



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:02 AM UTC

PDB ID : 8AM6 / pdb_00008am6
Title : Cyclohexanone dehydrogenase (CDH) from Alicyclophilus denitrificans K601 complexed with dehydrogenated substrate cyclohex-2-en-1-one - inactive mutant (Y195F)
Authors : Prior, S.H.; Taylor, E.J.
Deposited on : 2022-08-02
Resolution : 1.33 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

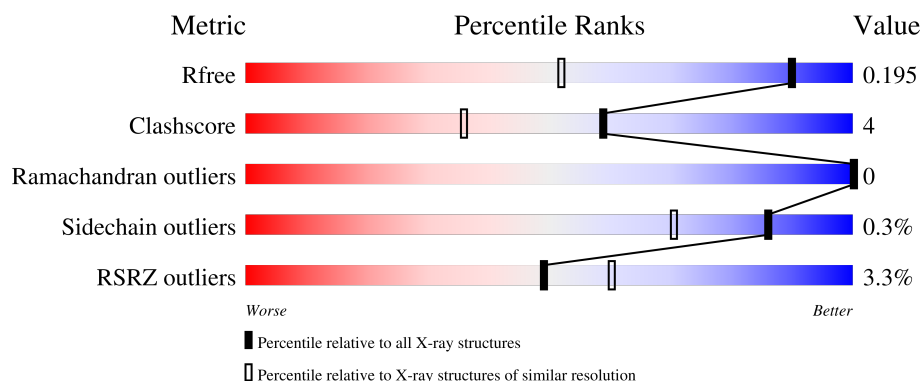
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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}	180053	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	AAA	598	4% 87% 9%
1	BaB	598	2% 81% 8% 11%

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	A2Q	AAA	602	-	X	-	-
3	A2Q	BaB	604	-	X	-	-
4	GOL	AAA	610	-	-	X	-
4	GOL	BaB	608	-	-	X	-
5	SO4	BaB	619	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10600 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 Fumarate reductase/succinate dehydrogenase flavoprotein domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	547	Total	C	N	O	S	0	43	0
			4503	2822	799	863	19			
1	BaB	535	Total	C	N	O	S	0	36	0
			4372	2745	779	831	17			

There are 42 discrepancies between the modelled and reference sequences:

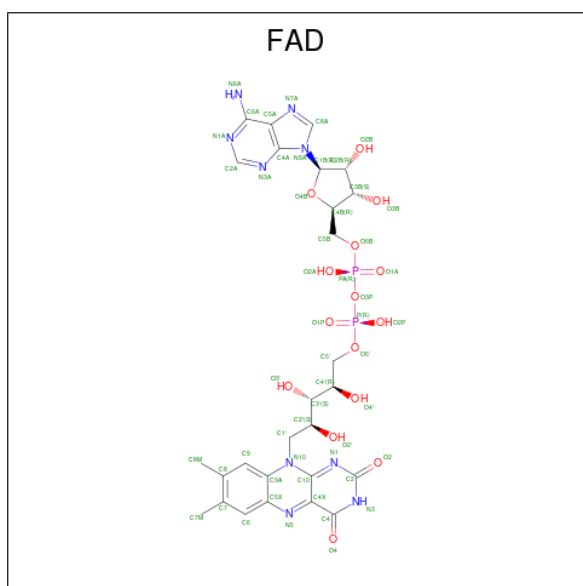
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP F4G7N3
AAA	2	GLY	-	expression tag	UNP F4G7N3
AAA	3	SER	-	expression tag	UNP F4G7N3
AAA	4	SER	-	expression tag	UNP F4G7N3
AAA	5	HIS	-	expression tag	UNP F4G7N3
AAA	6	HIS	-	expression tag	UNP F4G7N3
AAA	7	HIS	-	expression tag	UNP F4G7N3
AAA	8	HIS	-	expression tag	UNP F4G7N3
AAA	9	HIS	-	expression tag	UNP F4G7N3
AAA	10	HIS	-	expression tag	UNP F4G7N3
AAA	11	SER	-	expression tag	UNP F4G7N3
AAA	12	SER	-	expression tag	UNP F4G7N3
AAA	13	GLY	-	expression tag	UNP F4G7N3
AAA	14	LEU	-	expression tag	UNP F4G7N3
AAA	15	VAL	-	expression tag	UNP F4G7N3
AAA	16	PRO	-	expression tag	UNP F4G7N3
AAA	17	ARG	-	expression tag	UNP F4G7N3
AAA	18	GLY	-	expression tag	UNP F4G7N3
AAA	19	SER	-	expression tag	UNP F4G7N3
AAA	20	HIS	-	expression tag	UNP F4G7N3
AAA	195	PHE	TYR	engineered mutation	UNP F4G7N3
BaB	1	MET	-	initiating methionine	UNP F4G7N3
BaB	2	GLY	-	expression tag	UNP F4G7N3
BaB	3	SER	-	expression tag	UNP F4G7N3

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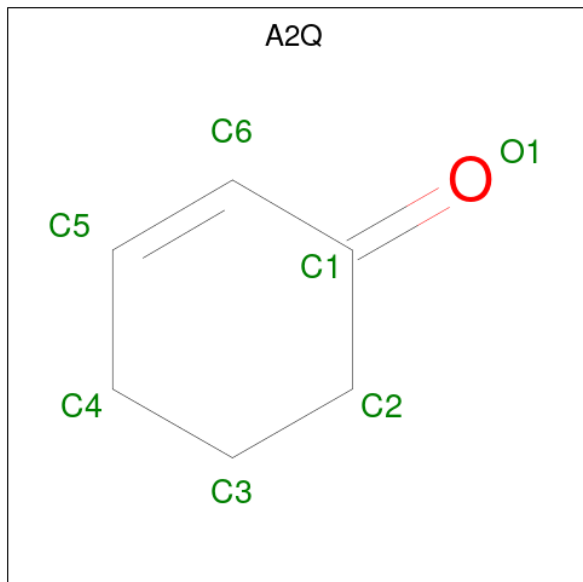
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Chain	Residue	Modelled	Actual	Comment	Reference
BaB	4	SER	-	expression tag	UNP F4G7N3
BaB	5	HIS	-	expression tag	UNP F4G7N3
BaB	6	HIS	-	expression tag	UNP F4G7N3
BaB	7	HIS	-	expression tag	UNP F4G7N3
BaB	8	HIS	-	expression tag	UNP F4G7N3
BaB	9	HIS	-	expression tag	UNP F4G7N3
BaB	10	HIS	-	expression tag	UNP F4G7N3
BaB	11	SER	-	expression tag	UNP F4G7N3
BaB	12	SER	-	expression tag	UNP F4G7N3
BaB	13	GLY	-	expression tag	UNP F4G7N3
BaB	14	LEU	-	expression tag	UNP F4G7N3
BaB	15	VAL	-	expression tag	UNP F4G7N3
BaB	16	PRO	-	expression tag	UNP F4G7N3
BaB	17	ARG	-	expression tag	UNP F4G7N3
BaB	18	GLY	-	expression tag	UNP F4G7N3
BaB	19	SER	-	expression tag	UNP F4G7N3
BaB	20	HIS	-	expression tag	UNP F4G7N3
BaB	195	PHE	TYR	engineered mutation	UNP F4G7N3

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



- Molecule 3 is cyclohex-2-en-1-one (CCD ID: A2Q) (formula: C_6H_8O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			7	6	1		
3	AAA	1	Total	C	O	0	0
			7	6	1		
3	AAA	1	Total	C	O	0	0
			7	6	1		
3	AAA	1	Total	C	O	0	1
			7	6	1		
3	BaB	1	Total	C	O	0	0
			7	6	1		
3	BaB	1	Total	C	O	0	0
			7	6	1		
3	BaB	1	Total	C	O	0	0
			7	6	1		
3	BaB	1	Total	C	O	0	1
			7	6	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	1
			6	3	3		
4	AAA	1	Total	C	O	0	1
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	1
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	1
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	1
			12	6	6		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		
4	AAA	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		
4	BaB	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	1
			5	4	1		
5	AAA	1	Total	O	S	0	1
			5	4	1		
5	AAA	1	Total	O	S	0	1
			5	4	1		
5	BaB	1	Total	O	S	0	0
			5	4	1		
5	BaB	1	Total	O	S	0	1
			5	4	1		
5	BaB	1	Total	O	S	0	1
			5	4	1		
5	BaB	1	Total	O	S	0	0
			5	4	1		
5	BaB	1	Total	O	S	0	1
			5	4	1		

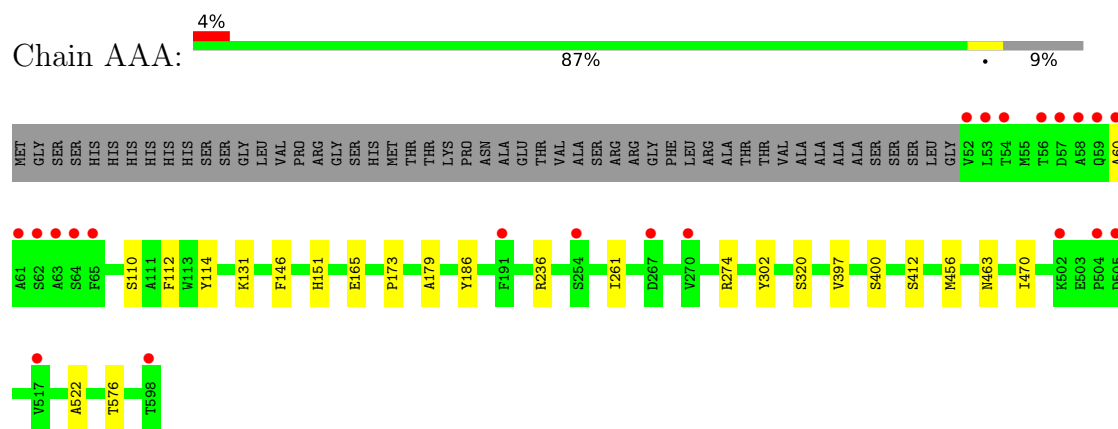
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	625	Total	O	0	48
			655	655		
6	BaB	667	Total	O	0	36
			695	695		

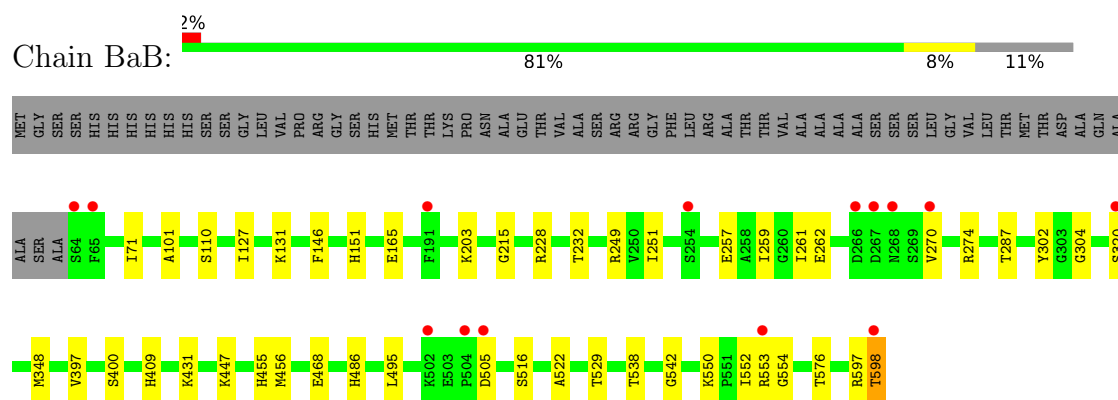
3 Residue-property plots

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: Fumarate reductase/succinate dehydrogenase flavoprotein domain protein



- Molecule 1: Fumarate reductase/succinate dehydrogenase flavoprotein domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.03Å 121.70Å 158.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.93 – 1.33 60.93 – 1.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.93-1.33) 99.9 (60.93-1.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.174 , 0.195 0.174 , 0.195	Depositor DCC
R_{free} test set	14422 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	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	0.98	EDS
Total number of atoms	10600	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8215e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, A2Q, SO4, FAD

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	1/4609 (0.0%)	0.99	0/6237
1	BaB	0.71	2/4480 (0.0%)	1.01	4/6063 (0.1%)
All	All	0.70	3/9089 (0.0%)	1.00	4/12300 (0.0%)

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	AAA	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	151	HIS	CE1-NE2	5.83	1.38	1.32
1	BaB	455	HIS	CE1-NE2	5.54	1.38	1.32
1	BaB	151	HIS	CE1-NE2	5.53	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BaB	598	THR	CB-CA-C	6.73	123.90	109.10
1	BaB	597	ARG	CA-C-N	5.24	131.14	121.70
1	BaB	597	ARG	C-N-CA	5.24	131.14	121.70
1	BaB	486	HIS	CA-CB-CG	-5.21	108.59	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	114	TYR	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	AAA	4503	0	4379	30	0
1	BaB	4372	0	4262	54	0
2	AAA	53	0	30	1	0
2	BaB	53	0	30	1	0
3	AAA	28	0	32	1	0
3	BaB	28	0	32	2	0
4	AAA	90	0	120	14	0
4	BaB	78	0	104	8	0
5	AAA	20	0	0	0	0
5	BaB	25	0	0	2	0
6	AAA	655	0	0	3	0
6	BaB	695	0	0	16	0
All	All	10600	0	8989	81	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.

The worst 5 of 81 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:AAA:463:ASN:HD22	4:AAA:610:GOL:H11	1.12	1.13
1:AAA:60:ALA:O	1:AAA:274:ARG:NH2	1.89	1.04
1:AAA:320[B]:SER:O	1:BaB:320[B]:SER:HB2	1.69	0.93
1:BaB:232[B]:THR:HG22	6:BaB:785:HOH:O	1.69	0.93
1:AAA:320[B]:SER:HB2	1:BaB:320[B]:SER:O	1.71	0.91

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	588/598 (98%)	578 (98%)	10 (2%)	0	100	100
1	BaB	570/598 (95%)	561 (98%)	9 (2%)	0	100	100
All	All	1158/1196 (97%)	1139 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	477/474 (101%)	475 (100%)	2 (0%)	84	67
1	BaB	463/474 (98%)	462 (100%)	1 (0%)	87	72
All	All	940/948 (99%)	937 (100%)	3 (0%)	86	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	112	PHE
1	AAA	576	THR
1	BaB	576	THR

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

47 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	BaB	606	-	5,5,5	0.14	0	5,5,5	0.65	0
5	SO4	AAA	622[A]	-	4,4,4	0.33	0	6,6,6	0.57	0
5	SO4	BaB	622	-	4,4,4	0.25	0	6,6,6	0.34	0
3	A2Q	BaB	603	-	7,7,7	4.34	7 (100%)	8,8,8	1.60	1 (12%)
5	SO4	BaB	619	-	4,4,4	0.31	0	6,6,6	0.17	0
4	GOL	AAA	612	-	5,5,5	0.11	0	5,5,5	0.17	0
4	GOL	AAA	619	-	5,5,5	0.17	0	5,5,5	0.65	0
4	GOL	AAA	606[B]	-	5,5,5	0.21	0	5,5,5	0.43	0
4	GOL	BaB	611	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	BaB	612	-	5,5,5	0.17	0	5,5,5	0.35	0
4	GOL	AAA	616[A]	-	5,5,5	0.11	0	5,5,5	0.18	0
3	A2Q	BaB	605[A]	-	7,7,7	4.84	6 (85%)	8,8,8	1.74	2 (25%)
4	GOL	BaB	615	-	5,5,5	0.17	0	5,5,5	0.34	0
4	GOL	BaB	613	-	5,5,5	0.41	0	5,5,5	0.67	0
4	GOL	BaB	610	-	5,5,5	0.10	0	5,5,5	0.28	0
4	GOL	AAA	614	-	5,5,5	0.24	0	5,5,5	0.31	0
3	A2Q	BaB	602	-	7,7,7	3.93	6 (85%)	8,8,8	1.81	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	AAA	618	-	5,5,5	0.26	0	5,5,5	0.39	0
4	GOL	BaB	607	-	5,5,5	0.15	0	5,5,5	0.27	0
5	SO4	BaB	623[A]	-	4,4,4	0.43	0	6,6,6	0.31	0
4	GOL	AAA	609[A]	-	5,5,5	0.20	0	5,5,5	0.77	0
5	SO4	AAA	621[A]	-	4,4,4	0.29	0	6,6,6	0.17	0
3	A2Q	AAA	605[A]	-	7,7,7	4.71	7 (100%)	8,8,8	1.84	2 (25%)
4	GOL	BaB	614	-	5,5,5	0.18	0	5,5,5	0.25	0
4	GOL	AAA	615	-	5,5,5	0.33	0	5,5,5	0.76	0
5	SO4	BaB	621[A]	-	4,4,4	0.35	0	6,6,6	0.58	0
4	GOL	AAA	608	-	5,5,5	0.12	0	5,5,5	0.35	0
4	GOL	AAA	610	-	5,5,5	0.10	0	5,5,5	0.60	0
4	GOL	BaB	609	-	5,5,5	0.09	0	5,5,5	0.29	0
3	A2Q	AAA	602	-	7,7,7	3.66	6 (85%)	8,8,8	2.19	4 (50%)
3	A2Q	BaB	604	-	7,7,7	4.64	7 (100%)	8,8,8	1.80	3 (37%)
4	GOL	BaB	618	-	5,5,5	0.19	0	5,5,5	0.42	0
2	FAD	AAA	601	1	58,58,58	0.81	3 (5%)	85,89,89	0.80	1 (1%)
4	GOL	AAA	617	-	5,5,5	0.28	0	5,5,5	0.46	0
4	GOL	AAA	607[A]	-	5,5,5	0.13	0	5,5,5	0.37	0
5	SO4	AAA	620	-	4,4,4	0.30	0	6,6,6	0.13	0
4	GOL	BaB	616	-	5,5,5	0.26	0	5,5,5	0.60	0
5	SO4	BaB	620[B]	-	4,4,4	0.07	0	6,6,6	0.21	0
3	A2Q	AAA	603	-	7,7,7	4.53	7 (100%)	8,8,8	1.62	1 (12%)
2	FAD	BaB	601	1	58,58,58	0.96	3 (5%)	85,89,89	0.71	0
3	A2Q	AAA	604	-	7,7,7	4.80	7 (100%)	8,8,8	1.71	2 (25%)
4	GOL	AAA	613[A]	-	5,5,5	0.18	0	5,5,5	0.57	0
4	GOL	BaB	608	-	5,5,5	0.22	0	5,5,5	0.86	0
4	GOL	AAA	616[B]	-	5,5,5	0.10	0	5,5,5	0.35	0
5	SO4	AAA	623[A]	-	4,4,4	0.24	0	6,6,6	0.42	0
4	GOL	AAA	611	-	5,5,5	0.14	0	5,5,5	0.61	0
4	GOL	BaB	617	-	5,5,5	0.32	0	5,5,5	0.48	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
4	GOL	BaB	606	-	-	4/4/4/4	-
3	A2Q	BaB	603	-	-	-	0/1/1/1
4	GOL	AAA	612	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	AAA	619	-	-	4/4/4/4	-
4	GOL	AAA	606[B]	-	-	4/4/4/4	-
4	GOL	BaB	611	-	-	2/4/4/4	-
4	GOL	BaB	612	-	-	0/4/4/4	-
4	GOL	AAA	616[A]	-	-	0/4/4/4	-
3	A2Q	BaB	605[A]	-	-	-	0/1/1/1
4	GOL	BaB	615	-	-	0/4/4/4	-
4	GOL	BaB	613	-	-	0/4/4/4	-
4	GOL	BaB	610	-	-	4/4/4/4	-
4	GOL	AAA	614	-	-	0/4/4/4	-
3	A2Q	BaB	602	-	-	-	0/1/1/1
4	GOL	AAA	618	-	-	0/4/4/4	-
4	GOL	BaB	607	-	-	4/4/4/4	-
4	GOL	AAA	609[A]	-	-	2/4/4/4	-
3	A2Q	AAA	605[A]	-	-	-	0/1/1/1
4	GOL	BaB	614	-	-	0/4/4/4	-
4	GOL	AAA	615	-	-	0/4/4/4	-
4	GOL	AAA	608	-	-	2/4/4/4	-
4	GOL	AAA	610	-	-	2/4/4/4	-
4	GOL	BaB	609	-	-	2/4/4/4	-
4	GOL	BaB	618	-	-	0/4/4/4	-
3	A2Q	AAA	602	-	-	-	0/1/1/1
3	A2Q	BaB	604	-	-	-	0/1/1/1
2	FAD	AAA	601	1	-	3/34/50/50	0/6/6/6
4	GOL	AAA	617	-	-	0/4/4/4	-
4	GOL	AAA	607[A]	-	-	2/4/4/4	-
4	GOL	BaB	616	-	-	0/4/4/4	-
3	A2Q	AAA	603	-	-	-	0/1/1/1
2	FAD	BaB	601	1	-	3/34/50/50	0/6/6/6
4	GOL	AAA	613[A]	-	-	4/4/4/4	-
4	GOL	BaB	608	-	-	2/4/4/4	-
3	A2Q	AAA	604	-	-	-	0/1/1/1
4	GOL	AAA	616[B]	-	-	2/4/4/4	-
4	GOL	AAA	611	-	-	3/4/4/4	-
4	GOL	BaB	617	-	-	0/4/4/4	-

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	603	A2Q	O1-C1	8.88	1.37	1.23
3	BaB	605[A]	A2Q	O1-C1	8.74	1.37	1.23
3	AAA	604	A2Q	O1-C1	8.71	1.37	1.23
3	BaB	603	A2Q	O1-C1	8.60	1.36	1.23
3	AAA	605[A]	A2Q	O1-C1	8.28	1.36	1.23

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	602	A2Q	O1-C1-C6	-3.15	116.47	121.88
3	AAA	602	A2Q	C2-C1-C6	2.92	123.46	116.75
3	AAA	602	A2Q	C5-C6-C1	-2.83	117.75	121.83
3	AAA	603	A2Q	O1-C1-C6	-2.72	117.20	121.88
3	AAA	605[A]	A2Q	C3-C4-C5	2.44	120.83	111.55

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	607[A]	GOL	O1-C1-C2-C3
4	AAA	608	GOL	C1-C2-C3-O3
4	AAA	609[A]	GOL	O1-C1-C2-C3
4	AAA	611	GOL	O1-C1-C2-C3
4	AAA	612	GOL	C1-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 29 short contacts:

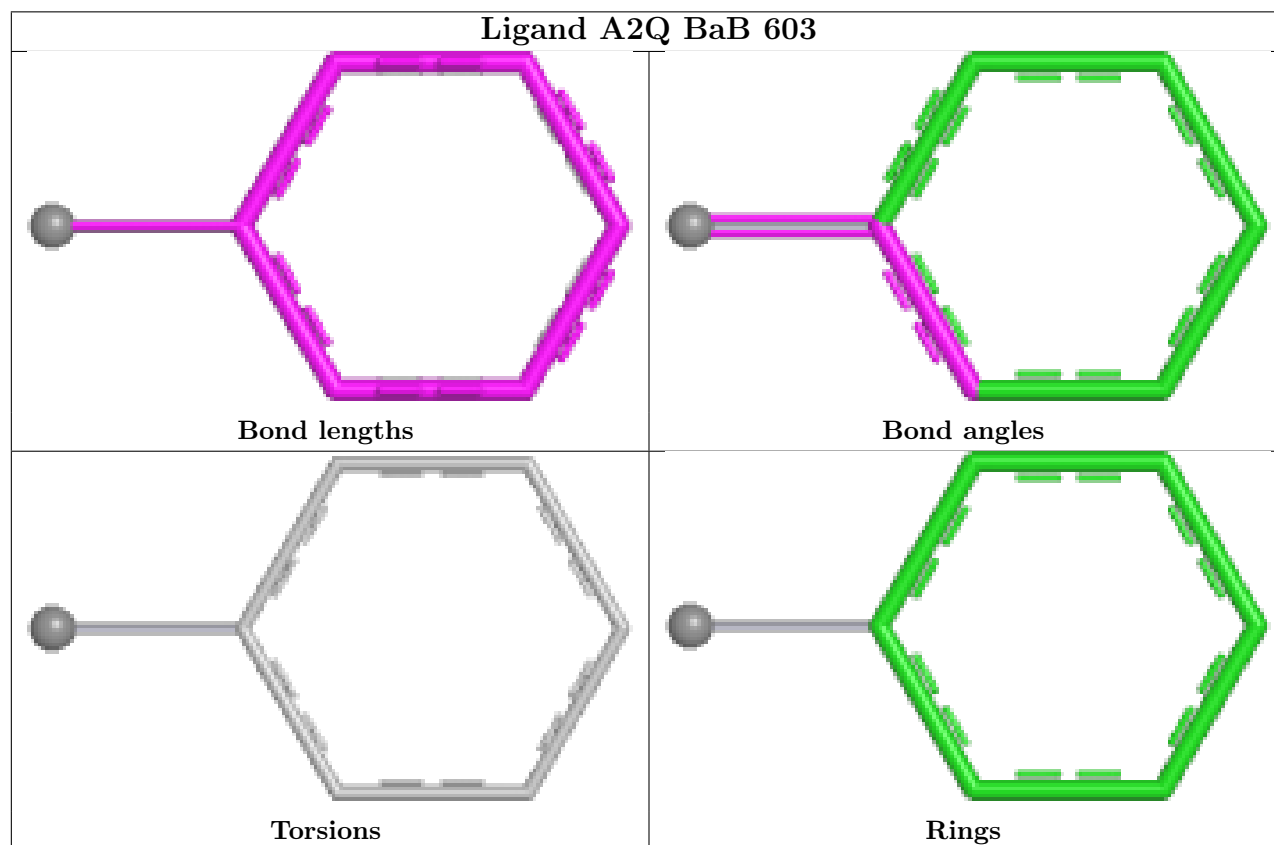
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BaB	606	GOL	1	0
5	BaB	619	SO4	2	0
4	AAA	606[B]	GOL	2	0
3	BaB	605[A]	A2Q	1	0
4	BaB	607	GOL	1	0
4	AAA	609[A]	GOL	3	0
4	AAA	610	GOL	5	0
4	BaB	609	GOL	1	0
3	BaB	604	A2Q	1	0
2	AAA	601	FAD	1	0
4	AAA	607[A]	GOL	1	0
2	BaB	601	FAD	1	0
3	AAA	604	A2Q	1	0

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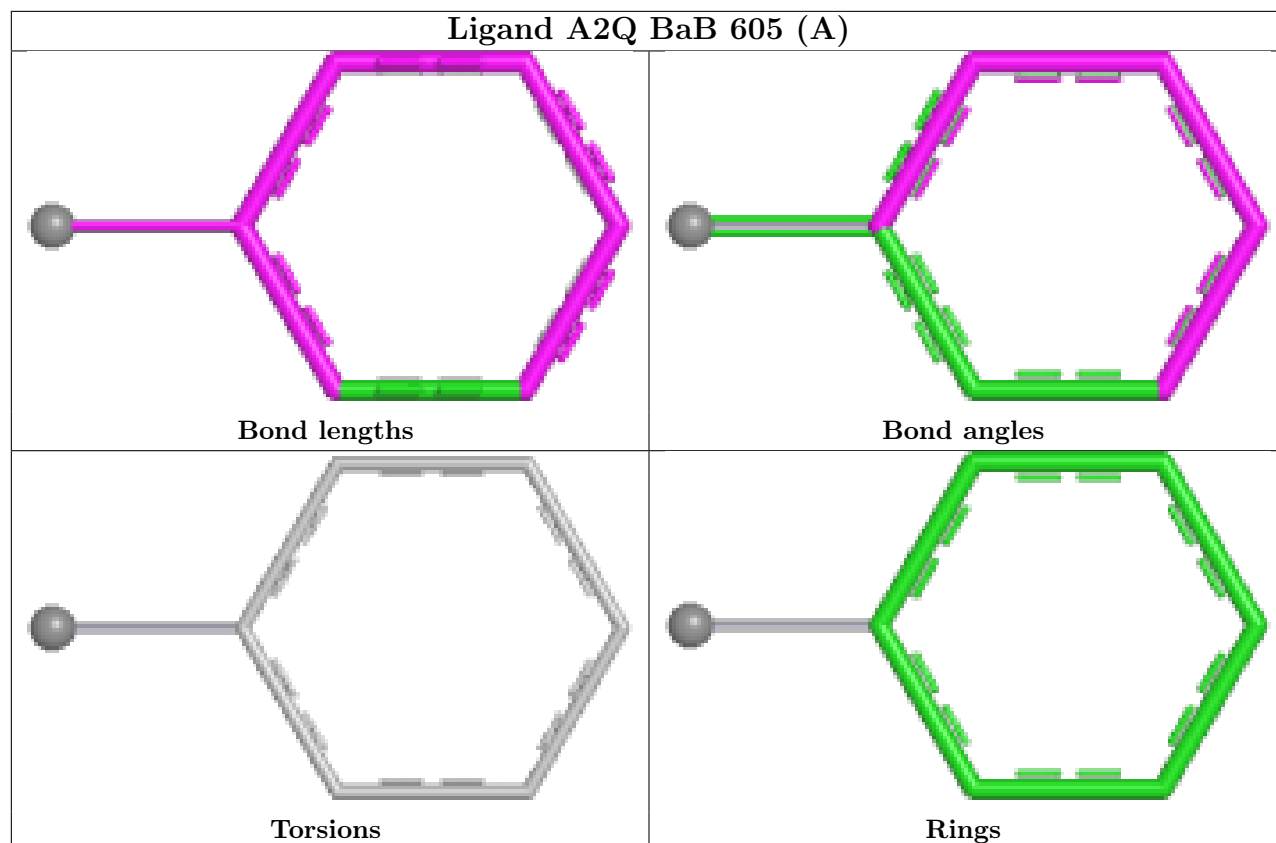
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	613[A]	GOL	1	0
4	BaB	608	GOL	5	0
4	AAA	611	GOL	2	0

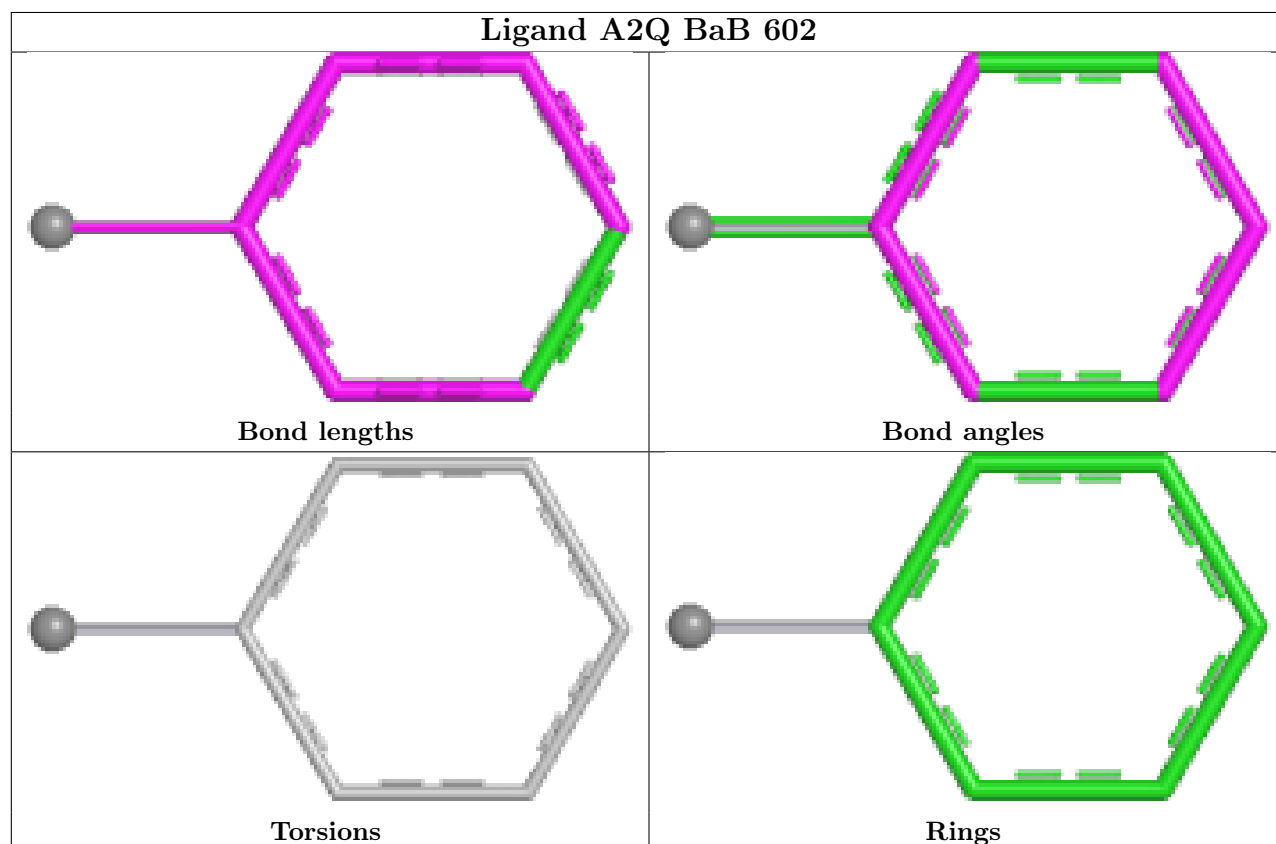
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

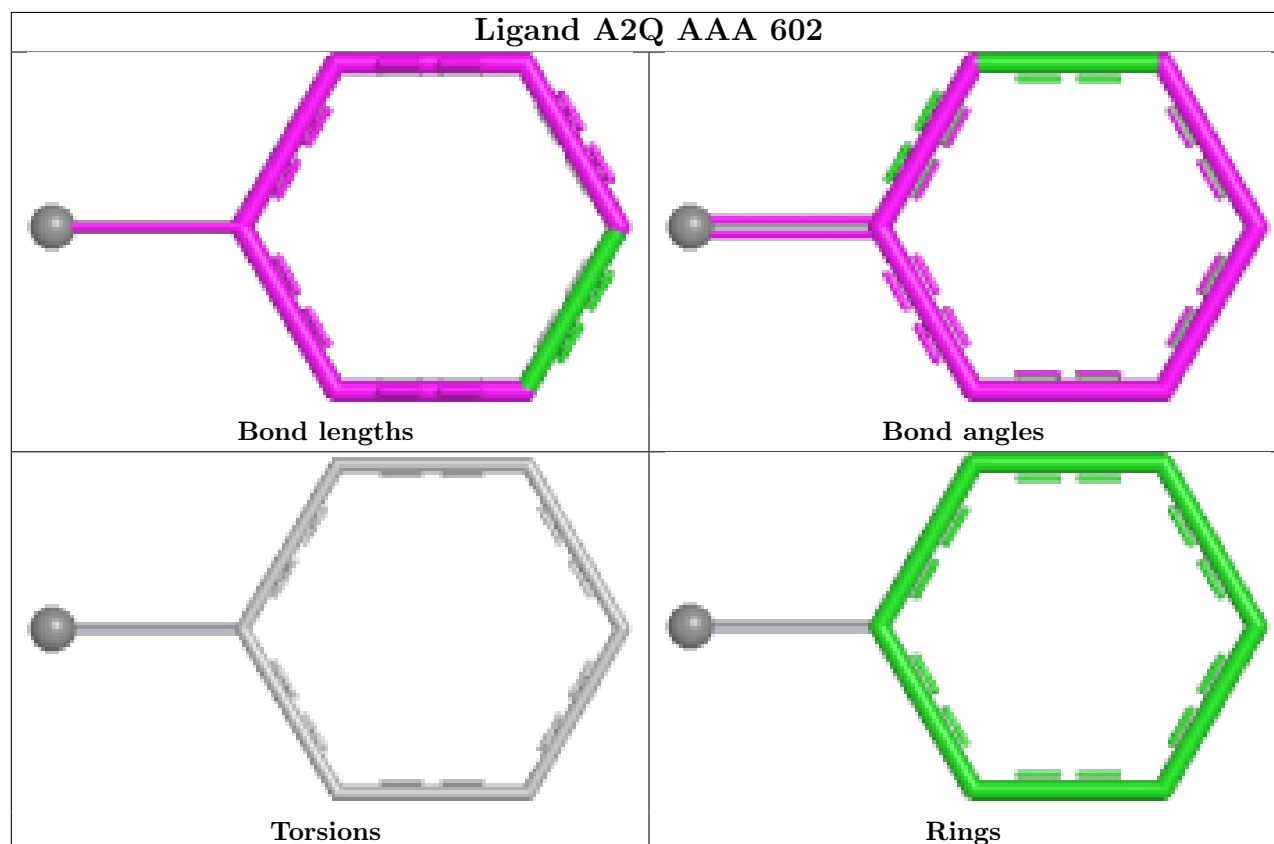
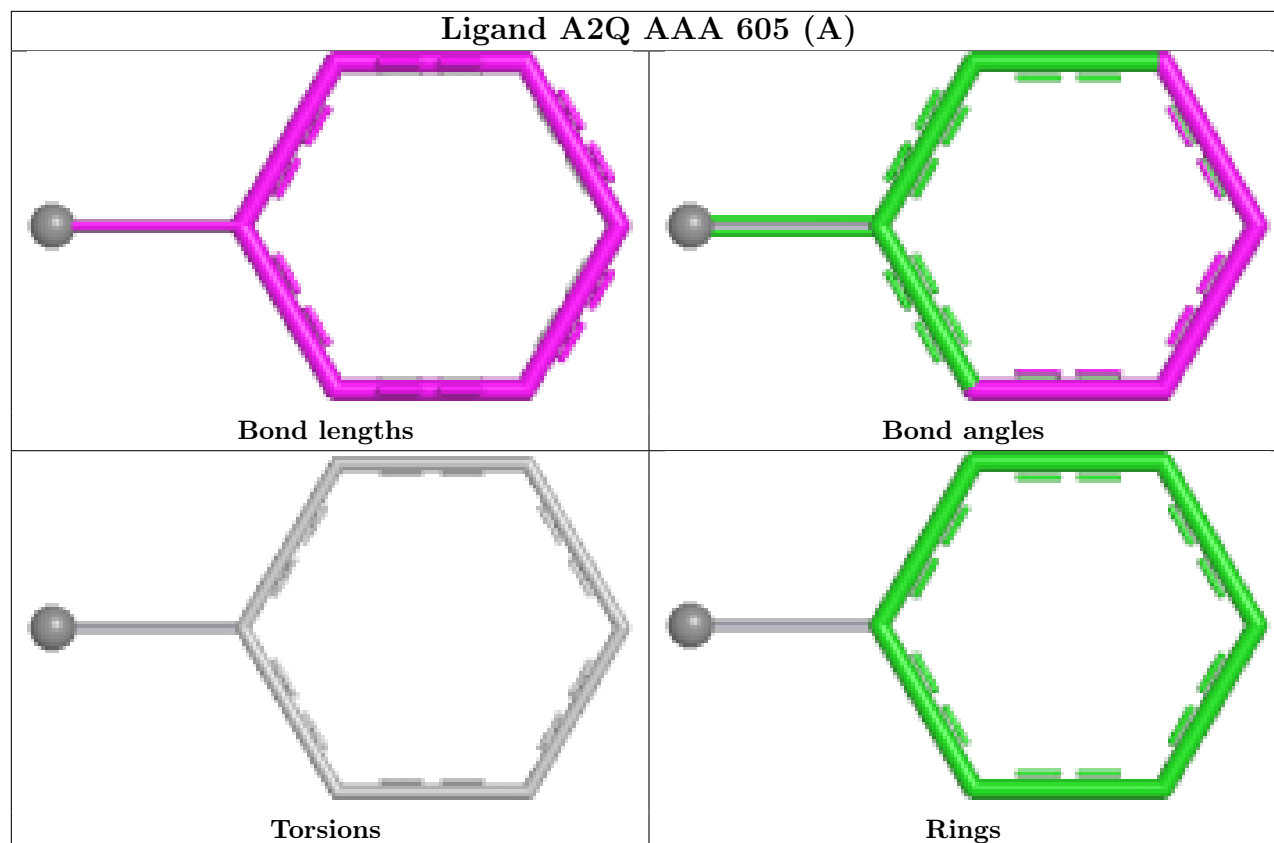


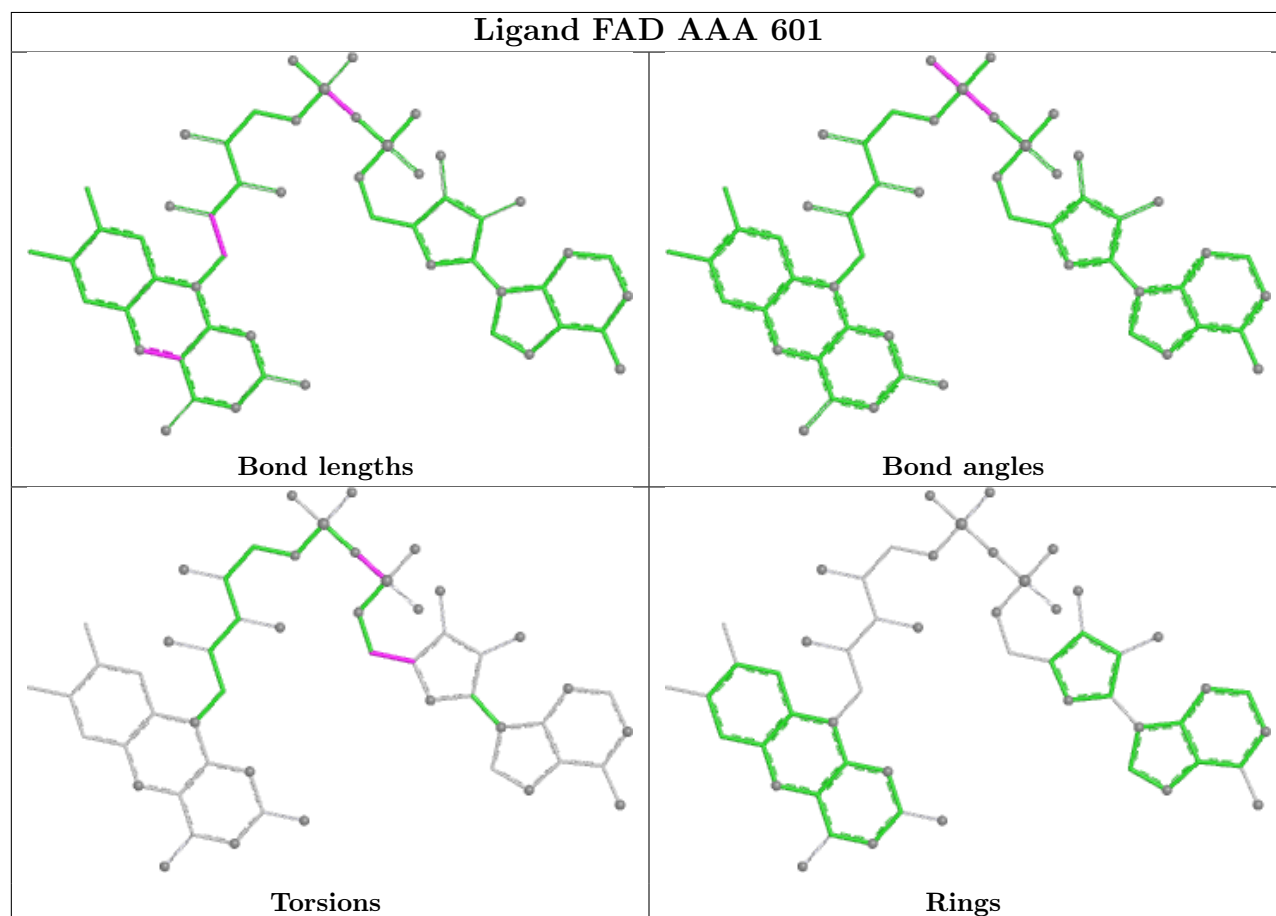
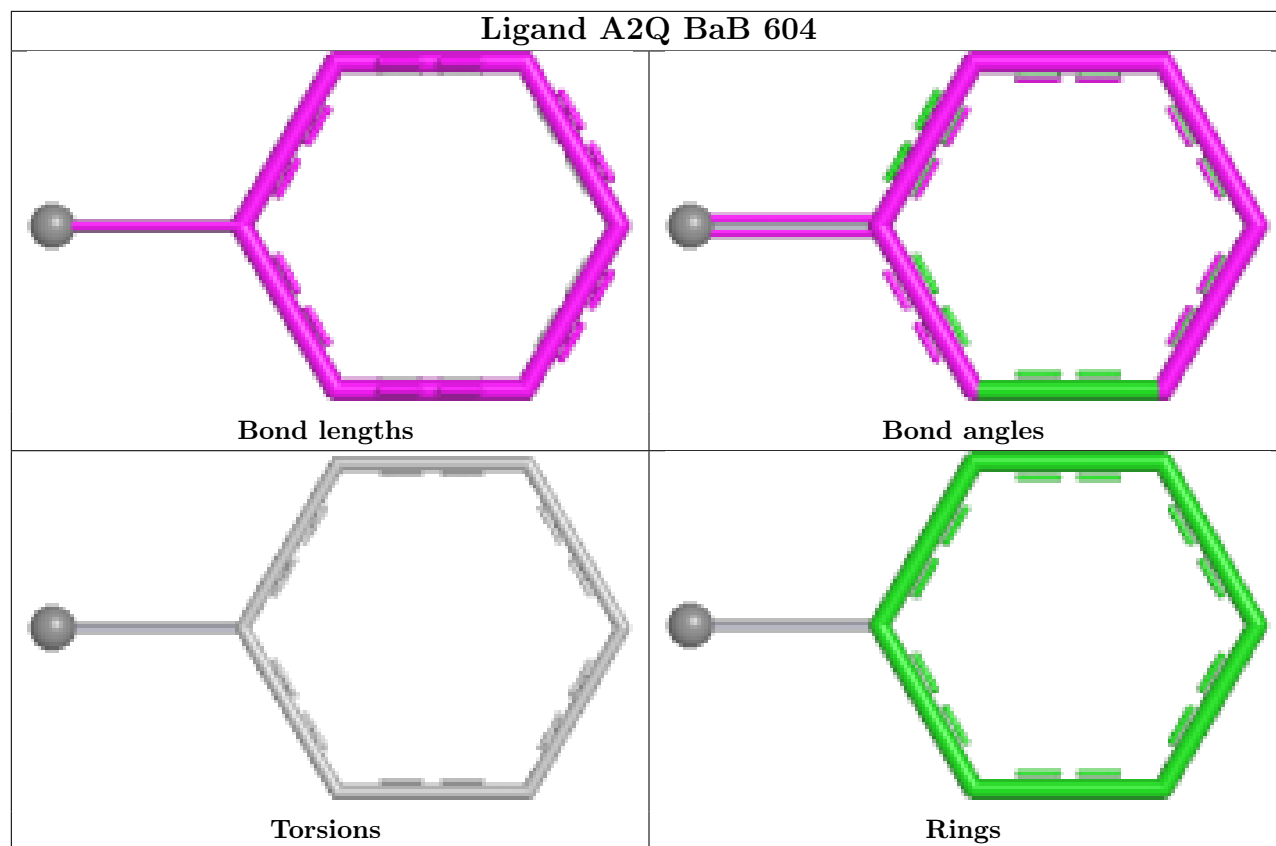
Ligand A2Q BaB 605 (A)

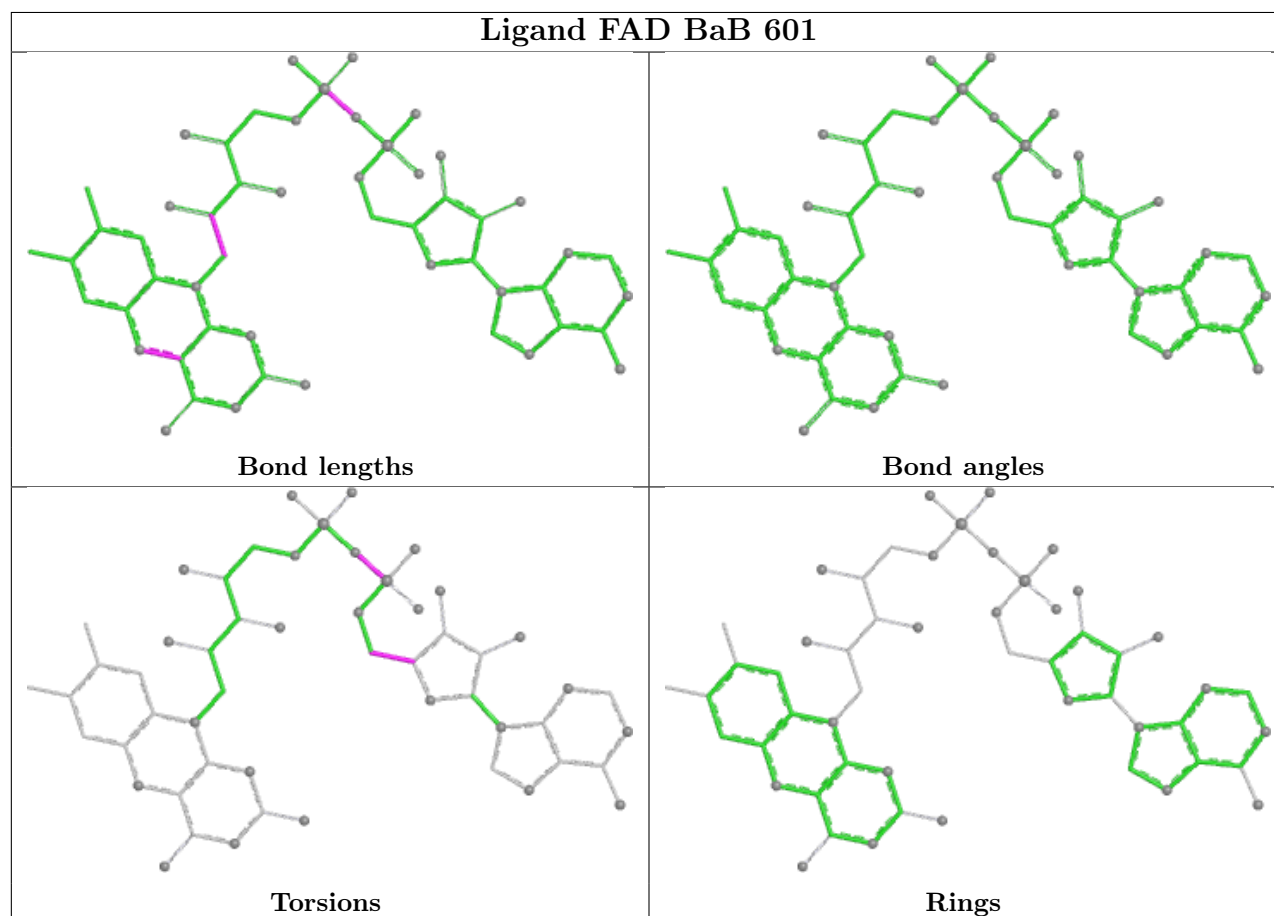
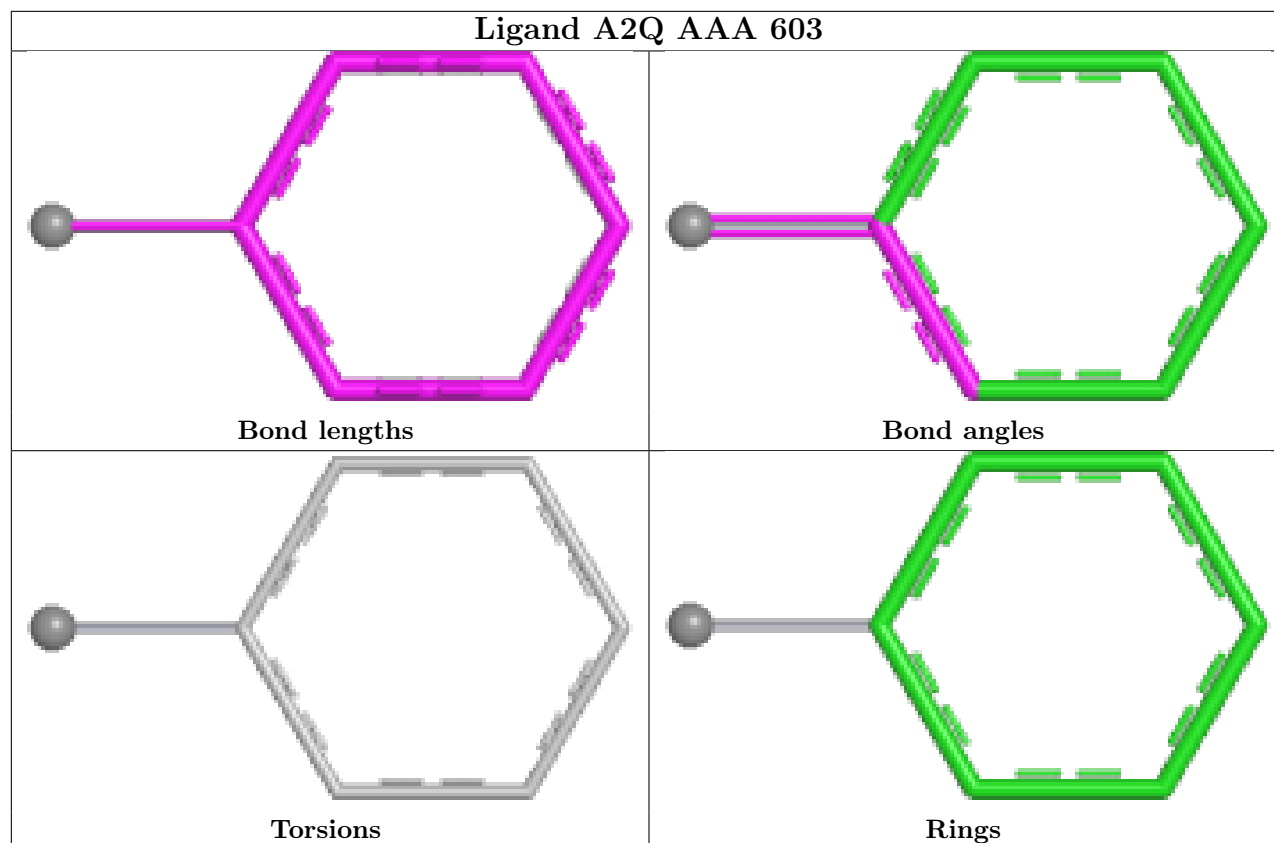


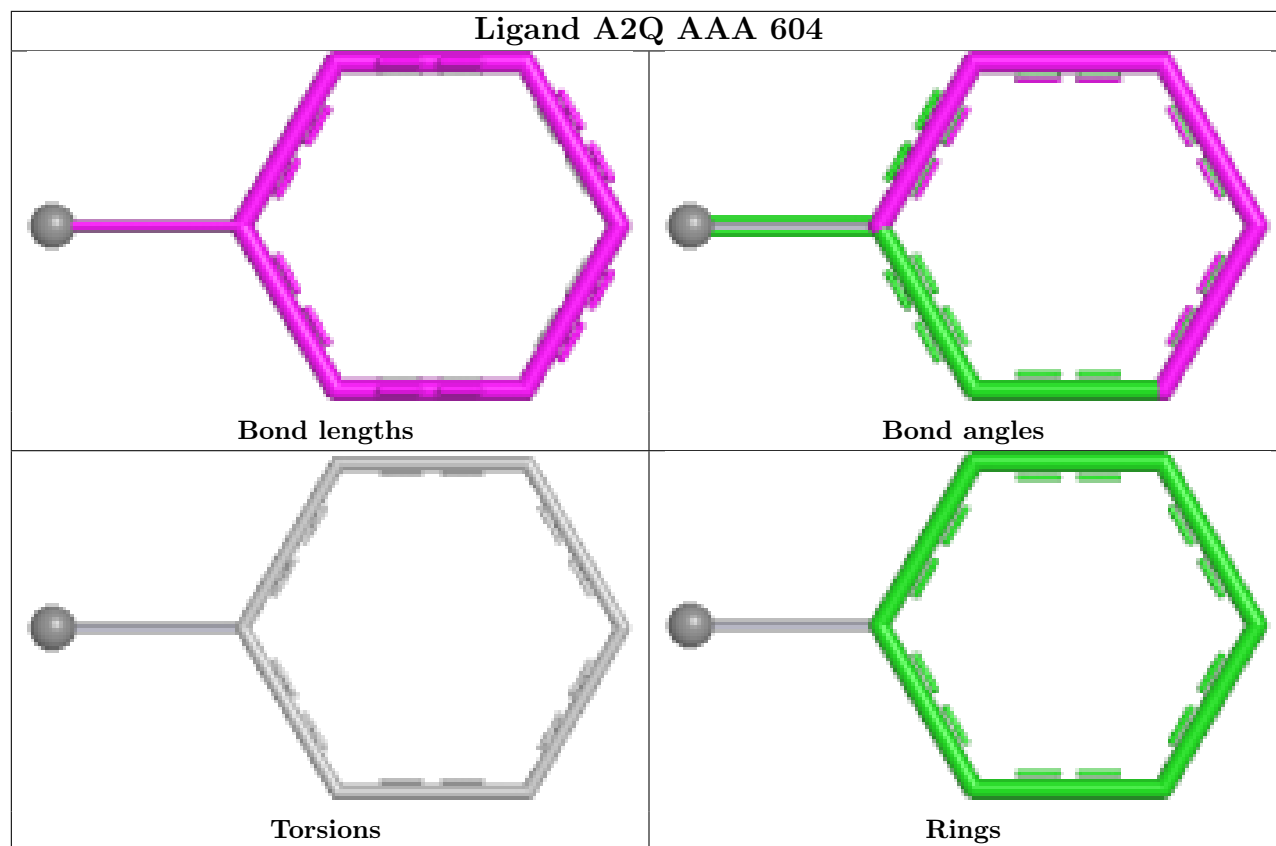
Ligand A2Q BaB 602











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	AAA	547/598 (91%)	-0.05	22 (4%)	42 54	6, 13, 24, 58	55 (10%)
1	BaB	535/598 (89%)	-0.14	14 (2%)	57 67	5, 13, 25, 53	36 (6%)
All	All	1082/1196 (90%)	-0.09	36 (3%)	49 60	5, 13, 25, 58	91 (8%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	58	ALA	12.2
1	AAA	60	ALA	8.5
1	AAA	52	VAL	7.6
1	AAA	53	LEU	6.9
1	AAA	598	THR	6.8

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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
4	GOL	AAA	607[A]	6/6	0.65	0.38	20,25,31,33	6
3	A2Q	AAA	604	7/7	0.71	0.30	21,24,26,32	7
4	GOL	BaB	609	6/6	0.71	0.18	53,55,57,65	0
5	SO4	BaB	619	5/5	0.71	0.13	77,78,86,86	0
3	A2Q	AAA	605[A]	7/7	0.72	0.26	15,17,17,18	7
4	GOL	AAA	608	6/6	0.74	0.21	40,59,60,64	0
4	GOL	BaB	607	6/6	0.74	0.19	38,56,68,72	0
3	A2Q	BaB	604	7/7	0.75	0.31	19,22,24,33	7
4	GOL	BaB	611	6/6	0.76	0.19	60,69,73,79	0
5	SO4	AAA	620	5/5	0.77	0.12	75,76,80,82	0
4	GOL	BaB	606	6/6	0.77	0.17	31,48,53,67	0
3	A2Q	BaB	605[A]	7/7	0.78	0.25	16,18,19,20	7
4	GOL	AAA	611	6/6	0.79	0.22	22,32,47,50	0
4	GOL	AAA	619	6/6	0.79	0.18	30,47,51,63	0
4	GOL	AAA	610	6/6	0.81	0.18	42,46,50,66	0
4	GOL	AAA	606[B]	6/6	0.82	0.25	20,21,27,31	6
4	GOL	BaB	608	6/6	0.82	0.16	33,34,39,42	0
5	SO4	AAA	621[A]	5/5	0.82	0.16	28,29,33,35	5
4	GOL	AAA	609[A]	6/6	0.82	0.21	20,20,23,24	6
5	SO4	BaB	620[B]	5/5	0.84	0.14	20,24,29,31	5
4	GOL	BaB	615	6/6	0.87	0.13	28,33,35,37	0
4	GOL	BaB	618	6/6	0.90	0.15	22,35,51,53	0
4	GOL	BaB	610	6/6	0.90	0.15	24,49,54,63	0
4	GOL	AAA	613[A]	6/6	0.90	0.19	13,22,24,27	6
4	GOL	BaB	614	6/6	0.90	0.12	19,20,21,23	6
4	GOL	AAA	612	6/6	0.90	0.14	24,47,53,65	0
3	A2Q	AAA	603	7/7	0.93	0.09	15,15,17,20	0
4	GOL	BaB	613	6/6	0.93	0.14	7,9,11,11	6
3	A2Q	BaB	603	7/7	0.93	0.08	15,16,19,19	0
4	GOL	AAA	618	6/6	0.93	0.09	21,22,26,27	0
4	GOL	BaB	617	6/6	0.93	0.09	22,22,24,25	0
5	SO4	BaB	621[A]	5/5	0.93	0.11	14,14,16,16	5
4	GOL	AAA	615	6/6	0.94	0.15	7,10,11,11	6
5	SO4	AAA	622[A]	5/5	0.95	0.09	14,15,15,17	5
4	GOL	BaB	616	6/6	0.95	0.09	17,24,25,26	0
4	GOL	AAA	614	6/6	0.96	0.06	15,15,15,19	0
4	GOL	AAA	616[A]	6/6	0.96	0.07	13,15,16,18	6
4	GOL	AAA	616[B]	6/6	0.96	0.07	30,49,53,54	6
4	GOL	AAA	617	6/6	0.96	0.08	17,22,23,28	0
5	SO4	BaB	622	5/5	0.96	0.14	13,14,16,17	5
3	A2Q	AAA	602	7/7	0.97	0.05	12,12,14,17	0
3	A2Q	BaB	602	7/7	0.97	0.06	12,13,16,16	0
4	GOL	BaB	612	6/6	0.97	0.06	14,15,16,19	0

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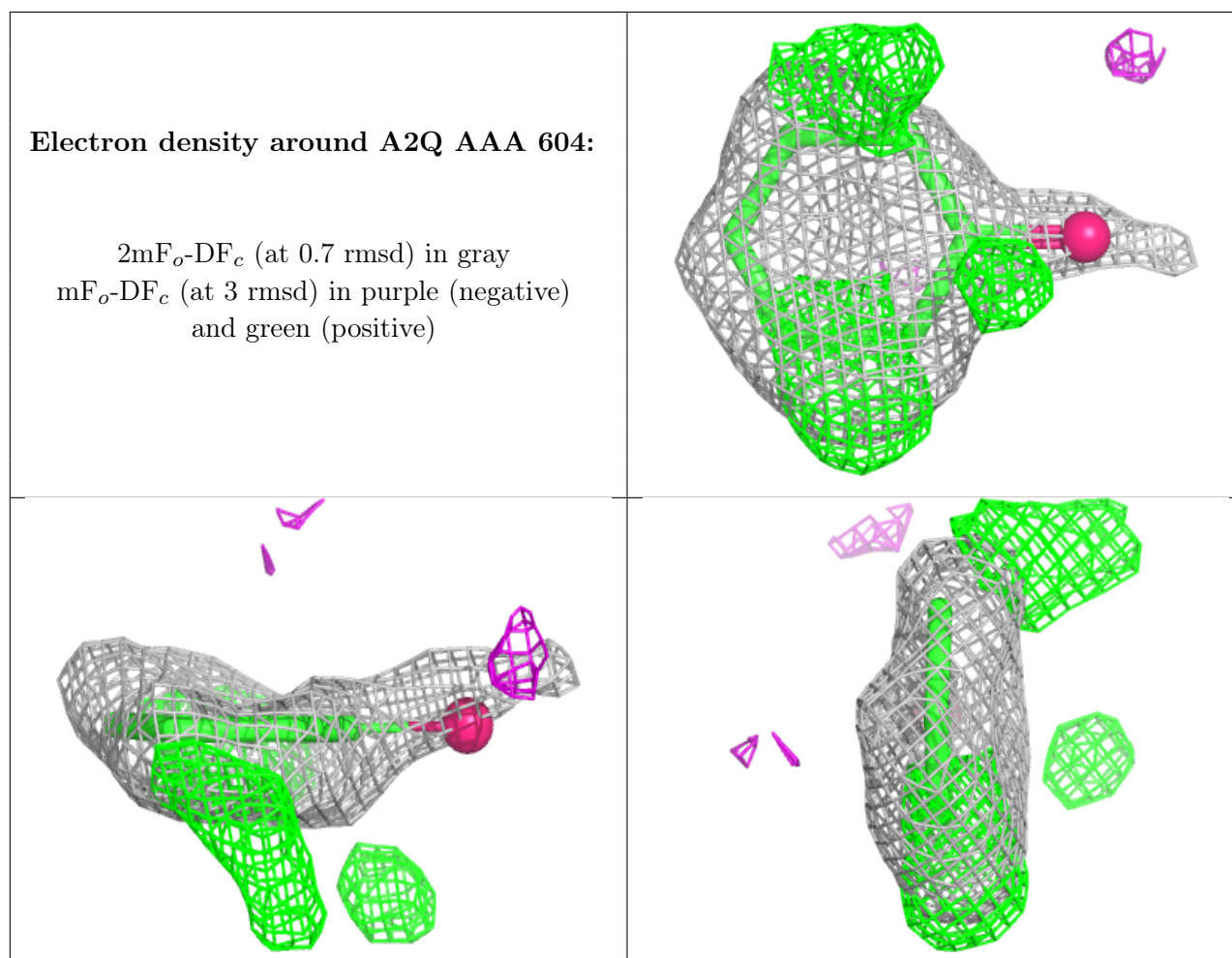
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	AAA	623[A]	5/5	0.97	0.11	13,14,15,16	5
5	SO4	BaB	623[A]	5/5	0.98	0.04	14,14,15,15	5
2	FAD	BaB	601	53/53	0.99	0.04	9,11,12,12	0
2	FAD	AAA	601	53/53	0.99	0.04	9,10,11,12	0

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.

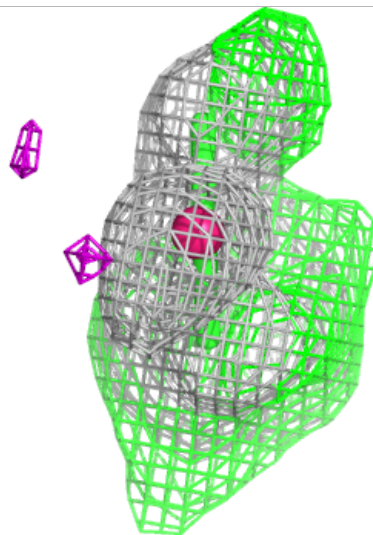
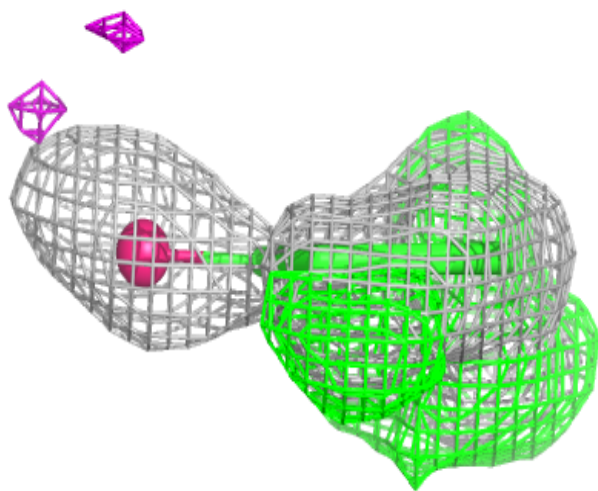
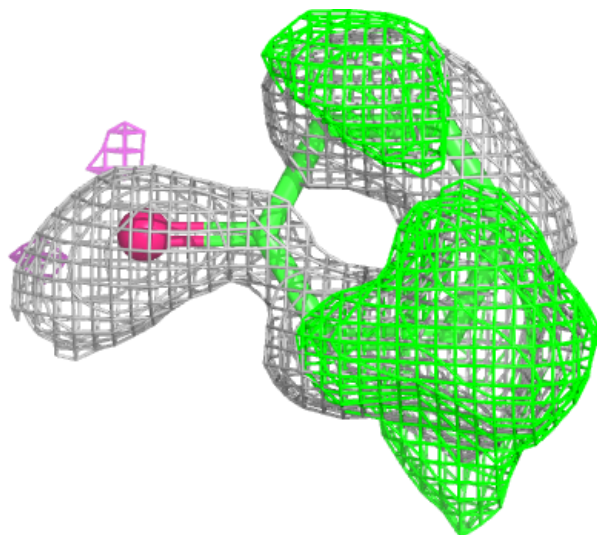
Electron density around A2Q AAA 604:

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



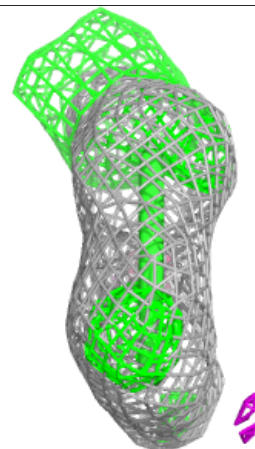
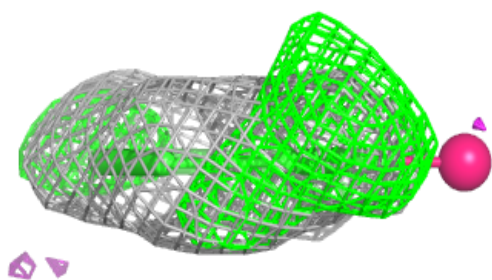
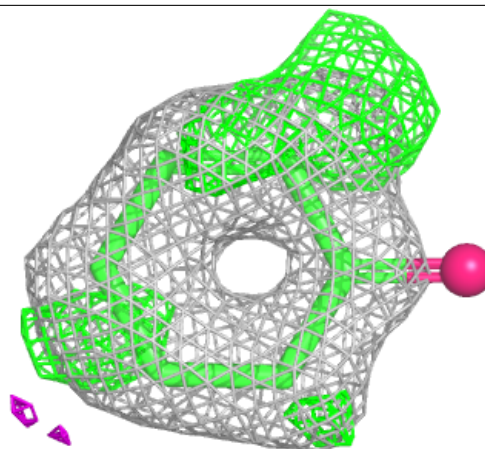
Electron density around A2Q AAA 605 (A):

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



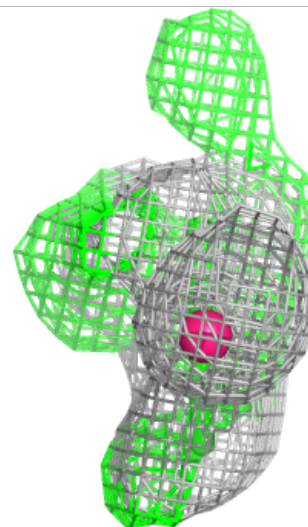
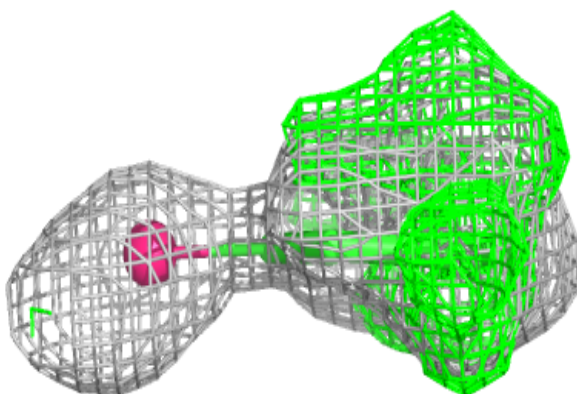
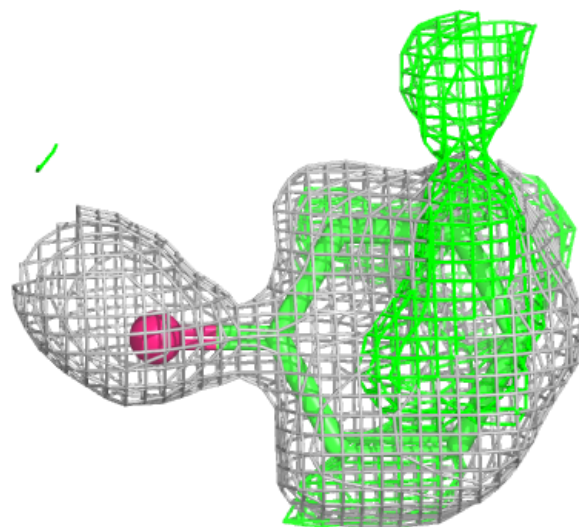
Electron density around A2Q BaB 604:

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



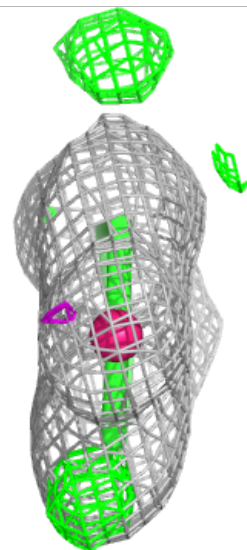
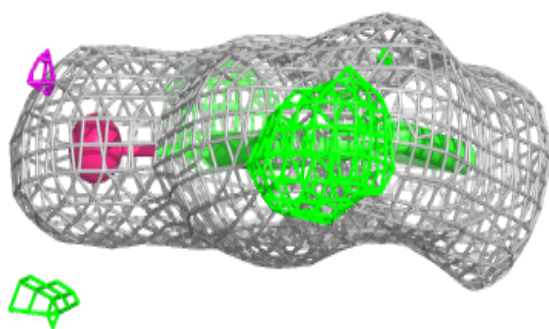
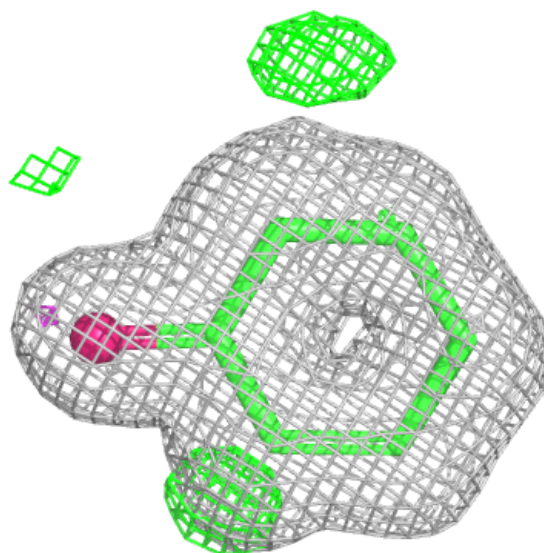
Electron density around A2Q BaB 605 (A):

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



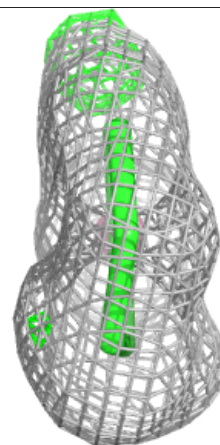
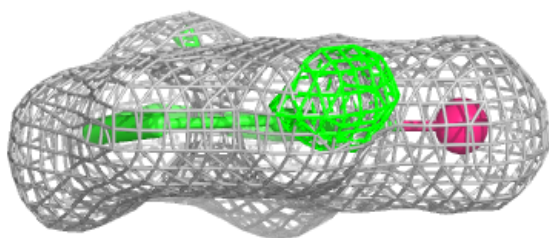
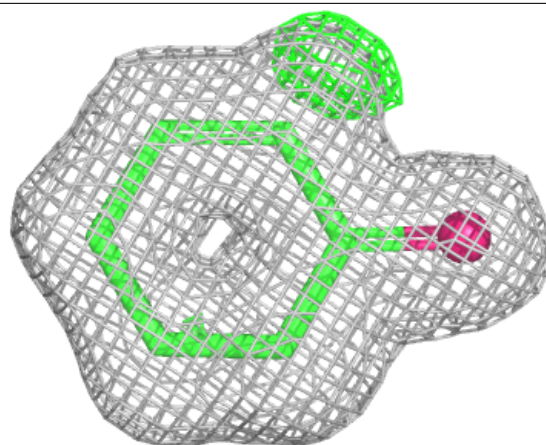
Electron density around A2Q AAA 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



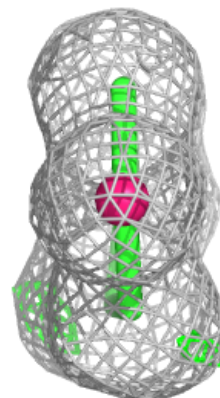
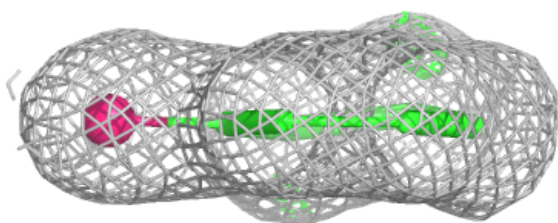
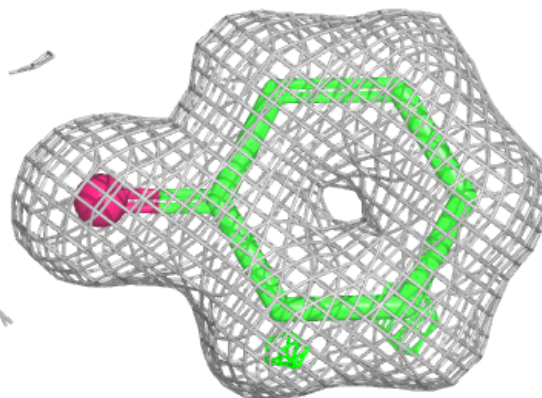
Electron density around A2Q BaB 603:

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

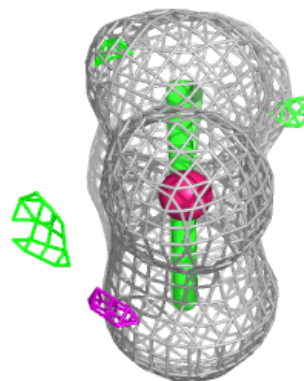
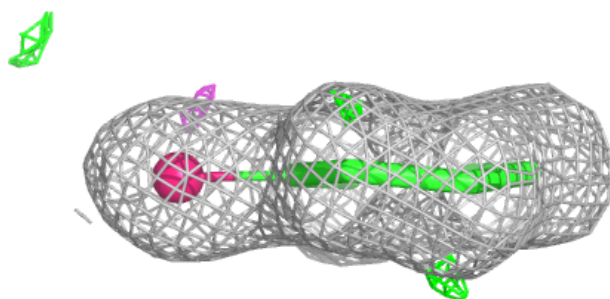
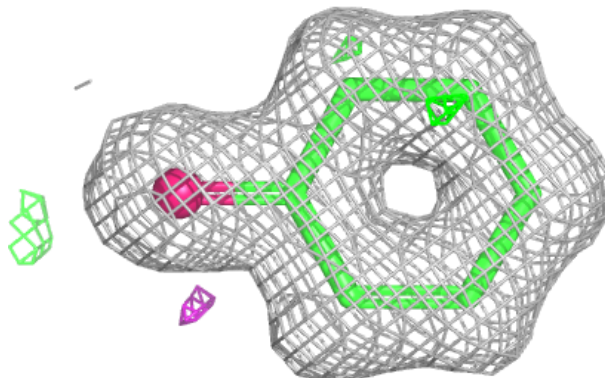


Electron density around A2Q AAA 602:

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

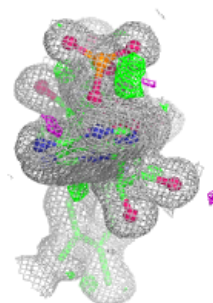
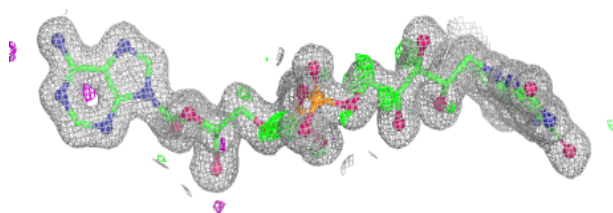
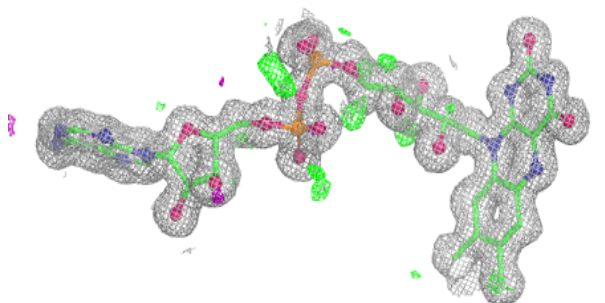
**Electron density around A2Q BaB 602:**

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

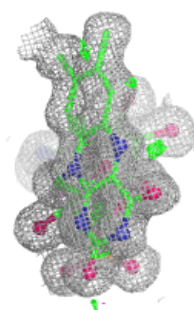
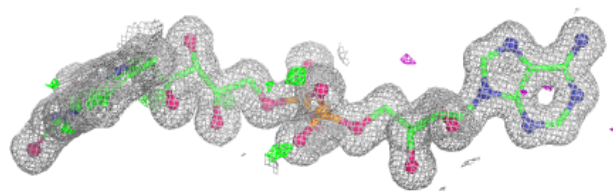
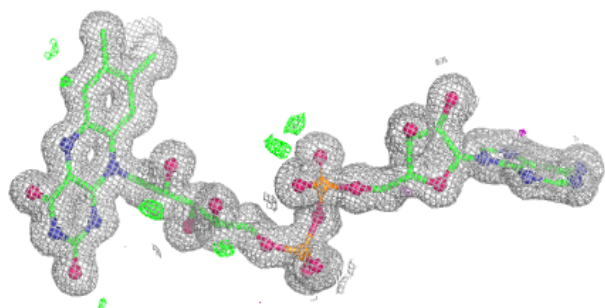


Electron density around FAD BaB 601:

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

**Electron density around FAD AAA 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.