



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:02 PM GMT

PDB ID : 3MZH
Title : Crystal structure of cAMP receptor protein from mycobacterium tuberculosis
in complex with cAMP and its DNA binding element
Authors : Akhter, Y.; Wilmanns, M.
Deposited on : 2010-05-12
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

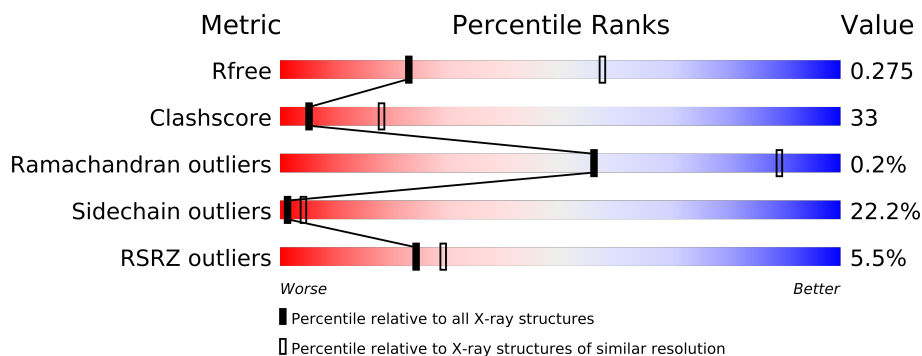
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	225	
1	B	225	
2	C	21	
3	D	20	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CMP	B	621	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4357 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/FNR-FAMILY).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1712	1070	326	312	4			
1	B	225	Total	C	N	O	S	0	2	0
			1739	1086	336	314	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	EXPRESSION TAG	UNP O69644
B	0	HIS	-	EXPRESSION TAG	UNP O69644

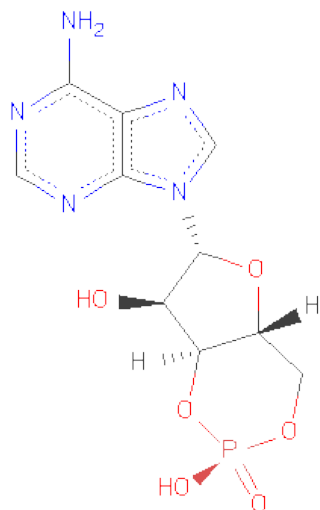
- Molecule 2 is a DNA chain called 5'-D(P*AP*AP*AP*TP*GP*TP*GP*AP*TP*CP*TP*AP*GP*GP*TP*CP*AP*CP*GP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	P	0	0	0
			435	207	81	126	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total	C	N	O	P	0	0	0
			405	193	74	118	20			

- Molecule 4 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C₁₀H₁₂N₅O₆P).



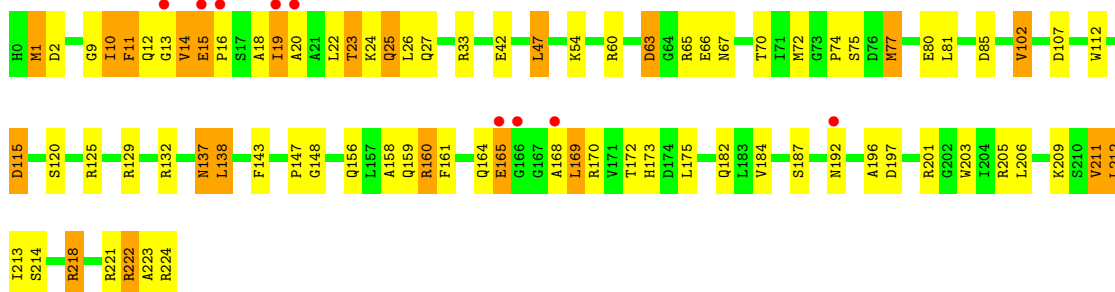
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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 errors 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.

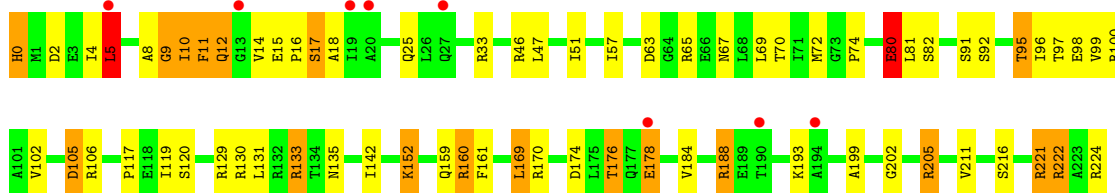
- Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/FNR-FAMILY)

Chain A: 



- Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN (PROBABLY CRP/FNR-FAMILY)

Chain B: 



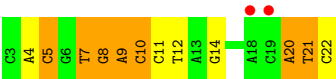
- Molecule 2: 5'-D(P*AP*AP*AP*TP*GP*TP*GP*AP*TP*CP*TP*AP*GP*GP*TP*CP*AP*CP*GP*TP*G)-3'

Chain C: 



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.13Å 61.25Å 89.94Å 90.00° 104.29° 90.00°	Depositor
Resolution (Å)	43.58 – 2.90 44.28 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.4 (43.58-2.90) 93.2 (44.28-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.247 , 0.279 0.250 , 0.275	Depositor DCC
R_{free} test set	726 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.922	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 14707 reflections (0.014%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4357	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.82	1/1737 (0.1%)	0.72	0/2349
1	B	0.80	1/1768 (0.1%)	0.70	3/2388 (0.1%)
2	C	0.57	0/488	1.42	8/752 (1.1%)
3	D	1.58	11/453 (2.4%)	2.18	29/695 (4.2%)
All	All	0.90	13/4446 (0.3%)	1.08	40/6184 (0.6%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	DC	C3'-O3'	-9.05	1.32	1.44
3	D	5	DC	N3-C4	-6.96	1.29	1.33
3	D	9	DA	C6-N1	-6.86	1.30	1.35
3	D	5	DC	N1-C6	-6.77	1.33	1.37
3	D	9	DA	N3-C4	-6.15	1.31	1.34
3	D	10	DC	N1-C6	-5.99	1.33	1.37
1	B	80	GLU	CG-CD	-5.98	1.43	1.51
3	D	5	DC	O3'-P	-5.91	1.54	1.61
3	D	8	DG	N3-C4	-5.62	1.31	1.35
3	D	5	DC	N1-C2	-5.50	1.34	1.40
3	D	10	DC	N1-C2	-5.19	1.34	1.40
3	D	5	DC	C2-N3	-5.18	1.31	1.35
1	A	14	VAL	CB-CG1	-5.11	1.42	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	DG	O4'-C4'-C3'	-15.88	96.47	106.00
3	D	5	DC	O4'-C4'-C3'	-15.17	96.90	106.00
3	D	10	DC	O4'-C4'-C3'	-12.82	98.31	106.00
3	D	10	DC	C1'-O4'-C4'	-11.54	98.56	110.10
3	D	7	DT	P-O3'-C3'	10.15	131.88	119.70
3	D	9	DA	O4'-C4'-C3'	-9.89	100.07	106.00
3	D	9	DA	C4'-C3'-C2'	-9.79	94.29	103.10
2	C	15	DG	O4'-C1'-N9	9.70	114.79	108.00
3	D	8	DG	C5-C6-O6	8.84	133.90	128.60
3	D	20	DA	O4'-C1'-N9	8.20	113.74	108.00
3	D	5	DC	O4'-C1'-N1	-7.71	102.60	108.00
3	D	5	DC	C1'-O4'-C4'	-7.58	102.52	110.10
3	D	8	DG	C4-C5-N7	-7.55	107.78	110.80
3	D	8	DG	C1'-O4'-C4'	-7.31	102.79	110.10
3	D	5	DC	O4'-C1'-C2'	-7.30	100.06	105.90
3	D	14	DG	O4'-C1'-N9	7.22	113.05	108.00
3	D	9	DA	O5'-P-OP1	-6.79	99.59	105.70
3	D	8	DG	N9-C4-C5	6.73	108.09	105.40
3	D	8	DG	O5'-P-OP2	6.45	118.44	110.70
3	D	8	DG	C5-C6-N1	-6.23	108.39	111.50
2	C	8	DT	P-O3'-C3'	6.18	127.11	119.70
2	C	3	DA	O4'-C1'-N9	6.14	112.30	108.00
2	C	4	DA	O4'-C1'-N9	6.11	112.28	108.00
2	C	16	DG	O4'-C1'-N9	-6.05	103.76	108.00
3	D	10	DC	C4'-C3'-C2'	-6.04	97.67	103.10
2	C	3	DA	C1'-O4'-C4'	-6.02	104.08	110.10
3	D	8	DG	O4'-C1'-N9	5.95	112.16	108.00
3	D	10	DC	C5'-C4'-C3'	5.86	124.64	114.10
3	D	10	DC	OP2-P-O3'	5.77	117.89	105.20
1	B	9	GLY	N-CA-C	5.47	126.77	113.10
3	D	9	DA	P-O5'-C5'	-5.40	112.25	120.90
3	D	9	DA	O4'-C1'-N9	5.40	111.78	108.00
3	D	8	DG	C4-C5-C6	5.36	122.02	118.80
1	B	5	LEU	CA-CB-CG	-5.34	103.02	115.30
3	D	9	DA	O5'-P-OP2	5.28	117.03	110.70
3	D	21	DT	N3-C4-O4	5.20	123.02	119.90
1	B	174	ASP	CB-CG-OD2	5.18	122.96	118.30
2	C	12	DC	O4'-C1'-N1	-5.14	104.40	108.00
3	D	8	DG	C8-N9-C4	-5.10	104.36	106.40
2	C	9	DG	O4'-C1'-N9	5.07	111.55	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	PHE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1712	0	39	67	0
1	B	1739	0	39	59	0
2	C	435	0	0	10	0
3	D	405	0	0	18	0
4	A	22	0	0	1	0
4	B	44	0	0	4	0
All	All	4357	0	78	146	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (146) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:TRP:CZ2	1:A:218:ARG:CG	2.23	1.20
1:B:10:ILE:CD1	1:B:11:PHE:CB	2.30	1.08
1:A:203:TRP:CE2	1:A:218:ARG:CG	2.38	1.06
3:D:10:DC:C2'	3:D:11:DC:O5'	2.03	1.06
1:B:10:ILE:CD1	1:B:11:PHE:CA	2.36	1.02
1:A:212:LEU:HD12	1:A:213:ILE:N	1.72	1.02
1:B:176:THR:OG1	1:B:178:GLU:HG2	1.60	1.01
1:B:80:GLU:OE2	1:B:81:LEU:N	1.95	0.99
1:B:10:ILE:CD1	1:B:10:ILE:C	2.30	0.99
1:A:223:ALA:O	1:A:224:ARG:C	2.01	0.98
2:C:16:DG:N1	3:D:10:DC:N4	2.13	0.95
1:B:10:ILE:CD1	1:B:11:PHE:N	2.30	0.94
1:B:97:THR:CG2	1:B:98:GLU:N	2.29	0.94
1:B:5:LEU:CD1	1:B:5:LEU:N	2.30	0.94
1:A:203:TRP:NE1	1:A:218:ARG:CG	2.30	0.93
1:B:10:ILE:CG1	1:B:11:PHE:N	2.30	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:18:DC:N3	3:D:8:DG:N1	2.16	0.92
1:B:5:LEU:O	1:B:11:PHE:CE1	2.23	0.91
1:A:169:LEU:C	1:A:169:LEU:CD2	2.45	0.85
1:A:125:ARG:NH2	1:A:129:ARG:HH12	1.76	0.83
1:B:14:VAL:O	1:B:14:VAL:CG1	2.30	0.80
1:A:169:LEU:O	1:A:169:LEU:CD2	2.29	0.80
1:A:138:LEU:O	1:A:138:LEU:CD1	2.30	0.80
1:B:222:ARG:O	1:B:222:ARG:CD	2.30	0.79
1:A:13:GLY:O	1:A:14:VAL:CG1	2.30	0.79
1:A:222:ARG:O	1:A:222:ARG:CD	2.30	0.79
1:A:1:MET:O	1:A:1:MET:CE	2.30	0.79
3:D:9:DA:O5'	3:D:9:DA:C2'	2.30	0.79
1:B:15:GLU:O	1:B:17:SER:N	2.15	0.78
1:A:218:ARG:CD	1:A:221:ARG:NH2	2.47	0.77
1:A:11:PHE:O	1:A:14:VAL:CG1	2.32	0.77
1:A:22:LEU:O	1:A:23:THR:C	2.19	0.77
2:C:18:DC:N3	3:D:8:DG:C6	2.42	0.77
1:A:164:GLN:NE2	1:A:168:ALA:C	2.39	0.76
1:A:14:VAL:CG1	1:A:14:VAL:O	2.30	0.76
1:A:26:LEU:CD1	1:A:102:VAL:CG2	2.63	0.76
1:B:80:GLU:CA	1:B:80:GLU:OE2	2.30	0.75
1:B:221:ARG:HG3	1:B:221:ARG:HH11	1.51	0.75
1:A:16:PRO:CA	1:A:19:ILE:CG2	2.65	0.75
1:B:12:GLN:CA	1:B:12:GLN:OE1	2.36	0.74
1:B:221:ARG:CG	1:B:221:ARG:HH11	2.03	0.71
1:A:11:PHE:O	1:A:12:GLN:O	2.09	0.71
1:B:80:GLU:OE2	1:B:80:GLU:C	2.29	0.70
1:A:63:ASP:OD1	1:A:63:ASP:C	2.29	0.70
3:D:7:DT:C2	3:D:8:DG:C8	2.81	0.69
1:B:82:SER:O	1:B:106:ARG:NH1	2.26	0.69
1:B:95:THR:CG2	1:B:99:VAL:CG2	2.71	0.68
1:B:133[B]:ARG:NH2	4:B:622:CMP:N1	2.42	0.68
2:C:4:DA:N1	3:D:22:DC:N3	2.41	0.68
1:B:11:PHE:CD1	1:B:11:PHE:O	2.47	0.67
1:B:15:GLU:O	1:B:18:ALA:N	2.28	0.67
2:C:16:DG:N2	3:D:10:DC:N3	2.43	0.67
1:B:33[A]:ARG:CA	1:B:97:THR:O	2.42	0.66
1:A:15:GLU:O	1:A:18:ALA:N	2.29	0.66
1:A:164:GLN:NE2	1:A:169:LEU:N	2.44	0.66
1:B:15:GLU:O	1:B:16:PRO:C	2.30	0.66
1:B:33[C]:ARG:CA	1:B:97:THR:O	2.42	0.65
3:D:4:DA:C2'	3:D:5:DC:O5'	2.44	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:LEU:CD2	1:A:211:VAL:CG2	2.73	0.65
1:B:14:VAL:O	1:B:15:GLU:C	2.34	0.65
1:B:80:GLU:OE2	1:B:80:GLU:N	2.30	0.65
1:A:205:ARG:N	1:A:212:LEU:O	2.30	0.65
1:A:11:PHE:O	1:A:12:GLN:C	2.34	0.65
1:B:0:HIS:CD2	1:B:0:HIS:N	2.64	0.65
1:B:9:GLY:O	1:B:10:ILE:C	2.30	0.64
1:A:23:THR:O	1:A:26:LEU:CB	2.44	0.64
1:B:222:ARG:CD	1:B:222:ARG:C	2.64	0.64
1:A:165:GLU:O	1:A:165:GLU:CG	2.46	0.64
1:A:212:LEU:HD12	1:A:212:LEU:C	2.16	0.63
1:A:2:ASP:N	1:A:2:ASP:OD2	2.30	0.63
1:B:15:GLU:C	1:B:17:SER:N	2.50	0.62
1:A:19:ILE:CD1	1:A:19:ILE:C	2.67	0.62
1:B:74:PRO:O	1:B:160:ARG:NH2	2.31	0.62
1:A:223:ALA:O	1:A:224:ARG:O	2.17	0.62
1:A:14:VAL:CG2	1:A:14:VAL:O	2.45	0.60
1:A:66:GLU:CG	1:A:182:GLN:NE2	2.65	0.60
1:B:221:ARG:CG	1:B:221:ARG:NH1	2.62	0.59
2:C:4:DA:N6	3:D:22:DC:N4	2.50	0.59
1:A:203:TRP:NE1	1:A:218:ARG:CB	2.66	0.59
1:B:205:ARG:CG	1:B:205:ARG:NH1	2.66	0.58
1:B:10:ILE:CG1	1:B:11:PHE:CG	2.87	0.58
3:D:21:DT:C2	3:D:22:DC:C5	2.93	0.57
1:B:80:GLU:OE1	4:B:622:CMP:O2'	2.22	0.57
1:A:10:ILE:CG1	1:A:11:PHE:N	2.65	0.57
1:A:63:ASP:OD1	1:A:65:ARG:HG3	2.06	0.56
1:A:160:ARG:NH1	1:A:161:PHE:CE1	2.74	0.56
1:A:138:LEU:CD1	1:A:138:LEU:C	2.69	0.56
1:A:33:ARG:NH2	1:A:209:LYS:NZ	2.55	0.55
1:B:160:ARG:CD	1:B:161:PHE:CE1	2.89	0.55
3:D:7:DT:O2	3:D:8:DG:C8	2.60	0.55
1:B:10:ILE:CG1	1:B:11:PHE:CB	2.84	0.55
1:A:158:ALA:O	1:A:159:GLN:C	2.45	0.54
1:A:13:GLY:C	1:A:14:VAL:CG1	2.76	0.54
1:B:188:ARG:CG	1:B:188:ARG:NH1	2.71	0.53
1:A:11:PHE:O	1:A:14:VAL:CB	2.57	0.53
1:B:152:LYS:CD	4:B:621:CMP:O1P	2.57	0.52
3:D:11:DC:C1'	3:D:12:DT:OP2	2.57	0.52
1:A:203:TRP:O	1:A:214:SER:N	2.42	0.52
1:A:74:PRO:O	1:A:160:ARG:NH2	2.43	0.52
1:A:192:ASN:O	1:A:196:ALA:N	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:ASP:OD2	1:A:115:ASP:N	2.43	0.51
1:B:0:HIS:N	1:B:0:HIS:HD2	2.08	0.51
3:D:21:DT:C6	3:D:21:DT:OP2	2.64	0.51
1:A:222:ARG:CD	1:A:222:ARG:C	2.72	0.50
2:C:18:DC:C2	3:D:8:DG:N1	2.78	0.50
2:C:8:DT:C2'	2:C:9:DG:OP2	2.59	0.50
1:B:2:ASP:OD1	1:B:2:ASP:O	2.29	0.49
3:D:7:DT:C2	3:D:8:DG:N7	2.80	0.49
1:A:173:HIS:ND1	1:A:175:LEU:N	2.60	0.49
1:A:25:GLN:OE1	1:A:112:TRP:CZ2	2.66	0.49
1:A:74:PRO:O	1:A:75:SER:CB	2.61	0.48
1:A:143:PHE:HE1	1:B:65:ARG:CB	2.25	0.48
1:A:201:ARG:NH1	1:A:201:ARG:CG	2.76	0.48
1:A:47:LEU:CD1	1:A:77:MET:SD	3.01	0.48
2:C:20:DC:C2'	2:C:21:DG:C8	2.98	0.47
1:B:5:LEU:O	1:B:8:ALA:CB	2.63	0.47
1:A:18:ALA:O	1:A:19:ILE:C	2.50	0.47
1:A:148:GLY:O	1:A:223:ALA:CB	2.63	0.47
1:A:9:GLY:O	1:A:12:GLN:N	2.49	0.46
1:A:81:LEU:O	1:A:85:ASP:N	2.49	0.46
2:C:6:DT:C2'	2:C:7:DG:C8	2.98	0.46
4:A:623:CMP:N6	1:B:135:ASN:OD1	2.49	0.46
3:D:12:DT:OP2	3:D:12:DT:O4'	2.34	0.46
1:B:96:ILE:O	1:B:97:THR:OG1	2.33	0.46
1:A:137:ASN:ND2	1:A:137:ASN:N	2.64	0.46
1:B:117:PRO:C	1:B:119:ILE:N	2.69	0.45
1:A:63:ASP:OD1	1:A:65:ARG:N	2.50	0.45
1:A:22:LEU:O	1:A:24:LYS:N	2.50	0.44
1:A:15:GLU:O	1:A:18:ALA:CB	2.65	0.44
1:B:10:ILE:CD1	1:B:10:ILE:O	2.65	0.44
1:A:54:LYS:NZ	1:A:172:THR:O	2.52	0.43
1:B:176:THR:OG1	1:B:178:GLU:CG	2.50	0.43
1:B:10:ILE:CG1	1:B:11:PHE:CD2	3.01	0.43
1:B:51:ILE:N	1:B:100:ARG:O	2.52	0.43
1:B:169:LEU:N	1:B:169:LEU:CD1	2.82	0.43
1:B:69:LEU:CA	4:B:621:CMP:N6	2.83	0.42
1:B:105:ASP:OD1	1:B:105:ASP:C	2.58	0.42
1:B:4:ILE:CD1	1:B:4:ILE:N	2.83	0.42
1:B:117:PRO:O	1:B:119:ILE:N	2.52	0.42
1:A:23:THR:O	1:A:26:LEU:N	2.52	0.41
1:B:80:GLU:CD	1:B:80:GLU:N	2.73	0.41
1:A:169:LEU:N	1:A:169:LEU:CD2	2.78	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:199:ALA:O	1:B:202:GLY:N	2.54	0.41
1:A:19:ILE:CG1	1:A:20:ALA:N	2.83	0.40
1:A:14:VAL:O	1:A:15:GLU:C	2.59	0.40
3:D:20:DA:C8	3:D:20:DA:OP2	2.74	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	223/225 (99%)	210 (94%)	12 (5%)	1 (0%)	43	82
1	B	225/225 (100%)	214 (95%)	11 (5%)	0	100	100
All	All	448/450 (100%)	424 (95%)	23 (5%)	1 (0%)	56	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	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	173/184 (94%)	138 (80%)	35 (20%)	2	5
1	B	176/184 (96%)	133 (76%)	43 (24%)	1	3
All	All	349/368 (95%)	271 (78%)	78 (22%)	1	4

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ILE
1	A	15	GLU
1	A	19	ILE
1	A	23	THR
1	A	25	GLN
1	A	27	GLN
1	A	42	GLU
1	A	47	LEU
1	A	60	ARG
1	A	63	ASP
1	A	67	ASN
1	A	70	THR
1	A	72	MET
1	A	77	MET
1	A	80	GLU
1	A	102	VAL
1	A	107	ASP
1	A	115	ASP
1	A	120	SER
1	A	132	ARG
1	A	137	ASN
1	A	138	LEU
1	A	156	GLN
1	A	160	ARG
1	A	165	GLU
1	A	169	LEU
1	A	170	ARG
1	A	184	VAL
1	A	187	SER
1	A	197	ASP
1	A	211	VAL
1	A	212	LEU
1	A	218	ARG
1	A	222	ARG
1	B	0	HIS
1	B	5	LEU
1	B	10	ILE
1	B	11	PHE
1	B	12	GLN
1	B	17	SER
1	B	25	GLN
1	B	46	ARG

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Mol	Chain	Res	Type
1	B	47	LEU
1	B	57	ILE
1	B	63	ASP
1	B	67	ASN
1	B	70	THR
1	B	72	MET
1	B	80	GLU
1	B	91	SER
1	B	92	SER
1	B	95	THR
1	B	102	VAL
1	B	105	ASP
1	B	120	SER
1	B	129	ARG
1	B	130	ARG
1	B	131	LEU
1	B	133[A]	ARG
1	B	133[B]	ARG
1	B	142	ILE
1	B	152	LYS
1	B	159	GLN
1	B	160	ARG
1	B	169	LEU
1	B	170	ARG
1	B	176	THR
1	B	178	GLU
1	B	184	VAL
1	B	188	ARG
1	B	193	LYS
1	B	205	ARG
1	B	211	VAL
1	B	216	SER
1	B	221	ARG
1	B	222	ARG
1	B	224	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	0	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 ligands 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	$\# Z > 2$
4	CMP	A	623	-	25,25,25	1.30	2 (8%)	39,39,39	1.95	8 (20%)
4	CMP	B	621	-	25,25,25	1.32	2 (8%)	39,39,39	2.05	12 (30%)
4	CMP	B	622	-	25,25,25	1.31	4 (16%)	39,39,39	2.03	8 (20%)

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
4	CMP	A	623	-	-	0/4/31/31	0/0/4/4
4	CMP	B	621	-	-	0/4/31/31	0/0/4/4
4	CMP	B	622	-	-	0/4/31/31	0/0/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	622	CMP	C5-C4	3.27	1.47	1.40
4	A	623	CMP	C5-C4	3.12	1.47	1.40
4	B	621	CMP	C5-C4	3.09	1.47	1.40
4	B	621	CMP	C4-N9	-2.91	1.33	1.37
4	A	623	CMP	C4-N9	-2.67	1.33	1.37
4	B	622	CMP	P-O3'	2.39	1.62	1.58
4	B	622	CMP	C4-N9	-2.16	1.34	1.37
4	B	622	CMP	P-O5'	2.03	1.61	1.58

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	623	CMP	N3-C2-N1	-5.86	123.81	128.71
4	B	622	CMP	N3-C4-N9	5.77	135.85	125.43
4	B	621	CMP	N3-C4-N9	5.49	135.35	125.43
4	B	621	CMP	N3-C2-N1	-5.29	124.28	128.71
4	A	623	CMP	N3-C4-N9	5.27	134.95	125.43
4	B	622	CMP	N3-C2-N1	-5.19	124.37	128.71
4	B	622	CMP	O3'-C3'-C2'	4.29	120.56	115.62
4	A	623	CMP	O3'-C3'-C4'	-4.27	107.31	110.73
4	B	621	CMP	O5'-P-O3'	-4.02	100.30	105.81
4	B	622	CMP	O3'-C3'-C4'	-3.92	107.58	110.73
4	A	623	CMP	C4-C5-N7	-3.75	106.31	109.52
4	B	622	CMP	C5-C4-N3	-3.52	118.04	125.70
4	B	621	CMP	O3'-C3'-C2'	3.46	119.60	115.62
4	A	623	CMP	C5-C4-N3	-3.36	118.38	125.70
4	B	622	CMP	C4-C5-N7	-3.34	106.66	109.52
4	B	621	CMP	C5-C4-N3	-3.26	118.60	125.70
4	B	621	CMP	O5'-P-O1P	3.20	116.83	109.99
4	B	621	CMP	C2'-C1'-N9	-3.13	105.23	113.27
4	B	621	CMP	C4-C5-N7	-2.86	107.07	109.52
4	B	622	CMP	O5'-P-O3'	-2.64	102.19	105.81
4	A	623	CMP	C2-N3-C4	2.53	121.22	114.01
4	B	622	CMP	C2-N3-C4	2.36	120.73	114.01
4	A	623	CMP	O3'-C3'-C2'	2.35	118.33	115.62
4	B	621	CMP	O3'-P-O1P	2.34	114.99	109.99
4	B	621	CMP	O3'-C3'-C4'	-2.29	108.89	110.73
4	B	621	CMP	C2-N3-C4	2.29	120.54	114.01
4	A	623	CMP	C5'-C4'-C3'	-2.26	107.84	112.62
4	B	621	CMP	P-O3'-C3'	-2.10	107.13	117.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	225/225 (100%)	0.31	9 (4%)	36 43	15, 53, 131, 248	0
1	B	225/225 (100%)	0.19	8 (3%)	41 48	11, 48, 110, 169	0
2	C	21/21 (100%)	1.36	7 (33%)	1 1	45, 82, 118, 162	0
3	D	20/20 (100%)	0.88	2 (10%)	8 10	55, 80, 116, 141	0
All	All	491/491 (100%)	0.32	26 (5%)	24 31	11, 54, 123, 248	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	GLY	6.8
1	A	19	ILE	4.7
1	B	19	ILE	4.5
1	A	20	ALA	4.5
1	A	16	PRO	4.4
1	A	13	GLY	3.2
1	B	27	GLN	3.1
2	C	23	DG	3.1
1	B	178	GLU	3.1
3	D	18	DA	3.0
2	C	20	DC	2.8
1	A	165	GLU	2.6
1	A	192	ASN	2.6
2	C	19	DA	2.5
3	D	19	DC	2.4
1	A	15	GLU	2.4
1	B	20	ALA	2.3
1	B	5	LEU	2.3
1	A	168	ALA	2.2
2	C	21	DG	2.2
1	B	194	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	190	THR	2.2
1	A	166	GLY	2.1
2	C	3	DA	2.1
2	C	7	DG	2.1
2	C	9	DG	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CMP	B	621	22/22	0.49	9.87	70,75,81,83	22
4	CMP	A	623	22/22	0.28	1.88	73,76,78,79	0
4	CMP	B	622	22/22	0.27	1.56	78,85,89,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.