



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:35 AM GMT

PDB ID : 3BDP
Title : DNA POLYMERASE I/DNA COMPLEX
Authors : Kiefer, J.R.; Mao, C.; Beese, L.S.
Deposited on : 1997-11-17
Resolution : 1.90 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

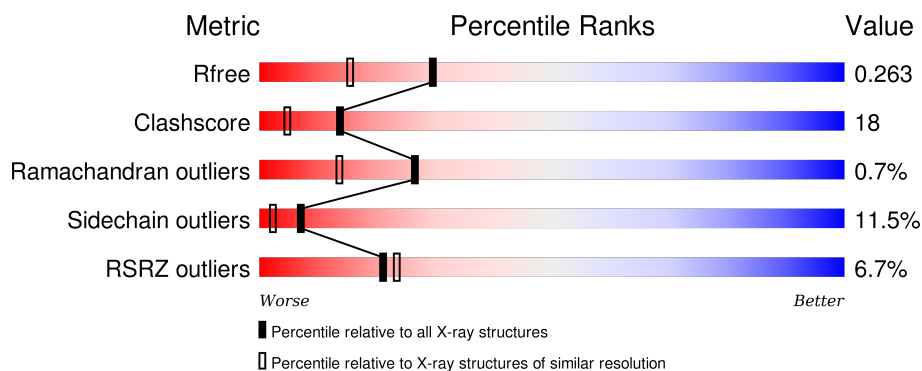
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	P	10	<div> <div>10%</div> <div>20%</div> <div>70%</div> <div>10%</div> </div>
2	T	10	<div> <div>10%</div> <div>40%</div> <div>50%</div> <div>10%</div> </div>
3	A	580	<div> <div>7%</div> <div>69%</div> <div>25%</div> <div>6%</div> </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	SO4	A	910	-	X	-	-
4	SO4	A	912	-	X	-	-
4	SO4	A	915	-	X	-	-
4	SO4	A	920	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5513 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 DNA (5'-D(*GP*CP*AP*TP*GP*AP*TP*GP*CP*2DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	10	Total	C	N	O	P	0	0	0
			202	98	37	58	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	10	Total	C	N	O	P	0	0	0
			201	97	38	57	9			

- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE I).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	580	Total	C	N	O	S	0	0	0
			4656	2959	810	870	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	ALA	LYS	CONFLICT	UNP P52026
A	411	ARG	ALA	CONFLICT	UNP P52026
A	456	GLU	ALA	CONFLICT	UNP P52026
A	505	LYS	GLU	CONFLICT	UNP P52026
A	512	GLY	ARG	CONFLICT	UNP P52026
A	550	THR	SER	CONFLICT	UNP P52026
A	?	-	GLN	DELETION	UNP P52026
A	823	HIS	ARG	CONFLICT	UNP P52026

- 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	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	402	Total	O	0	0
			402	402		
5	P	15	Total	O	0	0
			15	15		
5	T	17	Total	O	0	0
			17	17		

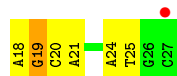
3 Residue-property plots

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.

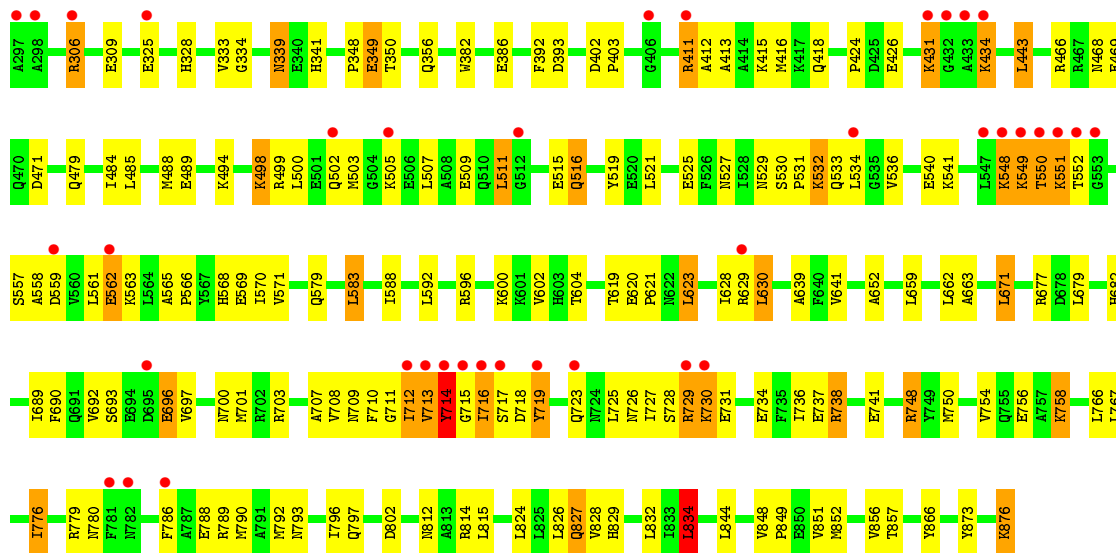
- Molecule 1: DNA (5'-D(*GP*CP*AP*TP*GP*AP*TP*GP*CP*2DT)-3')



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



- Molecule 3: PROTEIN (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	87.06Å 93.55Å 106.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.1 (20.00-1.90) 92.8 (19.73-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 1.90Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.250 , 0.294 0.208 , 0.263	Depositor DCC
R_{free} test set	3232 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 71.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63955 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5513	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 3.56% 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: 2DT, 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	P	0.56	0/205	0.81	0/315
2	T	0.61	0/225	0.84	0/345
3	A	0.55	0/4740	0.71	1/6405 (0.0%)
All	All	0.56	0/5170	0.73	1/7065 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
2	T	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	834	LEU	CA-CB-CG	7.76	133.14	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	13	DT	Sidechain
2	T	19	DG	Sidechain

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	P	202	0	115	12	0
2	T	201	0	114	6	0
3	A	4656	0	4709	173	0
4	A	20	0	0	0	0
5	A	402	0	0	18	1
5	P	15	0	0	2	0
5	T	17	0	0	1	0
All	All	5513	0	4938	185	1

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 18.

All (185) 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:692:VAL:HB	3:A:696:GLU:HG3	1.26	1.16
3:A:484:ILE:HG22	3:A:488:MET:CE	1.89	1.01
1:P:9:DA:H4'	1:P:10:DT:OP1	1.60	1.00
3:A:484:ILE:HG22	3:A:488:MET:HE2	1.46	0.95
3:A:719:TYR:H	3:A:719:TYR:HD1	1.16	0.94
3:A:411:ARG:NH1	3:A:412:ALA:HA	1.83	0.92
3:A:682:HIS:HD2	3:A:709:ASN:HD22	1.10	0.92
3:A:565:ALA:HB3	3:A:566:PRO:HD3	1.52	0.90
3:A:663:ALA:HB2	3:A:671:LEU:HD13	1.57	0.86
3:A:411:ARG:HD3	5:A:2703:HOH:O	1.75	0.85
1:P:7:DG:H2''	1:P:8:DC:H5'	1.60	0.83
3:A:700:ASN:HD21	3:A:703:ARG:HH21	1.25	0.82
3:A:848:VAL:CG1	3:A:852:MET:HE3	2.11	0.81
3:A:789:ARG:HA	3:A:792:MET:HE3	1.63	0.80
3:A:848:VAL:HG12	3:A:852:MET:HE3	1.65	0.79
3:A:550:THR:HG23	3:A:551:LYS:HG3	1.66	0.77
3:A:713:VAL:HG12	3:A:714:TYR:N	2.00	0.76
3:A:719:TYR:N	3:A:719:TYR:CD1	2.52	0.75
3:A:790:MET:HG2	5:A:2061:HOH:O	1.86	0.75
3:A:712:ILE:HG22	3:A:713:VAL:N	2.00	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:789:ARG:HA	3:A:792:MET:CE	2.17	0.74
3:A:682:HIS:CD2	3:A:709:ASN:HD22	2.02	0.74
3:A:431:LYS:H	3:A:434:LYS:NZ	1.87	0.73
1:P:7:DG:H2"	1:P:8:DC:C5'	2.19	0.72
3:A:629:ARG:HG2	5:A:2735:HOH:O	1.89	0.72
3:A:707:ALA:CB	3:A:725:LEU:HD21	2.20	0.72
2:T:24:DA:H2"	2:T:25:DT:H5'	1.71	0.72
3:A:714:TYR:HA	3:A:793:ASN:ND2	2.05	0.71
3:A:790:MET:HA	5:A:2061:HOH:O	1.90	0.70
3:A:536:VAL:HG23	5:A:2748:HOH:O	1.90	0.70
3:A:328:HIS:HD2	3:A:382:TRP:HE1	1.39	0.69
3:A:334:GLY:HA2	3:A:348:PRO:HD3	1.75	0.69
3:A:559:ASP:O	3:A:563:LYS:HG2	1.92	0.68
3:A:832:LEU:HB2	3:A:852:MET:HE1	1.75	0.67
3:A:411:ARG:C	3:A:411:ARG:HD2	2.15	0.66
3:A:411:ARG:HG2	3:A:424:PRO:HG3	1.76	0.66
3:A:521:LEU:HD13	3:A:569:GLU:HB3	1.78	0.66
3:A:719:TYR:N	3:A:719:TYR:HD1	1.88	0.65
3:A:521:LEU:CD1	3:A:569:GLU:HB3	2.27	0.64
3:A:550:THR:CG2	3:A:551:LYS:HE2	2.28	0.64
3:A:788:GLU:O	3:A:792:MET:HG3	1.97	0.63
3:A:707:ALA:HB3	3:A:725:LEU:HD21	1.80	0.63
3:A:623:LEU:HD23	3:A:826:LEU:HD21	1.80	0.62
3:A:499:ARG:HD3	5:A:2769:HOH:O	1.98	0.62
3:A:333:VAL:HG12	3:A:443:LEU:HD11	1.82	0.62
3:A:758:LYS:HG3	3:A:776:ILE:HG23	1.82	0.61
3:A:712:ILE:CG2	3:A:713:VAL:N	2.64	0.60
3:A:713:VAL:HG21	5:A:2797:HOH:O	2.00	0.60
3:A:718:ASP:OD1	3:A:719:TYR:CE1	2.54	0.60
3:A:548:LYS:HA	3:A:549:LYS:NZ	2.16	0.60
3:A:728:SER:OG	3:A:731:GLU:HG3	2.02	0.59
3:A:692:VAL:CB	3:A:696:GLU:HG3	2.16	0.59
1:P:7:DG:H1'	1:P:8:DC:H5"	1.82	0.59
3:A:550:THR:HG23	3:A:551:LYS:N	2.17	0.59
3:A:693:SER:H	3:A:696:GLU:CG	2.16	0.59
3:A:848:VAL:CG1	3:A:852:MET:CE	2.81	0.59
3:A:604:THR:HB	3:A:623:LEU:HD22	1.85	0.59
3:A:565:ALA:HB3	3:A:566:PRO:CD	2.30	0.58
3:A:750:MET:SD	3:A:792:MET:HB3	2.42	0.58
3:A:393:ASP:H	3:A:479:GLN:NE2	2.01	0.58
3:A:392:PHE:HA	3:A:479:GLN:HE22	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:530:SER:OG	3:A:533:GLN:HG3	2.04	0.57
3:A:548:LYS:HA	3:A:549:LYS:HZ1	1.69	0.57
3:A:652:ALA:HB3	3:A:852:MET:CE	2.35	0.57
2:T:24:DA:H2"	2:T:25:DT:C5'	2.35	0.57
3:A:786:PHE:CZ	3:A:790:MET:HE2	2.40	0.57
3:A:339:ASN:HD22	3:A:339:ASN:C	2.08	0.57
1:P:9:DA:H2"	1:P:10:DT:C7	2.35	0.57
3:A:652:ALA:HB3	3:A:852:MET:HE3	1.86	0.57
3:A:333:VAL:CG1	3:A:443:LEU:HD11	2.35	0.57
1:P:11:DG:OP1	3:A:551:LYS:HG3	2.05	0.56
3:A:700:ASN:ND2	3:A:703:ARG:HH21	1.99	0.56
3:A:737:GLU:O	3:A:741:GLU:HG3	2.05	0.56
3:A:349:GLU:H	3:A:349:GLU:CD	2.07	0.56
3:A:488:MET:HE1	3:A:824:LEU:HD13	1.87	0.56
3:A:559:ASP:HA	3:A:562:GLU:HB2	1.87	0.56
3:A:848:VAL:HB	3:A:849:PRO:HD3	1.88	0.56
3:A:411:ARG:HG3	5:A:2419:HOH:O	2.05	0.56
3:A:411:ARG:HD2	3:A:411:ARG:O	2.06	0.56
3:A:502:GLN:HG3	5:A:2762:HOH:O	2.04	0.55
3:A:873:TYR:O	3:A:876:LYS:HD3	2.06	0.55
3:A:718:ASP:OD1	3:A:719:TYR:HE1	1.89	0.55
3:A:519:TYR:CD1	3:A:525:GLU:HA	2.42	0.55
3:A:561:LEU:O	3:A:571:VAL:HG11	2.06	0.55
3:A:568:HIS:HD2	3:A:570:ILE:H	1.54	0.54
3:A:621:PRO:HG2	3:A:623:LEU:HD13	1.88	0.54
3:A:339:ASN:ND2	3:A:341:HIS:H	2.06	0.54
3:A:827:GLN:NE2	3:A:829:HIS:H	2.06	0.54
3:A:690:PHE:CB	3:A:701:MET:HE3	2.38	0.54
3:A:662:LEU:HD13	3:A:796:ILE:HD11	1.91	0.53
3:A:507:LEU:HD21	3:A:583:LEU:HB3	1.91	0.53
3:A:563:LYS:HE2	3:A:726:ASN:ND2	2.23	0.53
3:A:485:LEU:O	3:A:489:GLU:HG3	2.08	0.53
3:A:519:TYR:CG	3:A:525:GLU:HG2	2.44	0.53
3:A:730:LYS:HE3	3:A:730:LYS:O	2.09	0.53
3:A:588:ILE:O	3:A:592:LEU:HG	2.09	0.53
3:A:499:ARG:O	3:A:503:MET:HG3	2.09	0.52
3:A:527:ASN:H	3:A:533:GLN:NE2	2.08	0.52
3:A:411:ARG:CZ	3:A:412:ALA:HA	2.37	0.52
3:A:418:GLN:HA	5:A:2424:HOH:O	2.08	0.52
3:A:748:ARG:NH2	5:A:2138:HOH:O	2.43	0.52
3:A:550:THR:CG2	3:A:551:LYS:N	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:621:PRO:HG2	3:A:623:LEU:CD1	2.40	0.52
3:A:532:LYS:HB2	5:A:2701:HOH:O	2.11	0.51
3:A:710:PHE:O	3:A:714:TYR:CE1	2.63	0.51
3:A:411:ARG:HH11	3:A:415:LYS:HB2	1.76	0.51
5:P:2060:HOH:O	3:A:579:GLN:HG2	2.10	0.51
3:A:494:LYS:HG3	3:A:641:VAL:HG23	1.93	0.51
3:A:563:LYS:O	3:A:566:PRO:HD2	2.11	0.51
1:P:9:DA:C2'	1:P:10:DT:H72	2.40	0.51
3:A:494:LYS:HD3	5:A:2371:HOH:O	2.09	0.51
3:A:431:LYS:H	3:A:434:LYS:HZ3	1.58	0.51
3:A:718:ASP:HB3	3:A:736:ILE:HD13	1.93	0.50
3:A:565:ALA:CB	3:A:566:PRO:HD3	2.35	0.50
3:A:849:PRO:HG3	3:A:866:TYR:CD1	2.47	0.50
3:A:797:GLN:HG3	5:A:1002:HOH:O	2.10	0.50
3:A:716:ILE:HG13	3:A:716:ILE:O	2.12	0.49
1:P:11:DG:OP1	3:A:551:LYS:CG	2.60	0.49
2:T:19:DG:OP2	3:A:786:PHE:HZ	1.95	0.49
3:A:536:VAL:O	3:A:540:GLU:HB2	2.11	0.49
3:A:498:LYS:O	3:A:502:GLN:HG3	2.13	0.49
3:A:689:ILE:O	3:A:738:ARG:NH1	2.46	0.49
3:A:411:ARG:NH1	3:A:415:LYS:HB2	2.28	0.49
3:A:519:TYR:CD2	3:A:525:GLU:HG2	2.48	0.49
3:A:718:ASP:OD2	3:A:729:ARG:HD3	2.13	0.49
3:A:712:ILE:HA	3:A:716:ILE:HB	1.95	0.49
2:T:19:DG:H1'	2:T:20:DC:C6	2.48	0.49
1:P:9:DA:H2''	1:P:10:DT:H72	1.95	0.48
3:A:682:HIS:HE1	5:A:2301:HOH:O	1.96	0.48
3:A:500:LEU:HD13	3:A:639:ALA:CB	2.43	0.48
3:A:551:LYS:CD	3:A:552:THR:H	2.27	0.47
2:T:18:DA:H2''	2:T:19:DG:O5'	2.14	0.47
3:A:521:LEU:HD12	3:A:570:ILE:HA	1.96	0.47
3:A:716:ILE:CG1	3:A:736:ILE:HG12	2.44	0.47
3:A:532:LYS:HE3	3:A:532:LYS:C	2.35	0.47
3:A:790:MET:CG	5:A:2061:HOH:O	2.53	0.47
3:A:690:PHE:CD2	3:A:701:MET:HE3	2.50	0.47
3:A:559:ASP:HA	3:A:562:GLU:CD	2.36	0.47
1:P:13:DT:OP2	3:A:558:ALA:HB2	2.15	0.47
5:T:1007:HOH:O	3:A:620:GLU:HA	2.15	0.46
3:A:754:VAL:CG1	3:A:788:GLU:HG2	2.46	0.46
3:A:716:ILE:HG12	3:A:736:ILE:HG12	1.97	0.46
3:A:339:ASN:HD22	3:A:341:HIS:H	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:494:LYS:HG3	3:A:641:VAL:CG2	2.46	0.46
3:A:725:LEU:O	3:A:727:ILE:HG23	2.17	0.45
3:A:715:GLY:O	3:A:716:ILE:CG2	2.65	0.45
3:A:434:LYS:HE2	3:A:434:LYS:HB2	1.61	0.44
3:A:824:LEU:HD23	3:A:834:LEU:HD22	1.98	0.44
5:P:2147:HOH:O	3:A:630:LEU:HD22	2.18	0.44
3:A:711:GLY:O	3:A:712:ILE:C	2.56	0.44
3:A:529:ASN:O	3:A:531:PRO:HD3	2.17	0.44
3:A:411:ARG:C	3:A:411:ARG:CD	2.82	0.44
1:P:15:DC:H2'	1:P:16:2DT:C6	2.48	0.44
3:A:789:ARG:HA	3:A:792:MET:HE2	1.97	0.44
3:A:767:LEU:HG	3:A:802:ASP:HB3	2.00	0.44
3:A:712:ILE:HD13	3:A:716:ILE:HB	1.99	0.43
3:A:629:ARG:HG3	3:A:630:LEU:HD13	1.99	0.43
3:A:677:ARG:HB2	3:A:679:LEU:HG	1.99	0.43
3:A:550:THR:O	3:A:551:LYS:C	2.57	0.43
3:A:411:ARG:NH1	3:A:415:LYS:CB	2.82	0.43
3:A:780:ASN:OD1	3:A:780:ASN:C	2.57	0.43
3:A:712:ILE:O	3:A:713:VAL:C	2.58	0.42
1:P:11:DG:OP1	3:A:550:THR:HG23	2.19	0.42
3:A:494:LYS:CD	5:A:2371:HOH:O	2.67	0.42
3:A:413:ALA:O	3:A:416:MET:HB2	2.19	0.42
3:A:516:GLN:OE1	3:A:516:GLN:HA	2.18	0.42
3:A:730:LYS:HE3	3:A:734:GLU:OE1	2.20	0.42
3:A:426:GLU:CD	3:A:431:LYS:HG3	2.40	0.42
3:A:814:ARG:HG3	3:A:851:VAL:HG21	2.02	0.42
3:A:717:SER:HB2	3:A:789:ARG:HD3	2.02	0.42
3:A:402:ASP:HA	3:A:403:PRO:HD2	1.89	0.42
3:A:715:GLY:C	3:A:716:ILE:HG22	2.40	0.42
3:A:431:LYS:N	3:A:434:LYS:NZ	2.63	0.42
3:A:468:ASN:O	3:A:469:GLU:HB2	2.20	0.42
3:A:306:ARG:HD2	5:A:2148:HOH:O	2.18	0.42
3:A:498:LYS:HE2	3:A:600:LYS:NZ	2.35	0.41
2:T:21:DA:H3'	3:A:619:THR:HG22	2.01	0.41
3:A:393:ASP:H	3:A:479:GLN:HE21	1.68	0.41
3:A:550:THR:HG23	3:A:551:LYS:H	1.84	0.41
3:A:856:VAL:HG12	3:A:857:THR:N	2.34	0.41
3:A:339:ASN:HD22	3:A:341:HIS:N	2.18	0.40
3:A:507:LEU:O	3:A:511:LEU:HB2	2.21	0.40
3:A:708:VAL:O	3:A:712:ILE:HB	2.21	0.40
3:A:786:PHE:CZ	3:A:790:MET:CE	3.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:471:ASP:OD1	3:A:471:ASP:N	2.44	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	Interatomic distance (Å)	Clash overlap (Å)
5:A:2171:HOH:O	5:A:2385:HOH:O[3_555]	2.14	0.06

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%)	551 (95%)	23 (4%)	4 (1%)	26 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	713	VAL
3	A	714	TYR
3	A	628	ILE
3	A	716	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	496/496 (100%)	439 (88%)	57 (12%)	7 2

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	306	ARG
3	A	309	GLU
3	A	325	GLU
3	A	339	ASN
3	A	349	GLU
3	A	350	THR
3	A	356	GLN
3	A	386	GLU
3	A	411	ARG
3	A	431	LYS
3	A	434	LYS
3	A	443	LEU
3	A	466	ARG
3	A	498	LYS
3	A	505	LYS
3	A	509	GLU
3	A	511	LEU
3	A	515	GLU
3	A	516	GLN
3	A	532	LYS
3	A	534	LEU
3	A	541	LYS
3	A	548	LYS
3	A	549	LYS
3	A	550	THR
3	A	551	LYS
3	A	557	SER
3	A	562	GLU
3	A	583	LEU
3	A	596	ARG
3	A	602	VAL
3	A	623	LEU
3	A	630	LEU
3	A	659	LEU
3	A	671	LEU
3	A	696	GLU
3	A	697	VAL
3	A	712	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	714	TYR
3	A	719	TYR
3	A	723	GLN
3	A	729	ARG
3	A	730	LYS
3	A	738	ARG
3	A	748	ARG
3	A	756	GLU
3	A	758	LYS
3	A	766	LEU
3	A	776	ILE
3	A	779	ARG
3	A	812	ASN
3	A	815	LEU
3	A	827	GLN
3	A	828	VAL
3	A	834	LEU
3	A	844	LEU
3	A	876	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	328	HIS
3	A	339	ASN
3	A	479	GLN
3	A	533	GLN
3	A	543	GLN
3	A	568	HIS
3	A	576	HIS
3	A	656	GLN
3	A	682	HIS
3	A	700	ASN
3	A	704	GLN
3	A	723	GLN
3	A	793	ASN
3	A	812	ASN
3	A	827	GLN
3	A	854	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	2DT	P	16	1,2	11,20,21	1.25	2 (18%)	12,28,31	4.89	4 (33%)

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	2DT	P	16	1,2	-	0/3/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	16	2DT	C6-N1	2.23	1.38	1.35
1	P	16	2DT	C4-N3	2.67	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	16	2DT	C5-C4-N3	-9.09	115.02	125.14
1	P	16	2DT	C2'-C1'-N1	2.09	116.72	112.49
1	P	16	2DT	C5M-C5-C6	2.21	123.08	118.62
1	P	16	2DT	C4-N3-C2	13.84	127.21	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	16	2DT	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	910	-	4,4,4	4.95	4 (100%)	6,6,6	0.39	0
4	SO4	A	912	-	4,4,4	4.73	4 (100%)	6,6,6	0.33	0
4	SO4	A	915	-	4,4,4	5.18	4 (100%)	6,6,6	0.13	0
4	SO4	A	920	-	4,4,4	5.09	4 (100%)	6,6,6	0.21	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	910	-	-	0/0/0/0	0/0/0/0
4	SO4	A	912	-	-	0/0/0/0	0/0/0/0
4	SO4	A	915	-	-	0/0/0/0	0/0/0/0
4	SO4	A	920	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	912	SO4	O1-S	3.25	1.58	1.47
4	A	912	SO4	O2-S	3.31	1.58	1.47
4	A	910	SO4	O1-S	3.40	1.58	1.47
4	A	910	SO4	O2-S	3.75	1.60	1.47
4	A	920	SO4	O1-S	3.78	1.60	1.47
4	A	915	SO4	O1-S	3.85	1.60	1.47
4	A	920	SO4	O2-S	3.94	1.60	1.47
4	A	915	SO4	O2-S	4.28	1.61	1.47
4	A	912	SO4	O3-S	5.75	1.68	1.47
4	A	912	SO4	O4-S	5.92	1.68	1.47
4	A	910	SO4	O3-S	6.02	1.69	1.47
4	A	910	SO4	O4-S	6.02	1.69	1.47
4	A	920	SO4	O3-S	6.04	1.69	1.47
4	A	915	SO4	O4-S	6.04	1.69	1.47
4	A	920	SO4	O4-S	6.10	1.69	1.47
4	A	915	SO4	O3-S	6.15	1.69	1.47

There are no bond angle outliers.

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 [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	P	9/10 (90%)	0.47	1 (11%) 7 8	21, 30, 58, 60	0
2	T	10/10 (100%)	0.40	1 (10%) 9 10	23, 30, 44, 59	0
3	A	580/580 (100%)	0.40	38 (6%) 22 24	12, 22, 45, 63	0
All	All	599/600 (99%)	0.40	40 (6%) 21 23	12, 22, 46, 63	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	552	THR	10.4
3	A	550	THR	7.3
3	A	719	TYR	6.9
3	A	433	ALA	5.9
3	A	716	ILE	5.7
3	A	297	ALA	5.5
3	A	729	ARG	5.2
3	A	549	LYS	4.8
3	A	553	GLY	4.8
3	A	551	LYS	4.7
3	A	717	SER	4.6
3	A	712	ILE	4.5
3	A	306	ARG	4.4
3	A	715	GLY	4.3
3	A	432	GLY	4.3
3	A	431	LYS	4.2
3	A	298	ALA	3.9
3	A	713	VAL	3.8
3	A	714	TYR	3.6
3	A	559	ASP	3.6
3	A	434	LYS	3.6
3	A	562	GLU	3.5
3	A	629	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	547	LEU	3.0
2	T	27	DC	2.9
3	A	548	LYS	2.8
1	P	7	DG	2.8
3	A	723	GLN	2.7
3	A	782	ASN	2.6
3	A	534	LEU	2.5
3	A	786	PHE	2.5
3	A	411	ARG	2.4
3	A	512	GLY	2.4
3	A	695	ASP	2.4
3	A	502	GLN	2.4
3	A	730	LYS	2.3
3	A	781	PHE	2.2
3	A	505	LYS	2.1
3	A	406	GLY	2.1
3	A	325	GLU	2.1

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
1	2DT	P	16	19/20	0.97	0.09	-	19,20,21,21	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
4	SO4	A	912	5/5	0.95	0.12	-0.10	39,39,41,41	0
4	SO4	A	920	5/5	0.94	0.11	-0.63	52,52,52,52	0
4	SO4	A	915	5/5	0.93	0.17	-	44,44,44,45	0
4	SO4	A	910	5/5	0.94	0.17	-	45,45,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.