PRO	N-CA-C	-5.48	106.06	113.40
2	E	130	ILE	N-CA-C	-5.44	105.22	110.72
2	A	64	LYS	N-CA-C	5.43	119.08	112.23
5	D	57	LYS	N-CA-C	-5.23	105.66	111.36
5	D	123	SER	N-CA-C	5.18	116.73	111.14
2	E	130	ILE	N-CA-CB	5.13	118.27	110.58

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	I	2990	0	1652	88	0
1	J	2990	0	1652	98	0
2	A	807	0	844	24	0
2	E	816	0	856	23	0
3	B	627	0	663	9	0
3	F	703	0	755	10	0
4	C	819	0	879	14	0
4	G	844	0	910	18	0
5	D	797	0	833	26	0
5	H	746	0	768	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	1	0
6	G	1	0	0	0	0
6	I	11	0	0	0	0
6	J	6	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	2	0
7	I	2	0	0	0	0
7	J	2	0	0	1	0
8	A	3	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
8	E	4	0	0	0	0
8	F	4	0	0	0	0
8	G	1	0	0	0	0
8	I	12	0	0	3	0
8	J	5	0	0	0	0
All	All	12197	0	9812	275	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 13.

All (275) 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)
1:I:122:DG:H5''	5:H:33:ARG:NH2	1.35	1.36
1:I:122:DG:C5'	5:H:33:ARG:NH2	2.01	1.23
5:D:29:ARG:NH2	5:D:31:ARG:NH2	2.05	1.04
1:I:122:DG:C5'	5:H:33:ARG:HH21	1.75	0.96
6:D:201:MN:MN	7:D:202:CL:CL	1.64	0.93
5:D:29:ARG:NH2	5:D:31:ARG:HH21	1.61	0.92
5:D:29:ARG:HH22	5:D:31:ARG:HH21	0.97	0.90
5:D:29:ARG:HH22	5:D:31:ARG:NH2	1.64	0.89
1:J:206:DC:H4'	2:E:63:ARG:HH21	1.38	0.88
1:I:122:DG:H4'	5:H:33:ARG:NE	1.89	0.87
1:J:259:DA:H2''	1:J:260:DC:H5''	1.56	0.87
1:J:271:DG:OP1	5:D:31:ARG:NH2	2.09	0.86
1:I:122:DG:H5''	5:H:33:ARG:HH22	1.40	0.83
1:I:122:DG:H4'	5:H:33:ARG:CZ	2.10	0.82
1:I:100:DG:N7	8:I:301:HOH:O	2.12	0.81
1:I:144:DG:H1	1:J:149:DC:H42	1.29	0.79
1:J:282:DT:H2''	1:J:283:DG:H5'	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:193:DC:OP1	5:D:29:ARG:HG3	1.84	0.77
1:I:136:DT:H2'	1:I:137:DG:C8	2.20	0.77
1:I:5:DA:H2''	1:I:6:DT:H5''	1.67	0.76
1:J:217:DG:N7	7:J:308:CL:CL	2.55	0.76
5:D:31:ARG:HD3	5:D:32:CYS:H	1.50	0.74
4:C:40:SER:HA	4:G:38:ASN:OD1	1.89	0.72
1:I:136:DT:H2''	1:I:137:DG:H5'	1.71	0.72
1:I:122:DG:C4'	5:H:33:ARG:NH2	2.54	0.71
5:H:48:VAL:O	5:H:49:HIS:ND1	2.23	0.70
1:I:128:DT:H2''	1:I:129:DC:H5''	1.74	0.70
1:I:40:DG:H8	1:I:40:DG:H5''	1.56	0.70
1:I:117:DT:O3'	4:G:11:ARG:NH2	2.25	0.69
5:D:76:GLU:OE1	5:D:79:ARG:NH1	2.25	0.69
1:I:51:DA:H2''	1:I:52:DT:H5''	1.73	0.69
4:C:79:ILE:HG12	4:C:82:HIS:CE1	2.27	0.69
4:C:67:GLY:HA3	5:D:49:HIS:CD2	2.30	0.67
1:I:122:DG:H5''	5:H:33:ARG:CZ	2.21	0.67
1:J:250:DT:OP1	5:H:32:CYS:HA	1.94	0.66
1:I:139:DA:H1'	1:I:140:DT:H5'	1.76	0.66
1:J:181:DA:H2''	1:J:182:DT:H5''	1.78	0.65
1:J:197:DA:H2''	1:J:198:DT:H5''	1.78	0.65
5:D:29:ARG:HH21	5:D:31:ARG:NH2	1.94	0.64
1:I:121:DG:H1'	1:I:122:DG:H5'	1.79	0.64
1:J:275:DC:H2''	1:J:276:DT:H5'	1.80	0.62
1:I:58:DG:H2''	1:I:59:DG:C8	2.33	0.62
1:J:285:DA:H5'	1:J:285:DA:C8	2.35	0.62
3:F:20:LYS:NZ	3:F:21:VAL:O	2.32	0.62
1:J:238:DT:H1'	1:J:239:DT:H5'	1.81	0.62
1:I:130:DT:H2''	1:I:131:DG:N7	2.15	0.62
5:H:54:ILE:HG21	5:H:59:MET:HE2	1.82	0.61
1:I:36:DT:H2''	1:I:37:DT:H5''	1.81	0.61
1:I:144:DG:H1	1:J:149:DC:N4	1.98	0.61
1:J:246:DG:H2''	1:J:247:DC:H5''	1.81	0.61
1:I:115:DA:H2''	1:I:116:DC:H5''	1.83	0.61
1:I:122:DG:H5'	5:H:33:ARG:HH21	1.64	0.61
1:I:40:DG:H2''	1:I:41:DA:C8	2.36	0.61
1:J:148:DT:H2''	1:J:149:DC:H5'	1.82	0.60
1:J:198:DT:H2''	1:J:199:DC:H5'	1.82	0.60
5:D:31:ARG:CD	5:D:32:CYS:H	2.14	0.60
1:J:152:DT:H2''	1:J:153:DA:H5'	1.85	0.59
1:J:205:DG:H2''	1:J:206:DC:H5''	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:88:ARG:NH2	4:G:97:LEU:O	2.35	0.59
1:J:172:DC:H2''	1:J:173:DA:N7	2.18	0.59
4:G:79:ILE:HG12	4:G:82:HIS:CE1	2.38	0.58
1:J:226:DT:H2''	1:J:227:DG:C8	2.37	0.58
1:J:279:DA:H2''	1:J:280:DG:H5'	1.85	0.58
2:A:48:LEU:O	2:A:52:ARG:HG3	2.04	0.58
3:B:52:GLU:OE2	3:B:55:ARG:NH1	2.36	0.58
1:J:183:DT:H2''	1:J:184:DT:H5'	1.84	0.58
1:J:250:DT:H2''	1:J:251:DT:H5'	1.86	0.58
2:E:37:LYS:N	2:E:38:PRO:HD3	2.18	0.57
1:I:108:DC:H2''	1:I:109:DA:N7	2.20	0.57
1:I:122:DG:H1'	1:I:123:DT:H5'	1.86	0.57
2:E:63:ARG:NH1	2:E:63:ARG:HG2	2.20	0.57
1:I:40:DG:H5''	1:I:40:DG:C8	2.39	0.57
1:I:122:DG:C4'	5:H:33:ARG:HH21	2.15	0.57
2:E:120:MET:HE3	2:E:122:LYS:HE3	1.85	0.57
2:E:63:ARG:HG2	2:E:63:ARG:HH11	1.70	0.57
4:G:30:VAL:HG13	5:H:70:PHE:HE2	1.69	0.57
1:I:132:DC:H2''	1:I:133:DA:C8	2.40	0.56
2:A:57:SER:OG	2:A:59:GLU:OE1	2.22	0.56
1:J:164:DG:H2''	1:J:165:DA:H5''	1.87	0.56
1:I:121:DG:H5''	5:H:40:TYR:OH	2.06	0.56
2:A:71:VAL:HG13	3:B:66:ILE:HD11	1.87	0.55
1:J:216:DT:H2''	1:J:217:DG:C8	2.41	0.55
1:J:153:DA:H1'	1:J:154:DT:H5'	1.87	0.55
5:D:102:LEU:HB2	5:D:107:ALA:HB2	1.88	0.55
4:C:102:ILE:HG23	5:D:61:ILE:HD13	1.89	0.55
1:J:147:DA:C2	1:J:148:DT:C2	2.95	0.54
1:J:248:DA:OP1	3:B:79:LYS:N	2.31	0.54
1:I:135:DG:H2''	1:I:136:DT:C6	2.43	0.53
4:C:117:PRO:O	4:C:118:LYS:HB2	2.07	0.53
1:J:190:DC:H4'	1:J:190:DC:OP1	2.08	0.53
1:I:38:DT:H2''	1:I:39:DG:C8	2.43	0.53
1:I:34:DT:H1'	1:I:35:DA:H5'	1.91	0.53
4:C:55:LEU:O	4:C:59:THR:HG23	2.09	0.53
1:J:271:DG:H2''	1:J:272:DA:H8	1.73	0.53
1:J:277:DG:H8	1:J:277:DG:H5''	1.73	0.53
2:A:80:THR:HG22	2:A:81:ASP:N	2.24	0.53
1:J:185:DG:H1'	1:J:186:DG:H5'	1.91	0.52
2:E:37:LYS:N	2:E:37:LYS:HD3	2.24	0.52
2:E:116:ARG:CZ	2:E:120:MET:HE2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:DT:H2''	1:J:209:DG:C8	2.44	0.52
2:E:125:GLN:NE2	3:F:53:GLU:OE2	2.42	0.52
1:J:197:DA:C2'	1:J:198:DT:H5''	2.39	0.52
1:I:35:DA:H2''	1:I:36:DT:H5''	1.90	0.52
1:J:264:DT:H2''	1:J:265:DT:H5'	1.92	0.52
1:J:147:DA:C5	1:J:148:DT:C4	2.98	0.52
1:J:241:DA:H2''	1:J:242:DT:H5'	1.92	0.51
1:I:130:DT:H2''	1:I:131:DG:C8	2.45	0.51
3:F:17:ARG:CG	3:F:18:HIS:H	2.24	0.50
1:J:192:DG:H2''	1:J:193:DC:H5'	1.93	0.50
4:C:76:THR:O	5:D:52:THR:HG23	2.12	0.50
2:A:79:LYS:HG3	2:A:80:THR:N	2.27	0.50
1:I:99:DA:H2''	1:I:100:DG:C8	2.45	0.50
5:D:48:VAL:O	7:D:202:CL:CL	2.67	0.50
1:I:51:DA:C2'	1:I:52:DT:H5''	2.39	0.50
1:J:158:DC:H1'	1:J:159:DC:H5''	1.94	0.50
1:J:266:DT:H2''	1:J:267:DG:N7	2.26	0.50
4:G:84:GLN:NE2	4:G:106:GLY:O	2.42	0.50
1:I:95:DA:H2''	1:I:96:DT:H5'	1.94	0.49
2:A:79:LYS:HG3	2:A:80:THR:H	1.77	0.49
1:J:229:DA:H5''	2:A:43:PRO:HA	1.94	0.49
3:B:28:GLY:O	3:B:30:THR:HG23	2.12	0.49
4:C:65:LEU:HB2	4:C:86:ALA:HB1	1.93	0.49
1:I:115:DA:C2'	1:I:116:DC:H5''	2.42	0.49
5:D:31:ARG:HD3	5:D:32:CYS:N	2.26	0.49
1:J:155:DC:H5'	1:J:155:DC:H6	1.77	0.49
1:I:82:DA:H3'	2:E:46:VAL:HG21	1.94	0.48
1:J:285:DA:H5'	1:J:285:DA:H8	1.75	0.48
5:D:29:ARG:HG2	5:D:30:LYS:N	2.28	0.48
1:I:43:DA:H1'	1:I:44:DC:H5''	1.95	0.48
1:J:237:DT:P	2:A:69:ARG:HH22	2.36	0.48
1:J:238:DT:P	2:A:63:ARG:HE	2.36	0.48
1:I:139:DA:C1'	1:I:140:DT:H5'	2.42	0.48
1:I:2:DT:H2''	1:I:3:DC:H5'	1.96	0.48
1:I:38:DT:H2''	1:I:39:DG:N7	2.28	0.48
1:I:5:DA:C2'	1:I:6:DT:H5''	2.42	0.48
1:J:277:DG:H5''	1:J:277:DG:C8	2.49	0.48
2:E:99:TYR:OH	2:E:133:GLU:OE1	2.31	0.48
3:F:17:ARG:HD3	3:F:18:HIS:H	1.77	0.48
1:I:101:DC:H5''	1:I:101:DC:H6	1.78	0.48
1:I:118:DT:H4'	4:G:11:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:131:DG:H5''	1:I:131:DG:H8	1.80	0.47
1:J:176:DA:OP2	4:G:32:ARG:HD3	2.14	0.47
2:E:60:LEU:HD13	2:E:93:GLN:CD	2.39	0.47
1:I:48:DT:O3'	8:I:308:HOH:O	2.20	0.47
1:J:157:DA:H2''	1:J:158:DC:C6	2.50	0.47
2:A:123:ASP:OD1	2:E:113:HIS:NE2	2.43	0.47
1:I:85:DA:H1'	1:I:86:DT:H5'	1.97	0.47
1:I:122:DG:H4'	5:H:33:ARG:HE	1.72	0.47
1:I:89:DC:H2''	1:I:90:DT:H71	1.95	0.47
1:I:108:DC:H2''	1:I:109:DA:C8	2.50	0.47
5:D:29:ARG:HG2	5:D:30:LYS:H	1.80	0.47
1:I:122:DG:C4'	5:H:33:ARG:CZ	2.84	0.46
2:A:112:ILE:HD13	4:G:112:GLN:HG2	1.96	0.46
1:J:147:DA:C6	1:J:148:DT:C4	3.04	0.46
2:A:58:THR:HG22	4:G:106:GLY:HA3	1.96	0.46
1:I:68:DG:H5'	2:A:43:PRO:HG2	1.96	0.46
1:J:271:DG:OP1	5:D:31:ARG:CZ	2.61	0.46
1:I:29:DA:H8	1:I:29:DA:H5''	1.80	0.46
1:I:49:DC:O4'	2:A:83:ARG:NH2	2.49	0.46
1:J:270:DA:H2''	1:J:271:DG:O5'	2.16	0.46
1:J:274:DT:H2''	1:J:275:DC:C6	2.51	0.46
4:C:38:ASN:N	4:C:38:ASN:HD22	2.12	0.46
4:G:81:ARG:O	4:G:85:LEU:HG	2.15	0.46
1:I:103:DG:H1'	1:I:104:DT:H5''	1.98	0.46
1:I:118:DT:P	4:G:11:ARG:NH2	2.89	0.45
1:J:152:DT:C2'	1:J:153:DA:H5'	2.46	0.45
4:G:67:GLY:HA3	5:H:49:HIS:HD2	1.81	0.45
1:J:172:DC:H2''	1:J:173:DA:C8	2.51	0.45
2:A:80:THR:HG22	2:A:81:ASP:H	1.81	0.45
3:B:31:LYS:HG3	3:B:51:TYR:CZ	2.51	0.45
2:A:102:GLY:HA2	2:A:105:GLU:CD	2.41	0.45
2:E:119:ILE:HD13	3:F:43:VAL:HG21	1.97	0.45
1:J:260:DC:H2''	1:J:261:DA:C8	2.52	0.45
3:F:19:ARG:HG2	3:F:20:LYS:H	1.82	0.45
1:I:58:DG:O6	1:J:235:DC:N4	2.40	0.45
8:I:307:HOH:O	2:E:64:LYS:HG3	2.17	0.45
5:D:36:SER:HB2	5:D:63:ASN:ND2	2.32	0.45
1:J:238:DT:OP1	2:A:63:ARG:NE	2.51	0.45
1:J:271:DG:H2''	1:J:272:DA:C8	2.52	0.45
2:A:63:ARG:HD2	2:A:63:ARG:HA	1.62	0.45
1:I:129:DC:H2''	1:I:130:DT:C5	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:274:DT:H2''	1:J:275:DC:H5''	1.99	0.44
1:I:125:DG:H2''	1:I:126:DA:H8	1.83	0.44
1:J:206:DC:O5'	2:E:63:ARG:NH2	2.51	0.44
1:I:8:DT:H1'	1:I:9:DC:H5''	1.98	0.44
4:C:73:ASN:O	4:C:75:LYS:HG2	2.17	0.44
1:I:61:DA:H2''	1:I:62:DT:H5'	1.99	0.44
1:J:166:DT:H4'	4:G:77:ARG:NE	2.33	0.44
1:J:183:DT:C2'	1:J:184:DT:H5'	2.48	0.44
1:J:204:DG:H4'	1:J:205:DG:H5'	2.00	0.44
1:J:238:DT:C1'	1:J:239:DT:H5'	2.45	0.44
1:I:29:DA:OP1	4:C:32:ARG:NH1	2.51	0.44
1:J:249:DG:H1'	1:J:250:DT:H5''	1.99	0.44
1:I:20:DT:H1'	1:I:21:DT:H5'	1.99	0.44
1:J:266:DT:H2''	1:J:267:DG:C8	2.53	0.44
2:A:82:LEU:HD23	2:A:82:LEU:HA	1.76	0.44
5:H:34:LYS:O	5:H:35:GLU:CG	2.65	0.44
1:I:7:DA:H1'	1:I:8:DT:H5'	2.00	0.44
1:I:125:DG:H2''	1:I:126:DA:C8	2.53	0.44
1:J:220:DT:H1'	1:J:221:DT:H5'	2.00	0.44
3:B:82:THR:HG22	3:B:83:ALA:N	2.33	0.44
3:F:50:ILE:HD13	3:F:50:ILE:HA	1.85	0.44
1:I:105:DT:H1'	1:I:106:DT:H5'	1.99	0.43
5:D:54:ILE:HG21	5:D:59:MET:HE2	1.99	0.43
5:D:39:ILE:HG13	5:D:40:TYR:N	2.32	0.43
1:J:275:DC:C2'	1:J:276:DT:H5'	2.45	0.43
2:E:120:MET:CE	2:E:122:LYS:HE3	2.48	0.43
5:H:108:LYS:HE3	5:H:108:LYS:HB2	1.77	0.43
1:J:194:DT:H2''	1:J:195:DC:C6	2.54	0.43
1:J:196:DC:OP1	2:E:85:GLN:HA	2.19	0.43
2:E:56:LYS:HE3	2:E:56:LYS:HB2	1.73	0.43
4:C:26:PRO:O	4:C:30:VAL:HG23	2.19	0.43
3:B:90:LEU:HB3	3:B:95:ARG:O	2.19	0.43
3:B:102:GLY:HA2	5:H:64:SER:HB3	2.01	0.43
1:J:261:DA:H2''	1:J:262:DC:H5''	2.01	0.43
1:J:147:DA:C6	1:J:148:DT:N3	2.87	0.42
1:J:248:DA:H2''	1:J:249:DG:H8	1.84	0.42
1:J:250:DT:OP1	5:H:32:CYS:CA	2.65	0.42
5:H:102:LEU:HA	5:H:103:PRO:HD3	1.86	0.42
1:J:238:DT:OP1	2:A:63:ARG:HG3	2.19	0.42
1:J:165:DA:H2'	1:J:166:DT:H72	2.02	0.42
1:J:285:DA:H1'	1:J:286:DT:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:201:DA:OP2	1:J:201:DA:H8	2.03	0.42
1:J:237:DT:OP2	2:A:69:ARG:NH2	2.49	0.42
1:I:92:DT:H1'	1:I:93:DT:H5'	2.02	0.42
1:J:207:DA:H2''	1:J:208:DT:H5'	2.01	0.42
4:G:16:THR:O	4:G:20:ARG:HG3	2.19	0.42
1:I:91:DT:H2''	1:I:92:DT:H5'	2.02	0.42
2:A:73:GLU:O	2:A:76:GLN:HG2	2.20	0.42
1:J:196:DC:H2''	1:J:197:DA:C8	2.55	0.41
1:J:198:DT:C2'	1:J:199:DC:H5'	2.48	0.41
3:F:52:GLU:OE2	3:F:55:ARG:NH1	2.52	0.41
1:J:251:DT:H6	1:J:251:DT:H2'	1.75	0.41
4:G:38:ASN:N	4:G:38:ASN:HD22	2.17	0.41
1:I:131:DG:C8	1:I:131:DG:H5''	2.55	0.41
5:D:46:LYS:HD3	5:D:46:LYS:HA	1.86	0.41
1:J:155:DC:C2'	1:J:156:DC:H5'	2.50	0.41
3:F:67:ARG:HH11	3:F:67:ARG:HD2	1.76	0.41
1:I:139:DA:C8	1:I:139:DA:H5'	2.55	0.41
1:J:165:DA:H2''	1:J:166:DT:H5'	2.02	0.41
1:J:194:DT:H2''	1:J:195:DC:H5'	2.02	0.41
1:J:215:DC:C5'	2:E:43:PRO:HG2	2.51	0.41
2:E:129:ARG:CZ	2:E:134:ARG:HH22	2.34	0.41
3:F:17:ARG:HG3	3:F:18:HIS:H	1.84	0.41
1:I:83:DA:H5''	2:E:40:ARG:HG2	2.03	0.41
1:J:235:DC:H2''	1:J:236:DT:C7	2.51	0.41
1:J:154:DT:H1'	1:J:155:DC:H5''	2.02	0.41
1:J:155:DC:H1'	1:J:156:DC:H5'	2.03	0.41
1:J:247:DC:H2''	1:J:248:DA:C8	2.56	0.41
1:J:282:DT:H2'	1:J:283:DG:C8	2.56	0.41
2:A:79:LYS:HB3	2:A:82:LEU:HD11	2.03	0.41
1:I:128:DT:H2''	1:I:129:DC:C6	2.56	0.41
1:J:170:DA:H2''	1:J:171:DC:H5''	2.02	0.41
1:J:177:DG:OP1	4:G:17:ARG:HG3	2.21	0.41
1:J:267:DG:H5''	4:C:16:THR:HG21	2.02	0.41
4:C:118:LYS:HA	4:C:118:LYS:HD2	1.71	0.41
5:D:57:LYS:HD2	5:D:57:LYS:HA	1.91	0.41
1:I:122:DG:H5'	5:H:33:ARG:NH2	2.16	0.41
1:I:130:DT:H2''	1:I:131:DG:C5	2.56	0.41
1:I:133:DA:H2''	1:I:134:DG:H5'	2.03	0.41
1:J:206:DC:H4'	2:E:63:ARG:NH2	2.20	0.41
2:A:56:LYS:HE3	2:A:56:LYS:HB2	1.75	0.41
4:G:26:PRO:O	4:G:30:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:DT:H4'	2:E:63:ARG:HD3	2.03	0.41
1:I:141:DA:H2''	1:I:142:DT:H5'	2.04	0.41
1:I:122:DG:C4'	5:H:33:ARG:NE	2.73	0.40
1:I:9:DC:H6	1:I:9:DC:H5'	1.85	0.40
1:I:31:DG:H1'	1:I:32:DT:H5''	2.03	0.40
1:J:238:DT:H5'	1:J:238:DT:C6	2.56	0.40
5:D:106:LEU:HD12	5:D:106:LEU:HA	1.92	0.40
1:I:38:DT:H6	1:I:38:DT:H2'	1.74	0.40
3:B:62:LEU:HD23	3:B:62:LEU:HA	1.84	0.40
1:I:73:DA:H1'	1:I:74:DT:H5''	2.03	0.40
5:D:29:ARG:NH2	5:D:31:ARG:CZ	2.81	0.40
1:I:29:DA:H5''	1:I:29:DA:C8	2.56	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	
2	A	96/135 (71%)	96 (100%)	0	0	100	100
2	E	97/135 (72%)	97 (100%)	0	0	100	100
3	B	77/102 (76%)	75 (97%)	2 (3%)	0	100	100
3	F	85/102 (83%)	84 (99%)	1 (1%)	0	100	100
4	C	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
4	G	107/129 (83%)	106 (99%)	1 (1%)	0	100	100
5	D	98/126 (78%)	97 (99%)	1 (1%)	0	100	100
5	H	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
All	All	757/984 (77%)	748 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	85/110 (77%)	84 (99%)	1 (1%)	63	85
2	E	86/110 (78%)	83 (96%)	3 (4%)	32	64
3	B	64/78 (82%)	64 (100%)	0	100	100
3	F	72/78 (92%)	72 (100%)	0	100	100
4	C	84/99 (85%)	83 (99%)	1 (1%)	63	85
4	G	86/99 (87%)	85 (99%)	1 (1%)	63	85
5	D	89/109 (82%)	87 (98%)	2 (2%)	45	75
5	H	84/109 (77%)	81 (96%)	3 (4%)	31	63
All	All	650/792 (82%)	639 (98%)	11 (2%)	53	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	117	VAL
4	C	114	VAL
5	D	32	CYS
5	D	124	SER
2	E	37	LYS
2	E	115	LYS
2	E	117	VAL
4	G	88	ARG
5	H	48	VAL
5	H	98	VAL
5	H	119	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	38	ASN
5	D	47	GLN
5	D	95	GLN

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Mol	Chain	Res	Type
3	F	18	HIS
4	G	24	GLN
4	G	104	GLN
5	H	47	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	I	146/146 (100%)	0.28	5 (3%) 48 38	20, 61, 103, 115	0
1	J	146/146 (100%)	0.29	6 (4%) 41 33	26, 60, 102, 125	0
2	A	98/135 (72%)	-0.21	2 (2%) 65 56	13, 32, 69, 85	0
2	E	99/135 (73%)	-0.54	1 (1%) 79 72	8, 16, 36, 57	0
3	B	79/102 (77%)	-0.15	0 100 100	20, 30, 55, 74	0
3	F	87/102 (85%)	-0.51	1 (1%) 78 71	8, 14, 37, 84	0
4	C	106/129 (82%)	-0.42	0 100 100	9, 21, 42, 60	0
4	G	109/129 (84%)	-0.24	2 (1%) 67 59	12, 28, 70, 82	0
5	D	99/126 (78%)	-0.23	2 (2%) 65 56	11, 23, 77, 91	1 (1%)
5	H	94/126 (74%)	-0.21	2 (2%) 63 54	10, 25, 58, 100	1 (1%)
All	All	1063/1276 (83%)	-0.15	21 (1%) 65 56	8, 30, 85, 125	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	102	GLY	3.5
1	J	148	DT	3.4
1	J	147	DA	3.4
1	I	55	DA	3.3
5	H	33	ARG	3.3
4	G	13	LYS	3.0
1	I	1	DA	2.9
1	J	242	DT	2.8
5	D	27	ARG	2.7
1	I	136	DT	2.6
1	J	292	DT	2.5
5	H	32	CYS	2.5
2	A	38	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	135	ALA	2.4
2	A	63	ARG	2.4
5	D	28	LYS	2.4
1	I	2	DT	2.3
1	J	161	DG	2.2
1	I	135	DG	2.2
1	J	201	DA	2.1
4	G	77	ARG	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(Å ²)	Q<0.9
6	MN	J	301	1/1	0.59	0.14	120,120,120,120	0
6	MN	I	203	1/1	0.79	0.09	113,113,113,113	0
6	MN	I	209	1/1	0.82	0.15	98,98,98,98	0
7	CL	I	212	1/1	0.82	0.11	64,64,64,64	0
7	CL	J	308	1/1	0.83	0.09	37,37,37,37	0
6	MN	I	206	1/1	0.85	0.10	106,106,106,106	0
7	CL	I	213	1/1	0.87	0.12	82,82,82,82	0
6	MN	I	210	1/1	0.88	0.07	83,83,83,83	0
6	MN	J	306	1/1	0.89	0.11	77,77,77,77	0
6	MN	I	211	1/1	0.89	0.09	137,137,137,137	0
6	MN	I	208	1/1	0.91	0.07	63,63,63,63	0
6	MN	J	302	1/1	0.92	0.15	65,65,65,65	0
7	CL	J	307	1/1	0.93	0.20	50,50,50,50	0
6	MN	J	303	1/1	0.94	0.08	68,68,68,68	0
6	MN	I	202	1/1	0.94	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MN	J	305	1/1	0.95	0.06	68,68,68,68	0
6	MN	I	205	1/1	0.95	0.06	81,81,81,81	0
7	CL	B	201	1/1	0.95	0.10	54,54,54,54	0
6	MN	I	201	1/1	0.96	0.05	66,66,66,66	0
6	MN	I	204	1/1	0.97	0.04	55,55,55,55	0
6	MN	G	201	1/1	0.98	0.09	43,43,43,43	0
6	MN	I	207	1/1	0.98	0.05	44,44,44,44	0
6	MN	J	304	1/1	0.98	0.10	49,49,49,49	0
6	MN	D	201	1/1	0.99	0.05	29,29,29,29	0
7	CL	D	202	1/1	0.99	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.