



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:56 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

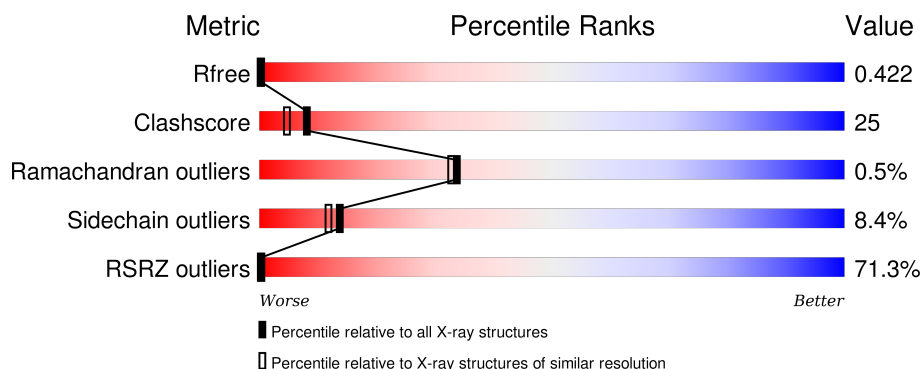
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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	-
1	U31	B	1005[B]	-	-	X	-
1	C31	B	1006[B]	-	-	X	-
4	MG	A	321	-	-	-	X
5	SO4	A	32	-	-	X	-
5	SO4	A	38	-	-	X	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	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: 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		

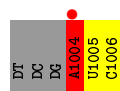
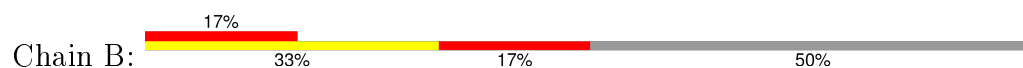
- Molecule 6 is water.

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

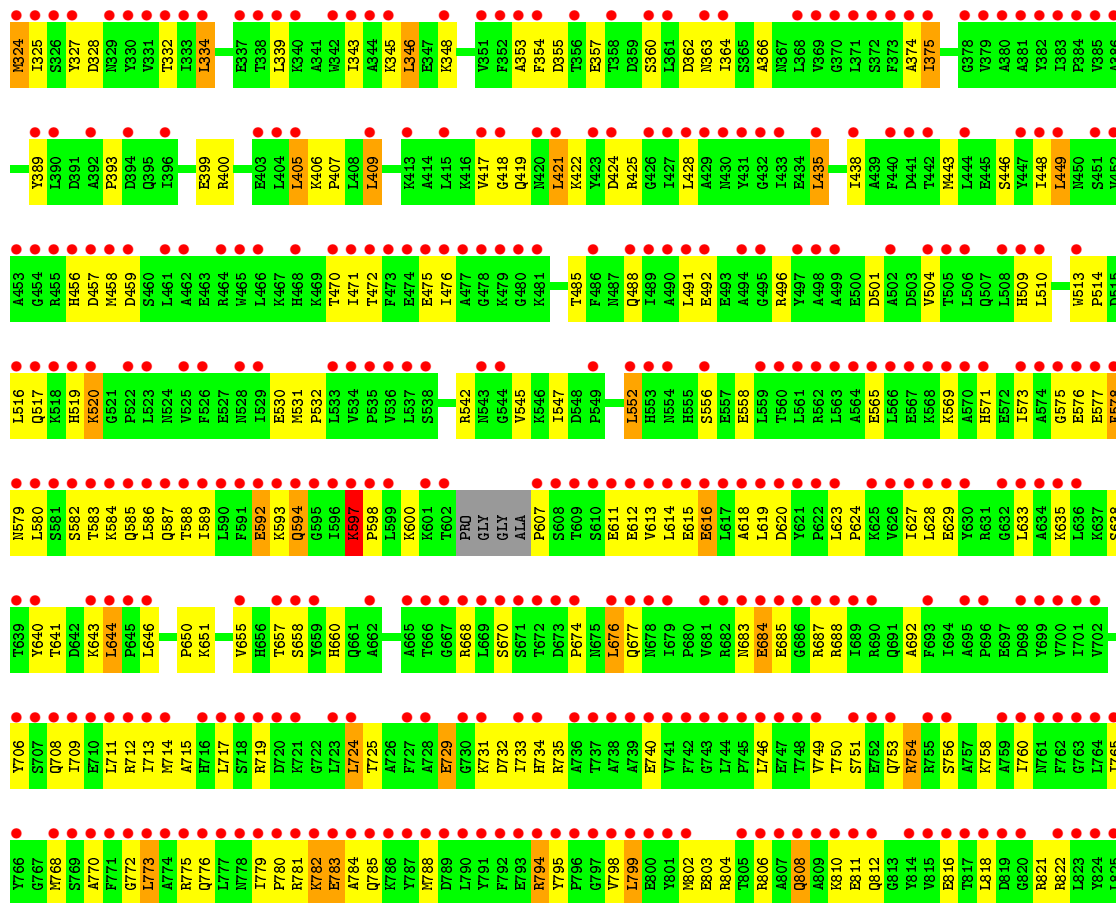
3 Residue-property plots

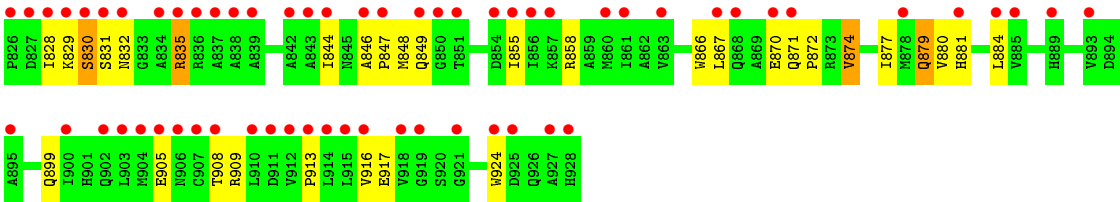
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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'



- 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 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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	26.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 76.0	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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 (239) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:830:SER:C	2:A:832:ASN:H	2.01	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	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:558:GLU:OE1	2:A:719:ARG:CG[2_765]	2.13	0.07
2:A:492:GLU:N	2:A:651:LYS:O[3_654]	2.13	0.07
2:A:345:LYS:NZ	6:A:1060:HOH:O[3_654]	2.14	0.06
2:A:651:LYS:NZ	6:A:1015:HOH:O[4_565]	2.17	0.03
2:A:345:LYS:CE	6:A:1060:HOH:O[3_654]	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%)	34	33

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	500/510 (98%)	458 (92%)	42 (8%)	14	12

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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	U31	B	1005[A]	1	15,25,26	1.46	3 (20%)	21,34,37	3.82	12 (57%)
1	U31	B	1005[B]	1	12,17,26	1.20	1 (8%)	17,24,37	3.50	2 (11%)
1	C31	B	1006[A]	1,3	16,25,26	1.44	2 (12%)	22,34,37	2.56	5 (22%)
1	C31	B	1006[B]	1	16,25,26	1.30	1 (6%)	22,34,37	2.37	4 (18%)

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	-	1/8/30/31	0/2/2/2
1	U31	B	1005[B]	1	-	0/2/18/31	0/2/2/2
1	C31	B	1006[A]	1,3	-	0/8/30/31	0/2/2/2
1	C31	B	1006[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	1006[B]	C31	C4-N4	-3.96	1.23	1.35
1	B	1006[A]	C31	C4-N4	-3.82	1.24	1.35
1	B	1005[A]	U31	C6-N1	-2.34	1.32	1.35
1	B	1005[A]	U31	CB'-CC	-2.00	1.41	1.51
1	B	1006[A]	C31	C6-N1	2.04	1.38	1.35
1	B	1005[B]	U31	C4-N3	2.57	1.37	1.33
1	B	1005[A]	U31	O2'-CA'	3.17	1.51	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1006[B]	C31	C5-C4-N3	-6.16	114.03	121.80
1	B	1006[A]	C31	C5-C4-N3	-5.85	114.42	121.80
1	B	1005[A]	U31	C5-C4-N3	-4.07	112.67	123.12
1	B	1005[B]	U31	C5-C4-N3	-3.38	114.44	123.12
1	B	1005[A]	U31	O3'-C3'-C4'	-2.93	102.26	111.05
1	B	1005[A]	U31	C3'-C2'-C1'	-2.78	97.36	102.73
1	B	1005[A]	U31	C6-N1-C2	-2.71	116.89	121.28
1	B	1006[A]	C31	CC-CB'-CA'	-2.61	104.18	113.88
1	B	1005[A]	U31	O4'-C1'-C2'	-2.39	102.29	106.60
1	B	1005[A]	U31	O4'-C1'-N1	-2.13	103.59	108.08
1	B	1006[A]	C31	O4'-C4'-C3'	2.05	109.27	105.15
1	B	1006[B]	C31	N4-C4-N3	2.12	120.36	116.50
1	B	1005[A]	U31	C4'-O4'-C1'	2.34	112.28	109.72
1	B	1005[A]	U31	C6-C5-C4	2.68	122.29	117.28
1	B	1006[B]	C31	C5-C4-N4	2.78	125.57	121.31
1	B	1005[A]	U31	CA'-O2'-C2'	3.10	122.90	114.40
1	B	1006[A]	C31	C5-C4-N4	3.14	126.12	121.31
1	B	1005[A]	U31	O2'-CA'-CB'	3.96	125.64	109.88
1	B	1005[A]	U31	C2'-C1'-N1	5.79	130.19	113.53
1	B	1006[B]	C31	C2-N3-C4	8.09	127.03	115.61
1	B	1006[A]	C31	C2-N3-C4	8.44	127.52	115.61
1	B	1005[A]	U31	C4-N3-C2	13.22	127.23	114.14
1	B	1005[B]	U31	C4-N3-C2	13.71	127.72	114.14

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.

4 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1005[A]	U31	22	0
1	B	1005[B]	U31	18	0
1	B	1006[A]	C31	7	0
1	B	1006[B]	C31	17	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	32	-	4,4,4	0.70	0	6,6,6	0.14	0
5	SO4	A	38	-	4,4,4	0.53	0	6,6,6	0.12	0
5	SO4	A	40	-	4,4,4	0.65	0	6,6,6	0.09	0
5	SO4	A	94	-	4,4,4	0.62	0	6,6,6	0.15	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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	32	SO4	2	0
5	A	38	SO4	3	0
5	A	94	SO4	1	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%)	3.72	1 (100%) 0 0	52, 52, 52, 52	1 (100%)
2	A	601/605 (99%)	3.09	428 (71%) 0 0	13, 30, 60, 60	0
All	All	602/611 (98%)	3.09	429 (71%) 0 0	13, 30, 60, 60	1 (0%)

All (429) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	582	SER	20.3
2	A	608	SER	14.0
2	A	602	THR	13.9
2	A	586	LEU	13.2
2	A	583	THR	12.6
2	A	596	ILE	10.8
2	A	779	ILE	10.7
2	A	597	LYS	10.5
2	A	609	THR	10.2
2	A	746	LEU	9.8
2	A	580	LEU	9.6
2	A	610	SER	9.0
2	A	621	TYR	9.0
2	A	589	ILE	8.7
2	A	773	LEU	8.7
2	A	581	SER	8.4
2	A	611	GLU	8.3
2	A	830	SER	8.2
2	A	730	GLY	7.9
2	A	578	PHE	7.8
2	A	598	PRO	7.8
2	A	590	LEU	7.7
2	A	617	LEU	7.5
2	A	781	ARG	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	795	TYR	7.3
2	A	744	LEU	7.1
2	A	614	LEU	7.0
2	A	832	ASN	7.0
2	A	834	ALA	6.9
2	A	595	GLY	6.9
2	A	784	ALA	6.8
2	A	785	GLN	6.7
2	A	792	PHE	6.7
2	A	465	TRP	6.6
2	A	783	GLU	6.5
2	A	607	PRO	6.4
2	A	778	ASN	6.2
2	A	798	VAL	6.1
2	A	594	GLN	6.1
2	A	809	ALA	6.1
2	A	577	GLU	6.0
2	A	835	ARG	5.9
2	A	591	PHE	5.9
2	A	741	VAL	5.7
2	A	569	LYS	5.6
2	A	828	ILE	5.5
2	A	623	LEU	5.5
2	A	751	SER	5.5
2	A	829	LYS	5.5
2	A	839	ALA	5.5
2	A	775	ARG	5.4
2	A	633	LEU	5.4
2	A	805	THR	5.4
2	A	364	ILE	5.3
2	A	814	TYR	5.3
2	A	912	VAL	5.3
2	A	924	TRP	5.3
2	A	794	ARG	5.3
2	A	766	TYR	5.3
2	A	327	TYR	5.2
2	A	615	GLU	5.2
2	A	689	ILE	5.2
2	A	786	LYS	5.2
2	A	630	TYR	5.2
2	A	777	LEU	5.1
2	A	903	LEU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	618	ALA	5.1
2	A	806	ARG	5.1
2	A	910	LEU	5.1
2	A	881	HIS	5.0
2	A	771	PHE	4.9
2	A	440	PHE	4.9
2	A	768	MET	4.9
2	A	451	SER	4.9
2	A	626	VAL	4.9
2	A	762	PHE	4.8
2	A	622	PRO	4.8
2	A	561	LEU	4.8
2	A	587	GLN	4.8
2	A	836	ARG	4.8
2	A	827	ASP	4.7
2	A	563	LEU	4.7
2	A	325	ILE	4.6
2	A	749	VAL	4.6
2	A	770	ALA	4.6
2	A	765	ILE	4.6
2	A	466	LEU	4.6
2	A	544	GLY	4.5
2	A	509	HIS	4.5
2	A	573	ILE	4.4
2	A	390	LEU	4.4
2	A	471	ILE	4.4
2	A	682	ARG	4.4
2	A	727	PHE	4.4
2	A	392	ALA	4.4
2	A	523	LEU	4.3
2	A	717	LEU	4.3
2	A	681	VAL	4.3
2	A	429	ALA	4.3
2	A	470	THR	4.3
2	A	789	ASP	4.3
2	A	477	ALA	4.3
2	A	628	LEU	4.2
2	A	826	PRO	4.2
2	A	454	GLY	4.2
2	A	640	TYR	4.2
2	A	739	ALA	4.1
2	A	428	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	491	LEU	4.1
2	A	721	LYS	4.1
2	A	668	ARG	4.0
2	A	861	ILE	4.0
2	A	799	LEU	4.0
2	A	566	LEU	4.0
2	A	856	ILE	4.0
2	A	334	LEU	4.0
2	A	619	LEU	4.0
2	A	728	ALA	4.0
2	A	736	ALA	4.0
2	A	447	TYR	4.0
2	A	914	LEU	3.9
2	A	854	ASP	3.9
2	A	417	VAL	3.9
2	A	772	GLY	3.9
2	A	787	TYR	3.9
2	A	711	LEU	3.9
2	A	919	GLY	3.9
2	A	863	VAL	3.9
2	A	709	ILE	3.9
2	A	802	MET	3.9
2	A	585	GLN	3.9
2	A	616	GLU	3.9
2	A	599	LEU	3.9
2	A	823	LEU	3.9
2	A	801	TYR	3.8
2	A	844	ILE	3.8
2	A	818	LEU	3.8
2	A	373	PHE	3.8
2	A	625	LYS	3.8
2	A	381	ALA	3.8
2	A	453	ALA	3.7
2	A	529	ILE	3.7
2	A	838	ALA	3.7
2	A	601	LYS	3.7
1	B	1004[A]	DA	3.7
2	A	423	TYR	3.7
2	A	537	LEU	3.7
2	A	764	LEU	3.7
2	A	788	MET	3.7
2	A	846	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	427	ILE	3.7
2	A	815	VAL	3.7
2	A	324	MET	3.6
2	A	884	LEU	3.6
2	A	354	PHE	3.6
2	A	571	HIS	3.6
2	A	776	GLN	3.6
2	A	812	GLN	3.6
2	A	383	ILE	3.6
2	A	669	LEU	3.6
2	A	678	ASN	3.6
2	A	761	ASN	3.6
2	A	473	PHE	3.6
2	A	662	ALA	3.6
2	A	916	VAL	3.6
2	A	790	LEU	3.5
2	A	358	THR	3.5
2	A	612	GLU	3.5
2	A	593	LYS	3.5
2	A	534	VAL	3.5
2	A	737	THR	3.5
2	A	742	PHE	3.5
2	A	368	LEU	3.5
2	A	733	ILE	3.5
2	A	343	ILE	3.4
2	A	344	ALA	3.4
2	A	576	GLU	3.4
2	A	331	VAL	3.4
2	A	677	GLN	3.4
2	A	513	TRP	3.4
2	A	413	LYS	3.4
2	A	431	TYR	3.4
2	A	699	TYR	3.4
2	A	481	LYS	3.4
2	A	731	LYS	3.4
2	A	824	TYR	3.4
2	A	505	THR	3.4
2	A	584	LYS	3.4
2	A	855	ILE	3.4
2	A	907	CYS	3.3
2	A	449	LEU	3.3
2	A	462	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	867	LEU	3.3
2	A	747	GLU	3.3
2	A	817	THR	3.3
2	A	461	LEU	3.3
2	A	636	LEU	3.3
2	A	900	ILE	3.3
2	A	831	SER	3.3
2	A	745	PRO	3.3
2	A	516	LEU	3.3
2	A	468	HIS	3.3
2	A	700	VAL	3.3
2	A	421	LEU	3.3
2	A	476	ILE	3.3
2	A	455	ARG	3.3
2	A	526	PHE	3.3
2	A	409	LEU	3.3
2	A	791	TYR	3.2
2	A	479	LYS	3.2
2	A	520	LYS	3.2
2	A	676	LEU	3.2
2	A	755	ARG	3.2
2	A	701	ILE	3.2
2	A	819	ASP	3.2
2	A	674	PRO	3.2
2	A	613	VAL	3.2
2	A	444	LEU	3.2
2	A	353	ALA	3.2
2	A	842	ALA	3.2
2	A	568	LYS	3.2
2	A	714	MET	3.2
2	A	822	ARG	3.2
2	A	724	LEU	3.2
2	A	374	ALA	3.2
2	A	333	ILE	3.2
2	A	352	PHE	3.2
2	A	404	LEU	3.2
2	A	902	GLN	3.2
2	A	915	LEU	3.2
2	A	620	ASP	3.1
2	A	672	THR	3.1
2	A	720	ASP	3.1
2	A	559	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	738	ALA	3.1
2	A	517	GLN	3.1
2	A	360	SER	3.1
2	A	659	TYR	3.1
2	A	361	LEU	3.1
2	A	424	ASP	3.1
2	A	666	THR	3.1
2	A	396	ILE	3.1
2	A	418	GLY	3.1
2	A	459	ASP	3.1
2	A	326	SER	3.1
2	A	433	ILE	3.1
2	A	438	ILE	3.1
2	A	927	ALA	3.0
2	A	330	TYR	3.0
2	A	808	GLN	3.0
2	A	895	ALA	3.0
2	A	426	GLY	3.0
2	A	371	LEU	3.0
2	A	510	LEU	3.0
2	A	562	ARG	3.0
2	A	502	ALA	3.0
2	A	574	ALA	3.0
2	A	627	ILE	3.0
2	A	643	LYS	3.0
2	A	490	ALA	3.0
2	A	843	ALA	3.0
2	A	632	GLY	2.9
2	A	518	LYS	2.9
2	A	556	SER	2.9
2	A	850	GLY	2.9
2	A	871	GLN	2.9
2	A	683	ASN	2.9
2	A	712	ARG	2.9
2	A	538	SER	2.9
2	A	452	VAL	2.9
2	A	702	VAL	2.9
2	A	592	GLU	2.9
2	A	552	LEU	2.9
2	A	575	GLY	2.9
2	A	644	LEU	2.9
2	A	519	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	756	SER	2.9
2	A	878	MET	2.9
2	A	710	GLU	2.8
2	A	382	TYR	2.8
2	A	820	GLY	2.8
2	A	716	HIS	2.8
2	A	474	GLU	2.8
2	A	673	ASP	2.8
2	A	384	PRO	2.8
2	A	687	ARG	2.8
2	A	489	ILE	2.8
2	A	658	SER	2.8
2	A	811	GLU	2.8
2	A	723	LEU	2.8
2	A	478	GLY	2.7
2	A	719	ARG	2.7
2	A	339	LEU	2.7
2	A	849	GLN	2.7
2	A	369	VAL	2.7
2	A	379	VAL	2.7
2	A	906	ASN	2.7
2	A	533	LEU	2.7
2	A	743	GLY	2.7
2	A	810	LYS	2.7
2	A	740	GLU	2.7
2	A	435	LEU	2.7
2	A	356	THR	2.7
2	A	588	THR	2.7
2	A	851	THR	2.7
2	A	332	THR	2.6
2	A	389	TYR	2.6
2	A	707	SER	2.6
2	A	348	LYS	2.6
2	A	472	THR	2.6
2	A	363	ASN	2.6
2	A	713	ILE	2.6
2	A	430	ASN	2.6
2	A	497	TYR	2.6
2	A	693	PHE	2.6
2	A	769	SER	2.6
2	A	695	ALA	2.6
2	A	458	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	918	VAL	2.6
2	A	670	SER	2.5
2	A	494	ALA	2.5
2	A	763	GLY	2.5
2	A	442	THR	2.5
2	A	560	THR	2.5
2	A	506	LEU	2.5
2	A	394	ASP	2.5
2	A	351	VAL	2.5
2	A	686	GLY	2.5
2	A	456	HIS	2.5
2	A	386	ALA	2.5
2	A	525	VAL	2.5
2	A	667	GLY	2.5
2	A	635	LYS	2.5
2	A	420	ASN	2.5
2	A	553	HIS	2.5
2	A	448	ILE	2.5
2	A	498	ALA	2.4
2	A	665	ALA	2.4
2	A	405	LEU	2.4
2	A	495	GLY	2.4
2	A	905	GLU	2.4
2	A	486	PHE	2.4
2	A	825	LEU	2.4
2	A	499	ALA	2.4
2	A	671	SER	2.4
2	A	782	LYS	2.4
2	A	329	ASN	2.4
2	A	816	GLU	2.4
2	A	760	ILE	2.4
2	A	342	TRP	2.4
2	A	752	GLU	2.4
2	A	536	VAL	2.4
2	A	554	ASN	2.4
2	A	340	LYS	2.4
2	A	793	GLU	2.4
2	A	800	GLU	2.4
2	A	570	ALA	2.3
2	A	432	GLY	2.3
2	A	904	MET	2.3
2	A	928	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	639	THR	2.3
2	A	684	GLU	2.3
2	A	718	SER	2.3
2	A	488	GLN	2.3
2	A	337	GLU	2.3
2	A	797	GLY	2.3
2	A	508	LEU	2.3
2	A	759	ALA	2.3
2	A	706	TYR	2.3
2	A	748	THR	2.3
2	A	796	PRO	2.3
2	A	698	ASP	2.3
2	A	646	LEU	2.3
2	A	564	ALA	2.2
2	A	837	ALA	2.2
2	A	480	GLY	2.2
2	A	634	ALA	2.2
2	A	690	ARG	2.2
2	A	657	THR	2.2
2	A	567	GLU	2.2
2	A	375	ILE	2.2
2	A	380	ALA	2.2
2	A	370	GLY	2.2
2	A	913	PRO	2.2
2	A	441	ASP	2.2
2	A	579	ASN	2.2
2	A	679	ILE	2.2
2	A	415	LEU	2.1
2	A	908	THR	2.1
2	A	911	ASP	2.1
2	A	543	ASN	2.1
2	A	464	ARG	2.1
2	A	535	PRO	2.1
2	A	696	PRO	2.1
2	A	868	GLN	2.1
2	A	753	GLN	2.1
2	A	565	GLU	2.1
2	A	645	PRO	2.1
2	A	345	LYS	2.1
2	A	860	MET	2.1
2	A	889	HIS	2.1
2	A	378	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	925	ASP	2.1
2	A	921	GLY	2.1
2	A	492	GLU	2.1
2	A	685	GLU	2.1
2	A	734	HIS	2.1
2	A	780	PRO	2.1
2	A	774	ALA	2.1
2	A	475	GLU	2.1
2	A	870	GLU	2.1
2	A	504	VAL	2.1
2	A	549	PRO	2.1
2	A	629	GLU	2.1
2	A	528	ASN	2.1
2	A	372	SER	2.1
2	A	847	PRO	2.0
2	A	457	ASP	2.0
2	A	338	THR	2.0
2	A	385	VAL	2.0
2	A	857	LYS	2.0
2	A	885	VAL	2.0
2	A	688	ARG	2.0
2	A	708	GLN	2.0
2	A	522	PRO	2.0
2	A	403	GLU	2.0
2	A	807	ALA	2.0
2	A	655	VAL	2.0
2	A	893	VAL	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	1005[A]	24/25	0.59	0.47	-	39,41,48,50	24
1	U31	B	1005[B]	16/25	0.59	0.47	-	48,50,52,53	16
1	C31	B	1006[B]	24/25	0.64	0.55	-	40,45,47,49	24
1	C31	B	1006[A]	24/25	0.64	0.55	-	28,34,37,40	24

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	A	321	1/1	0.42	1.10	12.60	50,50,50,50	0
5	SO4	A	38	5/5	0.59	0.47	2.24	32,33,35,35	5
5	SO4	A	32	5/5	0.62	0.31	-0.08	29,32,33,34	5
3	ZN	A	322	1/1	0.36	0.18	-1.15	42,42,42,42	1
3	ZN	A	1	1/1	0.89	0.11	-15.01	24,24,24,24	0
3	ZN	A	3	1/1	0.89	0.14	-	44,44,44,44	0
5	SO4	A	94	5/5	0.81	0.34	-	32,34,35,35	5
3	ZN	A	320	1/1	0.71	0.31	-	59,59,59,59	1
5	SO4	A	40	5/5	0.78	0.35	-	31,33,34,37	5

6.5 Other polymers [i](#)

There are no such residues in this entry.