



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:57 PM GMT

PDB ID : 4DSE  
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment F710Y, DNA duplex, and rCTP (paired with dG of template) in presence of Mg<sup>2+</sup>  
Authors : Wang, W.; Beese, L.S.  
Deposited on : 2012-02-18  
Resolution : 1.67 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

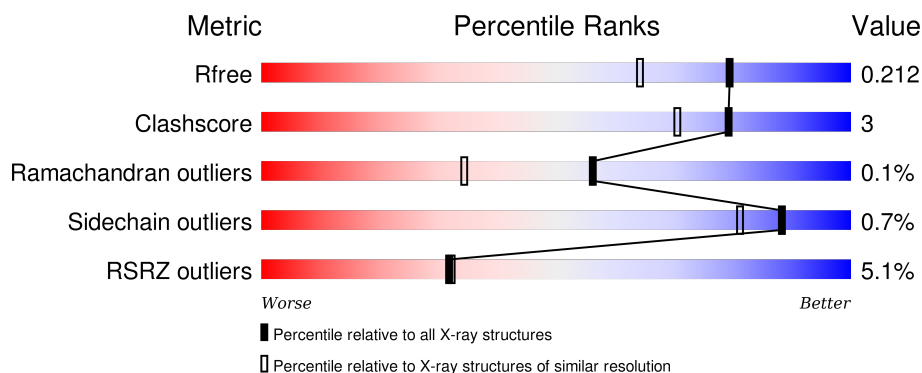
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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>7%</div> <div>87% 5% 8%</div> </div>
1	D	592	<div> <div>3%</div> <div>89% 8% .</div> </div>
2	B	9	<div> <div>44% 33% 22%</div> </div>
2	E	9	<div> <div>56% 44%</div> </div>
3	C	13	<div> <div>23% 46% 31%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	13	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a red segment at the start labeled '8%', a green segment labeled '54%', a yellow segment labeled '38%', and a grey segment at the end labeled '8%'.

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 20892 atoms, of which 9688 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	546	Total	C	H	N	O	S	0	6	0
			8882	2803	4479	766	819	15			
1	D	579	Total	C	H	N	O	S	0	14	0
			9459	2984	4763	814	881	17			

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	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
A	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1
D	598	ALA	ASP	ENGINEERED MUTATION	UNP Q5KWC1
D	710	TYR	PHE	ENGINEERED MUTATION	UNP Q5KWC1
D	823	HIS	ARG	SEE REMARK 999	UNP Q5KWC1

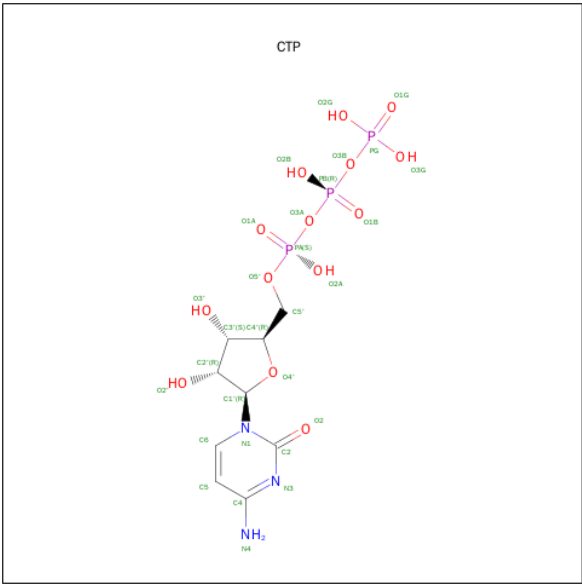
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DOC))-3').

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').

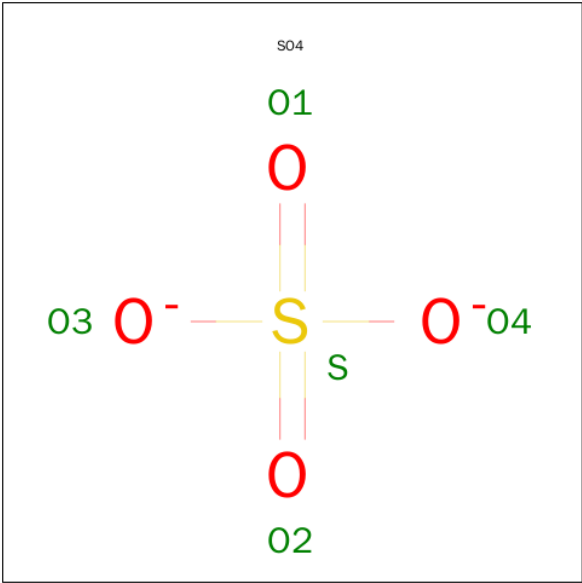
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O	P	0	0	0
			291	89	100	40	53	9			
3	F	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			

- 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	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	D	1	Total	O	S	0	0
			5	4	1		

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

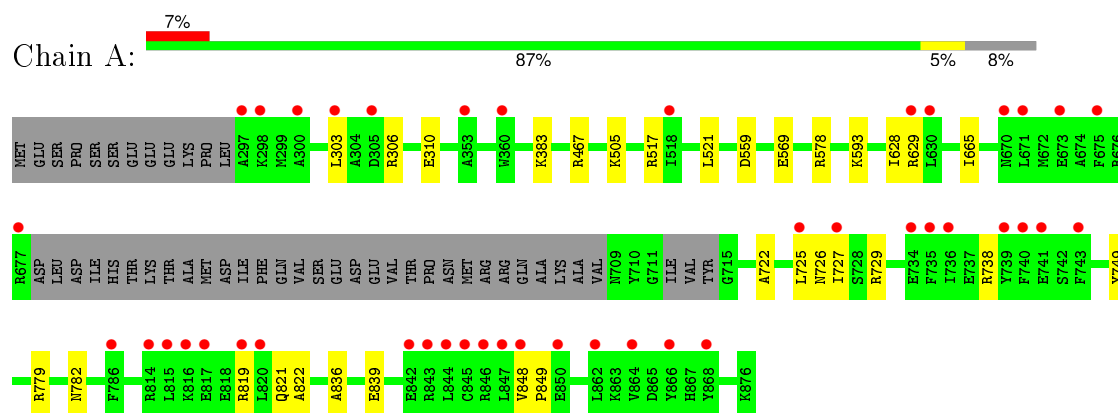
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	363	Total	O		0	0
			363	363			
6	D	723	Total	O		0	0
			723	723			
6	B	28	Total	O		0	0
			28	28			
6	C	55	Total	O		0	0
			55	55			
6	E	31	Total	O		0	0
			31	31			
6	F	66	Total	O		0	0
			66	66			

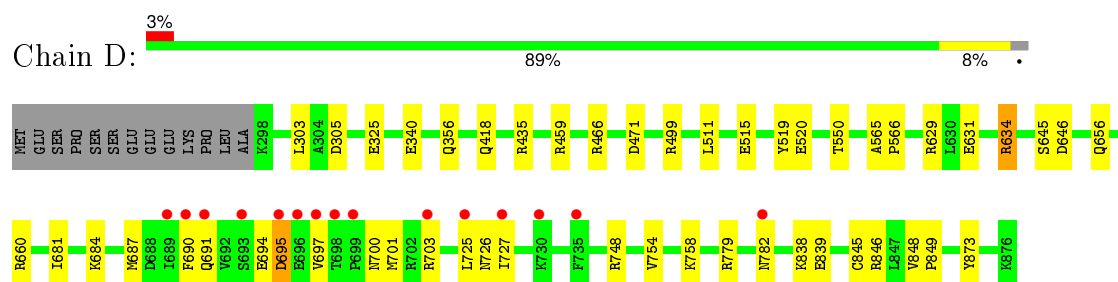
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

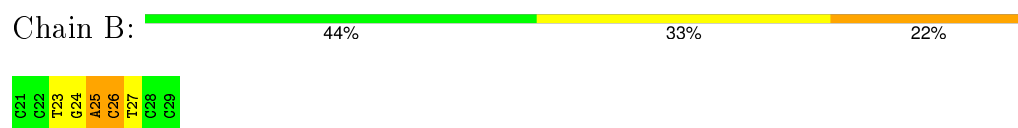
- Molecule 1: DNA polymerase



- Molecule 1: DNA polymerase



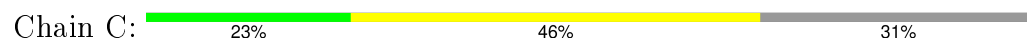
- Molecule 2: DNA (5'-D(\*CP\*CP\*TP\*GP\*AP\*CP\*TP\*CP\*(DOC))-3')



- 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, $\alpha$ , $\beta$ , $\gamma$	93.85Å 109.51Å 150.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.65 – 1.67 79.65 – 1.67	Depositor EDS
% Data completeness (in resolution range)	86.9 (79.65-1.67) 86.9 (79.65-1.67)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 1.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, $R_{free}$	0.175 , 0.200 0.188 , 0.212	Depositor DCC
$R_{free}$ test set	7004 reflections (4.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1402 of 156225 reflections (0.897%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: DOC, CTP, 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	0.43	0/4507	0.55	0/6085
1	D	0.63	0/4842	0.71	3/6544 (0.0%)
2	B	0.97	0/173	1.95	6/264 (2.3%)
2	E	1.20	0/173	1.92	6/264 (2.3%)
3	C	1.16	0/215	1.79	6/331 (1.8%)
3	F	1.25	0/283	1.93	9/437 (2.1%)
All	All	0.62	0/10193	0.84	30/13925 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8	DT	O4'-C1'-N1	-11.24	100.13	108.00
2	B	23	DT	O4'-C1'-N1	-10.12	100.91	108.00
3	C	8	DT	O4'-C1'-N1	-9.10	101.63	108.00
2	B	25	DA	O4'-C4'-C3'	-8.94	100.64	106.00
2	E	23	DT	O4'-C1'-N1	-8.81	101.84	108.00
2	B	25	DA	O5'-P-OP1	7.21	119.36	110.70
3	F	10	DA	O4'-C1'-N9	-6.98	103.11	108.00
3	C	7	DG	C2-N3-C4	6.96	115.38	111.90
3	F	4	DG	O5'-P-OP2	-6.94	99.45	105.70
2	E	23	DT	N3-C4-O4	6.87	124.02	119.90
3	F	6	DA	OP1-P-OP2	-6.79	109.42	119.60
3	F	6	DA	C5-N7-C8	-6.50	100.65	103.90
3	F	4	DG	O4'-C1'-N9	6.45	112.51	108.00
1	D	634	ARG	CG-CD-NE	-6.29	98.59	111.80
1	D	660	ARG	NE-CZ-NH1	6.19	123.39	120.30
3	C	5	DG	O4'-C4'-C3'	-6.10	102.06	104.50
2	B	26	DC	O4'-C1'-N1	5.83	112.08	108.00
3	C	12	DG	O4'-C1'-N9	5.78	112.04	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	23	DT	C5-C4-O4	-5.70	120.91	124.90
2	B	23	DT	N3-C4-O4	5.69	123.32	119.90
3	C	10	DA	O4'-C1'-N9	-5.57	104.10	108.00
1	D	471	ASP	CB-CG-OD1	5.48	123.23	118.30
3	C	11	DG	O4'-C1'-N9	-5.47	104.17	108.00
2	E	27	DT	C6-C5-C7	-5.44	119.63	122.90
2	E	26	DC	O4'-C1'-N1	5.36	111.75	108.00
3	F	4	DG	O4'-C1'-C2'	5.23	110.09	105.90
2	E	26	DC	N1-C2-O2	-5.21	115.77	118.90
3	F	8	DT	N3-C4-O4	5.14	122.99	119.90
2	B	24	DG	O4'-C1'-C2'	-5.12	101.80	105.90
3	F	9	DC	C4'-C3'-C2'	5.05	107.64	103.10

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	4403	4479	4438	25	1
1	D	4696	4763	4688	39	1
2	B	174	100	103	2	0
2	E	174	100	103	2	0
3	C	191	100	101	0	0
3	F	251	134	136	0	0
4	D	29	12	12	3	0
5	D	20	0	0	0	0
6	A	363	0	0	15	1
6	B	28	0	0	0	0
6	C	55	0	0	0	0
6	D	723	0	0	22	2
6	E	31	0	0	0	0
6	F	66	0	0	0	0
All	All	11204	9688	9581	68	3

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 3.

All (68) 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:845:CYS:SG	6:D:1121:HOH:O	2.32	0.88
1:A:821:GLN:O	6:A:1129:HOH:O	1.96	0.83
1:D:629:ARG:NH1	6:D:1383:HOH:O	2.10	0.83
1:A:839:GLU:HB2	6:A:1238:HOH:O	1.79	0.81
1:D:340:GLU:OE2	6:D:1600:HOH:O	2.04	0.75
1:D:418:GLN:NE2	6:D:1399:HOH:O	2.19	0.75
1:D:305:ASP:OD1	6:D:1641:HOH:O	2.05	0.74
1:A:467:ARG:HD2	6:A:1103:HOH:O	1.87	0.74
1:D:325:GLU:OE2	6:D:1119:HOH:O	2.08	0.72
1:D:550:THR:OG1	6:D:1637:HOH:O	2.09	0.70
4:D:901:CTP:O3G	6:D:1261:HOH:O	2.10	0.70
1:D:631:GLU:OE1	6:D:1660:HOH:O	2.09	0.69
1:A:559:ASP:OD2	6:A:1009:HOH:O	2.10	0.68
1:D:782:ASN:ND2	6:D:1691:HOH:O	2.26	0.66
1:D:779:ARG:NH1	6:D:1674:HOH:O	2.23	0.66
1:A:593:LYS:NZ	6:A:1232:HOH:O	2.28	0.66
1:D:846:ARG:HD2	6:D:1636:HOH:O	1.97	0.64
1:A:629:ARG:NH1	6:A:1076:HOH:O	2.32	0.62
1:A:726:ASN:ND2	6:A:1192:HOH:O	2.31	0.62
1:D:466:ARG:NH1	6:D:1232:HOH:O	2.34	0.61
1:D:499:ARG:NE	6:D:1386:HOH:O	2.23	0.60
1:A:738:ARG:HD3	6:A:1224:HOH:O	2.02	0.58
1:D:520:GLU:OE2	6:D:1492:HOH:O	2.16	0.58
1:A:819:ARG:NH2	6:A:1166:HOH:O	2.39	0.56
1:A:665:ILE:HG22	1:A:749:TYR:CE1	2.41	0.55
1:A:782:ASN:ND2	6:A:1246:HOH:O	2.34	0.55
1:D:325:GLU:CD	1:D:325:GLU:H	2.11	0.54
1:A:722:ALA:HB2	1:A:729:ARG:HA	1.91	0.52
1:D:634:ARG:NH1	1:D:873:TYR:CD1	2.78	0.52
1:D:435:ARG:NH2	6:D:1314:HOH:O	2.39	0.51
1:A:738:ARG:NH1	6:A:1224:HOH:O	2.44	0.51
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.92	0.51
1:A:310:GLU:HG2	6:A:1008:HOH:O	2.11	0.51
1:A:779:ARG:NH2	6:A:1236:HOH:O	2.44	0.50
1:D:656:GLN:OE1	1:D:681:ILE:HG22	2.12	0.50
1:D:690:PHE:CD1	1:D:701:MET:HE3	2.47	0.49
1:D:687:MET:HE2	1:D:694:GLU:HA	1.94	0.49
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:GLU:CD	6:D:1492:HOH:O	2.49	0.49
1:D:459:ARG:NH2	6:D:1589:HOH:O	2.45	0.48
1:D:838:LYS:NZ	1:D:839[B]:GLU:OE2	2.45	0.48
1:D:697:VAL:HA	1:D:701:MET:HE2	1.94	0.48
4:D:901:CTP:C4'	2:E:29:DOC:H2'	2.44	0.47
1:D:748:ARG:HD3	6:D:1418:HOH:O	2.14	0.47
1:A:569:GLU:HA	6:A:1097:HOH:O	2.13	0.47
1:D:848:VAL:HB	1:D:849:PRO:HD3	1.98	0.46
1:A:665:ILE:CG2	1:A:749:TYR:CE1	2.99	0.46
1:A:822:ALA:CB	1:A:836:ALA:HB2	2.46	0.46
1:A:578:ARG:NH1	2:B:25:DA:H5''	2.32	0.45
1:A:725:LEU:HB2	1:A:727:ILE:HG12	1.99	0.44
4:D:901:CTP:H4'	2:E:29:DOC:H2'	2.00	0.44
1:D:687:MET:CE	1:D:694:GLU:HA	2.48	0.44
1:D:725:LEU:HB2	1:D:727:ILE:HG12	2.00	0.43
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.54	0.43
1:D:550:THR:CG2	6:D:1637:HOH:O	2.67	0.42
1:D:645:SER:O	1:D:646:ASP:HB2	2.19	0.42
1:D:634:ARG:NE	6:D:1310:HOH:O	2.52	0.42
2:B:26:DC:H2''	2:B:27:DT:O5'	2.19	0.42
1:D:703:ARG:NH2	6:D:1294:HOH:O	2.53	0.42
1:A:383:LYS:HE2	6:A:1094:HOH:O	2.20	0.41
1:D:565:ALA:N	1:D:566:PRO:CD	2.83	0.41
1:A:517:ARG:NH2	1:A:521:LEU:HD21	2.35	0.41
1:A:665:ILE:HG21	1:A:749:TYR:CZ	2.55	0.41
1:D:754:VAL:HG12	1:D:758:LYS:HE2	2.04	0.40
1:A:822:ALA:HB2	1:A:836:ALA:HB2	2.01	0.40
1:D:695:ASP:OD1	1:D:695:ASP:N	2.46	0.40
1:D:725:LEU:O	1:D:726:ASN:C	2.59	0.40
1:D:684:LYS:O	1:D:687:MET:HG2	2.22	0.40

All (3) 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)
6:D:1171:HOH:O	6:D:1400:HOH:O[4_445]	1.53	0.67
6:A:997:HOH:O	6:D:1358:HOH:O[2_745]	1.71	0.49
1:A:505:LYS:HZ3	1:D:356:GLN:OE1[2_745]	1.55	0.05

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/592 (92%)	533 (98%)	12 (2%)	1 (0%)	52	31
1	D	591/592 (100%)	578 (98%)	13 (2%)	0	100	100
All	All	1137/1184 (96%)	1111 (98%)	25 (2%)	1 (0%)	56	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	ILE

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/507 (93%)	468 (100%)	2 (0%)	93	90
1	D	508/507 (100%)	503 (99%)	5 (1%)	82	71
All	All	978/1014 (96%)	971 (99%)	7 (1%)	88	81

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	306	ARG
1	D	303	LEU
1	D	511	LEU
1	D	691	GLN

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Mol	Chain	Res	Type
1	D	695	ASP
1	D	700	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	0.74	0	14,26,29	1.11	1 (7%)
2	DOC	E	29	3,2	11,19,20	1.05	1 (9%)	14,26,29	1.21	1 (7%)

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	-2.25	1.33	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	O4'-C4'-C5'	-2.47	105.90	109.54
2	B	29	DOC	C2-N3-C4	2.99	119.84	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
4	CTP	D	901	-	21,30,30	1.20	2 (9%)	31,47,47	1.27	3 (9%)
5	SO4	D	902	-	4,4,4	0.39	0	6,6,6	0.16	0
5	SO4	D	903	-	4,4,4	0.35	0	6,6,6	0.72	0
5	SO4	D	904	-	4,4,4	0.06	0	6,6,6	0.15	0
5	SO4	D	905	-	4,4,4	0.17	0	6,6,6	0.22	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	D	901	-	-	0/18/38/38	0/2/2/2
5	SO4	D	902	-	-	0/0/0/0	0/0/0/0
5	SO4	D	903	-	-	0/0/0/0	0/0/0/0
5	SO4	D	904	-	-	0/0/0/0	0/0/0/0
5	SO4	D	905	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	CTP	C3'-C2'	-2.03	1.47	1.53
4	D	901	CTP	C4-N4	2.83	1.43	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	CTP	C4'-O4'-C1'	-3.47	105.90	109.72
4	D	901	CTP	O2B-PB-O3B	2.49	116.40	105.09
4	D	901	CTP	C2-N3-C4	3.35	120.33	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	CTP	3	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	546/592 (92%)	0.51	43 (7%) 15 16	20, 40, 70, 99	0
1	D	579/592 (97%)	0.17	15 (2%) 59 62	10, 22, 45, 71	0
2	B	8/9 (88%)	-0.29	0 100 100	26, 30, 42, 48	0
2	E	8/9 (88%)	-0.33	0 100 100	17, 23, 38, 49	0
3	C	9/13 (69%)	-0.52	0 100 100	20, 25, 34, 42	0
3	F	12/13 (92%)	0.19	1 (8%) 14 14	14, 24, 62, 76	0
All	All	1162/1228 (94%)	0.32	59 (5%) 32 32	10, 31, 62, 99	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	816	LYS	6.2
1	A	297	ALA	5.8
1	A	298	LYS	5.5
1	D	698	THR	5.0
1	A	842	GLU	5.0
1	A	819	ARG	4.7
1	A	868	TYR	4.6
1	A	843	ARG	4.0
1	A	844	LEU	3.7
1	A	677	ARG	3.7
1	A	671	LEU	3.6
1	D	691	GLN	3.6
1	A	743	PHE	3.5
1	A	815	LEU	3.5
1	D	725	LEU	3.5
1	A	866	TYR	3.2
1	A	845	CYS	3.2
1	A	630	LEU	3.2
1	A	725	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	820	LEU	3.2
1	A	862	LEU	3.2
1	A	735	PHE	3.1
1	A	740	PHE	3.1
3	F	1	DA	3.0
1	A	360	TRP	3.0
1	D	730	LYS	3.0
1	A	727	ILE	2.9
1	D	727	ILE	2.9
1	A	629	ARG	2.9
1	A	846	ARG	2.9
1	A	673	GLU	2.8
1	A	864	VAL	2.8
1	A	739	TYR	2.8
1	D	695	ASP	2.8
1	D	782	ASN	2.7
1	A	741	GLU	2.7
1	A	850	GLU	2.6
1	A	303	LEU	2.6
1	D	693	SER	2.6
1	A	353	ALA	2.5
1	D	735	PHE	2.5
1	A	734	GLU	2.4
1	A	786	PHE	2.4
1	A	847	LEU	2.4
1	A	814	ARG	2.4
1	A	518	ILE	2.3
1	D	696	GLU	2.3
1	A	670	ASN	2.3
1	D	703	ARG	2.3
1	A	848	VAL	2.3
1	A	300	ALA	2.2
1	A	817	GLU	2.2
1	D	697	VAL	2.2
1	D	689	ILE	2.2
1	D	690	PHE	2.2
1	A	305	ASP	2.2
1	A	736	ILE	2.1
1	D	699	PRO	2.1
1	A	675	PHE	2.1

## 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(Å <sup>2</sup> )	Q<0.9
2	DOC	E	29	18/19	0.98	0.12	-	15,18,24,26	0
2	DOC	B	29	18/19	0.93	0.11	-	31,35,43,46	0

## 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. 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
4	CTP	D	901	29/29	0.97	0.08	-0.72	17,22,30,33	0
5	SO4	D	902	5/5	0.95	0.09	-1.20	32,35,43,51	0
5	SO4	D	904	5/5	0.96	0.19	-	60,62,66,67	0
5	SO4	D	903	5/5	0.97	0.09	-	30,33,41,44	0
5	SO4	D	905	5/5	0.93	0.26	-	56,60,66,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.