



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2022 – 06:26 PM JST

PDB ID : 7VW7  
Title : Crystal structure of the 2 ADP-AlF<sub>4</sub>-bound V1 complex  
Authors : Suzuki, K.; Shekhar, M.; Gupta, C.; Singharoy, A.; Murata, T.  
Deposited on : 2021-11-09  
Resolution : 3.82 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](mailto: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.

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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 : 2.28.1  
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) : 2.28.1

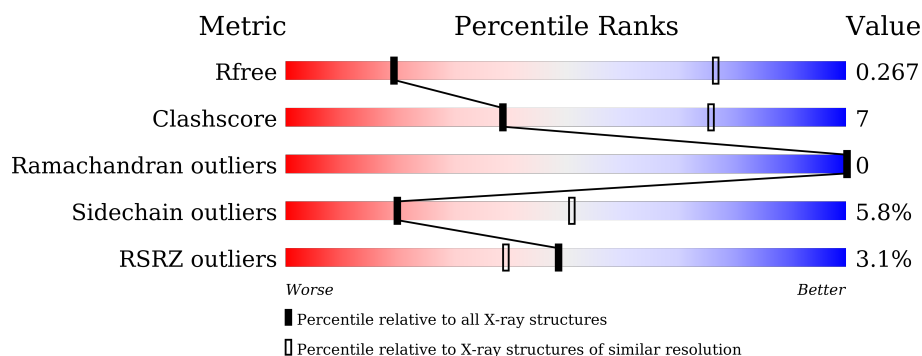
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.82 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	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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  $\geq 3$ , 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>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	600	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	600	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
2	D	465	<div> <div></div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
2	E	465	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
2	F	465	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>..</div> </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ALF	B	603	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25072 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	Se	0	0	0
			4320	2718	724	852	3	23			
1	B	593	Total	C	N	O	S	Se	0	0	0
			4370	2732	740	872	3	23			
1	C	579	Total	C	N	O	S	Se	0	0	0
			4220	2604	729	861	3	23			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A0A1V8WY35
A	-5	SER	-	expression tag	UNP A0A1V8WY35
A	-4	SER	-	expression tag	UNP A0A1V8WY35
A	-3	GLY	-	expression tag	UNP A0A1V8WY35
A	-2	SER	-	expression tag	UNP A0A1V8WY35
A	-1	SER	-	expression tag	UNP A0A1V8WY35
A	0	GLY	-	expression tag	UNP A0A1V8WY35
B	-6	GLY	-	expression tag	UNP A0A1V8WY35
B	-5	SER	-	expression tag	UNP A0A1V8WY35
B	-4	SER	-	expression tag	UNP A0A1V8WY35
B	-3	GLY	-	expression tag	UNP A0A1V8WY35
B	-2	SER	-	expression tag	UNP A0A1V8WY35
B	-1	SER	-	expression tag	UNP A0A1V8WY35
B	0	GLY	-	expression tag	UNP A0A1V8WY35
C	-6	GLY	-	expression tag	UNP A0A1V8WY35
C	-5	SER	-	expression tag	UNP A0A1V8WY35
C	-4	SER	-	expression tag	UNP A0A1V8WY35
C	-3	GLY	-	expression tag	UNP A0A1V8WY35
C	-2	SER	-	expression tag	UNP A0A1V8WY35
C	-1	SER	-	expression tag	UNP A0A1V8WY35
C	0	GLY	-	expression tag	UNP A0A1V8WY35

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	452	Total	C	N	O	Se	0	0	0
			3375	2121	587	653	14			
2	E	452	Total	C	N	O	Se	0	0	0
			3423	2153	587	669	14			
2	F	453	Total	C	N	O	Se	0	0	0
			3445	2181	589	661	14			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP A0A1V8XC32
D	-5	SER	-	expression tag	UNP A0A1V8XC32
D	-4	SER	-	expression tag	UNP A0A1V8XC32
D	-3	GLY	-	expression tag	UNP A0A1V8XC32
D	-2	SER	-	expression tag	UNP A0A1V8XC32
D	-1	SER	-	expression tag	UNP A0A1V8XC32
D	0	GLY	-	expression tag	UNP A0A1V8XC32
E	-6	GLY	-	expression tag	UNP A0A1V8XC32
E	-5	SER	-	expression tag	UNP A0A1V8XC32
E	-4	SER	-	expression tag	UNP A0A1V8XC32
E	-3	GLY	-	expression tag	UNP A0A1V8XC32
E	-2	SER	-	expression tag	UNP A0A1V8XC32
E	-1	SER	-	expression tag	UNP A0A1V8XC32
E	0	GLY	-	expression tag	UNP A0A1V8XC32
F	-6	GLY	-	expression tag	UNP A0A1V8XC32
F	-5	SER	-	expression tag	UNP A0A1V8XC32
F	-4	SER	-	expression tag	UNP A0A1V8XC32
F	-3	GLY	-	expression tag	UNP A0A1V8XC32
F	-2	SER	-	expression tag	UNP A0A1V8XC32
F	-1	SER	-	expression tag	UNP A0A1V8XC32
F	0	GLY	-	expression tag	UNP A0A1V8XC32

- Molecule 3 is a protein called V-type sodium ATPase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	165	Total	C	N	O	S Se	0	0	0
			1207	750	219	230	1 7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	expression tag	UNP A0A7Z9AX30
G	-5	SER	-	expression tag	UNP A0A7Z9AX30

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	SER	-	expression tag	UNP A0A7Z9AX30
G	-3	GLY	-	expression tag	UNP A0A7Z9AX30
G	-2	SER	-	expression tag	UNP A0A7Z9AX30
G	-1	SER	-	expression tag	UNP A0A7Z9AX30
G	0	GLY	-	expression tag	UNP A0A7Z9AX30

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	99	Total	C	N	O	S	Se	0	0	0
			639	402	107	128	1	1			

There are 12 discrepancies between the modelled and reference sequences:

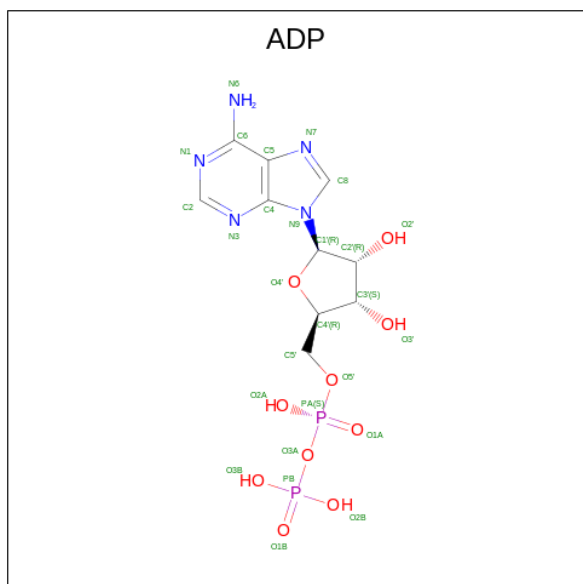
Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	-	expression tag	UNP A0A1V8XC17
H	105	GLY	-	expression tag	UNP A0A1V8XC17
H	106	PRO	-	expression tag	UNP A0A1V8XC17
H	107	SER	-	expression tag	UNP A0A1V8XC17
H	108	SER	-	expression tag	UNP A0A1V8XC17
H	109	GLY	-	expression tag	UNP A0A1V8XC17
H	110	GLU	-	expression tag	UNP A0A1V8XC17
H	111	ASN	-	expression tag	UNP A0A1V8XC17
H	112	LEU	-	expression tag	UNP A0A1V8XC17
H	113	TYR	-	expression tag	UNP A0A1V8XC17
H	114	PHE	-	expression tag	UNP A0A1V8XC17
H	115	GLN	-	expression tag	UNP A0A1V8XC17

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

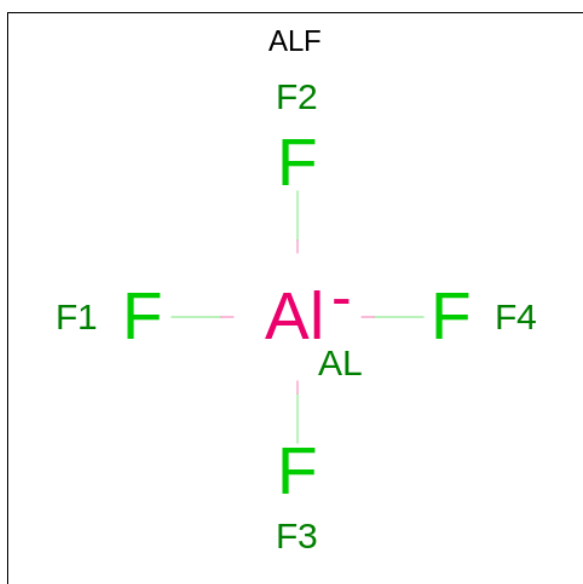


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 8 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Al	F	0	0
			5	1	4		
8	C	1	Total	Al	F	0	0
			5	1	4		

- Molecule 9 is water.

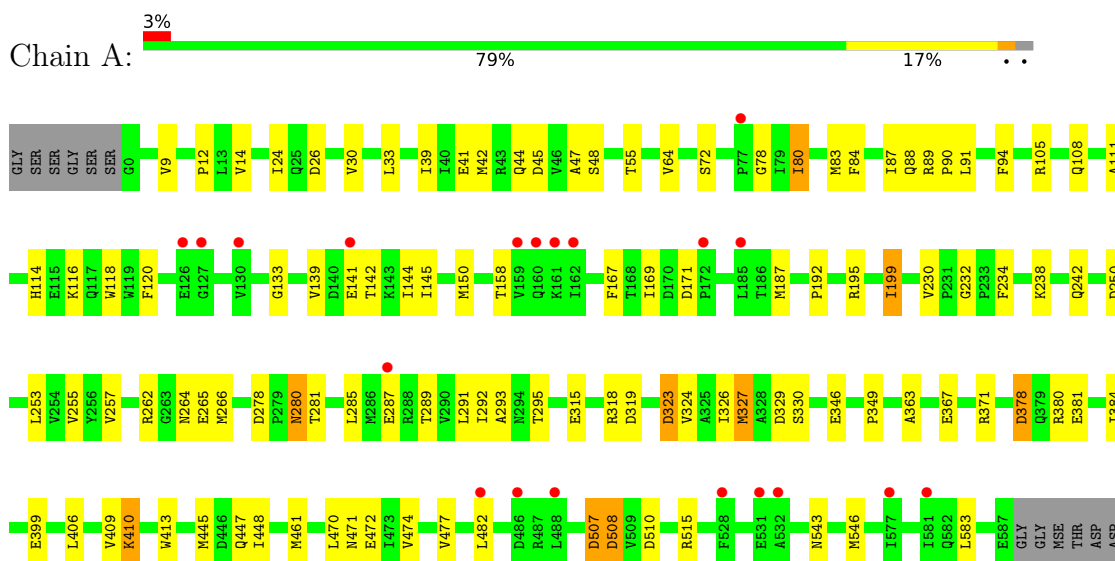
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O	0	0
			1	1		



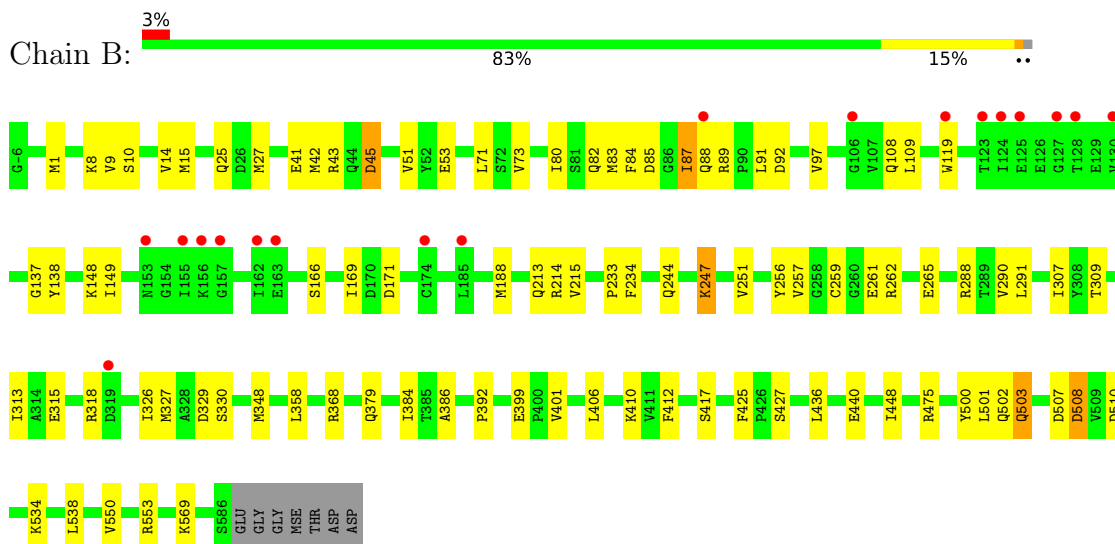
### 3 Residue-property plots [i](#)

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.

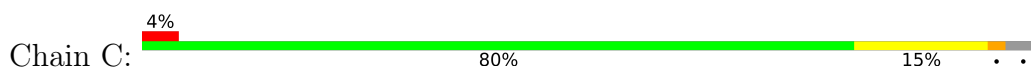
#### • Molecule 1: V-type sodium ATPase catalytic subunit A

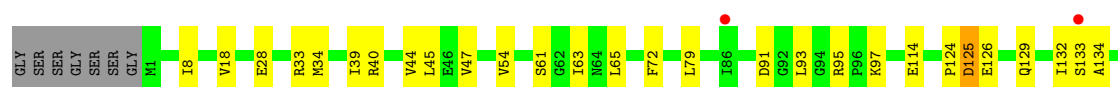


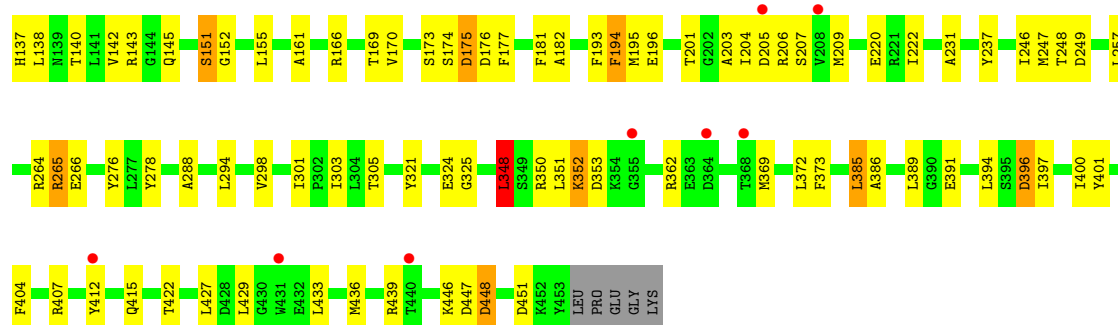
#### • Molecule 1: V-type sodium ATPase catalytic subunit A



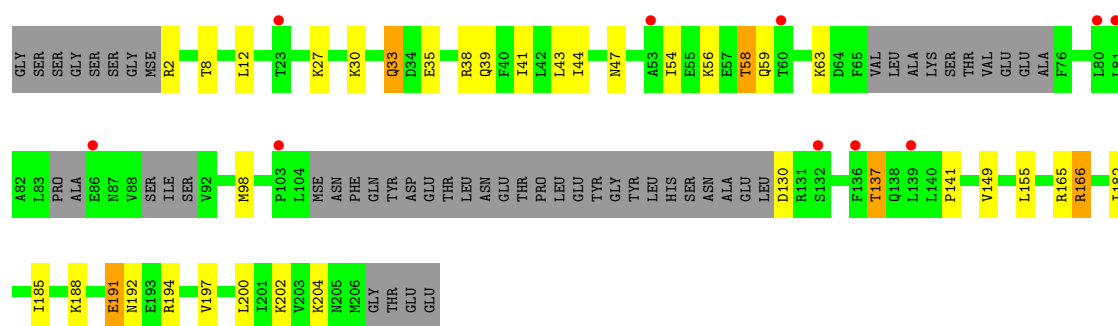
#### • Molecule 1: V-type sodium ATPase catalytic subunit A



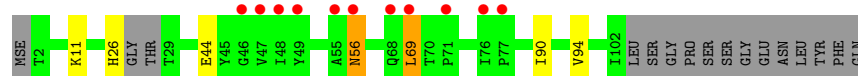
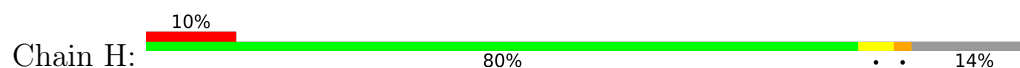




• Molecule 3: V-type sodium ATPase subunit D



• 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, $\alpha$ , $\beta$ , $\gamma$	127.74Å 128.87Å 231.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 3.82 46.13 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.13-3.82) 99.5 (46.13-3.82)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, $R_{free}$	0.226 , 0.267 0.226 , 0.267	Depositor DCC
$R_{free}$ test set	1884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.1	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 107.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	25072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: ALF, GOL, ADP, 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	0.24	0/4373	0.42	0/5921
1	B	0.25	0/4422	0.43	0/5974
1	C	0.25	0/4271	0.42	0/5774
2	D	0.25	0/3423	0.43	0/4628
2	E	0.26	0/3472	0.44	0/4693
2	F	0.26	0/3492	0.46	1/4715 (0.0%)
3	G	0.24	0/1204	0.41	0/1612
4	H	0.25	0/645	0.45	0/887
All	All	0.25	0/25302	0.43	1/34204 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	348	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4320	0	4062	68	0
1	B	4370	0	4075	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4220	0	3737	58	0
2	D	3375	0	3136	50	0
2	E	3423	0	3194	52	0
2	F	3445	0	3355	83	0
3	G	1207	0	1119	23	0
4	H	639	0	539	6	0
5	A	6	0	8	0	0
6	B	27	0	12	2	0
6	C	27	0	12	3	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	5	0	0	3	0
8	C	5	0	0	0	0
9	B	1	0	0	0	0
All	All	25072	0	23249	360	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 7.

The worst 5 of 360 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:MSE:HG2	2:E:65:LEU:HD21	1.49	0.93
1:C:509:VAL:HG11	1:C:561:TYR:HA	1.53	0.88
2:F:195:MSE:HA	2:F:195:MSE:HE2	1.57	0.87
2:F:385:LEU:HB3	2:F:394:LEU:HD21	1.65	0.79
1:B:214:ARG:NH1	1:B:510:ASP:OD1	2.16	0.78

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%)	568 (97%)	18 (3%)	0	100	100
1	B	591/600 (98%)	575 (97%)	16 (3%)	0	100	100
1	C	577/600 (96%)	560 (97%)	17 (3%)	0	100	100
2	D	450/465 (97%)	438 (97%)	12 (3%)	0	100	100
2	E	450/465 (97%)	438 (97%)	12 (3%)	0	100	100
2	F	451/465 (97%)	441 (98%)	10 (2%)	0	100	100
3	G	155/217 (71%)	153 (99%)	2 (1%)	0	100	100
4	H	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
All	All	3355/3527 (95%)	3262 (97%)	93 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	437/487 (90%)	414 (95%)	23 (5%)	22	54
1	B	437/487 (90%)	419 (96%)	18 (4%)	30	59
1	C	394/487 (81%)	366 (93%)	28 (7%)	14	45
2	D	313/372 (84%)	299 (96%)	14 (4%)	27	57
2	E	324/372 (87%)	307 (95%)	17 (5%)	23	54
2	F	349/372 (94%)	326 (93%)	23 (7%)	16	47
3	G	111/188 (59%)	97 (87%)	14 (13%)	4	23
4	H	53/97 (55%)	50 (94%)	3 (6%)	20	52
All	All	2418/2862 (84%)	2278 (94%)	140 (6%)	20	51

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	352	LYS
2	F	396	ASP

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Mol	Chain	Res	Type
3	G	58	THR
1	C	304	GLU
1	C	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	280	ASN
2	F	129	GLN
3	G	47	ASN

### 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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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$
6	ADP	B	601	7	24,29,29	0.97	1 (4%)	29,45,45	1.48	5 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ALF	B	603	-	0,4,4	-	-	-		
5	GOL	A	601	-	5,5,5	0.89	0	5,5,5	1.13	0
8	ALF	C	603	-	0,4,4	-	-	-		
6	ADP	C	601	7	24,29,29	0.97	1 (4%)	29,45,45	1.39	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
6	ADP	B	601	7	-	3/12/32/32	0/3/3/3
5	GOL	A	601	-	-	0/4/4/4	-
6	ADP	C	601	7	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	ADP	C5-C4	2.53	1.47	1.40
6	C	601	ADP	C5-C4	2.51	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	ADP	C3'-C2'-C1'	3.20	105.79	100.98
6	B	601	ADP	N3-C2-N1	-3.13	123.79	128.68
6	C	601	ADP	N3-C2-N1	-3.09	123.84	128.68
6	B	601	ADP	PA-O3A-PB	-3.07	122.31	132.83
6	C	601	ADP	PA-O3A-PB	-3.04	122.41	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

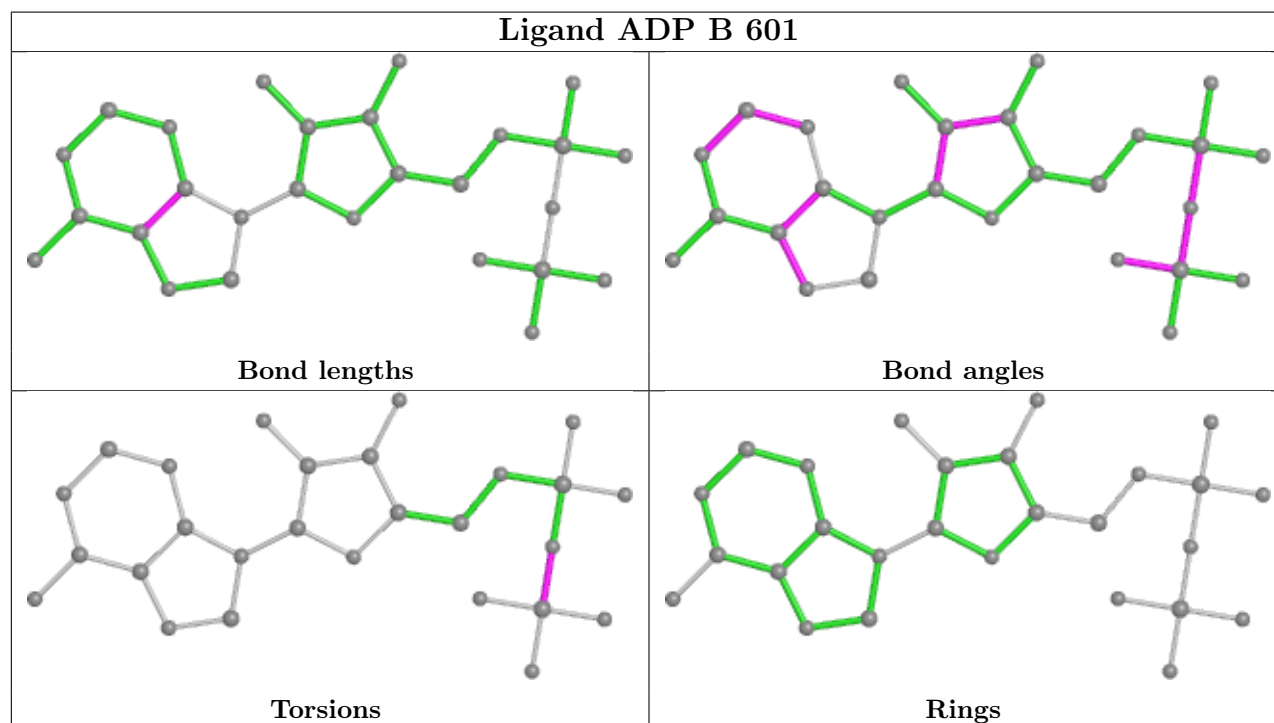
Mol	Chain	Res	Type	Atoms
6	B	601	ADP	PA-O3A-PB-O2B
6	C	601	ADP	PA-O3A-PB-O2B
6	B	601	ADP	PA-O3A-PB-O1B
6	C	601	ADP	PA-O3A-PB-O1B
6	B	601	ADP	PA-O3A-PB-O3B

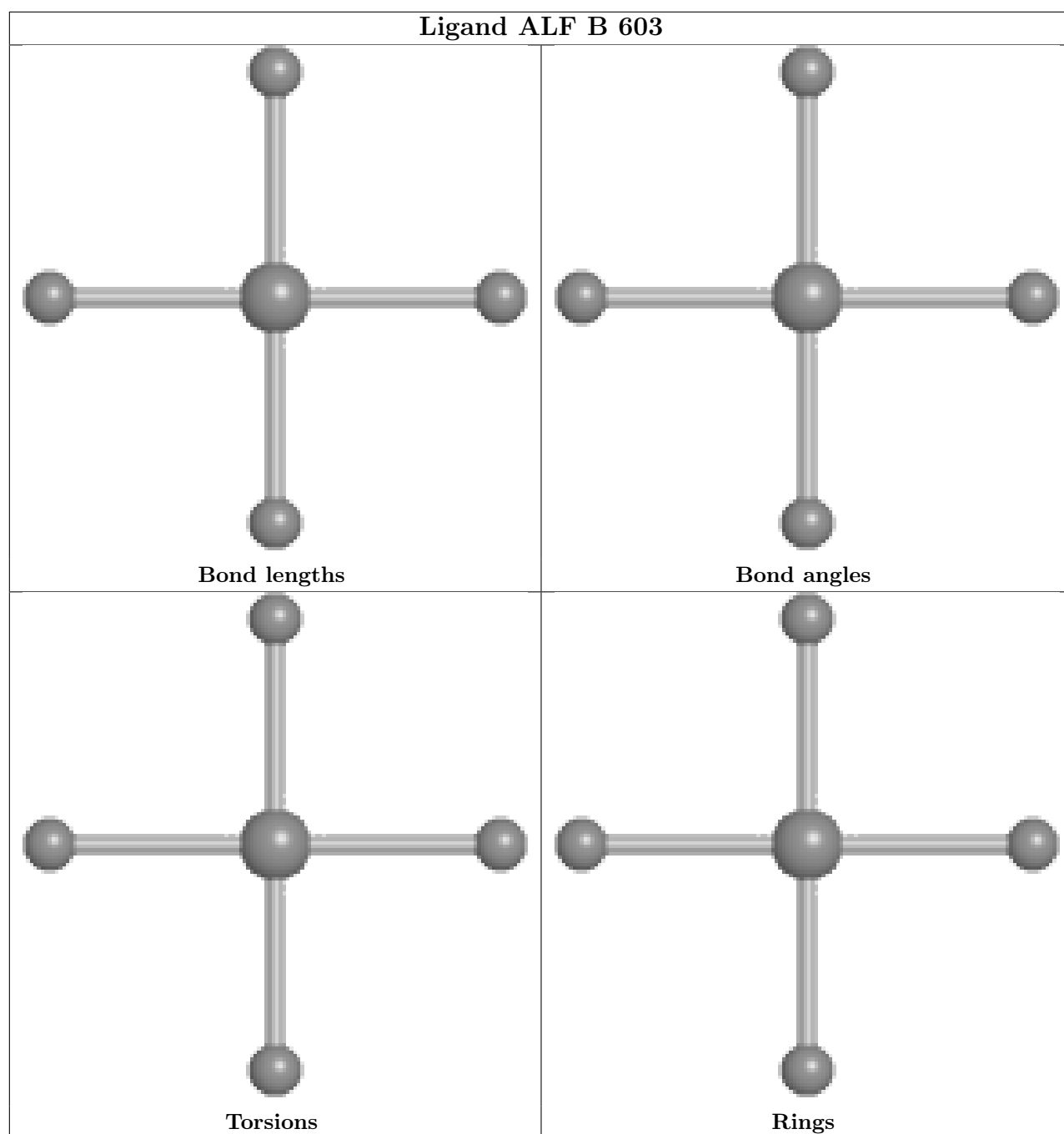
There are no ring outliers.

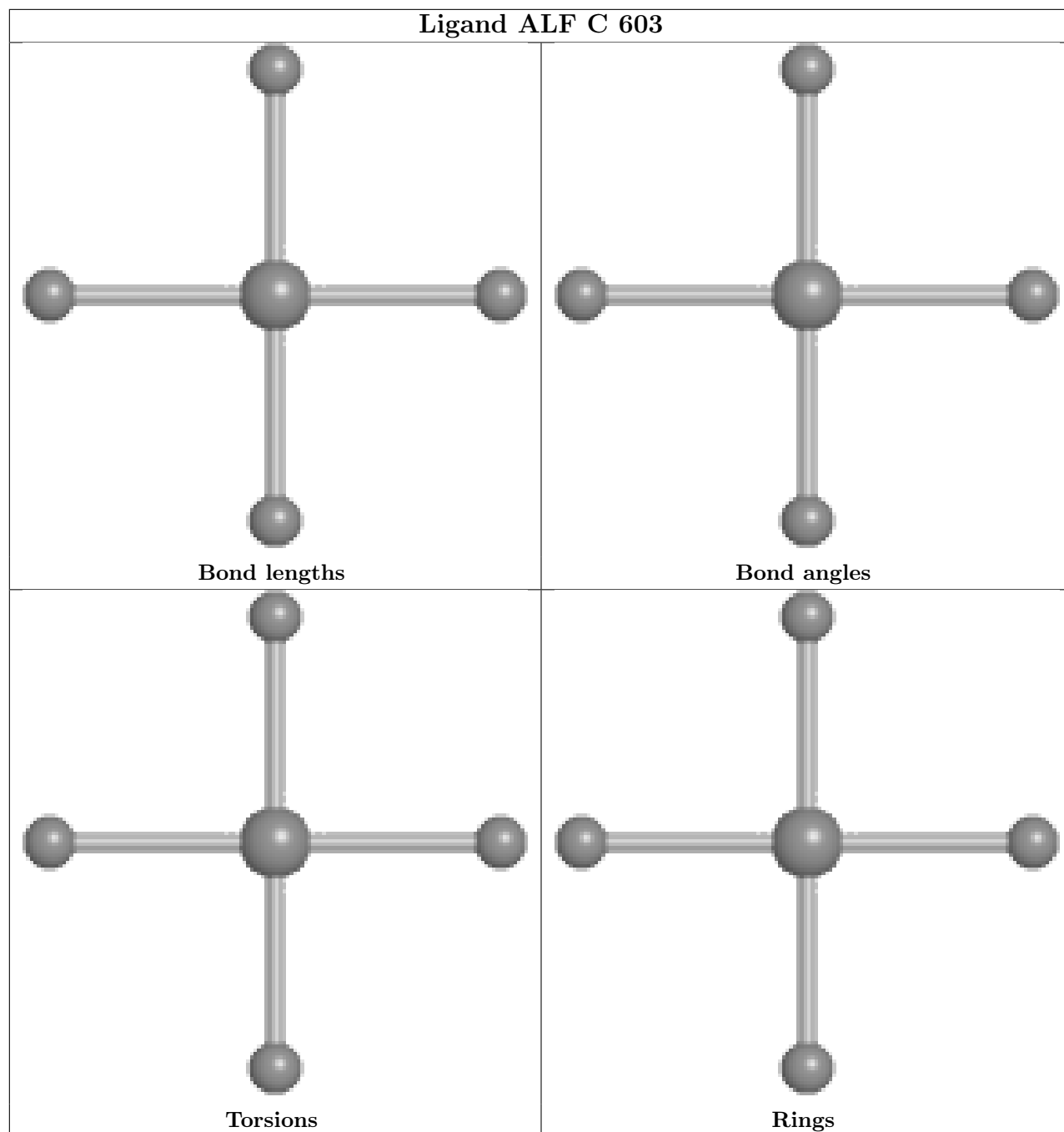
3 monomers are involved in 7 short contacts:

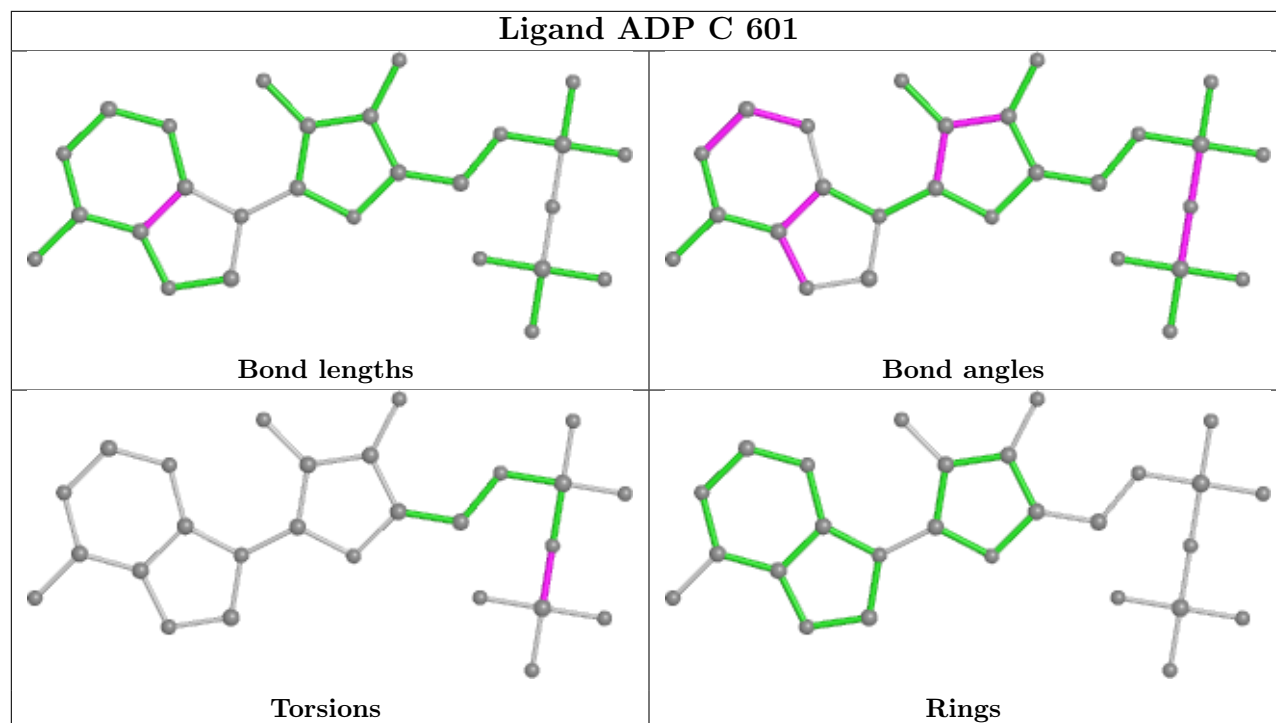
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	ADP	2	0
8	B	603	ALF	3	0
6	C	601	ADP	3	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	565/600 (94%)	0.03	20 (3%)	44	35	83, 140, 192, 219	0
1	B	570/600 (95%)	0.10	18 (3%)	47	38	82, 142, 215, 264	0
1	C	556/600 (92%)	0.10	23 (4%)	37	31	99, 150, 229, 266	0
2	D	438/465 (94%)	-0.10	2 (0%)	91	86	84, 138, 201, 228	0
2	E	438/465 (94%)	-0.15	7 (1%)	72	64	70, 122, 169, 218	0
2	F	438/465 (94%)	-0.01	10 (2%)	60	52	87, 151, 218, 240	0
3	G	157/217 (72%)	0.29	10 (6%)	19	14	97, 164, 282, 304	0
4	H	98/115 (85%)	0.62	11 (11%)	5	5	108, 221, 271, 277	0
All	All	3260/3527 (92%)	0.04	101 (3%)	49	39	70, 142, 221, 304	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	5.9
2	F	364	ASP	5.3
1	B	174	CYS	4.7
1	B	125	GLU	4.5
1	C	174	CYS	4.5

### 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 ⓘ

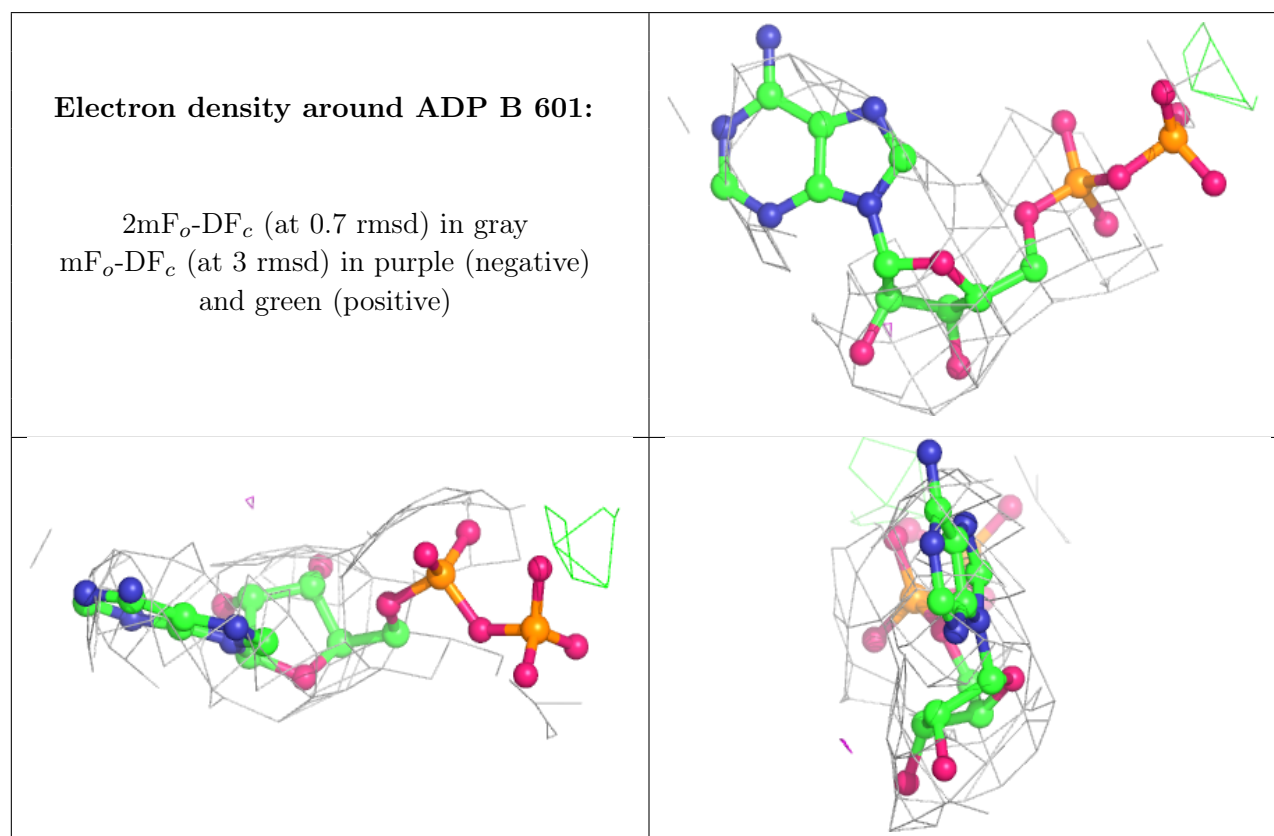
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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.

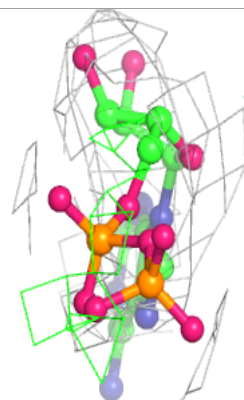
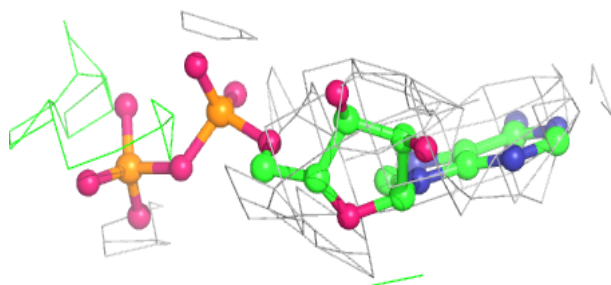
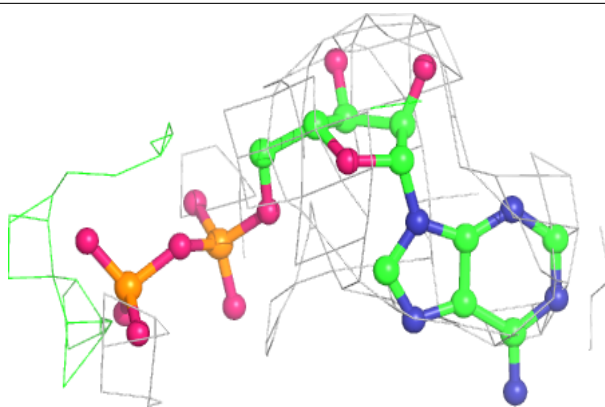
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	601	6/6	0.80	0.57	101,108,117,121	0
6	ADP	B	601	27/27	0.91	0.30	78,107,126,134	0
6	ADP	C	601	27/27	0.91	0.32	95,127,151,162	0
7	MG	C	602	1/1	0.91	0.70	144,144,144,144	0
8	ALF	C	603	5/5	0.91	0.52	101,110,129,135	0
8	ALF	B	603	5/5	0.93	0.41	111,112,155,160	0
7	MG	B	602	1/1	0.98	0.47	76,76,76,76	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 ADP C 601:**

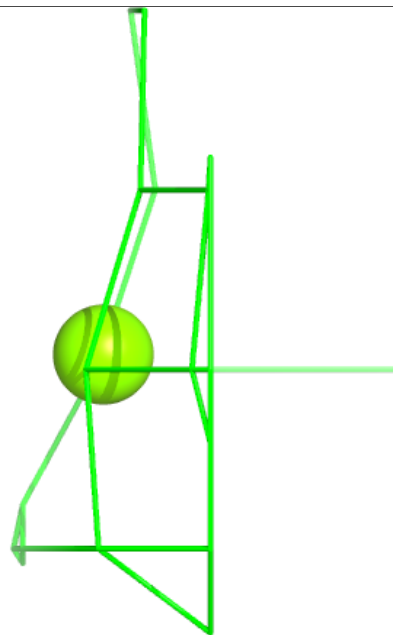
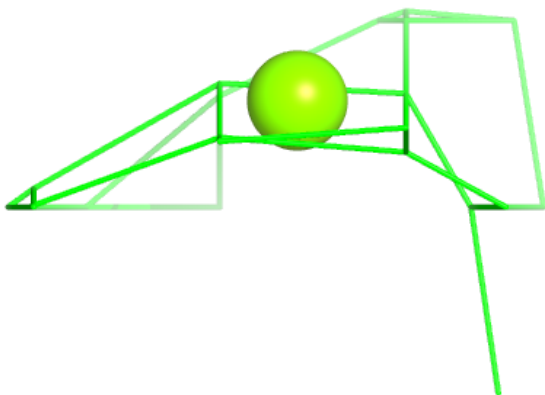
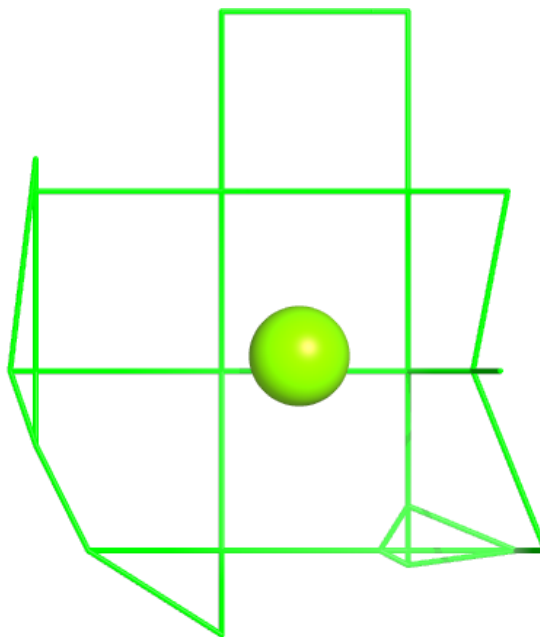
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





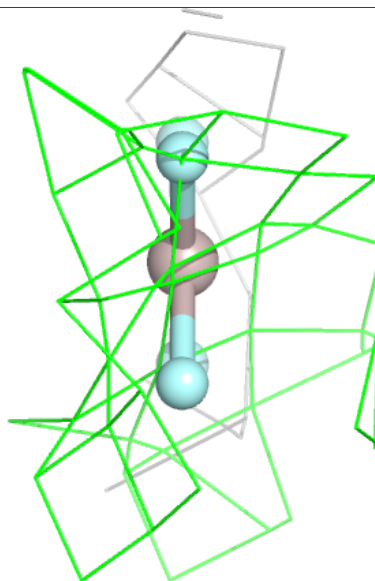
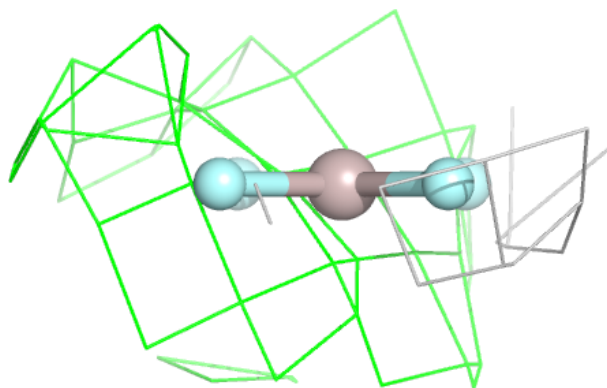
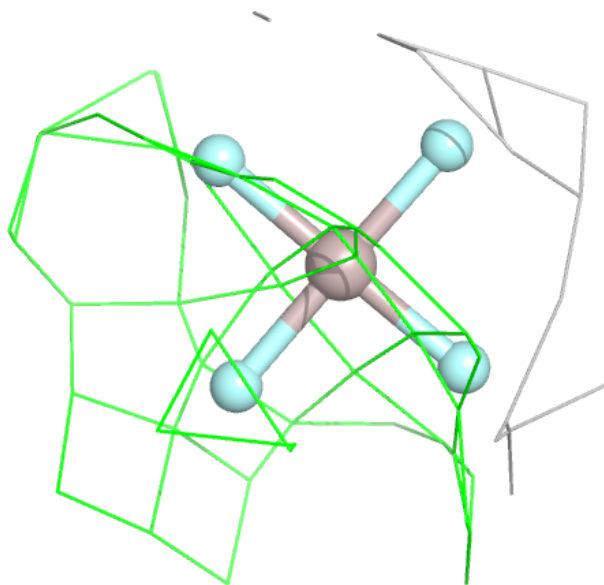
**Electron density around MG C 602:**

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



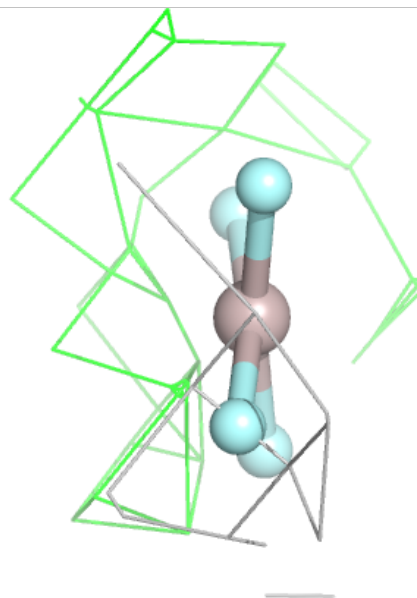
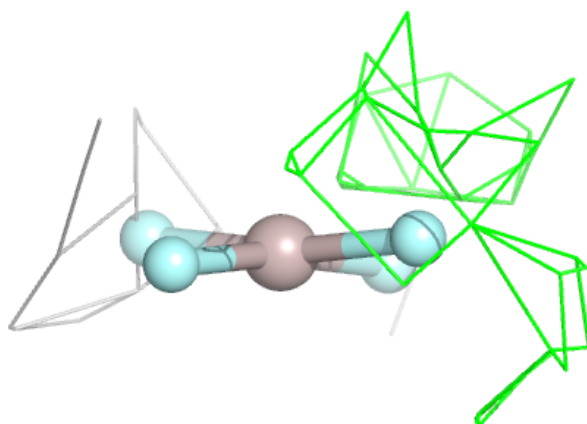
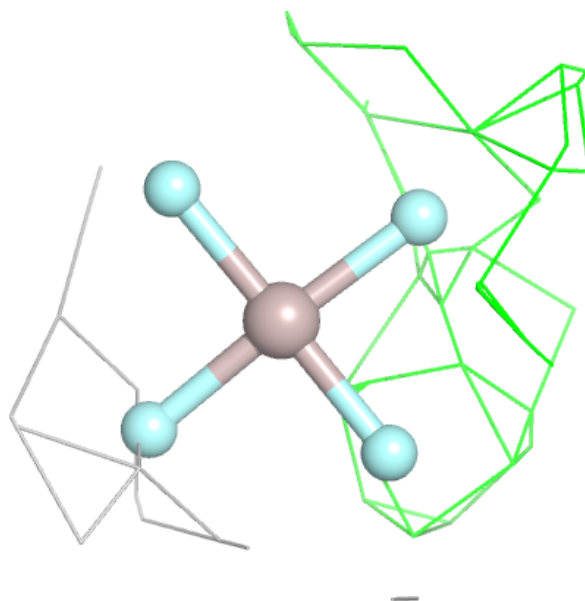
**Electron density around ALF C 603:**

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



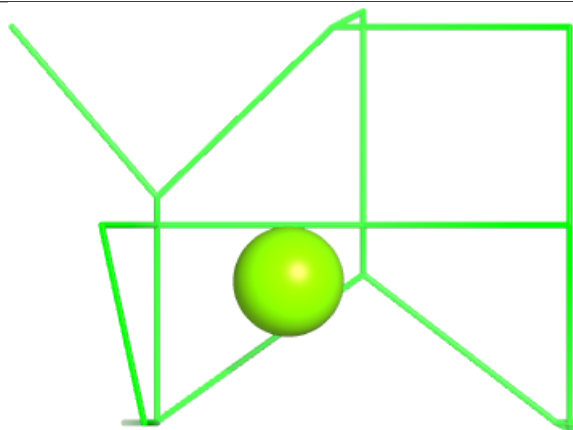
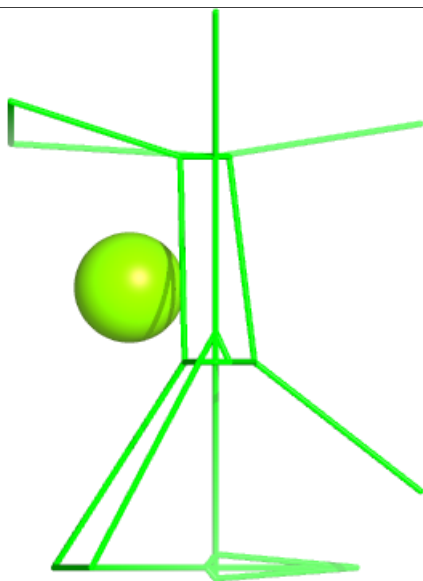
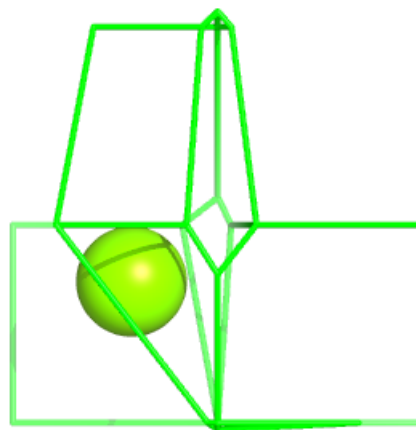
**Electron density around ALF B 603:**

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



**Electron density around MG B 602:**

$2mF_o-DF_c$  (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.