



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:54 PM GMT

PDB ID : 4DQI
Title : Ternary complex of Bacillus DNA Polymerase I Large Fragment, DNA duplex,
and dCTP (paired with dG of template)
Authors : Wang, W.; Beese, L.S.
Deposited on : 2012-02-15
Resolution : 1.69 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

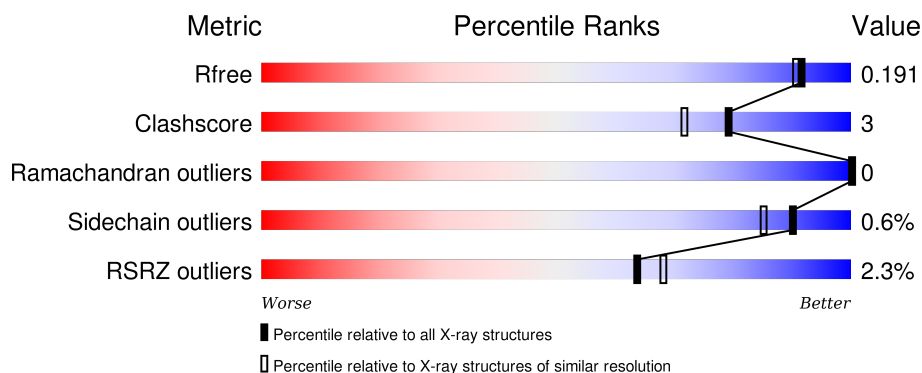
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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>3%</div> <div>92%</div> <div>6%</div> </div>
1	D	592	<div> <div>2%</div> <div>90%</div> <div>8%</div> </div>
2	B	9	<div> <div>67%</div> <div>22%</div> <div>11%</div> </div>
2	E	9	<div> <div>56%</div> <div>33%</div> <div>11%</div> </div>
3	C	13	<div> <div>69%</div> <div>23%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	901	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22370 atoms, of which 10238 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 I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	579	Total	C	H	N	O	S	20	16	0
			9534	3001	4810	825	880	18			
1	D	579	Total	C	H	N	O	S	0	39	0
			9750	3065	4924	841	903	17			

There are 4 discrepancies between the modelled and reference sequences:

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

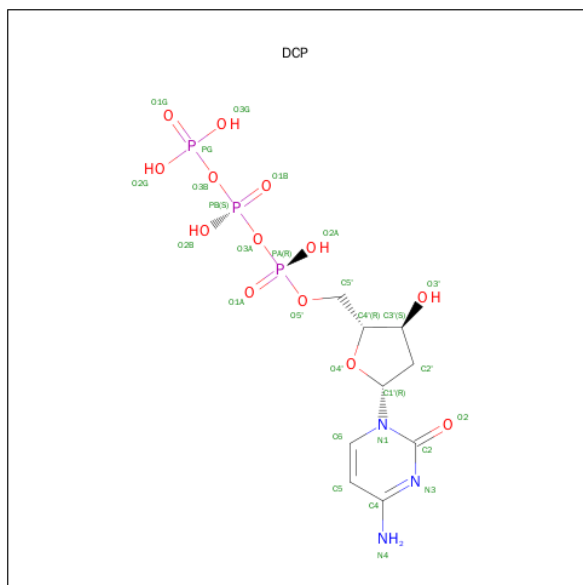
- Molecule 3 is a DNA chain called DNA (5'-D(*C*AP*TP*GP*GP*GP*AP*GP*TP*CP*AP*GP*G)-3').

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H N O P 40 9 12 3 13 3	0	0
5	A	1	Total C H N O P 40 9 12 3 13 3	0	0
5	D	1	Total C H N O P 40 9 12 3 13 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

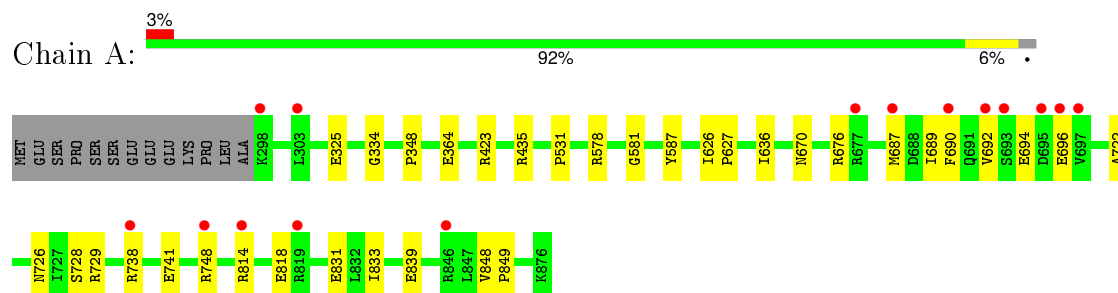
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	583	Total	O	0	0
			583	583		
7	D	820	Total	O	0	0
			820	820		
7	B	38	Total	O	0	0
			38	38		
7	C	77	Total	O	0	0
			77	77		
7	E	40	Total	O	0	0
			40	40		
7	F	78	Total	O	0	0
			78	78		

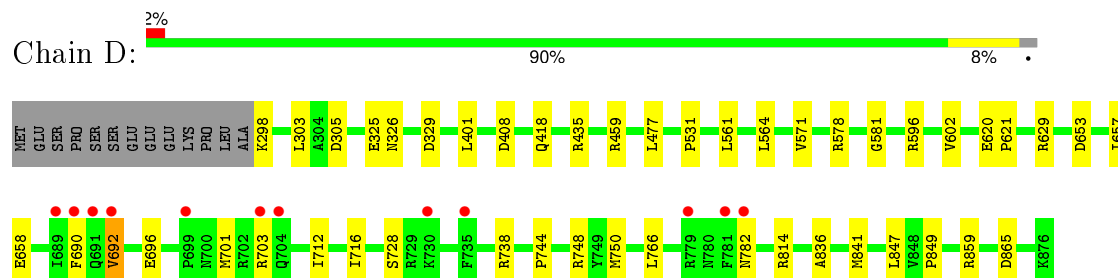
3 Residue-property plots [i](#)

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

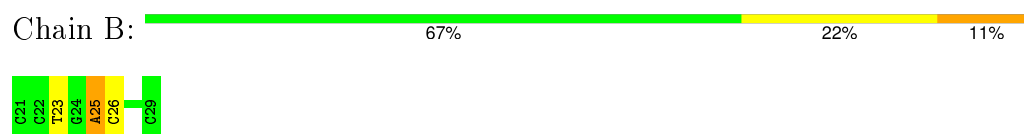
- Molecule 1: DNA polymerase I



- Molecule 1: DNA polymerase I



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

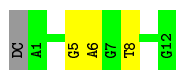


- Molecule 2: DNA (5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DOC))-3')



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





- Molecule 3: DNA (5'-D(*C*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, α , β , γ	93.68Å 109.36Å 150.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.77 – 1.69 47.22 – 1.69	Depositor EDS
% Data completeness (in resolution range)	86.0 (28.77-1.69) 86.0 (47.22-1.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1026)	Depositor
R, R_{free}	0.158 , 0.185 0.169 , 0.191	Depositor DCC
R_{free} test set	6645 reflections (4.69%)	DCC
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 148432 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22370	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, MG, SO4, DCP

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	0.45	0/4882	0.56	0/6594
1	D	0.57	0/5058	0.66	2/6838 (0.0%)
2	B	0.99	0/173	1.95	4/264 (1.5%)
2	E	1.26	0/173	2.15	9/264 (3.4%)
3	C	1.06	0/283	1.50	3/437 (0.7%)
3	F	1.09	0/283	1.74	5/437 (1.1%)
All	All	0.58	0/10852	0.80	23/14834 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	DT	O4'-C1'-N1	-9.85	101.10	108.00
2	B	26	DC	O4'-C1'-N1	8.89	114.23	108.00
2	E	25	DA	O5'-P-OP2	-7.95	98.55	105.70
2	E	23	DT	O4'-C1'-N1	-7.90	102.47	108.00
3	C	8	DT	O4'-C1'-N1	-7.86	102.50	108.00
2	E	25	DA	C5'-C4'-C3'	7.41	127.45	114.10
3	F	8	DT	O4'-C1'-N1	-7.24	102.93	108.00
2	E	25	DA	P-O5'-C5'	7.03	132.14	120.90
2	E	25	DA	O5'-P-OP1	6.87	118.95	110.70
3	F	10	DA	O4'-C1'-N9	-6.70	103.31	108.00
3	C	5	DG	O4'-C4'-C3'	-6.62	101.85	104.50
2	E	25	DA	O4'-C4'-C3'	-6.31	101.98	104.50
2	E	26	DC	O4'-C1'-N1	6.17	112.32	108.00
2	E	27	DT	OP1-P-OP2	5.95	128.53	119.60
2	B	25	DA	C5'-C4'-C3'	5.90	124.72	114.10
2	E	27	DT	O4'-C4'-C3'	-5.87	102.15	104.50
1	D	859	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	B	25	DA	O4'-C4'-C3'	-5.67	102.23	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	DT	C4-C5-C7	5.45	122.27	119.00
3	F	4	DG	N3-C4-C5	5.44	131.32	128.60
1	D	859	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	F	9	DC	O4'-C1'-C2'	5.17	110.03	105.90
3	C	6	DA	C5-N7-C8	-5.06	101.37	103.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4724	4810	4737	28	0
1	D	4826	4924	4751	41	0
2	B	174	100	103	2	0
2	E	174	100	103	2	0
3	C	251	134	136	0	0
3	F	251	134	136	3	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	56	24	24	0	0
5	D	28	12	12	0	0
6	A	5	0	0	0	0
6	D	5	0	0	0	0
7	A	583	0	0	12	4
7	B	38	0	0	0	0
7	C	77	0	0	0	0
7	D	820	0	0	24	4
7	E	40	0	0	0	0
7	F	78	0	0	3	0
All	All	12132	10238	10002	72	4

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 (72) 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)
3:F:2:DT:O4	7:F:169:HOH:O	1.83	0.97
1:A:839:GLU:OE1	7:A:1424:HOH:O	1.94	0.86
3:F:2:DT:C4	7:F:169:HOH:O	2.30	0.83
1:D:298:LYS:NZ	7:D:1768:HOH:O	1.96	0.79
1:D:750:MET:HG3	7:D:1764:HOH:O	1.80	0.79
1:D:782:ASN:HB2	7:D:1781:HOH:O	1.82	0.78
1:A:626:ILE:HG23	1:A:636[B]:ILE:HD11	1.68	0.76
1:D:865:ASP:OD2	7:D:1275:HOH:O	2.03	0.76
1:A:325:GLU:OE2	7:A:1463:HOH:O	2.05	0.74
1:D:782:ASN:CB	7:D:1781:HOH:O	2.34	0.74
1:D:408:ASP:OD1	7:D:1249:HOH:O	2.07	0.72
1:D:602[B]:VAL:HG11	1:D:621:PRO:HG3	1.74	0.70
1:D:561:LEU:O	1:D:571[A]:VAL:HG11	1.91	0.69
1:A:587:TYR:HB3	1:A:636[B]:ILE:HD13	1.75	0.69
1:A:696:GLU:OE2	7:A:1510:HOH:O	2.11	0.69
1:D:581:GLY:HA3	7:D:1743:HOH:O	1.92	0.69
1:D:325:GLU:OE1	7:D:1751:HOH:O	2.10	0.69
1:D:435:ARG:NH1	7:D:1816:HOH:O	2.17	0.68
1:D:766:LEU:HD23	7:D:1707:HOH:O	1.93	0.68
1:A:738:ARG:NE	7:A:1376:HOH:O	2.22	0.66
1:A:627:PRO:HD2	1:A:636[B]:ILE:HD11	1.78	0.64
3:F:2:DT:N3	7:F:169:HOH:O	2.24	0.64
1:A:676:ARG:NH1	7:A:1186:HOH:O	2.32	0.63
1:A:814:ARG:NH1	1:A:818:GLU:OE2	2.32	0.62
1:D:459[A]:ARG:NH2	7:D:1300:HOH:O	2.33	0.61
1:A:581:GLY:HA3	7:A:1563:HOH:O	2.00	0.61
1:A:692:VAL:HG13	1:A:696:GLU:HB2	1.85	0.58
1:D:703:ARG:NE	7:D:1742:HOH:O	2.21	0.57
1:D:782:ASN:OD1	7:D:1781:HOH:O	2.17	0.56
1:A:364:GLU:HG2	7:A:1522:HOH:O	2.06	0.56
1:D:561:LEU:HB3	1:D:571[A]:VAL:HG13	1.87	0.56
1:A:687:MET:HE2	1:A:694:GLU:HG3	1.88	0.55
1:A:578:ARG:NH1	2:B:25:DA:H5"	2.23	0.54
1:D:703:ARG:NH2	7:D:1742:HOH:O	2.37	0.54
1:D:814:ARG:NH2	1:D:847[A]:LEU:HD13	2.23	0.53
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.90	0.53
1:D:435:ARG:NH2	7:D:1280:HOH:O	2.42	0.53
1:D:418:GLN:NE2	7:D:1337:HOH:O	2.26	0.52
1:A:423:ARG:NE	7:A:1479:HOH:O	2.43	0.51
1:A:738:ARG:O	1:A:741:GLU:HG2	2.10	0.51
1:D:578:ARG:NH1	2:E:25:DA:H5"	2.26	0.51
1:A:435:ARG:NH1	7:A:1417:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:ARG:HD3	7:D:1808:HOH:O	2.11	0.50
1:D:782:ASN:CG	7:D:1781:HOH:O	2.48	0.50
1:D:744:PRO:O	1:D:748[A]:ARG:HG3	2.12	0.48
1:D:653:ASP:HB2	7:D:1741:HOH:O	2.13	0.48
1:A:831:GLU:HB3	7:A:1534:HOH:O	2.13	0.48
1:D:305:ASP:OD1	7:D:1795:HOH:O	2.20	0.47
1:D:305:ASP:CG	7:D:1795:HOH:O	2.52	0.47
1:D:329:ASP:OD2	1:D:596:ARG:NH2	2.48	0.47
1:A:587:TYR:HB3	1:A:636[B]:ILE:CD1	2.44	0.46
1:D:712:ILE:HA	1:D:716:ILE:HG22	1.98	0.46
1:D:629:ARG:NH1	7:D:1685:HOH:O	2.38	0.45
1:A:627:PRO:HD2	1:A:636[B]:ILE:CD1	2.44	0.45
1:D:459[C]:ARG:HG2	7:D:1300:HOH:O	2.16	0.45
1:D:418:GLN:HA	7:D:1239:HOH:O	2.17	0.44
1:D:657:ILE:HG23	1:D:658:GLU:N	2.34	0.43
1:A:748[A]:ARG:HG2	7:A:1402:HOH:O	2.19	0.43
1:D:531:PRO:HG3	2:E:25:DA:H5'	2.01	0.43
1:A:334:GLY:HA2	1:A:348:PRO:HD3	2.00	0.42
1:D:564:LEU:HB2	1:D:571[A]:VAL:HG21	2.00	0.42
1:A:689:ILE:HG13	1:A:690:PHE:CD1	2.54	0.42
1:D:401:LEU:HD23	1:D:401:LEU:HA	1.91	0.42
1:D:690:PHE:CD2	1:D:701:MET:HE2	2.54	0.42
1:A:833:ILE:HD12	1:A:833:ILE:N	2.34	0.42
1:A:531:PRO:HG3	2:B:25:DA:H5'	2.01	0.41
1:D:692:VAL:HG22	1:D:696:GLU:HB2	2.02	0.41
1:D:326:ASN:HD22	1:D:620[A]:GLU:CD	2.25	0.41
1:A:722:ALA:HB2	1:A:729:ARG:HA	2.03	0.40
1:A:670:ASN:HB3	7:A:1413:HOH:O	2.20	0.40
1:D:836:ALA:HB3	1:D:841:MET:CE	2.52	0.40

All (4) 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)
7:A:1155:HOH:O	7:D:1340:HOH:O[2_745]	1.76	0.44
7:A:1571:HOH:O	7:D:1794:HOH:O[2_745]	1.92	0.28
7:A:1155:HOH:O	7:D:1189:HOH:O[2_745]	2.05	0.15
7:A:1481:HOH:O	7:D:1696:HOH:O[2_745]	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	595/592 (100%)	582 (98%)	13 (2%)	0	100	100
1	D	617/592 (104%)	604 (98%)	13 (2%)	0	100	100
All	All	1212/1184 (102%)	1186 (98%)	26 (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	510/507 (101%)	508 (100%)	2 (0%)	93	90
1	D	534/507 (105%)	530 (99%)	4 (1%)	88	82
All	All	1044/1014 (103%)	1038 (99%)	6 (1%)	90	85

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

Mol	Chain	Res	Type
1	A	726	ASN
1	A	728	SER
1	D	303	LEU
1	D	477	LEU
1	D	692	VAL
1	D	728	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	502	GLN

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	0.76	0	14,26,29	1.34	2 (14%)
2	DOC	E	29	3,2	11,19,20	0.73	0	14,26,29	1.49	3 (21%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	DOC	C3'-C2'-C1'	-2.17	100.28	102.71
2	B	29	DOC	C2'-C1'-N1	2.14	116.81	112.49
2	E	29	DOC	C2-N3-C4	3.16	120.07	115.61
2	E	29	DOC	O4'-C1'-C2'	3.33	110.28	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	29	DOC	C2-N3-C4	3.94	121.17	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
5	DCP	A	902	4	21,29,29	1.34	2 (9%)	33,45,45	1.63	7 (21%)
5	DCP	A	903	-	21,29,29	1.45	3 (14%)	33,45,45	1.43	5 (15%)
6	SO4	A	904	-	4,4,4	0.11	0	6,6,6	0.14	0
5	DCP	D	902	4	21,29,29	1.29	3 (14%)	33,45,45	1.44	4 (12%)
6	SO4	D	903	-	4,4,4	0.28	0	6,6,6	0.48	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
5	DCP	A	902	4	-	0/18/34/34	0/2/2/2
5	DCP	A	903	-	-	0/18/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	A	904	-	-	0/0/0/0	0/0/0/0
5	DCP	D	902	4	-	0/18/34/34	0/2/2/2
6	SO4	D	903	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	903	DCP	C2'-C3'	-4.04	1.41	1.52
5	A	902	DCP	C2'-C3'	-3.53	1.43	1.52
5	A	902	DCP	PB-O2B	-3.25	1.41	1.54
5	D	902	DCP	C2'-C3'	-3.08	1.44	1.52
5	A	903	DCP	PB-O2B	-2.57	1.44	1.54
5	A	903	DCP	C3'-C4'	-2.33	1.46	1.53
5	D	902	DCP	PB-O2B	-2.19	1.45	1.54
5	D	902	DCP	C3'-C4'	-2.14	1.47	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	903	DCP	PB-O3A-PA	-4.41	120.34	132.73
5	A	903	DCP	PB-O3B-PG	-2.72	123.56	132.67
5	D	902	DCP	C2'-C1'-N1	-2.60	107.83	114.16
5	D	902	DCP	PB-O3A-PA	-2.16	126.66	132.73
5	A	902	DCP	PB-O3A-PA	-2.07	126.91	132.73
5	A	902	DCP	N4-C4-N3	2.04	120.22	116.50
5	A	902	DCP	O3A-PA-O5'	2.12	108.56	102.94
5	A	903	DCP	O3A-PA-O5'	2.21	108.80	102.94
5	A	902	DCP	O2B-PB-O3B	2.25	115.28	105.09
5	A	902	DCP	O5'-C5'-C4'	2.36	117.81	109.12
5	A	903	DCP	O4'-C1'-N1	2.91	112.76	107.72
5	D	902	DCP	C2-N3-C4	3.25	120.20	115.61
5	A	903	DCP	C2-N3-C4	3.38	120.38	115.61
5	D	902	DCP	O4'-C1'-N1	3.81	114.31	107.72
5	A	902	DCP	O4'-C1'-N1	4.14	114.88	107.72
5	A	902	DCP	C2-N3-C4	4.31	121.69	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	579/592 (97%)	-0.05	15 (2%) 59 64	13, 27, 51, 80	0
1	D	579/592 (97%)	-0.22	12 (2%) 67 71	6, 16, 36, 51	0
2	B	8/9 (88%)	-0.43	0 100 100	16, 21, 31, 38	0
2	E	8/9 (88%)	-0.54	0 100 100	10, 15, 26, 35	0
3	C	12/13 (92%)	-0.33	0 100 100	14, 18, 50, 63	0
3	F	12/13 (92%)	-0.30	1 (8%) 14 16	9, 15, 44, 56	0
All	All	1198/1228 (97%)	-0.15	28 (2%) 64 68	6, 22, 45, 80	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	LYS	6.3
1	A	695	ASP	4.2
1	A	693	SER	3.8
1	D	689	ILE	3.6
1	A	697	VAL	3.5
1	D	691	GLN	3.5
1	A	846	ARG	3.4
1	D	692	VAL	3.1
1	A	819	ARG	3.1
1	A	738	ARG	2.8
1	D	782	ASN	2.7
1	D	730	LYS	2.7
1	D	704	GLN	2.7
1	A	696	GLU	2.6
1	A	748[A]	ARG	2.6
1	D	779	ARG	2.6
1	A	690	PHE	2.5
1	D	690	PHE	2.4
1	A	692	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	703	ARG	2.3
3	F	1	DA	2.2
1	A	677	ARG	2.1
1	A	687	MET	2.1
1	D	781	PHE	2.1
1	D	699	PRO	2.1
1	A	303	LEU	2.0
1	A	814	ARG	2.0
1	D	735	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	DOC	B	29	18/19	0.98	0.07	-	16,17,20,22	0
2	DOC	E	29	18/19	0.99	0.09	-	8,10,15,18	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	901	1/1	0.99	0.09	2.21	23,23,23,23	0
5	DCP	A	903	28/28	0.87	0.14	1.85	24,50,119,120	0
4	MG	D	901	1/1	0.98	0.10	0.68	17,17,17,17	0
5	DCP	D	902	28/28	0.98	0.08	-0.38	7,13,24,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	SO4	D	903	5/5	0.98	0.08	-0.39	26,29,44,47	0
5	DCP	A	902	28/28	0.97	0.07	-0.96	14,18,25,35	0
6	SO4	A	904	5/5	0.95	0.14	-	40,57,58,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.