



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 03:04 PM EDT

PDB ID : 6PCM  
Title : Crystal Structure of Mycobacterium smegmatis Topoisomerase I with ssDNA bound to both N- and C-terminal domains  
Authors : Tan, K.; Cao, N.; Tse-Dinh, Y.C.  
Deposited on : 2019-06-17  
Resolution : 3.11 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

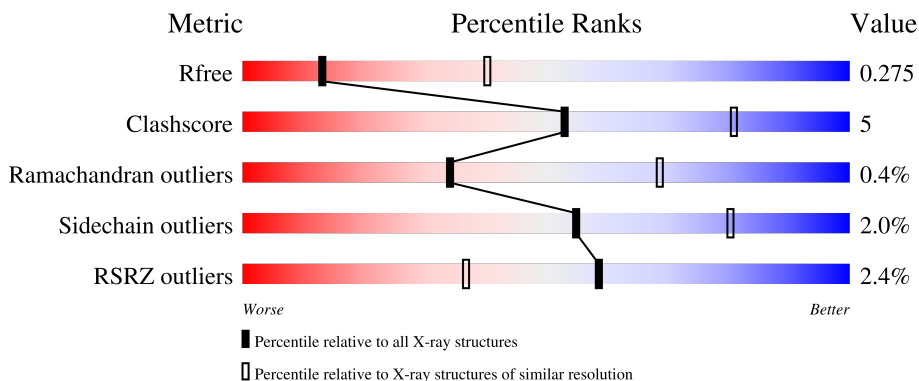
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of 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	842	 2% 80% 14% 6%
1	B	842	 2% 82% 11% 7%
2	C	25	 60% 36%
2	D	25	 56% 40%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	908	-	-	X	-
3	SO4	A	909	-	-	-	X
3	SO4	D	102	-	-	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 12445 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
			Total	C	N	O	S			
1	A	793	Total	C	N	O	S	0	0	0
			5753	3604	1014	1126	9			
1	B	783	Total	C	N	O	S	0	0	0
			5598	3510	994	1085	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0R5D9
A	-1	ASN	-	expression tag	UNP A0R5D9
A	0	ALA	-	expression tag	UNP A0R5D9
B	-2	SER	-	expression tag	UNP A0R5D9
B	-1	ASN	-	expression tag	UNP A0R5D9
B	0	ALA	-	expression tag	UNP A0R5D9

- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*AP\*G P\*CP\*TP\*TP\*CP\*CP\*GP\*CP\*TP\*TP\*GP\*AP\*CP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	24	Total	C	N	O	P	0	0	0
			492	234	87	147	24			
2	D	24	Total	C	N	O	P	0	0	0
			492	234	87	147	24			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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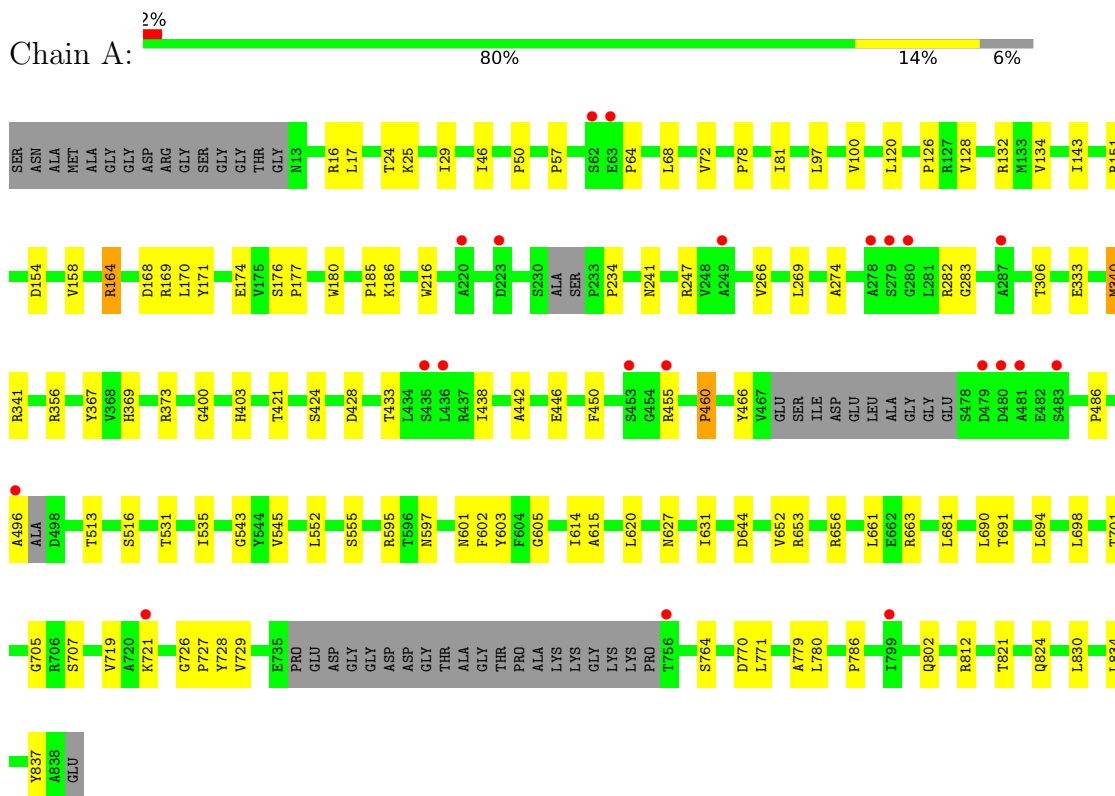
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

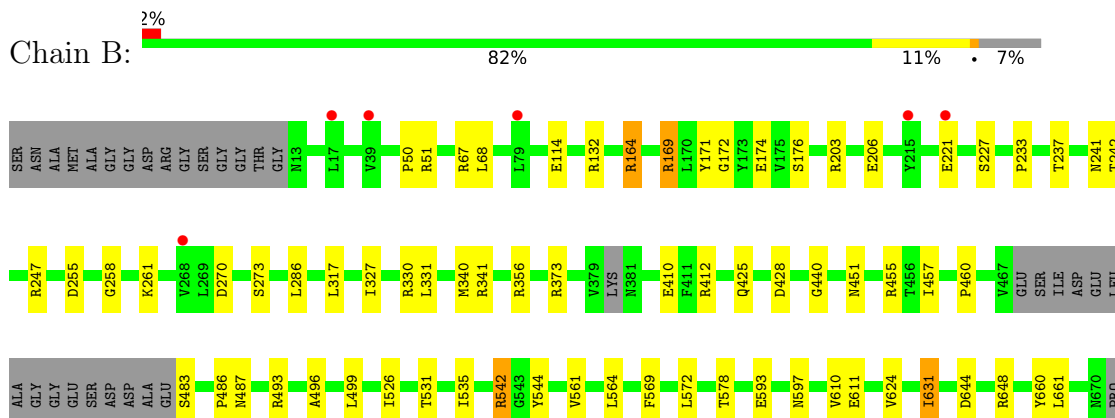
### 3 Residue-property plots [i](#)

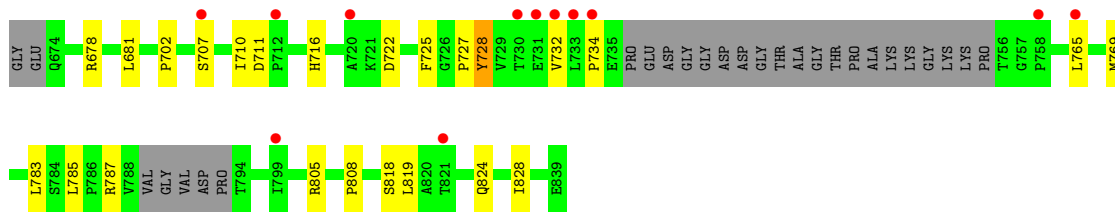
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1: DNA topoisomerase 1





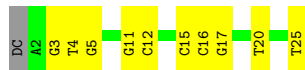
- Molecule 2: DNA (5'-D(P\*AP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*AP\*GP\*CP\*TP\*TP\*CP\*CP\*GP\*CP\*TP\*TP\*GP\*AP\*CP\*TP\*T)-3')

Chain C: 60% 36%



- Molecule 2: DNA (5'-D(P\*AP\*GP\*TP\*GP\*AP\*GP\*CP\*GP\*AP\*GP\*CP\*TP\*TP\*CP\*CP\*GP\*CP\*TP\*TP\*GP\*AP\*CP\*TP\*T)-3')

Chain D: 56% 40%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.32Å 135.07Å 145.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.44 – 3.11 47.44 – 3.11	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.44-3.11) 98.7 (47.44-3.11)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, $R_{free}$	0.225 , 0.275 0.225 , 0.275	Depositor DCC
$R_{free}$ test set	2282 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.8	Xtrriage
Anisotropy	0.534	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 111.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.026 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: SO4

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	0.23	0/5858	0.42	0/8001
1	B	0.24	0/5706	0.40	0/7802
2	C	0.45	0/550	0.89	0/847
2	D	0.46	0/550	0.91	0/847
All	All	0.26	0/12664	0.48	0/17497

There are no bond length outliers.

There are no bond angle outliers.

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	5753	0	5288	66	0
1	B	5598	0	5079	55	0
2	C	492	0	272	9	0
2	D	492	0	272	13	0
3	A	50	0	0	3	0
3	B	40	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
All	All	12445	0	10911	127	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 5.

All (127) 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)
2:C:16:DC:H2''	2:C:17:DG:H5''	1.64	0.79
1:B:255:ASP:HA	1:B:261:LYS:HE3	1.70	0.72
1:B:50:PRO:O	1:B:169:ARG:NH1	2.23	0.71
1:B:242:THR:HA	1:B:247:ARG:HA	1.72	0.71
1:A:729:VAL:HG11	1:A:779:ALA:HB1	1.74	0.68
1:A:50:PRO:O	1:A:169:ARG:NH2	2.26	0.68
1:B:174:GLU:HG3	1:B:624:VAL:HG11	1.77	0.66
1:A:356:ARG:NH1	1:A:369:HIS:O	2.29	0.66
1:B:765:LEU:HB3	1:B:769:MET:HB2	1.80	0.64
1:B:824:GLN:O	1:B:828:ILE:N	2.28	0.62
1:A:727:PRO:HB3	1:A:771:LEU:HD13	1.82	0.61
1:A:29:ILE:HD12	1:A:143:ILE:HG21	1.83	0.61
1:A:269:LEU:HB3	1:A:274:ALA:HB2	1.83	0.61
1:A:185:PRO:HG3	2:D:3:DG:H1'	1.83	0.61
1:A:653:ARG:NH2	3:A:908:SO4:O3	2.34	0.61
1:B:593:GLU:OE1	1:B:597:ASN:ND2	2.33	0.61
1:B:67:ARG:HG3	1:B:68:LEU:HD22	1.83	0.60
1:A:72:VAL:HG11	1:A:603:TYR:HD2	1.67	0.59
1:A:373:ARG:NH2	1:A:428:ASP:OD1	2.36	0.59
1:A:134:VAL:HG11	1:A:151:ARG:HH11	1.68	0.58
1:B:457:ILE:HD11	1:B:460:PRO:HA	1.85	0.58
1:A:373:ARG:NH1	3:A:901:SO4:O3	2.37	0.58
2:C:15:DC:H2'	2:C:16:DC:H5''	1.85	0.57
1:B:808:PRO:HG2	1:B:819:LEU:HB2	1.86	0.57
1:B:526:ILE:HA	1:B:578:THR:HG21	1.87	0.57
1:A:438:ILE:O	1:A:450:PHE:N	2.37	0.56
1:A:661:LEU:HD21	1:A:690:LEU:HD21	1.86	0.56
1:A:656:ARG:NH2	3:A:908:SO4:O1	2.37	0.55
1:B:169:ARG:NH2	2:D:15:DC:N3	2.54	0.55
1:B:114:GLU:OE1	1:B:132:ARG:NH1	2.32	0.55
1:A:367:TYR:HE2	1:A:460:PRO:HG2	1.72	0.55
1:B:164:ARG:NH1	2:D:16:DC:O2	2.31	0.55
1:B:496:ALA:HB1	1:B:499:LEU:HD11	1.89	0.55
1:A:597:ASN:O	1:A:601:ASN:ND2	2.39	0.54
1:A:726:GLY:H	2:D:25:DT:H3	1.54	0.54
1:B:172:GLY:O	1:B:176:SER:OG	2.24	0.54
1:B:542:ARG:NH1	2:D:15:DC:OP1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD21	1:A:126:PRO:HB3	1.90	0.54
1:A:17:LEU:HB2	1:A:100:VAL:HG21	1.90	0.54
1:A:513:THR:H	1:A:516:SER:HG	1.55	0.53
1:B:711:ASP:OD1	1:B:716:HIS:N	2.32	0.53
1:B:702:PRO:HG3	1:B:707:SER:HB3	1.91	0.53
1:B:564:LEU:HD11	1:B:631:ILE:HD11	1.91	0.52
1:B:644:ASP:OD1	1:B:648:ARG:N	2.42	0.52
1:A:186:LYS:HG2	2:C:13:DT:H1'	1.91	0.52
1:B:242:THR:HG22	1:B:247:ARG:HB3	1.91	0.52
1:A:46:ILE:HD13	1:A:120:LEU:HD23	1.91	0.52
1:B:660:TYR:OH	1:B:678:ARG:NH2	2.43	0.51
1:A:164:ARG:NH1	1:A:168:ASP:OD2	2.37	0.51
1:B:728:TYR:CZ	2:C:25:DT:H2'	2.46	0.51
1:A:72:VAL:HG11	1:A:603:TYR:CD2	2.46	0.51
1:A:78:PRO:HD3	1:A:595:ARG:HH22	1.75	0.51
1:A:707:SER:HA	1:A:719:VAL:HG12	1.93	0.51
1:B:722:ASP:N	1:B:722:ASP:OD1	2.43	0.51
1:B:661:LEU:HB2	1:B:681:LEU:HD21	1.93	0.51
1:A:68:LEU:HD21	1:A:174:GLU:HG2	1.92	0.50
1:B:221:GLU:HA	1:B:237:THR:HA	1.93	0.50
1:A:661:LEU:HG	1:A:681:LEU:HD21	1.92	0.50
1:A:821:THR:HB	1:A:824:GLN:HB3	1.93	0.50
1:A:247:ARG:H	1:A:266:VAL:HA	1.76	0.50
1:B:317:LEU:HD12	1:B:412:ARG:HD2	1.93	0.49
1:A:705:GLY:HA3	1:A:721:LYS:HG2	1.93	0.49
1:B:203:ARG:NH2	1:B:206:GLU:OE1	2.46	0.48
1:A:340:MET:SD	1:A:340:MET:N	2.82	0.48
1:A:442:ALA:N	1:A:446:GLU:O	2.46	0.48
1:B:544:TYR:HE1	1:B:561:VAL:HG21	1.78	0.48
1:A:543:GLY:O	1:A:555:SER:OG	2.23	0.48
1:B:569:PHE:HB3	1:B:572:LEU:HD12	1.96	0.48
1:B:805:ARG:NE	2:C:23:DC:OP2	2.46	0.48
1:A:25:LYS:O	1:A:29:ILE:HG12	2.14	0.48
1:A:605:GLY:HA2	1:A:615:ALA:HA	1.96	0.48
1:A:603:TYR:HD1	1:A:620:LEU:HB3	1.79	0.47
1:A:821:THR:O	1:A:824:GLN:HG2	2.14	0.47
1:A:283:GLY:HA2	1:A:496:ALA:HB3	1.96	0.47
1:B:227:SER:OG	1:B:493:ARG:O	2.33	0.47
1:B:341:ARG:NH1	2:D:20:DT:OP2	2.48	0.47
1:B:270:ASP:H	1:B:273:SER:HB2	1.79	0.46
1:A:545:VAL:HG21	1:A:552:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:PRO:HB2	1:B:486:PRO:HD3	1.97	0.46
1:B:327:ILE:HG12	1:B:330:ARG:HH21	1.81	0.46
1:B:610:VAL:HG12	1:B:611:GLU:H	1.81	0.46
2:C:12:DC:H2'	2:C:13:DT:C6	2.51	0.46
1:B:51:ARG:NH1	2:D:17:DG:O6	2.49	0.45
1:B:356:ARG:HG2	1:B:425:GLN:HB3	1.98	0.45
1:A:602:PHE:HE1	1:A:614:ILE:HD13	1.80	0.45
1:A:341:ARG:NH2	2:C:20:DT:OP2	2.49	0.45
1:B:725:PHE:H	2:C:25:DT:H3	1.64	0.45
1:A:400:GLY:O	1:A:403:HIS:ND1	2.50	0.45
1:A:644:ASP:OD2	1:A:663:ARG:NH2	2.49	0.45
1:A:614:ILE:HD12	1:A:614:ILE:H	1.82	0.45
1:B:51:ARG:HG2	2:D:15:DC:N4	2.32	0.45
1:B:51:ARG:HG2	2:D:15:DC:H41	1.82	0.45
1:B:331:LEU:HD21	1:B:410:GLU:HB3	1.99	0.45
2:D:4:DT:H2''	2:D:5:DG:O4'	2.17	0.45
1:B:727:PRO:HB2	1:B:765:LEU:HG	1.99	0.44
1:A:691:THR:HG23	1:A:694:LEU:H	1.83	0.44
1:A:306:THR:OG1	1:A:340:MET:O	2.27	0.44
1:A:602:PHE:CE1	1:A:614:ILE:HD13	2.53	0.43
1:B:818:SER:OG	2:C:21:DG:OP2	2.36	0.43
1:A:830:LEU:O	1:A:834:LEU:HG	2.19	0.43
1:B:373:ARG:NH2	1:B:428:ASP:OD1	2.26	0.43
1:B:542:ARG:HB3	1:B:544:TYR:CD2	2.54	0.43
1:A:176:SER:OG	1:A:177:PRO:HD3	2.18	0.42
1:A:531:THR:O	1:A:535:ILE:HG13	2.19	0.42
1:A:770:ASP:OD1	1:A:771:LEU:N	2.51	0.42
1:B:732:VAL:HG13	1:B:734:PRO:HD3	2.01	0.42
2:D:11:DG:H2''	2:D:12:DC:H5''	2.01	0.42
1:A:24:THR:HG21	1:A:333:GLU:HA	2.01	0.42
1:B:455:ARG:N	1:B:483:SER:O	2.33	0.42
1:A:57:PRO:HD3	1:A:81:ILE:HG21	2.00	0.42
1:A:421:THR:O	1:A:424:SER:OG	2.29	0.42
1:A:728:TYR:HB3	2:D:25:DT:C4	2.55	0.42
1:B:785:LEU:O	1:B:787:ARG:N	2.53	0.42
1:B:710:ILE:H	1:B:710:ILE:HG13	1.76	0.41
1:A:170:LEU:O	1:A:174:GLU:HB2	2.20	0.41
1:A:177:PRO:HA	1:A:180:TRP:CD2	2.55	0.41
1:B:286:LEU:HD22	1:B:440:GLY:HA3	2.02	0.41
1:B:531:THR:O	1:B:535:ILE:HG13	2.20	0.41
1:A:433:THR:HA	1:A:455:ARG:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:ARG:NH1	1:A:837:TYR:O	2.54	0.41
1:A:627:ASN:O	1:A:631:ILE:HG13	2.20	0.41
1:A:132:ARG:O	1:A:151:ARG:N	2.52	0.41
1:A:698:LEU:O	1:A:701:THR:OG1	2.34	0.41
1:B:241:ASN:ND2	1:B:451:ASN:OD1	2.54	0.41
1:A:154:ASP:O	1:A:158:VAL:HG23	2.21	0.40
1:A:652:VAL:HG22	1:A:661:LEU:HD23	2.03	0.40
2:D:16:DC:H2''	2:D:17:DG:H5''	2.02	0.40

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	783/842 (93%)	723 (92%)	55 (7%)	5 (1%)	25	59
1	B	771/842 (92%)	720 (93%)	50 (6%)	1 (0%)	51	83
All	All	1554/1684 (92%)	1443 (93%)	105 (7%)	6 (0%)	34	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	PRO
1	A	486	PRO
1	B	258	GLY
1	A	64	PRO
1	A	460	PRO
1	A	786	PRO

### 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	537/692 (78%)	525 (98%)	12 (2%)	52	78
1	B	510/692 (74%)	501 (98%)	9 (2%)	59	82
All	All	1047/1384 (76%)	1026 (98%)	21 (2%)	55	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	128	VAL
1	A	164	ARG
1	A	171	TYR
1	A	216	TRP
1	A	241	ASN
1	A	282	ARG
1	A	340	MET
1	A	466	TYR
1	A	764	SER
1	A	780	LEU
1	A	802	GLN
1	B	164	ARG
1	B	169	ARG
1	B	171	TYR
1	B	340	MET
1	B	487	ASN
1	B	542	ARG
1	B	631	ILE
1	B	728	TYR
1	B	783	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 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	$\# Z  > 2$
3	SO4	B	904	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	901	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	A	903	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	C	102	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	901	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	903	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	902	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	101	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	908	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	101	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	908	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	904	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	907	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	905	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	902	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	D	102	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	B	906	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	906	-	4,4,4	0.14	0	6,6,6	0.05	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	905	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	909	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	907	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	910	-	4,4,4	0.14	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	SO4	1	0
3	A	908	SO4	2	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	793/842 (94%)	0.05	21 (2%) 56 33	84, 132, 232, 311	0
1	B	783/842 (92%)	-0.05	18 (2%) 60 39	84, 141, 208, 259	0
2	C	24/25 (96%)	-0.11	0 100 100	101, 126, 182, 191	0
2	D	24/25 (96%)	-0.05	0 100 100	97, 136, 153, 161	0
All	All	1624/1734 (93%)	-0.00	39 (2%) 59 37	84, 136, 220, 311	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	SER	11.1
1	A	483	SER	10.9
1	A	481	ALA	8.9
1	A	480	ASP	6.5
1	A	249	ALA	5.8
1	A	756	THR	5.7
1	B	732	VAL	5.0
1	A	479	ASP	5.0
1	B	734	PRO	4.8
1	A	496	ALA	4.4
1	B	17	LEU	4.3
1	B	733	LEU	4.1
1	A	280	GLY	3.5
1	A	63	GLU	3.5
1	A	287	ALA	3.4
1	B	731	GLU	3.3
1	B	39	VAL	3.2
1	B	221	GLU	3.1
1	A	435	SER	3.1
1	A	279	SER	2.9
1	B	821	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	799	ILE	2.7
1	B	712	PRO	2.7
1	B	720	ALA	2.6
1	B	765	LEU	2.6
1	A	436	LEU	2.6
1	A	223	ASP	2.5
1	B	79	LEU	2.4
1	A	453	SER	2.4
1	B	730	THR	2.4
1	B	758	PRO	2.3
1	A	278	ALA	2.3
1	B	215	TYR	2.2
1	A	455	ARG	2.2
1	A	721	LYS	2.2
1	A	220	ALA	2.1
1	B	268	VAL	2.1
1	A	799	ILE	2.1
1	B	707	SER	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
3	SO4	B	902	5/5	0.72	0.14	185,189,193,200	0
3	SO4	A	909	5/5	0.75	0.42	219,224,226,227	0
3	SO4	B	907	5/5	0.77	0.27	221,225,229,234	0
3	SO4	A	907	5/5	0.80	0.31	170,171,174,175	5
3	SO4	D	102	5/5	0.80	0.49	142,149,153,156	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	901	5/5	0.83	0.13	182,182,189,189	5
3	SO4	A	908	5/5	0.83	0.30	239,240,241,242	0
3	SO4	A	910	5/5	0.84	0.11	217,219,220,221	5
3	SO4	B	903	5/5	0.84	0.17	170,177,182,190	5
3	SO4	B	906	5/5	0.85	0.26	171,177,180,187	5
3	SO4	A	905	5/5	0.85	0.24	150,154,165,167	5
3	SO4	C	101	5/5	0.85	0.47	165,168,174,174	0
3	SO4	D	101	5/5	0.85	0.39	201,207,211,215	0
3	SO4	B	904	5/5	0.85	0.12	187,191,194,197	0
3	SO4	A	903	5/5	0.86	0.40	185,189,196,201	0
3	SO4	A	906	5/5	0.88	0.23	195,199,202,205	0
3	SO4	A	904	5/5	0.89	0.09	186,189,191,193	5
3	SO4	C	102	5/5	0.90	0.29	129,137,141,142	5
3	SO4	B	901	5/5	0.91	0.46	215,216,221,222	0
3	SO4	A	902	5/5	0.91	0.36	127,139,142,143	5
3	SO4	B	908	5/5	0.95	0.21	175,177,182,182	5
3	SO4	B	905	5/5	0.96	0.20	193,194,196,196	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.