



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2021 – 07:29 am BST

PDB ID : 7AKR  
Title : Human ADP-ribosylserine hydrolase ARH3 mutant E41A in complex with ADP-ribose dimer  
Authors : Ariza, A.  
Deposited on : 2020-10-02  
Resolution : 1.95 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](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	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

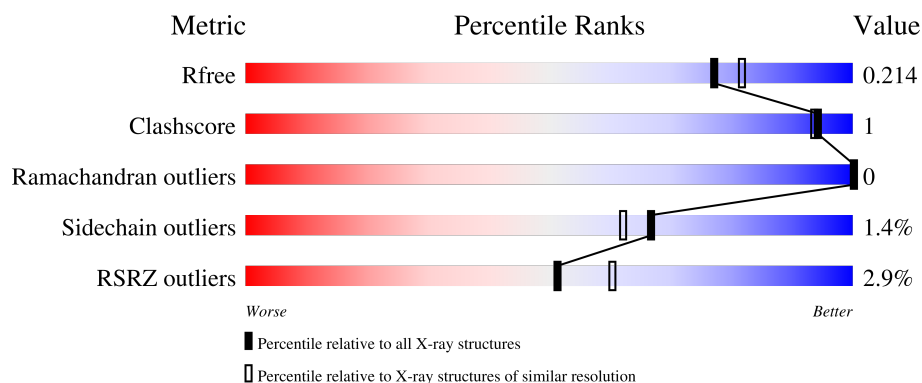
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	AAA	349	<div> <div>%</div> <div>95%</div> </div>
1	BBB	349	<div> <div>4%</div> <div>92%</div> </div>
1	CCC	349	<div> <div>%</div> <div>97%</div> </div>
1	DDD	349	<div> <div>5%</div> <div>92%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11206 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 ADP-ribose glycohydrolase ARH3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	344	Total	C	N	O	S	0	4	0
			2647	1654	454	525	14			
1	BBB	334	Total	C	N	O	S	0	3	0
			2568	1609	439	506	14			
1	CCC	344	Total	C	N	O	S	0	5	0
			2652	1657	455	526	14			
1	DDD	335	Total	C	N	O	S	0	2	0
			2574	1611	441	508	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	15	GLY	-	expression tag	UNP Q9NX46
AAA	16	PRO	-	expression tag	UNP Q9NX46
AAA	17	GLY	-	expression tag	UNP Q9NX46
AAA	18	SER	-	expression tag	UNP Q9NX46
AAA	41	ALA	GLU	engineered mutation	UNP Q9NX46
BBB	15	GLY	-	expression tag	UNP Q9NX46
BBB	16	PRO	-	expression tag	UNP Q9NX46
BBB	17	GLY	-	expression tag	UNP Q9NX46
BBB	18	SER	-	expression tag	UNP Q9NX46
BBB	41	ALA	GLU	engineered mutation	UNP Q9NX46
CCC	15	GLY	-	expression tag	UNP Q9NX46
CCC	16	PRO	-	expression tag	UNP Q9NX46
CCC	17	GLY	-	expression tag	UNP Q9NX46
CCC	18	SER	-	expression tag	UNP Q9NX46
CCC	41	ALA	GLU	engineered mutation	UNP Q9NX46
DDD	15	GLY	-	expression tag	UNP Q9NX46
DDD	16	PRO	-	expression tag	UNP Q9NX46
DDD	17	GLY	-	expression tag	UNP Q9NX46
DDD	18	SER	-	expression tag	UNP Q9NX46
DDD	41	ALA	GLU	engineered mutation	UNP Q9NX46

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | AAA   | 2        | Total Mg<br>2 2 | 0       | 0       |
| 2   | BBB   | 2        | Total Mg<br>2 2 | 0       | 0       |
| 2   | CCC   | 2        | Total Mg<br>2 2 | 0       | 0       |
| 2   | DDD   | 2        | Total Mg<br>2 2 | 0       | 0       |

- # AR6
- 
- The chemical structure of AR6 is a complex molecule. It features a purine base (top) connected to a ribose sugar (middle) via a glycosidic bond. The ribose sugar is further connected to a pyranose sugar (bottom) via a phosphate group. The purine base is labeled with atoms N1, C2, N3, C4, C5, N7, C8, and N9. The ribose sugar is labeled with atoms C1', C2', C3', C4', and C5'. The pyranose sugar is labeled with atoms C1, C2, C3, C4, and C5. The phosphate group is labeled with atoms P1, P2, and P3. The molecule is shown in a 3D representation with stereochemistry indicated by wedge and dash bonds.
- Nc1ncnc2c1ncn2[C@@H]3O[C@H](COP(=O)(O)OP(=O)(O)OP(=O)(O)O)[C@H](O)[C@@H](O)[C@H]3O

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total 35	C 15	N 5	O 13	P 2	0	0
3	AAA	1	Total 24	C 10	N 5	O 7	P 2	0	0
3	BBB	1	Total 35	C 15	N 5	O 13	P 2	0	0
3	BBB	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	CCC	1	Total 35	C 15	N 5	O 13	P 2	0	0



WORLD WIDE  
PDB  
PROTEIN DATA BANK

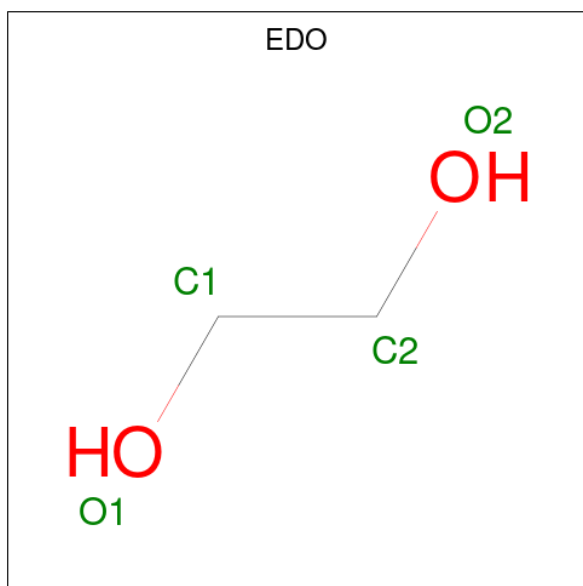
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	CCC	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	DDD	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	DDD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		
4	BBB	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	179	Total O 179 179	0	0
6	BBB	82	Total O 82 82	0	0
6	CCC	114	Total O 115 115	0	1
6	DDD	62	Total O 62 62	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.

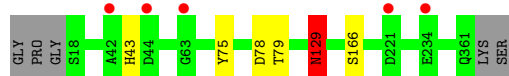
- Molecule 1: ADP-ribose glycohydrolase ARH3



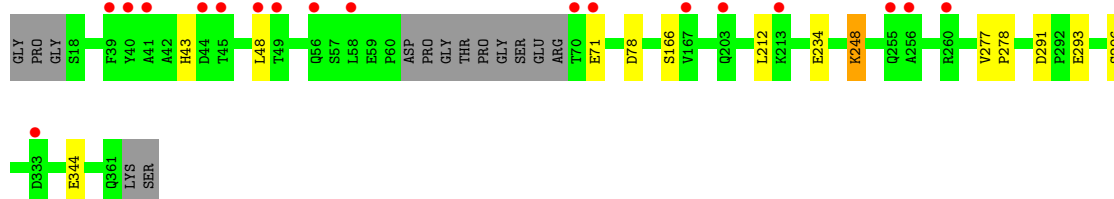
- Molecule 1: ADP-ribose glycohydrolase ARH3



- Molecule 1: ADP-ribose glycohydrolase ARH3



- Molecule 1: ADP-ribose glycohydrolase ARH3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.62Å 91.60Å 91.09Å 90.00° 105.47° 90.00°	Depositor
Resolution (Å)	70.63 – 1.95 70.63 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.63-1.95) 92.4 (70.63-1.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.187 , 0.211 0.192 , 0.214	Depositor DCC
$R_{free}$ test set	4757 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: MG, CL, EDO, 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	AAA	0.69	0/2705	0.76	0/3659
1	BBB	0.69	0/2622	0.75	1/3542 (0.0%)
1	CCC	0.68	0/2713	0.74	1/3670 (0.0%)
1	DDD	0.66	0/2623	0.72	0/3545
All	All	0.68	0/10663	0.74	2/14416 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	129	ASN	CB-CA-C	5.03	120.45	110.40
1	CCC	129	ASN	CB-CA-C	5.03	120.45	110.40

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	AAA	2647	0	2567	10	0
1	BBB	2568	0	2502	8	0
1	CCC	2652	0	2573	2	0
1	DDD	2574	0	2496	7	0
2	AAA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	2	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	2	0	0	0	0
3	AAA	59	0	28	2	0
3	BBB	62	0	28	0	0
3	CCC	62	0	28	0	0
3	DDD	62	0	28	1	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	1	0
5	AAA	28	0	42	3	0
5	BBB	8	0	12	0	0
5	CCC	20	0	30	0	0
5	DDD	16	0	24	0	0
6	AAA	179	0	0	1	0
6	BBB	82	0	0	1	0
6	CCC	115	0	0	1	0
6	DDD	62	0	0	0	0
All	All	11206	0	10358	27	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 1.

All (27) 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:BBB:213:LYS:HG2	1:DDD:296:SER:HB3	1.59	0.85
1:AAA:71:GLU:OE2	1:BBB:18:SER:HA	1.86	0.76
1:CCC:129:ASN:ND2	6:CCC:501:HOH:O	2.25	0.69
1:DDD:71:GLU:HB3	1:DDD:344:GLU:HA	1.76	0.68
1:BBB:248[A]:LYS:HE3	1:BBB:266:GLU:OE1	1.97	0.63
1:AAA:27:LEU:HD13	5:AAA:406:EDO:H11	1.83	0.58
1:AAA:83:ARG:HG3	5:AAA:406:EDO:H22	1.85	0.58
1:AAA:230:LEU:C	1:AAA:230:LEU:HD23	2.29	0.53
1:AAA:44:ASP:OD1	5:AAA:409:EDO:H11	2.14	0.47
3:AAA:404:AR6:C5'	3:AAA:404:AR6:PB	3.03	0.47
1:AAA:230:LEU:CD2	6:AAA:534:HOH:O	2.64	0.45
1:BBB:133:ARG:NH1	4:BBB:405:CL:CL	2.83	0.44
1:AAA:43:HIS:O	1:AAA:44:ASP:HB3	2.18	0.43
1:AAA:49:THR:HG22	1:AAA:53:ARG:NH1	2.34	0.43
3:DDD:404:AR6:PB	3:DDD:404:AR6:H5'A	2.58	0.43
1:DDD:48:LEU:CD2	1:DDD:293:GLU:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AAA:404:AR6:PB	3:AAA:404:AR6:H5'A	2.59	0.42
1:DDD:212:LEU:HD23	1:DDD:212:LEU:HA	1.89	0.42
1:CCC:75:TYR:HB2	1:CCC:79:THR:HB	2.01	0.42
1:AAA:48:LEU:CD2	1:AAA:293:GLU:HB3	2.50	0.42
1:BBB:212:LEU:HD23	1:BBB:212:LEU:HA	1.89	0.41
1:BBB:277:VAL:HB	1:BBB:278:PRO:HD3	2.02	0.41
1:DDD:277:VAL:HB	1:DDD:278:PRO:HD3	2.01	0.41
1:BBB:213:LYS:NZ	1:DDD:291:ASP:O	2.43	0.40
1:DDD:248:LYS:HE3	1:DDD:248:LYS:HB2	1.92	0.40
1:BBB:144[A]:ASN:ND2	6:BBB:504:HOH:O	2.54	0.40
1:AAA:277:VAL:HB	1:AAA:278:PRO:HD3	2.04	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	AAA	346/349 (99%)	338 (98%)	8 (2%)	0	100	100
1	BBB	333/349 (95%)	327 (98%)	6 (2%)	0	100	100
1	CCC	347/349 (99%)	340 (98%)	7 (2%)	0	100	100
1	DDD	333/349 (95%)	328 (98%)	5 (2%)	0	100	100
All	All	1359/1396 (97%)	1333 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	280/279 (100%)	278 (99%)	2 (1%)	84	82
1	BBB	271/279 (97%)	267 (98%)	4 (2%)	65	60
1	CCC	281/279 (101%)	277 (99%)	4 (1%)	67	62
1	DDD	271/279 (97%)	266 (98%)	5 (2%)	59	53
All	All	1103/1116 (99%)	1088 (99%)	15 (1%)	67	62

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	78	ASP
1	AAA	166	SER
1	BBB	43	HIS
1	BBB	78	ASP
1	BBB	129	ASN
1	BBB	166	SER
1	CCC	43	HIS
1	CCC	78	ASP
1	CCC	129	ASN
1	CCC	166	SER
1	DDD	43	HIS
1	DDD	78	ASP
1	DDD	166	SER
1	DDD	234	GLU
1	DDD	248	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 36 ligands modelled in this entry, 10 are monoatomic - leaving 26 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	$\# Z  > 2$
3	AR6	BBB	404	3	24,29,39	0.69	0	29,45,60	0.91	2 (6%)
3	AR6	DDD	403	2,3	33,38,39	0.62	0	37,58,60	0.92	1 (2%)
5	EDO	CCC	408	-	3,3,3	0.12	0	2,2,2	0.19	0
3	AR6	BBB	403	2,3	33,38,39	0.66	0	37,58,60	0.93	2 (5%)
5	EDO	AAA	409	-	3,3,3	0.15	0	2,2,2	0.24	0
5	EDO	DDD	405	-	3,3,3	0.17	0	2,2,2	0.77	0
3	AR6	AAA	403	2,3	33,38,39	0.70	0	37,58,60	0.78	0
5	EDO	AAA	411	-	3,3,3	0.25	0	2,2,2	0.34	0
5	EDO	AAA	412	-	3,3,3	0.03	0	2,2,2	0.05	0
5	EDO	CCC	406	-	3,3,3	0.24	0	2,2,2	0.65	0
3	AR6	AAA	404	3	21,26,39	0.72	0	24,39,60	0.78	1 (4%)
3	AR6	CCC	403	2,3	33,38,39	0.59	0	37,58,60	0.86	2 (5%)
5	EDO	BBB	407	-	3,3,3	0.16	0	2,2,2	0.17	0
5	EDO	DDD	407	-	3,3,3	0.04	0	2,2,2	0.07	0
5	EDO	DDD	406	-	3,3,3	0.17	0	2,2,2	0.27	0
5	EDO	AAA	410	-	3,3,3	0.06	0	2,2,2	0.31	0
5	EDO	CCC	407	-	3,3,3	0.12	0	2,2,2	0.42	0
5	EDO	AAA	408	-	3,3,3	0.04	0	2,2,2	0.18	0
5	EDO	CCC	405	-	3,3,3	0.15	0	2,2,2	0.43	0
5	EDO	BBB	406	-	3,3,3	0.27	0	2,2,2	0.47	0
5	EDO	CCC	409	-	3,3,3	0.08	0	2,2,2	0.36	0
5	EDO	DDD	408	-	3,3,3	0.07	0	2,2,2	0.17	0
3	AR6	CCC	404	3	24,29,39	0.74	0	29,45,60	0.94	2 (6%)
5	EDO	AAA	407	-	3,3,3	0.22	0	2,2,2	0.19	0
3	AR6	DDD	404	3	24,29,39	1.00	1 (4%)	29,45,60	1.11	2 (6%)
5	EDO	AAA	406	-	3,3,3	0.31	0	2,2,2	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AR6	BBB	404	3	-	3/12/32/54	0/3/3/4
3	AR6	DDD	403	2,3	-	4/18/51/54	0/4/4/4
5	EDO	CCC	408	-	-	1/1/1/1	-
3	AR6	BBB	403	2,3	-	2/18/51/54	0/4/4/4
5	EDO	AAA	409	-	-	1/1/1/1	-
5	EDO	DDD	405	-	-	0/1/1/1	-
3	AR6	AAA	403	2,3	-	3/18/51/54	0/4/4/4
5	EDO	AAA	411	-	-	1/1/1/1	-
5	EDO	AAA	412	-	-	1/1/1/1	-
5	EDO	CCC	406	-	-	0/1/1/1	-
3	AR6	AAA	404	3	-	0/6/29/54	0/3/3/4
3	AR6	CCC	403	2,3	-	4/18/51/54	0/4/4/4
5	EDO	BBB	407	-	-	1/1/1/1	-
5	EDO	DDD	407	-	-	1/1/1/1	-
5	EDO	DDD	406	-	-	1/1/1/1	-
5	EDO	AAA	410	-	-	1/1/1/1	-
5	EDO	CCC	407	-	-	0/1/1/1	-
5	EDO	AAA	408	-	-	1/1/1/1	-
5	EDO	CCC	405	-	-	1/1/1/1	-
5	EDO	BBB	406	-	-	0/1/1/1	-
5	EDO	CCC	409	-	-	0/1/1/1	-
5	EDO	DDD	408	-	-	1/1/1/1	-
3	AR6	CCC	404	3	-	6/12/32/54	0/3/3/4
5	EDO	AAA	407	-	-	1/1/1/1	-
3	AR6	DDD	404	3	-	5/12/32/54	0/3/3/4
5	EDO	AAA	406	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DDD	404	AR6	PB-O2B	3.41	1.61	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DDD	403	AR6	O4D-C4D-C3D	2.74	107.13	104.70
3	DDD	404	AR6	PA-O3A-PB	2.63	141.84	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	404	AR6	PA-O3A-PB	2.44	141.22	132.83
3	DDD	404	AR6	O5D-PB-O1B	2.39	116.78	107.64
3	CCC	403	AR6	O4D-C4D-C3D	2.32	106.76	104.70
3	BBB	404	AR6	C5-C6-N6	2.28	123.82	120.35
3	AAA	404	AR6	C5-C6-N6	2.23	123.74	120.35
3	BBB	403	AR6	O4D-C4D-C3D	2.19	106.64	104.70
3	BBB	404	AR6	O1B-PB-O2B	2.08	118.82	110.68
3	BBB	403	AR6	C5-C6-N6	2.07	123.49	120.35
3	CCC	403	AR6	C5-C6-N6	2.06	123.48	120.35
3	CCC	404	AR6	O1B-PB-O2B	2.02	118.59	110.68

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	403	AR6	PB-O3A-PA-O5'
3	BBB	404	AR6	C5'-O5'-PA-O1A
3	BBB	404	AR6	C5'-O5'-PA-O3A
3	CCC	403	AR6	PB-O3A-PA-O5'
3	CCC	404	AR6	PB-O3A-PA-O5'
3	CCC	404	AR6	C5'-O5'-PA-O1A
3	CCC	404	AR6	C5'-O5'-PA-O2A
3	CCC	404	AR6	C5'-O5'-PA-O3A
3	CCC	404	AR6	PA-O3A-PB-O1B
3	DDD	403	AR6	PB-O3A-PA-O5'
3	DDD	403	AR6	C5D-O5D-PB-O2B
3	DDD	404	AR6	PA-O3A-PB-O1B
3	DDD	404	AR6	PA-O3A-PB-O5D
5	AAA	408	EDO	O1-C1-C2-O2
5	AAA	412	EDO	O1-C1-C2-O2
5	AAA	409	EDO	O1-C1-C2-O2
5	AAA	410	EDO	O1-C1-C2-O2
5	CCC	408	EDO	O1-C1-C2-O2
5	DDD	408	EDO	O1-C1-C2-O2
5	AAA	411	EDO	O1-C1-C2-O2
3	DDD	404	AR6	PB-O3A-PA-O5'
3	CCC	403	AR6	PA-O3A-PB-O1B
3	BBB	404	AR6	C5'-O5'-PA-O2A
5	BBB	407	EDO	O1-C1-C2-O2
5	DDD	406	EDO	O1-C1-C2-O2
3	AAA	403	AR6	PA-O3A-PB-O1B
3	AAA	403	AR6	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	BBB	403	AR6	PA-O3A-PB-O1B
3	CCC	404	AR6	PA-O3A-PB-O2B
3	CCC	403	AR6	PA-O3A-PB-O2B
3	CCC	403	AR6	C4'-C5'-O5'-PA
3	DDD	403	AR6	PA-O3A-PB-O2B
3	DDD	404	AR6	PA-O3A-PB-O2B
5	CCC	405	EDO	O1-C1-C2-O2
5	DDD	407	EDO	O1-C1-C2-O2
3	DDD	403	AR6	C5D-O5D-PB-O3A
3	BBB	403	AR6	PA-O3A-PB-O2B
3	DDD	404	AR6	PB-O3A-PA-O1A
5	AAA	407	EDO	O1-C1-C2-O2

There are no ring outliers.

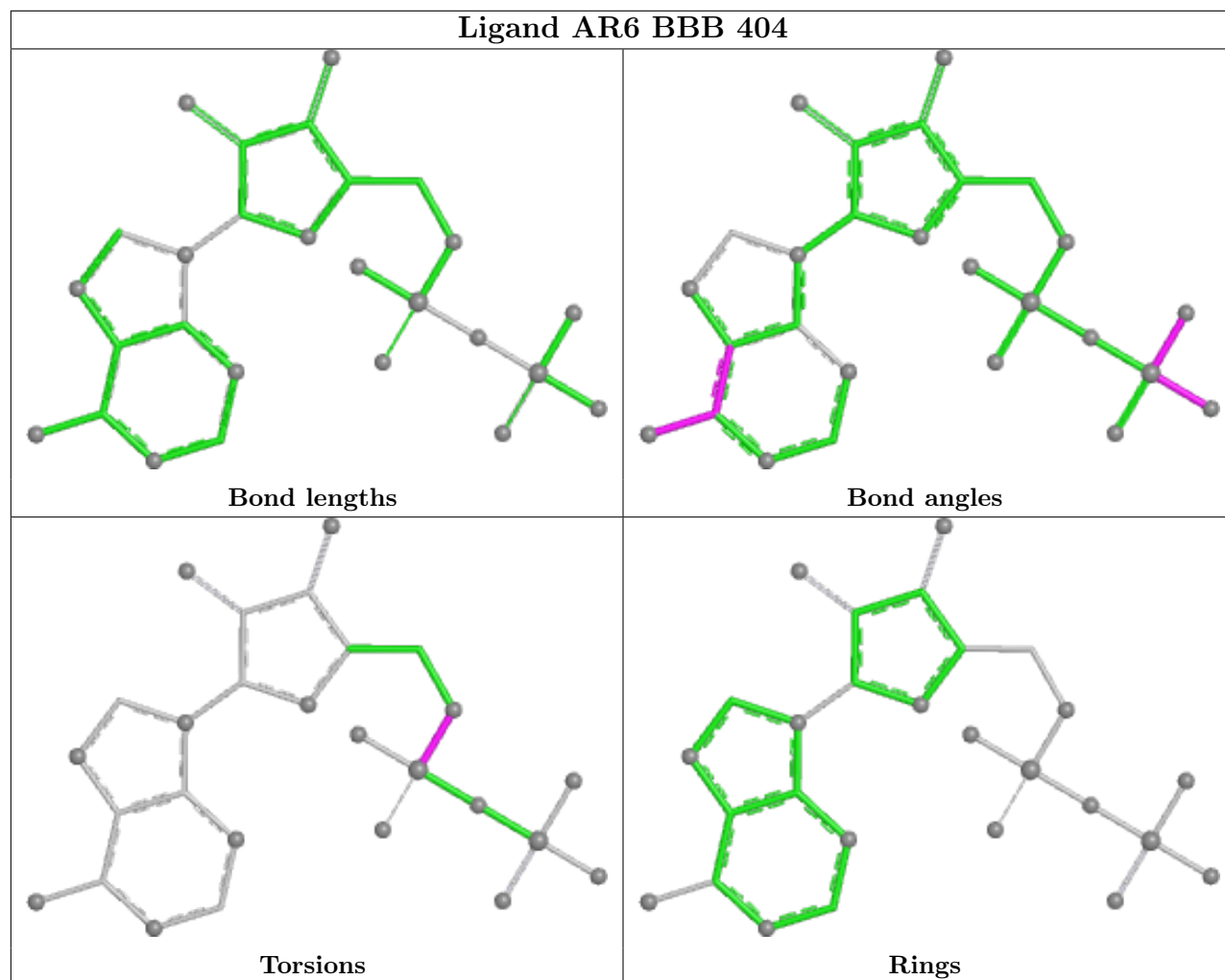
4 monomers are involved in 6 short contacts:

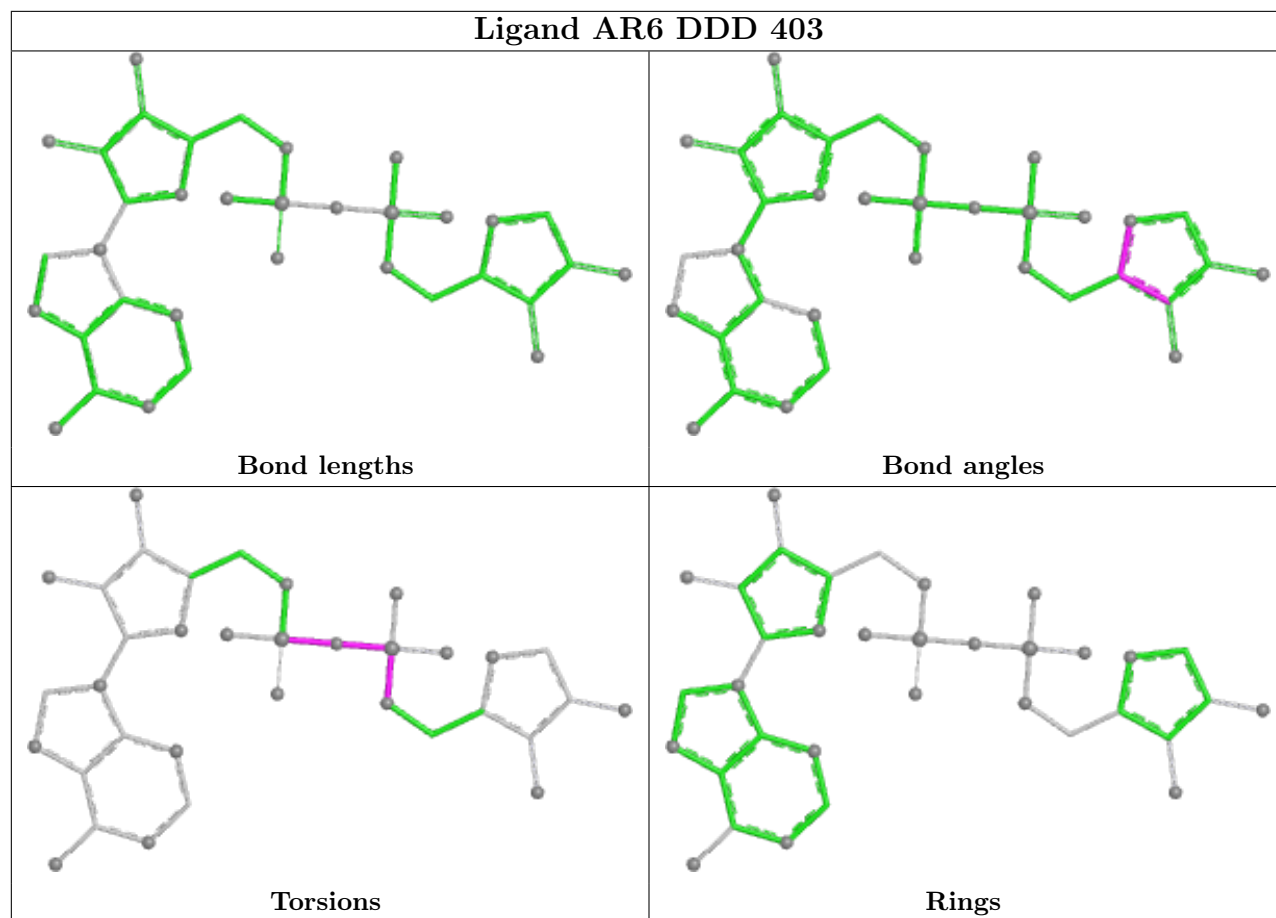
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	409	EDO	1	0
3	AAA	404	AR6	2	0
3	DDD	404	AR6	1	0
5	AAA	406	EDO	2	0

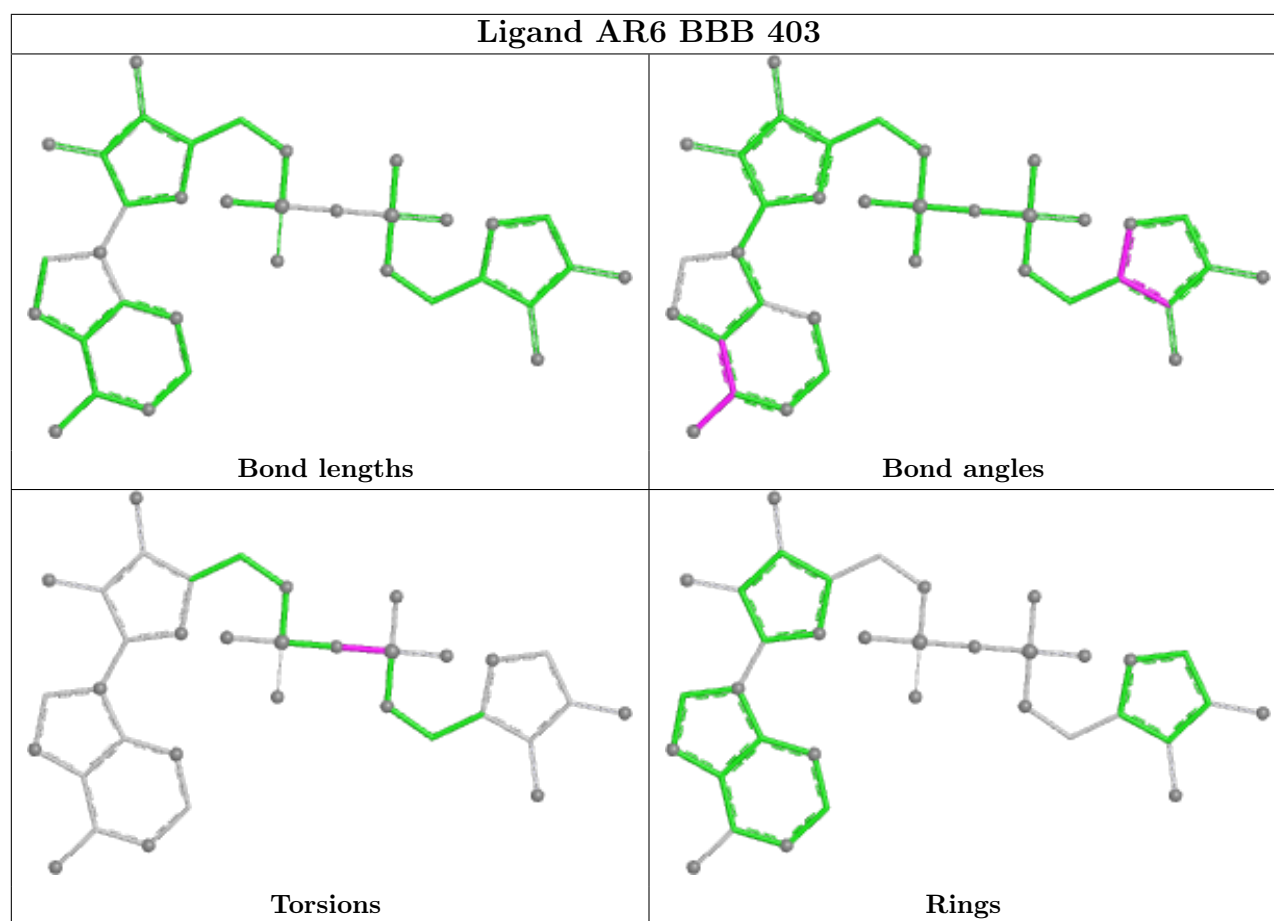
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



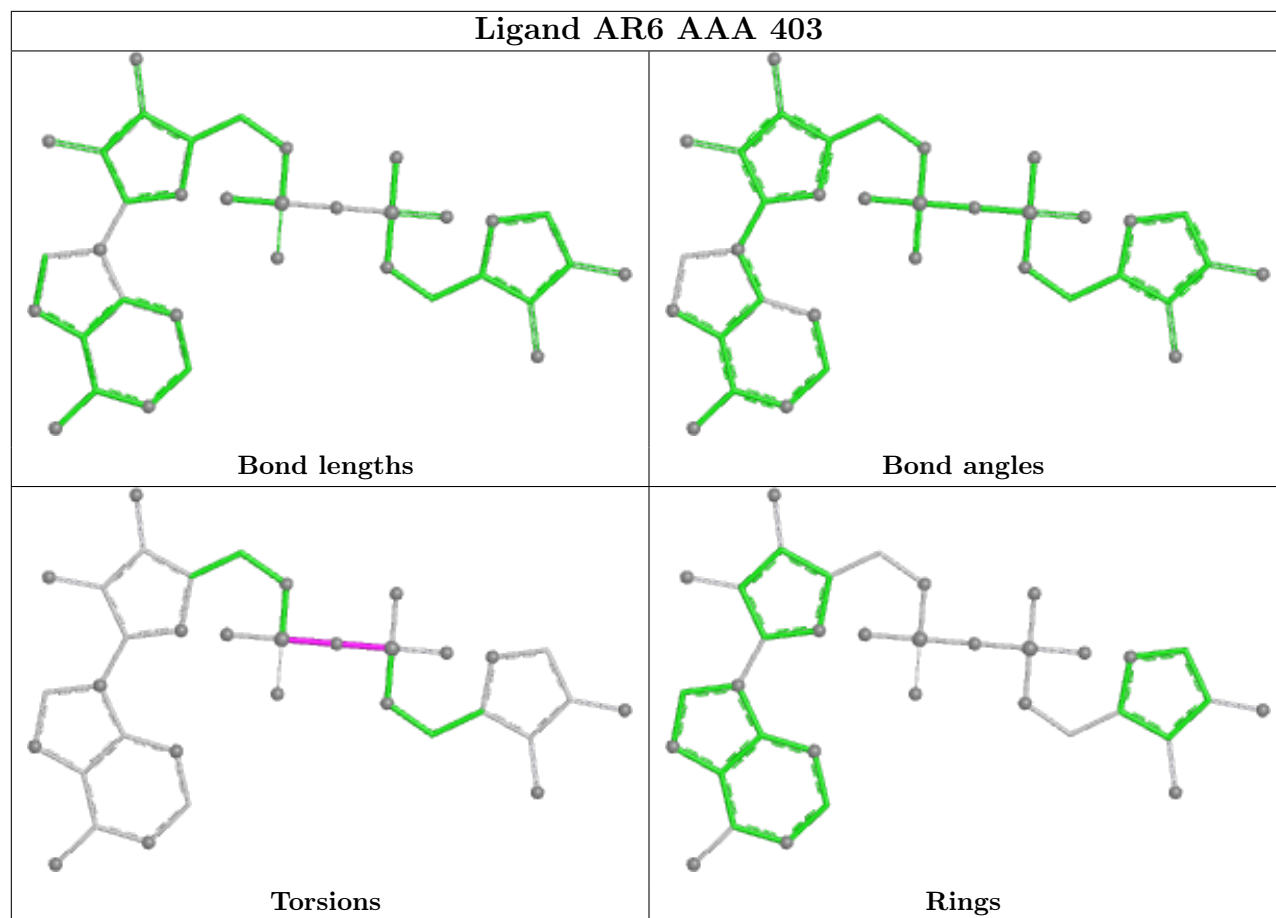
## Ligand AR6 BBB 404



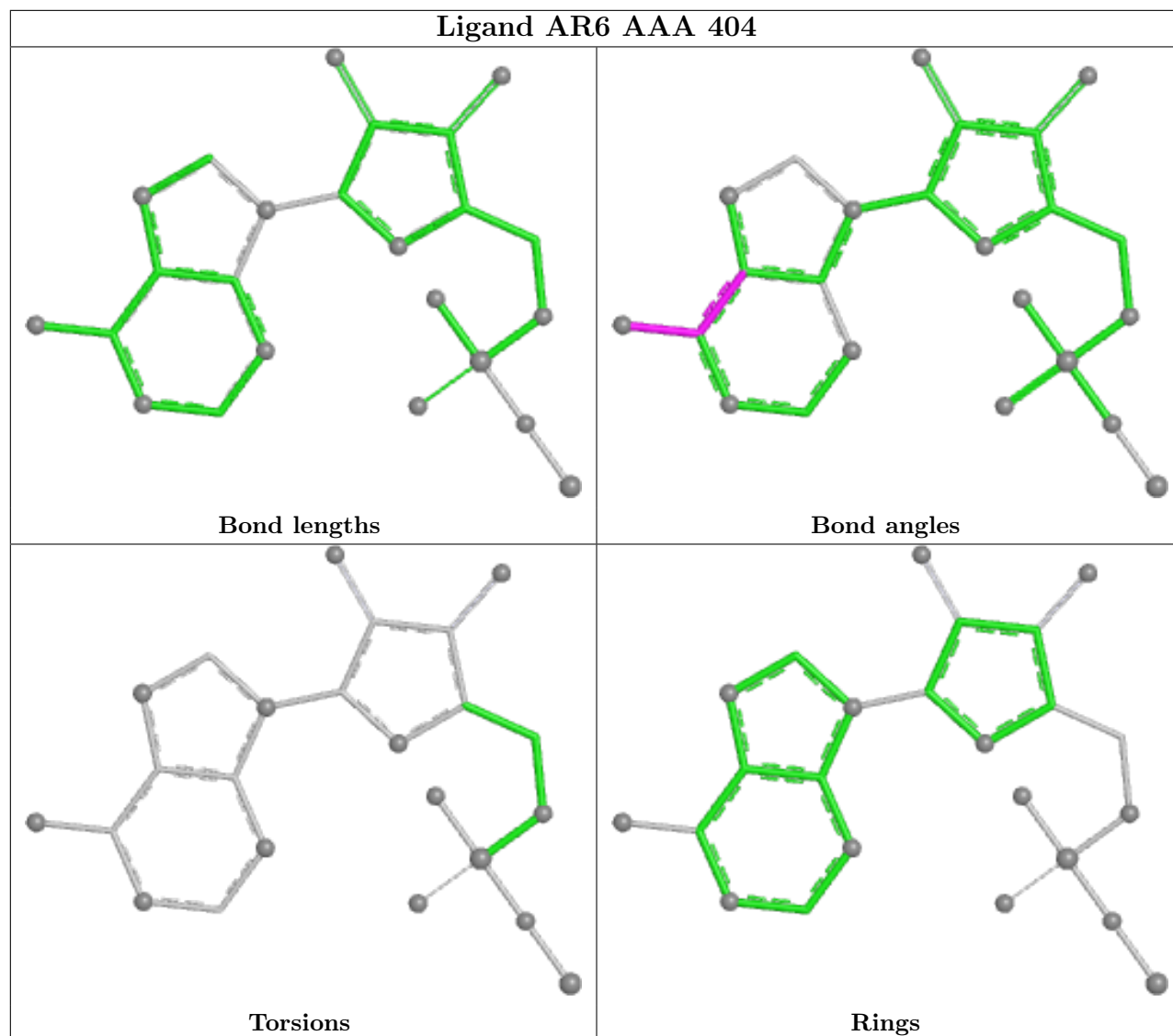


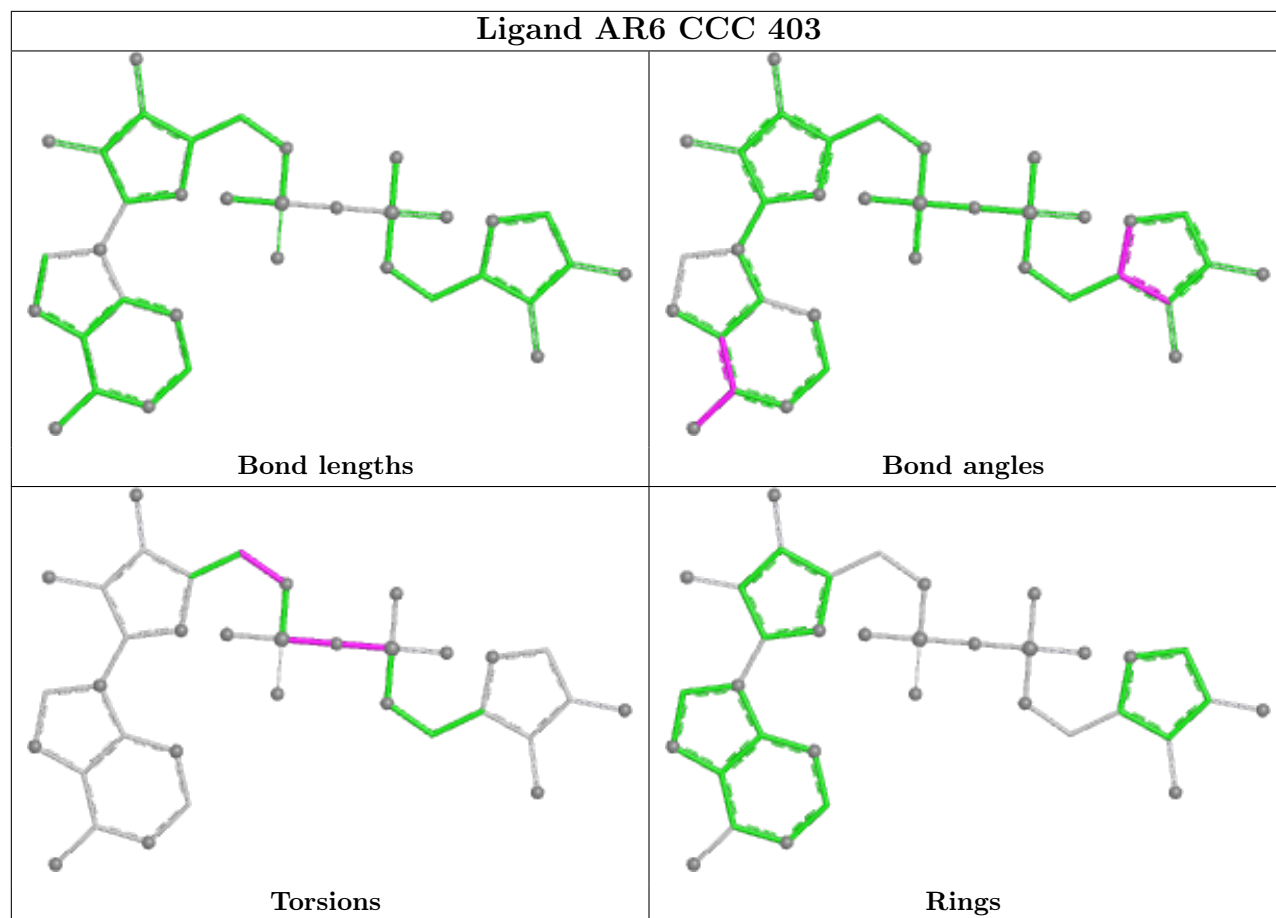


## Ligand AR6 AAA 403

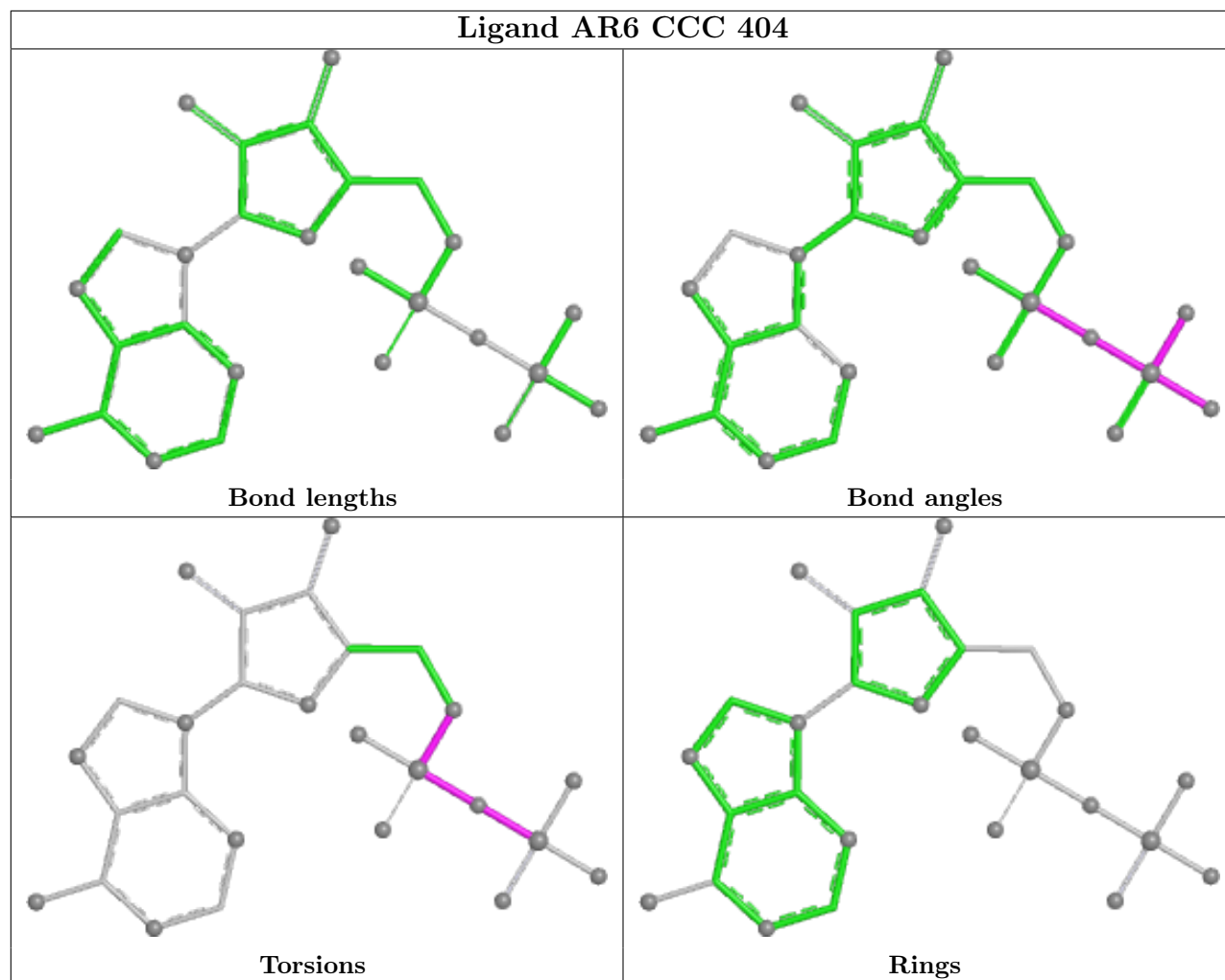


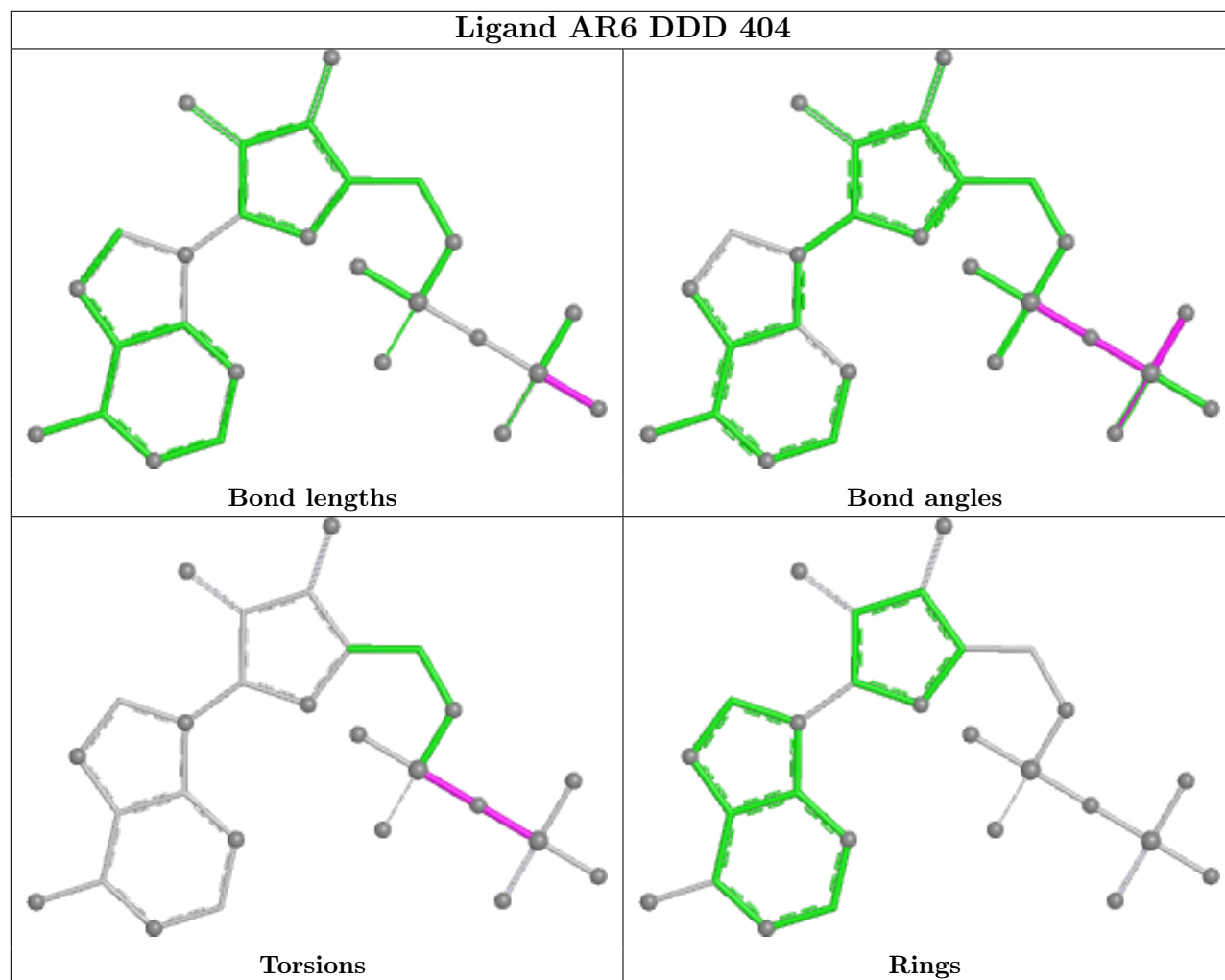
## Ligand AR6 AAA 404





## Ligand AR6 CCC 404





## 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	AAA	344/349 (98%)	0.09	3 (0%) 84 89	21, 32, 52, 65	0
1	BBB	334/349 (95%)	0.09	13 (3%) 39 49	29, 43, 80, 114	0
1	CCC	344/349 (98%)	0.01	5 (1%) 73 81	29, 41, 72, 91	0
1	DDD	335/349 (95%)	0.24	18 (5%) 25 34	37, 52, 85, 103	0
All	All	1357/1396 (97%)	0.11	39 (2%) 51 60	21, 42, 77, 114	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	44	ASP	8.8
1	DDD	44	ASP	6.5
1	BBB	42	ALA	5.5
1	DDD	70	THR	4.9
1	BBB	45	THR	4.7
1	DDD	256	ALA	4.6
1	BBB	59	GLU	3.7
1	CCC	63	GLY	3.6
1	DDD	58	LEU	3.5
1	DDD	45	THR	3.5
1	DDD	48	LEU	3.4
1	BBB	56	GLN	3.3
1	CCC	44	ASP	3.1
1	CCC	42	ALA	3.0
1	DDD	41	ALA	2.7
1	DDD	39	PHE	2.6
1	DDD	333	ASP	2.6
1	BBB	239	GLU	2.5
1	BBB	43	HIS	2.5
1	BBB	292	PRO	2.5
1	DDD	71	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	DDD	255	GLN	2.5
1	BBB	221	ASP	2.4
1	AAA	63	GLY	2.4
1	DDD	213	LYS	2.3
1	BBB	240	ARG	2.3
1	AAA	256	ALA	2.3
1	CCC	221	ASP	2.3
1	AAA	65	PRO	2.3
1	BBB	49	THR	2.3
1	BBB	53	ARG	2.3
1	DDD	260	ARG	2.3
1	DDD	167	VAL	2.2
1	BBB	47	ASP	2.2
1	DDD	203	GLN	2.2
1	CCC	234	GLU	2.1
1	DDD	40	TYR	2.0
1	DDD	56	GLN	2.0
1	DDD	49	THR	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<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	EDO	AAA	411	4/4	0.76	0.19	60,65,65,69	0
5	EDO	AAA	409	4/4	0.80	0.26	50,55,58,62	0
4	CL	AAA	405	1/1	0.81	0.07	61,61,61,61	0
5	EDO	AAA	408	4/4	0.83	0.14	58,58,59,59	0
5	EDO	DDD	408	4/4	0.85	0.13	68,69,69,70	0

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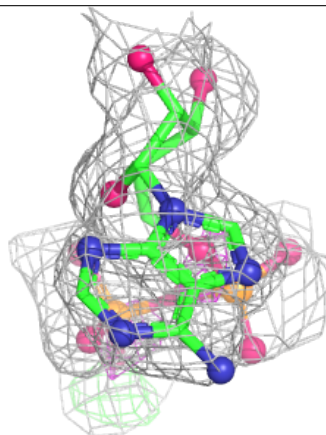
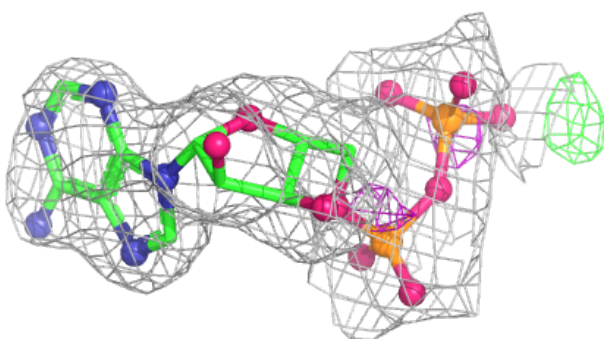
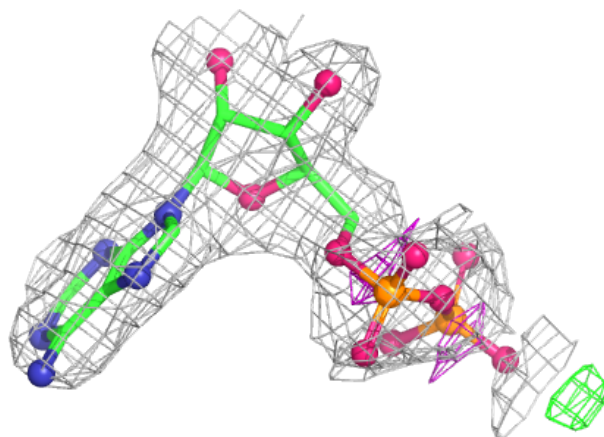
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	CCC	408	4/4	0.86	0.17	62,66,66,67	0
3	AR6	CCC	404	27/36	0.87	0.15	39,56,90,95	0
5	EDO	AAA	412	4/4	0.87	0.27	55,59,61,61	0
5	EDO	BBB	407	4/4	0.87	0.21	59,60,60,60	0
3	AR6	BBB	404	27/36	0.87	0.14	39,57,96,100	0
5	EDO	AAA	410	4/4	0.87	0.18	68,70,72,73	0
3	AR6	DDD	404	27/36	0.88	0.14	44,57,94,100	0
5	EDO	DDD	405	4/4	0.89	0.13	48,48,49,52	0
4	CL	BBB	405	1/1	0.92	0.12	67,67,67,67	0
5	EDO	CCC	409	4/4	0.92	0.14	51,52,53,54	0
5	EDO	DDD	406	4/4	0.93	0.25	52,53,54,56	0
5	EDO	AAA	406	4/4	0.93	0.23	39,42,44,44	0
5	EDO	CCC	405	4/4	0.94	0.17	54,55,57,57	0
5	EDO	BBB	406	4/4	0.94	0.12	46,46,46,47	0
2	MG	DDD	401	1/1	0.95	0.09	39,39,39,39	0
3	AR6	AAA	404	24/36	0.95	0.11	27,34,45,70	0
5	EDO	CCC	407	4/4	0.95	0.11	43,44,44,47	0
5	EDO	AAA	407	4/4	0.95	0.15	49,51,52,54	0
2	MG	CCC	402	1/1	0.96	0.03	29,29,29,29	0
5	EDO	DDD	407	4/4	0.96	0.10	62,63,63,64	0
2	MG	AAA	402	1/1	0.96	0.13	23,23,23,23	0
2	MG	DDD	402	1/1	0.97	0.06	42,42,42,42	0
2	MG	BBB	402	1/1	0.97	0.03	34,34,34,34	0
5	EDO	CCC	406	4/4	0.97	0.08	42,47,47,48	0
2	MG	CCC	401	1/1	0.97	0.08	29,29,29,29	0
3	AR6	CCC	403	35/36	0.97	0.08	29,38,46,47	0
3	AR6	AAA	403	35/36	0.98	0.11	23,26,30,30	0
2	MG	BBB	401	1/1	0.98	0.14	32,32,32,32	0
3	AR6	DDD	403	35/36	0.98	0.07	38,41,45,45	0
2	MG	AAA	401	1/1	0.98	0.11	23,23,23,23	0
3	AR6	BBB	403	35/36	0.99	0.08	29,32,35,37	0

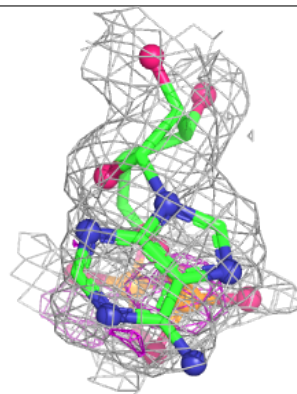
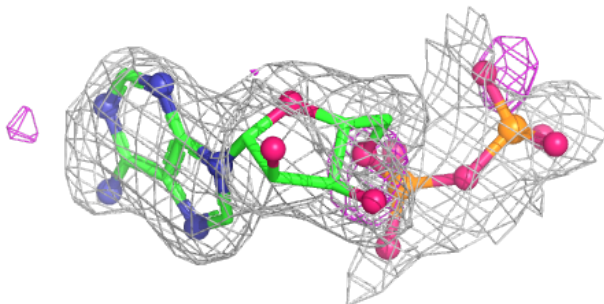
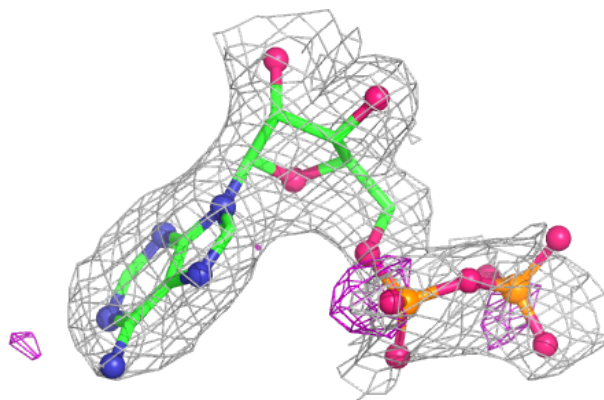
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around AR6 CCC 404:**

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

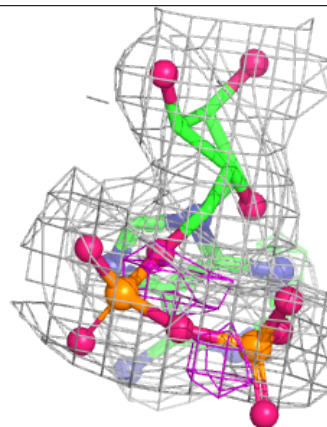
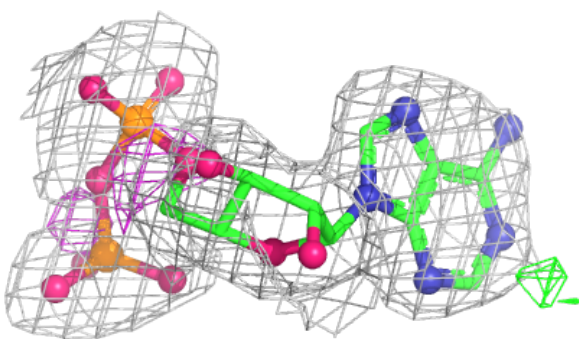
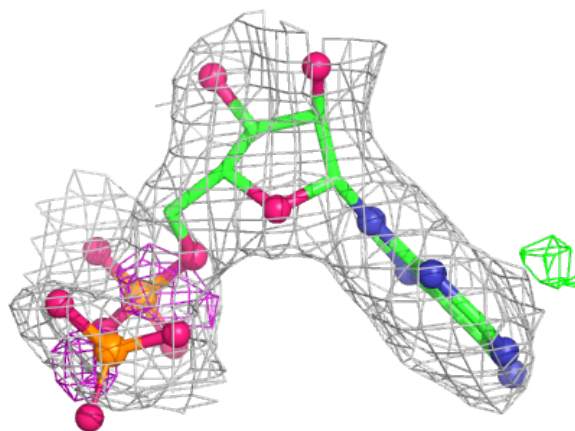
**Electron density around AR6 BBB 404:**

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



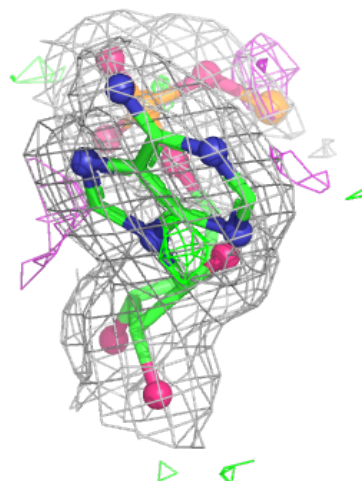
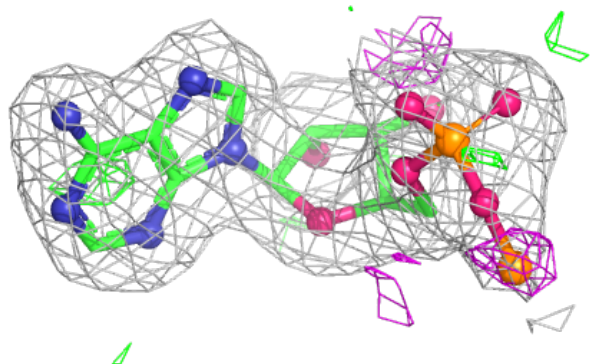
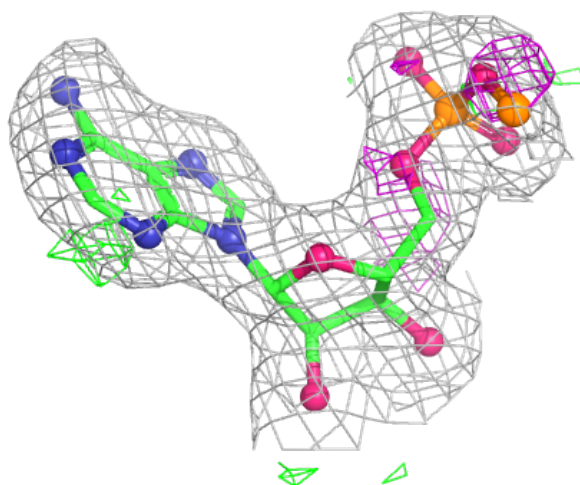
**Electron density around AR6 DDD 404:**

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



**Electron density around AR6 AAA 404:**

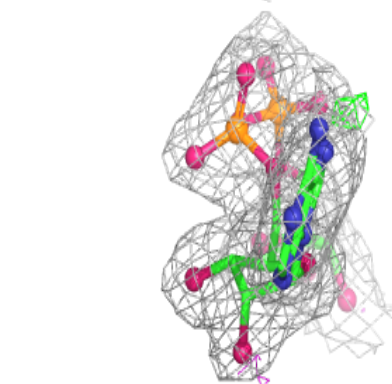
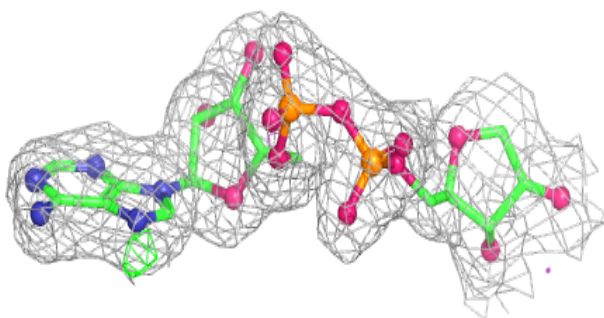
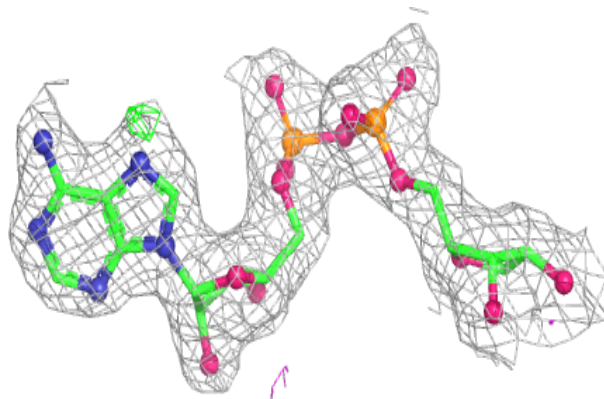
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



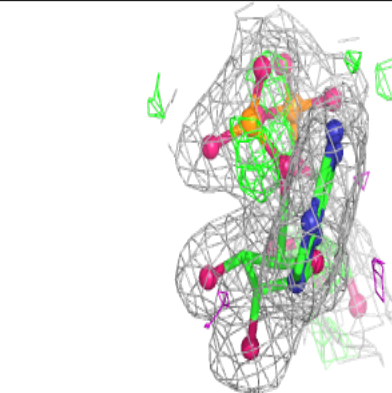
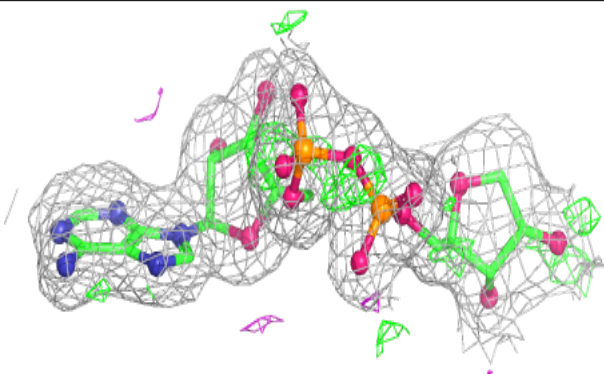
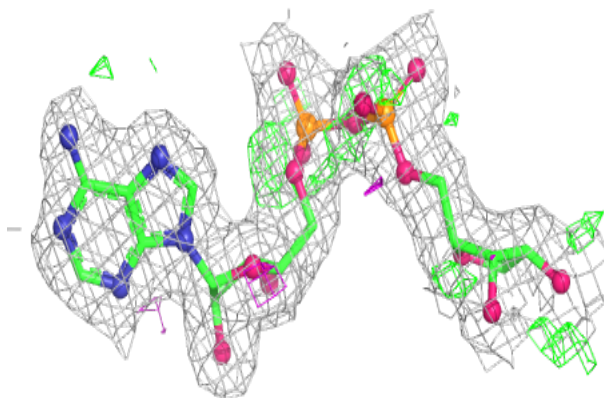


**Electron density around AR6 CCC 403:**

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

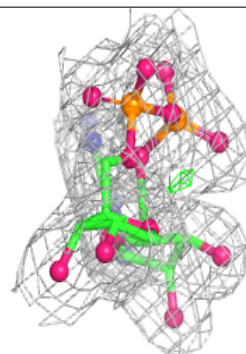
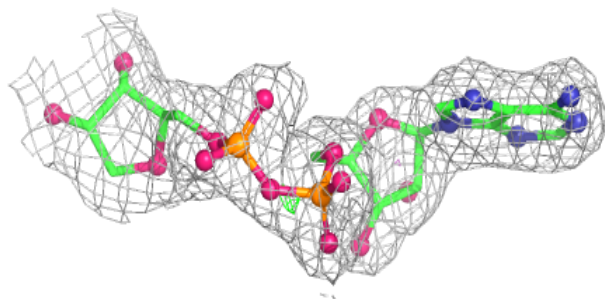
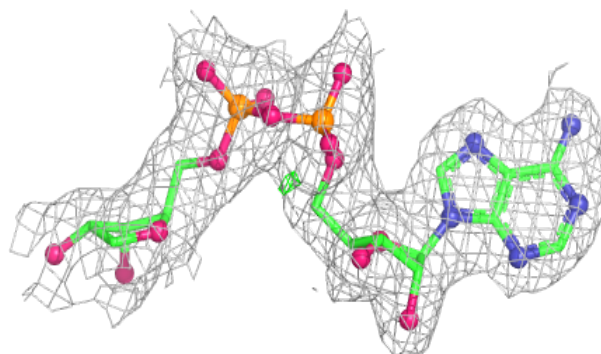
**Electron density around AR6 AAA 403:**

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

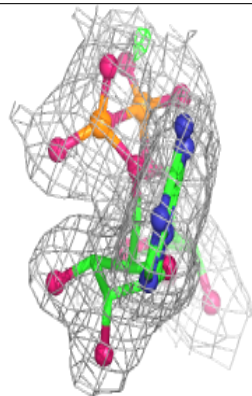
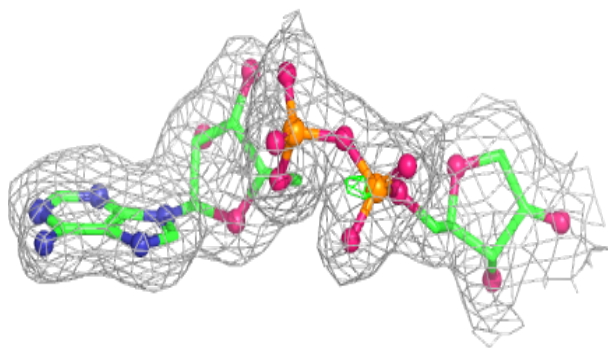
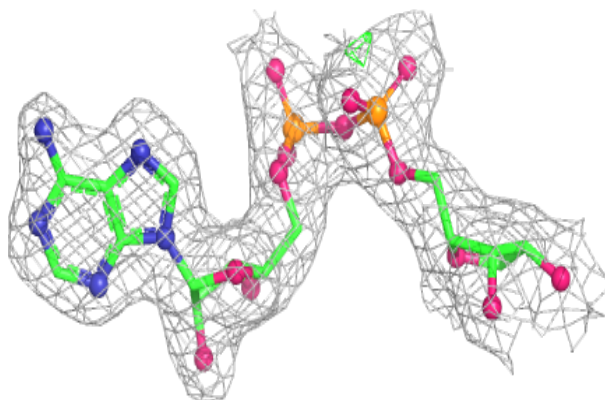


**Electron density around AR6 DDD 403:**

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

**Electron density around AR6 BBB 403:**

$2mF_o-DF_c$  (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.