



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:51 AM GMT

PDB ID : 2JG3  
Title : MTAQI WITH BAZ  
Authors : Pljevaljcic, G.; Scheidig, A.J.; Weinhold, E.  
Deposited on : 2007-02-07  
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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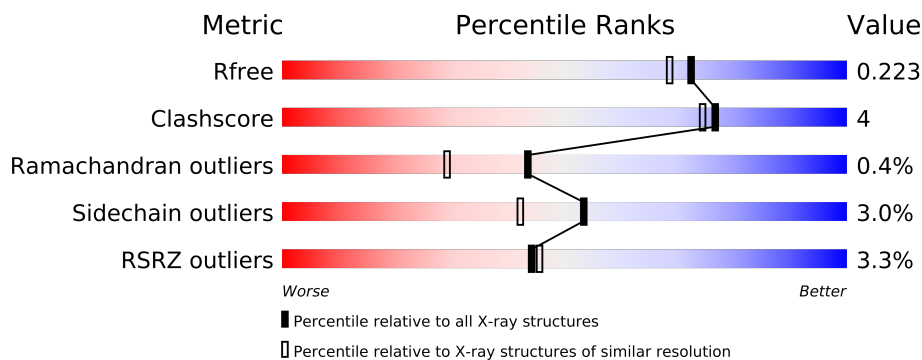
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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  $\geq 3$ , 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	421	
1	D	421	
2	B	10	
2	E	10	
3	C	10	
3	F	10	

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	BA2	D	1416	-	X
5	GOL	A	1416	-	X
6	K	D	1415	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7895 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 MODIFICATION METHYLASE TAQI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	1
			3168	2074	544	544	6			
1	D	392	Total	C	N	O	S	0	0	1
			3174	2077	547	544	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ALA	GLY	CONFLICT	UNP P14385
D	64	ALA	GLY	CONFLICT	UNP P14385

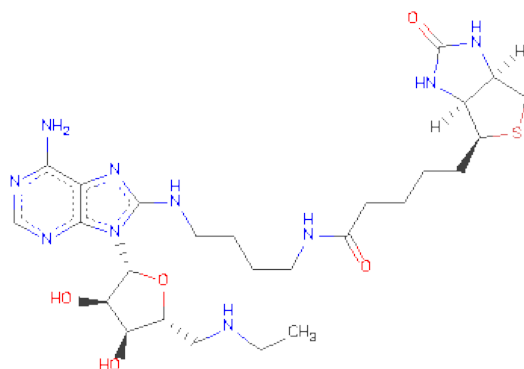
- Molecule 2 is a DNA chain called 5'-D(\*GP\*TP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			202	98	34	61	9			
2	E	10	Total	C	N	O	P	0	0	0
			202	98	34	61	9			

- Molecule 3 is a DNA chain called 5'-D(\*GP\*AP\*CP\*AP\*TP\*CP\*GP\*6MAP\*AP\*CP)-3'.

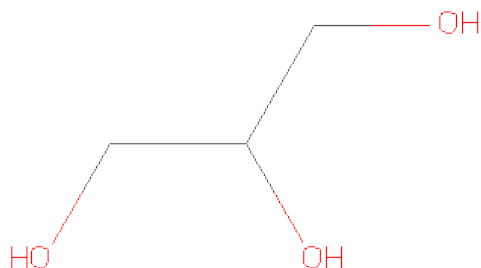
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	P	0	0	0
			203	98	41	55	9			
3	F	10	Total	C	N	O	P	0	0	0
			203	98	41	55	9			

- Molecule 4 is 5'-DEOXY-5'-(ETHYLAMINO)-8-{[4-({5-[(3AS,4S,6AR)-2-OXOHEXAHYDRO-1H-THIENO[3,4-D]IMIDAZOL-4-YL]PENTANOYL}AMINO)BUTYL]AMINO}ADENOSINE (three-letter code: BA2) (formula: C<sub>26</sub>H<sub>42</sub>N<sub>10</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	13	7	3		
4	D	1	Total	C	N	O	0	0
			26	16	7	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is water.

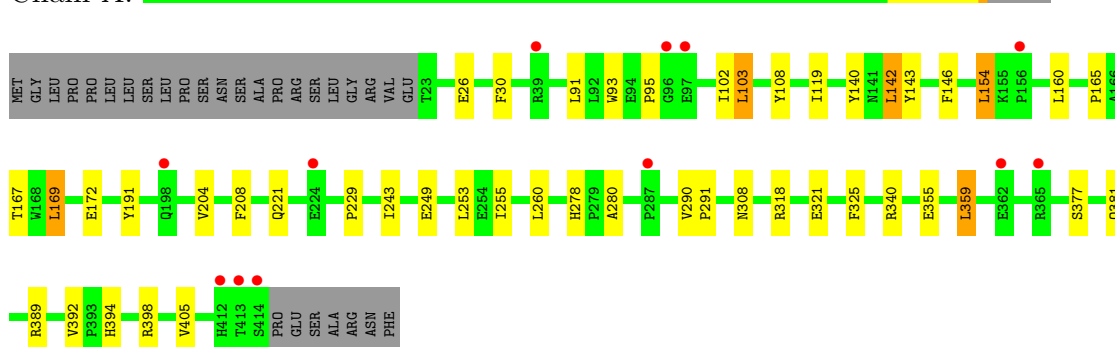
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	287	Total O 287 287	0	0
7	B	48	Total O 48 48	0	0
7	C	28	Total O 28 28	0	0
7	D	259	Total O 259 259	0	0
7	E	30	Total O 30 30	0	0
7	F	28	Total O 28 28	0	0

### 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 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.

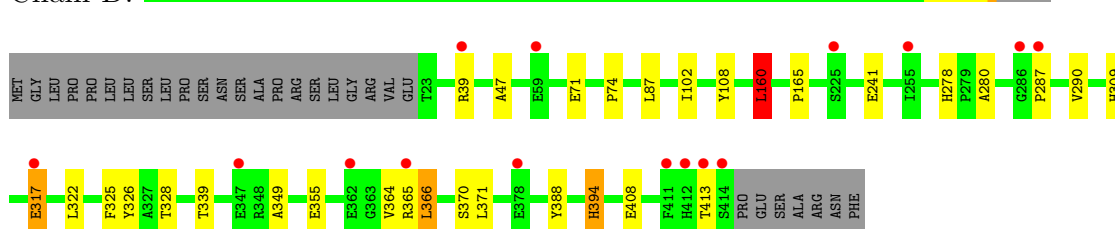
#### • Molecule 1: MODIFICATION METHYLASE TAQI

Chain A:



#### • Molecule 1: MODIFICATION METHYLASE TAQI

Chain D:



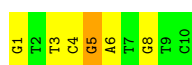
#### • Molecule 2: 5'-D(\*GP\*TP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*CP)-3'

Chain B:



#### • Molecule 2: 5'-D(\*GP\*TP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*CP)-3'

Chain E:



#### • Molecule 3: 5'-D(\*GP\*AP\*CP\*AP\*TP\*CP\*GP\*6MAP\*AP\*CP)-3'

Chain C:



- Molecule 3: 5'-D(\*GP\*AP\*CP\*AP\*TP\*CP\*GP\*6MAP\*AP\*CP)-3'

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.40Å 69.19Å 114.39Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	19.73 – 1.90 19.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.73-1.90) 99.5 (19.73-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.226 0.184 , 0.223	Depositor DCC
$R_{free}$ test set	3639 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 27.8	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 72768 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: GOL, K, BA2, 6MA

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	0.60	0/3272	0.69	2/4448 (0.0%)
1	D	0.61	1/3278 (0.0%)	0.72	2/4455 (0.0%)
2	B	1.10	0/225	2.04	10/346 (2.9%)
2	E	1.08	0/225	1.91	8/346 (2.3%)
3	C	1.01	0/202	1.77	5/307 (1.6%)
3	F	1.08	0/202	1.93	8/307 (2.6%)
All	All	0.68	1/7404 (0.0%)	0.95	35/10209 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	370	SER	C-N	-7.24	1.17	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	PRO	CB-CA-C	-11.89	82.27	112.00
2	E	8	DG	O4'-C1'-N9	-11.62	99.86	108.00
2	B	5	DG	O4'-C1'-N9	9.88	114.91	108.00
3	F	20	DC	O4'-C1'-N1	9.88	114.91	108.00
1	D	160	LEU	CA-CB-CG	8.76	135.45	115.30
2	B	2	DT	P-O3'-C3'	8.57	129.98	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	DG	O4'-C1'-N9	-8.48	102.06	108.00
3	F	19	DA	O4'-C1'-N9	8.29	113.80	108.00
3	F	12	DA	O4'-C1'-N9	-8.07	102.35	108.00
3	C	12	DA	O4'-C1'-N9	-7.44	102.79	108.00
2	E	3	DT	O4'-C1'-N1	-7.33	102.87	108.00
2	B	2	DT	C6-C5-C7	-7.09	118.65	122.90
2	E	4	DC	O4'-C1'-N1	-7.04	103.07	108.00
3	C	20	DC	O4'-C1'-N1	6.88	112.81	108.00
2	B	9	DT	P-O3'-C3'	6.67	127.71	119.70
2	B	2	DT	N3-C4-O4	6.38	123.73	119.90
3	F	15	DT	N3-C4-O4	6.36	123.71	119.90
2	B	9	DT	C1'-O4'-C4'	-6.22	103.88	110.10
3	C	13	DC	C1'-O4'-C4'	-6.11	103.99	110.10
1	A	169	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	103	LEU	CA-CB-CG	5.87	128.81	115.30
3	F	11	DG	P-O3'-C3'	5.87	126.74	119.70
3	F	15	DT	C5-C4-O4	-5.64	120.95	124.90
2	E	1	DG	P-O3'-C3'	5.63	126.45	119.70
2	B	4	DC	P-O3'-C3'	5.62	126.44	119.70
3	C	15	DT	C5-C4-O4	-5.61	120.97	124.90
3	C	15	DT	N3-C4-O4	5.53	123.22	119.90
2	E	5	DG	C5-C6-O6	-5.53	125.28	128.60
2	B	3	DT	O4'-C1'-N1	-5.45	104.19	108.00
2	E	3	DT	C4'-C3'-C2'	5.42	107.98	103.10
2	B	2	DT	C4-C5-C7	5.36	122.22	119.00
3	F	16	DC	C6-N1-C2	-5.19	118.23	120.30
2	E	5	DG	C5-C6-N1	5.12	114.06	111.50
3	F	13	DC	C1'-O4'-C4'	-5.11	104.99	110.10
2	E	3	DT	N1-C1'-C2'	5.05	122.20	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	394	HIS	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	3168	0	3158	25	0
1	D	3174	0	3168	15	0
2	B	202	0	116	10	0
2	E	202	0	116	5	0
3	C	203	0	114	1	0
3	F	203	0	114	1	0
4	A	23	0	18	8	0
4	D	26	0	24	6	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	287	0	0	3	0
7	B	48	0	0	0	0
7	C	28	0	0	0	0
7	D	259	0	0	2	0
7	E	30	0	0	0	0
7	F	28	0	0	0	0
All	All	7895	0	6844	54	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 4.

All (54) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1415:BA2:C12	2:B:6:DA:H61	1.33	1.40
4:A:1415:BA2:H123	2:B:6:DA:N6	1.62	1.14
4:A:1415:BA2:H123	2:B:6:DA:H61	0.95	1.10
4:D:1416:BA2:H111	2:E:6:DA:H61	1.15	1.08
4:D:1416:BA2:H111	2:E:6:DA:N6	1.70	1.04
4:A:1415:BA2:C12	2:B:6:DA:N6	2.18	0.97
4:A:1415:BA2:H121	2:B:6:DA:H61	1.46	0.81
1:A:394:HIS:HE1	2:B:5:DG:N7	1.89	0.69
4:A:1415:BA2:C11	2:B:6:DA:H61	2.05	0.68
7:A:2153:HOH:O	1:D:317:GLU:HG2	1.96	0.66
1:A:160:LEU:HG	1:A:208:PHE:HB3	1.80	0.63
1:D:394:HIS:HE1	2:E:5:DG:N7	1.96	0.62
4:A:1415:BA2:C11	2:B:6:DA:N6	2.63	0.59
1:D:365:ARG:NH1	7:D:2226:HOH:O	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:1416:BA2:C11	2:E:6:DA:H61	2.04	0.59
1:D:339:THR:HG21	1:D:388:TYR:HB2	1.85	0.59
1:A:119:ILE:HG13	1:A:142:LEU:HD22	1.85	0.57
3:F:18:6MA:H2'	3:F:19:DA:O5'	2.03	0.57
1:A:169:LEU:HB3	1:A:243:ILE:HB	1.86	0.57
1:A:255:ILE:HD11	7:A:2073:HOH:O	2.03	0.57
3:C:18:6MA:H2'	3:C:19:DA:O5'	2.05	0.57
1:A:30:PHE:HE1	1:A:229:PRO:HG3	1.73	0.54
1:D:309:HIS:HE1	7:D:2194:HOH:O	1.91	0.52
1:A:278:HIS:CD2	1:A:280:ALA:H	2.28	0.51
4:A:1415:BA2:H111	2:B:6:DA:N6	2.27	0.50
1:A:249:GLU:HG2	7:A:2177:HOH:O	2.10	0.50
1:A:318:ARG:HD2	1:A:321:GLU:OE2	2.11	0.50
1:A:191:TYR:HA	1:A:204:VAL:HG12	1.95	0.48
1:A:260:LEU:HD13	1:A:405:VAL:HG21	1.95	0.48
1:A:26:GLU:CD	1:A:26:GLU:H	2.17	0.47
1:A:394:HIS:CE1	2:B:5:DG:N7	2.77	0.47
1:D:74:PRO:HA	1:D:87:LEU:HD21	1.96	0.47
1:D:47:ALA:HB1	4:D:1416:BA2:O4'	2.15	0.46
1:A:325:PHE:HB2	1:A:359:LEU:HD11	1.98	0.45
4:D:1416:BA2:C11	2:E:6:DA:N6	2.60	0.45
1:A:93:TRP:CZ2	1:A:95:PRO:HB3	2.52	0.45
1:A:278:HIS:HD2	1:A:280:ALA:H	1.64	0.44
1:A:167:THR:HG22	1:A:392:VAL:HG12	1.98	0.44
1:D:326:TYR:O	1:D:349:ALA:HB1	2.17	0.44
1:D:102:ILE:O	1:D:160:LEU:HA	2.16	0.44
1:A:377:SER:O	1:A:381:GLN:HG2	2.18	0.44
1:D:278:HIS:HD2	1:D:280:ALA:H	1.65	0.43
1:D:364:VAL:HG12	1:D:366:LEU:HD13	2.00	0.42
1:D:278:HIS:CD2	1:D:280:ALA:H	2.37	0.42
1:A:102:ILE:O	1:A:160:LEU:HA	2.20	0.42
1:A:291:PRO:HB3	1:A:308:ASN:HD22	1.84	0.42
1:A:108:TYR:CE1	1:A:165:PRO:HD3	2.55	0.41
1:D:71:GLU:OE2	4:D:1416:BA2:O2'	2.33	0.41
1:A:91:LEU:HD21	1:A:146:PHE:CD1	2.55	0.41
1:A:102:ILE:HD12	1:A:154:LEU:HD13	2.02	0.41
1:A:172:GLU:OE2	1:A:398:ARG:NE	2.51	0.41
1:D:325:PHE:O	1:D:328:THR:HG22	2.21	0.41
1:D:108:TYR:CE1	1:D:165:PRO:HD3	2.55	0.40
1:A:30:PHE:CE1	1:A:229:PRO:HG3	2.54	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	390/421 (93%)	378 (97%)	10 (3%)	2 (0%)	38	23
1	D	390/421 (93%)	377 (97%)	12 (3%)	1 (0%)	50	37
All	All	780/842 (93%)	755 (97%)	22 (3%)	3 (0%)	43	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	355	GLU
1	A	389	ARG
1	A	355	GLU

### 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	329/356 (92%)	319 (97%)	10 (3%)	53	42
1	D	330/356 (93%)	320 (97%)	10 (3%)	53	42
All	All	659/712 (93%)	639 (97%)	20 (3%)	53	42

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	140	TYR
1	A	142	LEU
1	A	143	TYR
1	A	154	LEU
1	A	221	GLN

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Mol	Chain	Res	Type
1	A	253	LEU
1	A	290	VAL
1	A	340	ARG
1	A	359	LEU
1	D	39	ARG
1	D	160	LEU
1	D	241	GLU
1	D	290	VAL
1	D	317	GLU
1	D	322	LEU
1	D	366	LEU
1	D	371	LEU
1	D	408	GLU
1	D	413	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	278	HIS
1	A	394	HIS
1	D	278	HIS
1	D	309	HIS
1	D	394	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	6MA	C	18	3,2	22,24,25	0.93	1 (4%)	31,34,37	2.17	9 (29%)
3	6MA	F	18	3,2	22,24,25	0.77	0	31,34,37	2.21	11 (35%)

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
3	6MA	C	18	3,2	-	0/8/23/24	0/1/3/3
3	6MA	F	18	3,2	-	0/8/23/24	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	18	6MA	O4'-C4'	-2.24	1.39	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	18	6MA	C2-N1-C6	6.94	121.05	116.69
3	F	18	6MA	C2-N1-C6	5.79	120.33	116.69
3	F	18	6MA	C1-N6-C6	5.29	127.49	122.85
3	F	18	6MA	C5-C6-N6	3.95	127.11	120.44
3	C	18	6MA	C8-N9-C1'	3.52	132.78	126.15
3	F	18	6MA	O4'-C4'-C3'	3.34	114.12	105.66
3	C	18	6MA	O4'-C4'-C3'	3.20	113.78	105.66
3	C	18	6MA	C5-C6-N6	3.20	125.85	120.44
3	F	18	6MA	C8-N9-C1'	3.18	132.15	126.15
3	C	18	6MA	O3'-C3'-C2'	-2.92	99.77	110.78
3	C	18	6MA	C1'-N9-C4	-2.79	120.06	126.84
3	C	18	6MA	O4'-C1'-C2'	2.66	111.49	106.25
3	F	18	6MA	O4'-C1'-C2'	2.65	111.47	106.25
3	F	18	6MA	N6-C6-N1	-2.65	115.36	118.61
3	C	18	6MA	C1-N6-C6	2.39	124.95	122.85
3	F	18	6MA	O3'-C3'-C2'	-2.25	102.29	110.78
3	C	18	6MA	C5'-C4'-C3'	2.18	128.41	114.76
3	F	18	6MA	C1'-N9-C4	-2.15	121.60	126.84
3	F	18	6MA	O4'-C4'-C5'	2.13	116.95	109.36
3	F	18	6MA	C4'-O4'-C1'	-2.00	104.37	109.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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
4	BA2	A	1415	6	24,25,46	3.90	9 (37%)	34,36,64	4.12	17 (50%)
5	GOL	A	1416	-	5,5,5	0.48	0	5,5,5	0.65	0
5	GOL	B	1012	-	5,5,5	0.31	0	5,5,5	0.82	0
4	BA2	D	1416	6	28,28,46	3.83	11 (39%)	38,39,64	4.48	17 (44%)

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	BA2	A	1415	6	-	0/9/26/61	0/1/3/5
5	GOL	A	1416	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1012	-	-	0/4/4/4	0/0/0/0
4	BA2	D	1416	6	-	0/13/29/61	0/1/3/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1415	BA2	C8-N9	11.12	1.46	1.35
4	D	1416	BA2	C8-N9	10.35	1.45	1.35
4	A	1415	BA2	C8-N7	7.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1416	BA2	C2-N3	7.19	1.46	1.32
4	D	1416	BA2	C2-N1	6.88	1.47	1.33
4	A	1415	BA2	C2-N3	6.80	1.45	1.32
4	D	1416	BA2	C4-N3	6.77	1.46	1.35
4	A	1415	BA2	C2-N1	6.15	1.46	1.33
4	D	1416	BA2	C8-N7	6.12	1.44	1.34
4	D	1416	BA2	C8-N13	6.10	1.44	1.33
4	A	1415	BA2	C4-N3	5.48	1.44	1.35
4	A	1415	BA2	C8-N13	5.00	1.45	1.35
4	D	1416	BA2	C4-N9	4.96	1.45	1.37
4	D	1416	BA2	C5-C4	4.49	1.50	1.40
4	D	1416	BA2	C17-C16	-4.02	1.53	1.55
4	A	1415	BA2	C5-C4	3.90	1.49	1.40
4	A	1415	BA2	C4-N9	3.63	1.43	1.37
4	A	1415	BA2	C6-N6	2.72	1.43	1.35
4	D	1416	BA2	C6-N6	2.65	1.43	1.35
4	D	1416	BA2	C6-N1	2.25	1.47	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1416	BA2	N3-C2-N1	-14.75	116.38	128.71
4	A	1415	BA2	N3-C2-N1	-14.38	116.69	128.71
4	D	1416	BA2	O4'-C1'-N9	13.07	125.12	108.34
4	D	1416	BA2	N7-C8-N9	-12.47	104.57	111.55
4	A	1415	BA2	O4'-C1'-N9	10.36	121.65	108.34
4	A	1415	BA2	N7-C8-N9	-8.22	106.95	111.55
4	D	1416	BA2	C2-N1-C6	6.18	129.94	118.77
4	A	1415	BA2	O4'-C4'-C5'	6.04	116.97	108.56
4	D	1416	BA2	O4'-C4'-C5'	5.80	116.64	108.56
4	A	1415	BA2	C1'-N9-C4	-5.40	117.26	126.71
4	D	1416	BA2	C8-N7-C5	4.90	111.23	106.71
4	A	1415	BA2	C2-N1-C6	4.60	127.08	118.77
4	A	1415	BA2	N3-C4-N9	4.55	133.53	126.68
4	D	1416	BA2	C5'-C4'-C3'	-4.22	108.98	116.76
4	D	1416	BA2	C4-C5-N7	-3.80	106.49	109.58
4	A	1415	BA2	C5'-C4'-C3'	-3.76	109.84	116.76
4	D	1416	BA2	N3-C4-N9	2.98	131.16	126.68
4	D	1416	BA2	C1'-N9-C4	-2.98	121.50	126.71
4	D	1416	BA2	O2'-C2'-C1'	2.90	120.00	111.23
4	A	1415	BA2	O4'-C1'-C2'	2.87	111.17	106.77
4	D	1416	BA2	C5-C6-N1	-2.53	110.78	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1415	BA2	C5-C6-N6	-2.51	115.04	120.72
4	A	1415	BA2	C2-N3-C4	2.32	120.61	114.01
4	D	1416	BA2	N13-C8-N9	2.31	125.43	122.24
4	A	1415	BA2	C5-C4-N3	-2.29	120.72	125.70
4	A	1415	BA2	O3'-C3'-C4'	-2.20	104.59	111.08
4	D	1416	BA2	C2'-C1'-N9	-2.16	112.69	115.76
4	D	1416	BA2	C3'-C2'-C1'	2.14	104.26	100.91
4	A	1415	BA2	O4'-C4'-C3'	2.11	109.45	105.17
4	A	1415	BA2	C5-C4-N9	-2.11	104.33	106.67
4	D	1416	BA2	O4'-C4'-C3'	2.09	109.41	105.17
4	A	1415	BA2	C2'-C3'-C4'	2.09	106.81	102.65
4	A	1415	BA2	C5-C6-N1	-2.06	112.35	119.27
4	D	1416	BA2	O3'-C3'-C2'	-2.06	105.14	111.83

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, 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	392/421 (93%)	0.18	12 (3%) 47 48	4, 10, 22, 36	0
1	D	392/421 (93%)	0.30	15 (3%) 38 40	5, 11, 21, 36	0
2	B	10/10 (100%)	-0.50	0 100 100	4, 6, 10, 11	0
2	E	10/10 (100%)	-0.43	0 100 100	5, 8, 10, 11	0
3	C	10/10 (100%)	-0.47	0 100 100	4, 6, 7, 13	0
3	F	10/10 (100%)	-0.24	0 100 100	7, 9, 14, 19	0
All	All	824/882 (93%)	0.21	27 (3%) 44 45	4, 10, 21, 36	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	413	THR	4.9
1	D	414	SER	4.8
1	D	287	PRO	4.1
1	A	287	PRO	3.4
1	A	198	GLN	3.3
1	A	96	GLY	3.0
1	D	286	GLY	3.0
1	A	362	GLU	2.9
1	A	224	GLU	2.8
1	D	255	ILE	2.8
1	A	412	HIS	2.7
1	A	413	THR	2.7
1	D	365	ARG	2.7
1	A	365	ARG	2.6
1	D	362	GLU	2.5
1	A	97	GLU	2.5
1	D	412	HIS	2.5
1	D	378	GLU	2.4
1	A	39	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	225	SER	2.3
1	A	414	SER	2.3
1	A	156	PRO	2.2
1	D	317	GLU	2.1
1	D	347	GLU	2.1
1	D	39	ARG	2.1
1	D	59	GLU	2.1
1	D	411	PHE	2.1

## 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. 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	6MA	F	18	22/23	0.10	-0.48	3,8,10,13	0
3	6MA	C	18	22/23	0.09	-0.71	2,3,6,7	0

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	K	D	1415	1/1	0.14	20.83	22,22,22,22	0
5	GOL	A	1416	6/6	0.28	3.02	28,31,32,33	0
4	BA2	D	1416	26/42	0.15	2.92	5,10,22,24	0
5	GOL	B	1012	6/6	0.14	1.36	22,22,23,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BA2	A	1415	23/42	0.13	1.23	4,8,15,19	0
6	K	B	1011	1/1	0.09	0.83	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.