Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 05:16 PM EDT

PDB ID	:	3O0N
Title	:	Thermotoga maritima Ribonucleotide Reductase, NrdJ, in complex with dTTP and Adenosylcobalamin
Authors	:	Larsson, K.-M.; Logan, D.T.; Nordlund, P.
Deposited on	:	2010-07-19
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

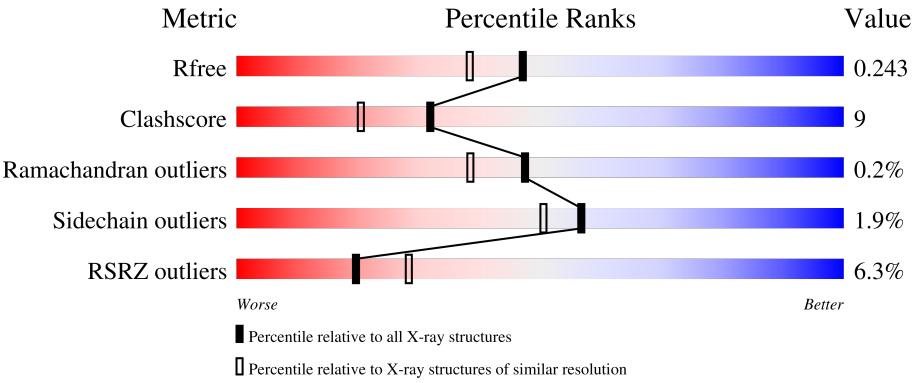
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	9% 74% 20% • 6%
1	B	644	3% 82% 13% 5%

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
6	B12	B	1003	X	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10466 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.

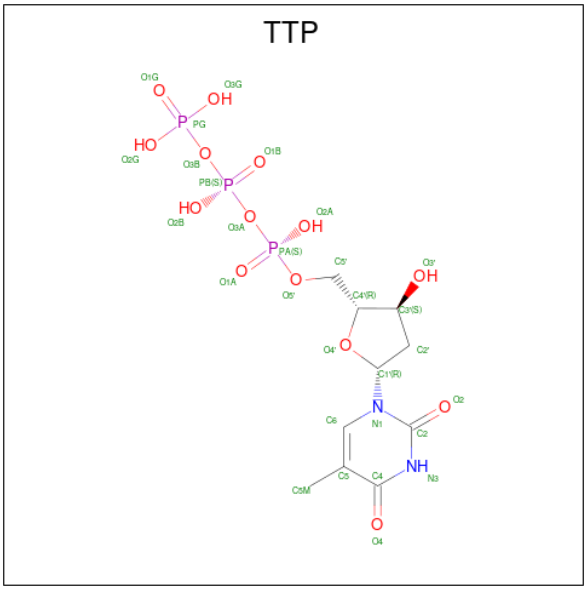
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4872	3127	824	901	20			
1	B	611	Total	C	N	O	S	0	0	0
			4910	3153	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 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 COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		

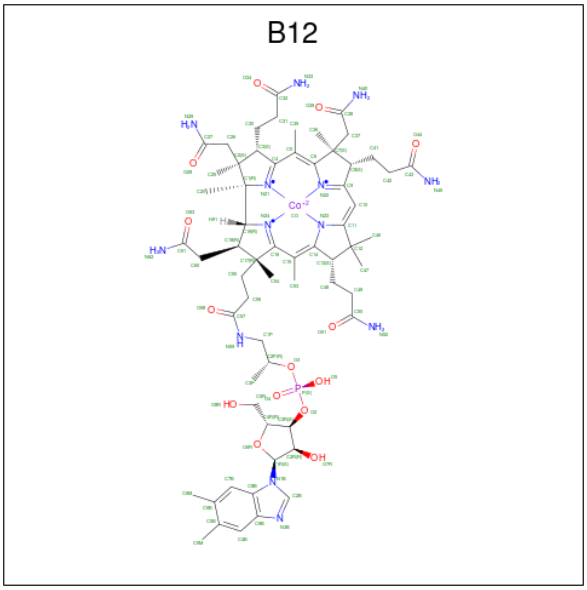
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

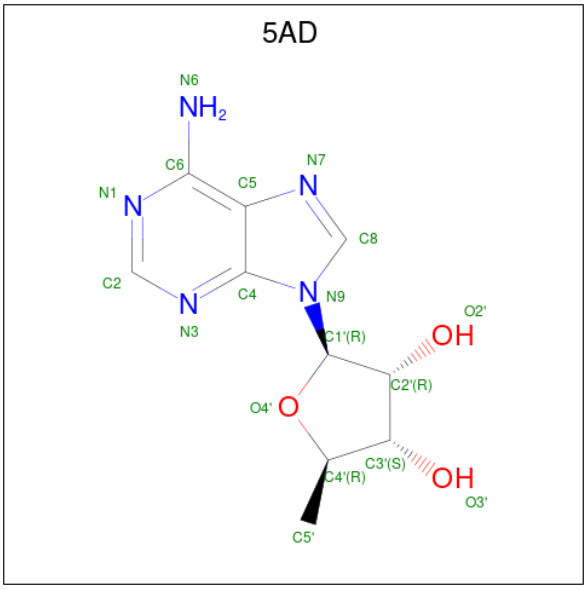
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	Co	N	O	P	4	0
			91	62	1	13	14	1		

- Molecule 7 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



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

- Molecule 8 is water.

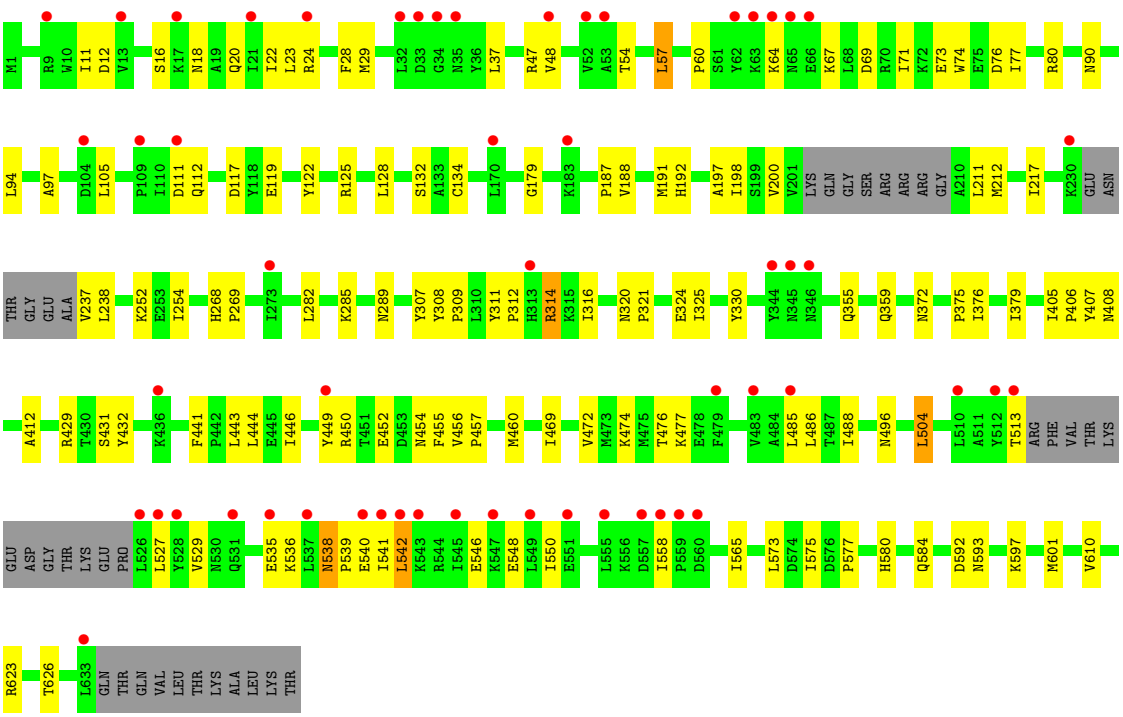
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	193	Total	O	0	0
			193	193		
8	B	320	Total	O	0	0
			320	320		

3 Residue-property plots (i)

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

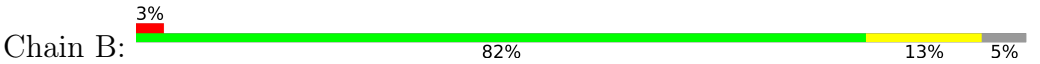
• Molecule 1: Ribonucleoside-diphosphate reductase

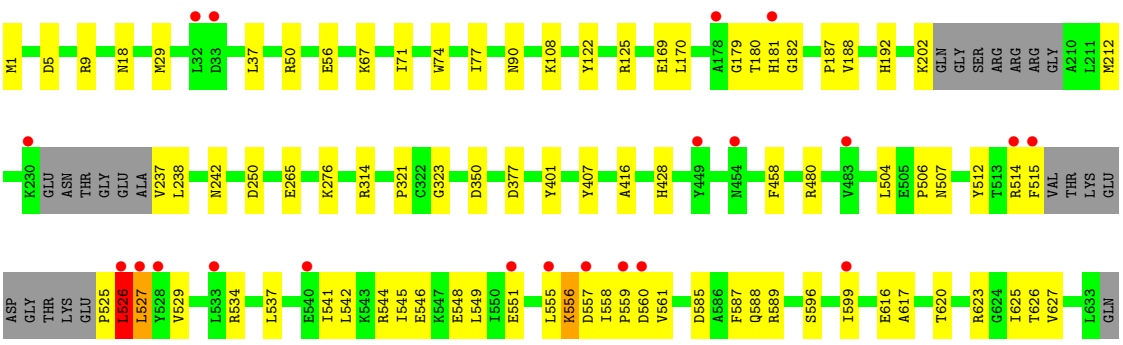
Chain A:



• Molecule 1: Ribonucleoside-diphosphate reductase

Chain B:





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	119.01Å 123.82Å 106.44Å 90.00° 103.10° 90.00°	Depositor
Resolution (Å)	19.97 – 1.95 19.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.97-1.95) 99.1 (19.97-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432), REFMAC	Depositor
R, R_{free}	0.203 , 0.249 0.197 , 0.243	Depositor DCC
R_{free} test set	5408 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10466	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TTP, 5AD, CL, B12, CO, MG

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	0.34	0/4968	0.49	0/6708
1	B	0.39	0/5008	0.54	0/6760
All	All	0.37	0/9976	0.52	0/13468

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4872	0	4926	103	0
1	B	4910	0	4969	60	0
2	A	29	0	13	1	0
2	B	29	0	13	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	91	0	86	22	0
7	B	18	0	13	3	0
8	A	193	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	320	0	0	8	0
All	All	10466	0	10020	177	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 9.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:HIS:HD2	1:B:480:ARG:HH22	1.09	0.96
1:A:237:VAL:HG13	1:A:238:LEU:H	1.30	0.94
1:B:237:VAL:HG23	1:B:238:LEU:H	1.34	0.92
1:A:314:ARG:HH11	1:A:314:ARG:HG3	1.35	0.91
1:B:428:HIS:CD2	1:B:480:ARG:HH22	1.97	0.82
1:A:314:ARG:HH11	1:A:314:ARG:CG	1.92	0.81
6:B:1003:B12:H552	6:B:1003:B12:H531	1.62	0.80
1:B:250:ASP:HB3	8:B:846:HOH:O	1.83	0.77
1:A:431:SER:HB2	1:A:485:LEU:HD21	1.69	0.75
1:B:525:PRO:O	1:B:526:LEU:HB2	1.85	0.74
1:B:212:MET:HB2	1:B:321:PRO:HA	1.69	0.73
6:B:1003:B12:N45	6:B:1003:B12:H363	2.03	0.73
1:A:324:GLU:HG2	1:A:325:ILE:HG12	1.72	0.71
1:A:592:ASP:HA	8:A:656:HOH:O	1.91	0.71
1:A:536:LYS:HG2	8:A:760:HOH:O	1.92	0.68
1:A:237:VAL:HG13	1:A:238:LEU:N	2.06	0.67
1:B:428:HIS:HD2	1:B:480:ARG:NH2	1.88	0.66
1:A:488:ILE:HG21	1:A:504:LEU:HG	1.76	0.66
1:B:242:ASN:HD21	6:B:1003:B12:C46	2.09	0.66
6:B:1003:B12:H8	6:B:1003:B12:O39	1.96	0.66
1:A:577:PRO:HG3	1:A:601:MET:HG2	1.78	0.66
1:A:212:MET:HB2	1:A:321:PRO:HA	1.78	0.66
1:A:237:VAL:CG1	1:A:238:LEU:H	2.09	0.65
6:B:1003:B12:H302	6:B:1003:B12:HM53	1.79	0.65
1:B:242:ASN:HD21	6:B:1003:B12:H461	1.62	0.65
1:B:512:TYR:HE1	1:B:514:ARG:HE	1.45	0.64
1:A:20:GLN:HB3	1:A:24:ARG:HH22	1.63	0.62
6:B:1003:B12:H451	6:B:1003:B12:C6	2.11	0.62
6:B:1003:B12:H552	6:B:1003:B12:C53	2.30	0.62
6:B:1003:B12:H601	6:B:1003:B12:H252	1.81	0.61
1:A:408:ASN:HB3	1:A:575:ILE:HG23	1.83	0.60
1:A:626:THR:HG23	8:A:810:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:PRO:HD2	8:B:844:HOH:O	2.02	0.60
1:A:486:LEU:O	1:A:593:ASN:HB2	2.02	0.60
6:B:1003:B12:N45	6:B:1003:B12:C4B	2.64	0.60
6:B:1003:B12:H362	6:B:1003:B12:H351	1.84	0.59
1:A:527:LEU:HD21	1:A:529:VAL:HG23	1.85	0.59
1:B:559:PRO:O	1:B:560:ASP:HB2	2.03	0.58
1:A:76:ASP:O	1:A:80:ARG:HG3	2.04	0.58
1:B:544:ARG:HH11	1:B:560:ASP:HB3	1.69	0.56
1:A:74:TRP:HA	1:A:77:ILE:HG22	1.88	0.56
1:A:584:GLN:HB2	1:A:597:LYS:HG3	1.87	0.56
1:B:50:ARG:NH2	1:B:108:LYS:O	2.34	0.56
1:A:535:GLU:HB2	8:A:760:HOH:O	2.06	0.56
1:A:64:LYS:HD3	1:A:67:LYS:HD3	1.89	0.55
1:A:538:ASN:HD22	1:A:539:PRO:N	2.04	0.55
1:B:50:ARG:HH12	1:B:108:LYS:HB3	1.70	0.55
1:A:623:ARG:HD2	8:A:688:HOH:O	2.06	0.55
1:A:601:MET:CE	1:A:610:VAL:HG22	2.36	0.55
6:B:1003:B12:N24	7:B:1004:5AD:H5'1	2.22	0.55
1:A:128:LEU:HD11	1:B:179:GLY:HA2	1.88	0.55
1:A:11:ILE:HG23	1:A:12:ASP:OD1	2.07	0.54
1:A:308:TYR:HD1	1:A:309:PRO:HD2	1.72	0.54
1:A:407:TYR:HB2	8:A:822:HOH:O	2.05	0.54
1:A:455:PHE:HA	8:A:696:HOH:O	2.06	0.54
1:B:407:TYR:CZ	1:B:506:PRO:HD3	2.43	0.54
1:A:449:TYR:OH	1:A:457:PRO:HG3	2.08	0.54
1:A:314:ARG:HG3	1:A:314:ARG:NH1	2.14	0.53
1:A:538:ASN:HD22	1:A:539:PRO:HD2	1.73	0.53
1:A:601:MET:HE1	1:A:610:VAL:HG22	1.90	0.53
1:B:237:VAL:HG23	1:B:238:LEU:N	2.15	0.53
1:A:538:ASN:HD22	1:A:539:PRO:CD	2.22	0.52
1:A:308:TYR:CD2	1:A:316:ILE:HG13	2.44	0.52
1:A:472:VAL:O	1:A:476:THR:HG23	2.10	0.52
1:B:169:GLU:HG3	8:B:883:HOH:O	2.09	0.52
1:A:314:ARG:CG	1:A:314:ARG:NH1	2.61	0.51
1:A:48:VAL:HG21	1:A:94:LEU:HD23	1.92	0.51
1:B:616:GLU:O	1:B:620:THR:HG23	2.10	0.51
1:A:20:GLN:HB3	1:A:24:ARG:NH2	2.25	0.51
6:B:1003:B12:N23	7:B:1004:5AD:H5'1	2.26	0.51
1:B:541:ILE:O	1:B:545:ILE:HG12	2.11	0.50
1:A:450:ARG:NH1	1:A:477:LYS:O	2.44	0.50
1:A:469:ILE:HA	1:A:472:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1003:B12:C4B	6:B:1003:B12:H452	2.25	0.50
1:A:538:ASN:HD22	1:A:538:ASN:C	2.13	0.50
1:A:198:ILE:HG13	1:A:211:LEU:HD11	1.94	0.50
6:B:1003:B12:H531	6:B:1003:B12:C55	2.34	0.49
1:A:452:GLU:OE1	1:A:455:PHE:HB2	2.12	0.49
1:A:29:MET:HG2	1:A:37:LEU:HD12	1.94	0.49
1:A:542:LEU:HD22	1:A:542:LEU:O	2.13	0.49
1:A:407:TYR:CD1	1:A:575:ILE:HD13	2.48	0.48
1:B:527:LEU:HD23	1:B:529:VAL:HG23	1.95	0.48
1:A:406:PRO:O	1:A:412:ALA:HB2	2.13	0.48
1:A:57:LEU:HD21	1:A:119:GLU:HA	1.95	0.48
1:A:69:ASP:O	1:A:73:GLU:HG3	2.13	0.48
1:A:592:ASP:O	1:A:623:ARG:NH2	2.47	0.48
1:A:623:ARG:NH1	8:A:656:HOH:O	2.22	0.47
1:A:307:TYR:HE2	8:A:697:HOH:O	1.96	0.47
1:A:217:ILE:HG13	1:A:217:ILE:O	2.14	0.47
1:A:542:LEU:O	1:A:546:GLU:HB3	2.14	0.47
1:B:401:TYR:CE2	1:B:507:ASN:ND2	2.82	0.47
1:B:188:VAL:O	1:B:192:HIS:HD2	1.98	0.47
1:A:320:ASN:HB2	1:A:321:PRO:HD2	1.95	0.47
1:A:454:ASN:HD22	1:A:474:LYS:NZ	2.12	0.47
1:B:537:LEU:HD23	1:B:542:LEU:HD13	1.94	0.47
1:A:355:GLN:O	1:A:359:GLN:HG3	2.14	0.47
1:B:265:GLU:OE1	1:B:276:LYS:HG3	2.14	0.47
1:A:454:ASN:ND2	1:A:474:LYS:NZ	2.63	0.46
1:A:314:ARG:HD3	8:A:823:HOH:O	2.15	0.46
1:B:529:VAL:HB	1:B:534:ARG:HH22	1.78	0.46
1:B:377:ASP:HB2	8:B:865:HOH:O	2.15	0.46
1:B:555:LEU:O	1:B:556:LYS:C	2.54	0.46
1:A:105:LEU:HD21	1:A:117:ASP:OD1	2.15	0.46
1:A:187:PRO:O	1:A:191:MET:HG3	2.16	0.46
1:B:537:LEU:HD21	1:B:545:ILE:HD11	1.97	0.46
1:B:542:LEU:O	1:B:546:GLU:HB2	2.16	0.46
6:B:1003:B12:H202	6:B:1003:B12:C9B	2.46	0.46
1:B:323:GLY:HA3	7:B:1004:5AD:H2	1.99	0.45
1:B:599:ILE:HB	1:B:627:VAL:HG12	1.98	0.45
1:A:188:VAL:O	1:A:192:HIS:HD2	1.99	0.45
1:B:9:ARG:O	1:B:9:ARG:HD3	2.17	0.45
1:A:22:ILE:CD1	1:A:496:ASN:HB3	2.47	0.45
1:B:515:PHE:CD2	1:B:525:PRO:HB3	2.52	0.45
1:A:513:THR:HA	1:A:527:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HB3	1:B:350:ASP:OD1	2.16	0.45
1:A:429:ARG:O	1:A:432:TYR:HB3	2.17	0.45
1:B:416:ALA:HB1	1:B:587:PHE:CE2	2.52	0.44
1:A:443:LEU:HD22	1:A:446:ILE:HD11	2.00	0.44
1:A:122:TYR:O	1:A:125:ARG:HD3	2.18	0.44
1:A:128:LEU:CD1	1:B:179:GLY:HA2	2.47	0.44
1:B:242:ASN:ND2	6:B:1003:B12:C46	2.79	0.44
1:A:197:ALA:O	1:A:200:VAL:HG22	2.18	0.43
1:A:285:LYS:HE3	1:A:285:LYS:HB2	1.82	0.43
1:B:545:ILE:HG21	1:B:561:VAL:CG2	2.48	0.43
1:B:585:ASP:O	1:B:589:ARG:HG3	2.19	0.43
1:A:252:LYS:HB2	1:A:252:LYS:NZ	2.34	0.43
1:A:527:LEU:C	1:A:527:LEU:HD23	2.38	0.43
1:B:314:ARG:HD3	8:B:755:HOH:O	2.18	0.43
1:A:134:CYS:HB3	1:A:320:ASN:HB3	2.01	0.43
1:A:529:VAL:HG21	1:A:542:LEU:HD21	2.01	0.43
1:B:242:ASN:ND2	6:B:1003:B12:H463	2.33	0.43
1:B:548:GLU:OE1	1:B:558:ILE:HG23	2.19	0.43
1:B:623:ARG:HD2	8:B:650:HOH:O	2.18	0.43
1:A:580:HIS:ND1	1:A:597:LYS:NZ	2.67	0.43
1:A:538:ASN:HB3	1:A:541:ILE:HG13	2.01	0.43
1:A:47:ARG:HD2	1:A:97:ALA:O	2.18	0.43
1:A:527:LEU:CD1	1:A:550:ILE:HD11	2.49	0.43
1:A:16:SER:OG	1:A:18:ASN:HB3	2.18	0.42
1:A:54:THR:O	1:A:57:LEU:HB2	2.18	0.42
1:B:428:HIS:CD2	1:B:480:ARG:HH12	2.37	0.42
1:A:268:HIS:ND1	1:A:269:PRO:HD2	2.33	0.42
1:A:456:VAL:HG11	1:A:460:MET:HE2	2.01	0.42
1:B:67:LYS:O	1:B:71:ILE:HG13	2.20	0.42
1:A:64:LYS:HD3	1:A:64:LYS:HA	1.83	0.42
1:A:311:TYR:CD1	1:A:312:PRO:HA	2.55	0.42
1:B:321:PRO:HD2	8:B:653:HOH:O	2.20	0.42
1:A:254:ILE:HD13	1:A:254:ILE:HA	1.92	0.42
1:A:548:GLU:OE2	1:A:558:ILE:HG12	2.19	0.42
1:B:56:GLU:HB2	1:B:71:ILE:HG12	2.02	0.42
1:B:549:LEU:HD13	1:B:555:LEU:HD23	2.01	0.42
1:B:74:TRP:HA	1:B:77:ILE:HG22	2.02	0.41
1:A:23:LEU:HB3	1:A:28:PHE:CZ	2.55	0.41
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.81	0.41
1:B:588:GLN:CD	1:B:623:ARG:HD3	2.40	0.41
1:B:180:THR:C	1:B:182:GLY:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:PRO:C	1:A:376:ILE:HG13	2.40	0.41
1:A:268:HIS:CG	1:A:269:PRO:HD2	2.56	0.41
1:A:504:LEU:HD11	1:A:597:LYS:HG2	2.01	0.41
1:B:626:THR:HG23	6:B:1003:B12:H402	1.84	0.41
1:A:573:LEU:HD23	1:A:573:LEU:HA	1.90	0.41
6:B:1003:B12:N45	6:B:1003:B12:H4B	2.35	0.41
1:A:67:LYS:O	1:A:71:ILE:HG13	2.20	0.41
1:A:111:ASP:OD1	1:A:112:GLN:HG3	2.21	0.41
1:B:170:LEU:HD12	1:B:187:PRO:HA	2.03	0.41
1:B:617:ALA:CB	1:B:625:ILE:HG13	2.51	0.41
1:A:330:TYR:O	1:A:379:ILE:HA	2.21	0.40
1:A:441:PHE:CZ	1:A:444:LEU:HA	2.56	0.40
1:A:538:ASN:ND2	1:A:540:GLU:H	2.19	0.40
1:B:626:THR:HG21	8:B:953:HOH:O	2.20	0.40
1:A:132:SER:OG	1:A:372:ASN:ND2	2.54	0.40
1:A:179:GLY:HA3	2:A:1001:TTP:O1B	2.21	0.40
6:B:1003:B12:H4B	6:B:1003:B12:C4	2.51	0.40
1:A:405:ILE:HA	1:A:406:PRO:HD3	1.98	0.40
1:B:29:MET:HG2	1:B:37:LEU:HD12	2.03	0.40
1:B:122:TYR:O	1:B:125:ARG:HD3	2.21	0.40
1:B:626:THR:CG2	6:B:1003:B12:N40	2.84	0.40
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.94	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	599/644 (93%)	580 (97%)	19 (3%)	0	100	100
1	B	603/644 (94%)	579 (96%)	21 (4%)	3 (0%)	29	17
All	All	1202/1288 (93%)	1159 (96%)	40 (3%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	526	LEU
1	B	556	LYS
1	B	181	HIS

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	535/566 (94%)	526 (98%)	9 (2%)	60	55
1	B	539/566 (95%)	528 (98%)	11 (2%)	55	48
All	All	1074/1132 (95%)	1054 (98%)	20 (2%)	57	50

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	60	PRO
1	A	90	ASN
1	A	289	ASN
1	A	314	ARG
1	A	504	LEU
1	A	538	ASN
1	A	542	LEU
1	A	565	ILE
1	B	5	ASP
1	B	18	ASN
1	B	90	ASN
1	B	202	LYS
1	B	458	PHE
1	B	504	LEU
1	B	526	LEU
1	B	527	LEU
1	B	551	GLU
1	B	557	ASP
1	B	596	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	90	ASN
1	A	192	HIS
1	A	355	GLN
1	A	359	GLN
1	A	454	ASN
1	A	531	GLN
1	A	538	ASN
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	242	ASN
1	B	345	ASN
1	B	359	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
2	TTP	B	1001	5	26,30,30	1.26	6 (23%)	39,47,47	1.87	8 (20%)
6	B12	B	1003	7	90,101,101	1.02	5 (5%)	137,166,166	1.54	12 (8%)
7	5AD	B	1004	6	17,20,20	1.85	5 (29%)	15,30,30	3.07	4 (26%)
2	TTP	A	1001	5	26,30,30	1.25	5 (19%)	39,47,47	2.03	9 (23%)

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	B	1001	5	-	7/22/34/34	0/2/2/2
6	B12	B	1003	7	1/1/36/38	14/52/223/223	0/3/11/11
7	5AD	B	1004	6	-	0/0/20/20	0/3/3/3
2	TTP	A	1001	5	-	4/22/34/34	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1004	5AD	C2-N3	4.84	1.39	1.32
6	B	1003	B12	C5M-C5B	-3.67	1.43	1.51
6	B	1003	B12	C53-C15	3.44	1.58	1.50
6	B	1003	B12	C14-N23	3.16	1.39	1.35
6	B	1003	B12	C6B-C5B	3.07	1.48	1.40
7	B	1004	5AD	C2-N1	3.06	1.39	1.33
2	A	1001	TTP	C6-C5	2.92	1.39	1.34
2	B	1001	TTP	C6-C5	2.83	1.39	1.34
2	B	1001	TTP	C4-N3	-2.74	1.33	1.38
6	B	1003	B12	C48-C13	2.71	1.60	1.54
7	B	1004	5AD	C5-C4	-2.62	1.34	1.40
2	A	1001	TTP	C4-N3	-2.58	1.34	1.38
7	B	1004	5AD	C6-C5	-2.47	1.34	1.43
2	A	1001	TTP	C2-N1	2.34	1.42	1.38
2	A	1001	TTP	C4-C5	2.32	1.48	1.44
7	B	1004	5AD	O4'-C1'	2.09	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	TTP	C4-C5	2.08	1.48	1.44
2	B	1001	TTP	C2-N1	2.05	1.41	1.38
2	A	1001	TTP	C6-N1	-2.03	1.34	1.38
2	B	1001	TTP	C6-N1	-2.02	1.34	1.38
2	B	1001	TTP	C2-N3	-2.01	1.34	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1003	B12	C1-C19-N24	8.47	115.77	106.24
7	B	1004	5AD	C5'-C4'-C3'	-7.91	107.39	115.70
6	B	1003	B12	C1-C19-C18	7.61	134.37	121.88
7	B	1004	5AD	N3-C2-N1	-7.03	117.70	128.68
2	A	1001	TTP	C4-N3-C2	-5.36	120.42	127.35
2	A	1001	TTP	N3-C2-N1	5.14	121.71	114.89
6	B	1003	B12	C18-C19-N24	4.88	109.73	102.31
2	A	1001	TTP	C5-C4-N3	4.66	119.29	115.31
2	B	1001	TTP	N3-C2-N1	4.63	121.03	114.89
2	B	1001	TTP	C4-N3-C2	-4.50	121.53	127.35
2	B	1001	TTP	PB-O3B-PG	-4.40	117.71	132.83
6	B	1003	B12	C20-C1-C19	-4.35	105.16	109.36
7	B	1004	5AD	C1'-N9-C4	-3.82	119.92	126.64
2	B	1001	TTP	C5-C4-N3	3.78	118.53	115.31
2	B	1001	TTP	C5-C6-N1	-3.65	119.59	123.34
2	A	1001	TTP	O4-C4-C5	-3.62	120.70	124.90
2	A	1001	TTP	C5-C6-N1	-3.60	119.63	123.34
2	A	1001	TTP	PB-O3B-PG	-3.49	120.84	132.83
6	B	1003	B12	C48-C13-C12	3.44	126.28	116.63
6	B	1003	B12	C7-C37-C38	3.33	124.26	114.25
2	B	1001	TTP	PB-O3A-PA	-3.21	121.81	132.83
6	B	1003	B12	O6R-C4R-C3R	3.14	111.59	104.87
6	B	1003	B12	O6R-C1R-C2R	2.94	111.22	106.93
2	B	1001	TTP	O4-C4-C5	-2.81	121.64	124.90
6	B	1003	B12	C7B-C8B-C9B	2.76	123.27	120.54
6	B	1003	B12	O6R-C4R-C5R	2.74	115.14	109.21
6	B	1003	B12	C18-C17-C16	2.70	103.95	100.67
2	A	1001	TTP	O3G-PG-O3B	2.47	112.92	104.64
2	B	1001	TTP	O3G-PG-O3B	2.25	112.18	104.64
2	A	1001	TTP	O2-C2-N1	-2.22	119.83	122.79
7	B	1004	5AD	C3'-C2'-C1'	2.20	104.28	100.98
6	B	1003	B12	C2-C1-C19	2.07	121.87	118.60
2	A	1001	TTP	C5M-C5-C4	2.03	121.00	118.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1003	B12	C19

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	TTP	C5'-O5'-PA-O1A
6	B	1003	B12	C38-C37-C7-C6
6	B	1003	B12	C38-C37-C7-C36
6	B	1003	B12	C38-C37-C7-C8
6	B	1003	B12	C42-C41-C8-C9
6	B	1003	B12	C16-C17-C55-C56
6	B	1003	B12	C18-C17-C55-C56
6	B	1003	B12	C2P-O3-P-O2
6	B	1003	B12	C54-C17-C55-C56
6	B	1003	B12	C18-C60-C61-O63
6	B	1003	B12	C8-C41-C42-C43
6	B	1003	B12	C2-C3-C30-C31
6	B	1003	B12	C4-C3-C30-C31
6	B	1003	B12	C18-C60-C61-N62
2	B	1001	TTP	C5'-O5'-PA-O3A
2	B	1001	TTP	PG-O3B-PB-O2B
2	B	1001	TTP	C5'-O5'-PA-O2A
2	A	1001	TTP	PA-O3A-PB-O2B
2	B	1001	TTP	PA-O3A-PB-O2B
2	A	1001	TTP	C5'-O5'-PA-O3A
2	A	1001	TTP	PA-O3A-PB-O1B
2	B	1001	TTP	PA-O3A-PB-O1B
2	B	1001	TTP	PG-O3B-PB-O1B
2	A	1001	TTP	C5'-O5'-PA-O2A
6	B	1003	B12	C41-C42-C43-O44

There are no ring outliers.

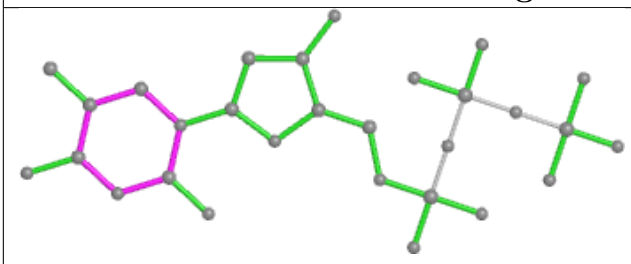
3 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1003	B12	22	0
7	B	1004	5AD	3	0
2	A	1001	TTP	1	0

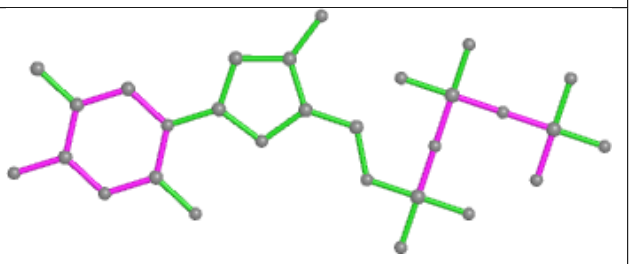
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

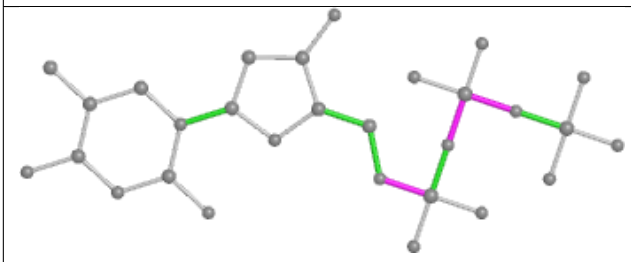
Ligand TTP B 1001



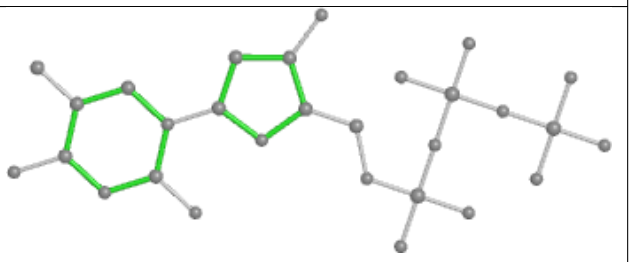
Bond lengths



Bond angles

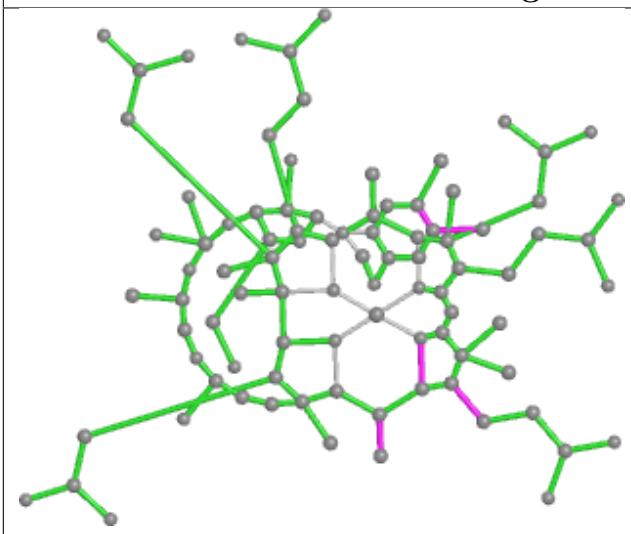


Torsions

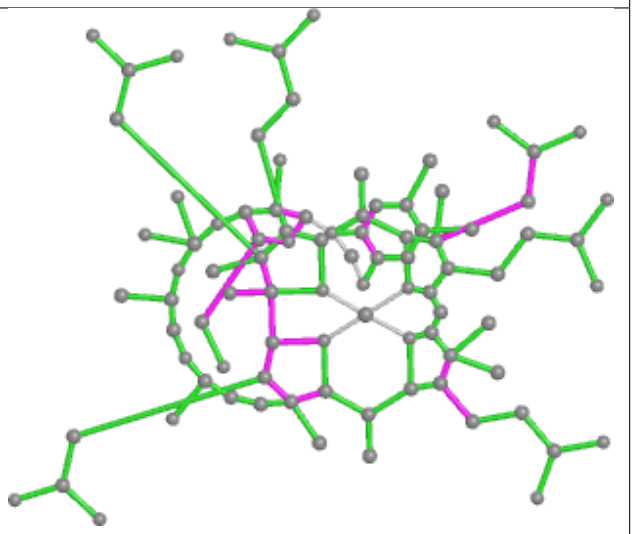


Rings

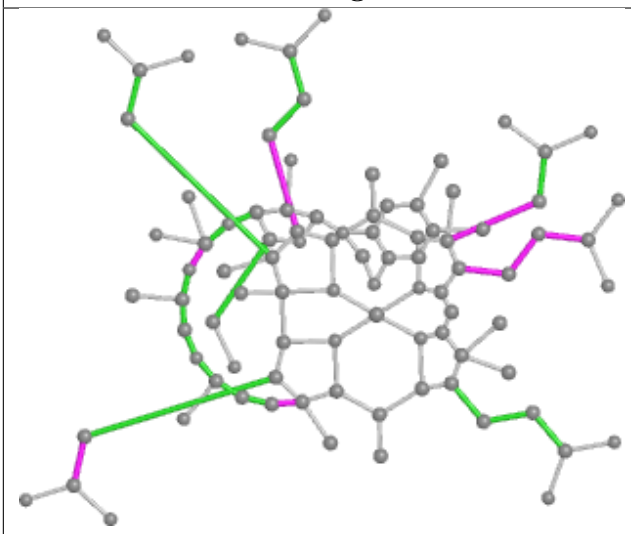
Ligand B12 B 1003



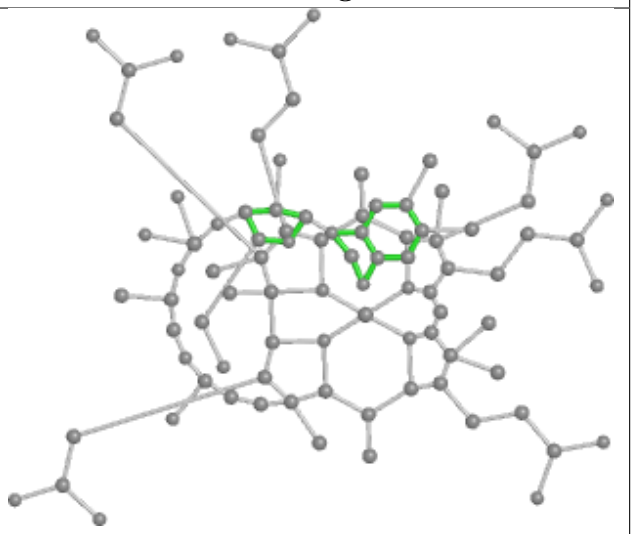
Bond lengths



Bond angles

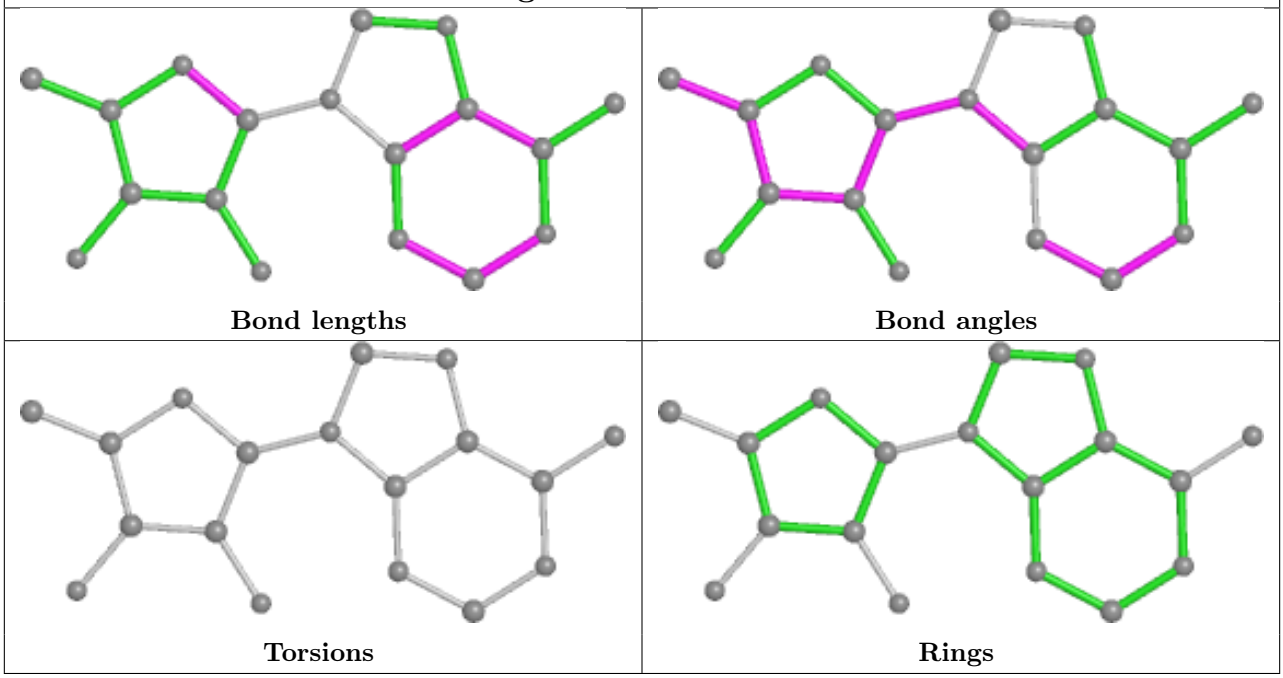


Torsions

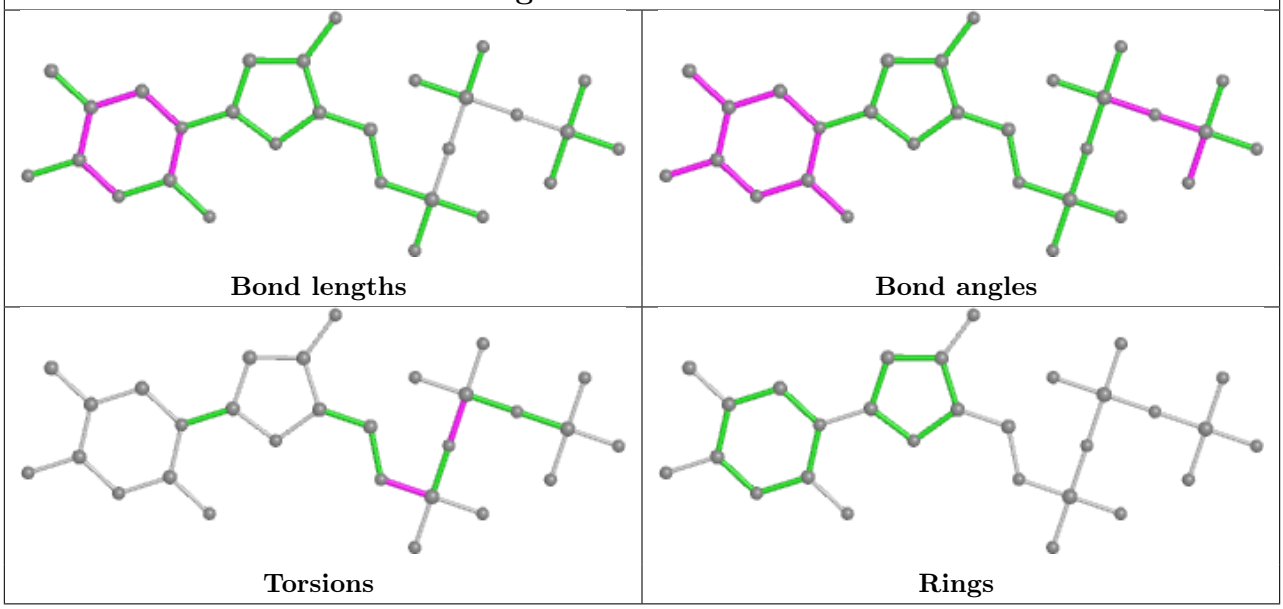


Rings

Ligand 5AD B 1004



Ligand TTP A 1001



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	607/644 (94%)	0.33	56 (9%)	9	14	27, 56, 103, 152	0
1	B	611/644 (94%)	-0.01	21 (3%)	45	55	25, 41, 87, 118	0
All	All	1218/1288 (94%)	0.16	77 (6%)	20	28	25, 48, 96, 152	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	LEU	8.5
1	A	65	ASN	5.1
1	A	64	LYS	4.9
1	A	32	LEU	4.7
1	A	527	LEU	4.4
1	A	543	LYS	4.3
1	A	62	TYR	4.2
1	A	513	THR	4.2
1	A	33	ASP	3.9
1	B	32	LEU	3.8
1	A	540	GLU	3.8
1	B	528	TYR	3.7
1	A	34	GLY	3.7
1	B	540	GLU	3.7
1	A	111	ASP	3.7
1	A	35	ASN	3.6
1	A	53	ALA	3.6
1	B	526	LEU	3.5
1	A	104	ASP	3.2
1	A	510	LEU	3.2
1	A	449	TYR	3.2
1	B	181	HIS	3.2
1	A	551	GLU	3.2
1	B	515	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	633	LEU	3.1
1	A	66	GLU	3.0
1	B	527	LEU	3.0
1	A	48	VAL	3.0
1	B	483	VAL	2.9
1	B	230	LYS	2.9
1	A	13	VAL	2.9
1	B	33	ASP	2.9
1	A	512	TYR	2.9
1	A	559	PRO	2.9
1	A	531	GLN	2.8
1	A	528	TYR	2.8
1	A	555	LEU	2.7
1	A	436	LYS	2.7
1	A	346	ASN	2.7
1	A	17	LYS	2.7
1	A	24	ARG	2.6
1	A	63	LYS	2.6
1	A	183	LYS	2.6
1	A	479	PHE	2.6
1	B	449	TYR	2.5
1	A	9	ARG	2.5
1	A	558	ILE	2.5
1	A	560	ASP	2.4
1	A	545	ILE	2.4
1	A	547	LYS	2.4
1	A	21	ILE	2.4
1	B	514	ARG	2.4
1	A	230	LYS	2.4
1	A	273	ILE	2.3
1	B	599	ILE	2.3
1	A	345	ASN	2.3
1	B	551	GLU	2.3
1	A	535	GLU	2.2
1	B	178	ALA	2.2
1	A	313	HIS	2.2
1	A	549	LEU	2.2
1	A	542	LEU	2.2
1	A	537	LEU	2.2
1	B	533	LEU	2.2
1	B	557	ASP	2.2
1	A	344	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	109	PRO	2.1
1	B	559	PRO	2.1
1	B	454	ASN	2.1
1	B	555	LEU	2.1
1	B	560	ASP	2.1
1	A	483	VAL	2.1
1	A	557	ASP	2.1
1	A	541	ILE	2.1
1	A	170	LEU	2.0
1	A	52	VAL	2.0
1	A	485	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 monosaccharides in this entry.

6.4 Ligands (i)

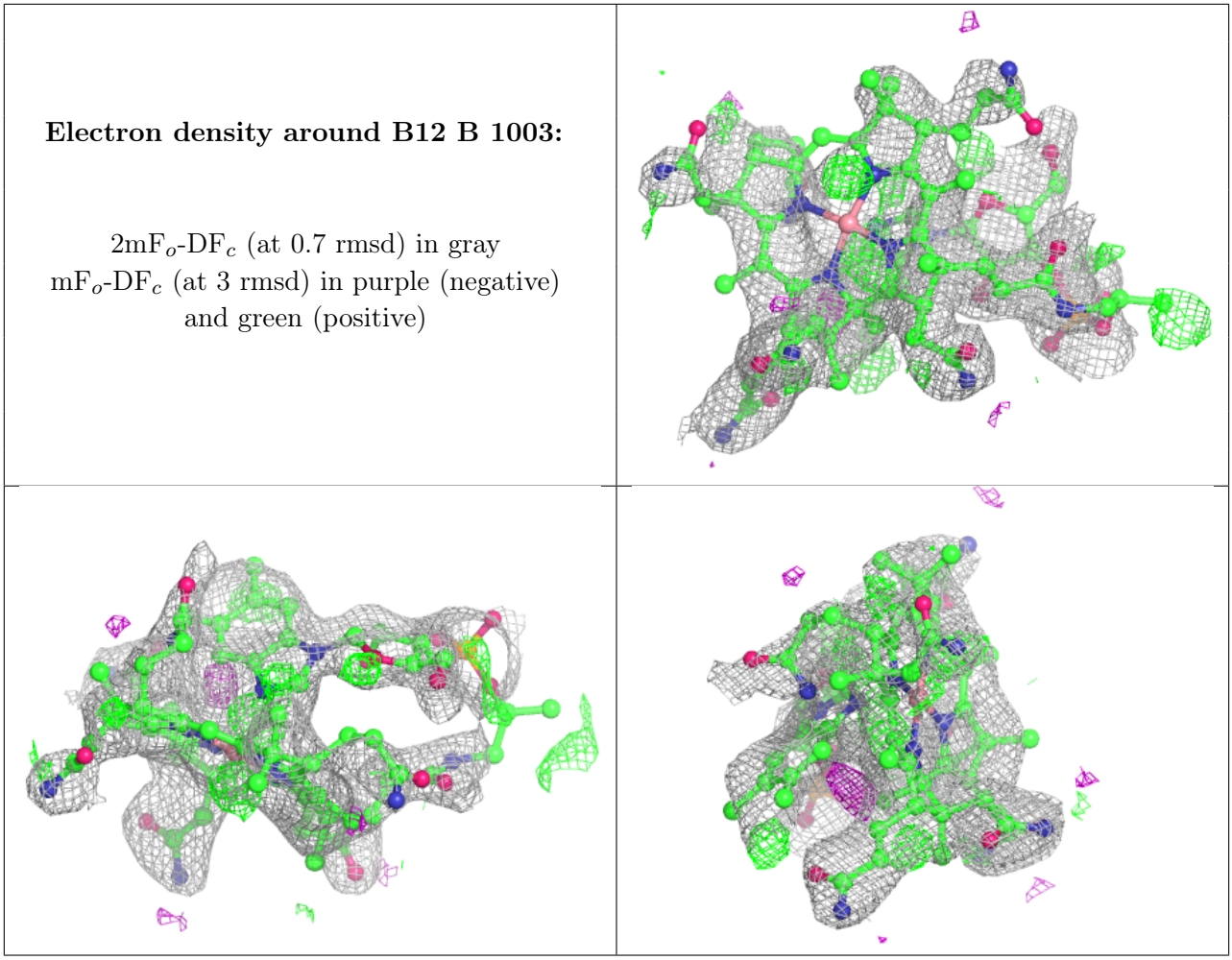
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	B	1002	1/1	0.90	0.07	46,46,46,46	0
6	B12	B	1003	91/91	0.91	0.17	30,68,95,143	30
7	5AD	B	1004	18/18	0.91	0.19	33,59,73,74	10
2	TTP	B	1001	29/29	0.94	0.10	26,39,68,76	0
5	MG	A	1002	1/1	0.95	0.04	33,33,33,33	0
3	CO	A	1003	1/1	0.96	0.04	89,89,89,89	0
2	TTP	A	1001	29/29	0.97	0.08	26,38,46,52	0
4	CL	A	1004	1/1	0.99	0.14	48,48,48,48	1

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.

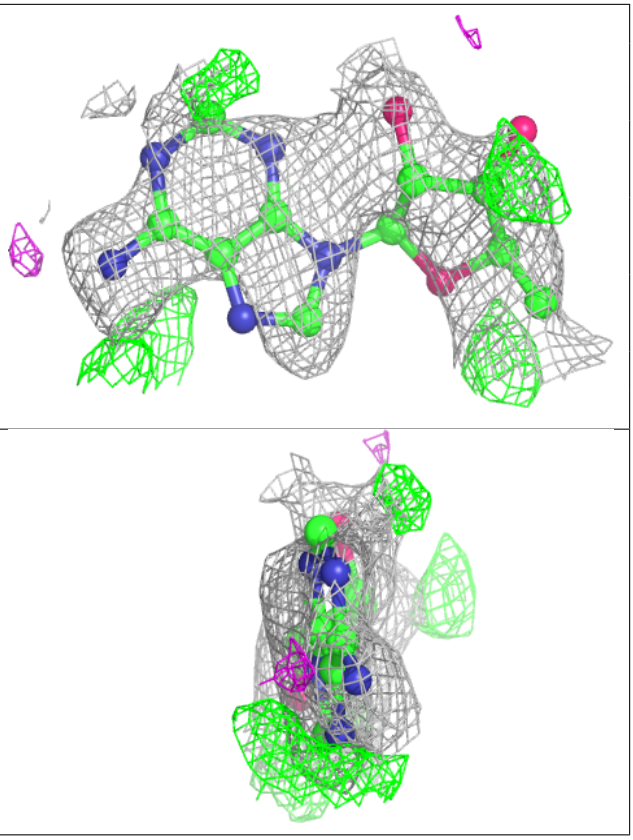
Electron density around B12 B 1003:

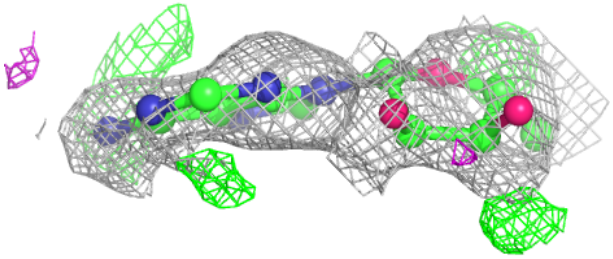
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 5AD B 1004:

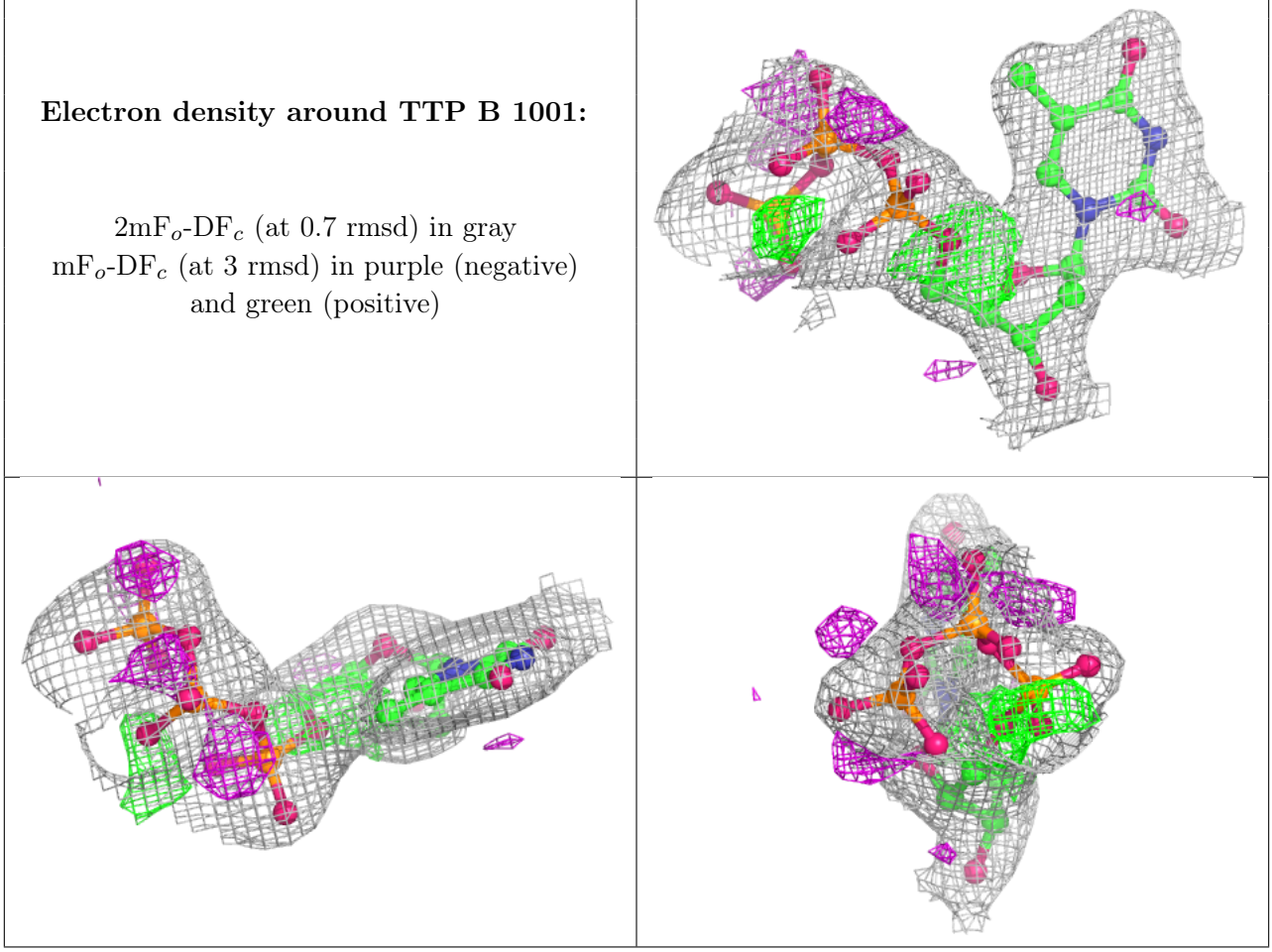
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





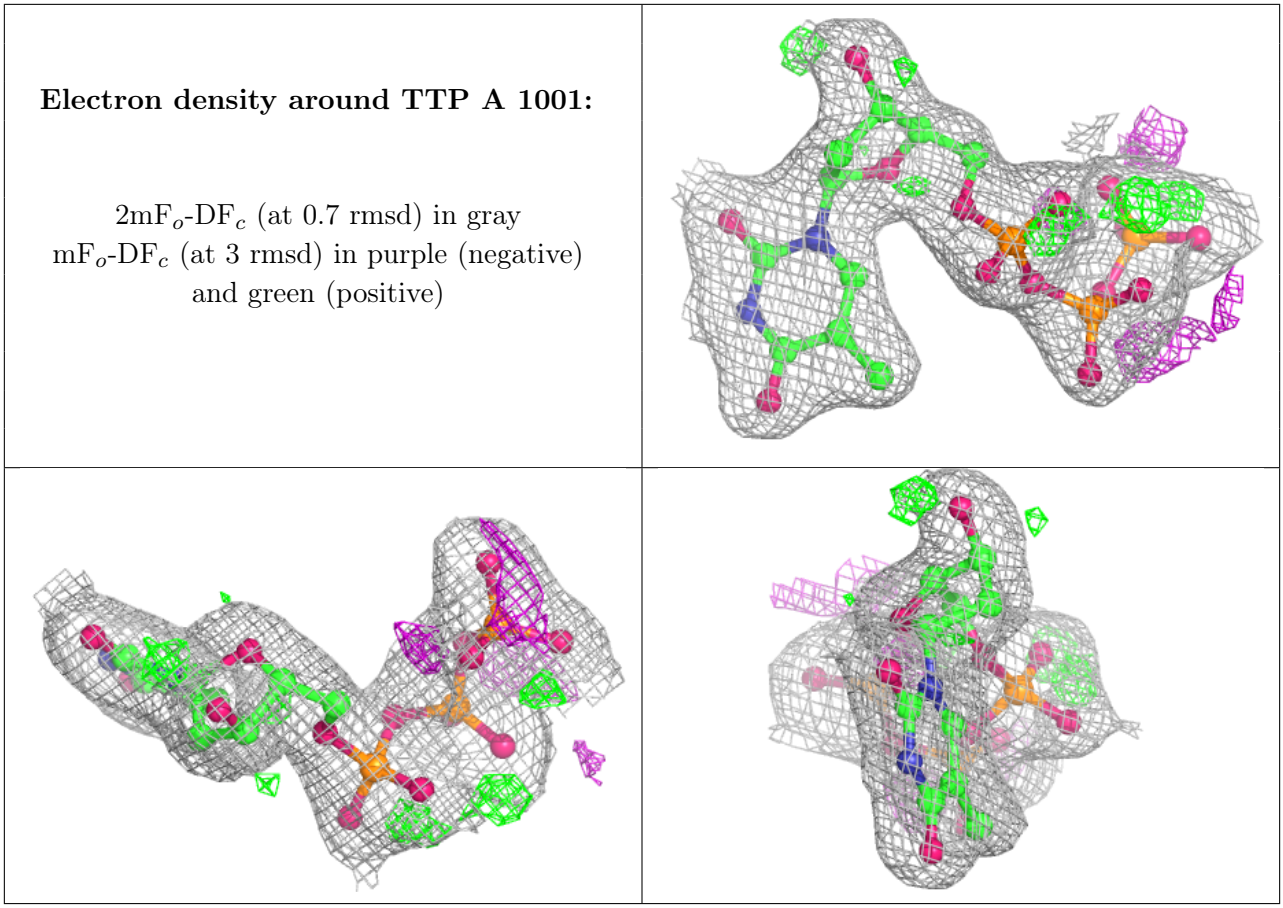
Electron density around TTP B 1001:

$2mF_o$-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

There are no such residues in this entry.