



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:37 AM GMT

PDB ID : 2HVH
Title : ddCTP:O6MeG pair in the polymerase active site (0 position)
Authors : Warren, J.J.; Forsberg, L.J.; Beese, L.S.
Deposited on : 2006-07-28
Resolution : 2.49 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

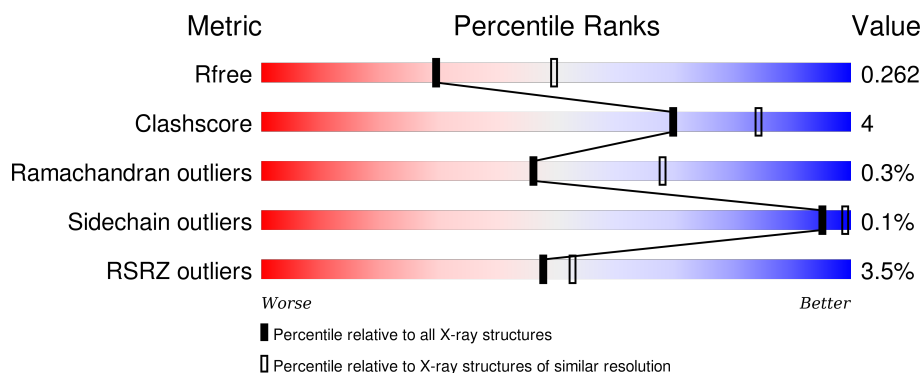
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	B	9	<div> <div>56%</div> <div>33%</div> <div>11%</div> </div>
1	E	9	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
2	C	13	<div> <div>69%</div> <div>15%</div> <div>15%</div> </div>
2	F	13	<div> <div>46%</div> <div>31%</div> <div>8%</div> <div>15%</div> </div>
3	A	580	<div> <div>7%</div> <div>87%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	580	 <div>93%7%</div>

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	SUC	A	877	-	-	-	X
4	SUC	A	878	-	-	-	X
4	SUC	D	877	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10548 atoms, of which 0 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 DNA chain called 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			
1	E	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			

- Molecule 2 is a DNA chain called 5'-D(*CP*A*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			228	109	45	64	10			
2	F	11	Total	C	N	O	P	0	0	0
			228	109	45	64	10			

- Molecule 3 is a protein called DNA Polymerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	580	Total	C	N	O	S	0	0	0
			4652	2958	808	869	17			
3	D	580	Total	C	N	O	S	0	1	0
			4658	2962	808	871	17			

- Molecule 4 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		
4	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

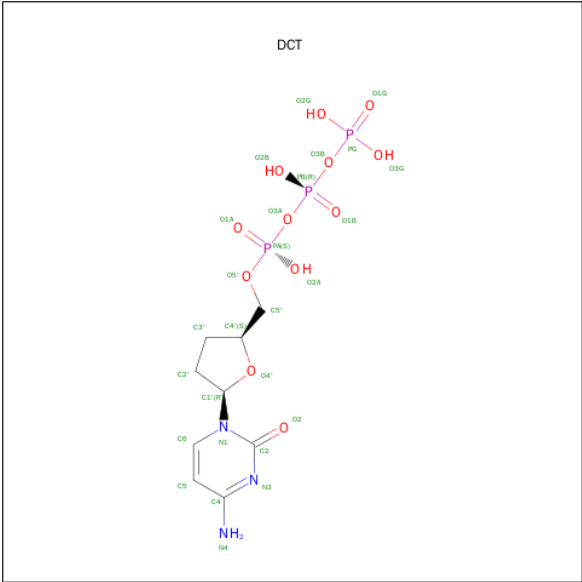
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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		
6	D	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT) (formula: $C_9H_{16}N_3O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	9	3	12	3		
7	D	1	Total	C	N	O	P	0	0
			27	9	3	12	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	86	Total	O	0	0
			86	86		
8	B	5	Total	O	0	0
			5	5		
8	C	11	Total	O	0	0
			11	11		
8	D	150	Total	O	0	0
			150	150		
8	E	10	Total	O	0	0
			10	10		
8	F	16	Total	O	0	0
			16	16		

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: 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3'

Chain B: 



- Molecule 1: 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3'

Chain E: 



- Molecule 2: 5'-D(*CP*A*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'

Chain C: 




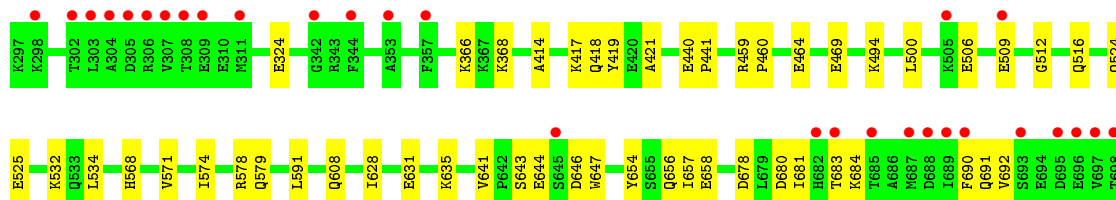
- Molecule 2: 5'-D(*CP*A*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'

Chain F: 



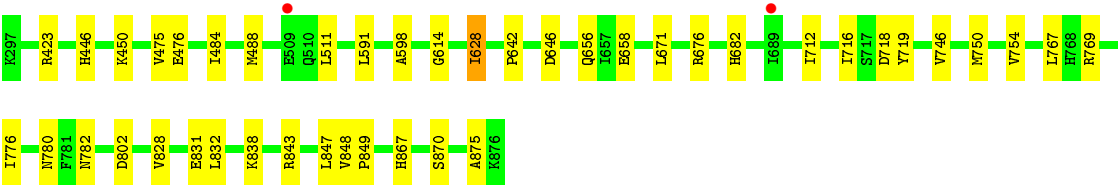
- Molecule 3: DNA Polymerase I

Chain A: 





● Molecule 3: DNA Polymerase I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.06Å 109.39Å 151.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.49 47.28 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.30-2.49) 98.8 (47.28-2.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.201 , 0.262 0.201 , 0.262	Depositor DCC
R_{free} test set	2765 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 54529 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10548	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 6OG, SUC, MN, SO4, DCT, DDG

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	B	0.73	0/173	1.55	4/264 (1.5%)
1	E	0.82	0/173	1.62	7/264 (2.7%)
2	C	0.80	0/229	1.38	2/350 (0.6%)
2	F	0.95	0/229	1.50	2/350 (0.6%)
3	A	0.37	0/4736	0.56	0/6400
3	D	0.44	0/4745	0.61	0/6412
All	All	0.45	0/10285	0.71	15/14040 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	DG	O4'-C1'-N9	-8.81	101.83	108.00
1	B	27	DT	O4'-C4'-C3'	-8.50	100.90	106.00
1	E	28	DC	O4'-C4'-C3'	-7.86	101.28	106.00
1	B	25	DA	O4'-C4'-C3'	-7.85	101.29	106.00
1	E	21	DC	O4'-C4'-C3'	-7.00	101.70	104.50
1	E	27	DT	O4'-C4'-C3'	-6.76	101.80	104.50
2	C	11	DG	O4'-C1'-N9	-6.34	103.56	108.00
1	B	26	DC	O4'-C1'-N1	6.21	112.35	108.00
2	C	12	DG	O4'-C1'-N9	6.09	112.26	108.00
1	E	21	DC	P-O3'-C3'	5.91	126.79	119.70
1	E	21	DC	O4'-C1'-N1	5.64	111.95	108.00
2	F	9	DC	O4'-C1'-N1	5.31	111.72	108.00
1	E	26	DC	O4'-C1'-N1	5.11	111.58	108.00
1	E	22	DC	O4'-C1'-N1	-5.07	104.45	108.00
1	B	27	DT	O4'-C1'-N1	5.07	111.55	108.00

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	B	177	0	103	2	0
1	E	177	0	103	4	0
2	C	228	0	127	0	0
2	F	228	0	127	3	0
3	A	4652	0	4707	49	0
3	D	4658	0	4713	29	0
4	A	46	0	44	6	0
4	D	23	0	22	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	0	0	0
6	D	10	0	0	0	0
7	A	27	0	12	7	0
7	D	27	0	12	6	0
8	A	86	0	0	5	0
8	B	5	0	0	0	0
8	C	11	0	0	0	0
8	D	150	0	0	4	0
8	E	10	0	0	0	0
8	F	16	0	0	1	0
All	All	10548	0	9970	90	0

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 4.

All (90) 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)
4:A:878:SUC:O1'	4:A:878:SUC:H1	1.51	1.10
3:A:830:ASP:OD2	7:A:883:DCT:H5"	1.77	0.85
3:D:867:HIS:HB2	3:D:875:ALA:O	1.81	0.80
3:A:658:GLU:OE2	7:A:883:DCT:H2"	1.85	0.77
3:A:789:ARG:HG2	3:A:792:MET:HE3	1.67	0.77
3:A:608:GLN:O	8:A:88:HOH:O	2.10	0.69
3:A:853:GLU:HG2	3:A:862:LEU:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:843:ARG:HD2	8:D:196:HOH:O	1.97	0.64
3:A:506:GLU:O	3:A:509:GLU:HG2	1.99	0.62
3:A:830:ASP:OD2	7:A:883:DCT:C5'	2.47	0.61
3:D:676:ARG:NH1	8:D:230:HOH:O	2.29	0.61
3:D:656:GLN:HA	7:D:881:DCT:O1B	2.00	0.61
3:A:324:GLU:OE1	8:A:201:HOH:O	2.16	0.60
3:A:421:ALA:O	8:A:51:HOH:O	2.16	0.60
3:D:767:LEU:HD12	3:D:802:ASP:HB3	1.83	0.59
3:A:469:GLU:O	4:A:878:SUC:H6'1	2.05	0.57
1:B:25:DA:H5''	3:A:578:ARG:NH2	2.19	0.57
3:D:658:GLU:CD	7:D:881:DCT:H2''	2.25	0.57
3:A:440:GLU:HB3	3:A:441:PRO:HD3	1.87	0.56
3:A:524:GLN:HG2	3:A:525:GLU:N	2.20	0.56
3:A:631:GLU:OE2	3:A:635:LYS:HE3	2.06	0.55
4:A:878:SUC:H1	4:A:878:SUC:HO1'	1.69	0.53
3:D:754:VAL:HG13	3:D:776:ILE:HD11	1.91	0.53
3:D:656:GLN:HA	7:D:881:DCT:PB	2.49	0.52
3:D:848:VAL:HB	3:D:849:PRO:HD3	1.92	0.52
3:A:709:ASN:O	3:A:713:VAL:HG13	2.10	0.52
3:A:512:GLY:O	3:A:516:GLN:HG2	2.11	0.51
3:A:754:VAL:HG12	3:A:758:LYS:HE2	1.92	0.51
3:A:680:ASP:HB3	3:A:683:THR:HB	1.92	0.51
3:A:658:GLU:HB2	3:A:710:TYR:CE1	2.45	0.50
3:A:532:LYS:NZ	8:A:268:HOH:O	2.15	0.50
1:E:21:DC:H2'	1:E:22:DC:C6	2.46	0.50
3:A:681:ILE:HA	3:A:684:LYS:HB3	1.94	0.50
3:A:767:LEU:HG	3:A:802:ASP:HB3	1.92	0.50
3:A:417:LYS:NZ	3:A:464:GLU:OE2	2.31	0.50
3:A:658:GLU:HB2	3:A:710:TYR:HE1	1.76	0.49
7:D:881:DCT:O2A	8:D:77:HOH:O	2.19	0.49
3:A:500:LEU:HD21	3:A:591:LEU:HD23	1.94	0.49
3:D:828:VAL:HB	3:D:831:GLU:HG2	1.94	0.48
3:D:646:ASP:O	3:D:838:LYS:HG3	2.13	0.48
3:D:484:ILE:O	3:D:488:MET:HG3	2.14	0.48
3:A:644:GLU:HB2	3:A:647:TRP:CG	2.49	0.48
2:F:3:6OG:H2	7:D:881:DCT:HN41	1.78	0.48
1:B:29:DDG:H2''	7:A:883:DCT:O4'	2.14	0.47
3:D:712:ILE:HA	3:D:716:ILE:HG22	1.96	0.47
3:A:579:GLN:HB2	8:A:162:HOH:O	2.14	0.47
3:A:656:GLN:HA	7:A:883:DCT:O1B	2.14	0.47
3:A:417:LYS:O	3:A:418:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:690:PHE:C	3:A:692:VAL:H	2.18	0.47
2:F:9:DC:H2"	2:F:10:DA:C8	2.50	0.46
3:D:642:PRO:HD3	3:D:870:SER:O	2.16	0.46
3:A:789:ARG:HA	3:A:792:MET:HE3	1.99	0.45
3:A:712:ILE:HA	3:A:716:ILE:HG22	1.98	0.45
3:A:459:ARG:HB3	3:A:460:PRO:HD3	1.99	0.45
3:D:780:ASN:OD1	3:D:782:ASN:N	2.50	0.44
1:E:28:DC:H2'	1:E:29:DDG:H8	1.98	0.44
3:A:641:VAL:HG12	3:A:871:THR:HG22	2.00	0.44
3:D:656:GLN:HG2	3:D:682:HIS:CD2	2.53	0.44
3:D:831:GLU:O	3:D:832:LEU:HD23	2.18	0.44
3:D:718:ASP:OD2	3:D:719:TYR:N	2.51	0.44
4:A:877:SUC:H1'2	4:A:877:SUC:H1	1.78	0.44
3:D:423:ARG:HG2	3:D:423:ARG:HH11	1.82	0.43
3:D:598:ALA:HB3	8:D:107:HOH:O	2.17	0.43
3:A:804:ILE:HD12	3:A:830:ASP:HA	1.99	0.43
3:D:446:HIS:O	3:D:450:LYS:HG3	2.18	0.43
3:D:591:LEU:HA	3:D:591:LEU:HD12	1.90	0.43
3:A:690:PHE:O	3:A:692:VAL:N	2.52	0.43
3:A:768:HIS:NE2	4:A:878:SUC:H5	2.34	0.42
3:A:830:ASP:OD2	7:A:883:DCT:O2A	2.36	0.42
3:A:494:LYS:HD3	3:A:643:SER:HA	2.00	0.42
3:A:366:LYS:O	3:A:368:LYS:HD2	2.19	0.42
3:A:702:ARG:O	3:A:706:LYS:HB2	2.19	0.42
2:F:2:DT:O5'	8:F:135:HOH:O	1.99	0.42
3:A:658:GLU:CD	7:A:883:DCT:H2"	2.40	0.42
3:A:534:LEU:HD11	3:A:574:ILE:HD13	2.00	0.42
3:D:614:GLY:HA3	3:D:769:ARG:CD	2.49	0.42
3:D:847:LEU:HD23	3:D:847:LEU:C	2.40	0.42
3:A:414:ALA:HB1	3:A:419:TYR:HB3	2.00	0.42
3:A:680:ASP:O	3:A:684:LYS:N	2.52	0.41
3:A:654:TYR:HB3	3:A:657:ILE:HB	2.02	0.41
1:E:28:DC:H5"	3:D:628:ILE:HG22	2.02	0.41
3:A:568:HIS:O	3:A:571:VAL:HG22	2.21	0.41
3:A:646:ASP:O	3:A:838:LYS:HB2	2.21	0.41
3:D:746:VAL:O	3:D:750:MET:HG2	2.20	0.41
3:A:799:SER:O	3:A:803:ILE:HG13	2.21	0.41
3:D:511:LEU:HA	3:D:511:LEU:HD23	1.75	0.41
4:A:878:SUC:O1'	4:A:878:SUC:C1	2.42	0.41
1:E:29:DDG:H2"	7:D:881:DCT:O4'	2.21	0.41
3:D:671:LEU:HA	3:D:671:LEU:HD12	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:475:VAL:HG12	3:D:476:GLU:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
3	A	578/580 (100%)	543 (94%)	32 (6%)	3 (0%)	34	55
3	D	579/580 (100%)	564 (97%)	14 (2%)	1 (0%)	52	75
All	All	1157/1160 (100%)	1107 (96%)	46 (4%)	4 (0%)	46	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	628	ILE
3	A	678	ASP
3	A	691	GLN
3	A	628	ILE

5.3.2 Protein sidechains [i](#)

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	
3	A	495/496 (100%)	494 (100%)	1 (0%)	95	99

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	496/496 (100%)	496 (100%)	0	100	100
All	All	991/992 (100%)	990 (100%)	1 (0%)	95	99

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	827	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	576	HIS
3	A	759	GLN
3	D	867	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
1	DDG	B	29	1,2	15,23,24	1.28	2 (13%)	16,33,36	2.66	2 (12%)
2	6OG	C	3	2	16,25,26	1.64	1 (6%)	21,36,39	2.52	4 (19%)
1	DDG	E	29	1,2	15,23,24	1.17	1 (6%)	16,33,36	2.61	4 (25%)
2	6OG	F	3	2	16,25,26	1.58	2 (12%)	21,36,39	2.50	6 (28%)

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
1	DDG	B	29	1,2	-	0/3/18/19	0/3/3/3
2	6OG	C	3	2	-	0/5/23/24	0/3/3/3
1	DDG	E	29	1,2	-	0/3/18/19	0/3/3/3
2	6OG	F	3	2	-	0/5/23/24	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	DDG	C8-N7	-2.15	1.30	1.34
2	F	3	6OG	C8-N7	-2.14	1.30	1.34
1	E	29	DDG	C6-N1	3.58	1.39	1.33
1	B	29	DDG	C6-N1	3.59	1.39	1.33
2	F	3	6OG	C6-N1	5.36	1.41	1.31
2	C	3	6OG	C6-N1	5.51	1.41	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	DDG	C5-C6-N1	-8.33	112.20	123.59
1	E	29	DDG	C5-C6-N1	-7.51	113.33	123.59
2	F	3	6OG	C5-C6-N1	-6.95	111.53	123.81
2	C	3	6OG	C5-C6-N1	-6.93	111.57	123.81
2	C	3	6OG	N3-C2-N1	-3.23	122.53	127.44
1	E	29	DDG	N3-C2-N1	-2.74	123.28	127.44
2	F	3	6OG	N3-C2-N1	-2.65	123.42	127.44
1	E	29	DDG	C6-C5-C4	-2.07	118.42	120.90
2	F	3	6OG	C4-C5-N7	2.09	111.40	109.48
2	F	3	6OG	O6-C6-N1	2.42	122.48	119.01
2	C	3	6OG	C-O6-C6	3.74	121.14	117.26
2	F	3	6OG	C-O6-C6	3.85	121.26	117.26
1	B	29	DDG	C6-N1-C2	5.74	123.90	115.94
1	E	29	DDG	C6-N1-C2	5.81	124.01	115.94
2	F	3	6OG	C2-N1-C6	6.72	125.27	116.03
2	C	3	6OG	C2-N1-C6	7.16	125.88	116.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	29	DDG	1	0
1	E	29	DDG	2	0
2	F	3	6OG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	SUC	A	877	-	24,24,24	0.73	0	36,36,36	0.91	1 (2%)
4	SUC	A	878	-	24,24,24	0.87	1 (4%)	36,36,36	1.53	6 (16%)
6	SO4	A	880	-	4,4,4	0.20	0	6,6,6	0.09	0
6	SO4	A	881	-	4,4,4	0.26	0	6,6,6	0.26	0
6	SO4	A	882	-	4,4,4	0.18	0	6,6,6	0.11	0
7	DCT	A	883	-	20,28,28	1.78	5 (25%)	29,43,43	1.75	7 (24%)
4	SUC	D	877	-	24,24,24	0.81	1 (4%)	36,36,36	0.72	0
6	SO4	D	879	-	4,4,4	0.26	0	6,6,6	0.21	0
6	SO4	D	880	-	4,4,4	0.21	0	6,6,6	0.19	0
7	DCT	D	881	5	20,28,28	1.71	4 (20%)	29,43,43	1.48	6 (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
4	SUC	A	877	-	-	0/12/51/51	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SUC	A	878	-	-	0/12/51/51	0/2/2/2
6	SO4	A	880	-	-	0/0/0/0	0/0/0/0
6	SO4	A	881	-	-	0/0/0/0	0/0/0/0
6	SO4	A	882	-	-	0/0/0/0	0/0/0/0
7	DCT	A	883	-	-	0/18/31/31	0/2/2/2
4	SUC	D	877	-	-	0/12/51/51	0/2/2/2
6	SO4	D	879	-	-	0/0/0/0	0/0/0/0
6	SO4	D	880	-	-	0/0/0/0	0/0/0/0
7	DCT	D	881	5	-	0/18/31/31	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	883	DCT	O4'-C1'	2.01	1.47	1.42
4	D	877	SUC	O5-C1	2.09	1.47	1.41
7	D	881	DCT	PG-O3G	2.17	1.62	1.54
7	A	883	DCT	PG-O3G	2.33	1.63	1.54
7	A	883	DCT	C4-N3	2.76	1.40	1.35
4	A	878	SUC	O2'-C2'	3.12	1.50	1.42
7	D	881	DCT	C4-N3	3.26	1.41	1.35
7	D	881	DCT	PG-O1G	3.43	1.62	1.51
7	A	883	DCT	PG-O1G	3.83	1.63	1.51
7	A	883	DCT	C6-N1	4.15	1.41	1.35
7	D	881	DCT	C6-N1	4.21	1.41	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	883	DCT	C2'-C1'-N1	-3.33	105.74	112.49
7	A	883	DCT	C3'-C4'-C5'	-3.01	103.78	116.05
4	A	878	SUC	C6-C5-C4	-2.98	105.67	113.02
4	A	878	SUC	C2'-O1-C1	-2.81	110.11	117.53
7	A	883	DCT	PB-O3B-PG	-2.45	124.45	132.67
7	D	881	DCT	C2'-C1'-N1	-2.40	107.63	112.49
7	D	881	DCT	O3G-PG-O1G	-2.09	103.84	110.58
7	D	881	DCT	PB-O3A-PA	-2.06	126.94	132.73
7	A	883	DCT	O3G-PG-O1G	-2.04	104.03	110.58
7	D	881	DCT	O2G-PG-O3B	2.24	115.25	105.09
4	A	877	SUC	O5-C5-C6	2.26	112.06	106.36
4	A	878	SUC	O2'-C2'-C1'	2.28	114.19	107.98
7	D	881	DCT	O2A-PA-O3A	2.47	116.29	105.09
4	A	878	SUC	O2'-C5'-C6'	2.60	116.43	108.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	883	DCT	O4'-C4'-C5'	2.66	113.47	109.54
7	D	881	DCT	C2-N3-C4	2.74	119.47	115.61
4	A	878	SUC	C3-C4-C5	2.85	115.16	110.20
7	A	883	DCT	C2-N3-C4	3.18	120.09	115.61
4	A	878	SUC	O5-C5-C4	3.98	117.16	109.68
7	A	883	DCT	O4'-C1'-N1	4.34	115.24	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	877	SUC	1	0
4	A	878	SUC	5	0
7	A	883	DCT	7	0
7	D	881	DCT	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	8/9 (88%)	-0.46	0 100 100	25, 27, 41, 46	0
1	E	8/9 (88%)	-0.68	0 100 100	15, 21, 31, 45	0
2	C	10/13 (76%)	-0.56	0 100 100	19, 24, 31, 62	0
2	F	10/13 (76%)	-0.57	0 100 100	9, 17, 25, 54	0
3	A	580/580 (100%)	0.34	40 (6%) 20 22	20, 37, 67, 91	0
3	D	580/580 (100%)	-0.18	2 (0%) 94 95	6, 21, 40, 52	0
All	All	1196/1204 (99%)	0.06	42 (3%) 48 53	6, 30, 54, 91	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	701	MET	6.4
3	A	688	ASP	6.0
3	A	687	MET	5.5
3	A	707	ALA	5.4
3	A	298	LYS	4.8
3	A	693	SER	4.3
3	A	698	THR	4.2
3	A	695	ASP	4.2
3	A	683	THR	3.9
3	A	696	GLU	3.7
3	A	697	VAL	3.4
3	A	685	THR	3.3
3	A	689	ILE	3.3
3	A	713	VAL	3.2
3	A	866	TYR	3.2
3	A	306	ARG	3.2
3	A	344	PHE	3.0
3	A	353	ALA	3.0
3	A	690	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	846	ARG	2.8
3	A	311	MET	2.7
3	A	645	SER	2.6
3	A	307	VAL	2.6
3	A	303	LEU	2.6
3	D	689	ILE	2.5
3	A	714	TYR	2.5
3	A	309	GLU	2.4
3	A	704	GLN	2.4
3	A	699	PRO	2.4
3	A	682	HIS	2.3
3	A	700	ASN	2.3
3	A	843	ARG	2.3
3	A	305	ASP	2.3
3	A	505	LYS	2.3
3	A	842	GLU	2.2
3	A	342	GLY	2.2
3	A	357	PHE	2.2
3	A	302	THR	2.2
3	A	304	ALA	2.1
3	A	509	GLU	2.1
3	A	308	THR	2.1
3	D	509	GLU	2.1

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	DDG	B	29	21/22	0.97	0.13	-	14,15,22,24	0
1	DDG	E	29	21/22	0.99	0.12	-	12,13,14,15	0
2	6OG	F	3	23/24	0.95	0.13	-	25,29,40,41	0
2	6OG	C	3	23/24	0.89	0.17	-	37,44,49,49	0

6.3 Carbohydrates ⓘ

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	SUC	D	877	23/23	0.87	0.22	6.04	51,53,53,54	0
4	SUC	A	877	23/23	0.76	0.28	5.13	88,90,91,91	0
4	SUC	A	878	23/23	0.76	0.26	3.34	39,45,46,47	0
7	DCT	A	883	27/27	0.89	0.20	0.10	56,58,61,61	0
7	DCT	D	881	27/27	0.98	0.11	-1.55	17,19,23,24	0
6	SO4	A	881	5/5	0.97	0.12	-1.66	43,44,44,44	0
5	MN	D	878	1/1	0.98	0.09	-4.84	23,23,23,23	0
5	MN	A	879	1/1	0.96	0.04	-5.64	64,64,64,64	0
6	SO4	A	882	5/5	0.95	0.20	-	61,62,62,62	0
6	SO4	D	880	5/5	0.95	0.27	-	70,70,71,71	0
6	SO4	A	880	5/5	0.83	0.35	-	112,112,112,112	0
6	SO4	D	879	5/5	0.98	0.12	-	29,30,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.