WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 10:42 am GMT

PDB ID	:	4K1Y
Title	:	Crystal structure of Canavalia boliviana lectin in complex with Man1-3Man-OMe
Authors	:	Bezerra, G.A.; Viertlmayr, R.; Moura, T.R.; Delatorre, P.; Rocha, B.A.M.; Cavada, B.S.; Gruber, K.
Deposited on	:	2013-04-07
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.50 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.
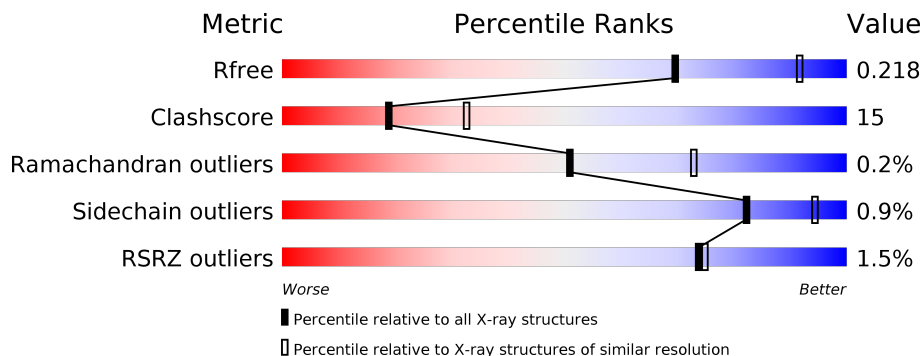
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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 <=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	237	% 73% 25% •
1	B	237	2% 77% 23%
1	C	237	69% 31%
1	D	237	3% 76% 23% •

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	C	301	-	-	-	X
2	MN	D	301	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7529 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 Canavalia boliviana lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total 1807	C 1138	N 305	O 362	S 2	0	0	0
1	B	237	Total 1807	C 1138	N 305	O 362	S 2	0	0	0
1	C	237	Total 1807	C 1138	N 305	O 362	S 2	0	0	0
1	D	237	Total 1807	C 1138	N 305	O 362	S 2	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Cd 2	0	0
4	A	2	Total 2	Cd 2	0	0
4	D	2	Total 2	Cd 2	0	0
4	C	3	Total 3	Cd 3	0	0

- Molecule 5 is SUGAR (METHYL-O3-(ALPHA-D-MANNOSE)-ALPHA-D-MANNOSE) (three-letter code: MDM) (formula: $C_{13}H_{24}O_{11}$).
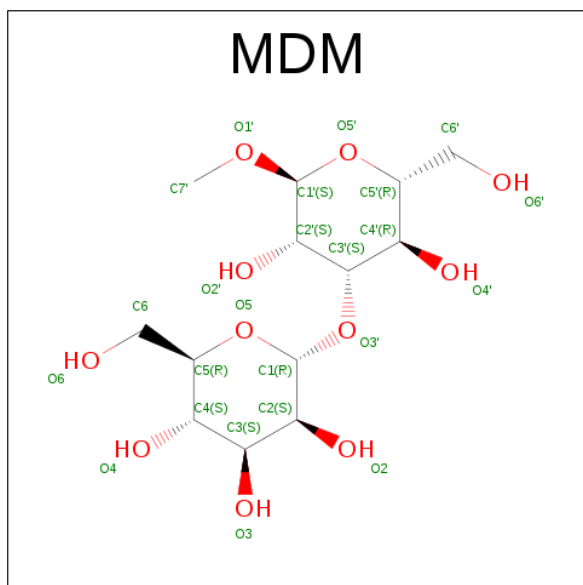
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 24	C 13	O 11	0	0
5	B	1	Total 24	C 13	O 11	0	0
5	C	1	Total 24	C 13	O 11	0	0
5	D	1	Total 24	C 13	O 11	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total 48	O 48	0	0
6	B	45	Total 45	O 45	0	0
6	C	55	Total 55	O 55	0	0
6	D	40	Total 40	O 40	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Canavalia boliviana lectin
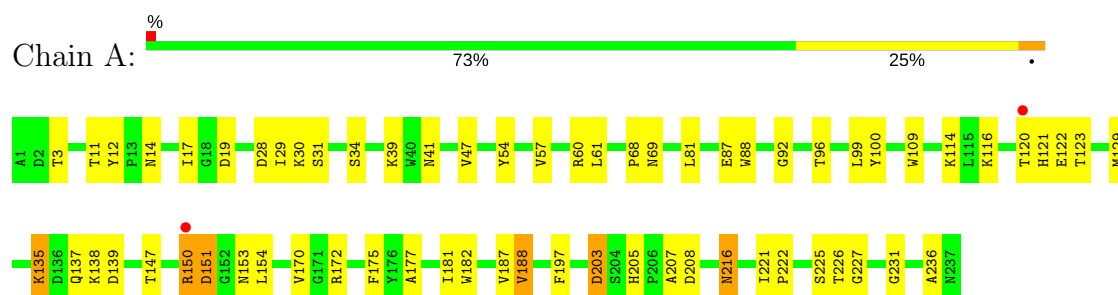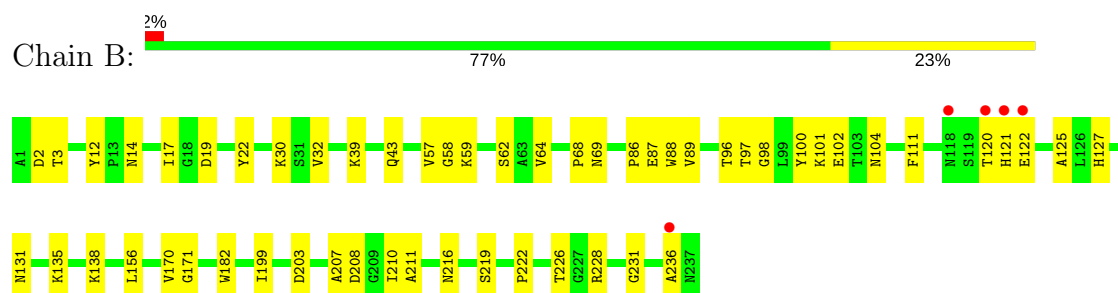
Chain A:

- Molecule 1: Canavalia boliviana lectin

Chain B:

- Molecule 1: Canavalia boliviana lectin

Chain C:

- Molecule 1: Canavalia boliviana lectin

Chain D:

A1 I4 V5 E8 L9 D10 T11 Y12 P13 N14 D19 P23 H24 I25 I29 W40 I52 V57 G58 K59 R60 L61 S62 A63 V64 P68 N69 G70 V79 D80 V91 E102 T103 N104 F111 T112 S113 S117 N118 S119 T120 H121 E122 T123 K135

D136 Q137 L140 I141 L142 T148 G149 L154 E155 L156 V170 G171 A177 A186 V187 V188 I199 S204 A207 D208 I214 S215 I221 L229 F233 N237
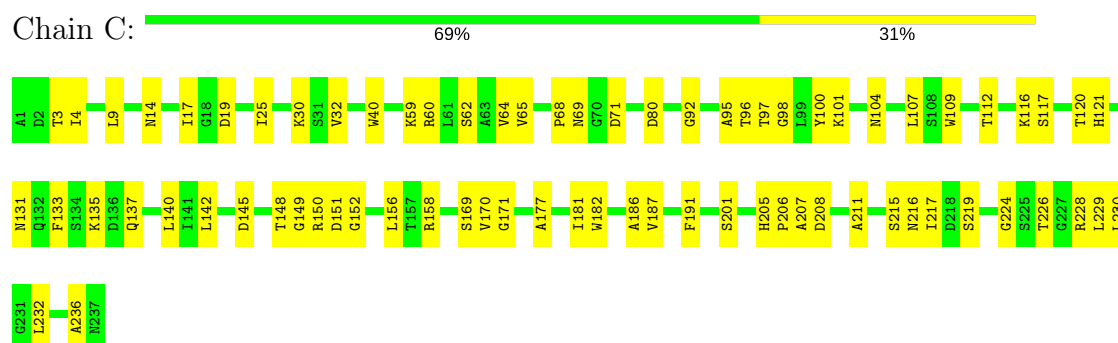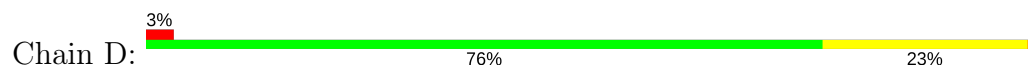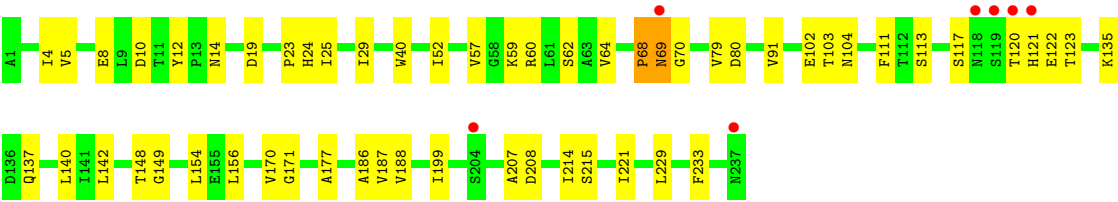
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.88Å 95.66Å 94.61Å 90.00° 132.29° 90.00°	Depositor
Resolution (Å)	40.94 – 2.50 40.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.94-2.50) 98.7 (40.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.204 , 0.228 0.196 , 0.218	Depositor DCC
R_{free} test set	1613 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 19.2	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.058 for -h+k-l,-l,-k 0.049 for -h-k-l,l,k 0.259 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.296 for -h-2*l,-k,l	Depositor
Outliers	0 of 31960 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7529	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, MN, CD, MDM

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	0.28	0/1848	0.52	0/2515
1	B	0.27	0/1848	0.50	0/2515
1	C	0.29	0/1848	0.51	0/2515
1	D	0.27	0/1848	0.52	0/2515
All	All	0.28	0/7392	0.51	0/10060

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	68	PRO	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1807	0	1756	62	0
1	B	1807	0	1756	57	0
1	C	1807	0	1756	64	0
1	D	1807	0	1756	53	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
5	A	24	0	24	4	0
5	B	24	0	24	7	0
5	C	24	0	24	2	0
5	D	24	0	24	2	0
6	A	48	0	0	3	0
6	B	45	0	0	2	0
6	C	55	0	0	4	0
6	D	40	0	0	1	0
All	All	7529	0	7120	212	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 15.

All (212) 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:69:ASN:HB3	1:D:70:GLY:HA3	1.36	1.07
1:D:69:ASN:HB3	1:D:70:GLY:CA	1.92	0.99
1:A:123:THR:H	1:B:131:ASN:HD22	0.98	0.95
1:C:131:ASN:HD22	1:D:123:THR:H	1.18	0.92
1:C:135:LYS:HD3	1:C:149:GLY:HA3	1.54	0.89
1:C:135:LYS:NZ	1:C:150:ARG:HG2	1.92	0.84
1:A:123:THR:N	1:B:131:ASN:HD22	1.76	0.83
1:C:68:PRO:O	1:C:69:ASN:HB3	1.81	0.81
1:C:120:THR:O	1:C:121:HIS:HB2	1.83	0.77
1:A:123:THR:H	1:B:131:ASN:ND2	1.81	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ASN:CB	1:D:70:GLY:CA	2.64	0.76
1:B:100:TYR:HE1	5:B:305:MDM:C7'	1.98	0.76
1:B:96:THR:HG22	1:B:170:VAL:HG23	1.68	0.75
1:B:121:HIS:HB2	1:B:122:GLU:HA	1.69	0.74
1:C:145:ASP:HB3	1:C:158:ARG:HG2	1.69	0.73
1:D:120:THR:HA	1:D:121:HIS:C	2.10	0.72
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.72	0.71
1:B:100:TYR:CE1	5:B:305:MDM:C7'	2.74	0.71
1:C:14:ASN:O	1:C:19:ASP:HB2	1.92	0.70
1:D:14:ASN:O	1:D:19:ASP:HB2	1.91	0.69
1:A:88:TRP:CG	1:B:138:LYS:HD2	2.28	0.69
1:D:187:VAL:HG23	1:D:188:VAL:HG23	1.75	0.69
1:B:14:ASN:O	1:B:19:ASP:HB2	1.94	0.68
1:B:120:THR:HA	1:B:121:HIS:C	2.15	0.67
1:D:137:GLN:HG2	1:D:140:LEU:HD12	1.76	0.66
1:C:131:ASN:ND2	1:D:123:THR:H	1.93	0.66
1:A:96:THR:HG22	1:A:170:VAL:HG23	1.76	0.66
1:A:151:ASP:OD2	6:A:426:HOH:O	2.14	0.65
1:A:57:VAL:HG13	1:C:64:VAL:HG23	1.79	0.64
1:C:68:PRO:O	1:C:69:ASN:CB	2.46	0.64
1:B:100:TYR:CE1	5:B:305:MDM:H7'1	2.32	0.64
1:C:135:LYS:CE	1:C:150:ARG:HG2	2.28	0.64
1:C:17:ILE:HD11	6:C:455:HOH:O	1.98	0.63
1:C:145:ASP:CB	1:C:158:ARG:HG2	2.28	0.63
1:A:12:TYR:CD1	5:A:305:MDM:H61	2.34	0.62
1:C:135:LYS:HZ1	1:C:150:ARG:HG2	1.63	0.62
1:B:17:ILE:HD13	1:B:228:ARG:HD2	1.81	0.62
1:C:131:ASN:HD22	1:D:123:THR:N	1.93	0.61
1:B:121:HIS:CB	1:B:122:GLU:HA	2.29	0.61
1:A:92:GLY:HA2	1:A:109:TRP:CH2	2.36	0.61
1:C:208:ASP:HB3	6:C:411:HOH:O	2.00	0.61
1:C:97:THR:OG1	1:C:169:SER:HB3	2.00	0.60
1:C:224:GLY:O	1:C:229:LEU:HD12	2.00	0.60
1:A:60:ARG:HB2	1:C:60:ARG:NH1	2.15	0.60
1:A:150:ARG:O	1:A:151:ASP:CG	2.40	0.60
1:B:62:SER:HB3	1:D:57:VAL:HG12	1.84	0.60
1:C:25:ILE:HG21	1:C:65:VAL:HG11	1.83	0.59
1:B:62:SER:HB3	1:D:57:VAL:CG1	2.32	0.59
1:C:120:THR:HA	6:C:430:HOH:O	2.02	0.59
1:A:121:HIS:HB2	1:A:122:GLU:HA	1.85	0.58
1:A:17:ILE:HG13	1:A:236:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:CB	1:A:122:GLU:HA	2.33	0.58
1:A:120:THR:HA	1:A:121:HIS:C	2.23	0.58
1:A:170:VAL:HB	1:A:226:THR:HG22	1.85	0.58
1:D:121:HIS:CB	1:D:122:GLU:HA	2.34	0.57
1:D:59:LYS:NZ	6:D:424:HOH:O	2.36	0.57
1:B:120:THR:HA	1:B:121:HIS:O	2.05	0.57
1:A:116:LYS:O	1:A:187:VAL:HG22	2.05	0.56
1:C:100:TYR:HD1	5:C:306:MDM:H62	1.70	0.56
1:C:59:LYS:HD3	1:C:80:ASP:HB2	1.88	0.56
1:D:12:TYR:HB2	1:D:207:ALA:HB2	1.87	0.56
1:D:148:THR:HG22	1:D:154:LEU:HD13	1.86	0.56
1:B:57:VAL:HG12	1:D:62:SER:HB3	1.88	0.56
1:A:28:ASP:HB3	1:A:31:SER:O	2.06	0.56
1:C:145:ASP:CG	1:C:158:ARG:HG2	2.26	0.55
1:B:3:THR:HG23	1:B:30:LYS:HD3	1.88	0.55
1:D:170:VAL:HG22	1:D:221:ILE:HD13	1.89	0.55
1:B:68:PRO:O	1:B:69:ASN:CG	2.44	0.55
1:C:4:ILE:HD13	1:C:215:SER:HB3	1.89	0.55
1:B:98:GLY:HA3	5:B:305:MDM:H4	1.89	0.54
1:C:96:THR:HG22	1:C:170:VAL:HG23	1.90	0.54
1:D:121:HIS:HB2	1:D:122:GLU:HA	1.88	0.54
1:D:120:THR:HA	1:D:121:HIS:O	2.06	0.54
1:B:57:VAL:HG13	1:D:64:VAL:HG23	1.90	0.54
1:C:116:LYS:O	1:C:187:VAL:HG22	2.07	0.54
1:A:208:ASP:OD2	1:A:227:GLY:HA2	2.08	0.54
1:B:86:PRO:HG2	1:B:89:VAL:HG12	1.89	0.53
1:C:228:ARG:O	1:C:230:LEU:HG	2.08	0.53
1:A:100:TYR:CE2	1:A:205:HIS:HB2	2.43	0.53
1:B:87:GLU:HG3	1:B:182:TRP:O	2.09	0.53
1:C:25:ILE:HG21	1:C:65:VAL:CG1	2.38	0.53
1:D:68:PRO:O	1:D:69:ASN:CB	2.56	0.53
1:A:150:ARG:O	1:A:151:ASP:CB	2.56	0.53
1:A:181:ILE:HG23	1:A:182:TRP:CD1	2.43	0.53
1:C:142:LEU:HD11	1:C:148:THR:HG23	1.91	0.52
1:C:216:ASN:OD1	1:C:219:SER:HB2	2.09	0.52
1:C:135:LYS:CD	1:C:149:GLY:HA3	2.32	0.52
1:A:181:ILE:HG23	1:A:182:TRP:HD1	1.75	0.52
1:C:150:ARG:O	1:C:151:ASP:OD1	2.27	0.52
1:B:97:THR:HB	1:B:101:LYS:HA	1.92	0.52
1:C:95:ALA:HB1	1:C:104:ASN:OD1	2.10	0.52
1:A:225:SER:OG	1:A:231:GLY:HA2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LYS:HE2	1:C:150:ARG:HG2	1.90	0.51
1:B:208:ASP:OD1	5:B:305:MDM:O4	2.23	0.51
1:B:216:ASN:OD1	1:B:219:SER:HB2	2.10	0.51
1:D:69:ASN:CB	1:D:70:GLY:HA2	2.41	0.50
1:B:102:GLU:HG2	1:B:207:ALA:O	2.11	0.50
1:C:120:THR:O	1:C:121:HIS:CB	2.55	0.50
1:C:117:SER:HA	1:C:186:ALA:HA	1.94	0.49
1:B:59:LYS:NZ	6:B:427:HOH:O	2.44	0.49
1:A:175:PHE:CE2	1:A:177:ALA:HB3	2.47	0.49
1:A:39:LYS:HE2	1:A:41:ASN:HD21	1.77	0.49
1:B:222:PRO:HD2	1:B:231:GLY:O	2.12	0.49
1:B:69:ASN:OD1	1:B:69:ASN:C	2.50	0.49
1:A:14:ASN:O	1:A:17:ILE:HG22	2.13	0.49
1:A:14:ASN:O	1:A:19:ASP:HB2	2.12	0.49
1:B:32:VAL:HG11	1:B:236:ALA:HA	1.95	0.49
1:C:150:ARG:O	1:C:151:ASP:CG	2.51	0.49
1:C:3:THR:HG23	1:C:30:LYS:HD3	1.94	0.49
1:C:98:GLY:HA3	5:C:306:MDM:H4	1.95	0.49
1:D:156:LEU:O	1:D:171:GLY:HA3	2.13	0.49
1:A:137:GLN:HG3	1:A:139:ASP:OD1	2.12	0.49
1:D:12:TYR:HB2	1:D:207:ALA:CB	2.43	0.49
1:A:147:THR:O	1:A:154:LEU:HD12	2.13	0.48
1:A:54:TYR:CE2	1:A:81:LEU:HD12	2.48	0.48
1:A:216:ASN:OD1	1:A:216:ASN:N	2.41	0.48
1:B:2:ASP:HA	1:B:216:ASN:HD21	1.79	0.48
1:C:32:VAL:HG11	1:C:236:ALA:HA	1.95	0.48
1:D:229:LEU:HD13	1:D:233:PHE:O	2.14	0.48
1:A:187:VAL:HG23	1:A:188:VAL:CG1	2.44	0.48
1:C:9:LEU:HB3	1:C:40:TRP:CZ3	2.48	0.48
1:A:120:THR:HA	1:A:121:HIS:O	2.14	0.47
1:B:12:TYR:HB2	1:B:207:ALA:HB2	1.96	0.47
1:C:135:LYS:HE2	1:C:150:ARG:CD	2.45	0.47
1:C:170:VAL:HB	1:C:226:THR:HG22	1.97	0.47
1:D:12:TYR:HD1	1:D:14:ASN:OD1	1.98	0.46
5:A:305:MDM:H2'	5:A:305:MDM:H5	1.97	0.46
1:B:156:LEU:O	1:B:171:GLY:HA3	2.16	0.46
1:B:104:ASN:HD22	1:B:210:ILE:CG1	2.28	0.46
1:A:114:LYS:NZ	6:A:418:HOH:O	2.45	0.46
1:B:100:TYR:HE1	5:B:305:MDM:H7'2	1.80	0.46
1:C:101:LYS:HG3	6:C:431:HOH:O	2.16	0.46
1:B:64:VAL:HG23	1:D:57:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:O	1:C:171:GLY:HA3	2.16	0.46
1:B:207:ALA:HA	1:B:208:ASP:HA	1.77	0.46
1:A:12:TYR:CE1	5:A:305:MDM:H61	2.50	0.45
1:C:92:GLY:HA2	1:C:109:TRP:CH2	2.51	0.45
1:A:92:GLY:HA2	1:A:109:TRP:HH2	1.79	0.45
1:B:57:VAL:HG13	1:D:64:VAL:CG2	2.46	0.45
1:A:14:ASN:HA	6:A:436:HOH:O	2.17	0.45
1:A:87:GLU:HG3	1:A:182:TRP:O	2.16	0.45
1:B:210:ILE:HG22	1:B:211:ALA:N	2.32	0.44
1:D:111:PHE:CE2	1:D:113:SER:HB2	2.51	0.44
1:A:47:VAL:HA	1:A:197:PHE:O	2.18	0.44
1:A:129:MET:HE3	1:B:125:ALA:HB3	1.98	0.44
1:B:100:TYR:HD2	1:B:203:ASP:OD2	2.00	0.44
1:D:135:LYS:HD3	1:D:149:GLY:HA3	1.99	0.44
1:C:150:ARG:O	1:C:151:ASP:CB	2.65	0.44
1:A:203:ASP:OD1	1:A:203:ASP:N	2.48	0.44
1:A:3:THR:HG23	1:A:30:LYS:HD2	1.98	0.44
1:A:29:ILE:HG22	1:A:30:LYS:HG3	1.99	0.44
1:B:97:THR:HG22	1:B:207:ALA:O	2.18	0.44
1:B:57:VAL:CG1	1:D:62:SER:HB3	2.47	0.44
1:C:207:ALA:HB1	1:C:208:ASP:CG	2.38	0.44
1:D:69:ASN:CG	1:D:70:GLY:HA2	2.37	0.44
1:A:57:VAL:HG13	1:C:64:VAL:CG2	2.47	0.44
1:B:58:GLY:O	1:D:60:ARG:NH1	2.49	0.44
1:D:52:ILE:N	1:D:52:ILE:HD12	2.32	0.44
1:A:57:VAL:HG12	1:C:62:SER:HB3	1.99	0.43
1:B:100:TYR:CE1	5:B:305:MDM:H7'2	2.52	0.43
1:C:107:LEU:HD12	1:C:107:LEU:N	2.32	0.43
1:D:4:ILE:CD1	1:D:215:SER:HB3	2.46	0.43
1:A:28:ASP:OD1	1:A:34:SER:HA	2.18	0.43
1:B:64:VAL:CG2	1:D:57:VAL:HG13	2.48	0.43
1:A:99:LEU:HB2	5:A:305:MDM:H1	2.01	0.43
1:D:208:ASP:OD1	5:D:305:MDM:O4	2.36	0.43
1:A:135:LYS:HD2	1:A:135:LYS:HA	1.78	0.43
1:A:54:TYR:HB2	1:A:61:LEU:HD12	2.00	0.43
1:C:137:GLN:HG2	1:C:140:LEU:HD12	2.00	0.43
1:A:54:TYR:CD2	1:A:81:LEU:HD12	2.54	0.43
1:C:181:ILE:HG23	1:C:182:TRP:CD1	2.53	0.43
1:C:97:THR:HG22	1:C:207:ALA:O	2.18	0.43
1:C:177:ALA:HB2	1:D:177:ALA:HB2	2.01	0.42
1:A:221:ILE:HA	1:A:222:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:CG1	1:C:64:VAL:HG23	2.46	0.42
1:D:117:SER:HA	1:D:186:ALA:HA	2.01	0.42
1:D:5:VAL:HG13	1:D:29:ILE:HD13	2.01	0.42
1:C:135:LYS:HD3	1:C:149:GLY:CA	2.36	0.42
1:D:91:VAL:HG12	1:D:214:ILE:HG12	2.02	0.42
1:B:135:LYS:HD3	1:B:135:LYS:HA	1.83	0.42
1:C:112:THR:O	1:C:191:PHE:HA	2.20	0.42
5:D:305:MDM:H1	5:D:305:MDM:O4'	2.19	0.42
1:B:22:TYR:CD1	1:B:39:LYS:HG3	2.55	0.42
1:A:11:THR:OG1	1:A:207:ALA:HA	2.20	0.41
1:A:54:TYR:HB2	1:A:61:LEU:CD1	2.50	0.41
1:A:172:ARG:HG3	1:A:221:ILE:HD11	2.01	0.41
1:B:111:PHE:O	1:B:127:HIS:HA	2.20	0.41
1:D:103:THR:O	1:D:199:ILE:HA	2.20	0.41
1:A:151:ASP:OD2	1:A:153:ASN:HB2	2.21	0.41
1:B:64:VAL:HG23	1:D:57:VAL:CG1	2.50	0.41
1:C:133:PHE:O	1:C:152:GLY:HA2	2.20	0.41
1:D:10:ASP:HB3	1:D:24:HIS:CE1	2.56	0.41
1:B:57:VAL:CG1	1:D:64:VAL:HG23	2.49	0.41
1:D:59:LYS:HD3	1:D:80:ASP:HB2	2.03	0.41
1:B:14:ASN:HB2	1:B:17:ILE:HD11	2.02	0.41
1:A:138:LYS:HD2	1:B:88:TRP:HB3	2.02	0.41
1:B:170:VAL:HB	1:B:226:THR:HG22	2.02	0.41
1:D:23:PRO:HB2	1:D:40:TRP:O	2.21	0.41
1:A:187:VAL:HG23	1:A:188:VAL:HG13	2.02	0.41
1:A:68:PRO:O	1:A:69:ASN:CB	2.70	0.41
1:B:102:GLU:OE2	1:B:199:ILE:HD13	2.21	0.41
1:C:135:LYS:HE2	1:C:150:ARG:NE	2.36	0.41
1:D:142:LEU:HD11	1:D:148:THR:HG23	2.03	0.41
1:D:8:GLU:O	1:D:25:ILE:HA	2.21	0.41
1:A:69:ASN:C	1:A:69:ASN:OD1	2.59	0.40
1:A:99:LEU:HD13	1:A:99:LEU:C	2.42	0.40
1:C:100:TYR:CD2	1:C:205:HIS:HB2	2.57	0.40
1:D:102:GLU:OE2	1:D:104:ASN:ND2	2.49	0.40
1:D:79:VAL:HG22	1:D:80:ASP:N	2.35	0.40
1:C:201:SER:CB	1:C:206:PRO:HB3	2.52	0.40
1:C:211:ALA:CB	1:C:232:LEU:HD11	2.52	0.40
1:B:43:GLN:NE2	6:B:422:HOH:O	2.55	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	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	38	59
1	B	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
1	C	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
1	D	235/237 (99%)	225 (96%)	9 (4%)	1 (0%)	38	59
All	All	940/948 (99%)	899 (96%)	39 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASP
1	D	69	ASN

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	202/202 (100%)	197 (98%)	5 (2%)	53	79
1	B	202/202 (100%)	202 (100%)	0	100	100
1	C	202/202 (100%)	200 (99%)	2 (1%)	80	93
1	D	202/202 (100%)	202 (100%)	0	100	100
All	All	808/808 (100%)	801 (99%)	7 (1%)	82	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LYS
1	A	150	ARG
1	A	188	VAL
1	A	203	ASP
1	A	216	ASN
1	C	71	ASP
1	C	217	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	43	GLN
1	A	83	ASN
1	A	132	GLN
1	A	205	HIS
1	B	43	GLN
1	B	104	ASN
1	B	131	ASN
1	B	132	GLN
1	B	166	GLN
1	B	237	ASN
1	C	118	ASN
1	C	131	ASN
1	C	132	GLN
1	C	237	ASN
1	D	43	GLN
1	D	216	ASN
1	D	237	ASN

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 21 ligands modelled in this entry, 17 are monoatomic - leaving 4 for Mogul analysis.

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	$\#|Z| > 2$
5	MDM	A	305	-	25,25,25	1.09	2 (8%)	36,36,36	1.42	5 (13%)
5	MDM	B	305	-	25,25,25	1.10	3 (12%)	36,36,36	1.98	11 (30%)
5	MDM	C	306	-	25,25,25	1.17	2 (8%)	36,36,36	1.65	10 (27%)
5	MDM	D	305	-	25,25,25	0.90	1 (4%)	36,36,36	1.64	8 (22%)

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
5	MDM	A	305	-	-	0/10/50/50	0/2/2/2
5	MDM	B	305	-	-	0/10/50/50	0/2/2/2
5	MDM	C	306	-	-	0/10/50/50	0/2/2/2
5	MDM	D	305	-	-	0/10/50/50	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	305	MDM	C4'-C5'	-2.63	1.47	1.53
5	B	305	MDM	C4-C3	-2.23	1.46	1.52
5	B	305	MDM	O5'-C1'	2.00	1.46	1.41
5	A	305	MDM	O1'-C1'	2.08	1.43	1.40
5	D	305	MDM	O5-C1	2.25	1.47	1.41
5	C	306	MDM	O5'-C1'	2.59	1.48	1.41
5	A	305	MDM	O5'-C1'	3.16	1.49	1.41
5	C	306	MDM	O1'-C1'	3.44	1.46	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	305	MDM	O5'-C5'-C6'	-5.15	94.07	106.41
5	B	305	MDM	O3'-C1-O5	-4.64	99.43	110.70
5	A	305	MDM	C7'-O1'-C1'	-4.12	106.85	113.29
5	B	305	MDM	C6'-C5'-C4'	-4.02	103.60	113.00
5	C	306	MDM	C4'-C3'-C2'	-3.88	105.24	110.83
5	D	305	MDM	C7'-O1'-C1'	-3.70	107.52	113.29
5	A	305	MDM	C1'-O5'-C5'	-3.43	107.25	113.72
5	B	305	MDM	C4'-C3'-C2'	-3.22	106.19	110.83
5	D	305	MDM	C6'-C5'-C4'	-2.67	106.76	113.00
5	C	306	MDM	O3'-C1-O5	-2.60	104.39	110.70
5	D	305	MDM	O3'-C1-O5	-2.57	104.45	110.70
5	C	306	MDM	C7'-O1'-C1'	-2.53	109.34	113.29
5	C	306	MDM	C1-O3'-C3'	-2.51	111.88	118.00
5	B	305	MDM	O5'-C1'-C2'	-2.42	105.63	110.30
5	D	305	MDM	C6-C5-C4	-2.40	107.38	113.00
5	C	306	MDM	C6'-C5'-C4'	-2.39	107.41	113.00
5	D	305	MDM	C3-C4-C5	-2.37	106.04	110.22
5	D	305	MDM	O4'-C4'-C5'	-2.36	103.33	109.28
5	B	305	MDM	O3-C3-C4	-2.26	105.45	110.36
5	B	305	MDM	C3-C4-C5	-2.19	106.36	110.22
5	C	306	MDM	C1'-C2'-C3'	-2.14	106.31	110.04
5	C	306	MDM	O4-C4-C3	-2.08	105.83	110.36
5	B	305	MDM	O2-C2-C1	-2.07	105.70	110.03
5	A	305	MDM	O4'-C4'-C5'	2.00	114.33	109.28
5	A	305	MDM	O3'-C3'-C2'	2.05	112.13	107.19
5	C	306	MDM	O2-C2-C3	2.07	114.86	110.36
5	C	306	MDM	O5'-C1'-O1'	2.23	116.14	110.92
5	D	305	MDM	O2'-C2'-C1'	2.27	114.78	110.03
5	B	305	MDM	O2-C2-C3	2.32	115.41	110.36
5	A	305	MDM	O2'-C2'-C3'	2.59	115.75	109.87
5	B	305	MDM	O1'-C1'-C2'	2.80	111.47	108.14
5	C	306	MDM	O5'-C5'-C6'	2.83	113.19	106.41
5	B	305	MDM	O5-C5-C6	3.34	114.41	106.41
5	D	305	MDM	O5-C5-C6	4.36	116.86	106.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	305	MDM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	305	MDM	7	0
5	C	306	MDM	2	0
5	D	305	MDM	2	0

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(Å²)	Q<0.9
1	A	237/237 (100%)	-0.08	2 (0%)	86	86	19, 30, 45, 63	0
1	B	237/237 (100%)	0.01	5 (2%)	64	66	20, 30, 48, 67	0
1	C	237/237 (100%)	-0.13	0	100	100	19, 28, 45, 60	0
1	D	237/237 (100%)	0.10	7 (2%)	51	53	19, 32, 54, 63	0
All	All	948/948 (100%)	-0.03	14 (1%)	74	75	19, 30, 48, 67	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	THR	4.7
1	B	121	HIS	3.8
1	B	236	ALA	3.4
1	D	118	ASN	3.3
1	D	121	HIS	3.0
1	A	120	THR	3.0
1	D	204	SER	2.8
1	B	122	GLU	2.6
1	D	119	SER	2.4
1	B	120	THR	2.3
1	B	118	ASN	2.3
1	D	237	ASN	2.2
1	A	150	ARG	2.0
1	D	69	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	MN	C	301	1/1	0.99	0.18	2.79	24,24,24,24	0
2	MN	D	301	1/1	0.98	0.17	2.04	30,30,30,30	0
2	MN	A	301	1/1	0.99	0.17	1.68	23,23,23,23	0
3	CA	D	302	1/1	0.87	0.17	1.08	36,36,36,36	0
3	CA	B	302	1/1	0.94	0.17	0.17	30,30,30,30	0
5	MDM	D	305	24/24	0.89	0.14	-0.18	29,39,47,57	0
2	MN	B	301	1/1	0.99	0.14	-0.49	22,22,22,22	0
3	CA	C	302	1/1	0.81	0.14	-0.66	32,32,32,32	0
5	MDM	B	305	24/24	0.91	0.13	-0.69	23,33,42,45	0
4	CD	D	303	1/1	0.96	0.10	-0.93	56,56,56,56	0
5	MDM	A	305	24/24	0.92	0.12	-1.16	26,31,37,38	0
5	MDM	C	306	24/24	0.93	0.11	-1.34	30,37,44,48	0
3	CA	A	302	1/1	0.96	0.12	-1.57	29,29,29,29	0
4	CD	B	303	1/1	0.91	0.11	-2.13	54,54,54,54	0
4	CD	A	303	1/1	0.99	0.11	-2.73	45,45,45,45	0
4	CD	A	304	1/1	0.99	0.05	-	61,61,61,61	1
4	CD	B	304	1/1	0.99	0.04	-	57,57,57,57	1
4	CD	C	304	1/1	0.95	0.06	-	73,73,73,73	1
4	CD	C	305	1/1	0.90	0.07	-	83,83,83,83	1
4	CD	C	303	1/1	0.99	0.09	-	40,40,40,40	0
4	CD	D	304	1/1	0.95	0.04	-	86,86,86,86	1

6.5 Other polymers ⓘ

There are no such residues in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK