



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:53 PM GMT

PDB ID : 4DQQ  
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment E658A, DNA duplex, and rCTP (paired with dG of template) in presence of Mg<sup>2+</sup>  
Authors : Wang, W.; Beese, L.S.  
Deposited on : 2012-02-16  
Resolution : 1.59 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

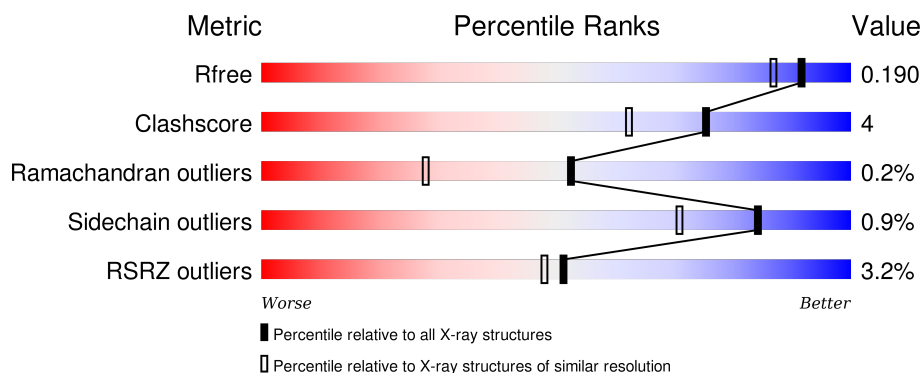
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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))
$R_{free}$	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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. 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	592	<div> <div>2%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	D	592	<div> <div>4%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
2	B	9	<div> <div>44%</div> <div>22%</div> <div>33%</div> </div>
2	E	9	<div> <div>33%</div> <div>67%</div> </div>
3	C	13	<div> <div>31%</div> <div>54%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	13	

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
6	MPD	A	903	-	-	-	X
6	MPD	A	904	-	-	-	X
6	MPD	D	904	-	-	-	X
6	MPD	D	905	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 21874 atoms, of which 10212 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 polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	580	Total	C	H	N	O	S	0	16	0
			9514	2995	4801	822	878	18			
1	D	584	Total	C	H	N	O	S	0	27	0
			9640	3040	4861	829	892	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
A	658	ALA	GLU	ENGINEERED MUTATION	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
D	658	ALA	GLU	ENGINEERED MUTATION	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

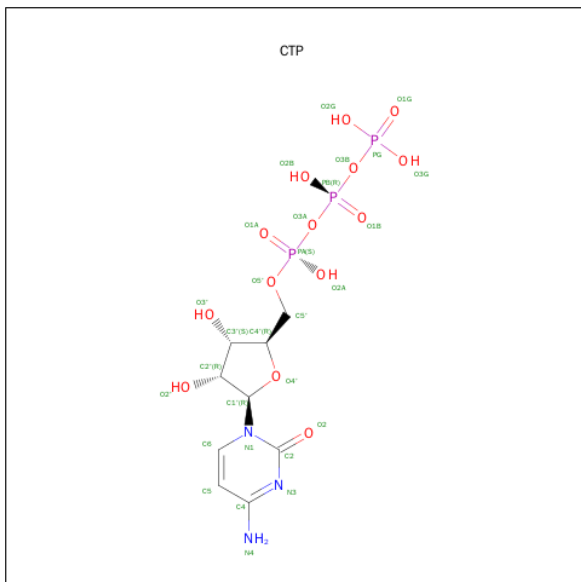
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DOC))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			274	85	100	29	52	8			

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

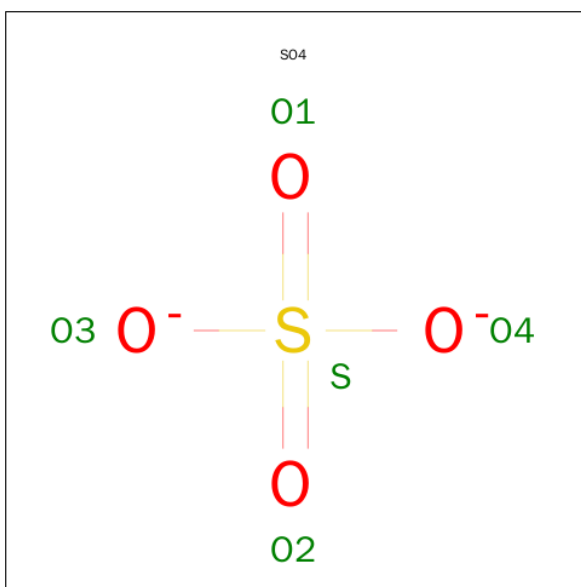
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	0
			356	109	123	47	66	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula:  $C_9H_{16}N_3O_{14}P_3$ ).



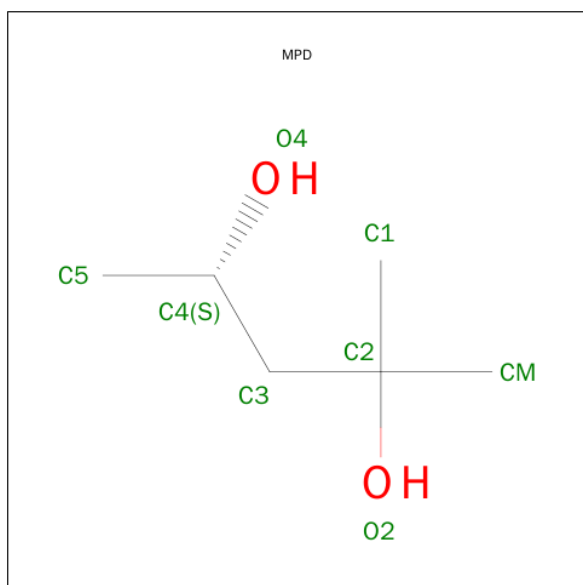
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			33	9	12	3	8	1		
4	D	1	Total	C	H	N	O	P	0	0
			41	9	12	3	14	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



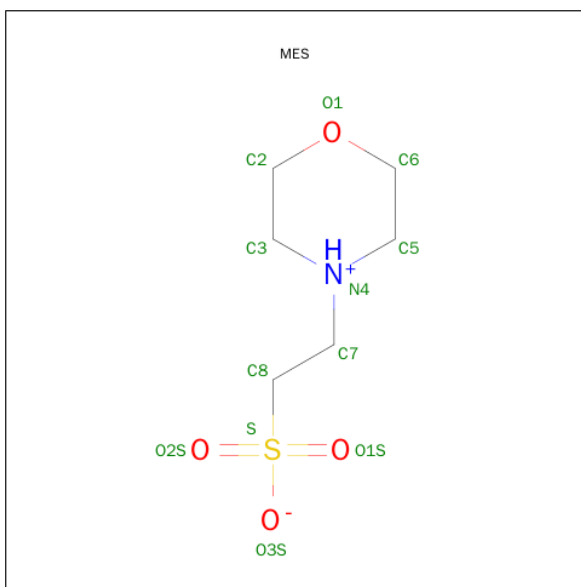
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			22	6	14	2		
6	A	1	Total	C	H	O	0	0
			22	6	14	2		
6	D	1	Total	C	H	O	0	0
			22	6	14	2		
6	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Mg		
			1	1	0	0

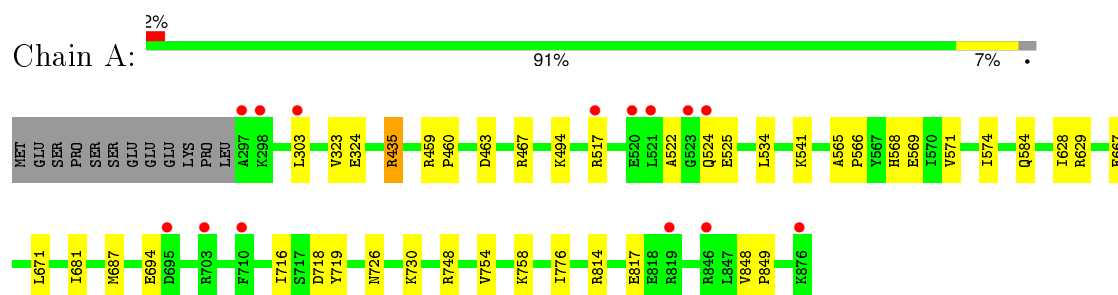
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	465	Total	O		
			465	465	0	0
9	D	595	Total	O		
			595	595	0	0
9	B	34	Total	O		
			34	34	0	0
9	C	47	Total	O		
			47	47	0	0
9	E	29	Total	O		
			29	29	0	0
9	F	63	Total	O		
			63	63	0	0

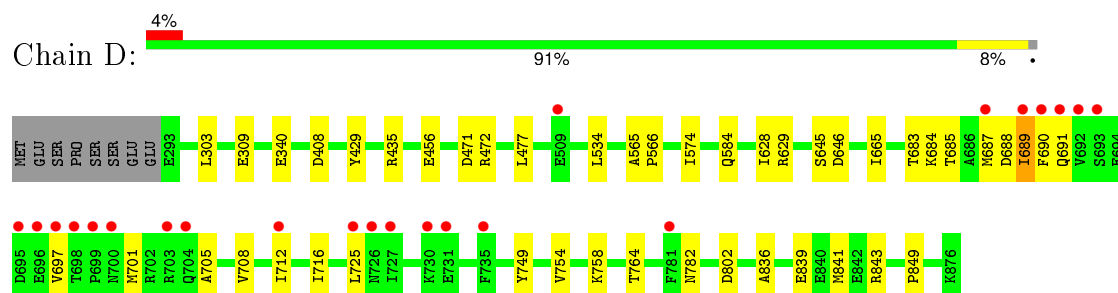
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

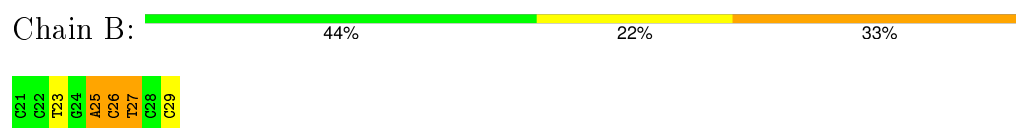
- Molecule 1: DNA polymerase



- Molecule 1: DNA polymerase



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



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



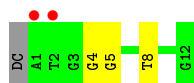
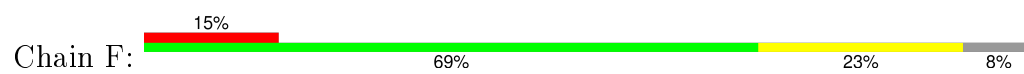
- Molecule 3: DNA (5'-D(\*CP\*AP\*TP\*GP\*GP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*G)-3')







- Molecule 3: DNA (5'-D(\*CP\*AP\*TP\*GP\*GP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.54Å 107.97Å 149.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.35 – 1.59 79.35 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (79.35-1.59) 95.8 (79.35-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.59Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, $R_{free}$	0.160 , 0.179 0.173 , 0.190	Depositor DCC
$R_{free}$ test set	8769 reflections (4.76%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 192920 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	21874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CTP, DOC, MPD, SO4, MES

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	0.43	0/4854	0.58	0/6558
1	D	0.54	0/4968	0.65	3/6720 (0.0%)
2	B	1.01	0/173	1.87	5/264 (1.9%)
2	E	1.03	1/173 (0.6%)	1.87	5/264 (1.9%)
3	C	0.96	0/262	1.67	4/404 (1.0%)
3	F	1.07	0/283	1.56	5/437 (1.1%)
All	All	0.55	1/10713 (0.0%)	0.79	22/14647 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	DA	C3'-O3'	-5.85	1.36	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8	DT	O4'-C1'-N1	-10.01	101.00	108.00
2	E	23	DT	O4'-C1'-N1	-9.03	101.68	108.00
3	F	8	DT	O4'-C1'-N1	-8.82	101.82	108.00
2	B	25	DA	O5'-P-OP2	-8.57	97.98	105.70
2	B	23	DT	O4'-C1'-N1	-7.59	102.68	108.00
2	B	26	DC	O4'-C1'-N1	6.46	112.52	108.00
2	E	22	DC	O4'-C1'-N1	-6.37	103.54	108.00
1	D	471	ASP	CB-CG-OD1	6.30	123.97	118.30
3	F	4	DG	O5'-P-OP2	-6.16	100.16	105.70
2	B	27	DT	O4'-C4'-C3'	-5.82	102.17	104.50
3	F	5	DG	N1-C6-O6	5.81	123.38	119.90
2	E	26	DC	C6-N1-C2	5.75	122.60	120.30
1	D	802	ASP	CB-CG-OD1	-5.69	113.17	118.30
3	C	11	DG	N3-C4-N9	-5.67	122.60	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	DG	C2-N3-C4	-5.65	109.08	111.90
1	D	471	ASP	CB-CG-OD2	-5.53	113.33	118.30
2	E	26	DC	C2-N1-C1'	-5.48	112.77	118.80
3	C	11	DG	N9-C4-C5	5.45	107.58	105.40
2	B	25	DA	O5'-P-OP1	5.43	117.22	110.70
2	E	24	DG	O5'-P-OP2	-5.16	101.05	105.70
3	F	5	DG	N3-C4-N9	-5.14	122.91	126.00
3	C	5	DG	N1-C6-O6	5.11	122.97	119.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	4713	4801	4726	30	0
1	D	4779	4861	4727	43	0
2	B	174	100	103	5	0
2	E	174	100	103	2	0
3	C	233	123	124	3	0
3	F	251	134	136	0	0
4	A	21	12	12	0	0
4	D	29	12	12	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
6	A	16	28	28	2	0
6	D	16	28	28	1	0
7	A	12	13	12	2	0
8	D	1	0	0	0	0
9	A	465	0	0	10	1
9	B	34	0	0	0	0
9	C	47	0	0	1	0
9	D	595	0	0	19	2
9	E	29	0	0	0	0
9	F	63	0	0	0	0
All	All	11662	10212	10011	81	2

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 (81) 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:D:839:GLU:OE2	9:D:1563:HOH:O	1.95	0.83
1:D:685:THR:HG21	9:D:1571:HOH:O	1.85	0.76
1:D:705:ALA:O	9:D:1571:HOH:O	2.02	0.76
6:D:904:MPD:HM2	9:D:1065:HOH:O	1.87	0.74
1:A:565:ALA:HA	1:A:571:VAL:HG21	1.70	0.73
1:D:839:GLU:HG3	9:D:1563:HOH:O	1.88	0.73
1:A:324:GLU:OE2	9:A:1384:HOH:O	2.06	0.73
1:A:565:ALA:HA	1:A:571:VAL:CG2	2.17	0.73
1:D:684:LYS:NZ	9:D:1221:HOH:O	2.22	0.72
1:A:323:VAL:O	1:A:435:ARG:NH2	2.24	0.71
1:D:683:THR:HG22	1:D:687:MET:CE	2.24	0.68
1:D:456:GLU:HG2	9:D:1302:HOH:O	1.97	0.65
1:D:408:ASP:OD1	9:D:1163:HOH:O	2.13	0.65
1:A:323:VAL:O	6:A:904:MPD:H52	1.98	0.64
1:D:309:GLU:OE1	9:D:1367:HOH:O	2.15	0.64
7:A:905:MES:H72	9:A:1398:HOH:O	1.99	0.63
1:D:754:VAL:HG12	1:D:758:LYS:HE2	1.81	0.62
1:A:748:ARG:HD2	9:A:1445:HOH:O	1.99	0.62
1:D:708:VAL:HB	9:D:1571:HOH:O	1.99	0.61
1:D:683:THR:HG22	1:D:687:MET:HE3	1.84	0.60
1:A:667:GLU:OE1	9:A:1293:HOH:O	2.16	0.60
1:D:584:GLN:HG3	9:D:1175:HOH:O	2.00	0.60
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.33	0.58
1:D:839:GLU:CG	9:D:1563:HOH:O	2.47	0.58
1:A:522:ALA:O	1:A:541:LYS:HE2	2.03	0.58
6:A:904:MPD:H53	6:A:904:MPD:HM1	1.86	0.57
1:D:836:ALA:HB3	1:D:841:MET:CE	2.35	0.57
1:D:764[B]:THR:HG21	9:D:1502:HOH:O	2.03	0.56
1:D:683:THR:HG22	1:D:687:MET:HE2	1.88	0.56
1:A:517:ARG:NH2	1:A:569:GLU:OE2	2.41	0.54
1:A:494:LYS:HE2	9:A:1461:HOH:O	2.08	0.53
1:D:565:ALA:N	1:D:566:PRO:HD2	2.23	0.53
1:D:629:ARG:HH22	2:E:29:DOC:H5	1.73	0.52
1:D:843:ARG:HD2	9:D:1156:HOH:O	2.11	0.51
1:D:472:ARG:NH1	9:D:1432:HOH:O	2.19	0.51
1:D:836:ALA:HB3	1:D:841:MET:HE1	1.92	0.50
1:D:665:ILE:HG22	1:D:749[A]:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:THR:O	1:D:687:MET:HG3	2.11	0.50
1:A:494:LYS:NZ	9:A:1130:HOH:O	2.44	0.50
1:D:689:ILE:HG23	1:D:690:PHE:CD1	2.46	0.49
1:D:690:PHE:O	1:D:691:GLN:HG2	2.11	0.49
1:A:435:ARG:NH1	9:A:1359:HOH:O	2.37	0.49
1:D:534:LEU:HD11	1:D:574[A]:ILE:HD13	1.95	0.49
2:B:25:DA:H2'	2:B:26:DC:C6	2.48	0.49
1:D:685:THR:CG2	9:D:1571:HOH:O	2.55	0.48
1:A:629:ARG:HH22	2:B:29:DOC:H5	1.78	0.48
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.96	0.48
1:A:629:ARG:NH1	9:A:1283:HOH:O	2.47	0.48
7:A:905:MES:H32	2:B:29:DOC:H2'	1.97	0.47
1:A:730:LYS:NZ	9:A:1420:HOH:O	2.47	0.47
1:A:584:GLN:HG3	9:A:1102:HOH:O	2.14	0.47
1:A:629:ARG:NH2	2:B:29:DOC:H5	2.30	0.47
1:A:671:LEU:HD12	1:A:681:ILE:HD11	1.96	0.46
1:D:725:LEU:N	1:D:725:LEU:HD12	2.31	0.46
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.97	0.46
1:A:534:LEU:HD11	1:A:574:ILE:HD13	1.98	0.45
1:A:754:VAL:CG1	1:A:758[B]:LYS:HE2	2.45	0.45
1:A:718:ASP:OD1	1:A:719:TYR:N	2.49	0.45
1:D:629:ARG:NH2	2:E:29:DOC:H5	2.31	0.45
3:C:12:DG:N7	9:C:127:HOH:O	2.35	0.45
1:A:814:ARG:HA	1:A:817:GLU:HG2	2.00	0.44
1:A:568:HIS:O	1:A:571:VAL:HG22	2.18	0.44
1:D:565:ALA:N	1:D:566:PRO:CD	2.80	0.44
1:D:749[A]:TYR:HA	9:D:1373:HOH:O	2.16	0.44
1:D:697:VAL:HA	1:D:701:MET:HE1	2.00	0.44
1:A:524:GLN:HG2	1:A:525:GLU:N	2.33	0.43
1:D:712:ILE:HA	1:D:716:ILE:HG22	2.00	0.43
1:A:565:ALA:N	1:A:566:PRO:CD	2.81	0.43
1:D:645:SER:O	1:D:646:ASP:HB2	2.18	0.42
1:A:716:ILE:HA	3:C:3:DG:H5'	2.01	0.42
1:D:725:LEU:CD1	1:D:725:LEU:N	2.83	0.42
1:A:463:ASP:O	1:A:467[A]:ARG:HG3	2.19	0.42
1:D:472:ARG:HD3	9:D:1432:HOH:O	2.20	0.41
1:D:429:TYR:O	1:D:435:ARG:HA	2.20	0.41
3:C:9:DC:H2'	3:C:10:DA:C8	2.56	0.41
1:D:340:GLU:OE2	9:D:1478:HOH:O	2.22	0.41
1:D:685:THR:O	1:D:689:ILE:HG22	2.21	0.41
1:D:665:ILE:CG2	1:D:749[A]:TYR:CE1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:DC:H2''	2:B:27:DT:O5'	2.21	0.41
1:A:687:MET:SD	1:A:694:GLU:HA	2.61	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1420:HOH:O	9:D:1542:HOH:O[2_755]	1.75	0.45
9:D:1574:HOH:O	9:D:1576:HOH:O[4_545]	2.16	0.04

## 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	594/592 (100%)	583 (98%)	10 (2%)	1 (0%)	52	28
1	D	609/592 (103%)	594 (98%)	14 (2%)	1 (0%)	52	28
All	All	1203/1184 (102%)	1177 (98%)	24 (2%)	2 (0%)	52	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	ILE
1	D	628	ILE

### 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	508/506 (100%)	504 (99%)	4 (1%)	86	75
1	D	522/506 (103%)	517 (99%)	5 (1%)	82	67
All	All	1030/1012 (102%)	1021 (99%)	9 (1%)	84	71

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	435	ARG
1	A	726	ASN
1	A	776	ILE
1	D	303	LEU
1	D	477	LEU
1	D	688	ASP
1	D	689	ILE
1	D	782	ASN

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

### 5.3.3 RNA ⓘ

There are no RNA molecules 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$
2	DOC	B	29	3,2	11,19,20	0.81	0	14,26,29	1.01	0
2	DOC	E	29	3,2	11,19,20	0.87	1 (9%)	14,26,29	1.14	2 (14%)



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
2	DOC	B	29	3,2	-	0/3/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/3/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	DOC	C6-C5	-2.40	1.32	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	O4'-C1'-C2'	2.24	109.09	106.67
2	E	29	DOC	C2-N3-C4	3.17	120.08	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	29	DOC	3	0
2	E	29	DOC	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	CTP	A	901	-	17,22,30	1.51	3 (17%)	22,33,47	1.25	2 (9%)
5	SO4	A	902	-	4,4,4	0.48	0	6,6,6	0.55	0
6	MPD	A	903	-	6,7,7	0.42	0	7,10,10	1.05	0
6	MPD	A	904	-	6,7,7	0.49	0	7,10,10	0.51	0
7	MES	A	905	-	12,12,12	2.04	3 (25%)	16,16,16	2.67	5 (31%)
4	CTP	D	901	8	21,30,30	1.43	3 (14%)	31,47,47	0.80	1 (3%)
5	SO4	D	903	-	4,4,4	0.35	0	6,6,6	0.52	0
6	MPD	D	904	-	6,7,7	0.35	0	7,10,10	0.79	0
6	MPD	D	905	-	6,7,7	0.37	0	7,10,10	0.40	0

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	CTP	A	901	-	-	0/6/26/38	0/2/2/2
5	SO4	A	902	-	-	0/0/0/0	0/0/0/0
6	MPD	A	903	-	-	0/5/5/5	0/0/0/0
6	MPD	A	904	-	-	0/5/5/5	0/0/0/0
7	MES	A	905	-	-	0/6/14/14	0/1/1/1
4	CTP	D	901	8	-	0/18/38/38	0/2/2/2
5	SO4	D	903	-	-	0/0/0/0	0/0/0/0
6	MPD	D	904	-	-	0/5/5/5	0/0/0/0
6	MPD	D	905	-	-	0/5/5/5	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	905	MES	C8-S	-5.37	1.68	1.78
7	A	905	MES	C7-N4	-2.15	1.45	1.50
4	D	901	CTP	C3'-C4'	-2.12	1.47	1.53
4	A	901	CTP	O3'-C3'	-2.06	1.38	1.43
4	A	901	CTP	C4-N4	2.32	1.42	1.35
7	A	905	MES	O1S-S	2.49	1.51	1.45
4	D	901	CTP	C4-N4	2.88	1.43	1.35
4	D	901	CTP	C6-N1	3.24	1.40	1.35
4	A	901	CTP	C6-N1	3.32	1.40	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	905	MES	O1-C2-C3	-4.71	106.48	111.41
4	A	901	CTP	O2A-PA-O1A	-2.40	102.84	110.58
7	A	905	MES	O3S-S-O1S	-2.03	107.52	112.47
4	D	901	CTP	O2B-PB-O3B	2.07	114.49	105.09
4	A	901	CTP	O4'-C1'-N1	3.63	115.73	108.08
7	A	905	MES	C5-N4-C3	3.72	117.59	109.76
7	A	905	MES	C6-C5-N4	4.15	115.17	109.98
7	A	905	MES	O1-C6-C5	6.43	118.14	111.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	904	MPD	2	0
7	A	905	MES	2	0
6	D	904	MPD	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	580/592 (97%)	-0.08	14 (2%) 62 60	13, 28, 48, 67	0
1	D	584/592 (98%)	0.20	23 (3%) 43 40	10, 22, 45, 70	0
2	B	8/9 (88%)	-0.40	0 100 100	18, 24, 45, 56	0
2	E	8/9 (88%)	-0.33	0 100 100	17, 25, 42, 51	0
3	C	11/13 (84%)	-0.23	0 100 100	15, 20, 43, 61	0
3	F	12/13 (92%)	0.44	2 (16%) 2 2	15, 24, 63, 73	0
All	All	1203/1228 (97%)	0.06	39 (3%) 51 48	10, 25, 47, 73	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	689	ILE	9.4
1	D	691	GLN	6.7
1	A	297	ALA	6.3
1	A	298	LYS	4.9
3	F	1	DA	4.9
1	D	699	PRO	4.8
1	D	695	ASP	4.7
1	A	521	LEU	4.6
1	D	698	THR	4.5
1	D	687	MET	4.2
1	D	697	VAL	4.2
1	D	690	PHE	4.1
1	A	520	GLU	3.8
1	A	710	PHE	3.7
1	D	692	VAL	3.7
1	D	735	PHE	3.6
1	D	712	ILE	3.5
1	A	703	ARG	3.5
1	D	704	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	2	DT	3.3
1	D	700	ASN	3.2
1	A	695	ASP	3.2
1	D	725	LEU	3.2
1	D	727	ILE	3.1
1	D	693	SER	3.1
1	D	703	ARG	2.9
1	A	819	ARG	2.8
1	D	730	LYS	2.7
1	D	726	ASN	2.7
1	D	731	GLU	2.6
1	A	524	GLN	2.5
1	A	517	ARG	2.4
1	A	303	LEU	2.3
1	D	509	GLU	2.3
1	D	781	PHE	2.3
1	A	523	GLY	2.2
1	A	876	LYS	2.1
1	A	846	ARG	2.0
1	D	696	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DOC	B	29	18/19	0.98	0.06	-	17,22,28,29	0
2	DOC	E	29	18/19	0.98	0.10	-	12,18,23,28	0

## 6.3 Carbohydrates [i](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MPD	A	904	8/8	0.82	0.23	5.28	29,41,49,60	0
6	MPD	D	905	8/8	0.85	0.16	3.39	30,37,43,46	0
6	MPD	A	903	8/8	0.91	0.14	2.70	22,31,36,44	0
6	MPD	D	904	8/8	0.88	0.12	2.21	19,36,56,63	0
4	CTP	A	901	21/29	0.79	0.16	1.90	23,41,92,113	0
7	MES	A	905	12/12	0.90	0.15	1.18	17,26,49,59	25
5	SO4	A	902	5/5	0.97	0.07	-0.75	24,24,25,26	0
4	CTP	D	901	29/29	0.96	0.07	-1.40	14,20,27,37	0
5	SO4	D	903	5/5	0.99	0.08	-	25,25,37,38	0
8	MG	D	902	1/1	0.88	0.12	-	22,22,22,22	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.