



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:33 AM UTC

PDB ID : 7PSX / pdb_00007psx
Title : Structure of HOXB13 bound to hydroxymethylated DNA
Authors : Morgunova, E.; Popov, A.; Yin, Y.; Taipale, J.
Deposited on : 2021-09-24
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

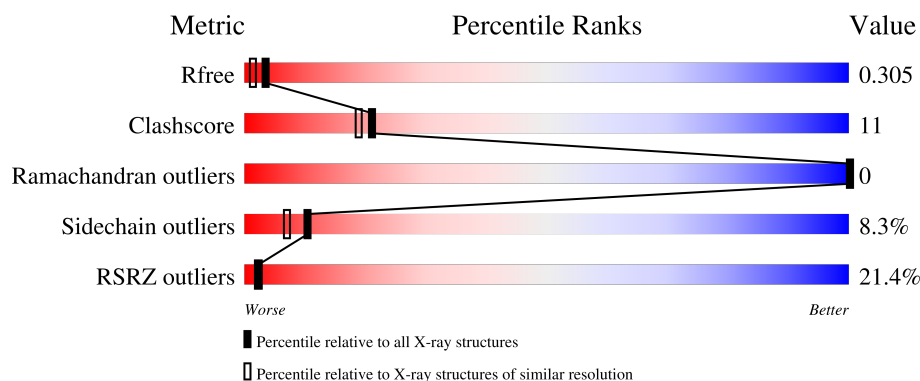
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	61	16% 77% 21% .
1	B	61	15% 79% 18% ..
1	G	61	28% 72% 18% 8% .
1	J	61	16% 72% 20% 5%
2	C	18	22% 72% 28%

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Mol	Chain	Length	Quality of chain
2	D	18	28%61%39%
2	H	18	28%61%39%
2	K	18	28%61%39%
3	E	18	28%61%39%
3	F	18	17%72%28%
3	I	18	28%67%28%6%
3	L	18	17%61%39%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5413 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 Homeobox protein Hox-B13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	0	0	0
			521	329	105	87			
1	B	60	Total	C	N	O	0	3	0
			538	339	108	91			
1	G	60	Total	C	N	O	0	2	0
			532	334	108	90			
1	J	58	Total	C	N	O	0	0	0
			496	314	98	84			

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*AP*CP*GP*AP*GP*GP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			371	178	59	116	18			
2	D	18	Total	C	N	O	P	0	0	0
			371	178	59	116	18			
2	H	18	Total	C	N	O	P	0	0	0
			371	178	59	116	18			
2	K	18	Total	C	N	O	P	0	0	0
			371	178	59	116	18			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*AP*CP*CP*TP*5HCP*AP*TP*AP*AP*AP*AP*CP*AP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	18	Total	C	N	O	P	5	0	0
			371	176	74	103	18			
3	E	18	Total	C	N	O	P	5	0	0
			371	176	74	103	18			
3	I	18	Total	C	N	O	P	5	0	0
			371	176	74	103	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	18	Total	C	N	O	P	5	0	0
			371	176	74	103	18			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total	O	0	0
			45	45		
5	C	39	Total	O	0	0
			39	39		
5	F	24	Total	O	0	0
			24	24		
5	B	53	Total	O	0	0
			53	53		
5	D	38	Total	O	0	0
			38	38		
5	E	28	Total	O	0	0
			28	28		
5	G	32	Total	O	0	0
			32	32		
5	H	25	Total	O	0	0
			25	25		
5	I	19	Total	O	0	0
			19	19		
5	J	21	Total	O	0	0
			21	21		
5	K	14	Total	O	0	0
			14	14		
5	L	18	Total	O	0	0
			18	18		

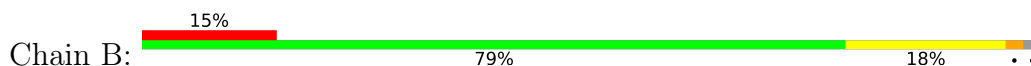
3 Residue-property plots [i](#)

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.

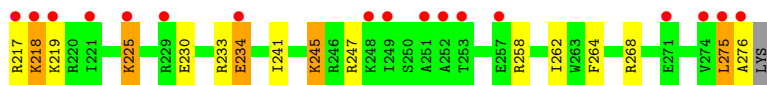
- Molecule 1: Homeobox protein Hox-B13



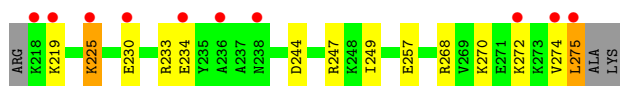
- Molecule 1: Homeobox protein Hox-B13



- Molecule 1: Homeobox protein Hox-B13



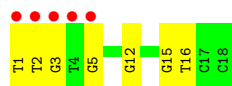
- Molecule 1: Homeobox protein Hox-B13



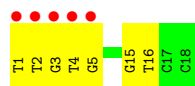
- Molecule 2: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*CP*GP*AP*GP*GP*T P*CP*C)-3')



- Molecule 2: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*CP*GP*AP*GP*GP*TP*CP*C)-3')



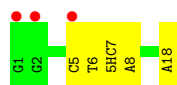
- Molecule 2: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*CP*GP*AP*GP*GP*TP*CP*C)-3')



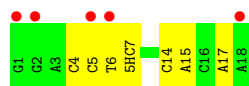
- Molecule 2: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*CP*GP*AP*GP*GP*TP*CP*C)-3')



- Molecule 3: DNA (5'-D(P*GP*GP*AP*CP*CP*TP*5HCP*AP*TP*AP*AP*AP*AP*CP*AP*CP*AP*A)-3')

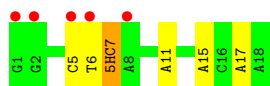


- Molecule 3: DNA (5'-D(P*GP*GP*AP*CP*CP*TP*5HCP*AP*TP*AP*AP*AP*AP*CP*AP*CP*AP*A)-3')

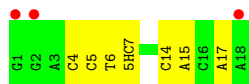


- Molecule 3: DNA (5'-D(P*GP*GP*AP*CP*CP*TP*5HCP*AP*TP*AP*AP*AP*AP*CP*AP*CP*AP*A)-3')





- Molecule 3: DNA (5'-D(P*GP*GP*AP*CP*CP*TP*5HCP*AP*TP*AP*AP*AP*AP*CP*AP*CP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.15Å 55.54Å 101.08Å 88.02° 81.46° 84.94°	Depositor
Resolution (Å)	47.00 – 2.00 47.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.00-2.00) 98.6 (47.00-2.00)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.260 , 0.283 0.277 , 0.305	Depositor DCC
R_{free} test set	1642 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5413	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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, 5HC

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	1.10	0/527	1.43	0/697
1	B	1.08	0/544	1.40	0/719
1	G	1.02	0/538	1.39	0/712
1	J	1.07	0/502	1.37	0/665
2	C	0.45	0/413	0.87	0/635
2	D	0.41	0/413	0.84	1/635 (0.2%)
2	H	0.43	0/413	0.85	0/635
2	K	0.42	0/413	0.81	0/635
3	E	0.40	0/393	0.77	0/599
3	F	0.39	0/393	0.81	0/599
3	I	0.39	0/393	0.77	0/599
3	L	0.37	0/393	0.74	0/599
All	All	0.74	0/5335	1.06	1/7729 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	DG	C4'-C3'-O3'	-5.28	102.08	110.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	521	0	568	11	0
1	B	538	0	582	16	0
1	G	532	0	572	15	0
1	J	496	0	537	12	0
2	C	371	0	208	4	0
2	D	371	0	208	4	0
2	H	371	0	208	10	0
2	K	371	0	208	5	0
3	E	371	0	203	13	0
3	F	371	0	203	11	0
3	I	371	0	203	18	0
3	L	371	0	203	7	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	45	0	0	4	0
5	B	53	0	0	1	0
5	C	39	0	0	1	0
5	D	38	0	0	0	0
5	E	28	0	0	7	0
5	F	24	0	0	1	0
5	G	32	0	0	1	0
5	H	25	0	0	2	0
5	I	19	0	0	5	0
5	J	21	0	0	3	0
5	K	14	0	0	0	0
5	L	18	0	0	0	0
All	All	5413	0	3903	98	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 11.

All (98) 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)
2:H:5:DG:N2	3:I:15:DA:C2	2.01	1.28
2:H:3:DG:N2	3:I:17:DA:N7	2.03	1.04
1:B:248[A]:LYS:HE3	1:B:248[A]:LYS:HA	1.44	1.00
3:E:5:DC:OP2	5:E:101:HOH:O	1.80	0.99
1:G:268:ARG:HH21	3:I:5:DC:H3'	1.32	0.94
1:G:268:ARG:NH2	3:I:5:DC:H3'	1.85	0.91
1:B:248[A]:LYS:HE3	1:B:248[A]:LYS:CA	2.04	0.88
1:A:268:ARG:HH21	3:F:5:DC:H3'	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:5:DC:H5	5:E:101:HOH:O	1.60	0.84
3:F:5:DC:H2'	3:F:6:DT:H71	1.62	0.81
1:A:268:ARG:NH2	3:F:5:DC:H3'	1.95	0.81
1:G:268:ARG:HE	3:I:6:DT:P	2.06	0.79
2:H:3:DG:N2	3:I:17:DA:C8	2.51	0.77
3:I:5:DC:H2'	3:I:6:DT:H71	1.66	0.77
3:F:18:DA:N3	5:F:101:HOH:O	2.21	0.73
2:H:5:DG:C2	3:I:15:DA:C2	2.74	0.73
3:E:5:DC:OP1	5:E:102:HOH:O	2.06	0.72
3:E:5:DC:C5	5:E:101:HOH:O	2.38	0.71
1:B:248[A]:LYS:HE3	1:B:248[A]:LYS:O	1.91	0.70
1:A:268:ARG:HE	3:F:6:DT:P	2.14	0.70
1:B:248[A]:LYS:O	1:B:248[A]:LYS:CE	2.39	0.69
2:D:3:DG:N2	3:E:17:DA:N7	2.41	0.68
2:H:5:DG:N2	3:I:15:DA:N3	2.41	0.67
1:G:225:LYS:O	1:G:225:LYS:HE3	1.96	0.66
1:B:248[A]:LYS:CA	1:B:248[A]:LYS:CE	2.72	0.65
1:B:248[A]:LYS:HE3	1:B:248[A]:LYS:C	2.21	0.65
3:E:4:DC:N4	5:E:103:HOH:O	2.28	0.65
3:E:5:DC:N4	5:E:104:HOH:O	2.30	0.65
2:H:3:DG:H1'	2:H:4:DT:H5'	1.80	0.64
1:G:262:ILE:HG21	5:H:122:HOH:O	2.00	0.60
1:J:268:ARG:NE	3:L:6:DT:OP1	2.34	0.60
5:A:311:HOH:O	3:F:5:DC:C6	2.52	0.59
1:B:248[A]:LYS:CE	1:B:248[A]:LYS:C	2.76	0.58
1:B:274:VAL:HG23	5:B:416:HOH:O	2.03	0.58
1:J:274:VAL:HG12	1:J:274:VAL:O	2.03	0.58
1:J:244:ASP:HB2	5:J:304:HOH:O	2.04	0.58
1:G:275:LEU:O	1:G:276:ALA:O	2.21	0.57
1:A:230:GLU:OE2	1:A:233:ARG:NH2	2.35	0.57
5:A:311:HOH:O	3:F:5:DC:H6	1.87	0.57
3:I:7:5HC:H1'	5:I:106:HOH:O	2.04	0.57
2:H:5:DG:N2	3:I:15:DA:N1	2.50	0.56
1:B:248[A]:LYS:O	1:B:248[A]:LYS:HE2	2.05	0.56
1:G:268:ARG:NE	3:I:6:DT:OP2	2.34	0.55
1:A:217:ARG:N	5:A:302:HOH:O	2.40	0.55
2:K:5:DG:N2	3:L:15:DA:C2	2.74	0.55
1:B:268:ARG:HE	3:E:6:DT:P	2.29	0.55
3:I:17:DA:H8	5:I:116:HOH:O	1.89	0.55
2:K:3:DG:N2	3:L:17:DA:N7	2.56	0.54
1:A:268:ARG:NE	3:F:6:DT:OP2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:270:LYS:NZ	2:K:8:DT:OP1	2.42	0.52
3:L:4:DC:H2'	3:L:5:DC:C6	2.45	0.52
1:B:268:ARG:NE	3:E:6:DT:OP1	2.41	0.52
1:J:234:GLU:HG3	1:J:249:ILE:HD11	1.92	0.50
1:G:230:GLU:OE2	1:G:233:ARG:NH2	2.44	0.50
1:G:234[B]:GLU:HG3	1:G:264:PHE:HZ	1.77	0.50
1:B:265:GLN:NE2	5:E:101:HOH:O	2.31	0.49
1:J:230:GLU:OE2	1:J:233:ARG:NH2	2.46	0.49
1:G:241:ILE:HD11	1:G:245:LYS:HB3	1.95	0.49
1:G:247[B]:ARG:NH1	5:G:303:HOH:O	2.45	0.49
1:J:275:LEU:HD23	5:J:320:HOH:O	2.12	0.49
2:D:1:DT:H1'	2:D:2:DT:C5	2.48	0.48
2:K:1:DT:H2''	2:K:2:DT:H72	1.94	0.48
1:A:234:GLU:HG3	1:A:249:ILE:HD11	1.95	0.48
1:G:258:ARG:HE	1:G:262:ILE:HD11	1.78	0.48
1:G:268:ARG:NH2	3:I:6:DT:OP2	2.46	0.48
1:G:217:ARG:C	1:G:218:LYS:HG3	2.39	0.47
1:A:241:ILE:HD11	1:A:245:LYS:HB3	1.96	0.47
1:B:241:ILE:HD11	1:B:245:LYS:HB3	1.96	0.47
1:B:233[B]:ARG:HG2	1:B:233[B]:ARG:HH11	1.78	0.47
1:J:275:LEU:HD23	1:J:275:LEU:C	2.38	0.47
3:L:5:DC:H2'	3:L:6:DT:C6	2.50	0.47
2:D:15:DG:H2''	2:D:16:DT:H5'	1.97	0.47
2:H:1:DT:H2''	2:H:2:DT:H72	1.95	0.47
1:J:275:LEU:CD2	5:J:320:HOH:O	2.62	0.47
2:D:5:DG:N2	3:E:15:DA:C2	2.83	0.47
5:A:311:HOH:O	3:F:5:DC:C5	2.69	0.46
3:I:5:DC:H6	5:I:109:HOH:O	1.98	0.46
2:H:16:DT:H5''	5:H:101:HOH:O	2.15	0.46
3:E:5:DC:H2''	3:E:6:DT:H5'	1.98	0.46
1:J:225:LYS:HA	1:J:225:LYS:CE	2.47	0.45
2:H:15:DG:H2''	2:H:16:DT:H5'	1.99	0.45
1:J:268:ARG:HE	3:L:6:DT:P	2.40	0.45
1:G:268:ARG:NE	3:I:6:DT:P	2.85	0.44
1:A:268:ARG:NH2	3:F:6:DT:OP2	2.49	0.44
1:A:220:ARG:HD2	2:C:9:DT:O4'	2.17	0.43
3:L:14:DC:H2''	3:L:15:DA:C8	2.53	0.43
1:J:247:ARG:HG2	1:J:257:GLU:OE2	2.18	0.43
3:E:14:DC:H2''	3:E:15:DA:C8	2.54	0.43
3:I:7:5HC:C1'	5:I:106:HOH:O	2.66	0.43
2:C:15:DG:H2''	2:C:16:DT:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:DG:N2	3:F:8:DA:C2	2.88	0.42
1:B:233[B]:ARG:HG2	1:B:233[B]:ARG:NH1	2.35	0.41
1:B:247:ARG:HG2	1:B:257:GLU:OE2	2.20	0.41
1:A:247:ARG:HG2	1:A:257:GLU:OE2	2.19	0.41
3:E:4:DC:H2'	3:E:5:DC:C6	2.56	0.41
2:C:13:DA:H2''	5:C:201:HOH:O	2.22	0.40
3:I:11:DA:P	5:I:101:HOH:O	2.80	0.40
2:K:15:DG:H2''	2:K:16:DT:H5'	2.03	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	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
1	B	61/61 (100%)	61 (100%)	0	0	100	100
1	G	60/61 (98%)	56 (93%)	4 (7%)	0	100	100
1	J	56/61 (92%)	55 (98%)	1 (2%)	0	100	100
All	All	236/244 (97%)	230 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	55/55 (100%)	51 (93%)	4 (7%)	13	9
1	B	57/55 (104%)	52 (91%)	5 (9%)	9	6
1	G	56/55 (102%)	49 (88%)	7 (12%)	4	2
1	J	53/55 (96%)	49 (92%)	4 (8%)	12	9
All	All	221/220 (100%)	201 (91%)	20 (9%)	10	6

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	LYS
1	A	245	LYS
1	A	275	LEU
1	A	277	LYS
1	B	219	LYS
1	B	225	LYS
1	B	248[A]	LYS
1	B	248[B]	LYS
1	B	275	LEU
1	G	218	LYS
1	G	219	LYS
1	G	225	LYS
1	G	234[A]	GLU
1	G	234[B]	GLU
1	G	245	LYS
1	G	275	LEU
1	J	219	LYS
1	J	225	LYS
1	J	272	LYS
1	J	275	LEU

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 ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	5HC	F	7	3,2	18,22,23	0.81	1 (5%)	22,31,34	1.05	1 (4%)
3	5HC	L	7	3,2	18,22,23	0.81	1 (5%)	22,31,34	1.07	1 (4%)
3	5HC	E	7	3,2	18,22,23	0.83	1 (5%)	22,31,34	1.04	1 (4%)
3	5HC	I	7	3,2	18,22,23	0.82	1 (5%)	22,31,34	1.05	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5HC	F	7	3,2	-	2/9/23/24	0/2/2/2
3	5HC	L	7	3,2	-	4/9/23/24	0/2/2/2
3	5HC	E	7	3,2	-	2/9/23/24	0/2/2/2
3	5HC	I	7	3,2	-	2/9/23/24	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	7	5HC	C6-N1	-2.32	1.34	1.38
3	E	7	5HC	C6-N1	-2.31	1.34	1.38
3	L	7	5HC	C6-N1	-2.27	1.34	1.38
3	F	7	5HC	C6-N1	-2.25	1.34	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	7	5HC	C5-C6-N1	-2.46	119.63	122.94
3	F	7	5HC	C5-C6-N1	-2.41	119.70	122.94
3	I	7	5HC	C5-C6-N1	-2.40	119.71	122.94
3	E	7	5HC	C5-C6-N1	-2.40	119.72	122.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	7	5HC	O4'-C4'-C5'-O5'
3	F	7	5HC	C4-C5-C5M-O5
3	E	7	5HC	C4-C5-C5M-O5
3	I	7	5HC	C4-C5-C5M-O5
3	L	7	5HC	C4-C5-C5M-O5
3	L	7	5HC	C3'-C4'-C5'-O5'
3	F	7	5HC	C6-C5-C5M-O5
3	E	7	5HC	C6-C5-C5M-O5
3	I	7	5HC	C6-C5-C5M-O5
3	L	7	5HC	C6-C5-C5M-O5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	7	5HC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

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	61/61 (100%)	1.05	10 (16%)	4 4	19, 31, 69, 99	0
1	B	60/61 (98%)	1.01	9 (15%)	5 5	15, 30, 64, 81	3 (5%)
1	G	60/61 (98%)	1.62	17 (28%)	1 1	18, 40, 63, 97	2 (3%)
1	J	58/61 (95%)	1.39	10 (17%)	4 3	30, 38, 60, 87	0
2	C	18/18 (100%)	0.86	4 (22%)	2 2	22, 36, 83, 90	0
2	D	18/18 (100%)	0.87	5 (27%)	1 1	23, 36, 97, 130	0
2	H	18/18 (100%)	0.87	5 (27%)	1 1	28, 37, 65, 80	0
2	K	18/18 (100%)	1.16	5 (27%)	1 1	32, 47, 83, 115	0
3	E	17/18 (94%)	1.43	5 (29%)	1 1	26, 34, 66, 67	0
3	F	17/18 (94%)	1.17	3 (17%)	4 3	27, 35, 56, 63	0
3	I	17/18 (94%)	1.42	5 (29%)	1 1	31, 40, 59, 60	0
3	L	17/18 (94%)	1.50	3 (17%)	4 3	35, 44, 70, 70	0
All	All	379/388 (97%)	1.22	81 (21%)	2 2	15, 37, 73, 130	5 (1%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	4	DT	5.5
1	J	275	LEU	5.4
1	A	275	LEU	5.1
1	J	225	LYS	5.0
3	I	5	DC	4.8
1	B	275	LEU	4.8
1	G	252	ALA	4.6
2	D	1	DT	4.5
1	G	253	THR	4.5
3	F	5	DC	4.5
1	A	217	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	3	DG	4.4
2	K	1	DT	4.2
1	B	276	ALA	4.1
1	G	225	LYS	4.0
1	A	276	ALA	3.8
2	C	1	DT	3.8
2	H	1	DT	3.8
2	K	3	DG	3.7
1	G	218	LYS	3.7
3	F	1	DG	3.7
2	C	2	DT	3.7
1	J	238	ASN	3.6
1	J	274	VAL	3.6
1	G	276	ALA	3.6
2	H	4	DT	3.5
3	L	2	DG	3.5
1	G	251	ALA	3.5
2	H	3	DG	3.5
3	E	2	DG	3.4
1	B	218	LYS	3.4
2	C	3	DG	3.4
3	I	2	DG	3.3
3	E	5	DC	3.3
1	B	277	LYS	3.3
3	E	1	DG	3.2
1	A	219	LYS	3.2
3	L	1	DG	3.1
1	B	219	LYS	3.1
1	J	230	GLU	3.1
1	G	229	ARG	3.1
3	I	1	DG	3.0
1	J	218	LYS	3.0
1	A	277	LYS	2.9
1	J	219	LYS	2.9
2	D	2	DT	2.9
2	H	2	DT	2.9
1	G	217	ARG	2.9
2	H	5	DG	2.9
2	K	4	DT	2.9
3	I	6	DT	2.9
1	G	219	LYS	2.9
1	G	275	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	234	GLU	2.8
1	A	229	ARG	2.7
2	D	4	DT	2.7
3	E	6	DT	2.6
3	E	18	DA	2.6
1	G	271	GLU	2.6
1	A	225	LYS	2.5
1	B	240	PHE	2.5
1	G	221	ILE	2.4
1	G	257	GLU	2.3
2	K	5	DG	2.3
1	G	274	VAL	2.3
1	A	218	LYS	2.3
2	K	2	DT	2.3
3	F	2	DG	2.3
1	G	234[A]	GLU	2.3
1	G	249	ILE	2.2
3	I	8	DA	2.2
1	B	249	ILE	2.1
1	A	274	VAL	2.1
1	B	274	VAL	2.1
1	J	236	ALA	2.1
1	A	249	ILE	2.1
2	D	5	DG	2.1
3	L	18	DA	2.1
1	G	248	LYS	2.1
1	J	272	LYS	2.1
1	B	234	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	5HC	I	7	21/22	0.71	0.18	31,42,49,52	5
3	5HC	E	7	21/22	0.73	0.18	29,34,38,45	5
3	5HC	F	7	21/22	0.75	0.16	31,36,40,42	5
3	5HC	L	7	21/22	0.77	0.16	36,40,46,48	5

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
4	MG	B	301	1/1	0.94	0.13	52,52,52,52	0
4	MG	C	101	1/1	0.98	0.03	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.