



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:20 am BST

PDB ID : 5YBI
Title : Structure of the bacterial pathogens ATPase with substrate AMPPNP
Authors : Mu, Z.X.; Gao, X.P.; Cui, S.
Deposited on : 2017-09-05
Resolution : 2.27 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

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

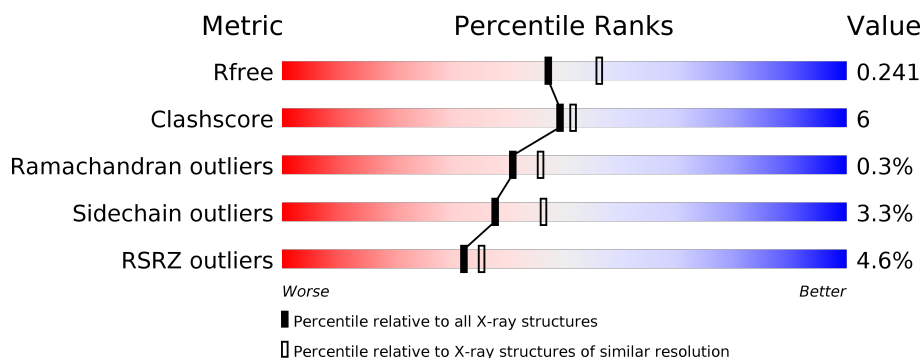
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	368	
1	B	368	

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
4	MG	A	520	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11266 atoms, of which 5435 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 Probable ATP synthase SpaL/MxiB.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	337	Total	C	H	N	O	S	Se	0	7	0
			5361	1690	2690	460	510	4	7			
1	B	345	Total	C	H	N	O	S	Se	0	3	0
			5436	1713	2729	468	516	4	6			

There are 42 discrepancies between the modelled and reference sequences:

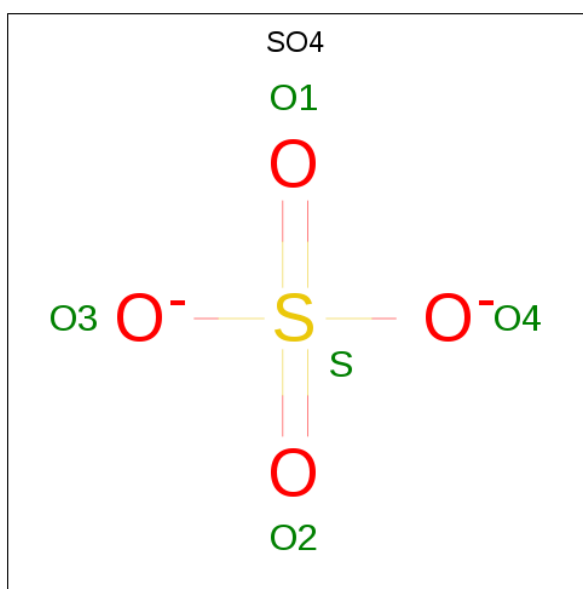
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	initiating methionine	UNP P0A1C1
A	-20	GLY	-	expression tag	UNP P0A1C1
A	-19	SER	-	expression tag	UNP P0A1C1
A	-18	SER	-	expression tag	UNP P0A1C1
A	-17	HIS	-	expression tag	UNP P0A1C1
A	-16	HIS	-	expression tag	UNP P0A1C1
A	-15	HIS	-	expression tag	UNP P0A1C1
A	-14	HIS	-	expression tag	UNP P0A1C1
A	-13	HIS	-	expression tag	UNP P0A1C1
A	-12	HIS	-	expression tag	UNP P0A1C1
A	-11	SER	-	expression tag	UNP P0A1C1
A	-10	SER	-	expression tag	UNP P0A1C1
A	-9	GLY	-	expression tag	UNP P0A1C1
A	-8	LEU	-	expression tag	UNP P0A1C1
A	-7	VAL	-	expression tag	UNP P0A1C1
A	-6	PRO	-	expression tag	UNP P0A1C1
A	-5	ARG	-	expression tag	UNP P0A1C1
A	-4	GLY	-	expression tag	UNP P0A1C1
A	-3	SER	-	expression tag	UNP P0A1C1
A	-2	HIS	-	expression tag	UNP P0A1C1
A	-1	MSE	-	expression tag	UNP P0A1C1
B	-15	MSE	-	initiating methionine	UNP P0A1C1
B	-14	GLY	-	expression tag	UNP P0A1C1
B	-13	SER	-	expression tag	UNP P0A1C1
B	-12	SER	-	expression tag	UNP P0A1C1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P0A1C1
B	-10	HIS	-	expression tag	UNP P0A1C1
B	-9	HIS	-	expression tag	UNP P0A1C1
B	-8	HIS	-	expression tag	UNP P0A1C1
B	-7	HIS	-	expression tag	UNP P0A1C1
B	-6	HIS	-	expression tag	UNP P0A1C1
B	-5	SER	-	expression tag	UNP P0A1C1
B	-4	SER	-	expression tag	UNP P0A1C1
B	-3	GLY	-	expression tag	UNP P0A1C1
B	-2	LEU	-	expression tag	UNP P0A1C1
B	-1	VAL	-	expression tag	UNP P0A1C1
B	0	PRO	-	expression tag	UNP P0A1C1
B	1	ARG	-	expression tag	UNP P0A1C1
B	2	GLY	-	expression tag	UNP P0A1C1
B	3	SER	-	expression tag	UNP P0A1C1
B	4	HIS	-	expression tag	UNP P0A1C1
B	5	MSE	-	expression tag	UNP P0A1C1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



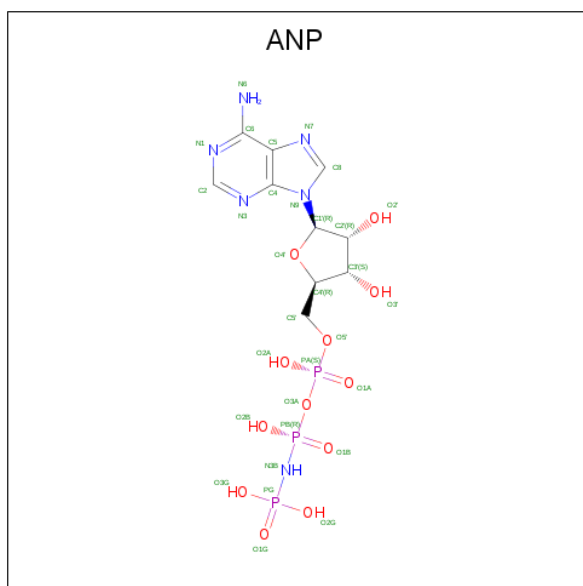
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			47	10	16	6	12	3		

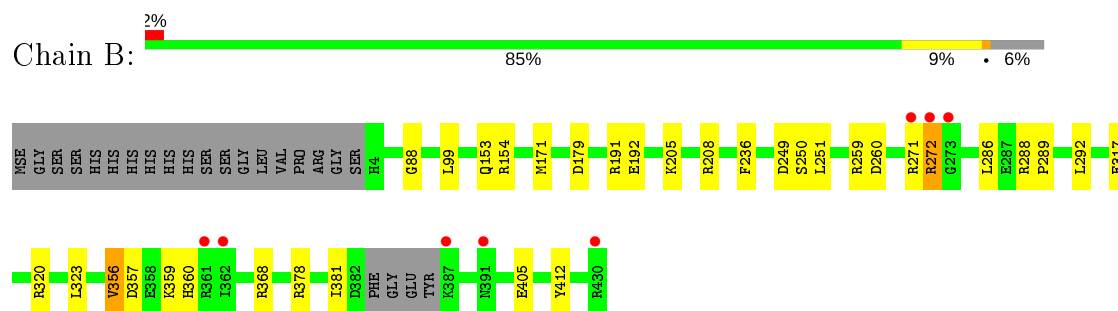
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	22	Total	Mg	0	0
			22	22		
4	A	16	Total	Mg	0	0
			16	16		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total 160	O 160	0	0
5	B	189	Total 189	O 189	0	0

- Molecule 1: Probable ATP synthase SpaL/MxiB



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.02Å 105.02Å 146.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.00 – 2.27 43.43 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.00-2.27) 98.6 (43.43-2.27)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, R_{free}	0.179 , 0.227 0.194 , 0.241	Depositor DCC
R_{free} test set	2178 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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, ANP, 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	0.48	0/2728	0.58	0/3669
1	B	0.56	0/2748	0.61	2/3701 (0.1%)
All	All	0.52	0/5476	0.59	2/7370 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ASP	C-N-CA	9.59	145.68	121.70
1	B	249	ASP	CB-CG-OD1	5.25	123.02	118.30

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	2671	2690	2665	38	0
1	B	2707	2729	2721	23	0
2	A	20	0	0	1	0
2	B	15	0	0	1	0
3	A	31	16	13	6	0
4	A	16	0	0	0	0
4	B	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	160	0	0	16	2
5	B	189	0	0	10	3
All	All	5831	5435	5399	64	3

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 (64) 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:208[B]:ARG:NH1	5:B:604:HOH:O	2.15	0.78
3:A:505:ANP:O1B	5:A:601:HOH:O	2.01	0.78
1:A:310:ASP:O	5:A:603:HOH:O	2.02	0.78
1:A:259:ARG:NE	5:A:607:HOH:O	2.17	0.77
1:A:199:TYR:OH	5:A:602:HOH:O	2.01	0.75
1:A:324:ASP:OD2	5:A:604:HOH:O	2.06	0.74
1:A:259:ARG:NH1	1:A:260:ASP:OD1	2.22	0.72
1:A:324:ASP:OD1	5:A:604:HOH:O	2.08	0.71
1:A:169[A]:MSE:HE1	1:A:249:ASP:HB2	1.71	0.70
1:B:271:ARG:O	5:B:601:HOH:O	2.08	0.70
1:A:402:SER:OG	5:A:605:HOH:O	2.10	0.69
1:B:317:GLU:OE1	5:B:602:HOH:O	2.10	0.69
1:B:259:ARG:NH1	1:B:260:ASP:OD1	2.27	0.68
1:A:117[A]:ARG:NH2	5:A:612:HOH:O	2.31	0.64
1:A:411:ASP:OD1	5:A:606:HOH:O	2.13	0.64
1:A:259:ARG:NH2	5:A:607:HOH:O	2.31	0.63
1:A:324:ASP:CG	5:A:604:HOH:O	2.35	0.63
2:B:503:SO4:O3	5:B:603:HOH:O	2.13	0.62
1:B:171:MSE:CE	1:B:412:TYR:HA	2.32	0.59
1:A:259:ARG:CZ	5:A:607:HOH:O	2.51	0.59
1:B:292:LEU:O	5:B:605:HOH:O	2.17	0.58
1:A:169[B]:MSE:CE	1:A:247:PHE:HB3	2.36	0.55
1:B:405:GLU:OE2	5:B:607:HOH:O	2.18	0.54
1:B:260:ASP:OD2	5:B:606:HOH:O	2.17	0.53
1:B:171:MSE:HE2	1:B:412:TYR:HA	1.90	0.53
1:A:272:ARG:O	1:A:274:TYR:N	2.42	0.53
1:B:192:GLU:OE1	5:B:608:HOH:O	2.19	0.52
1:A:324:ASP:HA	1:A:350:ARG:HD2	1.92	0.51
1:B:378:ARG:O	1:B:381:ILE:HG13	2.11	0.50
1:A:154:ARG:HB3	1:A:323:LEU:HD22	1.92	0.50
1:B:368:ARG:NE	5:B:616:HOH:O	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PHE:CD2	3:A:505:ANP:H5'1	2.49	0.47
1:A:153:GLN:HG3	1:A:324:ASP:OD1	2.13	0.47
1:A:117[A]:ARG:NE	5:A:627:HOH:O	2.47	0.47
1:A:165:LYS:O	1:A:169[B]:MSE:HG2	2.14	0.47
1:B:357:ASP:OD2	1:B:359:LYS:NZ	2.35	0.47
1:A:155:MSE:HE1	1:A:325:GLY:HA3	1.98	0.46
3:A:505:ANP:O1G	3:A:505:ANP:O2B	2.33	0.45
1:B:179:ASP:O	1:B:208[B]:ARG:HD2	2.16	0.45
1:A:167:PHE:HE2	3:A:505:ANP:H2'	1.81	0.45
1:A:107:ALA:HB2	1:A:206:LYS:HG3	1.99	0.44
1:A:351:VAL:O	1:A:354:GLN:HG2	2.17	0.44
1:A:320:ARG:HE	1:A:326:HIS:CE1	2.36	0.44
1:B:205:LYS:HG2	1:B:208[B]:ARG:NH2	2.33	0.44
1:B:356:VAL:CG2	1:B:360:HIS:ND1	2.82	0.43
1:A:288:ARG:N	1:A:289:PRO:CD	2.82	0.43
1:B:205:LYS:HE2	1:B:208[B]:ARG:HH21	1.84	0.43
1:A:169[B]:MSE:CE	1:A:247:PHE:HD2	2.32	0.42
1:B:288:ARG:N	1:B:289:PRO:CD	2.82	0.42
1:B:191:ARG:HD3	5:B:632:HOH:O	2.19	0.42
1:A:169[A]:MSE:HE2	1:A:247:PHE:HB3	2.01	0.42
1:B:88:GLY:HA2	1:B:236:PHE:CE2	2.55	0.41
1:A:190:GLY:O	1:A:194:THR:HG23	2.21	0.41
1:B:271:ARG:O	1:B:272:ARG:HB2	2.21	0.41
1:A:189:ARG:CG	5:A:620:HOH:O	2.68	0.41
1:A:167:PHE:HE2	3:A:505:ANP:H3'	1.85	0.41
1:A:180:ILE:HG21	1:A:237:PHE:CD2	2.55	0.41
1:B:286:LEU:HD13	1:B:323:LEU:HD21	2.03	0.41
1:A:167:PHE:CE2	3:A:505:ANP:H2'	2.56	0.41
1:A:217:ASP:N	1:A:217:ASP:OD1	2.48	0.41
1:A:-2:HIS:ND1	2:A:503:SO4:O4	2.46	0.40
1:A:189:ARG:NE	5:A:620:HOH:O	2.41	0.40
1:A:199:TYR:O	5:A:609:HOH:O	2.22	0.40
1:B:251:LEU:HD11	1:B:286:LEU:HD21	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:721:HOH:O	5:B:771:HOH:O[4_555]	2.04	0.16
5:A:695:HOH:O	5:B:764:HOH:O[6_655]	2.09	0.11
5:A:738:HOH:O	5:B:602:HOH:O[3_665]	2.12	0.08

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	338/368 (92%)	325 (96%)	12 (4%)	1 (0%)	41	46
1	B	343/368 (93%)	333 (97%)	9 (3%)	1 (0%)	41	46
All	All	681/736 (92%)	658 (97%)	21 (3%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	ARG
1	A	273	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	289/301 (96%)	276 (96%)	13 (4%)	27	31
1	B	290/301 (96%)	284 (98%)	6 (2%)	53	62
All	All	579/602 (96%)	560 (97%)	19 (3%)	38	46

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	154	ARG
1	A	167	PHE
1	A	206	LYS

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Mol	Chain	Res	Type
1	A	215	THR
1	A	268	SER
1	A	271	ARG
1	A	282	LEU
1	A	291	LYS
1	A	321	SER
1	A	324	ASP
1	A	329	LEU
1	A	378	ARG
1	B	99	LEU
1	B	153	GLN
1	B	154	ARG
1	B	250	SER
1	B	320	ARG
1	B	356	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	HIS

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 46 ligands modelled in this entry, 38 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
2	SO4	B	503	4	4,4,4	0.15	0	6,6,6	0.40	0
2	SO4	A	503	-	4,4,4	0.17	0	6,6,6	0.29	0
3	ANP	A	505	4	29,33,33	1.14	3 (10%)	31,52,52	1.24	4 (12%)
2	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.39	0
2	SO4	B	501	-	4,4,4	0.18	0	6,6,6	0.95	0
2	SO4	B	502	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	501	-	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
3	ANP	A	505	4	-	8/14/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	ANP	PB-O3A	-3.15	1.55	1.59
3	A	505	ANP	PG-O1G	2.84	1.50	1.46
3	A	505	ANP	PB-O1B	2.12	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	ANP	O1G-PG-N3B	-3.00	107.35	111.77
3	A	505	ANP	PA-O3A-PB	-2.93	122.30	132.62
3	A	505	ANP	C3'-C2'-C1'	2.77	105.15	100.98
3	A	505	ANP	C5-C6-N6	2.37	123.96	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

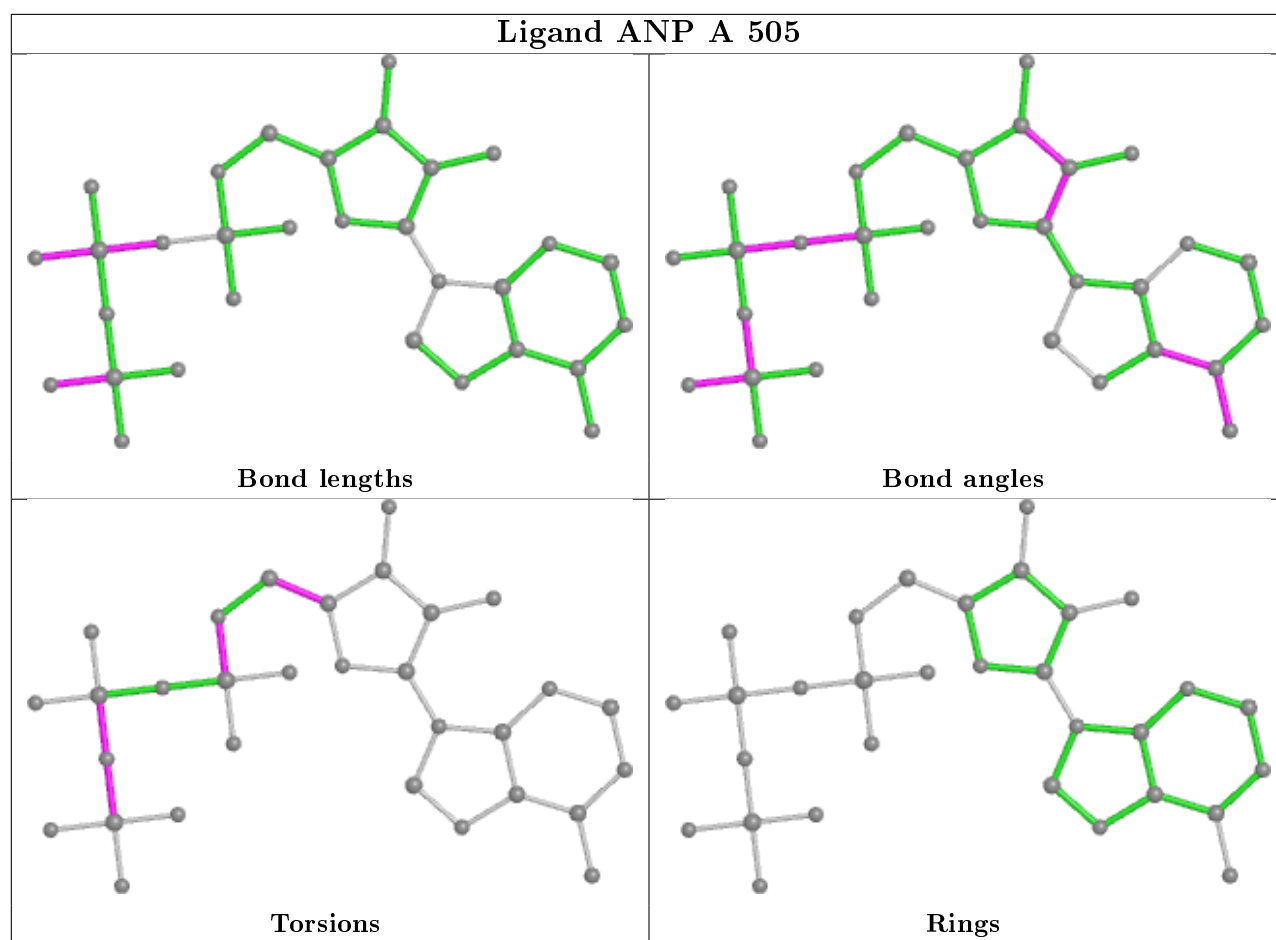
Mol	Chain	Res	Type	Atoms
3	A	505	ANP	PB-N3B-PG-O1G
3	A	505	ANP	PG-N3B-PB-O1B
3	A	505	ANP	PG-N3B-PB-O3A
3	A	505	ANP	C5'-O5'-PA-O1A
3	A	505	ANP	C5'-O5'-PA-O2A
3	A	505	ANP	C3'-C4'-C5'-O5'
3	A	505	ANP	O4'-C4'-C5'-O5'
3	A	505	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	SO4	1	0
2	A	503	SO4	1	0
3	A	505	ANP	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, 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	331/368 (89%)	0.14	23 (6%) 16 18	19, 37, 84, 123	0
1	B	339/368 (92%)	-0.17	8 (2%) 59 62	17, 32, 61, 88	0
All	All	670/736 (91%)	-0.02	31 (4%) 32 35	17, 34, 69, 123	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	PHE	13.9
1	A	271	ARG	8.8
1	A	398	TYR	7.2
1	A	310	ASP	6.3
1	A	272	ARG	5.3
1	A	393	SER	5.1
1	A	377	LEU	5.1
1	A	397	ILE	4.8
1	A	270	ALA	4.7
1	A	378	ARG	4.3
1	A	395	ASP	4.1
1	A	394	GLN	4.1
1	A	110	ASP	3.7
1	A	403	VAL	3.6
1	A	380	ILE	3.5
1	B	271	ARG	3.4
1	A	309	ASP	3.4
1	A	396	LYS	3.4
1	A	371	LEU	3.2
1	A	379	THR	3.1
1	B	387	LYS	3.1
1	A	430	ARG	2.9
1	B	430	ARG	2.8
1	B	361	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	399	ASN	2.6
1	A	314	PRO	2.6
1	B	362	ILE	2.5
1	B	272	ARG	2.4
1	A	374	ILE	2.4
1	B	273	GLY	2.1
1	B	391	ASN	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, 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.

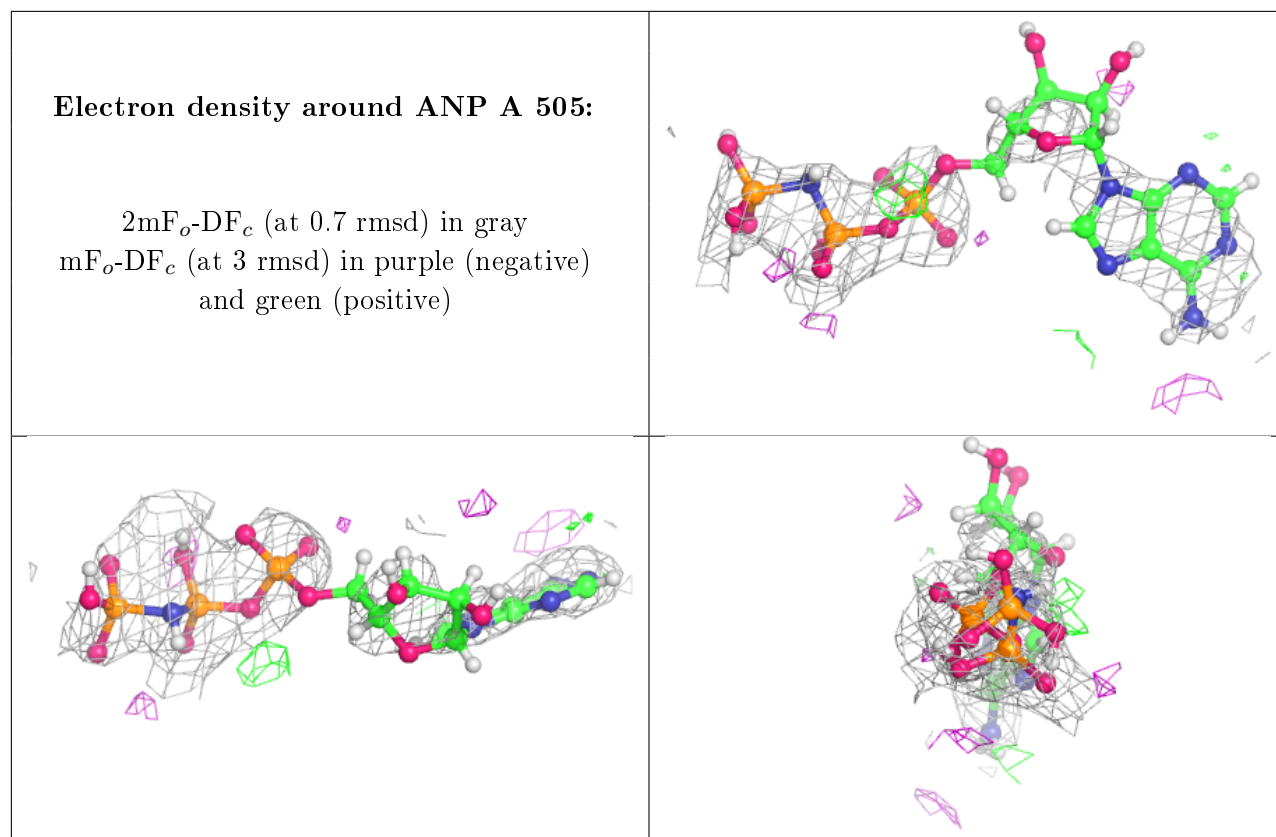
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	506	1/1	0.72	0.18	59,59,59,59	0
4	MG	B	523	1/1	0.74	0.37	59,59,59,59	0
4	MG	A	520	1/1	0.78	0.41	55,55,55,55	0
4	MG	A	511	1/1	0.79	0.16	51,51,51,51	0
4	MG	B	509	1/1	0.82	0.26	45,45,45,45	0
4	MG	B	510	1/1	0.83	0.28	52,52,52,52	0
4	MG	A	510	1/1	0.84	0.15	42,42,42,42	0
4	MG	B	516	1/1	0.86	0.33	54,54,54,54	0
4	MG	A	518	1/1	0.87	0.34	48,48,48,48	0
4	MG	A	509	1/1	0.88	0.12	45,45,45,45	0
4	MG	A	517	1/1	0.89	0.26	61,61,61,61	0
3	ANP	A	505	31/31	0.90	0.27	37,59,77,89	47
4	MG	B	513	1/1	0.91	0.26	51,51,51,51	0
4	MG	A	514	1/1	0.91	0.51	60,60,60,60	0
4	MG	B	525	1/1	0.91	0.08	63,63,63,63	0
4	MG	B	518	1/1	0.92	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	519	1/1	0.92	0.21	77,77,77,77	0
4	MG	B	519	1/1	0.92	0.16	52,52,52,52	0
4	MG	A	513	1/1	0.92	0.07	53,53,53,53	0
4	MG	B	508	1/1	0.92	0.11	44,44,44,44	0
4	MG	A	508	1/1	0.93	0.29	49,49,49,49	0
4	MG	B	512	1/1	0.93	0.13	44,44,44,44	0
2	SO4	A	502	5/5	0.94	0.12	52,59,70,81	0
2	SO4	A	504	5/5	0.94	0.14	55,62,70,83	0
4	MG	B	520	1/1	0.94	0.12	55,55,55,55	0
2	SO4	B	503	5/5	0.94	0.13	32,48,58,68	0
4	MG	B	524	1/1	0.95	0.20	64,64,64,64	0
4	MG	B	514	1/1	0.95	0.07	46,46,46,46	0
2	SO4	B	502	5/5	0.95	0.12	54,58,76,79	0
2	SO4	B	501	5/5	0.95	0.16	25,35,46,47	0
4	MG	B	521	1/1	0.95	0.25	52,52,52,52	0
4	MG	B	504	1/1	0.95	0.23	40,40,40,40	0
4	MG	B	506	1/1	0.96	0.16	42,42,42,42	0
4	MG	B	517	1/1	0.96	0.08	54,54,54,54	0
4	MG	A	516	1/1	0.96	0.43	59,59,59,59	0
2	SO4	A	503	5/5	0.96	0.11	60,61,75,80	0
2	SO4	A	501	5/5	0.97	0.08	54,55,62,63	0
4	MG	B	507	1/1	0.97	0.14	45,45,45,45	0
4	MG	B	522	1/1	0.97	0.15	79,79,79,79	0
4	MG	B	511	1/1	0.97	0.15	41,41,41,41	0
4	MG	A	515	1/1	0.97	0.09	48,48,48,48	0
4	MG	A	507	1/1	0.97	0.17	42,42,42,42	0
4	MG	B	515	1/1	0.97	0.21	54,54,54,54	0
4	MG	A	521	1/1	0.98	0.36	49,49,49,49	0
4	MG	B	505	1/1	0.99	0.12	34,34,34,34	0
4	MG	A	512	1/1	0.99	0.11	48,48,48,48	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.