



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 06:46 AM EDT

PDB ID : 3HNE
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 : 4.02b-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

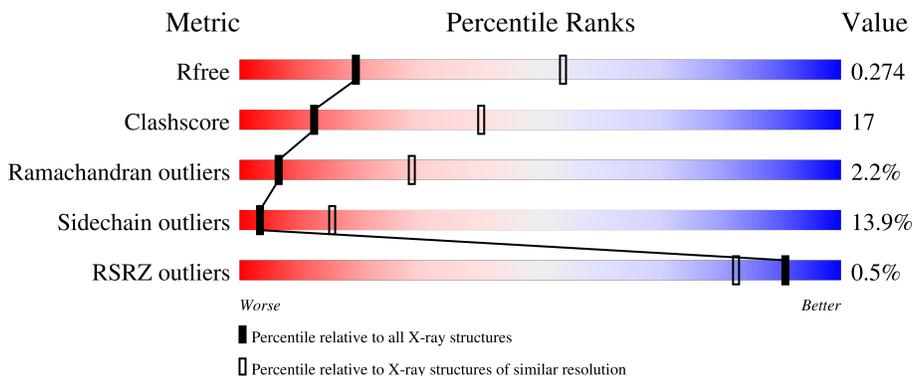
1 Overall quality at a glance

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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (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](#)

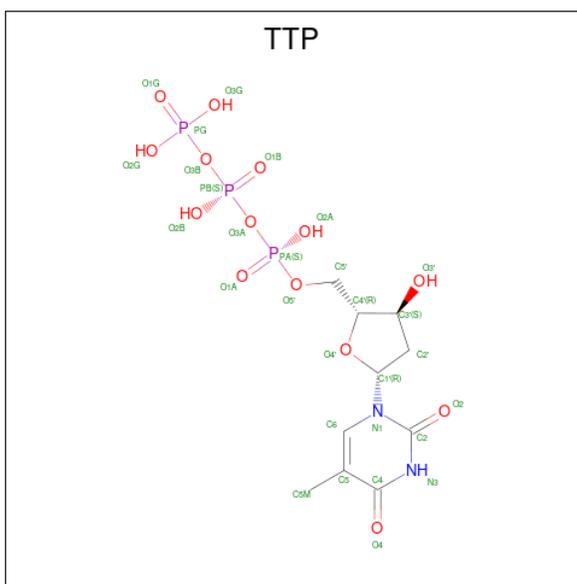
There are 6 unique types of molecules in this entry. The entry contains 11380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
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 (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

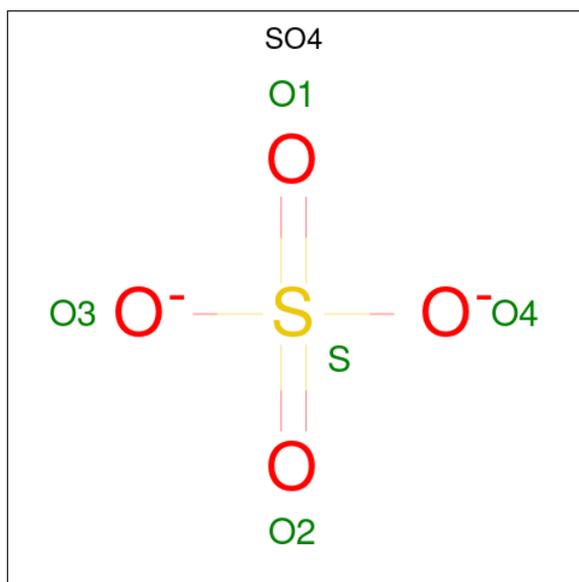


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



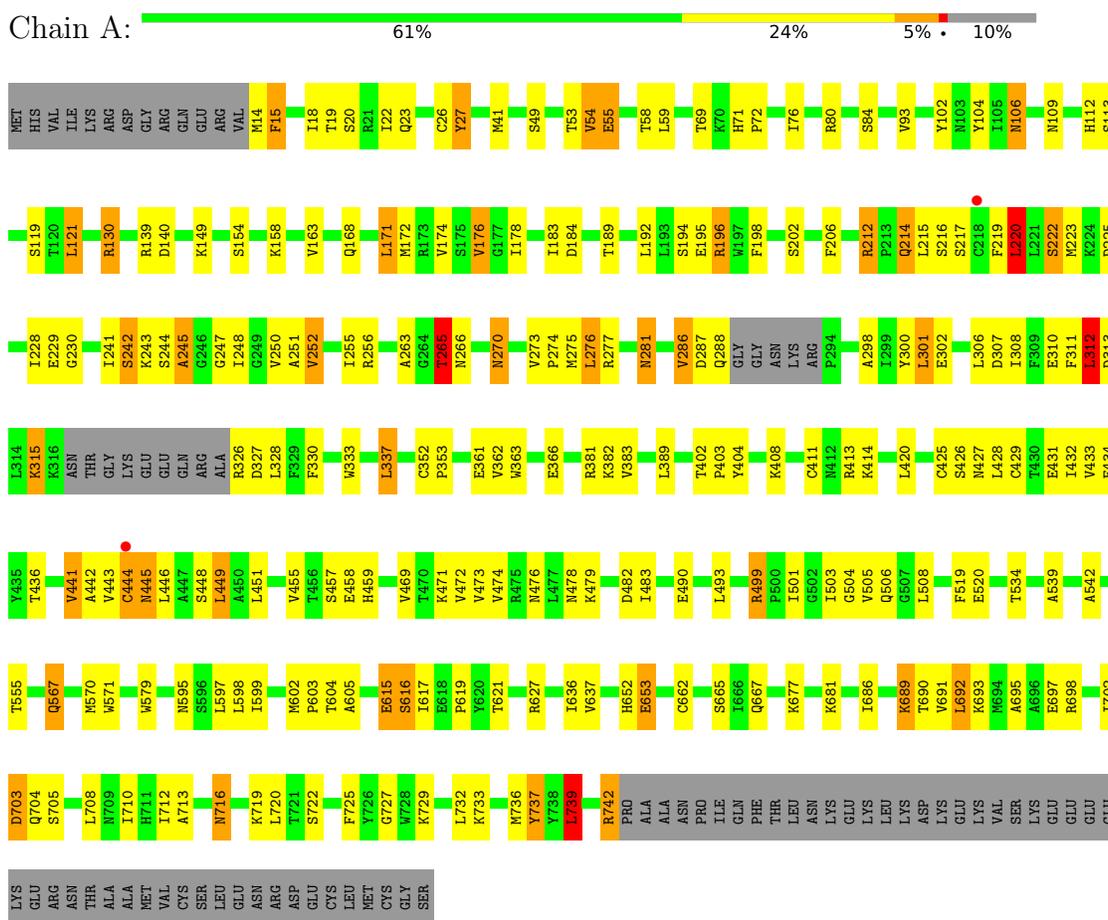
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

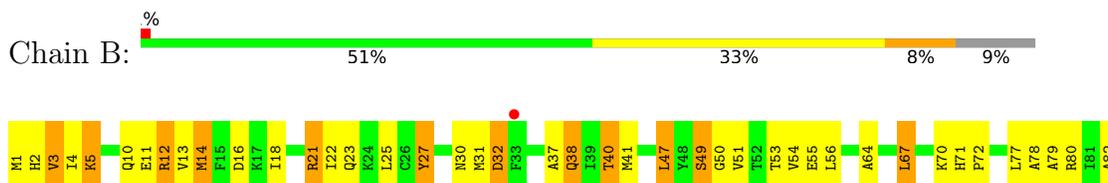
3 Residue-property plots [i](#)

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 large subunit



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



ASP	E685	E686	G687	Q688	K689	T690	V691	L692	A695	A696	R697	R698	G699	A700	F701	I702	D703	M704	S705	Q706	S707	L708	Y717	G718	K719	M723	H724	M725	G727	Q730	T734	G735	M736	Y737	Y738	L739	R740	T741	R742	PRO	ALA	ALA	ASN	ASN	PRO	ILE	GLN	PHE	THR	LEU	LEU	ASN	LYS	GLU	LYS	LEU	LYS																																		
	P601	M602	P603	K607	L610	L611	N612	N613	N614	E615	S616	L617	E618	P619	Y620	S622	N623	L624	Y625	T626	ARG	ARG	VAL	LEU	SER	GLY	GLU	F684	Q635	L645	V651	H652	E653	E654	M655	R656	N657	Q658	I659	A661	G664	P673	D674	D675	L676	K677	O678	L679	V683	M684	L560	Q567	Y568	D569	M570	Y573	T574	T575	T576	K587	R594	I501	L598																												
	K414	S415	N416	Q417	Q418	N419	L420	S426	R427	Y428	I432	D439	E440	Y441	A442	Y443	C444	N445	L446	A447	S448	L451	Y454	S457	Y461	R464	E468	K471	V474	R475	N476	L477	D482	I483	N484	Y485	E490	A491	C492	L493	R497	H498	R499	P500	I501	O502	K315	K316	N317	THR	GLY	LYS	GLU	GLU	GLN	R324	A325	R326	D327	F330	V333	L337	Q346	D347	C352	F353	N354	L359	V362	E365	E366	F367	E368	Y374	R379	V383	A386	L389	I393	I394	E395	S396	Q397	P403	Y404	M405	L406	Y487	K408	D409	S410
	V250	A251	V252	S253	C254	I255	R256	A257	T258	G259	S260	Y261	L262	A263	G264	T265	N266	M270	G271	L272	V273	P274	M275	L276	R277	N281	T282	A283	R284	Y285	V286	D287	Q288	G289	GLY	ASN	LYS	ARG	PRO	G295	A296	F297	A298	I299	Y300	L301	E302	P303	L306	D307	I308	F309	E310	F311	L312	D313	S154	Y155																																	
	V83	S84	N85	L86	H87	K88	E89	T90	F91	K92	V93	F94	S95	D96	L101	Y102	F107	H108	N109	H112	S113	P114	M115	V116	A117	T120	L121	V124	L125	A126	N127	K128	D129	R130	L131	N132	I135	L136	Y137	D138	R139	D140	Y145	F146	G147	F148	K149	T150	L151	E152	R153	S154	Y155																																						
	I159	K162	R166	H169	M170	L171	M172	R173	V174	S175	V176	I187	E188	E195	R196	T199	S202	P203	F206	N207	T210	R211	R212	Q214	L215	S216	Q218	S217	F219	L220	L221	S222	M223	D226	E229	T234	Q237	I241	S244	A245	T248	G249																																																	

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) 88.5 (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)	Xtrriage
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 (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TTP, MG, ATP

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	0.74	3/5696 (0.1%)	0.78	4/7749 (0.1%)
1	B	0.71	2/5767 (0.0%)	0.80	1/7840 (0.0%)
All	All	0.72	5/11463 (0.0%)	0.79	5/15589 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	615	GLU	CB-CG	6.68	1.64	1.52
1	B	218	CYS	CB-SG	-6.52	1.71	1.82
1	A	662	CYS	CB-SG	-6.20	1.71	1.82
1	A	615	GLU	CG-CD	5.86	1.60	1.51
1	B	365	GLU	CB-CG	5.49	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	LEU	CA-CB-CG	7.33	132.16	115.30
1	A	312	LEU	CA-CB-CG	6.74	130.81	115.30
1	A	220	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	739	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	221	LEU	CA-CB-CG	5.14	127.13	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	5568	0	5368	166	0
1	B	5644	0	5448	208	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	374	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 17.

The worst 5 of 374 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	1.44
1:A:445:ASN:O	1:A:446:LEU:HD23	1.50	1.11
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
1:A:445:ASN:C	1:A:446:LEU:CD2	2.30	0.98

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%)	8	33
1	B	716/792 (90%)	616 (86%)	82 (12%)	18 (2%)	5	26
All	All	1426/1584 (90%)	1252 (88%)	143 (10%)	31 (2%)	6	28

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 [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	586/693 (85%)	523 (89%)	63 (11%)	6	25
1	B	593/693 (86%)	492 (83%)	101 (17%)	2	9
All	All	1179/1386 (85%)	1015 (86%)	164 (14%)	3	15

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314	LEU
1	B	615	GLU
1	B	352	CYS
1	B	445	ASN
1	B	675	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN

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Mol	Chain	Res	Type
1	B	214	GLN
1	B	207	ASN
1	B	281	ASN
1	A	387	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	810	-	4,4,4	0.21	0	6,6,6	0.34	0
4	SO4	B	811	-	4,4,4	0.18	0	6,6,6	0.53	0
2	TTP	B	805	3	26,30,30	1.35	5 (19%)	39,47,47	1.88	9 (23%)
4	SO4	A	808	-	4,4,4	0.18	0	6,6,6	0.40	0
2	TTP	A	806	3	26,30,30	1.36	6 (23%)	39,47,47	2.08	9 (23%)
5	ATP	B	807	3	26,33,33	1.30	2 (7%)	31,52,52	1.79	8 (25%)
4	SO4	B	813	-	4,4,4	0.17	0	6,6,6	0.57	0
4	SO4	A	812	-	4,4,4	0.14	0	6,6,6	0.47	0
4	SO4	A	809	-	4,4,4	0.13	0	6,6,6	0.28	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
5	ATP	B	807	3	-	4/18/38/38	0/3/3/3
2	TTP	A	806	3	-	11/22/34/34	0/2/2/2
2	TTP	B	805	3	-	1/22/34/34	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807	ATP	O4'-C1'	4.57	1.47	1.41
2	A	806	TTP	C4-C5	2.93	1.49	1.44
2	A	806	TTP	C4-N3	-2.89	1.33	1.38
2	B	805	TTP	C6-C5	2.84	1.39	1.34
2	B	805	TTP	C4-C5	2.78	1.49	1.44

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	806	TTP	C4-N3-C2	-5.43	120.32	127.35
2	A	806	TTP	C5-C6-N1	-5.42	117.76	123.34
2	B	805	TTP	C4-N3-C2	-4.73	121.22	127.35
2	A	806	TTP	N3-C2-N1	4.65	121.06	114.89
2	B	805	TTP	C5-C6-N1	-4.45	118.76	123.34

There are no chirality outliers.

5 of 16 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
5	B	807	ATP	C5'-O5'-PA-O1A
5	B	807	ATP	C5'-O5'-PA-O2A
5	B	807	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

6 monomers are involved in 11 short contacts:

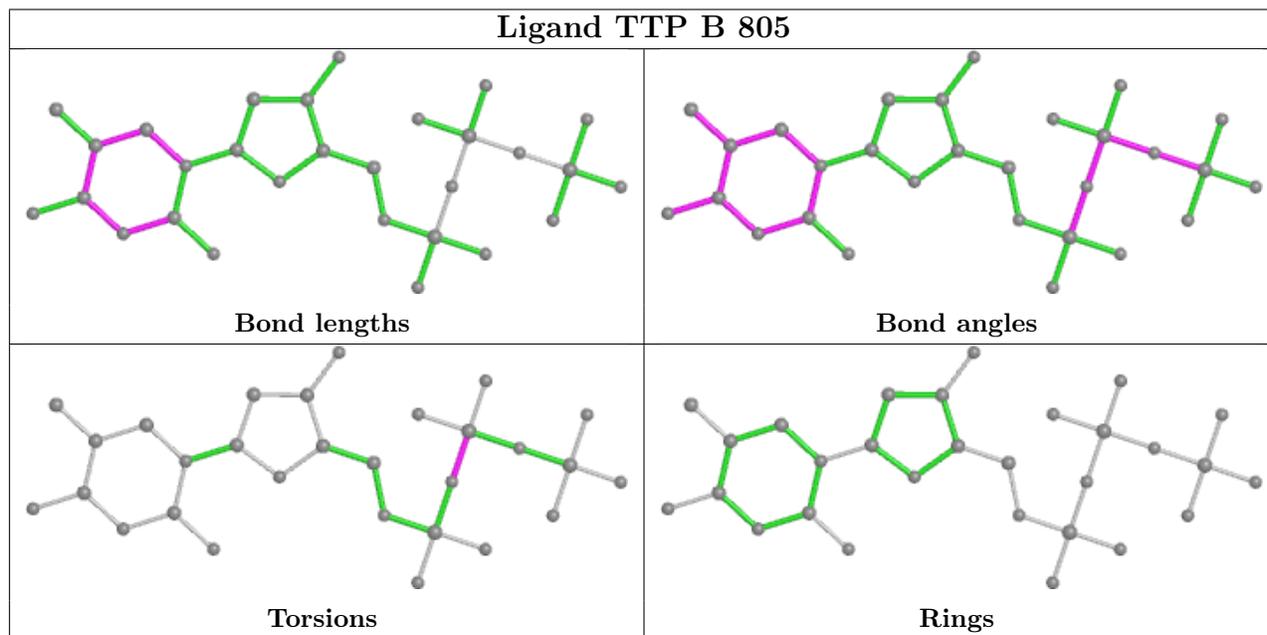
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	810	SO4	1	0

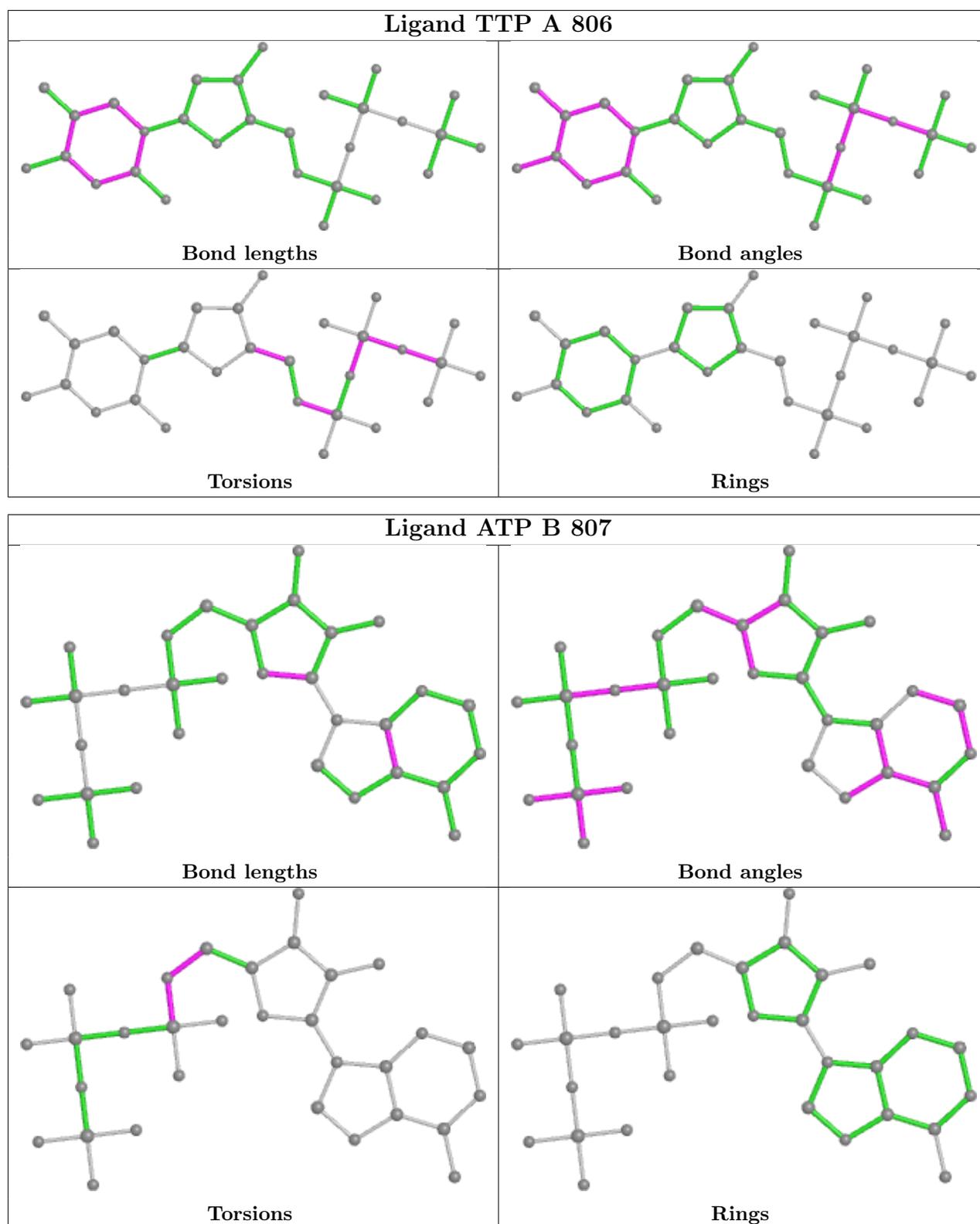
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	805	TTP	4	0
2	A	806	TTP	1	0
5	B	807	ATP	3	0
4	A	812	SO4	1	0
4	A	809	SO4	1	0

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 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

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%)	-0.47	2 (0%) 94 89	46, 61, 81, 110	2 (0%)
1	B	724/792 (91%)	-0.42	5 (0%) 87 77	46, 65, 94, 126	0
All	All	1439/1584 (90%)	-0.45	7 (0%) 91 82	46, 63, 90, 126	2 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	6.4
1	A	218	CYS	6.1
1	B	107	PRO	2.5
1	B	676	LEU	2.2
1	B	659	ILE	2.2

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](#)

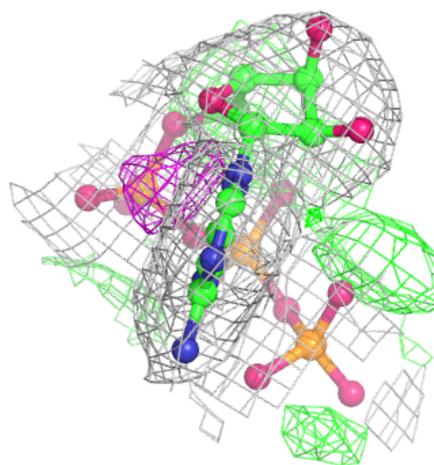
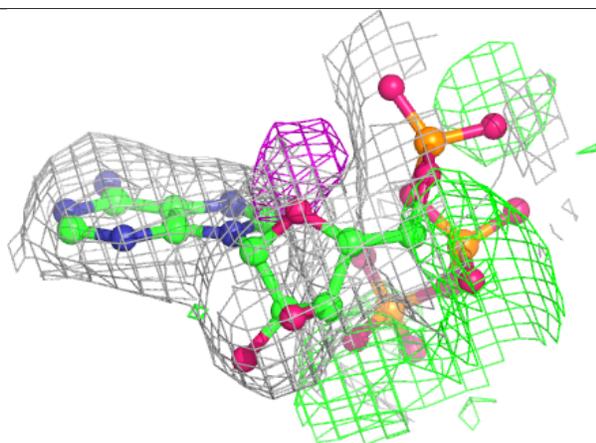
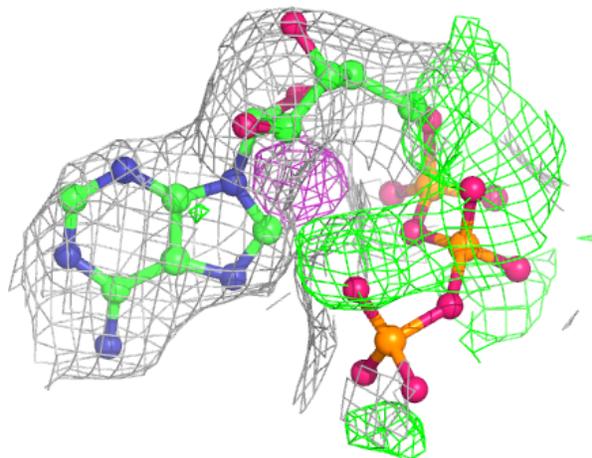
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	809	5/5	0.89	0.13	127,127,127,127	0
5	ATP	B	807	31/31	0.91	0.15	65,69,76,76	0
3	MG	B	804	1/1	0.92	0.12	47,47,47,47	0
4	SO4	B	813	5/5	0.93	0.27	70,70,72,72	0
4	SO4	B	811	5/5	0.94	0.13	99,100,100,100	0
4	SO4	A	808	5/5	0.94	0.16	86,87,87,87	0
3	MG	B	803	1/1	0.94	0.19	42,42,42,42	0
3	MG	B	802	1/1	0.95	0.10	62,62,62,62	0
4	SO4	A	812	5/5	0.96	0.21	83,83,85,86	0
2	TTP	A	806	29/29	0.96	0.14	59,63,74,75	0
4	SO4	B	810	5/5	0.97	0.13	79,79,80,81	0
2	TTP	B	805	29/29	0.97	0.13	72,75,83,85	0
3	MG	A	801	1/1	0.98	0.20	56,56,56,56	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.

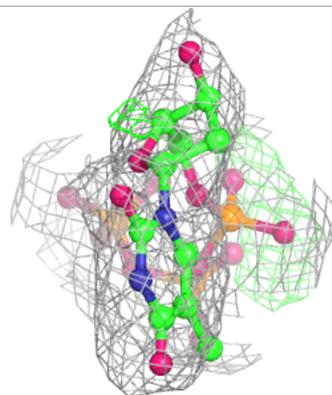
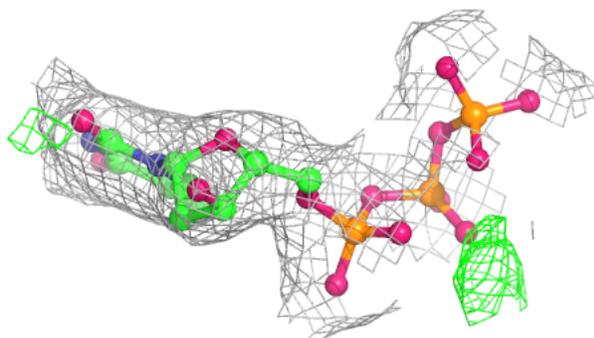
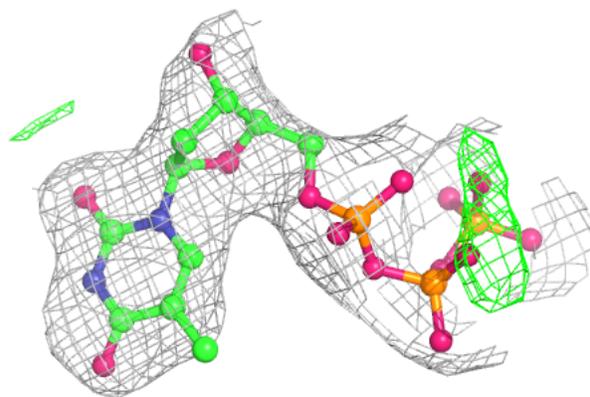
Electron density around ATP B 807:

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

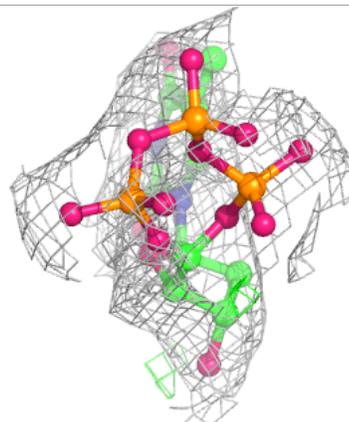
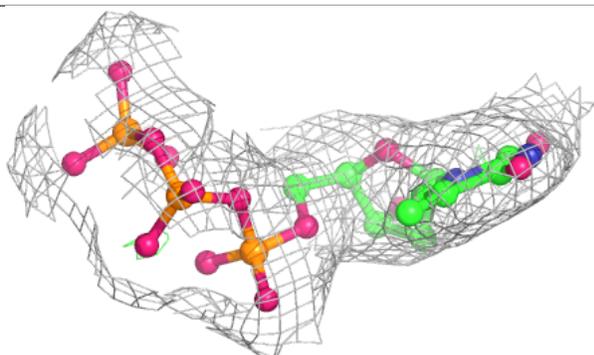
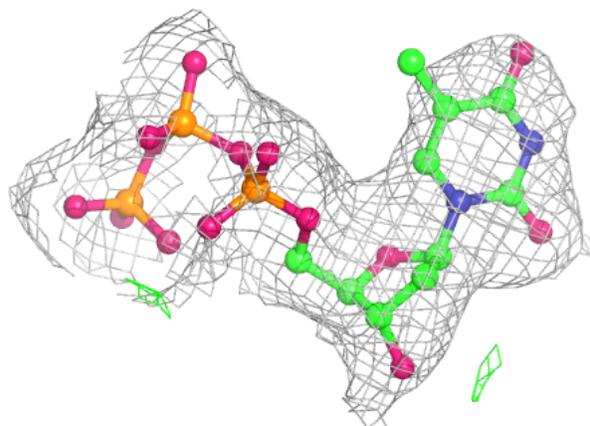


Electron density around TTP A 806:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.