



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:58 pm BST

PDB ID : 6CQI  
Title : 2.42Å Crystal structure of Mycobacterium tuberculosis Topoisomerase I in complex with an oligonucleotide MTS2-11  
Authors : Cao, N.; Thirunavukkarasu, A.; Tan, K.; Tse-Dinh, Y.-C.  
Deposited on : 2018-03-15  
Resolution : 2.42 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

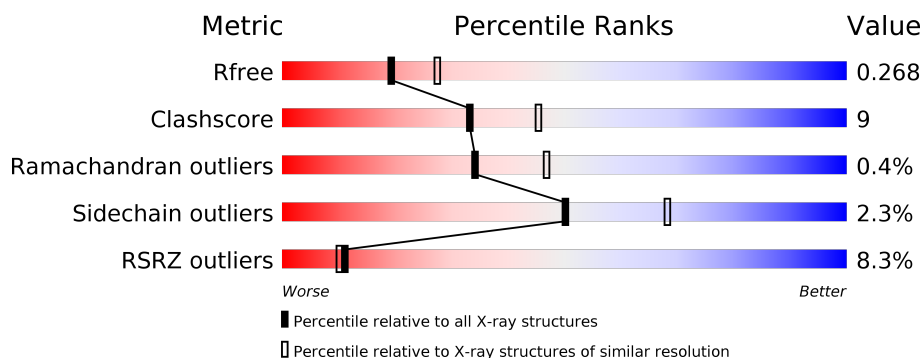
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	706	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>
2	B	11	<div> <div>64%</div> <div>27%</div> <div>9%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5279 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 DNA topoisomerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	0	0
			5035	3171	898	959	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P9WG49
A	0	ASN	-	expression tag	UNP P9WG49
A	1	ALA	-	expression tag	UNP P9WG49

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			202	97	32	63	10			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

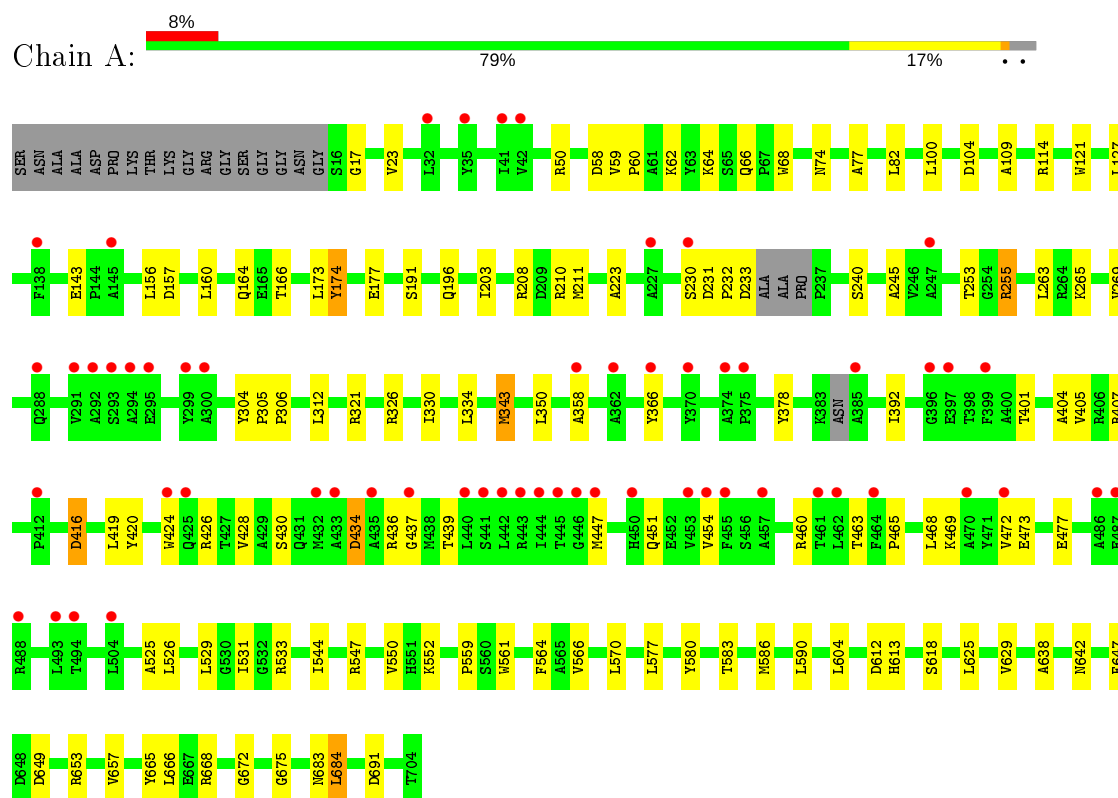
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total	O	0	0
			15	15		
6	B	3	Total	O	0	0
			3	3		

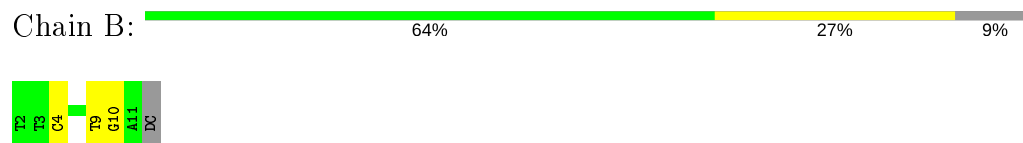
### 3 Residue-property plots [i](#)

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: DNA topoisomerase 1



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.78 Å 44.98 Å 129.23 Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	47.00 – 2.42 47.34 – 2.42	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.00-2.42) 96.5 (47.34-2.42)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.42 Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.224 , 0.269 0.223 , 0.268	Depositor DCC
$R_{free}$ test set	1488 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 62.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, ACT

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	0.27	0/5135	0.49	3/7001 (0.0%)
2	B	0.62	0/224	1.06	0/343
All	All	0.30	0/5359	0.53	3/7344 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	LEU	CB-CG-CD2	-8.18	97.10	111.00
1	A	612	ASP	CB-CG-OD2	7.43	124.99	118.30
1	A	612	ASP	CB-CG-OD1	-5.64	113.22	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5035	0	4730	86	0
2	B	202	0	115	2	0
3	A	6	0	2	1	0
4	A	6	0	8	1	0
5	A	12	0	9	2	0
6	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	3	0	0	0	0
All	All	5279	0	4864	87	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 9.

All (87) 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:A:649:ASP:CB	1:A:668:ARG:NH1	2.04	1.19
1:A:649:ASP:CB	1:A:668:ARG:HH11	1.58	1.16
1:A:649:ASP:HB3	1:A:668:ARG:NH1	1.64	1.13
1:A:649:ASP:CG	1:A:668:ARG:HH11	1.54	1.10
1:A:649:ASP:OD2	1:A:668:ARG:NH1	1.90	1.03
1:A:526:LEU:HD22	1:A:531:ILE:HD11	1.52	0.90
1:A:665:TYR:HA	1:A:683:ASN:HA	1.60	0.83
1:A:649:ASP:HB3	1:A:668:ARG:HH11	1.31	0.81
1:A:231:ASP:O	1:A:233:ASP:N	2.14	0.80
1:A:649:ASP:CB	1:A:668:ARG:HH12	1.98	0.76
1:A:434:ASP:N	1:A:434:ASP:OD1	2.24	0.71
1:A:366:TYR:HD2	1:A:469:LYS:HD3	1.56	0.70
1:A:649:ASP:CG	1:A:668:ARG:NH1	2.27	0.69
1:A:378:TYR:OH	1:A:430:SER:O	2.07	0.69
1:A:321:ARG:NH2	1:A:477:GLU:OE2	2.28	0.67
1:A:306:PRO:HD3	1:A:378:TYR:CD2	2.30	0.66
1:A:649:ASP:HB2	1:A:668:ARG:NH1	2.09	0.64
1:A:306:PRO:HD3	1:A:378:TYR:HD2	1.64	0.63
1:A:437:GLY:HA2	1:A:463:THR:H	1.64	0.63
1:A:525:ALA:O	1:A:529:LEU:HD12	2.02	0.59
1:A:533:ARG:HH11	1:A:533:ARG:HG2	1.68	0.59
1:A:531:ILE:HG22	1:A:583:THR:HB	1.85	0.58
1:A:468:LEU:HD12	1:A:472:VAL:HG22	1.84	0.58
1:A:436:ARG:O	1:A:463:THR:OG1	2.16	0.58
1:A:649:ASP:OD2	1:A:668:ARG:CZ	2.51	0.58
1:A:62:LYS:NZ	6:A:901:HOH:O	2.37	0.56
1:A:649:ASP:HB2	1:A:668:ARG:HH12	1.66	0.56
1:A:638:ALA:O	1:A:642:ASN:ND2	2.36	0.56
1:A:401:THR:HG23	1:A:404:ALA:H	1.72	0.55
1:A:210:ARG:NH2	1:A:691:ASP:OD2	2.41	0.54
1:A:378:TYR:HE2	1:A:430:SER:HB2	1.71	0.54
1:A:263:LEU:HD21	1:A:269:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:NE2	3:A:802:FMT:O1	2.36	0.53
1:A:245:ALA:HB3	1:A:454:VAL:HB	1.91	0.53
1:A:306:PRO:HG2	1:A:350:LEU:HD11	1.91	0.52
1:A:343:MET:HA	1:A:392:ILE:HG12	1.92	0.52
1:A:424:TRP:O	1:A:428:VAL:HG12	2.10	0.52
1:A:437:GLY:HA2	1:A:463:THR:HG23	1.92	0.52
1:A:50:ARG:NH2	5:A:804:ACT:O	2.40	0.51
1:A:649:ASP:OD1	1:A:653:ARG:N	2.38	0.51
1:A:17:GLY:N	1:A:104:ASP:OD2	2.32	0.51
1:A:544:ILE:HD12	1:A:550:VAL:HG21	1.93	0.51
1:A:405:VAL:HG21	1:A:420:TYR:CE1	2.46	0.51
1:A:625:LEU:O	1:A:629:VAL:HG23	2.11	0.51
1:A:174:TYR:CZ	1:A:577:LEU:HB3	2.45	0.50
1:A:529:LEU:CD2	1:A:580:TYR:HB3	2.42	0.50
1:A:366:TYR:CD2	1:A:469:LYS:HD3	2.42	0.49
1:A:114:ARG:HG2	1:A:164:GLN:HB2	1.94	0.49
1:A:312:LEU:HD11	1:A:419:LEU:HD11	1.94	0.49
1:A:304:TYR:CE2	1:A:473:GLU:HG3	2.48	0.49
1:A:330:ILE:CG2	1:A:416:ASP:HA	2.43	0.48
1:A:358:ALA:HB1	1:A:428:VAL:HA	1.95	0.48
1:A:566:VAL:O	1:A:570:LEU:HD22	2.13	0.48
1:A:334:LEU:HD21	1:A:416:ASP:HB3	1.96	0.48
1:A:439:THR:HA	1:A:460:ARG:HB2	1.95	0.48
1:A:552:LYS:NZ	5:A:806:ACT:OXT	2.48	0.46
1:A:672:GLY:N	1:A:675:GLY:O	2.49	0.46
1:A:173:LEU:O	1:A:177:GLU:HB2	2.16	0.45
1:A:166:THR:HG23	1:A:604:LEU:HG	1.99	0.45
1:A:59:VAL:O	1:A:64:LYS:NZ	2.50	0.45
1:A:66:GLN:HG2	1:A:68:TRP:CZ2	2.52	0.45
1:A:60:PRO:HD2	1:A:82:LEU:HD21	1.99	0.45
1:A:174:TYR:OH	1:A:577:LEU:HB3	2.17	0.45
1:A:561:TRP:CD2	1:A:657:VAL:HG11	2.52	0.45
1:A:253:THR:HB	1:A:255:ARG:NH1	2.32	0.44
1:A:305:PRO:O	1:A:426:ARG:NE	2.39	0.44
1:A:547:ARG:HH21	2:B:4:DC:P	2.40	0.44
1:A:666:LEU:HB2	1:A:684:LEU:HD11	2.00	0.44
1:A:618:SER:HB2	4:A:803:GOL:O3	2.18	0.44
1:A:561:TRP:O	1:A:564:PHE:HB2	2.19	0.43
1:A:531:ILE:HG22	1:A:583:THR:CB	2.50	0.42
2:B:9:DT:H2"	2:B:10:DG:C8	2.54	0.42
1:A:23:VAL:HG12	1:A:109:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:MET:O	1:A:590:LEU:HG	2.19	0.42
1:A:465:PRO:O	1:A:468:LEU:HB2	2.20	0.42
1:A:191:SER:OG	1:A:196:GLN:NE2	2.51	0.42
1:A:74:ASN:ND2	1:A:77:ALA:HB3	2.35	0.41
1:A:223:ALA:O	1:A:240:SER:HA	2.20	0.41
1:A:203:ILE:HG22	1:A:559:PRO:HB3	2.01	0.41
1:A:321:ARG:HH22	1:A:477:GLU:CD	2.23	0.41
1:A:665:TYR:HB3	1:A:683:ASN:HB3	2.02	0.41
1:A:157:ASP:HB3	1:A:160:LEU:HB2	2.02	0.41
1:A:100:LEU:HD22	1:A:127:LEU:HB3	2.01	0.41
1:A:306:PRO:CG	1:A:350:LEU:HD11	2.50	0.41
1:A:447:MET:HA	1:A:451:GLN:O	2.21	0.41
1:A:208:ARG:HA	1:A:211:MET:HE2	2.01	0.41
1:A:121:TRP:HB2	1:A:156:LEU:HD21	2.03	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	679/706 (96%)	641 (94%)	35 (5%)	3 (0%)	34	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	A	232	PRO
1	A	265	LYS

### 5.3.2 Protein sidechains [i](#)

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	470/574 (82%)	459 (98%)	11 (2%)	50 68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	143	GLU
1	A	174	TYR
1	A	255	ARG
1	A	326	ARG
1	A	343	MET
1	A	407	ARG
1	A	416	ASP
1	A	434	ASP
1	A	613	HIS
1	A	647	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	431	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6 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	$\# Z  > 2$
5	ACT	A	806	-	1,3,3	1.35	0	0,3,3	0.00	-
5	ACT	A	805	-	1,3,3	1.38	0	0,3,3	0.00	-
5	ACT	A	804	-	1,3,3	1.35	0	0,3,3	0.00	-
3	FMT	A	802	-	0,2,2	0.00	-	0,1,1	0.00	-
4	GOL	A	803	-	5,5,5	0.38	0	5,5,5	0.27	0
3	FMT	A	801	-	0,2,2	0.00	-	0,1,1	0.00	-

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	GOL	A	803	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	O1-C1-C2-C3
4	A	803	GOL	O1-C1-C2-O2
4	A	803	GOL	C1-C2-C3-O3
4	A	803	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	806	ACT	1	0
5	A	804	ACT	1	0
3	A	802	FMT	1	0
4	A	803	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	685/706 (97%)	0.34	58 (8%) 10 9	43, 87, 174, 241	0
2	B	10/11 (90%)	0.31	0 100 100	53, 72, 135, 207	0
All	All	695/717 (96%)	0.34	58 (8%) 11 10	43, 87, 175, 241	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	15.3
1	A	453	VAL	12.3
1	A	375	PRO	9.2
1	A	444	ILE	8.5
1	A	454	VAL	6.5
1	A	300	ALA	6.4
1	A	486	ALA	6.1
1	A	487	GLU	5.7
1	A	374	ALA	5.5
1	A	230	SER	5.3
1	A	294	ALA	5.1
1	A	446	GLY	4.9
1	A	288	GLN	4.8
1	A	397	GLU	4.6
1	A	412	PRO	4.6
1	A	440	LEU	4.4
1	A	293	SER	4.2
1	A	442	LEU	4.1
1	A	443	ARG	4.1
1	A	488	ARG	4.0
1	A	291	VAL	3.9
1	A	455	PHE	3.8
1	A	35	TYR	3.7
1	A	396	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	227	ALA	3.5
1	A	457	ALA	3.4
1	A	461	THR	3.4
1	A	358	ALA	3.4
1	A	41	ILE	3.3
1	A	385	ALA	3.2
1	A	433	ALA	3.1
1	A	435	ALA	3.1
1	A	32	LEU	3.0
1	A	424	TRP	2.9
1	A	445	THR	2.8
1	A	138	PHE	2.7
1	A	464	PHE	2.7
1	A	295	GLU	2.7
1	A	366	TYR	2.7
1	A	399	PHE	2.6
1	A	494	THR	2.6
1	A	432	MET	2.5
1	A	441	SER	2.5
1	A	450	HIS	2.5
1	A	292	ALA	2.5
1	A	447	MET	2.4
1	A	247	ALA	2.4
1	A	42	VAL	2.3
1	A	370	TYR	2.3
1	A	437	GLY	2.3
1	A	299	TYR	2.2
1	A	145	ALA	2.2
1	A	362	ALA	2.2
1	A	425	GLN	2.1
1	A	470	ALA	2.1
1	A	462	LEU	2.1
1	A	472	VAL	2.1
1	A	504	LEU	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 [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
4	GOL	A	803	6/6	0.55	0.37	99,110,111,111	0
5	ACT	A	804	4/4	0.68	0.36	106,113,116,116	0
3	FMT	A	801	3/3	0.88	0.18	96,96,98,99	0
5	ACT	A	806	4/4	0.89	0.15	93,99,102,103	0
5	ACT	A	805	4/4	0.91	0.12	87,91,93,95	0
3	FMT	A	802	3/3	0.96	0.20	101,101,102,102	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.