



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 07:55 PM UTC

PDB ID : 3HNE / pdb_00003hne
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors
TTP and ATP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : 2009-05-31
Resolution : 3.11 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

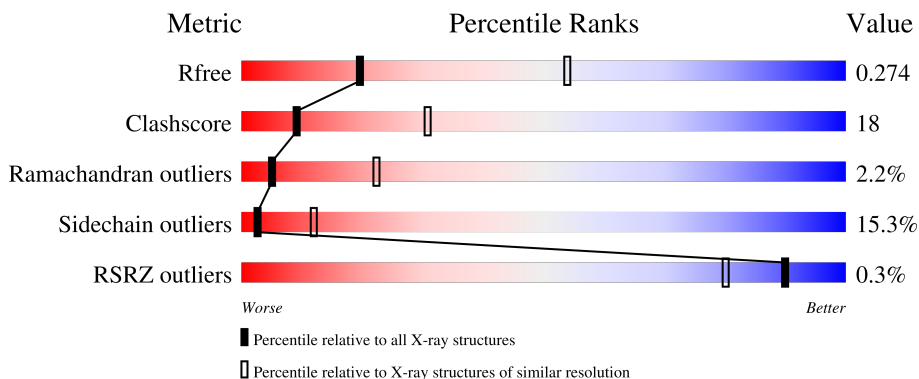
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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 $\leq 5\%$. 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	
1	B	792	

2 Entry composition [i](#)

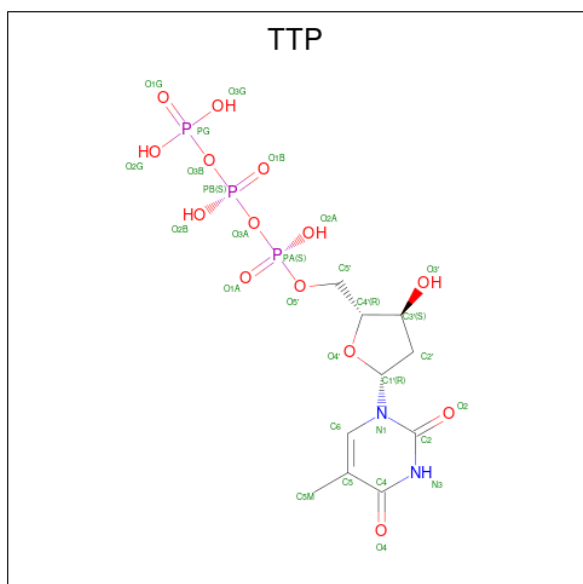
There are 6 unique types of molecules in this entry. The entry contains 11380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	715	Total	C	N	O	S	6	1	0
			5568	3557	927	1051	33			
1	B	724	Total	C	N	O	S	0	0	0
			5644	3593	955	1062	34			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

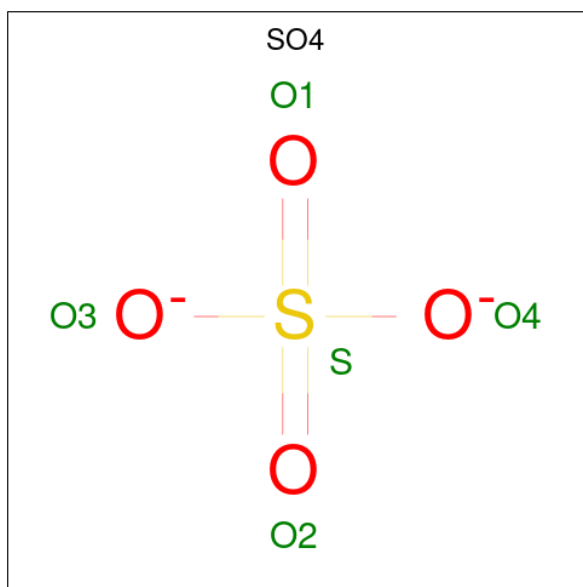


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

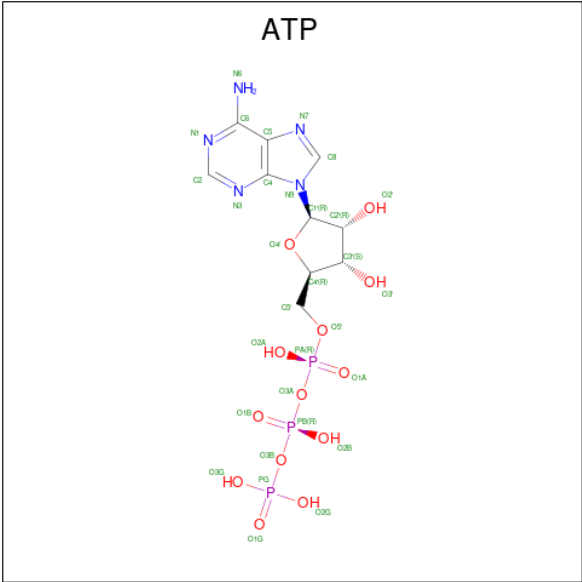
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	3	Total	Mg	0	0
			3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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 ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

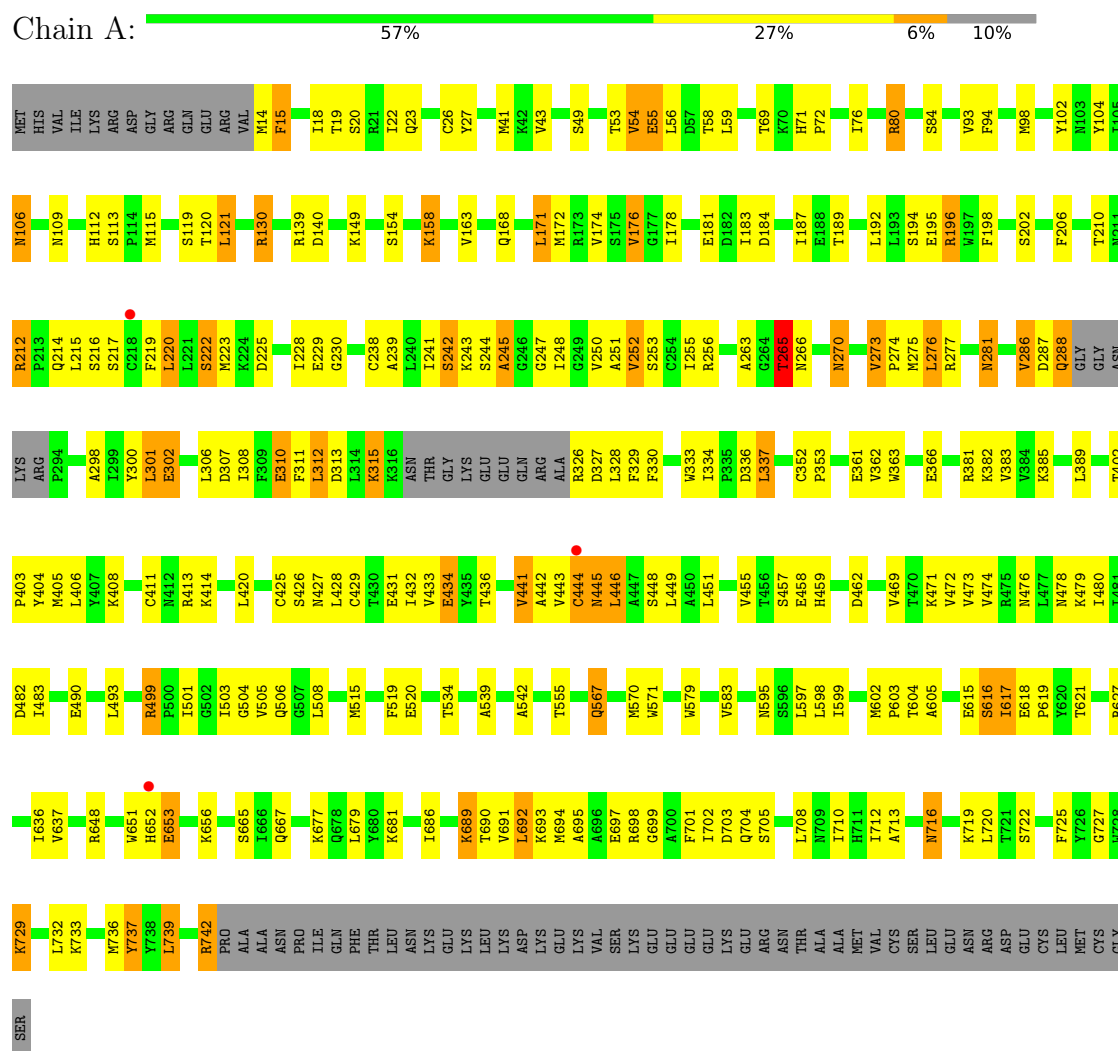
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		
6	B	18	Total	O	0	0
			18	18		

3 Residue-property plots

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 large subunit



Y737	H652	E653	L739	E654	E655	P566	Y566	I481	D482	I393	L306	Q237	L151	R80
R740	K655	E656	T741	N657	L566	Y486	Q397	E395	I483	I394	D307	I241	R153	A82
R742	N657	K656	T741	N657	L566	Y486	Q397	E395	I483	I394	D307	I241	Y155	V83
PRO	A661	E661	ALA	A661	Y568	E568	P403	Y404	E490	P403	L312	A244	I159	N85
ALA	A661	Y568	ALA	A661	Y568	E568	P403	Y404	E490	P403	L312	A244	I159	L86
ASN	G664	E569	ASN	G664	Y569	E569	P403	Y404	E490	P403	L312	A244	I159	H87
PRO	E671	E672	ILE	E671	E672	W570	L493	M405	C492	M405	L314	G249	K162	E89
GLN	E671	E672	GLN	E671	E672	W570	L493	M405	C492	M405	L314	G249	K162	T90
PHE	P673	E673	PHE	P673	E673	W573	N495	K408	S494	N495	K316	V250	R166	K91
THR	D674	E674	THR	D674	E674	T576	N496	K409	S495	N496	K317	V252	H169	K92
LEU	D675	E675	LEU	D675	E675	T576	N497	K496	S496	N497	THR	S253	M170	V93
ASN	D678	E678	ASN	D678	E678	K587	R497	H498	R499	S410	GLY	C254	L171	F94
LYS	D678	E678	LYS	D678	E678	K587	R497	H498	R499	S410	GLY	C254	L171	S95
GLU	L679	E679	GLU	L679	E679	I588	R499	K414	R499	K414	GLU	I255	M172	D96
LYS	V683	E683	LYS	V683	E683	I588	R499	K414	R499	K414	GLU	I255	M172	D96
LYS	V683	E683	LYS	V683	E683	I588	R499	K414	R499	K414	GLU	I255	M172	D96
ASP	E684	E684	ASP	E684	E684	L596	G504	Q418	G502	Q417	R324	G259	V176	V97
LYS	E684	E684	LYS	E684	E684	L596	G504	Q418	G502	Q417	R324	G259	V176	M98
GLU	E686	E686	GLU	E686	E686	P601	Q506	Q418	G502	Q417	R324	G259	V176	V97
P603	E687	E687	P603	E687	E687	M602	G507	Q418	G502	Q417	R324	G259	V176	V97
LYS	E688	E688	LYS	E688	E688	M602	G507	Q418	G502	Q417	R324	G259	V176	V97
VAL	K689	E689	VAL	K689	E689	T604	L508	M427	S507	S426	F330	T265	E195	K111
SER	T690	E690	SER	T690	E690	T604	L508	M427	S507	S426	F330	T265	E195	K111
LYS	V691	E691	LYS	V691	E691	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
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GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
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GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
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GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
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GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112
GLU	L692	E692	GLU	L692	E692	T607	F512	I432	P518	V441	L337	N270	R196	H112

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.15Å 114.37Å 222.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 3.11 44.07 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.5 (44.07-3.11) 88.4 (44.07-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.275 0.188 , 0.274	Depositor DCC
R_{free} test set	1440 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11380	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, TTP, SO4, 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	0.89	1/5696 (0.0%)	1.10	9/7749 (0.1%)
1	B	0.88	1/5767 (0.0%)	1.15	19/7840 (0.2%)
All	All	0.89	2/11463 (0.0%)	1.12	28/15589 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	CYS	CA-C	-6.36	1.44	1.52
1	A	273	VAL	CA-CB	5.84	1.57	1.54

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ILE	N-CA-C	9.11	116.46	108.63
1	B	334	ILE	N-CA-C	8.83	116.68	107.76
1	B	302	GLU	CA-C-N	7.81	129.60	119.84
1	B	302	GLU	C-N-CA	7.81	129.60	119.84
1	B	556	TYR	N-CA-C	7.10	118.67	111.07

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	5568	0	5368	179	0
1	B	5644	0	5448	227	0
2	A	29	0	13	1	0
2	B	29	0	13	4	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	15	0	0	2	0
4	B	15	0	0	1	0
5	B	31	0	12	3	0
6	A	27	0	0	3	0
6	B	18	0	0	3	0
All	All	11380	0	10854	406	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 18.

The worst 5 of 406 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:445:ASN:C	1:A:446:LEU:HD23	1.34	1.49
1:A:445:ASN:O	1:A:446:LEU:HD23	1.50	1.11
1:A:445:ASN:C	1:A:446:LEU:CD2	2.30	1.03
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.18	1.01
1:A:443:VAL:HG12	1:A:444:CYS:H	1.23	0.99

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	710/792 (90%)	636 (90%)	61 (9%)	13 (2%)	6	26
1	B	716/792 (90%)	616 (86%)	82 (12%)	18 (2%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1426/1584 (90%)	1252 (88%)	143 (10%)	31 (2%)	5	22

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	B	130	ARG
1	B	288	GLN
1	B	316	LYS
1	B	327	ASP

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	586/693 (85%)	509 (87%)	77 (13%)	4	17
1	B	593/693 (86%)	490 (83%)	103 (17%)	2	9
All	All	1179/1386 (85%)	999 (85%)	180 (15%)	3	12

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	216	SER
1	B	426	SER
1	B	234	THR
1	B	313	ASP
1	B	508	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	ASN
1	B	711	HIS
1	B	38	GLN

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Mol	Chain	Res	Type
1	B	614	ASN
1	B	23	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	B	813	-	4,4,4	0.27	0	6,6,6	0.56	0
4	SO4	B	810	-	4,4,4	0.31	0	6,6,6	0.30	0
4	SO4	A	808	-	4,4,4	0.29	0	6,6,6	0.41	0
4	SO4	A	812	-	4,4,4	0.25	0	6,6,6	0.39	0
4	SO4	A	809	-	4,4,4	0.24	0	6,6,6	0.30	0
2	TTP	A	806	3	29,30,30	1.32	6 (20%)	43,47,47	1.93	9 (20%)
5	ATP	B	807	3	32,33,33	1.96	8 (25%)	48,52,52	2.06	16 (33%)
4	SO4	B	811	-	4,4,4	0.28	0	6,6,6	0.53	0
2	TTP	B	805	3	29,30,30	1.41	6 (20%)	43,47,47	1.68	7 (16%)

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	806	3	-	11/22/34/34	0/2/2/2
5	ATP	B	807	3	-	5/22/38/38	0/3/3/3
2	TTP	B	805	3	-	1/22/34/34	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807	ATP	PB-O3B	5.59	1.65	1.59
5	B	807	ATP	C5-C4	4.89	1.47	1.39
5	B	807	ATP	PA-O3A	3.77	1.63	1.59
5	B	807	ATP	PB-O3A	3.52	1.63	1.59
5	B	807	ATP	C5-C6	3.05	1.49	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	807	ATP	C5-C4-N3	-5.73	118.83	126.72
2	A	806	TTP	C4-N3-C2	-5.35	120.32	127.34
2	A	806	TTP	C5-C6-N1	-5.11	117.76	123.31
2	A	806	TTP	N3-C2-N1	4.74	121.06	114.89
2	B	805	TTP	C4-N3-C2	-4.66	121.22	127.34

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	806	TTP	C5'-O5'-PA-O1A
2	A	806	TTP	C5'-O5'-PA-O2A
2	A	806	TTP	C5'-O5'-PA-O3A
5	B	807	ATP	C5'-O5'-PA-O1A
5	B	807	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 11 short contacts:

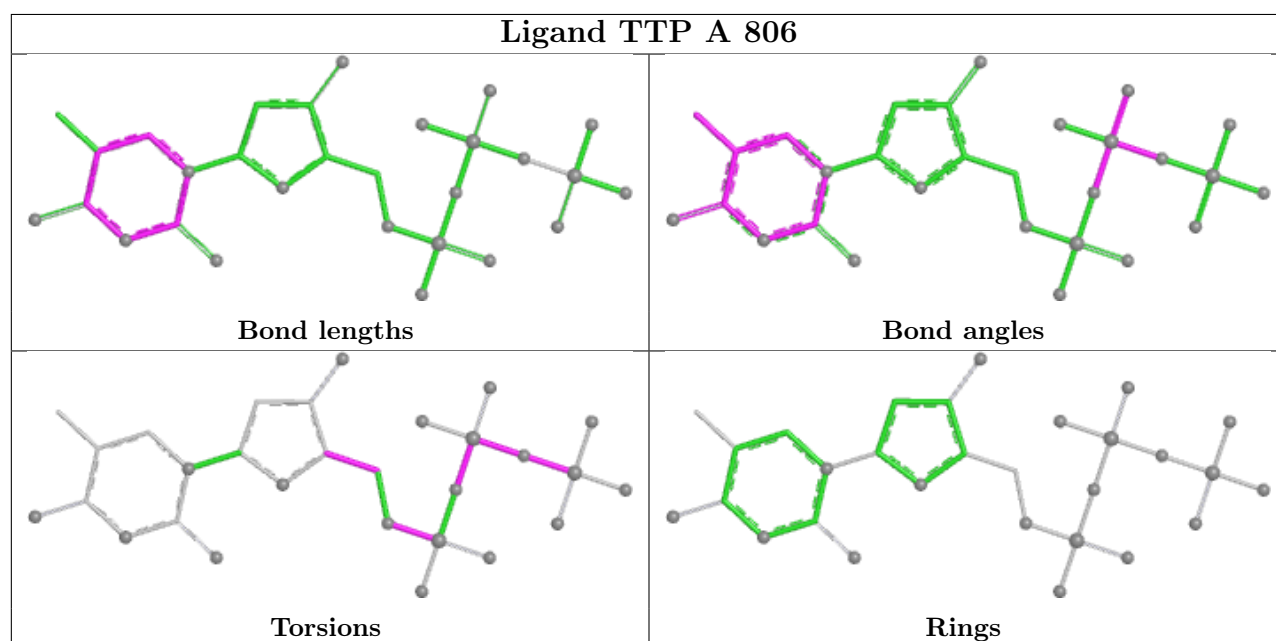
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	810	SO4	1	0
4	A	812	SO4	1	0

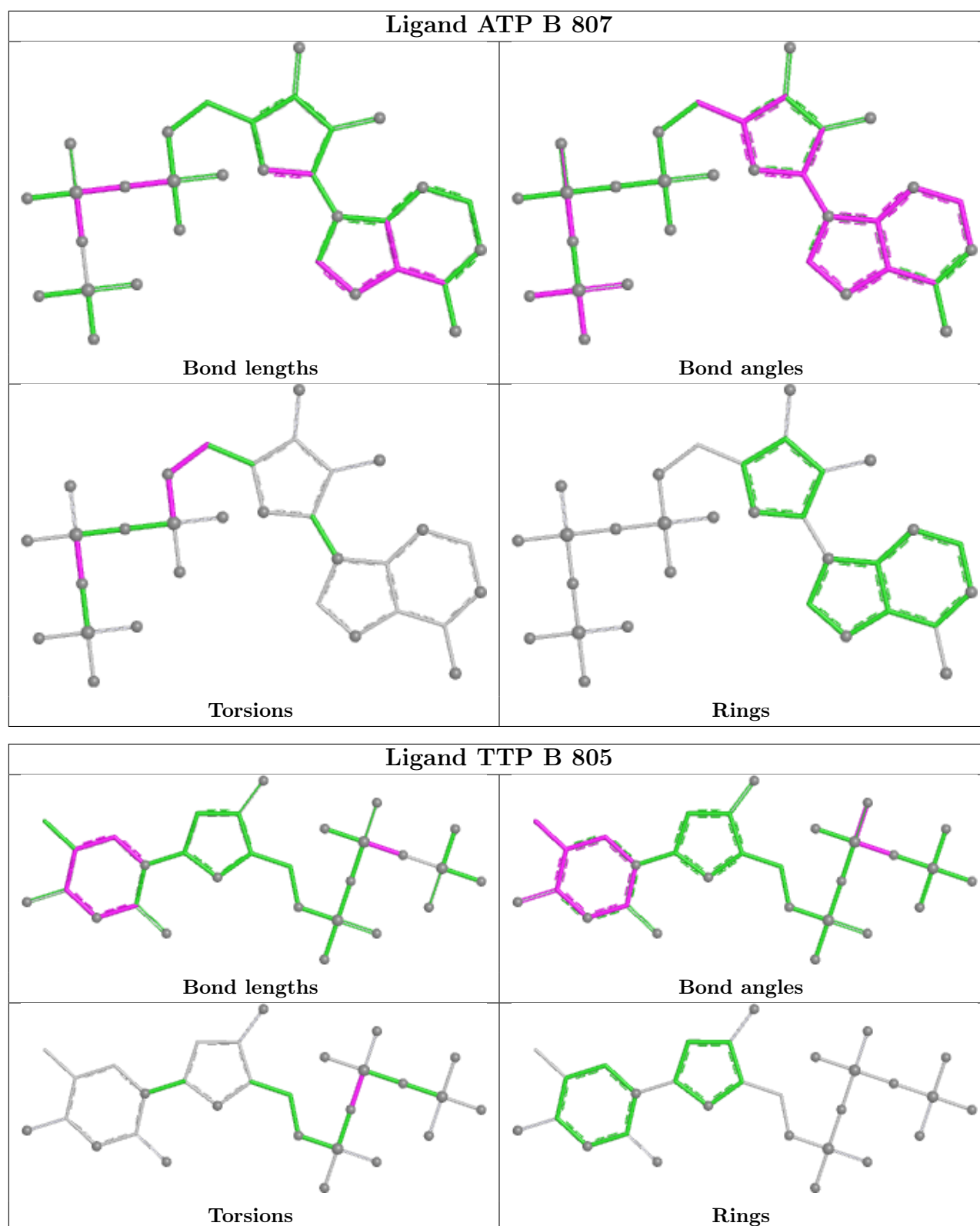
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	809	SO4	1	0
2	A	806	TTP	1	0
5	B	807	ATP	3	0
2	B	805	TTP	4	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	715/792 (90%)	-0.54	3 (0%)	88 76	13, 61, 81, 110	3 (0%)
1	B	724/792 (91%)	-0.52	1 (0%)	92 86	46, 65, 94, 126	0
All	All	1439/1584 (90%)	-0.53	4 (0%)	90 80	13, 63, 90, 126	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	8.5
1	A	218	CYS	6.5
1	B	634	PHE	2.6
1	A	652[A]	HIS	2.4

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 oligosaccharides 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
3	MG	B	804	1/1	0.85	0.15	47,47,47,47	0

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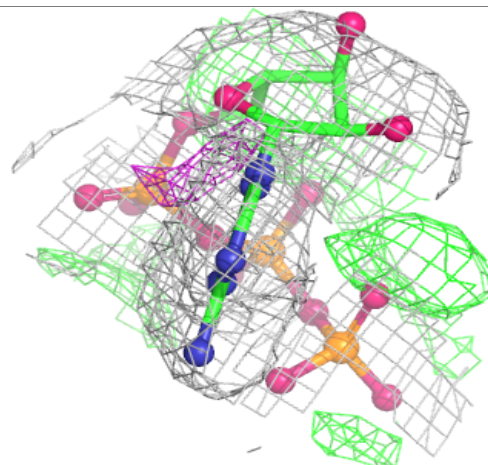
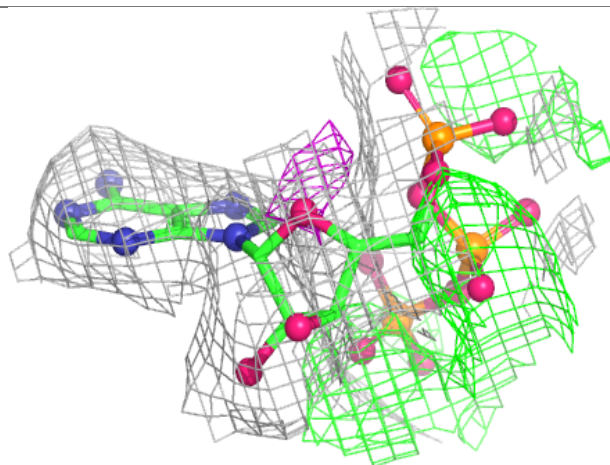
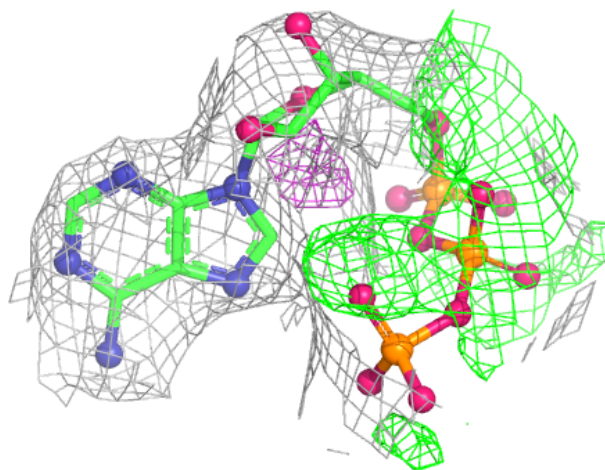
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	803	1/1	0.86	0.19	42,42,42,42	0
4	SO4	A	809	5/5	0.86	0.08	127,127,127,127	0
5	ATP	B	807	31/31	0.87	0.10	65,69,76,76	0
3	MG	A	801	1/1	0.88	0.13	56,56,56,56	0
4	SO4	B	813	5/5	0.90	0.07	70,70,72,72	0
4	SO4	B	811	5/5	0.90	0.08	99,100,100,100	0
3	MG	B	802	1/1	0.91	0.08	62,62,62,62	0
4	SO4	A	812	5/5	0.92	0.09	83,83,85,86	0
4	SO4	B	810	5/5	0.93	0.06	79,79,80,81	0
4	SO4	A	808	5/5	0.93	0.08	86,87,87,87	0
2	TTP	B	805	29/29	0.96	0.07	72,75,83,85	0
2	TTP	A	806	29/29	0.96	0.07	59,63,74,75	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.

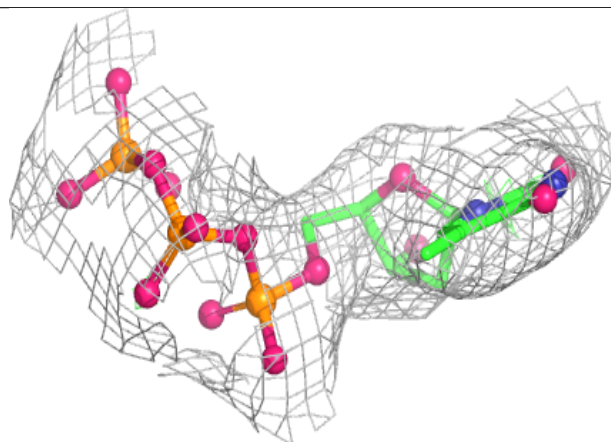
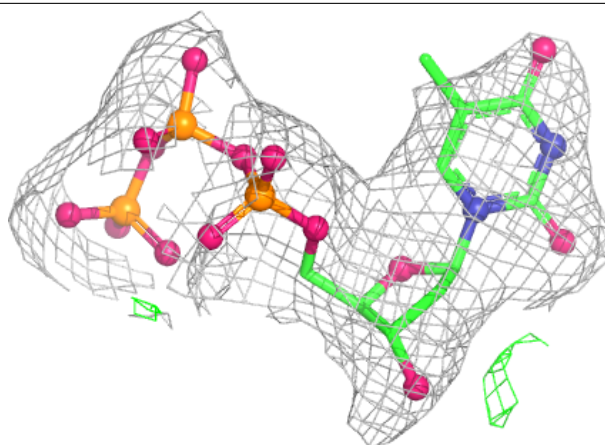
Electron density around ATP B 807:

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

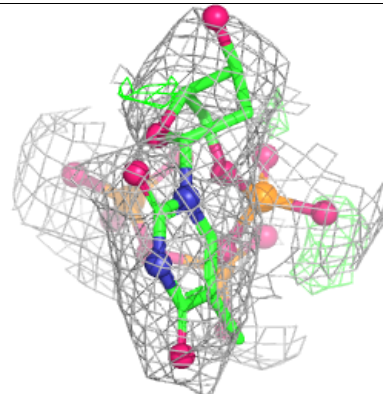
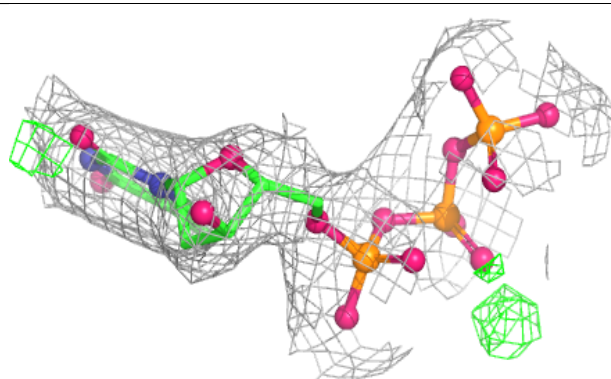
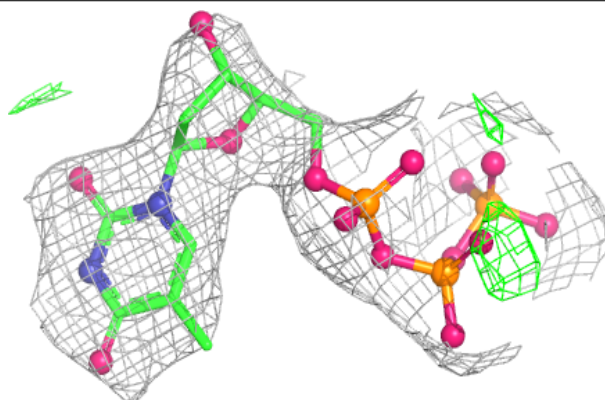


Electron density around TTP B 805:

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

**Electron density around TTP A 806:**

$2mF_o-DF_c$ (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.