Full wwPDB X-ray Structure Validation Report (i)

Mar 28, 2023 – 01:53 PM JST

PDB ID	:	8IPW
Title	:	The sturecture of Legionella effector protein MavL with ADPR
Deposited on	:	2023-03-15
Resolution	:	2.35 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) 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	:	2.32.2
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)

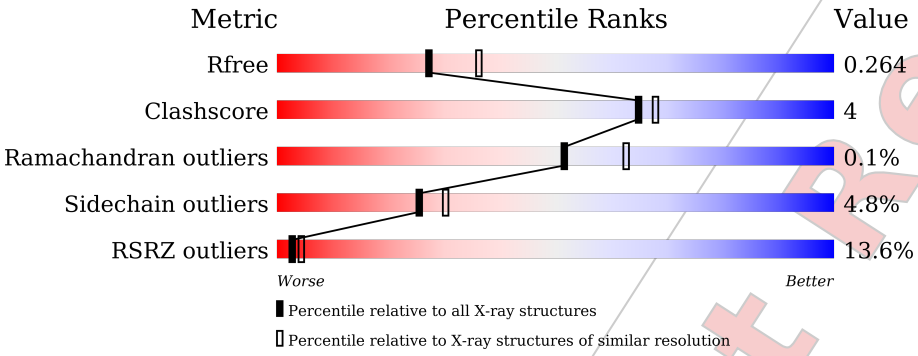
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1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	363	10% 88% 11%
1	B	363	17% 83% 15%

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2 Entry composition (i)

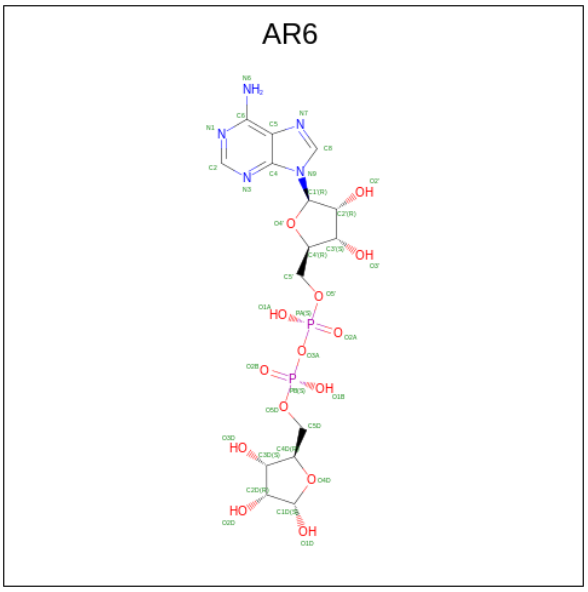
There are 3 unique types of molecules in this entry. The entry contains 5684 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MavL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2796	1781	464	541	10			
1	B	361	Total	C	N	O	S	0	0	0
			2801	1779	471	541	10			

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: $C_{15}H_{23}N_5O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is water.

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	6	Total O 6 6	0	0

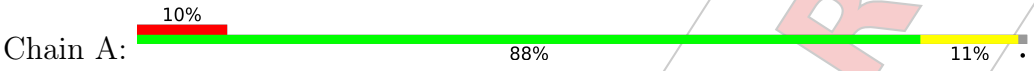
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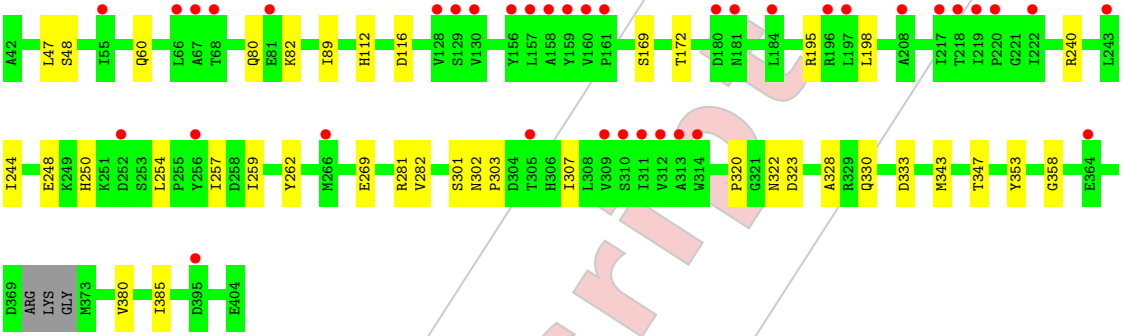
3 Residue-property plots (i)

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: MavL

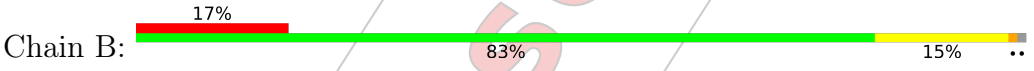
Chain A:

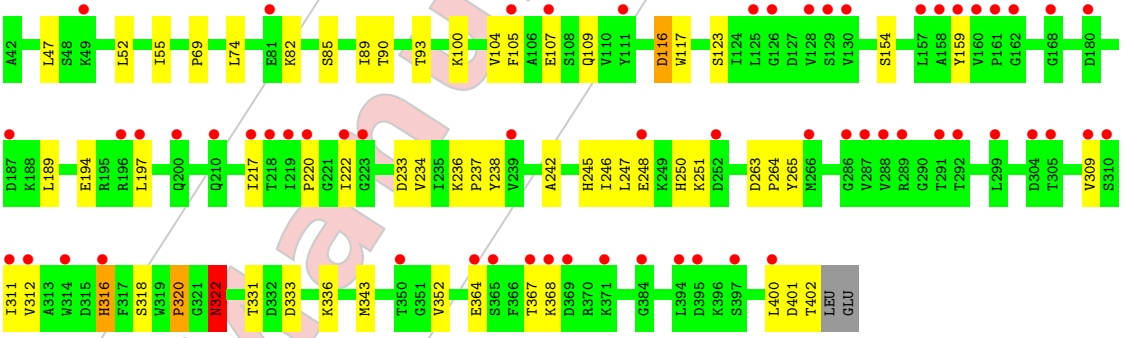




- Molecule 1: MavL

Chain B:





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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.79Å 108.32Å 129.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.24 – 2.35 25.24 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.24-2.35) 98.4 (25.24-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.36Å)	Xtriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
R, R_{free}	0.209 , 0.257 0.219 , 0.264	Depositor DCC
R_{free} test set	1998 reflections (6.63%)	wwPDB-VP
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5684	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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.

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5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AR6

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	0.44	0/2865	0.62	0/3889
1	B	0.41	0/2870	0.63	2/3895 (0.1%)
All	All	0.43	0/5735	0.62	2/7784 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	367	THR	CB-CA-C	-5.87	95.75	111.60
1	B	320	PRO	N-CA-C	5.13	125.44	112.10

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	2796	0	2709	13	0
1	B	2801	0	2708	31	0
2	A	36	0	19	1	0
2	B	36	0	19	3	0
3	A	9	0	0	0	0
3	B	6	0	0	0	0
All	All	5684	0	5455	46	0

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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 4.

All (46) 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)
2:A:501:AR6:C1D	2:A:501:AR6:O4D	1.66	1.29
2:B:501:AR6:C1D	2:B:501:AR6:O4D	1.64	1.16
1:B:55:ILE:HG21	1:B:93:THR:OG1	1.85	0.76
1:B:364:GLU:O	1:B:368:LYS:HG2	1.88	0.73
1:A:262:TYR:HD2	1:A:282:VAL:HG22	1.57	0.69
1:B:400:LEU:HG	1:B:401:ASP:H	1.58	0.67
1:B:100:LYS:HE3	1:B:316:HIS:O	1.95	0.66
1:B:352:VAL:HG21	1:B:364:GLU:HG3	1.75	0.66
1:B:159:TYR:CE2	1:B:320:PRO:O	2.50	0.65
1:B:52:LEU:HD13	1:B:402:THR:HG23	1.79	0.65
1:B:52:LEU:CD1	1:B:402:THR:HG23	2.30	0.60
1:A:240:ARG:O	1:A:244:ILE:HG12	2.01	0.60
1:A:328:ALA:HB1	1:A:330:GLN:HG3	1.83	0.60
1:B:320:PRO:O	1:B:333:ASP:OD1	2.20	0.59
1:B:242:ALA:O	1:B:246:ILE:HG12	2.03	0.59
1:A:259:ILE:HD12	1:A:301:SER:HB3	1.85	0.56
1:B:69:PRO:HG2	1:B:74:LEU:HD13	1.90	0.54
1:B:400:LEU:HG	1:B:401:ASP:N	2.23	0.54
1:B:189:LEU:HD23	1:B:238:TYR:HB3	1.90	0.53
1:B:233:ASP:HA	1:B:236:LYS:NZ	2.25	0.52
1:A:254:LEU:HB3	1:A:257:ILE:HD12	1.92	0.52
1:B:234:VAL:O	1:B:237:PRO:HD2	2.10	0.51
1:B:100:LYS:HE2	1:B:318:SER:O	2.11	0.50
1:A:302:ASN:HB2	1:A:303:PRO:HD2	1.94	0.49
1:A:198:LEU:HD22	1:A:250:HIS:NE2	2.28	0.49
1:B:245:HIS:HA	1:B:248:GLU:HG2	1.93	0.49
1:B:55:ILE:HG21	1:B:93:THR:HG1	1.79	0.48
1:B:104:VAL:H	1:B:322:ASN:HD21	1.62	0.48
1:B:194:GLU:OE2	1:B:250:HIS:HE1	1.97	0.47
1:B:116:ASP:HB2	1:B:117:TRP:CE3	2.49	0.47
1:B:55:ILE:HG22	1:B:89:ILE:HD11	1.96	0.47
1:A:347:THR:HB	1:A:385:ILE:HD13	1.97	0.47
1:A:320:PRO:O	1:A:333:ASP:OD1	2.33	0.47
1:B:312:VAL:HG22	1:B:336:LYS:HD3	1.96	0.47
1:B:222:ILE:HD11	1:B:311:ILE:HG22	1.98	0.46
1:B:220:PRO:HD3	1:B:311:ILE:O	2.17	0.44
1:B:331:THR:HG21	2:B:501:AR6:H1D	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:HIS:CE1	1:A:172:THR:HG22	2.52	0.44
1:B:233:ASP:HA	1:B:236:LYS:HZ1	1.82	0.44
1:A:353:TYR:OH	1:A:358:GLY:HA2	2.18	0.43
1:A:48:SER:OG	1:A:195:ARG:HG2	2.18	0.42
1:A:262:TYR:CD2	1:A:282:VAL:HG22	2.46	0.42
1:B:217:ILE:HA	1:B:309:VAL:O	2.19	0.42
1:B:263:ASP:OD1	1:B:264:PRO:O	2.37	0.42
1:B:265:TYR:HB2	2:B:501:AR6:H1'	2.01	0.41
1:B:247:LEU:O	1:B:251:LYS:HB3	2.22	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	356/363 (98%)	347 (98%)	9 (2%)	0	100 100
1	B	359/363 (99%)	344 (96%)	14 (4%)	1 (0%)	41 47
All	All	715/726 (98%)	691 (97%)	23 (3%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	ASN

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

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analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/309 (97%)	286 (95%)	15 (5%)	24	28
1	B	299/309 (97%)	285 (95%)	14 (5%)	26	31
All	All	600/618 (97%)	571 (95%)	29 (5%)	25	30

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	60	GLN
1	A	80	GLN
1	A	82	LYS
1	A	89	ILE
1	A	116	ASP
1	A	169	SER
1	A	248	GLU
1	A	269	GLU
1	A	281	ARG
1	A	307	ILE
1	A	322	ASN
1	A	323	ASP
1	A	343	MET
1	A	380	VAL
1	B	47	LEU
1	B	82	LYS
1	B	85	SER
1	B	90	THR
1	B	105	PHE
1	B	107	GLU
1	B	109	GLN
1	B	116	ASP
1	B	123	SER
1	B	154	SER
1	B	197	LEU
1	B	316	HIS
1	B	322	ASN
1	B	343	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

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Mol	Chain	Res	Type
1	A	302	ASN
1	A	322	ASN
1	A	345	GLN
1	B	109	GLN
1	B	250	HIS
1	B	322	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AR6	B	501	-	34,39,39	5.55	12 (35%)	40,60,60	2.18	7 (17%)
2	AR6	A	501	-	34,39,39	5.53	13 (38%)	40,60,60	2.41	7 (17%)

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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AR6	B	501	-	-	1/18/54/54	0/4/4/4
2	AR6	A	501	-	-	2/18/54/54	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AR6	O4D-C1D	19.00	1.66	1.43
2	B	501	AR6	O4D-C1D	17.87	1.64	1.43
2	B	501	AR6	C1D-C2D	-15.43	1.34	1.52
2	A	501	AR6	O4'-C1'	13.30	1.59	1.41
2	A	501	AR6	C1D-C2D	-12.99	1.37	1.52
2	A	501	AR6	C2'-C1'	-12.94	1.34	1.53
2	B	501	AR6	C2'-C1'	-12.85	1.34	1.53
2	B	501	AR6	O4'-C1'	12.49	1.58	1.41
2	A	501	AR6	C3'-C4'	-5.88	1.38	1.53
2	B	501	AR6	C3'-C4'	-5.81	1.38	1.53
2	B	501	AR6	O4D-C4D	-5.68	1.32	1.45
2	A	501	AR6	O4D-C4D	-5.64	1.32	1.45
2	B	501	AR6	O3D-C3D	-4.78	1.31	1.43
2	B	501	AR6	O4'-C4'	4.55	1.55	1.45
2	A	501	AR6	O3D-C3D	-4.29	1.32	1.43
2	A	501	AR6	O4'-C4'	4.28	1.54	1.45
2	B	501	AR6	C5-C4	-3.36	1.32	1.40
2	A	501	AR6	C5-C4	-3.21	1.32	1.40
2	A	501	AR6	C6-N6	3.02	1.45	1.34
2	A	501	AR6	C3'-C2'	2.99	1.61	1.53
2	B	501	AR6	C6-N6	2.98	1.44	1.34
2	B	501	AR6	C3'-C2'	2.96	1.61	1.53
2	A	501	AR6	O2D-C2D	2.87	1.49	1.43
2	A	501	AR6	C3D-C4D	2.79	1.60	1.53
2	B	501	AR6	O2D-C2D	2.05	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	AR6	C5-C6-N6	10.00	135.56	120.35
2	B	501	AR6	C5-C6-N6	9.05	134.10	120.35
2	A	501	AR6	N6-C6-N1	-6.92	104.22	118.57
2	B	501	AR6	N6-C6-N1	-6.04	106.03	118.57
2	A	501	AR6	N3-C2-N1	-5.72	119.73	128.68
2	B	501	AR6	N3-C2-N1	-4.91	121.01	128.68
2	A	501	AR6	O1D-C1D-O4D	-3.06	107.21	111.13
2	B	501	AR6	O4'-C1'-C2'	-3.04	102.48	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	AR6	C2'-C3'-C4'	2.73	107.95	102.64
2	A	501	AR6	C1'-N9-C4	-2.61	122.05	126.64
2	A	501	AR6	C3'-C2'-C1'	2.09	104.12	100.98
2	B	501	AR6	O3D-C3D-C4D	-2.04	105.14	111.05
2	B	501	AR6	C1'-N9-C4	-2.04	123.06	126.64
2	B	501	AR6	C5D-C4D-C3D	-2.02	107.60	115.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AR6	PB-O3A-PA-O2A
2	B	501	AR6	C3D-C4D-C5D-O5D
2	A	501	AR6	PB-O3A-PA-O1A

There are no ring outliers.

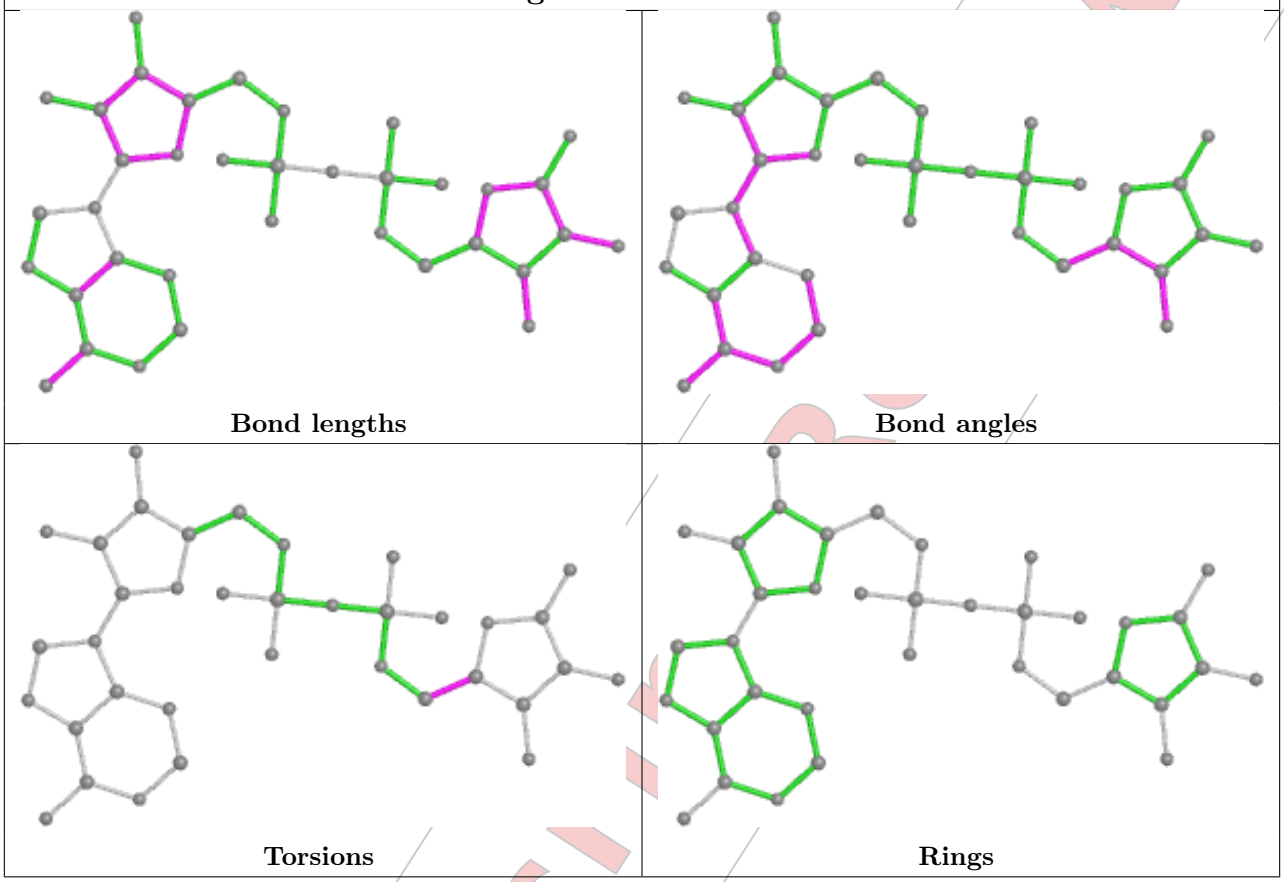
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	AR6	3	0
2	A	501	AR6	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.

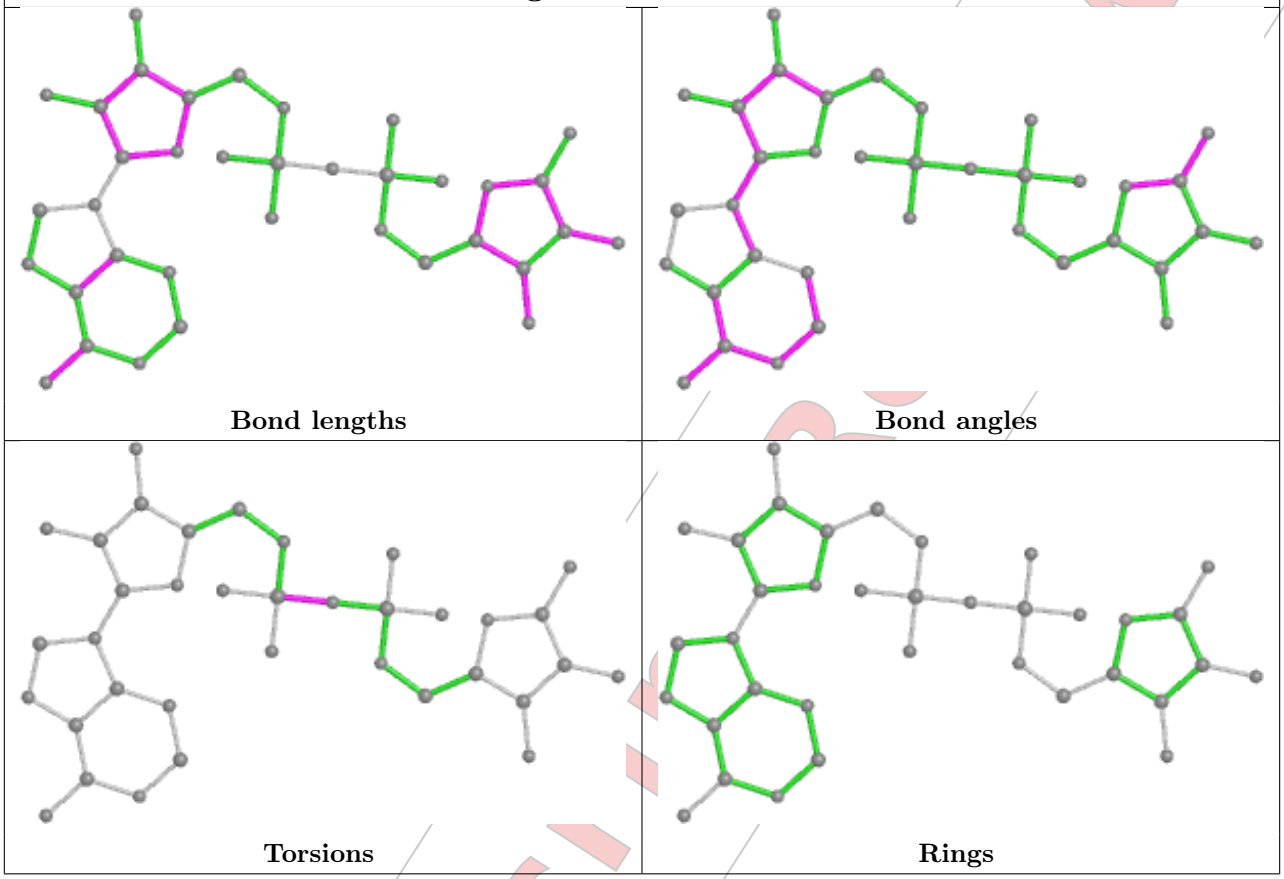
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Ligand AR6 B 501



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Ligand AR6 A 501



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.

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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	360/363 (99%)	0.56	38 (10%)	6	9	47, 71, 92, 105	0
1	B	361/363 (99%)	0.84	60 (16%)	1	2	51, 76, 98, 114	0
All	All	721/726 (99%)	0.70	98 (13%)	3	4	47, 73, 95, 114	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	PHE	7.4
1	B	311	ILE	7.1
1	A	256	TYR	5.9
1	A	311	ILE	5.7
1	A	160	VAL	5.7
1	B	125	LEU	5.2
1	B	160	VAL	5.0
1	A	222	ILE	4.7
1	B	309	VAL	4.6
1	A	180	ASP	4.6
1	A	66	LEU	4.3
1	B	288	VAL	4.1
1	B	367	THR	4.0
1	B	310	SER	4.0
1	A	181	ASN	3.9
1	A	312	VAL	3.9
1	B	219	ILE	3.9
1	A	252	ASP	3.9
1	B	395	ASP	3.9
1	A	219	ILE	3.9
1	B	161	PRO	3.8
1	B	266	MET	3.8
1	A	81	GLU	3.8
1	A	310	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	111	TYR	3.7
1	B	159	TYR	3.7
1	B	312	VAL	3.7
1	B	162	GLY	3.6
1	B	217	ILE	3.6
1	A	161	PRO	3.6
1	A	197	LEU	3.5
1	B	371	LYS	3.5
1	A	220	PRO	3.4
1	B	292	THR	3.4
1	A	157	LEU	3.3
1	B	168	GLY	3.3
1	B	220	PRO	3.3
1	B	397	SER	3.2
1	B	128	VAL	3.2
1	B	210	GLN	3.2
1	B	305	THR	3.1
1	B	158	ALA	3.1
1	B	369	ASP	3.1
1	A	67	ALA	3.1
1	B	316	HIS	3.1
1	B	157	LEU	3.1
1	B	394	LEU	3.1
1	A	158	ALA	3.1
1	B	222	ILE	3.1
1	B	248	GLU	3.0
1	B	291	THR	3.0
1	B	180	ASP	3.0
1	B	384	GLY	3.0
1	B	364	GLU	2.9
1	B	130	VAL	2.9
1	B	49	LYS	2.9
1	B	252	ASP	2.9
1	B	350	THR	2.8
1	B	287	VAL	2.7
1	A	395	ASP	2.7
1	A	218	THR	2.7
1	B	126	GLY	2.7
1	A	309	VAL	2.7
1	A	305	THR	2.6
1	A	314	TRP	2.5
1	B	368	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	130	VAL	2.5
1	B	218	THR	2.5
1	A	364	GLU	2.4
1	B	107	GLU	2.4
1	B	196	ARG	2.4
1	A	208	ALA	2.4
1	B	299	LEU	2.4
1	B	314	TRP	2.4
1	B	286	GLY	2.3
1	A	184	LEU	2.3
1	B	129	SER	2.3
1	B	289	ARG	2.3
1	A	313	ALA	2.3
1	B	400	LEU	2.3
1	A	129	SER	2.3
1	A	128	VAL	2.3
1	B	239	VAL	2.3
1	A	196	ARG	2.3
1	A	159	TYR	2.3
1	B	187	ASP	2.2
1	A	55	ILE	2.2
1	A	266	MET	2.2
1	B	200	GLN	2.2
1	A	217	ILE	2.2
1	B	304	ASP	2.2
1	A	156	TYR	2.1
1	B	365	SER	2.1
1	A	68	THR	2.1
1	A	243	LEU	2.1
1	B	197	LEU	2.1
1	B	81	GLU	2.0
1	B	223	GLY	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.

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6.4 Ligands

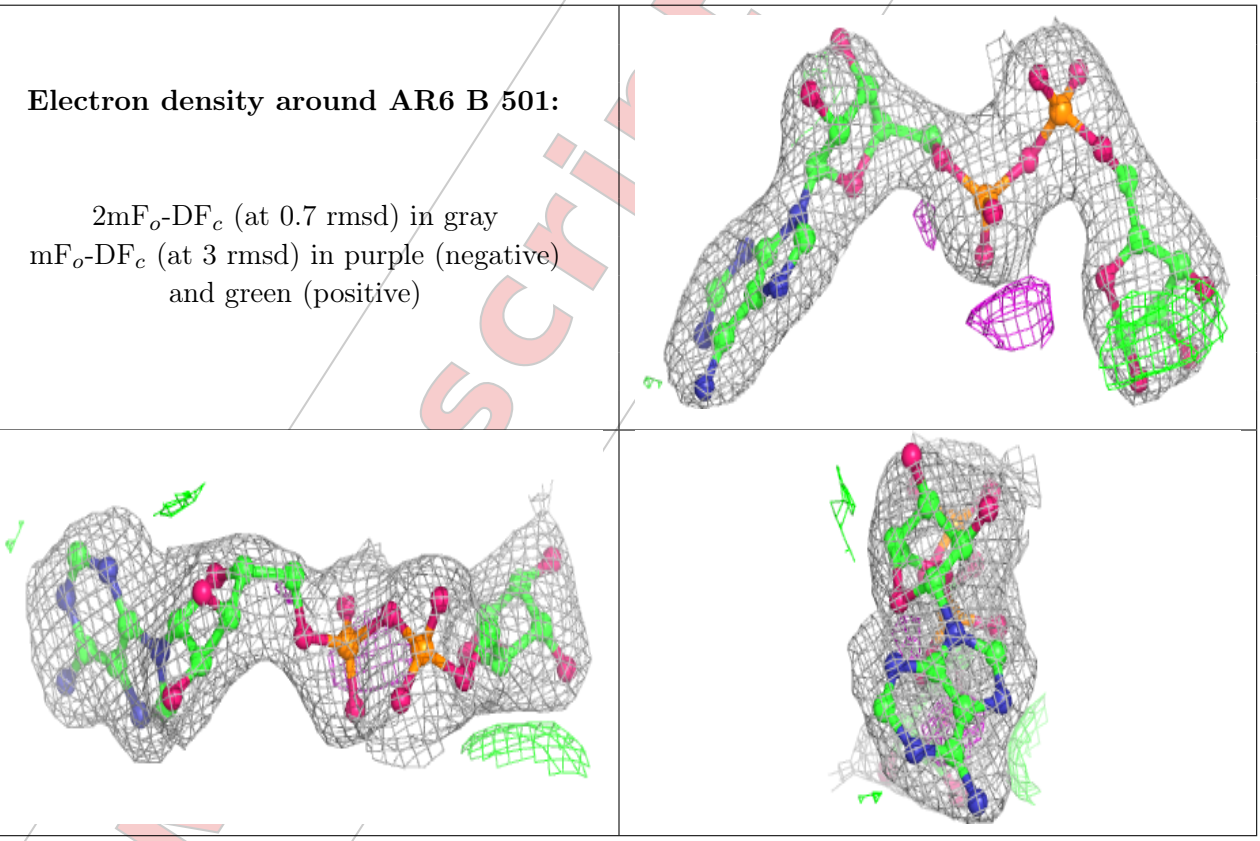
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	AR6	B	501	36/36	0.94	0.13	62,64,66,66	0
2	AR6	A	501	36/36	0.95	0.12	58,64,72,72	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 AR6 B 501:

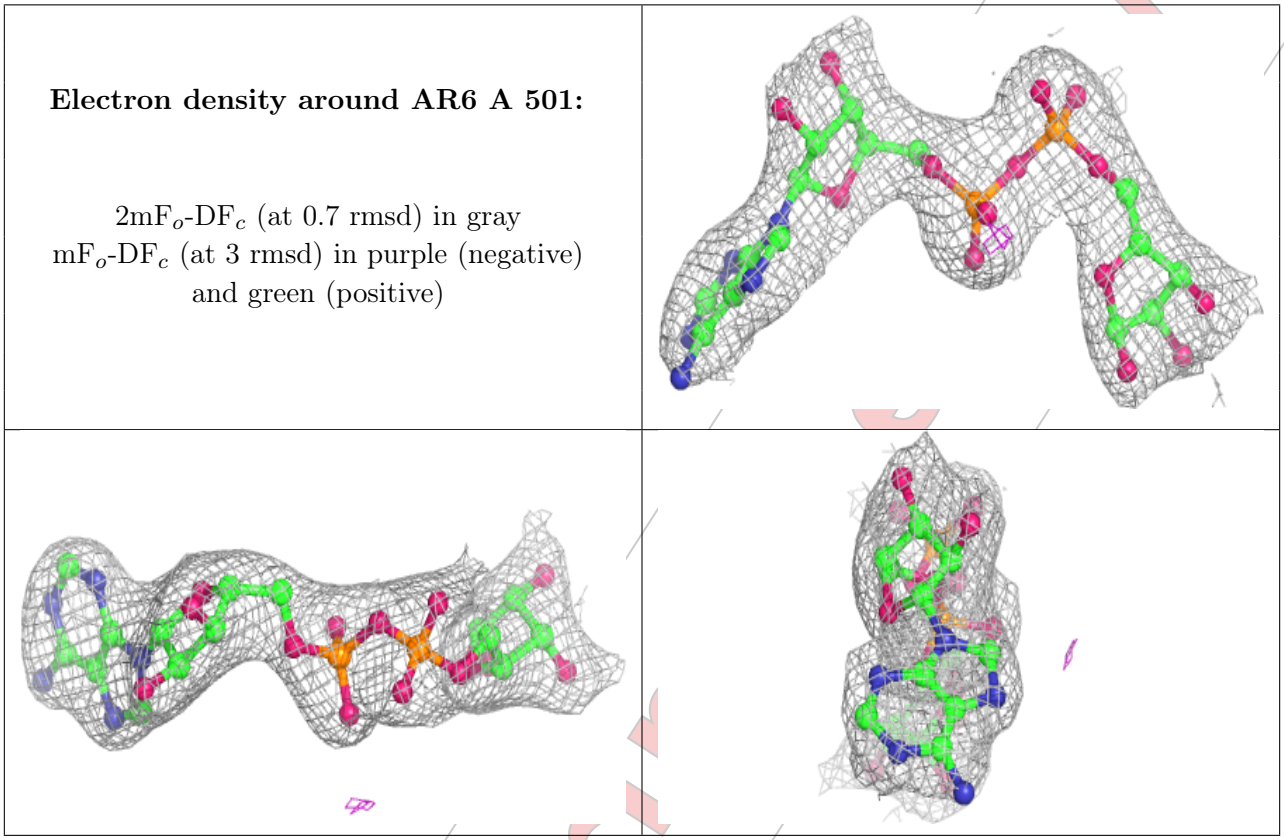
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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Electron density around AR6 A 501:

$2mF_o$-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.

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