



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:37 AM GMT

PDB ID : 4DSF
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment F710Y, DNA duplex, and rCTP (paired with dG of template) in presence of Mn²⁺
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-02-18
Resolution : 1.66 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

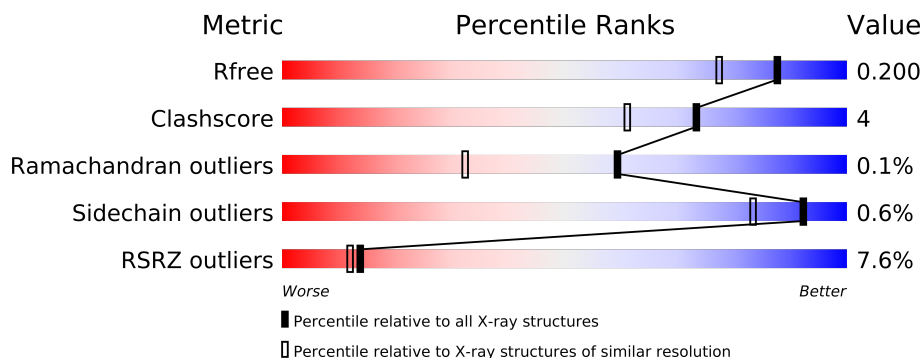
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.66 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}	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	592	
1	D	592	
2	B	9	
2	E	9	
3	C	13	
3	F	13	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	D	904	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20794 atoms, of which 9688 are hydrogens and 0 are deuterium.

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

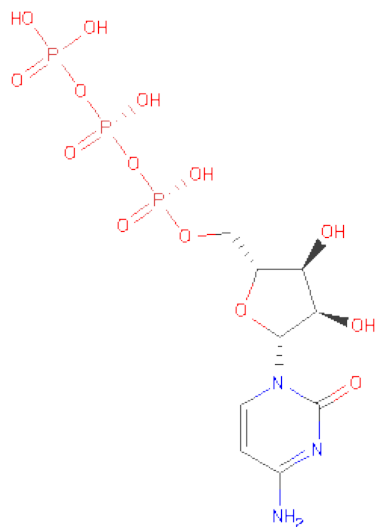
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3').

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').

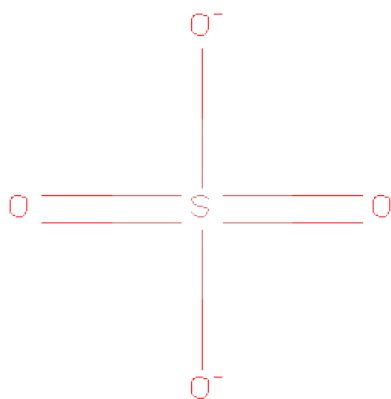
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O	P	0	0	0
			291	89	100	40	53	9			
3	F	12	Total	C	H	N	O	P	0	0	0
			385	119	134	52	69	11			

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_{14}\text{P}_3$).



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: SO_4) (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	343	Total	O		0	0
			343	343			
6	D	659	Total	O		0	0
			659	659			
6	B	29	Total	O		0	0
			29	29			
6	C	48	Total	O		0	0
			48	48			
6	E	30	Total	O		0	0
			30	30			
6	F	59	Total	O		0	0
			59	59			

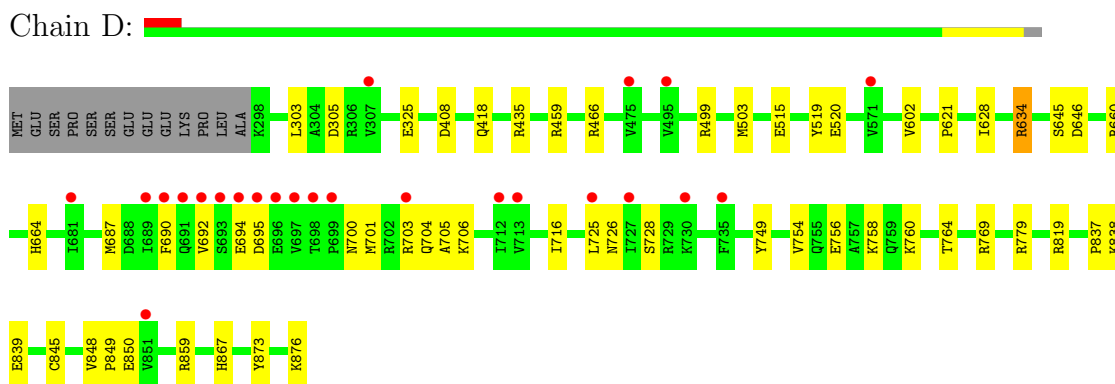
3 Residue-property plots

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.

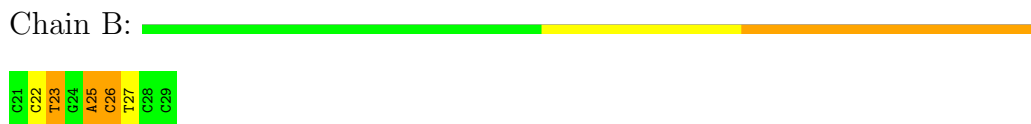
- Molecule 1: DNA polymerase



- 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')

Chain C:



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

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.68Å 109.06Å 150.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.06 – 1.66 71.06 – 1.66	Depositor EDS
% Data completeness (in resolution range)	86.5 (71.06-1.66) 86.5 (71.06-1.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.177 , 0.200 0.178 , 0.200	Depositor DCC
R_{free} test set	6759 reflections (4.32%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 156490 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20794	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.56	0/6085
1	D	0.62	1/4842 (0.0%)	0.71	2/6544 (0.0%)
2	B	1.02	0/173	1.92	9/264 (3.4%)
2	E	1.13	0/173	1.97	5/264 (1.9%)
3	C	1.22	1/215 (0.5%)	1.79	4/331 (1.2%)
3	F	1.24	1/283 (0.4%)	1.88	10/437 (2.3%)
All	All	0.62	3/10193 (0.0%)	0.84	30/13925 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6	DA	N9-C4	-7.53	1.33	1.37
1	D	749	TYR	CB-CG	-5.29	1.43	1.51
3	C	6	DA	N9-C4	-5.00	1.34	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8	DT	O4'-C1'-N1	-12.94	98.94	108.00
3	C	8	DT	O4'-C1'-N1	-9.12	101.61	108.00
2	E	23	DT	O4'-C1'-N1	-8.44	102.09	108.00
2	B	23	DT	O4'-C1'-N1	-7.86	102.50	108.00
2	B	25	DA	O4'-C4'-C3'	-7.33	101.57	104.50
2	B	23	DT	N3-C4-O4	6.90	124.04	119.90
3	F	6	DA	OP1-P-OP2	-6.87	109.30	119.60
3	F	6	DA	C2-N3-C4	-6.72	107.24	110.60
2	E	23	DT	N3-C4-O4	6.52	123.81	119.90
2	E	27	DT	C6-C5-C7	-6.33	119.11	122.90
3	F	10	DA	O4'-C1'-N9	-6.31	103.58	108.00
2	E	23	DT	C5-C4-O4	-6.17	120.58	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	DG	O4'-C4'-C3'	-5.99	102.10	104.50
2	B	25	DA	C5'-C4'-C3'	5.97	124.84	114.10
3	C	12	DG	O4'-C1'-N9	5.88	112.12	108.00
3	F	7	DG	N1-C6-O6	-5.75	116.45	119.90
1	D	634	ARG	CG-CD-NE	-5.62	99.99	111.80
2	B	23	DT	C5-C4-O4	-5.59	120.99	124.90
3	F	6	DA	C5-N7-C8	-5.57	101.11	103.90
1	D	660	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	B	26	DC	O4'-C1'-N1	5.48	111.84	108.00
3	F	4	DG	O5'-P-OP2	-5.42	100.82	105.70
2	E	26	DC	O4'-C1'-N1	5.41	111.78	108.00
2	B	25	DA	O4'-C1'-C2'	5.38	110.20	105.90
3	F	2	DT	O4'-C1'-N1	5.34	111.74	108.00
3	C	11	DG	O4'-C1'-N9	-5.25	104.33	108.00
3	F	9	DC	C2-N3-C4	5.20	122.50	119.90
3	F	4	DG	O4'-C1'-C2'	5.17	110.04	105.90
2	B	25	DA	O5'-P-OP1	5.14	116.87	110.70
2	B	26	DC	N1-C1'-C2'	-5.13	102.85	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4403	4479	0	26	0
1	D	4696	4763	0	47	0
2	B	174	100	0	4	0
2	E	174	100	0	6	0
3	C	191	100	0	0	0
3	F	251	134	0	1	0
4	D	29	12	0	4	0
5	D	20	0	0	0	0
6	A	343	0	0	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	29	0	0	1	0
6	C	48	0	0	0	0
6	D	659	0	0	21	1
6	E	30	0	0	0	0
6	F	59	0	0	0	0
All	All	11106	9688	0	82	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:845:CYS:SG	6:D:1411:HOH:O	2.30	0.85
1:D:705:ALA:N	6:D:1612:HOH:O	2.10	0.84
1:A:821:GLN:O	6:A:1183:HOH:O	2.01	0.79
1:A:676:ARG:HD2	6:A:1220:HOH:O	1.83	0.77
1:D:845:CYS:SG	6:D:1168:HOH:O	2.38	0.76
2:B:27:DT:OP1	6:B:128:HOH:O	2.07	0.72
1:A:408:ASP:OD1	6:A:996:HOH:O	2.06	0.71
1:A:676:ARG:NH1	6:A:1220:HOH:O	2.26	0.68
1:D:305:ASP:OD1	6:D:1627:HOH:O	2.12	0.67
1:D:408:ASP:OD1	6:D:1181:HOH:O	2.13	0.67
1:A:749:TYR:CE2	6:A:951:HOH:O	2.48	0.66
1:D:664:HIS:HD1	1:D:859:ARG:H	1.44	0.65
1:D:459:ARG:NH2	6:D:1489:HOH:O	2.29	0.64
1:A:559:ASP:OD2	6:A:1005:HOH:O	2.14	0.64
1:D:466:ARG:NH1	6:D:1227:HOH:O	2.29	0.64
1:D:779:ARG:NH1	6:D:1590:HOH:O	2.24	0.64
1:D:602[B]:VAL:HG21	1:D:621:PRO:HG3	1.79	0.63
1:D:325:GLU:OE2	6:D:1133:HOH:O	2.15	0.63
1:A:839:GLU:HB2	6:A:1156:HOH:O	1.99	0.61
1:D:418:GLN:OE1	6:D:1261:HOH:O	2.16	0.61
1:A:738:ARG:NH1	6:A:1198:HOH:O	2.32	0.61
1:D:520:GLU:OE2	6:D:1577:HOH:O	2.15	0.61
1:D:706:LYS:NZ	4:D:901:CTP:O1A	2.31	0.61
1:D:692:VAL:HG21	1:D:701:MET:HE1	1.84	0.60
1:D:867:HIS:HD2	6:D:1410:HOH:O	1.84	0.59
1:D:705:ALA:CA	6:D:1612:HOH:O	2.50	0.58
1:A:578:ARG:NH1	2:B:25:DA:H5"	2.22	0.55
1:A:665:ILE:HG22	1:A:749:TYR:CE1	2.43	0.54
1:A:749:TYR:CZ	6:A:951:HOH:O	2.61	0.53
2:B:26:DC:H2'	2:B:27:DT:H73	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:325:GLU:CD	1:D:325:GLU:H	2.12	0.53
4:D:901:CTP:C4'	2:E:29:DOC:H2'	2.38	0.52
1:D:645:SER:O	1:D:646:ASP:HB2	2.10	0.51
1:D:520:GLU:CD	6:D:1577:HOH:O	2.48	0.51
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.94	0.49
1:D:704:GLN:C	6:D:1612:HOH:O	2.48	0.49
4:D:901:CTP:H4'	2:E:29:DOC:H2'	1.94	0.49
2:E:26:DC:H2'	2:E:27:DT:H71	1.94	0.48
1:D:634:ARG:NH1	1:D:873:TYR:CD1	2.82	0.48
1:D:690:PHE:CD1	1:D:701:MET:HE3	2.48	0.48
1:D:876:LYS:NZ	6:D:1471:HOH:O	2.46	0.48
1:D:690:PHE:HB2	1:D:701:MET:HE3	1.97	0.47
1:D:687:MET:HE2	1:D:694:GLU:HA	1.96	0.47
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.44	0.47
1:A:738:ARG:HD3	6:A:1198:HOH:O	2.15	0.47
1:D:754:VAL:HG12	1:D:758:LYS:HE2	1.96	0.46
1:D:837:PRO:HB2	1:D:839[A]:GLU:HG2	1.97	0.46
1:A:519:TYR:CD2	1:A:525:GLU:HG2	2.49	0.46
1:D:850:GLU:OE2	6:D:1538:HOH:O	2.21	0.46
1:D:819:ARG:NE	6:D:1530:HOH:O	2.48	0.46
1:D:756:GLU:OE2	1:D:760:LYS:HE2	2.16	0.46
1:D:695:ASP:OD1	1:D:695:ASP:N	2.48	0.45
1:A:665:ILE:CG2	1:A:749:TYR:CE1	2.99	0.45
1:D:687:MET:HA	1:D:692:VAL:HG22	2.00	0.45
1:D:725:LEU:O	1:D:726:ASN:C	2.54	0.45
1:A:631:GLU:OE2	1:A:635:LYS:NZ	2.46	0.44
1:A:738:ARG:CZ	6:A:1198:HOH:O	2.65	0.44
2:B:22:DC:H2'	2:B:23:DT:H73	1.99	0.44
1:A:340:GLU:HG2	6:A:1216:HOH:O	2.17	0.44
4:D:901:CTP:O4'	2:E:29:DOC:H2'	2.18	0.44
1:D:515:GLU:HG2	1:D:519:TYR:CE2	2.52	0.44
1:A:739:TYR:C	1:A:739:TYR:CD2	2.91	0.44
1:A:749:TYR:OH	6:A:951:HOH:O	2.19	0.43
1:A:541:LYS:HE3	6:A:1211:HOH:O	2.18	0.43
1:D:838:LYS:NZ	1:D:839[B]:GLU:OE2	2.48	0.43
1:D:602[B]:VAL:O	1:D:602[B]:VAL:HG13	2.19	0.43
1:D:848:VAL:HB	1:D:849:PRO:HD3	2.01	0.42
2:E:21:DC:H2'	2:E:22:DC:C6	2.54	0.42
1:A:517:ARG:NH2	1:A:521:LEU:HD21	2.33	0.42
1:D:716:ILE:HD12	3:F:3:DG:C8	2.54	0.42
1:A:722:ALA:HB2	1:A:729:ARG:HA	2.01	0.42
1:D:703:ARG:NH2	6:D:1291:HOH:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:602[B]:VAL:CG2	1:D:621:PRO:HG3	2.49	0.41
1:D:435:ARG:NH2	6:D:1247:HOH:O	2.37	0.41
2:E:26:DC:H2"	2:E:27:DT:O5'	2.21	0.41
1:D:499:ARG:HG2	1:D:503:MET:HE2	2.02	0.41
1:A:725:LEU:HB2	1:A:727:ILE:HG12	2.03	0.41
1:D:705:ALA:HA	6:D:1612:HOH:O	2.19	0.41
1:A:440:GLU:HB3	1:A:441:PRO:HD3	2.03	0.41
1:D:764:THR:HA	1:D:769:ARG:O	2.21	0.41
1:D:692:VAL:CG2	1:D:701:MET:HE1	2.51	0.40
1:A:459:ARG:HB3	1:A:460:PRO:HD3	2.03	0.40

All (1) 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	Distance(Å)	Clash(Å)
6:A:1027:HOH:O	6:D:1404:HOH:O[2_745]	1.88	0.32

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%)	13 (2%)	0	100	100
1	D	591/592 (100%)	576 (98%)	14 (2%)	1 (0%)	56	29
All	All	1137/1184 (96%)	1109 (98%)	27 (2%)	1 (0%)	59	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	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%)	467 (99%)	3 (1%)	92	83
1	D	508/507 (100%)	505 (99%)	3 (1%)	92	83
All	All	978/1014 (96%)	972 (99%)	6 (1%)	92	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ARG
1	A	477	LEU
1	A	544	LEU
1	D	303	LEU
1	D	700	ASN
1	D	728	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	A	479	GLN
1	A	502	GLN
1	A	510	GLN
1	A	573	ASN
1	A	670	ASN
1	A	724	ASN
1	D	405	GLN
1	D	502	GLN
1	D	670	ASN
1	D	726	ASN
1	D	755	GLN
1	D	782	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	17,19,20	0.81	0	20,26,29	1.30	2 (10%)
2	DOC	E	29	3,2	17,19,20	0.88	2 (11%)	20,26,29	2.40	4 (20%)

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	-	0/5/18/19	0/2/2/2
2	DOC	E	29	3,2	-	0/5/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	DOC	C6-C5	-2.07	1.33	1.38
2	E	29	DOC	C2-N1	2.01	1.40	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	C6-C5-C4	6.88	120.33	117.47
2	E	29	DOC	C4'-O4'-C1'	-5.69	107.68	110.05
2	B	29	DOC	C4'-O4'-C1'	-3.44	108.61	110.05
2	E	29	DOC	O4'-C4'-C5'	-3.34	105.00	109.67
2	E	29	DOC	C5-C6-N1	-3.28	117.50	121.21
2	B	29	DOC	C2-N3-C4	2.80	119.63	115.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	30,30,30	1.78	5 (16%)	44,47,47	1.48	5 (11%)
5	SO4	D	902	-	4,4,4	0.35	0	6,6,6	0.12	0
5	SO4	D	903	-	4,4,4	0.38	0	6,6,6	0.61	0
5	SO4	D	904	-	4,4,4	0.21	0	6,6,6	0.18	0
5	SO4	D	905	-	4,4,4	0.09	0	6,6,6	0.14	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	-	-	0/20/38/38	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	CTP	O2-C2	5.39	1.34	1.23
4	D	901	CTP	C2'-C1'	-3.45	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	901	CTP	C4-N4	2.73	1.43	1.35
4	D	901	CTP	C2-N3	2.66	1.42	1.35
4	D	901	CTP	PA-O3A	-2.36	1.55	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	CTP	C6-C5-C4	5.65	119.82	117.47
4	D	901	CTP	C2-N3-C4	3.24	120.26	115.57
4	D	901	CTP	PB-O3B-PG	-2.72	123.72	131.68
4	D	901	CTP	O2B-PB-O3B	2.41	116.57	105.14
4	D	901	CTP	C2'-C1'-N1	2.17	118.84	113.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	546/592 (92%)	0.62	64 (11%) 5 4	22, 41, 67, 94	0
1	D	579/592 (97%)	0.21	24 (4%) 35 35	11, 24, 47, 84	0
2	B	9/9 (100%)	-0.34	0 100 100	27, 31, 42, 50	0
2	E	9/9 (100%)	-0.08	0 100 100	19, 24, 40, 50	0
3	C	9/13 (69%)	-0.58	0 100 100	21, 26, 34, 42	0
3	F	12/13 (92%)	0.06	1 (8%) 11 9	16, 25, 65, 76	0
All	All	1164/1228 (94%)	0.38	89 (7%) 14 12	11, 32, 62, 94	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	689	ILE	7.9
1	A	297	ALA	7.5
1	A	816	LYS	6.4
1	A	298	LYS	6.3
1	A	677	ARG	5.3
1	A	848	VAL	5.1
1	D	691	GLN	4.8
1	D	698	THR	4.7
1	A	842	GLU	4.6
1	D	727	ILE	4.6
1	A	864	VAL	4.6
1	A	736	ILE	4.5
1	D	697	VAL	4.5
1	D	725	LEU	4.4
1	A	819	ARG	4.3
1	A	844	LEU	4.2
1	A	495	VAL	4.2
1	A	636	ILE	4.2
1	D	735	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	338	VAL	4.0
1	A	868	TYR	3.9
1	A	518	ILE	3.9
1	A	866	TYR	3.8
1	A	862	LEU	3.8
1	A	588	ILE	3.8
1	A	448	VAL	3.7
1	A	337	VAL	3.6
1	A	514	VAL	3.6
1	A	528	ILE	3.6
1	D	699	PRO	3.5
1	A	475	VAL	3.5
1	D	695	ASP	3.4
1	A	846	ARG	3.3
1	A	571	VAL	3.2
1	A	442	VAL	3.2
1	A	727	ILE	3.2
1	A	845	CYS	3.1
1	D	712	ILE	3.1
1	D	693	SER	3.1
1	A	843	ARG	3.0
1	A	320	VAL	3.0
1	A	641	VAL	3.0
1	A	307	VAL	2.9
1	A	740	PHE	2.8
1	D	690	PHE	2.8
1	D	681	ILE	2.8
1	A	739	TYR	2.7
1	A	313	ALA	2.6
1	A	350	THR	2.6
1	A	360	TRP	2.6
1	A	828	VAL	2.5
1	A	851	VAL	2.5
1	A	860	VAL	2.5
1	A	820	LEU	2.5
1	A	661	VAL	2.4
1	D	307	VAL	2.4
1	D	730	LYS	2.4
1	D	696	GLU	2.4
1	D	692	VAL	2.4
1	A	847	LEU	2.4
3	F	1	DA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	513	THR	2.4
1	D	495	VAL	2.4
1	D	713	VAL	2.4
1	D	475[A]	VAL	2.3
1	A	303	LEU	2.3
1	A	809	ILE	2.3
1	D	703	ARG	2.3
1	A	716	ILE	2.3
1	A	725	LEU	2.3
1	A	306	ARG	2.3
1	A	302	THR	2.2
1	A	856	VAL	2.2
1	A	786	PHE	2.2
1	A	630	LEU	2.2
1	D	694	GLU	2.2
1	A	863	LYS	2.2
1	A	628	ILE	2.2
1	A	594	VAL	2.2
1	A	454	ILE	2.1
1	A	308	THR	2.1
1	A	353	ALA	2.1
1	A	814	ARG	2.1
1	A	815	LEU	2.1
1	A	833[A]	ILE	2.1
1	D	851[A]	VAL	2.1
1	D	571	VAL	2.0
1	A	665	ILE	2.0
1	A	657	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	DOC	E	29	18/19	0.12	0.06	15,19,26,26	0
2	DOC	B	29	18/19	0.10	-0.22	30,36,43,45	0

6.3 Carbohydrates ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	D	904	5/5	0.23	2.22	59,67,69,69	0
5	SO4	D	905	5/5	0.15	1.15	62,67,69,69	0
4	CTP	D	901	29/29	0.10	-0.03	21,28,42,50	0
5	SO4	D	903	5/5	0.08	-0.50	33,37,42,47	0
5	SO4	D	902	5/5	0.10	-0.53	40,40,45,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.