Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 03:02 am GMT

PDB ID	:	6Z6C
Title	:	Crystal structurel of FleA lectin in complex with a monovalent inhibitor
Authors	:	Varrot, A.
Deposited on	:	2020-05-28
Resolution	:	1.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

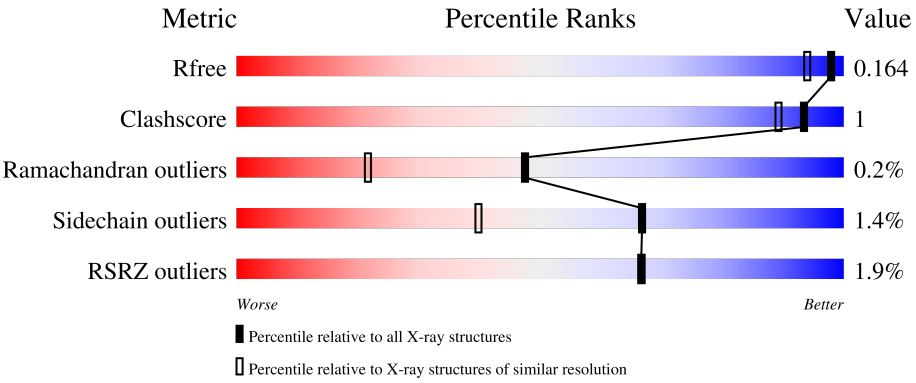
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	317	2% 96%
1	BBB	317	2% 96%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5929 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.

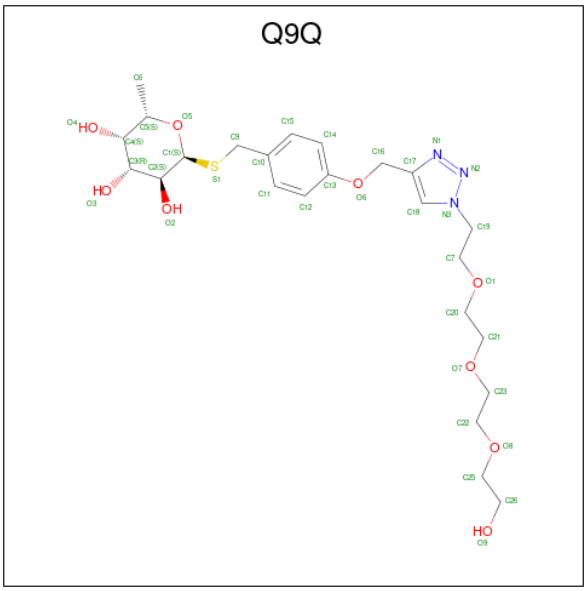
- Molecule 1 is a protein called Fucose-specific lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	315	Total	C	N	O	S	0	6	0
			2494	1587	430	472	5			
1	BBB	317	Total	C	N	O	S	0	7	0
			2522	1604	437	476	5			

There are 8 discrepancies between the modelled and reference sequences:

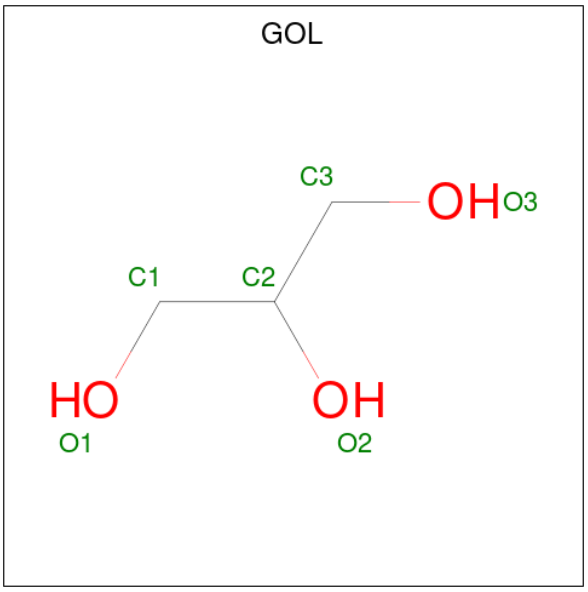
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	GLY	-	expression tag	UNP Q4WW81
AAA	0	HIS	-	expression tag	UNP Q4WW81
AAA	20	SER	LEU	conflict	UNP Q4WW81
AAA	111	CYS	ARG	conflict	UNP Q4WW81
BBB	-1	GLY	-	expression tag	UNP Q4WW81
BBB	0	HIS	-	expression tag	UNP Q4WW81
BBB	20	SER	LEU	conflict	UNP Q4WW81
BBB	111	CYS	ARG	conflict	UNP Q4WW81

- Molecule 2 is 4-((1-(2-(2-(2-(2-hydroxyethoxy)ethoxy)ethoxy)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)benzyl-a-L-thiofucoside (three-letter code: Q9Q) (formula: $C_{24}H_{37}N_3O_9S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C N O S 26 17 3 5 1	0	0
2	AAA	1	Total C O S 20 14 5 1	0	0
2	AAA	1	Total C O S 21 15 5 1	0	0
2	AAA	1	Total C O S 12 7 4 1	0	0
2	AAA	1	Total C O S 12 7 4 1	0	0
2	BBB	1	Total C O S 19 13 5 1	0	0
2	BBB	1	Total C O S 20 14 5 1	0	0
2	BBB	1	Total C O S 19 13 5 1	0	0
2	BBB	1	Total C O S 12 7 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

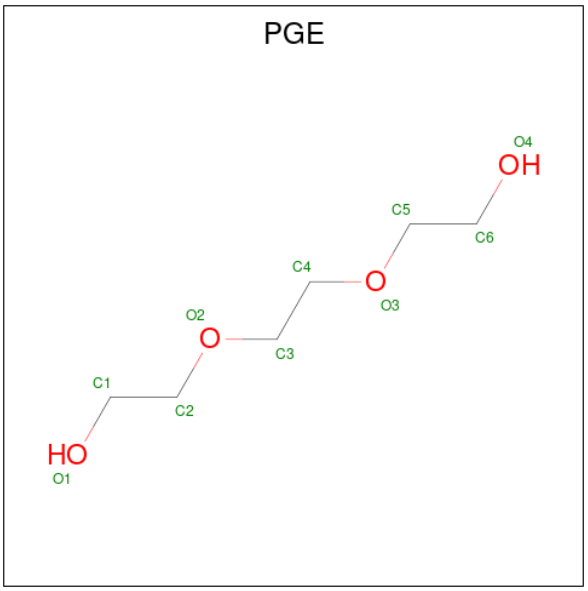


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Na 1 1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 10 6 4	0	0

- Molecule 6 is water.

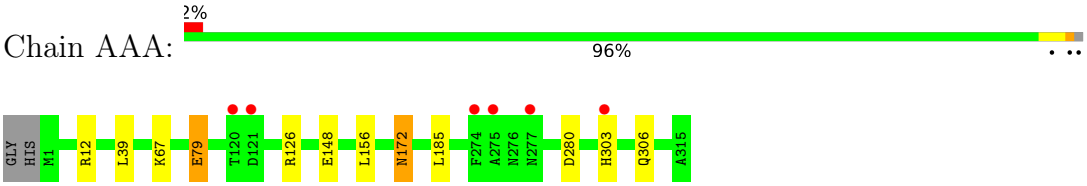
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	357	Total O 367 367	0	10
6	BBB	356	Total O 362 362	0	6

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.

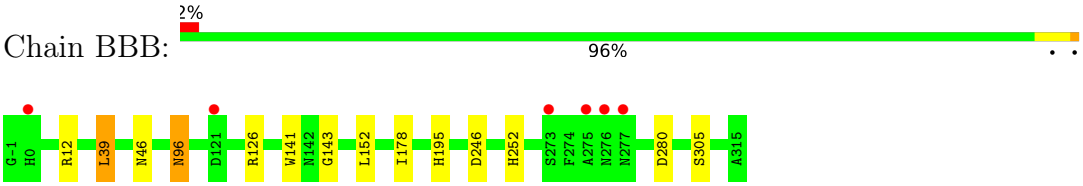
• Molecule 1: Fucose-specific lectin

Chain AAA:



• Molecule 1: Fucose-specific lectin

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.12Å 46.89Å 80.17Å 103.08° 98.54° 108.51°	Depositor
Resolution (Å)	42.53 – 1.40 42.53 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.53-1.40) 99.1 (42.53-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.118 , 0.158 0.127 , 0.164	Depositor DCC
R_{free} test set	5702 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.005 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	5929	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Q9Q, GOL, PGE, NA

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	0.77	2/2566 (0.1%)	0.93	2/3498 (0.1%)
1	BBB	0.76	0/2596	0.93	2/3538 (0.1%)
All	All	0.76	2/5162 (0.0%)	0.93	4/7036 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	79	GLU	CD-OE1	5.97	1.32	1.25
1	AAA	148	GLU	CD-OE2	-5.50	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	12	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	AAA	12	ARG	NE-CZ-NH2	-11.07	114.77	120.30
1	BBB	126	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	AAA	126	ARG	NE-CZ-NH1	5.53	123.06	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2494	0	2368	6	0
1	BBB	2522	0	2386	6	0
2	AAA	91	0	0	0	0
2	BBB	70	0	0	0	0
3	AAA	6	0	8	0	0
3	BBB	6	0	8	0	0
4	AAA	1	0	0	0	0
5	BBB	10	0	13	2	0
6	AAA	367	0	0	3	0
6	BBB	362	0	0	2	0
All	All	5929	0	4783	14	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 (14) 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:96[A]:ASN:ND2	6:BBB:502:HOH:O	2.28	0.66
1:AAA:79:GLU:OE2	6:AAA:501:HOH:O	2.14	0.64
1:AAA:303[A]:HIS:CE1	1:AAA:306:GLN:HG2	2.41	0.56
1:BBB:246:ASP:OD2	1:BBB:252:HIS:HE1	1.88	0.55
1:AAA:67:LYS:NZ	6:AAA:506:HOH:O	2.36	0.54
1:AAA:156[A]:LEU:CD1	1:AAA:185:LEU:HD23	2.40	0.51
1:BBB:152:LEU:HD13	1:BBB:178:ILE:HD11	1.93	0.50
1:BBB:141[A]:TRP:CH2	1:BBB:143:GLY:HA2	2.47	0.49
5:BBB:404:PGE:C3	5:BBB:404:PGE:H6	2.43	0.49
1:AAA:303[A]:HIS:CE1	1:AAA:306:GLN:CG	3.00	0.44
5:BBB:404:PGE:C6	5:BBB:404:PGE:H32	2.48	0.43
1:BBB:39:LEU:C	1:BBB:39:LEU:HD12	2.39	0.42
1:AAA:172:ASN:ND2	6:AAA:516:HOH:O	2.52	0.41
1:BBB:305[B]:SER:OG	6:BBB:501:HOH:O	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AAA	319/317 (101%)	313 (98%)	6 (2%)	0	100 100
1	BBB	322/317 (102%)	314 (98%)	7 (2%)	1 (0%)	41 18
All	All	641/634 (101%)	627 (98%)	13 (2%)	1 (0%)	47 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	46	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	255/251 (102%)	252 (99%)	3 (1%)	71 47
1	BBB	257/251 (102%)	252 (98%)	5 (2%)	57 25
All	All	512/502 (102%)	504 (98%)	8 (2%)	67 33

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	39	LEU
1	AAA	172	ASN
1	AAA	280	ASP
1	BBB	39	LEU
1	BBB	96[A]	ASN
1	BBB	96[B]	ASN
1	BBB	195	HIS
1	BBB	280	ASP

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	Q9Q	AAA	405	-	11,12,39	0.78	0	14,17,50	0.86	0
2	Q9Q	BBB	403	-	20,20,39	1.09	2 (10%)	25,28,50	1.87	10 (40%)
2	Q9Q	AAA	401	-	27,28,39	1.72	7 (25%)	30,39,50	1.63	8 (26%)
2	Q9Q	AAA	402	-	21,21,39	1.08	1 (4%)	26,29,50	1.49	7 (26%)
2	Q9Q	BBB	402	-	21,21,39	1.17	1 (4%)	26,29,50	1.79	5 (19%)
5	PGE	BBB	404	-	9,9,9	0.93	0	8,8,8	0.40	0
2	Q9Q	AAA	403	-	22,22,39	1.12	2 (9%)	27,30,50	1.72	8 (29%)
2	Q9Q	BBB	405	-	11,12,39	0.81	0	14,17,50	1.43	2 (14%)
3	GOL	AAA	404	-	5,5,5	0.61	0	5,5,5	0.75	0
3	GOL	BBB	406	-	5,5,5	0.21	0	5,5,5	0.43	0
2	Q9Q	BBB	401	-	20,20,39	0.93	0	25,28,50	1.43	6 (24%)
2	Q9Q	AAA	406	-	11,12,39	1.36	2 (18%)	14,17,50	1.36	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Q9Q	AAA	405	-	-	0/2/22/42	0/1/1/3
2	Q9Q	BBB	403	-	-	0/5/25/42	0/2/2/3
2	Q9Q	AAA	401	-	-	0/8/30/42	0/3/3/3
2	Q9Q	AAA	402	-	-	0/7/27/42	0/2/2/3
2	Q9Q	BBB	402	-	-	1/7/27/42	0/2/2/3
5	PGE	BBB	404	-	-	2/7/7/7	-
2	Q9Q	AAA	403	-	-	0/8/28/42	0/2/2/3
2	Q9Q	BBB	405	-	-	0/2/22/42	0/1/1/3
3	GOL	AAA	404	-	-	1/4/4/4	-
3	GOL	BBB	406	-	-	0/4/4/4	-
2	Q9Q	BBB	401	-	-	1/5/25/42	0/2/2/3
2	Q9Q	AAA	406	-	-	0/2/22/42	0/1/1/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401	Q9Q	C18-C17	5.05	1.43	1.36
2	AAA	401	Q9Q	C1-S1	3.78	1.86	1.80
2	BBB	402	Q9Q	C9-S1	-3.45	1.74	1.81
2	AAA	403	Q9Q	C6-C5	-2.85	1.44	1.51
2	AAA	402	Q9Q	C1-S1	2.63	1.84	1.80
2	BBB	403	Q9Q	O5-C1	2.63	1.46	1.42
2	AAA	406	Q9Q	O3-C3	-2.46	1.37	1.43
2	AAA	401	Q9Q	C17-N1	2.37	1.37	1.34
2	AAA	403	Q9Q	O5-C1	2.32	1.46	1.42
2	AAA	401	Q9Q	C1-C2	-2.20	1.49	1.53
2	AAA	401	Q9Q	C12-C13	-2.13	1.34	1.38
2	AAA	406	Q9Q	O2-C2	2.12	1.48	1.43
2	BBB	403	Q9Q	C9-S1	-2.12	1.77	1.81
2	AAA	401	Q9Q	O3-C3	-2.04	1.38	1.43
2	AAA	401	Q9Q	C11-C12	-2.00	1.35	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	402	Q9Q	C15-C14-C13	4.15	124.81	119.73
2	BBB	403	Q9Q	C10-C9-S1	3.56	123.85	111.61
2	BBB	405	Q9Q	O5-C1-C2	3.41	114.60	110.31
2	BBB	402	Q9Q	C14-C13-C12	-3.41	114.93	120.18
2	BBB	403	Q9Q	C15-C14-C13	3.34	123.54	119.88
2	BBB	402	Q9Q	O3-C3-C2	3.30	117.98	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	403	Q9Q	O6-C16-C17	3.25	119.33	108.21
2	BBB	402	Q9Q	C10-C9-S1	3.16	122.50	111.61
2	AAA	403	Q9Q	C16-O6-C13	3.14	126.03	117.99
2	AAA	401	Q9Q	C9-C10-C15	3.08	126.92	120.86
2	BBB	403	Q9Q	O2-C2-C1	3.08	115.93	110.27
2	BBB	403	Q9Q	O5-C1-C2	3.05	114.15	110.31
2	AAA	403	Q9Q	O5-C1-C2	3.04	114.13	110.31
2	AAA	402	Q9Q	C9-C10-C15	2.92	126.59	120.86
2	AAA	401	Q9Q	C9-C10-C11	-2.91	115.16	120.86
2	AAA	401	Q9Q	O5-C5-C4	2.90	114.73	109.52
2	BBB	402	Q9Q	C9-C10-C11	2.82	126.39	120.86
2	AAA	403	Q9Q	C3-C4-C5	2.78	114.10	109.77
2	BBB	405	Q9Q	O2-C2-C1	2.69	115.22	110.27
2	AAA	406	Q9Q	O2-C2-C1	2.58	115.01	110.27
2	AAA	401	Q9Q	O4-C4-C5	-2.57	103.97	109.67
2	AAA	403	Q9Q	C6-C5-C4	2.46	117.62	113.07
2	BBB	403	Q9Q	O3-C3-C4	2.45	116.02	110.35
2	BBB	403	Q9Q	O5-C1-S1	2.43	115.62	109.82
2	AAA	403	Q9Q	O3-C3-C4	2.42	115.94	110.35
2	BBB	401	Q9Q	C15-C14-C13	2.41	122.52	119.88
2	BBB	403	Q9Q	C12-C11-C10	2.41	124.34	121.03
2	AAA	402	Q9Q	O5-C1-S1	2.41	115.58	109.82
2	AAA	403	Q9Q	C9-C10-C15	2.40	125.57	120.86
2	AAA	401	Q9Q	C12-C11-C10	2.39	124.31	121.03
2	BBB	401	Q9Q	C9-C10-C15	2.37	125.52	120.86
2	AAA	401	Q9Q	C10-C9-S1	2.33	119.63	111.61
2	AAA	402	Q9Q	C9-C10-C11	-2.26	116.43	120.86
2	BBB	403	Q9Q	O4-C4-C5	-2.21	104.77	109.67
2	AAA	403	Q9Q	O5-C1-S1	2.21	115.11	109.82
2	AAA	401	Q9Q	C14-C15-C10	-2.15	118.07	121.03
2	BBB	401	Q9Q	O4-C4-C3	2.13	115.28	110.35
2	BBB	401	Q9Q	C10-C9-S1	2.13	118.95	111.61
2	AAA	402	Q9Q	C16-O6-C13	2.13	122.12	117.51
2	BBB	403	Q9Q	C11-C12-C13	-2.12	117.55	119.88
2	AAA	402	Q9Q	O2-C2-C1	2.12	114.16	110.27
2	AAA	402	Q9Q	C10-C9-S1	2.05	118.68	111.61
2	AAA	401	Q9Q	C1-C2-C3	2.05	114.63	110.59
2	BBB	403	Q9Q	O2-C2-C3	-2.03	105.65	110.35
2	AAA	402	Q9Q	O3-C3-C4	2.02	115.03	110.35
2	BBB	401	Q9Q	C12-C11-C10	2.01	123.80	121.03
2	BBB	401	Q9Q	C3-C4-C5	-2.01	106.65	109.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	404	GOL	C1-C2-C3-O3
5	BBB	404	PGE	O3-C5-C6-O4
5	BBB	404	PGE	C3-C4-O3-C5
2	BBB	402	Q9Q	C12-C13-O6-C16
2	BBB	401	Q9Q	C15-C10-C9-S1

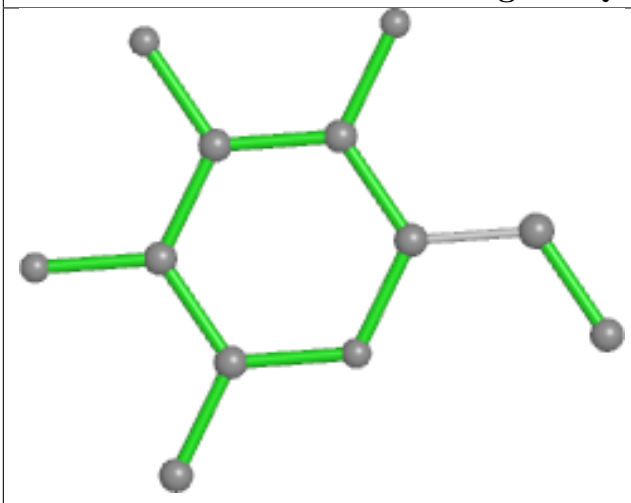
There are no ring outliers.

1 monomer is involved in 2 short contacts:

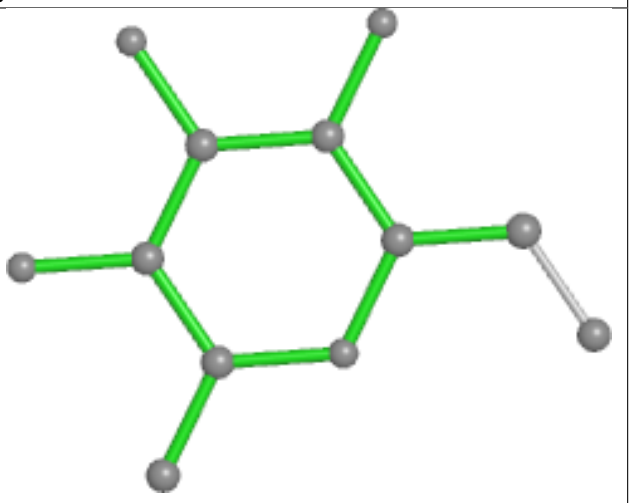
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	404	PGE	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

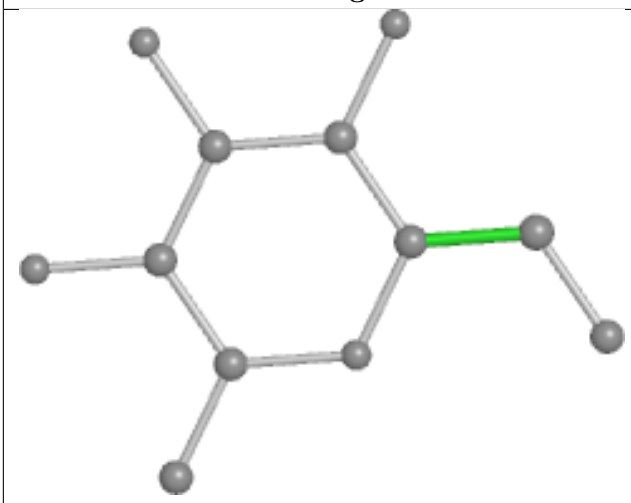
Ligand Q9Q AAA 405



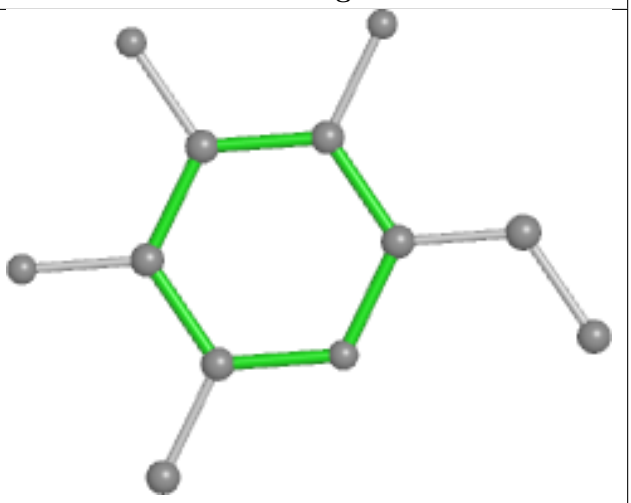
Bond lengths



Bond angles

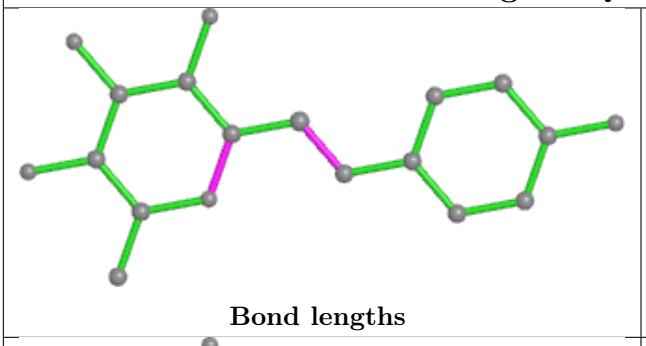


Torsions

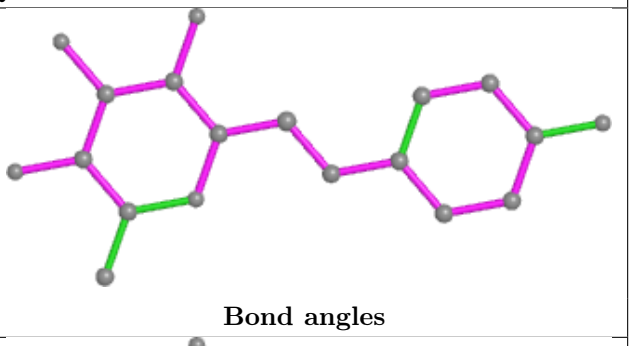


Rings

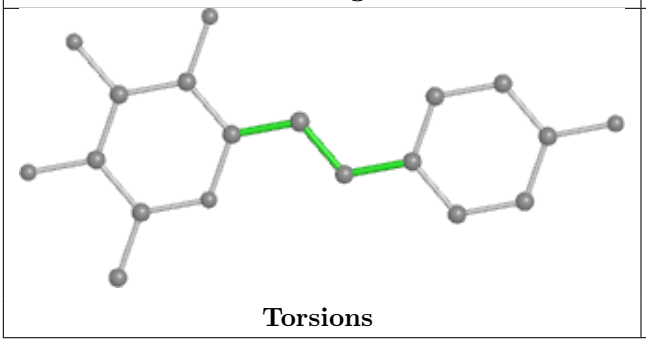
Ligand Q9Q BBB 403



Bond lengths



Bond angles



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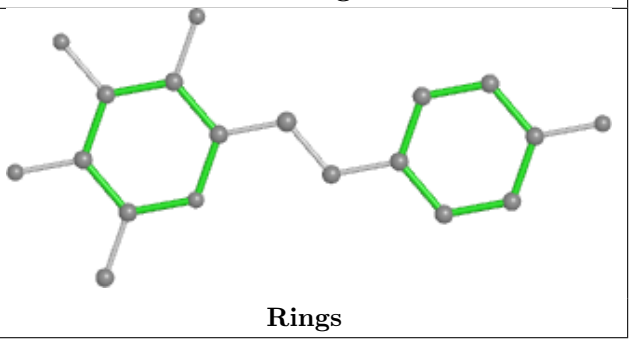
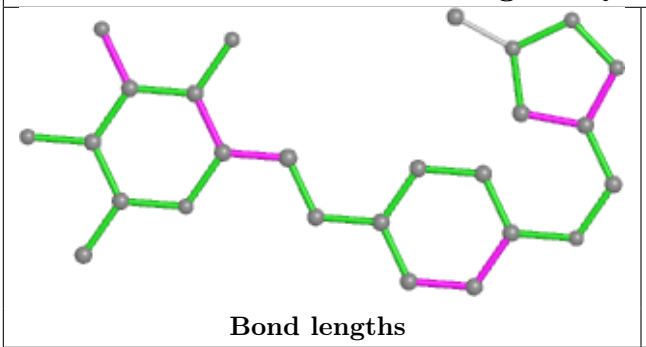


Rings

Ligand Q9Q AAA 401



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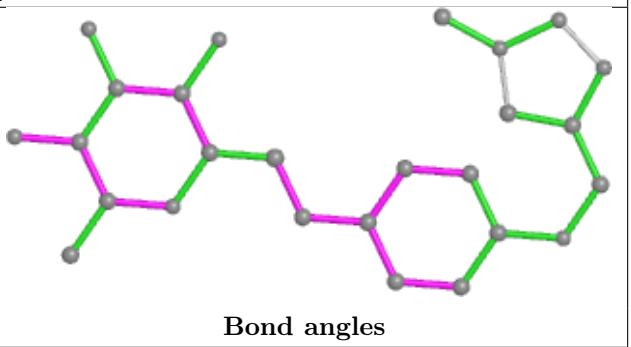
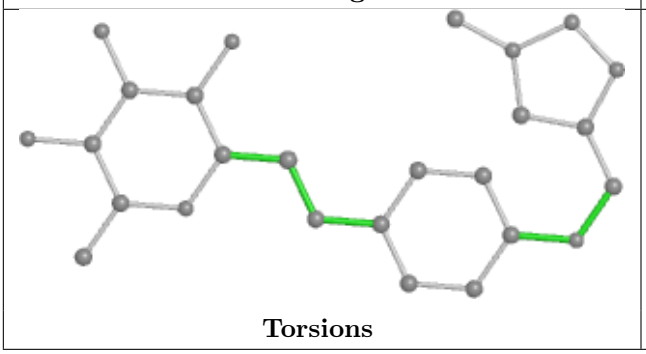
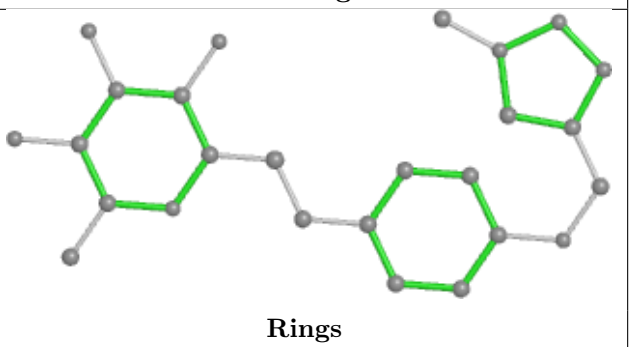


Bond angles

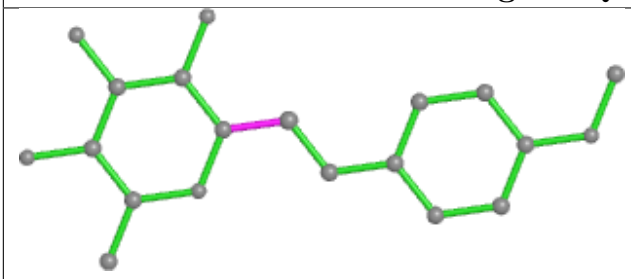


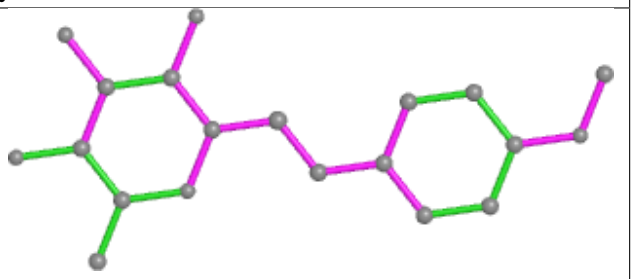
Torsions

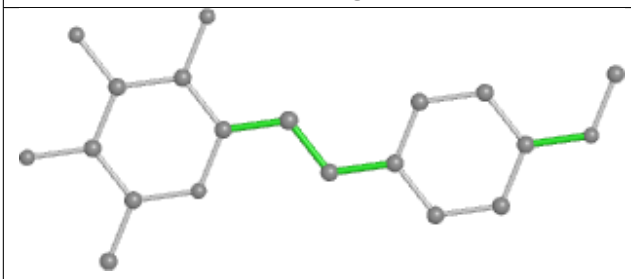


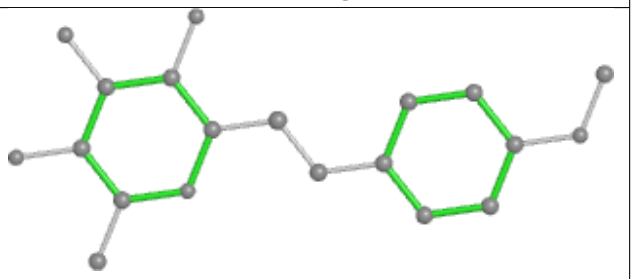
Rings

Ligand Q9Q AAA 402

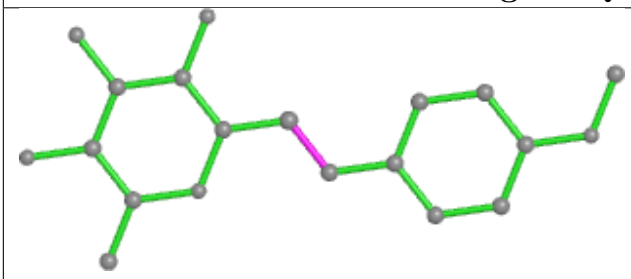

Bond lengths

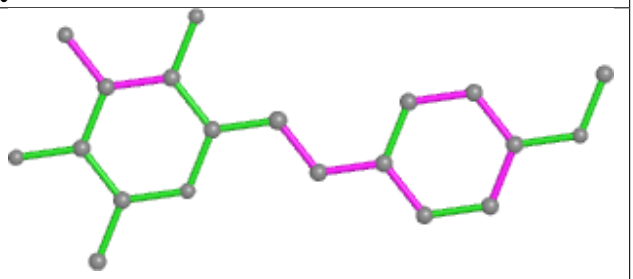

Bond angles

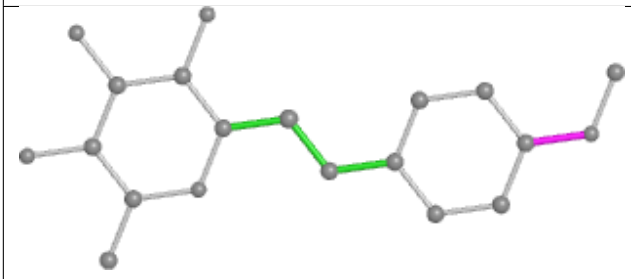

Torsions

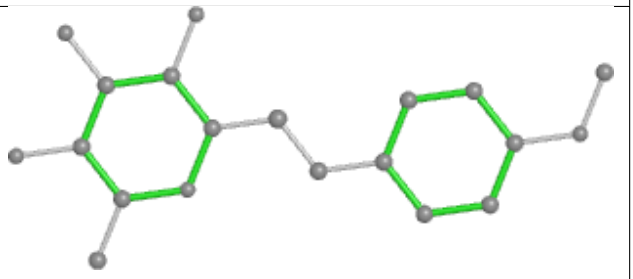

Rings

Ligand Q9Q BBB 402


Bond lengths


Bond angles

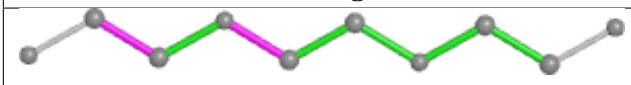

Torsions


Rings

Ligand PGE BBB 404


Bond lengths


Bond angles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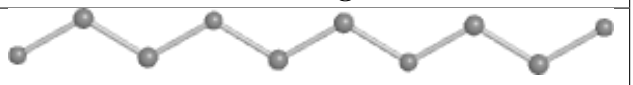
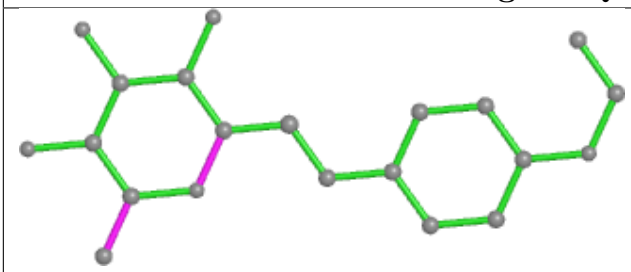
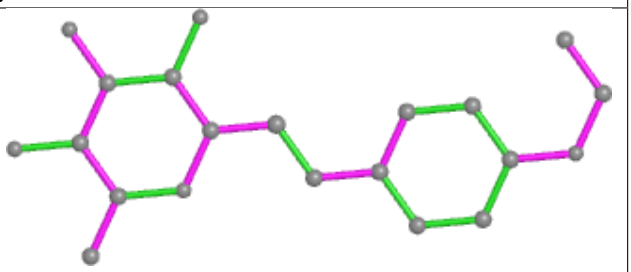

Rings

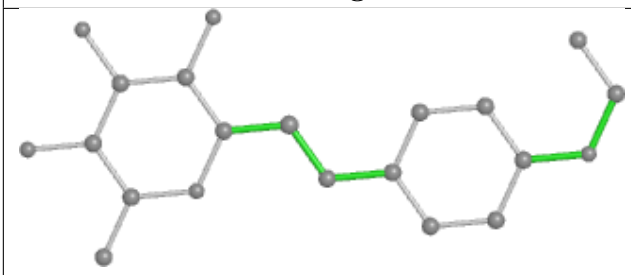
Ligand Q9Q AAA 403



Bond lengths



Bond angles



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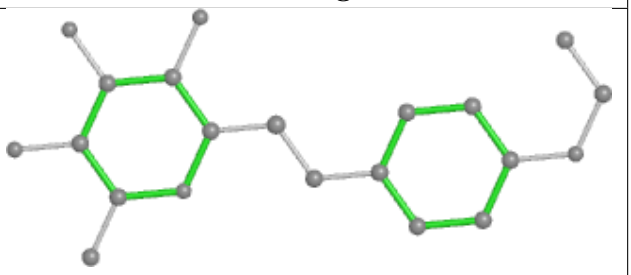
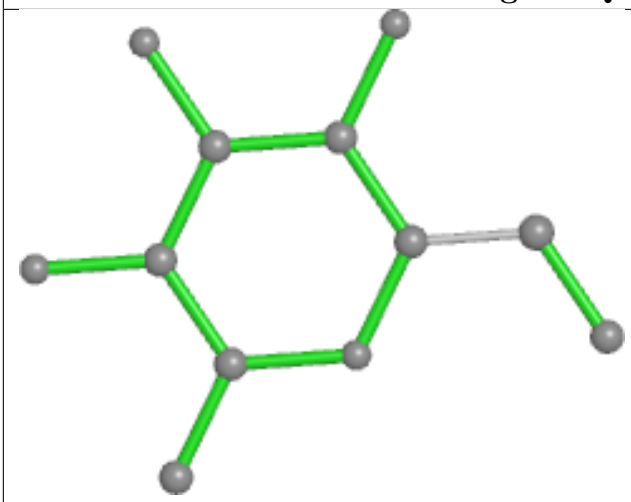


Rings

Ligand Q9Q BBB 405



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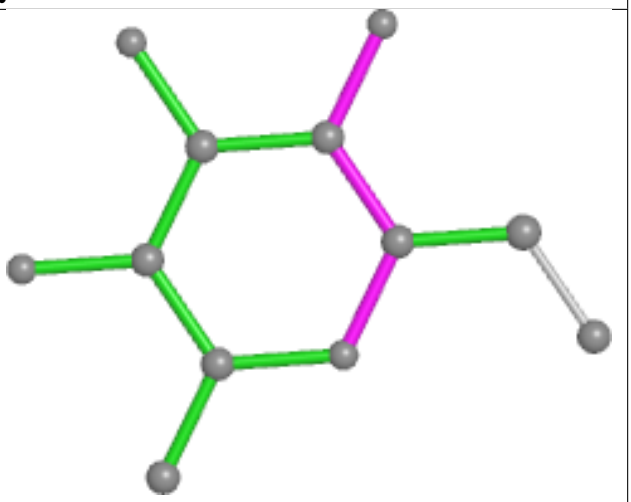
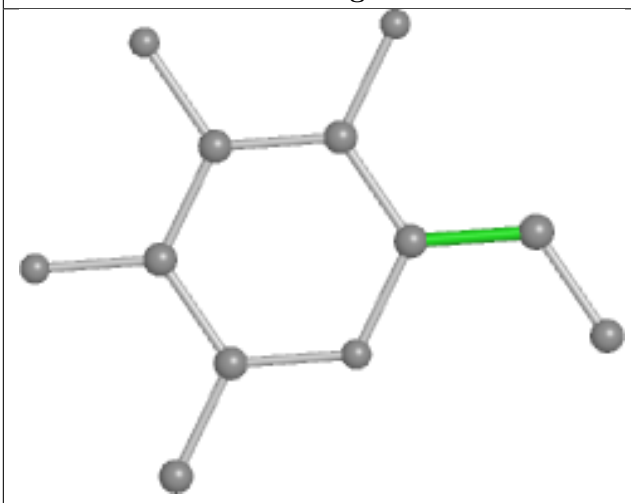
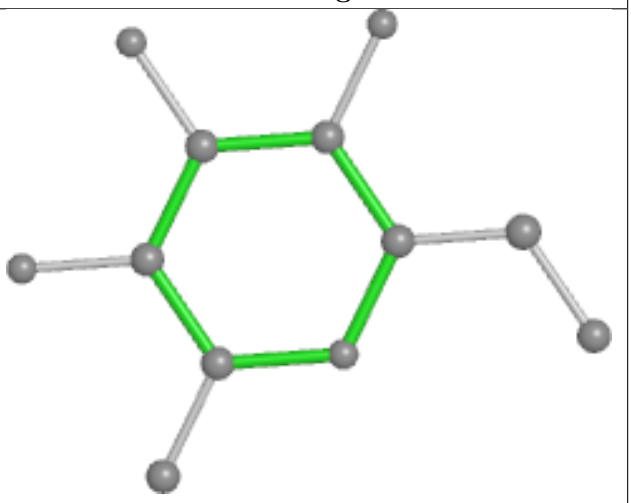


Bond angles

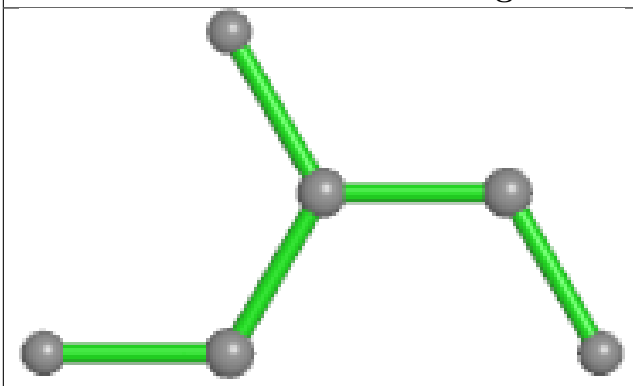


Torsions

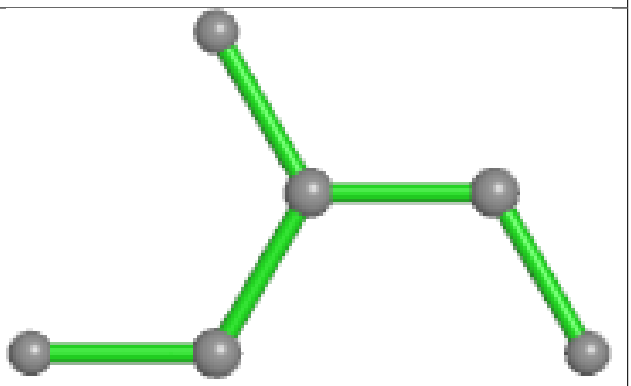


Rings

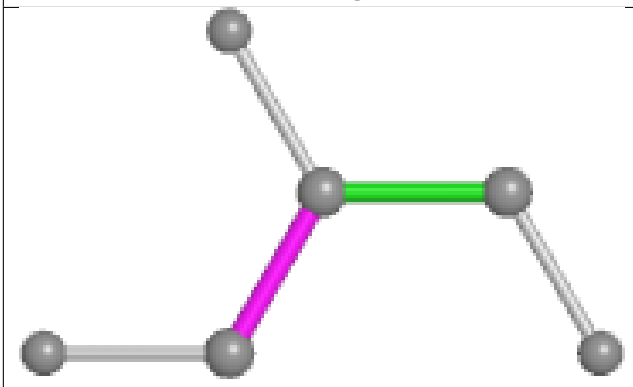
Ligand GOL AAA 404



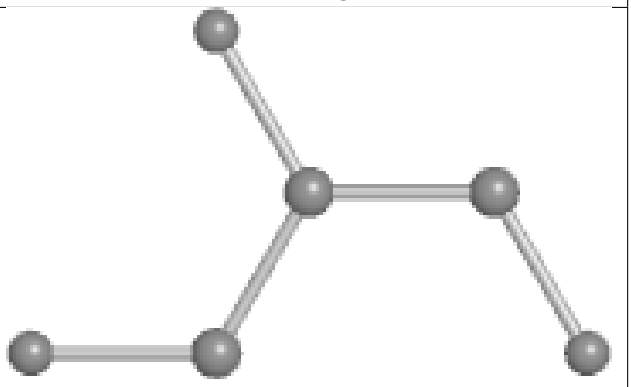
Bond lengths



Bond angles

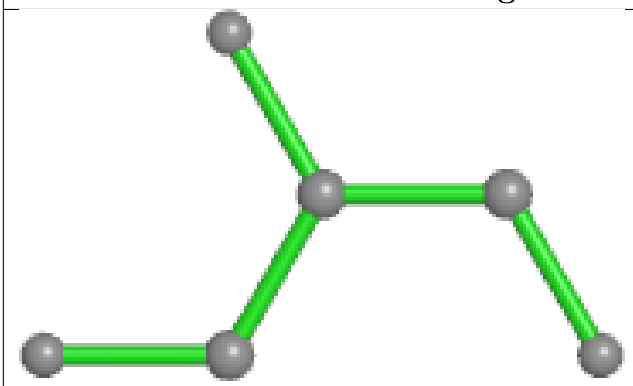


Torsions

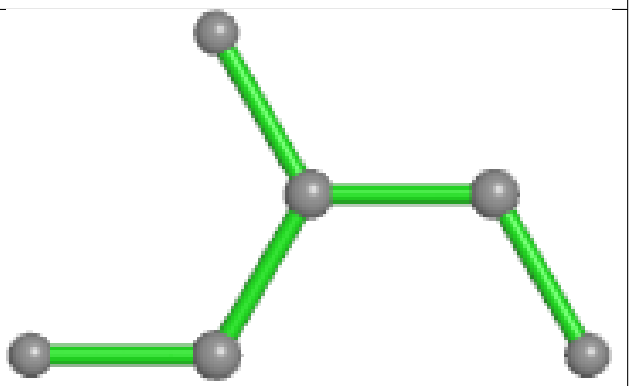


Rings

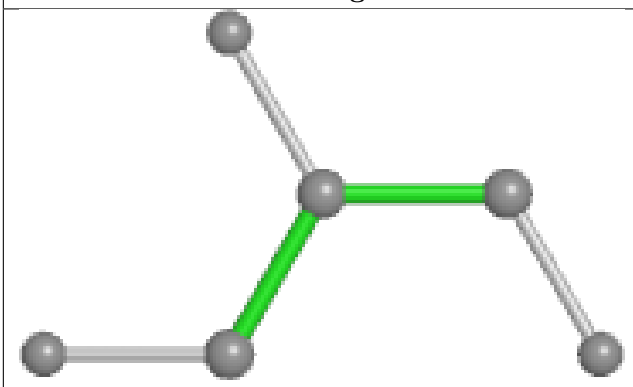
Ligand GOL BBB 406



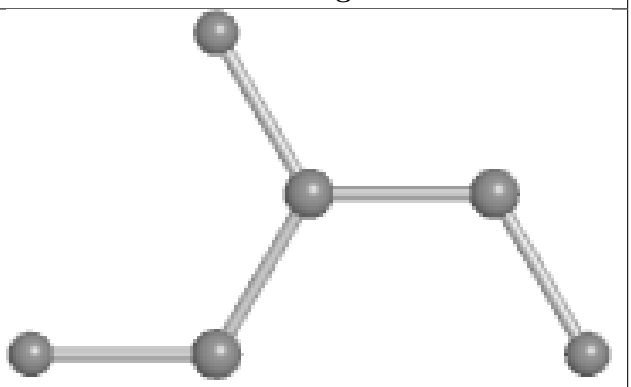
Bond lengths



Bond angles

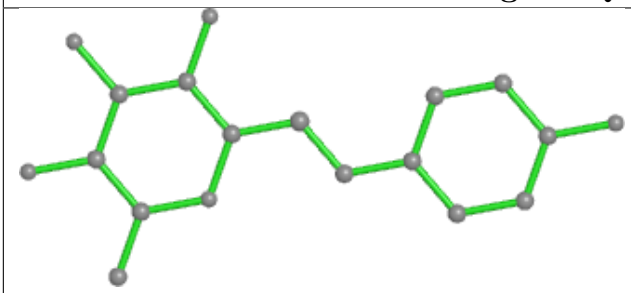


Torsions

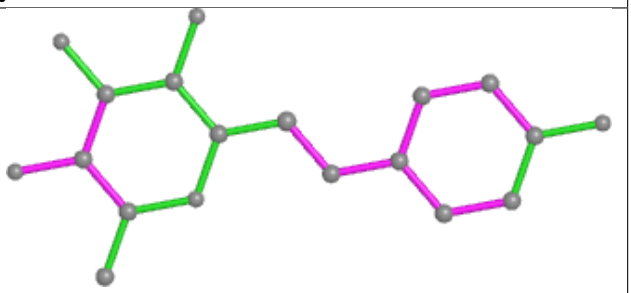


Rings

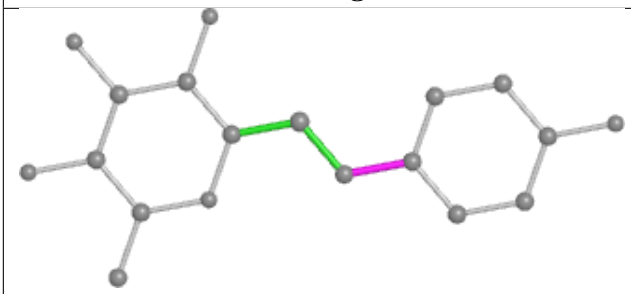
Ligand Q9Q BBB 401



Bond lengths



Bond angles



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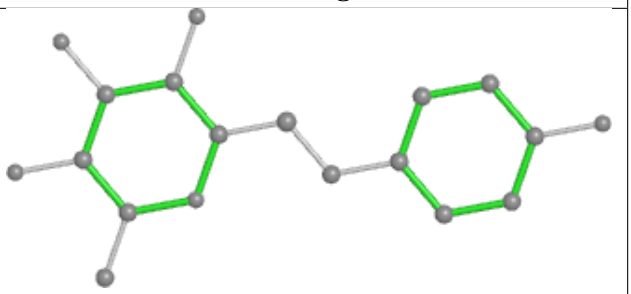
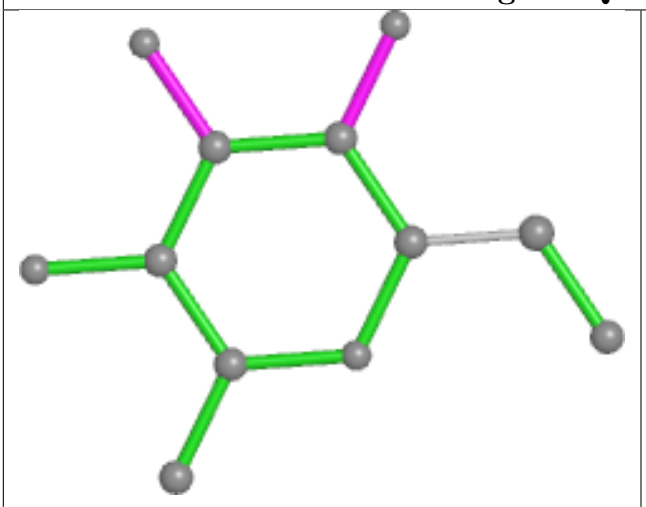
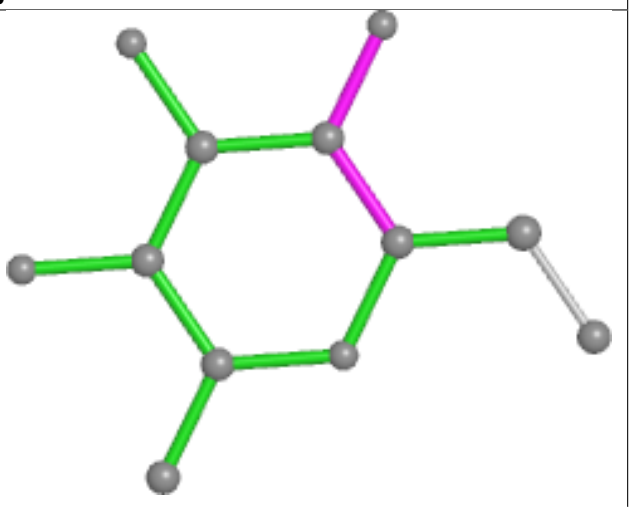


Rings

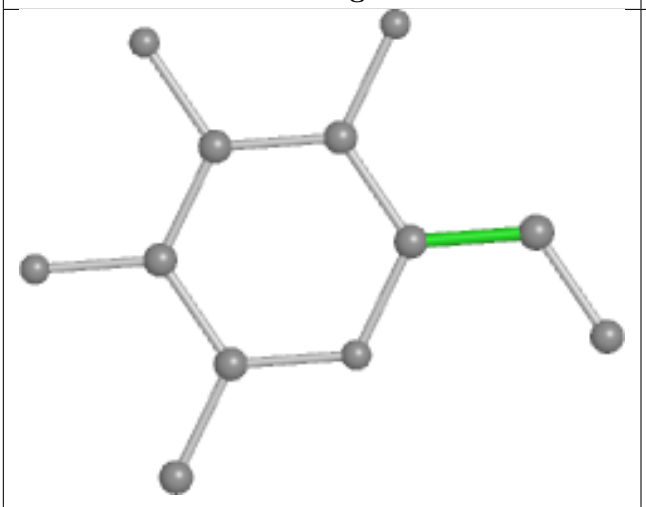
Ligand Q9Q AAA 406



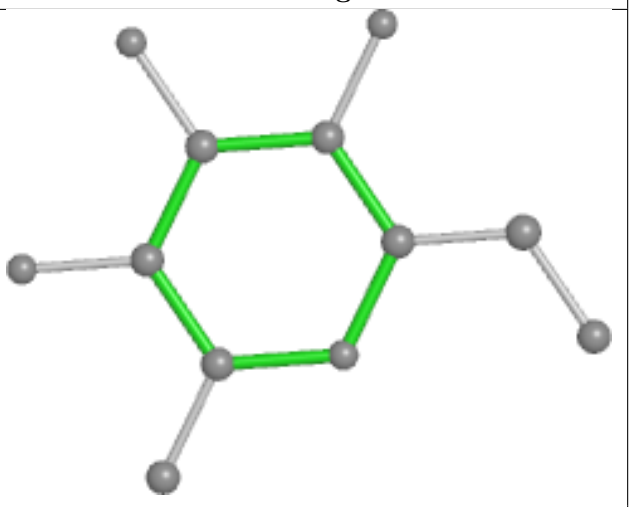
Bond lengths



Bond angles



Torsions



Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	315/317 (99%)	0.35	6 (1%)	66	67	12, 17, 30, 42	1 (0%)
1	BBB	317/317 (100%)	0.30	6 (1%)	66	67	13, 18, 30, 43	0
All	All	632/634 (99%)	0.33	12 (1%)	66	67	12, 17, 30, 43	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	275	ALA	5.1
1	AAA	121	ASP	4.6
1	AAA	274	PHE	3.7
1	BBB	121	ASP	3.7
1	BBB	276	ASN	3.4
1	BBB	273	SER	3.3
1	AAA	303[A]	HIS	2.8
1	BBB	0	HIS	2.8
1	AAA	120	THR	2.7
1	BBB	275	ALA	2.6
1	BBB	277	ASN	2.5
1	AAA	277	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

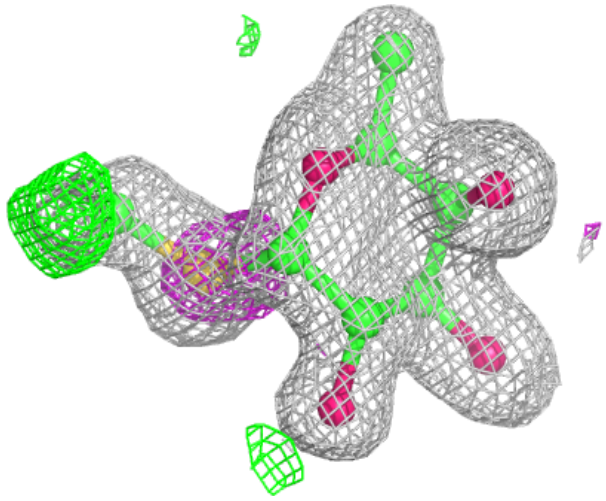
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

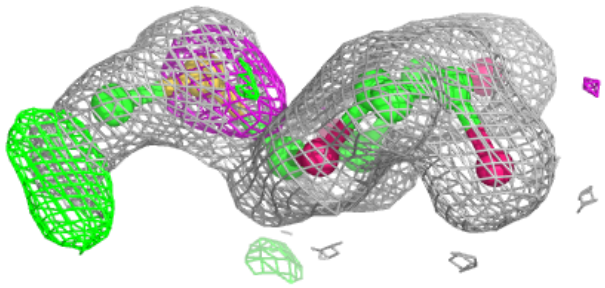
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	Q9Q	AAA	406	12/37	0.87	0.14	22,26,32,34	1
3	GOL	AAA	404	6/6	0.87	0.14	25,28,33,36	0
2	Q9Q	AAA	403	21/37	0.89	0.18	17,26,34,35	0
2	Q9Q	BBB	403	19/37	0.90	0.17	21,28,37,37	0
2	Q9Q	BBB	401	19/37	0.90	0.17	21,24,39,40	0
2	Q9Q	AAA	405	12/37	0.91	0.11	18,19,21,27	0
2	Q9Q	BBB	405	12/37	0.92	0.12	19,22,25,28	0
2	Q9Q	BBB	402	20/37	0.93	0.11	18,21,32,35	0
2	Q9Q	AAA	402	20/37	0.93	0.12	19,23,34,35	0
2	Q9Q	AAA	401	26/37	0.94	0.13	21,27,31,34	15
5	PGE	BBB	404	10/10	0.94	0.12	18,24,26,33	0
3	GOL	BBB	406	6/6	0.95	0.09	20,21,23,23	0
4	NA	AAA	407	1/1	0.99	0.07	24,24,24,24	0

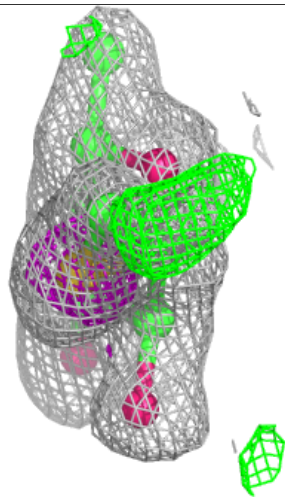
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Q9Q AAA 406:

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

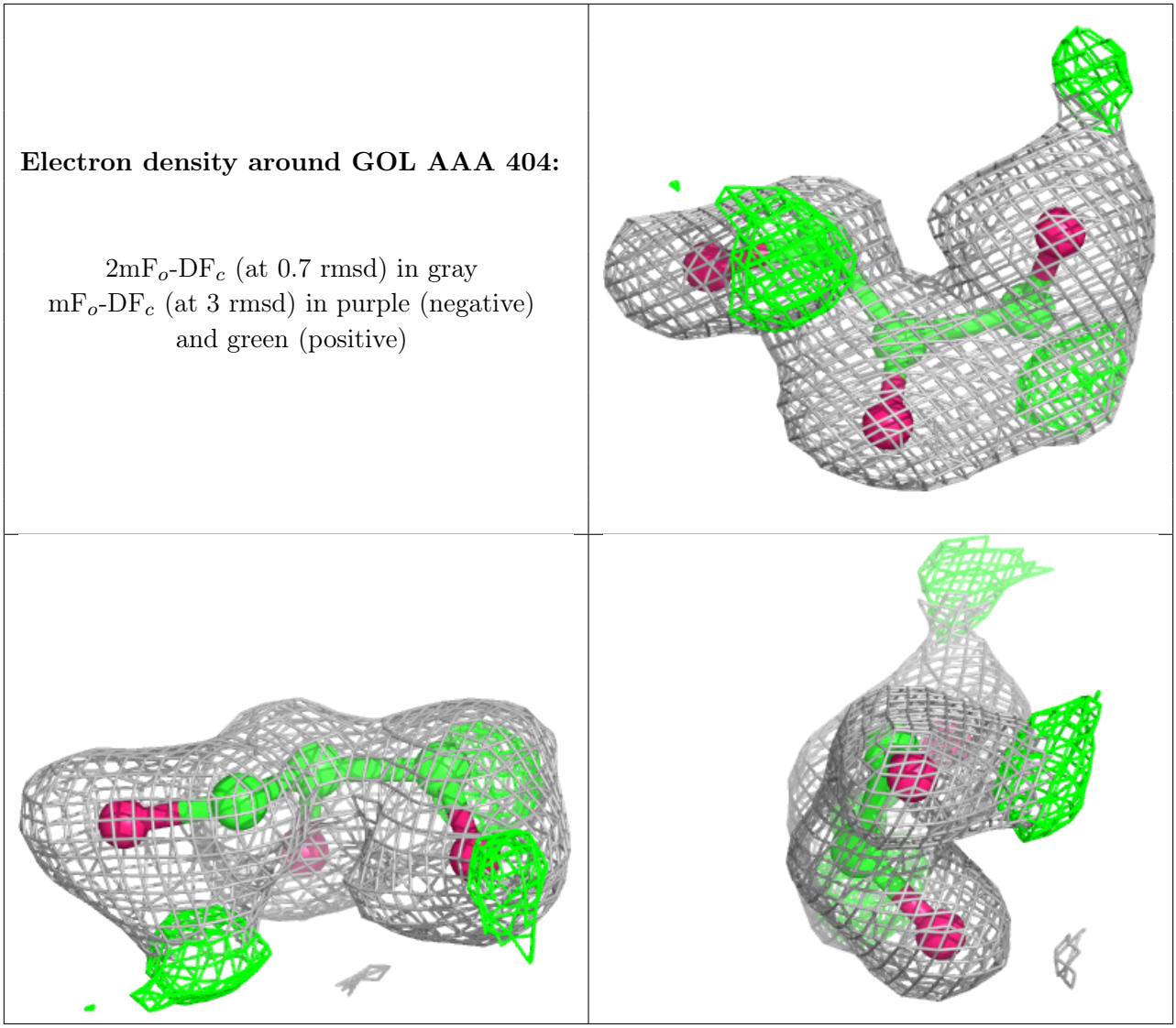






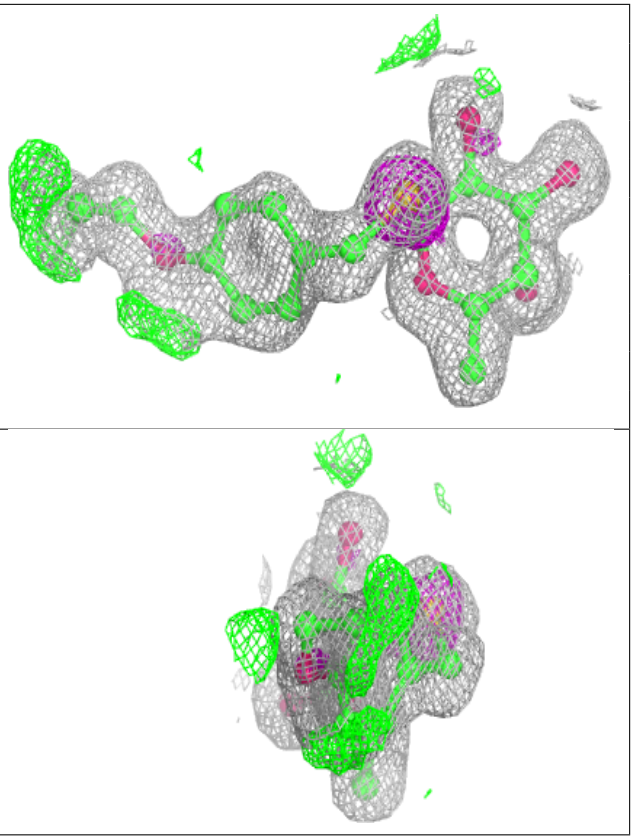
Electron density around GOL AAA 404:

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



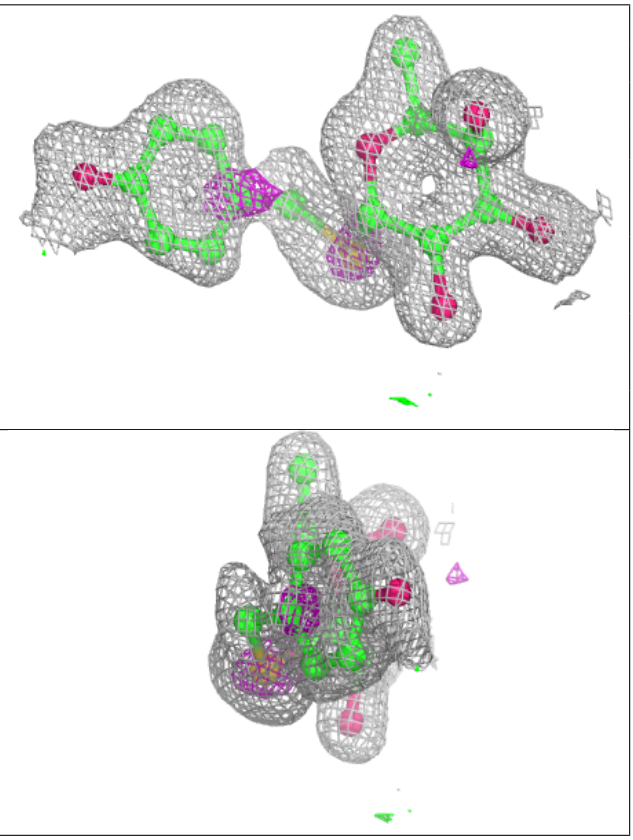
Electron density around Q9Q AAA 403:

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



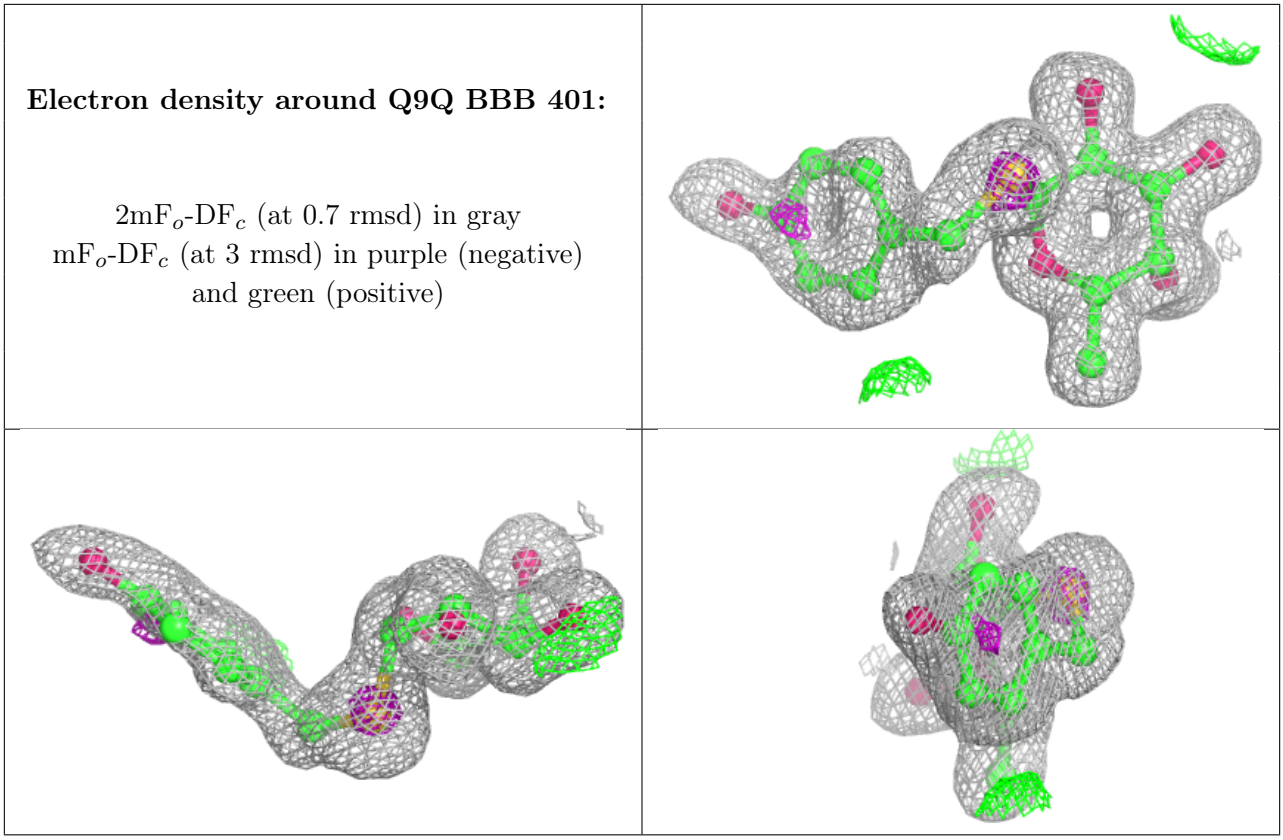
Electron density around Q9Q BBB 403:

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



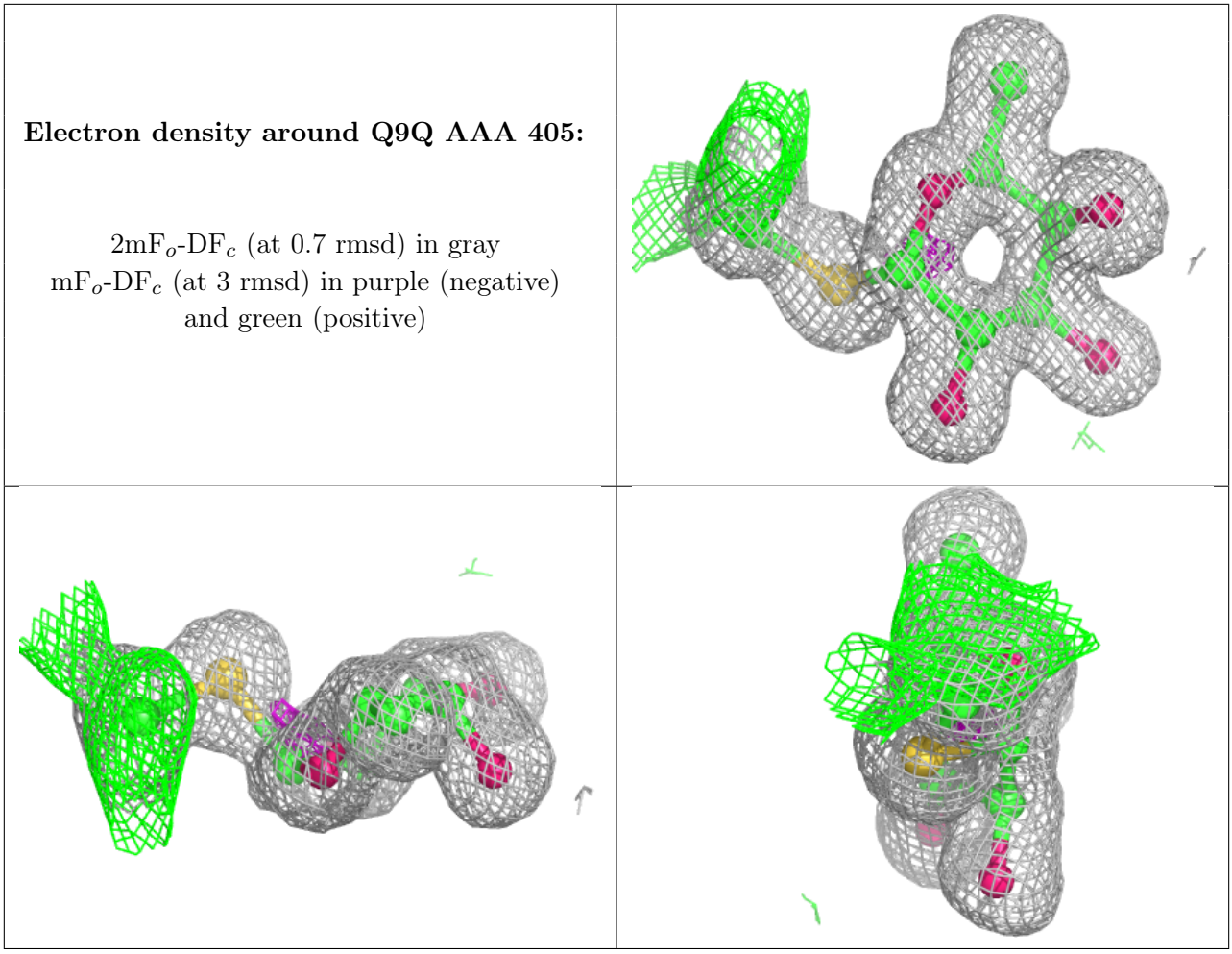
Electron density around Q9Q BBB 401:

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



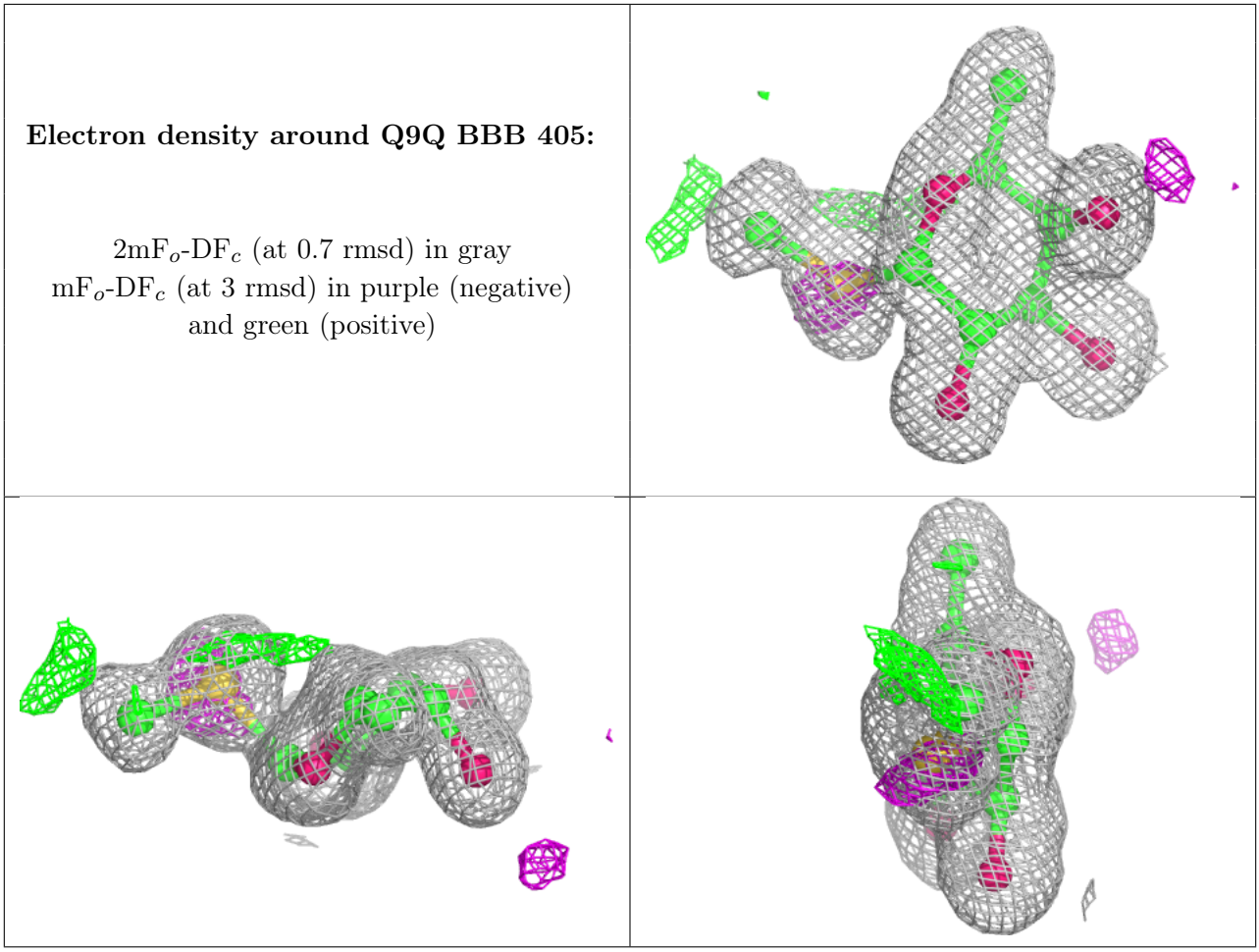
Electron density around Q9Q AAA 405:

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



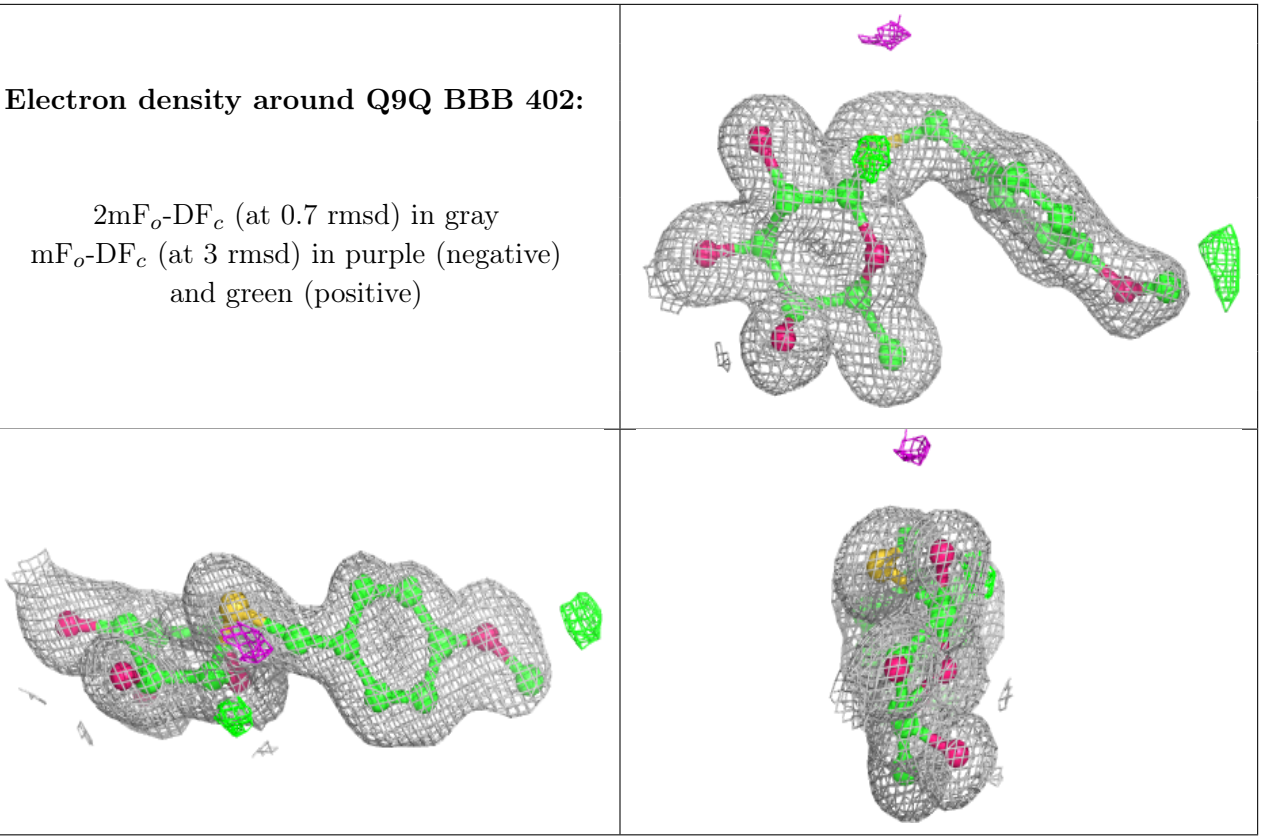
Electron density around Q9Q BBB 405:

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



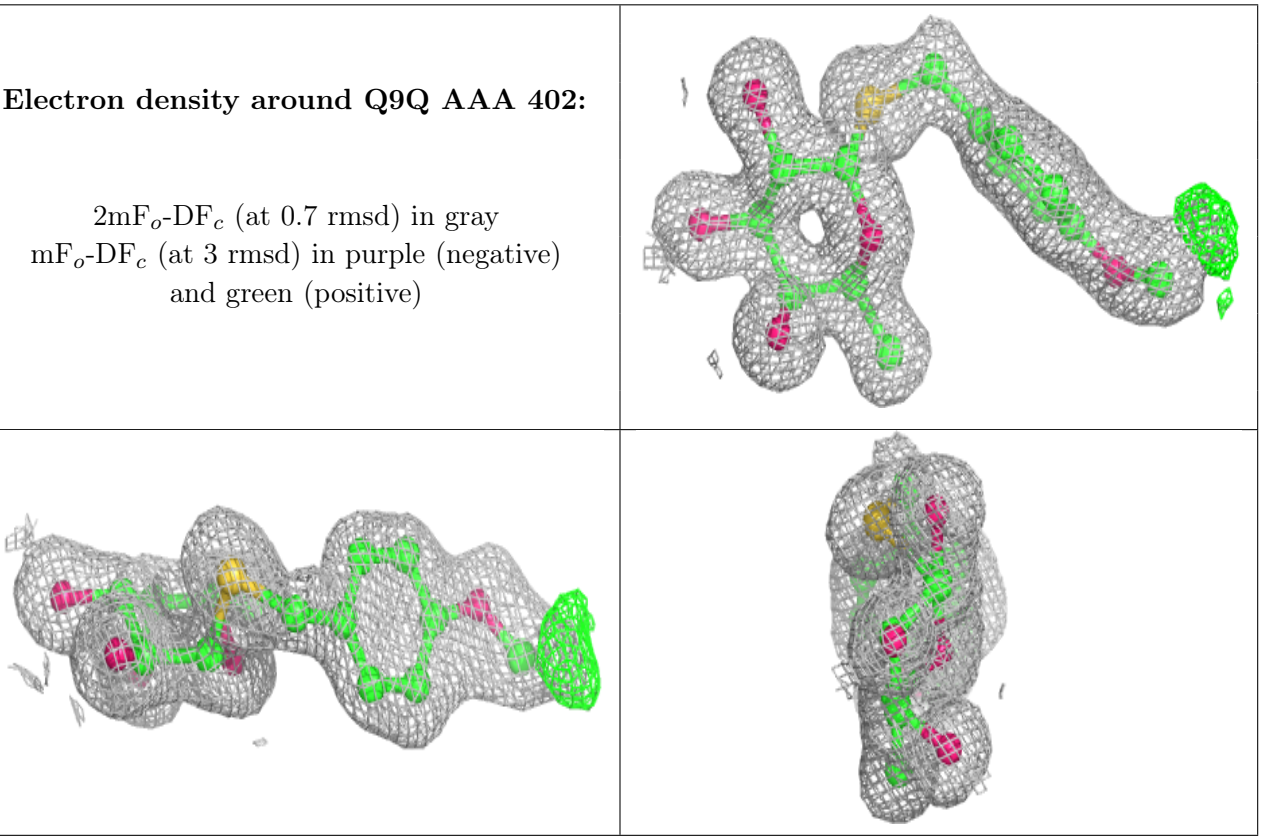
Electron density around Q9Q BBB 402:

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



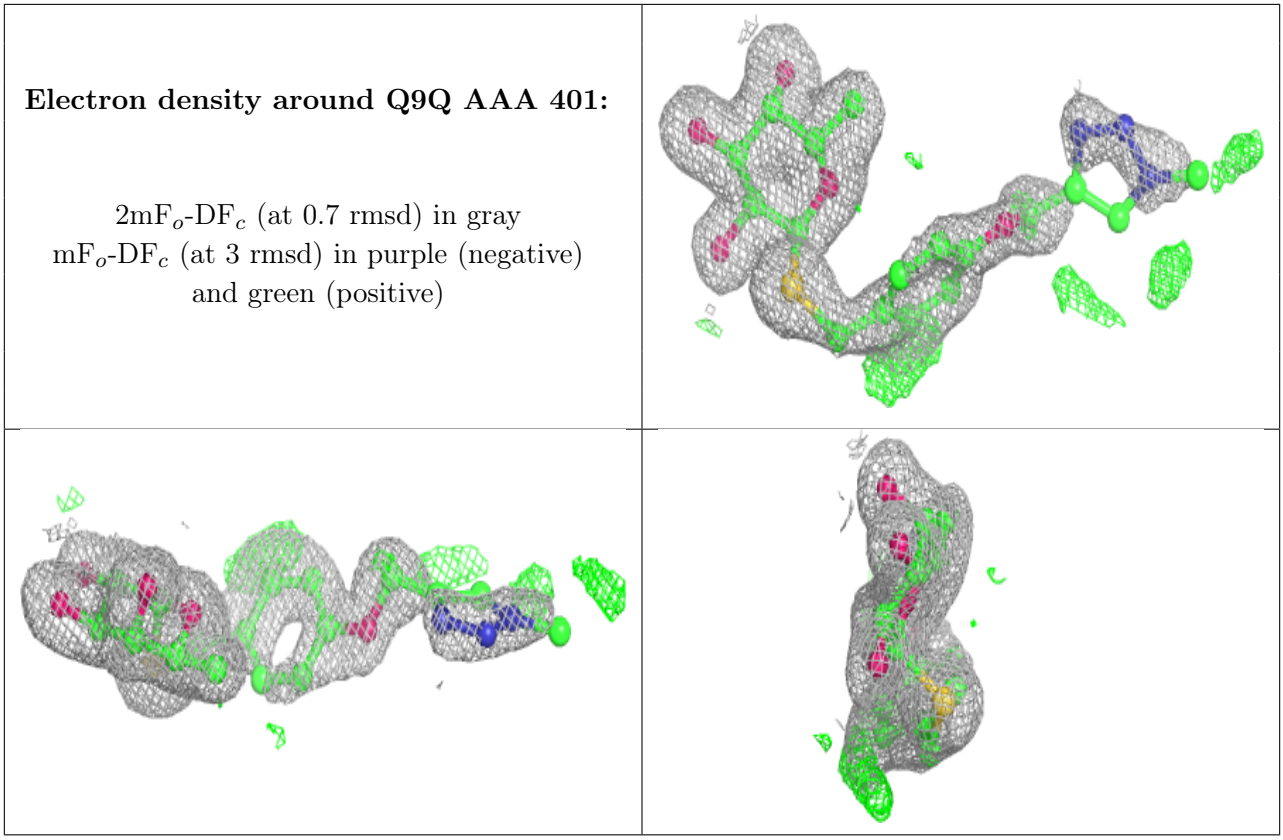
Electron density around Q9Q AAA 402:

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



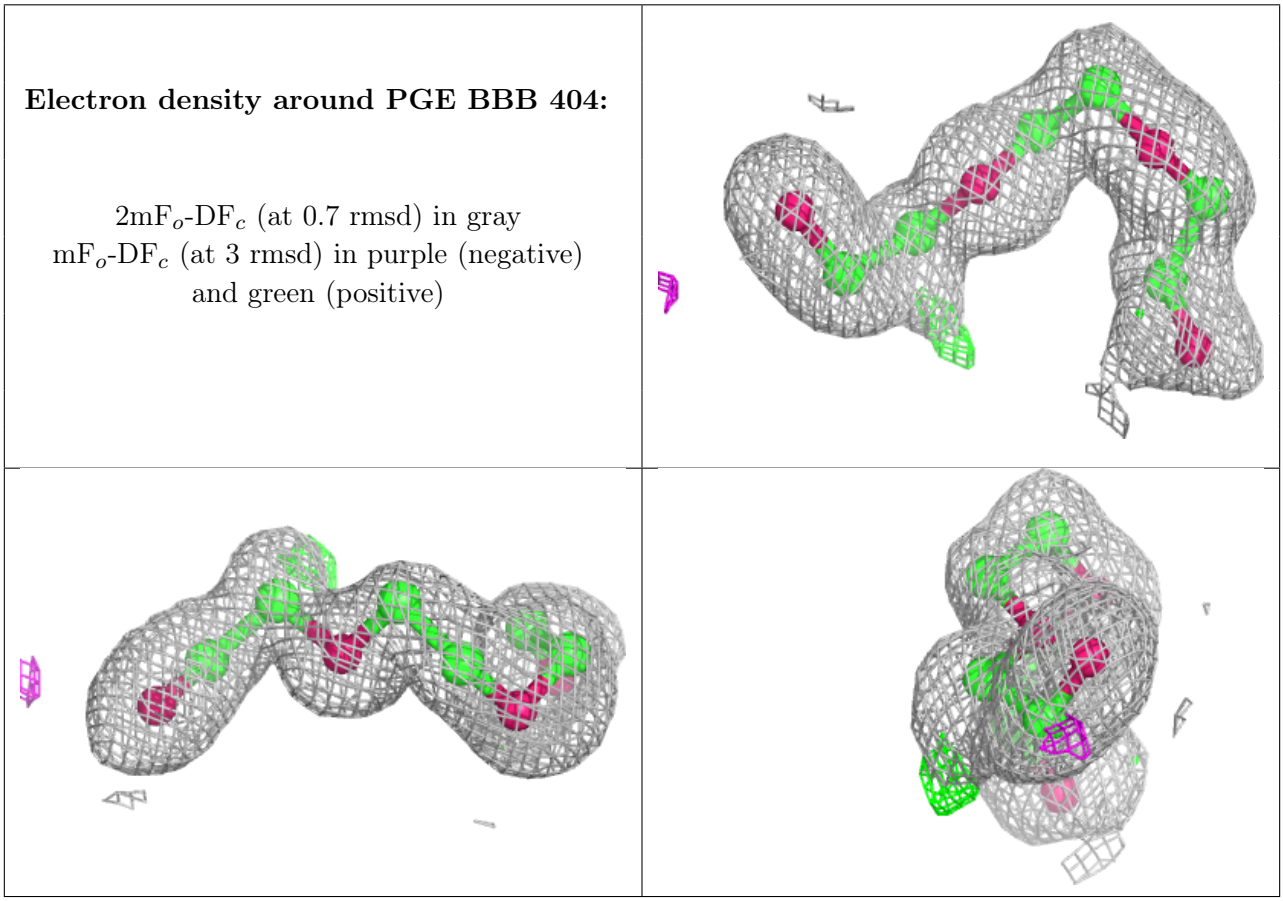
Electron density around Q9Q AAA 401:

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



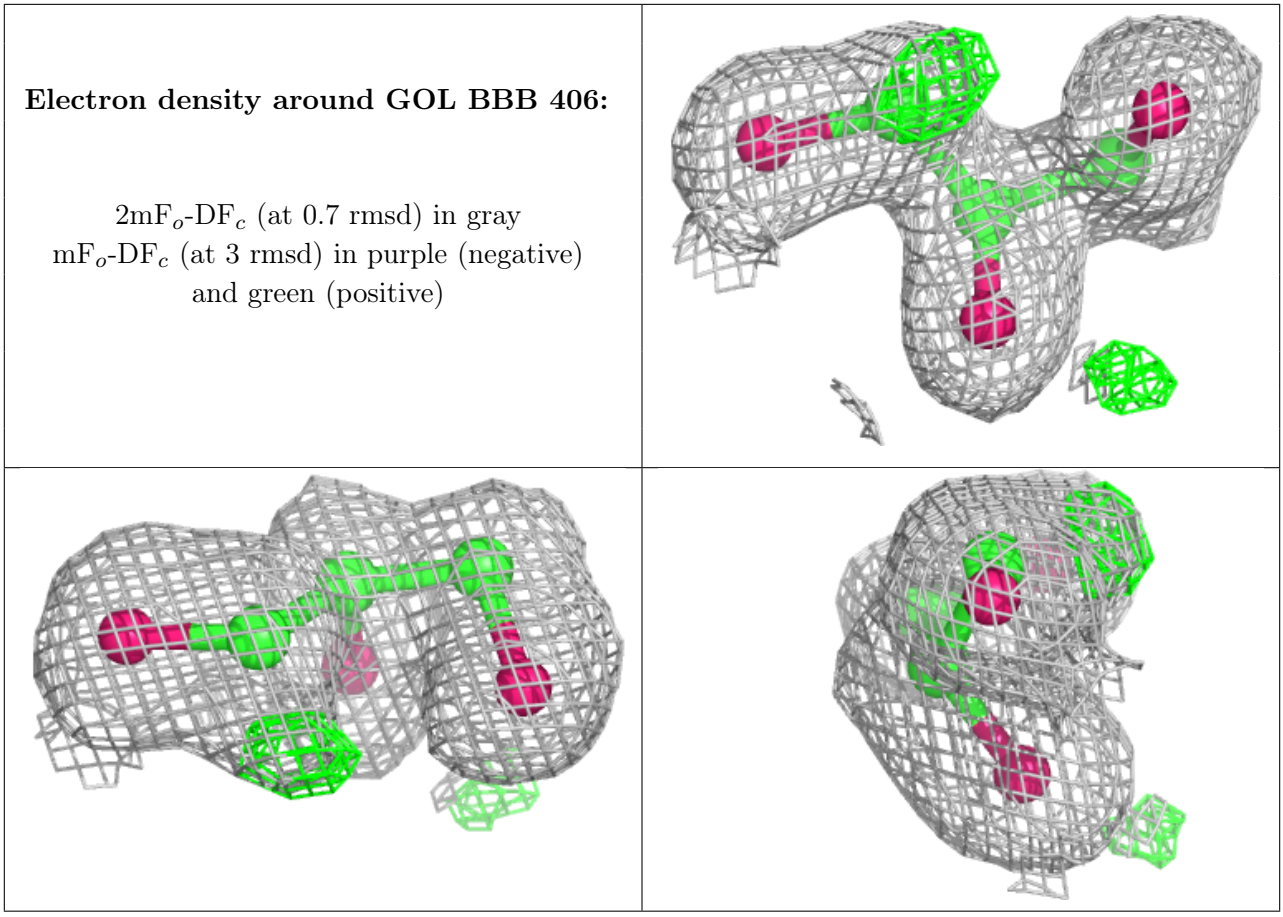
Electron density around PGE BBB 404:

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



Electron density around GOL BBB 406:

$2mF_o$-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

There are no such residues in this entry.