



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:04 PM UTC

PDB ID : 1D9D / pdb_00001d9d
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'
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Deposited on : 1999-10-27
Resolution : 2.18 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

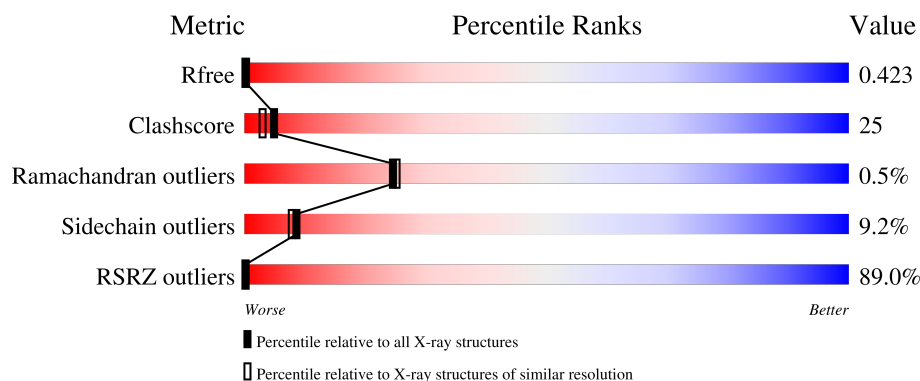
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (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 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	B	6	
2	A	605	

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	1005[A]	-	-	X	X
1	U31	B	1005[B]	-	-	X	X
1	C31	B	1006[B]	-	-	X	-
4	MG	A	321	-	-	-	X
5	SO4	A	32	-	-	X	-
5	SO4	A	38	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5149 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 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 mutation	UNP P00582

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Zn	0	0
			4	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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		

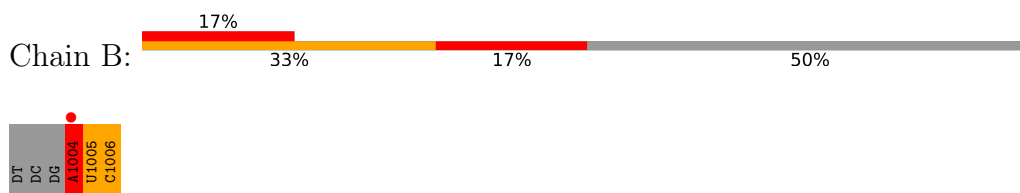
- Molecule 6 is water.

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

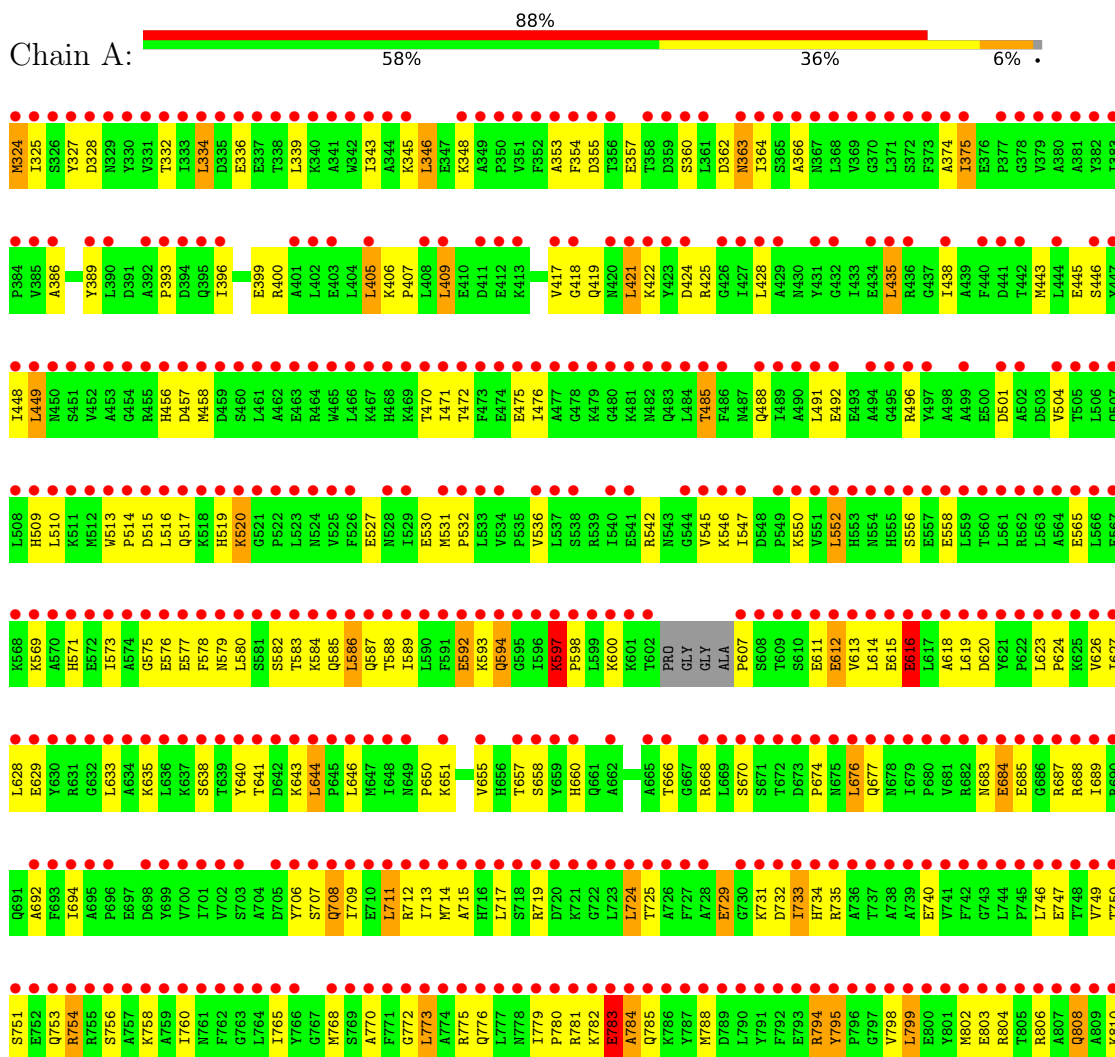
3 Residue-property plots

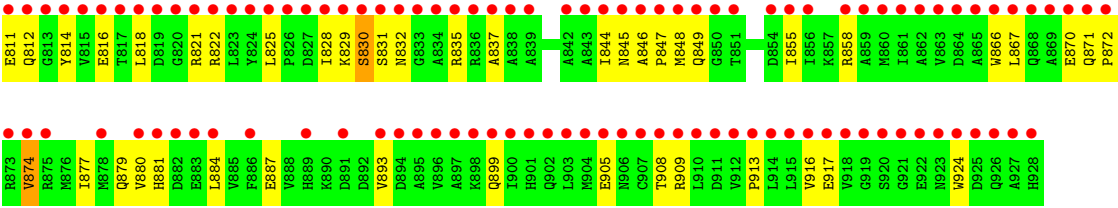
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-D(*TP*CP*GP)-R(AP*(U31)P*(C31))-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	102.55Å 102.55Å 86.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.18 20.00 – 2.18	Depositor EDS
% Data completeness (in resolution range)	84.5 (20.00-2.18) 92.5 (20.00-2.18)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.238 0.414 , 0.423	Depositor DCC
R_{free} test set	4799 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	5149	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: U31, ZN, MG, C31, 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	0.78	0/20	2.09	1/29 (3.4%)
2	A	0.41	0/4839	0.96	23/6547 (0.4%)
All	All	0.41	0/4859	0.97	24/6576 (0.4%)

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

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	783	GLU	N-CA-C	-10.61	99.00	112.90
2	A	597	LYS	N-CA-C	7.26	125.86	109.81
2	A	527	GLU	N-CA-C	7.04	118.75	111.14
2	A	887	GLU	N-CA-C	-6.67	98.03	108.90
2	A	893	VAL	N-CA-C	6.62	118.16	110.62
1	B	1004[A]	DA	O5'-C5'-C4'	6.60	120.70	110.80
2	A	607	PRO	N-CA-CB	6.35	109.99	103.00
2	A	616	GLU	N-CA-C	-6.28	104.06	111.03
2	A	694	ILE	N-CA-C	6.11	118.66	109.20
2	A	845	ASN	N-CA-C	6.10	117.73	111.14
2	A	795	TYR	CA-C-N	6.07	125.95	119.28
2	A	795	TYR	C-N-CA	6.07	125.95	119.28
2	A	689	ILE	N-CA-C	-5.83	104.82	110.42
2	A	396	ILE	N-CA-C	-5.63	101.53	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	825	LEU	CA-C-N	5.55	125.39	119.28
2	A	825	LEU	C-N-CA	5.55	125.39	119.28
2	A	837	ALA	N-CA-C	-5.48	105.22	111.14
2	A	586	LEU	N-CA-C	5.36	116.93	111.14
2	A	485	THR	N-CA-C	-5.29	101.66	110.17
2	A	363	ASN	N-CA-C	5.18	116.61	111.07
2	A	666	THR	N-CA-C	5.15	119.62	113.23
2	A	445	GLU	N-CA-C	-5.14	105.59	111.14
2	A	784	ALA	N-CA-C	-5.09	105.43	111.69
2	A	386	ALA	N-CA-C	5.03	117.31	110.88

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 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	106	0	73	66	0
2	A	4753	0	4752	209	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	13	11
6	B	10	0	0	10	0
All	All	5149	0	4825	246	16

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 25.

All (246) 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:1005[A]:U31:H5	2:A:458:MET:CE	1.75	1.16
1:B:1005[A]:U31:HB'1	1:B:1005[A]:U31:H3'	1.23	1.14
1:B:1005[B]:U31:O5'	6:B:189:HOH:O	1.64	1.13
1:B:1005[A]:U31:H5	2:A:458:MET:HE2	1.24	1.10
1:B:1005[A]:U31:HB'1	1:B:1005[A]:U31:C3'	1.86	1.05
1:B:1004[A]:DA:H2	2:A:422:LYS:NZ	1.55	1.05
1:B:1005[A]:U31:ND'	6:B:364:HOH:O	1.90	1.05
1:B:1006[A]:C31:ND'	6:B:35:HOH:O	1.92	1.01
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[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
1:B:1005[A]:U31:C5	2:A:458:MET:HE2	2.10	0.80
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:O2'	1:B:1006[B]:C31:ND'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:802:MET:HE2	2:A:844:ILE:HD13	1.73	0.70
2:A:520:LYS:HG2	5:A:32:SO4:O3	1.91	0.69
2:A:830:SER:C	2:A:832:ASN:H	2.01	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: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:O2	1:B:1006[A]:C31:C5'	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:583:THR:HA	2:A:587:GLN:CD	2.25	0.61
1:B:1005[A]:U31:H5	2:A:458:MET:HE1	1.78	0.60
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
2:A:324:MET:HE2	6:A:1092:HOH:O	2.03	0.59
1:B:1005[A]:U31:CC	6:B:364:HOH:O	2.39	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:588:THR:O	2:A:592:GLU:HB3	2.02	0.58
2:A:830:SER:OG	2:A:835:ARG:HD3	2.04	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:ND'	1:B:1006[B]:C31:O3'	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:H4'	1:B:1006[B]:C31:HB'2	1.87	0.56
2:A:586:LEU:HD22	2:A:627:ILE:CD1	2.35	0.56
2:A:770:ALA:HA	2:A:788:MET:SD	2.45	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:558:GLU:CD	2:A:688:ARG:HH12	2.15	0.55
2:A:660:HIS:HB2	2:A:670:SER:OG	2.07	0.54
2:A:589:ILE:O	2:A:593:LYS:HG2	2.08	0.54
2:A:616:GLU:O	2:A:619:LEU:HD23	2.07	0.54
2:A:458:MET:HE3	2:A:504:VAL:HG11	1.89	0.54
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:765:ILE:HA	2:A:848:MET:HE1	1.91	0.53
2:A:717:LEU:HD21	2:A:818:LEU:CD1	2.37	0.53
2:A:569:LYS:O	2:A:573:ILE:HG13	2.09	0.53
2:A:711:LEU:HD13	2:A:765:ILE:HD11	1.89	0.53
2:A:600:LYS:CB	2:A:614:LEU:H	2.21	0.53
2:A:612:GLU:HB3	2:A:615:GLU:CG	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H4'	1:B:1006[B]:C31:O1P	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:781:ARG:C	2:A:783:GLU:H	2.17	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:N	2:A:619:LEU:HD22	2.26	0.51
1:B:1005[A]:U31:O1P	2:A:457:ASP:HA	2.10	0.50
2:A:425:ARG:HD3	2:A:425:ARG:C	2.35	0.50
2:A:585:GLN:O	2:A:588:THR:OG1	2.29	0.50
2:A:816:GLU:HG2	2:A:822:ARG:HG2	1.92	0.50
2:A:324:MET:HA	2:A:324:MET:HE3	1.94	0.50
2:A:332:THR:HG22	2:A:334:LEU:HD13	1.92	0.50
2:A:830:SER:C	2:A:832:ASN:N	2.68	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
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:353:ALA:HB3	2:A:374:ALA:HB3	1.94	0.48
2:A:611:GLU:CB	2:A:775:ARG:NH2	2.77	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:657:THR:HG22	6:A:1033:HOH:O	2.14	0.48
2:A:808:GLN:O	2:A:812:GLN:HG2	2.13	0.48
2:A:715:ALA:HB1	2:A:724:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005[B]:U31:H3'	1:B:1006[B]:C31:C5'	2.42	0.47
2:A:579:ASN:C	2:A:580:LEU:HD22	2.39	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:399:GLU:HG2	6:A:1000:HOH:O	2.15	0.47
2:A:905:GLU:HB3	2:A:916:VAL:HG23	1.97	0.47
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:611:GLU:CB	2:A:775:ARG:HH22	2.29	0.46
2:A:749:VAL:HG23	2:A:753:GLN:HB2	1.98	0.46
1:B:1006[B]:C31:O2	1:B:1006[B]:C31:H3'	2.16	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:346:LEU:HD12	2:A:375:ILE:HG23	1.95	0.45
2:A:485:THR:H	2:A:488:GLN:NE2	2.03	0.45
2:A:740:GLU:HG3	2:A:795:TYR:OH	2.16	0.45
2:A:593:LYS:O	2:A:594:GLN:CB	2.64	0.45
2:A:735:ARG:CZ	2:A:749:VAL:HG13	2.46	0.45
2:A:799:LEU:HD22	2:A:803:GLU:HG3	1.98	0.45
1:B:1006[B]:C31:O2	1:B:1006[B]:C31:H2'	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
2:A:565:GLU:HG2	6:A:1037:HOH:O	2.17	0.44
2:A:515:ASP:C	2:A:517:GLN:H	2.24	0.44
2:A:756:SER:O	2:A:760:ILE:HG13	2.17	0.44
2:A:362:ASP:O	2:A:366:ALA:HB2	2.17	0.44
2:A:531:MET:HB2	2:A:532:PRO:HD3	2.00	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:405:LEU:HB3	2:A:409:LEU:HD22	1.99	0.44
2:A:683:ASN:OD1	2:A:684:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:336:GLU:CD	2:A:400:ARG:HE	2.26	0.43
2:A:814:TYR:CD1	2:A:814:TYR:C	2.97	0.43
2:A:472:THR:OG1	2:A:475:GLU:HG3	2.18	0.43
2:A:513:TRP:O	2:A:517:GLN:HG3	2.19	0.43
2:A:597:LYS:CG	2:A:598:PRO:HD3	2.49	0.43
1:B:1004[A]:DA:C6	2:A:658:SER:HB3	2.54	0.43
2:A:343:ILE:HD11	2:A:405:LEU:HD13	2.00	0.42
2:A:711:LEU:CD1	2:A:765:ILE:HD11	2.48	0.42
2:A:592:GLU:O	2:A:592:GLU:HG2	2.18	0.42
2:A:731:LYS:HD2	2:A:746:LEU:CD2	2.50	0.42
2:A:773:LEU:HD22	2:A:773:LEU:O	2.19	0.42
2:A:880:VAL:HG11	2:A:924:TRP:HZ2	1.84	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:406:LYS:NZ	6:A:1079:HOH:O	2.49	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:354:PHE:CZ	2:A:428:LEU:HD11	2.56	0.41
2:A:773:LEU:HD13	2:A:784:ALA:HB1	2.03	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:707:SER:C	2:A:708:GLN:HG2	2.46	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: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
2:A:782:LYS:N	2:A:782:LYS:HD2	2.36	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	Interatomic distance (Å)	Clash overlap (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 [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
2	A	597/605 (99%)	563 (94%)	31 (5%)	3 (0%)	24 25

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%)	454 (91%)	46 (9%)	8 8

All (46) 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	510	LEU
2	A	520	LYS
2	A	536	VAL
2	A	546	LYS
2	A	550	LYS
2	A	552	LEU
2	A	584	LYS
2	A	592	GLU
2	A	597	LYS
2	A	612	GLU
2	A	616	GLU
2	A	620	ASP
2	A	626	VAL
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	711	LEU

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Mol	Chain	Res	Type
2	A	724	LEU
2	A	729	GLU
2	A	733	ILE
2	A	747	GLU
2	A	754	ARG
2	A	773	LEU
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	917	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) 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	543	ASN
2	A	571	HIS
2	A	587	GLN
2	A	677	GLN
2	A	734	HIS
2	A	879	GLN
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 ⓘ

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	C31	B	1006[A]	3,1	22,25,26	1.40	4 (18%)	29,34,37	1.72	7 (24%)
1	C31	B	1006[B]	1	22,25,26	1.22	1 (4%)	29,34,37	1.64	6 (20%)
1	U31	B	1005[B]	1	17,17,26	0.67	0	24,24,37	0.64	0
1	U31	B	1005[A]	1	22,25,26	1.80	6 (27%)	29,34,37	2.91	11 (37%)

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	C31	B	1006[A]	3,1	-	5/12/30/31	0/2/2/2
1	C31	B	1006[B]	1	-	9/12/30/31	0/2/2/2
1	U31	B	1005[B]	1	-	4/6/18/31	0/2/2/2
1	U31	B	1005[A]	1	-	10/12/30/31	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1006[B]	C31	C4-N4	-4.21	1.23	1.33
1	B	1006[A]	C31	C4-N4	-4.05	1.24	1.33
1	B	1005[A]	U31	O2-C2	-3.89	1.16	1.23
1	B	1005[A]	U31	O2'-CA'	3.24	1.51	1.43
1	B	1005[A]	U31	C4-N3	-3.17	1.33	1.38
1	B	1005[A]	U31	C5-C4	-3.17	1.36	1.43
1	B	1006[A]	C31	O5'-C5'	3.07	1.52	1.44
1	B	1005[A]	U31	C6-N1	-2.34	1.32	1.38
1	B	1005[A]	U31	CB'-CC	-2.19	1.41	1.51
1	B	1006[A]	C31	CB'-CC	-2.16	1.41	1.51
1	B	1006[A]	C31	CB'-CA'	-2.16	1.42	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1005[A]	U31	C2'-C1'-N1	8.41	130.19	114.24
1	B	1005[A]	U31	O2'-C2'-C1'	7.81	123.04	108.97
1	B	1005[A]	U31	O2'-CA'-CB'	4.80	125.64	109.37
1	B	1006[A]	C31	C4-N3-C2	4.61	127.52	120.26
1	B	1006[B]	C31	C5-C4-N3	-4.33	114.03	121.32
1	B	1006[B]	C31	C4-N3-C2	4.30	127.03	120.26
1	B	1006[A]	C31	C5-C4-N3	-4.09	114.42	121.32
1	B	1005[A]	U31	CA'-O2'-C2'	4.00	122.90	114.02
1	B	1005[A]	U31	C1'-N1-C2	3.68	124.21	117.59
1	B	1005[A]	U31	C6-N1-C2	-3.38	116.89	121.00
1	B	1006[A]	C31	C5-C4-N4	3.14	126.12	120.63
1	B	1005[A]	U31	O3'-C3'-C4'	-3.07	102.26	111.08
1	B	1005[A]	U31	C3'-C2'-C1'	-2.85	97.36	102.81
1	B	1006[B]	C31	C5-C4-N4	2.82	125.57	120.63
1	B	1006[B]	C31	O2'-C2'-C3'	2.78	118.21	111.05
1	B	1006[A]	C31	CC-CB'-CA'	-2.72	104.18	113.53
1	B	1005[A]	U31	O4'-C1'-C2'	-2.50	102.29	106.59
1	B	1006[A]	C31	O2-C2-N1	2.36	123.53	118.90
1	B	1006[B]	C31	N1-C2-N3	-2.22	114.94	118.80
1	B	1006[B]	C31	O2-C2-N1	2.21	123.22	118.90
1	B	1005[A]	U31	C6-C5-C4	2.16	122.29	119.53
1	B	1005[A]	U31	O4'-C1'-N1	-2.10	103.59	108.36
1	B	1006[A]	C31	O4'-C4'-C3'	2.07	109.27	105.15
1	B	1006[A]	C31	N1-C2-N3	-2.04	115.27	118.80

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1005[A]	U31	C3'-C2'-O2'-CA'
1	B	1005[A]	U31	CB'-CA'-O2'-C2'
1	B	1005[A]	U31	C2'-C1'-N1-C2
1	B	1005[A]	U31	C2'-C1'-N1-C6
1	B	1005[B]	U31	O4'-C1'-N1-C2
1	B	1005[B]	U31	O4'-C1'-N1-C6
1	B	1006[A]	C31	C4'-C5'-O5'-P
1	B	1006[A]	C31	O4'-C1'-N1-C2
1	B	1006[A]	C31	O4'-C1'-N1-C6
1	B	1006[B]	C31	C4'-C5'-O5'-P
1	B	1006[B]	C31	C1'-C2'-O2'-CA'
1	B	1006[A]	C31	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	1006[B]	C31	O4'-C4'-C5'-O5'
1	B	1006[B]	C31	C3'-C4'-C5'-O5'
1	B	1005[A]	U31	O4'-C4'-C5'-O5'
1	B	1006[B]	C31	C2'-C1'-N1-C2
1	B	1005[A]	U31	C3'-C4'-C5'-O5'
1	B	1006[A]	C31	C3'-C4'-C5'-O5'
1	B	1005[A]	U31	O2'-CA'-CB'-CC
1	B	1005[B]	U31	O4'-C4'-C5'-O5'
1	B	1005[A]	U31	O4'-C1'-N1-C2
1	B	1005[B]	U31	C3'-C4'-C5'-O5'
1	B	1006[B]	C31	C2'-C1'-N1-C6
1	B	1005[A]	U31	O4'-C1'-N1-C6
1	B	1006[B]	C31	O4'-C1'-N1-C6
1	B	1006[B]	C31	CB'-CA'-O2'-C2'
1	B	1005[A]	U31	CA'-CB'-CC-ND'
1	B	1006[B]	C31	O4'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1006[A]	C31	7	0
1	B	1006[B]	C31	17	0
1	B	1005[B]	U31	18	0
1	B	1005[A]	U31	23	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	38	-	4,4,4	0.52	0	6,6,6	0.09	0
5	SO4	A	94	-	4,4,4	0.54	0	6,6,6	0.16	0
5	SO4	A	40	-	4,4,4	0.57	0	6,6,6	0.13	0
5	SO4	A	32	-	4,4,4	0.60	0	6,6,6	0.19	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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	38	SO4	3	0
5	A	94	SO4	1	0
5	A	32	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	1/6 (16%)	5.80	1 (100%) 0 0	26, 26, 26, 26	1 (100%)
2	A	601/605 (99%)	3.58	535 (89%) 0 0	13, 30, 60, 60	0
All	All	602/611 (98%)	3.59	536 (89%) 0 0	13, 30, 60, 60	1 (0%)

All (536) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	582	SER	13.2
2	A	608	SER	9.1
2	A	580	LEU	9.1
2	A	830	SER	8.5
2	A	586	LEU	8.2
2	A	746	LEU	8.0
2	A	832	ASN	7.9
2	A	792	PHE	7.6
2	A	622	PRO	7.6
2	A	583	THR	7.5
2	A	581	SER	7.5
2	A	730	GLY	7.3
2	A	610	SER	7.1
2	A	784	ALA	7.0
2	A	578	PHE	7.0
2	A	591	PHE	7.0
2	A	598	PRO	7.0
2	A	771	PHE	6.9
2	A	751	SER	6.9
2	A	596	ILE	6.8
2	A	798	VAL	6.8
2	A	623	LEU	6.8
2	A	454	GLY	6.8
2	A	614	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
2	A	786	LYS	6.7
2	A	770	ALA	6.7
2	A	465	TRP	6.6
2	A	779	ILE	6.4
2	A	617	LEU	6.3
2	A	773	LEU	6.2
2	A	785	GLN	6.1
2	A	477	ALA	6.1
2	A	744	LEU	6.1
2	A	621	TYR	6.1
2	A	741	VAL	6.1
2	A	626	VAL	6.1
2	A	790	LEU	6.1
2	A	392	ALA	6.0
2	A	774	ALA	5.9
2	A	569	LYS	5.9
2	A	588	THR	5.9
2	A	805	THR	5.9
2	A	625	LYS	5.9
2	A	777	LEU	5.8
2	A	831	SER	5.8
1	B	1004[A]	DA	5.8
2	A	633	LEU	5.8
2	A	844	ILE	5.7
2	A	597	LYS	5.7
2	A	810	LYS	5.7
2	A	727	PHE	5.7
2	A	924	TRP	5.6
2	A	628	LEU	5.6
2	A	609	THR	5.6
2	A	566	LEU	5.5
2	A	828	ILE	5.5
2	A	607	PRO	5.5
2	A	602	THR	5.5
2	A	914	LEU	5.5
2	A	829	LYS	5.5
2	A	795	TYR	5.4
2	A	518	LYS	5.4
2	A	559	LEU	5.4
2	A	689	ILE	5.4
2	A	574	ALA	5.3
2	A	517	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
2	A	912	VAL	5.3
2	A	769	SER	5.3
2	A	766	TYR	5.3
2	A	451	SER	5.3
2	A	587	GLN	5.2
2	A	787	TYR	5.2
2	A	471	ILE	5.2
2	A	717	LEU	5.2
2	A	768	MET	5.2
2	A	585	GLN	5.2
2	A	601	LYS	5.2
2	A	903	LEU	5.2
2	A	827	ASP	5.2
2	A	780	PRO	5.2
2	A	611	GLU	5.2
2	A	721	LYS	5.2
2	A	632	GLY	5.1
2	A	589	ILE	5.1
2	A	749	VAL	5.1
2	A	544	GLY	5.1
2	A	681	VAL	5.0
2	A	720	ASP	5.0
2	A	630	TYR	5.0
2	A	662	ALA	5.0
2	A	919	GLY	5.0
2	A	825	LEU	5.0
2	A	814	TYR	5.0
2	A	783	GLU	4.9
2	A	794	ARG	4.9
2	A	818	LEU	4.9
2	A	640	TYR	4.9
2	A	619	LEU	4.9
2	A	324	MET	4.9
2	A	327	TYR	4.9
2	A	806	ARG	4.9
2	A	556	SER	4.8
2	A	811	GLU	4.8
2	A	563	LEU	4.8
2	A	590	LEU	4.8
2	A	910	LEU	4.8
2	A	615	GLU	4.8
2	A	762	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
2	A	479	LYS	4.7
2	A	644	LEU	4.7
2	A	826	PRO	4.7
2	A	360	SER	4.7
2	A	552	LEU	4.7
2	A	835	ARG	4.6
2	A	447	TYR	4.6
2	A	561	LEU	4.6
2	A	325	ILE	4.6
2	A	634	ALA	4.6
2	A	815	VAL	4.6
2	A	836	ARG	4.6
2	A	373	PHE	4.6
2	A	613	VAL	4.5
2	A	328	ASP	4.5
2	A	429	ALA	4.5
2	A	461	LEU	4.5
2	A	627	ILE	4.5
2	A	440	PHE	4.5
2	A	915	LEU	4.5
2	A	573	ILE	4.5
2	A	577	GLU	4.5
2	A	739	ALA	4.5
2	A	843	ALA	4.5
2	A	364	ILE	4.4
2	A	791	TYR	4.4
2	A	820	GLY	4.4
2	A	599	LEU	4.4
2	A	671	SER	4.4
2	A	459	ASP	4.4
2	A	353	ALA	4.4
2	A	452	VAL	4.4
2	A	668	ARG	4.4
2	A	635	LYS	4.4
2	A	470	THR	4.3
2	A	478	GLY	4.3
2	A	666	THR	4.3
2	A	833	GLY	4.3
2	A	516	LEU	4.3
2	A	813	GLY	4.3
2	A	659	TYR	4.3
2	A	809	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	A	842	ALA	4.3
2	A	755	ARG	4.3
2	A	804	ARG	4.3
2	A	509	HIS	4.3
2	A	672	THR	4.3
2	A	466	LEU	4.2
2	A	926	GLN	4.2
2	A	520	LYS	4.2
2	A	789	ASP	4.2
2	A	742	PHE	4.2
2	A	834	ALA	4.2
2	A	639	THR	4.2
2	A	731	LYS	4.2
2	A	701	ILE	4.2
2	A	728	ALA	4.2
2	A	473	PHE	4.2
2	A	474	GLU	4.2
2	A	861	ILE	4.1
2	A	802	MET	4.1
2	A	902	GLN	4.1
2	A	616	GLU	4.1
2	A	801	TYR	4.1
2	A	839	ALA	4.1
2	A	368	LEU	4.1
2	A	823	LEU	4.1
2	A	916	VAL	4.1
2	A	379	VAL	4.1
2	A	505	THR	4.1
2	A	670	SER	4.1
2	A	568	LYS	4.1
2	A	796	PRO	4.1
2	A	502	ALA	4.1
2	A	772	GLY	4.1
2	A	468	HIS	4.1
2	A	488	GLN	4.1
2	A	658	SER	4.1
2	A	579	ASN	4.0
2	A	678	ASN	4.0
2	A	838	ALA	4.0
2	A	480	GLY	4.0
2	A	523	LEU	4.0
2	A	519	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
2	A	737	THR	4.0
2	A	824	TYR	4.0
2	A	680	PRO	4.0
2	A	453	ALA	4.0
2	A	869	ALA	4.0
2	A	690	ARG	4.0
2	A	641	THR	4.0
2	A	550	LYS	4.0
2	A	753	GLN	4.0
2	A	575	GLY	4.0
2	A	775	ARG	4.0
2	A	850	GLY	4.0
2	A	361	LEU	3.9
2	A	481	LYS	3.9
2	A	776	GLN	3.9
2	A	781	ARG	3.9
2	A	472	THR	3.9
2	A	513	TRP	3.9
2	A	554	ASN	3.9
2	A	868	GLN	3.9
2	A	854	ASP	3.9
2	A	426	GLY	3.9
2	A	881	HIS	3.9
2	A	722	GLY	3.9
2	A	867	LEU	3.9
2	A	870	GLU	3.9
2	A	759	ALA	3.8
2	A	444	LEU	3.8
2	A	676	LEU	3.8
2	A	557	GLU	3.8
2	A	374	ALA	3.8
2	A	724	LEU	3.8
2	A	413	LYS	3.8
2	A	592	GLU	3.8
2	A	927	ALA	3.8
2	A	571	HIS	3.8
2	A	891	ASP	3.8
2	A	748	THR	3.7
2	A	764	LEU	3.7
2	A	576	GLU	3.7
2	A	584	LYS	3.7
2	A	812	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	525	VAL	3.7
2	A	529	ILE	3.7
2	A	389	TYR	3.7
2	A	618	ALA	3.7
2	A	549	PRO	3.7
2	A	856	ILE	3.7
2	A	736	ALA	3.7
2	A	905	GLU	3.7
2	A	464	ARG	3.7
2	A	674	PRO	3.7
2	A	348	LYS	3.7
2	A	684	GLU	3.7
2	A	455	ARG	3.7
2	A	646	LEU	3.6
2	A	624	PRO	3.6
2	A	913	PRO	3.6
2	A	344	ALA	3.6
2	A	510	LEU	3.6
2	A	799	LEU	3.6
2	A	396	ILE	3.6
2	A	807	ALA	3.6
2	A	837	ALA	3.6
2	A	428	LEU	3.6
2	A	782	LYS	3.6
2	A	866	TRP	3.6
2	A	893	VAL	3.6
2	A	442	THR	3.6
2	A	449	LEU	3.6
2	A	636	LEU	3.6
2	A	803	GLU	3.6
2	A	756	SER	3.6
2	A	675	ASN	3.5
2	A	390	LEU	3.5
2	A	921	GLY	3.5
2	A	560	THR	3.5
2	A	515	ASP	3.5
2	A	673	ASP	3.5
2	A	747	GLU	3.5
2	A	863	VAL	3.5
2	A	900	ILE	3.5
2	A	645	PRO	3.5
2	A	370	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	A	898	LYS	3.5
2	A	526	PHE	3.4
2	A	695	ALA	3.4
2	A	334	LEU	3.4
2	A	435	LEU	3.4
2	A	920	SER	3.4
2	A	457	ASP	3.4
2	A	719	ARG	3.4
2	A	923	ASN	3.4
2	A	384	PRO	3.4
2	A	763	GLY	3.4
2	A	849	GLN	3.4
2	A	871	GLN	3.4
2	A	534	VAL	3.4
2	A	655	VAL	3.4
2	A	460	SER	3.4
2	A	682	ARG	3.4
2	A	743	GLY	3.4
2	A	760	ILE	3.4
2	A	883	GLU	3.4
2	A	884	LEU	3.4
2	A	808	GLN	3.4
2	A	716	HIS	3.4
2	A	489	ILE	3.4
2	A	494	ALA	3.4
2	A	687	ARG	3.3
2	A	793	GLU	3.3
2	A	365	SER	3.3
2	A	504	VAL	3.3
2	A	918	VAL	3.3
2	A	553	HIS	3.3
2	A	562	ARG	3.3
2	A	326	SER	3.3
2	A	393	PRO	3.3
2	A	386	ALA	3.3
2	A	862	ALA	3.3
2	A	354	PHE	3.3
2	A	565	GLU	3.3
2	A	514	PRO	3.3
2	A	331	VAL	3.3
2	A	570	ALA	3.3
2	A	491	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	816	GLU	3.3
2	A	620	ASP	3.3
2	A	358	THR	3.2
2	A	707	SER	3.2
2	A	522	PRO	3.2
2	A	874	VAL	3.2
2	A	336	GLU	3.2
2	A	497	TYR	3.2
2	A	685	GLU	3.2
2	A	800	GLU	3.2
2	A	846	ALA	3.2
2	A	448	ILE	3.2
2	A	788	MET	3.2
2	A	848	MET	3.2
2	A	797	GLY	3.2
2	A	712	ARG	3.2
2	A	745	PRO	3.2
2	A	922	GLU	3.2
2	A	456	HIS	3.2
2	A	752	GLU	3.2
2	A	683	ASN	3.2
2	A	700	VAL	3.2
2	A	409	LEU	3.2
2	A	484	LEU	3.2
2	A	699	TYR	3.2
2	A	706	TYR	3.2
2	A	894	ASP	3.2
2	A	342	TRP	3.1
2	A	533	LEU	3.1
2	A	330	TYR	3.1
2	A	649	ASN	3.1
2	A	692	ALA	3.1
2	A	895	ALA	3.1
2	A	710	GLU	3.1
2	A	765	ILE	3.1
2	A	423	TYR	3.1
2	A	446	SER	3.1
2	A	637	LYS	3.1
2	A	851	THR	3.1
2	A	819	ASP	3.1
2	A	403	GLU	3.1
2	A	490	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	711	LEU	3.1
2	A	343	ILE	3.1
2	A	476	ILE	3.1
2	A	855	ILE	3.1
2	A	345	LYS	3.1
2	A	638	SER	3.1
2	A	501	ASP	3.1
2	A	702	VAL	3.1
2	A	418	GLY	3.0
2	A	686	GLY	3.0
2	A	750	THR	3.0
2	A	761	ASN	3.0
2	A	696	PRO	3.0
2	A	821	ARG	3.0
2	A	925	ASP	3.0
2	A	462	ALA	3.0
2	A	679	ILE	3.0
2	A	495	GLY	3.0
2	A	431	TYR	3.0
2	A	369	VAL	3.0
2	A	536	VAL	3.0
2	A	778	ASN	3.0
2	A	424	ASP	3.0
2	A	928	HIS	3.0
2	A	507	GLN	3.0
2	A	594	GLN	3.0
2	A	822	ARG	3.0
2	A	669	LEU	3.0
2	A	612	GLU	3.0
2	A	709	ILE	3.0
2	A	733	ILE	3.0
2	A	564	ALA	2.9
2	A	408	LEU	2.9
2	A	383	ILE	2.9
2	A	901	HIS	2.9
2	A	708	GLN	2.9
2	A	475	GLU	2.9
2	A	528	ASN	2.9
2	A	467	LYS	2.9
2	A	911	ASP	2.9
2	A	356	THR	2.9
2	A	872	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	688	ARG	2.9
2	A	593	LYS	2.9
2	A	405	LEU	2.9
2	A	483	GLN	2.9
2	A	648	ILE	2.9
2	A	677	GLN	2.9
2	A	377	PRO	2.9
2	A	538	SER	2.9
2	A	858	ARG	2.8
2	A	906	ASN	2.8
2	A	381	ALA	2.8
2	A	595	GLY	2.8
2	A	351	VAL	2.8
2	A	657	THR	2.8
2	A	907	CYS	2.8
2	A	469	LYS	2.8
2	A	521	GLY	2.8
2	A	908	THR	2.8
2	A	917	GLU	2.8
2	A	665	ALA	2.8
2	A	421	LEU	2.8
2	A	600	LYS	2.8
2	A	817	THR	2.8
2	A	546	LYS	2.7
2	A	417	VAL	2.7
2	A	375	ILE	2.7
2	A	694	ILE	2.7
2	A	845	ASN	2.7
2	A	714	MET	2.7
2	A	629	GLU	2.7
2	A	718	SER	2.7
2	A	693	PHE	2.7
2	A	492	GLU	2.7
2	A	394	ASP	2.7
2	A	732	ASP	2.7
2	A	511	LYS	2.7
2	A	865	ALA	2.7
2	A	402	LEU	2.7
2	A	434	GLU	2.7
2	A	382	TYR	2.7
2	A	385	VAL	2.7
2	A	441	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	341	ALA	2.6
2	A	366	ALA	2.6
2	A	567	GLU	2.6
2	A	897	ALA	2.6
2	A	367	ASN	2.6
2	A	537	LEU	2.6
2	A	540	ILE	2.6
2	A	878	MET	2.6
2	A	726	ALA	2.6
2	A	651	LYS	2.6
2	A	899	GLN	2.6
2	A	572	GLU	2.6
2	A	329	ASN	2.6
2	A	363	ASN	2.6
2	A	380	ALA	2.6
2	A	754	ARG	2.6
2	A	512	MET	2.6
2	A	555	HIS	2.6
2	A	758	LYS	2.6
2	A	705	ASP	2.6
2	A	909	ARG	2.6
2	A	339	LEU	2.6
2	A	438	ILE	2.5
2	A	551	VAL	2.5
2	A	660	HIS	2.5
2	A	524	ASN	2.5
2	A	371	LEU	2.5
2	A	337	GLU	2.5
2	A	352	PHE	2.5
2	A	496	ARG	2.5
2	A	349	ALA	2.5
2	A	340	LYS	2.5
2	A	873	ARG	2.5
2	A	482	ASN	2.5
2	A	531	MET	2.5
2	A	875	ARG	2.5
2	A	642	ASP	2.4
2	A	740	GLU	2.4
2	A	725	THR	2.4
2	A	463	GLU	2.4
2	A	378	GLY	2.4
2	A	359	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	350	PRO	2.4
2	A	734	HIS	2.4
2	A	541	GLU	2.4
2	A	427	ILE	2.4
2	A	735	ARG	2.4
2	A	338	THR	2.4
2	A	757	ALA	2.3
2	A	859	ALA	2.3
2	A	335	ASP	2.3
2	A	896	VAL	2.3
2	A	532	PRO	2.3
2	A	395	GLN	2.3
2	A	506	LEU	2.3
2	A	698	ASP	2.3
2	A	889	HIS	2.3
2	A	333	ILE	2.3
2	A	713	ILE	2.3
2	A	631	ARG	2.3
2	A	864	ASP	2.3
2	A	860	MET	2.3
2	A	486	PHE	2.2
2	A	547	ILE	2.2
2	A	545	VAL	2.2
2	A	847	PRO	2.2
2	A	738	ALA	2.2
2	A	703	SER	2.2
2	A	485	THR	2.2
2	A	355	ASP	2.2
2	A	411	ASP	2.2
2	A	882	ASP	2.2
2	A	508	LEU	2.2
2	A	715	ALA	2.2
2	A	723	LEU	2.2
2	A	422	LYS	2.2
2	A	436	ARG	2.1
2	A	643	LYS	2.1
2	A	420	ASN	2.1
2	A	432	GLY	2.1
2	A	499	ALA	2.1
2	A	450	ASN	2.1
2	A	886	PHE	2.1
2	A	458	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	558	GLU	2.1
2	A	904	MET	2.1
2	A	880	VAL	2.1
2	A	412	GLU	2.0
2	A	332	THR	2.0
2	A	372	SER	2.0
2	A	647	MET	2.0
2	A	401	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
1	U31	B	1005[A]	24/25	0.58	0.44	39,41,48,50	24
1	U31	B	1005[B]	16/25	0.58	0.44	48,50,52,53	16
1	C31	B	1006[A]	24/25	0.65	0.39	28,34,37,40	24
1	C31	B	1006[B]	24/25	0.65	0.39	40,45,47,49	24

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(Å ²)	Q<0.9
5	SO4	A	38	5/5	0.41	0.32	32,33,35,35	5
4	MG	A	321	1/1	0.44	0.57	50,50,50,50	0
3	ZN	A	322	1/1	0.61	0.14	42,42,42,42	1
5	SO4	A	32	5/5	0.64	0.27	29,32,33,34	5
3	ZN	A	320	1/1	0.65	0.20	59,59,59,59	1
5	SO4	A	94	5/5	0.68	0.33	32,34,35,35	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	3	1/1	0.70	0.13	44,44,44,44	0
3	ZN	A	1	1/1	0.81	0.10	24,24,24,24	0
5	SO4	A	40	5/5	0.82	0.22	31,33,34,37	5

6.5 Other polymers [i](#)

There are no such residues in this entry.