

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 20, 2023 - 07:15 AM EDT

PDB ID	:	2O54
Title	:	Structure of E. coli topoisomerase III in complex with an 8-base single stranded
		oligonucleotide. Frozen in glycerol at pH 7.0
Authors	:	Changela, A.; Digate, R.J.; Mondragon, A.
Deposited on	:	2006-12-05
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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
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 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Motric	Whole archive	Similar resolution		
Wiethic	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$		
$R_{free}$	130704	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	5231 (2.50-2.50)		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	С	8	12%	50%	25%	12%		
1	D	8	25%	62%		12%		
2	А	659	9%	83%		11% • •		
2	В	659	4%	84%		11% • •		



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10538 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	C	7	Total	С	Ν	Ο	Р	0	0	0
		1	138	67	26	39	6	0		0
1	П	0	Total	С	Ν	0	Р	0	0	0
1	I D	8	158	77	28	46	7	0	0	0

• Molecule 1 is a DNA chain called 5'-D(\*CP\*GP\*CP\*AP\*AP\*CP\*TP\*T)-3'.

• Molecule 2 is a protein called DNA topoisomerase 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	А	630	Total 5013	C 3165	N 912	O 916	S 20	0	0	0
2	В	631	Total 5016	C 3168	N 913	0 915	S 20	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	654	HIS	-	expression tag	UNP P14294
А	655	HIS	-	expression tag	UNP P14294
А	656	HIS	-	expression tag	UNP P14294
А	657	HIS	-	expression tag	UNP P14294
А	658	HIS	-	expression tag	UNP P14294
А	659	HIS	-	expression tag	UNP P14294
В	654	HIS	-	expression tag	UNP P14294
В	655	HIS	-	expression tag	UNP P14294
В	656	HIS	-	expression tag	UNP P14294
В	657	HIS	-	expression tag	UNP P14294
В	658	HIS	-	expression tag	UNP P14294
В	659	HIS	-	expression tag	UNP P14294

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Cl 2 2	0	0

• Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total O 1 1	0	0
5	D	10	Total         O           10         10	0	0
5	А	79	Total O 79 79	0	0
5	В	117	Total O 117 117	0	0



## 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.

- 12% Chain C: 50% 25% 12% 12% • Molecule 1: 5'-D(\*CP\*GP\*CP\*AP\*AP\*CP\*TP\*T)-3' Chain D: 25% 62% 12% C1 C2 C3 C3 A5 A5 C3 T7 T7 T8 • Molecule 2: DNA topoisomerase 3 Chain A: 83% 11% . • Molecule 2: DNA topoisomerase 3 Chain B: 84% 11%
- Molecule 1: 5'-D(\*CP\*GP\*CP\*AP\*AP\*CP\*TP\*T)-3'



# SER A187 PR0 PR0 A187 ALA A465 5194 ALA A465 5194 ALA A465 5194 ALA A465 5194 ALA A465 8208 ALA A469 R208 AG43 L474 R219 AG43 L474 R219 AG43 L474 R219 AG5 L497 R219 AG5 L497 R219 AG5 Coor B233 H65 Coor B234 H65 Coor B235 H65 Coor B236 H65 Coor B236 H65 Coor</



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	101.83Å 101.83Å 452.38Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$Resolution(\AA)$	29.10 - 2.50	Depositor
Resolution (A)	29.10 - 2.50	EDS
% Data completeness	97.7 (29.10-2.50)	Depositor
(in resolution range)	97.7 (29.10-2.50)	EDS
R <sub>merge</sub>	0.07	Depositor
$R_{sym}$	0.07	Depositor
$< I/\sigma(I) > 1$	$2.88 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D .	0.222 , $0.269$	Depositor
$\Lambda, \Lambda_{free}$	0.222 , $0.264$	DCC
$R_{free}$ test set	4104 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.2	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , $45.8$	EDS
L-test for $twinning^2$	$ < L >=0.41, < L^2>=0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10538	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: ACY, CL

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	С	1.10	0/154	1.99	5/235~(2.1%)	
1	D	1.07	0/176	1.84	7/269~(2.6%)	
2	А	0.48	0/5123	0.61	2/6945~(0.0%)	
2	В	0.53	0/5127	0.63	1/6952~(0.0%)	
All	All	0.54	0/10580	0.70	15/14401~(0.1%)	

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	1	DC	O4'-C1'-N1	9.54	114.68	108.00
1	С	5	DA	O4'-C1'-N9	8.85	114.19	108.00
1	D	5	DA	O4'-C1'-N9	8.57	114.00	108.00
1	D	8	DT	O4'-C4'-C3'	-6.87	101.75	104.50
1	D	2	DG	P-O3'-C3'	6.67	127.70	119.70
1	С	6	DC	P-O3'-C3'	6.64	127.67	119.70
1	С	7	DT	C6-C5-C7	-6.18	119.19	122.90
1	D	3	DC	P-O3'-C3'	6.14	127.07	119.70
1	С	4	DA	O4'-C1'-N9	-6.05	103.76	108.00
1	D	1	DC	P-O3'-C3'	-5.39	113.23	119.70
2	А	178	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	В	455	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	А	178	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	8	DT	C6-C5-C7	-5.17	119.80	122.90
1	D	1	DC	O4'-C1'-N1	5.15	111.60	108.00

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	С	138	0	80	2	0
1	D	158	0	92	2	0
2	А	5013	0	5014	49	0
2	В	5016	0	5020	39	0
3	А	2	0	0	0	0
4	В	4	0	3	0	0
5	А	79	0	0	2	0
5	В	117	0	0	0	0
5	С	1	0	0	0	0
5	D	10	0	0	0	0
All	All	10538	0	10209	88	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 4.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ( { m \AA} )$	overlap (Å)
2:A:396:THR:OG1	2:A:399:GLU:HG3	1.78	0.83
2:A:588:TYR:HB3	2:A:656:HIS:HE1	1.47	0.80
2:A:197:ARG:HD2	2:A:574:TRP:CZ3	2.17	0.79
2:A:588:TYR:HB3	2:A:656:HIS:CE1	2.23	0.74
2:A:169:ASP:OD2	2:A:197:ARG:HG2	1.89	0.72
2:A:520:ASP:HB3	2:A:525:GLU:OE2	1.89	0.72
2:B:525:GLU:OE2	2:B:525:GLU:HA	1.91	0.70
2:B:219:LYS:NZ	2:B:251:ASP:OD1	2.25	0.69
2:A:646:GLU:HB2	2:A:649:SER:HB3	1.77	0.67
2:A:187:ALA:HB2	2:A:611:VAL:HG13	1.76	0.66
2:B:87:VAL:HG22	2:B:90:ARG:HH21	1.61	0.66
2:B:259:ARG:NH1	2:B:263:GLU:OE2	2.30	0.65
2:B:92:LEU:HG	2:B:121:LEU:HD13	1.77	0.64
2:A:197:ARG:CD	2:A:574:TRP:CZ3	2.81	0.64
2:A:21:LYS:HG3	2:A:22:PRO:HA	1.81	0.62
2:A:126:ARG:HH12	2:A:152:ASN:HD22	1.50	0.59
2:A:515:ILE:HD13	2:A:576:SER:HB2	1.83	0.59



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:98:ILE:HB	2:B:129:VAL:HG22	1.86	0.58	
2:A:169:ASP:OD2	2:A:197:ARG:CG	2.51	0.58	
1:D:7:DT:H5"	2:B:8:LYS:HE2	1.86	0.58	
2:A:503:ILE:HG23	2:A:516:LEU:HD13	1.87	0.57	
2:A:577:VAL:O	2:A:581:ILE:HG13	2.04	0.57	
2:A:169:ASP:OD2	2:A:197:ARG:HD3	2.04	0.56	
2:B:106:ARG:HG3	2:B:162:ALA:HB2	1.87	0.56	
2:B:221:PHE:CD1	2:B:255:ARG:HB3	2.41	0.56	
2:B:150:ARG:HH11	2:B:150:ARG:HG2	1.70	0.55	
2:A:58:TYR:O	2:A:178:ARG:NH2	2.26	0.55	
2:B:427:LEU:HD21	2:B:473:LEU:HD12	1.89	0.55	
2:B:583:GLU:O	2:B:584:LYS:HB2	2.08	0.54	
2:B:72:LYS:NZ	2:B:649:SER:HB2	2.23	0.54	
2:A:1:MET:HG2	2:A:35:GLY:O	2.08	0.54	
2:B:7:GLU:HB2	2:B:102:GLY:HA2	1.90	0.54	
2:A:419:VAL:HB	2:A:443:GLU:HB2	1.89	0.53	
2:A:453:LYS:O	2:A:457:GLU:HG2	2.09	0.52	
1:C:6:DC:H3'	1:C:7:DT:H5'	1.90	0.52	
2:B:277:THR:O	2:B:469:LYS:HD2	2.10	0.52	
2:A:520:ASP:CB	2:A:525:GLU:OE2	2.58	0.52	
2:A:106:ARG:HB2	2:A:162:ALA:HB2	1.92	0.51	
2:B:177:THR:HG23	2:B:194:SER:HA	1.92	0.51	
2:B:455:ARG:HD2	2:B:456:ASP:OD2	2.11	0.51	
1:C:2:DG:N7	2:A:178:ARG:HD2	2.26	0.51	
2:B:100:HIS:CE1	2:B:112:VAL:HB	2.45	0.50	
2:A:361:GLN:HG2	2:A:449:LEU:HD21	1.94	0.50	
2:B:46:LEU:HD12	2:B:114:GLU:HG3	1.93	0.50	
2:B:574:TRP:CZ2	2:B:595:LEU:CD1	2.96	0.49	
2:A:83:LYS:O	2:A:87:VAL:HG23	2.13	0.48	
2:A:197:ARG:HD2	2:A:574:TRP:CE3	2.49	0.48	
2:B:187:ALA:HB2	2:B:611:VAL:HB	1.94	0.48	
2:B:88:ILE:O	2:B:92:LEU:HB2	2.13	0.48	
2:A:276:VAL:HG21	2:A:467:VAL:HG13	1.96	0.48	
2:A:615:ARG:O	2:A:617:ILE:HG13	2.15	0.47	
2:B:100:HIS:NE2	2:B:112:VAL:HB	2.29	0.47	
2:A:509:ASP:HB3	2:A:512:LEU:HB2	1.95	0.47	
2:B:208:ARG:NH2	2:B:566:THR:O	2.48	0.46	
2:B:507:VAL:CG2	2:B:568:PRO:HG2	2.45	0.46	
2:B:232:ALA:HB3	2:B:234:GLU:OE1	2.15	0.46	
1:D:8:DT:O3'	2:B:321:GLU:OE1	2.30	0.46	
2:A:240:TRP:O	2:A:242:PRO:HD3	2.16	0.45	

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Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
2:B:229:VAL:HG12	2:B:474:LEU:HB3	1.98	0.45
2:A:169:ASP:OD2	2:A:197:ARG:CD	2.65	0.45
2:A:277:THR:O	2:A:469:LYS:HE2	2.17	0.45
2:B:525:GLU:OE2	2:B:525:GLU:CA	2.62	0.45
2:A:98:ILE:HB	2:A:129:VAL:HG22	1.99	0.45
2:B:7:GLU:HG3	2:B:111:LEU:HD11	1.98	0.44
2:B:444:ALA:O	2:B:447:ARG:HB2	2.17	0.44
2:B:247:GLU:N	2:B:248:PRO:HD2	2.32	0.44
2:B:574:TRP:CZ2	2:B:595:LEU:HD11	2.53	0.44
2:A:133:LEU:HD11	2:A:155:PHE:CZ	2.52	0.44
2:A:197:ARG:HH21	2:A:571:THR:HG23	1.83	0.44
2:A:268:ARG:HD3	5:A:861:HOH:O	2.17	0.44
2:B:89:LYS:HD3	2:B:119:LEU:HD22	1.98	0.44
2:A:450:LEU:HB3	2:A:454:GLU:HG3	2.00	0.43
2:A:588:TYR:CB	2:A:656:HIS:HE1	2.24	0.43
2:A:584:LYS:NZ	5:A:811:HOH:O	2.52	0.43
2:A:1:MET:HE1	2:A:3:LEU:HB2	2.00	0.42
2:B:327:THR:O	2:B:328:TYR:C	2.57	0.42
2:A:151:SER:O	2:A:154:GLU:HG2	2.20	0.42
2:B:579:THR:O	2:B:583:GLU:HG2	2.20	0.42
2:A:133:LEU:HD11	2:A:155:PHE:HZ	1.85	0.41
2:A:202:VAL:O	2:A:203:LEU:C	2.58	0.41
2:A:117:ASP:HB3	2:A:648:GLY:HA2	2.00	0.41
2:A:69:VAL:HB	2:B:593:GLN:OE1	2.20	0.41
2:A:265:VAL:O	2:A:269:ILE:HG12	2.21	0.41
2:A:88:ILE:O	2:A:92:LEU:HB2	2.20	0.41
2:B:6:ALA:HA	2:B:101:ALA:O	2.20	0.41
2:B:422:LYS:HA	2:B:438:ALA:O	2.21	0.41
2:A:276:VAL:HG21	2:A:467:VAL:CG1	2.52	0.40
2:A:428:ASP:HA	2:A:432:GLY:O	2.20	0.40

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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.



Mol	Chain	Analysed	Analysed Favoured Allowed		Outliers	Percentiles
2	А	626/659~(95%)	591~(94%)	28~(4%)	7(1%)	14 26
2	В	627/659~(95%)	608~(97%)	19(3%)	0	100 100
All	All	1253/1318~(95%)	1199 (96%)	47 (4%)	7 (1%)	25 43

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

All (7) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
2	А	455	ARG
2	А	615	ARG
2	А	616	GLY
2	А	463	PRO
2	А	525	GLU
2	А	453	LYS
2	А	647	VAL

#### 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		
2	А	535/555~(96%)	520~(97%)	15 (3%)	43	70	
2	В	535/555~(96%)	518~(97%)	17 (3%)	39	65	
All	All	1070/1110~(96%)	1038~(97%)	32 (3%)	41	68	

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	А	1	MET
2	А	126	ARG
2	А	140	GLN
2	А	153	SER
2	А	158	LEU
2	А	251	ASP



Mol	Chain	Res	Type
2	А	280	ASN
2	А	458	GLU
2	А	462	THR
2	А	467	VAL
2	А	520	ASP
2	А	527	THR
2	А	586	CYS
2	А	611	VAL
2	А	652	ILE
2	В	18	VAL
2	В	48	GLN
2	В	57	ARG
2	В	80	SER
2	В	98	ILE
2	В	127	GLN
2	В	246	CYS
2	В	263	GLU
2	В	270	SER
2	В	277	THR
2	В	285	SER
2	В	318	LYS
2	В	372	CYS
2	В	481	VAL
2	В	497	LEU
2	В	508	GLN
2	В	569	ASP

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	А	93	HIS
2	А	317	GLN
2	А	656	HIS
2	В	50	GLN
2	В	76	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 (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	Chain	Chain	Chain	Dog	Tink	B	ond leng	gths	E	ond ang	gles
	туре	res		LIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2			
4	ACY	В	803	-	3,3,3	1.10	0	$3,\!3,\!3$	0.71	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.

No monomer is involved in short contacts.

#### 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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	< <b>RSRZ</b> >	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	С	7/8~(87%)	-0.09	1 (14%) 2 2	24, 28, 62, 71	0
1	D	8/8~(100%)	-0.62	0 100 100	17, 24, 36, 44	0
2	А	630/659~(95%)	0.44	62 (9%) 7 7	14, 51, 104, 145	0
2	В	631/659~(95%)	0.04	24 (3%) 40 43	15, 35, 79, 138	0
All	All	1276/1334~(95%)	0.23	87 (6%) 17 17	14, 42, 95, 145	0

All (87) RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
2	В	657	HIS	7.9
2	А	249	TYR	7.5
2	А	658	HIS	6.4
2	В	658	HIS	6.0
2	А	654	HIS	5.9
2	А	218	ALA	5.4
2	А	647	VAL	5.3
2	А	544	LYS	5.3
2	А	508	GLN	5.3
2	А	547	TYR	5.0
2	В	656	HIS	5.0
2	А	456	ASP	5.0
2	А	657	HIS	4.6
2	А	22	PRO	4.4
2	А	612	ARG	4.4
2	В	654	HIS	4.3
2	А	252	GLU	4.3
2	А	458	GLU	4.3
2	А	459	ASN	3.9
2	А	440	PHE	3.9
2	А	248	PRO	3.8



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Mol	Chain	Res	Type	RSRZ
2	А	258	HIS	3.8
2	В	653	ALA	3.8
2	А	510	LYS	3.8
2	А	260	PRO	3.8
2	А	507	VAL	3.6
2	А	512	LEU	3.4
2	А	486	GLN	3.4
2	В	124	GLU	3.4
2	А	484	GLN	3.4
2	А	511	ASP	3.4
2	А	123	PRO	3.3
2	А	306	GLY	3.3
2	В	655	HIS	3.3
2	А	487	PRO	3.2
2	А	124	GLU	3.2
2	В	24	ARG	3.2
2	В	253	GLU	3.1
2	А	489	ARG	3.1
2	А	127	GLN	3.1
2	А	267	ASN	3.1
2	А	460	ASP	3.0
2	А	253	GLU	3.0
2	А	216	PHE	2.9
2	А	505	ARG	2.9
2	А	217	VAL	2.9
2	А	655	HIS	2.8
2	А	514	LYS	2.8
2	А	616	GLY	2.8
2	А	5	ILE	2.7
2	А	615	ARG	2.7
2	А	648	GLY	2.7
2	В	618	VAL	2.7
2	A	244	GLU	2.6
2	А	656	HIS	2.6
2	A	112	VAL	2.6
2	В	652	ILE	2.6
2	А	649	SER	2.6
2	В	392	ALA	2.5
2	A	455	ARG	2.4
2	В	21	LYS	2.4
2	А	34	ASN	2.4
2	В	612	ARG	2.4



and from			
Chain	$\frac{1 \text{ previol}}{\text{Res}}$	Type	RSRZ
В	394	ASN	2.4
А	215	ASN	2.3
В	619	ALA	2.3
А	546	ARG	2.3
В	252	GLU	2.3
А	517	ARG	2.3
А	221	PHE	2.3
А	264	HIS	2.3
А	650	GLY	2.3
В	81	VAL	2.2
А	504	ALA	2.2
В	123	PRO	2.2
В	283	ARG	2.1
А	245	ALA	2.1
В	648	GLY	2.1
А	617	ILE	2.1
В	649	SER	2.1
А	453	LYS	2.1
А	543	LYS	2.0
С	7	DT	2.0

PRO

LYS

THR

VAL

620

431

462

112

Conti

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

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

2.0

2.0

2.0

2.0

#### Carbohydrates (i) 6.3

There are no monosaccharides in this entry.

#### Ligands (i) **6.4**

В

А

А

В

2

2

2

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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	ACY	В	803	4/4	0.92	0.17	$23,\!23,\!24,\!25$	0
3	CL	А	800	1/1	0.99	0.15	23,23,23,23	0
3	CL	А	801	1/1	1.00	0.13	20,20,20,20	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

