



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 3, 2025 – 10:22 AM EST

PDB ID : 9DTS
Title : Crystal structure of the human eIF4A1/AMPPNP/amidino-rocaglate/polypurine RNA complex
Authors : Conley, J.F.; Allen, K.N.
Deposited on : 2024-10-01
Resolution : 1.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

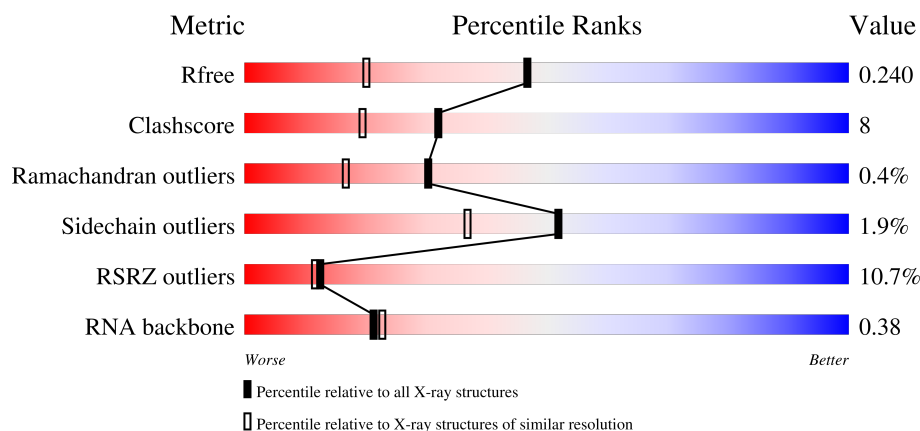
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)
RNA backbone	3690	1037 (2.20-1.20)

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 $\leq 5\%$. 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	388	<div> <div>8%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	B	388	<div> <div>7%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	C	388	<div> <div>6%</div> <div>86%</div> <div>11%</div> <div>• •</div> </div>
1	D	388	<div> <div>21%</div> <div>76%</div> <div>18%</div> <div>• • •</div> </div>

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Mol	Chain	Length	Quality of chain
2	W	10	<div><div></div><div></div><div></div><div></div><div></div></div>
2	X	10	<div><div></div><div></div><div></div><div></div><div></div></div>
2	Y	10	<div><div></div><div></div><div></div><div></div><div></div></div>
2	Z	10	<div><div></div><div></div><div></div><div></div><div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26889 atoms, of which 12860 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 Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	378	Total	C	H	N	O	S	30	4	0
			6144	1922	3101	528	573	20			
1	B	373	Total	C	H	N	O	S	0	3	0
			6061	1898	3053	525	565	20			
1	C	378	Total	C	H	N	O	S	28	5	0
			6166	1927	3114	531	574	20			
1	D	374	Total	C	H	N	O	S	0	3	0
			6075	1903	3060	526	566	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	cloning artifact	UNP P60842
A	20	SER	-	cloning artifact	UNP P60842
B	19	SER	-	cloning artifact	UNP P60842
B	20	SER	-	cloning artifact	UNP P60842
C	19	SER	-	cloning artifact	UNP P60842
C	20	SER	-	cloning artifact	UNP P60842
D	19	SER	-	cloning artifact	UNP P60842
D	20	SER	-	cloning artifact	UNP P60842

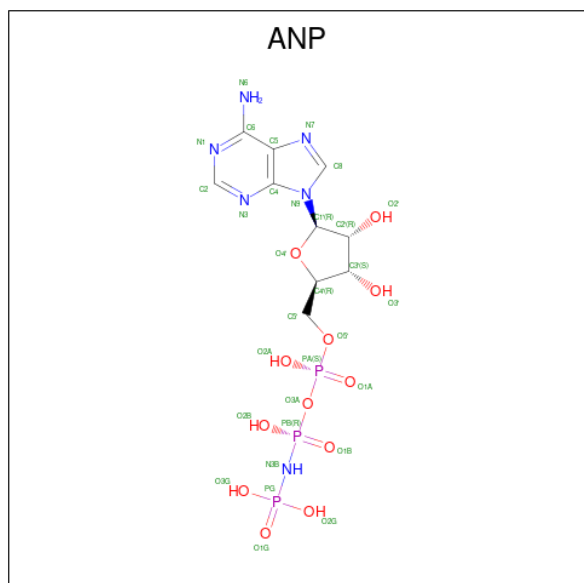
- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*GP*AP*GP*AP*GP*AP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	W	8	Total	C	H	N	O	P	0	0	0
			268	80	88	40	52	8			
2	X	8	Total	C	H	N	O	P	0	0	0
			268	80	88	40	52	8			
2	Y	8	Total	C	H	N	O	P	0	0	0
			268	80	88	40	52	8			
2	Z	8	Total	C	H	N	O	P	0	0	0
			268	80	88	40	52	8			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

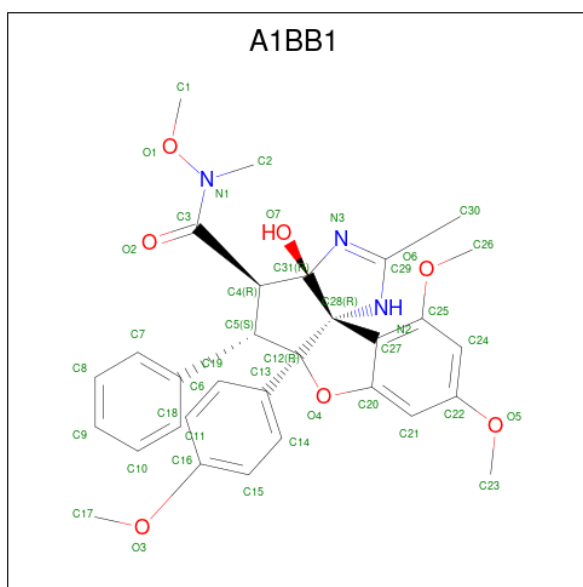
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0
4	B	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0
4	C	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0
4	D	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0

- Molecule 5 is (3aR,4R,5S,5aR,10bR)-3a-hydroxy-N,8,10-trimethoxy-5a-(4-methoxyphenyl)-N,2-dimethyl-5-phenyl-3a,4,5,5a-tetrahydro-1H-[1]benzofuro[3',2':1,5]cyclopenta[1,2-d]imidazole-4-carboxamide (three-letter code: A1BB1) (formula: C₃₁H₃₃N₃O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	0	0
			74	31	33	3	7		
5	W	1	Total	C	H	N	O	0	0
			74	31	33	3	7		
5	X	1	Total	C	H	N	O	0	0
			74	31	33	3	7		
5	Y	1	Total	C	H	N	O	0	0
			74	31	33	3	7		

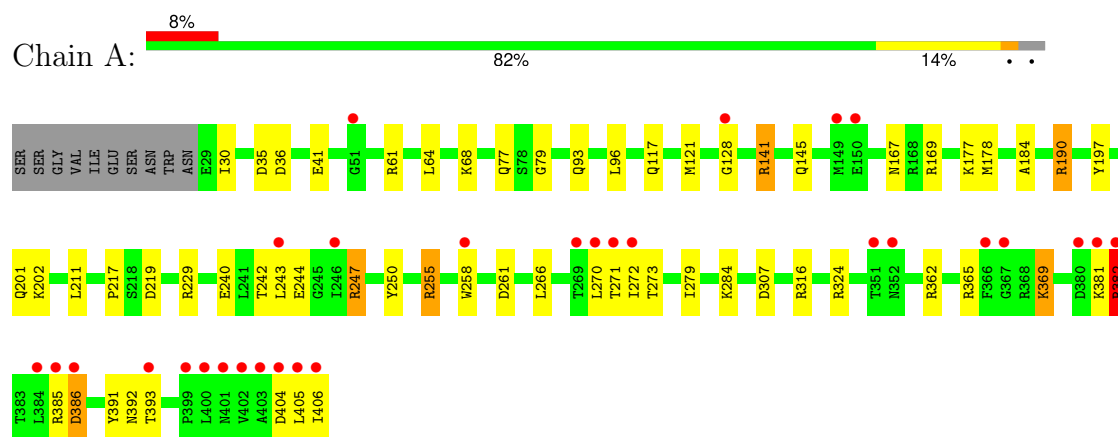
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total	O	0	0
			221	221		
6	B	220	Total	O	0	0
			220	220		
6	C	215	Total	O	0	0
			215	215		
6	D	155	Total	O	0	0
			155	155		
6	W	28	Total	O	0	0
			28	28		
6	X	22	Total	O	0	0
			22	22		
6	Y	21	Total	O	0	0
			21	21		
6	Z	17	Total	O	0	0
			17	17		

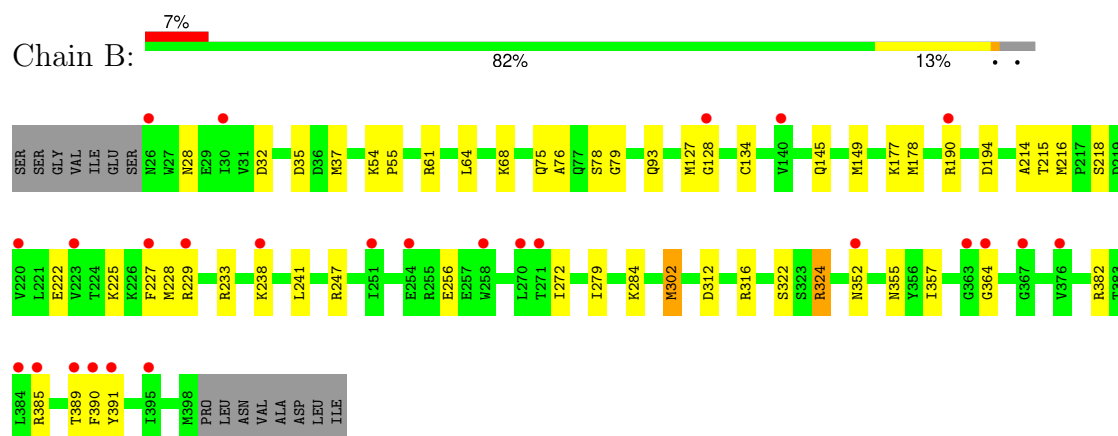
3 Residue-property plots [i](#)

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.

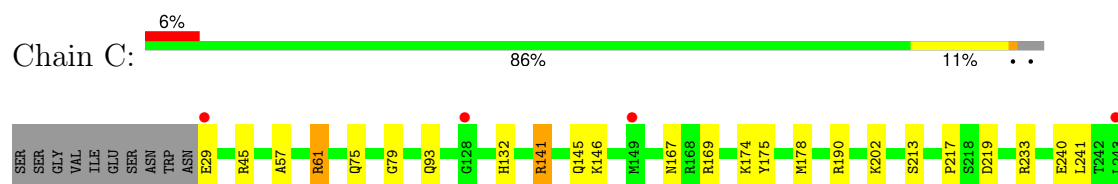
• Molecule 1: Eukaryotic initiation factor 4A-I



• Molecule 1: Eukaryotic initiation factor 4A-I

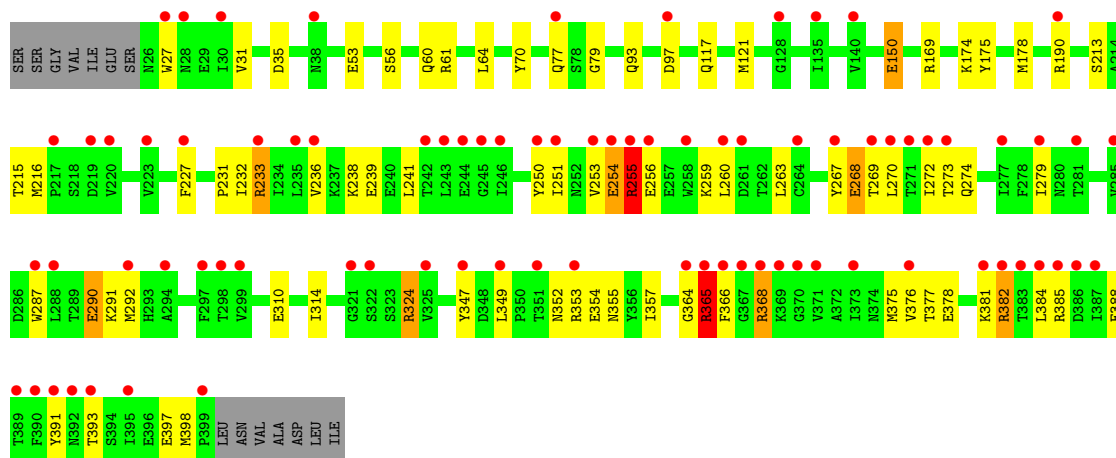
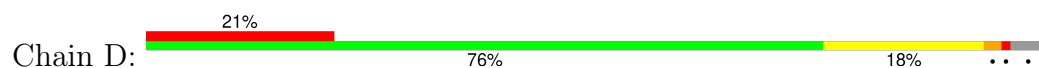


• Molecule 1: Eukaryotic initiation factor 4A-I





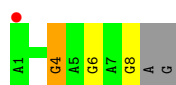
- Molecule 1: Eukaryotic initiation factor 4A-I



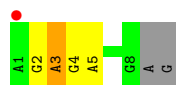
- Molecule 2: RNA (5'-R(P*AP*GP*AP*GP*AP*GP*AP*G)-3')



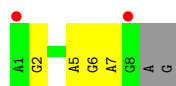
- Molecule 2: RNA (5'-R(P*AP*GP*AP*GP*AP*GP*AP*G)-3')



- Molecule 2: RNA (5'-R(P*AP*GP*AP*GP*AP*GP*AP*G)-3')



- Molecule 2: RNA (5'-R(P*AP*GP*AP*GP*AP*GP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.11Å 87.31Å 93.16Å 95.22° 105.29° 108.35°	Depositor
Resolution (Å)	40.68 – 1.69 40.68 – 1.69	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.68-1.69) 96.0 (40.68-1.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.240 0.203 , 0.240	Depositor DCC
R_{free} test set	207759 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26889	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A1BB1, ANP

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	0.56	0/3105	0.74	0/4187
1	B	0.61	1/3068 (0.0%)	0.78	2/4136 (0.0%)
1	C	0.59	0/3117	0.76	0/4201
1	D	0.51	0/3076	0.72	1/4148 (0.0%)
2	W	1.04	0/203	1.48	3/316 (0.9%)
2	X	1.21	0/203	1.70	6/316 (1.9%)
2	Y	1.03	0/203	1.34	2/316 (0.6%)
2	Z	1.04	0/203	1.41	3/316 (0.9%)
All	All	0.61	1/13178 (0.0%)	0.83	17/17936 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	D	0	6
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	CYS	CB-SG	-5.67	1.72	1.81

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	4	G	O5'-P-OP1	-8.48	98.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	2	G	N1-C6-O6	-7.06	115.67	119.90
2	W	6	G	C4-C5-N7	-6.68	108.13	110.80
2	X	6	G	N1-C6-O6	5.96	123.48	119.90
2	W	6	G	C5-N7-C8	5.91	107.25	104.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ARG	Sidechain
1	A	247	ARG	Sidechain
1	A	255	ARG	Sidechain
1	A	382	ARG	Sidechain
1	B	324	ARG	Sidechain

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	3043	3101	3091	59	0
1	B	3008	3053	3043	44	0
1	C	3052	3114	3104	30	0
1	D	3015	3060	3050	70	0
2	W	180	88	89	5	0
2	X	180	88	89	0	0
2	Y	180	88	89	1	0
2	Z	180	88	89	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	12	13	1	0
4	B	31	12	13	1	0
4	C	31	12	13	1	0
4	D	31	12	13	2	0
5	D	41	33	0	0	0
5	W	41	33	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	X	41	33	0	0	0
5	Y	41	33	0	0	0
6	A	221	0	0	16	0
6	B	220	0	0	10	0
6	C	215	0	0	7	0
6	D	155	0	0	5	0
6	W	28	0	0	1	0
6	X	22	0	0	0	0
6	Y	21	0	0	0	0
6	Z	17	0	0	1	0
All	All	14029	12860	12696	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 204 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:B:216:MET:N	6:B:601:HOH:O	1.74	1.17
1:D:169:ARG:O	6:D:601:HOH:O	1.81	0.98
1:A:244:GLU:OE2	6:A:601:HOH:O	1.85	0.95
1:A:242:THR:HG21	1:A:393:THR:HG21	1.47	0.94
1:B:382:ARG:NH1	6:B:603:HOH:O	2.05	0.88

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	380/388 (98%)	373 (98%)	7 (2%)	0	100 100
1	B	374/388 (96%)	367 (98%)	6 (2%)	1 (0%)	37 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	381/388 (98%)	372 (98%)	9 (2%)	0	100	100
1	D	375/388 (97%)	364 (97%)	6 (2%)	5 (1%)	10	2
All	All	1510/1552 (97%)	1476 (98%)	28 (2%)	6 (0%)	30	17

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	364	GLY
1	D	254	GLU
1	D	365	ARG
1	D	268	GLU
1	D	255	ARG

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	337/342 (98%)	331 (98%)	6 (2%)	54	39
1	B	332/342 (97%)	327 (98%)	5 (2%)	60	47
1	C	338/342 (99%)	331 (98%)	7 (2%)	48	32
1	D	333/342 (97%)	324 (97%)	9 (3%)	40	23
All	All	1340/1368 (98%)	1313 (98%)	27 (2%)	52	34

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	61[B]	ARG
1	C	406	ILE
1	D	365	ARG
1	C	382	ARG
1	D	150	GLU

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

Mol	Chain	Res	Type
1	A	355	ASN
1	B	28	ASN
1	B	75	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	W	7/10 (70%)	1 (14%)	0
2	X	7/10 (70%)	2 (28%)	0
2	Y	7/10 (70%)	1 (14%)	0
2	Z	7/10 (70%)	0	0
All	All	28/40 (70%)	4 (14%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	W	2	G
2	X	4	G
2	X	8	G
2	Y	2	G

There are no RNA pucker outliers to report.

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	ANP	A	502	3	29,33,33	1.64	3 (10%)	31,52,52	1.25	4 (12%)
5	A1BB1	X	101	-	39,46,46	0.93	2 (5%)	48,72,72	0.87	1 (2%)
4	ANP	C	502	3	29,33,33	1.70	5 (17%)	31,52,52	1.30	3 (9%)
5	A1BB1	W	101	-	39,46,46	0.84	2 (5%)	48,72,72	1.12	3 (6%)
4	ANP	B	502	3	29,33,33	1.56	4 (13%)	31,52,52	1.51	4 (12%)
5	A1BB1	Y	101	-	39,46,46	0.67	2 (5%)	48,72,72	1.05	3 (6%)
5	A1BB1	D	503	-	39,46,46	0.69	1 (2%)	48,72,72	1.14	3 (6%)
4	ANP	D	502	3	29,33,33	1.26	3 (10%)	31,52,52	1.13	3 (9%)

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
4	ANP	A	502	3	-	2/14/38/38	0/3/3/3
5	A1BB1	X	101	-	-	1/26/81/81	0/6/6/6
4	ANP	C	502	3	-	2/14/38/38	0/3/3/3
5	A1BB1	W	101	-	-	0/26/81/81	0/6/6/6
4	ANP	B	502	3	-	2/14/38/38	0/3/3/3
5	A1BB1	Y	101	-	-	0/26/81/81	0/6/6/6
5	A1BB1	D	503	-	-	1/26/81/81	0/6/6/6
4	ANP	D	502	3	-	2/14/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ANP	PB-O1B	6.34	1.55	1.46
4	B	502	ANP	PG-O1G	5.50	1.54	1.46
4	C	502	ANP	PB-O1B	5.14	1.54	1.46
4	C	502	ANP	PA-O3A	4.24	1.64	1.59
4	D	502	ANP	PB-O1B	3.48	1.51	1.46

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	ANP	O1G-PG-N3B	-5.77	103.27	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	ANP	O1G-PG-N3B	-4.59	105.02	111.77
5	W	101	A1BB1	C4-C3-N1	-3.51	113.58	117.78
4	B	502	ANP	O2B-PB-O1B	3.29	116.93	109.87
4	D	502	ANP	O1G-PG-N3B	-3.27	106.95	111.77

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

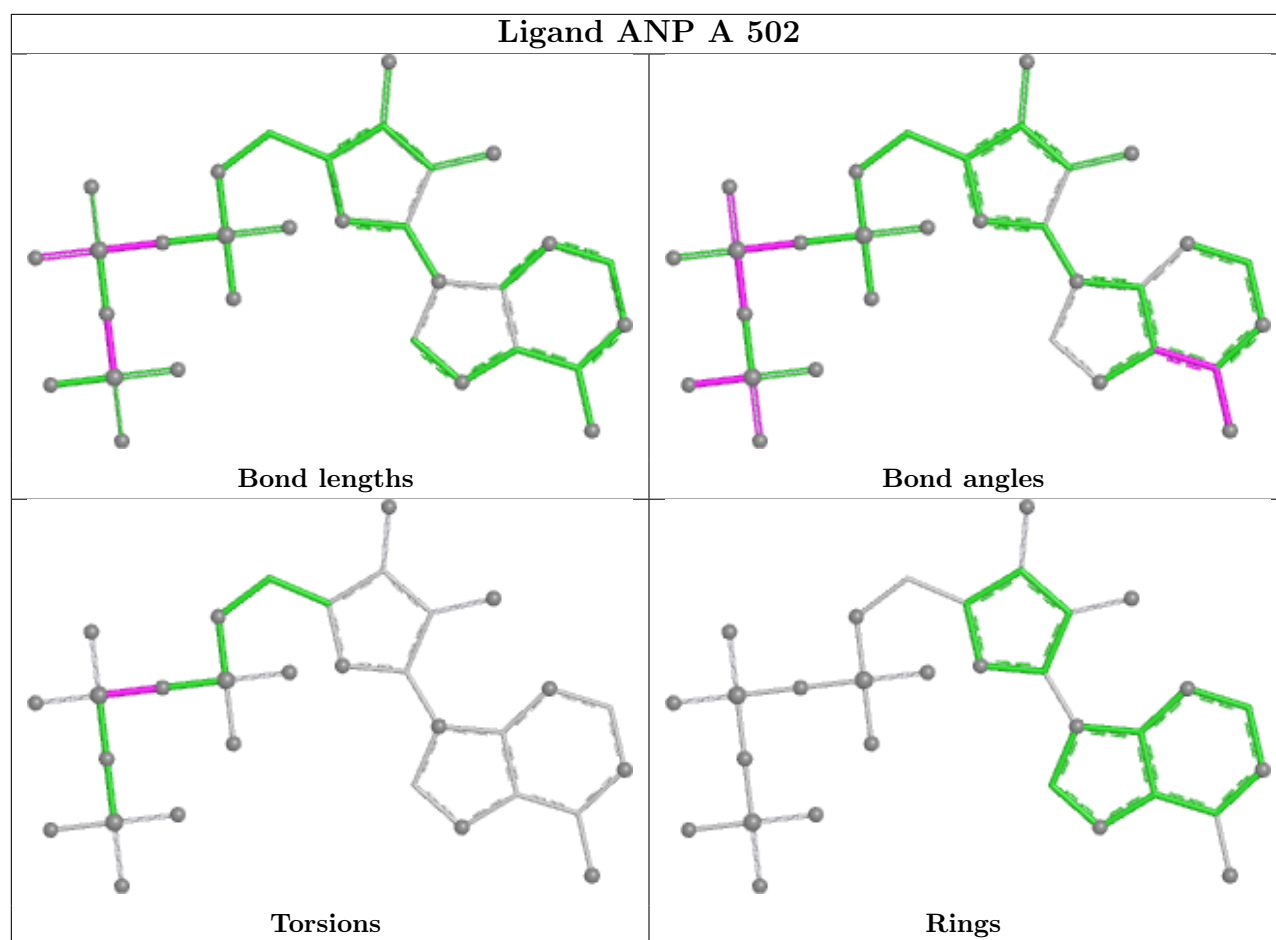
Mol	Chain	Res	Type	Atoms
4	A	502	ANP	PA-O3A-PB-O2B
4	B	502	ANP	PA-O3A-PB-O2B
4	C	502	ANP	PA-O3A-PB-O2B
4	D	502	ANP	PA-O3A-PB-O2B
5	D	503	A1BB1	C2-N1-O1-C1

There are no ring outliers.

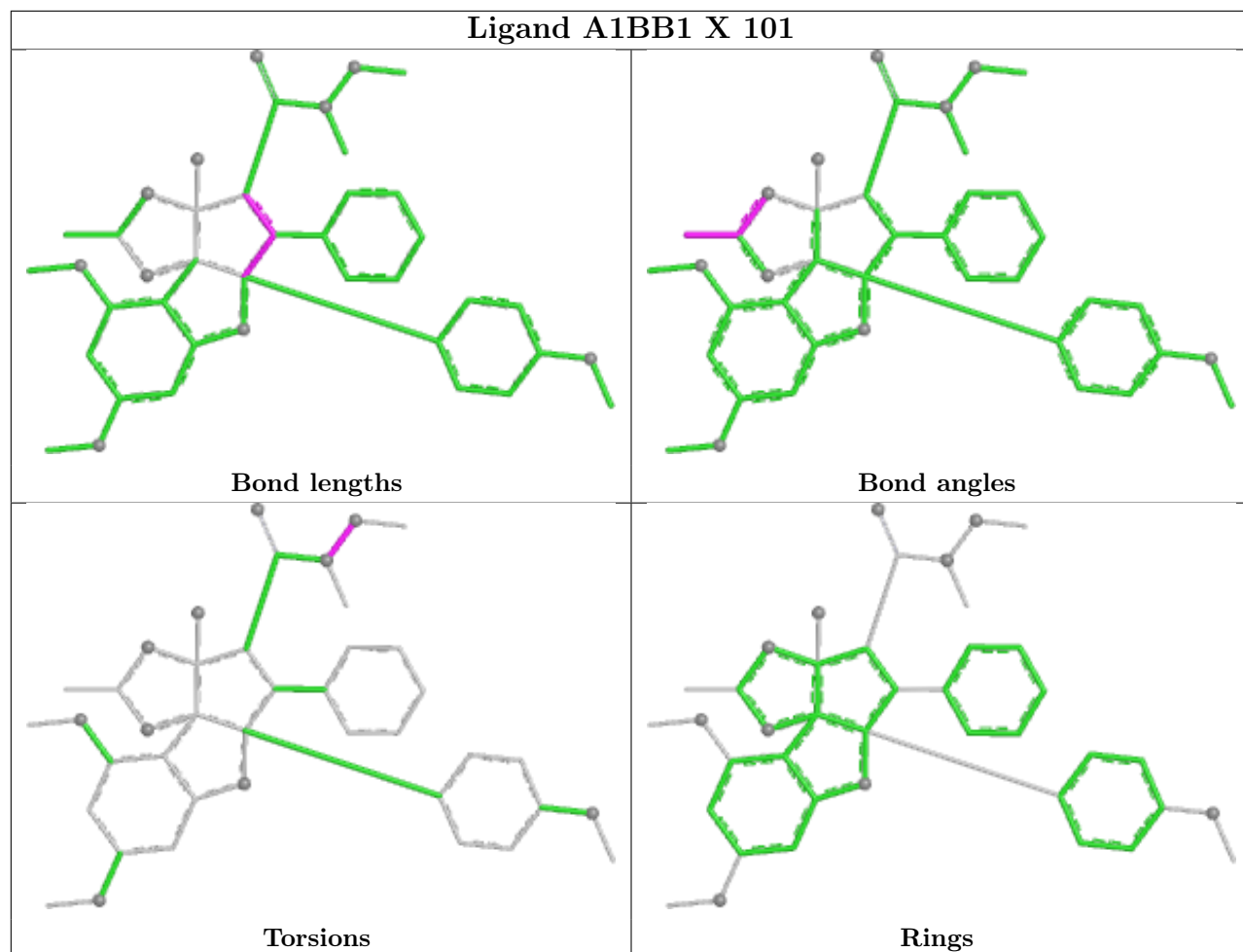
4 monomers are involved in 5 short contacts:

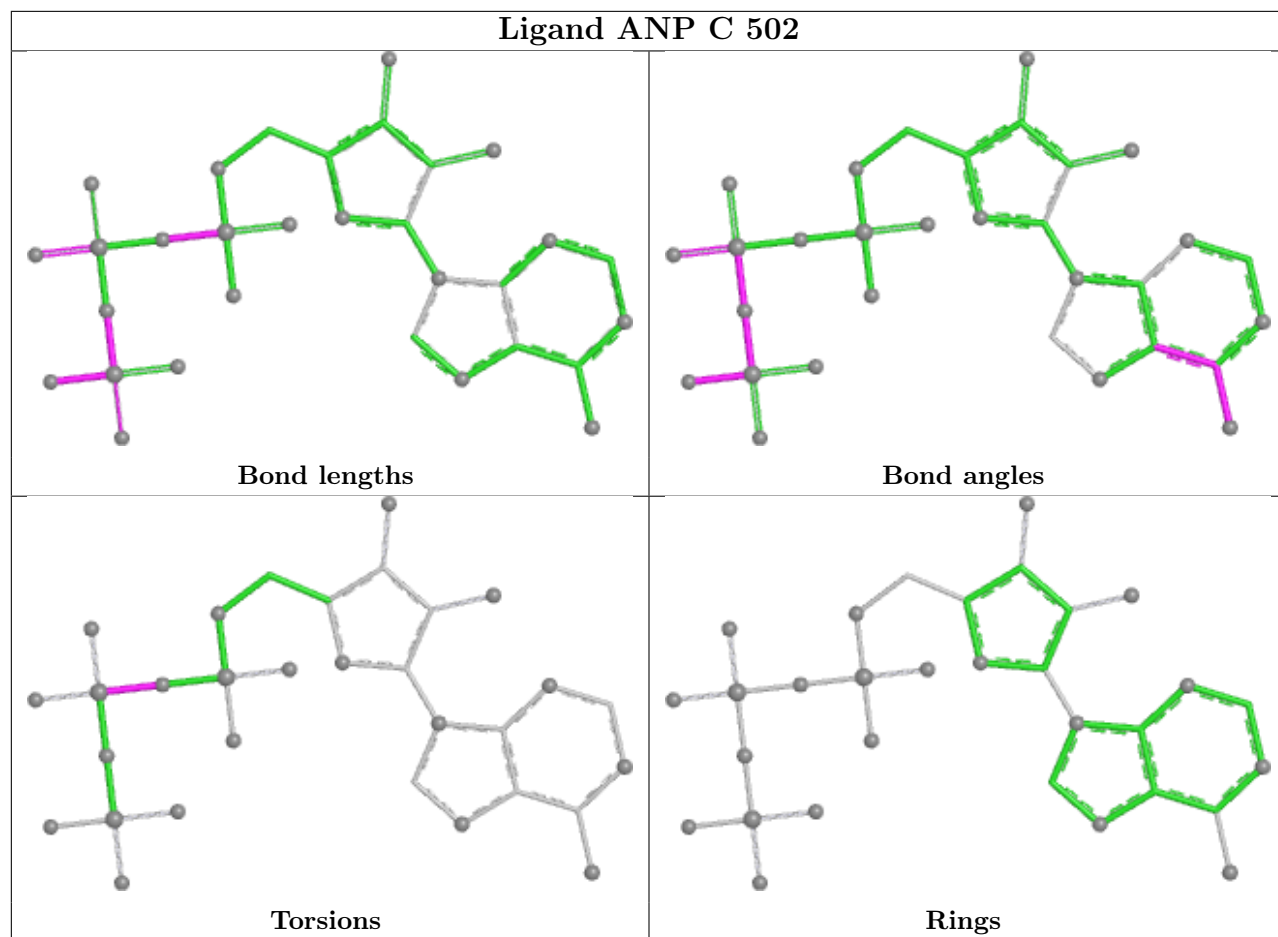
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	ANP	1	0
4	C	502	ANP	1	0
4	B	502	ANP	1	0
4	D	502	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

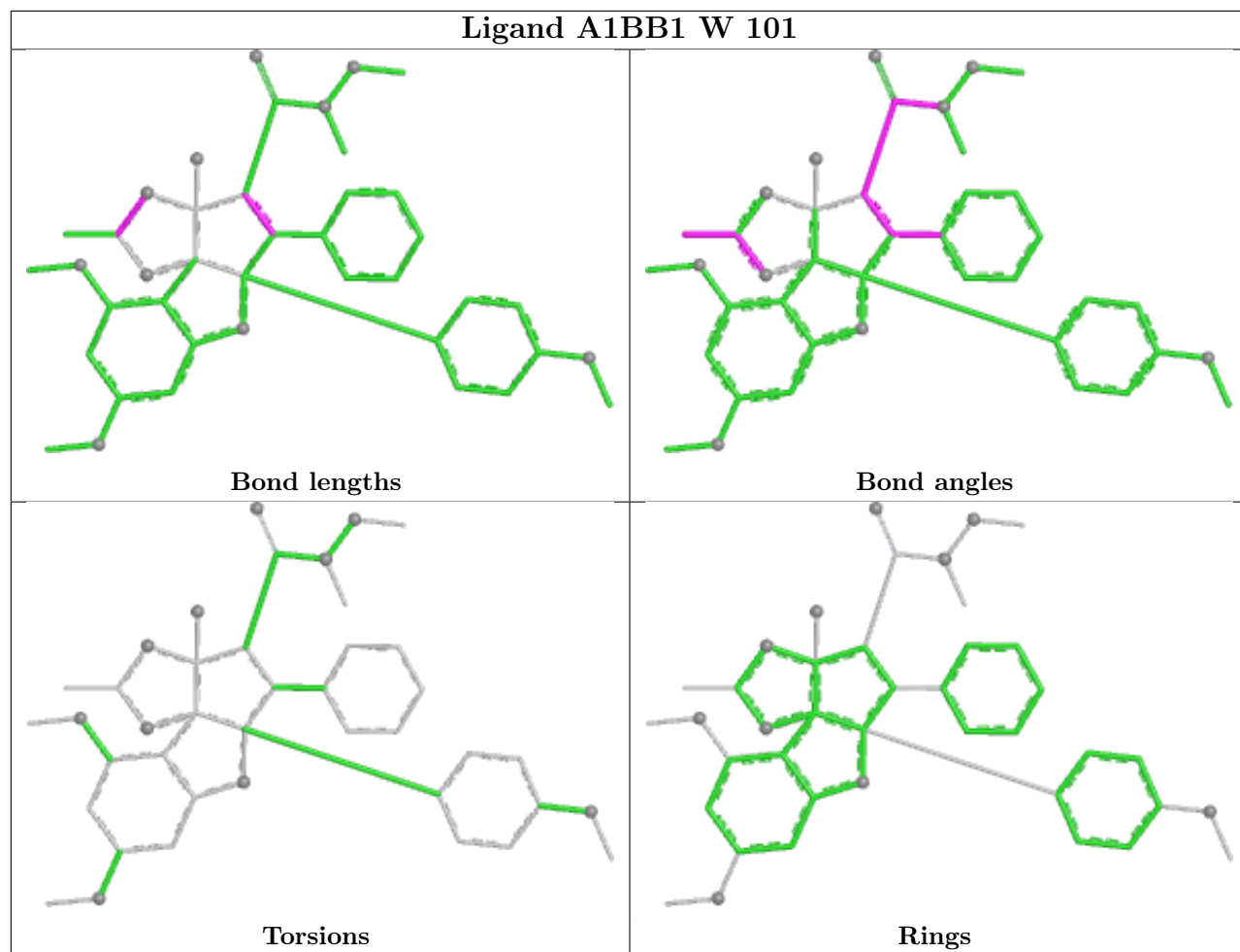


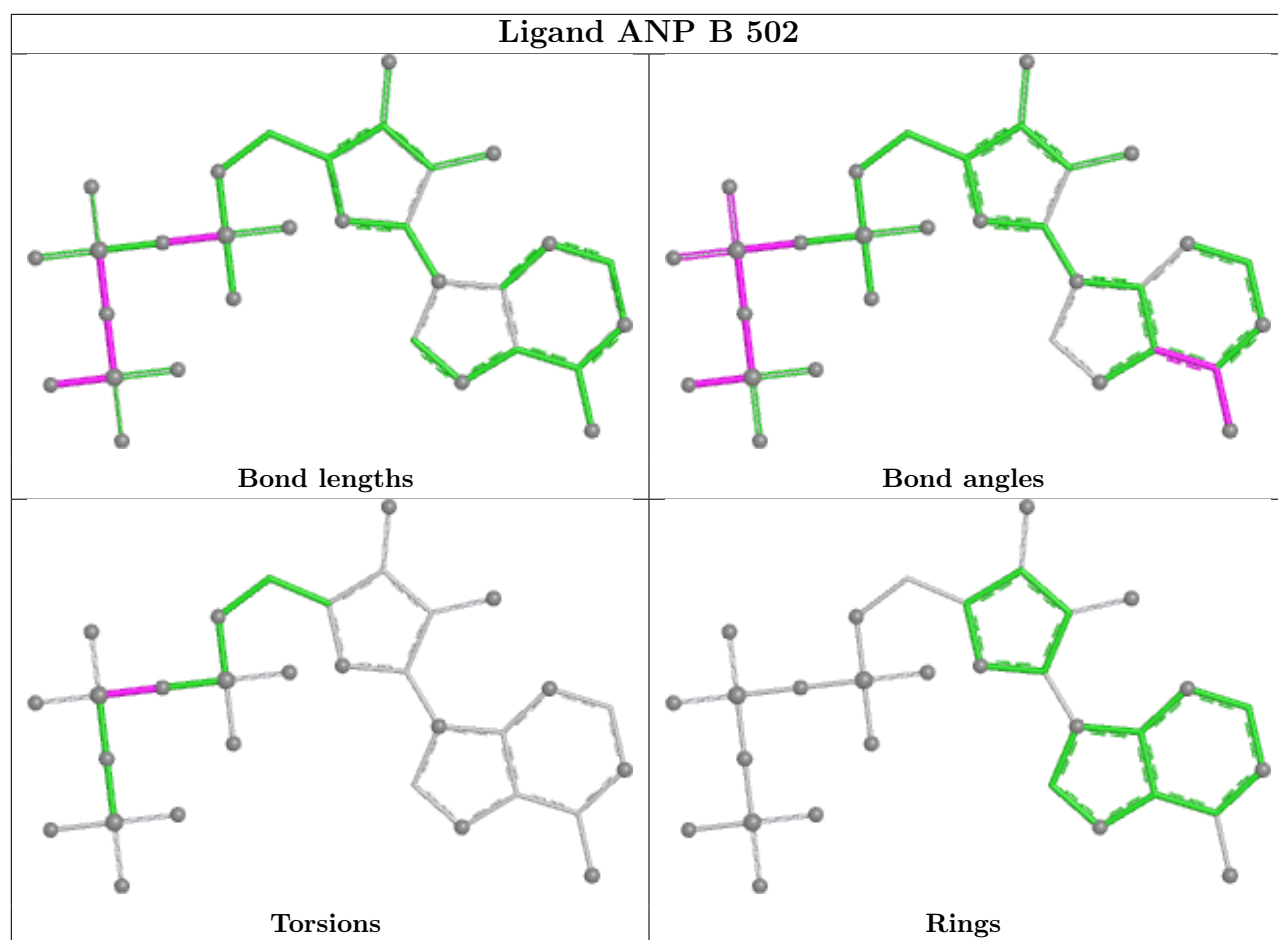
Ligand A1BB1 X 101



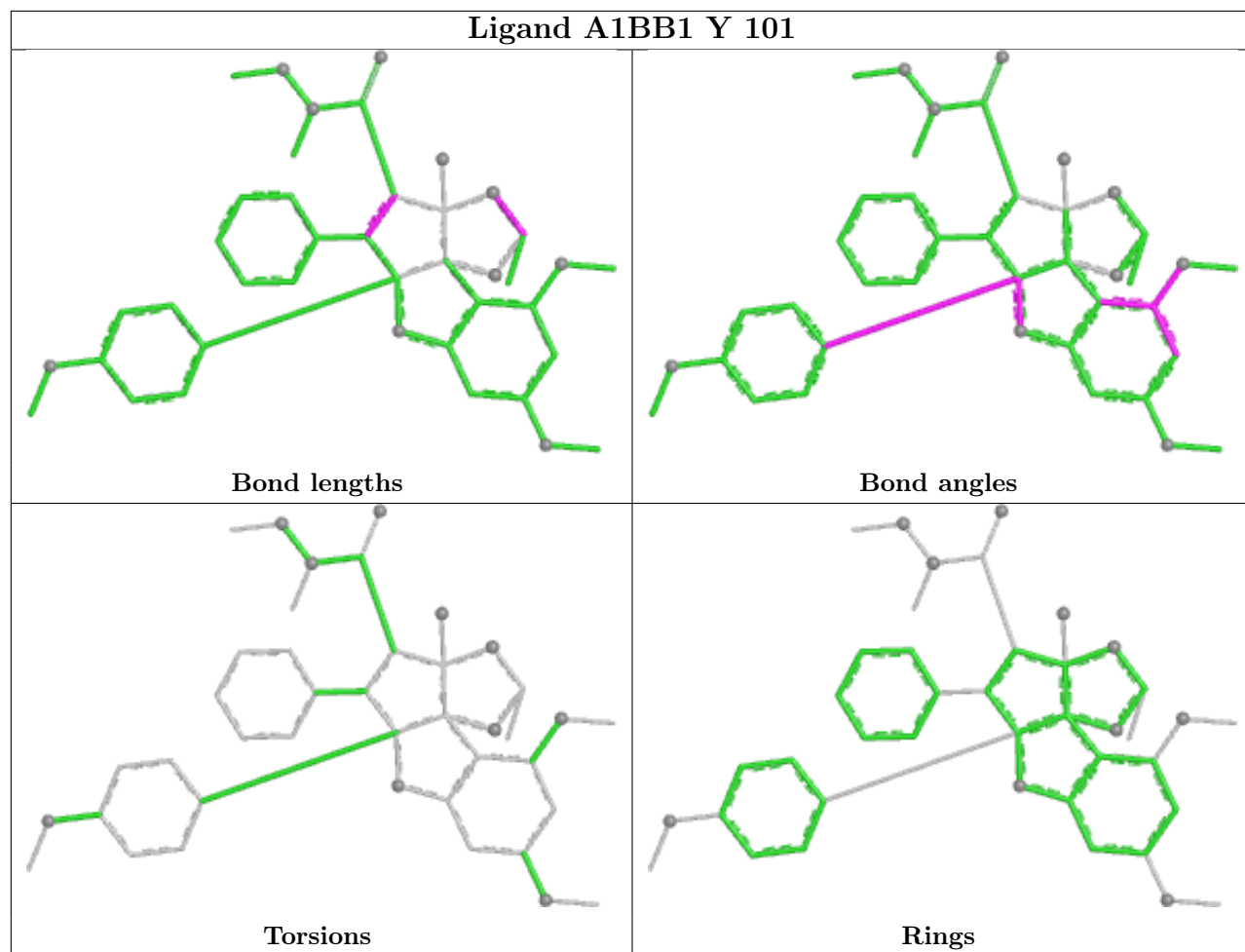


Ligand A1BB1 W 101

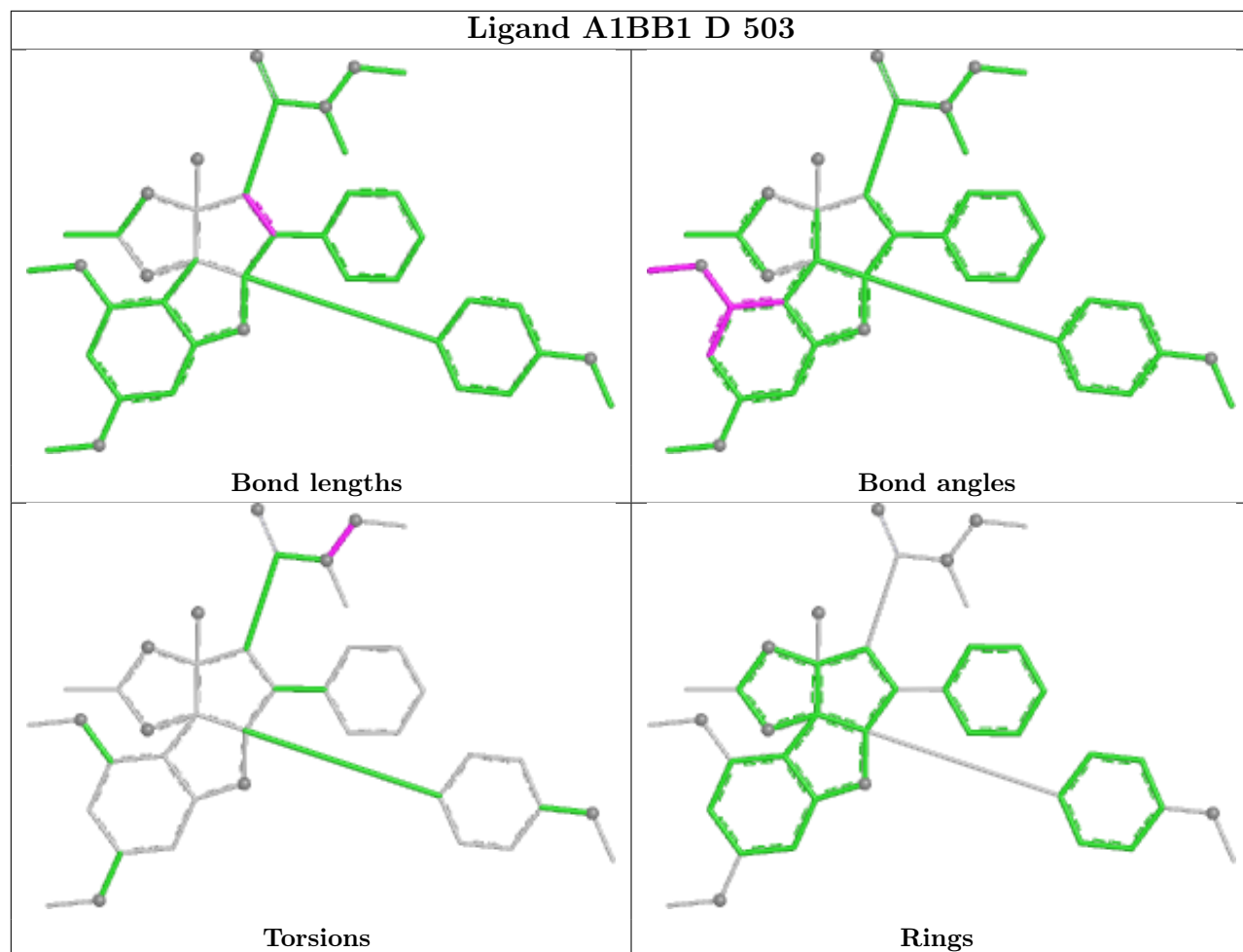


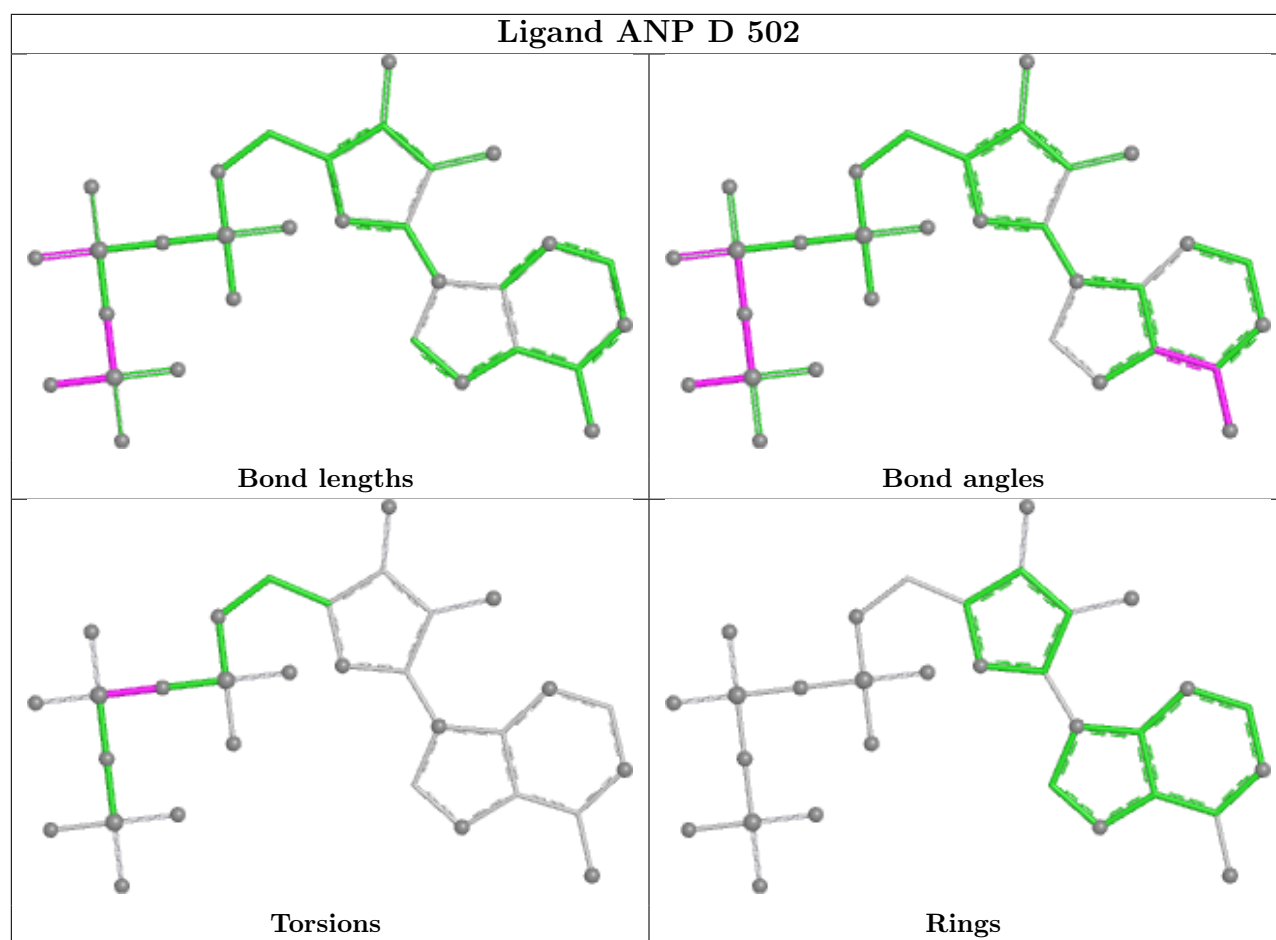


Ligand A1BB1 Y 101



Ligand A1BB1 D 503





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	378/388 (97%)	0.52	30 (7%)	20 20	15, 37, 68, 95	5 (1%)
1	B	373/388 (96%)	0.49	26 (6%)	24 24	13, 36, 66, 85	2 (0%)
1	C	378/388 (97%)	0.45	22 (5%)	30 31	16, 36, 67, 91	6 (1%)
1	D	374/388 (96%)	1.10	81 (21%)	3 2	16, 46, 88, 117	2 (0%)
2	W	8/10 (80%)	0.39	2 (25%)	2 2	25, 31, 69, 85	0
2	X	8/10 (80%)	0.37	1 (12%)	9 8	26, 35, 65, 82	0
2	Y	8/10 (80%)	0.26	1 (12%)	9 8	28, 33, 69, 90	0
2	Z	8/10 (80%)	0.94	2 (25%)	2 2	31, 44, 74, 87	0
All	All	1535/1592 (96%)	0.64	165 (10%)	12 12	13, 38, 78, 117	15 (0%)

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	365	ARG	6.1
1	D	366	PHE	5.9
1	D	258	TRP	5.3
1	D	390	PHE	5.2
1	A	272	ILE	4.8

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

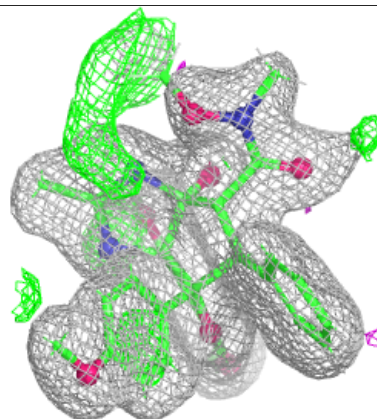
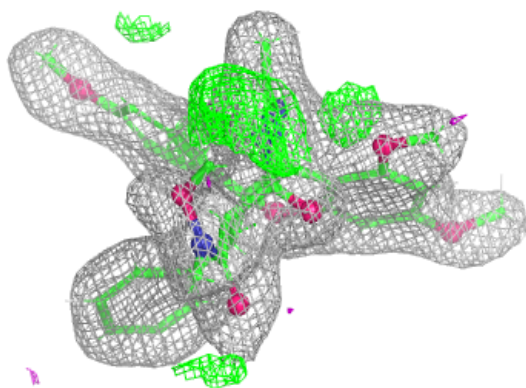
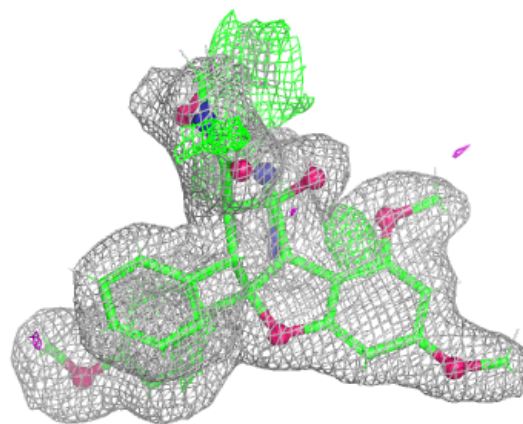
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	A1BB1	D	503	41/41	0.92	0.10	22,34,58,77	0
5	A1BB1	W	101	41/41	0.95	0.08	22,28,44,48	0
5	A1BB1	X	101	41/41	0.95	0.08	19,28,45,49	0
5	A1BB1	Y	101	41/41	0.95	0.09	23,32,49,59	0
4	ANP	D	502	31/31	0.97	0.07	23,29,38,42	0
4	ANP	C	502	31/31	0.98	0.05	20,28,35,38	0
4	ANP	A	502	31/31	0.98	0.06	22,30,36,39	0
4	ANP	B	502	31/31	0.98	0.05	18,24,30,34	0
3	MG	A	501	1/1	0.99	0.06	23,23,23,23	0
3	MG	B	501	1/1	0.99	0.05	21,21,21,21	0
3	MG	C	501	1/1	0.99	0.03	20,20,20,20	0
3	MG	D	501	1/1	0.99	0.03	22,22,22,22	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.

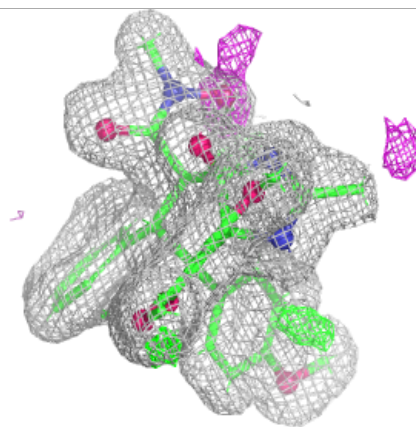
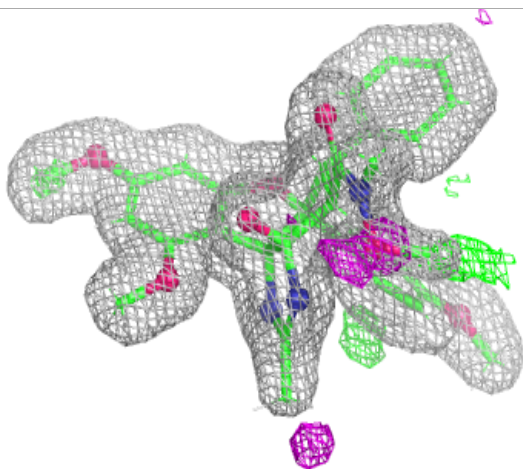
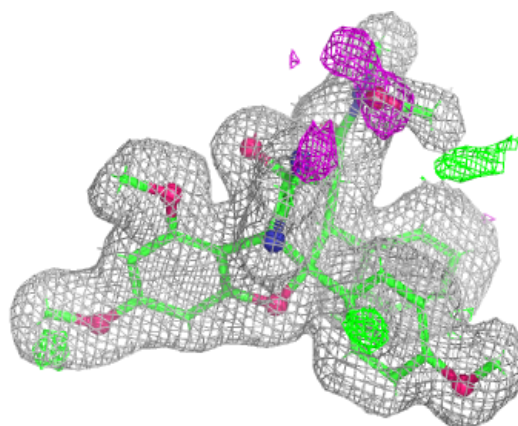
Electron density around A1BB1 D 503:

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



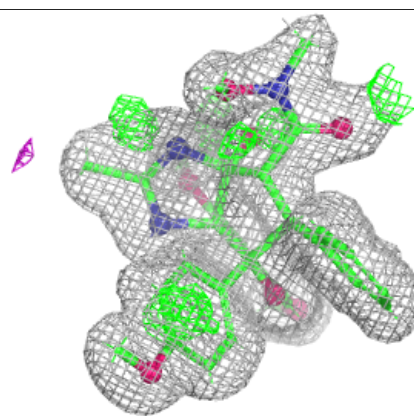
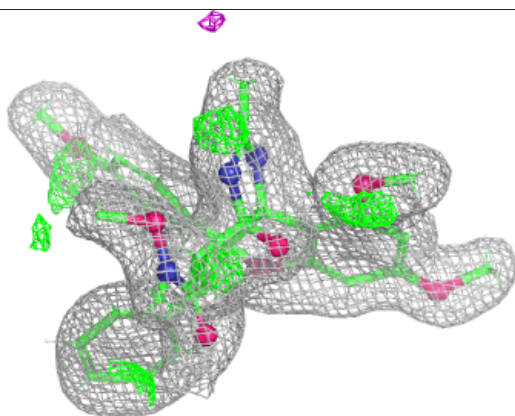
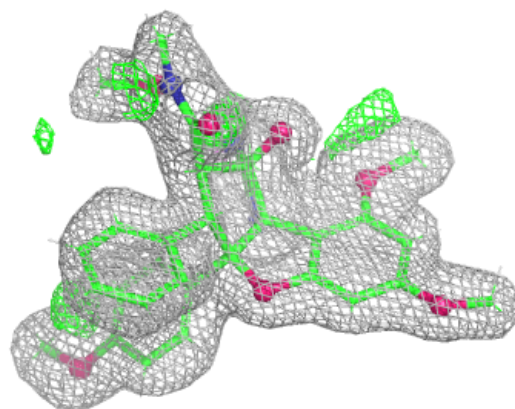
Electron density around A1BB1 W 101:

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

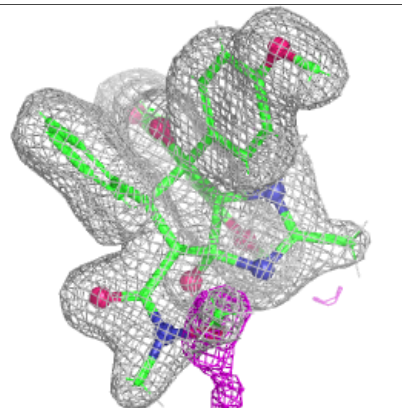
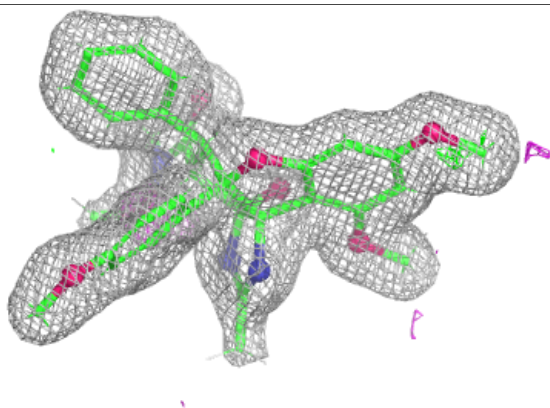
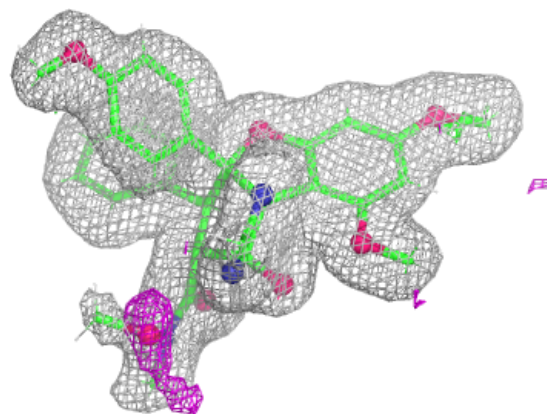


Electron density around A1BB1 X 101:

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

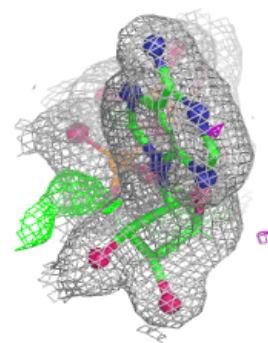
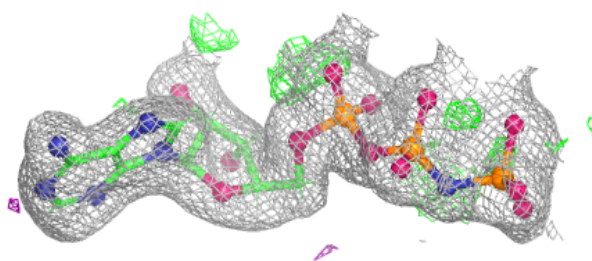
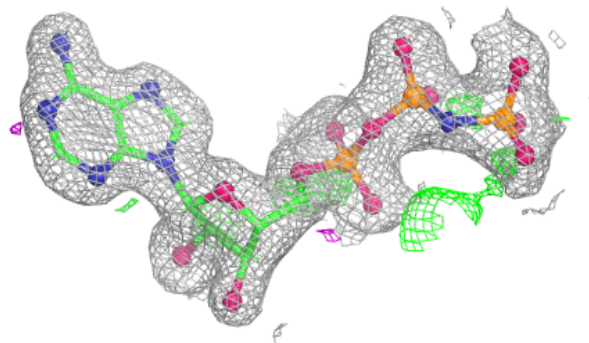
**Electron density around A1BB1 Y 101:**

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

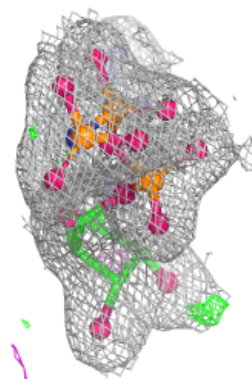
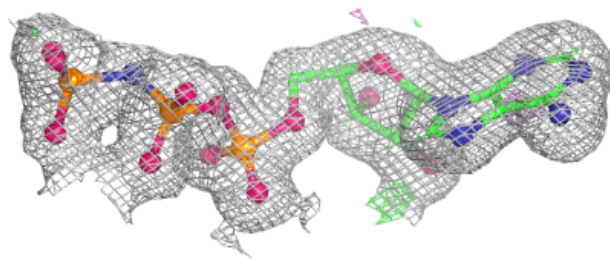
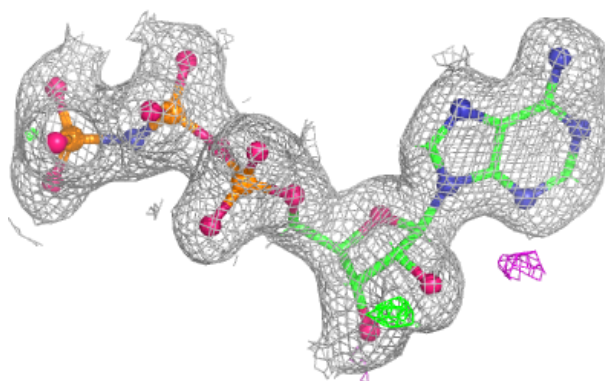


Electron density around ANP D 502:

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

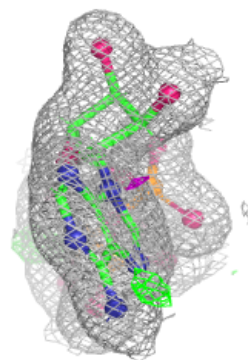
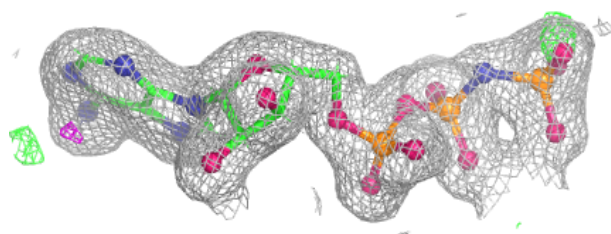
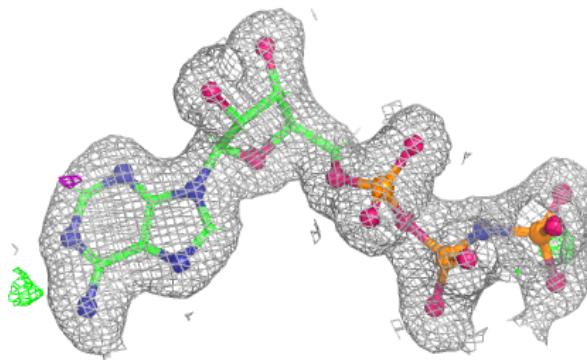
**Electron density around ANP C 502:**

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

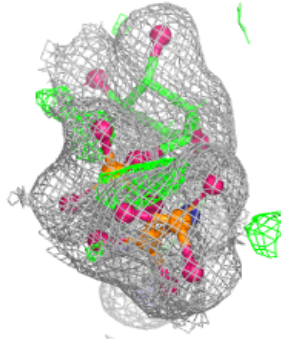
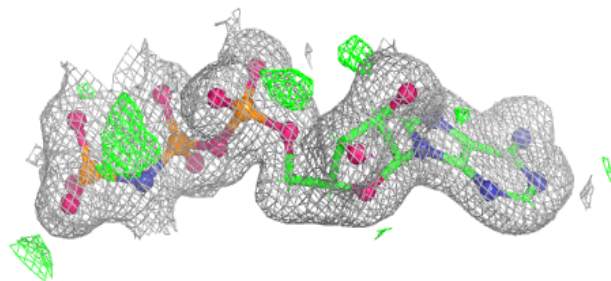
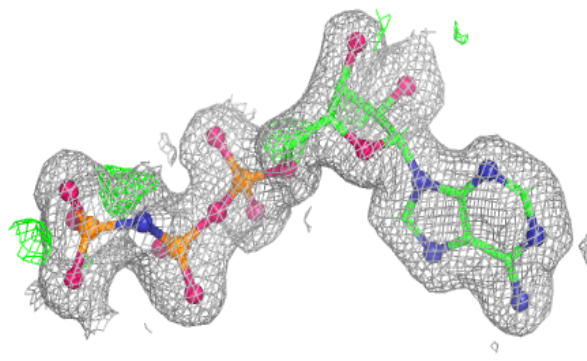


Electron density around ANP A 502:

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

**Electron density around ANP B 502:**

$2mF_o-DF_c$ (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.