



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:48 am BST

PDB ID : 6JNN
Title : REF6 ZnF2-4-NAC004-mC1 complex
Authors : Yao, Q.Q.; Wu, B.X.; Ma, J.B.
Deposited on : 2019-03-17
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

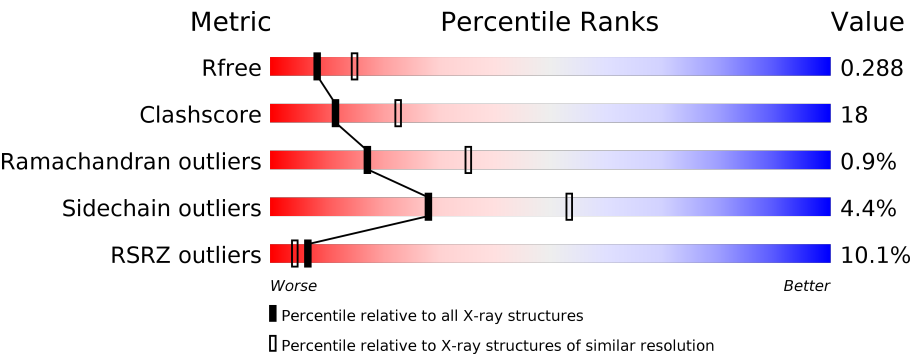
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	101	<div><div>%</div><div><div></div><div>67%</div><div>20%</div><div>•</div><div>12%</div></div></div>
1	B	101	<div><div>%</div><div><div></div><div>57%</div><div>29%</div><div>•</div><div>12%</div></div></div>
1	G	101	<div><div>26%</div><div><div></div><div>58%</div><div>26%</div><div>•</div><div>13%</div></div></div>
1	N	101	<div><div>16%</div><div><div></div><div>57%</div><div>26%</div><div>5%</div><div>12%</div></div></div>
2	D	12	<div><div></div><div><div></div><div>50%</div><div>50%</div></div></div>
2	F	12	<div><div></div><div><div></div><div>50%</div><div>42%</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	I	12	 75% 25%
2	L	12	 42% 58%
3	C	12	 58% 42%
3	E	12	 83% 17%
3	H	12	 50% 50%
3	K	12	 8% 58% 42%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4939 atoms, of which 39 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 Lysine-specific demethylase REF6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	0	0
			735	463	146	119	7			
1	B	89	Total	C	N	O	S	0	0	0
			739	466	147	119	7			
1	N	89	Total	C	N	O	S	0	0	0
			738	466	147	118	7			
1	G	88	Total	C	N	O	S	0	0	0
			728	460	143	118	7			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	12	Total	C	H	N	O	P	0	0	0
			253	119	13	32	78	11			
2	F	12	Total	C	H	N	O	P	0	0	0
			253	119	13	32	78	11			
2	I	12	Total	C	N	O	P		0	0	0
			240	119	32	78	11				
2	L	12	Total	C	H	N	O	P	0	0	0
			253	119	13	32	78	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			247	118	56	62	11			
3	E	12	Total	C	N	O	P	0	0	0
			247	118	56	62	11			
3	H	12	Total	C	N	O	P	0	0	0
			247	118	56	62	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	12	Total	C	N	O	P	0	0	0
			247	118	56	62	11			

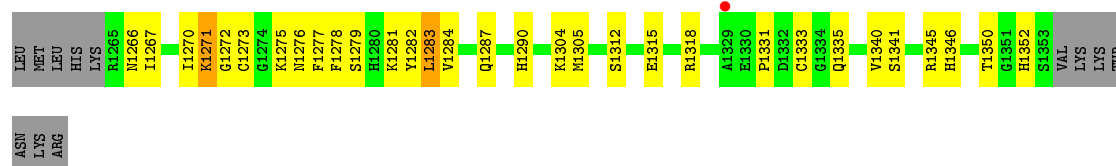
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	3	Total	Zn	0	0
			3	3		
4	B	3	Total	Zn	0	0
			3	3		
4	A	3	Total	Zn	0	0
			3	3		
4	N	3	Total	Zn	0	0
			3	3		

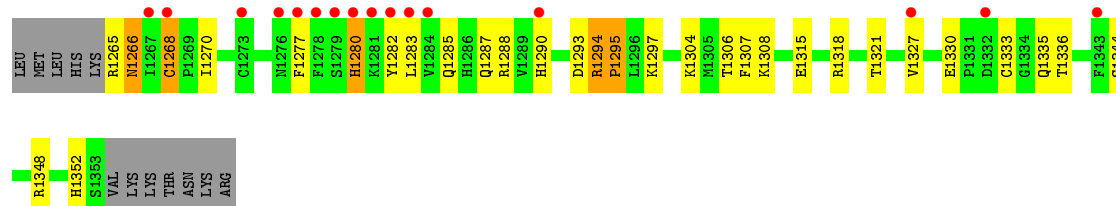
- Molecule 1: Lysine-specific demethylase REF6



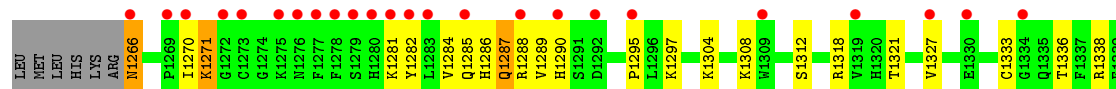
- Chain B:  %

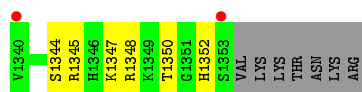


- Chain N: 



- Chain G: 

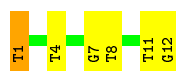




- Molecule 2: DNA (5'-D(*TP*TP*(5CM)P*TP*CP*TP*GP*TP*TP*TP*TP*G)-3')



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



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



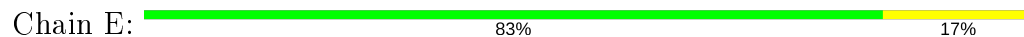
- Molecule 2: DNA (5'-D(*TP*TP*(5CM)P*TP*CP*TP*GP*TP*TP*TP*TP*G)-3')



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



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

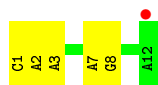


- Molecule 3: DNA (5'-D(*CP*AP*AP*AP*AP*CP*AP*GP*AP*GP*AP*A)-3')





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	70.97Å 70.97Å 141.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.03 – 2.58	Depositor EDS
% Data completeness (in resolution range)	85.0 (30.00-2.60) 80.4 (30.03-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.251 , 0.265 0.271 , 0.288	Depositor DCC
R_{free} test set	1053 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 8.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.227 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.537 for H, K, L 0.463 for K, H, -L	Depositor
Outliers	0 of 20070 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4939	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, 5CM

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	0.73	0/760	0.83	1/1022 (0.1%)
1	B	0.74	0/764	0.87	1/1026 (0.1%)
1	G	0.66	0/753	0.95	1/1012 (0.1%)
1	N	0.69	0/763	0.95	2/1024 (0.2%)
2	D	1.09	1/242 (0.4%)	0.98	0/370
2	F	1.12	2/242 (0.8%)	0.95	0/370
2	I	1.40	4/242 (1.7%)	1.05	0/370
2	L	0.86	1/242 (0.4%)	1.01	1/370 (0.3%)
3	C	0.59	0/280	0.85	0/430
3	E	0.56	0/280	0.86	0/430
3	H	0.60	0/280	0.90	0/430
3	K	0.47	0/280	0.87	0/430
All	All	0.78	8/5128 (0.2%)	0.91	6/7284 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	DT	O3'-P	-10.64	1.48	1.61
2	F	4	DT	O3'-P	-9.79	1.49	1.61
2	D	4	DT	O3'-P	-8.80	1.50	1.61
2	L	4	DT	O3'-P	-8.47	1.50	1.61
2	I	1	DT	O3'-P	-7.85	1.51	1.61
2	I	7	DG	O3'-P	-7.46	1.52	1.61
2	F	1	DT	O3'-P	-6.56	1.53	1.61
2	I	4	DT	O3'-P	-5.37	1.54	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1266	ASN	N-CA-CB	-13.79	85.78	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1266	ASN	N-CA-CB	-13.59	86.14	110.60
1	N	1266	ASN	N-CA-C	8.84	134.85	111.00
1	B	1283	LEU	CB-CG-CD2	6.62	122.26	111.00
2	L	6	DT	C1'-O4'-C4'	-5.35	104.75	110.10
1	A	1338	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	735	0	703	19	0
1	B	739	0	714	27	0
1	G	728	0	705	25	0
1	N	738	0	715	31	0
2	D	240	13	144	6	0
2	F	240	13	144	5	0
2	I	240	0	144	40	0
2	L	240	13	144	8	0
3	C	247	0	134	4	0
3	E	247	0	134	1	0
3	H	247	0	134	10	0
3	K	247	0	134	6	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	G	3	0	0	1	0
4	N	3	0	0	0	0
All	All	4900	39	3949	154	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 18.

All (154) 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:I:7:DG:O6	3:H:6:DC:N4	1.81	1.13
2:I:7:DG:N1	3:H:6:DC:N3	2.09	0.99
2:I:7:DG:H1'	2:I:8:DT:C6	2.00	0.96
2:L:1:DT:H6	2:L:1:DT:HO5'	1.09	0.93
1:G:1289:VAL:HG12	1:G:1290:HIS:HD2	1.31	0.92
2:F:1:DT:HO5'	2:F:1:DT:H6	1.10	0.91
1:A:1265:ARG:NH1	1:B:1305:MET:CE	2.33	0.91
2:I:7:DG:H2''	2:I:8:DT:C7	2.04	0.86
3:H:8:DG:OP2	1:N:1348:ARG:HD3	1.76	0.85
1:G:1289:VAL:HG12	1:G:1290:HIS:CD2	2.11	0.85
1:B:1346:HIS:O	1:B:1350:THR:HB	1.78	0.83
2:I:7:DG:H2''	2:I:8:DT:H73	1.62	0.81
1:A:1265:ARG:NH1	1:B:1305:MET:HE3	1.95	0.80
1:G:1347:LYS:HD3	1:G:1352:HIS:O	1.81	0.80
1:A:1265:ARG:NH1	1:B:1305:MET:HE1	1.96	0.79
2:D:1:DT:H2''	2:D:2:DT:H5'	1.66	0.78
2:I:7:DG:C2'	2:I:8:DT:H72	2.14	0.77
1:G:1270:ILE:HD11	1:G:1287:GLN:OE1	1.84	0.76
1:N:1327:VAL:HG22	1:N:1336:THR:HG22	1.67	0.75
1:A:1265:ARG:HH12	1:B:1305:MET:CE	1.94	0.75
2:I:6:DT:C2'	2:I:7:DG:C8	2.70	0.73
2:I:7:DG:H1'	2:I:8:DT:C5	2.24	0.73
2:I:10:DT:H1'	2:I:11:DT:H5'	1.72	0.72
2:I:8:DT:C2	2:I:9:DT:C5	2.78	0.71
1:G:1327:VAL:HG22	1:G:1336:THR:HG22	1.71	0.71
2:I:8:DT:O2	2:I:9:DT:C6	2.43	0.71
2:D:1:DT:H6	2:D:1:DT:HO5'	1.37	0.71
2:I:7:DG:H2'	2:I:7:DG:OP2	1.90	0.71
1:N:1293:ASP:O	1:N:1308:LYS:NZ	2.17	0.71
1:G:1270:ILE:HG22	1:G:1271:LYS:O	1.92	0.70
2:I:7:DG:C2'	2:I:8:DT:C7	2.70	0.70
2:I:8:DT:O2	2:I:9:DT:H5'	1.92	0.69
1:N:1266:ASN:ND2	1:N:1266:ASN:H	1.90	0.69
1:G:1288:ARG:HB2	1:G:1308:LYS:HE2	1.75	0.69
2:I:6:DT:H2''	2:I:7:DG:C8	2.27	0.68
2:I:8:DT:H2''	2:I:9:DT:O5'	1.95	0.67
1:B:1281:LYS:O	1:B:1284:VAL:HG12	1.94	0.67
1:G:1350:THR:HG23	1:G:1352:HIS:H	1.61	0.65
1:N:1287:GLN:NE2	1:N:1290:HIS:CD2	2.65	0.65
1:G:1270:ILE:CD1	1:G:1287:GLN:OE1	2.45	0.65
2:L:7:DG:OP2	1:G:1286:HIS:ND1	2.29	0.65
2:I:7:DG:C1'	2:I:8:DT:H72	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1266:ASN:HA	1:N:1280:HIS:CE1	2.32	0.64
2:I:6:DT:H2''	2:I:7:DG:H5'	1.79	0.62
1:N:1333:CYS:SG	1:N:1335:GLN:NE2	2.72	0.62
2:I:8:DT:N3	2:I:9:DT:C4	2.67	0.62
1:B:1333:CYS:SG	1:B:1335:GLN:NE2	2.72	0.61
1:G:1333:CYS:SG	4:G:1402:ZN:ZN	1.88	0.61
2:I:7:DG:N2	3:H:6:DC:O2	2.27	0.60
1:A:1333:CYS:SG	1:A:1335:GLN:NE2	2.74	0.60
2:I:7:DG:OP2	1:N:1282:TYR:OH	2.12	0.60
1:N:1270:ILE:HD11	1:N:1287:GLN:HE22	1.67	0.59
2:I:1:DT:H2''	2:I:2:DT:H5'	1.83	0.59
2:I:6:DT:C2'	2:I:7:DG:H8	2.16	0.59
2:I:6:DT:H2'	2:I:7:DG:C8	2.37	0.59
2:I:7:DG:C8	2:I:8:DT:H72	2.37	0.59
3:C:11:DA:OP1	1:G:1297:LYS:HD2	2.04	0.57
1:N:1315:GLU:HG2	1:N:1318:ARG:NH1	2.19	0.57
1:B:1270:ILE:HD13	1:B:1290:HIS:CD2	2.40	0.56
2:I:8:DT:C2	2:I:9:DT:C6	2.93	0.56
1:G:1281:LYS:O	1:G:1284:VAL:HB	2.06	0.56
1:G:1285:GLN:HB3	1:G:1288:ARG:HH21	1.70	0.56
2:I:12:DG:C2	3:H:2:DA:C2	2.95	0.55
2:I:7:DG:N9	2:I:8:DT:H72	2.21	0.55
2:I:6:DT:C2	2:I:7:DG:C5	2.95	0.54
2:I:7:DG:OP1	1:N:1277:PHE:HE1	1.91	0.54
1:G:1347:LYS:HA	1:G:1350:THR:HG22	1.89	0.54
1:N:1330:GLU:HG2	1:N:1352:HIS:CE1	2.43	0.54
2:D:1:DT:H6	2:D:1:DT:O5'	1.91	0.53
1:B:1267:ILE:CD1	1:B:1276:ASN:HB2	2.39	0.53
1:B:1266:ASN:HB3	1:B:1283:LEU:HD12	1.90	0.53
2:I:3:5CM:HN41	3:H:10:DG:H1	1.57	0.53
1:N:1294:ARG:HG2	1:N:1306:THR:OG1	2.09	0.52
1:N:1268:CYS:HA	1:N:1283:LEU:HD11	1.91	0.52
1:A:1278:PHE:HD1	2:D:8:DT:OP2	1.91	0.52
2:I:7:DG:C1'	2:I:8:DT:C7	2.87	0.52
1:N:1315:GLU:HG2	1:N:1318:ARG:HH12	1.75	0.51
1:A:1266:ASN:HB2	1:A:1277:PHE:O	2.11	0.51
2:F:11:DT:H2''	2:F:12:DG:C8	2.46	0.51
1:N:1297:LYS:HE2	1:N:1306:THR:HG22	1.93	0.51
1:G:1295:PRO:HD2	1:G:1308:LYS:HA	1.92	0.50
1:A:1267:ILE:CD1	1:A:1276:ASN:HB2	2.42	0.50
3:E:1:DC:H2''	3:E:2:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:DC:H2"	3:C:2:DA:C8	2.46	0.50
1:B:1282:TYR:OH	2:F:7:DG:OP2	2.27	0.49
2:I:6:DT:N3	2:I:7:DG:C6	2.80	0.49
1:G:1345:ARG:HA	1:G:1348:ARG:NH1	2.27	0.49
1:B:1271:LYS:CD	1:B:1271:LYS:N	2.72	0.49
1:B:1266:ASN:O	1:B:1276:ASN:HA	2.13	0.49
3:K:7:DA:OP2	1:G:1344:SER:OG	2.30	0.49
1:G:1318:ARG:HA	1:G:1321:THR:OG1	2.12	0.48
1:A:1315:GLU:HG2	1:A:1318:ARG:NH1	2.27	0.48
2:D:11:DT:H2"	2:D:12:DG:C8	2.48	0.48
2:L:7:DG:H2'	1:G:1282:TYR:CE2	2.49	0.48
1:N:1287:GLN:HE21	1:N:1290:HIS:CD2	2.32	0.48
1:B:1271:LYS:H	1:B:1271:LYS:CD	2.26	0.47
2:I:12:DG:N2	3:H:2:DA:C2	2.82	0.47
1:A:1265:ARG:HH12	1:B:1305:MET:HE1	1.68	0.47
1:N:1287:GLN:HE21	1:N:1290:HIS:HD2	1.61	0.47
1:B:1273:CYS:SG	1:B:1275:LYS:HG3	2.54	0.47
2:I:5:DC:H2"	2:I:6:DT:H5"	1.96	0.47
1:N:1344:SER:O	1:N:1348:ARG:HG3	2.15	0.47
1:B:1278:PHE:HD1	2:F:8:DT:OP2	1.98	0.46
3:H:7:DA:C6	3:H:8:DG:C6	3.03	0.46
2:L:12:DG:C2	3:K:2:DA:C2	3.04	0.46
1:A:1341:SER:OG	3:C:9:DA:N6	2.47	0.46
1:B:1267:ILE:HD13	1:B:1276:ASN:HB2	1.97	0.46
1:B:1315:GLU:HG2	1:B:1318:ARG:NH1	2.30	0.45
2:D:1:DT:H2'	2:D:2:DT:C6	2.51	0.45
2:L:12:DG:N2	3:K:2:DA:C2	2.84	0.45
2:I:6:DT:H2"	2:I:7:DG:H8	1.76	0.45
1:N:1330:GLU:HB3	1:N:1333:CYS:HB3	1.99	0.45
1:A:1266:ASN:O	1:A:1276:ASN:HA	2.17	0.45
1:A:1315:GLU:OE1	1:A:1340:VAL:HG22	2.17	0.45
1:G:1289:VAL:CG1	1:G:1290:HIS:CD2	2.93	0.45
1:N:1268:CYS:SG	1:N:1277:PHE:HE2	2.40	0.45
1:B:1284:VAL:O	1:B:1287:GLN:HG2	2.17	0.45
2:L:11:DT:H2"	2:L:12:DG:C8	2.52	0.45
1:A:1278:PHE:CD2	1:A:1279:SER:HB3	2.53	0.44
2:I:7:DG:C1'	2:I:8:DT:C5	2.96	0.44
1:N:1304:LYS:HD3	1:N:1304:LYS:HA	1.77	0.44
1:B:1278:PHE:CD2	1:B:1279:SER:HB3	2.53	0.44
1:G:1287:GLN:HG3	1:G:1287:GLN:O	2.18	0.44
1:G:1266:ASN:ND2	1:G:1266:ASN:N	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:ILE:HD13	1:A:1276:ASN:HB2	1.99	0.43
1:B:1271:LYS:HA	1:B:1271:LYS:HD2	1.64	0.43
1:G:1318:ARG:NH1	1:G:1338:ARG:O	2.52	0.43
3:H:1:DC:H2''	3:H:2:DA:C8	2.54	0.43
1:B:1350:THR:HG22	1:B:1352:HIS:CG	2.54	0.42
1:N:1270:ILE:HD11	1:N:1287:GLN:NE2	2.31	0.42
3:H:7:DA:OP2	1:N:1344:SER:OG	2.37	0.42
1:B:1282:TYR:CE2	2:F:7:DG:H2'	2.54	0.42
3:K:1:DC:H2''	3:K:2:DA:C8	2.55	0.42
1:A:1278:PHE:CE2	1:A:1279:SER:HB3	2.55	0.41
1:A:1330:GLU:HB2	1:A:1352:HIS:HB3	2.02	0.41
2:L:11:DT:O2	3:K:3:DA:H2	2.02	0.41
1:B:1266:ASN:HB2	1:B:1277:PHE:O	2.20	0.41
1:B:1340:VAL:HG23	1:B:1341:SER:N	2.35	0.41
1:N:1318:ARG:HA	1:N:1321:THR:OG1	2.20	0.41
1:N:1295:PRO:HD2	1:N:1308:LYS:HG2	2.02	0.41
1:N:1285:GLN:HB3	1:N:1288:ARG:HH21	1.85	0.41
1:A:1311:TRP:CZ3	3:C:5:DA:H2'	2.56	0.41
2:I:5:DC:H2''	2:I:6:DT:C6	2.56	0.41
1:N:1287:GLN:NE2	1:N:1290:HIS:HD2	2.15	0.41
2:L:1:DT:H2'	2:L:2:DT:C6	2.55	0.41
2:I:3:5CM:H2'	2:I:3:5CM:H6	1.85	0.41
1:N:1295:PRO:HD2	1:N:1307:PHE:O	2.21	0.41
1:N:1294:ARG:HG2	1:N:1306:THR:CB	2.51	0.41
3:K:7:DA:C6	3:K:8:DG:C6	3.09	0.40
1:B:1267:ILE:HD11	1:B:1276:ASN:HB2	2.04	0.40
1:G:1304:LYS:HD3	1:G:1304:LYS:HA	1.75	0.40
2:I:6:DT:H2'	2:I:7:DG:H8	1.78	0.40
1:A:1270:ILE:HG13	1:A:1290:HIS:CD2	2.56	0.40
1:N:1270:ILE:HD11	1:N:1287:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	87/101 (86%)	82 (94%)	5 (6%)	0	100	100
1	B	87/101 (86%)	79 (91%)	6 (7%)	2 (2%)	6	11
1	G	86/101 (85%)	79 (92%)	7 (8%)	0	100	100
1	N	87/101 (86%)	80 (92%)	6 (7%)	1 (1%)	14	30
All	All	347/404 (86%)	320 (92%)	24 (7%)	3 (1%)	17	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1271	LYS
1	B	1272	GLY
1	N	1295	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/92 (86%)	76 (96%)	3 (4%)	33	59
1	B	80/92 (87%)	76 (95%)	4 (5%)	24	47
1	G	79/92 (86%)	76 (96%)	3 (4%)	33	59
1	N	80/92 (87%)	76 (95%)	4 (5%)	24	47
All	All	318/368 (86%)	304 (96%)	14 (4%)	28	53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1265	ARG
1	A	1281	LYS
1	A	1312	SER
1	B	1304	LYS
1	B	1312	SER

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Mol	Chain	Res	Type
1	B	1331	PRO
1	B	1345	ARG
1	N	1265	ARG
1	N	1268	CYS
1	N	1280	HIS
1	N	1294	ARG
1	G	1271	LYS
1	G	1287	GLN
1	G	1312	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	1266	ASN
1	N	1280	HIS
1	N	1287	GLN
1	N	1290	HIS
1	G	1290	HIS

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
2	5CM	D	3	3,2	15,21,22	2.23	7 (46%)	19,30,33	1.63	2 (10%)
2	5CM	L	3	3,2	15,21,22	1.80	4 (26%)	19,30,33	1.52	5 (26%)
2	5CM	I	3	3,2	15,21,22	1.89	4 (26%)	19,30,33	1.69	4 (21%)
2	5CM	F	3	3,2	15,21,22	2.75	11 (73%)	19,30,33	1.54	3 (15%)

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	5CM	D	3	3,2	-	3/4/21/22	0/2/2/2
2	5CM	L	3	3,2	-	1/4/21/22	0/2/2/2
2	5CM	I	3	3,2	-	1/4/21/22	0/2/2/2
2	5CM	F	3	3,2	-	1/4/21/22	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	5CM	C2-N3	-5.47	1.27	1.38
2	D	3	5CM	C2-N3	-4.93	1.28	1.38
2	I	3	5CM	C2-N3	-4.24	1.29	1.38
2	L	3	5CM	C2-N3	-3.92	1.30	1.38
2	F	3	5CM	C4-N3	-3.79	1.29	1.35
2	F	3	5CM	O5'-C5'	-3.61	1.35	1.44
2	D	3	5CM	C4-N3	-3.35	1.30	1.35
2	I	3	5CM	C4-N3	-3.32	1.30	1.35
2	F	3	5CM	C5-C4	2.75	1.45	1.41
2	F	3	5CM	O3'-C3'	-2.73	1.37	1.43
2	F	3	5CM	C2'-C1'	-2.71	1.44	1.52
2	L	3	5CM	O5'-C5'	-2.64	1.38	1.44
2	L	3	5CM	C4-N3	-2.59	1.31	1.35
2	D	3	5CM	C5-C4	2.59	1.45	1.41
2	L	3	5CM	C5-C4	2.58	1.45	1.41
2	F	3	5CM	C5A-C5	-2.55	1.45	1.51
2	F	3	5CM	C2'-C3'	-2.53	1.46	1.52
2	F	3	5CM	C6-C5	-2.45	1.33	1.40
2	I	3	5CM	C1'-N1	-2.45	1.42	1.49
2	D	3	5CM	O5'-C5'	-2.37	1.38	1.44
2	D	3	5CM	O4'-C4'	-2.20	1.40	1.45
2	F	3	5CM	O4'-C4'	-2.18	1.40	1.45
2	I	3	5CM	O4'-C4'	-2.15	1.40	1.45
2	D	3	5CM	C6-C5	-2.12	1.34	1.40
2	D	3	5CM	C1'-N1	-2.11	1.43	1.49
2	F	3	5CM	C3'-C4'	-2.09	1.47	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	5CM	C5-C6-N1	-4.56	117.28	122.19
2	I	3	5CM	C5-C6-N1	-4.18	117.69	122.19
2	F	3	5CM	C5-C6-N1	-3.79	118.11	122.19
2	L	3	5CM	C5-C6-N1	-3.65	118.26	122.19
2	D	3	5CM	C2-N3-C4	3.40	120.13	116.02
2	I	3	5CM	C3'-C2'-C1'	-3.14	94.68	102.54
2	F	3	5CM	C3'-C2'-C1'	3.05	110.17	102.54
2	L	3	5CM	C2'-C1'-N1	-2.71	108.02	114.27
2	I	3	5CM	C2-N3-C4	2.61	119.17	116.02
2	L	3	5CM	N4-C4-N3	2.57	120.66	117.03
2	I	3	5CM	O4'-C1'-C2'	-2.39	101.74	106.25
2	L	3	5CM	C2-N3-C4	2.14	118.60	116.02
2	F	3	5CM	C5'-C4'-C3'	-2.10	102.39	114.74
2	L	3	5CM	C5'-C4'-C3'	-2.09	102.48	114.74

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	5CM	O4'-C1'-N1-C6
2	L	3	5CM	O4'-C1'-N1-C6
2	I	3	5CM	O4'-C1'-N1-C6
2	D	3	5CM	C3'-C4'-C5'-O5'
2	D	3	5CM	O4'-C4'-C5'-O5'
2	F	3	5CM	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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

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	89/101 (88%)	-0.01	1 (1%) 80 78	10, 35, 75, 103	0
1	B	89/101 (88%)	-0.21	1 (1%) 80 78	16, 33, 76, 92	0
1	G	88/101 (87%)	1.39	26 (29%) 0 0	27, 71, 130, 134	0
1	N	89/101 (88%)	0.65	16 (17%) 1 0	22, 59, 124, 143	0
2	D	11/12 (91%)	-0.71	0 100 100	17, 25, 36, 36	0
2	F	11/12 (91%)	-0.62	0 100 100	16, 26, 41, 44	0
2	I	11/12 (91%)	-0.37	0 100 100	20, 57, 74, 79	0
2	L	11/12 (91%)	0.18	0 100 100	52, 79, 98, 106	0
3	C	12/12 (100%)	-0.48	0 100 100	25, 35, 48, 49	0
3	E	12/12 (100%)	-0.62	0 100 100	23, 34, 53, 56	0
3	H	12/12 (100%)	-0.08	0 100 100	42, 64, 79, 81	0
3	K	12/12 (100%)	0.07	1 (8%) 11 8	55, 78, 102, 106	0
All	All	447/500 (89%)	0.29	45 (10%) 7 4	10, 48, 114, 143	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1353	SER	7.1
1	G	1276	ASN	6.1
1	N	1284	VAL	5.7
1	G	1275	LYS	5.2
1	G	1277	PHE	4.9
1	N	1283	LEU	4.7
1	G	1279	SER	4.5
1	N	1278	PHE	4.5
1	G	1272	GLY	4.3
1	G	1295	PRO	4.2
1	G	1285	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	1281	LYS	3.9
1	N	1267	ILE	3.7
1	G	1278	PHE	3.7
1	G	1282	TYR	3.5
1	G	1340	VAL	3.3
1	G	1283	LEU	3.1
1	G	1270	ILE	3.1
1	G	1266	ASN	3.0
1	B	1329	ALA	3.0
1	N	1343	PHE	2.9
1	N	1290	HIS	2.9
1	N	1276	ASN	2.9
1	A	1332	ASP	2.7
1	G	1309	TRP	2.6
1	G	1327	VAL	2.5
1	N	1273	CYS	2.5
1	N	1332	ASP	2.5
3	K	12	DA	2.5
1	G	1269	PRO	2.5
1	G	1334	GLY	2.5
1	N	1279	SER	2.4
1	G	1273	CYS	2.4
1	G	1290	HIS	2.4
1	N	1277	PHE	2.4
1	G	1292	ASP	2.3
1	N	1282	TYR	2.3
1	G	1280	HIS	2.3
1	N	1268	CYS	2.3
1	G	1288	ARG	2.3
1	N	1327	VAL	2.3
1	G	1319	VAL	2.2
1	N	1281	LYS	2.1
1	N	1280	HIS	2.1
1	G	1330	GLU	2.0

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

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(\AA^2)	Q<0.9
2	5CM	L	3	20/21	0.87	0.21	20,20,20,20	0
2	5CM	I	3	20/21	0.94	0.17	20,20,20,20	0
2	5CM	D	3	20/21	0.96	0.11	20,20,20,20	0
2	5CM	F	3	20/21	0.96	0.12	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
4	ZN	N	1403	1/1	0.69	0.10	153,153,153,153	0
4	ZN	G	1402	1/1	0.89	0.09	86,86,86,86	0
4	ZN	B	1403	1/1	0.90	0.08	81,81,81,81	0
4	ZN	A	1402	1/1	0.95	0.12	62,62,62,62	0
4	ZN	G	1403	1/1	0.96	0.10	112,112,112,112	0
4	ZN	A	1403	1/1	0.97	0.14	33,33,33,33	0
4	ZN	N	1402	1/1	0.98	0.05	70,70,70,70	0
4	ZN	B	1402	1/1	0.98	0.09	31,31,31,31	0
4	ZN	A	1401	1/1	0.99	0.10	21,21,21,21	0
4	ZN	B	1401	1/1	0.99	0.09	28,28,28,28	0
4	ZN	G	1401	1/1	0.99	0.12	46,46,46,46	0
4	ZN	N	1401	1/1	1.00	0.12	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.