Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 05:55 pm GMT

PDB ID	:	1D9F
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX OF DNA POLYMERASE I KLENOW FRAGMENT WITH DNA TETRAMER CARRYING 2'-O-(3-A MINOPROPYL)-RNA MODIFICATION 5'-D(TT)-AP(U)-D(T)-3'
Authors	:	Teplova, M.; Wallace, S.T.; Tereshko, V.; Minasov, G.; Simons, A.M.; Cook, P.D.; Manoharan, M.; Egli, M.
Deposited on	:	1999-10-27
Resolution	:	3.00 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 3.00 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		19
Ramachandran outliers		0.8%
Sidechain outliers		8.2%
RSRZ outliers		6.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
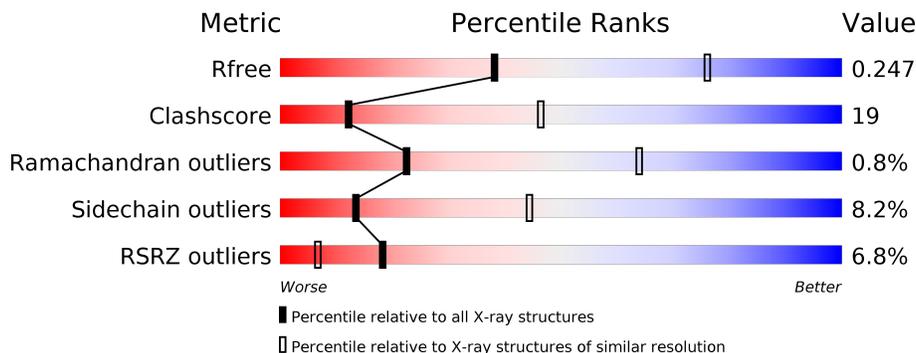
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 <=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	4	50% / 25% / 50% / 25%
2	A	605	6% / 70% / 25% / · ·

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
1	U31	B	1003[A]	-	-	X	-
1	U31	B	1003[B]	-	-	X	-
4	SO4	A	38	-	-	X	-
4	SO4	A	94	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4934 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 DNA/RNA hybrid called DNA/RNA (5'-D(*TP*TP)-R(*(U31)P)-D(*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	3	Total	C	N	O	P	0	3	0
			122	64	14	40	4			

- Molecule 2 is a protein called DNA POLYMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	601	Total	C	N	O	S	0	0	0
			4753	3008	830	899	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	MET	VAL	ENGINEERED	UNP P00582

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
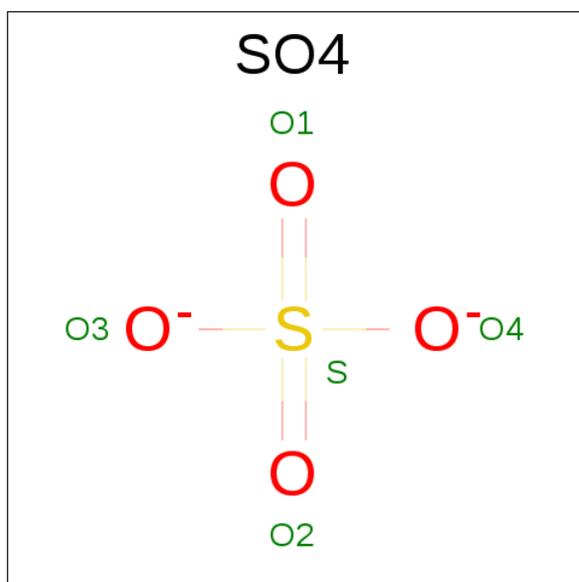
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total 37	O 37	0	0
5	B	1	Total 1	O 1	0	0

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 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/RNA (5'-D(*TP*TP)-R(*(U31)P)-D(*T)-3')
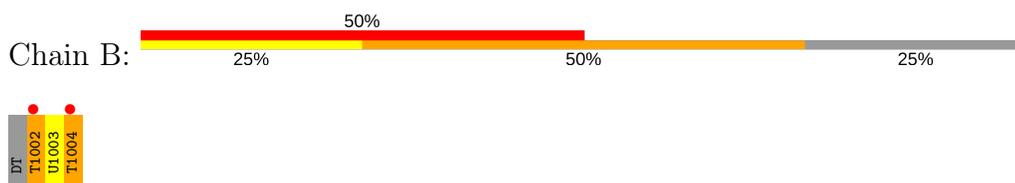
• Molecule 2: DNA POLYMERASE I
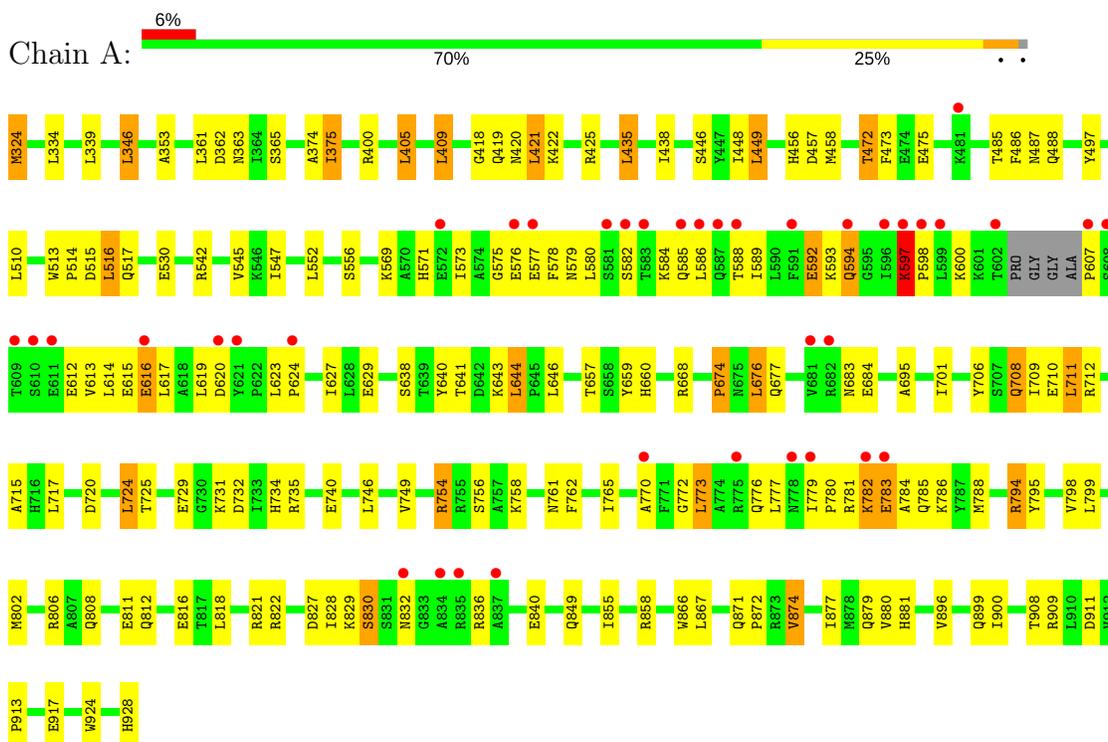
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	102.65Å 102.65Å 86.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 28.47 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.4 (20.00-3.00) 95.5 (28.47-2.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.243 0.232 , 0.247	Depositor DCC
R_{free} test set	1723 reflections (9.91%)	DCC
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 67.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4934	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, SO4, U31

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	4.54	8/78 (10.3%)	3.04	6/112 (5.4%)
2	A	0.41	0/4839	0.72	2/6547 (0.0%)
All	All	0.70	8/4917 (0.2%)	0.82	8/6659 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1002[A]	DT	C3'-O3'	-22.40	1.14	1.44
1	B	1002[B]	DT	C3'-O3'	-22.40	1.14	1.44
1	B	1004[A]	DT	O5'-C5'	11.30	1.70	1.42
1	B	1004[B]	DT	O5'-C5'	11.30	1.70	1.42
1	B	1002[A]	DT	C5-C7	-9.78	1.44	1.50
1	B	1002[B]	DT	C5-C7	-9.78	1.44	1.50
1	B	1002[A]	DT	C2-O2	-5.32	1.18	1.22
1	B	1002[B]	DT	C2-O2	-5.32	1.18	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1004[A]	DT	P-O5'-C5'	12.57	141.01	120.90
1	B	1004[B]	DT	P-O5'-C5'	12.57	141.01	120.90
1	B	1002[A]	DT	C2'-C3'-O3'	-11.94	73.21	112.60
1	B	1002[B]	DT	C2'-C3'-O3'	-11.94	73.21	112.60
1	B	1004[A]	DT	O5'-C5'-C4'	11.60	139.99	111.00
1	B	1004[B]	DT	O5'-C5'-C4'	11.60	139.99	111.00
2	A	607	PRO	N-CA-CB	5.40	109.78	103.30
2	A	597	LYS	N-CA-C	5.38	125.51	111.00

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	122	0	86	65	0
2	A	4753	0	4753	161	0
3	A	1	0	0	0	0
4	A	20	0	0	7	0
5	A	37	0	0	2	0
5	B	1	0	0	0	0
All	All	4934	0	4839	185	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 19.

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)
1:B:1002[B]:DT:C7	2:A:422:LYS:HZ1	1.03	1.59
1:B:1004[A]:DT:O5'	1:B:1004[A]:DT:C5'	1.70	1.36
1:B:1002[A]:DT:C7	2:A:422:LYS:NZ	1.85	1.34
1:B:1002[B]:DT:C7	2:A:422:LYS:NZ	1.85	1.34
1:B:1002[A]:DT:H73	2:A:422:LYS:NZ	1.40	1.27
1:B:1002[B]:DT:H73	2:A:422:LYS:NZ	1.40	1.27
1:B:1003[B]:U31:H6	1:B:1003[B]:U31:O5'	1.36	1.21
1:B:1003[B]:U31:H2'	2:A:361:LEU:CD2	1.75	1.17
1:B:1002[B]:DT:H2'	1:B:1003[B]:U31:O4'	1.49	1.10
1:B:1003[A]:U31:H5	2:A:458:MET:HE1	1.35	1.09
1:B:1003[B]:U31:H2'	2:A:361:LEU:HD22	1.34	1.05
1:B:1003[A]:U31:H5	2:A:458:MET:CE	1.90	1.01
1:B:1002[B]:DT:H72	2:A:422:LYS:HZ1	1.22	0.99
1:B:1003[B]:U31:C5'	1:B:1003[B]:U31:H6	1.95	0.96
1:B:1003[A]:U31:O1P	2:A:457:ASP:HB2	1.70	0.91
2:A:828:ILE:HG23	2:A:829:LYS:HE2	1.56	0.87
2:A:710:GLU:HG3	5:A:320:HOH:O	1.77	0.85
1:B:1002[B]:DT:H73	2:A:422:LYS:HZ1	0.69	0.84
2:A:485:THR:H	2:A:488:GLN:HE21	1.25	0.84
2:A:712:ARG:HD3	2:A:913:PRO:O	1.77	0.84
2:A:677:GLN:HE21	2:A:881:HIS:H	1.21	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:740:GLU:HB3	2:A:794:ARG:HG2	1.61	0.83
1:B:1002[A]:DT:H2"	1:B:1003[A]:U31:H5'1	1.60	0.81
2:A:575:GLY:O	2:A:576:GLU:HG2	1.80	0.80
1:B:1003[A]:U31:O1P	2:A:457:ASP:CB	2.30	0.79
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.63	0.79
1:B:1002[B]:DT:O2	1:B:1002[B]:DT:H3'	1.85	0.76
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.71	0.73
2:A:600:LYS:CB	2:A:614:LEU:HG	2.19	0.72
1:B:1002[B]:DT:H72	2:A:422:LYS:NZ	1.89	0.72
2:A:556:SER:HB2	2:A:641:THR:HG22	1.72	0.71
1:B:1003[A]:U31:C5	2:A:458:MET:HE1	2.17	0.71
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.72	0.70
2:A:677:GLN:NE2	2:A:881:HIS:H	1.88	0.70
2:A:556:SER:HB2	2:A:641:THR:CG2	2.21	0.70
2:A:677:GLN:HE21	2:A:881:HIS:N	1.88	0.70
1:B:1002[B]:DT:C2'	1:B:1003[B]:U31:O4'	2.34	0.70
1:B:1002[B]:DT:H2"	1:B:1003[B]:U31:O1P	1.91	0.70
1:B:1003[A]:U31:HCC2	2:A:419:GLN:O	1.92	0.69
2:A:421:LEU:HD23	2:A:438:ILE:HG23	1.73	0.68
2:A:782:LYS:HA	2:A:785:GLN:CB	2.23	0.68
1:B:1004[B]:DT:H2'	2:A:473:PHE:CE1	2.27	0.68
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.75	0.68
2:A:717:LEU:HD21	2:A:818:LEU:HD11	1.75	0.68
2:A:725:THR:O	2:A:729:GLU:HG2	1.94	0.67
1:B:1004[A]:DT:H2'	2:A:473:PHE:CE1	2.27	0.67
2:A:640:TYR:O	2:A:644:LEU:HB2	1.96	0.66
2:A:808:GLN:O	2:A:812:GLN:HG2	1.95	0.66
1:B:1002[B]:DT:O2	1:B:1002[B]:DT:C3'	2.44	0.66
1:B:1002[A]:DT:C3'	1:B:1002[A]:DT:O2	2.44	0.66
1:B:1003[A]:U31:H5	2:A:458:MET:HE2	1.77	0.66
2:A:400:ARG:NH2	4:A:94:SO4:O2	2.29	0.66
1:B:1003[A]:U31:HB'1	2:A:419:GLN:HB3	1.79	0.64
2:A:346:LEU:CD1	2:A:375:ILE:HG23	2.27	0.64
2:A:828:ILE:CG2	2:A:829:LYS:HE2	2.25	0.64
1:B:1003[B]:U31:C2'	2:A:361:LEU:HD22	2.19	0.64
2:A:758:LYS:NZ	4:A:38:SO4:O1	2.25	0.63
2:A:580:LEU:N	2:A:580:LEU:HD22	2.14	0.62
1:B:1002[B]:DT:H1'	2:A:420:ASN:OD1	1.99	0.62
1:B:1002[A]:DT:H1'	2:A:420:ASN:OD1	1.99	0.62
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.81	0.61
2:A:400:ARG:NH1	4:A:94:SO4:O2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003[B]:U31:H2'	2:A:361:LEU:HD21	1.77	0.60
2:A:746:LEU:O	2:A:749:VAL:HG12	2.02	0.59
1:B:1002[B]:DT:H71	2:A:422:LYS:NZ	2.08	0.59
1:B:1002[A]:DT:H71	2:A:659:TYR:O	2.02	0.59
1:B:1002[B]:DT:H71	2:A:659:TYR:O	2.02	0.59
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.85	0.59
2:A:808:GLN:OE1	2:A:812:GLN:NE2	2.37	0.57
2:A:582:SER:HA	2:A:586:LEU:HB2	1.86	0.57
1:B:1003[A]:U31:C2	2:A:497:TYR:OH	2.52	0.57
2:A:731:LYS:HD2	2:A:746:LEU:HD22	1.87	0.57
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.88	0.56
2:A:772:GLY:O	2:A:776:GLN:HG2	2.05	0.56
1:B:1002[A]:DT:H73	2:A:422:LYS:CE	2.31	0.56
1:B:1002[B]:DT:H73	2:A:422:LYS:CE	2.31	0.56
2:A:362:ASP:OD2	2:A:365:SER:OG	2.14	0.55
1:B:1002[B]:DT:O2	1:B:1002[B]:DT:H5"	2.07	0.55
1:B:1002[A]:DT:H5"	1:B:1002[A]:DT:O2	2.07	0.55
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.88	0.55
2:A:674:PRO:HG2	2:A:676:LEU:HD13	1.90	0.54
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.90	0.54
2:A:600:LYS:CB	2:A:613:VAL:HB	2.38	0.53
2:A:472:THR:HG22	2:A:475:GLU:H	1.74	0.53
2:A:657:THR:HG22	5:A:169:HOH:O	2.08	0.53
1:B:1002[B]:DT:O4	2:A:660:HIS:CE1	2.62	0.53
1:B:1002[A]:DT:O4	2:A:660:HIS:CE1	2.62	0.53
1:B:1003[B]:U31:C5'	1:B:1003[B]:U31:C6	2.81	0.53
2:A:576:GLU:HG3	2:A:577:GLU:O	2.09	0.53
1:B:1002[A]:DT:H3'	1:B:1002[A]:DT:O2	2.08	0.53
1:B:1003[A]:U31:C5	2:A:458:MET:CE	2.77	0.52
2:A:588:THR:O	2:A:592:GLU:HB3	2.10	0.52
2:A:827:ASP:HB3	2:A:830:SER:HB2	1.92	0.51
2:A:487:ASN:H	2:A:487:ASN:HD22	1.58	0.51
2:A:779:ILE:HB	2:A:783:GLU:HG2	1.93	0.51
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.93	0.50
2:A:798:VAL:O	2:A:802:MET:HG3	2.11	0.50
2:A:909:ARG:HB3	2:A:911:ASP:OD1	2.11	0.50
1:B:1003[A]:U31:CC	2:A:419:GLN:O	2.59	0.50
2:A:754:ARG:NH2	4:A:38:SO4:S	2.85	0.50
2:A:783:GLU:O	2:A:786:LYS:HB3	2.11	0.50
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.76	0.50
2:A:619:LEU:N	2:A:619:LEU:HD22	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:683:ASN:OD1	2:A:684:GLU:N	2.44	0.50
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.94	0.49
1:B:1003[B]:U31:O5'	1:B:1003[B]:U31:C6	2.31	0.49
2:A:446:SER:OG	2:A:456:HIS:HD2	1.94	0.49
1:B:1004[A]:DT:H2'	2:A:473:PHE:CZ	2.48	0.49
1:B:1004[B]:DT:H2'	2:A:473:PHE:CZ	2.48	0.49
2:A:513:TRP:HB3	2:A:514:PRO:HD3	1.94	0.48
2:A:353:ALA:HB3	2:A:374:ALA:HB3	1.95	0.48
2:A:715:ALA:HB1	2:A:724:LEU:HD13	1.95	0.48
2:A:836:ARG:O	2:A:840:GLU:HG3	2.14	0.48
2:A:924:TRP:O	2:A:928:HIS:HB2	2.14	0.48
2:A:487:ASN:H	2:A:487:ASN:ND2	2.11	0.47
2:A:580:LEU:CD2	2:A:580:LEU:N	2.77	0.47
2:A:779:ILE:HD12	2:A:783:GLU:HG3	1.96	0.47
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.62	0.47
1:B:1002[A]:DT:H73	2:A:422:LYS:HZ3	1.65	0.47
1:B:1002[B]:DT:H73	2:A:422:LYS:HZ3	1.65	0.47
2:A:324:MET:CE	2:A:324:MET:HA	2.43	0.47
2:A:556:SER:CA	2:A:641:THR:HG21	2.45	0.47
1:B:1003[A]:U31:C4'	1:B:1004[A]:DT:OP2	2.62	0.47
2:A:780:PRO:O	2:A:783:GLU:HB3	2.15	0.47
2:A:616:GLU:O	2:A:619:LEU:HD23	2.15	0.46
2:A:773:LEU:HD13	2:A:784:ALA:HB1	1.96	0.46
2:A:589:ILE:O	2:A:593:LYS:HG2	2.16	0.46
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.50	0.46
2:A:593:LYS:O	2:A:594:GLN:HB3	2.17	0.45
2:A:758:LYS:NZ	4:A:38:SO4:S	2.90	0.45
1:B:1002[A]:DT:C5'	1:B:1002[A]:DT:O2	2.65	0.45
1:B:1002[B]:DT:O2	1:B:1002[B]:DT:C5'	2.65	0.45
2:A:770:ALA:HA	2:A:788:MET:SD	2.57	0.45
2:A:449:LEU:HD13	2:A:516:LEU:HG	1.99	0.45
1:B:1003[B]:U31:H1'	1:B:1003[B]:U31:HA'2	1.36	0.45
2:A:472:THR:HG22	2:A:475:GLU:HG3	1.98	0.45
2:A:866:TRP:CE2	2:A:899:GLN:HG2	2.52	0.45
2:A:324:MET:HA	2:A:324:MET:HE2	1.98	0.45
2:A:571:HIS:CE1	2:A:577:GLU:HG3	2.53	0.44
2:A:580:LEU:HD12	2:A:627:ILE:HG12	1.99	0.44
2:A:623:LEU:N	2:A:624:PRO:HD2	2.32	0.44
2:A:638:SER:O	2:A:643:LYS:HG2	2.17	0.44
2:A:896:VAL:O	2:A:900:ILE:HG12	2.17	0.44
2:A:695:ALA:HB2	2:A:701:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:400:ARG:CZ	4:A:94:SO4:O2	2.66	0.44
1:B:1003[A]:U31:HCC2	2:A:419:GLN:H	1.83	0.43
2:A:597:LYS:HG2	2:A:598:PRO:HD3	1.99	0.43
2:A:547:ILE:HD13	2:A:644:LEU:HG	1.99	0.43
2:A:735:ARG:CZ	2:A:749:VAL:HG13	2.48	0.43
2:A:880:VAL:HG11	2:A:924:TRP:CZ2	2.53	0.43
1:B:1002[A]:DT:H72	2:A:422:LYS:NZ	1.89	0.43
2:A:740:GLU:HG3	2:A:795:TYR:OH	2.18	0.43
2:A:756:SER:HA	2:A:777:LEU:HD11	2.01	0.43
2:A:808:GLN:HA	2:A:811:GLU:HB3	1.99	0.43
2:A:830:SER:C	2:A:832:ASN:H	2.21	0.43
1:B:1003[A]:U31:O1P	2:A:457:ASP:HB3	2.12	0.43
2:A:734:HIS:HD2	2:A:761:ASN:HD22	1.67	0.43
2:A:515:ASP:C	2:A:517:GLN:H	2.21	0.42
2:A:802:MET:O	2:A:806:ARG:HG3	2.18	0.42
2:A:435:LEU:HD13	2:A:438:ILE:CG1	2.46	0.42
1:B:1002[B]:DT:C4	1:B:1003[B]:U31:HCC1	2.55	0.42
2:A:754:ARG:NH2	4:A:38:SO4:O4	2.53	0.42
2:A:762:PHE:HD1	2:A:765:ILE:HD12	1.84	0.42
2:A:720:ASP:O	2:A:724:LEU:HB2	2.19	0.42
2:A:729:GLU:HG2	2:A:729:GLU:H	1.71	0.42
2:A:866:TRP:CZ2	2:A:899:GLN:HG2	2.54	0.41
2:A:449:LEU:HA	2:A:449:LEU:HD12	1.91	0.41
2:A:569:LYS:O	2:A:573:ILE:HG13	2.21	0.41
2:A:735:ARG:NH2	2:A:749:VAL:HG13	2.35	0.41
2:A:773:LEU:HD22	2:A:773:LEU:O	2.20	0.41
2:A:586:LEU:HD22	2:A:627:ILE:HD13	2.02	0.41
2:A:585:GLN:O	2:A:588:THR:OG1	2.38	0.41
2:A:617:LEU:HB3	2:A:624:PRO:HG3	2.03	0.41
1:B:1003[A]:U31:H4'	1:B:1004[A]:DT:OP2	2.20	0.41
2:A:579:ASN:C	2:A:580:LEU:HD22	2.41	0.41
1:B:1003[B]:U31:O2	1:B:1003[B]:U31:HA'1	2.21	0.41
1:B:1002[A]:DT:H5"	1:B:1002[A]:DT:C2	2.55	0.41
1:B:1002[B]:DT:C2	1:B:1002[B]:DT:H5"	2.55	0.41
2:A:794:ARG:HB2	2:A:794:ARG:NH1	2.36	0.41
2:A:816:GLU:HG2	2:A:822:ARG:HG2	2.02	0.41
2:A:880:VAL:HG11	2:A:924:TRP:HZ2	1.86	0.41
2:A:706:TYR:HB3	2:A:709:ILE:HB	2.03	0.40
2:A:732:ASP:OD2	2:A:754:ARG:NH1	2.53	0.40
2:A:405:LEU:HB3	2:A:409:LEU:HD22	2.03	0.40
2:A:781:ARG:C	2:A:783:GLU:H	2.24	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	
2	A	597/605 (99%)	568 (95%)	24 (4%)	5 (1%)	22	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	830	SER
2	A	594	GLN
2	A	597	LYS
2	A	516	LEU
2	A	708	GLN

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	
2	A	500/510 (98%)	459 (92%)	41 (8%)	13	44

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	324	MET
2	A	334	LEU
2	A	339	LEU

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Mol	Chain	Res	Type
2	A	346	LEU
2	A	375	ILE
2	A	405	LEU
2	A	409	LEU
2	A	421	LEU
2	A	425	ARG
2	A	435	LEU
2	A	449	LEU
2	A	472	THR
2	A	486	PHE
2	A	510	LEU
2	A	552	LEU
2	A	578	PHE
2	A	584	LYS
2	A	592	GLU
2	A	597	LYS
2	A	616	GLU
2	A	620	ASP
2	A	629	GLU
2	A	644	LEU
2	A	646	LEU
2	A	674	PRO
2	A	676	LEU
2	A	708	GLN
2	A	711	LEU
2	A	724	LEU
2	A	754	ARG
2	A	773	LEU
2	A	782	LYS
2	A	783	GLU
2	A	794	ARG
2	A	799	LEU
2	A	821	ARG
2	A	867	LEU
2	A	871	GLN
2	A	874	VAL
2	A	879	GLN
2	A	917	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	363	ASN
2	A	456	HIS
2	A	487	ASN
2	A	488	GLN
2	A	543	ASN
2	A	571	HIS
2	A	677	GLN
2	A	708	GLN
2	A	734	HIS
2	A	812	GLN
2	A	845	ASN
2	A	899	GLN
2	A	901	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	U31	B	1003[A]	1	17,25,26	1.61	3 (17%)	21,34,37	3.98	7 (33%)
1	U31	B	1003[B]	1	17,25,26	1.43	4 (23%)	21,34,37	4.15	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	U31	B	1003[A]	1	-	0/8/30/31	0/2/2/2
1	U31	B	1003[B]	1	-	0/8/30/31	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1003[B]	U31	O5'-C5'	-3.11	1.40	1.44
1	B	1003[B]	U31	C6-C5	-2.51	1.32	1.38
1	B	1003[A]	U31	CB'-CC	-2.49	1.39	1.51
1	B	1003[B]	U31	CB'-CA'	-2.22	1.41	1.51
1	B	1003[A]	U31	C4-N3	2.77	1.38	1.33
1	B	1003[B]	U31	C4-N3	2.78	1.38	1.33
1	B	1003[A]	U31	O2'-CA'	3.33	1.51	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1003[B]	U31	C5-C4-N3	-3.64	114.42	123.12
1	B	1003[A]	U31	C5-C4-N3	-3.22	115.42	123.12
1	B	1003[B]	U31	CA'-O2'-C2'	-3.01	106.78	114.32
1	B	1003[A]	U31	C4'-O4'-C1'	-3.00	106.58	109.77
1	B	1003[A]	U31	C3'-C2'-C1'	-2.17	98.51	102.75
1	B	1003[A]	U31	O3'-C3'-C4'	2.28	117.73	111.09
1	B	1003[B]	U31	O2'-CA'-CB'	3.42	121.88	109.68
1	B	1003[A]	U31	O2'-CA'-CB'	4.73	126.54	109.68
1	B	1003[B]	U31	O2'-C2'-C3'	6.64	127.36	111.06
1	B	1003[B]	U31	O3'-C3'-C2'	6.83	130.59	111.18
1	B	1003[A]	U31	O2'-C2'-C1'	8.06	124.25	108.76
1	B	1003[A]	U31	C4-N3-C2	14.25	126.37	114.13
1	B	1003[B]	U31	C4-N3-C2	14.92	126.95	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1003[A]	U31	16	0
1	B	1003[B]	U31	14	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	SO4	A	32	-	4,4,4	0.60	0	6,6,6	0.17	0
4	SO4	A	38	-	4,4,4	0.50	0	6,6,6	0.14	0
4	SO4	A	40	-	4,4,4	0.57	0	6,6,6	0.14	0
4	SO4	A	94	-	4,4,4	0.53	0	6,6,6	0.14	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	32	-	-	0/0/0/0	0/0/0/0
4	SO4	A	38	-	-	0/0/0/0	0/0/0/0
4	SO4	A	40	-	-	0/0/0/0	0/0/0/0
4	SO4	A	94	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	38	SO4	4	0
4	A	94	SO4	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	2/4 (50%)	2.32	2 (100%)	0	0	45, 45, 45, 49	0
2	A	601/605 (99%)	-0.05	39 (6%)	20	7	16, 37, 82, 83	0
All	All	603/609 (99%)	-0.04	41 (6%)	18	7	16, 37, 82, 83	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	610	SER	9.2
2	A	608	SER	8.1
2	A	598	PRO	6.8
2	A	607	PRO	5.6
2	A	599	LEU	5.5
2	A	582	SER	5.4
2	A	611	GLU	4.9
2	A	609	THR	4.9
2	A	576	GLU	4.8
2	A	581	SER	4.6
2	A	583	THR	4.5
2	A	586	LEU	4.2
2	A	596	ILE	3.9
2	A	681	VAL	3.2
2	A	778	ASN	3.1
2	A	591	PHE	3.0
2	A	834	ALA	2.9
2	A	682	ARG	2.9
2	A	597	LYS	2.9
2	A	588	THR	2.9
2	A	775	ARG	2.9
2	A	594	GLN	2.8
2	A	621	TYR	2.7
2	A	835	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	577	GLU	2.6
2	A	572	GLU	2.6
2	A	620	ASP	2.5
2	A	602	THR	2.5
2	A	779	ILE	2.4
1	B	1002[A]	DT	2.4
2	A	616	GLU	2.4
2	A	832	ASN	2.2
1	B	1004[A]	DT	2.2
2	A	782	LYS	2.2
2	A	585	GLN	2.2
2	A	770	ALA	2.1
2	A	624	PRO	2.1
2	A	837	ALA	2.1
2	A	481	LYS	2.1
2	A	587	GLN	2.0
2	A	783	GLU	2.0

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	U31	B	1003[B]	24/25	0.62	0.51	-	44,44,45,45	24
1	U31	B	1003[A]	24/25	0.62	0.51	-	46,48,55,57	24

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(Å²)	Q<0.9
4	SO4	A	40	5/5	0.89	0.28	1.28	37,38,46,65	5
3	ZN	A	1	1/1	0.84	0.27	-0.05	31,31,31,31	1
4	SO4	A	38	5/5	0.83	0.22	-0.46	32,48,50,56	5
4	SO4	A	32	5/5	0.83	0.29	-	24,45,52,59	5
4	SO4	A	94	5/5	0.91	0.19	-	20,36,44,63	5

6.5 Other polymers ⓘ

There are no such residues in this entry.