Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2024 – 12:39 PM EDT

PDB ID	:	9CSI
Title	:	A. baumannii MsbA Bound to Cerastecin Compound 5
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Deposited on	:	2024-07-23
Resolution	:	2.80 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 (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:

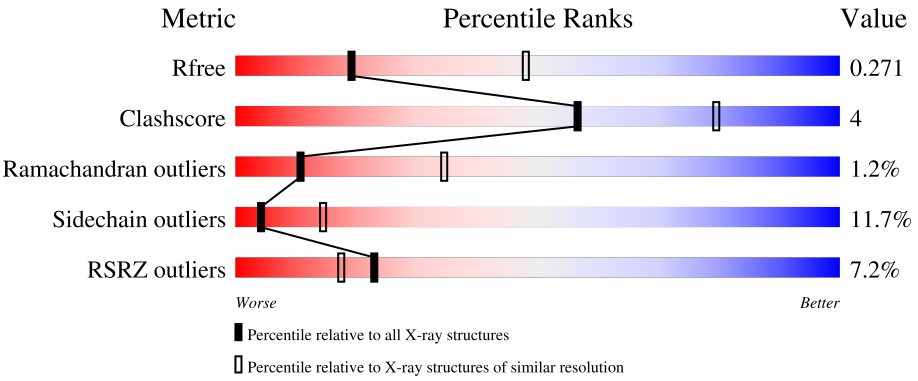
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	598	7% 77% 16% • 5%

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
3	MVC	A	602	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4619 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.

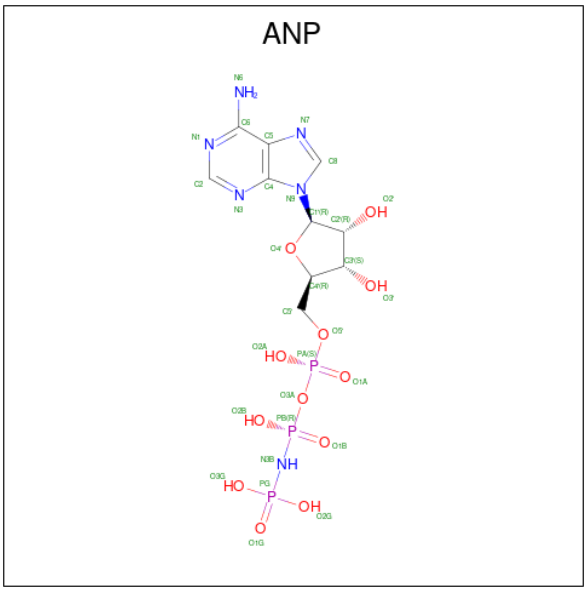
- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein MsbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	569	4452	2841	771	821	19	0	1	0

There are 23 discrepancies between the modelled and reference sequences:

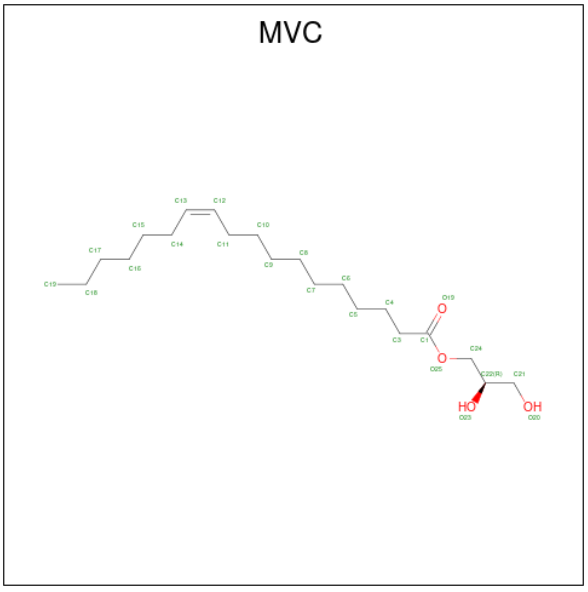
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0A6F8TGG1
A	-21	GLY	-	expression tag	UNP A0A6F8TGG1
A	-20	HIS	-	expression tag	UNP A0A6F8TGG1
A	-19	HIS	-	expression tag	UNP A0A6F8TGG1
A	-18	HIS	-	expression tag	UNP A0A6F8TGG1
A	-17	HIS	-	expression tag	UNP A0A6F8TGG1
A	-16	HIS	-	expression tag	UNP A0A6F8TGG1
A	-15	HIS	-	expression tag	UNP A0A6F8TGG1
A	-14	HIS	-	expression tag	UNP A0A6F8TGG1
A	-13	HIS	-	expression tag	UNP A0A6F8TGG1
A	-12	HIS	-	expression tag	UNP A0A6F8TGG1
A	-11	HIS	-	expression tag	UNP A0A6F8TGG1
A	-10	SER	-	expression tag	UNP A0A6F8TGG1
A	-9	SER	-	expression tag	UNP A0A6F8TGG1
A	-8	GLY	-	expression tag	UNP A0A6F8TGG1
A	-7	HIS	-	expression tag	UNP A0A6F8TGG1
A	-6	ILE	-	expression tag	UNP A0A6F8TGG1
A	-5	ASP	-	expression tag	UNP A0A6F8TGG1
A	-4	ASP	-	expression tag	UNP A0A6F8TGG1
A	-3	ASP	-	expression tag	UNP A0A6F8TGG1
A	-2	ASP	-	expression tag	UNP A0A6F8TGG1
A	-1	LYS	-	expression tag	UNP A0A6F8TGG1
A	0	HIS	-	expression tag	UNP A0A6F8TGG1

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MONOVACCENIN (three-letter code: MVC) (formula: $C_{21}H_{40}O_4$).

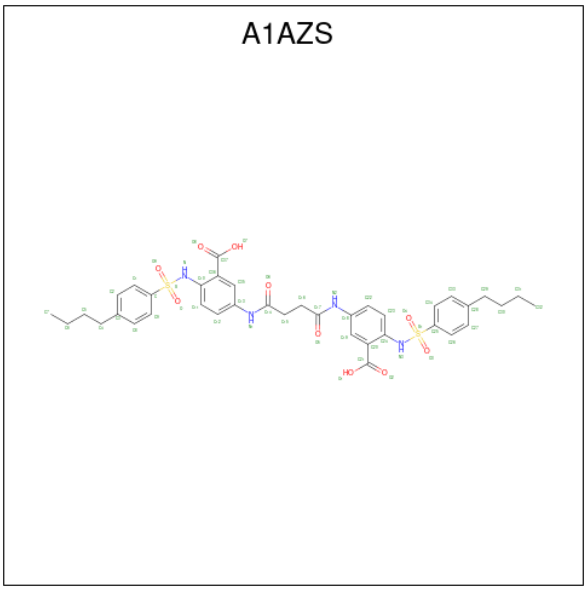


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			16	12	4			

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

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

- Molecule 5 is 3,3'-[(1,4-dioxobutane-1,4-diyl)bis(azanediyl)]bis[(4-butylbenzene-1-sulfonamido)benzoic acid] (three-letter code: A1AZS) (formula: $C_{38}H_{42}N_4O_{10}S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 54 38 4 10 2	0	1

- Molecule 6 is water.

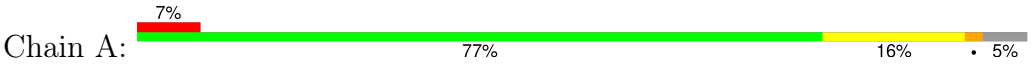
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	65	Total O 65 65	0	0

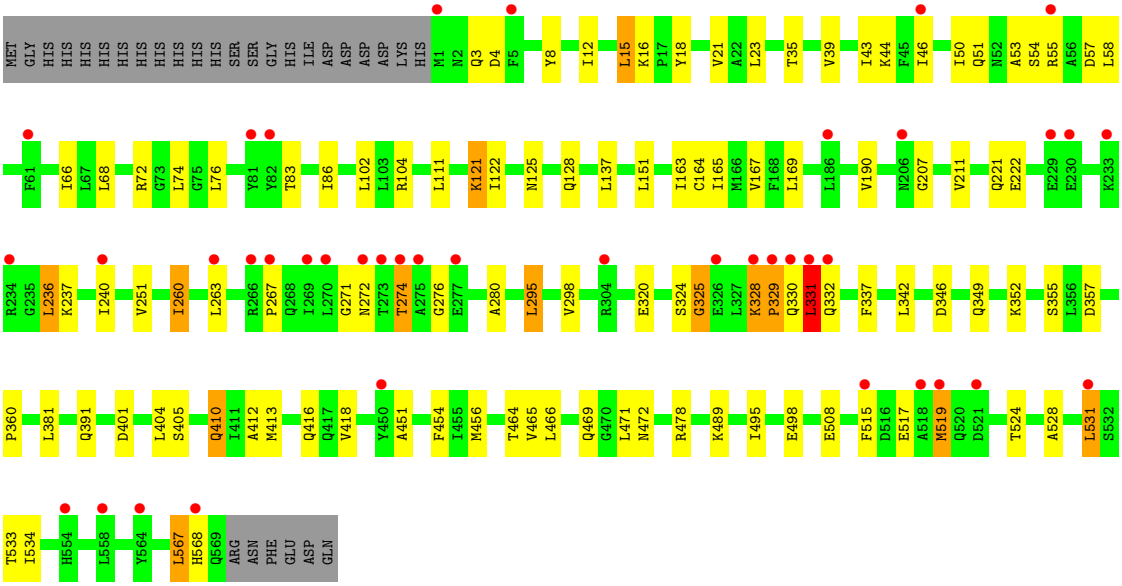
3 Residue-property plots (i)

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: Lipid A export ATP-binding/permease protein MsbA

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	70.28Å 83.16Å 338.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.38 – 2.80 40.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.38-2.80) 99.8 (40.38-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.204 , 0.252 0.221 , 0.271	Depositor DCC
R_{free} test set	1243 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.3	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	0.94	EDS
Total number of atoms	4619	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: MVC, ANP, MG, A1AZS

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	0.50	0/4524	0.73	1/6127 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	GLY	N-CA-C	6.41	129.11	113.10

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	4452	0	4543	38	0
2	A	31	0	13	1	0
3	A	16	0	21	0	0
4	A	1	0	0	0	0
5	A	54	0	0	3	0
6	A	65	0	0	0	0
All	All	4619	0	4577	41	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 4.

All (41) 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:35:THR:HG21	1:A:72:ARG:HB2	1.67	0.77
1:A:164:CYS:HB2	1:A:260:ILE:HD11	1.81	0.61
1:A:328:LYS:HG3	1:A:330:GLN:H	1.72	0.55
1:A:416:GLN:HG3	1:A:498:GLU:HB2	1.89	0.54
1:A:15:LEU:HA	1:A:18:TYR:HD2	1.74	0.52
1:A:55:ARG:HA	1:A:58:LEU:HD12	1.91	0.52
1:A:531:LEU:HD11	1:A:567:LEU:HD22	1.92	0.52
1:A:8:TYR:O	1:A:12:ILE:HG12	2.12	0.50
1:A:236:LEU:O	1:A:240:ILE:HG13	2.11	0.50
1:A:43:ILE:HA	1:A:46:ILE:HG22	1.94	0.50
1:A:466:LEU:HA	1:A:472:ASN:HD21	1.77	0.49
1:A:325:GLY:HA2	1:A:401:ASP:O	2.14	0.48
1:A:328:LYS:HD2	1:A:329:PRO:HD2	1.95	0.48
1:A:35:THR:HG23	1:A:68:LEU:HG	1.96	0.48
1:A:332:GLN:CB	1:A:360:PRO:HB3	2.44	0.47
1:A:451:ALA:HA	1:A:454:PHE:CE2	2.50	0.47
1:A:207:GLY:O	1:A:211:VAL:HG23	2.14	0.46
1:A:528:ALA:O	1:A:534:ILE:HD11	2.16	0.46
1:A:329:PRO:HA	1:A:410:GLN:NE2	2.30	0.46
1:A:329:PRO:HA	1:A:410:GLN:HE22	1.81	0.46
1:A:337:PHE:O	1:A:355:SER:HA	2.17	0.45
1:A:349[A]:GLN:HG2	1:A:352:LYS:HG2	1.97	0.45
1:A:44:LYS:HB2	1:A:280:ALA:HB2	1.99	0.45
1:A:413:MET:HG2	1:A:495:ILE:HB	1.99	0.45
5:A:604[A]:A1AZS:O1	5:A:604[A]:A1AZS:N3	2.50	0.45
1:A:346:ASP:OD2	2:A:601:ANP:H2	2.16	0.45
1:A:519:MET:O	1:A:519:MET:HG3	2.16	0.44
1:A:329:PRO:C	1:A:331:LEU:H	2.20	0.44
1:A:39:VAL:O	1:A:43:ILE:HG12	2.17	0.43
1:A:164:CYS:O	1:A:167:VAL:HG12	2.17	0.43
5:A:604[A]:A1AZS:N	5:A:604[A]:A1AZS:O7	2.51	0.43
5:A:604[A]:A1AZS:O6	5:A:604[A]:A1AZS:C12	2.65	0.42
1:A:469:GLN:HB3	1:A:471:LEU:HG	2.01	0.42
1:A:83:THR:HG23	1:A:137:LEU:HD23	2.01	0.42
1:A:237:LYS:HA	1:A:240:ILE:HD12	2.02	0.42
1:A:104:ARG:HD2	1:A:320:GLU:OE2	2.19	0.41
1:A:121:LYS:O	1:A:125:ASN:HB2	2.20	0.41
1:A:412:ALA:HA	1:A:489:LYS:HD3	2.02	0.41
1:A:18:TYR:HB3	1:A:86:ILE:HG12	2.02	0.41
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HD12	1:A:295:LEU:HA	1.96	0.41

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	568/598 (95%)	528 (93%)	33 (6%)	7 (1%)	11 34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ALA
1	A	271	GLY
1	A	274	THR
1	A	3	GLN
1	A	331	LEU
1	A	267	PRO
1	A	276	GLY

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	478/506 (94%)	422 (88%)	56 (12%)	4 14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	15	LEU
1	A	16	LYS
1	A	21	VAL
1	A	23	LEU
1	A	50	ILE
1	A	51	GLN
1	A	54	SER
1	A	57	ASP
1	A	66	ILE
1	A	74	LEU
1	A	102	LEU
1	A	111	LEU
1	A	121	LYS
1	A	122	ILE
1	A	128	GLN
1	A	151	LEU
1	A	163	ILE
1	A	165	ILE
1	A	169	LEU
1	A	190	VAL
1	A	221	GLN
1	A	222	GLU
1	A	236	LEU
1	A	251	VAL
1	A	260	ILE
1	A	263	LEU
1	A	272	ASN
1	A	274	THR
1	A	295	LEU
1	A	298	VAL
1	A	324	SER
1	A	328	LYS
1	A	329	PRO
1	A	331	LEU
1	A	342	LEU
1	A	357	ASP
1	A	381	LEU
1	A	391	GLN
1	A	404	LEU
1	A	405	SER
1	A	410	GLN

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Mol	Chain	Res	Type
1	A	418	VAL
1	A	456	MET
1	A	464	THR
1	A	465	VAL
1	A	478	ARG
1	A	508	GLU
1	A	515	PHE
1	A	517	GLU
1	A	519	MET
1	A	524	THR
1	A	531	LEU
1	A	533	THR
1	A	567	LEU
1	A	568	HIS

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	3	GLN
1	A	410	GLN
1	A	416	GLN
1	A	422	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	ANP	A	601	4	29,33,33	0.78	1 (3%)	31,52,52	1.12	3 (9%)
3	MVC	A	602	-	13,13,24	1.11	1 (7%)	12,12,25	0.82	1 (8%)
5	A1AZS	A	604[A]	-	57,57,57	1.77	4 (7%)	80,80,80	2.09	16 (20%)

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
2	ANP	A	601	4	-	5/14/38/38	0/3/3/3
3	MVC	A	602	-	1/1/1/4	5/10/10/24	-
5	A1AZS	A	604[A]	-	-	12/51/51/51	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604[A]	A1AZS	C25-S1	-8.31	1.63	1.76
5	A	604[A]	A1AZS	C-S	-7.82	1.64	1.76
3	A	602	MVC	C8-C9	-3.84	1.32	1.51
5	A	604[A]	A1AZS	S1-N3	2.64	1.67	1.63
2	A	601	ANP	PB-O3A	-2.26	1.56	1.59
5	A	604[A]	A1AZS	S-N	2.08	1.66	1.63

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	604[A]	A1AZS	C25-S1-N3	-10.67	93.64	106.88
5	A	604[A]	A1AZS	C-S-N	-9.02	95.69	106.88
5	A	604[A]	A1AZS	C35-C36-C10	3.40	122.15	119.09
5	A	604[A]	A1AZS	O7-C37-O8	-3.32	116.22	123.35
5	A	604[A]	A1AZS	C19-C20-C24	3.28	122.04	119.09
5	A	604[A]	A1AZS	O1-C21-O2	-3.19	116.49	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	604[A]	A1AZS	O3-S1-C25	2.59	111.25	107.98
5	A	604[A]	A1AZS	C33-C34-C25	2.56	121.93	119.44
5	A	604[A]	A1AZS	O4-S1-C25	2.54	111.19	107.98
5	A	604[A]	A1AZS	O-S-C	2.42	111.04	107.98
3	A	602	MVC	C7-C8-C9	2.37	126.37	114.37
2	A	601	ANP	O3G-PG-O1G	-2.36	107.53	113.45
5	A	604[A]	A1AZS	C2-C1-C	2.36	121.74	119.44
5	A	604[A]	A1AZS	C26-C25-C34	-2.32	117.45	120.47
2	A	601	ANP	O2G-PG-O1G	-2.23	107.86	113.45
5	A	604[A]	A1AZS	C18-N2-C17	-2.21	123.61	127.52
5	A	604[A]	A1AZS	C1-C-C9	-2.20	117.59	120.47
2	A	601	ANP	C5-C6-N6	2.20	123.66	120.31
5	A	604[A]	A1AZS	C15-C16-C17	-2.14	108.26	112.67
5	A	604[A]	A1AZS	O9-S-C	2.12	110.65	107.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	602	MVC	C22

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PB-N3B-PG-O1G
2	A	601	ANP	PG-N3B-PB-O1B
2	A	601	ANP	PA-O3A-PB-O2B
2	A	601	ANP	C5'-O5'-PA-O3A
3	A	602	MVC	O20-C21-C22-C24
5	A	604[A]	A1AZS	C14-C15-C16-C17
3	A	602	MVC	O20-C21-C22-O23
3	A	602	MVC	C4-C5-C6-C7
3	A	602	MVC	C11-C10-C9-C8
5	A	604[A]	A1AZS	C10-N-S-O9
5	A	604[A]	A1AZS	C24-N3-S1-O3
5	A	604[A]	A1AZS	C28-C29-C30-C31
5	A	604[A]	A1AZS	C2-C3-C4-C5
3	A	602	MVC	C3-C4-C5-C6
5	A	604[A]	A1AZS	C8-C3-C4-C5
5	A	604[A]	A1AZS	C10-N-S-O
5	A	604[A]	A1AZS	C10-N-S-C
5	A	604[A]	A1AZS	C4-C5-C6-C7
5	A	604[A]	A1AZS	C15-C16-C17-O5

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Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PA-O3A-PB-O1B
5	A	604[A]	A1AZS	C15-C16-C17-N2
5	A	604[A]	A1AZS	O6-C14-C15-C16

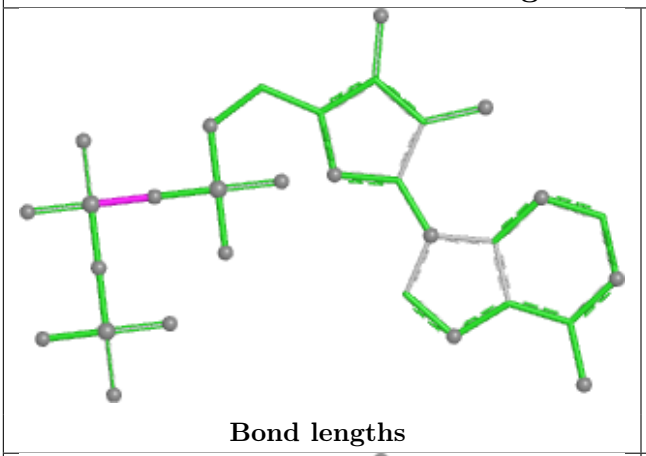
There are no ring outliers.

2 monomers are involved in 4 short contacts:

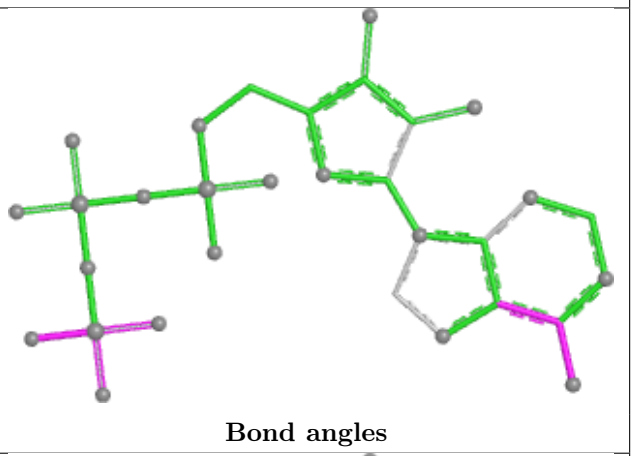
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ANP	1	0
5	A	604[A]	A1AZS	3	0

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 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.

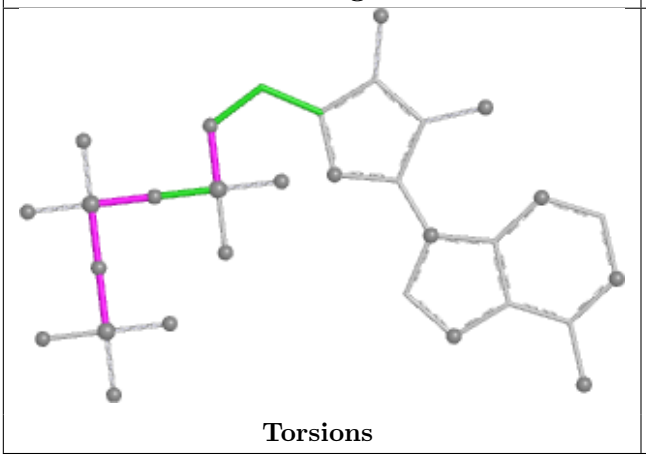
Ligand ANP A 601



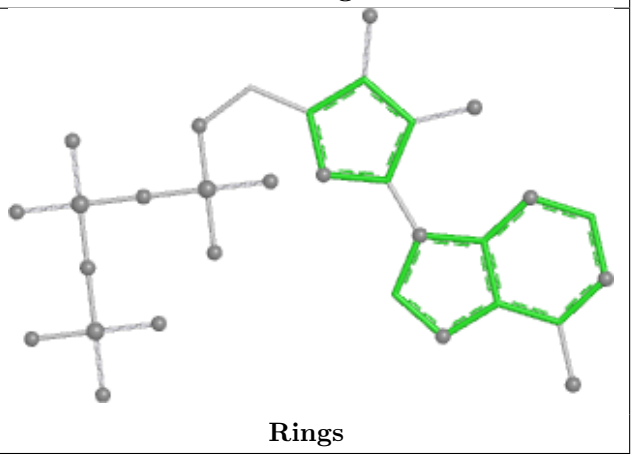
Bond lengths



Bond angles

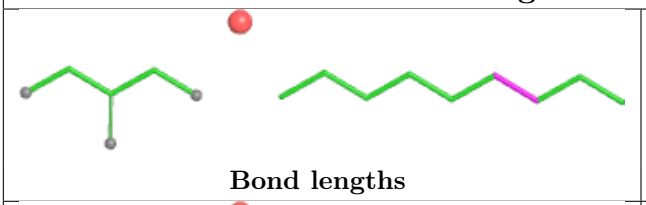


Torsions

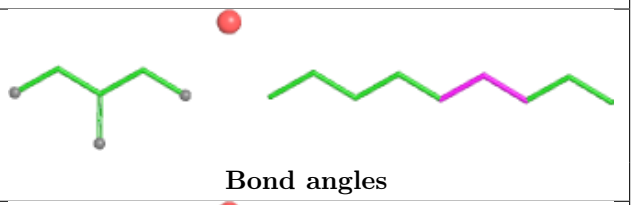


Rings

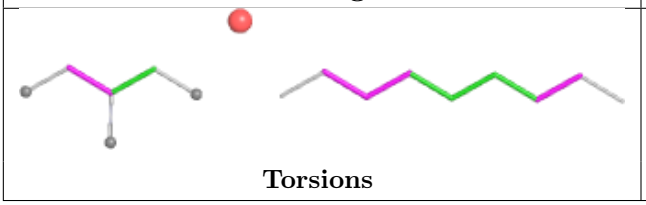
Ligand MVC A 602



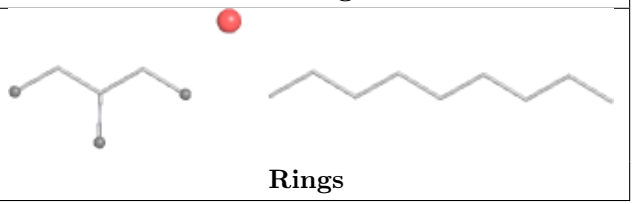
Bond lengths



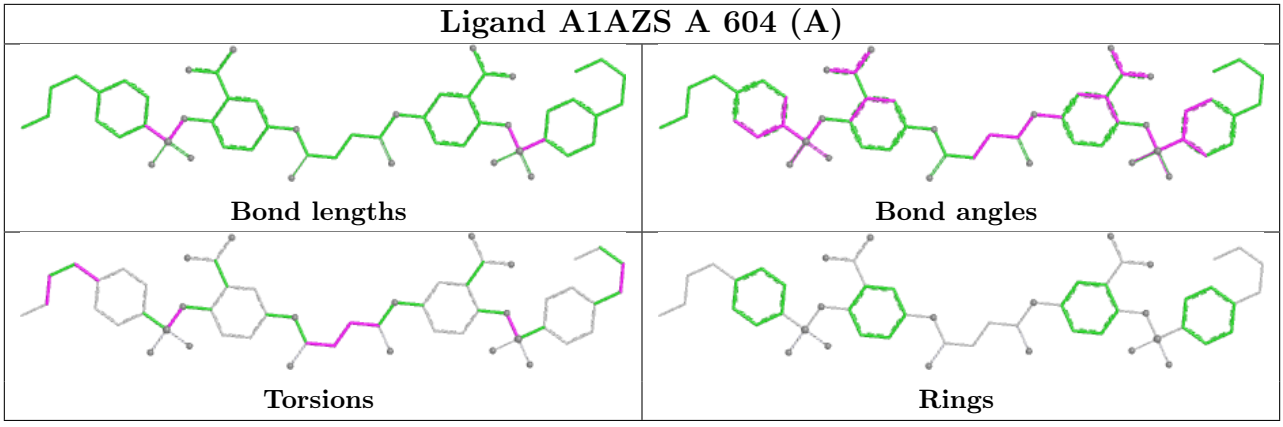
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	569/598 (95%)	0.40	41 (7%)	23	17	30, 82, 135, 169	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	THR	6.6
1	A	332	GLN	6.2
1	A	331	LEU	5.5
1	A	269	ILE	4.5
1	A	275	ALA	4.1
1	A	82	TYR	3.8
1	A	326	GLU	3.7
1	A	233	LYS	3.5
1	A	186	LEU	3.3
1	A	270	LEU	3.3
1	A	558	LEU	3.3
1	A	81	TYR	3.3
1	A	272	ASN	3.2
1	A	1	MET	3.2
1	A	277	GLU	3.1
1	A	55	ARG	2.9
1	A	61	PHE	2.8
1	A	263	LEU	2.7
1	A	330	GLN	2.7
1	A	273	THR	2.6
1	A	304	ARG	2.6
1	A	266	ARG	2.6
1	A	234	ARG	2.5
1	A	267	PRO	2.5
1	A	240	ILE	2.5
1	A	521	ASP	2.4
1	A	568	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	229	GLU	2.3
1	A	230	GLU	2.3
1	A	5	PHE	2.3
1	A	329	PRO	2.3
1	A	564	TYR	2.3
1	A	554	HIS	2.3
1	A	515	PHE	2.2
1	A	450	TYR	2.2
1	A	519	MET	2.2
1	A	518	ALA	2.2
1	A	46	ILE	2.1
1	A	328	LYS	2.1
1	A	531	LEU	2.0
1	A	206	ASN	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)

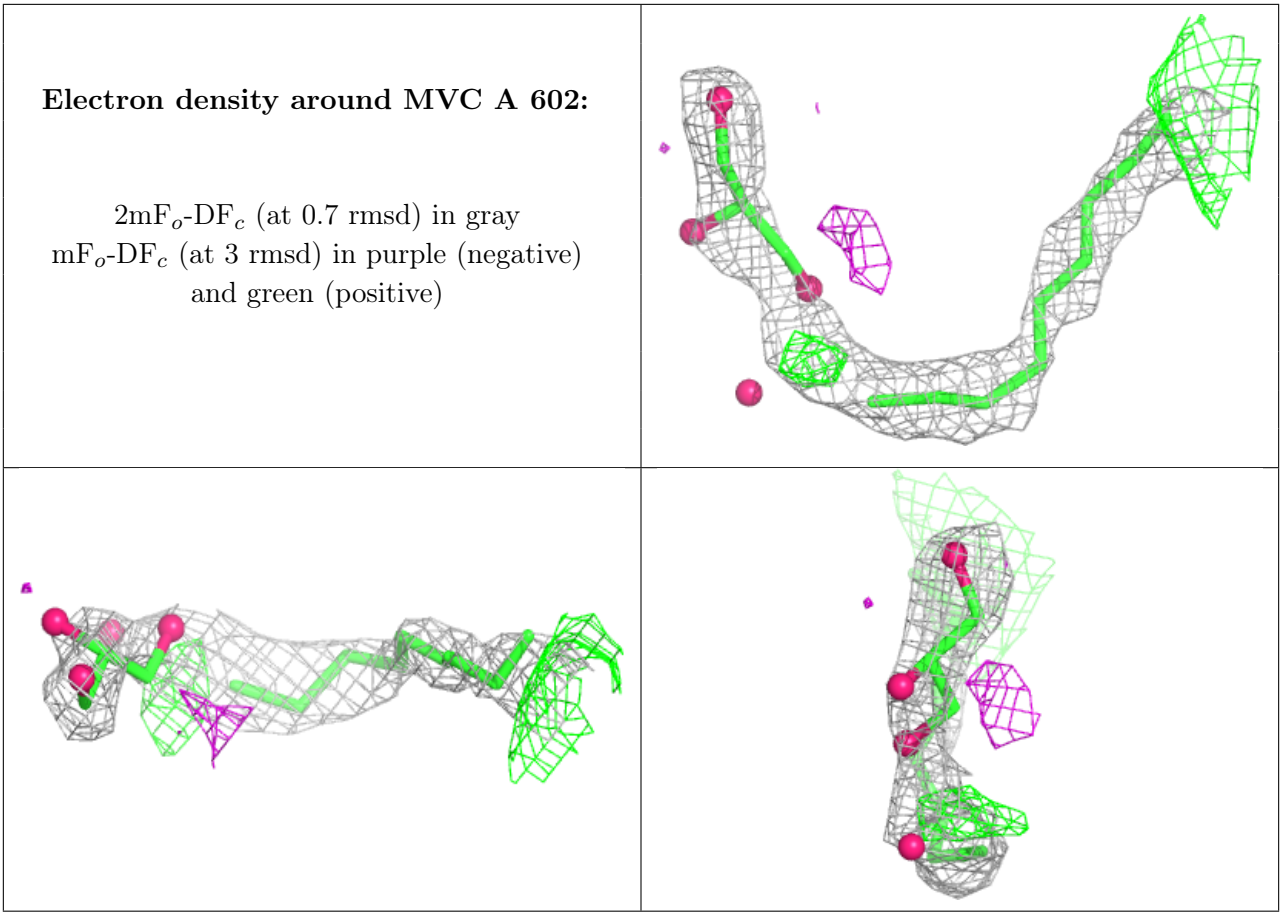
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MVC	A	602	16/25	0.82	0.26	57,72,95,95	0
5	A1AZS	A	604[A]	54/54	0.91	0.16	114,119,127,127	54
2	ANP	A	601	31/31	0.97	0.06	47,57,64,66	0
4	MG	A	603	1/1	0.99	0.06	71,71,71,71	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.

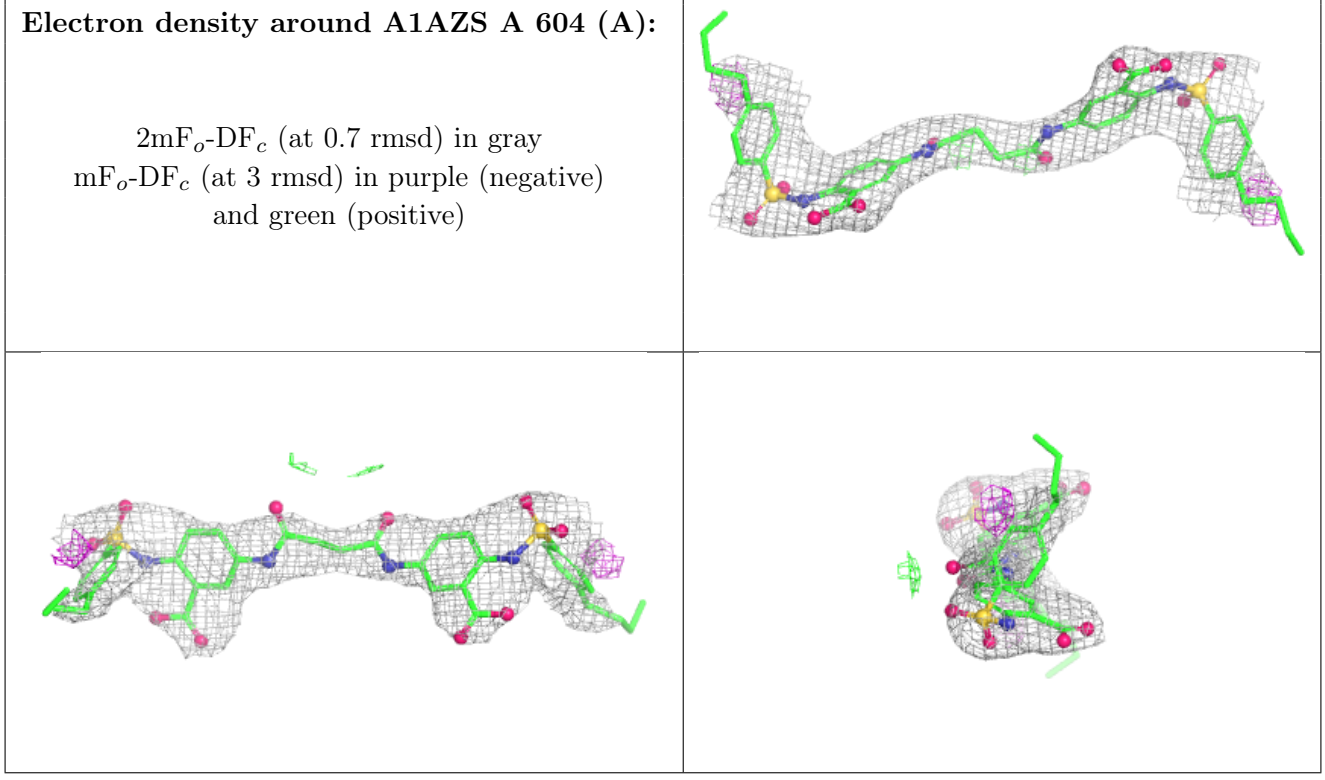
Electron density around MVC A 602:

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



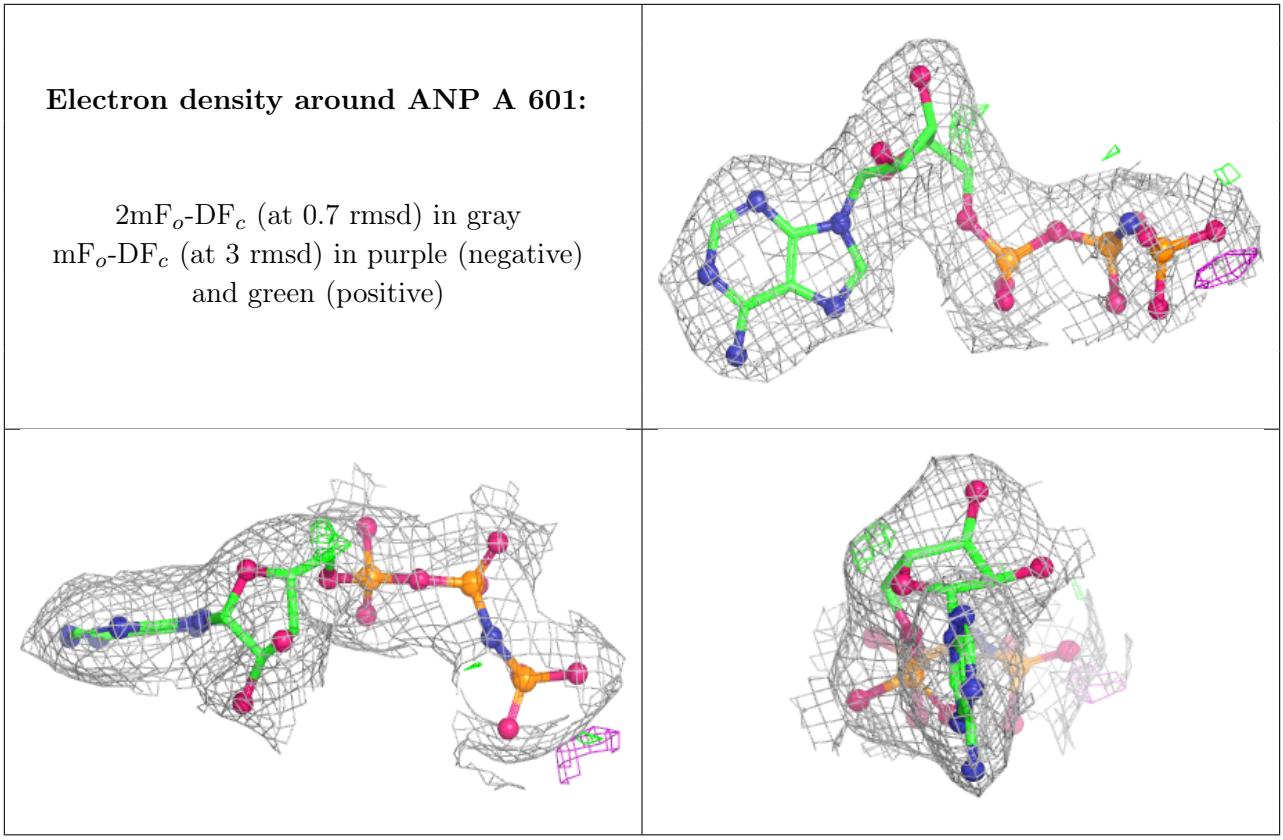
Electron density around A1AZS A 604 (A):

$2mF_o$-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.