



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:49 am BST

PDB ID : 3HNF
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors
TTP and dATP
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on : 2009-05-31
Resolution : 3.16 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 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

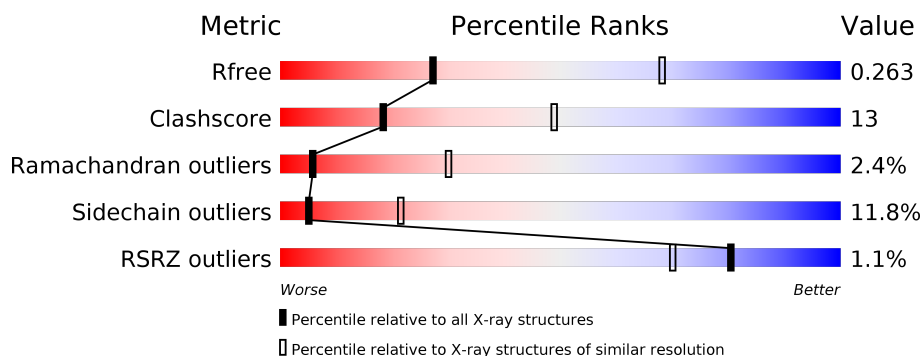
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	792	<div> <div></div> <div>58% 28% 10%</div> </div>
1	B	792	<div> <div></div> <div>61% 27% 5% 7%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11549 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.

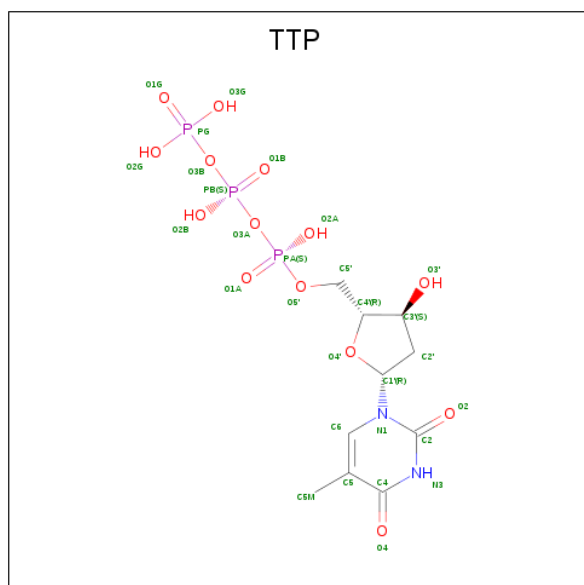
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	6	0	0
			5596	3579	925	1059	33			
1	B	737	Total	C	N	O	S	0	0	0
			5795	3698	980	1083	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: 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	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

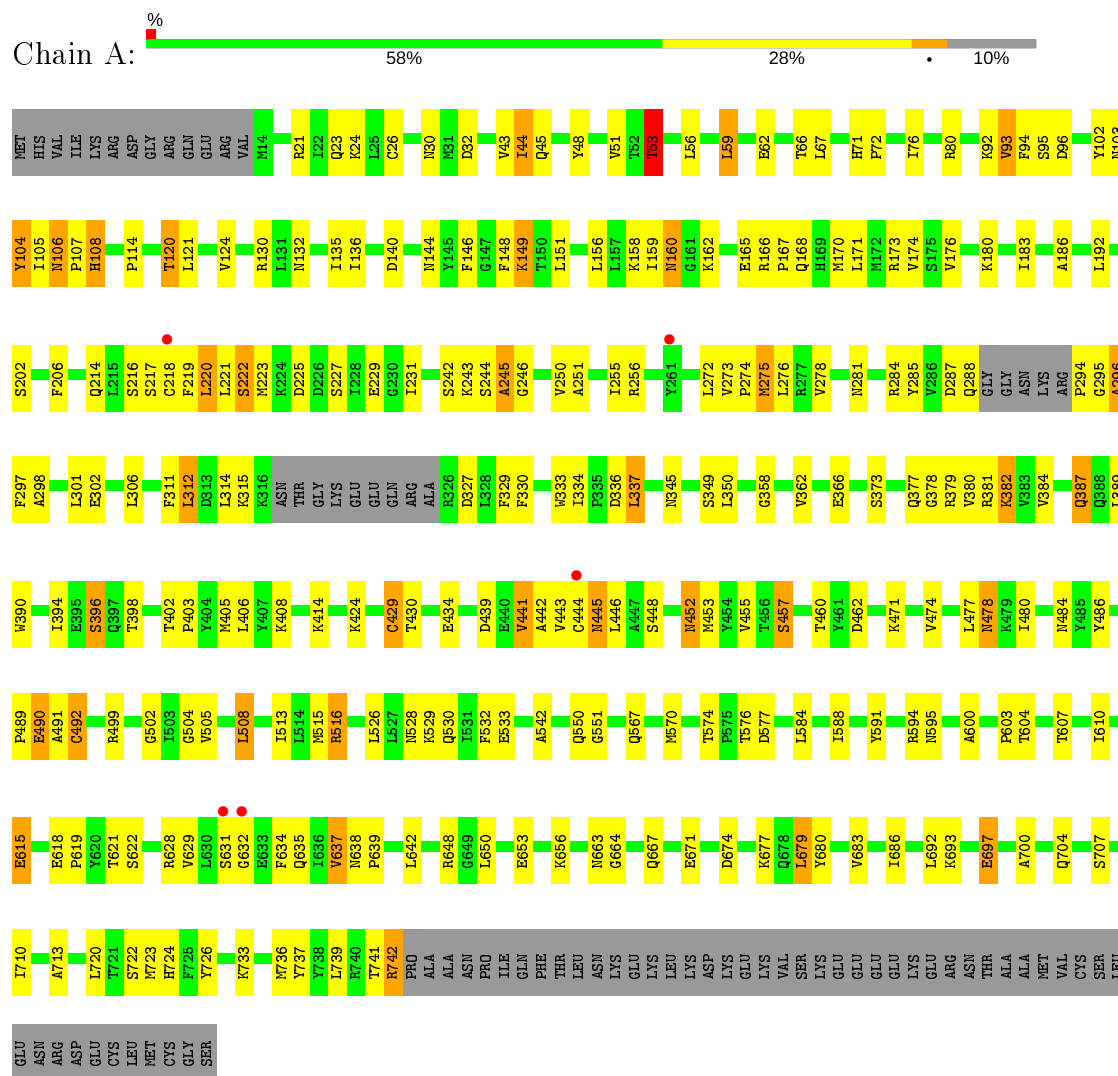
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O	0	0
			22 22		
6	B	26	Total O	0	0
			26 26		

3 Residue-property plots [i](#)

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

- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



M1	K92	S202	ASN	S373	F519	V629	M736
K5	V93	P203	K292	Q377	Q525	LEU	LEU
R6	V97	T204	A298	L389	I531	SER	L739
D7	M98	L205	I299	E395	T534	Q632	R740
G8	M106	A208	Y300	S396	I535	Q635	T741
R9	F107	R212	L301	E399	Y536	I636	R742
E11	H108	L215	E302	E399	L540	V637	PRO
D16	M109	S217	L308	E399	E541	M638	ALA
K17	G110	S217	F309	L406	A542	L642	ALA
I18	K111	S217	E310	Y407	E547	K643	ASN
T19	H112	S222	F311	K408	G551	D644	PRO
I22	S113	S222	L312	Q418	Y552	R648	ILE
C26	M114	M223	D313	S426	Y553	M655	GLN
Y27	M115	K224	L314	S426	E554	M655	THR
G28	L121	D225	K315	C429	G561	I659	ASN
Y27	L121	D226	K316	T430	S562	I660	LYS
L29	Y124	S227	K317	E431	K563	G664	GLU
N30	L125	I231	T318	Y441	G564	Q667	LEU
F33	D129	T234	K319	V443	L566	Q677	LYS
V34	R130	L240	E321	V443	D675	I672	LYS
D35	I136	K243	E322	C444	M570	D674	GLU
I39	I136	R243	K324	M445	V583	D675	LYS
T40	D140	I248	R326	L446	L584	K677	GLU
M41	G147	G249	D327	A447	L588	Q678	GLU
K42	F148	V256	L328	S448	I593	K681	GLU
Y43	K149	A251	F329	L449	R594	V683	LYS
L47	T150	R256	F330	M452	S596	T684	GLU
Y48	L151	S260	A331	K471	P601	K684	ARG
S49	E152	T261	L332	V455	M602	E685	ASN
T52	R153	I262	W333	K464	S606	K689	THR
T53	S154	T265	L337	K471	T607	L692	ALA
V54	Y155	N266	F338	M478	I610	A695	ALA
E55	L156	G267	T344	K479	E615	G699	VAL
L56	L157	T267	V342	I481	E618	I702	CYS
D57	M160	L272	E343	Y485	P619	L708	SER
T58	R166	V273	N345	E490	H710	M709	LEU
L59	P167	P274	Q346	L493	H711	I712	GLU
T66	Q168	R275	S349	S494	T621	A713	ASN
T69	H169	L276	G352	M495	S622	E714	ARG
M70	M170	R277	L359	L508	R627	P715	ASP
A79	L171	M172	V362	R516	R628	M723	GLU
R80	R173	N280	K363				CYS
V83	V174	N281	G364				LEU
S84	I187	R284	E365				MET
H87	L192	Q288	E366				CYS
T90	GLY	GLY	F367				GLY
K91	T199	GLY	E368				SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.86Å 114.39Å 220.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.86 – 3.16 40.85 – 3.16	Depositor EDS
% Data completeness (in resolution range)	89.4 (40.86-3.16) 89.4 (40.85-3.16)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.260 0.185 , 0.263	Depositor DCC
R_{free} test set	1335 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11549	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: MG, DTP, 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	0.59	1/5721 (0.0%)	0.70	1/7782 (0.0%)
1	B	0.57	0/5920	0.70	2/8035 (0.0%)
All	All	0.58	1/11641 (0.0%)	0.70	3/15817 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	CYS	CB-SG	-5.55	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	LEU	CA-CB-CG	7.19	131.84	115.30
1	B	449	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	508	LEU	CA-CB-CG	5.10	127.03	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	5596	0	5436	151	0
1	B	5795	0	5687	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	3	0
3	B	29	0	13	7	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
5	B	30	0	12	1	0
6	A	22	0	0	0	0
6	B	26	0	0	1	0
All	All	11549	0	11161	301	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 13.

The worst 5 of 301 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:219:PHE:C	1:A:220:LEU:HD23	1.40	1.42
1:A:443:VAL:HG12	1:A:444:CYS:N	1.67	1.10
1:A:220:LEU:N	1:A:220:LEU:HD23	1.48	1.09
1:B:416:ASN:OD1	1:B:561:VAL:CG2	2.09	1.00
1:A:219:PHE:C	1:A:220:LEU:CD2	2.30	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	709/792 (90%)	633 (89%)	54 (8%)	22 (3%)	4	23
1	B	731/792 (92%)	639 (87%)	79 (11%)	13 (2%)	8	37
All	All	1440/1584 (91%)	1272 (88%)	133 (9%)	35 (2%)	6	30

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	296	ALA
1	A	327	ASP
1	A	379	ARG
1	B	110	GLY

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	597/693 (86%)	533 (89%)	64 (11%)	6	25
1	B	617/693 (89%)	538 (87%)	79 (13%)	4	18
All	All	1214/1386 (88%)	1071 (88%)	143 (12%)	5	21

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	ARG
1	B	93	VAL
1	B	644	ASP
1	B	16	ASP
1	B	53	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2	HIS
1	B	106	ASN
1	B	459	HIS
1	A	595	ASN
1	A	652	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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$
3	TTP	A	804	2	23,30,30	1.06	1 (4%)	29,47,47	1.59	4 (13%)
4	SO4	B	809	-	4,4,4	0.20	0	6,6,6	0.18	0
4	SO4	A	807	-	4,4,4	0.17	0	6,6,6	0.20	0
4	SO4	A	808	-	4,4,4	0.14	0	6,6,6	0.29	0
4	SO4	B	806	-	4,4,4	0.18	0	6,6,6	0.47	0
5	DTP	B	805	-	26,32,32	0.92	2 (7%)	30,50,50	1.30	3 (10%)
3	TTP	B	803	2	23,30,30	1.06	1 (4%)	29,47,47	1.72	4 (13%)

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	804	2	-	10/19/34/34	0/2/2/2
5	DTP	B	805	-	-	3/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTP	B	803	2	-	4/19/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	TTP	C4-C5	4.10	1.50	1.41
3	A	804	TTP	C4-C5	3.93	1.49	1.41
5	B	805	DTP	C5-C4	2.51	1.47	1.40
5	B	805	DTP	C2-N3	2.07	1.35	1.32

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	TTP	C4-N3-C2	5.76	120.01	115.14
3	B	803	TTP	C4-N3-C2	4.71	119.12	115.14
3	B	803	TTP	PB-O3A-PA	-4.60	117.03	132.83
5	B	805	DTP	N3-C2-N1	-3.71	122.87	128.68
3	B	803	TTP	PB-O3B-PG	-3.57	120.57	132.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	TTP	C5'-O5'-PA-O1A
3	A	804	TTP	O4'-C1'-N1-C6
3	B	803	TTP	C5'-O5'-PA-O1A
3	B	803	TTP	O4'-C4'-C5'-O5'
3	B	803	TTP	C3'-C4'-C5'-O5'

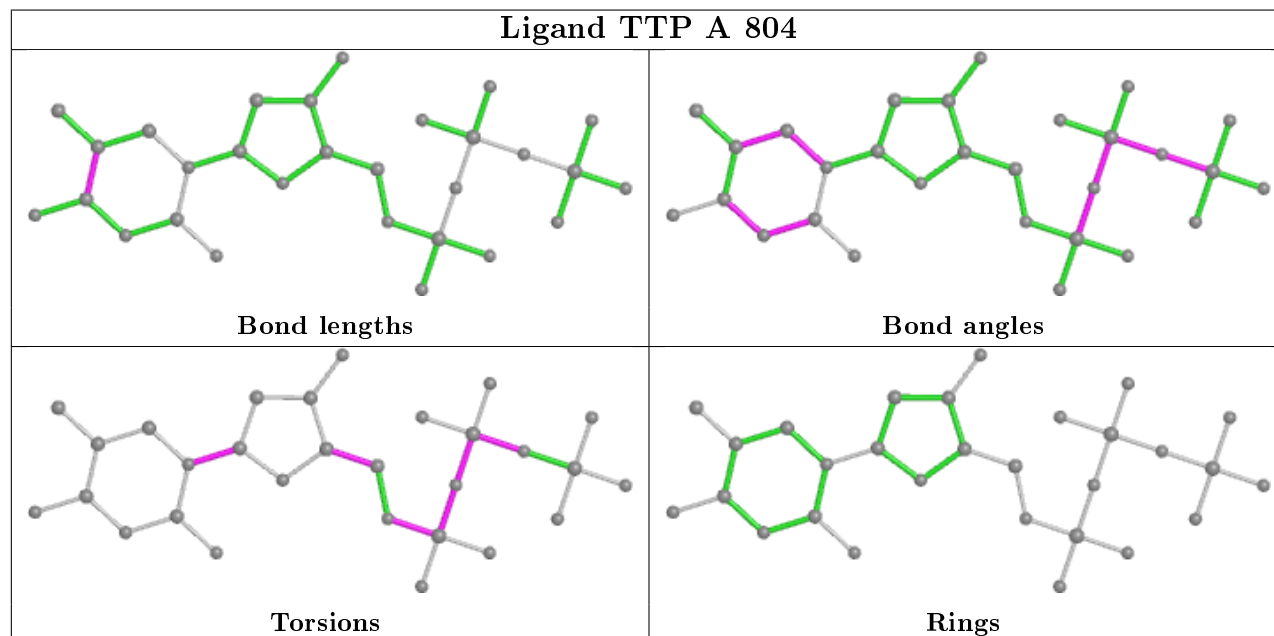
There are no ring outliers.

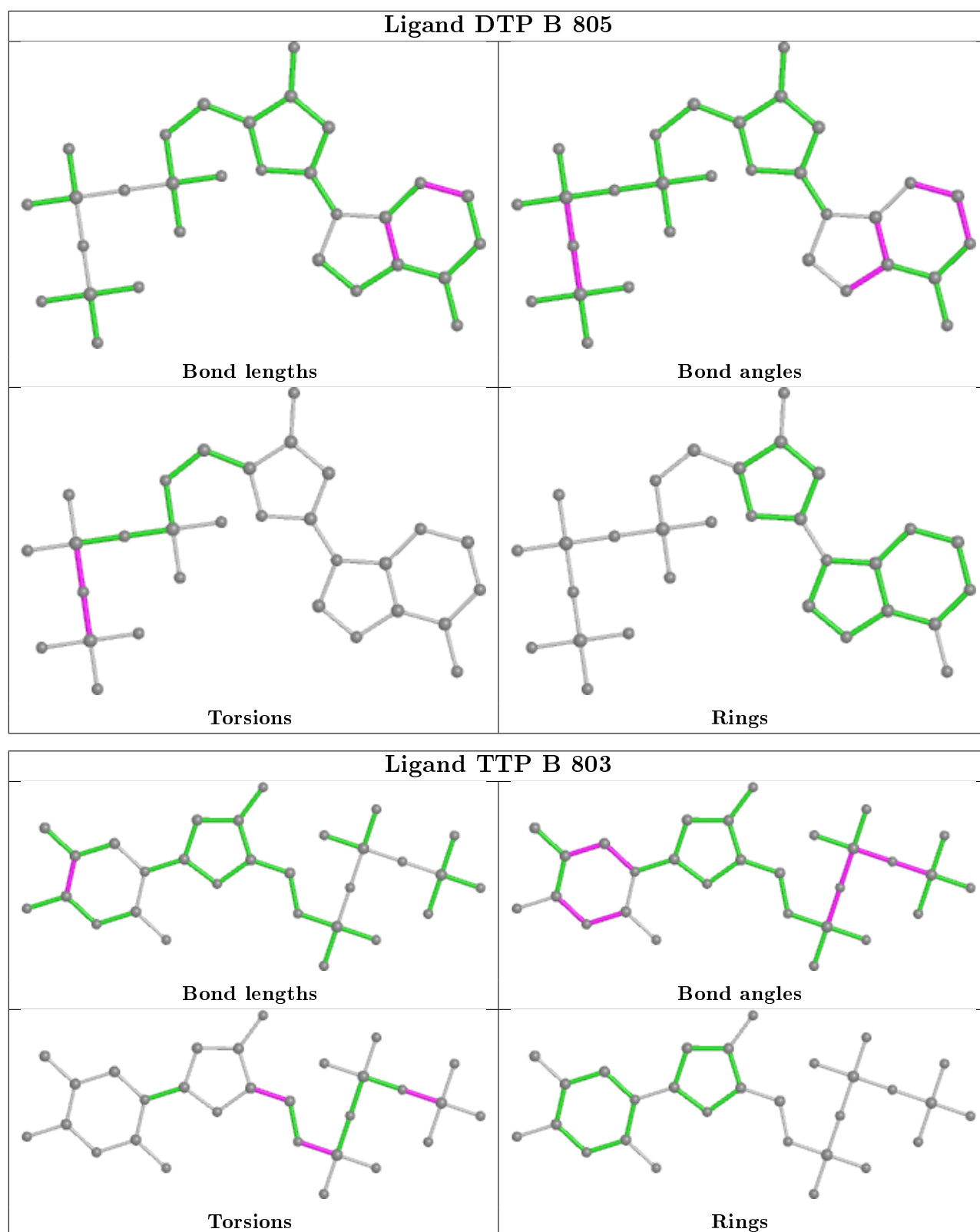
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	TTP	3	0
4	B	809	SO4	1	0
4	A	808	SO4	1	0
5	B	805	DTP	1	0
3	B	803	TTP	7	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%)	-0.36	5 (0%) 87 81	45, 63, 85, 123	2 (0%)
1	B	737/792 (93%)	-0.27	11 (1%) 73 61	38, 58, 94, 110	0
All	All	1452/1584 (91%)	-0.31	16 (1%) 80 70	38, 61, 91, 123	2 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	5.3
1	A	218	CYS	4.7
1	A	632	GLY	3.2
1	B	49	SER	2.9
1	B	323	GLN	2.6

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

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

6.3 Carbohydrates [i](#)

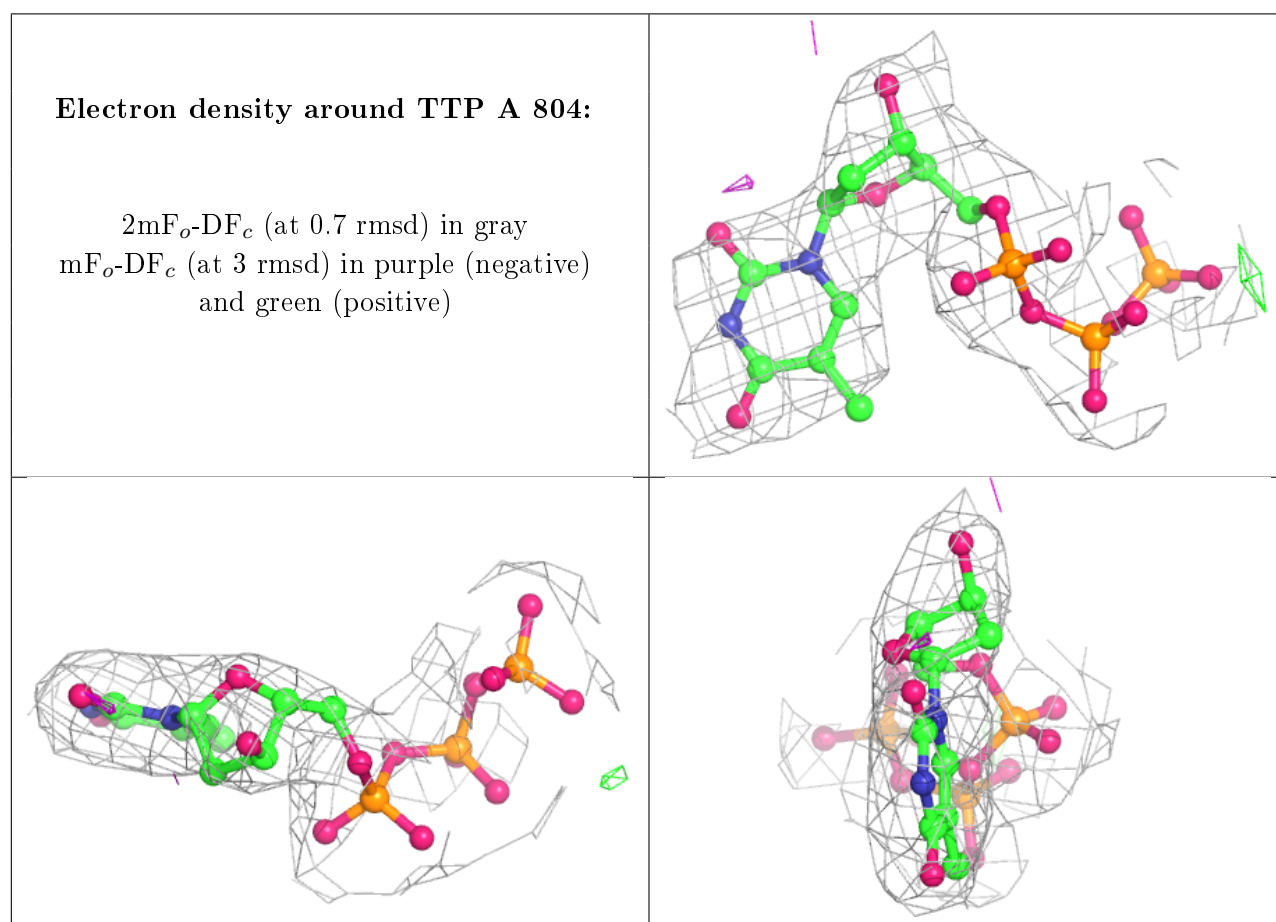
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

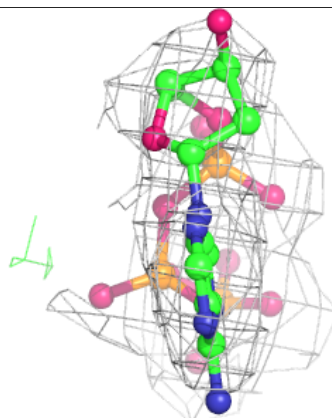
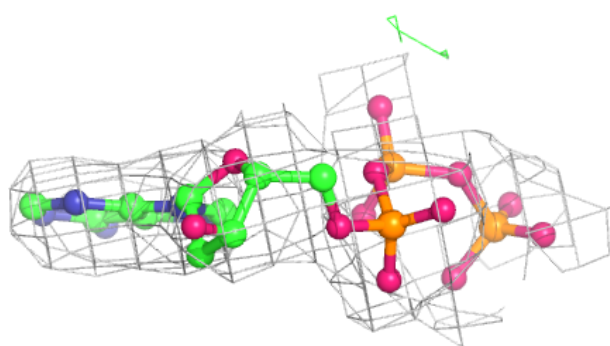
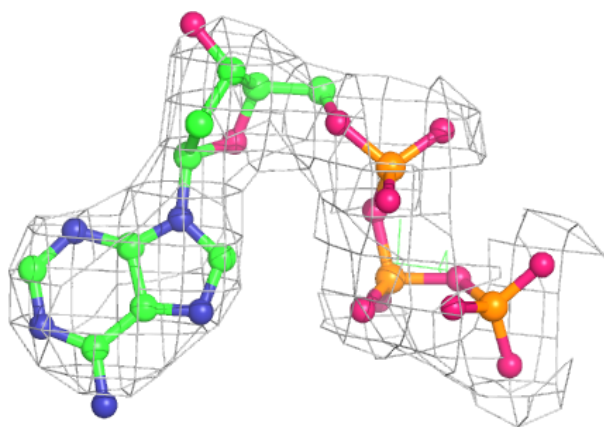
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	806	5/5	0.91	0.52	101,102,102,102	0
4	SO4	A	808	5/5	0.93	0.19	76,76,77,78	0
2	MG	B	802	1/1	0.94	0.18	48,48,48,48	0
3	TTP	A	804	29/29	0.95	0.14	58,60,66,67	0
5	DTP	B	805	30/30	0.96	0.17	83,84,88,89	0
2	MG	A	801	1/1	0.96	0.17	46,46,46,46	0
4	SO4	B	809	5/5	0.97	0.10	74,75,75,75	0
3	TTP	B	803	29/29	0.97	0.12	54,57,66,67	0
4	SO4	A	807	5/5	0.97	0.20	91,91,91,91	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.

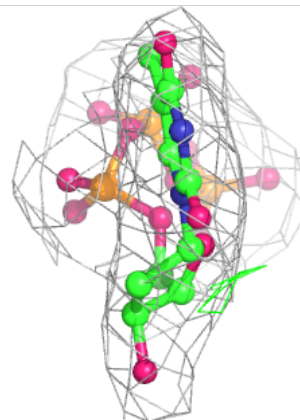
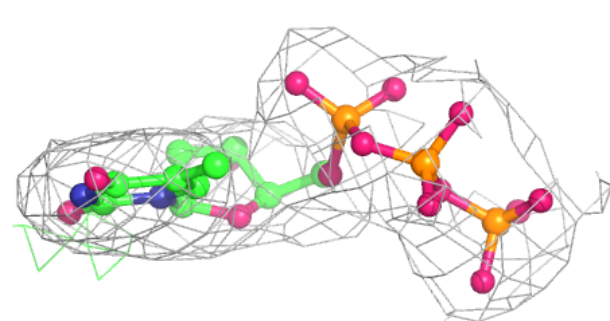
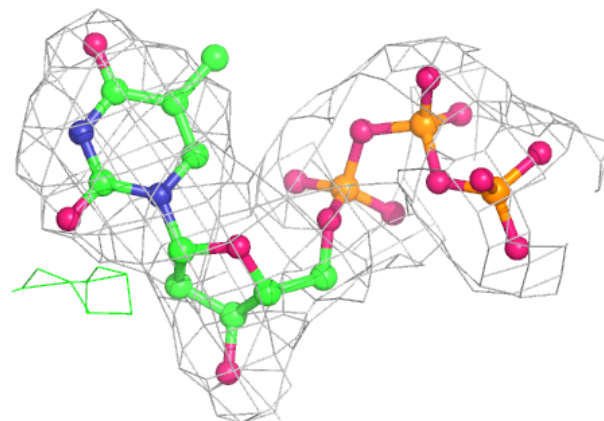


Electron density around DTP B 805:

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

**Electron density around TTP B 803:**

$2mF_o-DF_c$ (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.