



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 12:44 am BST

PDB ID : 3HNC  
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effector TTP  
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.  
Deposited on : 2009-05-31  
Resolution : 2.41 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

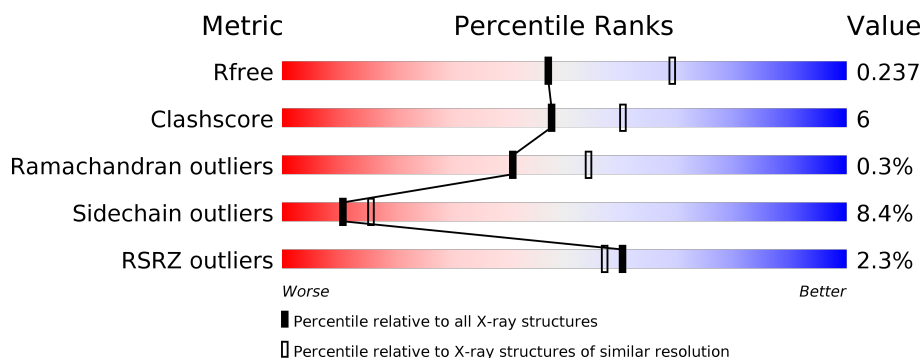
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	792	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	792	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11778 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.

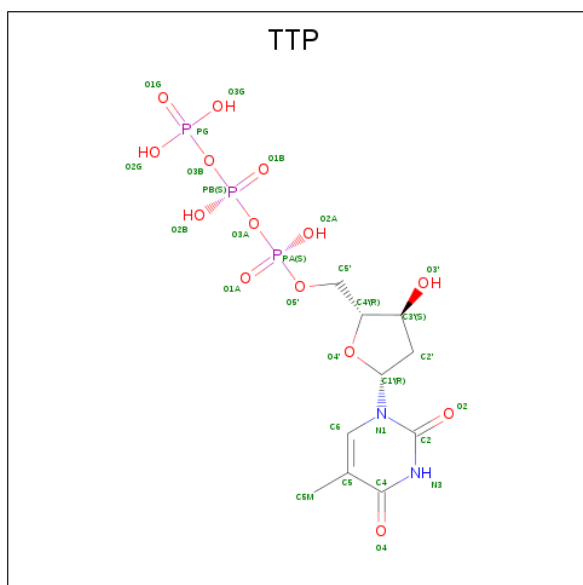
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	6	0	0
			5577	3567	926	1052	32			
1	B	738	Total	C	N	O	S	0	0	0
			5751	3669	968	1080	34			

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

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

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

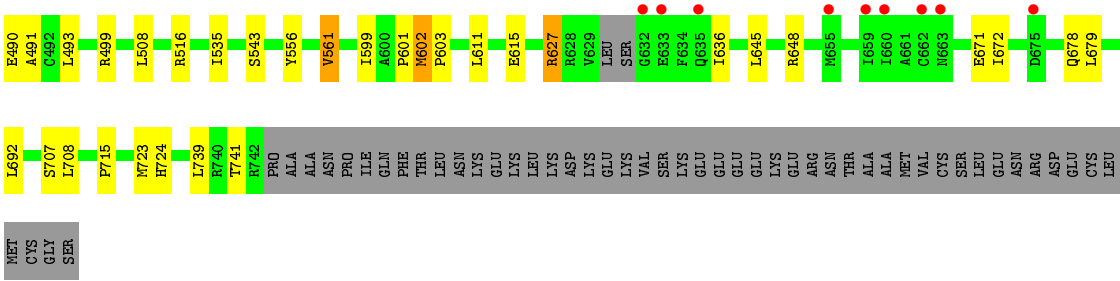
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	187	Total	O	0	0
			187	187		
5	B	173	Total	O	0	0
			173	173		

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 ( $\text{RSRZ} > 2$ ). 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:
- 
- 2% 74% 14% 10%
- 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100
- GLU LYS ARG ASN THR ALA MET VAL CYS LEU GLN ASP CYS LEU MET CYS GLY SER
- BE53 BE54 BE55 T669 P670 BE71 BE72 L679 V683 L692 K693 D703 L708 N709 I710 N716 L720 H724 M736 Y737 Y738 L739 R740 R741 R742 PRO ALA ASN ASN PRO ILE GLN PHE THR LEU ASN LYS GLU LYS LEU LYS ASP LYS GLU VAL SER LYS VAL LYS GLU CYS
- K149 L306 L449 V455 T456 S457 E458 V472 V473 V474 N478 D482 I483 N484 A491 C492 L493 H498 R499 L508 K529 E533 T534 I535 A539 Q577 G578 R579 T585 Y586 V581 L593 R594 N595 I599 S606 T607 T621 S631 V637 L642 H652
- HIS VAL ILE LYS ARG ASP GLY ARG GLN GLU ARG VAL F14 F15 I18 R21 I22 Y27 D35 Q38 R41 K42 V43 I44 L47 G50 V51 T52 T53 L56 L59 L67 I76 A79 R80 V83 V93 L121 L125 D140 K149 R153 Q168 L171 L192 T199 Q214 L215 S216 S217 C218 F219 L220 L221 S222 S223 K224 K243 I248 V252 T255 I256 S260 N270 P274 T275 L276 N281 T282 A283 R284 Y285 T286 P403 D287 Q288 G289 A296 F297 Y300 T301
- K149 L306 L449 V455 T456 S457 E458 V472 V473 V474 N478 D482 I483 N484 A491 C492 L493 H498 R499 L508 K529 E533 T534 I535 A539 Q577 G578 R579 T585 Y586 V581 L593 R594 N595 I599 S606 T607 T621 S631 V637 L642 H652
- HIS VAL ILE LYS ARG ASP GLY ARG GLN GLU ARG VAL F14 F15 I18 R21 I22 Y27 D35 Q38 R41 K42 V43 I44 L47 G50 V51 T52 T53 L56 L59 L67 I76 A79 R80 V83 V93 L121 L125 D140 K149 R153 Q168 L171 L192 T199 Q214 L215 S216 S217 C218 F219 L220 L221 S222 S223 K224 K243 I248 V252 T255 I256 S260 N270 P274 T275 L276 N281 T282 A283 R284 Y285 T286 P403 D287 Q288 G289 A296 F297 Y300 T301

- [illegible]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.98Å 114.10Å 219.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.41 37.67 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.53-2.41) 97.0 (37.67-2.41)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.236 0.187 , 0.237	Depositor DCC
$R_{free}$ test set	3306 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: MG, TTP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/5700	0.63	3/7754 (0.0%)
1	B	0.45	0/5877	0.60	1/7989 (0.0%)
All	All	0.49	0/11577	0.61	4/15743 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	CA-CB-CG	7.01	131.42	115.30
1	A	499	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	220	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	508	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5577	0	5418	64	0
1	B	5751	0	5586	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	13	6	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	187	0	0	3	0
5	B	173	0	0	3	0
All	All	11778	0	11030	136	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 6.

All (136) 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:123:ILE:CD1	1:B:180:LYS:HG2	1.86	1.06
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.69	0.75
1:B:448:SER:HB3	1:B:602:MET:CE	2.17	0.75
1:B:123:ILE:HD13	1:B:180:LYS:HG2	1.70	0.73
1:B:413:ARG:HD2	5:B:827:HOH:O	1.87	0.73
1:B:196:ARG:HG2	1:B:611:LEU:HD22	1.71	0.72
1:B:123:ILE:CD1	1:B:180:LYS:CG	2.70	0.68
1:B:402:THR:HB	1:B:403:PRO:HA	1.74	0.68
1:B:256:ARG:HD3	3:B:802:TTP:H4'	1.76	0.67
1:A:416:ASN:OD1	1:A:561:VAL:HG13	1.95	0.67
1:A:478:ASN:HD22	1:A:499:ARG:HH11	1.44	0.66
1:B:80:ARG:HD3	1:B:141:PHE:HB3	1.76	0.66
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.79	0.65
1:B:90:THR:HG21	1:B:166:ARG:HG3	1.77	0.65
1:B:123:ILE:HD13	1:B:180:LYS:CG	2.26	0.64
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.80	0.64
1:A:498:HIS:ND1	1:A:555:THR:HG21	2.13	0.63
1:B:180:LYS:HG3	5:B:935:HOH:O	2.00	0.62
1:B:220:LEU:HG	1:B:442:ALA:HB3	1.82	0.62
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.00	0.62
1:B:256:ARG:CD	3:B:802:TTP:H4'	2.28	0.62
1:B:218:CYS:HB3	1:B:444:CYS:SG	2.40	0.62
1:B:123:ILE:HD11	1:B:180:LYS:HG2	1.80	0.61
1:A:283:ALA:HB1	1:A:295:GLY:O	2.00	0.61
1:B:645:LEU:HD21	1:B:672:ILE:HD12	1.83	0.60
1:B:415:SER:O	1:B:418:GLN:HB2	2.02	0.60
1:B:221:LEU:HD13	1:B:248:ILE:HG21	1.84	0.60
1:B:448:SER:HB3	1:B:602:MET:HE1	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ALA:HB2	1:B:288:GLN:OE1	2.03	0.59
1:A:456:THR:HG23	1:A:458:GLU:H	1.68	0.59
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.66	0.58
1:A:482:ASP:OD2	1:A:499:ARG:NH2	2.32	0.58
1:B:535:ILE:HG22	1:B:599:ILE:HD12	1.86	0.58
1:A:456:THR:CG2	1:A:458:GLU:H	2.17	0.57
1:A:248:ILE:HD12	1:A:297:PHE:CE2	2.40	0.56
1:B:324:ARG:HG3	1:B:326:ARG:NH2	2.20	0.56
1:A:362:VAL:HG22	1:A:366:GLU:HB3	1.87	0.56
1:B:3:VAL:HG22	1:B:13:VAL:HG22	1.87	0.56
1:A:478:ASN:ND2	1:A:499:ARG:HH11	2.04	0.55
1:A:637:VAL:HG22	1:A:642:LEU:HB2	1.88	0.55
1:A:655:MET:HE3	1:A:672:ILE:HD11	1.89	0.55
1:A:281:ASN:ND2	1:B:281:ASN:OD1	2.31	0.55
1:A:27:TYR:O	1:A:80:ARG:NH2	2.39	0.54
1:B:448:SER:HB3	1:B:602:MET:HE3	1.87	0.54
1:B:221:LEU:HD13	1:B:248:ILE:CG2	2.38	0.54
1:A:153:ARG:NH1	1:A:153:ARG:HB2	2.23	0.54
1:A:402:THR:HB	1:A:403:PRO:HA	1.90	0.53
1:A:275:MET:CE	1:A:276:LEU:HD13	2.38	0.53
1:A:637:VAL:HG13	1:A:642:LEU:HD22	1.89	0.53
1:B:223:MET:HE2	1:B:231:ILE:HG12	1.92	0.52
1:B:362:VAL:CG1	1:B:367:PHE:HA	2.40	0.51
1:B:130:ARG:CG	1:B:130:ARG:HH11	2.22	0.51
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.44	0.51
1:A:121:LEU:HD22	1:A:125:LEU:HG	1.93	0.51
1:A:478:ASN:HD22	1:A:499:ARG:NH1	2.06	0.50
1:B:441:VAL:O	1:B:491:ALA:HA	2.11	0.50
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.10	0.50
1:A:260:SER:OG	1:A:381:ARG:NH2	2.44	0.50
1:B:444:CYS:HA	5:B:863:HOH:O	2.12	0.50
1:A:243:LYS:HG3	3:B:802:TTP:C5M	2.41	0.50
1:A:655:MET:CE	1:A:672:ILE:HD11	2.41	0.50
1:A:553:TYR:CE1	1:A:555:THR:HG22	2.47	0.50
1:A:652:HIS:O	1:A:655:MET:HB3	2.12	0.49
1:B:256:ARG:NH2	3:B:802:TTP:O2G	2.45	0.49
1:A:221:LEU:CD1	1:A:248:ILE:HG23	2.42	0.49
1:B:27:TYR:O	1:B:80:ARG:NH2	2.46	0.49
1:B:287:ASP:HB3	1:B:294:PRO:HA	1.94	0.48
1:A:535:ILE:HG22	1:A:599:ILE:HD12	1.95	0.48
1:A:18:ILE:O	1:A:22:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:CYS:HB3	1:B:374:TYR:CD1	2.49	0.48
1:A:359:LEU:HB2	5:A:800:HOH:O	2.14	0.48
1:A:35:ASP:HB3	1:A:38:GLN:HG3	1.96	0.47
1:A:364:GLY:O	1:A:368:GLU:HG3	2.14	0.47
1:B:80:ARG:CD	1:B:141:PHE:HB3	2.42	0.47
1:B:275:MET:HE2	1:B:276:LEU:HD13	1.96	0.47
1:A:416:ASN:CG	1:A:561:VAL:HG13	2.34	0.47
1:A:621:THR:HA	1:A:683:VAL:HG12	1.96	0.47
1:B:627:ARG:HB2	1:B:636:ILE:HD12	1.95	0.47
1:B:123:ILE:HD12	1:B:180:LYS:HG2	1.86	0.46
1:B:416:ASN:CG	1:B:561:VAL:HG13	2.36	0.46
1:B:341:ARG:HD2	1:B:347:ASP:O	2.16	0.46
1:A:362:VAL:HG13	1:A:367:PHE:HA	1.98	0.46
1:B:627:ARG:HB2	1:B:636:ILE:CD1	2.46	0.45
1:B:715:PRO:HG3	1:B:741:THR:HG21	1.98	0.45
1:B:223:MET:HE3	1:B:231:ILE:HA	1.98	0.45
1:B:556:TYR:HE2	1:B:561:VAL:CG2	2.29	0.45
1:A:285:TYR:O	1:B:270:ASN:ND2	2.50	0.45
1:B:406:LEU:HD22	1:B:426:SER:HB2	1.99	0.45
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.81	0.45
1:B:221:LEU:CD1	1:B:248:ILE:CG2	2.95	0.45
1:B:454:TYR:HB2	1:B:461:TYR:CZ	2.52	0.45
1:B:603:PRO:HD3	1:B:707:SER:OG	2.16	0.45
1:B:275:MET:CE	1:B:276:LEU:HD13	2.47	0.44
1:B:319:GLY:HA3	1:B:324:ARG:NH1	2.32	0.44
1:B:83:VAL:HG11	1:B:140:ASP:HB3	1.99	0.44
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.99	0.44
1:B:284:ARG:HD2	1:B:327:ASP:OD2	2.16	0.44
1:A:76:ILE:O	1:A:80:ARG:HG3	2.18	0.44
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.53	0.44
1:B:482:ASP:CG	1:B:499:ARG:HH22	2.20	0.44
1:B:256:ARG:HG3	1:B:354:ASN:HB2	1.99	0.43
1:A:427:ASN:HB2	5:A:920:HOH:O	2.18	0.43
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.18	0.43
1:B:432:ILE:HG13	1:B:444:CYS:SG	2.58	0.43
1:B:251:ALA:HB2	1:B:425:CYS:HB3	1.99	0.43
1:A:362:VAL:CG1	1:A:367:PHE:HA	2.49	0.43
1:A:270:ASN:HB3	1:A:274:PRO:HG3	2.01	0.43
1:A:441:VAL:HG22	1:A:491:ALA:HB2	2.01	0.42
1:A:199:THR:HG21	1:A:607:THR:HB	2.00	0.42
1:B:90:THR:HG22	1:B:91:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:VAL:HG13	1:B:490:GLU:HB2	2.01	0.42
1:A:306:LEU:HD22	1:A:381:ARG:HG2	2.02	0.42
1:A:192:LEU:HD23	1:A:472:VAL:HG11	2.02	0.42
1:A:220:LEU:HG	1:A:442:ALA:HB3	2.02	0.42
1:A:593:ILE:HD12	1:A:595:ASN:O	2.20	0.42
1:A:379:ARG:HG2	1:A:379:ARG:H	1.64	0.41
1:A:423:ILE:HA	5:A:926:HOH:O	2.18	0.41
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.55	0.41
1:B:35:ASP:O	1:B:38:GLN:HB2	2.21	0.41
1:A:362:VAL:HG13	1:A:367:PHE:CA	2.50	0.41
1:A:553:TYR:HE1	1:A:555:THR:HG22	1.85	0.41
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.84	0.41
1:B:221:LEU:CD1	1:B:248:ILE:HG23	2.51	0.41
1:A:243:LYS:HG3	3:B:802:TTP:HM53	2.03	0.41
1:A:373:SER:O	1:A:377:GLN:HG3	2.21	0.41
1:A:669:ILE:HA	1:A:670:PRO:HD3	1.96	0.41
1:A:529:LYS:O	1:A:533:GLU:HG3	2.21	0.41
1:A:275:MET:HE3	1:A:276:LEU:HD13	2.02	0.40
1:A:79:ALA:O	1:A:83:VAL:HG23	2.21	0.40
1:A:710:ILE:HG12	1:A:736:MET:HG3	2.04	0.40
1:B:130:ARG:NH1	1:B:130:ARG:CG	2.82	0.40
1:B:264:GLY:HA3	3:B:802:TTP:O1B	2.20	0.40
1:A:216:SER:OG	1:A:484:ASN:ND2	2.54	0.40
1:A:556:TYR:HE2	1:A:561:VAL:HG22	1.87	0.40
1:B:196:ARG:HG2	1:B:611:LEU:CD2	2.46	0.40
1:B:1:MET:HE3	1:B:47:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	708/792 (89%)	685 (97%)	21 (3%)	2 (0%)	41	54
1	B	732/792 (92%)	702 (96%)	28 (4%)	2 (0%)	41	54
All	All	1440/1584 (91%)	1387 (96%)	49 (3%)	4 (0%)	41	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	B	224	LYS
1	A	737	TYR
1	B	601	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/693 (85%)	545 (92%)	47 (8%)	12	18
1	B	607/693 (88%)	553 (91%)	54 (9%)	9	14
All	All	1199/1386 (86%)	1098 (92%)	101 (8%)	11	16

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	44	ILE
1	A	59	LEU
1	A	67	LEU
1	A	93	VAL
1	A	121	LEU
1	A	149	LYS
1	A	153	ARG
1	A	171	LEU
1	A	192	LEU
1	A	214	GLN
1	A	220	LEU

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Mol	Chain	Res	Type
1	A	252	VAL
1	A	276	LEU
1	A	286	VAL
1	A	287	ASP
1	A	301	LEU
1	A	312	LEU
1	A	327	ASP
1	A	337	LEU
1	A	359	LEU
1	A	362	VAL
1	A	379	ARG
1	A	383	VAL
1	A	389	LEU
1	A	441	VAL
1	A	443	VAL
1	A	444	CYS
1	A	449	LEU
1	A	455	VAL
1	A	456	THR
1	A	458	GLU
1	A	493	LEU
1	A	555	THR
1	A	606	SER
1	A	637	VAL
1	A	653	GLU
1	A	679	LEU
1	A	692	LEU
1	A	693	LYS
1	A	703	ASP
1	A	708	LEU
1	A	716	ASN
1	A	720	LEU
1	A	739	LEU
1	A	741	THR
1	A	742	ARG
1	B	3	VAL
1	B	12	ARG
1	B	47	LEU
1	B	56	LEU
1	B	59	LEU
1	B	67	LEU
1	B	80	ARG

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Mol	Chain	Res	Type
1	B	93	VAL
1	B	108	HIS
1	B	121	LEU
1	B	130	ARG
1	B	149	LYS
1	B	171	LEU
1	B	180	LYS
1	B	192	LEU
1	B	217	SER
1	B	218	CYS
1	B	220	LEU
1	B	225	ASP
1	B	252	VAL
1	B	256	ARG
1	B	276	LEU
1	B	286	VAL
1	B	301	LEU
1	B	312	LEU
1	B	316	LYS
1	B	318	THR
1	B	337	LEU
1	B	359	LEU
1	B	361	GLU
1	B	362	VAL
1	B	365	GLU
1	B	380	VAL
1	B	381	ARG
1	B	389	LEU
1	B	441	VAL
1	B	449	LEU
1	B	455	VAL
1	B	493	LEU
1	B	508	LEU
1	B	516	ARG
1	B	543	SER
1	B	561	VAL
1	B	602	MET
1	B	615	GLU
1	B	627	ARG
1	B	648	ARG
1	B	671	GLU
1	B	678	GLN

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Mol	Chain	Res	Type
1	B	679	LEU
1	B	692	LEU
1	B	708	LEU
1	B	723	MET
1	B	739	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	281	ASN
1	B	281	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z  > 2$
4	SO4	A	805	-	4,4,4	0.82	0	6,6,6	0.26	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TTP	A	802	2	23,30,30	0.94	1 (4%)	29,47,47	1.63	4 (13%)
4	SO4	B	806	-	4,4,4	0.78	0	6,6,6	0.10	0
4	SO4	A	804	-	4,4,4	0.15	0	6,6,6	0.20	0
4	SO4	B	807	-	4,4,4	0.84	0	6,6,6	0.20	0
4	SO4	B	803	-	4,4,4	0.17	0	6,6,6	0.19	0
3	TTP	B	802	2	23,30,30	0.94	1 (4%)	29,47,47	1.49	4 (13%)
4	SO4	A	809	-	4,4,4	0.79	0	6,6,6	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTP	A	802	2	-	5/19/34/34	0/2/2/2
3	TTP	B	802	2	-	4/19/34/34	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TTP	C4-C5	3.36	1.48	1.41
3	B	802	TTP	C4-C5	3.36	1.48	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	TTP	C4-N3-C2	6.61	120.72	115.14
3	B	802	TTP	C4-N3-C2	5.39	119.69	115.14
3	B	802	TTP	PB-O3B-PG	-3.13	122.07	132.83
3	B	802	TTP	C5-C6-N1	-2.66	119.33	122.19
3	A	802	TTP	PB-O3B-PG	-2.55	124.06	132.83
3	A	802	TTP	C5-C6-N1	-2.51	119.49	122.19
3	B	802	TTP	PB-O3A-PA	-2.39	124.63	132.83
3	A	802	TTP	PB-O3A-PA	-2.31	124.91	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	TTP	PA-O3A-PB-O1B

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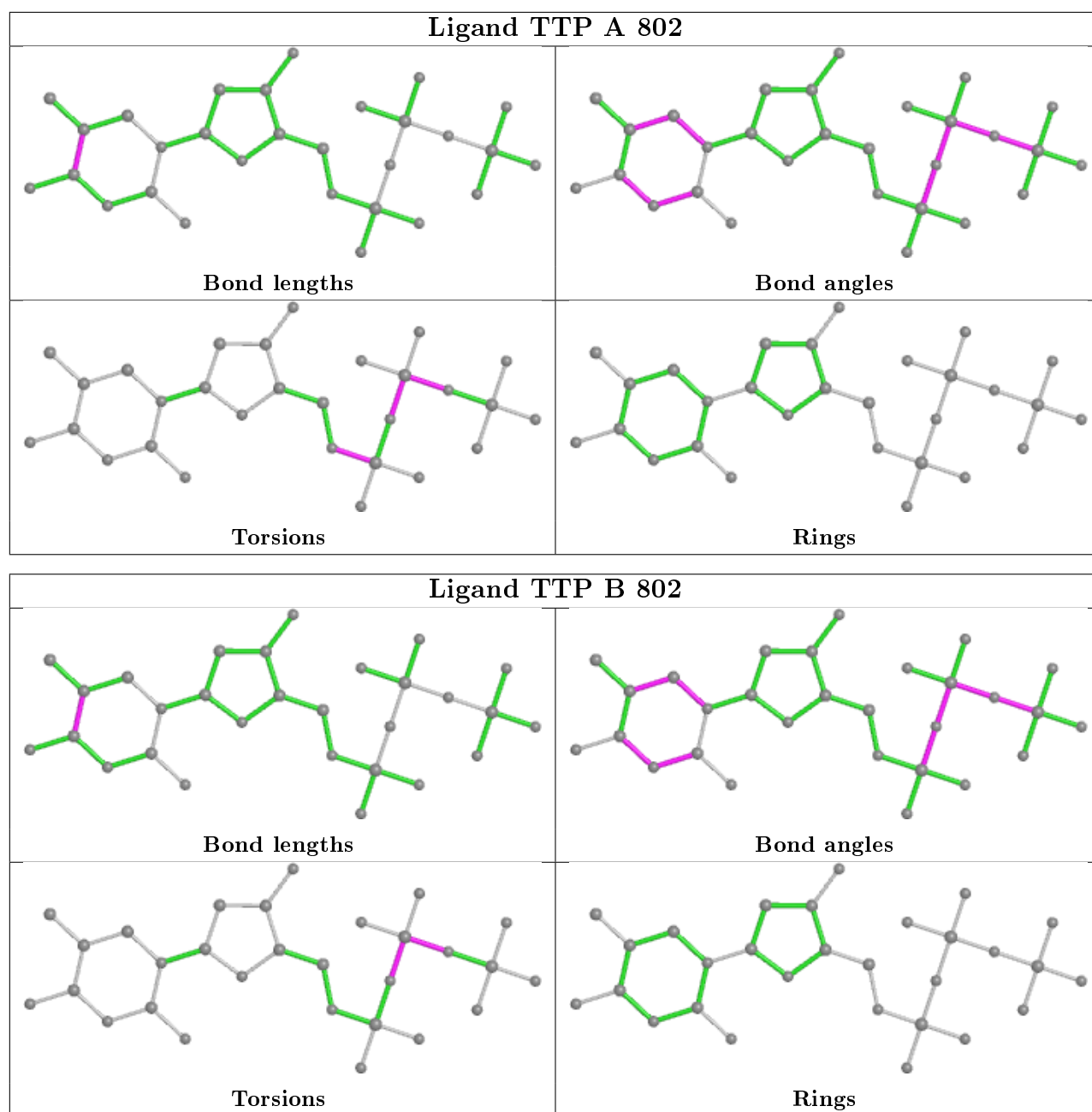
Mol	Chain	Res	Type	Atoms
3	A	802	TTP	PG-O3B-PB-O2B
3	B	802	TTP	PA-O3A-PB-O2B
3	B	802	TTP	PG-O3B-PB-O2B
3	A	802	TTP	PA-O3A-PB-O2B
3	B	802	TTP	PG-O3B-PB-O1B
3	A	802	TTP	C5'-O5'-PA-O3A
3	B	802	TTP	PA-O3A-PB-O1B
3	A	802	TTP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	TTP	6	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.



## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	714/792 (90%)	-0.19	12 (1%) 70 67	31, 44, 63, 87	2 (0%)
1	B	738/792 (93%)	-0.11	21 (2%) 53 50	31, 46, 74, 88	0
All	All	1452/1584 (91%)	-0.15	33 (2%) 60 57	31, 44, 71, 88	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	13.9
1	A	218	CYS	11.8
1	B	107	PRO	4.9
1	B	108	HIS	4.7
1	A	53	THR	3.7
1	A	43	VAL	3.6
1	B	48	TYR	3.4
1	A	314	LEU	3.3
1	B	318	THR	3.2
1	B	633	GLU	3.0
1	A	47	LEU	2.9
1	B	290	GLY	2.7
1	B	180	LYS	2.6
1	B	264	GLY	2.6
1	A	50	GLY	2.6
1	B	655	MET	2.6
1	B	675	ASP	2.5
1	B	27	TYR	2.5
1	B	105	ILE	2.5
1	B	663	ASN	2.4
1	B	113	SER	2.4
1	A	631	SER	2.3
1	B	291	ASN	2.3
1	B	635	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	659	ILE	2.3
1	B	660	ILE	2.2
1	A	56	LEU	2.2
1	B	632	GLY	2.1
1	A	41	MET	2.1
1	B	317	ASN	2.1
1	A	52	THR	2.1
1	B	662	CYS	2.0
1	A	15	PHE	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](#)

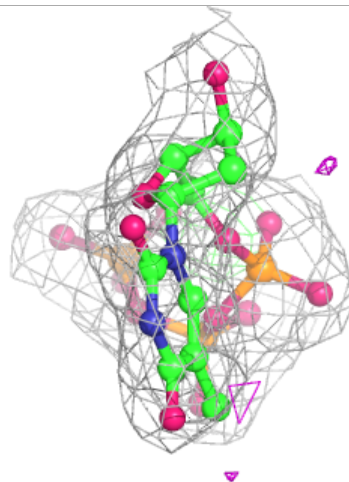
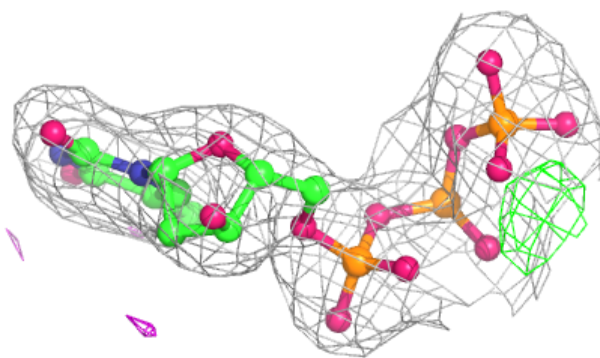
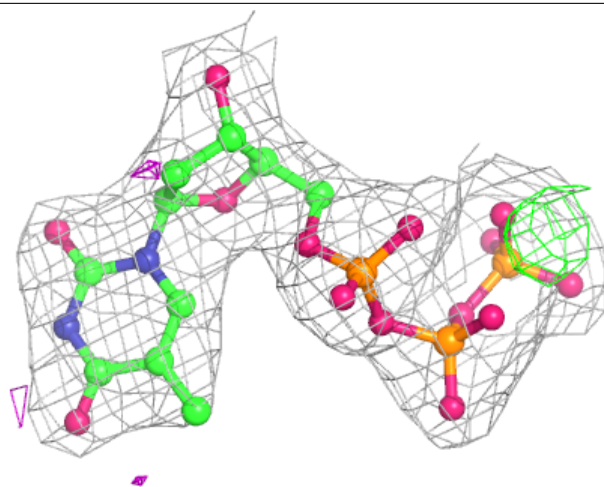
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

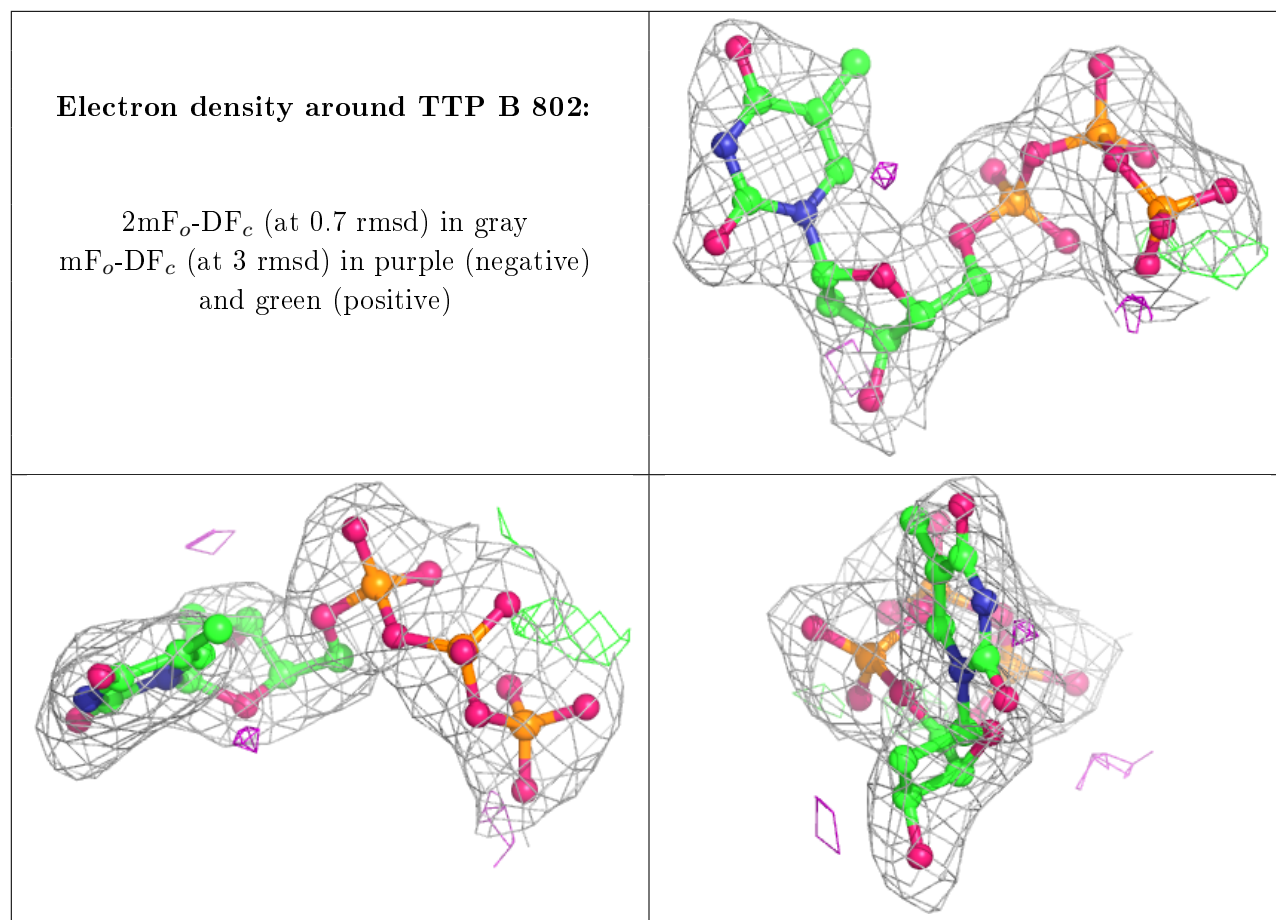
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	801	1/1	0.80	0.10	50,50,50,50	0
4	SO4	A	805	5/5	0.91	0.26	71,72,72,73	0
2	MG	A	801	1/1	0.91	0.09	52,52,52,52	0
4	SO4	A	809	5/5	0.93	0.18	83,83,84,85	0
4	SO4	B	807	5/5	0.94	0.20	75,75,76,77	0
3	TTP	A	802	29/29	0.97	0.09	37,40,49,49	0
3	TTP	B	802	29/29	0.97	0.10	39,41,54,55	0
4	SO4	B	806	5/5	0.97	0.09	82,82,83,83	0
4	SO4	A	804	5/5	0.98	0.08	48,48,49,50	0
4	SO4	B	803	5/5	0.99	0.07	49,50,50,51	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 TTP A 802:**

$2mF_o-DF_c$  (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.