



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:21 AM UTC

PDB ID : 3BDP / pdb_00003bdp
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

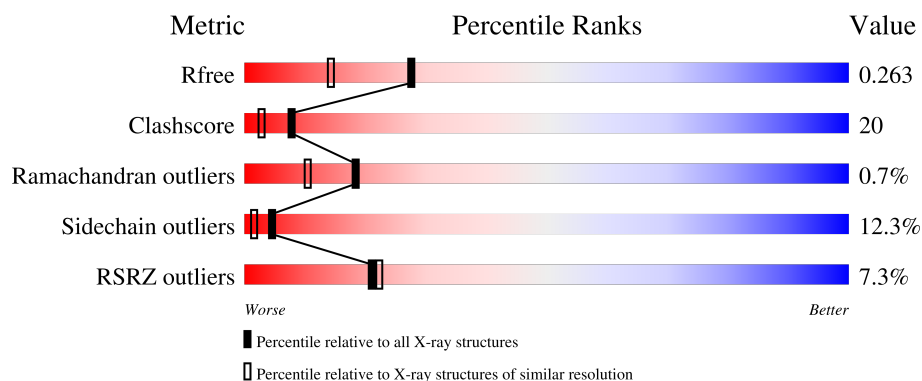
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
2	T	10	
3	A	580	

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 [i](#)

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			

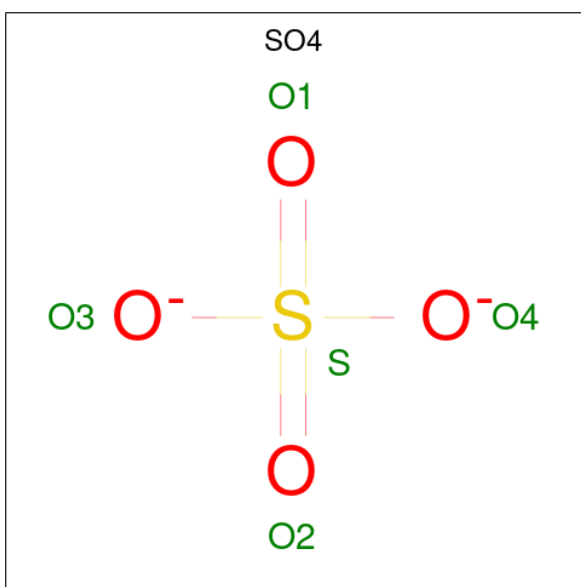
- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE I).

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 (CCD ID: 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		

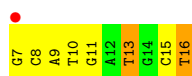
- Molecule 5 is water.

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

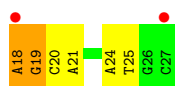
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

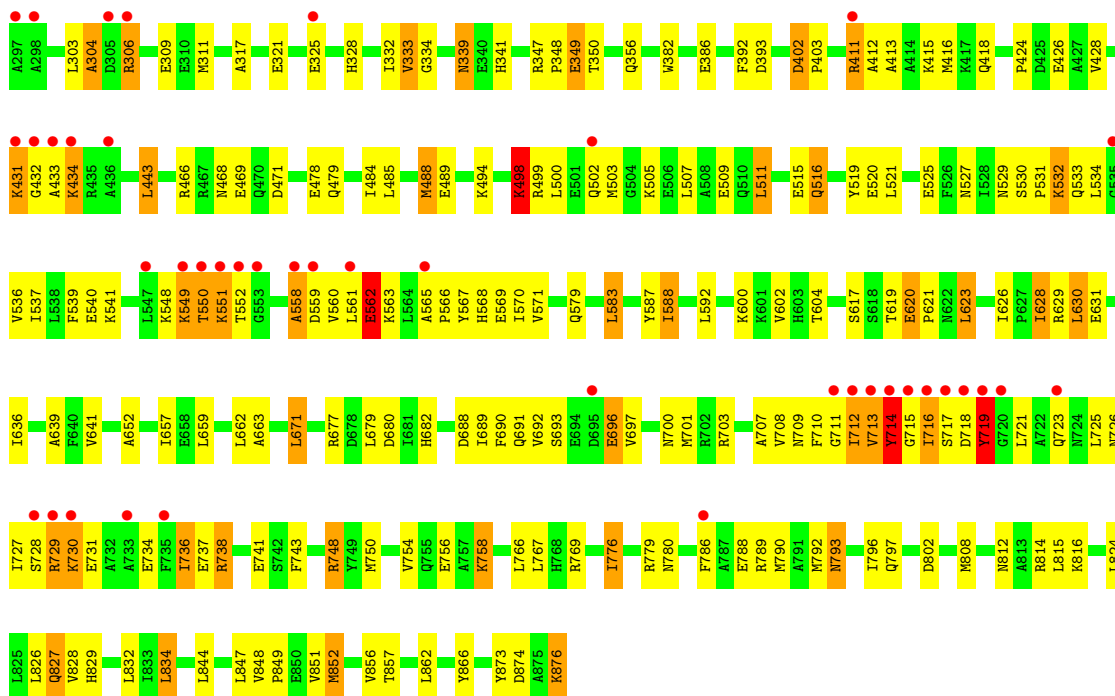
- Molecule 1: DNA (5'-D(*GP*CP*AP*TP*GP*AP*TP*GP*CP*2DT)-3')



- 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 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.1 (20.00-1.90) 92.7 (20.00-1.90)	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%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.37	0/205	0.89	0/315
2	T	0.40	0/225	0.92	1/345 (0.3%)
3	A	0.70	3/4740 (0.1%)	1.04	33/6405 (0.5%)
All	All	0.68	3/5170 (0.1%)	1.03	34/7065 (0.5%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	488	MET	SD-CE	-8.31	1.58	1.79
3	A	852	MET	SD-CE	-5.85	1.65	1.79
3	A	657	ILE	CA-CB	5.38	1.61	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	321	GLU	N-CA-C	8.75	122.45	109.59
3	A	567	TYR	N-CA-C	8.03	121.14	111.82
3	A	743	PHE	CA-C-N	7.51	127.38	119.05
3	A	743	PHE	C-N-CA	7.51	127.38	119.05
3	A	680	ASP	N-CA-C	-7.05	99.00	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	317	ALA	N-CA-C	-6.92	97.98	109.46
3	A	719	TYR	N-CA-C	-6.71	103.89	111.14
3	A	332	ILE	N-CA-C	-6.68	98.23	107.99
3	A	769	ARG	N-CA-C	-6.29	101.63	110.50
3	A	793	ASN	N-CA-C	6.28	120.15	112.23
3	A	587	TYR	N-CA-C	6.25	120.90	113.28
3	A	560	VAL	N-CA-C	-6.23	104.68	110.53
3	A	347	ARG	N-CA-C	-6.07	102.40	109.93
3	A	588	ILE	CB-CA-C	-6.07	106.55	111.71
3	A	478	GLU	N-CA-C	5.91	117.72	111.28
2	T	18	DA	O5'-C5'-C4'	5.89	119.64	110.80
3	A	558	ALA	N-CA-C	5.66	117.14	110.97
3	A	617	SER	N-CA-C	-5.62	100.81	109.52
3	A	304	ALA	N-CA-C	5.49	118.18	110.23
3	A	688	ASP	N-CA-C	5.44	117.01	111.14
3	A	847	LEU	N-CA-C	5.41	116.98	111.14
3	A	333	VAL	N-CA-C	5.35	119.94	112.50
3	A	562	GLU	N-CA-C	-5.32	105.38	111.07
3	A	631	GLU	N-CA-C	5.31	117.75	111.33
3	A	498	LYS	N-CA-C	-5.29	105.59	111.36
3	A	588	ILE	N-CA-C	-5.28	106.52	111.48
3	A	402	ASP	CA-C-N	5.26	124.92	119.56
3	A	402	ASP	C-N-CA	5.26	124.92	119.56
3	A	620	GLU	CB-CA-C	-5.18	106.49	111.00
3	A	721	LEU	N-CA-C	-5.08	105.39	111.03
3	A	862	LEU	N-CA-C	-5.08	101.41	109.59
3	A	626	ILE	N-CA-C	-5.07	104.31	109.02
3	A	539	PHE	N-CA-C	5.04	119.42	113.28
3	A	779	ARG	N-CA-C	-5.03	106.98	113.02

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 [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	P	202	0	115	12	0
2	T	201	0	114	6	0
3	A	4656	0	4709	187	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	199	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 20.

All (199) 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:848:VAL:CG1	3:A:852:MET:HE3	1.89	1.02
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:848:VAL:HG12	3:A:852:MET:HE3	1.49	0.95
3:A:719:TYR:HD1	3:A:719:TYR:H	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:789:ARG:HA	3:A:792:MET:HE3	1.56	0.87
3:A:663:ALA:HB2	3:A:671:LEU:HD13	1.57	0.86
3:A:652:ALA:HB3	3:A:852:MET:HE1	1.58	0.85
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:484:ILE:HG22	3:A:488:MET:HE3	1.60	0.82
3:A:700:ASN:HD21	3:A:703:ARG:HH21	1.25	0.82
3:A:488:MET:HE1	3:A:808:MET:HE2	1.66	0.78
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:832:LEU:HD12	3:A:852:MET:HE2	1.67	0.75
3:A:719:TYR:CD1	3:A:719:TYR:N	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
3:A:789:ARG:HA	3:A:792:MET:CE	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:411:ARG:HD2	3:A:411:ARG:C	2.15	0.71
3:A:714:TYR:HA	3:A:793:ASN:ND2	2.05	0.71
3:A:484:ILE:HG22	3:A:488:MET:HE2	1.73	0.70
3:A:536:VAL:HG23	5:A:2748:HOH:O	1.90	0.70
3:A:790:MET:HA	5:A:2061: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:488:MET:HE1	3:A:808:MET:CE	2.25	0.67
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:HD1	3:A:719:TYR:N	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:692:VAL:HG21	3:A:701:MET:HE1	1.80	0.63
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:431:LYS:H	3:A:434:LYS:HZ1	1.47	0.62
3:A:499:ARG:HD3	5:A:2769:HOH:O	1.98	0.62
3:A:623:LEU:HD23	3:A:826:LEU:HD21	1.80	0.62
3:A:333:VAL:HG12	3:A:443:LEU:HD11	1.82	0.62
3:A:339:ASN:C	3:A:339:ASN:HD22	2.08	0.62
3:A:758:LYS:HG3	3:A:776:ILE:HG23	1.82	0.61
3:A:503:MET:HE1	3:A:636:ILE:HA	1.81	0.61
3:A:349:GLU:H	3:A:349:GLU:CD	2.07	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:786:PHE:CZ	3:A:790:MET:HE2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:604:THR:HB	3:A:623:LEU:HD22	1.85	0.59
3:A:548:LYS:HA	3:A:549:LYS:HZ1	1.68	0.58
3:A:565:ALA:HB3	3:A:566:PRO:CD	2.30	0.58
3:A:848:VAL:HG13	3:A:852:MET:HE3	1.82	0.58
3:A:393:ASP:H	3:A:479:GLN:NE2	2.01	0.58
3:A:750:MET:SD	3:A:792:MET:HB3	2.42	0.58
3:A:392:PHE:HA	3:A:479:GLN:HE22	1.67	0.58
3:A:530:SER:OG	3:A:533:GLN:HG3	2.04	0.57
2:T:24:DA:H2''	2:T:25:DT:C5'	2.35	0.57
1:P:9:DA:H2''	1:P:10:DT:C7	2.35	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: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:690:PHE:CB	3:A:701:MET:HE3	2.36	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:339:ASN:ND2	3:A:341:HIS:H	2.06	0.54
3:A:621:PRO:HG2	3:A:623:LEU:HD13	1.88	0.54
3:A:827:GLN:NE2	3:A:829:HIS:H	2.06	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:485:LEU:O	3:A:489:GLU:HG3	2.08	0.53
3:A:563:LYS:HE2	3:A:726:ASN:ND2	2.23	0.53
3:A:519:TYR:CG	3:A:525:GLU:HG2	2.44	0.53
3:A:588:ILE:O	3:A:592:LEU:HG	2.09	0.53
3:A:730:LYS:O	3:A:730:LYS:HE3	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:304:ALA:CB	3:A:311:MET:HE1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:550:THR:CG2	3:A:551:LYS:N	2.73	0.52
3:A:411:ARG:C	3:A:411:ARG:CD	2.82	0.52
3:A:652:ALA:HB3	3:A:852:MET:CE	2.35	0.52
3:A:621:PRO:HG2	3:A:623:LEU:CD1	2.40	0.52
3:A:559:ASP:HA	3:A:562:GLU:CD	2.36	0.51
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
5:P:2060:HOH:O	3:A:579:GLN:HG2	2.10	0.51
3:A:411:ARG:HH11	3:A:415:LYS:HB2	1.76	0.51
3:A:494:LYS:HG3	3:A:641:VAL:HG23	1.93	0.51
3:A:532:LYS:HE3	3:A:532:LYS:C	2.35	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:565:ALA:CB	3:A:566:PRO:HD3	2.35	0.50
3:A:718:ASP:HB3	3:A:736:ILE:HD13	1.93	0.50
3:A:728:SER:HG	3:A:731:GLU:HG3	1.76	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
1:P:11:DG:OP1	3:A:551:LYS:CG	2.60	0.49
3:A:716:ILE:O	3:A:716:ILE:HG13	2.12	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
2:T:19:DG:H1'	2:T:20:DC:C6	2.48	0.49
3:A:711:GLY:O	3:A:712:ILE:C	2.56	0.49
3:A:712:ILE:HA	3:A:716:ILE:HB	1.95	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:431:LYS:N	3:A:434:LYS:HZ1	2.12	0.48
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:551:LYS:CD	3:A:552:THR:H	2.27	0.47
3:A:780:ASN:OD1	3:A:780:ASN:C	2.57	0.47
3:A:712:ILE:O	3:A:713:VAL:C	2.58	0.47
3:A:716:ILE:CG1	3:A:736:ILE:HG12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:426:GLU:CD	3:A:431:LYS:HG3	2.40	0.47
3:A:550:THR:O	3:A:551:LYS:C	2.57	0.47
3:A:790:MET:CG	5:A:2061:HOH:O	2.53	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:715:GLY:C	3:A:716:ILE:HG22	2.40	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
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:HB2	3:A:434:LYS:HE2	1.61	0.44
3:A:304:ALA:HB2	3:A:311:MET:HE1	1.99	0.44
5:P:2147:HOH:O	3:A:630:LEU:HD22	2.18	0.44
3:A:484:ILE:CG2	3:A:488:MET:HE2	2.44	0.44
3:A:824:LEU:HD23	3:A:834:LEU:HD22	1.98	0.44
3:A:529:ASN:O	3:A:531:PRO:HD3	2.17	0.44
1:P:15:DC:H2'	1:P:16:2DT:C6	2.48	0.44
3:A:874:ASP:C	3:A:876:LYS:H	2.26	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:690:PHE:HB3	3:A:701:MET:HE3	1.99	0.43
3:A:411:ARG:NH1	3:A:415:LYS:CB	2.82	0.43
1:P:11:DG:OP1	3:A:550:THR:HG23	2.19	0.42
3:A:432:GLY:O	3:A:433:ALA:C	2.61	0.42
3:A:494:LYS:CD	5:A:2371:HOH:O	2.67	0.42
3:A:713:VAL:C	3:A:793:ASN:HD22	2.27	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:692:VAL:CG2	3:A:701:MET:HE1	2.49	0.42
3:A:730:LYS:HE3	3:A:734:GLU:OE1	2.20	0.42
3:A:814:ARG:HG3	3:A:851:VAL:HG21	2.02	0.42
3:A:402:ASP:HA	3:A:403:PRO:HD2	1.89	0.42
3:A:717:SER:HB2	3:A:789:ARG:HD3	2.02	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:786:PHE:C	3:A:786:PHE:CD1	2.98	0.42
3:A:306:ARG:HD2	5:A:2148:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:21:DA:H3'	3:A:619:THR:HG22	2.01	0.41
3:A:498:LYS:HE2	3:A:600:LYS:NZ	2.35	0.41
3:A:393:ASP:H	3:A:479:GLN:HE21	1.68	0.41
3:A:530:SER:C	3:A:532:LYS:N	2.77	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
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%)	18 10

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 ⓘ

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%)	435 (88%)	61 (12%)	4 1

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	303	LEU
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	428	VAL
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	520	GLU
3	A	532	LYS
3	A	534	LEU
3	A	537	ILE
3	A	541	LYS
3	A	549	LYS
3	A	550	THR
3	A	551	LYS
3	A	562	GLU

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Mol	Chain	Res	Type
3	A	583	LEU
3	A	602	VAL
3	A	623	LEU
3	A	628	ILE
3	A	630	LEU
3	A	659	LEU
3	A	671	LEU
3	A	691	GLN
3	A	696	GLU
3	A	697	VAL
3	A	712	ILE
3	A	714	TYR
3	A	719	TYR
3	A	723	GLN
3	A	729	ARG
3	A	730	LYS
3	A	736	ILE
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	812	ASN
3	A	815	LEU
3	A	816	LYS
3	A	827	GLN
3	A	828	VAL
3	A	834	LEU
3	A	844	LEU
3	A	876	LYS

Sometimes 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	418	GLN
3	A	479	GLN
3	A	510	GLN
3	A	533	GLN
3	A	543	GLN

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Mol	Chain	Res	Type
3	A	568	HIS
3	A	576	HIS
3	A	624	GLN
3	A	682	HIS
3	A	700	ASN
3	A	723	GLN
3	A	793	ASN
3	A	812	ASN
3	A	827	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	2,1	17,20,21	0.44	0	22,28,31	0.58	1 (4%)

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	2,1	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	16	2DT	C2'-C1'-N1	2.28	116.72	112.40

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 oligosaccharides 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	915	-	4,4,4	2.66	4 (100%)	6,6,6	0.15	0
4	SO4	A	920	-	4,4,4	2.59	4 (100%)	6,6,6	0.18	0
4	SO4	A	912	-	4,4,4	2.37	4 (100%)	6,6,6	0.32	0
4	SO4	A	910	-	4,4,4	2.50	4 (100%)	6,6,6	0.31	0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	915	SO4	O2-S	2.86	1.61	1.44
4	A	920	SO4	O2-S	2.66	1.60	1.44
4	A	915	SO4	O1-S	2.61	1.60	1.44
4	A	915	SO4	O3-S	2.60	1.69	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	920	SO4	O4-S	2.58	1.69	1.48
4	A	920	SO4	O1-S	2.57	1.60	1.44
4	A	915	SO4	O4-S	2.55	1.69	1.48
4	A	920	SO4	O3-S	2.55	1.69	1.48
4	A	910	SO4	O2-S	2.55	1.60	1.44
4	A	910	SO4	O4-S	2.55	1.69	1.48
4	A	910	SO4	O3-S	2.55	1.69	1.48
4	A	912	SO4	O4-S	2.50	1.68	1.48
4	A	912	SO4	O3-S	2.43	1.68	1.48
4	A	910	SO4	O1-S	2.35	1.58	1.44
4	A	912	SO4	O2-S	2.30	1.58	1.44
4	A	912	SO4	O1-S	2.26	1.58	1.44

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%)	0.54	1 (11%) 10 11	21, 30, 58, 60	0
2	T	10/10 (100%)	0.61	2 (20%) 3 2	23, 30, 44, 59	0
3	A	580/580 (100%)	0.29	41 (7%) 22 23	12, 22, 45, 63	0
All	All	599/600 (99%)	0.30	44 (7%) 21 22	12, 22, 46, 63	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	715	GLY	7.3
3	A	716	ILE	6.5
3	A	550	THR	6.1
3	A	717	SER	5.8
3	A	552	THR	5.4
3	A	719	TYR	5.2
3	A	713	VAL	5.0
3	A	549	LYS	4.8
3	A	714	TYR	4.7
3	A	298	ALA	4.5
3	A	712	ILE	4.5
3	A	433	ALA	4.5
3	A	558	ALA	3.6
3	A	553	GLY	3.3
3	A	306	ARG	3.1
3	A	502	GLN	3.0
3	A	723	GLN	3.0
3	A	535	GLY	3.0
3	A	729	ARG	2.9
3	A	786	PHE	2.8
3	A	432	GLY	2.7
3	A	411	ARG	2.6
3	A	728	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	720	GLY	2.6
3	A	297	ALA	2.5
3	A	559	ASP	2.5
2	T	18	DA	2.5
2	T	27	DC	2.4
3	A	436	ALA	2.4
3	A	695	ASP	2.4
3	A	718	ASP	2.4
3	A	431	LYS	2.4
3	A	551	LYS	2.4
3	A	561	LEU	2.3
3	A	565	ALA	2.3
3	A	733	ALA	2.3
3	A	730	LYS	2.3
3	A	325	GLU	2.2
3	A	547	LEU	2.2
3	A	711	GLY	2.2
3	A	434	LYS	2.2
1	P	7	DG	2.1
3	A	735	PHE	2.1
3	A	305	ASP	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. 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	B-factors($\text{\AA}^2$)	Q<0.9
1	2DT	P	16	19/20	0.97	0.06	19,20,21,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	910	5/5	0.87	0.12	45,45,46,46	0
4	SO4	A	915	5/5	0.90	0.15	44,44,44,45	0
4	SO4	A	912	5/5	0.92	0.12	39,39,41,41	0
4	SO4	A	920	5/5	0.93	0.11	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.