Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 12:23 PM JST

PDB ID	:	5ZE9
Title	:	Crystal structure of AMP-PNP bound mutant A3B3 complex from Enterococcus hirae V-ATPase
Authors	:	Maruyama, S.; Suzuki, K.; Sasaki, H.; Mizutani, K.; Saito, Y.; Imai, F.L.; Ishizuka-Katsura, Y.; Shirouzu, M.; Ichiro, Y.; Murata, T.
Deposited on	:	2018-02-27
Resolution	:	2.10 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 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:

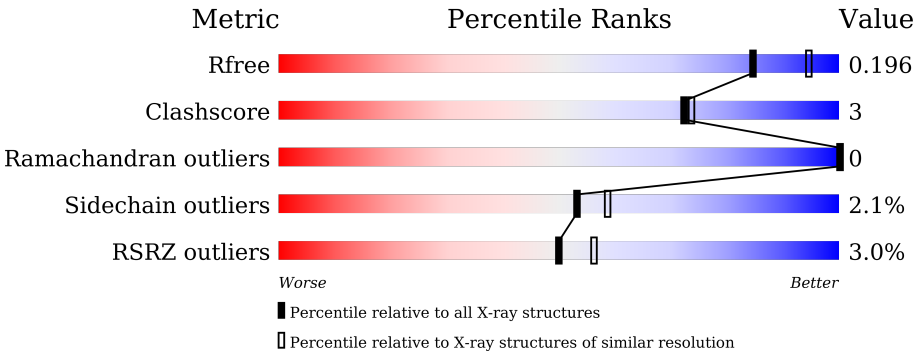
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	5% 87% 11%
1	B	600	93% 5%
1	C	600	91% 6%
2	D	600	6% 87% 9%
2	E	465	89% 9%

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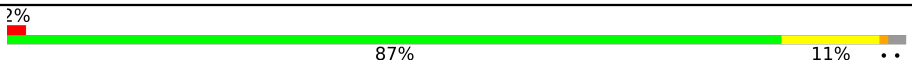
Mol	Chain	Length	Quality of chain
2	F	465	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 26108 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	588	Total	C	N	O	S	0	0	0
			4559	2865	766	902	26			
1	B	592	Total	C	N	O	S	0	4	0
			4622	2902	778	913	29			
1	C	587	Total	C	N	O	S	0	3	0
			4588	2882	770	910	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

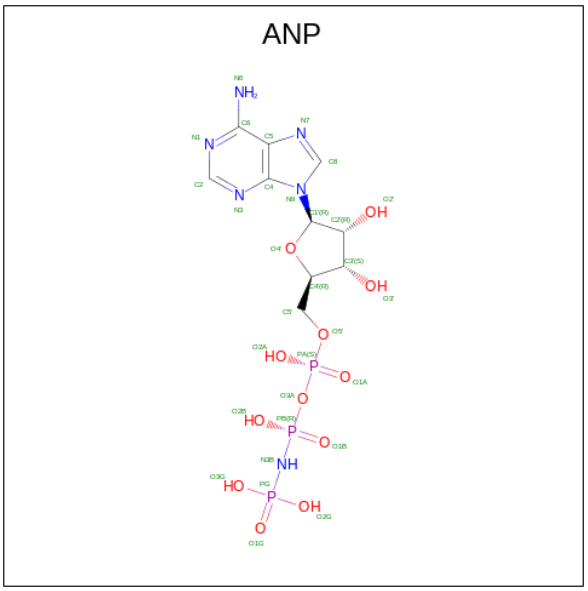
- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	453	Total	C	N	O	S	0	3	0
			3561	2258	604	685	14			
2	E	455	Total	C	N	O	S	0	0	0
			3565	2262	610	678	15			
2	F	456	Total	C	N	O	S	0	1	0
			3572	2269	608	679	16			

There are 24 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
D	65	TYR	LEU	engineered mutation	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
E	65	TYR	LEU	engineered mutation	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
F	65	TYR	LEU	engineered mutation	UNP Q08637

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

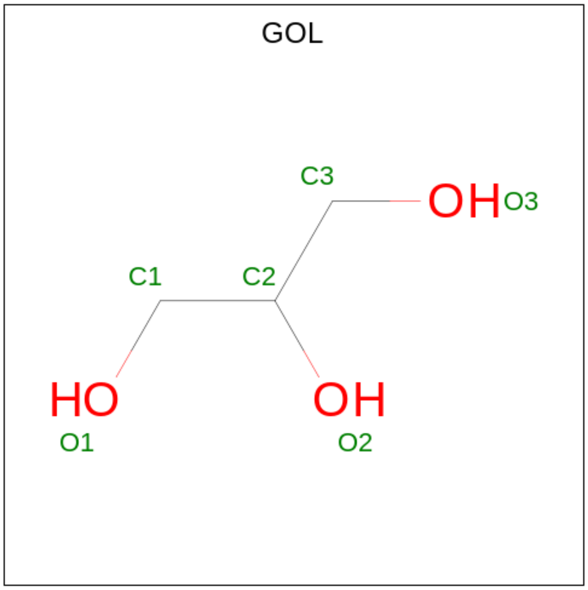


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

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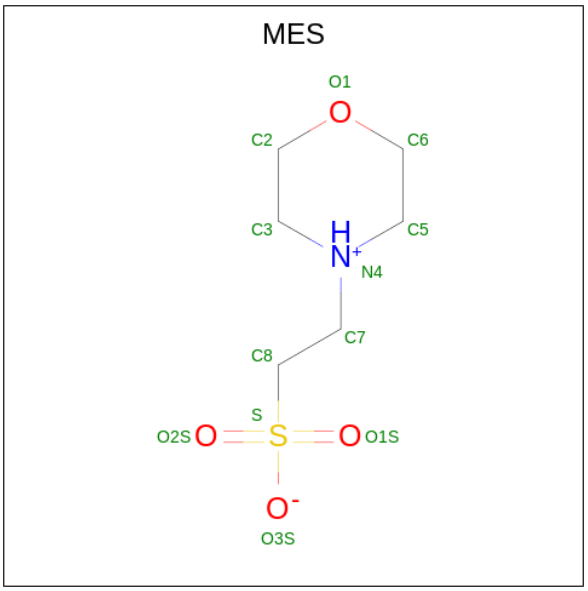
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	179	Total O 179 179	0	0
7	B	298	Total O 298 298	0	0
7	C	300	Total O 300 300	0	0
7	D	130	Total O 130 130	0	0

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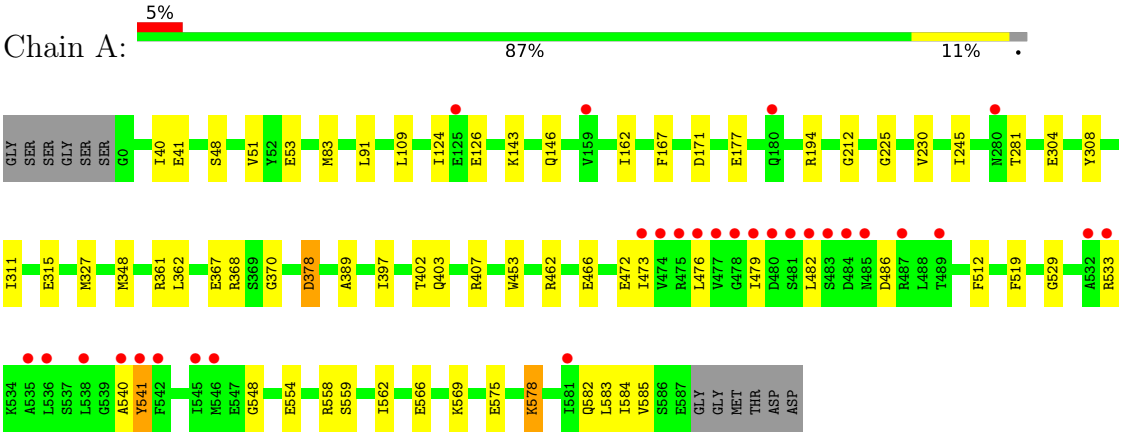
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	173	Total O 173 173	0	0
7	F	219	Total O 219 219	0	0

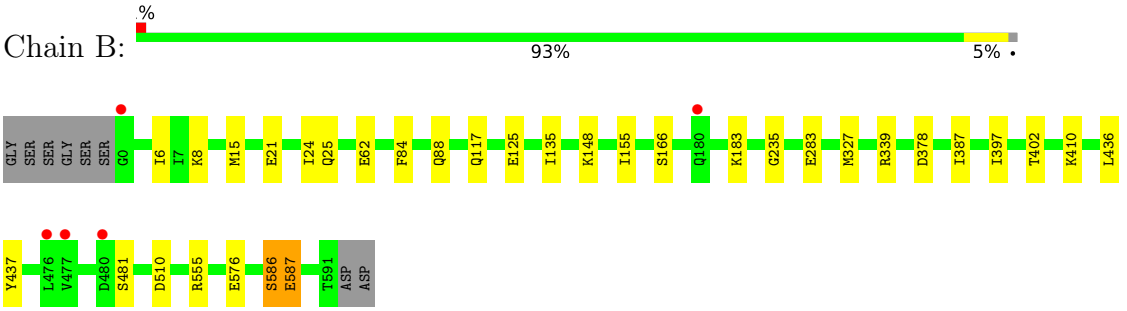
3 Residue-property plots (i)

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.

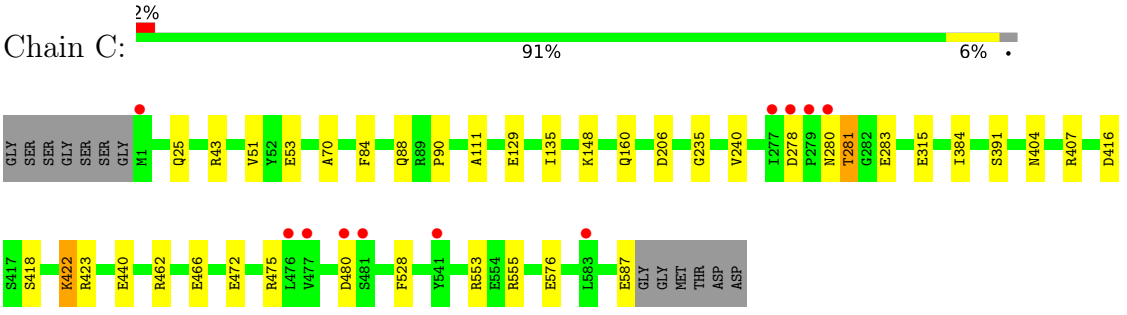
• Molecule 1: V-type sodium ATPase catalytic subunit A



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

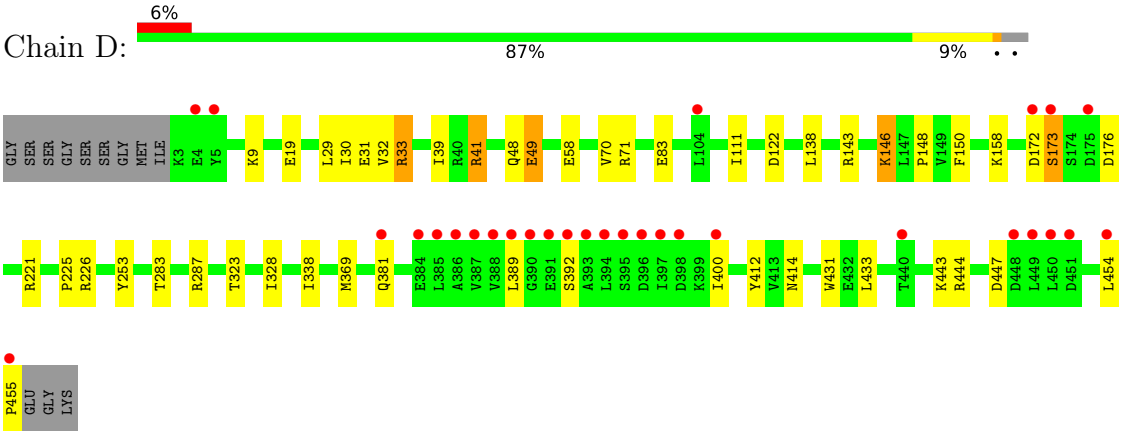


• Molecule 1: V-type sodium ATPase catalytic subunit A



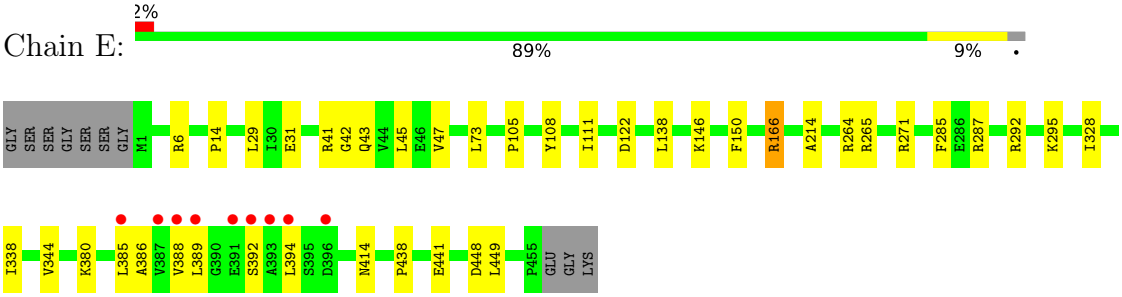
• Molecule 2: V-type sodium ATPase subunit B

Chain D:



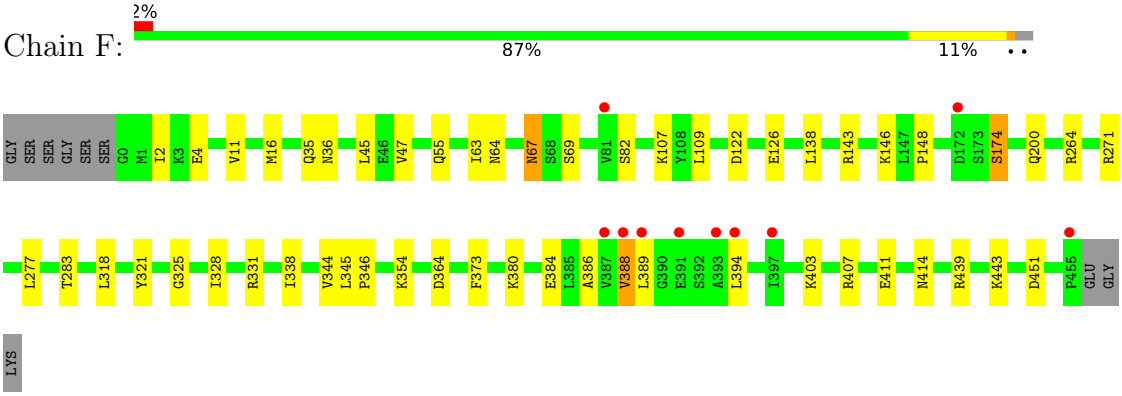
• Molecule 2: V-type sodium ATPase subunit B

Chain E:



• Molecule 2: V-type sodium ATPase subunit B

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.83Å 151.37Å 235.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.87 – 2.10 58.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (54.87-2.10) 99.5 (58.20-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.166 , 0.196 0.166 , 0.196	Depositor DCC
R_{free} test set	10953 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26108	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MES, MG, ANP, GOL

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	0.31	0/4635	0.48	0/6273
1	B	0.35	0/4710	0.52	0/6368
1	C	0.36	0/4673	0.53	0/6323
2	D	0.33	0/3634	0.51	0/4918
2	E	0.34	0/3629	0.53	0/4906
2	F	0.36	0/3639	0.54	0/4920
All	All	0.34	0/24920	0.52	0/33708

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

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	4559	0	4510	37	0
1	B	4622	0	4598	17	0
1	C	4588	0	4551	25	0
2	D	3561	0	3542	28	0
2	E	3565	0	3577	27	0
2	F	3572	0	3592	33	0
3	A	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	13	1	0
3	C	31	0	13	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	42	0	56	2	0
5	B	60	0	80	3	0
5	C	48	0	64	3	0
5	D	18	0	24	3	0
5	E	24	0	32	1	0
5	F	42	0	56	2	0
6	D	12	0	12	0	0
7	A	179	0	0	0	0
7	B	298	0	0	2	0
7	C	300	0	0	3	0
7	D	130	0	0	2	0
7	E	173	0	0	6	0
7	F	219	0	0	3	0
All	All	26108	0	24733	166	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 3.

All (166) 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:423[B]:ARG:NH2	7:C:701:HOH:O	2.03	0.89
1:B:235:GLY:H	3:B:601:ANP:HNB1	1.18	0.88
1:C:235:GLY:H	3:C:601:ANP:HNB1	1.20	0.88
1:C:462:ARG:NH1	1:C:466:GLU:OE2	2.15	0.78
1:B:24:ILE:HG22	1:B:25:GLN:HG2	1.68	0.75
2:E:271:ARG:NH2	7:E:603:HOH:O	2.22	0.72
3:C:601:ANP:O2G	7:C:702:HOH:O	2.07	0.71
2:D:454:LEU:HD12	2:D:455:PRO:HD2	1.73	0.70
1:C:278:ASP:HB3	1:C:281:THR:HG22	1.74	0.69
2:D:412:TYR:HB2	2:D:433:LEU:HD11	1.75	0.69
1:B:510:ASP:OD2	7:B:701:HOH:O	2.10	0.67
2:F:354:LYS:NZ	7:F:603:HOH:O	2.27	0.67
2:D:9:LYS:HB2	2:D:19:GLU:HG3	1.76	0.67
1:C:472:GLU:OE2	1:C:475:ARG:NH2	2.28	0.66
1:C:281:THR:HG23	1:C:283:GLU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:NH2	1:A:304:GLU:OE2	2.29	0.65
5:B:607:GOL:O1	5:B:607:GOL:O3	2.11	0.65
2:E:31:GLU:HG3	2:E:73:LEU:HD11	1.79	0.65
1:B:555:ARG:NH1	1:B:576:GLU:OE2	2.29	0.64
2:D:444:ARG:HE	5:D:504:GOL:H31	1.61	0.64
1:A:540:ALA:HB2	1:A:585:VAL:HG12	1.81	0.63
2:F:64:ASN:HB3	2:F:67:ASN:OD1	2.00	0.61
2:E:146:LYS:HD3	2:E:285:PHE:O	2.02	0.59
2:F:386:ALA:HB2	2:F:394:LEU:HD11	1.84	0.59
1:C:555:ARG:NH1	1:C:576:GLU:OE2	2.30	0.59
5:C:605:GOL:O3	5:C:605:GOL:O1	2.17	0.59
1:B:117:GLN:HG3	1:B:166:SER:OG	2.02	0.59
2:F:407:ARG:NH1	2:F:411:GLU:OE1	2.36	0.58
1:A:378:ASP:OD1	1:A:378:ASP:N	2.28	0.58
2:D:111:ILE:O	2:D:287:ARG:NH2	2.34	0.58
1:A:575:GLU:N	1:A:575:GLU:OE1	2.36	0.58
1:C:423[A]:ARG:HD3	2:F:373:PHE:CE1	2.39	0.57
1:A:361:ARG:HH21	5:A:604:GOL:H31	1.69	0.57
2:D:143:ARG:HH22	2:D:172:ASP:CB	2.18	0.57
2:F:283:THR:HB	5:F:501:GOL:H2	1.86	0.57
2:F:271:ARG:NH2	7:F:601:HOH:O	2.20	0.57
2:F:4:GLU:HB3	2:F:69:SER:HB2	1.86	0.57
2:E:448:ASP:OD1	2:E:449:LEU:N	2.39	0.56
2:F:345:LEU:HA	2:F:373:PHE:CZ	2.41	0.56
2:F:35:GLN:H	2:F:67:ASN:ND2	2.05	0.55
2:E:31:GLU:HG2	2:E:41:ARG:HE	1.72	0.55
1:A:482:LEU:HD12	1:A:486:ASP:HB3	1.87	0.54
2:E:166:ARG:HD2	7:E:623:HOH:O	2.07	0.54
1:B:397:ILE:HB	1:B:402:THR:HG21	1.89	0.54
5:B:607:GOL:HO1	5:B:607:GOL:HO3	1.55	0.53
7:C:867:HOH:O	5:F:507:GOL:H2	2.07	0.53
2:E:338:ILE:HG23	2:E:414:ASN:HB2	1.91	0.52
2:D:444:ARG:NE	5:D:504:GOL:H31	2.24	0.52
2:E:386:ALA:HB2	2:E:394:LEU:HD11	1.92	0.52
5:E:504:GOL:O1	7:E:601:HOH:O	2.19	0.52
1:C:84:PHE:HB3	1:C:88:GLN:HA	1.92	0.52
1:C:404:ASN:OD1	1:C:407:ARG:NH2	2.40	0.52
2:D:143:ARG:HH22	2:D:172:ASP:HB3	1.75	0.51
5:A:604:GOL:H12	2:E:14:PRO:HD3	1.92	0.51
1:A:348:MET:HG3	2:E:265:ARG:HA	1.93	0.51
5:B:604:GOL:H2	2:F:331:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLY:HA3	1:A:584:ILE:HD11	1.93	0.50
2:F:338:ILE:HG23	2:F:414:ASN:HB2	1.93	0.50
1:A:473:ILE:HD13	1:A:476:LEU:HD12	1.94	0.50
2:E:438:PRO:HG2	2:E:441:GLU:HG2	1.93	0.50
2:E:111:ILE:O	2:E:287:ARG:NH2	2.42	0.49
2:D:173:SER:HB2	2:D:176:ASP:OD1	2.12	0.49
2:E:271:ARG:NH1	7:E:611:HOH:O	2.45	0.49
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.94	0.49
1:A:83:MET:HG2	1:A:91:LEU:HD12	1.95	0.49
1:A:529:GLY:O	1:A:533:ARG:HG3	2.12	0.49
2:D:148:PRO:HD3	2:D:323:THR:HB	1.95	0.49
1:B:135:ILE:HD13	1:B:148:LYS:HD3	1.94	0.49
2:D:33:ARG:HG3	2:D:39:ILE:CD1	2.42	0.49
2:D:221:ARG:O	2:D:225:PRO:HD2	2.13	0.49
2:E:43:GLN:NE2	7:E:608:HOH:O	2.42	0.48
1:C:240:VAL:HG13	5:C:608:GOL:H11	1.96	0.48
2:D:150:PHE:HB2	2:D:328:ILE:HD13	1.95	0.48
2:D:338:ILE:HG23	2:D:414:ASN:HB2	1.95	0.48
2:F:45:LEU:HD11	2:F:55:GLN:HB3	1.95	0.48
2:F:138:LEU:HD12	2:F:344:VAL:HG11	1.96	0.48
1:A:167:PHE:HB3	1:A:171:ASP:HB2	1.96	0.48
1:A:367:GLU:HG3	2:E:214:ALA:HB3	1.94	0.48
1:B:155:ILE:HD12	1:B:183:LYS:HG2	1.95	0.48
1:B:6:ILE:HD12	1:B:62:GLU:HB2	1.96	0.48
2:D:146:LYS:HE2	7:D:635:HOH:O	2.13	0.48
2:D:226:ARG:NH2	2:D:253:TYR:OH	2.46	0.48
1:A:367:GLU:CG	2:E:214:ALA:HB3	2.44	0.47
1:C:391:SER:HB3	2:F:321:TYR:CE1	2.49	0.47
1:A:578:LYS:O	1:A:582:GLN:HG3	2.14	0.47
2:D:31:GLU:OE1	2:D:33:ARG:NH1	2.36	0.47
2:D:138:LEU:HD22	2:D:369:MET:HG3	1.97	0.47
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.50	0.46
1:C:423[A]:ARG:HD3	2:F:373:PHE:CD1	2.50	0.46
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.83	0.46
2:F:45:LEU:HD13	2:F:264:ARG:HD2	1.97	0.46
1:C:422:LYS:HB3	1:C:422:LYS:HE3	1.77	0.46
2:F:384:GLU:O	2:F:388:VAL:HG12	2.16	0.46
1:A:212:GLY:HA3	1:A:512:PHE:CD1	2.50	0.46
2:E:105:PRO:HG3	2:E:108:TYR:CZ	2.51	0.46
1:C:278:ASP:HB3	1:C:281:THR:CG2	2.43	0.46
2:E:295:LYS:HA	2:E:295:LYS:HD2	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:LEU:HD23	2:E:394:LEU:HD23	1.97	0.46
2:F:126:GLU:OE1	2:F:143:ARG:HD2	2.16	0.46
1:B:8:LYS:HB3	1:B:15:MET:HB2	1.97	0.45
2:E:138:LEU:HD12	2:E:344:VAL:HG11	1.98	0.45
2:F:35:GLN:H	2:F:67:ASN:HD22	1.62	0.45
1:C:51:VAL:HG12	1:C:53:GLU:H	1.82	0.45
2:D:143:ARG:HH22	2:D:172:ASP:HB2	1.82	0.45
2:F:16[A]:MET:HE1	2:F:63:ILE:HG21	1.99	0.45
1:A:143:LYS:NZ	1:A:281:THR:O	2.45	0.45
2:F:328:ILE:HD12	2:F:346:PRO:HB2	1.99	0.45
2:D:283:THR:HG22	5:D:503:GOL:H31	1.98	0.45
2:F:143:ARG:HH22	2:F:174:SER:CB	2.30	0.45
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.99	0.45
2:D:29:LEU:HD11	2:D:41:ARG:HG2	1.99	0.45
1:B:327:MET:HE3	1:B:387:ILE:HB	1.99	0.44
1:C:278:ASP:HB2	5:C:610:GOL:H2	1.99	0.44
2:D:158:LYS:HB3	2:D:158:LYS:HE2	1.84	0.44
2:E:385:LEU:HB3	2:E:394:LEU:HD21	1.99	0.44
1:A:315:GLU:OE2	1:A:368:ARG:HD2	2.17	0.44
2:E:45:LEU:HD13	2:E:264:ARG:HD2	1.98	0.44
1:A:51:VAL:HG12	1:A:53:GLU:H	1.82	0.44
1:A:194:ARG:HH22	1:A:304:GLU:CD	2.21	0.44
1:A:397:ILE:HB	1:A:402:THR:HG21	2.00	0.44
1:B:410:LYS:HE2	1:B:437:TYR:CE1	2.52	0.44
2:F:364:ASP:OD1	2:F:364:ASP:N	2.45	0.44
1:A:245:ILE:HG22	1:A:327:MET:HE1	2.00	0.44
1:A:559:SER:HA	1:A:562:ILE:HG12	1.99	0.44
1:A:566:GLU:O	1:A:569:LYS:HG3	2.17	0.44
1:C:25:GLN:O	1:C:70:ALA:HA	2.18	0.44
1:A:308:TYR:HA	1:A:311:ILE:HG22	2.00	0.43
1:B:339[B]:ARG:HD2	7:B:922:HOH:O	2.18	0.43
1:A:472:GLU:O	1:A:476:LEU:HG	2.18	0.43
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.83	0.43
1:A:124:ILE:HG22	1:A:162:ILE:HD13	2.00	0.43
2:F:443:LYS:HE2	2:F:443:LYS:HB2	1.75	0.43
1:A:41:GLU:HG2	1:A:48:SER:HB2	1.99	0.43
1:C:206:ASP:HB2	1:C:440:GLU:OE2	2.18	0.43
2:D:31:GLU:OE1	2:D:71:ARG:NH2	2.39	0.43
1:A:40:ILE:HG12	1:A:48:SER:O	2.18	0.43
1:A:462:ARG:NE	1:A:466:GLU:OE2	2.41	0.43
2:E:380:LYS:HB3	2:E:380:LYS:HE3	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:THR:HG23	1:C:283:GLU:N	2.31	0.43
1:C:135:ILE:HD13	1:C:148:LYS:HD2	2.00	0.43
2:F:107:LYS:HD2	2:F:109:LEU:HD21	2.01	0.43
2:D:48:GLN:C	2:D:49:GLU:HG2	2.38	0.42
2:F:277:LEU:HD23	2:F:318:LEU:HD12	2.00	0.42
1:A:225:GLY:O	1:A:370:GLY:HA2	2.19	0.42
1:C:528:PHE:CZ	1:C:553:ARG:HD3	2.54	0.42
2:E:6:ARG:NH2	7:E:615:HOH:O	2.49	0.42
2:D:58[B]:GLU:OE1	7:D:601:HOH:O	2.22	0.42
2:F:439:ARG:NH2	2:F:451:ASP:OD1	2.48	0.42
2:E:150:PHE:HB2	2:E:328:ILE:HG12	2.01	0.42
1:B:410:LYS:HB3	1:B:436:LEU:HB2	2.02	0.42
1:C:315:GLU:HA	1:C:384:ILE:HD11	2.01	0.42
1:B:21:GLU:O	2:F:64:ASN:ND2	2.45	0.42
1:C:416:ASP:OD2	1:C:418:SER:OG	2.27	0.41
2:F:148:PRO:HD2	2:F:325:GLY:O	2.19	0.41
1:A:541:TYR:HD1	1:A:541:TYR:HA	1.73	0.41
2:D:454:LEU:HD12	2:D:454:LEU:HA	1.94	0.41
1:A:403:GLN:O	1:A:407:ARG:HG3	2.20	0.41
2:E:29:LEU:HD12	2:E:42:GLY:O	2.21	0.41
2:F:2:ILE:HD12	7:F:777:HOH:O	2.21	0.41
2:E:388:VAL:C	2:E:389:LEU:HD23	2.40	0.41
2:F:11:VAL:HG22	2:F:16[B]:MET:HG2	2.01	0.41
1:B:586:SER:HB2	1:B:587:GLU:OE1	2.22	0.40
2:D:431:TRP:CE3	2:D:454:LEU:HD13	2.56	0.40
2:F:380:LYS:HD2	2:F:380:LYS:HA	1.91	0.40
1:A:230:VAL:HG13	1:A:389:ALA:HA	2.03	0.40
2:D:32:VAL:HG22	2:D:70:VAL:HG22	2.03	0.40

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	586/600 (98%)	577 (98%)	9 (2%)	0	100	100
1	B	594/600 (99%)	588 (99%)	6 (1%)	0	100	100
1	C	588/600 (98%)	579 (98%)	9 (2%)	0	100	100
2	D	454/465 (98%)	446 (98%)	8 (2%)	0	100	100
2	E	453/465 (97%)	443 (98%)	10 (2%)	0	100	100
2	F	455/465 (98%)	447 (98%)	8 (2%)	0	100	100
All	All	3130/3195 (98%)	3080 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	498/511 (98%)	487 (98%)	11 (2%)	52	57
1	B	509/511 (100%)	503 (99%)	6 (1%)	71	77
1	C	505/511 (99%)	497 (98%)	8 (2%)	62	69
2	D	375/387 (97%)	361 (96%)	14 (4%)	34	35
2	E	376/387 (97%)	371 (99%)	5 (1%)	69	75
2	F	378/387 (98%)	367 (97%)	11 (3%)	42	46
All	All	2641/2694 (98%)	2586 (98%)	55 (2%)	53	59

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLU
1	A	146	GLN
1	A	177	GLU
1	A	362	LEU
1	A	378	ASP
1	A	479	ILE
1	A	541	TYR

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Mol	Chain	Res	Type
1	A	554	GLU
1	A	558	ARG
1	A	578	LYS
1	A	583	LEU
1	B	125	GLU
1	B	283	GLU
1	B	378	ASP
1	B	481	SER
1	B	586	SER
1	B	587	GLU
1	C	43	ARG
1	C	129	GLU
1	C	160	GLN
1	C	280	ASN
1	C	281	THR
1	C	422	LYS
1	C	480	ASP
1	C	587	GLU
2	D	30	ILE
2	D	33	ARG
2	D	41	ARG
2	D	49	GLU
2	D	83	GLU
2	D	122	ASP
2	D	146	LYS
2	D	173	SER
2	D	381	GLN
2	D	389	LEU
2	D	392	SER
2	D	400	ILE
2	D	443	LYS
2	D	447	ASP
2	E	47	VAL
2	E	122	ASP
2	E	166	ARG
2	E	292	ARG
2	E	392	SER
2	F	36	ASN
2	F	47	VAL
2	F	67	ASN
2	F	82	SER
2	F	122	ASP

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Mol	Chain	Res	Type
2	F	146	LYS
2	F	174	SER
2	F	200	GLN
2	F	388	VAL
2	F	389	LEU
2	F	403	LYS

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

Mol	Chain	Res	Type
2	E	43	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 3 are monoatomic - leaving 43 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	$\#\|Z\| > 2$
5	GOL	B	611	-	5,5,5	0.35	0	5,5,5	0.32	0
5	GOL	C	606	-	5,5,5	0.33	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	F	505	-	5,5,5	0.34	0	5,5,5	0.21	0
5	GOL	B	607	-	5,5,5	0.42	0	5,5,5	0.21	0
5	GOL	F	503	-	5,5,5	0.40	0	5,5,5	0.27	0
5	GOL	E	504	-	5,5,5	0.49	0	5,5,5	0.32	0
5	GOL	A	608	-	5,5,5	0.37	0	5,5,5	0.40	0
5	GOL	B	603	-	5,5,5	0.37	0	5,5,5	0.47	0
5	GOL	B	612	-	5,5,5	0.35	0	5,5,5	0.27	0
5	GOL	D	503	-	5,5,5	0.36	0	5,5,5	0.21	0
3	ANP	A	601	4	29,33,33	1.04	2 (6%)	31,52,52	1.17	4 (12%)
5	GOL	C	604	-	5,5,5	0.39	0	5,5,5	0.39	0
6	MES	D	501	-	12,12,12	2.32	1 (8%)	14,16,16	1.87	3 (21%)
5	GOL	A	607	-	5,5,5	0.36	0	5,5,5	0.34	0
5	GOL	C	605	-	5,5,5	0.30	0	5,5,5	0.48	0
5	GOL	E	503	-	5,5,5	0.38	0	5,5,5	0.13	0
5	GOL	B	605	-	5,5,5	0.37	0	5,5,5	0.24	0
5	GOL	F	507	-	5,5,5	0.32	0	5,5,5	0.18	0
5	GOL	A	609	-	5,5,5	0.36	0	5,5,5	0.30	0
5	GOL	A	603	-	5,5,5	0.31	0	5,5,5	0.55	0
5	GOL	B	609	-	5,5,5	0.36	0	5,5,5	0.33	0
5	GOL	A	606	-	5,5,5	0.39	0	5,5,5	0.20	0
5	GOL	C	610	-	5,5,5	0.38	0	5,5,5	0.14	0
5	GOL	E	502	-	5,5,5	0.35	0	5,5,5	0.18	0
5	GOL	B	608	-	5,5,5	0.34	0	5,5,5	0.32	0
5	GOL	F	502	-	5,5,5	0.45	0	5,5,5	0.12	0
5	GOL	E	501	-	5,5,5	0.38	0	5,5,5	0.33	0
5	GOL	B	606	-	5,5,5	0.36	0	5,5,5	0.30	0
5	GOL	A	604	-	5,5,5	0.36	0	5,5,5	0.28	0
3	ANP	C	601	4	29,33,33	1.74	5 (17%)	31,52,52	0.98	3 (9%)
5	GOL	D	504	-	5,5,5	0.45	0	5,5,5	0.14	0
5	GOL	C	607	-	5,5,5	0.37	0	5,5,5	0.30	0
5	GOL	F	504	-	5,5,5	0.36	0	5,5,5	0.41	0
5	GOL	A	605	-	5,5,5	0.38	0	5,5,5	0.19	0
5	GOL	C	608	-	5,5,5	0.35	0	5,5,5	0.39	0
3	ANP	B	601	4	29,33,33	1.61	4 (13%)	31,52,52	1.05	3 (9%)
5	GOL	F	501	-	5,5,5	0.35	0	5,5,5	0.23	0
5	GOL	C	609	-	5,5,5	0.33	0	5,5,5	0.33	0
5	GOL	B	610	-	5,5,5	0.34	0	5,5,5	0.39	0
5	GOL	D	502	-	5,5,5	0.32	0	5,5,5	0.28	0
5	GOL	C	603	-	5,5,5	0.37	0	5,5,5	0.32	0
5	GOL	F	506	-	5,5,5	0.37	0	5,5,5	0.28	0
5	GOL	B	604	-	5,5,5	0.34	0	5,5,5	0.25	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
5	GOL	B	611	-	-	4/4/4/4	-
5	GOL	C	606	-	-	2/4/4/4	-
5	GOL	F	505	-	-	2/4/4/4	-
5	GOL	B	607	-	-	4/4/4/4	-
5	GOL	F	503	-	-	2/4/4/4	-
5	GOL	E	504	-	-	3/4/4/4	-
5	GOL	A	608	-	-	2/4/4/4	-
5	GOL	B	603	-	-	4/4/4/4	-
5	GOL	B	612	-	-	4/4/4/4	-
5	GOL	D	503	-	-	2/4/4/4	-
3	ANP	A	601	4	-	3/14/38/38	0/3/3/3
5	GOL	C	604	-	-	0/4/4/4	-
6	MES	D	501	-	-	2/6/14/14	0/1/1/1
5	GOL	A	607	-	-	4/4/4/4	-
5	GOL	C	605	-	-	2/4/4/4	-
5	GOL	E	503	-	-	2/4/4/4	-
5	GOL	B	605	-	-	2/4/4/4	-
5	GOL	F	507	-	-	2/4/4/4	-
5	GOL	A	609	-	-	4/4/4/4	-
5	GOL	A	603	-	-	2/4/4/4	-
5	GOL	B	609	-	-	1/4/4/4	-
5	GOL	A	606	-	-	0/4/4/4	-
5	GOL	C	610	-	-	2/4/4/4	-
5	GOL	E	502	-	-	0/4/4/4	-
5	GOL	B	608	-	-	2/4/4/4	-
5	GOL	F	502	-	-	1/4/4/4	-
5	GOL	E	501	-	-	1/4/4/4	-
5	GOL	B	606	-	-	2/4/4/4	-
5	GOL	A	604	-	-	2/4/4/4	-
3	ANP	C	601	4	-	3/14/38/38	0/3/3/3
5	GOL	D	504	-	-	4/4/4/4	-
5	GOL	C	607	-	-	2/4/4/4	-
5	GOL	F	504	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	605	-	-	2/4/4/4	-
5	GOL	C	608	-	-	2/4/4/4	-
3	ANP	B	601	4	-	4/14/38/38	0/3/3/3
5	GOL	F	501	-	-	2/4/4/4	-
5	GOL	C	609	-	-	1/4/4/4	-
5	GOL	B	610	-	-	2/4/4/4	-
5	GOL	D	502	-	-	2/4/4/4	-
5	GOL	C	603	-	-	0/4/4/4	-
5	GOL	F	506	-	-	2/4/4/4	-
5	GOL	B	604	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	501	MES	C8-S	-7.79	1.66	1.77
3	C	601	ANP	PG-O1G	7.27	1.57	1.46
3	B	601	ANP	PB-O1B	5.63	1.55	1.46
3	B	601	ANP	PG-O1G	3.46	1.51	1.46
3	A	601	ANP	PG-O1G	3.18	1.51	1.46
3	B	601	ANP	PG-N3B	2.90	1.70	1.63
3	B	601	ANP	PB-O2B	-2.90	1.49	1.56
3	A	601	ANP	PG-N3B	2.51	1.69	1.63
3	C	601	ANP	PG-N3B	2.43	1.69	1.63
3	C	601	ANP	PG-O2G	-2.41	1.50	1.56
3	C	601	ANP	PB-O3A	-2.33	1.56	1.59
3	C	601	ANP	PB-O1B	2.03	1.49	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	501	MES	C5-N4-C3	5.11	120.33	108.83
3	A	601	ANP	O1G-PG-N3B	-4.05	105.81	111.77
6	D	501	MES	O1S-S-C8	2.67	110.12	106.92
6	D	501	MES	O2S-S-C8	2.63	110.09	106.92
3	C	601	ANP	O3G-PG-O1G	-2.42	107.37	113.45
3	A	601	ANP	C5-C6-N6	2.28	123.82	120.35
3	A	601	ANP	O2G-PG-O1G	-2.24	107.81	113.45
3	C	601	ANP	C5-C6-N6	2.18	123.66	120.35
3	B	601	ANP	C5-C6-N6	2.13	123.58	120.35
3	B	601	ANP	O2B-PB-O1B	-2.12	105.48	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	ANP	PB-O3A-PA	-2.08	125.29	132.62
3	A	601	ANP	O2B-PB-O3A	2.04	111.45	104.64
3	B	601	ANP	O1G-PG-N3B	-2.04	108.77	111.77

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ANP	PG-N3B-PB-O1B
3	A	601	ANP	PG-N3B-PB-O3A
3	A	601	ANP	PA-O3A-PB-O1B
3	B	601	ANP	PB-N3B-PG-O1G
3	B	601	ANP	PG-N3B-PB-O1B
3	B	601	ANP	PA-O3A-PB-O1B
3	B	601	ANP	PA-O3A-PB-O2B
3	C	601	ANP	PB-N3B-PG-O1G
3	C	601	ANP	PA-O3A-PB-O1B
3	C	601	ANP	PA-O3A-PB-O2B
5	A	604	GOL	O1-C1-C2-C3
5	A	605	GOL	O1-C1-C2-O2
5	A	605	GOL	O1-C1-C2-C3
5	A	607	GOL	O1-C1-C2-C3
5	A	607	GOL	C1-C2-C3-O3
5	A	608	GOL	O1-C1-C2-C3
5	A	609	GOL	O1-C1-C2-O2
5	A	609	GOL	O1-C1-C2-C3
5	A	609	GOL	C1-C2-C3-O3
5	B	604	GOL	O1-C1-C2-C3
5	B	606	GOL	O1-C1-C2-C3
5	B	610	GOL	O1-C1-C2-C3
5	B	611	GOL	O1-C1-C2-C3
5	C	606	GOL	C1-C2-C3-O3
5	C	607	GOL	O1-C1-C2-C3
5	C	608	GOL	O1-C1-C2-C3
5	D	502	GOL	O1-C1-C2-C3
5	D	503	GOL	O1-C1-C2-C3
5	D	504	GOL	C1-C2-C3-O3
5	E	504	GOL	O1-C1-C2-C3
5	F	501	GOL	O1-C1-C2-C3
5	F	504	GOL	O1-C1-C2-C3
5	F	505	GOL	O1-C1-C2-C3
5	F	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	F	507	GOL	O1-C1-C2-C3
6	D	501	MES	C7-C8-S-O2S
5	A	607	GOL	O2-C2-C3-O3
5	A	608	GOL	O1-C1-C2-O2
5	C	606	GOL	O2-C2-C3-O3
5	D	504	GOL	O2-C2-C3-O3
5	E	503	GOL	O2-C2-C3-O3
5	F	507	GOL	O1-C1-C2-O2
5	A	603	GOL	O1-C1-C2-C3
5	B	603	GOL	O1-C1-C2-C3
5	B	603	GOL	C1-C2-C3-O3
5	B	607	GOL	O1-C1-C2-C3
5	B	607	GOL	C1-C2-C3-O3
5	B	608	GOL	O1-C1-C2-C3
5	B	612	GOL	O1-C1-C2-C3
5	C	605	GOL	O1-C1-C2-C3
5	C	609	GOL	O1-C1-C2-C3
5	D	504	GOL	O1-C1-C2-C3
5	E	503	GOL	C1-C2-C3-O3
5	F	503	GOL	O1-C1-C2-C3
5	A	604	GOL	O1-C1-C2-O2
5	A	607	GOL	O1-C1-C2-O2
5	B	604	GOL	O1-C1-C2-O2
5	B	610	GOL	O1-C1-C2-O2
5	B	611	GOL	O1-C1-C2-O2
5	C	607	GOL	O1-C1-C2-O2
5	D	502	GOL	O1-C1-C2-O2
5	D	503	GOL	O1-C1-C2-O2
5	E	504	GOL	O1-C1-C2-O2
5	F	503	GOL	O1-C1-C2-O2
5	F	505	GOL	O1-C1-C2-O2
5	A	609	GOL	O2-C2-C3-O3
5	B	603	GOL	O1-C1-C2-O2
5	C	608	GOL	O1-C1-C2-O2
5	D	504	GOL	O1-C1-C2-O2
5	F	504	GOL	O1-C1-C2-O2
5	F	506	GOL	O1-C1-C2-O2
5	B	603	GOL	O2-C2-C3-O3
5	B	607	GOL	O2-C2-C3-O3
5	B	608	GOL	O1-C1-C2-O2
5	F	501	GOL	O1-C1-C2-O2
5	B	605	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	606	GOL	O1-C1-C2-O2
5	B	611	GOL	O2-C2-C3-O3
5	B	612	GOL	O1-C1-C2-O2
5	C	610	GOL	O1-C1-C2-O2
5	C	610	GOL	O1-C1-C2-C3
6	D	501	MES	C7-C8-S-O1S
5	A	603	GOL	O1-C1-C2-O2
5	C	605	GOL	O1-C1-C2-O2
5	B	612	GOL	C1-C2-C3-O3
5	B	607	GOL	O1-C1-C2-O2
5	B	612	GOL	O2-C2-C3-O3
5	E	501	GOL	O1-C1-C2-O2
5	B	605	GOL	O1-C1-C2-C3
5	B	609	GOL	O1-C1-C2-C3
5	B	611	GOL	C1-C2-C3-O3
5	F	502	GOL	O1-C1-C2-C3
5	E	504	GOL	O2-C2-C3-O3

There are no ring outliers.

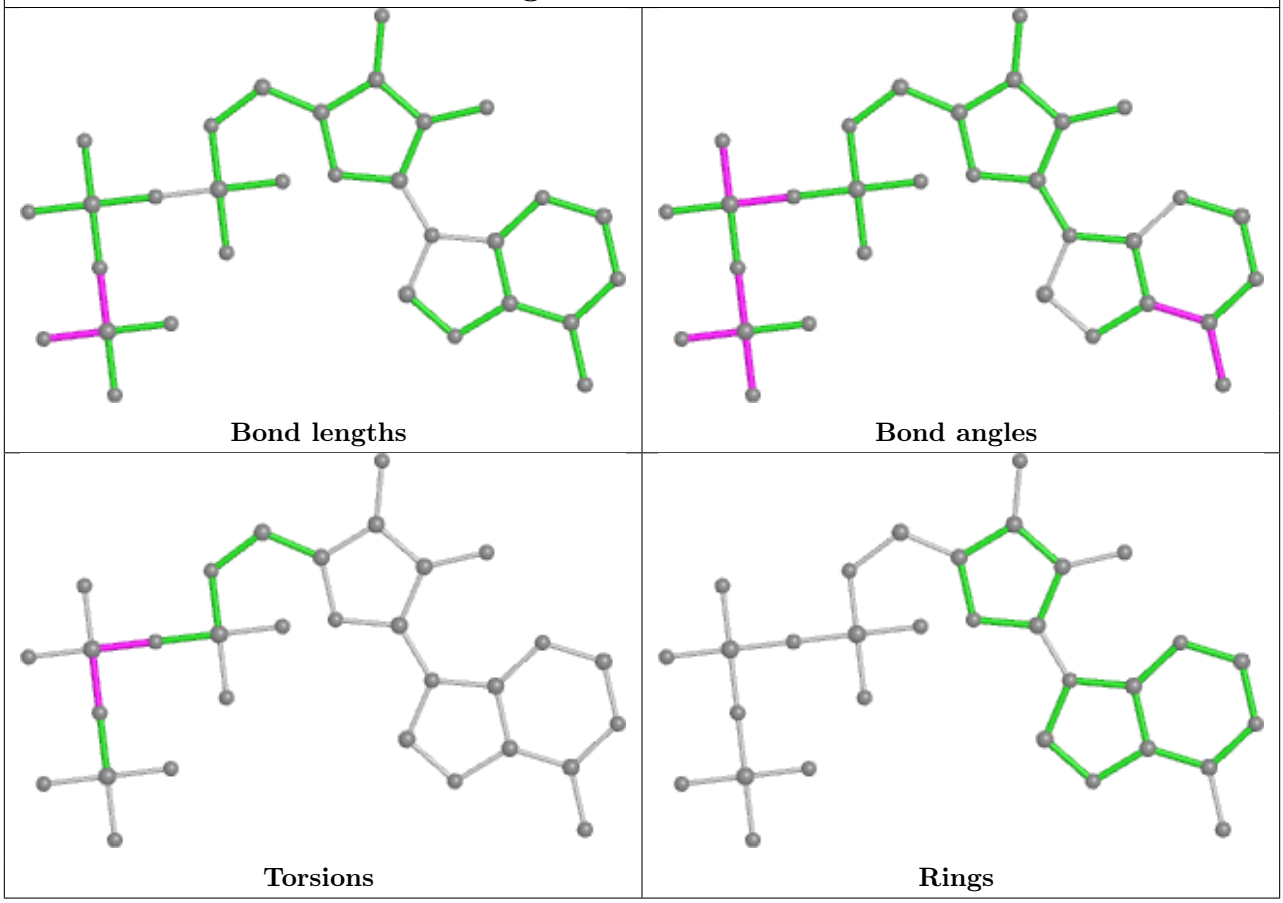
13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	607	GOL	2	0
5	E	504	GOL	1	0
5	D	503	GOL	1	0
5	C	605	GOL	1	0
5	F	507	GOL	1	0
5	C	610	GOL	1	0
5	A	604	GOL	2	0
3	C	601	ANP	2	0
5	D	504	GOL	2	0
5	C	608	GOL	1	0
3	B	601	ANP	1	0
5	F	501	GOL	1	0
5	B	604	GOL	1	0

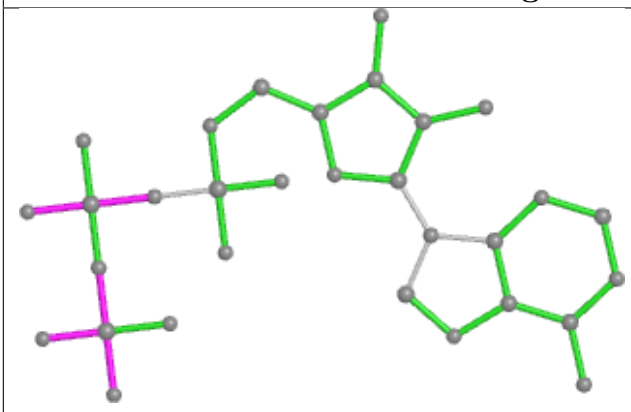
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

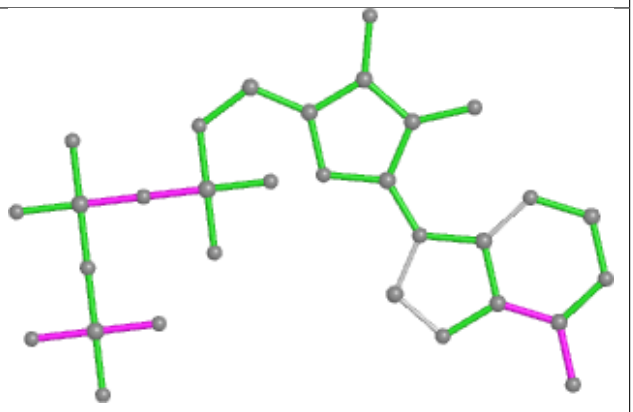
Ligand ANP A 601



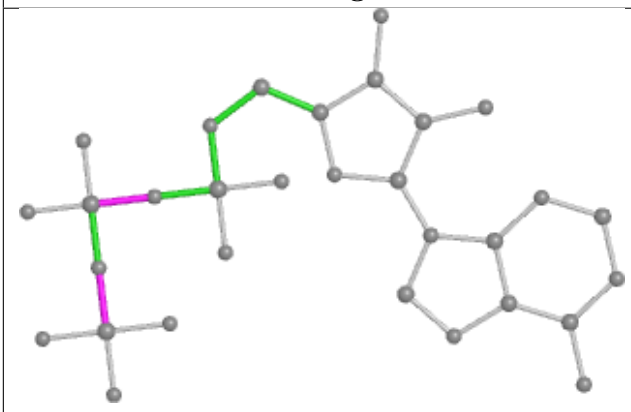
Ligand ANP C 601



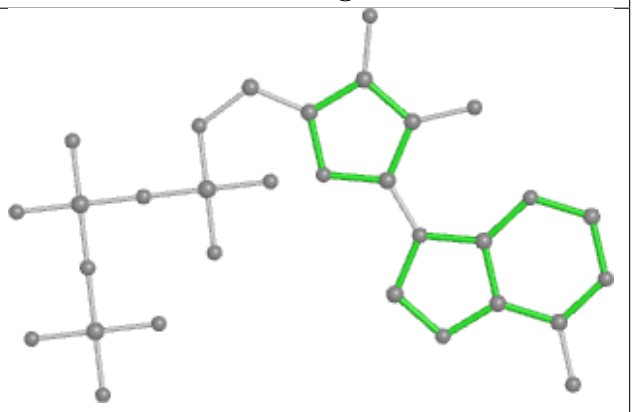
Bond lengths



Bond angles

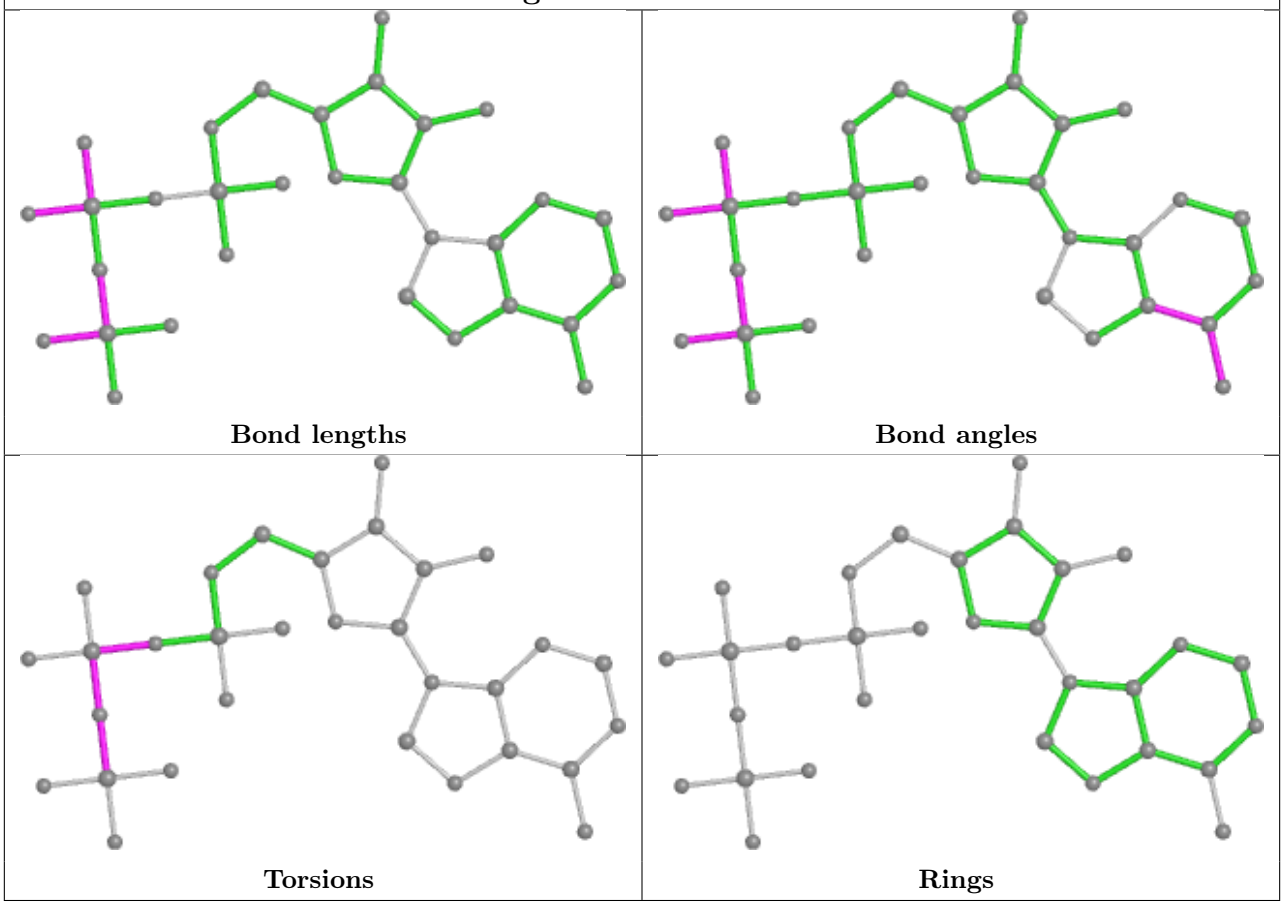


Torsions



Rings

Ligand ANP B 601



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, 95^{th} 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	588/600 (98%)	0.02	30 (5%)	28	33	25, 40, 82, 114	0
1	B	592/600 (98%)	-0.34	5 (0%)	86	88	19, 30, 60, 91	1 (0%)
1	C	587/600 (97%)	-0.19	11 (1%)	66	71	18, 30, 61, 116	0
2	D	453/465 (97%)	0.09	30 (6%)	18	23	25, 39, 91, 130	0
2	E	455/465 (97%)	-0.28	9 (1%)	65	69	19, 34, 63, 97	0
2	F	456/465 (98%)	-0.10	10 (2%)	62	66	18, 31, 63, 100	0
All	All	3131/3195 (97%)	-0.14	95 (3%)	50	56	18, 34, 72, 130	1 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	386	ALA	9.8
2	D	388	VAL	9.0
2	D	390	GLY	7.7
1	A	476	LEU	7.5
2	D	387	VAL	7.5
1	A	482	LEU	7.4
1	A	479	ILE	7.3
2	D	393	ALA	7.3
1	A	477	VAL	6.7
1	A	478	GLY	6.5
1	A	541	TYR	6.2
1	C	477	VAL	6.2
2	D	394	LEU	6.0
2	D	389	LEU	5.9
1	C	280	ASN	5.8
2	D	392	SER	5.8
1	A	542	PHE	5.4
1	A	535	ALA	5.2
2	E	389	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	480	ASP	5.0
2	D	454	LEU	4.9
2	D	385	LEU	4.7
1	C	279	PRO	4.6
1	A	481	SER	4.6
2	D	455	PRO	4.5
2	D	397	ILE	4.3
2	F	393	ALA	4.3
1	A	473	ILE	4.1
2	F	397	ILE	4.1
1	B	477	VAL	4.1
1	A	538	LEU	4.0
2	E	392	SER	3.9
2	D	440	THR	3.9
2	D	391	GLU	3.8
2	F	394	LEU	3.6
1	A	475	ARG	3.6
1	A	581	ILE	3.4
1	B	0	GLY	3.4
2	E	387	VAL	3.4
1	A	545	ILE	3.3
2	D	400	ILE	3.2
2	D	384	GLU	3.1
1	A	474	VAL	3.1
1	C	541	TYR	3.1
1	C	583	LEU	3.0
2	E	396	ASP	3.0
1	A	485	ASN	3.0
2	D	172	ASP	2.9
1	C	481	SER	2.9
2	D	451	ASP	2.9
1	A	487	ARG	2.9
2	F	172	ASP	2.9
1	A	280	ASN	2.9
1	B	476	LEU	2.9
1	A	540	ALA	2.8
1	C	476	LEU	2.8
2	D	104	LEU	2.8
2	F	389	LEU	2.7
2	F	388	VAL	2.7
2	E	385	LEU	2.7
1	A	546	MET	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	175	ASP	2.6
2	E	388	VAL	2.6
2	F	455	PRO	2.6
2	D	396	ASP	2.6
2	D	448	ASP	2.6
1	A	536	LEU	2.6
2	E	394	LEU	2.6
2	D	5	TYR	2.5
1	B	480	ASP	2.5
2	D	381	GLN	2.4
2	D	4	GLU	2.4
2	E	393	ALA	2.4
2	E	391	GLU	2.4
2	D	449	LEU	2.4
1	A	532	ALA	2.3
1	A	159	VAL	2.3
1	A	533	ARG	2.3
2	D	395	SER	2.3
1	C	277	ILE	2.3
1	C	278	ASP	2.2
2	D	450	LEU	2.2
1	B	180	GLN	2.2
1	A	125	GLU	2.2
1	C	480	ASP	2.2
1	A	484	ASP	2.2
2	D	398	ASP	2.2
2	F	81	VAL	2.1
1	C	1	MET	2.1
2	D	173	SER	2.1
1	A	483	SER	2.1
1	A	489	THR	2.1
1	A	180	GLN	2.1
2	F	387	VAL	2.1
2	F	391	GLU	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 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, 95^{th} 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	GOL	F	505	6/6	0.65	0.29	70,71,72,72	0
5	GOL	E	502	6/6	0.73	0.21	58,65,66,68	0
5	GOL	D	504	6/6	0.73	0.22	81,83,86,86	0
5	GOL	C	610	6/6	0.74	0.21	76,78,79,79	0
5	GOL	C	606	6/6	0.75	0.22	65,68,71,72	0
5	GOL	F	502	6/6	0.76	0.29	61,62,62,63	0
5	GOL	E	504	6/6	0.77	0.22	70,74,81,81	0
5	GOL	B	606	6/6	0.79	0.26	61,63,64,65	0
5	GOL	C	605	6/6	0.80	0.20	64,65,66,67	0
5	GOL	A	606	6/6	0.82	0.15	71,74,74,74	0
5	GOL	B	610	6/6	0.82	0.23	62,64,65,66	0
5	GOL	C	609	6/6	0.83	0.29	78,79,80,82	0
5	GOL	E	501	6/6	0.83	0.20	35,55,57,61	0
5	GOL	A	607	6/6	0.85	0.18	69,72,72,73	0
5	GOL	E	503	6/6	0.87	0.25	67,70,71,73	0
5	GOL	B	611	6/6	0.87	0.14	46,51,53,53	0
5	GOL	C	604	6/6	0.87	0.17	66,70,72,73	0
5	GOL	A	609	6/6	0.87	0.27	72,73,74,75	0
5	GOL	F	501	6/6	0.88	0.19	37,56,59,61	0
5	GOL	C	608	6/6	0.88	0.19	66,66,68,71	0
5	GOL	B	604	6/6	0.88	0.19	61,61,63,67	0
5	GOL	F	506	6/6	0.88	0.13	60,63,66,67	0
6	MES	D	501	12/12	0.88	0.14	42,45,68,69	0
5	GOL	B	609	6/6	0.89	0.18	77,80,80,80	0
5	GOL	D	502	6/6	0.89	0.15	58,63,64,66	0
5	GOL	C	607	6/6	0.89	0.19	63,66,68,69	0
5	GOL	B	607	6/6	0.90	0.18	57,61,64,65	0
5	GOL	D	503	6/6	0.90	0.19	33,53,58,59	0
5	GOL	B	608	6/6	0.90	0.18	48,51,55,58	0
5	GOL	A	604	6/6	0.90	0.17	66,70,71,71	0
5	GOL	F	504	6/6	0.91	0.16	56,57,60,66	0
5	GOL	F	507	6/6	0.91	0.20	62,64,68,69	0

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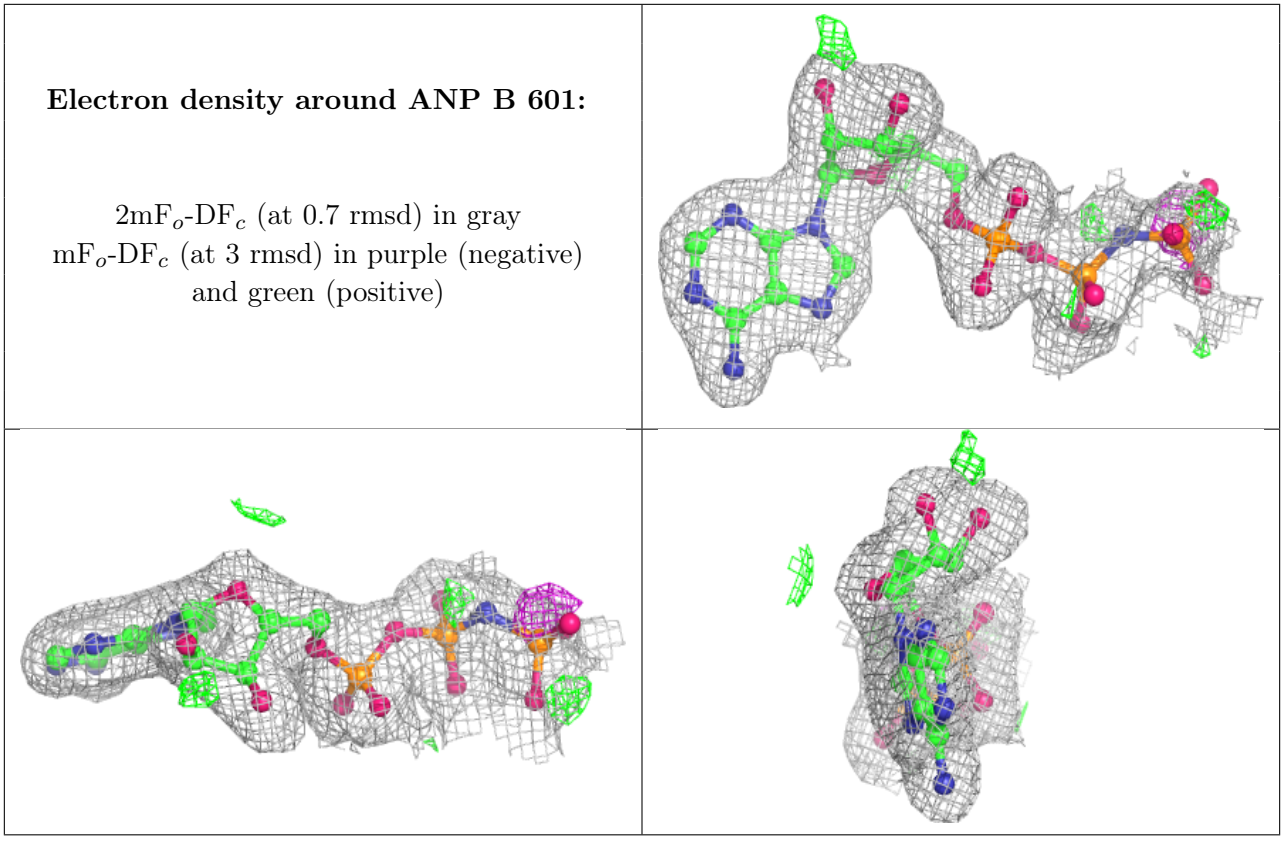
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	612	6/6	0.91	0.17	71,71,72,73	0
5	GOL	C	603	6/6	0.92	0.13	52,57,62,66	0
5	GOL	A	603	6/6	0.92	0.16	57,59,60,61	0
5	GOL	A	608	6/6	0.93	0.15	50,59,61,62	0
5	GOL	B	605	6/6	0.94	0.11	53,54,55,55	0
5	GOL	B	603	6/6	0.94	0.16	51,58,60,63	0
5	GOL	A	605	6/6	0.94	0.10	51,57,58,58	0
5	GOL	F	503	6/6	0.95	0.19	71,72,73,73	0
4	MG	B	602	1/1	0.96	0.10	24,24,24,24	0
4	MG	A	602	1/1	0.98	0.12	24,24,24,24	0
3	ANP	B	601	31/31	0.98	0.14	18,23,39,51	4
3	ANP	C	601	31/31	0.99	0.12	17,24,29,31	3
4	MG	C	602	1/1	0.99	0.10	21,21,21,21	0
3	ANP	A	601	31/31	0.99	0.09	20,30,34,36	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.

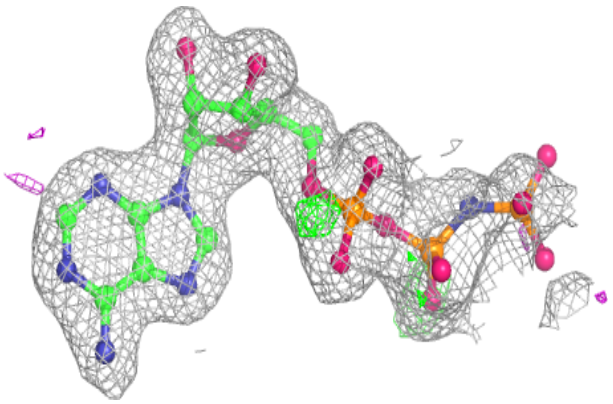
Electron density around ANP B 601:

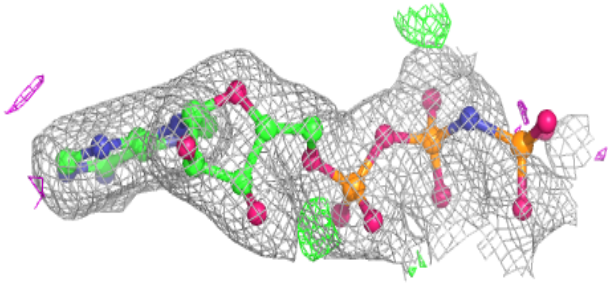
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

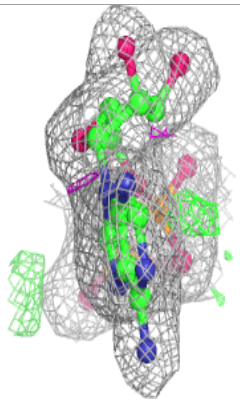


Electron density around ANP C 601:

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

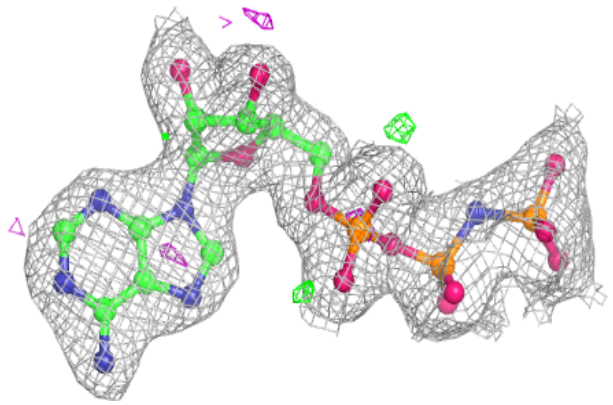


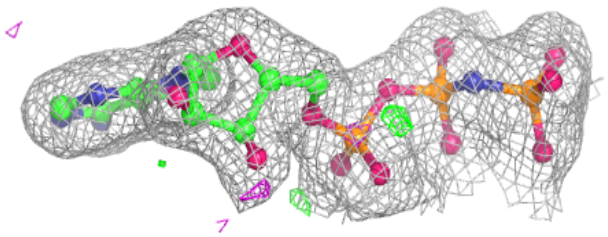


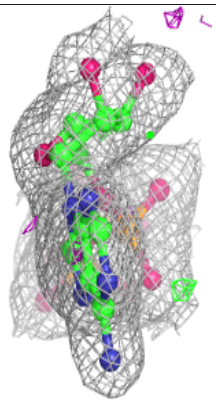


Electron density around ANP A 601:

$2mF_o$-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.