



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 02:32 PM BST

PDB ID : 5KNB
Title : Crystal structure of the 2 ADP-bound V1 complex
Authors : Suzuki, K.; Mizutani, K.; Maruyama, S.; Shimono, K.; Imai, F.L.; Muneyuki, E.; Kakinuma, Y.; Ishizuka-Katsura, Y.; Shirouzu, M.; Yokoyama, S.; Yamato, I.; Murata, T.
Deposited on : 2016-06-28
Resolution : 3.25 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 : 2.13.1
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) : 2.13.1

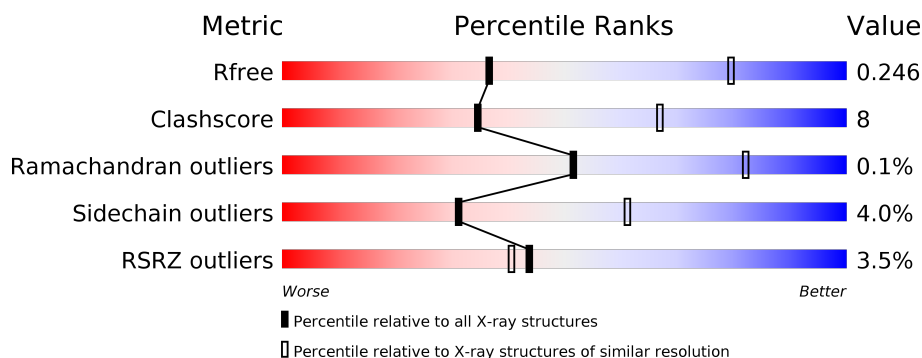
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.




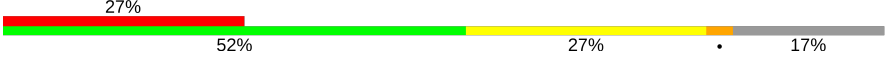
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	600	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	600	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
1	C	600	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>..</div> </div> </div>
2	D	465	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
2	E	465	<div> <div></div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>
2	F	465	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	217	
4	H	115	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26077 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	587	Total	C	N	O	S	0	0	0
			4431	2779	747	880	25			
1	B	592	Total	C	N	O	S	0	0	0
			4557	2858	763	910	26			
1	C	586	Total	C	N	O	S	0	0	0
			4428	2782	746	874	26			

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	453	Total	C	N	O	S	0	0	0
			3475	2201	589	671	14			
2	E	454	Total	C	N	O	S	0	1	0
			3552	2253	609	676	14			
2	F	455	Total	C	N	O	S	0	0	0
			3541	2243	606	677	15			

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 a protein called V-type sodium ATPase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	164	Total	C	N	O	S	0	0	0
			1308	822	233	244	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	expression tag	UNP P43435
G	-5	SER	-	expression tag	UNP P43435

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	SER	-	expression tag	UNP P43435
G	-3	GLY	-	expression tag	UNP P43435
G	-2	SER	-	expression tag	UNP P43435
G	-1	SER	-	expression tag	UNP P43435
G	0	GLY	-	expression tag	UNP P43435

- Molecule 4 is a protein called V-type sodium ATPase subunit NtpG (F).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	95	Total	C	N	O	S	0	0	0
			684	436	112	135	1			

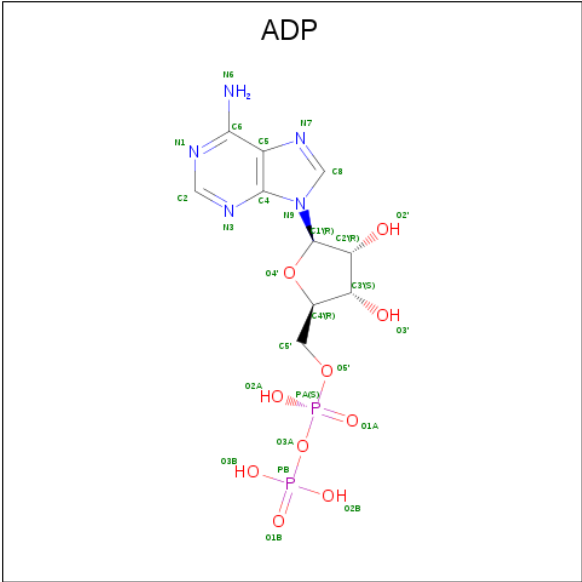
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	-	expression tag	UNP P43455
H	105	GLY	-	expression tag	UNP P43455
H	106	PRO	-	expression tag	UNP P43455
H	107	SER	-	expression tag	UNP P43455
H	108	SER	-	expression tag	UNP P43455
H	109	GLY	-	expression tag	UNP P43455
H	110	GLU	-	expression tag	UNP P43455
H	111	ASN	-	expression tag	UNP P43455
H	112	LEU	-	expression tag	UNP P43455
H	113	TYR	-	expression tag	UNP P43455
H	114	PHE	-	expression tag	UNP P43455
H	115	GLN	-	expression tag	UNP P43455

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

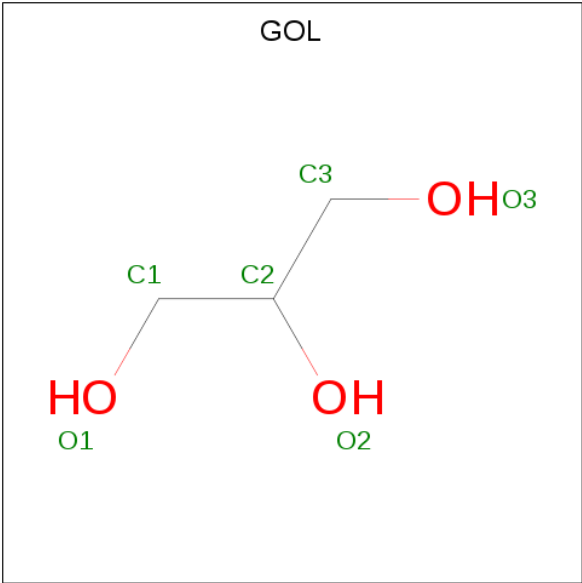
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

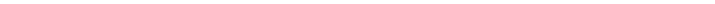
- Molecule 8 is water.

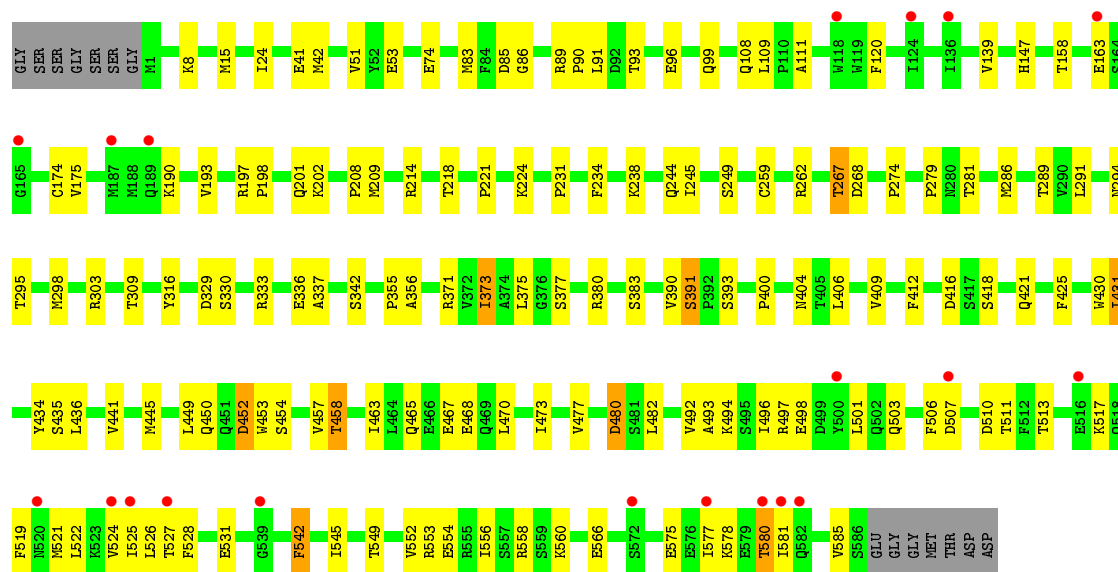
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total 7	O 7	0	0
8	B	10	Total 10	O 10	0	0
8	C	6	Total 6	O 6	0	0
8	D	1	Total 1	O 1	0	0
8	E	8	Total 8	O 8	0	0
8	F	1	Total 1	O 1	0	0

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.

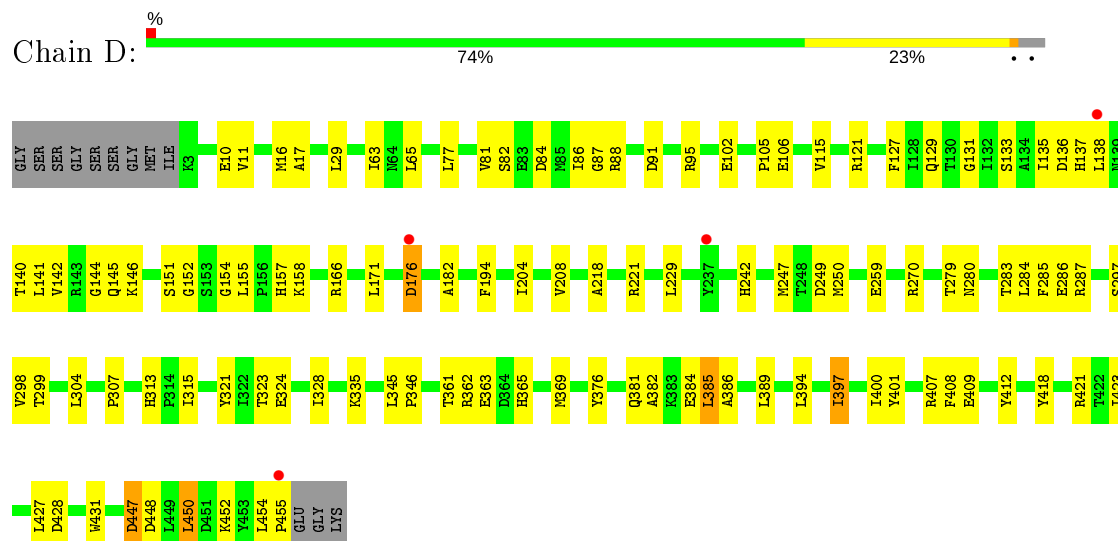
- Chain A:
-
- 5% 77% 20%
- GLY SER SER GLY SER SER GLY M1 I24 Q25 G34 I40 M42 R43 V73 P77 I80 F84 P90 T93 N101 F102 L103 Q108 F120 T128 S131 A132 G133 D140 I144 P152 V151 I155 Q160 K161 I162 I169
- R303 Y308 T309 T311 Y316 A325 D829 S330 R333 E336 E340 M341 S342 D851 E352 P355 R380 G394 L406 V409 K410 W413 G414 L415 D416 S427 L436 E439 V441 M445 I448 L449 Q451 Q457 Q465 E466 E467 E468
- Q469 R471 V474 V477 G478 S481 L482 S483 D484 N485 D486 R487 V492 R497 E498 D499 Y500 L501 D507 D510 T513 S514 K517 V524 E531 K534 A535 L536 S537 L538 G539 A540 Y541 F542 N543 E544 I545 G548 T549 V552 R553 E554 R555 I556
- P563 E564 E565 E566 I573 N574 E575 E576 I577 T580 I581 Q582 V585 S586 E587 GLY GLY MET THR ASP

- Chain B:
-
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| L436 | L453 | R462 | Q465 | E466 | E467 | A493 | R497 | T513 | K517 | Q518 | F519 | I545 | T549 | S586 | GLY | GLY | GLY | MET | THR | ASP | | | | | | | | | | | | | | | | | | | |
| P198 | L203 | P208 | T223 | P231 | G232 | P233 | V241 | I245 | A246 | K247 | R262 | T281 | G282 | E283 | S284 | L285 | E304 | E315 | D329 | S330 | W334 | H348 | D351 | R371 | D378 | E381 | I394 | P400 | N404 | K410 | Y411 | F412 | D416 | S417 | S427 | | | | |
| GLY | S-5 | Q2 | K8 | S20 | E38 | E41 | H42 | R43 | S48 | V51 | E52 | E53 | S56 | H83 | F84 | Q88 | R89 | P90 | L91 | D92 | R105 | A111 | E121 | E122 | T123 | I124 | F125 | E126 | G127 | T128 | E129 | V130 | I135 | K148 | I162 | I169 | Q180 | M188 | P197 |

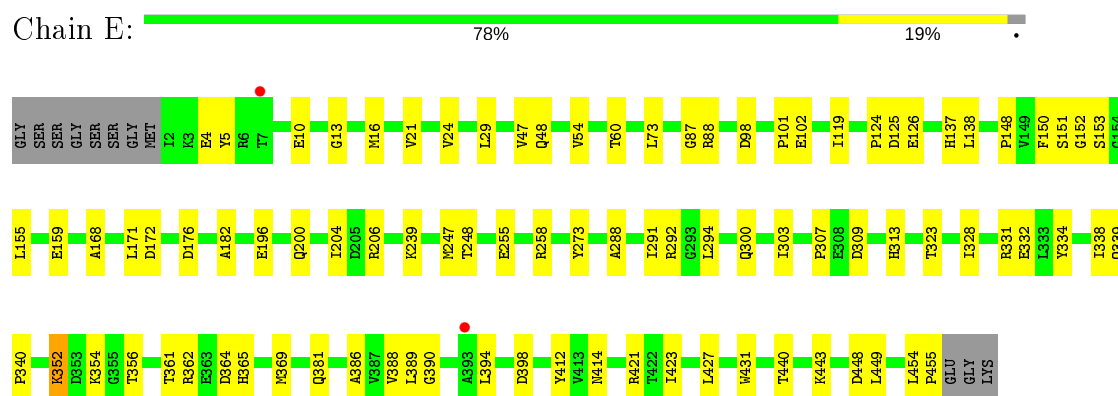
- Chain C:  3% 73% 23%



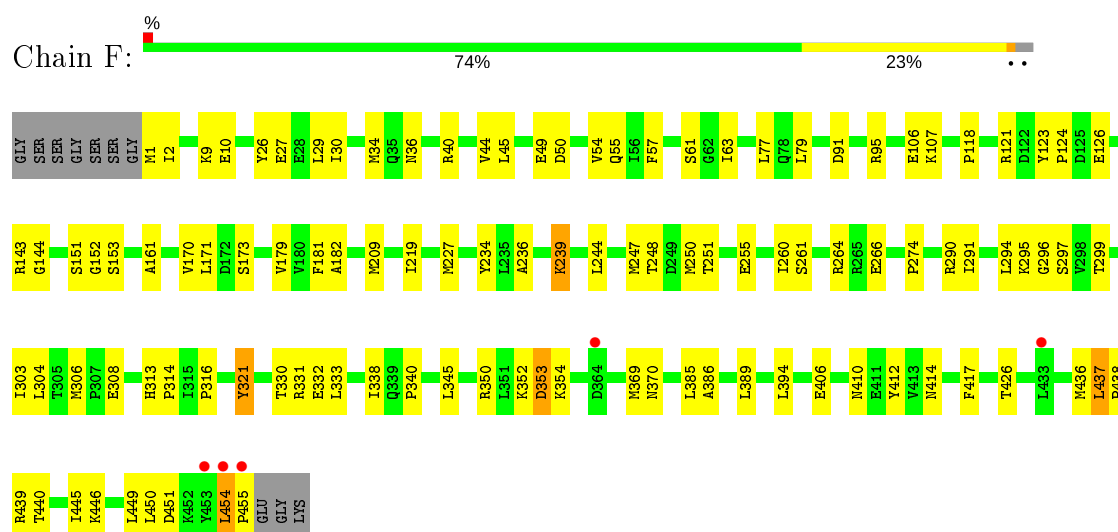
• Molecule 2: V-type sodium ATPase subunit B



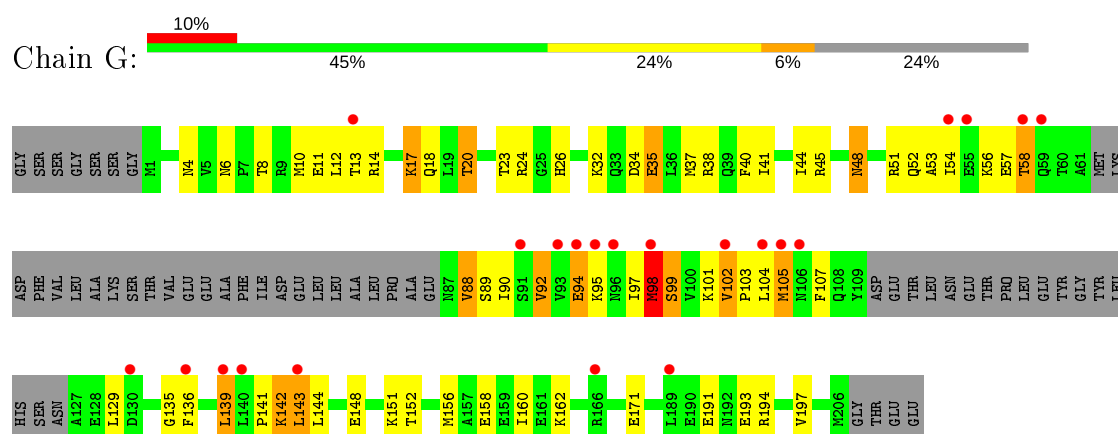
• Molecule 2: V-type sodium ATPase subunit B



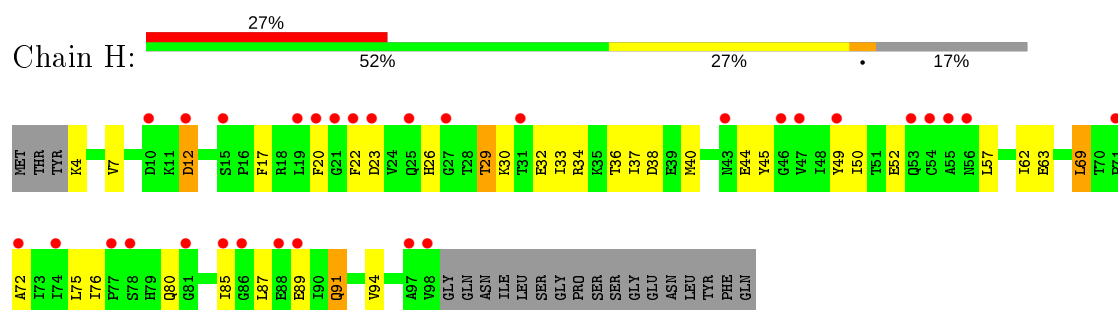
• Molecule 2: V-type sodium ATPase subunit B



- Molecule 3: V-type sodium ATPase subunit D



- Molecule 4: V-type sodium ATPase subunit NtpG (F)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.35Å 129.62Å 237.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.55 – 3.25 46.64 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.55-3.25) 99.4 (46.64-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.209 , 0.245 0.211 , 0.246	Depositor DCC
R_{free} test set	3106 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
Reported twinning fraction	0.050 for k,h,-l	Depositor
Outliers	1 of 62128 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26077	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, MG, ADP

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	0/4507	0.40	0/6119
1	B	0.21	0/4633	0.38	0/6275
1	C	0.23	0/4503	0.41	0/6109
2	D	0.21	0/3538	0.42	0/4801
2	E	0.21	0/3615	0.39	0/4893
2	F	0.21	0/3604	0.41	0/4879
3	G	0.24	0/1316	0.49	0/1764
4	H	0.24	0/695	0.45	0/947
All	All	0.22	0/26411	0.41	0/35787

There are no bond length outliers.

There are no bond angle outliers.

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	4431	0	4235	73	0
1	B	4557	0	4458	40	0
1	C	4428	0	4264	92	0
2	D	3475	0	3388	68	0
2	E	3552	0	3548	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3541	0	3527	70	0
3	G	1308	0	1353	44	0
4	H	684	0	635	25	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	27	0	12	0	0
6	C	27	0	12	2	0
7	B	6	0	8	0	0
7	E	6	0	8	0	0
8	A	7	0	0	3	0
8	B	10	0	0	1	0
8	C	6	0	0	2	0
8	D	1	0	0	0	0
8	E	8	0	0	0	0
8	F	1	0	0	0	0
All	All	26077	0	25448	427	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 8.

The worst 5 of 427 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)
3:G:89:SER:HG	4:H:4:LYS:N	1.56	1.02
2:F:106:GLU:HG2	2:F:107:LYS:HG2	1.55	0.85
2:E:88:ARG:NH1	2:E:101:PRO:O	2.15	0.79
1:A:214:ARG:NH2	1:A:510:ASP:OD1	2.17	0.77
1:C:558:ARG:NH2	2:F:445:ILE:O	2.17	0.76

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	585/600 (98%)	556 (95%)	28 (5%)	1 (0%)	47	77
1	B	590/600 (98%)	570 (97%)	20 (3%)	0	100	100
1	C	584/600 (97%)	562 (96%)	22 (4%)	0	100	100
2	D	451/465 (97%)	431 (96%)	20 (4%)	0	100	100
2	E	453/465 (97%)	442 (98%)	10 (2%)	1 (0%)	47	77
2	F	453/465 (97%)	441 (97%)	11 (2%)	1 (0%)	47	77
3	G	158/217 (73%)	146 (92%)	11 (7%)	1 (1%)	25	59
4	H	93/115 (81%)	89 (96%)	3 (3%)	1 (1%)	14	46
All	All	3367/3527 (96%)	3237 (96%)	125 (4%)	5 (0%)	51	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	98	MET
2	F	353	ASP
4	H	23	ASP
2	E	124	PRO
1	A	477	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	461/511 (90%)	448 (97%)	13 (3%)	43	69
1	B	493/511 (96%)	487 (99%)	6 (1%)	71	83
1	C	462/511 (90%)	436 (94%)	26 (6%)	21	52
2	D	356/387 (92%)	344 (97%)	12 (3%)	37	64
2	E	373/387 (96%)	367 (98%)	6 (2%)	62	79
2	F	372/387 (96%)	364 (98%)	8 (2%)	52	74
3	G	141/198 (71%)	113 (80%)	28 (20%)	1	5
4	H	66/99 (67%)	57 (86%)	9 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2724/2991 (91%)	2616 (96%)	108 (4%)	31 61

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	176	ASP
2	E	172	ASP
4	H	12	ASP
2	D	363	GLU
2	D	407	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
2	F	410	ASN
3	G	48	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
7	GOL	E	501	-	5,5,5	0.37	0	5,5,5	0.31	0
6	ADP	C	602	5	24,29,29	1.04	2 (8%)	29,45,45	1.50	5 (17%)
7	GOL	B	603	-	5,5,5	0.37	0	5,5,5	0.29	0
6	ADP	B	602	5	24,29,29	0.97	1 (4%)	29,45,45	1.42	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
7	GOL	E	501	-	-	2/4/4/4	-
6	ADP	C	602	5	-	6/12/32/32	0/3/3/3
7	GOL	B	603	-	-	2/4/4/4	-
6	ADP	B	602	5	-	7/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	602	ADP	C5-C4	2.84	1.48	1.40
6	B	602	ADP	C5-C4	2.53	1.47	1.40
6	C	602	ADP	O4'-C1'	2.02	1.43	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	602	ADP	N3-C2-N1	-3.82	122.71	128.68
6	B	602	ADP	C3'-C2'-C1'	3.46	106.18	100.98
6	C	602	ADP	C3'-C2'-C1'	3.28	105.91	100.98
6	C	602	ADP	PA-O3A-PB	-3.19	121.89	132.83
6	B	602	ADP	PA-O3A-PB	-3.16	121.99	132.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	602	ADP	PA-O3A-PB-O2B

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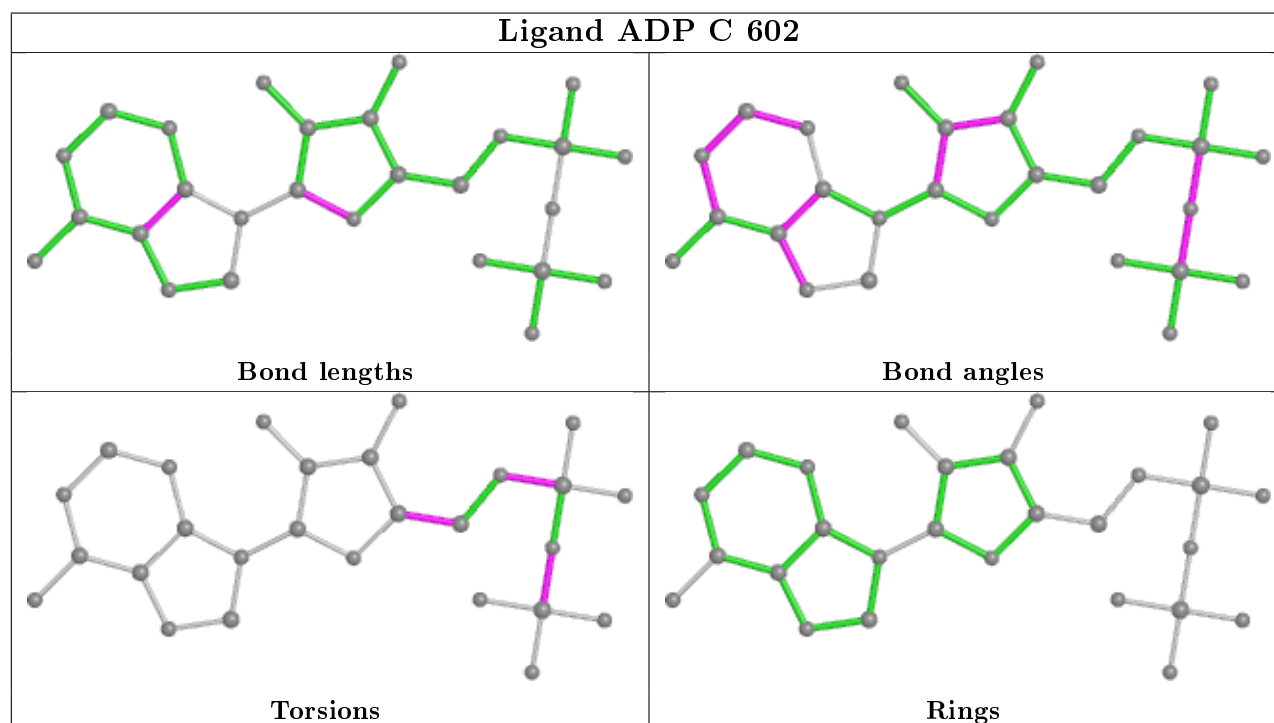
Mol	Chain	Res	Type	Atoms
6	B	602	ADP	C5'-O5'-PA-O1A
6	B	602	ADP	C5'-O5'-PA-O2A
6	B	602	ADP	C5'-O5'-PA-O3A
6	C	602	ADP	C5'-O5'-PA-O3A

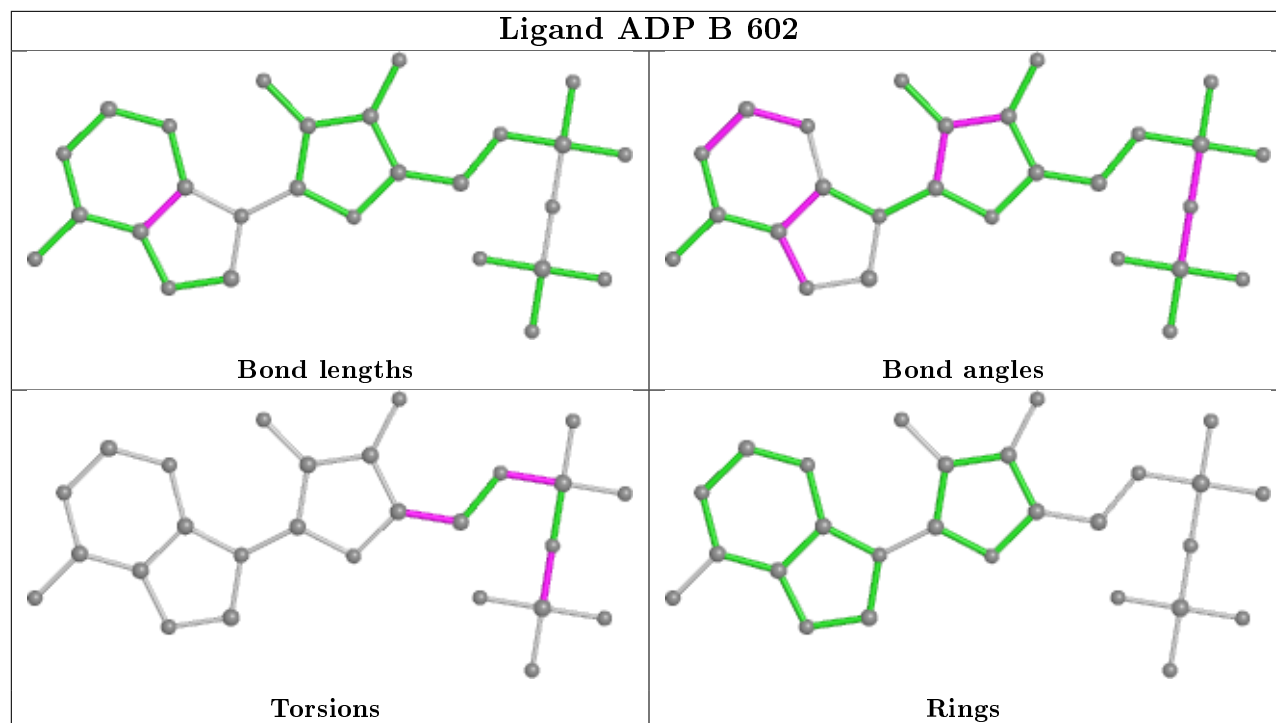
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	602	ADP	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 ⓘ

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	587/600 (97%)	0.15	30 (5%) 28 26	40, 81, 144, 184	0
1	B	592/600 (98%)	-0.11	4 (0%) 87 88	27, 54, 91, 124	0
1	C	586/600 (97%)	0.23	20 (3%) 45 42	41, 93, 152, 185	0
2	D	453/465 (97%)	0.07	4 (0%) 84 84	63, 90, 128, 144	0
2	E	454/465 (97%)	-0.20	2 (0%) 92 92	29, 54, 93, 159	0
2	F	455/465 (97%)	-0.06	5 (1%) 80 80	41, 76, 120, 145	0
3	G	164/217 (75%)	0.69	22 (13%) 3 3	71, 119, 183, 202	0
4	H	95/115 (82%)	1.67	31 (32%) 0 0	126, 157, 190, 203	0
All	All	3386/3527 (96%)	0.10	118 (3%) 44 40	27, 79, 149, 203	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	47	VAL	9.5
4	H	55	ALA	7.2
1	A	542	PHE	5.9
1	C	520	ASN	5.4
4	H	54	CYS	5.0

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

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

6.3 Carbohydrates ⓘ

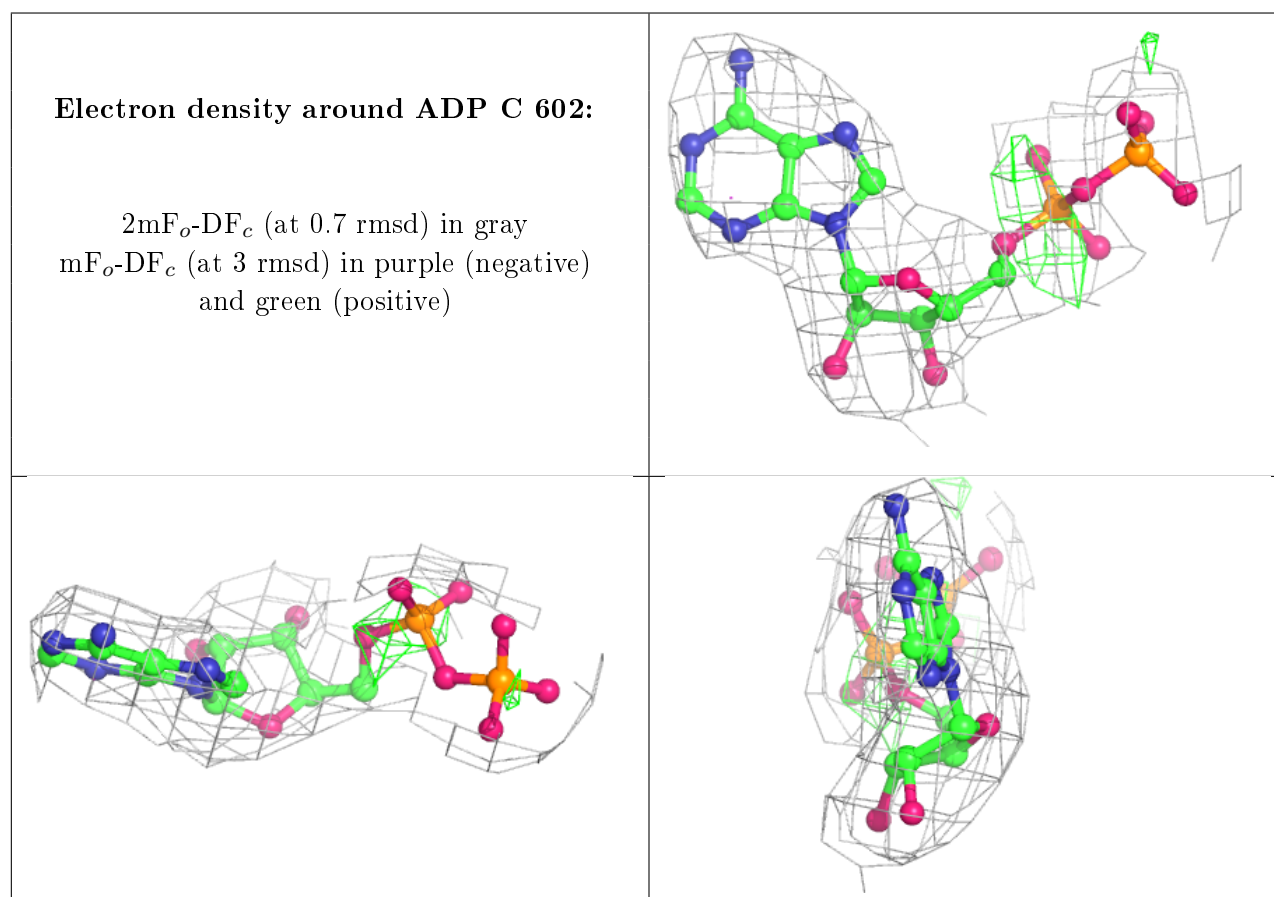
There are no monosaccharides in this entry.

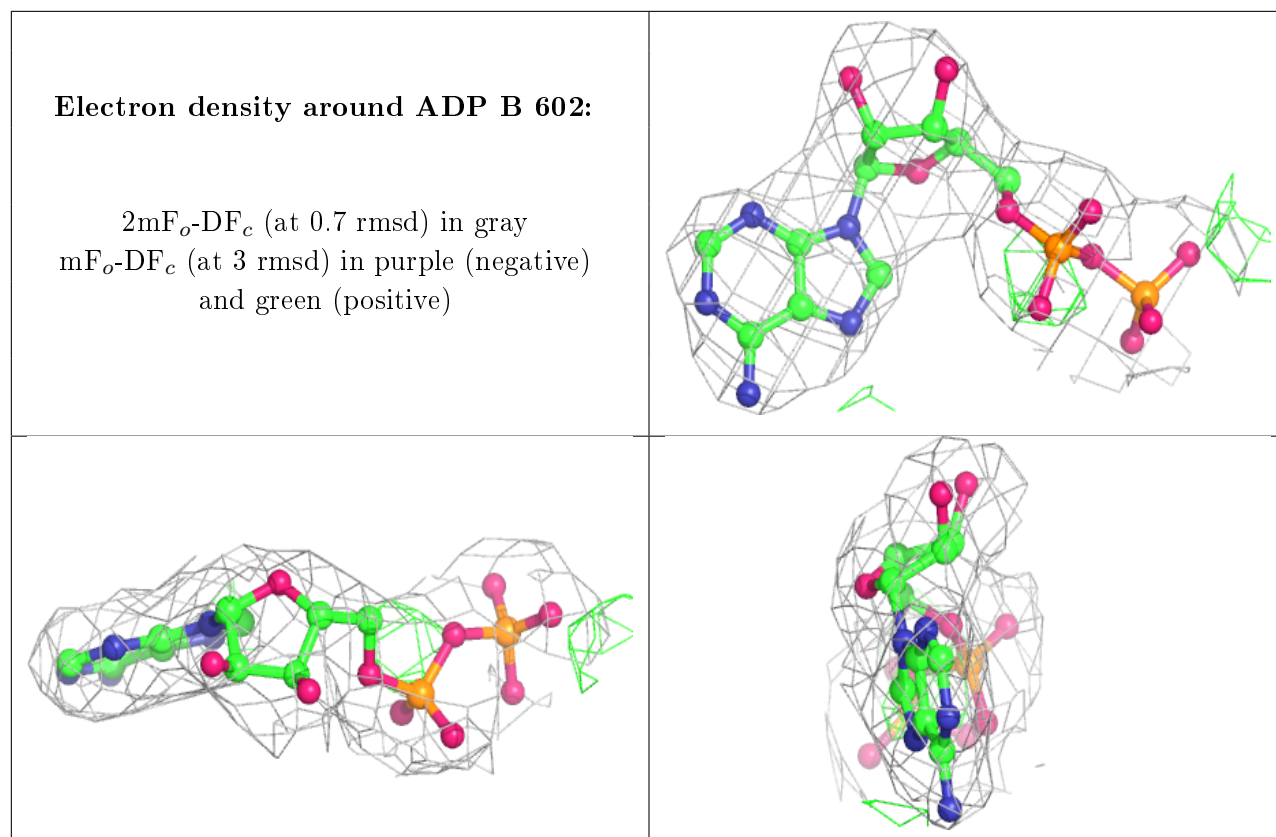
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
7	GOL	E	501	6/6	0.88	0.29	62,63,63,64	0
6	ADP	C	602	27/27	0.92	0.28	54,59,117,120	0
7	GOL	B	603	6/6	0.95	0.19	55,58,60,61	0
6	ADP	B	602	27/27	0.96	0.25	40,45,54,68	0
5	MG	C	601	1/1	0.97	0.23	52,52,52,52	0
5	MG	B	601	1/1	0.99	0.32	14,14,14,14	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.