



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:48 pm BST

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

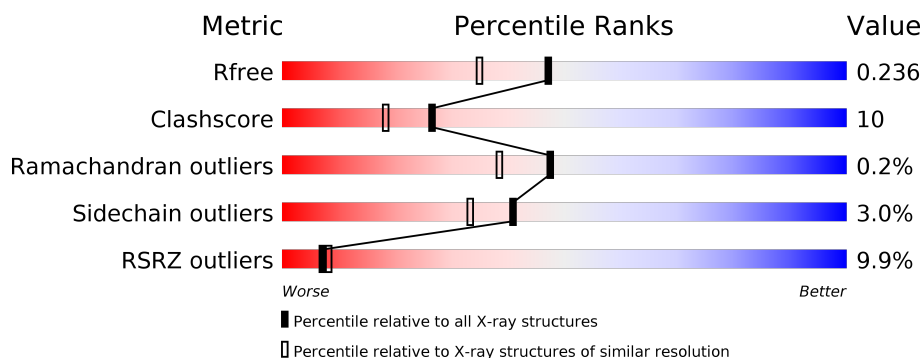
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	644	<div> <div>15%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	B	644	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>

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
5	B12	A	1004	X	-	-	-
5	B12	B	1004	X	-	X	-

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.

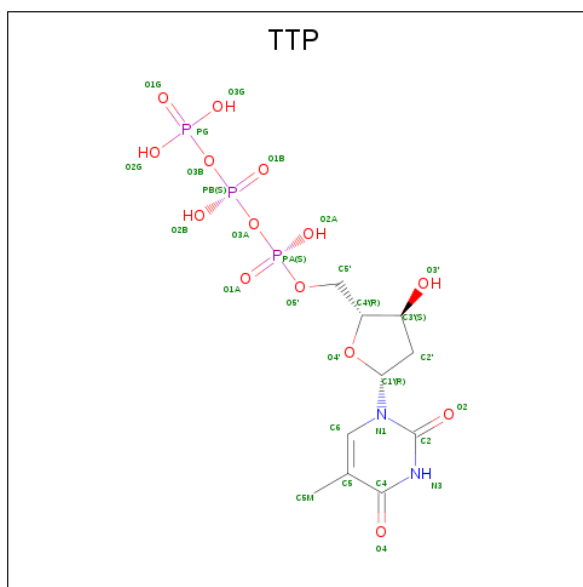
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase.

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

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: $\text{C}_{10}\text{H}_{17}\text{N}_2\text{O}_{14}\text{P}_3$).



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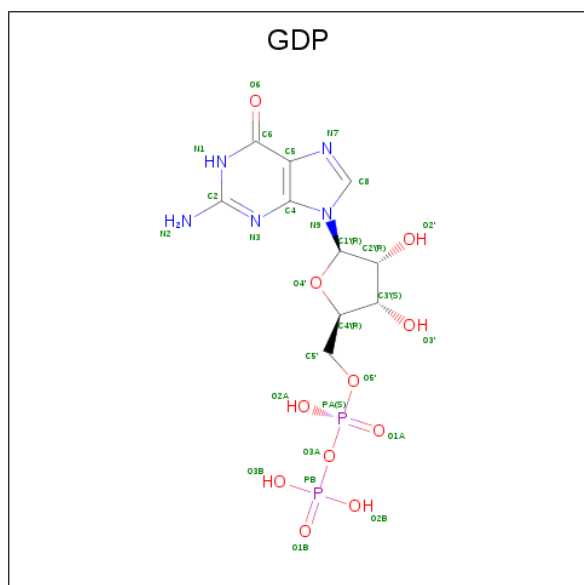
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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

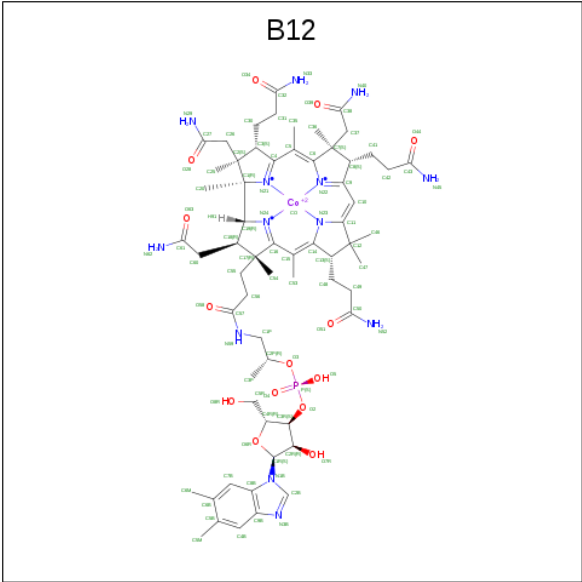
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



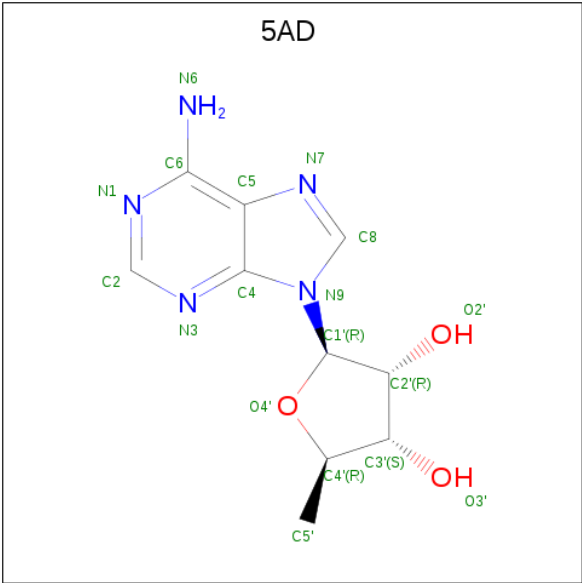
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			56	20	10	22	4		
4	B	1	Total	C	N	O	P	0	1
			56	20	10	22	4		

- Molecule 5 is COBALAMIN (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



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: C₁₀H₁₃N₅O₃).



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		

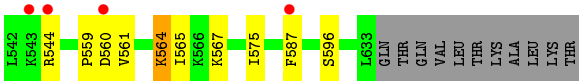
- Molecule 7 is water.

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

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

- Chain A:
-
- 15% 73% 20% 5%
- GLY THR LYS GLU P525 L532 L533 R534 E535 K536 L537 N538 P539 E540 L541 L542 K543 R544 L545 E546 E547 K548 L549 I550 E551 K552 L555 K556 L557 D557 P559 E559 D560 V561 K564 I565 K566 F569 I575 D576 P577 M578 M583 F587 Q588 I593 D592 N593 Q594 L595 E596
- M1 Q12 M13 T114 Y116 Y122 R125 L128 Q129 Q20 L23 R24 F28 M29 K30 D31 L32 N38 Y36 L37 R47 S61 TTR LYS LYS ASN GLU K67 L68 D69 R70 I71 K72 E73 W74 D76 F79 R80 N90 A97 D104 W107 K108 P109 I110 R111 Q112 T114 Y116 Y122 R125 L128 Q129 Q20 L23 R24 F28 M29 K30 D31 L32 N38 Y36 L37 R47 S61 TTR LYS LYS ASN GLU K67 L68 D69 R70 I71 K72 E73 W74 D76 F79 R80 N90 A97 D104 W107 K108 P109 I110 R111
- G435 K436 N440 F441 F442 L443 L444 E445 L446 R447 R448 Y449 R450 T451 F452 D453 D454 K455 V456 M460 D466 D467 E471 W472 W473 K474 W475 W476 K477 E478 F479 R480 L486 L488 P490 T491 T494 L504 N507 F508 L509 A511 A512 Y513 T514 R514 F515 VAL THR LYS GLU K52
- K1273 K285 L298 E303 Y308 P309 L310 H313 N320 P321 E324 I325 G326 L327 E331 A332 K333 N334 F348 Q355 Q359 Q363 P375 I376 K381 E385 Y401 Y407 M408 R413 A416 H426 R429 T430 Y432 E433 L434

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 200. A color scale at the top indicates conservation levels: 4% (red), 82% (green), and 13% (yellow).
- Key residues (positions and amino acids) with high information content (bits) are highlighted:
- Position 1: M1 (0.24 bits)
 - Position 118: N18 (0.24 bits)
 - Position 119: A19 (0.24 bits)
 - Position 120: Q20 (0.24 bits)
 - Position 124: R24 (0.24 bits)
 - Position 150: R50 (0.24 bits)
 - Position 163: K63 (0.24 bits)
 - Position 164: K64 (0.24 bits)
 - Position 167: K67 (0.24 bits)
 - Position 168: L68 (0.24 bits)
 - Position 169: D69 (0.24 bits)
 - Position 170: F70 (0.24 bits)
 - Position 171: I71 (0.24 bits)
 - Position 172: E72 (0.24 bits)
 - Position 173: V73 (0.24 bits)
 - Position 174: W74 (0.24 bits)
 - Position 177: I77 (0.24 bits)
 - Position 190: N90 (0.24 bits)
 - Position 191: S91 (0.24 bits)
 - Position 192: P92 (0.24 bits)
 - Position 199: L99 (0.24 bits)
 - Position 200: L100 (0.24 bits)
 - Position 201: K108 (0.24 bits)
 - Position 202: E120 (0.24 bits)
 - Position 203: I121 (0.24 bits)
 - Position 204: Y122 (0.24 bits)
 - Position 205: R125 (0.24 bits)
 - Position 206: H126 (0.24 bits)
 - Position 207: H127 (0.24 bits)
 - Position 208: S132 (0.24 bits)
 - Position 209: A133 (0.24 bits)
 - Position 210: I156 (0.24 bits)
 - Position 211: V163 (0.24 bits)
 - Position 212: E169 (0.24 bits)
 - Position 213: L170 (0.24 bits)
 - Position 214: F176 (0.24 bits)
 - Position 215: G179 (0.24 bits)
 - Position 216: T180 (0.24 bits)
 - Position 217: H181 (0.24 bits)
 - Position 218: P187 (0.24 bits)



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432), REFMAC	Depositor
R, R_{free}	0.202 , 0.238 0.200 , 0.236	Depositor DCC
R_{free} test set	5994 reflections (5.00%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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:A:440:ASN:HB3	1:A:444:LEU:HD13	1.57	0.86
1:B:206:ARG:HD3	4:B:1003[B]:GDP:HN21	1.41	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:HA	1:A:583:MET:HE3	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:324:GLU:HG2	1:A:325:ILE:HG12	1.79	0.64
1:A:74:TRP:HZ3	1:A:363:ARG:HD3	1.59	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:564:LYS:HB3	1:A:564:LYS:HZ2	1.73	0.54
1:A:298:LEU:HD12	1:A:625:ILE:HD12	1.89	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:A:74:TRP:HH2	1:A:363:ARG:HE	1.57	0.52
1:B:428:HIS:CD2	1:B:480:ARG:HH12	2.28	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:A:588:GLN:HB2	1:A:595:ILE:HD12	1.93	0.51
1:B:206:ARG:CD	4:B:1003[B]:GDP:HN21	2.18	0.51
1:A:527:LEU:HG	1:A:528:TYR:N	2.26	0.51
5:B:1004:B12:H353	5:B:1004:B12:H302	1.92	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:20:GLN:HB3	1:A:24:ARG:NH2	2.25	0.50
1:A:592:ASP:O	1:A:623:ARG:NH2	2.45	0.50
1:B:470:ARG:HD3	7:B:831:HOH:O	2.11	0.50
1:A:407:TYR:CD1	1:A:575:ILE:HD13	2.46	0.50
5:B:1004:B12:H372	7:B:812:HOH:O	2.10	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:490:PRO:HB2	4:A:1003[B]:GDP:O2B	2.13	0.49
1:A:202:LYS:HE3	1:A:207:ARG:CZ	2.43	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:308:TYR:HD1	1:A:309:PRO:HD2	1.77	0.48
1:A:491:THR:HG22	1:A:494:ILE:HD11	1.96	0.48
1:A:617:ALA:HB2	1:A:625:ILE:HD11	1.89	0.48
1:B:416:ALA:HB1	1:B:587:PHE:CE2	2.48	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:327:LEU:HD22	1:A:331:GLU:HB3	1.96	0.46
1:A:359:GLN:O	1:A:363:ARG:HG3	2.15	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:B:314:ARG:NH1	1:B:314:ARG:HG3	2.30	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:C6	5:B:1004:B12:H4B	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:A:504:LEU:HD12	1:A:587:PHE:CD2	2.51	0.45
1:B:170:LEU:HD12	1:B:187:PRO:HA	1.98	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
1:A:401:TYR:CE1	1:A:569:PHE:HA	2.51	0.45
5:B:1004:B12:C53	5:B:1004:B12:H482	2.46	0.45
5:A:1004:B12:O28	5:A:1004:B12:H3	2.15	0.45
1:A:158:LYS:O	1:A:203:GLN:HG2	2.16	0.45
1:B:50:ARG:NH2	1:B:108:LYS:O	2.43	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:237:VAL:HB	1:B:238:LEU:H	1.46	0.44
1:B:492:GLY:O	5:B:1004:B12:H1P2	2.18	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:92:PRO:HG2	1:B:133:ALA:HA	2.00	0.43
1:B:229:LYS:HD3	1:B:238:LEU:HB2	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:187:PRO:O	1:A:191:MET:HG3	2.19	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:A:476:THR:HG21	1:A:480:ARG:HE	1.76	0.42
1:B:122:TYR:O	1:B:125:ARG:HD3	2.18	0.42
1:A:401:TYR:CE2	1:A:507:ASN:ND2	2.88	0.42
1:A:122:TYR:O	1:A:125:ARG:HD3	2.19	0.42
1:A:508:PHE:O	1:A:509:LEU:HD23	2.20	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:A:545:ILE:O	1:A:546:GLU:C	2.59	0.42
1:B:202[A]:LYS:HG2	1:B:205:SER:CB	2.50	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:20:GLN:O	1:B:24:ARG:HG3	2.21	0.41
1:B:514:ARG:HA	1:B:514:ARG:HD2	1.76	0.41
5:B:1004:B12:H4B	5:B:1004:B12:C5	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:A:152:GLU:HG2	1:A:376:ILE:HD13	2.03	0.40
1:A:76:ASP:O	1:A:80:ARG:HG3	2.21	0.40
1:B:18:ASN:HD21	1:B:496:ASN:HD22	1.70	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:334:ASN:N	1:A:334:ASN:OD1	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

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%)	41	31
1	B	620/644 (96%)	600 (97%)	20 (3%)	0	100	100
All	All	1223/1288 (95%)	1178 (96%)	43 (4%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	GLU
1	A	2	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	539/566 (95%)	516 (96%)	23 (4%)	29	19
1	B	551/566 (97%)	540 (98%)	11 (2%)	55	51
All	All	1090/1132 (96%)	1056 (97%)	34 (3%)	41	32

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	23,30,30	0.98	1 (4%)	29,47,47	1.67	4 (13%)
2	TTP	B	1001	3	23,30,30	0.97	2 (8%)	29,47,47	1.87	6 (20%)
6	5AD	A	1005	-	17,20,20	1.90	5 (29%)	15,30,30	2.75	4 (26%)
6	5AD	B	1005	5	17,20,20	1.90	5 (29%)	15,30,30	3.10	4 (26%)
5	B12	A	1004	-	80,101,101	0.92	3 (3%)	101,166,166	1.50	9 (8%)
4	GDP	B	1003[B]	-	24,30,30	1.23	2 (8%)	31,47,47	1.95	7 (22%)
4	GDP	B	1003[A]	-	24,30,30	1.14	2 (8%)	31,47,47	1.94	7 (22%)
4	GDP	A	1003[A]	-	24,30,30	1.20	2 (8%)	31,47,47	1.79	8 (25%)
5	B12	B	1004	6	80,101,101	0.93	3 (3%)	101,166,166	1.58	13 (12%)
4	GDP	A	1003[B]	-	24,30,30	1.17	2 (8%)	31,47,47	1.88	8 (25%)

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	-	3/19/34/34	0/2/2/2
2	TTP	B	1001	3	-	6/19/34/34	0/2/2/2
6	5AD	A	1005	-	-	0/0/20/20	0/3/3/3
6	5AD	B	1005	5	-	0/0/20/20	0/3/3/3
5	B12	A	1004	-	1/1/36/38	10/51/223/223	0/3/11/11
4	GDP	B	1003[B]	-	-	7/12/32/32	0/3/3/3
4	GDP	B	1003[A]	-	-	7/12/32/32	0/3/3/3
4	GDP	A	1003[A]	-	-	7/12/32/32	0/3/3/3
5	B12	B	1004	6	1/1/36/38	2/51/223/223	0/3/11/11
4	GDP	A	1003[B]	-	-	3/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1005	5AD	C2-N3	4.99	1.40	1.32
6	B	1005	5AD	C2-N3	4.95	1.40	1.32
4	A	1003[A]	GDP	C6-C5	4.14	1.48	1.41
4	B	1003[B]	GDP	C6-C5	4.08	1.48	1.41
4	A	1003[B]	GDP	C6-C5	3.95	1.48	1.41
5	B	1004	B12	C5M-C5B	-3.58	1.43	1.51
4	B	1003[A]	GDP	C6-C5	3.57	1.47	1.41
5	A	1004	B12	C5M-C5B	-3.51	1.44	1.51
5	B	1004	B12	C6B-C5B	3.39	1.49	1.40
6	A	1005	5AD	C2-N1	3.35	1.40	1.33
6	B	1005	5AD	C2-N1	3.33	1.40	1.33
2	A	1001	TTP	C4-C5	3.30	1.48	1.41
5	A	1004	B12	C6B-C5B	3.24	1.49	1.40
5	B	1004	B12	C53-C15	3.22	1.58	1.52
2	B	1001	TTP	C4-C5	3.19	1.48	1.41
5	A	1004	B12	C53-C15	2.99	1.58	1.52
6	A	1005	5AD	C5-C4	-2.62	1.34	1.40
6	B	1005	5AD	C6-C5	-2.57	1.33	1.43
6	A	1005	5AD	C6-C5	-2.56	1.33	1.43
6	B	1005	5AD	O4'-C1'	2.55	1.44	1.41
4	B	1003[A]	GDP	C5-C4	2.53	1.47	1.40
4	A	1003[B]	GDP	C5-C4	2.53	1.47	1.40
4	A	1003[A]	GDP	C5-C4	2.51	1.47	1.40
4	B	1003[B]	GDP	C5-C4	2.49	1.47	1.40
6	B	1005	5AD	C5-C4	-2.41	1.34	1.40
6	A	1005	5AD	O4'-C1'	2.25	1.44	1.41
2	B	1001	TTP	C2-N3	-2.23	1.33	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1005	5AD	C5'-C4'-C3'	-8.87	106.39	115.70
5	A	1004	B12	C1-C19-C18	8.26	135.58	121.93
5	B	1004	B12	C1-C19-N24	8.02	115.27	106.24
5	B	1004	B12	C1-C19-C18	7.57	134.44	121.93
5	A	1004	B12	C1-C19-N24	7.47	114.65	106.24
2	B	1001	TTP	C4-N3-C2	7.06	121.11	115.14
6	A	1005	5AD	C5'-C4'-C3'	-6.83	108.52	115.70
6	B	1005	5AD	N3-C2-N1	-6.81	118.03	128.68
6	A	1005	5AD	N3-C2-N1	-6.80	118.05	128.68
2	A	1001	TTP	C4-N3-C2	6.14	120.33	115.14
4	B	1003[A]	GDP	C2-N3-C4	5.12	121.20	115.36
4	A	1003[A]	GDP	C2-N3-C4	4.98	121.04	115.36
4	A	1003[B]	GDP	C2-N3-C4	4.77	120.81	115.36
4	B	1003[B]	GDP	C6-C5-C4	-4.75	116.27	120.80
4	B	1003[B]	GDP	C6-N1-C2	4.38	122.89	115.93
4	B	1003[B]	GDP	C5-C6-N1	-4.22	117.66	123.43
4	B	1003[B]	GDP	C2-N3-C4	4.15	120.09	115.36
5	B	1004	B12	C20-C1-C19	-3.96	105.54	109.36
4	A	1003[B]	GDP	C6-N1-C2	3.95	122.20	115.93
4	A	1003[A]	GDP	C6-N1-C2	3.91	122.14	115.93
4	A	1003[A]	GDP	C5-C6-N1	-3.85	118.17	123.43
4	B	1003[A]	GDP	C6-N1-C2	3.85	122.04	115.93
4	A	1003[B]	GDP	C6-C5-C4	-3.84	117.13	120.80
4	A	1003[B]	GDP	C5-C6-N1	-3.82	118.20	123.43
4	B	1003[A]	GDP	C5-C6-N1	-3.64	118.45	123.43
2	A	1001	TTP	PB-O3B-PG	-3.60	120.47	132.83
4	B	1003[B]	GDP	O3B-PB-O3A	3.57	116.61	104.64
4	B	1003[A]	GDP	N3-C2-N1	-3.57	122.46	127.22
5	A	1004	B12	C48-C13-C12	3.46	126.22	116.59
4	A	1003[A]	GDP	C6-C5-C4	-3.39	117.56	120.80
4	B	1003[B]	GDP	N3-C2-N1	-3.35	122.75	127.22
5	A	1004	B12	O6R-C4R-C5R	3.32	116.39	109.21
4	A	1003[B]	GDP	N3-C2-N1	-3.26	122.87	127.22
4	A	1003[A]	GDP	N3-C2-N1	-3.26	122.88	127.22
2	B	1001	TTP	PB-O3B-PG	-3.25	121.69	132.83
5	B	1004	B12	O6R-C4R-C5R	3.17	116.07	109.21
4	A	1003[B]	GDP	PA-O3A-PB	-3.12	122.10	132.83
4	B	1003[A]	GDP	O2'-C2'-C3'	-3.05	101.95	111.82
4	B	1003[A]	GDP	C6-C5-C4	-3.05	117.89	120.80
2	B	1001	TTP	PB-O3A-PA	-2.93	122.76	132.83
2	B	1001	TTP	O3G-PG-O3B	2.78	113.97	104.64
4	A	1003[B]	GDP	C3'-C2'-C1'	2.77	105.16	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1004	B12	O6R-C4R-C3R	2.76	110.79	104.87
5	B	1004	B12	C48-C13-C12	2.75	124.23	116.59
2	B	1001	TTP	C5-C6-N1	-2.74	119.25	122.19
2	A	1001	TTP	O3G-PG-O3B	2.65	113.53	104.64
5	B	1004	B12	O6R-C1R-C2R	2.63	110.77	106.93
5	B	1004	B12	C18-C60-C61	-2.62	107.44	113.97
6	A	1005	5AD	C5-C6-N6	-2.49	116.57	120.35
2	B	1001	TTP	C2'-C1'-N1	-2.47	108.57	114.27
6	B	1005	5AD	C3'-C2'-C1'	2.42	104.63	100.98
5	B	1004	B12	C26-C2-C1	2.41	113.77	110.02
2	A	1001	TTP	C5-C6-N1	-2.39	119.62	122.19
5	B	1004	B12	C3-C4-C5	-2.38	123.06	131.68
5	A	1004	B12	O6R-C4R-C3R	2.36	109.92	104.87
5	B	1004	B12	C7B-C8B-C9B	2.29	122.81	120.54
5	A	1004	B12	O6R-C1R-C2R	2.28	110.25	106.93
4	B	1003[B]	GDP	C4-C5-N7	-2.25	107.06	109.40
4	A	1003[A]	GDP	C4-C5-N7	-2.21	107.10	109.40
5	A	1004	B12	C7B-C8B-C9B	2.20	122.72	120.54
4	A	1003[A]	GDP	C3'-C2'-C1'	2.19	104.27	100.98
6	A	1005	5AD	C3'-C2'-C1'	2.18	104.27	100.98
5	A	1004	B12	C13-C14-C15	-2.15	123.90	131.68
4	A	1003[A]	GDP	O3B-PB-O3A	2.13	111.77	104.64
5	A	1004	B12	C3-C4-C5	-2.11	124.02	131.68
6	B	1005	5AD	C5-C6-N6	-2.11	117.15	120.35
5	B	1004	B12	C2-C1-C19	2.10	121.92	118.60
4	A	1003[B]	GDP	C4-C5-N7	-2.09	107.22	109.40
4	B	1003[A]	GDP	O3B-PB-O3A	2.08	111.61	104.64
5	B	1004	B12	C13-C14-C15	-2.04	124.29	131.68

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1004	B12	C19
5	B	1004	B12	C19

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	TTP	C5'-O5'-PA-O1A
5	A	1004	B12	C2P-O3-P-O2
4	B	1003[B]	GDP	C5'-O5'-PA-O3A
4	B	1003[B]	GDP	C5'-O5'-PA-O2A

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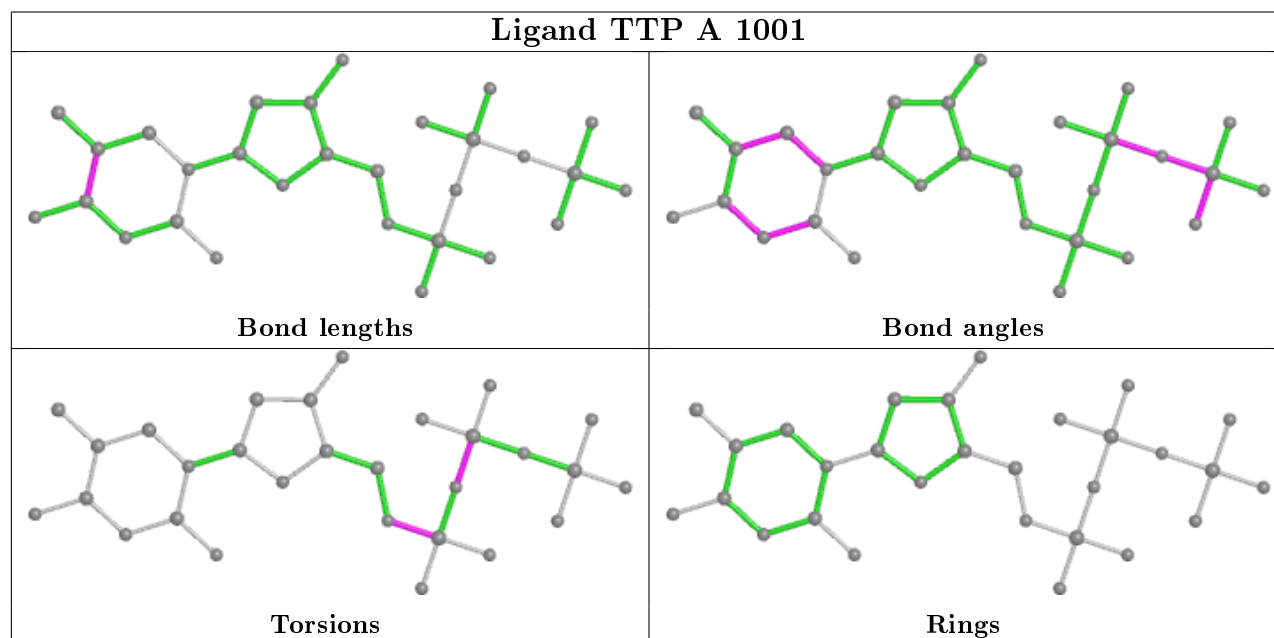
Mol	Chain	Res	Type	Atoms
4	B	1003[B]	GDP	C3'-C4'-C5'-O5'
4	B	1003[A]	GDP	C5'-O5'-PA-O1A
4	A	1003[A]	GDP	C5'-O5'-PA-O3A
4	A	1003[A]	GDP	C5'-O5'-PA-O1A
4	A	1003[A]	GDP	C5'-O5'-PA-O2A
4	A	1003[A]	GDP	O4'-C4'-C5'-O5'
4	A	1003[A]	GDP	C3'-C4'-C5'-O5'
4	B	1003[A]	GDP	O4'-C4'-C5'-O5'
4	B	1003[B]	GDP	O4'-C4'-C5'-O5'
4	B	1003[A]	GDP	C3'-C4'-C5'-O5'
5	A	1004	B12	C18-C17-C55-C56
5	A	1004	B12	C16-C17-C55-C56
5	A	1004	B12	C2P-C1P-N59-C57
4	B	1003[B]	GDP	PA-O3A-PB-O1B
4	A	1003[B]	GDP	PA-O3A-PB-O1B
5	A	1004	B12	C2P-O3-P-O4
4	B	1003[B]	GDP	PA-O3A-PB-O3B
2	B	1001	TTP	C5'-O5'-PA-O3A
4	B	1003[A]	GDP	C5'-O5'-PA-O3A
4	A	1003[B]	GDP	C5'-O5'-PA-O3A
2	B	1001	TTP	PG-O3B-PB-O1B
4	A	1003[A]	GDP	PB-O3A-PA-O2A
2	B	1001	TTP	C5'-O5'-PA-O2A
4	B	1003[B]	GDP	C5'-O5'-PA-O1A
4	B	1003[A]	GDP	C5'-O5'-PA-O2A
4	A	1003[B]	GDP	C3'-C4'-C5'-O5'
5	A	1004	B12	C18-C60-C61-O63
2	A	1001	TTP	PA-O3A-PB-O2B
2	B	1001	TTP	PA-O3A-PB-O2B
4	B	1003[A]	GDP	PB-O3A-PA-O2A
5	A	1004	B12	C18-C60-C61-N62
5	A	1004	B12	C17-C18-C60-C61
5	A	1004	B12	C19-C18-C60-C61
5	B	1004	B12	C17-C18-C60-C61
5	B	1004	B12	C19-C18-C60-C61
2	A	1001	TTP	PA-O3A-PB-O1B
5	A	1004	B12	C38-C37-C7-C8
2	B	1001	TTP	PG-O3B-PB-O2B
4	B	1003[A]	GDP	PB-O3A-PA-O1A
4	A	1003[A]	GDP	PB-O3A-PA-O1A
2	A	1001	TTP	C5'-O5'-PA-O2A

There are no ring outliers.

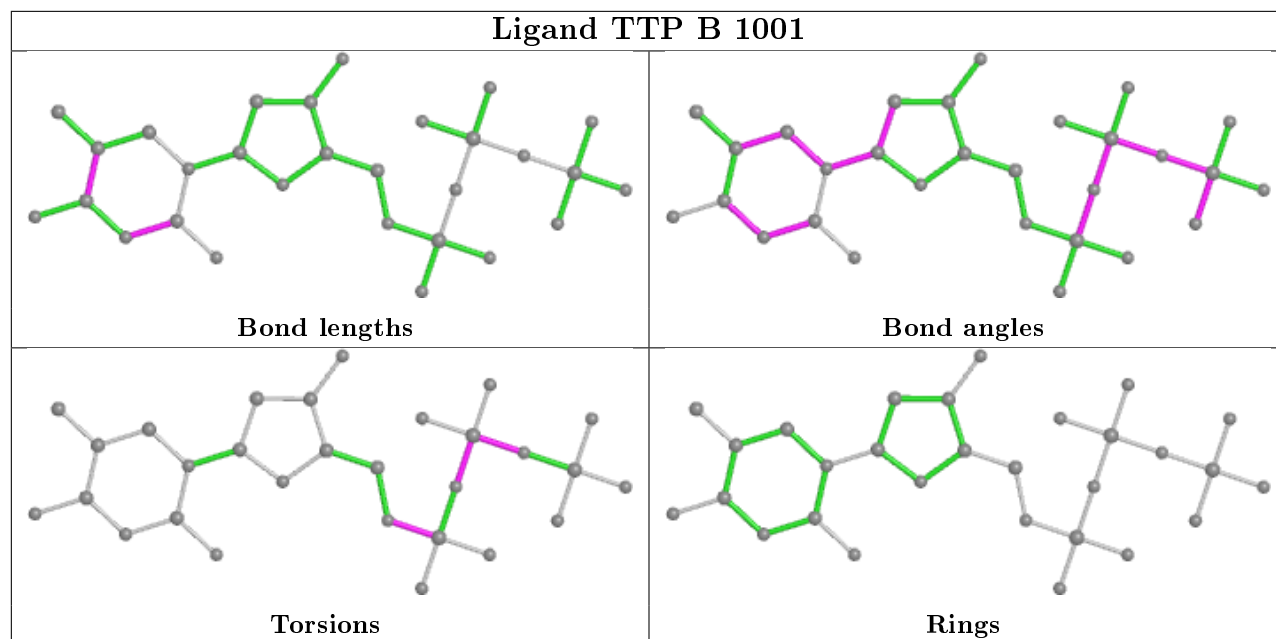
8 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	TTP	1	0
6	A	1005	5AD	1	0
6	B	1005	5AD	3	0
5	A	1004	B12	14	0
4	B	1003[B]	GDP	5	0
4	B	1003[A]	GDP	1	0
5	B	1004	B12	21	0
4	A	1003[B]	GDP	3	0

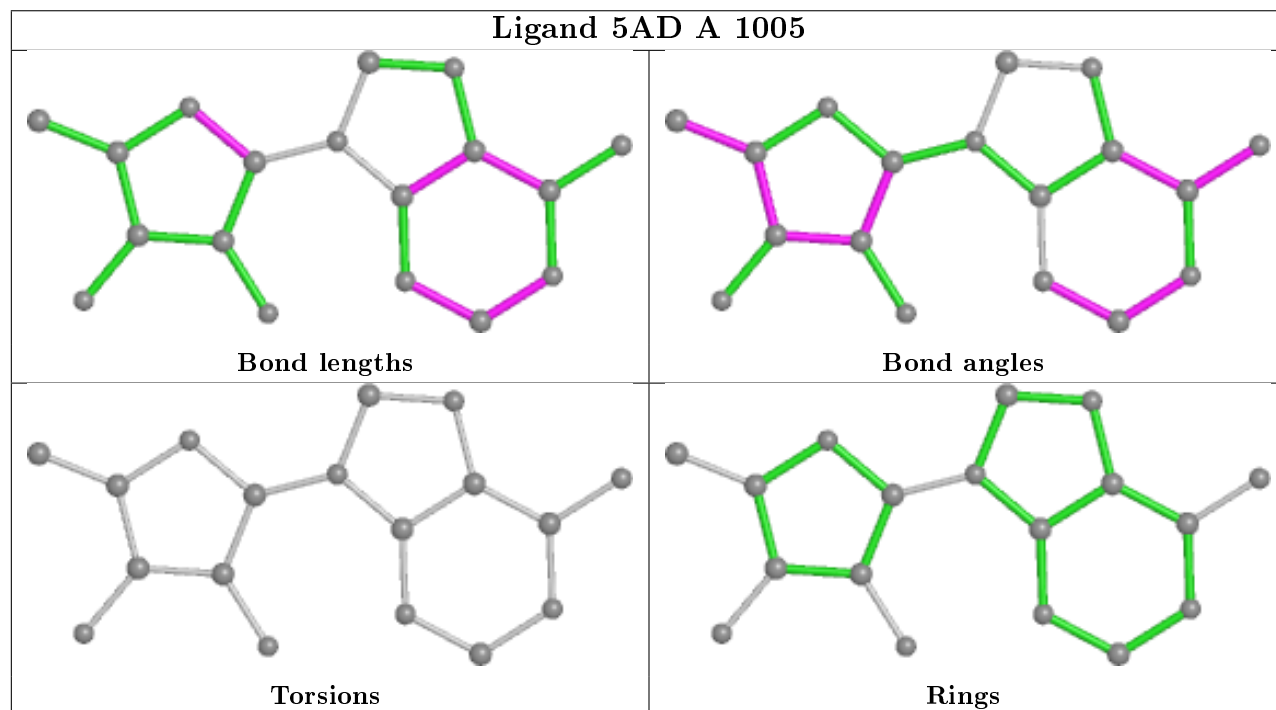
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

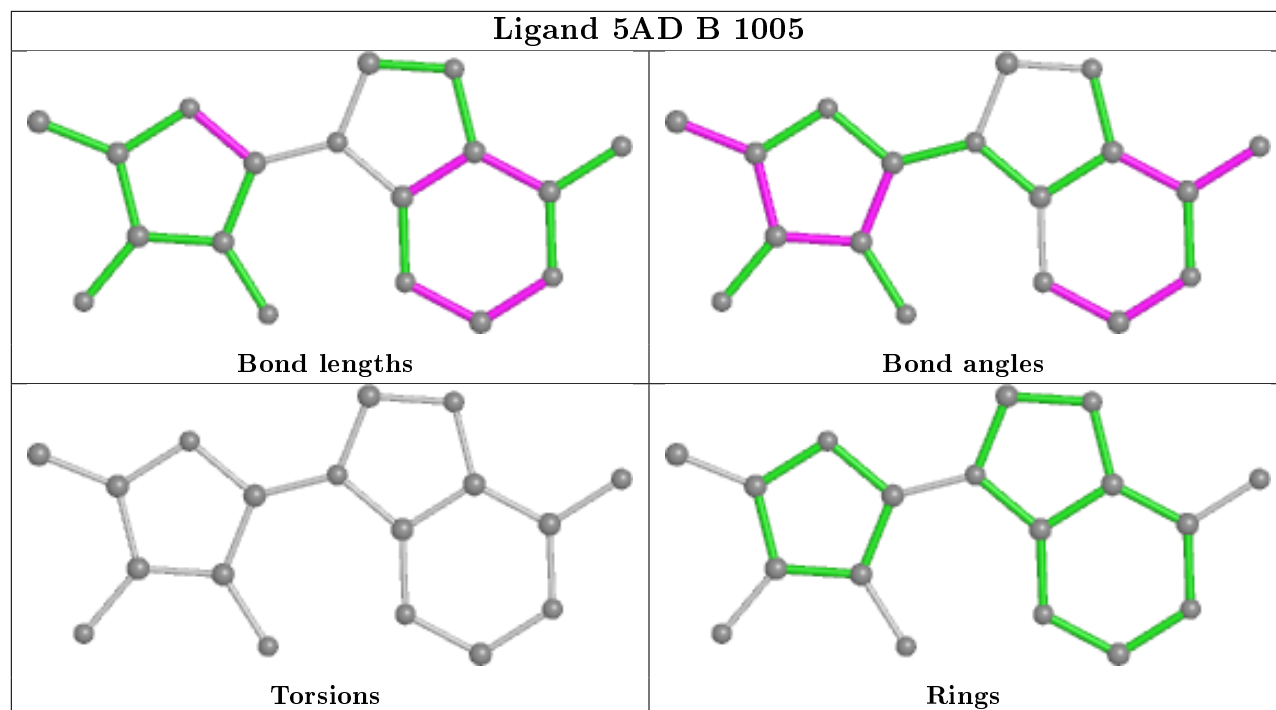


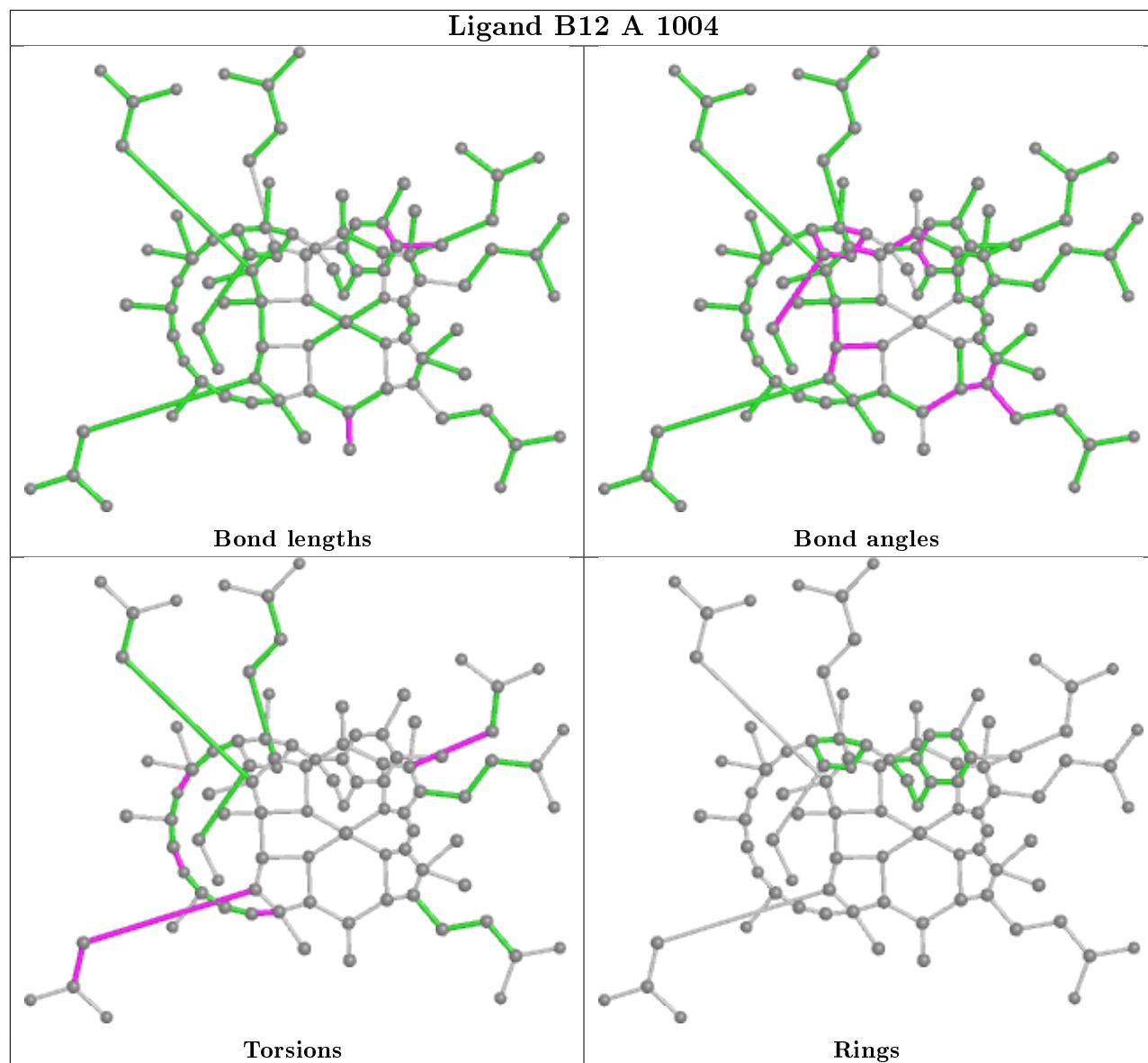
Ligand TTP B 1001



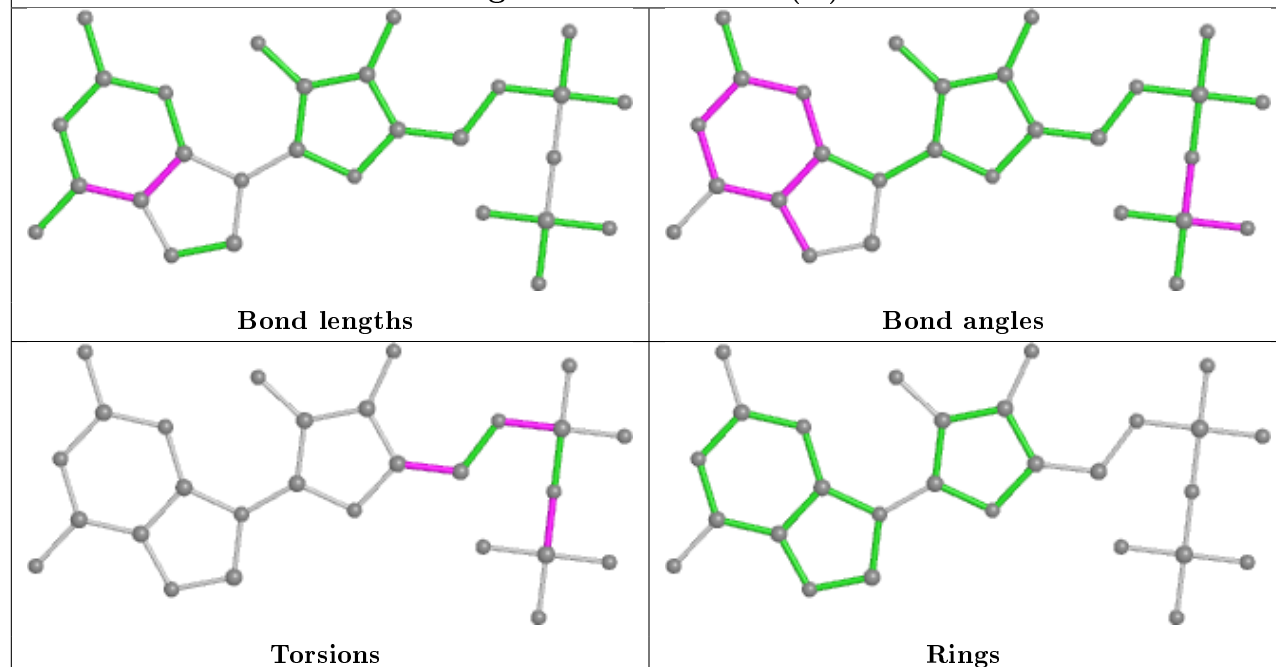
Ligand 5AD A 1005



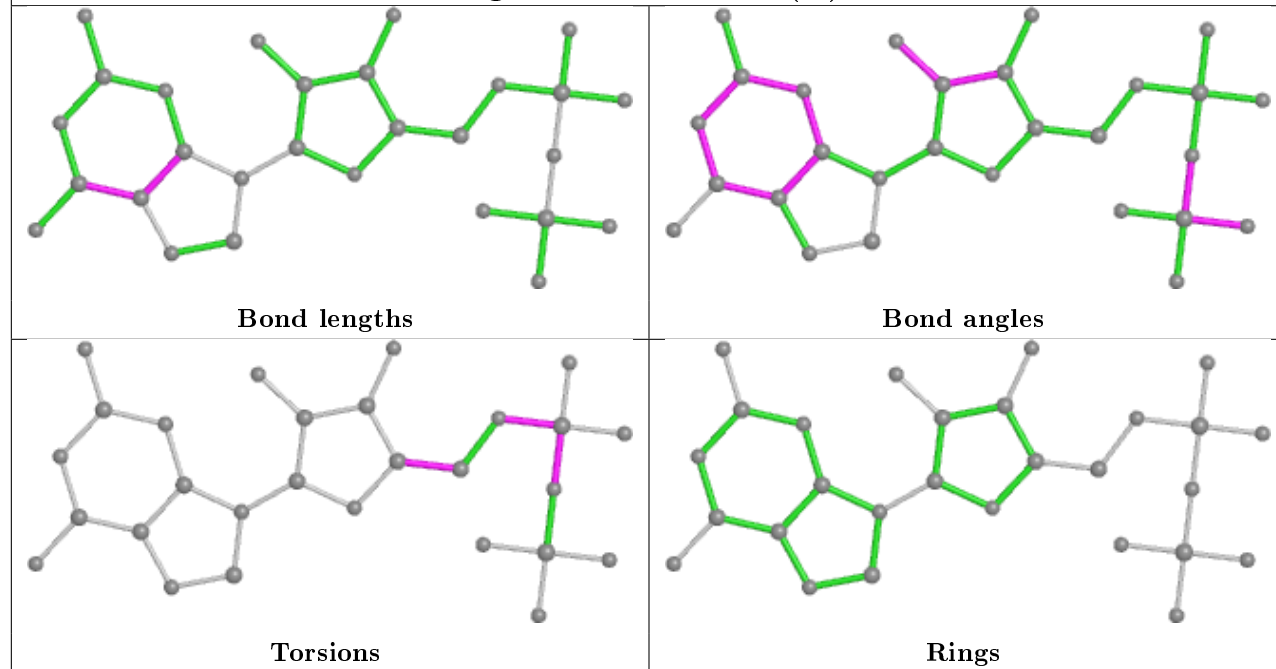


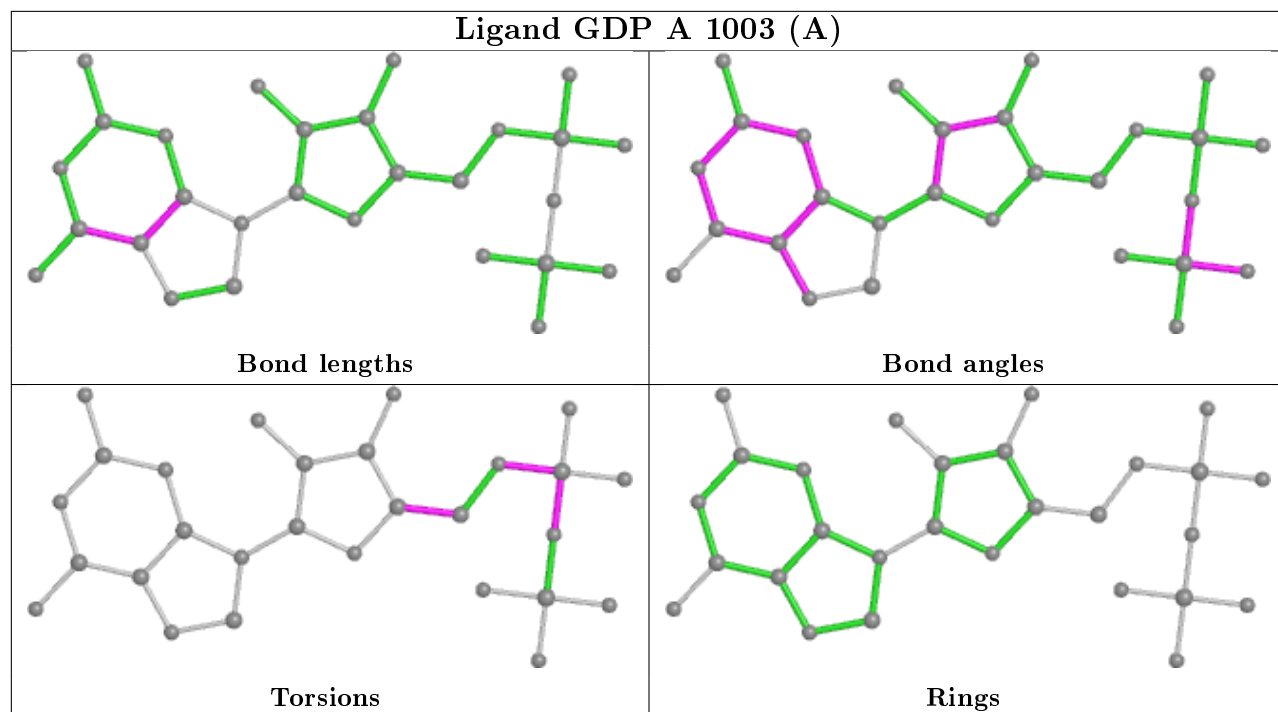


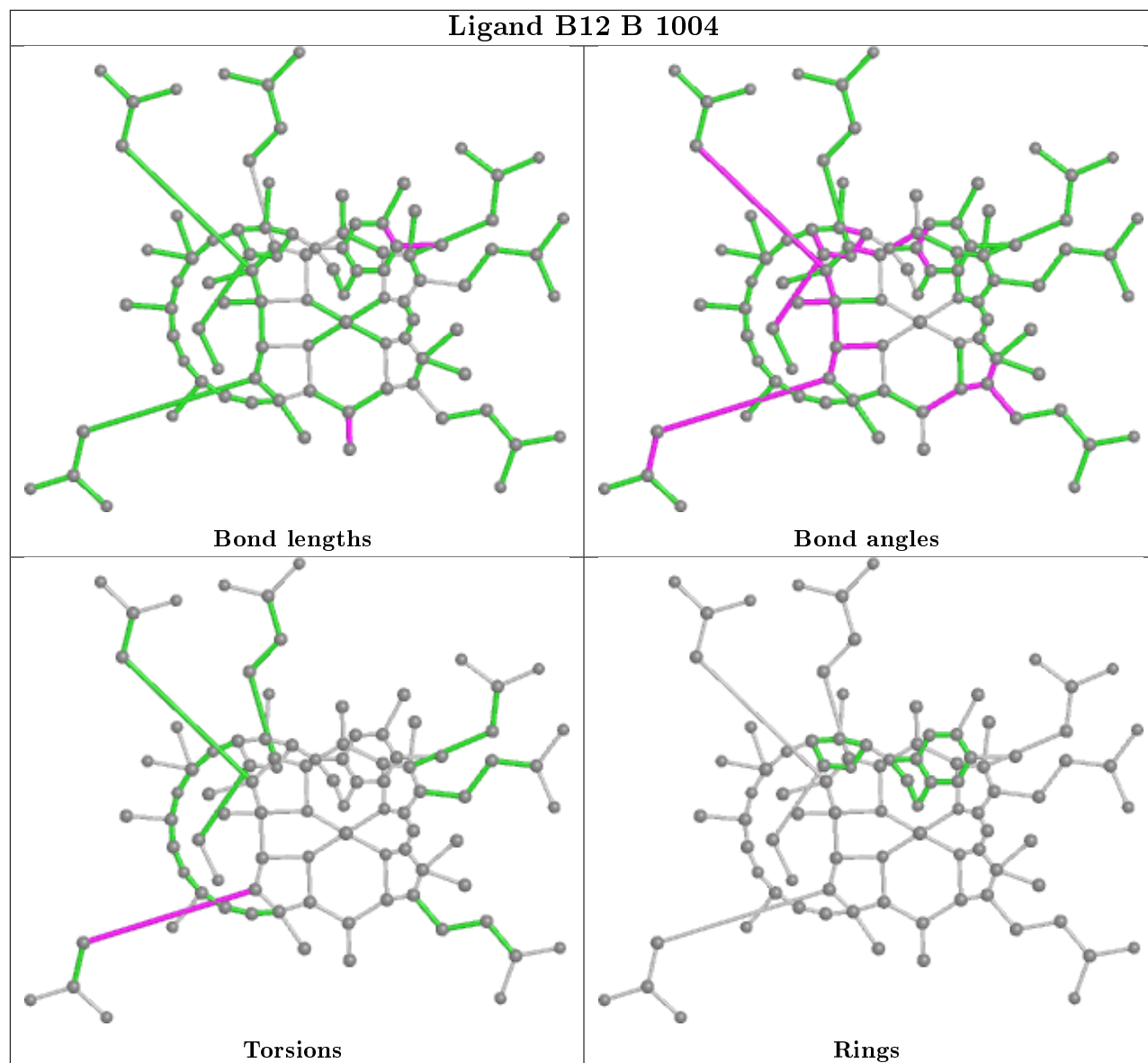
Ligand GDP B 1003 (B)

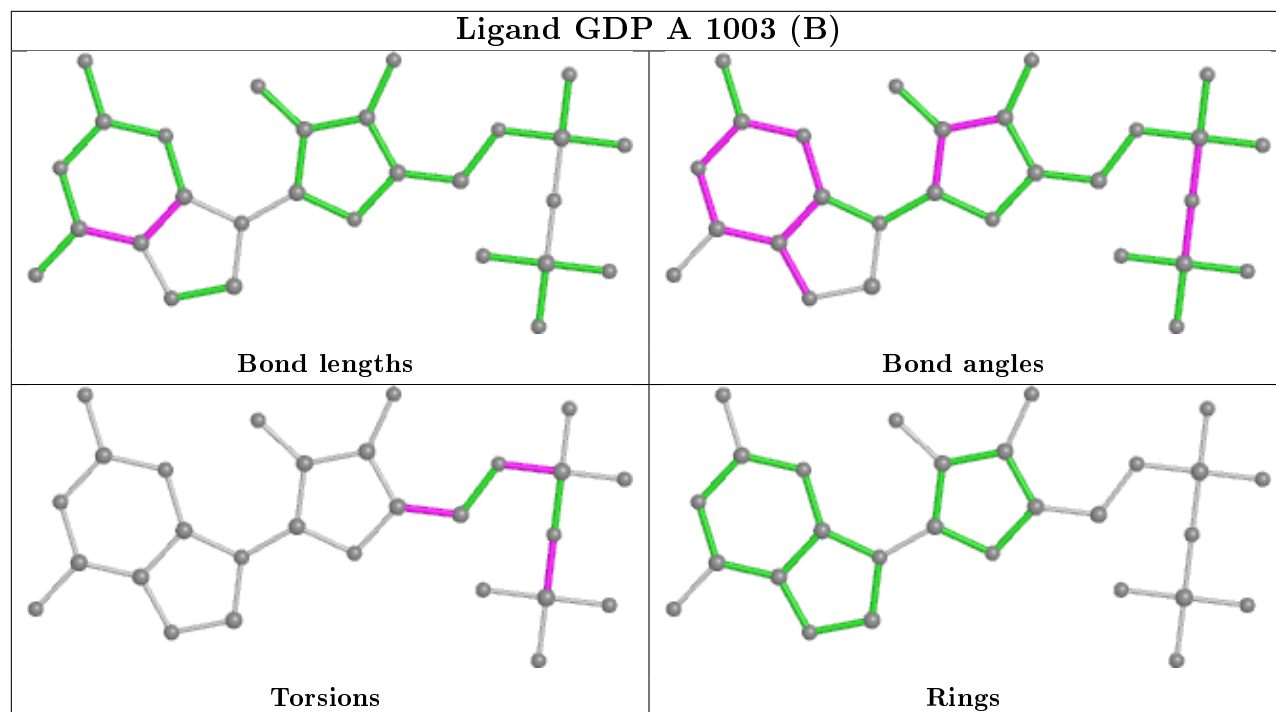


Ligand GDP B 1003 (A)









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	A	612/644 (95%)	0.75	94 (15%) 2 2	34, 68, 122, 153	0
1	B	618/644 (95%)	0.10	28 (4%) 33 36	24, 41, 82, 110	0
All	All	1230/1288 (95%)	0.42	122 (9%) 7 8	24, 53, 113, 153	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	PHE	11.8
1	A	526	LEU	7.9
1	B	526	LEU	7.4
1	A	558	ILE	6.6
1	A	559	PRO	6.5
1	A	476	THR	5.8
1	A	479	PHE	5.5
1	A	561	VAL	5.5
1	A	71	ILE	5.0
1	A	111	ASP	5.0
1	A	560	ASP	5.0
1	A	525	PRO	5.0
1	A	118	TYR	5.0
1	A	550	ILE	4.9
1	A	549	LEU	4.9
1	A	551	GLU	4.9
1	A	68	LEU	4.8
1	A	513	THR	4.8
1	A	110	ILE	4.8
1	A	32	LEU	4.6
1	A	449	TYR	4.6
1	A	313	HIS	4.5
1	A	545	ILE	4.5
1	A	446	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	471	GLU	4.4
1	A	548	GLU	4.3
1	A	107	TRP	4.3
1	A	527	LEU	4.2
1	A	555	LEU	4.2
1	A	474	LYS	4.1
1	A	544	ARG	4.1
1	A	540	GLU	4.0
1	A	204	GLY	4.0
1	B	204	GLY	4.0
1	A	80	ARG	4.0
1	A	70	ARG	3.9
1	A	543	LYS	3.8
1	A	537	LEU	3.8
1	A	208	ARG	3.8
1	A	478	GLU	3.8
1	A	444	LEU	3.7
1	A	113	MET	3.6
1	A	566	LYS	3.6
1	A	363	ARG	3.6
1	A	547	LYS	3.6
1	A	109	PRO	3.5
1	A	565	ILE	3.4
1	A	76	ASP	3.4
1	B	64	LYS	3.4
1	A	451	THR	3.3
1	A	455	PHE	3.3
1	A	441	PHE	3.2
1	B	515	PHE	3.2
1	A	541	ILE	3.2
1	A	445	GLU	3.2
1	A	104	ASP	3.2
1	B	540	GLU	3.2
1	B	333[A]	CYS	3.2
1	A	542	LEU	3.1
1	A	511	ALA	3.1
1	A	112	GLN	3.1
1	A	114	THR	3.1
1	A	310	LEU	3.0
1	A	528	TYR	3.0
1	A	447	SER	3.0
1	B	206	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	443	LEU	2.9
1	B	543	LYS	2.9
1	A	450	ARG	2.9
1	B	63	LYS	2.9
1	B	391	LEU	2.9
1	A	477	LYS	2.8
1	A	480	ARG	2.8
1	A	72	LYS	2.8
1	A	73	GLU	2.8
1	A	69	ASP	2.8
1	A	452	GLU	2.8
1	B	273	ILE	2.7
1	B	203	GLN	2.7
1	A	454	ASN	2.7
1	A	514[A]	ARG	2.7
1	A	5	ASP	2.7
1	A	448	ARG	2.7
1	A	512	TYR	2.7
1	A	546	GLU	2.7
1	B	358	VAL	2.6
1	A	203	GLN	2.6
1	A	1	MET	2.6
1	A	108	LYS	2.5
1	B	528	TYR	2.5
1	A	79	PHE	2.5
1	A	24	ARG	2.4
1	A	4	SER	2.4
1	B	587	PHE	2.4
1	A	453	ASP	2.3
1	A	534	ARG	2.3
1	A	348	PHE	2.3
1	A	333	CYS	2.3
1	B	527	LEU	2.3
1	B	393	ILE	2.3
1	A	475	MET	2.2
1	A	552	LYS	2.2
1	B	560	ASP	2.2
1	A	209	GLY	2.2
1	B	544	ARG	2.2
1	B	453	ASP	2.2
1	B	338	ILE	2.2
1	A	436	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	135	PHE	2.2
1	A	529	VAL	2.1
1	B	274	ARG	2.1
1	B	354	LEU	2.1
1	B	485	LEU	2.1
1	B	230	LYS	2.1
1	B	423	ILE	2.1
1	A	557	ASP	2.0
1	A	456	VAL	2.0
1	A	7	ILE	2.0
1	A	273	ILE	2.0
1	B	340	VAL	2.0
1	A	35	ASN	2.0
1	B	504	LEU	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

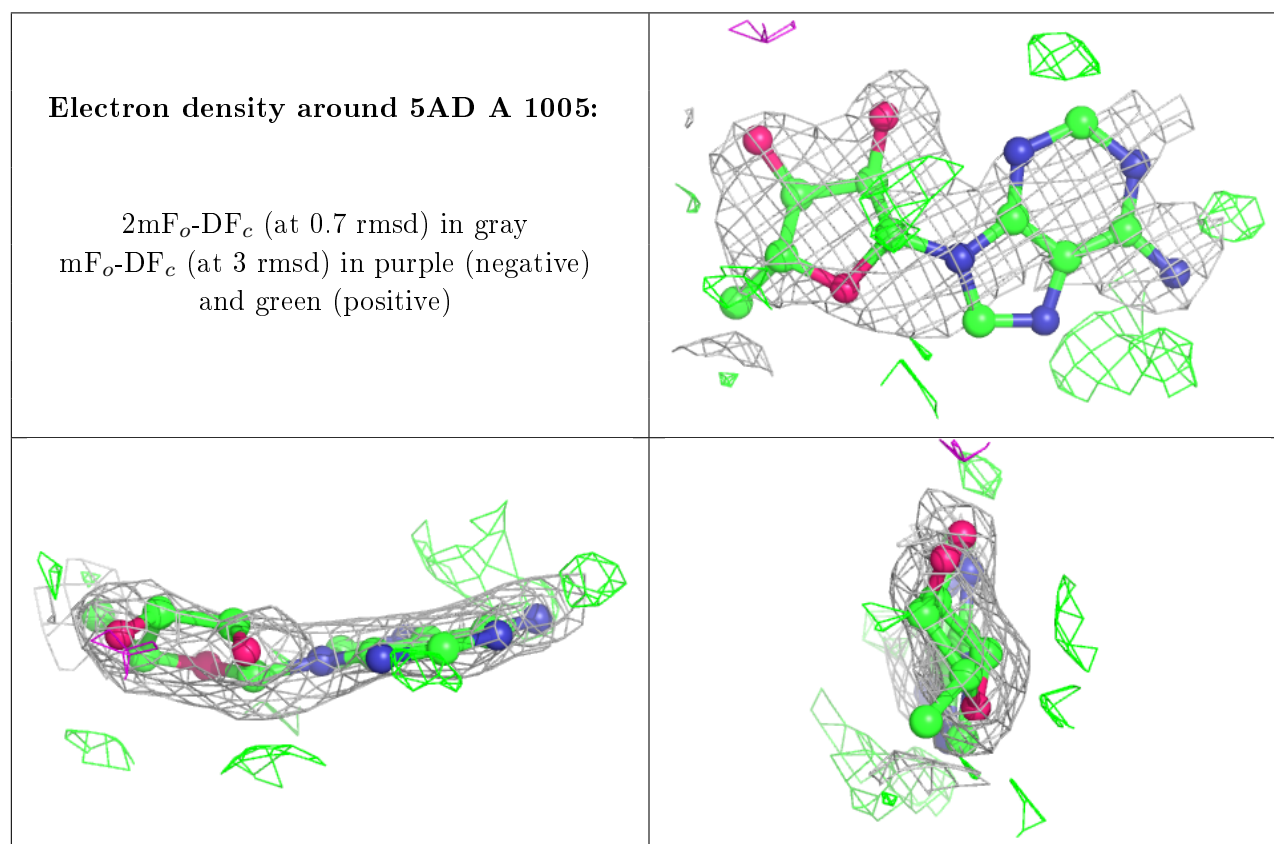
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	5AD	A	1005	18/18	0.81	0.32	54,69,71,72	16
5	B12	A	1004	91/91	0.90	0.21	33,71,88,99	81
4	GDP	A	1003[A]	28/28	0.91	0.30	36,64,72,73	28
4	GDP	A	1003[B]	28/28	0.91	0.30	31,51,65,68	28
3	MG	B	1002	1/1	0.92	0.22	57,57,57,57	0
6	5AD	B	1005	18/18	0.94	0.15	41,56,67,69	12
4	GDP	B	1003[B]	28/28	0.95	0.21	15,28,49,54	28
5	B12	B	1004	91/91	0.95	0.13	27,52,72,90	65
4	GDP	B	1003[A]	28/28	0.95	0.21	13,35,46,51	28

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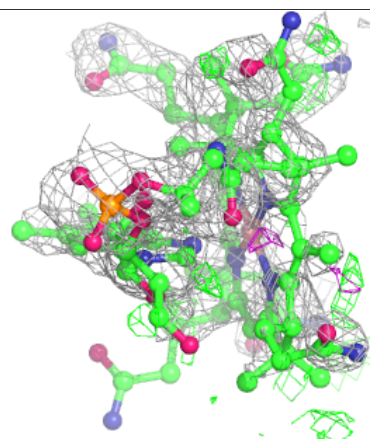
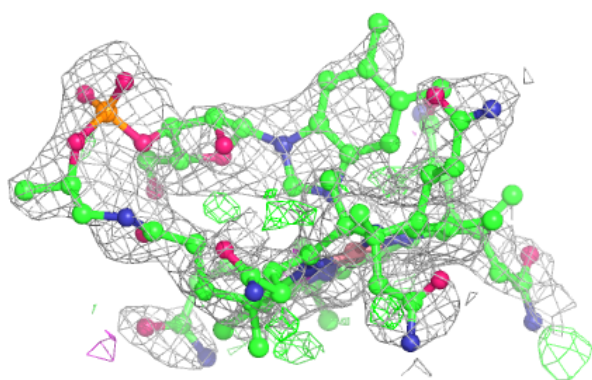
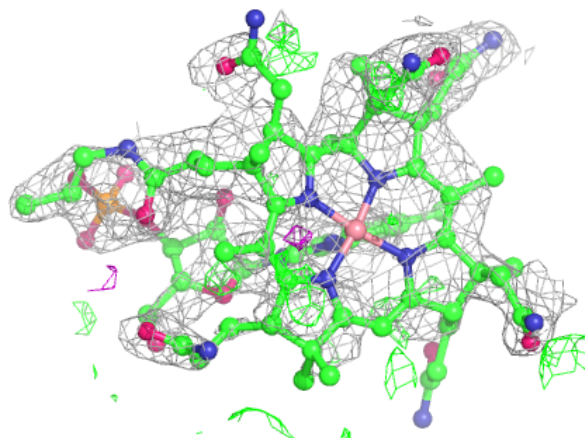
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TTP	B	1001	29/29	0.96	0.10	31,40,60,63	0
3	MG	A	1002	1/1	0.96	0.10	36,36,36,36	0
2	TTP	A	1001	29/29	0.97	0.07	20,38,44,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



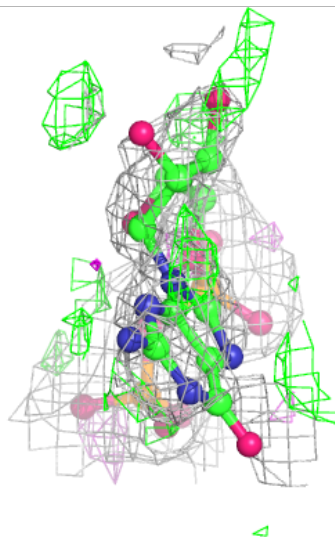
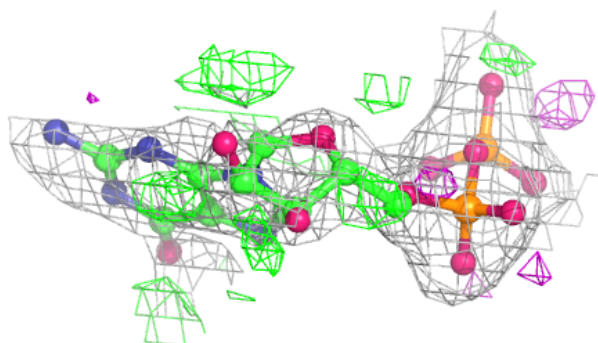
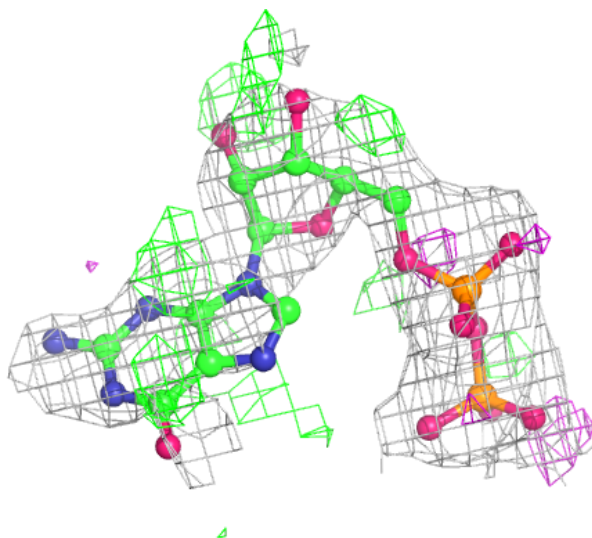
Electron density around B12 A 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



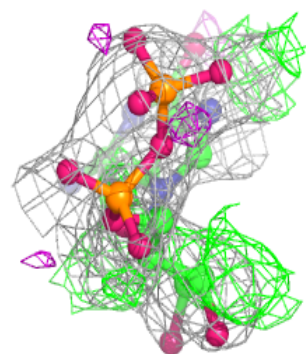
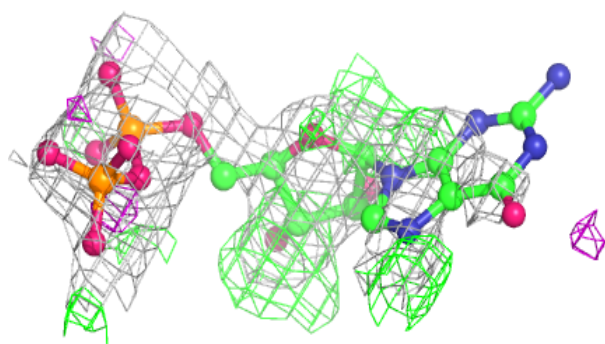
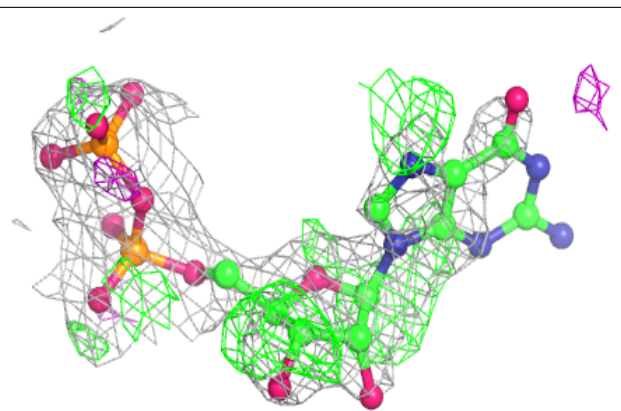
Electron density around GDP A 1003 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

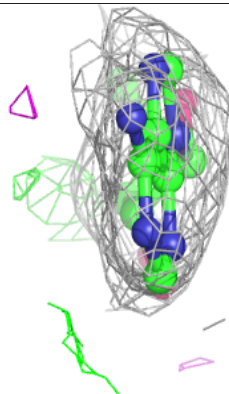
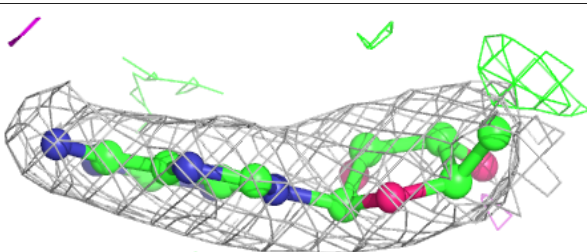
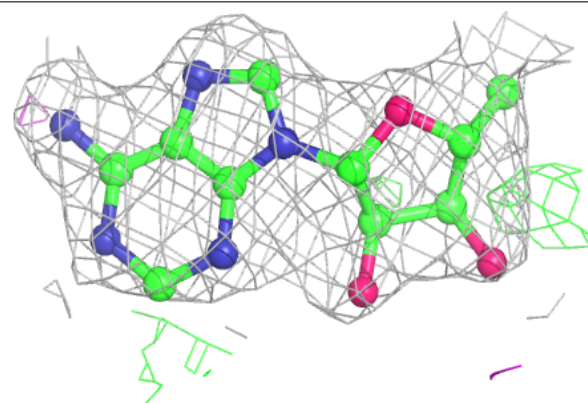


Electron density around GDP A 1003 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

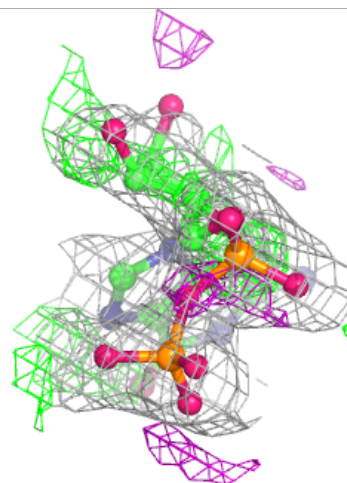
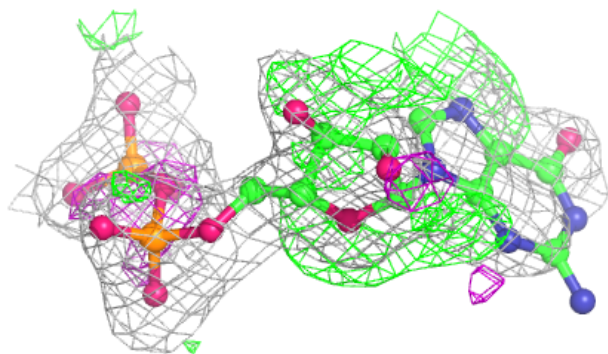
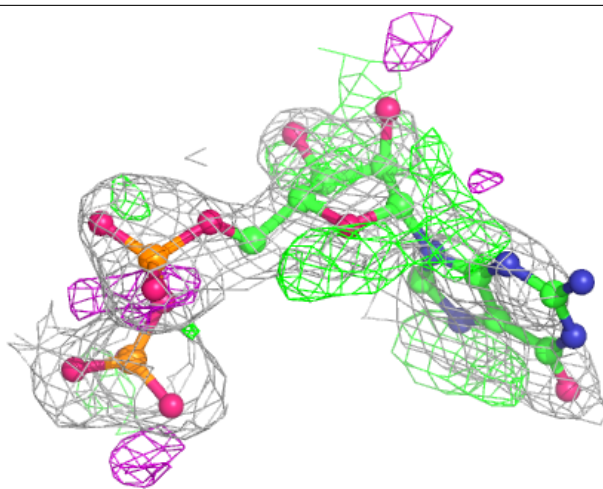
**Electron density around 5AD B 1005:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



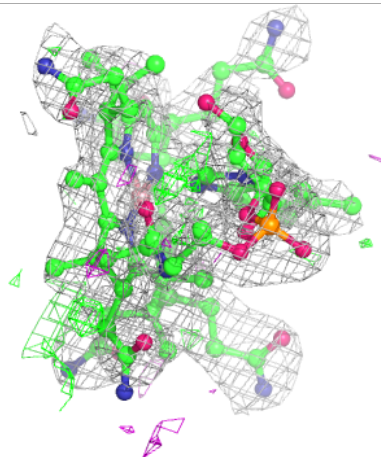
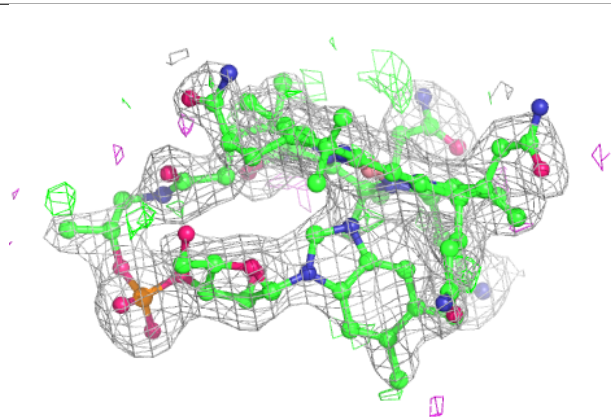
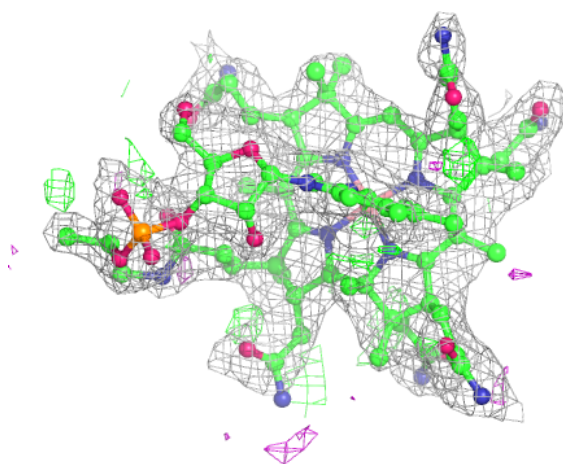
Electron density around GDP B 1003 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



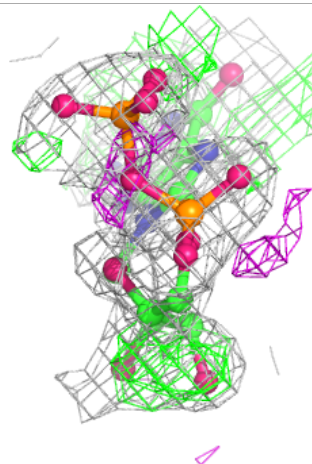
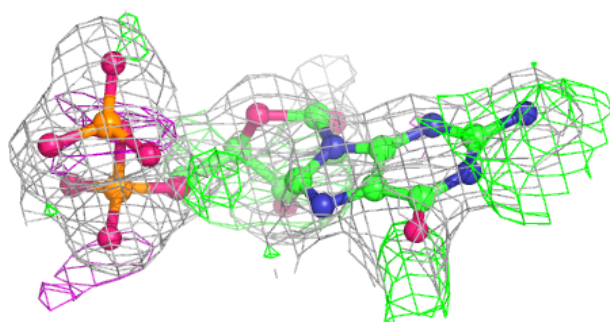
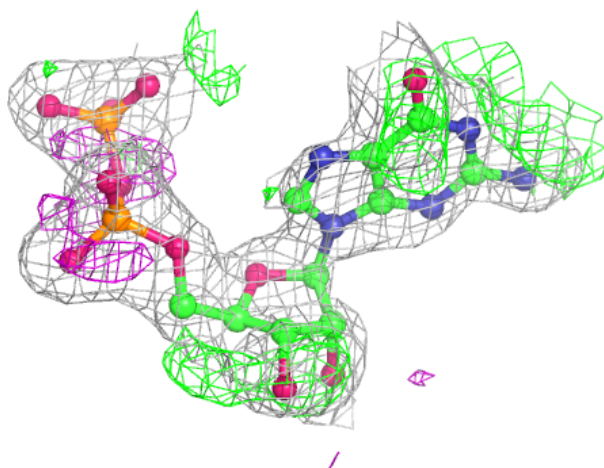
Electron density around B12 B 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



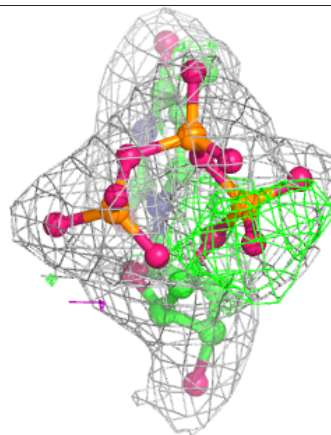
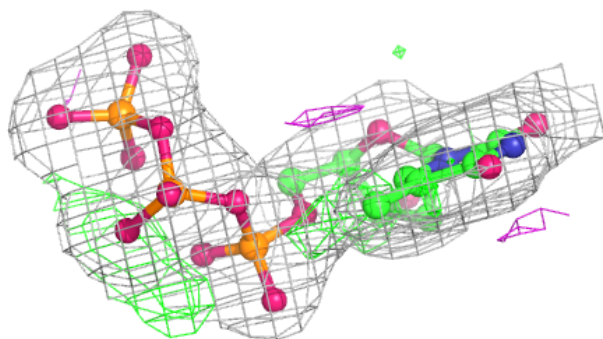
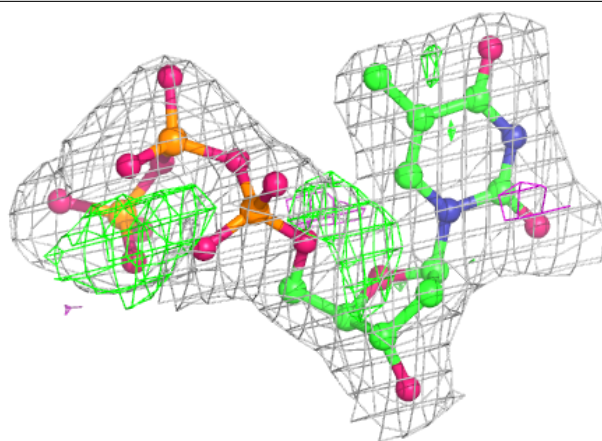
Electron density around GDP B 1003 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



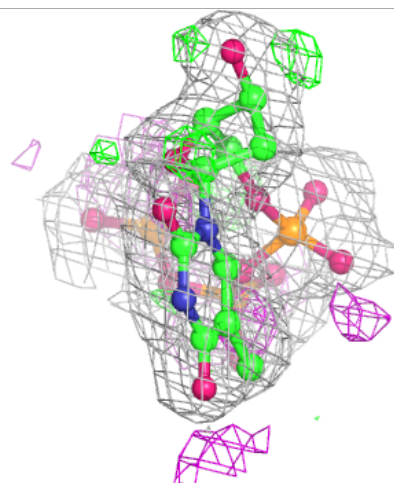
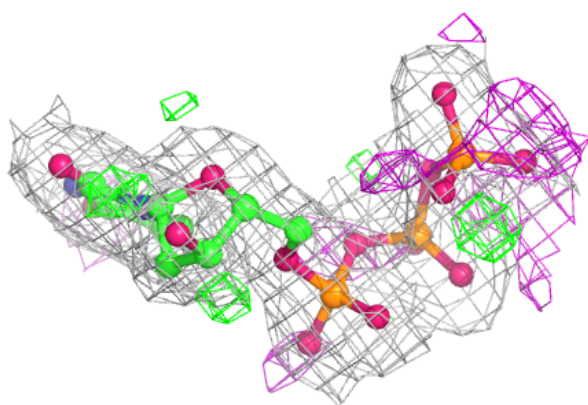
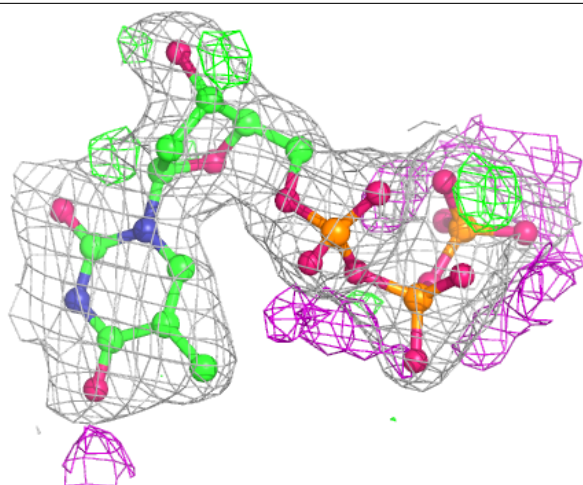
Electron density around TTP B 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TTP A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.