



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XJG  
Title : Structural mechanism of allosteric substrate specificity in a ribonucleotide reductase: dATP-UDP complex  
Authors : Larsson, K.-M.; Jordan, A.; Eliasson, R.; Reichard, P.; Logan, D.T.; Nordlund, P.  
Deposited on : 2004-09-23  
Resolution : 2.50 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](mailto: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.

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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 : 1.7 (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

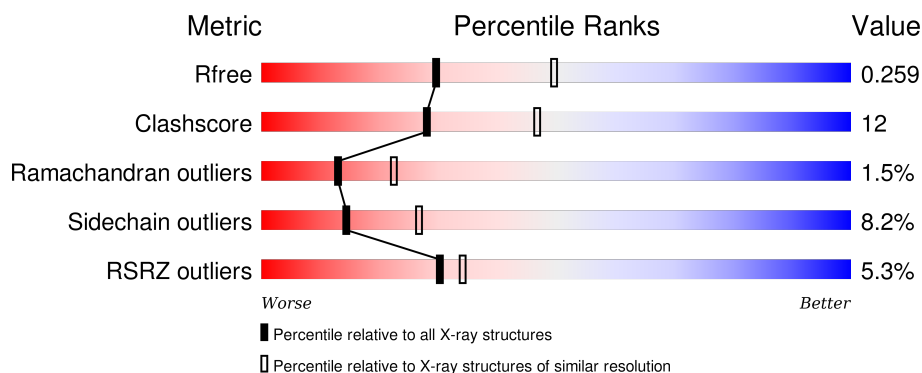
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	A	644	
1	B	644	

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
3	UDP	A	1001	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10209 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ribonucleotide reductase, B12-dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4942	3173	837	912	20			
1	B	610	Total	C	N	O	S	0	0	0
			4907	3150	832	905	20			

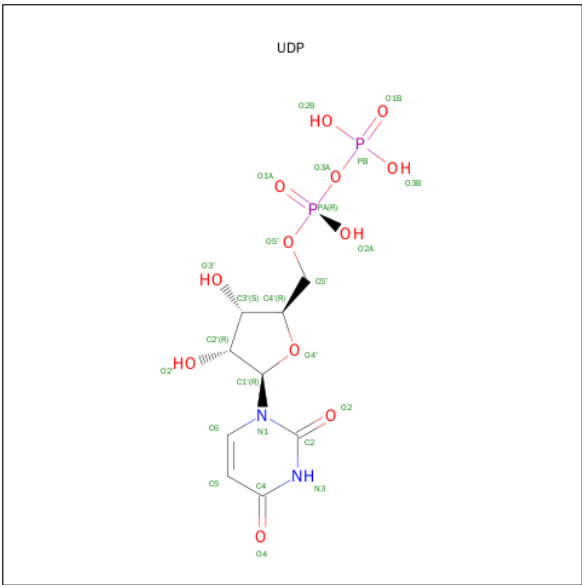
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	TYR	SEE REMARK 999	UNP O33839
B	205	SER	TYR	SEE REMARK 999	UNP O33839

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

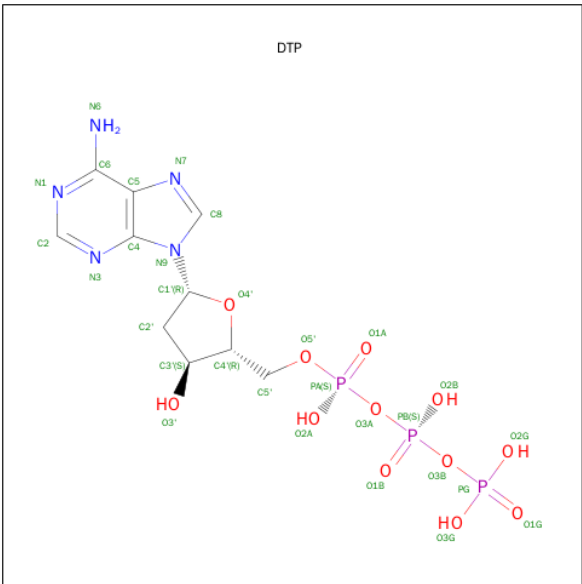
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

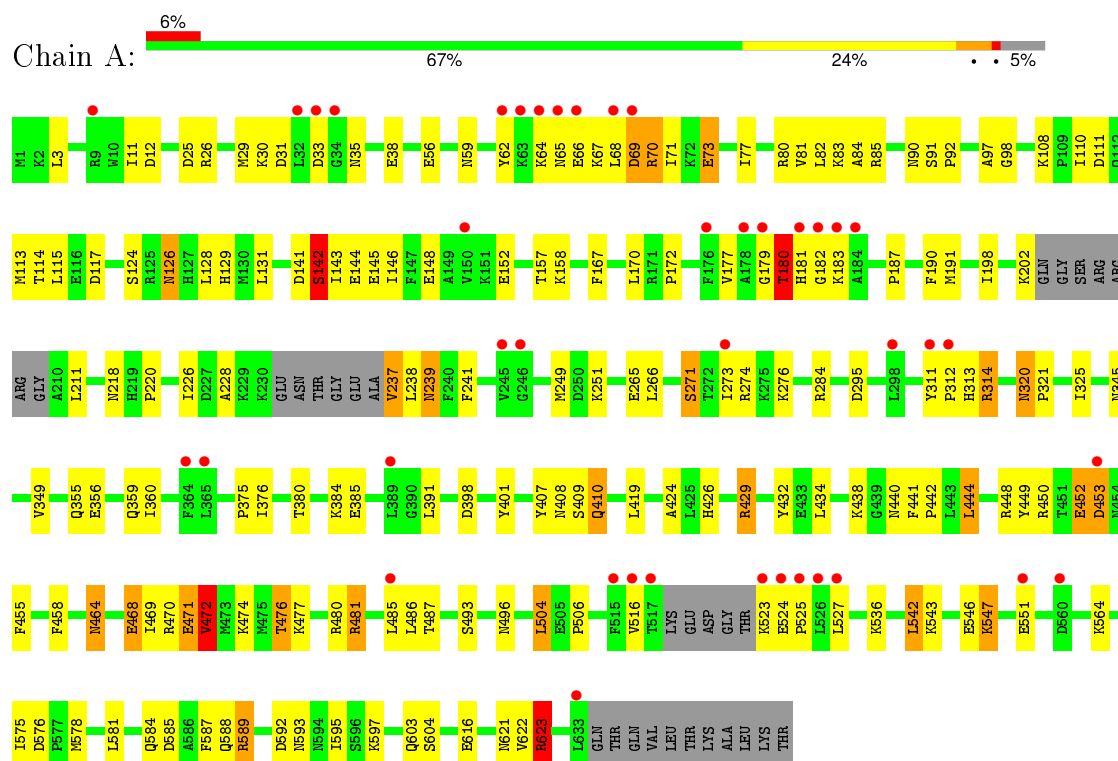
- Molecule 5 is water.

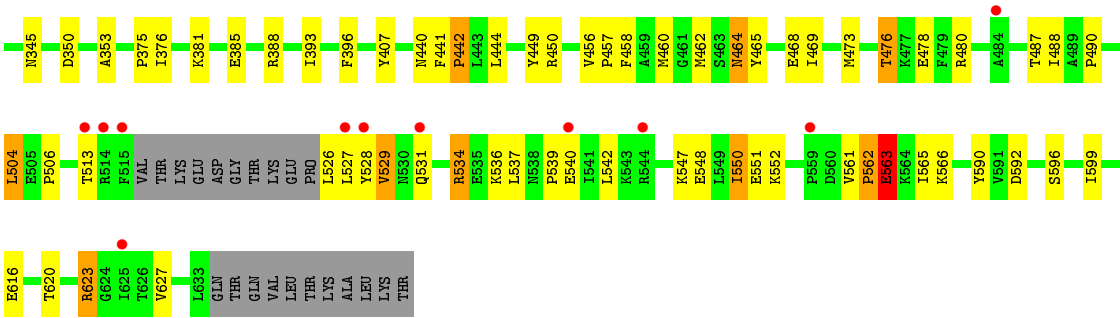
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total	O	0	0
			109	109		
5	B	139	Total	O	0	0
			139	139		

### 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: ribonucleotide reductase, B12-dependent







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.54Å 123.51Å 105.89Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	24.87 – 2.50 24.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.87-2.50) 100.0 (24.87-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.07 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.195 , 0.264 0.193 , 0.259	Depositor DCC
$R_{free}$ test set	2628 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 51410 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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, DTP, UDP

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	A	0.86	0/5040	0.89	6/6804 (0.1%)
1	B	0.95	3/5001 (0.1%)	0.91	4/6749 (0.1%)
All	All	0.91	3/10041 (0.0%)	0.90	10/13553 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	468	GLU	CD-OE1	5.37	1.31	1.25
1	B	465	TYR	CE1-CZ	5.27	1.45	1.38
1	B	81	VAL	CB-CG1	-5.10	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	462	MET	CG-SD-CE	7.02	111.44	100.20
1	A	82	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	B	623	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	142	SER	N-CA-C	5.47	125.78	111.00
1	B	388	ARG	NE-CZ-NH2	-5.43	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	623	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	589	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	215	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	82	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PHE	Peptide
1	B	562	PRO	Peptide

## 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	A	4942	0	5003	137	0
1	B	4907	0	4963	103	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	11	0	0
3	B	25	0	11	2	0
4	A	30	0	12	5	0
4	B	30	0	12	1	0
5	A	109	0	0	15	0
5	B	139	0	0	11	0
All	All	10209	0	10012	234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (234) 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:A:128:LEU:HD13	1:B:179:GLY:O	1.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLU:O	1:A:472:VAL:HB	1.48	1.06
1:A:126:ASN:HD22	1:A:128:LEU:H	1.13	0.95
1:B:457:PRO:HD3	5:B:1141:HOH:O	1.68	0.93
1:A:440:ASN:ND2	1:A:444:LEU:HD23	1.86	0.90
1:A:441:PHE:HB3	1:A:481:ARG:O	1.72	0.88
1:A:148:GLU:O	1:A:152:GLU:HG3	1.74	0.88
1:A:424:ALA:HA	1:A:486:LEU:HD11	1.55	0.88
1:B:456:VAL:HA	5:B:1141:HOH:O	1.74	0.87
1:A:452:GLU:O	1:A:453:ASP:HB2	1.75	0.87
1:B:70:ARG:NH2	5:B:1105:HOH:O	2.07	0.87
1:A:295:ASP:HB2	5:A:1107:HOH:O	1.75	0.87
1:B:528:TYR:O	1:B:529:VAL:HG23	1.75	0.87
1:B:73:GLU:CG	1:B:73:GLU:OE2	2.26	0.83
1:A:126:ASN:ND2	1:A:128:LEU:H	1.78	0.81
1:A:271:SER:OG	1:A:273:ILE:HD12	1.81	0.80
1:A:438:LYS:HD3	1:A:481:ARG:HH21	1.47	0.79
1:A:438:LYS:HD3	1:A:481:ARG:NH2	1.98	0.79
1:B:73:GLU:HB2	5:B:1125:HOH:O	1.82	0.79
1:B:563:GLU:HA	1:B:563:GLU:OE1	1.83	0.78
1:A:542:LEU:O	1:A:546:GLU:HG3	1.84	0.78
1:A:455:PHE:CE2	5:A:1113:HOH:O	2.37	0.78
1:A:536:LYS:HB3	5:A:1105:HOH:O	1.83	0.77
1:B:473:MET:HG3	5:B:1141:HOH:O	1.84	0.76
4:A:1004:DTP:O5'	4:A:1004:DTP:H8	1.85	0.76
1:B:67:LYS:O	1:B:71:ILE:HG13	1.86	0.75
1:A:450:ARG:NH1	1:A:477:LYS:O	2.20	0.74
1:A:128:LEU:CD1	1:B:179:GLY:O	2.35	0.73
1:B:381:LYS:O	1:B:385:GLU:HG3	1.87	0.73
1:B:195:ASN:HD21	1:B:239:ASN:ND2	1.88	0.72
1:B:141:ASP:O	4:B:1003:DTP:H5'2	1.89	0.72
1:A:448:ARG:O	1:A:452:GLU:HB2	1.88	0.71
1:A:472:VAL:O	1:A:476:THR:HB	1.90	0.71
1:B:473:MET:O	1:B:476:THR:HG22	1.90	0.71
1:A:64:LYS:O	1:A:65:ASN:HB2	1.91	0.70
1:B:146:ILE:O	1:B:150:VAL:HG23	1.92	0.70
1:A:464:ASN:HA	5:A:1044:HOH:O	1.91	0.69
1:B:229:LYS:HD2	1:B:243:LEU:HD22	1.75	0.69
1:A:468:GLU:O	1:A:471:GLU:O	2.11	0.67
1:A:587:PHE:HB3	1:A:595:ILE:HD11	1.77	0.67
1:A:455:PHE:CD2	5:A:1113:HOH:O	2.47	0.66
1:A:320:ASN:HB2	1:A:321:PRO:HD2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASN:HD21	1:B:239:ASN:HD21	1.43	0.66
1:A:265:GLU:OE1	1:A:276:LYS:HG2	1.96	0.66
1:A:251:LYS:NZ	1:A:622:VAL:O	2.28	0.65
1:A:438:LYS:CD	1:A:481:ARG:HH21	2.09	0.65
1:B:241:PHE:HB3	1:B:243:LEU:HD13	1.77	0.65
1:A:190:PHE:CD1	1:B:200:VAL:HG11	2.32	0.65
1:A:265:GLU:O	5:A:1097:HOH:O	2.15	0.64
1:B:1:MET:HB3	1:B:350:ASP:OD2	1.98	0.64
1:A:471:GLU:O	1:A:472:VAL:CB	2.33	0.64
1:B:449:TYR:OH	1:B:457:PRO:HG3	1.98	0.64
1:A:128:LEU:HD11	1:B:179:GLY:HA2	1.80	0.64
1:A:182:GLY:O	1:A:183:LYS:HB2	1.98	0.63
1:B:531:GLN:HG3	1:B:534:ARG:HH12	1.64	0.62
1:B:460:MET:HG2	1:B:590:TYR:CE1	2.34	0.62
1:A:98:GLY:H	1:A:129:HIS:CD2	2.18	0.62
1:B:182:GLY:O	1:B:183:LYS:HB2	2.00	0.61
1:A:126:ASN:C	1:A:126:ASN:HD22	2.04	0.61
1:A:239:ASN:HD22	1:A:239:ASN:H	1.48	0.61
1:A:143:ILE:H	1:A:146:ILE:HG13	1.66	0.61
1:A:408:ASN:HB3	1:A:575:ILE:HG23	1.82	0.61
1:A:190:PHE:CE1	1:B:200:VAL:CG1	2.84	0.60
1:A:69:ASP:O	1:A:70:ARG:HB2	2.02	0.60
1:A:449:TYR:CE1	5:A:1113:HOH:O	2.54	0.60
1:A:470:ARG:HG2	5:A:1073:HOH:O	2.00	0.60
1:A:218:ASN:O	1:A:266:LEU:HA	2.00	0.60
1:B:592:ASP:O	1:B:623:ARG:NH2	2.34	0.60
1:A:320:ASN:H	1:A:320:ASN:HD22	1.48	0.60
1:B:476:THR:CG2	1:B:480:ARG:HE	2.15	0.59
1:B:623:ARG:HD2	5:B:1011:HOH:O	2.02	0.59
1:B:464:ASN:H	1:B:464:ASN:ND2	1.99	0.59
1:B:198:ILE:HG13	1:B:211:LEU:HD11	1.83	0.59
1:B:537:LEU:HD23	1:B:542:LEU:HB2	1.85	0.59
1:A:265:GLU:OE2	1:A:274:ARG:HD2	2.03	0.59
1:A:180:THR:HG22	1:A:182:GLY:N	2.17	0.59
1:A:585:ASP:OD1	1:A:589:ARG:HD2	2.03	0.58
1:B:306:LYS:HA	5:B:1118:HOH:O	2.02	0.58
1:B:227:ASP:OD2	1:B:285:LYS:NZ	2.31	0.58
1:A:449:TYR:CZ	5:A:1113:HOH:O	2.51	0.58
1:B:177:VAL:HG22	1:B:183:LYS:H	1.69	0.57
1:B:487:THR:O	1:B:488:ILE:HD13	2.04	0.57
1:A:142:SER:O	1:A:143:ILE:HB	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LYS:O	1:B:550:ILE:HG22	2.05	0.57
1:A:429:ARG:O	1:A:432:TYR:HB3	2.04	0.57
1:A:73:GLU:O	1:A:77:ILE:HG13	2.05	0.57
1:A:142:SER:HB3	1:A:145:GLU:OE2	2.04	0.56
1:A:440:ASN:HD22	1:A:444:LEU:HD23	1.66	0.56
1:A:59:ASN:ND2	1:A:62:TYR:CE1	2.72	0.56
1:A:190:PHE:CD1	1:B:200:VAL:CG1	2.89	0.56
1:B:476:THR:HG21	1:B:480:ARG:HH21	1.70	0.55
1:B:460:MET:HG2	1:B:590:TYR:HE1	1.71	0.55
1:A:66:GLU:HG2	1:A:70:ARG:HD3	1.88	0.54
1:A:31:ASP:OD1	1:A:35:ASN:HB2	2.07	0.54
1:A:547:LYS:H	1:A:547:LYS:HD2	1.73	0.54
1:A:98:GLY:N	1:A:129:HIS:CD2	2.77	0.54
1:B:103:HIS:C	1:B:105:LEU:H	2.10	0.54
1:B:1:MET:HG3	1:B:5:ASP:HB2	1.90	0.53
1:B:513:THR:HG23	1:B:526:LEU:HA	1.90	0.53
1:A:592:ASP:O	1:A:623:ARG:NH2	2.41	0.53
1:B:527:LEU:HD23	1:B:528:TYR:O	2.08	0.53
1:A:587:PHE:HB3	1:A:595:ILE:CD1	2.37	0.53
1:B:488:ILE:HG21	1:B:504:LEU:HG	1.90	0.53
1:A:144:GLU:OE2	1:B:151:LYS:CE	2.56	0.53
1:B:616:GLU:O	1:B:620:THR:HG23	2.09	0.53
1:B:599:ILE:HB	1:B:627:VAL:HG12	1.90	0.52
1:A:295:ASP:N	5:A:1107:HOH:O	2.38	0.52
1:B:142:SER:O	1:B:146:ILE:HG13	2.09	0.52
1:A:448:ARG:HG2	1:A:452:GLU:HG3	1.90	0.52
1:A:157:THR:O	1:A:158:LYS:C	2.47	0.52
1:A:476:THR:CG2	1:A:480:ARG:HE	2.23	0.52
1:A:356:GLU:O	1:A:359:GLN:HB2	2.09	0.52
1:B:490:PRO:HD2	3:B:1002:UDP:H5'1	1.90	0.51
1:A:126:ASN:HD22	1:A:128:LEU:N	1.95	0.51
1:A:128:LEU:HD21	1:A:158:LYS:HE2	1.92	0.51
1:A:407:TYR:CZ	1:A:506:PRO:HD3	2.45	0.51
1:A:320:ASN:HB2	1:A:321:PRO:CD	2.40	0.51
1:B:407:TYR:CZ	1:B:506:PRO:HD3	2.45	0.51
1:B:250:ASP:OD1	1:B:252:LYS:HB2	2.10	0.51
4:A:1004:DTP:O2B	4:A:1004:DTP:O1A	2.30	0.50
1:A:584:GLN:HB2	1:A:597:LYS:HG2	1.93	0.50
1:A:576:ASP:C	1:A:576:ASP:OD1	2.50	0.50
1:B:473:MET:CG	5:B:1141:HOH:O	2.50	0.50
1:A:239:ASN:H	1:A:239:ASN:ND2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:HD12	1:A:444:LEU:O	2.13	0.49
1:B:551:GLU:HG2	1:B:552:LYS:N	2.27	0.49
1:A:311:TYR:CD1	1:A:312:PRO:HA	2.46	0.49
1:B:257:LEU:HD22	1:B:262:GLY:HA3	1.93	0.49
1:A:623:ARG:HD2	5:A:1024:HOH:O	2.13	0.49
1:A:398:ASP:O	1:A:401:TYR:HB2	2.12	0.49
1:A:380:THR:O	1:A:384:LYS:HG3	2.13	0.49
1:A:320:ASN:ND2	1:A:325:ILE:H	2.11	0.49
1:B:375:PRO:O	1:B:376:ILE:HG13	2.13	0.49
1:B:122:TYR:O	1:B:125:ARG:HD3	2.13	0.49
1:A:56:GLU:HB2	1:A:71:ILE:HG12	1.95	0.49
1:B:31:ASP:C	1:B:31:ASP:OD1	2.52	0.48
1:B:171:ARG:HH21	1:B:270:ARG:HD2	1.77	0.48
1:A:320:ASN:HD21	1:A:325:ILE:H	1.62	0.48
1:A:11:ILE:HG12	1:A:83:LYS:HD3	1.95	0.48
1:A:409:SER:O	1:A:410:GLN:CB	2.62	0.47
1:B:457:PRO:CD	5:B:1141:HOH:O	2.42	0.47
1:B:441:PHE:O	1:B:442:PRO:C	2.52	0.47
1:A:126:ASN:ND2	1:A:126:ASN:C	2.67	0.47
1:B:311:TYR:CD1	1:B:312:PRO:HA	2.49	0.47
1:A:452:GLU:O	1:A:453:ASP:CB	2.53	0.47
1:B:91:SER:OG	3:B:1002:UDP:O1B	2.23	0.47
1:A:198:ILE:HG13	1:A:211:LEU:HD21	1.96	0.47
1:A:141:ASP:O	4:A:1004:DTP:H5'2	2.13	0.47
1:A:313:HIS:HB2	5:A:1099:HOH:O	2.15	0.47
1:B:327:LEU:HD22	1:B:331:GLU:HB3	1.97	0.47
1:A:455:PHE:HE2	5:A:1113:HOH:O	1.83	0.47
1:A:487:THR:HG23	5:A:1045:HOH:O	2.15	0.47
1:A:97:ALA:HA	1:A:131:LEU:HD21	1.96	0.47
1:B:563:GLU:H	1:B:566:LYS:HB2	1.79	0.46
1:B:91:SER:HB2	1:B:92:PRO:HD3	1.98	0.46
1:A:179:GLY:O	1:B:128:LEU:HD22	2.15	0.46
1:B:151:LYS:O	1:B:154:ALA:HB3	2.16	0.46
1:A:29:MET:N	1:A:38:GLU:OE1	2.45	0.46
1:A:474:LYS:C	1:A:476:THR:H	2.17	0.46
1:B:70:ARG:HD2	1:B:70:ARG:HA	1.67	0.46
1:A:62:TYR:HB3	1:A:67:LYS:HG2	1.97	0.46
1:A:167:PHE:CE2	1:A:191:MET:HG2	2.51	0.46
1:B:6:LEU:HD23	1:B:353:ALA:HB1	1.97	0.46
1:B:172:PRO:O	1:B:175:SER:HB2	2.16	0.46
1:A:11:ILE:HG23	1:A:12:ASP:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:GLU:HA	1:A:616:GLU:OE1	2.16	0.45
1:A:444:LEU:HD12	1:A:444:LEU:C	2.37	0.45
1:A:66:GLU:O	1:A:70:ARG:HB2	2.15	0.45
1:B:90:ASN:HB3	1:B:335:LEU:HB2	1.99	0.45
1:B:528:TYR:O	1:B:529:VAL:CG2	2.57	0.45
1:A:542:LEU:HD13	1:A:546:GLU:OE2	2.17	0.45
1:B:440:ASN:ND2	1:B:444:LEU:HD23	2.32	0.45
1:A:114:THR:O	1:A:117:ASP:HB2	2.17	0.45
1:A:493:SER:O	1:A:496:ASN:HB2	2.17	0.44
1:A:355:GLN:HG3	1:A:426:HIS:ND1	2.32	0.44
1:A:170:LEU:HD12	1:A:187:PRO:HA	1.98	0.44
1:B:539:PRO:O	1:B:540:GLU:HB2	2.17	0.44
1:A:486:LEU:O	1:A:593:ASN:ND2	2.48	0.44
1:A:375:PRO:HG2	1:A:376:ILE:HG13	1.99	0.44
1:A:177:VAL:HG12	1:A:179:GLY:HA3	2.00	0.43
1:B:177:VAL:C	1:B:179:GLY:N	2.71	0.43
1:B:469:ILE:O	1:B:473:MET:HG2	2.19	0.43
1:B:31:ASP:CG	1:B:35:ASN:HB2	2.38	0.43
1:B:325:ILE:HG22	1:B:327:LEU:HG	1.99	0.43
1:B:393:ILE:HD12	1:B:396:PHE:HB2	2.00	0.43
1:A:449:TYR:CD1	1:A:476:THR:HG21	2.54	0.43
1:A:449:TYR:CD1	1:A:476:THR:CG2	3.01	0.43
1:A:581:LEU:HD12	1:A:622:VAL:HG11	2.01	0.43
1:A:588:GLN:HG2	1:A:621:ASN:O	2.18	0.43
1:B:15:PRO:HB2	1:B:20:GLN:HG2	1.99	0.43
1:B:265:GLU:OE1	1:B:276:LYS:HG3	2.18	0.43
1:A:143:ILE:HG12	4:A:1004:DTP:H2'2	1.99	0.43
1:A:144:GLU:OE2	1:B:151:LYS:HE2	2.18	0.43
1:A:527:LEU:HD23	1:A:527:LEU:O	2.19	0.43
4:A:1004:DTP:O2B	4:A:1004:DTP:O2G	2.36	0.42
1:B:213:GLY:O	1:B:243:LEU:HA	2.19	0.42
1:B:285:LYS:O	1:B:286:ILE:C	2.56	0.42
1:A:237:VAL:HB	1:A:238:LEU:H	1.48	0.42
1:A:585:ASP:O	1:A:589:ARG:HG3	2.20	0.42
1:A:30:LYS:HA	1:A:35:ASN:O	2.19	0.42
1:B:218:ASN:H	1:B:218:ASN:HD22	1.67	0.42
1:A:523:LYS:HE3	1:A:523:LYS:HB3	1.86	0.42
1:B:251:LYS:HG3	5:B:1102:HOH:O	2.19	0.42
1:A:91:SER:HB2	1:A:92:PRO:HD3	2.02	0.42
1:B:306:LYS:HE3	5:B:1107:HOH:O	2.18	0.42
1:B:531:GLN:HG3	1:B:534:ARG:NH1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:PRO:O	1:B:565:ILE:HB	2.19	0.42
1:A:115:LEU:HD13	1:A:115:LEU:O	2.19	0.42
1:A:172:PRO:HG3	1:A:220:PRO:HD2	2.01	0.42
1:A:313:HIS:CE1	1:A:314:ARG:HH12	2.37	0.42
1:B:217:ILE:HD13	1:B:245:VAL:HG11	2.02	0.42
1:A:77:ILE:CG2	1:A:360:ILE:HD13	2.50	0.42
1:A:504:LEU:HD13	1:A:597:LYS:HD3	2.02	0.42
1:B:74:TRP:HA	1:B:77:ILE:HG22	2.02	0.42
1:A:476:THR:HG23	1:A:480:ARG:HE	1.85	0.41
1:A:355:GLN:O	1:A:356:GLU:C	2.56	0.41
1:A:84:ALA:O	1:A:85:ARG:HB2	2.20	0.41
1:A:320:ASN:H	1:A:320:ASN:ND2	2.16	0.41
1:A:167:PHE:CZ	1:A:191:MET:HG2	2.56	0.41
1:B:476:THR:HG21	1:B:480:ARG:HE	1.83	0.41
1:B:527:LEU:CD2	1:B:528:TYR:O	2.69	0.41
1:A:110:ILE:O	1:A:113:MET:HB2	2.20	0.41
1:B:72:LYS:O	1:B:110:ILE:HD11	2.21	0.41
1:A:59:ASN:HB3	1:A:62:TYR:HD1	1.85	0.41
1:B:563:GLU:N	1:B:566:LYS:HB2	2.36	0.40
1:B:16:SER:O	1:B:20:GLN:HG3	2.22	0.40
1:A:516:VAL:HG22	1:A:524:GLU:N	2.37	0.40
1:B:157:THR:O	1:B:203:GLN:HA	2.22	0.40
1:A:91:SER:O	1:A:92:PRO:C	2.56	0.40
1:B:26:ARG:HH11	1:B:26:ARG:HG3	1.87	0.40
1:B:237:VAL:HB	1:B:238:LEU:H	1.45	0.40
1:B:26:ARG:HG3	1:B:26:ARG:NH1	2.37	0.40
1:A:604:SER:HB3	5:A:1104:HOH:O	2.21	0.40
1:B:220:PRO:HA	1:B:266:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

## 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	
1	A	607/644 (94%)	528 (87%)	68 (11%)	11 (2%)	11	18
1	B	600/644 (93%)	558 (93%)	35 (6%)	7 (1%)	16	29
All	All	1207/1288 (94%)	1086 (90%)	103 (8%)	18 (2%)	13	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	410	GLN
1	A	453	ASP
1	A	472	VAL
1	B	529	VAL
1	B	104	ASP
1	B	228	ALA
1	A	180	THR
1	A	564	LYS
1	A	68	LEU
1	B	183	LYS
1	B	563	GLU
1	A	69	ASP
1	A	228	ALA
1	A	525	PRO
1	B	182	GLY
1	A	226	ILE
1	B	442	PRO

### 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	
1	A	543/566 (96%)	493 (91%)	50 (9%)	11	21
1	B	538/566 (95%)	499 (93%)	39 (7%)	18	33
All	All	1081/1132 (96%)	992 (92%)	89 (8%)	14	27

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	25	ASP
1	A	26	ARG
1	A	33	ASP
1	A	73	GLU
1	A	80	ARG
1	A	81	VAL
1	A	90	ASN
1	A	108	LYS
1	A	111	ASP
1	A	124	SER
1	A	126	ASN
1	A	142	SER
1	A	180	THR
1	A	181	HIS
1	A	202	LYS
1	A	237	VAL
1	A	239	ASN
1	A	249	MET
1	A	271	SER
1	A	284	ARG
1	A	314	ARG
1	A	320	ASN
1	A	345	ASN
1	A	349	VAL
1	A	385	GLU
1	A	391	LEU
1	A	419	LEU
1	A	429	ARG
1	A	434	LEU
1	A	442	PRO
1	A	444	LEU
1	A	452	GLU
1	A	458	PHE
1	A	464	ASN
1	A	468	GLU
1	A	469	ILE
1	A	471	GLU
1	A	472	VAL
1	A	476	THR
1	A	481	ARG
1	A	485	LEU
1	A	504	LEU

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Mol	Chain	Res	Type
1	A	542	LEU
1	A	543	LYS
1	A	547	LYS
1	A	551	GLU
1	A	578	MET
1	A	603	GLN
1	A	623	ARG
1	B	3	LEU
1	B	9	ARG
1	B	17	LYS
1	B	26	ARG
1	B	40	LYS
1	B	57	LEU
1	B	64	LYS
1	B	70	ARG
1	B	90	ASN
1	B	105	LEU
1	B	108	LYS
1	B	111	ASP
1	B	112	GLN
1	B	119	GLU
1	B	158	LYS
1	B	175	SER
1	B	180	THR
1	B	202	LYS
1	B	215	LEU
1	B	218	ASN
1	B	243	LEU
1	B	249	MET
1	B	257	LEU
1	B	284	ARG
1	B	289	ASN
1	B	345	ASN
1	B	450	ARG
1	B	458	PHE
1	B	464	ASN
1	B	476	THR
1	B	478	GLU
1	B	504	LEU
1	B	534	ARG
1	B	536	LYS
1	B	548	GLU

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Mol	Chain	Res	Type
1	B	550	ILE
1	B	561	VAL
1	B	563	GLU
1	B	596	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	126	ASN
1	A	239	ASN
1	A	320	ASN
1	A	345	ASN
1	A	355	GLN
1	A	359	GLN
1	A	464	ASN
1	A	496	ASN
1	A	531	GLN
1	B	203	GLN
1	B	218	ASN
1	B	239	ASN
1	B	345	ASN
1	B	359	GLN
1	B	426	HIS
1	B	464	ASN
1	B	496	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 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$
3	UDP	A	1001	-	18,26,26	2.44	5 (27%)	26,40,40	1.36	3 (11%)
4	DTP	A	1004	2	24,32,32	1.20	3 (12%)	32,50,50	2.23	5 (15%)
3	UDP	B	1002	-	18,26,26	2.83	4 (22%)	26,40,40	1.64	3 (11%)
4	DTP	B	1003	2	24,32,32	1.23	3 (12%)	32,50,50	2.25	6 (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
3	UDP	A	1001	-	-	0/12/32/32	0/2/2/2
4	DTP	A	1004	2	-	0/18/34/34	0/3/3/3
3	UDP	B	1002	-	-	0/12/32/32	0/2/2/2
4	DTP	B	1003	2	-	0/18/34/34	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	DTP	C5-N7	-2.29	1.31	1.39
4	A	1004	DTP	PG-O2G	-2.23	1.46	1.54
4	A	1004	DTP	C5-N7	-2.17	1.32	1.39
4	B	1003	DTP	PG-O2G	-2.12	1.47	1.54
4	A	1004	DTP	PA-O2A	-2.10	1.46	1.54
4	B	1003	DTP	PA-O2A	-2.03	1.46	1.54
3	A	1001	UDP	PB-O2B	2.83	1.64	1.54
3	A	1001	UDP	PB-O3B	3.30	1.66	1.54
3	A	1001	UDP	C6-N1	3.91	1.41	1.35
3	B	1002	UDP	C4-N3	4.80	1.42	1.33
3	B	1002	UDP	PB-O3B	5.03	1.72	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	UDP	C4-N3	5.03	1.42	1.33
3	B	1002	UDP	C6-N1	5.35	1.43	1.35
3	A	1001	UDP	O4'-C1'	6.42	1.49	1.41
3	B	1002	UDP	O4'-C1'	7.16	1.50	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	DTP	N3-C2-N1	-9.08	121.94	128.89
4	A	1004	DTP	N3-C2-N1	-8.91	122.07	128.89
4	B	1003	DTP	PA-O3A-PB	-5.30	117.86	132.73
4	A	1004	DTP	PA-O3A-PB	-4.21	120.91	132.73
4	B	1003	DTP	PB-O3B-PG	-4.05	119.08	132.67
3	B	1002	UDP	C4'-O4'-C1'	-3.94	105.39	109.72
4	A	1004	DTP	PB-O3B-PG	-3.90	119.59	132.67
4	A	1004	DTP	C2'-C1'-N9	-3.86	104.77	114.16
4	B	1003	DTP	C2'-C1'-N9	-2.64	107.73	114.16
3	B	1002	UDP	O4'-C4'-C5'	-2.54	100.23	109.32
3	A	1001	UDP	C4'-O4'-C1'	-2.28	107.21	109.72
4	B	1003	DTP	O4'-C1'-N9	-2.06	104.14	107.72
3	A	1001	UDP	O3B-PB-O2B	2.12	115.44	107.38
4	A	1004	DTP	O2G-PG-O1G	3.02	120.31	110.58
4	B	1003	DTP	O2G-PG-O1G	3.18	120.83	110.58
3	A	1001	UDP	C4-N3-C2	4.30	118.40	114.14
3	B	1002	UDP	C4-N3-C2	5.34	119.43	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DTP	5	0
3	B	1002	UDP	2	0
4	B	1003	DTP	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	615/644 (95%)	0.21	41 (6%) 21 23	31, 49, 76, 97	0
1	B	610/644 (94%)	0.11	24 (3%) 43 48	23, 42, 72, 86	0
All	All	1225/1288 (95%)	0.16	65 (5%) 30 34	23, 46, 75, 97	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	VAL	6.9
1	A	65	ASN	5.8
1	B	515	PHE	5.7
1	B	179	GLY	5.5
1	A	179	GLY	5.0
1	A	517	THR	5.0
1	A	515	PHE	4.8
1	B	527	LEU	4.6
1	A	526	LEU	4.2
1	B	514	ARG	4.1
1	A	182	GLY	4.0
1	A	34	GLY	4.0
1	A	32	LEU	3.9
1	A	523	LYS	3.9
1	A	525	PRO	3.8
1	B	178	ALA	3.7
1	A	527	LEU	3.6
1	A	524	GLU	3.5
1	A	63	LYS	3.4
1	A	62	TYR	3.2
1	B	540	GLU	3.1
1	A	273	ILE	3.1
1	A	312	PRO	3.0
1	A	68	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	245	VAL	2.9
1	A	33	ASP	2.9
1	A	150	VAL	2.9
1	B	528	TYR	2.8
1	A	69	ASP	2.8
1	A	184	ALA	2.8
1	A	246	GLY	2.6
1	B	45	ALA	2.6
1	A	560	ASP	2.6
1	A	364	PHE	2.6
1	B	245	VAL	2.6
1	A	176	PHE	2.5
1	B	183	LYS	2.5
1	A	183	LYS	2.5
1	B	531	GLN	2.4
1	A	633	LEU	2.4
1	A	311	TYR	2.4
1	B	36	TYR	2.4
1	B	21	ILE	2.4
1	B	484	ALA	2.4
1	A	178	ALA	2.4
1	B	297	GLY	2.3
1	A	181	HIS	2.3
1	A	365	LEU	2.3
1	A	9	ARG	2.3
1	B	513	THR	2.3
1	B	32	LEU	2.3
1	B	35	ASN	2.3
1	A	551	GLU	2.2
1	A	66	GLU	2.2
1	A	485	LEU	2.2
1	B	150	VAL	2.2
1	B	48	VAL	2.1
1	A	298	LEU	2.1
1	A	389	LEU	2.1
1	B	33	ASP	2.1
1	A	453	ASP	2.0
1	B	544	ARG	2.0
1	A	64	LYS	2.0
1	B	625	ILE	2.0
1	B	559	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UDP	A	1001	25/25	0.94	0.19	2.10	48,70,76,76	0
3	UDP	B	1002	25/25	0.96	0.20	1.98	31,52,58,59	0
4	DTP	B	1003	30/30	0.94	0.11	-0.97	40,48,66,68	0
4	DTP	A	1004	30/30	0.92	0.13	-1.08	48,56,58,58	0
2	MG	A	1006	1/1	0.86	0.10	-	58,58,58,58	0
2	MG	B	1005	1/1	0.96	0.10	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.