



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:25 PM GMT

PDB ID : 1D9D  
Title : CRYSTALL STRUCTURE OF THE COMPLEX OF DNA POLYMERASE I KLENOW FRAGMENT WITH SHORT DNA FRAGMENT CARRYING 2'-O-AMINOPROPYL-RNA MODIFICATIONS 5'-D(TCG)-AP(AUC)-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 : 2.18 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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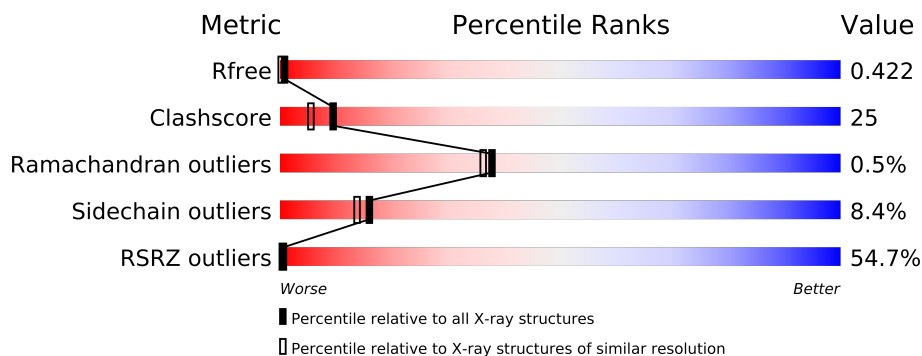
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.18 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))
$R_{free}$	66092	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	6	
2	A	605	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	321	-	X
5	SO4	A	38	-	X
5	SO4	A	40	-	X
5	SO4	A	94	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5149 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5'-D(\*TP\*CP\*GP)-R(AP\*(U31)P\*(C31))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	3	Total	C	N	O	P	0	3	0
			106	55	18	30	3			

- 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	4	Total	Zn	0	0
			4	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is water.

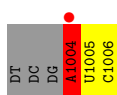
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	255	Total	O	0	0
			255	255		
6	B	10	Total	O	0	0
			10	10		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

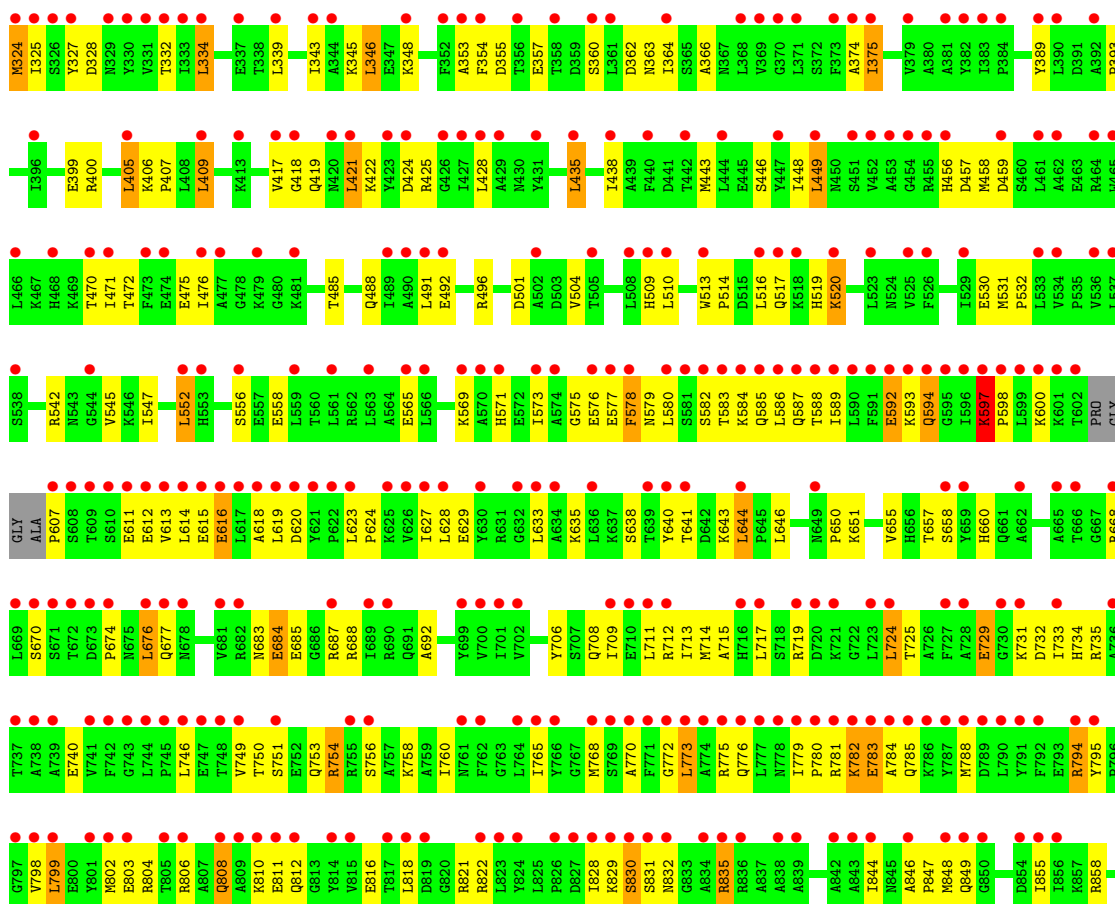
- Molecule 1: 5'-D(\*TP\*CP\*GP)-R(AP\*(U31)P\*(C31))-3'

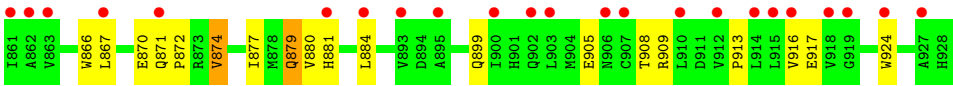
Chain B: 



- Molecule 2: DNA POLYMERASE I

Chain A: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.55Å 102.55Å 86.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.18 34.18 – 2.11	Depositor EDS
% Data completeness (in resolution range)	84.5 (20.00-2.18) 91.3 (34.18-2.11)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.238 0.409 , 0.422	Depositor DCC
$R_{free}$ test set	4023 reflections (8.56%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 59.3	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 46985 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	5149	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, C31, ZN, U31, 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	B	1.96	1/20 (5.0%)	2.55	0/29
2	A	0.33	0/4839	0.66	3/6547 (0.0%)
All	All	0.36	1/4859 (0.0%)	0.68	3/6576 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1004[A]	DA	C6-N1	-5.56	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	835	ARG	NE-CZ-NH1	7.13	123.86	120.30
2	A	607	PRO	N-CA-CB	5.57	109.99	103.30
2	A	597	LYS	N-CA-C	5.51	125.86	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1004[A]	DA	Sidechain



## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	106	0	73	65	0
2	A	4753	0	4752	202	13
3	A	4	0	0	0	0
4	A	1	0	0	0	0
5	A	20	0	0	6	0
6	A	255	0	0	12	11
6	B	10	0	0	10	0
All	All	5149	0	4825	239	16

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (239) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1005[A]:U31:H5	2:A:458:MET:CE	1.75	1.16
1:B:1005[A]:U31:H3'	1:B:1005[A]:U31:HB'1	1.23	1.14
1:B:1005[B]:U31:O5'	6:B:189:HOH:O	1.64	1.13
1:B:1005[A]:U31:HB'1	1:B:1005[A]:U31:C3'	1.86	1.05
1:B:1005[A]:U31:ND'	6:B:364:HOH:O	1.90	1.05
1:B:1004[A]:DA:H2	2:A:422:LYS:NZ	1.55	1.05
1:B:1006[A]:C31:ND'	6:B:35:HOH:O	1.92	1.01
1:B:1005[A]:U31:H5	2:A:458:MET:HE1	1.45	0.97
1:B:1005[A]:U31:HB'2	2:A:419:GLN:O	1.66	0.96
1:B:1004[A]:DA:C2	2:A:422:LYS:NZ	2.29	0.95
1:B:1005[B]:U31:C4	1:B:1006[B]:C31:H6	1.96	0.95
1:B:1005[A]:U31:H3'	1:B:1005[A]:U31:CB'	1.95	0.94
1:B:1005[B]:U31:H3	2:A:660:HIS:CE1	1.86	0.92
2:A:575:GLY:O	2:A:576:GLU:HG2	1.68	0.92
1:B:1004[A]:DA:N1	6:B:326:HOH:O	2.03	0.91
2:A:740:GLU:HB3	2:A:794:ARG:HG2	1.53	0.89
1:B:1006[A]:C31:H5'2	1:B:1006[A]:C31:O2	1.73	0.87
2:A:782:LYS:HA	2:A:785:GLN:HB3	1.55	0.87
2:A:485:THR:H	2:A:488:GLN:HE21	1.22	0.86
1:B:1005[A]:U31:H5	2:A:458:MET:HE2	1.57	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1005[B]:U31:N3	2:A:660:HIS:ND1	2.24	0.84
1:B:1005[A]:U31:HA'2	2:A:355:ASP:OD1	1.77	0.84
2:A:612:GLU:HB3	2:A:615:GLU:HG2	1.61	0.82
2:A:677:GLN:HE21	2:A:881:HIS:H	1.27	0.79
1:B:1005[A]:U31:HCC1	2:A:424:ASP:OD2	1.84	0.77
2:A:746:LEU:O	2:A:749:VAL:HG12	1.84	0.77
1:B:1004[A]:DA:H2	2:A:422:LYS:HZ1	0.86	0.77
2:A:519:HIS:HA	5:A:32:SO4:O4	1.83	0.77
1:B:1005[B]:U31:O4	1:B:1006[B]:C31:H5	1.85	0.76
2:A:717:LEU:HD21	2:A:818:LEU:HD11	1.68	0.76
1:B:1005[B]:U31:H3'	1:B:1006[B]:C31:H5'2	1.68	0.75
1:B:1004[A]:DA:H2	2:A:422:LYS:CE	2.00	0.75
1:B:1005[B]:U31:C4	1:B:1006[B]:C31:C6	2.64	0.75
1:B:1004[A]:DA:C2	6:B:205:HOH:O	2.40	0.73
2:A:772:GLY:O	2:A:776:GLN:HG2	1.87	0.73
2:A:677:GLN:HG3	6:A:1171:HOH:O	1.87	0.73
1:B:1006[B]:C31:ND'	1:B:1006[B]:C31:O2'	2.19	0.72
2:A:346:LEU:CD1	2:A:375:ILE:HG23	2.18	0.72
2:A:725:THR:O	2:A:729:GLU:HG2	1.90	0.72
2:A:421:LEU:HD23	2:A:438:ILE:HG23	1.69	0.72
2:A:908:THR:HG22	2:A:909:ARG:H	1.54	0.72
1:B:1005[B]:U31:C5	1:B:1006[B]:C31:H6	2.20	0.71
2:A:520:LYS:HG2	5:A:32:SO4:O3	1.91	0.69
1:B:1006[A]:C31:HA'2	2:A:360:SER:N	2.08	0.69
2:A:600:LYS:CB	2:A:614:LEU:HG	2.23	0.68
1:B:1005[B]:U31:C1'	6:B:324:HOH:O	2.40	0.68
2:A:446:SER:OG	2:A:456:HIS:HD2	1.77	0.68
2:A:418:GLY:HA3	2:A:421:LEU:HD13	1.75	0.68
2:A:435:LEU:HD13	2:A:438:ILE:HG12	1.75	0.68
1:B:1005[B]:U31:C2'	2:A:443:MET:SD	2.82	0.68
2:A:719:ARG:CZ	2:A:804:ARG:HH12	2.07	0.67
2:A:782:LYS:HA	2:A:785:GLN:CB	2.23	0.67
2:A:600:LYS:CB	2:A:613:VAL:HB	2.25	0.67
1:B:1004[A]:DA:N6	6:B:326:HOH:O	2.25	0.66
2:A:586:LEU:HD22	2:A:627:ILE:HD13	1.77	0.66
2:A:556:SER:HB2	2:A:641:THR:HG22	1.78	0.66
1:B:1005[A]:U31:HCC2	2:A:355:ASP:OD1	1.96	0.66
2:A:719:ARG:NH2	2:A:804:ARG:HH12	1.94	0.65
2:A:779:ILE:HD12	2:A:783:GLU:HG3	1.79	0.65
1:B:1005[B]:U31:H1'	6:B:324:HOH:O	1.96	0.64
2:A:580:LEU:HD12	2:A:627:ILE:HG12	1.79	0.64
2:A:830:SER:C	2:A:832:ASN:H	2.01	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:586:LEU:HD11	2:A:627:ILE:HG21	1.80	0.64
2:A:640:TYR:O	2:A:644:LEU:HB2	1.98	0.63
2:A:780:PRO:O	2:A:783:GLU:HB3	1.98	0.62
1:B:1005[A]:U31:H6	2:A:458:MET:SD	2.38	0.62
1:B:1006[A]:C31:C5'	1:B:1006[A]:C31:O2	2.45	0.62
2:A:677:GLN:HE21	2:A:881:HIS:N	1.98	0.62
2:A:881:HIS:ND1	6:A:1173:HOH:O	2.31	0.62
2:A:855:ILE:HG23	2:A:908:THR:HG21	1.82	0.61
2:A:580:LEU:N	2:A:580:LEU:HD22	2.14	0.61
2:A:677:GLN:HG2	2:A:880:VAL:HG23	1.84	0.60
2:A:872:PRO:HG2	2:A:874:VAL:HG13	1.83	0.60
2:A:677:GLN:NE2	2:A:881:HIS:H	1.97	0.60
2:A:547:ILE:HD12	2:A:655:VAL:HG21	1.83	0.60
2:A:364:ILE:HB	6:A:1061:HOH:O	2.02	0.60
1:B:1005[B]:U31:H1'	2:A:443:MET:SD	2.43	0.59
2:A:363:ASN:HD22	2:A:542:ARG:HH11	1.51	0.59
1:B:1005[A]:U31:CC	6:B:364:HOH:O	2.39	0.59
2:A:576:GLU:HG3	2:A:577:GLU:O	2.03	0.58
2:A:586:LEU:CD1	2:A:627:ILE:HG21	2.34	0.58
2:A:830:SER:OG	2:A:835:ARG:HD3	2.04	0.58
2:A:588:THR:O	2:A:592:GLU:HB3	2.02	0.58
1:B:1005[A]:U31:HA'1	6:A:1168:HOH:O	2.03	0.58
2:A:731:LYS:HD2	2:A:746:LEU:HD22	1.86	0.57
2:A:779:ILE:HB	2:A:783:GLU:HG2	1.86	0.57
2:A:519:HIS:CD2	2:A:822:ARG:HH22	2.22	0.57
2:A:712:ARG:HD3	2:A:913:PRO:O	2.05	0.57
1:B:1005[A]:U31:C5	2:A:501:ASP:OD1	2.53	0.57
1:B:1006[B]:C31:O3'	1:B:1006[B]:C31:ND'	2.37	0.57
2:A:393:PRO:HD2	2:A:491:LEU:HD22	1.87	0.57
1:B:1005[A]:U31:O4	2:A:470:THR:HB	2.05	0.57
1:B:1006[B]:C31:HB'2	1:B:1006[B]:C31:H4'	1.87	0.56
2:A:586:LEU:HD22	2:A:627:ILE:CD1	2.35	0.56
2:A:324:MET:HE2	6:A:1092:HOH:O	2.05	0.56
2:A:770:ALA:HA	2:A:788:MET:SD	2.45	0.56
2:A:583:THR:HA	2:A:587:GLN:CD	2.25	0.56
2:A:346:LEU:HD13	2:A:375:ILE:HG23	1.87	0.56
1:B:1005[B]:U31:O4	1:B:1006[B]:C31:C5	2.53	0.56
2:A:363:ASN:ND2	2:A:542:ARG:HH11	2.03	0.56
2:A:908:THR:HG22	2:A:909:ARG:N	2.20	0.56
2:A:660:HIS:HB2	2:A:670:SER:OG	2.07	0.54
2:A:616:GLU:O	2:A:619:LEU:HD23	2.07	0.54
2:A:589:ILE:O	2:A:593:LYS:HG2	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:597:LYS:HG2	2:A:598:PRO:HD3	1.89	0.54
2:A:545:VAL:HG23	2:A:877:ILE:HD12	1.90	0.54
2:A:325:ILE:HB	2:A:471:ILE:HD11	1.89	0.54
2:A:582:SER:HA	2:A:586:LEU:HB2	1.90	0.54
2:A:419:GLN:HG2	2:A:458:MET:HB2	1.89	0.54
2:A:798:VAL:O	2:A:802:MET:HG3	2.06	0.54
2:A:684:GLU:O	2:A:687:ARG:HB2	2.07	0.53
1:B:1005[B]:U31:O2	1:B:1005[B]:U31:O4'	2.25	0.53
2:A:768:MET:SD	6:A:1147:HOH:O	2.59	0.53
2:A:556:SER:HB2	2:A:641:THR:CG2	2.38	0.53
2:A:717:LEU:HD21	2:A:818:LEU:CD1	2.37	0.53
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.89	0.53
2:A:569:LYS:O	2:A:573:ILE:HG13	2.09	0.53
2:A:612:GLU:HB3	2:A:615:GLU:CG	2.37	0.53
2:A:600:LYS:CB	2:A:614:LEU:H	2.21	0.53
2:A:754:ARG:NH2	5:A:38:SO4:O4	2.42	0.53
2:A:734:HIS:CD2	2:A:758:LYS:HA	2.44	0.52
2:A:406:LYS:HB3	2:A:407:PRO:HD3	1.90	0.52
2:A:668:ARG:HE	2:A:849:GLN:HG3	1.75	0.52
1:B:1006[B]:C31:HD'1	1:B:1006[B]:C31:C2'	2.23	0.52
1:B:1006[B]:C31:O1P	1:B:1006[B]:C31:H4'	2.10	0.52
2:A:586:LEU:CD2	2:A:627:ILE:HD13	2.40	0.52
1:B:1005[A]:U31:HCC2	6:B:364:HOH:O	2.05	0.51
1:B:1006[B]:C31:C2'	1:B:1006[B]:C31:O2	2.58	0.51
2:A:624:PRO:O	2:A:628:LEU:HB2	2.09	0.51
2:A:357:GLU:HG2	6:A:1143:HOH:O	2.09	0.51
2:A:449:LEU:HD13	2:A:516:LEU:HG	1.92	0.51
2:A:418:GLY:HA3	2:A:421:LEU:CD1	2.40	0.51
2:A:619:LEU:HD22	2:A:619:LEU:N	2.26	0.51
1:B:1005[A]:U31:O1P	2:A:457:ASP:HA	2.10	0.50
2:A:816:GLU:HG2	2:A:822:ARG:HG2	1.92	0.50
2:A:585:GLN:O	2:A:588:THR:OG1	2.29	0.50
2:A:332:THR:HG22	2:A:334:LEU:HD13	1.92	0.50
2:A:558:GLU:CD	2:A:688:ARG:HH12	2.15	0.50
2:A:802:MET:O	2:A:806:ARG:HG3	2.11	0.50
2:A:583:THR:HA	2:A:587:GLN:NE2	2.26	0.50
2:A:732:ASP:OD2	2:A:754:ARG:NH1	2.45	0.50
2:A:580:LEU:N	2:A:580:LEU:CD2	2.75	0.49
2:A:448:ILE:HD11	2:A:530:GLU:HG3	1.93	0.49
2:A:593:LYS:O	2:A:594:GLN:HB3	2.12	0.49
1:B:1005[A]:U31:C5	2:A:458:MET:CE	2.68	0.49
1:B:1006[A]:C31:HA'2	2:A:360:SER:CA	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:623:LEU:N	2:A:624:PRO:HD2	2.28	0.48
2:A:623:LEU:HG	2:A:627:ILE:HD11	1.94	0.48
2:A:674:PRO:HG2	2:A:676:LEU:HD13	1.95	0.48
1:B:1005[B]:U31:C4	1:B:1006[B]:C31:C5	2.92	0.48
2:A:611:GLU:CB	2:A:775:ARG:NH2	2.77	0.48
2:A:353:ALA:HB3	2:A:374:ALA:HB3	1.94	0.48
2:A:623:LEU:HG	2:A:627:ILE:CD1	2.44	0.48
1:B:1005[A]:U31:H1'	1:B:1006[A]:C31:P	2.54	0.48
2:A:808:GLN:O	2:A:812:GLN:HG2	2.13	0.48
2:A:657:THR:HG22	6:A:1033:HOH:O	2.14	0.48
2:A:715:ALA:HB1	2:A:724:LEU:HD13	1.96	0.47
1:B:1005[B]:U31:H3'	1:B:1006[B]:C31:C5'	2.42	0.47
1:B:1005[A]:U31:HB'1	1:B:1005[A]:U31:O3'	2.12	0.47
2:A:735:ARG:HB3	2:A:749:VAL:HG11	1.97	0.47
1:B:1005[B]:U31:C1'	2:A:443:MET:SD	3.02	0.47
2:A:400:ARG:NH2	5:A:94:SO4:O2	2.44	0.47
2:A:638:SER:O	2:A:643:LYS:HG2	2.15	0.47
2:A:327:TYR:CE1	2:A:496:ARG:HD2	2.50	0.47
2:A:905:GLU:HB3	2:A:916:VAL:HG23	1.97	0.47
2:A:399:GLU:HG2	6:A:1000:HOH:O	2.15	0.47
2:A:781:ARG:C	2:A:783:GLU:H	2.17	0.46
2:A:829:LYS:O	2:A:831:SER:N	2.48	0.46
2:A:810:LYS:HG2	2:A:828:ILE:HG13	1.97	0.46
1:B:1004[A]:DA:N6	2:A:658:SER:OG	2.48	0.46
2:A:571:HIS:HD2	2:A:578:PHE:CE1	2.33	0.46
1:B:1005[B]:U31:C2	2:A:660:HIS:ND1	2.77	0.46
2:A:749:VAL:HG23	2:A:753:GLN:HB2	1.98	0.46
2:A:611:GLU:CB	2:A:775:ARG:HH22	2.29	0.46
1:B:1006[B]:C31:H3'	1:B:1006[B]:C31:O2	2.16	0.46
2:A:425:ARG:HD3	2:A:425:ARG:C	2.35	0.46
2:A:858:ARG:HB2	2:A:908:THR:HG23	1.98	0.46
1:B:1006[A]:C31:O2	1:B:1006[A]:C31:O4'	2.32	0.45
2:A:740:GLU:HG3	2:A:795:TYR:OH	2.16	0.45
2:A:485:THR:H	2:A:488:GLN:NE2	2.03	0.45
2:A:346:LEU:HD12	2:A:375:ILE:HG23	1.95	0.45
2:A:735:ARG:CZ	2:A:749:VAL:HG13	2.46	0.45
2:A:593:LYS:O	2:A:594:GLN:CB	2.64	0.45
2:A:799:LEU:HD22	2:A:803:GLU:HG3	1.98	0.45
1:B:1006[B]:C31:H2'	1:B:1006[B]:C31:O2	2.17	0.45
2:A:633:LEU:CD2	2:A:685:GLU:HG3	2.47	0.45
2:A:714:MET:HB2	2:A:848:MET:SD	2.56	0.44
1:B:1006[B]:C31:H1'	1:B:1006[B]:C31:HA'2	1.63	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:830:SER:C	2:A:832:ASN:N	2.68	0.44
2:A:565:GLU:HG2	6:A:1037:HOH:O	2.17	0.44
2:A:756:SER:O	2:A:760:ILE:HG13	2.17	0.44
2:A:531:MET:HB2	2:A:532:PRO:HD3	2.00	0.44
2:A:362:ASP:O	2:A:366:ALA:HB2	2.17	0.44
2:A:733:ILE:HG13	6:A:991:HOH:O	2.18	0.44
2:A:846:ALA:HB3	2:A:847:PRO:HD3	1.99	0.44
2:A:750:THR:OG1	2:A:753:GLN:HG3	2.18	0.44
2:A:556:SER:CA	2:A:641:THR:HG21	2.48	0.44
2:A:683:ASN:OD1	2:A:684:GLU:N	2.51	0.44
2:A:405:LEU:HB3	2:A:409:LEU:HD22	1.99	0.44
2:A:709:ILE:O	2:A:713:ILE:HG13	2.18	0.43
1:B:1004[A]:DA:N6	2:A:658:SER:HB3	2.34	0.43
2:A:472:THR:OG1	2:A:475:GLU:HG3	2.18	0.43
2:A:597:LYS:CG	2:A:598:PRO:HD3	2.49	0.43
2:A:513:TRP:O	2:A:517:GLN:HG3	2.19	0.43
1:B:1004[A]:DA:C6	2:A:658:SER:HB3	2.54	0.43
2:A:711:LEU:CD1	2:A:765:ILE:HD11	2.48	0.42
2:A:343:ILE:HD11	2:A:405:LEU:HD13	2.00	0.42
2:A:458:MET:HE3	2:A:504:VAL:HG11	2.00	0.42
2:A:579:ASN:C	2:A:580:LEU:HD22	2.39	0.42
2:A:731:LYS:HD2	2:A:746:LEU:CD2	2.50	0.42
2:A:592:GLU:HG2	2:A:592:GLU:O	2.18	0.42
2:A:880:VAL:HG11	2:A:924:TRP:HZ2	1.84	0.42
2:A:773:LEU:O	2:A:773:LEU:HD22	2.19	0.42
2:A:635:LYS:HE3	2:A:635:LYS:HB3	1.95	0.42
2:A:345:LYS:HA	2:A:348:LYS:HE2	2.01	0.42
2:A:324:MET:HA	2:A:324:MET:HE2	2.02	0.41
2:A:706:TYR:HB3	2:A:709:ILE:HB	2.01	0.41
2:A:683:ASN:ND2	6:A:1161:HOH:O	2.52	0.41
2:A:733:ILE:HG13	2:A:733:ILE:H	1.64	0.41
2:A:735:ARG:NH2	2:A:749:VAL:HG13	2.35	0.41
2:A:758:LYS:NZ	5:A:38:SO4:O4	2.53	0.41
2:A:899:GLN:HA	2:A:899:GLN:NE2	2.36	0.41
2:A:615:GLU:O	2:A:618:ALA:HB3	2.20	0.41
2:A:417:VAL:HG11	2:A:509:HIS:HB2	2.02	0.41
2:A:577:GLU:O	2:A:578:PHE:HB3	2.21	0.41
2:A:754:ARG:NH2	5:A:38:SO4:S	2.90	0.41
2:A:879:GLN:HG2	2:A:884:LEU:HD23	2.03	0.41
1:B:1005[A]:U31:O2P	2:A:457:ASP:HB2	2.21	0.41
2:A:556:SER:HA	2:A:641:THR:HG21	2.03	0.41
2:A:773:LEU:HD13	2:A:784:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:354:PHE:CZ	2:A:428:LEU:HD11	2.56	0.41
2:A:485:THR:N	2:A:488:GLN:HE21	2.04	0.41
2:A:799:LEU:O	2:A:803:GLU:HG3	2.21	0.41
2:A:844:ILE:O	2:A:848:MET:HE2	2.22	0.40
2:A:808:GLN:HA	2:A:811:GLU:HB3	2.03	0.40
2:A:866:TRP:CE2	2:A:899:GLN:HG2	2.56	0.40
2:A:782:LYS:HD2	2:A:782:LYS:N	2.36	0.40
2:A:513:TRP:HB3	2:A:514:PRO:HD3	2.03	0.40
2:A:552:LEU:HD13	2:A:692:ALA:HB2	2.04	0.40

All (16) 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	Distance(Å)	Clash(Å)
2:A:517:GLN:OE1	6:A:973:HOH:O[2_764]	1.67	0.53
2:A:565:GLU:OE2	6:A:1027:HOH:O[2_765]	1.87	0.33
2:A:751:SER:CA	6:A:1056:HOH:O[2_765]	1.95	0.25
6:A:1010:HOH:O	6:A:1026:HOH:O[3_654]	1.97	0.23
2:A:476:ILE:O	6:A:1128:HOH:O[3_654]	2.01	0.19
6:A:942:HOH:O	6:A:1073:HOH:O[4_565]	2.09	0.11
2:A:328:ASP:OD1	2:A:542:ARG:NE[3_654]	2.10	0.10
6:A:953:HOH:O	6:A:1014:HOH:O[4_565]	2.12	0.08
2:A:492:GLU:N	2:A:651:LYS:O[3_654]	2.13	0.07
2:A:558:GLU:OE1	2:A:719:ARG:CG[2_765]	2.13	0.07
2:A:345:LYS:NZ	6:A:1060:HOH:O[3_654]	2.14	0.06
2:A:345:LYS:CE	6:A:1060:HOH:O[3_654]	2.17	0.03
2:A:651:LYS:NZ	6:A:1015:HOH:O[4_565]	2.17	0.03
2:A:751:SER:N	6:A:1056:HOH:O[2_765]	2.17	0.03
2:A:558:GLU:OE1	2:A:719:ARG:CB[2_765]	2.18	0.02
2:A:389:TYR:OH	2:A:650:PRO:O[3_654]	2.19	0.01

## 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%)	563 (94%)	31 (5%)	3 (0%)	38	36

All (3) Ramachandran outliers are listed below:

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

### 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%)	458 (92%)	42 (8%)	16	14

All (42) 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
2	A	346	LEU
2	A	375	ILE
2	A	405	LEU
2	A	409	LEU
2	A	421	LEU
2	A	435	LEU
2	A	449	LEU
2	A	459	ASP
2	A	510	LEU
2	A	520	LYS
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

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Mol	Chain	Res	Type
2	A	629	GLU
2	A	644	LEU
2	A	646	LEU
2	A	676	LEU
2	A	684	GLU
2	A	708	GLN
2	A	724	LEU
2	A	729	GLU
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	808	GLN
2	A	821	ARG
2	A	867	LEU
2	A	870	GLU
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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	363	ASN
2	A	420	ASN
2	A	456	HIS
2	A	487	ASN
2	A	488	GLN
2	A	519	HIS
2	A	528	ASN
2	A	543	ASN
2	A	571	HIS
2	A	587	GLN
2	A	677	GLN
2	A	734	HIS
2	A	776	GLN
2	A	845	ASN
2	A	879	GLN
2	A	899	GLN

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Mol	Chain	Res	Type
2	A	901	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	U31	B	1005[A]	1	23,25,26	1.55	5 (21%)	27,34,37	3.23	13 (48%)
1	U31	B	1005[B]	1	16,17,26	1.11	0	16,24,37	0.88	0
1	C31	B	1006[A]	1,3	23,25,26	1.26	1 (4%)	28,34,37	2.46	7 (25%)
1	C31	B	1006[B]	1	23,25,26	1.22	2 (8%)	28,34,37	2.52	6 (21%)

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	1005[A]	1	-	1/11/30/31	0/2/2/2
1	U31	B	1005[B]	1	-	0/3/18/31	0/2/2/2
1	C31	B	1006[A]	1,3	-	0/11/30/31	0/2/2/2
1	C31	B	1006[B]	1	-	0/11/30/31	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006[B]	C31	C4-N4	-3.76	1.23	1.35
1	B	1006[A]	C31	C4-N4	-3.63	1.24	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1005[A]	U31	O2-C2	-3.39	1.16	1.23
1	B	1005[A]	U31	O2'-CA'	3.10	1.51	1.42
1	B	1006[B]	C31	P-O2P	2.84	1.50	1.46
1	B	1005[A]	U31	C2'-C1'	2.46	1.57	1.52
1	B	1005[A]	U31	C4-N3	-2.43	1.33	1.37
1	B	1005[A]	U31	C6-N1	-2.04	1.32	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1005[A]	U31	C2-N1-C1'	9.57	124.21	118.21
1	B	1006[A]	C31	C2-N3-C4	8.26	127.52	115.57
1	B	1006[B]	C31	C2-N3-C4	7.92	127.03	115.57
1	B	1005[A]	U31	O2'-C2'-C1'	7.71	123.04	108.78
1	B	1006[B]	C31	C6-C5-C4	6.76	120.28	117.47
1	B	1006[B]	C31	C5-C4-N3	-5.66	114.03	121.68
1	B	1006[A]	C31	C6-C5-C4	5.44	119.73	117.47
1	B	1006[A]	C31	C5-C4-N3	-5.37	114.42	121.68
1	B	1005[A]	U31	O4'-C1'-C2'	-4.99	102.29	106.95
1	B	1005[A]	U31	C2'-C1'-N1	4.22	130.19	113.73
1	B	1005[A]	U31	O2'-CA'-CB'	4.04	125.64	109.87
1	B	1006[B]	C31	O2'-C2'-C3'	3.26	118.21	110.76
1	B	1005[A]	U31	P-O5'-C5'	-3.24	110.54	123.19
1	B	1005[A]	U31	CA'-O2'-C2'	3.14	122.90	114.31
1	B	1005[A]	U31	O3'-C3'-C4'	-2.99	102.26	111.08
1	B	1005[A]	U31	C3'-C2'-C1'	-2.76	97.36	102.73
1	B	1006[A]	C31	O4'-C1'-C2'	2.73	109.50	106.95
1	B	1006[A]	C31	C5-C4-N4	2.66	126.12	121.33
1	B	1006[A]	C31	CC-CB'-CA'	-2.59	104.18	113.92
1	B	1006[B]	C31	C5-C4-N4	2.35	125.57	121.33
1	B	1005[A]	U31	C4'-O4'-C1'	2.33	112.28	109.75
1	B	1005[A]	U31	C5-C6-N1	2.30	123.81	121.21
1	B	1005[A]	U31	C5-C4-N3	-2.14	112.67	116.70
1	B	1005[A]	U31	O4'-C1'-N1	-2.12	103.59	108.06
1	B	1006[B]	C31	C5-C6-N1	2.06	123.55	121.21
1	B	1006[A]	C31	O4'-C4'-C3'	2.02	109.27	105.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1005[A]	U31	C2'-O2'-CA'-CB'

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are 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	$\# Z  > 2$
5	SO4	A	32	-	4,4,4	0.77	0	6,6,6	0.13	0
5	SO4	A	38	-	4,4,4	0.59	0	6,6,6	0.12	0
5	SO4	A	40	-	4,4,4	0.71	0	6,6,6	0.09	0
5	SO4	A	94	-	4,4,4	0.68	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
5	SO4	A	32	-	-	0/0/0/0	0/0/0/0
5	SO4	A	38	-	-	0/0/0/0	0/0/0/0
5	SO4	A	40	-	-	0/0/0/0	0/0/0/0
5	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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	2/6 (33%)	1.69	1 (50%)  	46, 46, 46, 52	2 (100%)
2	A	601/605 (99%)	2.51	329 (54%)  	13, 30, 60, 60	0
All	All	603/611 (98%)	2.51	330 (54%)  	13, 30, 60, 60	2 (0%)

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	582	SER	17.3
2	A	586	LEU	13.1
2	A	583	THR	13.0
2	A	608	SER	11.0
2	A	779	ILE	9.5
2	A	611	GLU	9.5
2	A	610	SER	9.4
2	A	602	THR	8.9
2	A	589	ILE	8.1
2	A	581	SER	8.1
2	A	580	LEU	8.0
2	A	596	ILE	8.0
2	A	746	LEU	8.0
2	A	597	LYS	7.7
2	A	830	SER	7.7
2	A	617	LEU	7.3
2	A	609	THR	7.3
2	A	578	PHE	6.7
2	A	730	GLY	6.6
2	A	621	TYR	6.6
2	A	591	PHE	6.5
2	A	598	PRO	6.4
2	A	832	ASN	6.3
2	A	783	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
2	A	781	ARG	6.0
2	A	590	LEU	5.9
2	A	775	ARG	5.9
2	A	784	ALA	5.8
2	A	785	GLN	5.8
2	A	607	PRO	5.6
2	A	465	TRP	5.5
2	A	594	GLN	5.5
2	A	744	LEU	5.4
2	A	773	LEU	5.4
2	A	595	GLY	5.4
2	A	623	LEU	5.4
2	A	829	LYS	5.3
2	A	614	LEU	5.2
2	A	835	ARG	5.2
2	A	828	ILE	5.1
2	A	770	ALA	5.1
2	A	834	ALA	5.1
2	A	792	PHE	5.0
2	A	798	VAL	5.0
2	A	771	PHE	4.9
2	A	795	TYR	4.9
2	A	786	LYS	4.8
2	A	741	VAL	4.8
2	A	577	GLU	4.8
2	A	910	LEU	4.8
2	A	587	GLN	4.7
2	A	618	ALA	4.7
2	A	794	ARG	4.7
2	A	451	SER	4.7
2	A	681	VAL	4.7
2	A	751	SER	4.6
2	A	477	ALA	4.5
2	A	768	MET	4.5
2	A	777	LEU	4.5
2	A	622	PRO	4.5
2	A	689	ILE	4.5
2	A	809	ALA	4.5
2	A	839	ALA	4.3
2	A	626	VAL	4.3
2	A	881	HIS	4.2
2	A	827	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
2	A	573	ILE	4.2
2	A	633	LEU	4.1
2	A	717	LEU	4.1
2	A	628	LEU	4.1
2	A	778	ASN	4.0
2	A	806	ARG	4.0
2	A	454	GLY	4.0
2	A	630	TYR	4.0
2	A	429	ALA	4.0
2	A	727	PHE	4.0
2	A	327	TYR	4.0
2	A	814	TYR	4.0
2	A	574	ALA	3.9
2	A	585	GLN	3.9
2	A	615	GLU	3.9
2	A	903	LEU	3.9
2	A	766	TYR	3.9
2	A	924	TRP	3.9
2	A	805	THR	3.9
2	A	544	GLY	3.8
2	A	325	ILE	3.8
2	A	912	VAL	3.8
2	A	599	LEU	3.8
2	A	749	VAL	3.8
2	A	762	PHE	3.8
2	A	601	LYS	3.7
2	A	373	PHE	3.7
2	A	836	ARG	3.7
2	A	584	LYS	3.7
2	A	428	LEU	3.6
2	A	466	LEU	3.6
2	A	640	TYR	3.6
2	A	563	LEU	3.6
2	A	780	PRO	3.6
2	A	561	LEU	3.6
2	A	625	LYS	3.6
2	A	844	ILE	3.6
2	A	374	ALA	3.5
2	A	678	ASN	3.5
2	A	914	LEU	3.5
2	A	471	ILE	3.4
2	A	856	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	A	802	MET	3.4
2	A	453	ALA	3.4
2	A	324	MET	3.3
2	A	534	VAL	3.3
2	A	368	LEU	3.3
2	A	593	LYS	3.3
2	A	509	HIS	3.3
2	A	569	LYS	3.3
2	A	344	ALA	3.2
2	A	789	ASP	3.2
2	A	787	TYR	3.2
2	A	676	LEU	3.2
2	A	644	LEU	3.2
2	A	861	ILE	3.2
2	A	588	THR	3.2
2	A	440	PHE	3.2
2	A	619	LEU	3.2
2	A	823	LEU	3.2
2	A	353	ALA	3.2
2	A	739	ALA	3.2
2	A	473	PHE	3.1
2	A	826	PRO	3.1
2	A	831	SER	3.1
2	A	364	ILE	3.1
2	A	354	PHE	3.1
2	A	479	LYS	3.1
2	A	731	LYS	3.1
2	A	627	ILE	3.1
2	A	566	LEU	3.1
2	A	808	GLN	3.1
2	A	383	ILE	3.1
2	A	505	THR	3.0
2	A	884	LEU	3.0
2	A	612	GLU	3.0
2	A	491	LEU	3.0
2	A	799	LEU	3.0
2	A	812	GLN	3.0
2	A	636	LEU	3.0
2	A	481	LYS	3.0
2	A	916	VAL	3.0
2	A	552	LEU	3.0
2	A	423	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	343	ILE	3.0
2	A	390	LEU	3.0
2	A	427	ILE	3.0
2	A	855	ILE	3.0
2	A	392	ALA	3.0
2	A	867	LEU	3.0
2	A	765	ILE	2.9
2	A	444	LEU	2.9
2	A	854	ASP	2.9
2	A	782	LYS	2.9
2	A	620	ASP	2.9
2	A	711	LEU	2.9
2	A	919	GLY	2.9
2	A	470	THR	2.9
2	A	810	LYS	2.9
2	A	791	TYR	2.9
2	A	571	HIS	2.8
2	A	455	ARG	2.8
2	A	459	ASP	2.8
2	A	902	GLN	2.8
2	A	801	TYR	2.8
2	A	592	GLU	2.8
2	A	721	LYS	2.8
2	A	818	LEU	2.8
2	A	709	ILE	2.8
2	A	662	ALA	2.8
2	A	449	LEU	2.8
2	A	733	ILE	2.8
2	A	523	LEU	2.8
2	A	843	ALA	2.8
2	A	447	TYR	2.8
2	A	824	TYR	2.8
2	A	849	GLN	2.7
2	A	474	GLU	2.7
2	A	668	ARG	2.7
2	A	468	HIS	2.7
2	A	517	GLN	2.7
2	A	331	VAL	2.7
1	B	1004[A]	DA	2.7
2	A	728	ALA	2.7
2	A	431	TYR	2.7
2	A	761	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	720	ASP	2.7
2	A	371	LEU	2.7
2	A	424	ASP	2.6
2	A	452	VAL	2.6
2	A	435	LEU	2.6
2	A	510	LEU	2.6
2	A	326	SER	2.6
2	A	907	CYS	2.6
2	A	846	ALA	2.6
2	A	417	VAL	2.6
2	A	461	LEU	2.6
2	A	790	LEU	2.6
2	A	632	GLY	2.6
2	A	536	VAL	2.6
2	A	815	VAL	2.6
2	A	529	ILE	2.6
2	A	426	GLY	2.6
2	A	716	HIS	2.6
2	A	659	TYR	2.6
2	A	538	SER	2.5
2	A	513	TRP	2.5
2	A	330	TYR	2.5
2	A	490	ALA	2.5
2	A	525	VAL	2.5
2	A	674	PRO	2.5
2	A	389	TYR	2.5
2	A	817	THR	2.5
2	A	413	LYS	2.5
2	A	797	GLY	2.5
2	A	476	ILE	2.5
2	A	701	ILE	2.5
2	A	665	ALA	2.5
2	A	421	LEU	2.5
2	A	516	LEU	2.5
2	A	677	GLN	2.5
2	A	863	VAL	2.5
2	A	356	THR	2.5
2	A	672	THR	2.5
2	A	361	LEU	2.5
2	A	409	LEU	2.5
2	A	379	VAL	2.4
2	A	613	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	702	VAL	2.4
2	A	358	THR	2.4
2	A	616	GLU	2.4
2	A	842	ALA	2.4
2	A	369	VAL	2.4
2	A	772	GLY	2.4
2	A	396	ILE	2.4
2	A	489	ILE	2.4
2	A	719	ARG	2.4
2	A	774	ALA	2.4
2	A	900	ILE	2.4
2	A	788	MET	2.4
2	A	418	GLY	2.4
2	A	723	LEU	2.3
2	A	915	LEU	2.3
2	A	556	SER	2.3
2	A	747	GLU	2.3
2	A	502	ALA	2.3
2	A	850	GLY	2.3
2	A	533	LEU	2.3
2	A	442	THR	2.3
2	A	819	ASP	2.3
2	A	776	GLN	2.3
2	A	537	LEU	2.3
2	A	755	ARG	2.3
2	A	634	ALA	2.3
2	A	333	ILE	2.3
2	A	456	HIS	2.3
2	A	743	GLY	2.3
2	A	520	LYS	2.3
2	A	600	LYS	2.3
2	A	742	PHE	2.3
2	A	906	ASN	2.3
2	A	332	THR	2.3
2	A	559	LEU	2.3
2	A	381	ALA	2.2
2	A	838	ALA	2.2
2	A	334	LEU	2.2
2	A	438	ILE	2.2
2	A	384	PRO	2.2
2	A	382	TYR	2.2
2	A	699	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	352	PHE	2.2
2	A	518	LYS	2.2
2	A	724	LEU	2.2
2	A	736	ALA	2.2
2	A	360	SER	2.2
2	A	764	LEU	2.2
2	A	738	ALA	2.2
2	A	737	THR	2.2
2	A	769	SER	2.2
2	A	822	ARG	2.2
2	A	570	ALA	2.2
2	A	927	ALA	2.2
2	A	576	GLU	2.2
2	A	803	GLU	2.2
2	A	748	THR	2.2
2	A	670	SER	2.2
2	A	348	LYS	2.1
2	A	682	ARG	2.1
2	A	756	SER	2.1
2	A	700	VAL	2.1
2	A	811	GLU	2.1
2	A	639	THR	2.1
2	A	526	PHE	2.1
2	A	464	ARG	2.1
2	A	669	LEU	2.1
2	A	492	GLU	2.1
2	A	862	ALA	2.1
2	A	649	ASN	2.1
2	A	710	GLU	2.1
2	A	508	LEU	2.1
2	A	671	SER	2.1
2	A	895	ALA	2.1
2	A	687	ARG	2.1
2	A	893	VAL	2.1
2	A	658	SER	2.1
2	A	370	GLY	2.1
2	A	405	LEU	2.1
2	A	641	THR	2.1
2	A	673	ASP	2.1
2	A	337	GLU	2.1
2	A	375	ILE	2.1
2	A	420	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	553	HIS	2.1
2	A	712	ARG	2.1
2	A	339	LEU	2.0
2	A	462	ALA	2.0
2	A	329	ASN	2.0
2	A	918	VAL	2.0
2	A	871	GLN	2.0
2	A	565	GLU	2.0
2	A	666	THR	2.0
2	A	690	ARG	2.0
2	A	745	PRO	2.0
2	A	848	MET	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	C31	B	1006[B]	24/25	0.51	7.53	40,45,47,49	24
1	C31	B	1006[A]	24/25	0.51	6.14	28,34,37,40	24
1	U31	B	1005[A]	24/25	0.42	4.02	39,41,48,50	24
1	U31	B	1005[B]	16/25	0.42	3.50	48,50,52,53	16

## 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	321	1/1	0.92	14.91	50,50,50,50	0
5	SO4	A	94	5/5	0.30	5.71	32,34,35,35	5
5	SO4	A	40	5/5	0.39	3.46	31,33,34,37	5
5	SO4	A	38	5/5	0.41	3.02	32,33,35,35	5
5	SO4	A	32	5/5	0.36	1.32	29,32,33,34	5
3	ZN	A	320	1/1	0.34	1.09	59,59,59,59	1
3	ZN	A	322	1/1	0.17	-1.21	42,42,42,42	1
3	ZN	A	3	1/1	0.12	-3.63	44,44,44,44	0
3	ZN	A	1	1/1	0.10	-5.72	24,24,24,24	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.