



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:33 AM GMT

PDB ID : 4EZ9
Title : Bacillus DNA Polymerase I Large Fragment Complex 2
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-05-02
Resolution : 1.64 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>

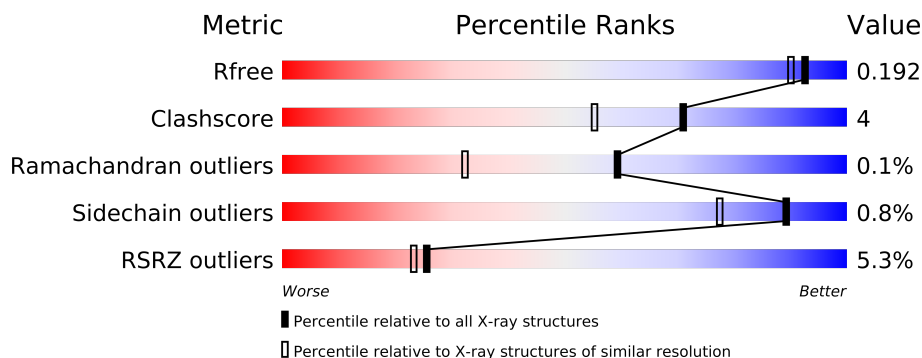
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.64 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	1326 (1.66-1.62)
Clashscore	79885	1525 (1.66-1.62)
Ramachandran outliers	78287	1490 (1.66-1.62)
Sidechain outliers	78261	1490 (1.66-1.62)
RSRZ outliers	66119	1326 (1.66-1.62)

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	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21531 atoms, of which 9964 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	578	Total	C	H	N	O	S	0	2	0
			9362	2955	4718	805	867	17			
1	D	579	Total	C	H	N	O	S	0	9	0
			9457	2986	4771	809	873	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	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*(2DT))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	9	Total	C	H	N	O	P	0	0	0
			276	86	101	28	53	8			
2	E	9	Total	C	H	N	O	P	0	0	0
			276	86	101	28	53	8			

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

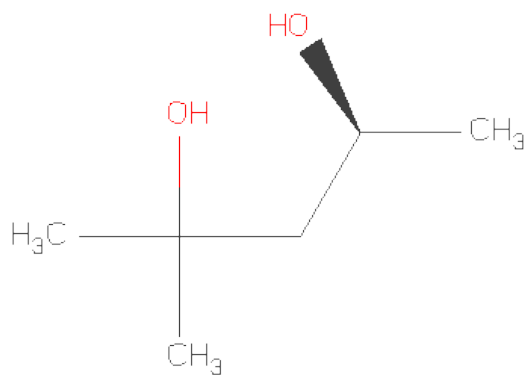
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	0
			354	109	124	44	66	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			383	119	135	49	69	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



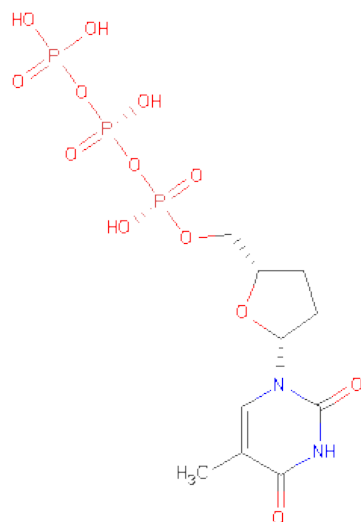
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 6 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: D3T) (formula: $C_{10}H_{17}N_2O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			28	10	2	13	3		

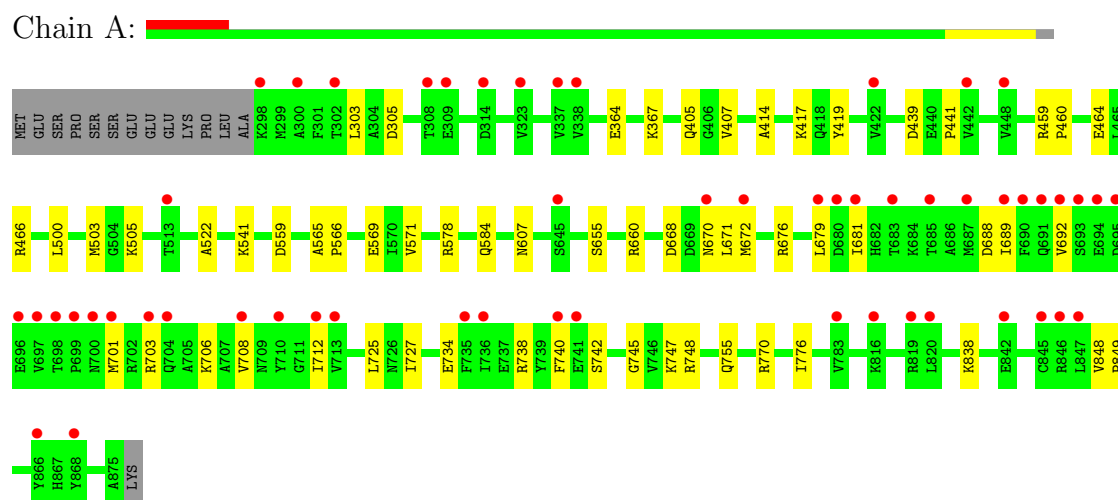
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	442	Total	O	0	0
			442	442		
7	D	710	Total	O	0	0
			710	710		
7	B	39	Total	O	0	0
			39	39		
7	C	69	Total	O	0	0
			69	69		
7	E	34	Total	O	0	0
			34	34		
7	F	69	Total	O	0	0
			69	69		

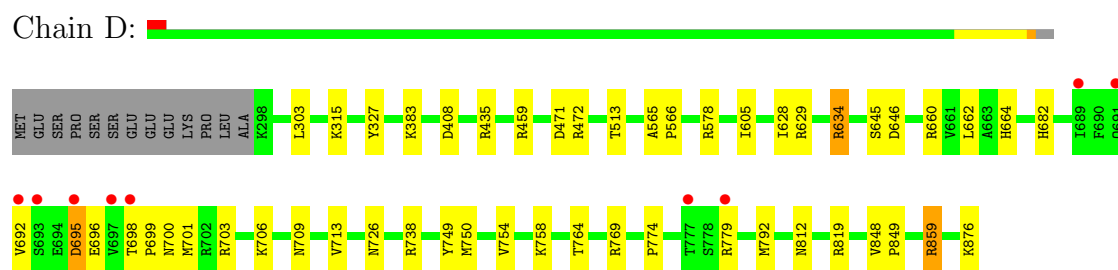
3 Residue-property plots

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*(2DT))-3')

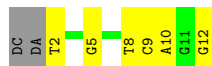


- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(2DT))-3')



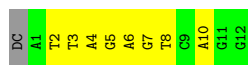
- Molecule 3: DNA (5'-D(*CP*AP*TP*TP*AP*GP*AP*GP*TP*CP*AP*GP*G)-3')

Chain C: 



- Molecule 3: DNA (5'-D(*CP*AP*TP*TP*AP*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	93.92Å 108.96Å 149.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 1.64 43.13 – 1.64	Depositor EDS
% Data completeness (in resolution range)	86.2 (43.12-1.64) 86.2 (43.13-1.64)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 1.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.168 , 0.191 0.169 , 0.192	Depositor DCC
R_{free} test set	7356 reflections (4.55%)	DCC
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 161682 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21531	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: 2DT, D3T, SO4, MPD

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	0.42	0/4734	0.56	0/6400
1	D	0.59	0/4801	0.71	4/6489 (0.1%)
2	B	1.12	0/173	1.95	7/264 (2.7%)
2	E	1.10	0/173	2.02	7/264 (2.7%)
3	C	1.07	0/258	1.76	4/397 (1.0%)
3	F	1.11	1/279 (0.4%)	1.72	8/430 (1.9%)
All	All	0.58	1/10418 (0.0%)	0.83	30/14244 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	7	DG	N7-C5	6.06	1.42	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	DT	O4'-C1'-N1	-9.98	101.01	108.00
3	F	8	DT	O4'-C1'-N1	-9.80	101.14	108.00
2	E	23	DT	O4'-C1'-N1	-9.63	101.26	108.00
3	C	8	DT	O4'-C1'-N1	-8.29	102.20	108.00
2	E	25	DA	O5'-P-OP2	-7.87	98.62	105.70
1	D	634	ARG	NE-CZ-NH1	7.78	124.19	120.30
3	C	2	DT	O4'-C1'-N1	7.37	113.16	108.00
1	D	634	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	E	25	DA	C5'-C4'-C3'	7.08	126.84	114.10
2	E	26	DC	O4'-C4'-C3'	6.97	110.19	106.00
2	B	23	DT	N3-C4-O4	6.93	124.06	119.90
3	F	10	DA	O4'-C1'-N9	-6.59	103.39	108.00
2	E	25	DA	O4'-C4'-C3'	-6.38	101.95	104.50
3	C	5	DG	O4'-C4'-C3'	-6.38	101.95	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	DT	O4'-C1'-N1	6.34	112.44	108.00
2	B	25	DA	C5'-C4'-C3'	6.16	125.19	114.10
1	D	859	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	B	25	DA	O4'-C4'-C3'	-5.94	102.12	104.50
2	E	26	DC	O4'-C1'-N1	5.73	112.01	108.00
3	F	6	DA	C5-C6-N1	-5.52	114.94	117.70
2	B	21	DC	O4'-C1'-C2'	5.48	110.28	105.90
2	B	25	DA	C1'-O4'-C4'	-5.48	104.62	110.10
3	F	6	DA	C2-N3-C4	-5.47	107.86	110.60
2	B	23	DT	C6-C5-C7	-5.42	119.64	122.90
3	C	5	DG	N3-C4-N9	-5.42	122.75	126.00
2	E	25	DA	O5'-P-OP1	5.41	117.19	110.70
1	D	660	ARG	NE-CZ-NH1	5.40	123.00	120.30
3	F	5	DG	O4'-C4'-C3'	-5.39	102.34	104.50
3	F	4	DA	O4'-C1'-C2'	5.19	110.05	105.90
3	F	3	DT	O4'-C1'-C2'	5.08	109.97	105.90

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	4644	4718	0	38	0
1	D	4686	4771	0	48	0
2	B	175	101	0	3	0
2	E	175	101	0	1	0
3	C	230	124	0	2	0
3	F	248	135	0	0	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	8	14	0	0	0
6	D	28	0	13	0	0
7	A	442	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	39	0	0	1	0
7	C	69	0	0	1	0
7	D	710	0	0	19	1
7	E	34	0	0	0	0
7	F	69	0	0	0	0
All	All	11567	9964	13	90	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 (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:749[A]:TYR:CE2	1:D:750[A]:MET:SD	2.57	0.97
1:D:459:ARG:NH1	7:D:1617:HOH:O	2.08	0.86
1:D:812[A]:ASN:OD1	7:D:1422:HOH:O	1.94	0.84
1:D:629:ARG:NH1	7:D:1218:HOH:O	2.11	0.84
1:D:472:ARG:NH2	7:D:1167:HOH:O	2.12	0.83
1:D:749[A]:TYR:CD2	1:D:750[A]:MET:SD	2.71	0.83
1:D:726:ASN:HB3	7:D:1614:HOH:O	1.80	0.80
1:D:471:ASP:OD2	7:D:1475:HOH:O	2.02	0.76
1:D:459:ARG:NH2	7:D:1657:HOH:O	2.19	0.75
1:D:749[A]:TYR:HE2	1:D:750[A]:MET:SD	2.09	0.74
1:D:408:ASP:OD1	7:D:1552:HOH:O	2.07	0.72
1:D:662:LEU:HD22	1:D:713[B]:VAL:HG21	1.72	0.71
1:A:607:ASN:OD1	7:A:1330:HOH:O	2.13	0.66
1:D:513:THR:OG1	7:D:1493:HOH:O	2.14	0.66
1:D:664:HIS:HD1	1:D:859:ARG:H	1.43	0.66
1:A:584:GLN:HG3	7:A:1353:HOH:O	1.96	0.65
1:A:770:ARG:NH2	7:A:1422:HOH:O	2.29	0.64
1:A:367:LYS:NZ	7:A:1439:HOH:O	2.31	0.62
1:A:703:ARG:NH2	7:A:1200:HOH:O	2.26	0.61
1:D:749[A]:TYR:CE2	1:D:750[A]:MET:CE	2.83	0.61
1:D:738:ARG:HD3	7:D:1411:HOH:O	2.01	0.61
1:D:383:LYS:HE3	7:D:1416:HOH:O	2.01	0.60
1:D:749[A]:TYR:HE2	1:D:750[A]:MET:CE	2.15	0.60
1:A:655:SER:O	1:A:660:ARG:NH1	2.35	0.59
1:D:754:VAL:HG12	1:D:758:LYS:HE2	1.86	0.58
1:A:672:MET:CE	1:A:676:ARG:NH2	2.68	0.57
1:D:819:ARG:NH1	7:D:1611:HOH:O	2.39	0.55
1:D:315:LYS:HD2	7:D:1405:HOH:O	2.07	0.54
1:D:383:LYS:NZ	7:D:1362:HOH:O	2.41	0.54
1:D:709:ASN:O	1:D:713[B]:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:22:DC:H2'	2:B:23:DT:H71	1.90	0.52
1:D:578:ARG:NH1	2:E:25:DA:H5''	2.24	0.52
1:D:692:VAL:HB	1:D:696:GLU:HB2	1.92	0.52
1:D:682:HIS:CG	1:D:706:LYS:HG2	2.44	0.52
1:A:364:GLU:HG2	7:A:1439:HOH:O	2.10	0.51
1:D:726:ASN:CB	7:D:1614:HOH:O	2.47	0.51
1:A:708:VAL:O	1:A:712:ILE:HG12	2.12	0.50
1:A:689:ILE:O	1:A:738:ARG:NH1	2.44	0.49
1:A:740:PHE:CG	1:A:747:LYS:HD3	2.47	0.49
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.93	0.49
1:D:695:ASP:N	1:D:695:ASP:OD2	2.45	0.49
1:D:698:THR:HB	1:D:701:MET:SD	2.53	0.49
3:C:12:DG:H1'	7:C:141:HOH:O	2.13	0.49
1:A:464:GLU:OE1	7:A:1189:HOH:O	2.20	0.48
1:A:565:ALA:HA	1:A:571:VAL:CG2	2.43	0.48
1:A:671:LEU:HD12	1:A:681:ILE:HD11	1.96	0.48
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.42	0.48
1:D:435:ARG:NH2	7:D:1495:HOH:O	2.43	0.47
1:A:522:ALA:O	1:A:541:LYS:HE2	2.14	0.47
1:D:698:THR:HG22	1:D:700:ASN:H	1.78	0.47
1:A:838:LYS:NZ	7:A:1349:HOH:O	2.33	0.47
1:D:698:THR:HG23	1:D:699:PRO:HD2	1.97	0.47
1:A:670:ASN:ND2	1:A:742:SER:O	2.48	0.47
1:A:459:ARG:HB3	1:A:460:PRO:HD3	1.97	0.47
1:A:569:GLU:HA	7:A:1298:HOH:O	2.14	0.46
1:A:688:ASP:HB3	1:A:742:SER:HG	1.80	0.46
1:A:405:GLN:HB3	1:A:407:VAL:HG23	1.97	0.46
1:D:749[A]:TYR:HD2	1:D:750[A]:MET:SD	2.36	0.46
1:D:565:ALA:N	1:D:566:PRO:CD	2.79	0.46
1:D:764:THR:HA	1:D:769:ARG:O	2.16	0.46
1:D:315:LYS:NZ	7:D:1405:HOH:O	2.41	0.45
3:C:9:DC:H2'	3:C:10:DA:C8	2.52	0.45
1:D:848:VAL:HB	1:D:849:PRO:HD3	1.98	0.45
1:A:668:ASP:OD2	1:A:745:GLY:N	2.50	0.45
1:A:738:ARG:O	1:A:742:SER:OG	2.35	0.44
1:A:692:VAL:HG21	1:A:701:MET:HE1	1.99	0.44
1:A:734:GLU:O	1:A:738:ARG:HG3	2.17	0.43
1:D:645:SER:O	1:D:646:ASP:HB2	2.18	0.43
1:D:634:ARG:HH22	1:D:876:LYS:HA	1.84	0.43
1:A:565:ALA:N	1:A:566:PRO:CD	2.82	0.43
1:A:505:LYS:NZ	7:A:1136:HOH:O	2.41	0.43
1:A:755:GLN:HG2	7:A:1112:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:776:ILE:HG13	1:A:776:ILE:O	2.18	0.42
1:A:748:ARG:NE	7:A:1417:HOH:O	2.47	0.42
2:B:22:DC:P	7:B:137:HOH:O	2.77	0.42
1:A:466:ARG:NH1	7:A:1424:HOH:O	2.51	0.41
1:A:500:LEU:HA	1:A:503:MET:HE3	2.01	0.41
1:A:578:ARG:NH1	2:B:25:DA:H5"	2.35	0.41
1:D:749[A]:TYR:CD2	1:D:750[A]:MET:CE	3.03	0.41
1:D:774:PRO:HA	7:D:1446:HOH:O	2.20	0.41
1:D:749[A]:TYR:HE2	1:D:750[A]:MET:HE3	1.84	0.41
1:D:700:ASN:OD1	1:D:703:ARG:NH2	2.54	0.40
1:A:747:LYS:HD2	1:A:747:LYS:HA	1.80	0.40
1:D:327:TYR:HH	1:D:605:ILE:HG23	1.86	0.40
1:D:750[A]:MET:SD	1:D:792:MET:HB3	2.61	0.40
1:A:439:ASP:OD2	1:A:441:PRO:HD2	2.21	0.40
1:A:725:LEU:HB2	1:A:727:ILE:HG12	2.04	0.40
1:A:414:ALA:HB1	1:A:419:TYR:HB3	2.03	0.40
1:D:779:ARG:NH1	7:D:1636:HOH:O	2.53	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)
7:D:1649:HOH:O	7:D:1659:HOH:O[3_854]	2.18	0.02

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	578/592 (98%)	564 (98%)	14 (2%)	0	100	100
1	D	586/592 (99%)	572 (98%)	13 (2%)	1 (0%)	56	29
All	All	1164/1184 (98%)	1136 (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	496/507 (98%)	490 (99%)	6 (1%)	82	62
1	D	503/507 (99%)	501 (100%)	2 (0%)	95	91
All	All	999/1014 (98%)	991 (99%)	8 (1%)	89	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	305	ASP
1	A	417	LYS
1	A	559	ASP
1	A	679	LEU
1	A	706	LYS
1	D	303	LEU
1	D	695	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	A	470	GLN
1	A	516	GLN
1	A	529	ASN
1	A	573	ASN
1	A	584	GLN
1	A	670	ASN
1	A	724	ASN
1	D	405	GLN
1	D	502	GLN
1	D	670	ASN
1	D	724	ASN

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Mol	Chain	Res	Type
1	D	755	GLN
1	D	793	ASN
1	D	854	GLN

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	2DT	B	29	3,2	18,20,21	1.03	0	20,28,31	1.72	4 (20%)
2	2DT	E	29	3,2	18,20,21	0.89	1 (5%)	20,28,31	1.94	3 (15%)

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	2DT	B	29	3,2	-	0/5/18/19	0/2/2/2
2	2DT	E	29	3,2	-	0/5/18/19	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	2DT	C6-C5	-2.19	1.34	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	2DT	C6-N1-C2	-6.58	120.54	122.41
2	B	29	2DT	C6-N1-C2	-5.51	120.84	122.41
2	E	29	2DT	C4'-O4'-C1'	-2.95	108.82	110.05
2	B	29	2DT	C5M-C5-C6	2.51	123.92	118.59
2	B	29	2DT	C5M-C5-C4	-2.42	118.58	121.04
2	B	29	2DT	C5-C6-N1	2.28	123.81	121.59
2	E	29	2DT	C3'-C2'-C1'	2.22	105.25	102.80

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 ⓘ

4 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	SO4	A	901	-	4,4,4	0.15	0	6,6,6	0.25	0
5	MPD	A	902	-	7,7,7	0.32	0	10,10,10	0.78	0
6	D3T	D	901	-	29,29,29	1.72	4 (13%)	40,45,45	1.41	4 (10%)
4	SO4	D	902	-	4,4,4	0.43	0	6,6,6	0.54	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	SO4	A	901	-	-	0/0/0/0	0/0/0/0
5	MPD	A	902	-	-	0/5/5/5	0/0/0/0
6	D3T	D	901	-	-	0/19/31/31	0/2/2/2
4	SO4	D	902	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	901	D3T	O4-C4	5.04	1.34	1.24
6	D	901	D3T	C2-N1	-4.92	1.33	1.38
6	D	901	D3T	PA-O3A	-2.74	1.54	1.59
6	D	901	D3T	C3'-C2'	-2.72	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	901	D3T	N3-C2-N1	5.09	120.22	115.97
6	D	901	D3T	C5-C6-N1	-3.95	117.74	121.59
6	D	901	D3T	C4-N3-C2	-2.10	121.08	125.39
6	D	901	D3T	C3'-C2'-C1'	2.05	105.07	102.80

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	578/592 (97%)	0.46	55 (9%) 8 7	14, 34, 66, 108	0
1	D	579/592 (97%)	0.03	9 (1%) 68 71	9, 21, 38, 56	0
2	B	9/9 (100%)	-0.18	0 100 100	19, 22, 40, 48	0
2	E	9/9 (100%)	-0.32	0 100 100	13, 17, 37, 48	0
3	C	11/13 (84%)	-0.12	0 100 100	16, 20, 49, 59	0
3	F	12/13 (92%)	-0.24	0 100 100	12, 17, 37, 48	0
All	All	1198/1228 (97%)	0.23	64 (5%) 25 23	9, 27, 56, 108	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	PRO	9.8
1	A	689	ILE	9.2
1	A	697	VAL	8.4
1	A	692	VAL	8.2
1	A	703	ARG	7.2
1	A	679	LEU	6.9
1	A	690	PHE	6.3
1	A	698	THR	5.6
1	A	298	LYS	5.1
1	A	816	LYS	5.0
1	A	691	GLN	4.8
1	A	819	ARG	4.5
1	D	692	VAL	4.3
1	A	846	ARG	4.1
1	A	708	VAL	3.9
1	A	842	GLU	3.6
1	A	681	ILE	3.5
1	A	448	VAL	3.4
1	A	694	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	735	PHE	3.3
1	A	337	VAL	3.3
1	A	868	TYR	3.1
1	D	691	GLN	3.1
1	A	740	PHE	3.1
1	A	845	CYS	3.0
1	A	736	ILE	2.9
1	A	687	MET	2.9
1	A	866	TYR	2.9
1	A	683	THR	2.9
1	A	695	ASP	2.9
1	A	700	ASN	2.8
1	A	713	VAL	2.8
1	A	847	LEU	2.8
1	A	701	MET	2.8
1	A	309	GLU	2.7
1	D	689	ILE	2.7
1	A	672	MET	2.6
1	A	820	LEU	2.6
1	A	783	VAL	2.6
1	A	741	GLU	2.6
1	A	704	GLN	2.5
1	D	698	THR	2.5
1	D	779	ARG	2.5
1	A	710	TYR	2.5
1	A	693	SER	2.4
1	A	338	VAL	2.4
1	A	422	VAL	2.4
1	A	680	ASP	2.4
1	A	513	THR	2.4
1	D	695	ASP	2.4
1	D	697	VAL	2.3
1	A	685	THR	2.3
1	A	645	SER	2.3
1	A	696	GLU	2.2
1	D	777	THR	2.2
1	A	300	ALA	2.2
1	A	670	ASN	2.2
1	A	314	ASP	2.1
1	A	712	ILE	2.1
1	A	308	THR	2.1
1	D	693	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	323[A]	VAL	2.0
1	A	302	THR	2.0
1	A	442	VAL	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	2DT	E	29	19/20	0.11	0.27	12,15,19,19	0
2	2DT	B	29	19/20	0.09	-0.36	17,23,29,34	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
6	D3T	D	901	28/28	0.11	0.50	12,16,22,24	0
4	SO4	A	901	5/5	0.11	0.29	30,33,35,35	0
4	SO4	D	902	5/5	0.07	-0.53	25,26,35,40	0
5	MPD	A	902	8/8	0.09	-1.10	16,26,38,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.