



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:45 am BST

PDB ID : 2OKV  
Title : c-Myc DNA Unwinding Element Binding Protein  
Authors : Bae, B.; Nair, S.K.  
Deposited on : 2007-01-17  
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](mailto: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.

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

MolProbity	:	4.02b-467
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

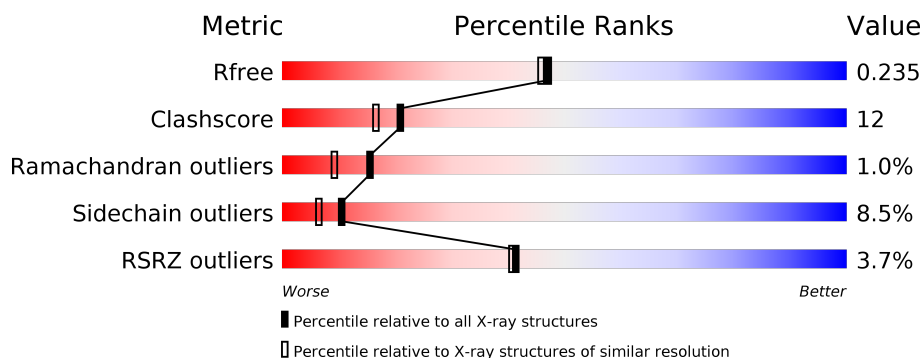
# 1 Overall quality at a glance

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	209	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>11%</div> <div>•</div> <div>29%</div> </div> </div>
1	B	209	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>12%</div> <div>•</div> <div>28%</div> </div> </div>
1	C	209	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>16%</div> <div>•</div> <div>29%</div> </div> </div>
1	D	209	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>8%</div> <div>• •</div> <div>29%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5076 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 Probable D-tyrosyl-tRNA(Tyr) deacylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1175	742	204	221	8			
1	B	150	Total	C	N	O	S	0	0	0
			1183	749	204	222	8			
1	C	149	Total	C	N	O	S	0	0	0
			1177	744	204	221	8			
1	D	149	Total	C	N	O	S	0	0	0
			1177	744	204	221	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

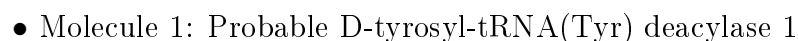
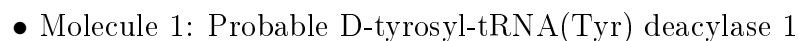
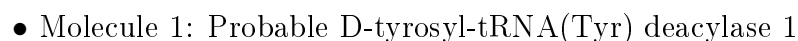
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

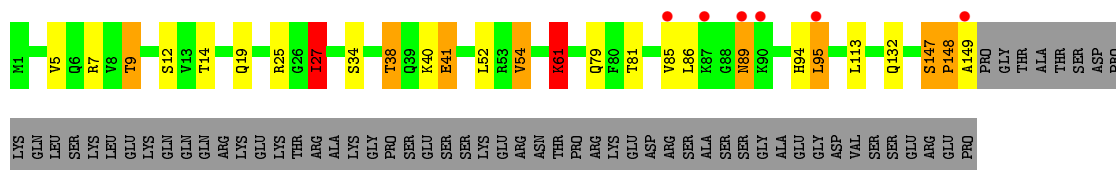
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		
3	B	73	Total	O	0	0
			73	73		
3	C	101	Total	O	0	0
			101	101		
3	D	80	Total	O	0	0
			80	80		



- Molecule 1: Probable D-tyrosyl-tRNA(Tyr) deacylase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.81Å 77.81Å 106.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.00 38.91 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-2.00) 99.3 (38.91-1.98)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.60 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.205 , 0.237 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	2528 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.490 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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

### 5.1 Standard geometry

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

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	0.55	0/1195	0.73	2/1607 (0.1%)
1	B	0.59	0/1204	0.70	0/1621
1	C	0.54	0/1197	0.75	3/1610 (0.2%)
1	D	0.86	4/1197 (0.3%)	0.74	1/1610 (0.1%)
All	All	0.65	4/4793 (0.1%)	0.73	6/6448 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	61	LYS	CE-NZ	14.37	1.84	1.49
1	D	61	LYS	CB-CG	12.09	1.85	1.52
1	D	61	LYS	CD-CE	11.52	1.80	1.51
1	D	61	LYS	CG-CD	5.26	1.70	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	A	114	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	D	27	ILE	CG1-CB-CG2	-6.30	97.53	111.40
1	C	118	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	114	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	1175	0	1180	37	0
1	B	1183	0	1189	28	0
1	C	1177	0	1187	33	0
1	D	1177	0	1187	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	106	0	0	3	0
3	B	73	0	0	3	0
3	C	101	0	0	2	0
3	D	80	0	0	4	0
All	All	5076	0	4743	115	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 12.

All (115) 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:D:61:LYS:CD	1:D:61:LYS:CE	1.80	1.56
1:D:61:LYS:CB	1:D:61:LYS:CG	1.85	1.53
1:D:61:LYS:NZ	1:D:61:LYS:CE	1.85	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:CE	1:A:102:ALA:HA	1.87	1.04
1:A:97:MET:HE3	1:A:102:ALA:HA	1.44	0.95
1:A:33:ILE:HG21	1:A:97:MET:HE1	1.49	0.94
1:C:38:THR:HG22	1:C:40:LYS:H	1.40	0.87
1:A:71:GLN:HE22	1:A:118:ARG:HE	1.26	0.83
1:A:33:ILE:HG21	1:A:97:MET:CE	2.07	0.83
1:A:97:MET:HE2	1:A:102:ALA:HA	1.65	0.79
1:A:6:GLN:HE21	1:A:137:ASN:HD22	1.32	0.77
1:B:1:MET:H3	1:B:148:PRO:HD3	1.50	0.76
1:C:142:THR:H	1:D:81:THR:HG21	1.51	0.76
1:C:142:THR:O	1:D:81:THR:HG23	1.88	0.74
1:C:114:ARG:HD3	3:C:1227:HOH:O	1.89	0.73
1:D:5:VAL:HG13	1:D:27:ILE:HG13	1.75	0.68
1:C:10:ARG:HH11	1:C:136:GLN:HE22	1.42	0.68
1:C:113:LEU:HD12	1:C:122:ILE:CD1	2.24	0.68
1:D:38:THR:HG23	1:D:40:LYS:H	1.60	0.67
1:A:100:GLU:HB2	3:A:1247:HOH:O	1.96	0.65
1:B:38:THR:HG23	1:B:40:LYS:H	1.61	0.65
1:A:91:PRO:HB2	1:A:93:PHE:CZ	2.31	0.65
1:C:4:VAL:HG13	1:C:30:LEU:HB2	1.78	0.64
1:B:38:THR:H	1:B:41:GLU:HG3	1.64	0.63
1:C:113:LEU:HD12	1:C:122:ILE:HD13	1.80	0.63
1:A:80:PHE:CE1	1:A:93:PHE:CE2	2.87	0.62
1:B:10:ARG:HH11	1:B:136:GLN:HE22	1.47	0.61
1:D:61:LYS:CA	1:D:61:LYS:CG	2.76	0.61
1:D:14:THR:HG23	3:D:1217:HOH:O	2.00	0.58
1:B:1:MET:H3	1:B:148:PRO:CD	2.17	0.58
1:C:91:PRO:HA	1:C:92:ASP:HB2	1.84	0.58
1:D:12:SER:HB2	1:D:19:GLN:HE22	1.67	0.58
1:A:114:ARG:HD3	3:A:1221:HOH:O	2.04	0.57
1:B:14:THR:HG22	3:B:1212:HOH:O	2.04	0.57
1:D:147:SER:O	1:D:149:ALA:N	2.39	0.56
1:A:97:MET:HE3	1:A:102:ALA:CA	2.28	0.55
1:D:14:THR:HG22	1:D:132:GLN:HB2	1.87	0.55
1:A:2:LYS:HG2	1:A:146:GLU:HG3	1.88	0.55
1:A:6:GLN:HE22	1:B:6:GLN:HE22	1.55	0.55
1:D:147:SER:HB3	1:D:148:PRO:CD	2.36	0.55
1:A:147:SER:CB	1:A:148:PRO:HD3	2.37	0.54
1:C:148:PRO:O	1:C:149:ALA:HB2	2.07	0.53
1:B:38:THR:HG21	3:B:1229:HOH:O	2.08	0.53
1:A:91:PRO:HG3	1:B:143:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLN:HE22	1:B:118:ARG:NE	2.07	0.52
1:A:9:THR:HG23	1:B:132:GLN:OE1	2.09	0.52
1:C:148:PRO:O	1:C:149:ALA:CB	2.57	0.52
1:D:61:LYS:CG	1:D:61:LYS:CE	2.85	0.52
1:D:61:LYS:CD	1:D:61:LYS:CB	2.87	0.50
1:A:97:MET:HE2	1:A:102:ALA:CA	2.40	0.50
1:A:80:PHE:CE1	1:A:93:PHE:CD2	3.00	0.50
1:B:10:ARG:HH11	1:B:136:GLN:NE2	2.10	0.50
1:C:9:THR:HG23	1:D:132:GLN:OE1	2.12	0.49
1:A:9:THR:CG2	1:B:132:GLN:OE1	2.59	0.49
1:D:7:ARG:HD3	1:D:54:VAL:HG13	1.95	0.49
1:A:53:ARG:HD2	3:A:1232:HOH:O	2.12	0.49
1:C:38:THR:HB	1:C:41:GLU:OE2	2.12	0.49
1:B:71:GLN:HE22	1:B:118:ARG:HE	1.59	0.49
1:A:97:MET:CE	1:A:102:ALA:CA	2.76	0.49
1:D:38:THR:H	1:D:41:GLU:HG2	1.78	0.49
1:D:61:LYS:HE2	1:D:61:LYS:HB3	1.95	0.48
1:C:108:SER:HA	1:C:111:GLU:HG2	1.94	0.48
1:C:9:THR:CG2	1:D:132:GLN:OE1	2.61	0.48
1:A:7:ARG:HD3	1:A:54:VAL:HG13	1.95	0.48
1:A:33:ILE:CG2	1:A:97:MET:HE1	2.34	0.48
1:C:4:VAL:CG1	1:C:30:LEU:HB2	2.44	0.48
1:C:51:ASN:ND2	1:D:89:ASN:HB3	2.28	0.48
1:A:120:GLU:HG2	1:A:121:LEU:HD13	1.96	0.47
1:D:94:HIS:CE1	1:D:95:LEU:HD13	2.49	0.47
1:A:147:SER:CB	1:A:148:PRO:CD	2.91	0.47
1:C:10:ARG:HH11	1:C:136:GLN:NE2	2.11	0.47
1:A:147:SER:HB3	1:A:148:PRO:HD3	1.97	0.46
1:A:33:ILE:HG21	1:A:97:MET:HE2	1.94	0.46
1:D:147:SER:HB3	1:D:148:PRO:HD3	1.98	0.46
1:C:132:GLN:OE1	1:D:9:THR:CG2	2.64	0.46
1:B:147:SER:O	1:B:148:PRO:C	2.54	0.46
1:D:38:THR:HG21	3:D:1235:HOH:O	2.16	0.46
1:A:71:GLN:HE22	1:A:118:ARG:NE	2.05	0.45
1:B:90:LYS:HG2	3:B:1250:HOH:O	2.15	0.45
1:D:25:ARG:NH2	3:D:1273:HOH:O	2.49	0.45
1:A:132:GLN:OE1	1:B:9:THR:CG2	2.64	0.45
1:B:7:ARG:HD3	1:B:54:VAL:HG13	1.98	0.45
1:C:9:THR:HG22	1:C:138:ASP:HB2	1.98	0.45
1:C:41:GLU:HG2	1:C:148:PRO:HG3	1.98	0.44
1:C:38:THR:CG2	1:C:39:GLN:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:HD12	1:C:113:LEU:HD11	2.00	0.44
1:B:46:VAL:HG13	1:B:113:LEU:HD23	1.99	0.44
1:B:5:VAL:CG1	1:B:27:ILE:HG12	2.48	0.44
1:B:41:GLU:H	1:B:41:GLU:HG2	1.36	0.43
1:B:1:MET:N	1:B:148:PRO:CD	2.82	0.43
1:D:79:GLN:NE2	1:D:81:THR:HG22	2.34	0.43
1:C:120:GLU:H	1:C:120:GLU:CD	2.22	0.43
1:D:148:PRO:HG3	3:D:1281:HOH:O	2.18	0.43
1:A:9:THR:HG22	1:A:138:ASP:HB2	2.00	0.43
1:C:84:CYS:O	1:C:92:ASP:OD2	2.37	0.42
1:D:61:LYS:CB	1:D:61:LYS:CE	2.97	0.42
1:A:80:PHE:HE1	1:A:93:PHE:CD2	2.37	0.42
1:C:2:LYS:HG2	1:C:146:GLU:HG3	2.00	0.42
1:A:118:ARG:HD2	1:A:121:LEU:HD22	2.02	0.42
1:C:143:ILE:HD11	1:D:81:THR:OG1	2.20	0.42
1:D:14:THR:CG2	1:D:132:GLN:HB2	2.48	0.42
1:A:6:GLN:HE21	1:A:137:ASN:ND2	2.09	0.42
1:C:142:THR:H	1:D:81:THR:CG2	2.26	0.42
1:C:132:GLN:OE1	1:D:9:THR:HG21	2.20	0.41
1:C:114:ARG:CD	3:C:1227:HOH:O	2.59	0.41
1:A:80:PHE:HE1	1:A:93:PHE:CE2	2.36	0.41
1:A:132:GLN:OE1	1:B:9:THR:HG21	2.21	0.41
1:B:5:VAL:HG13	1:B:27:ILE:HG12	2.02	0.41
1:B:27:ILE:HG22	1:B:74:ILE:HG12	2.02	0.41
1:C:42:LEU:HD21	1:C:109:PHE:HA	2.03	0.41
1:B:147:SER:H	1:B:148:PRO:HD2	1.86	0.41
1:C:10:ARG:NH1	1:C:136:GLN:HE22	2.15	0.41
1:C:46:VAL:HG13	1:C:113:LEU:HD22	2.02	0.41
1:A:6:GLN:NE2	1:B:6:GLN:HE22	2.18	0.41
1:B:1:MET:HE3	1:B:41:GLU:HB2	2.02	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	147/209 (70%)	141 (96%)	3 (2%)	3 (2%)	7	3
1	B	148/209 (71%)	140 (95%)	8 (5%)	0	100	100
1	C	147/209 (70%)	139 (95%)	8 (5%)	0	100	100
1	D	147/209 (70%)	139 (95%)	5 (3%)	3 (2%)	7	3
All	All	589/836 (70%)	559 (95%)	24 (4%)	6 (1%)	15	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	D	86	LEU
1	A	148	PRO
1	A	86	LEU
1	D	147	SER
1	D	148	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	129/183 (70%)	123 (95%)	6 (5%)	26	22
1	B	130/183 (71%)	116 (89%)	14 (11%)	6	3
1	C	130/183 (71%)	118 (91%)	12 (9%)	9	5
1	D	130/183 (71%)	118 (91%)	12 (9%)	9	5
All	All	519/732 (71%)	475 (92%)	44 (8%)	10	6

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	52	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	62	HIS
1	A	94	HIS
1	A	121	LEU
1	A	147	SER
1	B	9	THR
1	B	27	ILE
1	B	31	LEU
1	B	34	SER
1	B	38	THR
1	B	41	GLU
1	B	52	LEU
1	B	54	VAL
1	B	58	GLU
1	B	84	CYS
1	B	95	LEU
1	B	112	GLN
1	B	113	LEU
1	B	123	LYS
1	C	9	THR
1	C	31	LEU
1	C	40	LYS
1	C	52	LEU
1	C	54	VAL
1	C	87	LYS
1	C	90	LYS
1	C	99	THR
1	C	101	GLN
1	C	108	SER
1	C	113	LEU
1	C	120	GLU
1	D	9	THR
1	D	27	ILE
1	D	34	SER
1	D	38	THR
1	D	41	GLU
1	D	52	LEU
1	D	54	VAL
1	D	61	LYS
1	D	85	VAL
1	D	89	ASN
1	D	95	LEU
1	D	113	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	71	GLN
1	A	83	GLN
1	A	101	GLN
1	B	71	GLN
1	B	83	GLN
1	B	89	ASN
1	B	136	GLN
1	C	71	GLN
1	C	101	GLN
1	C	112	GLN
1	C	136	GLN
1	D	19	GLN
1	D	51	ASN
1	D	71	GLN
1	D	94	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	149/209 (71%)	-0.05	5 (3%)	45	44	37, 43, 55, 61	1 (0%)
1	B	150/209 (71%)	-0.00	6 (4%)	38	37	35, 42, 56, 63	1 (0%)
1	C	149/209 (71%)	-0.01	5 (3%)	45	44	37, 42, 56, 61	1 (0%)
1	D	149/209 (71%)	0.05	6 (4%)	38	37	36, 43, 54, 58	1 (0%)
All	All	597/836 (71%)	-0.00	22 (3%)	41	41	35, 43, 56, 63	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	87	LYS	5.0
1	B	86	LEU	4.1
1	A	149	ALA	3.1
1	D	149	ALA	3.0
1	B	95	LEU	3.0
1	D	90	LYS	3.0
1	C	87	LYS	3.0
1	A	88	GLY	2.8
1	D	89	ASN	2.7
1	B	150	PRO	2.6
1	B	84	CYS	2.6
1	A	84	CYS	2.5
1	A	87	LYS	2.4
1	C	86	LEU	2.4
1	B	87	LYS	2.3
1	D	95	LEU	2.2
1	C	149	ALA	2.2
1	D	85	VAL	2.2
1	C	84	CYS	2.1
1	B	148	PRO	2.0
1	A	51	ASN	2.0
1	C	51	ASN	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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
2	MG	D	1204	1/1	0.97	0.30	39,39,39,39	0
2	MG	B	1203	1/1	0.98	0.29	36,36,36,36	0
2	MG	A	1201	1/1	0.98	0.27	36,36,36,36	0
2	MG	C	1202	1/1	0.99	0.28	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.