



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:31 AM GMT

PDB ID : 2HHW
Title : ddTTP:O6-methyl-guanine pair in the polymerase active site, in the closed conformation
Authors : Warren, J.J.; Forsberg, L.J.; Beese, L.S.
Deposited on : 2006-06-28
Resolution : 1.88 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

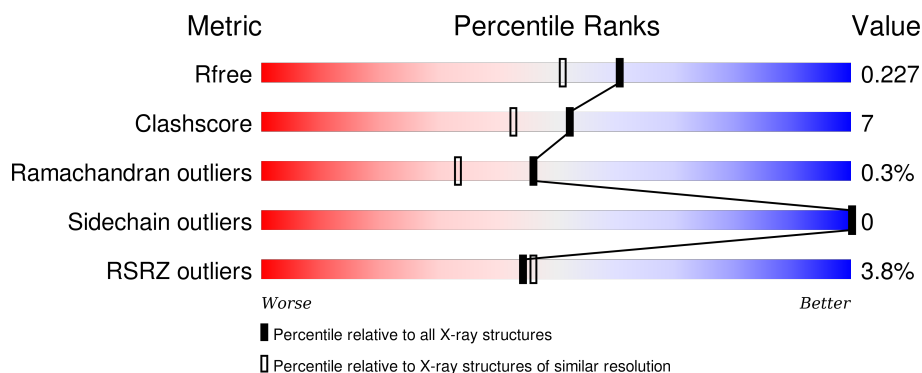
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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>11%</div> <div> <div>33%</div> <div>67%</div> </div> </div>
1	E	9	<div> <div>67%</div> <div>33%</div> </div>
2	C	13	<div> <div>69%</div> <div>15%</div> <div>15%</div> </div>
2	F	13	<div> <div>69%</div> <div>15%</div> <div>15%</div> </div>
3	A	580	<div> <div>7%</div> <div> <div>79%</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	580	<div><div>%</div><div><div></div><div>88%</div><div>12%</div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11027 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	E	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			
1	B	9	Total	C	N	O	P	0	0	0
			177	86	31	52	8			

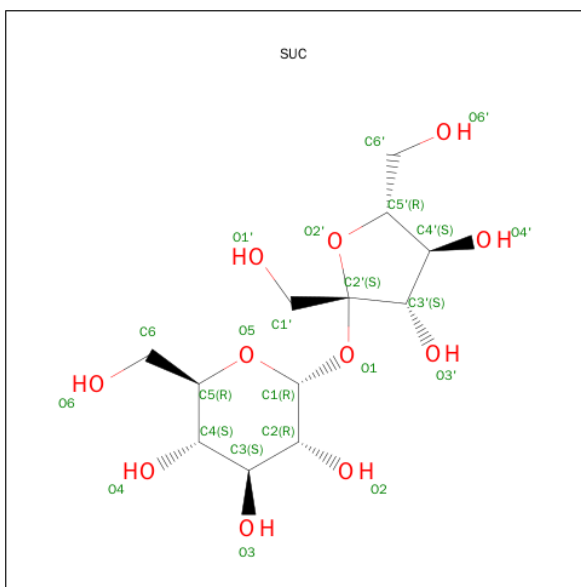
- Molecule 2 is a DNA chain called 5'-D(*CP*AP*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	11	Total	C	N	O	P	0	0	0
			228	109	45	64	10			
2	C	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	0	0
			4652	2958	808	869	17			

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

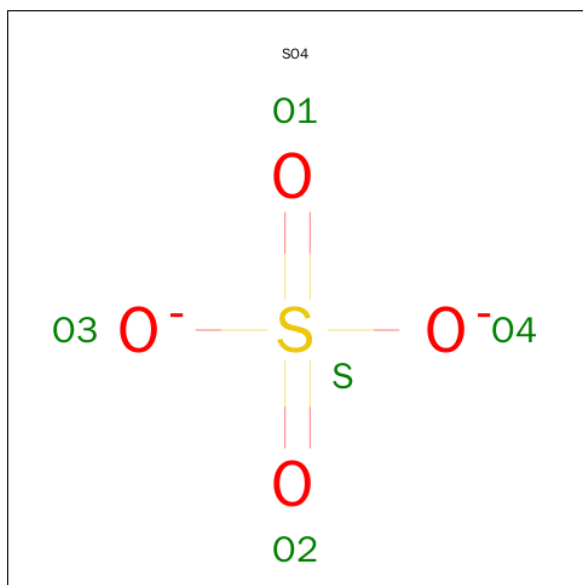


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		

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

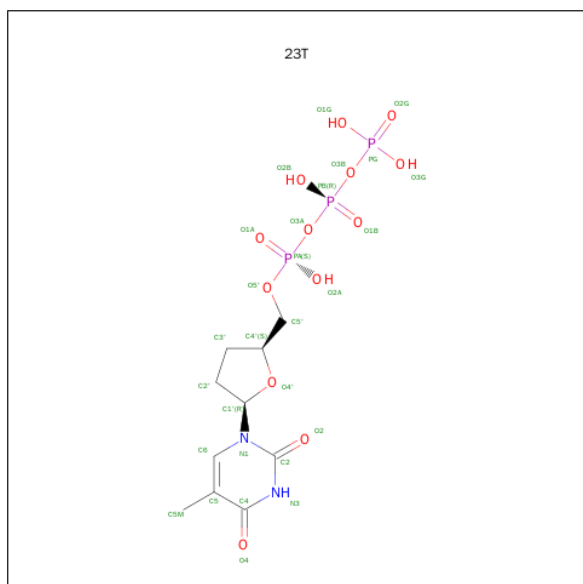
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- 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	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2',3'-DIDEOXY-THYMIDINE-5'-TRIPHOSPHATE (three-letter code: 23T) (formula: $C_{10}H_{17}N_2O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			28	10	2	13	3		
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	239	Total	O	0	0
			239	239		
8	B	30	Total	O	0	0
			30	30		
8	C	42	Total	O	0	0
			42	42		
8	D	416	Total	O	0	0
			416	416		
8	E	28	Total	O	0	0
			28	28		
8	F	39	Total	O	0	0
			39	39		

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.

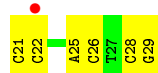
- Molecule 1: 5'-D(*CP*CP*TP*GP*AP*CP*TP*CP*(DDG))-3'

Chain E: 



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

Chain B: 



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

Chain F: 




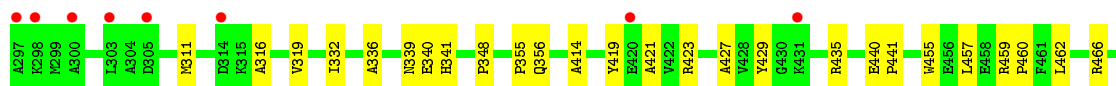
- Molecule 2: 5'-D(*CP*AP*TP*(6OG)P*CP*GP*AP*GP*TP*CP*AP*GP*G)-3'

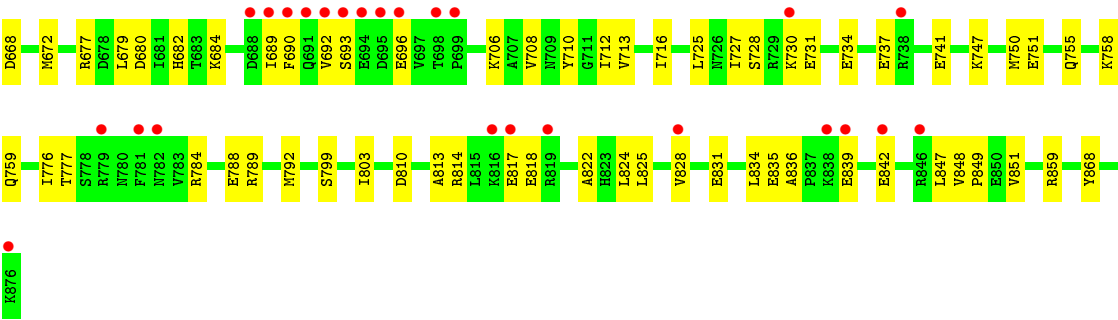
Chain C: 



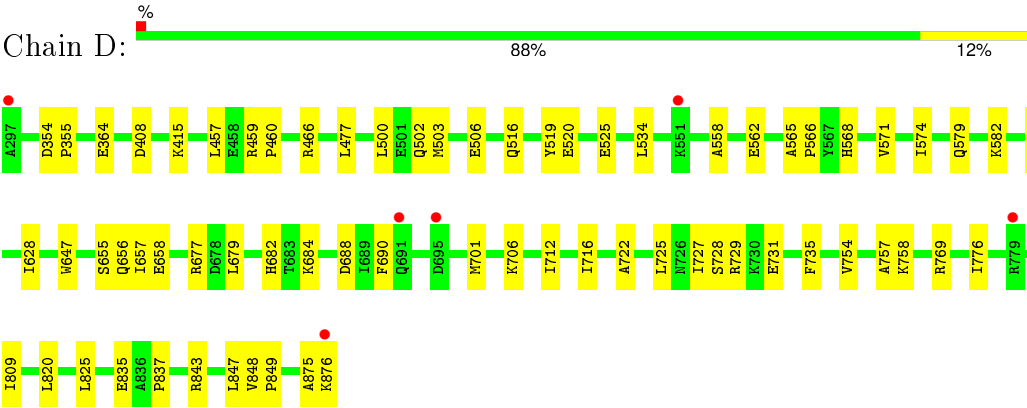
- Molecule 3: DNA Polymerase I

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	93.83Å 108.90Å 150.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.88 36.84 – 1.88	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-1.88) 90.6 (36.84-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.225 0.197 , 0.227	Depositor DCC
R_{free} test set	5689 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 57.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 113560 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11027	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6OG, SUC, MN, SO4, 23T, 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	0.36	0/173	0.81	0/264
1	E	0.45	0/173	0.73	0/264
2	C	0.36	0/229	0.72	0/350
2	F	0.39	0/229	0.71	0/350
3	A	0.28	0/4736	0.53	0/6400
3	D	0.32	0/4736	0.58	0/6400
All	All	0.31	0/10276	0.58	0/14028

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	9	0
1	E	177	0	103	2	0
2	C	228	0	127	1	0
2	F	228	0	127	1	0
3	A	4652	0	4710	77	0
3	D	4652	0	4710	53	0
4	A	23	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	23	0	22	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	10	0	0	0	0
6	D	5	0	0	0	0
7	A	28	0	13	2	0
7	D	28	0	13	3	0
8	A	239	0	0	2	0
8	B	30	0	0	0	0
8	C	42	0	0	0	0
8	D	416	0	0	3	0
8	E	28	0	0	1	0
8	F	39	0	0	0	0
All	All	11027	0	9950	136	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 7.

All (136) 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:A:828:VAL:HB	3:A:831:GLU:CG	2.21	0.71
3:A:558:ALA:O	3:A:562:GLU:HG3	1.90	0.71
3:D:534:LEU:HD11	3:D:574:ILE:HD13	1.73	0.70
3:D:558:ALA:O	3:D:562:GLU:HG3	1.92	0.69
3:A:842:GLU:HG3	8:A:1066:HOH:O	1.94	0.69
3:D:875:ALA:O	3:D:876:LYS:O	2.13	0.66
3:D:658:GLU:CD	7:D:880:23T:H2'2	2.17	0.65
3:A:737:GLU:O	3:A:741:GLU:HG3	1.97	0.65
3:D:679:LEU:HD13	3:D:684:LYS:NZ	2.13	0.64
3:A:725:LEU:O	3:A:727:ILE:HG23	1.98	0.64
3:A:789:ARG:HA	3:A:792:MET:HE3	1.79	0.63
3:D:459:ARG:HB3	3:D:460:PRO:HD3	1.80	0.62
3:D:656:GLN:HA	7:D:880:23T:O2B	1.99	0.62
3:A:658:GLU:CD	7:A:881:23T:H2'2	2.19	0.62
3:A:828:VAL:HB	3:A:831:GLU:HG2	1.83	0.61
3:A:730:LYS:O	3:A:734:GLU:HG3	1.99	0.61
3:A:459:ARG:HB3	3:A:460:PRO:HD3	1.82	0.61
3:A:462:LEU:O	3:A:466:ARG:HG3	2.01	0.60
3:D:754:VAL:HG12	3:D:758:LYS:HE2	1.84	0.60
3:A:747:LYS:O	3:A:751:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:784:ARG:O	3:A:788:GLU:HG3	2.02	0.59
3:A:664:HIS:ND1	3:A:859:ARG:HG3	2.17	0.59
3:D:843:ARG:HD2	8:D:931:HOH:O	2.02	0.59
3:A:680:ASP:O	3:A:684:LYS:HD3	2.03	0.58
3:A:839:GLU:CD	3:A:839:GLU:H	2.07	0.58
3:D:516:GLN:O	3:D:520:GLU:HG3	2.03	0.58
3:A:848:VAL:HB	3:A:849:PRO:HD3	1.84	0.58
3:D:725:LEU:O	3:D:727:ILE:HG23	2.04	0.57
3:A:825:LEU:HD11	3:A:835:GLU:HB3	1.86	0.57
1:B:26:DC:H1'	3:A:582:LYS:HG3	1.88	0.56
3:A:414:ALA:HB1	3:A:419:TYR:HB3	1.87	0.56
3:D:688:ASP:OD2	3:D:735:PHE:HE1	1.87	0.55
8:E:295:HOH:O	3:D:579:GLN:HG2	2.06	0.55
3:D:848:VAL:HB	3:D:849:PRO:HD3	1.87	0.55
3:A:319:VAL:HB	3:A:336:ALA:HB3	1.88	0.55
1:B:25:DA:H5''	3:A:578:ARG:NH2	2.22	0.54
3:D:825:LEU:HD11	3:D:835:GLU:HB3	1.89	0.54
3:A:500:LEU:HA	3:A:503:MET:HE2	1.90	0.54
3:A:502:GLN:O	3:A:506:GLU:HG3	2.08	0.53
3:D:679:LEU:HD13	3:D:684:LYS:HZ3	1.72	0.53
3:D:847:LEU:HD23	3:D:847:LEU:C	2.28	0.53
3:A:507:LEU:HD22	3:A:584:GLN:HB2	1.90	0.53
3:A:589:GLU:O	3:A:593:LYS:HG3	2.08	0.53
3:A:657:ILE:HG23	3:A:658:GLU:N	2.24	0.52
3:D:565:ALA:HA	3:D:571:VAL:HG21	1.90	0.52
3:A:682:HIS:CE1	3:A:706:LYS:HG3	2.45	0.52
3:A:667:GLU:HG2	3:A:859:ARG:HE	1.75	0.52
3:A:776:ILE:HG23	3:A:777:THR:HG23	1.91	0.51
3:D:593:LYS:HB3	3:D:593:LYS:NZ	2.26	0.51
3:D:754:VAL:CG1	3:D:758:LYS:HE2	2.40	0.50
1:B:25:DA:H2'	1:B:26:DC:C6	2.46	0.50
3:A:644:GLU:HB2	3:A:647:TRP:CG	2.47	0.50
3:D:690:PHE:CD2	3:D:701:MET:HE2	2.46	0.50
3:A:534:LEU:HD11	3:A:574:ILE:HD13	1.93	0.50
3:A:668:ASP:O	3:A:672:MET:HG3	2.11	0.50
3:A:584:GLN:O	3:A:589:GLU:HG3	2.13	0.49
3:A:355:PRO:HG2	3:A:356:GLN:OE1	2.12	0.49
1:B:26:DC:H5'	3:A:578:ARG:HB3	1.94	0.49
3:A:758:LYS:HG2	3:A:776:ILE:HG13	1.94	0.48
3:A:515:GLU:HG2	3:A:519:TYR:CE2	2.48	0.48
3:D:457:LEU:C	3:D:460:PRO:HD2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:568:HIS:O	3:D:571:VAL:HG22	2.12	0.48
3:D:589:GLU:O	3:D:593:LYS:HG3	2.12	0.48
3:D:657:ILE:HG23	3:D:658:GLU:N	2.29	0.48
3:D:784:ARG:O	3:D:788:GLU:HG3	2.14	0.48
1:B:21:DC:H2'	1:B:22:DC:C6	2.48	0.48
3:A:755:GLN:O	3:A:759:GLN:HG3	2.14	0.48
3:D:757:ALA:HB3	3:D:776:ILE:HD13	1.95	0.48
3:A:457:LEU:C	3:A:460:PRO:HD2	2.35	0.47
2:C:9:DC:H2'	2:C:10:DA:C8	2.50	0.47
3:D:502:GLN:O	3:D:506:GLU:HG3	2.15	0.47
3:D:677:ARG:HB2	3:D:679:LEU:HG	1.97	0.47
3:D:690:PHE:CG	3:D:701:MET:HE2	2.49	0.47
3:A:728:SER:HB3	3:A:731:GLU:HG3	1.96	0.47
3:A:693:SER:OG	3:A:696:GLU:HG3	2.15	0.47
3:A:610:LEU:C	3:A:610:LEU:HD23	2.35	0.47
1:E:28:DC:H2'	1:E:29:DDG:H8	1.96	0.46
3:A:824:LEU:HD23	3:A:834:LEU:HG	1.98	0.46
3:D:647:TRP:CE2	3:D:837:PRO:HG3	2.51	0.46
3:A:810:ASP:O	3:A:814:ARG:HG2	2.16	0.45
3:A:814:ARG:O	3:A:818:GLU:HG3	2.16	0.45
3:A:340:GLU:HG3	3:A:341:HIS:CD2	2.52	0.45
2:F:9:DC:H2'	2:F:10:DA:C8	2.51	0.45
3:A:429:TYR:O	3:A:435:ARG:HA	2.16	0.45
3:D:457:LEU:O	3:D:460:PRO:HD2	2.17	0.45
3:A:690:PHE:O	3:A:692:VAL:HG13	2.17	0.44
3:A:847:LEU:O	3:A:851:VAL:HG23	2.18	0.44
3:D:500:LEU:HD12	3:D:503:MET:HE3	2.00	0.44
3:A:667:GLU:HG2	3:A:859:ARG:NE	2.32	0.44
1:B:25:DA:H5''	3:A:578:ARG:CZ	2.47	0.44
3:D:354:ASP:HA	3:D:355:PRO:HD3	1.89	0.44
3:D:679:LEU:HD13	3:D:684:LYS:HZ1	1.82	0.44
3:A:710:TYR:HA	3:A:713:VAL:HG22	1.98	0.44
3:A:332:ILE:O	3:A:348:PRO:HG2	2.18	0.44
3:A:813:ALA:O	3:A:817:GLU:HG3	2.17	0.44
3:A:799:SER:O	3:A:803:ILE:HG13	2.18	0.43
3:D:712:ILE:HA	3:D:716:ILE:HG22	2.00	0.43
3:D:614:GLY:HA3	3:D:769:ARG:HD3	2.01	0.43
3:D:466:ARG:HG2	3:D:466:ARG:HH11	1.84	0.43
3:A:507:LEU:HD23	3:A:507:LEU:C	2.39	0.43
3:D:477:LEU:HD12	3:D:809:ILE:HD12	1.99	0.43
3:A:712:ILE:HA	3:A:716:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:505:LYS:O	3:A:509:GLU:HG3	2.19	0.43
1:B:26:DC:C1'	3:A:582:LYS:HG3	2.49	0.43
3:A:656:GLN:HA	7:A:881:23T:O1B	2.19	0.42
3:A:457:LEU:O	3:A:460:PRO:HD2	2.19	0.42
3:A:311:MET:HA	3:A:339:ASN:HD21	1.84	0.42
3:A:517:ARG:NH2	3:A:521:LEU:HD21	2.34	0.42
3:A:859:ARG:HH11	3:A:859:ARG:HG2	1.83	0.42
3:D:706:LYS:HD2	7:D:880:23T:H5M2	2.02	0.42
1:E:26:DC:H2''	3:D:582:LYS:HG2	2.02	0.42
1:B:28:DC:H2'	1:B:29:DDG:H8	2.01	0.42
3:D:364:GLU:HG2	8:D:1054:HOH:O	2.19	0.42
3:D:415:LYS:HE3	8:D:1245:HOH:O	2.19	0.42
3:A:423:ARG:NH2	3:A:427:ALA:O	2.53	0.42
3:D:408:ASP:HB2	4:D:877:SUC:H1'1	2.01	0.42
3:A:507:LEU:HD23	3:A:507:LEU:O	2.19	0.41
3:A:677:ARG:CB	3:A:679:LEU:HD13	2.49	0.41
3:D:728:SER:HB3	3:D:731:GLU:CD	2.40	0.41
3:A:657:ILE:HG23	3:A:658:GLU:H	1.84	0.41
3:A:822:ALA:CB	3:A:836:ALA:HB2	2.51	0.41
3:A:649:ILE:O	3:A:868:TYR:HA	2.20	0.41
3:D:682:HIS:CE1	3:D:706:LYS:HG3	2.55	0.41
3:D:614:GLY:HA3	3:D:769:ARG:CD	2.50	0.41
3:A:750:MET:HG3	8:A:1051:HOH:O	2.21	0.41
3:D:722:ALA:HB2	3:D:729:ARG:HA	2.02	0.41
3:D:820:LEU:HD21	3:D:843:ARG:CZ	2.51	0.41
1:B:26:DC:H2''	3:A:582:LYS:HG3	2.03	0.41
3:A:689:ILE:HD11	3:A:708:VAL:HG11	2.03	0.40
3:D:519:TYR:CD1	3:D:525:GLU:HA	2.56	0.40
3:A:542:LEU:HB2	3:A:544:LEU:HD13	2.03	0.40
3:D:565:ALA:N	3:D:566:PRO:CD	2.85	0.40
3:A:316:ALA:HA	3:A:455:TRP:CZ3	2.56	0.40
3:D:655:SER:O	3:D:656:GLN:C	2.60	0.40
3:D:593:LYS:NZ	3:D:593:LYS:CB	2.84	0.40
3:A:440:GLU:HB3	3:A:441:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

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	
3	A	578/580 (100%)	559 (97%)	17 (3%)	2 (0%)	46	33
3	D	578/580 (100%)	564 (98%)	13 (2%)	1 (0%)	52	40
All	All	1156/1160 (100%)	1123 (97%)	30 (3%)	3 (0%)	46	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	628	ILE
3	A	628	ILE
3	A	421	ALA

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	
3	A	495/495 (100%)	495 (100%)	0	100	100
3	D	495/495 (100%)	495 (100%)	0	100	100
All	All	990/990 (100%)	990 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	1.14	1 (6%)	16,33,36	2.92	3 (18%)
2	6OG	C	3	2	16,25,26	1.40	1 (6%)	21,36,39	2.28	3 (14%)
1	DDG	E	29	1,2	15,23,24	1.21	1 (6%)	16,33,36	2.92	3 (18%)
2	6OG	F	3	2	16,25,26	1.40	2 (12%)	21,36,39	2.26	3 (14%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	6OG	C8-N7	-2.01	1.30	1.34
1	B	29	DDG	C6-N1	3.40	1.39	1.33
1	E	29	DDG	C6-N1	3.72	1.40	1.33
2	C	3	6OG	C6-N1	4.82	1.40	1.31
2	F	3	6OG	C6-N1	4.84	1.40	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	DDG	C5-C6-N1	-8.88	111.44	123.59
1	E	29	DDG	C5-C6-N1	-8.84	111.50	123.59
2	C	3	6OG	C5-C6-N1	-7.11	111.25	123.81
2	F	3	6OG	C5-C6-N1	-7.07	111.32	123.81
1	E	29	DDG	N3-C2-N1	-2.43	123.75	127.44
2	C	3	6OG	N3-C2-N1	-2.35	123.87	127.44
2	F	3	6OG	N3-C2-N1	-2.34	123.88	127.44
1	B	29	DDG	N3-C2-N1	-2.27	123.99	127.44
2	F	3	6OG	C2-N1-C6	6.53	125.01	116.03
2	C	3	6OG	C2-N1-C6	6.61	125.13	116.03
1	E	29	DDG	C6-N1-C2	6.61	125.12	115.94
1	B	29	DDG	C6-N1-C2	6.65	125.17	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	29	DDG	1	0
1	E	29	DDG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	1.53	3 (12%)	36,36,36	0.91	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	879	-	4,4,4	0.20	0	6,6,6	0.08	0
6	SO4	A	880	-	4,4,4	0.22	0	6,6,6	0.08	0
7	23T	A	881	5	20,29,29	1.79	4 (20%)	27,45,45	2.14	8 (29%)
4	SUC	D	877	-	24,24,24	1.48	4 (16%)	36,36,36	0.89	1 (2%)
6	SO4	D	879	-	4,4,4	0.14	0	6,6,6	0.10	0
7	23T	D	880	5	20,29,29	1.78	4 (20%)	27,45,45	1.86	5 (18%)

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
6	SO4	A	879	-	-	0/0/0/0	0/0/0/0
6	SO4	A	880	-	-	0/0/0/0	0/0/0/0
7	23T	A	881	5	-	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
7	23T	D	880	5	-	0/18/31/31	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	877	SUC	O5-C5	2.00	1.49	1.44
4	D	877	SUC	O5-C1	2.17	1.47	1.41
4	D	877	SUC	C4-C5	2.37	1.58	1.53
4	A	877	SUC	C4-C5	2.50	1.58	1.53
4	A	877	SUC	O5-C1	2.53	1.48	1.41
7	D	880	23T	PB-O1B	2.77	1.61	1.51
7	A	881	23T	PB-O1B	2.84	1.61	1.51
7	D	880	23T	PG-O2G	3.11	1.61	1.51
7	A	881	23T	PG-O2G	3.12	1.61	1.51
7	D	880	23T	C6-N1	3.67	1.40	1.35
7	A	881	23T	C6-N1	3.68	1.40	1.35
7	D	880	23T	C4-N3	4.00	1.40	1.33
7	A	881	23T	C4-N3	4.02	1.40	1.33
4	D	877	SUC	C3-C2	5.24	1.66	1.52
4	A	877	SUC	C3-C2	5.38	1.66	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	880	23T	C5-C4-N3	-4.51	120.11	125.14
7	A	881	23T	C5-C4-N3	-4.39	120.25	125.14
7	A	881	23T	PB-O3B-PG	-3.52	120.86	132.67
7	A	881	23T	PB-O3A-PA	-3.47	122.98	132.73
7	D	880	23T	PB-O3A-PA	-3.00	124.31	132.73
7	A	881	23T	C2'-C3'-C4'	-2.91	96.91	102.59
7	D	880	23T	C2'-C3'-C4'	-2.88	96.97	102.59
7	A	881	23T	C3'-C2'-C1'	-2.55	99.86	102.71
4	D	877	SUC	O3-C3-C2	-2.13	105.54	110.34
7	D	880	23T	C3'-C2'-C1'	-2.07	100.39	102.71
4	A	877	SUC	C1-C2-C3	-2.04	105.95	109.97
4	A	877	SUC	O3-C3-C2	-2.04	105.75	110.34
7	A	881	23T	C2'-C1'-N1	-2.01	108.42	112.49
7	A	881	23T	O2B-PB-O3B	3.78	122.24	105.09
7	A	881	23T	C4-N3-C2	5.14	119.69	115.25
7	D	880	23T	C4-N3-C2	5.40	119.91	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	881	23T	2	0
4	D	877	SUC	1	0
7	D	880	23T	3	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%)	0.37	1 (12%) 5 5	16, 21, 52, 64	0
1	E	8/9 (88%)	0.04	0 100 100	11, 19, 39, 63	0
2	C	10/13 (76%)	-0.38	0 100 100	14, 19, 33, 50	0
2	F	10/13 (76%)	-0.15	0 100 100	10, 14, 30, 51	0
3	A	580/580 (100%)	0.40	38 (6%) 22 23	13, 26, 48, 67	0
3	D	580/580 (100%)	-0.08	6 (1%) 84 85	6, 17, 33, 49	0
All	All	1196/1204 (99%)	0.15	45 (3%) 44 46	6, 22, 44, 67	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	297	ALA	14.6
3	D	297	ALA	7.9
3	A	645	SER	6.9
3	A	298	LYS	5.7
3	A	695	ASP	5.2
3	D	691	GLN	4.8
3	D	876	LYS	4.7
3	A	842	GLU	4.0
3	A	819	ARG	3.9
3	A	696	GLU	3.9
3	A	692	VAL	3.8
3	A	846	ARG	3.6
3	A	816	LYS	3.6
3	A	691	GLN	3.2
3	A	646	ASP	3.2
3	D	779	ARG	3.1
3	A	876	LYS	3.1
3	A	781	PHE	3.0
3	A	300	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	817	GLU	2.9
3	A	690	PHE	2.8
3	A	420	GLU	2.8
3	A	779	ARG	2.8
3	A	838	LYS	2.7
3	D	695	ASP	2.7
3	A	689	ILE	2.6
3	A	644	GLU	2.6
3	A	693	SER	2.6
3	A	305	ASP	2.5
3	A	509	GLU	2.5
3	A	431	LYS	2.4
3	A	839	GLU	2.4
3	A	694	GLU	2.4
3	A	303	LEU	2.3
3	A	688	ASP	2.3
3	D	551	LYS	2.2
3	A	698	THR	2.2
3	A	559	ASP	2.2
1	B	22	DC	2.1
3	A	730	LYS	2.1
3	A	699	PRO	2.1
3	A	782	ASN	2.1
3	A	828	VAL	2.1
3	A	738	ARG	2.0
3	A	314	ASP	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	6OG	C	3	23/24	0.96	0.09	-	18,20,28,30	0
1	DDG	B	29	21/22	0.98	0.14	-	15,16,18,18	0
2	6OG	F	3	23/24	0.97	0.10	-	11,14,20,22	0
1	DDG	E	29	21/22	0.98	0.12	-	4,8,12,12	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(\AA^2)	Q<0.9
7	23T	D	880	28/28	0.98	0.13	0.55	9,11,14,15	0
7	23T	A	881	28/28	0.96	0.12	-0.08	17,19,24,25	0
4	SUC	A	877	23/23	0.92	0.11	-0.18	25,28,28,30	0
4	SUC	D	877	23/23	0.96	0.08	-0.64	14,18,19,20	0
5	MN	D	878	1/1	1.00	0.07	-2.00	10,10,10,10	0
5	MN	A	878	1/1	1.00	0.06	-5.21	21,21,21,21	0
6	SO4	D	879	5/5	0.91	0.27	-	76,77,78,78	0
6	SO4	A	879	5/5	0.78	0.36	-	94,95,95,95	0
6	SO4	A	880	5/5	0.85	0.34	-	97,97,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.