



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:35 AM UTC

PDB ID : 3VR3 / pdb_00003vr3
Title : Crystal structure of AMP-PNP bound A3B3 complex from *Enterococcus hirae* V-ATPase [bA3B3]
Authors : Arai, S.; Saijo, S.; Suzuki, K.; Mizutani, K.; Kakinuma, Y.; Ishizuka-Katsura, Y.; Ohsawa, N.; Terada, T.; Shirouzu, M.; Yokoyama, S.; Iwata, S.; Yamato, I.; Murata, T.
Deposited on : 2012-04-03
Resolution : 3.40 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](#) ①) 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

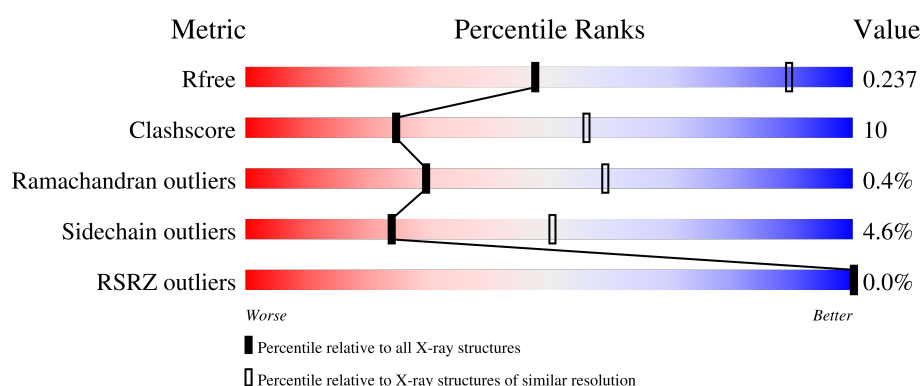
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	600	 72% 23% . .
1	B	600	 77% 19% . .
1	C	600	 74% 21% . .
2	D	465	 75% 20% . .
2	E	465	 74% 22% . .

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Mol	Chain	Length	Quality of chain
2	F	465	74% 22% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24266 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	Se	0	0	0
			4562	2866	766	904	3	23			
1	B	586	Total	C	N	O	S	Se	0	0	0
			4539	2851	763	899	3	23			
1	C	584	Total	C	N	O	S	Se	0	0	0
			4525	2844	758	897	3	23			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636
C	-3	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

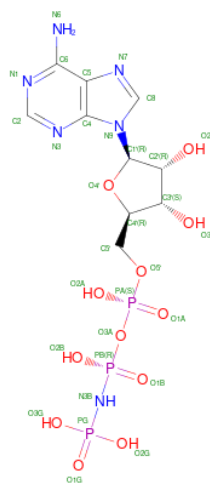
- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	447	Total 3449	C 2179	N 596	O 660	Se 14	0	0	0
2	E	451	Total 3533	C 2238	N 606	O 675	Se 14	0	0	0
2	F	451	Total 3523	C 2233	N 602	O 674	Se 14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	C	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	6	Total O 6 6	0	0
5	C	16	Total O 16 16	0	0
5	D	13	Total O 13 13	0	0
5	E	10	Total O 10 10	0	0

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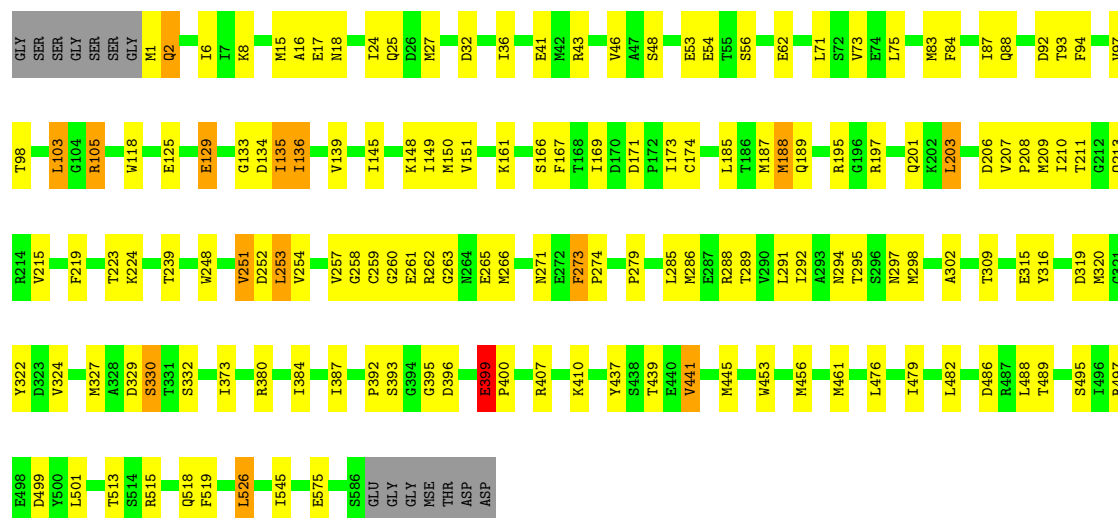
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	14	Total	O	0	0
			14	14		

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.

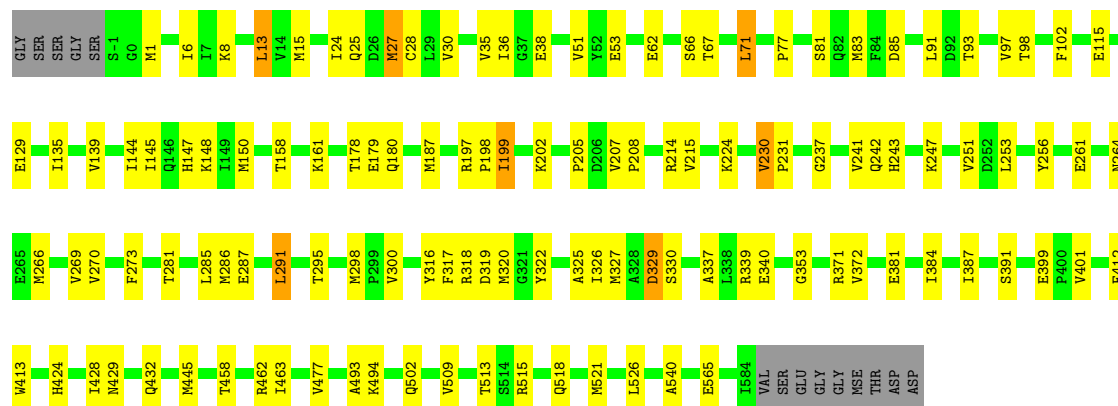
- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain A: 



- Molecule 1: V-type sodium ATPase catalytic subunit A

Chain B: 



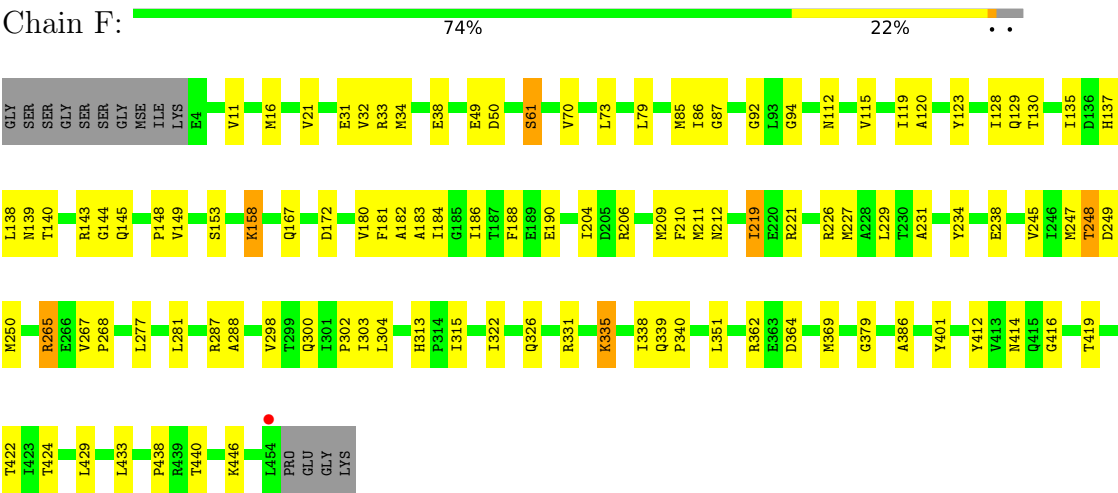
- Molecule 1: V-type sodium ATPase catalytic subunit A

E564	E399	D278	GLY
E565	P400	I144	SER
E566	K410	T281	SER
L567	V411	Q146	GLY
N574	F412	H147	SER
I577	W413	K148	SER
I584	L291	I149	GLY
VAL	I292	M150	M1
GLU	A293	T158	Q2
SER	H424	N294	K8
GLY	F425	T295	K8
GLY	P426	S296	P12
MSE	I428	N297	L13
THR	L436	M298	L13
ASP	L445	P299	V14
ASP	L449	V300	M15
	E467	I173	
	L470	T187	T24
	V474	M188	Q25
	R475	Q189	D26
	L476	K190	M27
	V477	M209	C28
	L488	R197	E41
	T489	P198	
	F491	I199	Q44
	L490	P208	S48
	R493	M209	
	K494	R214	R65
	R497	D329	S66
	L501	C225	
	Q502	T331	L71
	Q503	A228	M83
	N504	A229	F94
	D507	V230	D95
	T513	P231	
	R515	V241	Q88
	Q518	Q242	R89
	M521	H243	
	N543	Q244	D92
	I562	I245	M95
	E563	A246	
	E564	K247	N101
	E565	V248	
	E566	S249	H114
	E567	D250	M119
	E568	V251	E121
	E569	D252	E129
	E570	L253	I135
	E571	R262	V139
	E572	A389	D140
	E573	V390	E411
	E574	S391	
	E575	P392	
	E576	V270	
	E577	F273	
	E578	S397	
	E579	E399	

L433	N280	Q167	GLY
M436	F285	V170	SER
L442	R292	L171	GLY
LYS	Q300	D172	SER
R444	M306	S173	SER
D448	L328	S174	GLY
L449	L329	D175	MSE
L450	L338	D176	ILE
D451	P241	F177	LVS
R452	V344	F181	GLU
LEU	L345	A182	YS
PRO	P346	A183	K9
GLY	L351	I184	E10
LYS	R352	D187	V11
	D353	F198	V12
	R362	T201	G13
	R363	G202	M16
	D364	A203	E19
	Q371	R206	E27
	L385	S207	M34
	A386	V208	V44
	V387	M209	L45
	L388	F210	V54
	G390	M211	T60
	E391	I219	I63
	S392	T222	L79
	A393	M227	I86
	L394	Y234	P101
	T400	R239	E102
	K403	T248	I103
	F404	D249	V115
	F408	R250	I119
	E409	L257	P124
	N410	R258	L138
	N414	F259	R143
	F432	G269	F150
		R270	A162
		Y273	Q163
		L277	P165

E411	R258	L138	GLY
Y412	R264	L139	SER
Y413	R267	L140	SER
N414	V267	R143	GLY
Q415			SER
T419	Y273	P148	SER
		V149	GLY
R439	L277	S153	MSE
K443	V278		ILE
K444	T279	K158	LVS
K445	S297	V180	E4
K446	P302	F181	T7
D447	I303	A182	E10
	L304	A183	
L450		I184	L29
L454	H313	M195	R33
PRO	P314		
GLU	I315	R199	V44
GLY	P316		
LVS	D317	A203	Q48
	L318		
		R206	V54
	Y321		Q55
	L322	M209	I56
	T323	F210	F57
		M211	
	T330	M212	L77
			Q78
	L338	I219	L79
	D343	T224	E83
		P225	D84
	P346	R226	M85
		M227	
	L351	A228	V89
	K352	L229	F90
	D353	T230	
		A231	G94
	A367		R95
	T368	Y234	P96
	M369		K97
		E238	D98
	L372	K239	
			E102
	L385	H242	
	A386		I111
	V387	V245	N112
	V388	I246	G113
	L389	M247	E114
		T248	
	I400	D249	R121
		M250	
	F404		E126
	F408	Y253	F127
	F409	A254	I128
	N410	E255	T129

● Molecule 2: V-type sodium ATPase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.11Å 124.13Å 245.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.99 – 3.40 70.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.99-3.40) 99.6 (70.99-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.239 0.200 , 0.237	Depositor DCC
R_{free} test set	2653 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.030 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24266	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: ANP, 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	0.49	0/4616	0.83	2/6209 (0.0%)
1	B	0.50	0/4592	0.81	0/6176
1	C	0.48	0/4579	0.83	4/6162 (0.1%)
2	D	0.48	0/3494	0.83	0/4699
2	E	0.48	0/3581	0.83	1/4818 (0.0%)
2	F	0.47	0/3571	0.81	0/4806
All	All	0.48	0/24433	0.82	7/32870 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	564	GLU	N-CA-C	5.65	117.12	110.97
1	A	399	GLU	CA-C-N	5.62	125.08	119.24
1	A	399	GLU	C-N-CA	5.62	125.08	119.24
1	C	44	GLN	CB-CA-C	-5.25	110.09	117.23
2	E	447	ASP	N-CA-C	5.19	116.62	111.07

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	4562	0	4528	95	0
1	B	4539	0	4483	91	0
1	C	4525	0	4468	92	0
2	D	3449	0	3425	66	0
2	E	3533	0	3543	74	0
2	F	3523	0	3526	74	0
3	B	31	0	13	0	0
3	C	31	0	13	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	12	0	0	0	0
5	B	6	0	0	0	0
5	C	16	0	0	0	0
5	D	13	0	0	1	0
5	E	10	0	0	0	0
5	F	14	0	0	0	0
All	All	24266	0	23999	471	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 10.

The worst 5 of 471 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:C:27:MSE:HE3	1:C:71:LEU:HB2	1.23	1.15
2:E:77:LEU:HD23	2:E:111:ILE:CD1	1.76	1.14
2:E:77:LEU:HD23	2:E:111:ILE:HD11	1.10	1.09
1:B:242:GLN:OE1	1:B:329:ASP:HB2	1.58	1.04
1:A:320:MSE:HE2	1:A:322:TYR:HE2	1.28	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	584/600 (97%)	542 (93%)	38 (6%)	4 (1%)	18	47
1	B	584/600 (97%)	548 (94%)	35 (6%)	1 (0%)	43	71
1	C	582/600 (97%)	549 (94%)	33 (6%)	0	100	100
2	D	443/465 (95%)	403 (91%)	38 (9%)	2 (0%)	24	54
2	E	449/465 (97%)	420 (94%)	26 (6%)	3 (1%)	18	47
2	F	449/465 (97%)	422 (94%)	25 (6%)	2 (0%)	30	59
All	All	3091/3195 (97%)	2884 (93%)	195 (6%)	12 (0%)	30	59

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	SER
2	F	172	ASP
2	E	126	GLU
2	F	386	ALA
2	E	249	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	502/487 (103%)	469 (93%)	33 (7%)	15	41
1	B	495/487 (102%)	474 (96%)	21 (4%)	26	52
1	C	494/487 (101%)	473 (96%)	21 (4%)	26	51
2	D	360/372 (97%)	344 (96%)	16 (4%)	25	51
2	E	374/372 (100%)	357 (96%)	17 (4%)	24	51
2	F	372/372 (100%)	360 (97%)	12 (3%)	34	58
All	All	2597/2577 (101%)	2477 (95%)	120 (5%)	24	50

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	ARG

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Mol	Chain	Res	Type
2	F	86	ILE
1	C	399	GLU
2	F	61	SER
2	F	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	147	HIS
2	F	137	HIS
1	C	520	ASN
2	F	112	ASN
2	F	339	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ANP	C	601	4	33,33,33	2.00	10 (30%)	45,52,52	2.01	13 (28%)
3	ANP	B	601	4	33,33,33	2.16	10 (30%)	45,52,52	2.00	13 (28%)

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	C	601	4	-	5/18/38/38	0/3/3/3
3	ANP	B	601	4	-	5/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ANP	C5-C4	5.26	1.48	1.39
3	B	601	ANP	C5-C4	5.09	1.48	1.39
3	B	601	ANP	PG-N3B	4.91	1.76	1.63
3	B	601	ANP	PB-N3B	4.63	1.75	1.63
3	C	601	ANP	PG-N3B	4.25	1.74	1.63

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	ANP	C5-C4-N3	-5.51	119.13	126.72
3	C	601	ANP	C5-C4-N3	-5.38	119.31	126.72
3	B	601	ANP	O1G-PG-N3B	-4.52	105.11	111.77
3	B	601	ANP	N3-C4-N9	4.41	134.67	127.17
3	C	601	ANP	O2B-PB-O1B	4.41	119.33	109.87

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

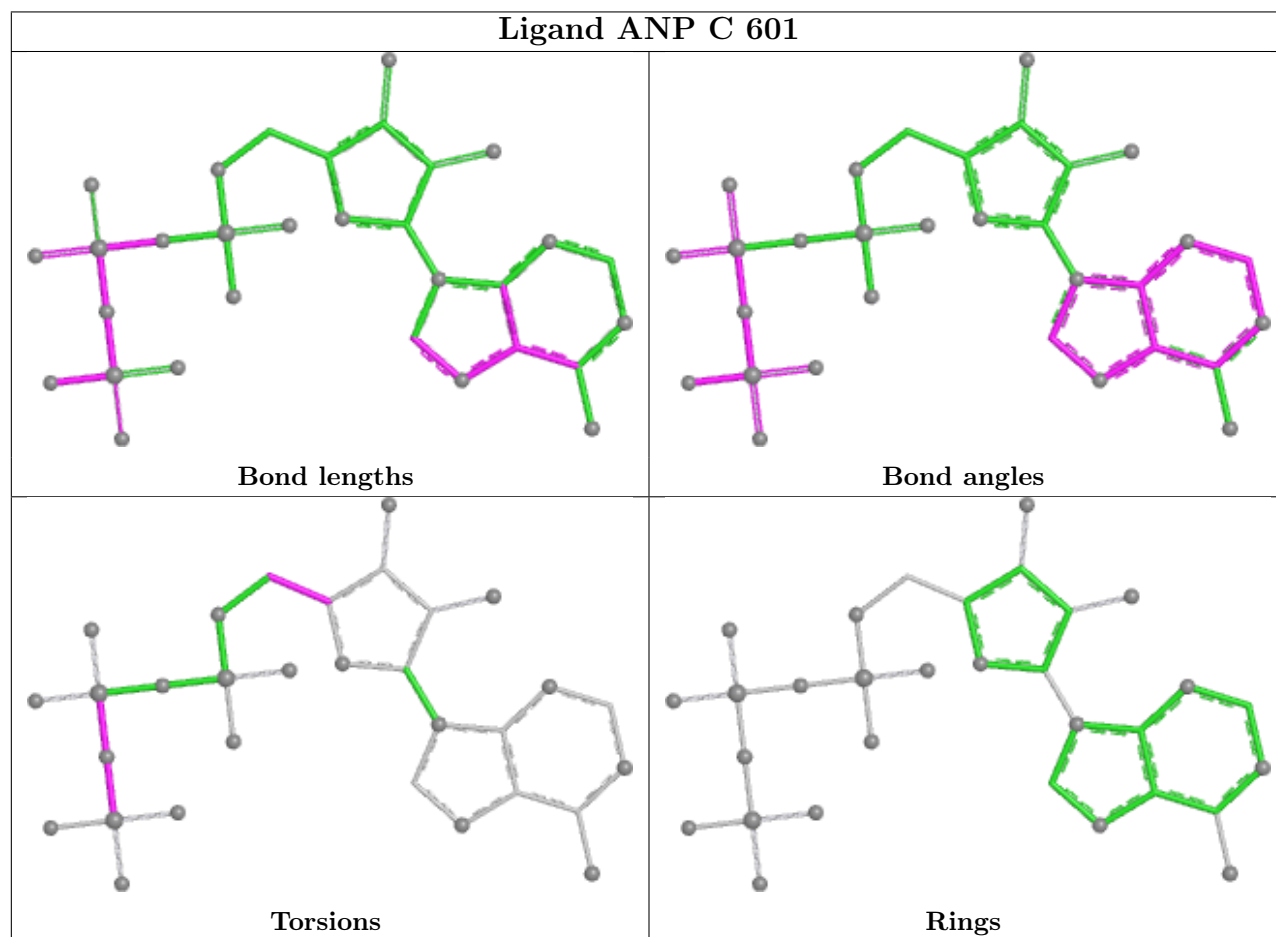
Mol	Chain	Res	Type	Atoms
3	B	601	ANP	PB-N3B-PG-O1G
3	B	601	ANP	PG-N3B-PB-O1B
3	B	601	ANP	PG-N3B-PB-O3A
3	C	601	ANP	PB-N3B-PG-O1G
3	C	601	ANP	PG-N3B-PB-O1B

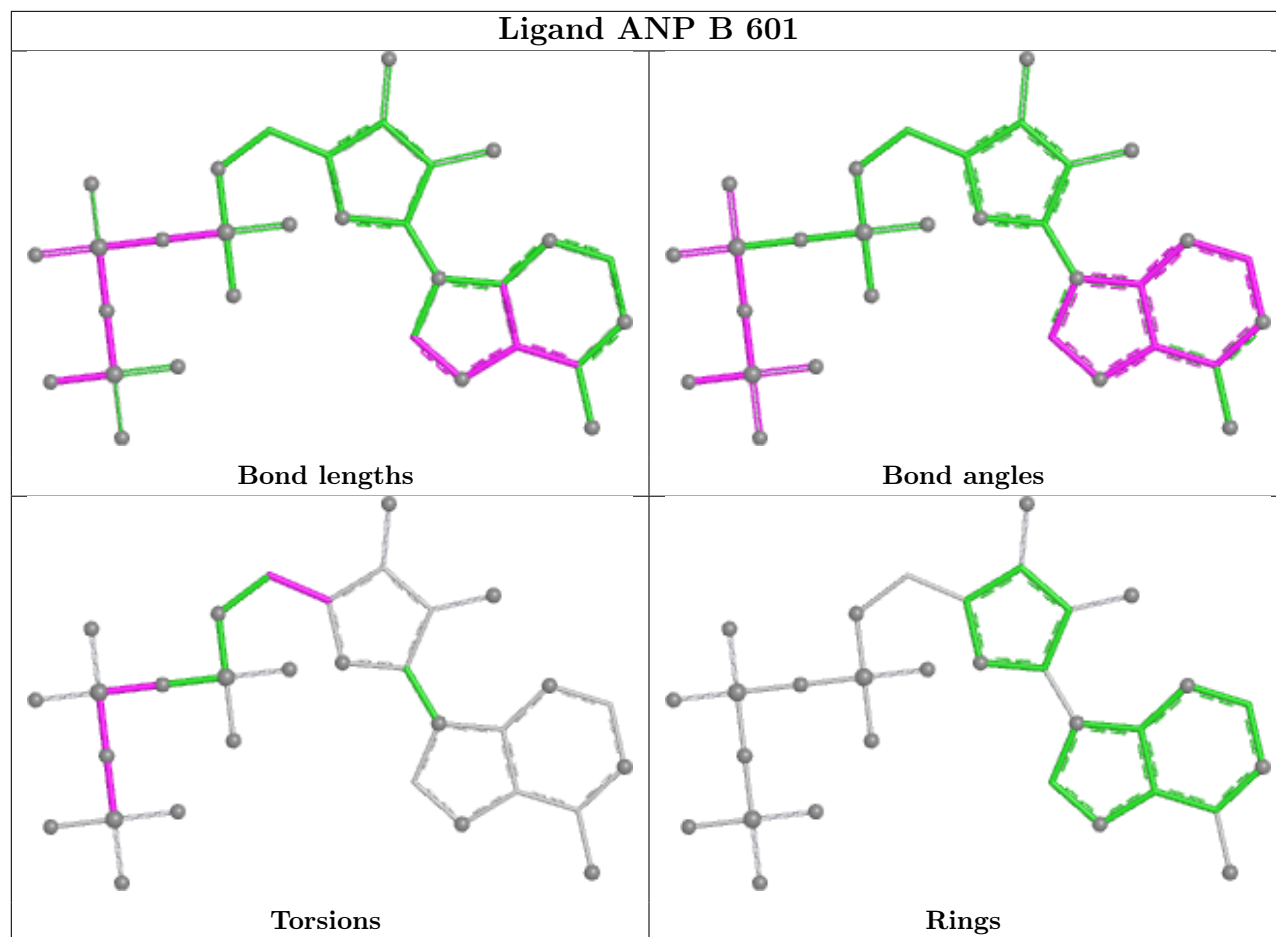
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	ANP	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 [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(Å²)	Q<0.9	
1	A	563/600 (93%)	-0.44	0	100	100	51, 82, 151, 165	0
1	B	563/600 (93%)	-0.39	0	100	100	61, 105, 153, 204	0
1	C	561/600 (93%)	-0.58	0	100	100	39, 71, 123, 153	0
2	D	433/465 (93%)	-0.43	0	100	100	47, 77, 156, 193	0
2	E	437/465 (93%)	-0.35	0	100	100	58, 102, 168, 193	0
2	F	437/465 (93%)	-0.51	1 (0%)	91	87	47, 84, 141, 173	0
All	All	2994/3195 (93%)	-0.45	1 (0%)	100	100	39, 87, 150, 204	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	454	LEU	2.7

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](#)

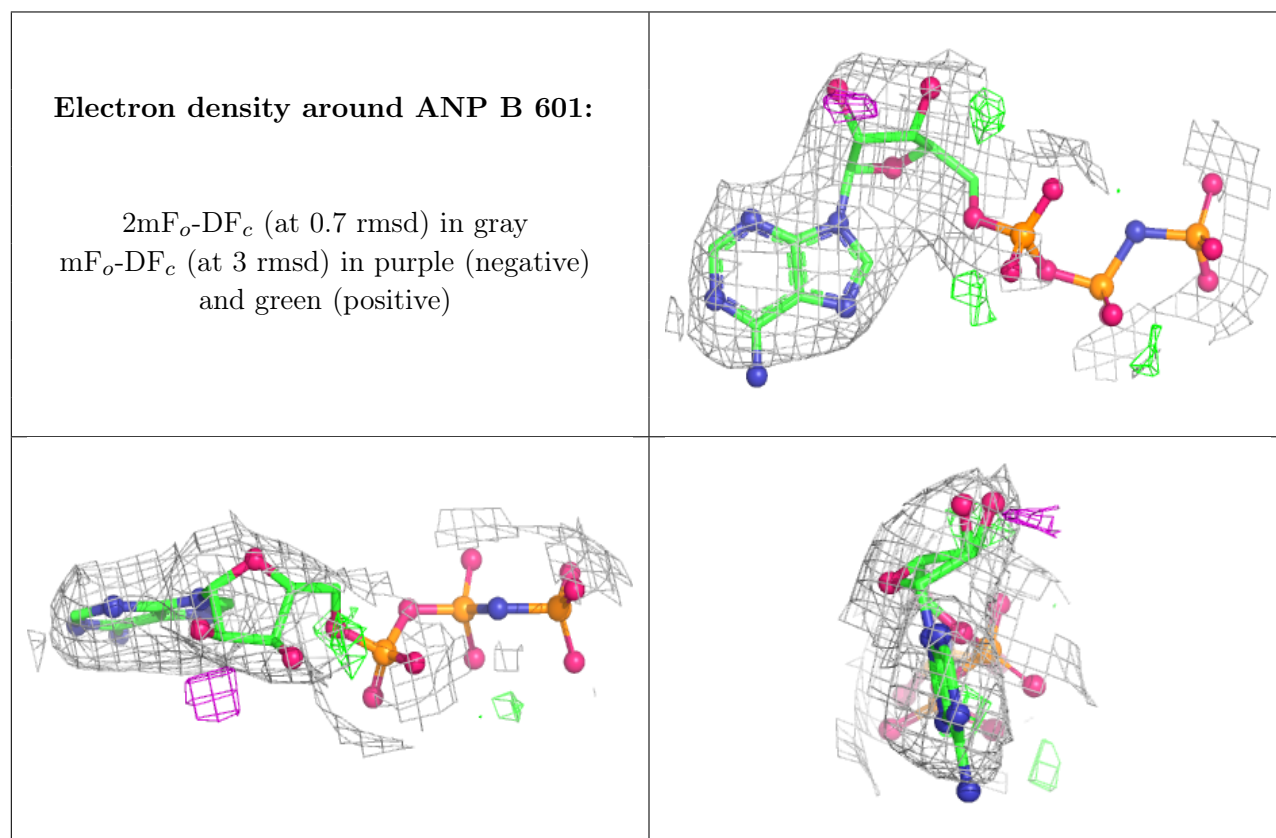
There are no oligosaccharides in this entry.

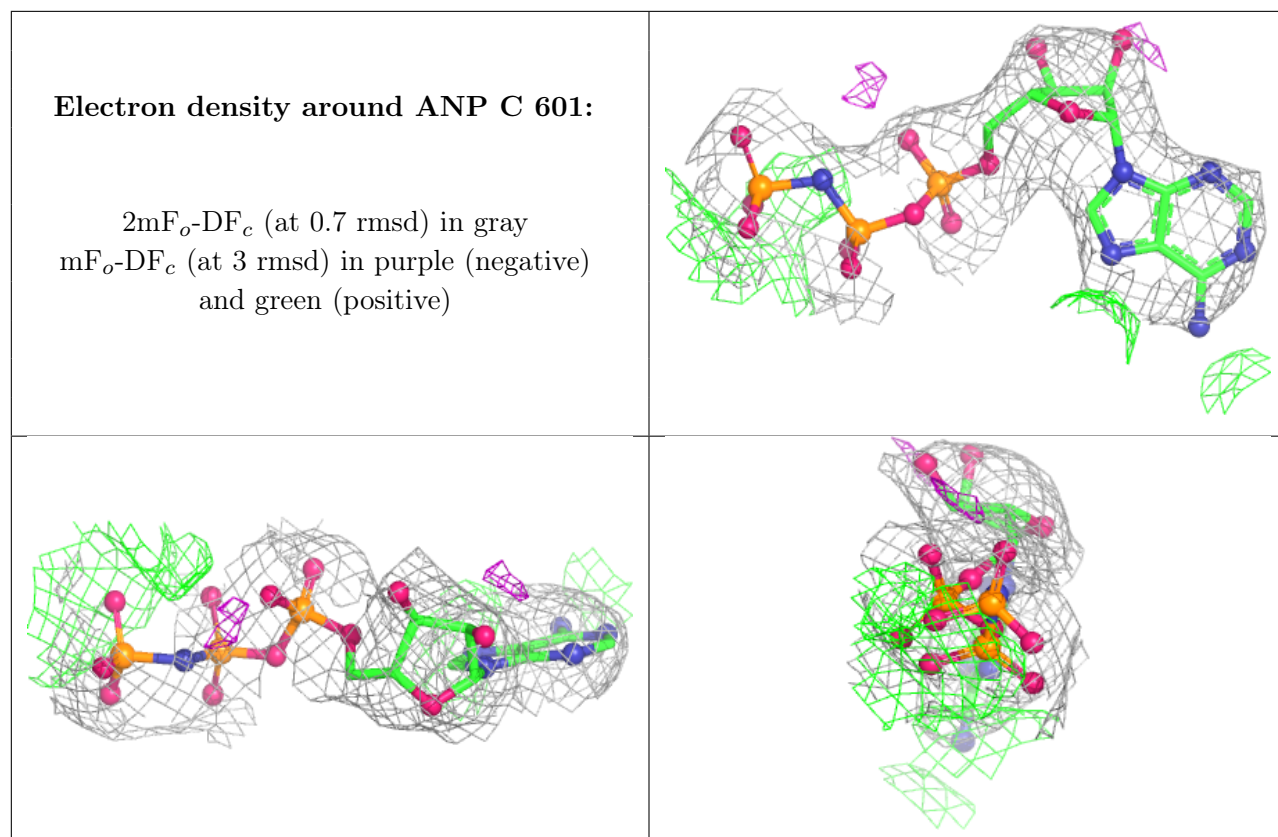
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	MG	C	602	1/1	0.86	0.17	46,46,46,46	0
4	MG	B	602	1/1	0.92	0.10	62,62,62,62	0
3	ANP	B	601	31/31	0.95	0.06	64,67,72,73	0
3	ANP	C	601	31/31	0.95	0.07	53,54,57,58	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.