



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:18 AM GMT

PDB ID : 4F3O
Title : DNA Polymerase I Large Fragment Complex 5
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-05-09
Resolution : 1.57 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>

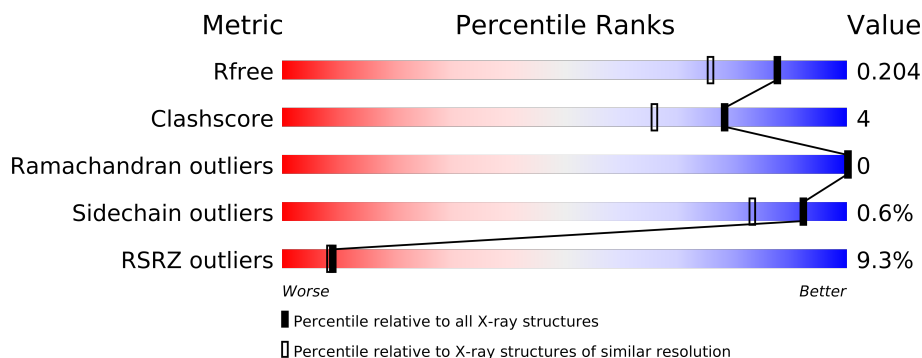
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.57 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	2778 (1.60-1.56)
Clashscore	79885	3207 (1.60-1.56)
Ramachandran outliers	78287	3107 (1.60-1.56)
Sidechain outliers	78261	3104 (1.60-1.56)
RSRZ outliers	66119	2778 (1.60-1.56)

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	MPD	A	903	-	X
6	MN	D	904	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21393 atoms, of which 9882 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	566	Total	C	H	N	O	S	0	2	0
			9177	2894	4628	794	845	16			
1	D	579	Total	C	H	N	O	S	0	9	0
			9459	2985	4770	812	875	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

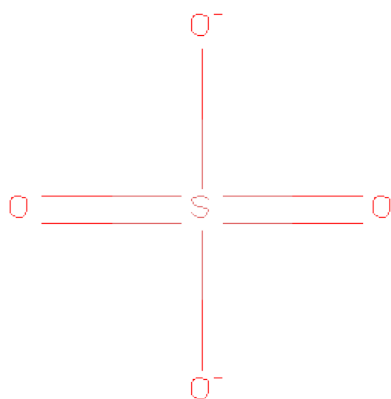
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(2DT))-3').

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(*C*AP*TP*GP*AP*GP*AP*GP*TP*CP*AP*GP*G)-3').

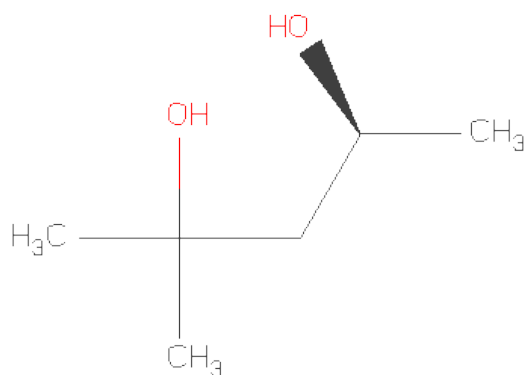
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	12	Total	C	H	N	O	P	0	0	0
			384	119	134	52	68	11			
3	F	12	Total	C	H	N	O	P	0	0	0
			384	119	134	52	68	11			

- 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	A	1	Total	O	S	0	0
			5	4	1		
4	D	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).

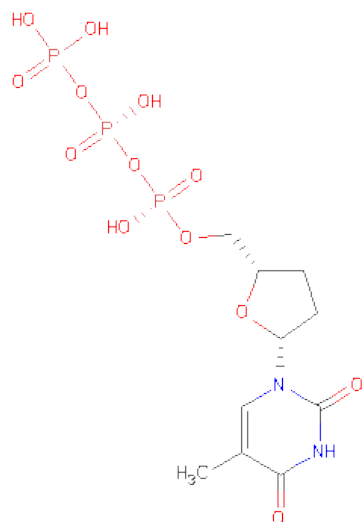


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn	0	0
			1	1		
6	D	1	Total	Mn	0	0
			1	1		

- Molecule 7 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: D3T) (formula: C₁₀H₁₇N₂O₁₃P₃).



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

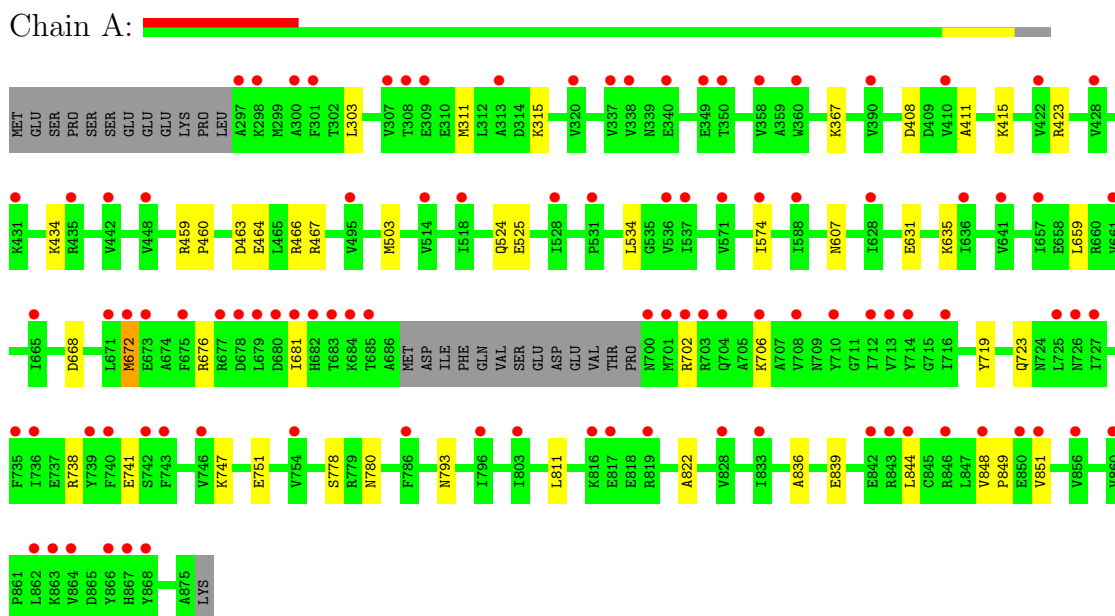
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	406	Total	O	0	0
			406	406		
8	C	64	Total	O	0	0
			64	64		
8	D	762	Total	O	0	0
			762	762		
8	B	31	Total	O	0	0
			31	31		
8	E	32	Total	O	0	0
			32	32		
8	F	70	Total	O	0	0
			70	70		

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

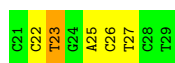


- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(2DT))-3')



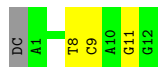
- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(2DT))-3')





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

Chain C:
Sequence logo for Chain C. The y-axis represents the conservation of each nucleotide position. The x-axis lists the positions: C21, C22, T23, G24, A25, C26, T27, C28, T29. The colors of the bars indicate the nucleotide: C (green), T (yellow), G (orange), and A (red).



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

Chain F:
Sequence logo for Chain F. The y-axis represents the conservation of each nucleotide position. The x-axis lists the positions: DC, A1, T8, C9, A10, G11, G12. The colors of the bars indicate the nucleotide: C (green), T (yellow), G (orange), and A (red).



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.83Å 109.33Å 150.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.56 – 1.57 79.57 – 1.57	Depositor EDS
% Data completeness (in resolution range)	89.3 (79.56-1.57) 89.3 (79.57-1.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.179 , 0.204 0.180 , 0.204	Depositor DCC
R_{free} test set	8784 reflections (4.58%)	DCC
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.3	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 191803 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21393	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, MPD, MN, D3T, 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	0.41	0/4636	0.56	0/6264
1	D	0.60	0/4800	0.69	3/6487 (0.0%)
2	B	1.03	0/173	1.89	7/264 (2.7%)
2	E	1.08	0/173	2.09	8/264 (3.0%)
3	C	0.88	0/282	1.50	4/435 (0.9%)
3	F	1.14	1/282 (0.4%)	1.77	8/435 (1.8%)
All	All	0.58	1/10346 (0.0%)	0.82	30/14149 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	DG	N7-C5	5.09	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	-10.09	100.94	108.00
3	F	8	DT	O4'-C1'-N1	-9.60	101.28	108.00
3	C	8	DT	O4'-C1'-N1	-9.43	101.40	108.00
2	E	27	DT	N3-C4-O4	8.90	125.24	119.90
2	E	25	DA	O5'-P-OP2	-8.60	97.96	105.70
2	E	26	DC	O4'-C1'-N1	8.21	113.75	108.00
3	F	2	DT	O4'-C1'-N1	7.51	113.25	108.00
1	D	634	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	B	27	DT	O4'-C4'-C3'	-7.22	101.61	104.50
3	F	11	DG	O4'-C1'-N9	-7.00	103.10	108.00
1	D	634	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	E	23	DT	O4'-C1'-N1	-6.55	103.41	108.00
3	F	4	DA	O4'-C4'-C3'	6.37	109.82	106.00
2	E	22	DC	O4'-C1'-N1	-6.35	103.55	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	27	DT	C4'-C3'-C2'	-6.19	97.53	103.10
2	E	27	DT	C5-C4-O4	-6.00	120.70	124.90
3	F	9	DC	C2-N3-C4	5.57	122.69	119.90
2	E	25	DA	O5'-P-OP1	5.55	117.36	110.70
2	B	25	DA	O4'-C4'-C3'	-5.55	102.28	104.50
2	B	26	DC	O4'-C4'-C3'	5.53	109.32	106.00
3	F	5	DG	N9-C4-C5	5.40	107.56	105.40
3	F	10	DA	O4'-C1'-N9	-5.38	104.24	108.00
1	D	653	ASP	CB-CG-OD1	5.33	123.10	118.30
2	B	23	DT	N3-C4-O4	5.31	123.09	119.90
3	C	9	DC	C1'-O4'-C4'	-5.28	104.82	110.10
3	C	11	DG	O4'-C1'-N9	-5.23	104.34	108.00
3	F	2	DT	C4-C5-C7	5.20	122.12	119.00
2	B	25	DA	O5'-P-OP1	5.20	116.94	110.70
2	B	23	DT	C5-C4-O4	-5.12	121.31	124.90
3	C	9	DC	O4'-C1'-N1	-5.01	104.50	108.00

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	4549	4628	0	34	0
1	D	4689	4770	0	34	0
2	B	175	101	0	0	0
2	E	175	101	0	1	0
3	C	250	134	0	0	0
3	F	250	134	0	1	0
4	A	10	0	0	0	0
4	D	10	0	0	1	0
5	A	8	14	0	1	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	28	0	13	1	0
8	A	406	0	0	17	0
8	B	31	0	0	0	0
8	C	64	0	0	0	0
8	D	762	0	0	18	1
8	E	32	0	0	1	0
8	F	70	0	0	1	0
All	All	11511	9882	13	71	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 (71) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:702:ARG:NH2	7:D:901:D3T:O2G	1.96	0.98
3:F:11:DG:OP1	8:F:149:HOH:O	1.84	0.95
1:D:750:MET:HG3	8:D:1355:HOH:O	1.67	0.93
1:A:607[A]:ASN:OD1	8:A:1172:HOH:O	1.99	0.78
1:A:676:ARG:NH1	8:A:1141:HOH:O	2.19	0.75
1:A:459:ARG:NH2	8:A:1070:HOH:O	2.19	0.75
5:A:903:MPD:HM2	8:A:1380:HOH:O	1.88	0.74
1:A:839:GLU:HB2	8:A:1385:HOH:O	1.92	0.70
1:A:408:ASP:OD1	8:A:1116:HOH:O	2.11	0.69
1:D:664:HIS:HD1	1:D:859:ARG:H	1.40	0.67
1:D:408:ASP:OD1	8:D:1174:HOH:O	2.13	0.65
1:A:315:LYS:HB2	8:A:1264:HOH:O	1.97	0.62
4:D:903:SO4:O1	8:D:1610:HOH:O	2.15	0.61
1:D:466:ARG:NE	8:D:1334:HOH:O	2.33	0.60
1:A:463:ASP:HB2	8:A:1250:HOH:O	2.00	0.60
1:A:311:MET:O	8:A:1134:HOH:O	2.16	0.60
1:D:459:ARG:NH2	8:D:1540:HOH:O	2.35	0.60
1:A:747:LYS:HE3	1:A:751:GLU:OE1	2.02	0.60
1:D:698:THR:OG1	1:D:701:MET:HG3	2.03	0.58
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.89	0.55
1:D:748:ARG:HD3	8:D:1501:HOH:O	2.07	0.55
1:D:305:ASP:OD1	8:D:1564:HOH:O	2.18	0.55
1:A:466:ARG:NH1	8:A:1324:HOH:O	2.39	0.55
1:A:631:GLU:OE2	1:A:635:LYS:HE3	2.08	0.53
1:A:668:ASP:O	1:A:672:MET:HB2	2.08	0.53
1:A:659:LEU:HD13	1:A:681:ILE:HG21	1.90	0.52
1:D:418:GLN:HA	8:D:1227:HOH:O	2.10	0.52
1:D:779:ARG:NH1	8:D:1552:HOH:O	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:467:ARG:HD2	8:A:1350:HOH:O	2.11	0.50
1:D:703:ARG:NH2	8:D:1199:HOH:O	2.44	0.50
1:A:434:LYS:NZ	8:A:1369:HOH:O	2.34	0.48
1:A:459:ARG:HB2	1:A:460:PRO:HD3	1.95	0.48
1:D:494:LYS:HE3	8:D:1649:HOH:O	2.14	0.47
1:D:435:ARG:NH2	8:D:1385:HOH:O	2.45	0.47
1:A:793:ASN:HB2	8:A:1008:HOH:O	2.15	0.46
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.30	0.46
1:D:754:VAL:CG1	1:D:758:LYS:HE2	2.45	0.46
1:D:583:LEU:HG	8:E:219:HOH:O	2.15	0.46
1:A:464:GLU:OE1	8:A:1287:HOH:O	2.21	0.46
1:D:764:THR:HA	1:D:769:ARG:O	2.16	0.46
1:D:596[B]:ARG:HD3	8:D:1028:HOH:O	2.15	0.45
1:D:607[A]:ASN:ND2	1:D:610:LEU:HD12	2.31	0.45
1:A:738:ARG:O	1:A:741:GLU:HB3	2.16	0.45
1:D:656:GLN:OE1	1:D:681:ILE:HG22	2.16	0.45
1:D:703:ARG:NH2	8:D:1237:HOH:O	2.50	0.45
1:D:551:LYS:NZ	2:E:23:DT:OP1	2.47	0.45
1:D:754:VAL:HG12	1:D:758:LYS:HE2	1.98	0.45
1:D:814:ARG:CZ	1:D:847[A]:LEU:HD13	2.47	0.45
1:D:782:ASN:ND2	8:D:1754:HOH:O	2.51	0.44
1:D:725:LEU:O	1:D:727:ILE:HG23	2.18	0.44
1:D:463:ASP:OD2	1:D:466:ARG:NH2	2.51	0.44
1:A:778:SER:HG	1:A:780:ASN:H	1.66	0.44
1:A:467:ARG:NH2	8:A:1189:HOH:O	2.51	0.43
1:D:680:ASP:OD2	1:D:702:ARG:NE	2.52	0.43
1:D:565:ALA:N	1:D:566:PRO:CD	2.82	0.43
1:A:367:LYS:NZ	8:A:1371:HOH:O	2.51	0.43
1:A:702:ARG:CZ	1:A:706:LYS:HE3	2.49	0.43
1:D:383:LYS:NZ	8:D:1262:HOH:O	2.51	0.42
1:D:383:LYS:HE3	8:D:1494:HOH:O	2.19	0.42
1:A:631:GLU:O	1:A:635:LYS:HG2	2.19	0.42
1:A:411:ALA:O	1:A:415:LYS:HG2	2.20	0.42
1:A:524:GLN:HG2	1:A:525:GLU:O	2.20	0.42
1:A:822:ALA:CB	1:A:836:ALA:HB2	2.50	0.41
1:D:645:SER:O	1:D:646:ASP:HB2	2.20	0.41
1:A:423:ARG:NH1	8:A:1401:HOH:O	2.53	0.41
1:A:463:ASP:O	1:A:467:ARG:HG3	2.21	0.41
1:A:811:LEU:HA	1:A:851:VAL:HG11	2.03	0.41
1:A:503:MET:HE1	1:A:635:LYS:O	2.21	0.41
1:A:534:LEU:HD11	1:A:574:ILE:HD13	2.03	0.41
1:D:774:PRO:HA	8:D:1545:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:719:TYR:O	1:A:723:GLN:HG2	2.21	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)
8:D:1161:HOH:O	8:D:1195:HOH:O[4_445]	2.06	0.14

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	564/592 (95%)	553 (98%)	11 (2%)	0	100	100
1	D	586/592 (99%)	572 (98%)	14 (2%)	0	100	100
All	All	1150/1184 (97%)	1125 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	483/507 (95%)	480 (99%)	3 (1%)	92	83
1	D	504/507 (99%)	501 (99%)	3 (1%)	92	83
All	All	987/1014 (97%)	981 (99%)	6 (1%)	92	83

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

Mol	Chain	Res	Type
1	A	303	LEU
1	A	672	MET
1	A	844	LEU
1	D	695	ASP
1	D	703	ARG
1	D	728	SER

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	510	GLN
1	A	543	GLN
1	A	573	ASN
1	A	579	GLN
1	A	755	GLN
1	D	405	GLN
1	D	502	GLN
1	D	516	GLN
1	D	573	ASN
1	D	670	ASN
1	D	726	ASN
1	D	821	GLN
1	D	854	GLN
1	D	867	HIS

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	1.02	2 (11%)	20,28,31	1.41	3 (15%)
2	2DT	E	29	3,2	18,20,21	1.18	2 (11%)	20,28,31	1.63	2 (10%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	2DT	C6-C5	-2.66	1.32	1.40
2	B	29	2DT	P-OP1	2.31	1.49	1.46
2	B	29	2DT	C6-C5	-2.15	1.34	1.40
2	E	29	2DT	C6-N1	2.03	1.39	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	2DT	C4'-O4'-C1'	5.98	112.54	110.05
2	B	29	2DT	C5M-C5-C4	-3.14	117.83	121.04
2	B	29	2DT	C6-N1-C2	-3.13	121.52	122.41
2	B	29	2DT	C5M-C5-C6	2.59	124.10	118.59
2	E	29	2DT	O4'-C4'-C3'	-2.40	100.76	104.80

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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	SO4	A	901	-	4,4,4	0.09	0	6,6,6	0.05	0
4	SO4	A	902	-	4,4,4	0.33	0	6,6,6	0.28	0
5	MPD	A	903	-	7,7,7	0.37	0	10,10,10	0.90	1 (10%)
7	D3T	D	901	6	29,29,29	1.84	4 (13%)	40,45,45	2.50	12 (30%)
4	SO4	D	902	-	4,4,4	0.32	0	6,6,6	0.56	0
4	SO4	D	903	-	4,4,4	0.22	0	6,6,6	0.08	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
4	SO4	A	902	-	-	0/0/0/0	0/0/0/0
5	MPD	A	903	-	-	0/5/5/5	0/0/0/0
7	D3T	D	901	6	-	0/19/31/31	0/2/2/2
4	SO4	D	902	-	-	0/0/0/0	0/0/0/0
4	SO4	D	903	-	-	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)
7	D	901	D3T	O4-C4	6.61	1.37	1.24
7	D	901	D3T	PB-O3B	3.72	1.66	1.59
7	D	901	D3T	C2-N1	-3.72	1.34	1.38
7	D	901	D3T	C3'-C2'	-2.69	1.46	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	901	D3T	C4'-O4'-C1'	9.24	113.90	110.05
7	D	901	D3T	N3-C2-N1	5.99	120.97	115.97
7	D	901	D3T	O4'-C4'-C5'	4.64	116.15	109.67
7	D	901	D3T	O4'-C1'-C2'	-3.93	101.67	106.37
7	D	901	D3T	C4-N3-C2	-3.29	118.65	125.39
7	D	901	D3T	C3'-C2'-C1'	3.23	106.38	102.80
7	D	901	D3T	O4'-C4'-C3'	-3.20	99.41	104.80
7	D	901	D3T	C6-N1-C2	-2.80	121.61	122.41
7	D	901	D3T	O4'-C1'-N1	2.60	112.57	107.68
7	D	901	D3T	PB-O3A-PA	2.22	138.19	131.68
7	D	901	D3T	C5-C6-N1	-2.16	119.48	121.59
7	D	901	D3T	O2B-PB-O3A	2.16	115.37	105.14
5	A	903	MPD	O2-C2-C3	2.00	116.19	109.16

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	566/592 (95%)	0.82	99 (17%) 2 2	16, 38, 62, 81	0
1	D	579/592 (97%)	0.28	11 (1%) 64 66	9, 19, 37, 49	0
2	B	9/9 (100%)	-0.26	0 100 100	22, 26, 46, 59	0
2	E	9/9 (100%)	-0.30	0 100 100	13, 20, 42, 51	0
3	C	12/13 (92%)	-0.22	0 100 100	18, 27, 66, 75	0
3	F	12/13 (92%)	-0.09	0 100 100	12, 20, 44, 51	0
All	All	1187/1228 (96%)	0.52	110 (9%) 9 8	9, 28, 57, 81	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	681	ILE	8.6
1	A	297	ALA	6.7
1	A	727	ILE	6.7
1	A	679	LEU	6.5
1	A	866	TYR	5.8
1	A	864	VAL	5.3
1	A	736	ILE	5.2
1	A	713	VAL	5.1
1	A	298	LYS	5.1
1	A	700	ASN	5.0
1	A	851	VAL	5.0
1	A	448	VAL	4.6
1	A	735	PHE	4.5
1	A	746	VAL	4.5
1	A	848	VAL	4.5
1	A	683	THR	4.4
1	D	689	ILE	4.4
1	A	338	VAL	4.3
1	A	743	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	675	PHE	4.2
1	A	842	GLU	4.1
1	A	740	PHE	4.1
1	A	844	LEU	4.1
1	A	860	VAL	4.0
1	A	665	ILE	3.9
1	D	681	ILE	3.6
1	A	358	VAL	3.6
1	A	703	ARG	3.6
1	A	636	ILE	3.5
1	A	531	PRO	3.5
1	A	537	ILE	3.5
1	D	698	THR	3.4
1	A	657	ILE	3.4
1	A	628	ILE	3.3
1	A	673	GLU	3.3
1	A	819	ARG	3.2
1	A	704	GLN	3.2
1	A	725	LEU	3.2
1	A	856	VAL	3.2
1	A	307	VAL	3.2
1	A	495	VAL	3.2
1	A	678	ASP	3.1
1	A	680	ASP	3.1
1	A	337	VAL	3.1
1	A	661	VAL	3.1
1	A	816	LYS	3.0
1	A	712	ILE	3.0
1	A	833	ILE	3.0
1	A	350	THR	2.9
1	A	817	GLU	2.9
1	D	697	VAL	2.9
1	A	706	LYS	2.8
1	A	708	VAL	2.8
1	A	682	HIS	2.8
1	D	735	PHE	2.8
1	A	862	LEU	2.8
1	A	300	ALA	2.8
1	A	641	VAL	2.8
1	A	867	HIS	2.8
1	A	677	ARG	2.7
1	A	309	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	301	PHE	2.7
1	A	796	ILE	2.7
1	D	692	VAL	2.7
1	A	863	LYS	2.7
1	A	846	ARG	2.7
1	A	726	ASN	2.6
1	A	685	THR	2.6
1	A	320	VAL	2.6
1	A	868	TYR	2.6
1	A	671	LEU	2.6
1	A	410	VAL	2.5
1	A	528	ILE	2.5
1	A	701	MET	2.5
1	A	714	TYR	2.5
1	A	702	ARG	2.5
1	A	754	VAL	2.5
1	A	428	VAL	2.4
1	A	360	TRP	2.4
1	D	571	VAL	2.4
1	A	574	ILE	2.3
1	A	850	GLU	2.3
1	D	727	ILE	2.3
1	A	742	SER	2.3
1	A	672	MET	2.3
1	A	739	TYR	2.3
1	D	531	PRO	2.3
1	A	442	VAL	2.3
1	A	828	VAL	2.3
1	A	514	VAL	2.2
1	A	786	PHE	2.2
1	A	684	LYS	2.2
1	A	716	ILE	2.2
1	A	710	TYR	2.2
1	A	536	VAL	2.2
1	A	588	ILE	2.2
1	A	422	VAL	2.1
1	A	313	ALA	2.1
1	A	518	ILE	2.1
1	A	803	ILE	2.0
1	A	308	THR	2.0
1	A	340	GLU	2.0
1	A	349	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	843	ARG	2.0
1	A	390	VAL	2.0
1	A	571	VAL	2.0
1	D	307	VAL	2.0
1	A	435	ARG	2.0
1	A	431	LYS	2.0
1	D	693	SER	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	0.10	-0.39	11,13,16,19	0
2	2DT	B	29	19/20	0.07	-0.68	22,26,32,32	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	MN	D	904	1/1	0.19	6.58	8,8,8,8	1
5	MPD	A	903	8/8	0.19	3.12	20,27,40,50	0
7	D3T	D	901	28/28	0.12	0.91	11,16,21,21	28
4	SO4	A	902	5/5	0.14	0.88	42,42,44,46	0
4	SO4	D	903	5/5	0.18	0.68	66,69,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	901	5/5	0.19	0.59	46,65,74,76	0
4	SO4	D	902	5/5	0.07	-0.59	25,33,37,43	0
6	MN	A	904	1/1	0.09	-1.08	16,16,16,16	1

6.5 Other polymers

There are no such residues in this entry.