



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:22 PM UTC

PDB ID : 7Q4N / pdb_00007q4n
Title : transcription factor CDX2 bound to hydroxymethylated DNA
Authors : Morgunova, E.; Yin, Y.; Popov, A.; Taipale, J.
Deposited on : 2021-11-01
Resolution : 3.20 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:

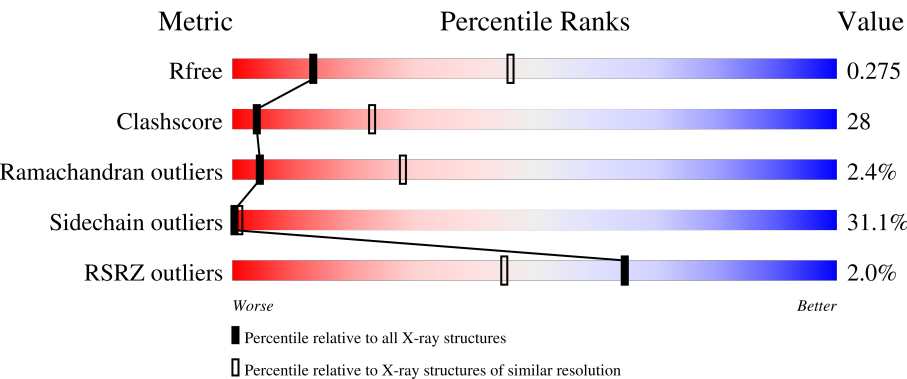
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	18	39% 50% 11%
1	B	18	6% 33% 61% 6%
2	D	18	6% 22% 39% 39%
2	E	18	6% 22% 44% 33%
3	C	67	33% 37% 21% • 6%

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Mol	Chain	Length	Quality of chain
3	K	67	% 39% 45% 15% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2634 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 (18-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	18	Total	C	N	O	P	0	0	0
			368	177	57	116	18			
1	B	18	Total	C	N	O	P	0	0	0
			368	177	57	116	18			

- Molecule 2 is a DNA chain called DNA (18-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	0
			373	177	76	102	18			
2	E	18	Total	C	N	O	P	0	0	0
			373	177	76	102	18			

- Molecule 3 is a protein called Homeobox protein CDX-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	66	Total	C	N	O	0	0	0
			582	368	115	99			
3	C	63	Total	C	N	O	0	0	0
			556	353	110	93			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total 2 O	0	0
4	D	1	Total 1 O	0	0
4	K	4	Total 4 O	0	0
4	B	2	Total 2 O	0	0

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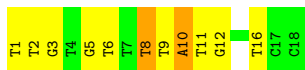
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total	O	0	0
			2	2		
4	C	3	Total	O	0	0
			3	3		

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: DNA (18-MER)

Chain A: 



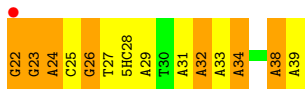
- Molecule 1: DNA (18-MER)

Chain B: 



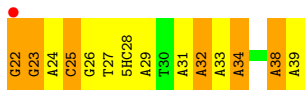
- Molecule 2: DNA (18-MER)

Chain D: 

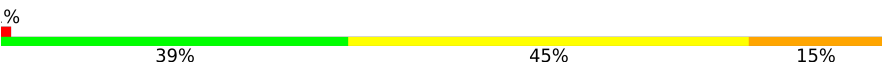


- Molecule 2: DNA (18-MER)

Chain E: 



- Molecule 3: Homeobox protein CDX-2

Chain K: 



ASP	L189	V192	V193	T194	D195	H196	L197	R198	L199	E200	L201	E202	K203	E204	F205	R209	I213	R214	R215	K216	L219	A220	L223	G224	L225	S226	E227	R228	Q229	V230	K231	L232	W233	F234	Q235	N236	R237	R238	E241	R242	K243	L244	N245	K246	K247	K248	L249	Q250	Q251	GLN	GLN
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4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.90Å 46.63Å 120.05Å 90.00° 98.25° 90.00°	Depositor
Resolution (Å)	43.45 – 3.20 43.45 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.45-3.20) 98.2 (43.45-3.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.279 0.238 , 0.275	Depositor DCC
R_{free} test set	385 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	1.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2634	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.33% 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: 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	0.84	0/409	1.37	3/628 (0.5%)
1	B	0.86	0/409	1.31	2/628 (0.3%)
2	D	0.80	0/396	1.52	8/606 (1.3%)
2	E	0.86	1/396 (0.3%)	1.41	6/606 (1.0%)
3	C	1.06	0/565	1.57	7/752 (0.9%)
3	K	1.01	0/591	1.61	2/786 (0.3%)
All	All	0.93	1/2766 (0.0%)	1.48	28/4006 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	22	DG	P-OP1	6.08	1.60	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	22	DG	P-O3'-C3'	8.46	132.89	120.20
2	D	32	DA	P-O3'-C3'	-8.12	108.02	120.20
2	D	24	DA	O3'-P-O5'	-7.65	92.53	104.00
2	D	34	DA	C4'-C3'-O3'	-7.60	98.60	110.00
2	E	34	DA	C4'-C3'-O3'	-7.43	98.85	110.00
2	E	32	DA	P-O3'-C3'	-7.31	109.23	120.20
1	A	16	DT	P-O3'-C3'	-7.05	109.62	120.20
1	B	16	DT	P-O3'-C3'	-7.01	109.68	120.20
3	C	235	GLN	CA-C-N	6.47	128.85	120.44
3	C	235	GLN	C-N-CA	6.47	128.85	120.44
3	C	195	ASP	CA-CB-CG	6.30	118.90	112.60
2	D	38	DA	P-O3'-C3'	-6.26	110.81	120.20
2	E	22	DG	P-O3'-C3'	6.19	129.48	120.20
3	K	235	GLN	CA-C-N	5.91	128.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	235	GLN	C-N-CA	5.91	128.13	120.44
1	A	10	DA	O3'-P-O5'	-5.63	95.55	104.00
3	C	197	GLN	CB-CA-C	5.57	120.32	110.85
2	D	22	DG	N9-C1'-C2'	5.56	121.84	113.50
2	D	26	DG	P-O3'-C3'	-5.54	111.89	120.20
1	A	8	DT	O3'-P-O5'	-5.47	95.80	104.00
2	E	38	DA	P-O3'-C3'	-5.36	112.16	120.20
3	C	238	ARG	CA-C-O	-5.36	115.20	120.82
3	C	220	ALA	CA-C-N	5.35	127.72	120.44
3	C	220	ALA	C-N-CA	5.35	127.72	120.44
2	D	23	DG	P-O3'-C3'	5.29	128.14	120.20
1	B	10	DA	O3'-P-O5'	-5.28	96.08	104.00
2	E	23	DG	C4'-C3'-O3'	5.27	117.90	110.00
2	E	25	DC	P-O3'-C3'	-5.03	112.66	120.20

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	368	0	208	18	0
1	B	368	0	208	17	1
2	D	373	0	203	14	1
2	E	373	0	203	16	0
3	C	556	0	581	45	0
3	K	582	0	606	32	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	1	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	K	4	0	0	0	0
All	All	2634	0	2009	127	1

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 28.

All (127) 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:B:18:DC:N4	2:E:22:DG:O6	1.87	1.07
3:C:202:GLU:OE2	3:C:237:ARG:HD2	1.63	0.98
2:D:22:DG:H2'	2:D:23:DG:C8	2.10	0.86
2:E:22:DG:OP1	2:E:22:DG:C5	2.33	0.81
1:A:1:DT:H2'	1:A:2:DT:C6	2.19	0.78
1:B:1:DT:H2'	1:B:2:DT:C6	2.19	0.76
1:A:9:DT:H1'	3:K:190:ARG:HG2	1.67	0.76
3:K:225:LEU:HD11	3:K:229:GLN:OE1	1.86	0.76
3:C:248:LYS:HE3	3:C:250:GLN:CG	2.18	0.74
2:E:22:DG:OP1	2:E:22:DG:C4	2.41	0.73
3:K:201:LEU:HG	3:K:233:TRP:CD2	2.24	0.72
1:B:17:DC:C6	1:B:18:DC:H2'	2.26	0.71
1:A:9:DT:H5'	3:K:193:TYR:CE1	2.26	0.71
1:A:1:DT:C2'	1:A:2:DT:C6	2.75	0.70
3:C:246:LYS:O	3:C:249:LEU:HG	1.90	0.69
1:B:1:DT:C2'	1:B:2:DT:C6	2.75	0.69
2:D:22:DG:H2''	2:D:23:DG:O4'	1.92	0.68
3:C:241:GLU:OE1	4:C:301:HOH:O	2.11	0.68
2:E:25:DC:OP1	3:C:213:ILE:HD13	1.95	0.67
2:D:22:DG:C2'	2:D:23:DG:C8	2.79	0.66
3:K:200:GLU:HB3	3:K:223:LEU:HD11	1.78	0.66
1:A:9:DT:H4'	3:K:191:VAL:O	1.96	0.65
3:C:226:SER:N	3:C:229:GLN:OE1	2.30	0.64
2:D:22:DG:H2''	2:D:23:DG:C1'	2.27	0.63
3:C:228:ARG:O	3:C:232:ILE:HG12	1.99	0.62
2:D:24:DA:H2''	2:D:25:DC:OP2	2.01	0.60
3:K:201:LEU:HG	3:K:233:TRP:CE3	2.37	0.59
3:C:248:LYS:HE3	3:C:250:GLN:NE2	2.18	0.59
2:E:28:5HC:OP2	3:C:242:ARG:NH1	2.34	0.58
2:E:22:DG:C6	2:E:23:DG:C6	2.92	0.58
2:E:28:5HC:P	3:C:242:ARG:HH12	2.27	0.58
3:C:250:GLN:O	3:C:251:GLN:NE2	2.37	0.57
3:K:228:ARG:O	3:K:232:ILE:HG12	2.04	0.57
1:B:1:DT:H2'	1:B:2:DT:C5	2.39	0.57
3:C:205:PHE:CE1	3:C:237:ARG:HB3	2.40	0.57
2:D:31:DA:H2''	2:D:32:DA:C8	2.40	0.57
3:K:218:GLU:O	3:K:222:THR:HG22	2.05	0.57
1:A:8:DT:H1'	3:K:190:ARG:NH1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:225:LEU:CD1	3:K:229:GLN:OE1	2.53	0.56
3:K:244:ILE:O	3:K:248:LYS:HG3	2.06	0.55
1:A:1:DT:H2'	1:A:2:DT:C5	2.42	0.55
3:C:243:LYS:HD2	3:C:246:LYS:HZ2	1.72	0.55
3:C:201:LEU:HD22	3:C:233:TRP:CD2	2.43	0.54
3:C:192:VAL:O	3:C:193:TYR:O	2.25	0.54
3:K:215:ARG:HA	3:K:218:GLU:HB2	1.90	0.53
2:E:31:DA:H2''	2:E:32:DA:C8	2.43	0.53
2:D:31:DA:H2''	2:D:32:DA:H8	1.74	0.53
1:A:1:DT:H2''	1:A:2:DT:C6	2.44	0.53
1:B:2:DT:H2''	1:B:3:DG:C8	2.45	0.53
1:B:11:DT:H2''	1:B:12:DG:C8	2.45	0.53
3:C:219:LEU:HD13	3:C:223:LEU:CD2	2.39	0.52
3:C:225:LEU:HG	3:C:229:GLN:OE1	2.10	0.52
3:K:201:LEU:HG	3:K:233:TRP:CE2	2.44	0.52
1:B:1:DT:H2''	1:B:2:DT:C6	2.44	0.52
2:D:26:DG:H2'	2:D:27:DT:C6	2.45	0.51
3:K:209:ARG:NH1	3:K:241:GLU:OE1	2.38	0.51
2:E:26:DG:H2'	2:E:27:DT:C6	2.45	0.51
1:B:1:DT:H2'	1:B:2:DT:C7	2.40	0.51
2:D:33:DA:H2''	2:D:34:DA:O5'	2.10	0.51
2:E:24:DA:H2''	2:E:25:DC:OP2	2.11	0.51
3:C:200:GLU:OE2	3:C:203:LYS:HE2	2.12	0.50
3:C:219:LEU:HD13	3:C:223:LEU:HD23	1.93	0.50
3:K:199:LEU:C	3:K:199:LEU:HD22	2.37	0.50
3:K:206:HIS:CE1	3:C:241:GLU:CD	2.90	0.49
1:A:11:DT:H2''	1:A:12:DG:C8	2.47	0.49
2:E:31:DA:H2''	2:E:32:DA:H8	1.78	0.49
2:E:33:DA:H2''	2:E:34:DA:O5'	2.11	0.48
3:K:193:TYR:HB2	3:K:198:ARG:NE	2.29	0.48
1:A:2:DT:H2''	1:A:3:DG:C8	2.48	0.48
2:E:22:DG:C2	2:E:23:DG:C2	3.02	0.48
3:K:197:GLN:O	3:K:201:LEU:HB2	2.13	0.47
3:C:247:LYS:C	3:C:249:LEU:H	2.20	0.47
3:C:246:LYS:HZ1	3:C:247:LYS:HE3	1.79	0.47
1:A:1:DT:H2'	1:A:2:DT:C7	2.45	0.47
1:B:17:DC:C2'	1:B:18:DC:H5'	2.44	0.47
3:C:243:LYS:HD2	3:C:246:LYS:NZ	2.30	0.47
1:B:17:DC:H6	1:B:18:DC:H2'	1.75	0.47
3:C:201:LEU:HB3	3:C:233:TRP:CZ2	2.50	0.47
3:C:225:LEU:HD12	3:C:229:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:248:LYS:HE3	3:C:250:GLN:CD	2.39	0.46
3:C:248:LYS:HE3	3:C:250:GLN:HE21	1.80	0.46
1:B:9:DT:H2''	1:B:10:DA:O5'	2.16	0.46
1:A:9:DT:P	3:K:198:ARG:NH2	2.89	0.46
3:C:248:LYS:HE3	3:C:250:GLN:HG2	1.95	0.46
3:C:194:THR:HG23	3:C:197:GLN:HB3	1.97	0.45
3:C:225:LEU:CD1	3:C:229:GLN:OE1	2.63	0.45
3:C:248:LYS:CE	3:C:250:GLN:HG3	2.47	0.45
3:C:248:LYS:CE	3:C:250:GLN:CG	2.90	0.45
1:A:9:DT:H5'	3:K:193:TYR:CD1	2.51	0.45
3:C:248:LYS:HD2	3:C:250:GLN:HG3	1.98	0.45
1:B:2:DT:H2''	1:B:3:DG:N7	2.32	0.44
2:D:38:DA:H2''	2:D:39:DA:C8	2.53	0.44
3:K:206:HIS:HE1	3:C:241:GLU:CD	2.25	0.44
2:E:38:DA:H2''	2:E:39:DA:C8	2.52	0.44
2:D:22:DG:H2''	2:D:23:DG:C2'	2.47	0.44
1:A:9:DT:H2''	1:A:10:DA:O5'	2.18	0.44
3:C:231:LYS:O	3:C:235:GLN:HG3	2.18	0.44
3:C:226:SER:O	3:C:229:GLN:HB2	2.17	0.43
1:B:17:DC:H2'	1:B:18:DC:H5'	2.00	0.43
1:A:2:DT:H4'	1:A:3:DG:OP1	2.18	0.43
3:K:195:ASP:OD2	3:C:196:HIS:HB2	2.19	0.43
1:B:5:DG:C2	1:B:6:DT:C2	3.06	0.43
2:D:22:DG:H2''	2:D:23:DG:H2'	2.00	0.43
2:D:26:DG:C2'	2:D:27:DT:O5'	2.67	0.43
3:C:248:LYS:CE	3:C:250:GLN:NE2	2.82	0.42
3:C:198:ARG:HA	3:C:201:LEU:HD12	2.00	0.42
1:A:5:DG:C2	1:A:6:DT:C2	3.07	0.42
3:K:220:ALA:HB1	3:K:225:LEU:O	2.19	0.42
2:E:28:5HC:H2''	2:E:29:DA:C8	2.54	0.42
3:C:200:GLU:O	3:C:201:LEU:C	2.63	0.42
3:C:233:TRP:CZ2	3:C:237:ARG:HG3	2.55	0.42
1:A:8:DT:H1'	3:K:190:ARG:HH12	1.84	0.41
3:K:199:LEU:C	3:K:199:LEU:CD2	2.92	0.41
2:D:28:5HC:H2''	2:D:29:DA:C8	2.55	0.41
3:K:195:ASP:O	3:K:199:LEU:N	2.43	0.41
3:K:240:LYS:HD3	3:K:240:LYS:HA	1.76	0.41
1:B:5:DG:H2''	1:B:6:DT:OP2	2.21	0.41
3:C:248:LYS:CD	3:C:250:GLN:HG3	2.51	0.41
1:A:2:DT:H2''	1:A:3:DG:N7	2.36	0.41
3:K:200:GLU:O	3:K:201:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:231:LYS:HE2	3:K:235:GLN:HE22	1.86	0.40
2:E:29:DA:OP2	2:E:29:DA:H8	2.04	0.40
3:K:207:TYR:CE1	3:C:244:ILE:HD13	2.57	0.40
3:K:216:LYS:HE2	3:K:216:LYS:HB2	1.86	0.40
1:B:2:DT:H4'	1:B:3:DG:OP1	2.21	0.40
3:C:225:LEU:HD12	3:C:225:LEU:HA	1.80	0.40
3:C:236:ASN:HD22	3:C:236:ASN:HA	1.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:DG:OP1	1:B:18:DC:O3'[2_465]	2.19	0.01

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	
3	C	61/67 (91%)	51 (84%)	7 (12%)	3 (5%)	1	13
3	K	64/67 (96%)	56 (88%)	8 (12%)	0	100	100
All	All	125/134 (93%)	107 (86%)	15 (12%)	3 (2%)	4	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	193	TYR
3	C	248	LYS
3	C	250	GLN

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	
3	C	58/62 (94%)	41 (71%)	17 (29%)	0	1
3	K	61/62 (98%)	41 (67%)	20 (33%)	0	1
All	All	119/124 (96%)	82 (69%)	37 (31%)	0	1

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	188	LYS
3	K	190	ARG
3	K	191	VAL
3	K	194	THR
3	K	199	LEU
3	K	200	GLU
3	K	201	LEU
3	K	203	LYS
3	K	211	ILE
3	K	218	GLU
3	K	226	SER
3	K	228	ARG
3	K	229	GLN
3	K	230	VAL
3	K	240	LYS
3	K	242	ARG
3	K	243	LYS
3	K	246	LYS
3	K	247	LYS
3	K	250	GLN
3	C	192	VAL
3	C	194	THR
3	C	197	GLN
3	C	198	ARG
3	C	209	ARG
3	C	214	ARG
3	C	216	LYS

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Mol	Chain	Res	Type
3	C	219	LEU
3	C	223	LEU
3	C	226	SER
3	C	230	VAL
3	C	237	ARG
3	C	242	ARG
3	C	243	LYS
3	C	244	ILE
3	C	246	LYS
3	C	248	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	197	GLN
3	K	236	ASN
3	K	250	GLN
3	C	196	HIS
3	C	197	GLN
3	C	236	ASN
3	C	250	GLN
3	C	251	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	$\# Z > 2$
2	5HC	D	28	1,2	18,22,23	0.41	0	22,31,34	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5HC	E	28	1,2	18,22,23	0.35	0	22,31,34	0.50	0

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
2	5HC	D	28	1,2	-	4/9/23/24	0/2/2/2
2	5HC	E	28	1,2	-	4/9/23/24	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	28	5HC	O4'-C4'-C5'-O5'
2	D	28	5HC	C4-C5-C5M-O5
2	D	28	5HC	C6-C5-C5M-O5
2	E	28	5HC	O4'-C4'-C5'-O5'
2	E	28	5HC	C3'-C4'-C5'-O5'
2	E	28	5HC	C4-C5-C5M-O5
2	E	28	5HC	C6-C5-C5M-O5
2	D	28	5HC	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	28	5HC	1	0
2	E	28	5HC	3	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	18/18 (100%)	0.43	0 100 100	48, 77, 130, 139	0
1	B	18/18 (100%)	0.36	1 (5%) 30 19	55, 76, 120, 144	0
2	D	17/18 (94%)	0.21	1 (5%) 28 18	53, 73, 123, 131	0
2	E	17/18 (94%)	0.57	1 (5%) 28 18	47, 76, 131, 160	0
3	C	63/67 (94%)	0.24	0 100 100	45, 65, 81, 100	0
3	K	66/67 (98%)	0.30	1 (1%) 72 52	41, 62, 88, 102	0
All	All	199/206 (96%)	0.31	4 (2%) 65 45	41, 67, 116, 160	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	22	DG	4.9
2	D	22	DG	3.4
3	K	245	ASN	2.3
1	B	1	DT	2.2

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
2	5HC	D	28	21/22	0.92	0.09	53,58,64,68	0
2	5HC	E	28	21/22	0.94	0.08	47,54,59,67	0

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.