Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:05 AM GMT

PDB ID	:	3O0O
Title	:	Thermotoga maritima Ribonucleotide Reductase, NrdJ, in complex with dTTP, GDP and Adenosylcobalamin
Authors	:	Larsson, K.-M.; Logan, D.T.; Nordlund, P.
Deposited on	:	2010-07-19
Resolution	:	1.90 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 ①) were used in the production of this report:

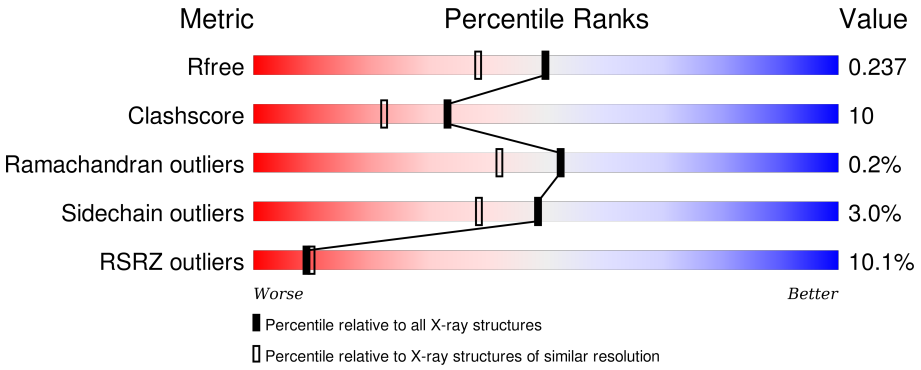
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	644	15%, 73%, 20%, 5%
1	B	644	5%, 82%, 13%

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
4	GDP	A	1003[A]	-	-	-	X
4	GDP	A	1003[B]	-	-	-	X
5	B12	A	1004	X	-	-	-
5	B12	B	1004	X	-	X	-
6	5AD	A	1005	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10787 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.

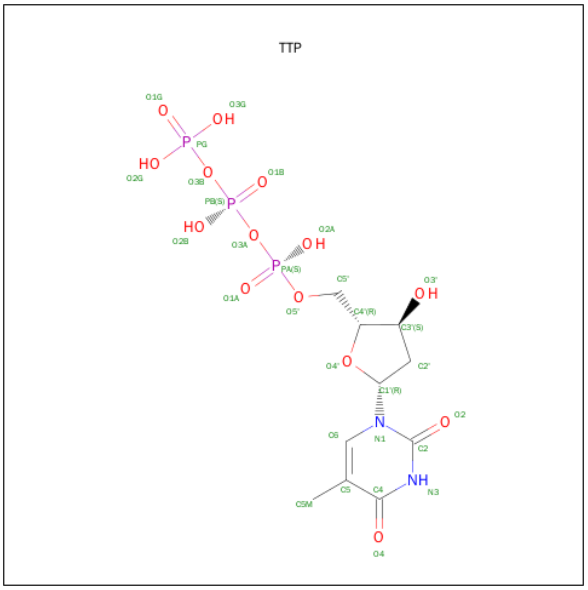
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	1	0
			4916	3152	840	904	20			
1	B	618	Total	C	N	O	S	0	8	0
			5018	3216	858	921	23			

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 THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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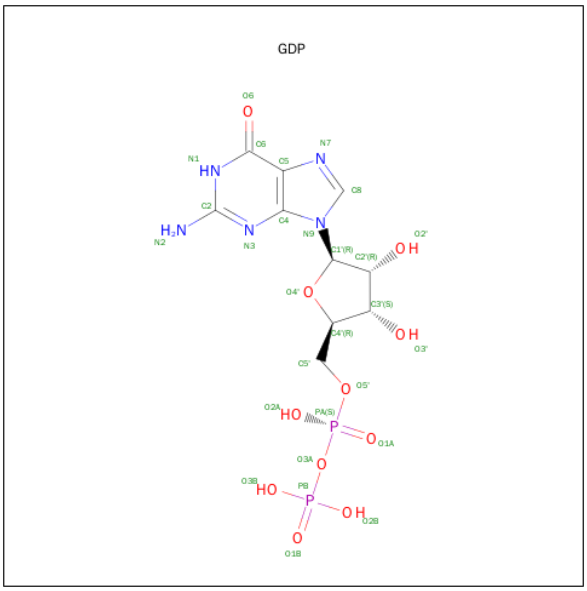
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

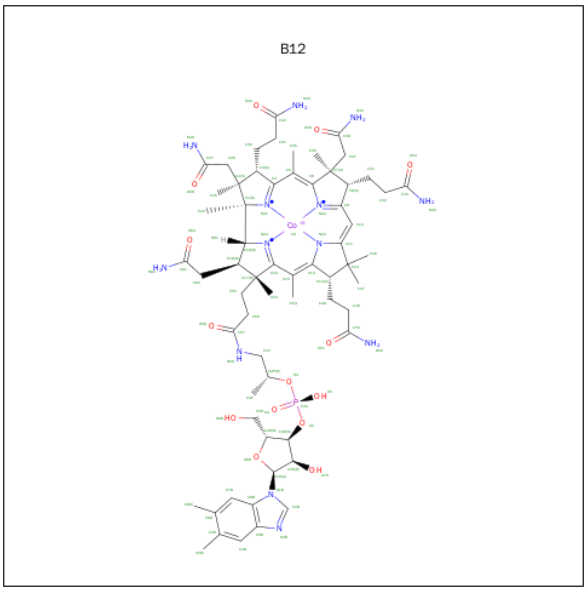
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



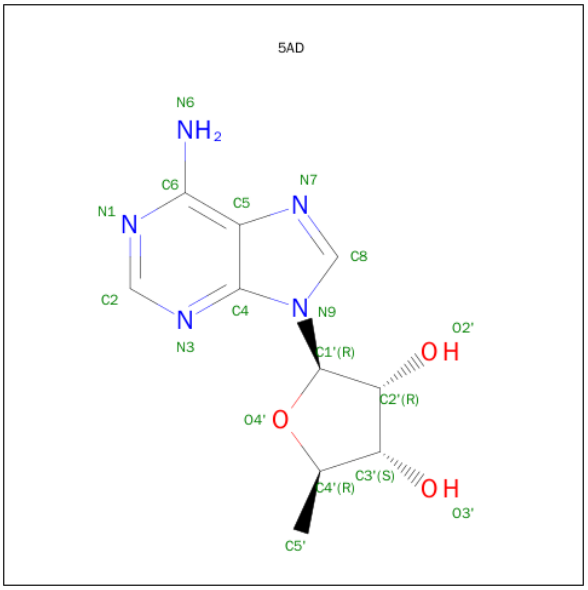
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			56	20	10	22	4		
4	B	1	Total	C	N	O	P	0	1
			56	20	10	22	4		

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
5	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 6 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	10	5	3		
6	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 7 is water.

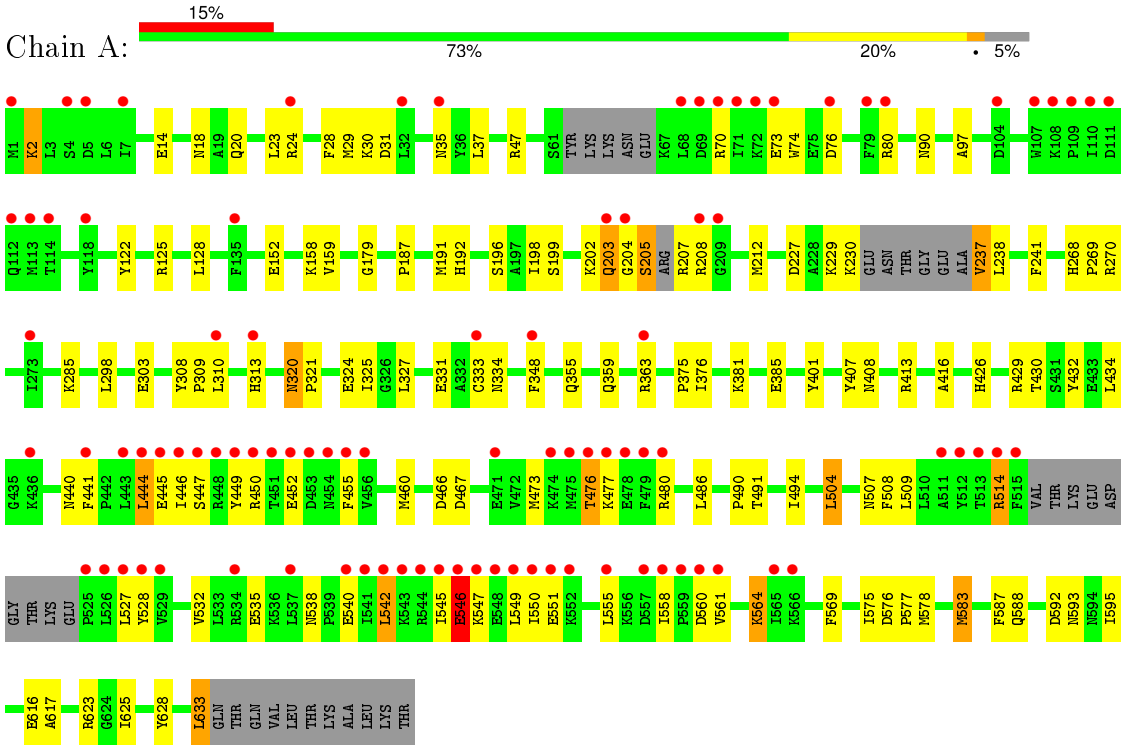
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	151	Total O 151 151	0	0
7	B	312	Total O 312 312	0	0

3 Residue-property plots (i)

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.

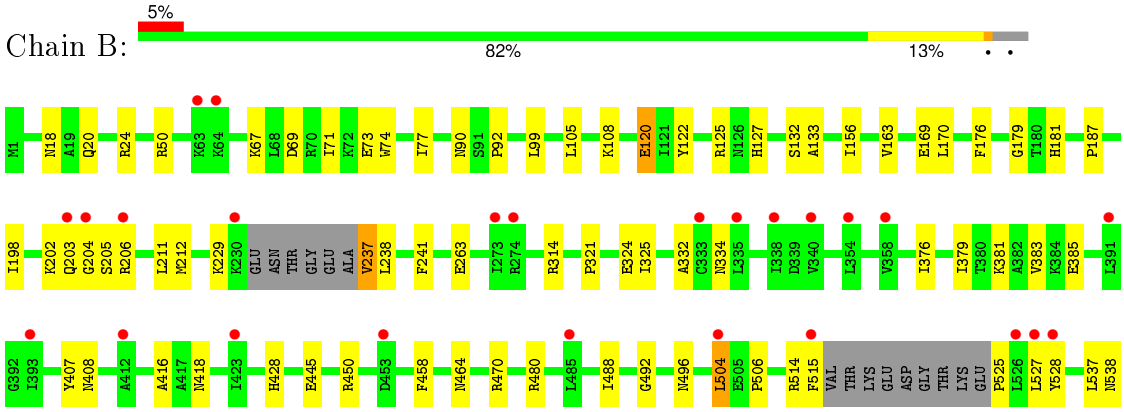
- Molecule 1: Ribonucleoside-diphosphate reductase

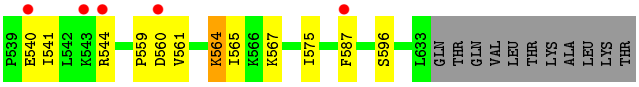
Chain A:



- Molecule 1: Ribonucleoside-diphosphate reductase

Chain B:




P539
E540
T541
L542
K543
R544
P559
D560
V561
K564
I565
K566
K567
I575
F587
S596
L633
GLN
THR
GLN
VAL
LEU
THR
LYS
ALA
LEU
LYS
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.02Å 124.23Å 107.17Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	46.94 – 1.90 48.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.94-1.90) 99.5 (48.10-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.202 , 0.238 0.202 , 0.237	Depositor DCC
R_{free} test set	5994 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 119789 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10787	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GDP, MG, TTP, B12, 5AD

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	0.33	0/5015	0.49	0/6766
1	B	0.43	0/5129	0.54	0/6918
All	All	0.39	0/10144	0.52	0/13684

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	241	PHE	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	4916	0	4979	112	0
1	B	5018	0	5091	67	0
2	A	29	0	13	1	0
2	B	29	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	56	0	24	3	0
4	B	56	0	24	6	0
5	A	91	0	86	14	0
5	B	91	0	86	21	0
6	A	18	0	13	1	0
6	B	18	0	13	3	0
7	A	151	0	0	4	0
7	B	312	0	0	4	0
All	All	10787	0	10342	212	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 10.

All (212) 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:617:ALA:CB	1:A:625:ILE:HD11	1.86	1.05
5:A:1004:B12:H262	5:A:1004:B12:H601	1.42	0.99
5:B:1004:B12:H351	5:B:1004:B12:H362	1.51	0.93
1:B:428:HIS:HD2	1:B:480:ARG:HH22	1.20	0.90
1:A:18:ASN:HD21	1:A:514[B]:ARG:HE	1.21	0.88
1:B:206:ARG:HD3	4:B:1003[B]:GDP:HN21	1.41	0.86
1:A:440:ASN:HB3	1:A:444:LEU:HD13	1.57	0.86
5:B:1004:B12:H531	5:B:1004:B12:H552	1.58	0.85
5:A:1004:B12:H362	5:A:1004:B12:H351	1.61	0.83
1:A:583:MET:HE3	1:A:583:MET:HA	1.60	0.82
1:B:203:GLN:H	1:B:204:GLY:HA2	1.45	0.82
1:A:204:GLY:O	1:A:205:SER:HB2	1.78	0.82
1:A:18:ASN:ND2	1:A:514[B]:ARG:HE	1.77	0.81
1:A:441:PHE:CE1	1:A:444:LEU:HD12	2.16	0.80
1:A:476:THR:CG2	1:A:480:ARG:HE	1.95	0.79
1:B:537:LEU:HD13	1:B:565:ILE:HD13	1.62	0.78
5:A:1004:B12:H531	5:A:1004:B12:H552	1.65	0.77
1:B:206:ARG:HD3	4:B:1003[B]:GDP:N2	1.99	0.77
1:A:363:ARG:HG2	1:A:434:LEU:HD11	1.66	0.77
1:A:617:ALA:HB3	1:A:625:ILE:HD11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TRP:CZ3	1:A:363:ARG:HD3	2.19	0.76
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.51	0.76
1:A:444:LEU:HD11	1:A:480:ARG:HB3	1.69	0.75
1:B:428:HIS:CD2	1:B:480:ARG:HH22	2.06	0.73
1:B:203:GLN:N	1:B:204:GLY:HA2	2.04	0.72
1:A:476:THR:HG23	1:A:480:ARG:HE	1.54	0.72
1:A:202:LYS:HD3	1:A:205:SER:HA	1.72	0.71
1:A:583:MET:HA	1:A:583:MET:CE	2.21	0.70
1:B:212:MET:HB2	1:B:321:PRO:HA	1.74	0.69
4:B:1003[A]:GDP:C8	5:B:1004:B12:N52	2.61	0.68
5:B:1004:B12:H533	5:B:1004:B12:H482	1.74	0.68
5:A:1004:B12:N23	6:A:1005:5AD:H5'1	2.10	0.67
1:A:545:ILE:HD11	1:A:561:VAL:HG22	1.78	0.66
1:A:202:LYS:HB3	1:A:207:ARG:HD3	1.76	0.66
1:A:564:LYS:H	1:A:564:LYS:HZ3	1.43	0.65
1:A:74:TRP:HZ3	1:A:363:ARG:HD3	1.59	0.64
1:A:324:GLU:HG2	1:A:325:ILE:HG12	1.79	0.64
1:A:237:VAL:HG23	1:A:238:LEU:H	1.60	0.64
1:A:320:ASN:HD21	1:A:325:ILE:H	1.45	0.64
1:A:532:VAL:O	1:A:535:GLU:HG2	1.98	0.63
1:B:381:LYS:O	1:B:385:GLU:HG3	1.99	0.63
1:A:628:TYR:HE1	1:A:633:LEU:HD22	1.63	0.63
1:A:70:ARG:O	1:A:74:TRP:HD1	1.82	0.62
1:A:212:MET:HB2	1:A:321:PRO:HA	1.82	0.62
1:A:320:ASN:H	1:A:320:ASN:HD22	1.48	0.61
1:A:413:ARG:HA	1:A:583:MET:HE1	1.82	0.61
5:B:1004:B12:O28	5:B:1004:B12:H3	2.00	0.61
1:B:105:LEU:CD1	1:B:120:GLU:HG2	2.31	0.61
1:B:464:ASN:HB2	7:B:860:HOH:O	2.02	0.59
1:B:332[A]:ALA:HB3	1:B:383:VAL:CG2	2.32	0.59
1:A:159:VAL:HG21	1:A:375:PRO:HG3	1.84	0.59
1:A:617:ALA:HB1	1:A:625:ILE:HD11	1.82	0.59
1:B:206:ARG:HB3	4:B:1003[B]:GDP:N1	2.18	0.58
1:A:413:ARG:HG2	1:A:583:MET:HE3	1.85	0.58
1:B:202[B]:LYS:HB3	1:B:204:GLY:HA3	1.85	0.58
1:B:314:ARG:HH11	1:B:314:ARG:HG3	1.67	0.58
1:B:428:HIS:HD2	1:B:480:ARG:NH2	1.95	0.58
1:B:156:ILE:HG21	1:B:163:VAL:HG22	1.85	0.58
5:A:1004:B12:N52	5:A:1004:B12:H13	2.19	0.58
5:B:1004:B12:H262	5:B:1004:B12:H601	1.86	0.57
1:B:203:GLN:N	1:B:204:GLY:CA	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202[A]:LYS:HB3	1:B:204:GLY:HA3	1.85	0.57
1:A:426:HIS:O	1:A:430:THR:HG22	2.04	0.57
1:A:208:ARG:HG3	1:A:208:ARG:NH1	2.19	0.57
1:A:196:SER:O	1:A:199:SER:HB3	2.04	0.57
5:A:1004:B12:H552	5:A:1004:B12:C53	2.34	0.56
1:A:452:GLU:OE1	1:A:455:PHE:HB2	2.06	0.56
5:B:1004:B12:H301	5:B:1004:B12:H203	1.88	0.56
5:A:1004:B12:H521	5:A:1004:B12:H13	1.69	0.56
1:B:537:LEU:HD13	1:B:565:ILE:CD1	2.35	0.55
1:B:564:LYS:H	1:B:564:LYS:HE2	1.69	0.55
1:A:320:ASN:ND2	1:A:325:ILE:H	2.04	0.55
1:B:538:ASN:OD1	1:B:540:GLU:HG2	2.06	0.55
1:A:473:MET:O	1:A:476:THR:HB	2.06	0.55
1:A:298:LEU:HD12	1:A:625:ILE:HD12	1.89	0.54
1:A:564:LYS:HB3	1:A:564:LYS:HZ2	1.73	0.54
1:A:31:ASP:OD2	1:A:35:ASN:HB2	2.09	0.53
1:B:564:LYS:N	1:B:564:LYS:HE2	2.23	0.53
1:A:14:GLU:HB2	7:A:757:HOH:O	2.07	0.53
1:A:460:MET:HB3	1:A:466:ASP:OD1	2.10	0.52
1:A:18:ASN:HD21	1:A:514[B]:ARG:NE	1.99	0.52
1:A:490:PRO:HD2	4:A:1003[B]:GDP:PB	2.50	0.52
1:A:47:ARG:HD2	1:A:97:ALA:O	2.09	0.52
1:B:428:HIS:CD2	1:B:480:ARG:HH12	2.28	0.52
1:A:74:TRP:HH2	1:A:363:ARG:HE	1.57	0.52
1:A:538:ASN:OD1	1:A:540:GLU:HB3	2.10	0.52
1:B:561:VAL:HG13	1:B:565:ILE:HD11	1.92	0.51
1:B:332[A]:ALA:HB3	1:B:383:VAL:HG21	1.92	0.51
1:B:407:TYR:CZ	1:B:506:PRO:HD3	2.46	0.51
1:B:206:ARG:CD	4:B:1003[B]:GDP:HN21	2.18	0.51
1:A:588:GLN:HB2	1:A:595:ILE:HD12	1.93	0.51
5:B:1004:B12:H353	5:B:1004:B12:H302	1.92	0.51
1:A:527:LEU:HG	1:A:528:TYR:N	2.26	0.51
1:B:69:ASP:O	1:B:73:GLU:HG3	2.10	0.51
1:A:547:LYS:O	1:A:550:ILE:HG22	2.10	0.51
5:A:1004:B12:H203	5:A:1004:B12:H301	1.93	0.51
1:A:320:ASN:HB2	1:A:321:PRO:HD2	1.91	0.51
1:A:592:ASP:O	1:A:623:ARG:NH2	2.45	0.50
1:A:20:GLN:HB3	1:A:24:ARG:NH2	2.25	0.50
1:B:470:ARG:HD3	7:B:831:HOH:O	2.11	0.50
5:B:1004:B12:H372	7:B:812:HOH:O	2.10	0.50
1:A:407:TYR:CD1	1:A:575:ILE:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:HG2	1:A:623:ARG:HG3	1.93	0.50
1:B:324:GLU:HG2	1:B:325:ILE:HG12	1.93	0.50
1:A:355:GLN:HE21	1:A:359:GLN:NE2	2.10	0.50
1:B:105:LEU:HD11	1:B:120:GLU:HG2	1.93	0.50
1:B:527:LEU:O	1:B:527:LEU:HD12	2.11	0.50
5:A:1004:B12:H262	5:A:1004:B12:C60	2.29	0.50
1:A:486:LEU:O	1:A:593:ASN:HB2	2.12	0.50
1:A:202:LYS:HE3	1:A:207:ARG:CZ	2.43	0.49
1:A:490:PRO:HB2	4:A:1003[B]:GDP:O2B	2.13	0.49
1:B:198:ILE:HG13	1:B:211:LEU:HD11	1.94	0.49
5:B:1004:B12:C55	5:B:1004:B12:H531	2.30	0.49
5:A:1004:B12:H353	5:A:1004:B12:H302	1.94	0.49
1:B:18:ASN:CG	1:B:528:TYR:OH	2.51	0.49
1:B:408:ASN:HB3	1:B:575:ILE:HG23	1.94	0.48
1:A:30:LYS:HE3	7:A:712:HOH:O	2.13	0.48
5:B:1004:B12:H351	5:B:1004:B12:C36	2.29	0.48
1:A:381:LYS:HE2	1:A:385:GLU:OE2	2.13	0.48
1:A:449:TYR:CD1	1:A:476:THR:HG21	2.49	0.48
1:A:617:ALA:HB2	1:A:625:ILE:HD11	1.89	0.48
1:A:308:TYR:HD1	1:A:309:PRO:HD2	1.77	0.48
1:B:416:ALA:HB1	1:B:587:PHE:CE2	2.48	0.48
1:A:491:THR:HG22	1:A:494:ILE:HD11	1.96	0.48
1:A:128:LEU:HD11	1:B:179:GLY:HA2	1.95	0.48
1:A:29:MET:HG2	1:A:37:LEU:HD12	1.96	0.47
1:A:558:ILE:O	1:A:561:VAL:HG23	2.13	0.47
5:A:1004:B12:H533	5:A:1004:B12:H482	1.96	0.47
1:A:268:HIS:CG	1:A:269:PRO:HD2	2.50	0.47
1:A:204:GLY:O	1:A:205:SER:CB	2.58	0.47
1:A:623:ARG:HD2	7:A:664:HOH:O	2.15	0.47
1:A:564:LYS:HB3	1:A:564:LYS:NZ	2.30	0.47
1:B:176:PHE:CE2	1:B:181:HIS:HA	2.50	0.47
1:A:359:GLN:O	1:A:363:ARG:HG3	2.15	0.46
1:A:327:LEU:HD22	1:A:331:GLU:HB3	1.96	0.46
1:B:314:ARG:NH1	1:B:314:ARG:HG3	2.30	0.46
1:A:429:ARG:O	1:A:432:TYR:HB3	2.14	0.46
1:A:549:LEU:HD13	1:A:555:LEU:HD23	1.97	0.46
1:A:545:ILE:HG22	1:A:546:GLU:N	2.30	0.46
1:B:202[B]:LYS:HE3	1:B:205:SER:HB3	1.97	0.46
5:B:1004:B12:H4B	5:B:1004:B12:C6	2.45	0.46
1:A:227:ASP:O	1:A:230:LYS:HG2	2.16	0.46
1:B:515:PHE:HD2	1:B:525:PRO:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:HG2	1:A:450:ARG:HH21	1.80	0.45
1:A:576:ASP:HB2	1:A:577:PRO:HD2	1.98	0.45
1:A:450:ARG:NH1	1:A:477:LYS:O	2.49	0.45
1:B:376:ILE:HB	1:B:379:ILE:HD12	1.98	0.45
1:B:170:LEU:HD12	1:B:187:PRO:HA	1.98	0.45
1:A:504:LEU:HD12	1:A:587:PHE:CD2	2.51	0.45
1:B:18:ASN:ND2	1:B:528:TYR:OH	2.49	0.45
1:B:514:ARG:O	1:B:525:PRO:HA	2.17	0.45
5:B:1004:B12:C53	5:B:1004:B12:H482	2.46	0.45
1:A:401:TYR:CE1	1:A:569:PHE:HA	2.51	0.45
5:A:1004:B12:O28	5:A:1004:B12:H3	2.15	0.45
1:B:50:ARG:NH2	1:B:108:LYS:O	2.43	0.45
1:A:158:LYS:O	1:A:203:GLN:HG2	2.16	0.45
5:A:1004:B12:C6	5:A:1004:B12:H4B	2.47	0.45
1:A:549:LEU:HD13	1:A:555:LEU:CD2	2.47	0.45
1:A:348:PHE:HA	7:A:714:HOH:O	2.17	0.44
1:A:179:GLY:HA3	2:A:1001:TTP:O1B	2.18	0.44
4:B:1003[B]:GDP:C2	5:B:1004:B12:C5R	3.00	0.44
1:B:541:ILE:O	1:B:544:ARG:HB3	2.18	0.44
5:B:1004:B12:C25	5:B:1004:B12:H312	2.48	0.44
1:B:492:GLY:O	5:B:1004:B12:H1P2	2.18	0.44
1:B:237:VAL:HB	1:B:238:LEU:H	1.46	0.44
1:B:132:SER:OG	1:B:334[B]:ASN:ND2	2.51	0.43
1:B:99:LEU:HD23	1:B:99:LEU:HA	1.89	0.43
5:B:1004:B12:H361	5:B:1004:B12:O39	2.17	0.43
1:B:229:LYS:HD3	1:B:238:LEU:HB2	2.00	0.43
1:B:92:PRO:HG2	1:B:133:ALA:HA	2.00	0.43
1:B:559:PRO:O	1:B:560:ASP:HB2	2.18	0.43
1:A:408:ASN:HB3	1:A:575:ILE:HG23	2.00	0.43
1:A:320:ASN:HB2	1:A:321:PRO:CD	2.49	0.43
1:A:578:MET:SD	1:A:616:GLU:HG2	2.59	0.43
1:A:476:THR:HG21	1:A:480:ARG:HE	1.76	0.42
1:A:192:HIS:CD2	1:A:238:LEU:HD21	2.54	0.42
1:A:313:HIS:ND1	1:A:446:ILE:HD11	2.34	0.42
1:B:122:TYR:O	1:B:125:ARG:HD3	2.18	0.42
1:A:187:PRO:O	1:A:191:MET:HG3	2.19	0.42
1:A:401:TYR:CE2	1:A:507:ASN:ND2	2.88	0.42
1:A:508:PHE:O	1:A:509:LEU:HD23	2.20	0.42
1:A:122:TYR:O	1:A:125:ARG:HD3	2.19	0.42
1:A:310:LEU:HD23	1:A:447:SER:HA	2.02	0.42
1:A:542:LEU:O	1:A:542:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202[A]:LYS:HG2	1:B:205:SER:CB	2.50	0.42
1:A:545:ILE:O	1:A:546:GLU:C	2.59	0.42
1:A:446:ILE:O	1:A:446:ILE:HG12	2.20	0.41
1:B:169:GLU:HB2	7:B:662:HOH:O	2.20	0.41
5:B:1004:B12:N23	6:B:1005:5AD:H5'1	2.34	0.41
1:B:514:ARG:HA	1:B:514:ARG:HD2	1.76	0.41
1:B:20:GLN:O	1:B:24:ARG:HG3	2.21	0.41
5:B:1004:B12:C5	5:B:1004:B12:H4B	2.50	0.41
1:B:74:TRP:HA	1:B:77:ILE:HG22	2.02	0.41
1:A:23:LEU:HB3	1:A:28:PHE:CE1	2.55	0.41
5:B:1004:B12:N24	6:B:1005:5AD:H5'1	2.36	0.41
1:B:488:ILE:HG21	1:B:504:LEU:HG	2.02	0.41
1:B:67:LYS:O	1:B:71:ILE:HG13	2.20	0.41
1:A:416:ALA:HB3	1:A:583:MET:HE1	2.02	0.41
1:B:332[A]:ALA:HB3	1:B:383:VAL:HG22	2.03	0.41
5:B:1004:B12:N40	6:B:1005:5AD:N7	2.68	0.41
1:A:363:ARG:CG	1:A:434:LEU:HD11	2.45	0.41
1:A:208:ARG:HB2	4:A:1003[B]:GDP:O6	2.21	0.41
1:B:567:LYS:HD3	1:B:567:LYS:HA	1.87	0.41
1:B:18:ASN:HD21	1:B:496:ASN:HD22	1.70	0.40
1:A:76:ASP:O	1:A:80:ARG:HG3	2.21	0.40
1:A:152:GLU:HG2	1:A:376:ILE:HD13	2.03	0.40
1:A:70:ARG:HA	1:A:70:ARG:NE	2.36	0.40
1:A:229:LYS:NZ	1:A:241:PHE:O	2.53	0.40
5:A:1004:B12:C5	5:A:1004:B12:H4B	2.51	0.40
1:A:70:ARG:O	1:A:73:GLU:HB3	2.21	0.40
1:B:127:HIS:H	1:B:127:HIS:CD2	2.40	0.40
1:A:334:ASN:N	1:A:334:ASN:OD1	2.51	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	603/644 (94%)	578 (96%)	23 (4%)	2 (0%)	46 35
1	B	620/644 (96%)	600 (97%)	20 (3%)	0	100 100
All	All	1223/1288 (95%)	1178 (96%)	43 (4%)	2 (0%)	52 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	GLU
1	A	2	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
1	A	539/566 (95%)	516 (96%)	23 (4%)	35 23
1	B	551/566 (97%)	540 (98%)	11 (2%)	63 57
All	All	1090/1132 (96%)	1056 (97%)	34 (3%)	48 37

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	90	ASN
1	A	198	ILE
1	A	203	GLN
1	A	205	SER
1	A	237	VAL
1	A	270	ARG
1	A	285	LYS
1	A	320	ASN
1	A	333	CYS
1	A	444	LEU
1	A	467	ASP
1	A	476	THR
1	A	504	LEU

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Mol	Chain	Res	Type
1	A	514[A]	ARG
1	A	514[B]	ARG
1	A	542	LEU
1	A	546	GLU
1	A	551	GLU
1	A	560	ASP
1	A	564	LYS
1	A	583	MET
1	A	633	LEU
1	B	90	ASN
1	B	120	GLU
1	B	237	VAL
1	B	263	GLU
1	B	418	ASN
1	B	445	GLU
1	B	450	ARG
1	B	458	PHE
1	B	504	LEU
1	B	564	LYS
1	B	596	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	192	HIS
1	A	320	ASN
1	A	346	ASN
1	A	359	GLN
1	A	600	ASN
1	A	603	GLN
1	A	612	ASN
1	B	18	ASN
1	B	65	ASN
1	B	127	HIS
1	B	192	HIS
1	B	289	ASN
1	B	359	GLN
1	B	418	ASN
1	B	428	HIS
1	B	584	GLN

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
2	TTP	A	1001	3	21,30,30	0.61	0	31,47,47	1.93	8 (25%)
4	GDP	A	1003[A]	-	23,30,30	1.19	2 (8%)	30,47,47	1.69	6 (20%)
4	GDP	A	1003[B]	-	23,30,30	1.17	2 (8%)	30,47,47	1.86	7 (23%)
5	B12	A	1004	-	74,101,101	1.01	4 (5%)	111,166,166	1.45	12 (10%)
6	5AD	A	1005	-	15,20,20	1.84	4 (26%)	14,30,30	4.51	4 (28%)
2	TTP	B	1001	3	21,30,30	0.48	0	31,47,47	1.99	6 (19%)
4	GDP	B	1003[A]	-	23,30,30	1.17	2 (8%)	30,47,47	2.04	6 (20%)
4	GDP	B	1003[B]	-	23,30,30	1.21	2 (8%)	30,47,47	2.05	9 (30%)
5	B12	B	1004	6	74,101,101	1.02	4 (5%)	111,166,166	1.54	17 (15%)
6	5AD	B	1005	5	15,20,20	1.86	4 (26%)	14,30,30	4.68	5 (35%)

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
2	TTP	A	1001	3	-	0/18/34/34	0/2/2/2
4	GDP	A	1003[A]	-	-	0/12/32/32	0/3/3/3
4	GDP	A	1003[B]	-	-	0/12/32/32	0/3/3/3
5	B12	A	1004	-	1/1/36/38	0/51/223/223	0/3/11/11
6	5AD	A	1005	-	-	0/0/20/20	0/3/3/3
2	TTP	B	1001	3	-	0/18/34/34	0/2/2/2
4	GDP	B	1003[A]	-	-	0/12/32/32	0/3/3/3
4	GDP	B	1003[B]	-	-	0/12/32/32	0/3/3/3
5	B12	B	1004	6	1/1/36/38	0/51/223/223	0/3/11/11
6	5AD	B	1005	5	-	0/0/20/20	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	B12	C5M-C5B	-3.54	1.43	1.51
5	A	1004	B12	C5M-C5B	-3.47	1.44	1.51
6	A	1005	5AD	C5-C4	-2.89	1.34	1.40
6	B	1005	5AD	C5-C4	-2.64	1.34	1.40
6	A	1005	5AD	O4'-C1'	2.38	1.44	1.41
5	A	1004	B12	C53-C15	2.60	1.58	1.51
6	B	1005	5AD	O4'-C1'	2.72	1.44	1.41
5	B	1004	B12	C53-C15	2.78	1.58	1.51
5	A	1004	B12	C6B-C5B	2.98	1.49	1.41
4	B	1003[B]	GDP	C5-C4	3.11	1.47	1.40
5	B	1004	B12	C6B-C5B	3.12	1.49	1.41
4	B	1003[A]	GDP	C6-C5	3.13	1.47	1.41
4	A	1003[A]	GDP	C5-C4	3.13	1.47	1.40
4	A	1003[B]	GDP	C5-C4	3.16	1.47	1.40
4	B	1003[A]	GDP	C5-C4	3.16	1.47	1.40
6	B	1005	5AD	C2-N1	3.26	1.40	1.33
6	A	1005	5AD	C2-N1	3.28	1.40	1.33
4	A	1003[B]	GDP	C6-C5	3.46	1.48	1.41
4	B	1003[B]	GDP	C6-C5	3.56	1.48	1.41
4	A	1003[A]	GDP	C6-C5	3.62	1.48	1.41
5	B	1004	B12	C48-C13	4.36	1.61	1.54
6	B	1005	5AD	C2-N3	4.46	1.40	1.32
5	A	1004	B12	C48-C13	4.50	1.61	1.54
6	A	1005	5AD	C2-N3	4.50	1.40	1.32

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1005	5AD	N3-C2-N1	-14.19	118.03	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1005	5AD	N3-C2-N1	-14.16	118.05	128.89
6	B	1005	5AD	C5'-C4'-C3'	-9.01	106.39	115.80
6	A	1005	5AD	C5'-C4'-C3'	-6.97	108.52	115.80
4	B	1003[A]	GDP	C2'-C1'-N9	-5.82	105.39	114.29
4	B	1003[B]	GDP	C2'-C1'-N9	-5.26	106.25	114.29
2	B	1001	TTP	C5-C4-N3	-5.08	119.48	125.14
2	A	1001	TTP	C5-C4-N3	-4.97	119.60	125.14
4	A	1003[B]	GDP	C2'-C1'-N9	-4.62	107.23	114.29
4	B	1003[B]	GDP	C5-C6-N1	-4.34	117.66	123.59
6	A	1005	5AD	C4'-O4'-C1'	-4.15	105.16	109.72
4	A	1003[A]	GDP	C5-C6-N1	-3.96	118.17	123.59
4	A	1003[B]	GDP	C5-C6-N1	-3.94	118.20	123.59
5	B	1004	B12	C20-C1-C19	-3.92	105.54	109.38
4	B	1003[B]	GDP	C6-C5-C4	-3.87	116.27	120.90
4	B	1003[A]	GDP	C5-C6-N1	-3.76	118.45	123.59
2	A	1001	TTP	PB-O3B-PG	-3.64	120.47	132.67
2	B	1001	TTP	PB-O3A-PA	-3.55	122.76	132.73
4	A	1003[A]	GDP	C2'-C1'-N9	-3.39	109.11	114.29
2	B	1001	TTP	PB-O3B-PG	-3.28	121.69	132.67
4	B	1003[A]	GDP	N3-C2-N1	-3.27	122.46	127.44
6	A	1005	5AD	C2'-C1'-N9	-3.23	109.36	114.29
4	A	1003[B]	GDP	C6-C5-C4	-3.15	117.13	120.90
4	A	1003[B]	GDP	PA-O3A-PB	-3.15	122.10	132.67
4	B	1003[B]	GDP	N3-C2-N1	-3.08	122.75	127.44
4	B	1003[A]	GDP	O2'-C2'-C3'	-3.04	101.95	111.83
4	A	1003[B]	GDP	N3-C2-N1	-3.00	122.87	127.44
4	A	1003[A]	GDP	N3-C2-N1	-3.00	122.88	127.44
4	A	1003[A]	GDP	C6-C5-C4	-2.79	117.56	120.90
6	B	1005	5AD	C4'-O4'-C1'	-2.75	106.69	109.72
6	B	1005	5AD	C2'-C1'-N9	-2.72	110.13	114.29
4	B	1003[B]	GDP	C4-C5-N7	-2.63	107.06	109.48
5	B	1004	B12	C18-C60-C61	-2.62	107.44	113.92
5	B	1004	B12	C3-C4-C5	-2.61	123.06	131.88
4	A	1003[A]	GDP	C4-C5-N7	-2.59	107.10	109.48
4	B	1003[A]	GDP	C6-C5-C4	-2.52	117.89	120.90
4	A	1003[B]	GDP	C4-C5-N7	-2.45	107.22	109.48
5	B	1004	B12	C4R-O6R-C1R	-2.40	107.08	109.72
5	A	1004	B12	C13-C14-C15	-2.36	123.90	131.88
5	A	1004	B12	C9-C10-C11	-2.34	126.41	132.28
5	A	1004	B12	C3-C4-C5	-2.33	124.02	131.88
2	A	1001	TTP	O3A-PA-O5'	-2.31	96.81	102.94
2	B	1001	TTP	C2'-C1'-N1	-2.30	108.57	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1004	B12	C13-C14-C15	-2.25	124.29	131.88
5	B	1004	B12	C9-C10-C11	-2.18	126.82	132.28
2	A	1001	TTP	PB-O3A-PA	-2.17	126.63	132.73
4	B	1003[B]	GDP	O3A-PA-O5'	-2.15	97.22	102.94
4	B	1003[B]	GDP	C1'-N9-C4	-2.11	123.76	126.94
6	B	1005	5AD	C4-C5-N7	-2.03	107.62	109.48
5	B	1004	B12	C18-C17-C16	2.02	103.27	100.54
2	A	1001	TTP	O2A-PA-O3A	2.10	114.64	105.09
5	A	1004	B12	C35-C5-C6	2.16	122.11	118.25
5	A	1004	B12	O6R-C4R-C3R	2.20	109.92	104.86
5	A	1004	B12	C7B-C8B-C9B	2.20	122.72	120.54
5	B	1004	B12	C7B-C8B-C9B	2.29	122.81	120.54
5	A	1004	B12	O2-P-O3	2.31	102.26	100.07
2	A	1001	TTP	O2B-PB-O3A	2.32	115.64	105.09
5	B	1004	B12	C26-C2-C1	2.37	113.77	110.00
2	A	1001	TTP	O4'-C1'-N1	2.39	111.86	107.72
5	A	1004	B12	C18-C17-C16	2.53	103.97	100.54
4	B	1003[B]	GDP	O3B-PB-O3A	2.54	116.61	105.09
5	B	1004	B12	C35-C5-C6	2.56	122.84	118.25
5	B	1004	B12	O6R-C4R-C3R	2.57	110.79	104.86
5	B	1004	B12	C53-C15-C14	2.63	122.96	118.25
2	B	1001	TTP	O2B-PB-O3A	2.66	117.16	105.09
5	B	1004	B12	O2-P-O3	2.69	102.63	100.07
5	B	1004	B12	C48-C13-C12	2.81	124.23	116.53
5	B	1004	B12	O6R-C4R-C5R	3.18	116.07	109.17
5	A	1004	B12	O6R-C4R-C5R	3.33	116.39	109.17
5	A	1004	B12	C48-C13-C12	3.54	126.22	116.53
4	B	1003[A]	GDP	C6-N1-C2	4.40	122.04	115.94
4	A	1003[A]	GDP	C6-N1-C2	4.47	122.14	115.94
4	A	1003[B]	GDP	C6-N1-C2	4.51	122.20	115.94
4	B	1003[B]	GDP	C6-N1-C2	5.01	122.89	115.94
2	A	1001	TTP	C4-N3-C2	5.88	120.33	115.25
2	B	1001	TTP	C4-N3-C2	6.78	121.11	115.25
5	A	1004	B12	C1-C19-N24	6.96	114.65	106.20
5	B	1004	B12	C1-C19-C18	7.17	134.44	121.85
5	B	1004	B12	C1-C19-N24	7.48	115.27	106.20
5	A	1004	B12	C1-C19-C18	7.82	135.58	121.85

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1004	B12	C19

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Mol	Chain	Res	Type	Atom
5	B	1004	B12	C19

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	TTP	1	0
4	A	1003[B]	GDP	3	0
5	A	1004	B12	14	0
6	A	1005	5AD	1	0
4	B	1003[A]	GDP	1	0
4	B	1003[B]	GDP	5	0
5	B	1004	B12	21	0
6	B	1005	5AD	3	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, 95^{th} 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	A	612/644 (95%)	0.79	94 (15%) 3 3	34, 68, 122, 153	0
1	B	618/644 (95%)	0.13	30 (4%) 33 36	24, 41, 82, 110	0
All	All	1230/1288 (95%)	0.46	124 (10%) 9 10	24, 53, 113, 153	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	PHE	12.0
1	A	526	LEU	8.1
1	B	526	LEU	7.6
1	A	558	ILE	6.8
1	A	559	PRO	6.7
1	A	476	THR	5.9
1	A	561	VAL	5.7
1	A	479	PHE	5.7
1	A	71	ILE	5.2
1	A	111	ASP	5.1
1	A	560	ASP	5.1
1	A	525	PRO	5.1
1	A	550	ILE	5.0
1	A	118	TYR	5.0
1	A	549	LEU	5.0
1	A	110	ILE	4.9
1	A	68	LEU	4.9
1	A	551	GLU	4.9
1	A	513	THR	4.9
1	A	32	LEU	4.7
1	A	449	TYR	4.6
1	A	545	ILE	4.6
1	A	313	HIS	4.6
1	A	446	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	471	GLU	4.5
1	A	107	TRP	4.4
1	A	527	LEU	4.4
1	A	548	GLU	4.3
1	A	555	LEU	4.3
1	A	474	LYS	4.2
1	B	204	GLY	4.1
1	A	544	ARG	4.1
1	A	204	GLY	4.1
1	A	540	GLU	4.1
1	A	80	ARG	4.0
1	A	70	ARG	3.9
1	A	537	LEU	3.9
1	A	543	LYS	3.9
1	A	478	GLU	3.9
1	A	208	ARG	3.8
1	A	444	LEU	3.8
1	A	113	MET	3.7
1	A	566	LYS	3.6
1	A	547	LYS	3.6
1	A	363	ARG	3.6
1	A	565	ILE	3.6
1	A	109	PRO	3.5
1	A	76	ASP	3.5
1	B	64	LYS	3.4
1	A	455	PHE	3.4
1	A	451	THR	3.4
1	A	441	PHE	3.3
1	A	541	ILE	3.3
1	B	515	PHE	3.3
1	A	445	GLU	3.3
1	A	542	LEU	3.2
1	B	333[A]	CYS	3.2
1	A	104	ASP	3.2
1	B	540	GLU	3.2
1	A	511	ALA	3.2
1	A	310	LEU	3.1
1	A	112	GLN	3.1
1	A	114	THR	3.1
1	A	528	TYR	3.1
1	A	447	SER	3.1
1	A	443	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	206	ARG	3.0
1	B	543	LYS	3.0
1	B	391	LEU	3.0
1	A	450	ARG	2.9
1	B	63	LYS	2.9
1	A	477	LYS	2.9
1	A	480	ARG	2.9
1	A	69	ASP	2.8
1	B	273	ILE	2.8
1	A	72	LYS	2.8
1	A	73	GLU	2.8
1	A	452	GLU	2.8
1	B	203	GLN	2.8
1	A	454	ASN	2.8
1	A	5	ASP	2.8
1	B	358	VAL	2.7
1	A	514[A]	ARG	2.7
1	A	448	ARG	2.7
1	A	512	TYR	2.7
1	A	546	GLU	2.7
1	A	203	GLN	2.7
1	A	1	MET	2.6
1	A	108	LYS	2.6
1	A	79	PHE	2.5
1	B	528	TYR	2.5
1	A	4	SER	2.5
1	B	587	PHE	2.5
1	A	24	ARG	2.4
1	A	348	PHE	2.4
1	A	453	ASP	2.4
1	B	393	ILE	2.3
1	A	333	CYS	2.3
1	B	527	LEU	2.3
1	A	534	ARG	2.3
1	B	560	ASP	2.3
1	A	209	GLY	2.3
1	B	338	ILE	2.3
1	A	135	PHE	2.2
1	A	475	MET	2.2
1	B	453	ASP	2.2
1	A	552	LYS	2.2
1	A	529	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	436	LYS	2.2
1	B	354	LEU	2.2
1	B	544	ARG	2.2
1	B	274	ARG	2.2
1	B	485	LEU	2.2
1	B	423	ILE	2.1
1	A	7	ILE	2.1
1	A	273	ILE	2.1
1	A	456	VAL	2.1
1	B	335	LEU	2.1
1	B	504	LEU	2.1
1	B	340	VAL	2.1
1	A	557	ASP	2.1
1	B	230	LYS	2.1
1	A	35	ASN	2.0
1	B	412	ALA	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^{th} 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
6	5AD	A	1005	18/18	0.81	0.32	9.49	54,69,71,72	16
4	GDP	A	1003[A]	28/28	0.91	0.30	2.61	36,64,72,73	28
4	GDP	A	1003[B]	28/28	0.91	0.30	2.17	31,51,65,68	28
6	5AD	B	1005	18/18	0.94	0.15	1.68	41,56,67,69	12
4	GDP	B	1003[A]	28/28	0.95	0.21	1.46	13,35,46,51	28

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	B12	A	1004	91/91	0.90	0.21	1.45	33,71,88,99	81
4	GDP	B	1003[B]	28/28	0.95	0.21	1.01	15,28,49,54	28
5	B12	B	1004	91/91	0.95	0.13	0.05	27,52,72,90	65
2	TTP	B	1001	29/29	0.96	0.10	-0.32	31,40,60,63	0
2	TTP	A	1001	29/29	0.97	0.07	-1.02	20,38,44,47	0
3	MG	B	1002	1/1	0.92	0.22	-	57,57,57,57	0
3	MG	A	1002	1/1	0.96	0.10	-	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.