



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 22, 2025 – 12:21 PM EDT

PDB ID : 9Y43 / pdb_00009y43
Title : 3-hydroxypropionyl-CoA Synthetase (ADP-forming) from *Nitrosopumilus maritimus*.
Authors : Johnson, J.A.; Yilmaz, M.; Tosun, B.; Wakatsuki, S.; Demirci, H.
Deposited on : 2025-09-02
Resolution : 2.80 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	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

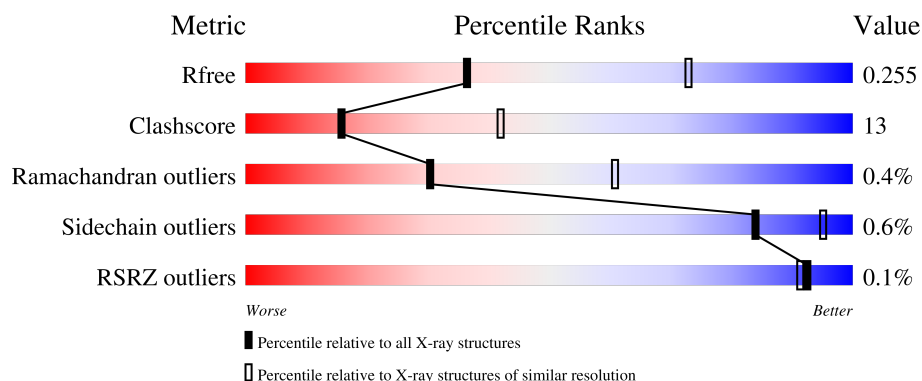
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	705	 68% 29% ..
1	B	705	 73% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3OH	A	802[A]	-	X	-	-
3	3OH	A	802[B]	-	X	-	-
3	3OH	B	801[A]	-	X	-	-
3	3OH	B	801[B]	-	X	-	-

2 Entry composition [i](#)

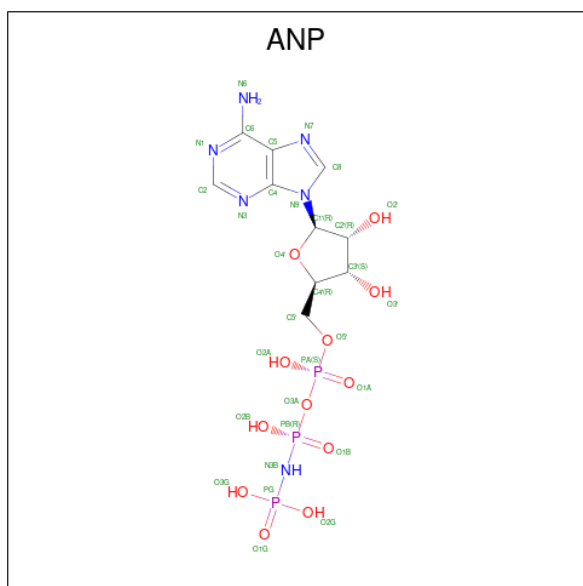
There are 6 unique types of molecules in this entry. The entry contains 10810 atoms, of which 13 are hydrogens and 0 are deuteriums.

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 3-hydroxypropionate--CoA ligase [ADP-forming].

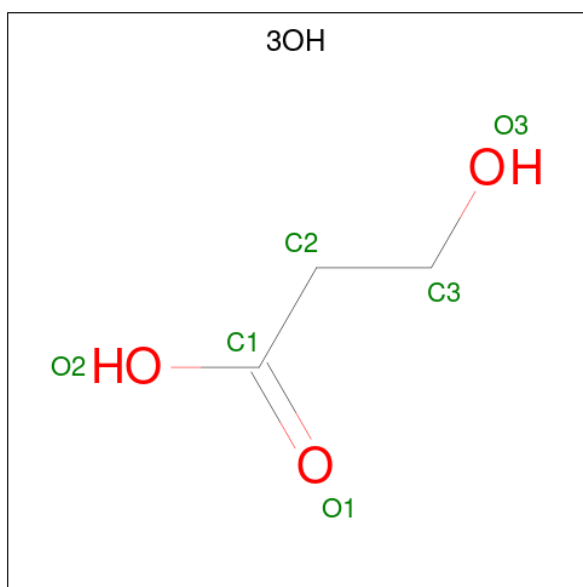
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	1	0
			5255	3370	893	960	32			
1	B	703	Total	C	N	O	S	0	2	0
			5342	3422	905	983	32			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



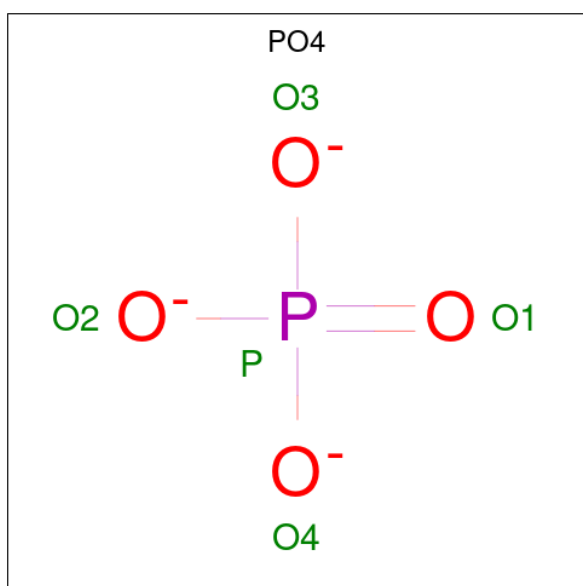
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			44	10	13	6	12		

- Molecule 3 is 3-HYDROXY-PROPANOIC ACID (CCD ID: 3OH) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

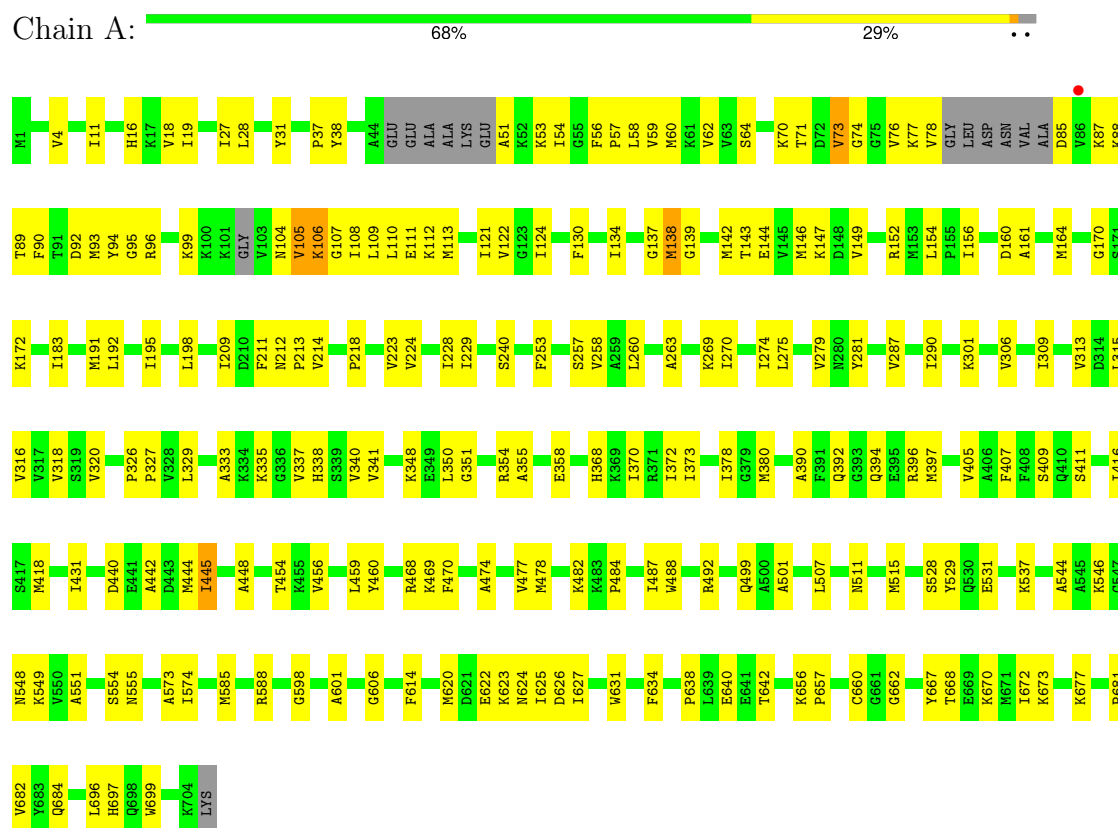
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total 61	O 61	0	0
6	B	73	Total 73	O 73	0	0

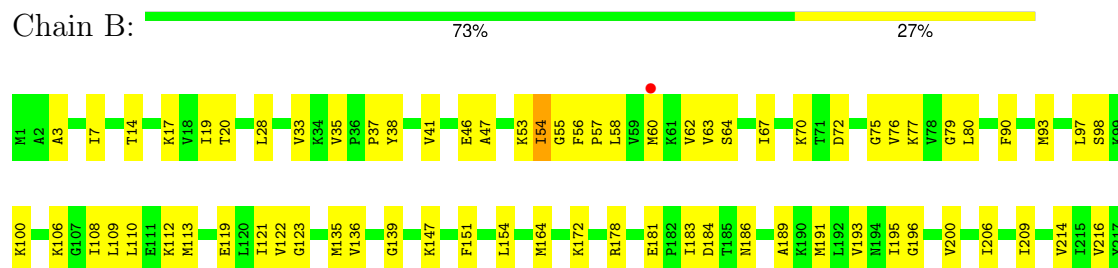
3 Residue-property plots

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: 3-hydroxypropionate--CoA ligase [ADP-forming]



- Molecule 1: 3-hydroxypropionate--CoA ligase [ADP-forming]



P637	N511	Q392	P218
P638	A512	R396	H221
K653	I513	M397	V222
K656	I514		V223
P657	Y529	K401	K232
L658	A538	F408	F253
L659	A545	S409	V251
C660	V550	Q410	
G661	A551	M414	
T668	M552	L419	P267
K673	T553		N272
L674	S554	K429	S273
L675	M560	M430	I274
E676	I564	I431	L275
K677	L567	S432	
	L572	F433	I290
V680	L581	D438	K296
P681	M585	V439	I297
V682	G598	D440	F298
A692	N599	E441	
	P600	A442	I309
L696	A601	D443	P310
H697	G606	M444	G311
S703	F614	Y447	K312
LYS	Q618	A448	V313
LYS	F619		V316
	M620	T454	V317
	D621	K455	V318
	E622	V456	S319
	W623	F470	V320
	N624		P326
	I625	V473	E330
	D626	Y477	
	I627		V337
	A628	P484	E358
	M629	L485	A359
	P630	V486	E360
	W631	I487	V361
	F634	W488	
	Q635	K489	L364
	D636	R492	I372
		T493	
		A494	G379
		K498	R386
		A501	L387
		T504	D388
		L507	C389
			A390
			F391

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.88Å 127.59Å 137.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.80 48.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	73.2 (48.72-2.80) 73.3 (48.72-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.210 , 0.250 0.212 , 0.255	Depositor DCC
R_{free} test set	1296 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: PO4, ANP, 3OH, 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	0.21	0/5351	0.66	5/7201 (0.1%)
1	B	0.19	0/5441	0.64	7/7329 (0.1%)
All	All	0.20	0/10792	0.65	12/14530 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	GLY	CA-C-N	6.79	134.19	121.97
1	B	75	GLY	C-N-CA	6.79	134.19	121.97
1	B	296	LYS	CA-C-N	6.08	132.92	121.97
1	B	296	LYS	C-N-CA	6.08	132.92	121.97
1	A	105	VAL	CA-C-N	5.99	132.58	122.15

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	5255	0	5467	155	0
1	B	5342	0	5544	133	0
2	A	31	13	13	2	0
3	A	12	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	3	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	1	0	0	0	0
6	A	61	0	0	1	0
6	B	73	0	0	0	0
All	All	10797	13	11030	284	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 284 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:56:PHE:HB2	1:A:57:PRO:HD3	1.41	1.03
1:B:54:ILE:HG23	1:B:112:LYS:HD2	1.55	0.87
1:B:470:PHE:HZ	1:B:487:ILE:HD11	1.47	0.79
1:A:253:PHE:HZ	1:A:431:ILE:HD11	1.48	0.78
1:B:390:ALA:HB1	1:B:392:GLN:HE21	1.49	0.77

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	684/705 (97%)	673 (98%)	9 (1%)	2 (0%)	37 67
1	B	703/705 (100%)	685 (97%)	15 (2%)	3 (0%)	30 61
All	All	1387/1410 (98%)	1358 (98%)	24 (2%)	5 (0%)	30 61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	B	178	ARG
1	A	71	THR
1	B	54	ILE
1	B	313	VAL

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	569/577 (99%)	566 (100%)	3 (0%)	86	95
1	B	577/577 (100%)	573 (99%)	4 (1%)	81	94
All	All	1146/1154 (99%)	1139 (99%)	7 (1%)	84	95

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19	ILE
1	B	76	VAL
1	B	386	ARG
1	B	172	LYS
1	A	555	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	B	624	ASN
1	A	697	HIS
1	B	186	ASN
1	B	202	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is 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$
2	ANP	A	801	-	29,33,33	1.25	5 (17%)	31,52,52	1.21	5 (16%)
3	3OH	A	802[A]	-	5,5,5	23.80	4 (80%)	5,5,5	30.02	5 (100%)
3	3OH	A	802[B]	-	5,5,5	23.93	4 (80%)	5,5,5	28.61	4 (80%)
4	PO4	A	803	-	4,4,4	1.44	1 (25%)	6,6,6	0.54	0
4	PO4	B	802	-	4,4,4	1.50	1 (25%)	6,6,6	0.39	0
3	3OH	B	801[A]	-	5,5,5	23.71	4 (80%)	5,5,5	28.54	4 (80%)
3	3OH	B	801[B]	-	5,5,5	23.87	4 (80%)	5,5,5	28.69	5 (100%)

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	ANP	A	801	-	-	8/14/38/38	0/3/3/3
3	3OH	A	802[A]	-	-	3/3/3/3	-
3	3OH	A	802[B]	-	-	3/3/3/3	-
3	3OH	B	801[A]	-	-	3/3/3/3	-
3	3OH	B	801[B]	-	-	2/3/3/3	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802[B]	3OH	O1-C1	36.16	2.40	1.22
3	B	801[B]	3OH	O1-C1	36.06	2.39	1.22
3	A	802[A]	3OH	O1-C1	36.04	2.39	1.22
3	B	801[A]	3OH	O1-C1	35.57	2.38	1.22
3	A	802[B]	3OH	O2-C1	33.64	2.42	1.30

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802[B]	3OH	C3-C2-C1	-56.94	34.96	113.11
3	B	801[B]	3OH	C3-C2-C1	-56.91	34.99	113.11
3	B	801[A]	3OH	C3-C2-C1	-56.80	35.14	113.11
3	A	802[A]	3OH	C3-C2-C1	-56.57	35.46	113.11
3	A	802[B]	3OH	O1-C1-C2	-28.28	33.38	123.09

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	O4'-C4'-C5'-O5'
2	A	801	ANP	C3'-C4'-C5'-O5'
3	A	802[A]	3OH	C1-C2-C3-O3
3	A	802[B]	3OH	C1-C2-C3-O3

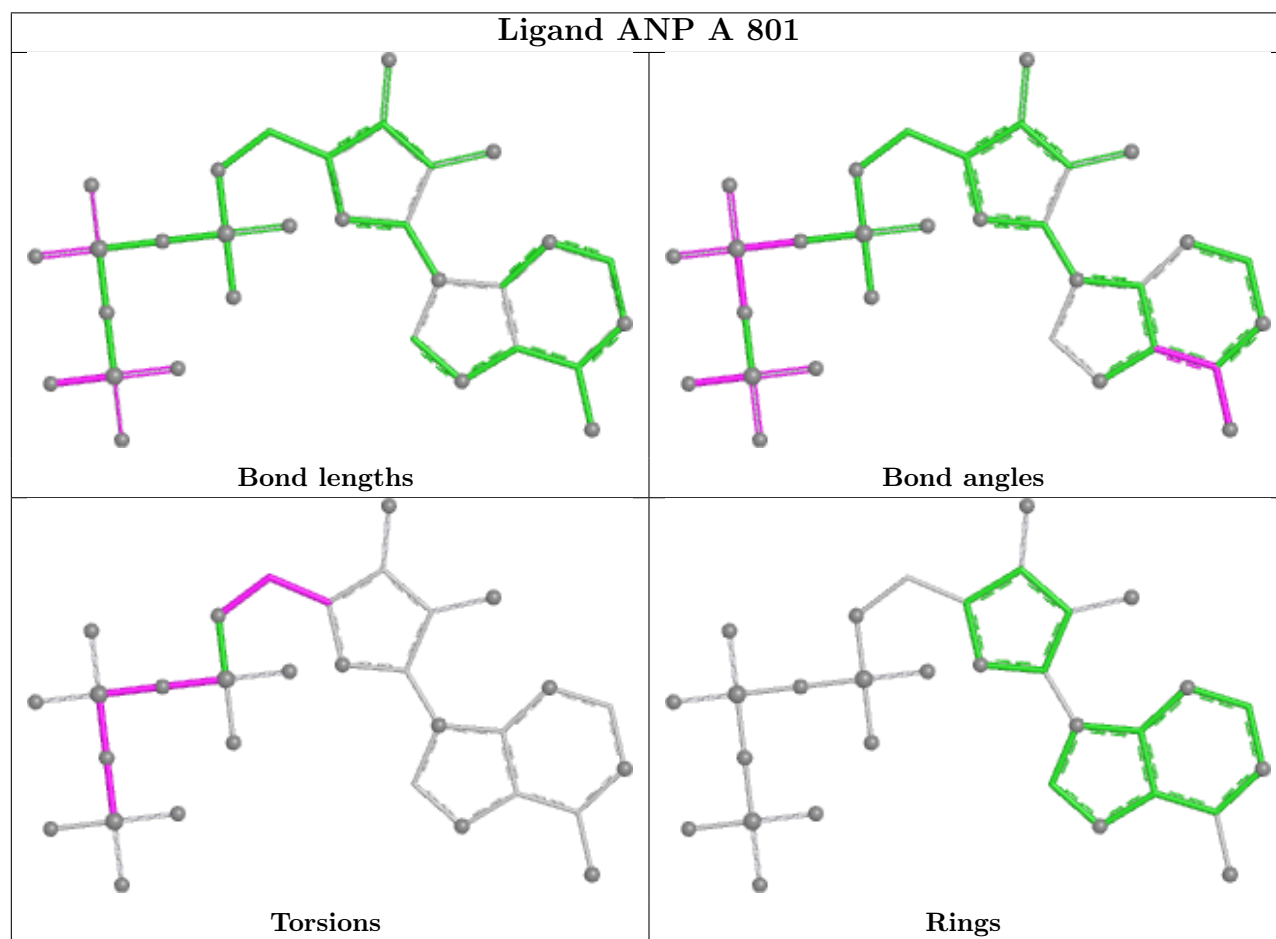
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	2	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 [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	691/705 (98%)	-0.09	1 (0%) 92 91	21, 52, 88, 123	1 (0%)
1	B	703/705 (99%)	-0.24	1 (0%) 92 91	18, 48, 74, 95	2 (0%)
All	All	1394/1410 (98%)	-0.17	2 (0%) 92 91	18, 50, 81, 123	3 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	VAL	2.4
1	B	60	MET	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
5	MG	A	804	1/1	0.65	0.17	108,108,108,108	0
2	ANP	A	801	31/31	0.67	0.12	64,86,128,181	0
3	3OH	B	801[B]	6/6	0.88	0.12	39,41,44,44	6

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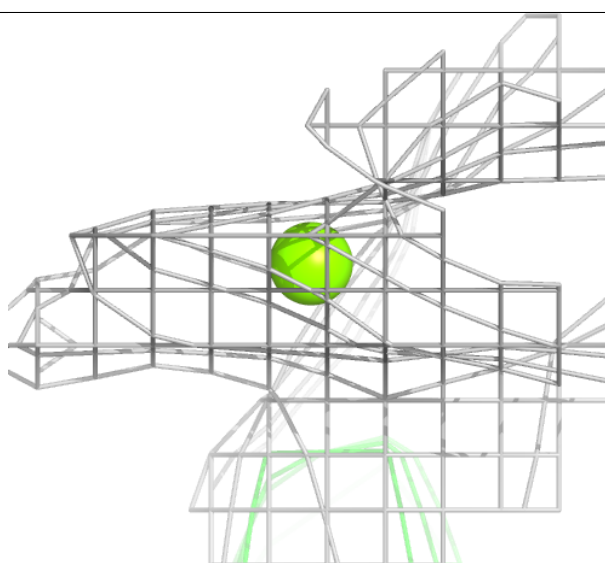
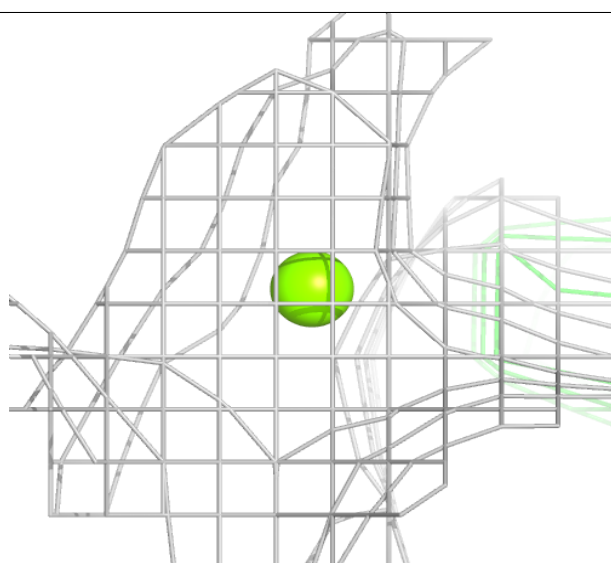
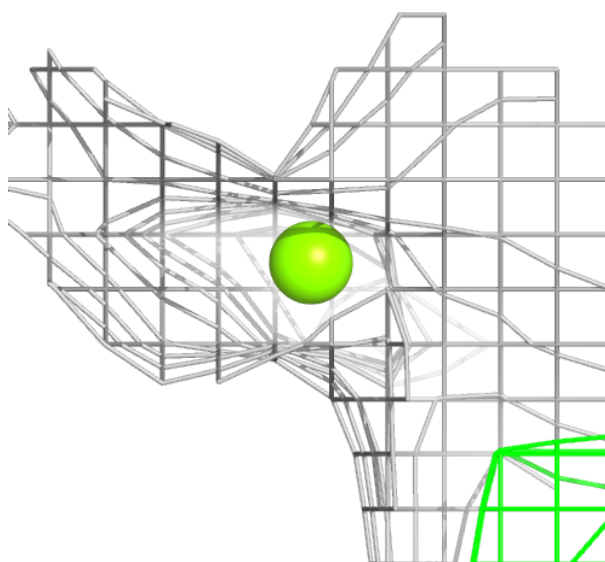
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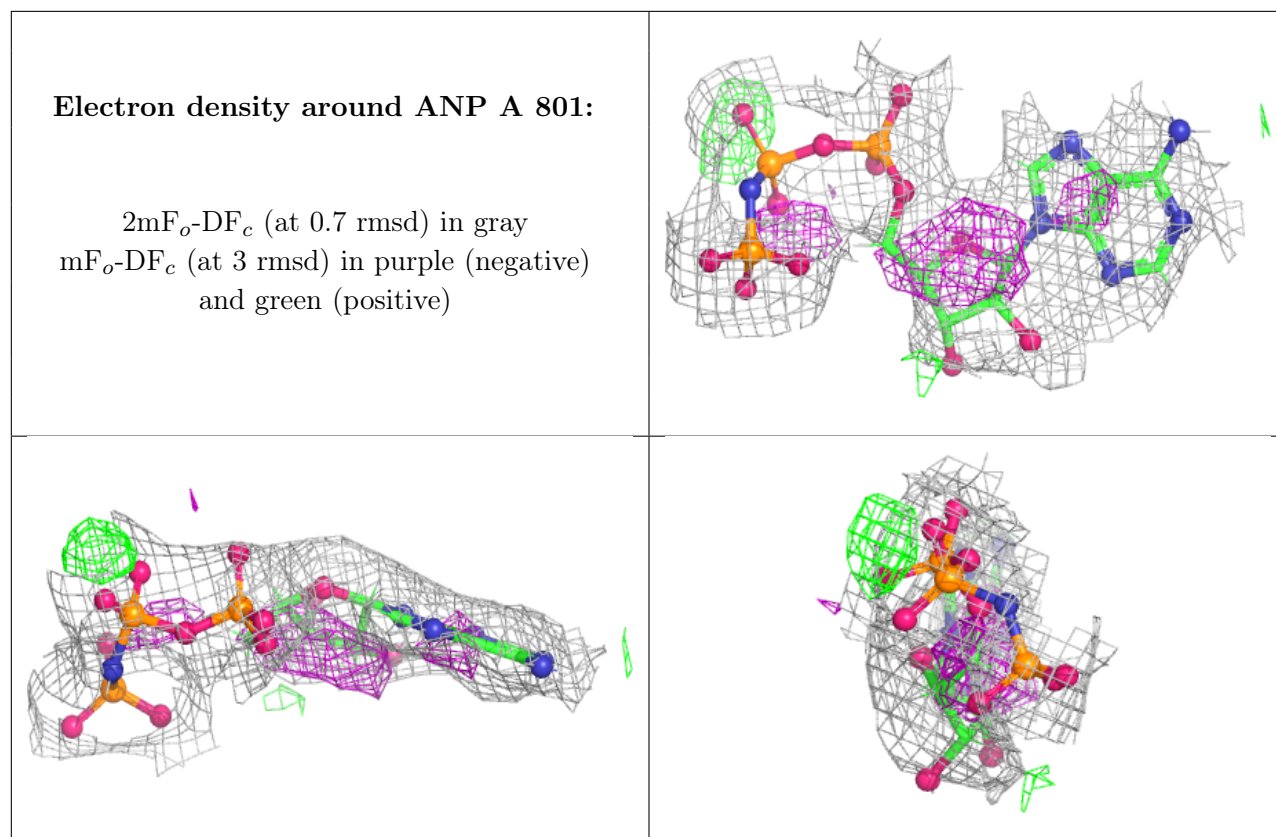
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3OH	B	801[A]	6/6	0.88	0.12	38,42,49,49	0
3	3OH	A	802[B]	6/6	0.93	0.09	55,57,58,60	6
3	3OH	A	802[A]	6/6	0.93	0.09	57,57,58,58	6
4	PO4	B	802	5/5	0.95	0.09	38,46,47,61	0
4	PO4	A	803	5/5	0.98	0.06	27,33,43,50	0

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 MG A 804:

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.