wwPDB X-ray Structure Validation Summary Report (i)

Feb 7, 2024 – 03:27 pm GMT

PDB ID	:	8AM8
Title	:	Cyclohexanone dehydrogenase (CDH) from Alicycliphilus denitrificans K601 complexed with dehydrogenated substrate - W113A mutant
Authors	:	Prior, S.H.; Taylor, E.J.
Deposited on	:	2022-08-03
Resolution	:	1.85 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 (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:

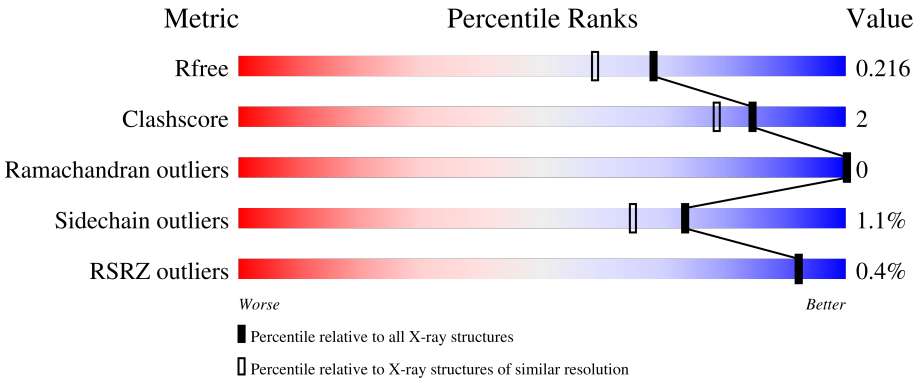
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

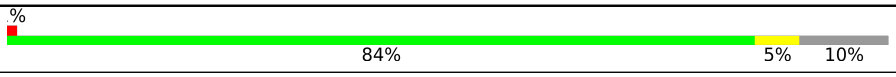
The reported resolution of this entry is 1.85 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	598	
1	BBB	598	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9076 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	BBB	535	Total	C	N	O	S	0	4	0
			4115	2590	733	776	16			
1	AAA	536	Total	C	N	O	S	0	3	0
			4107	2587	729	775	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	1	MET	-	initiating methionine	UNP F4G7N3
BBB	2	GLY	-	expression tag	UNP F4G7N3
BBB	3	SER	-	expression tag	UNP F4G7N3
BBB	4	SER	-	expression tag	UNP F4G7N3
BBB	5	HIS	-	expression tag	UNP F4G7N3
BBB	6	HIS	-	expression tag	UNP F4G7N3
BBB	7	HIS	-	expression tag	UNP F4G7N3
BBB	8	HIS	-	expression tag	UNP F4G7N3
BBB	9	HIS	-	expression tag	UNP F4G7N3
BBB	10	HIS	-	expression tag	UNP F4G7N3
BBB	11	SER	-	expression tag	UNP F4G7N3
BBB	12	SER	-	expression tag	UNP F4G7N3
BBB	13	GLY	-	expression tag	UNP F4G7N3
BBB	14	LEU	-	expression tag	UNP F4G7N3
BBB	15	VAL	-	expression tag	UNP F4G7N3
BBB	16	PRO	-	expression tag	UNP F4G7N3
BBB	17	ARG	-	expression tag	UNP F4G7N3
BBB	18	GLY	-	expression tag	UNP F4G7N3
BBB	19	SER	-	expression tag	UNP F4G7N3
BBB	20	HIS	-	expression tag	UNP F4G7N3
BBB	113	ALA	TRP	engineered mutation	UNP F4G7N3
AAA	1	MET	-	initiating methionine	UNP F4G7N3
AAA	2	GLY	-	expression tag	UNP F4G7N3
AAA	3	SER	-	expression tag	UNP F4G7N3

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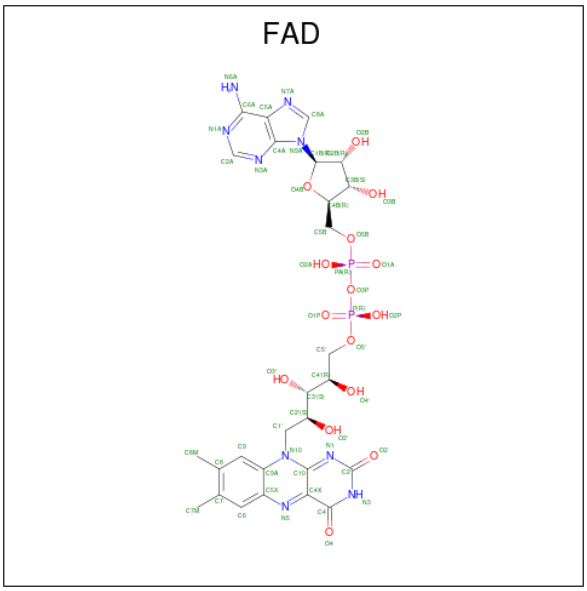
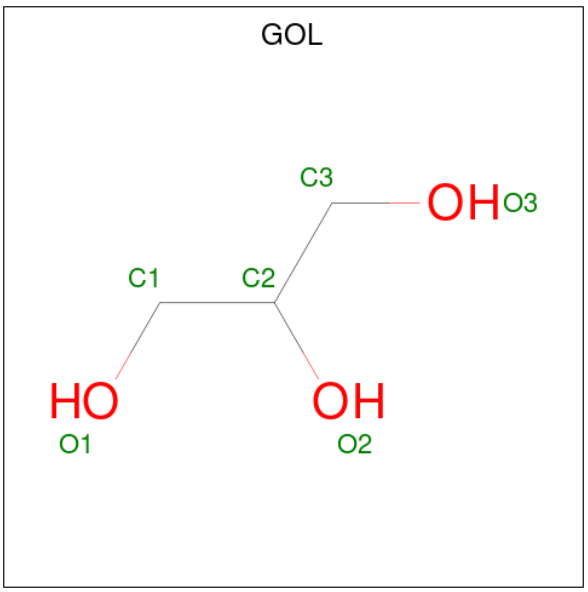
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	4	SER	-	expression tag	UNP F4G7N3
AAA	5	HIS	-	expression tag	UNP F4G7N3
AAA	6	HIS	-	expression tag	UNP F4G7N3
AAA	7	HIS	-	expression tag	UNP F4G7N3
AAA	8	HIS	-	expression tag	UNP F4G7N3
AAA	9	HIS	-	expression tag	UNP F4G7N3
AAA	10	HIS	-	expression tag	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	113	ALA	TRP	engineered mutation	UNP F4G7N3

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



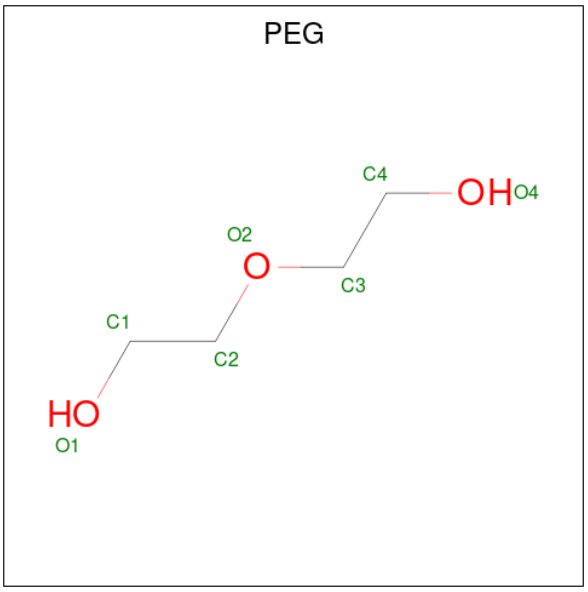
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	BBB	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	AAA	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



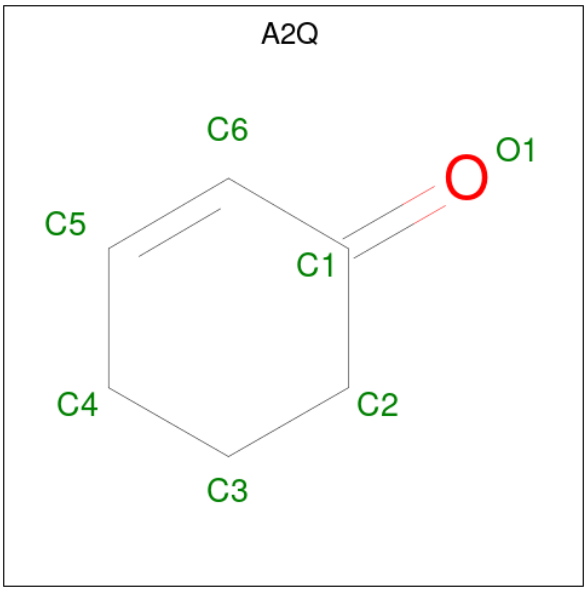
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C O 7 4 3	0	0
4	AAA	1	Total C O 7 4 3	0	0

- Molecule 5 is cyclohex-2-en-1-one (three-letter code: A2Q) (formula: C_6H_8O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 7 6 1	0	0

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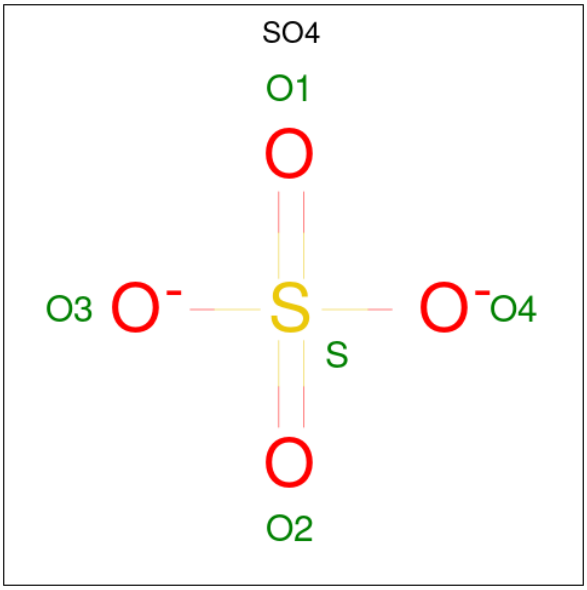
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 7 6 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

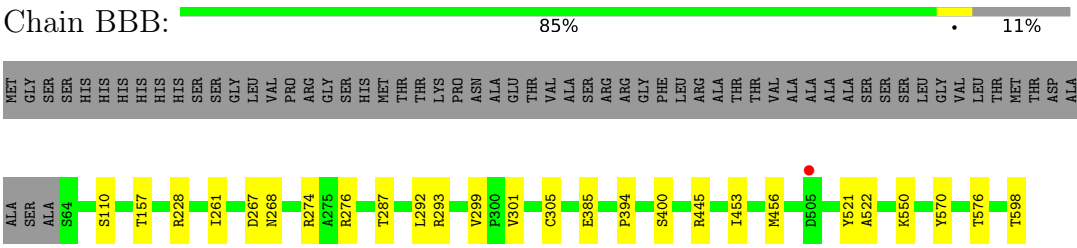
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	BBB	340	Total O 340 340	0	0
7	AAA	317	Total O 317 317	0	0

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.

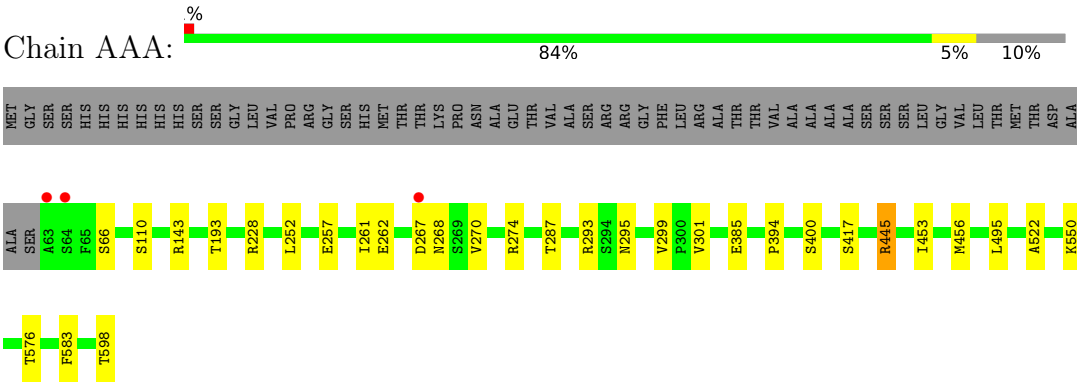
• Molecule 1: Fumarate reductase/succinate dehydrogenase flavoprotein domain protein

Chain BBB:



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

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.05Å 90.05Å 277.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.65 – 1.85 85.65 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.65-1.85) 99.9 (85.65-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.173 , 0.215 0.173 , 0.216	Depositor DCC
R_{free} test set	4802 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: GOL, A2Q, FAD, SO4, PEG

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	0.42	0/4206	0.69	1/5699 (0.0%)
1	BBB	0.42	0/4220	0.67	0/5716
All	All	0.42	0/8426	0.68	1/11415 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	228	ARG	CG-CD-NE	7.29	127.12	111.80

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	4107	0	4023	19	0
1	BBB	4115	0	4032	19	0
2	AAA	53	0	30	1	0
2	BBB	53	0	30	5	0
3	AAA	18	0	24	3	0
3	BBB	30	0	40	2	0
4	AAA	7	0	10	2	0
4	BBB	7	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	7	0	8	0	0
5	BBB	7	0	8	0	0
6	AAA	10	0	0	0	0
6	BBB	5	0	0	1	0
7	AAA	317	0	0	1	0
7	BBB	340	0	0	1	0
All	All	9076	0	8215	39	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 2.

The worst 5 of 39 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:305:CYS:SG	2:BBB:601:FAD:C8M	2.02	1.45
1:BBB:292:LEU:HD21	4:AAA:605:PEG:H11	1.65	0.78
1:BBB:276:ARG:NH2	6:BBB:609:SO4:O2	2.26	0.68
1:AAA:274:ARG:HH12	1:AAA:598:THR:HG22	1.62	0.65
1:AAA:143:ARG:HH21	3:AAA:603:GOL:H32	1.66	0.59

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	537/598 (90%)	528 (98%)	9 (2%)	0	100	100
1	BBB	537/598 (90%)	530 (99%)	7 (1%)	0	100	100
All	All	1074/1196 (90%)	1058 (98%)	16 (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	429/473 (91%)	424 (99%)	5 (1%)	71	62
1	BBB	430/473 (91%)	426 (99%)	4 (1%)	78	72
All	All	859/946 (91%)	850 (99%)	9 (1%)	73	69

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	570	TYR
1	AAA	576	THR
1	BBB	576	THR
1	AAA	66	SER
1	AAA	445	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
6	SO4	BBB	609	-	4,4,4	0.25	0	6,6,6	0.17	0
3	GOL	BBB	606	-	5,5,5	0.07	0	5,5,5	0.25	0
3	GOL	AAA	604	-	5,5,5	0.11	0	5,5,5	0.69	0
2	FAD	BBB	601	-	53,58,58	0.72	1 (1%)	68,89,89	0.91	3 (4%)
3	GOL	BBB	602	-	5,5,5	0.18	0	5,5,5	0.36	0
3	GOL	AAA	603	-	5,5,5	0.23	0	5,5,5	0.59	0
4	PEG	AAA	605	-	6,6,6	0.32	0	5,5,5	0.39	0
5	A2Q	BBB	608	-	7,7,7	4.71	7 (100%)	8,8,8	1.92	2 (25%)
6	SO4	AAA	608	-	4,4,4	0.24	0	6,6,6	0.14	0
3	GOL	BBB	603	-	5,5,5	0.28	0	5,5,5	0.71	0
4	PEG	BBB	607	-	6,6,6	0.17	0	5,5,5	0.36	0
5	A2Q	AAA	606	-	7,7,7	4.84	7 (100%)	8,8,8	1.83	2 (25%)
6	SO4	AAA	607	-	4,4,4	0.32	0	6,6,6	0.08	0
3	GOL	BBB	605	-	5,5,5	0.15	0	5,5,5	0.99	0
3	GOL	BBB	604	-	5,5,5	0.12	0	5,5,5	0.32	0
3	GOL	AAA	602	-	5,5,5	0.13	0	5,5,5	0.80	0
2	FAD	AAA	601	1	53,58,58	0.82	1 (1%)	68,89,89	0.89	4 (5%)

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	GOL	BBB	606	-	-	3/4/4/4	-
3	GOL	AAA	604	-	-	3/4/4/4	-
2	FAD	BBB	601	-	-	4/30/50/50	0/6/6/6
3	GOL	BBB	602	-	-	0/4/4/4	-
3	GOL	AAA	603	-	-	3/4/4/4	-
4	PEG	AAA	605	-	-	3/4/4/4	-
5	A2Q	BBB	608	-	-	-	0/1/1/1
3	GOL	BBB	603	-	-	3/4/4/4	-
4	PEG	BBB	607	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A2Q	AAA	606	-	-	-	0/1/1/1
3	GOL	BBB	605	-	-	4/4/4/4	-
3	GOL	BBB	604	-	-	4/4/4/4	-
3	GOL	AAA	602	-	-	1/4/4/4	-
2	FAD	AAA	601	1	-	1/30/50/50	0/6/6/6

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	606	A2Q	O1-C1	9.48	1.38	1.23
5	BBB	608	A2Q	O1-C1	9.16	1.38	1.23
5	AAA	606	A2Q	C2-C1	-4.64	1.39	1.49
5	BBB	608	A2Q	C2-C1	-4.59	1.39	1.49
5	AAA	606	A2Q	C3-C2	-3.85	1.39	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BBB	608	A2Q	C3-C4-C5	3.57	119.90	111.70
5	AAA	606	A2Q	C3-C4-C5	3.27	119.21	111.70
2	AAA	601	FAD	C1'-C2'-C3'	2.93	117.97	109.79
2	BBB	601	FAD	C1'-C2'-C3'	2.67	117.23	109.79
5	AAA	606	A2Q	C3-C2-C1	2.56	120.32	113.93

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	603	GOL	O1-C1-C2-O2
3	BBB	604	GOL	O1-C1-C2-C3
3	BBB	605	GOL	O1-C1-C2-O2
3	BBB	605	GOL	C1-C2-C3-O3
3	BBB	606	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BBB	609	SO4	1	0
2	BBB	601	FAD	5	0

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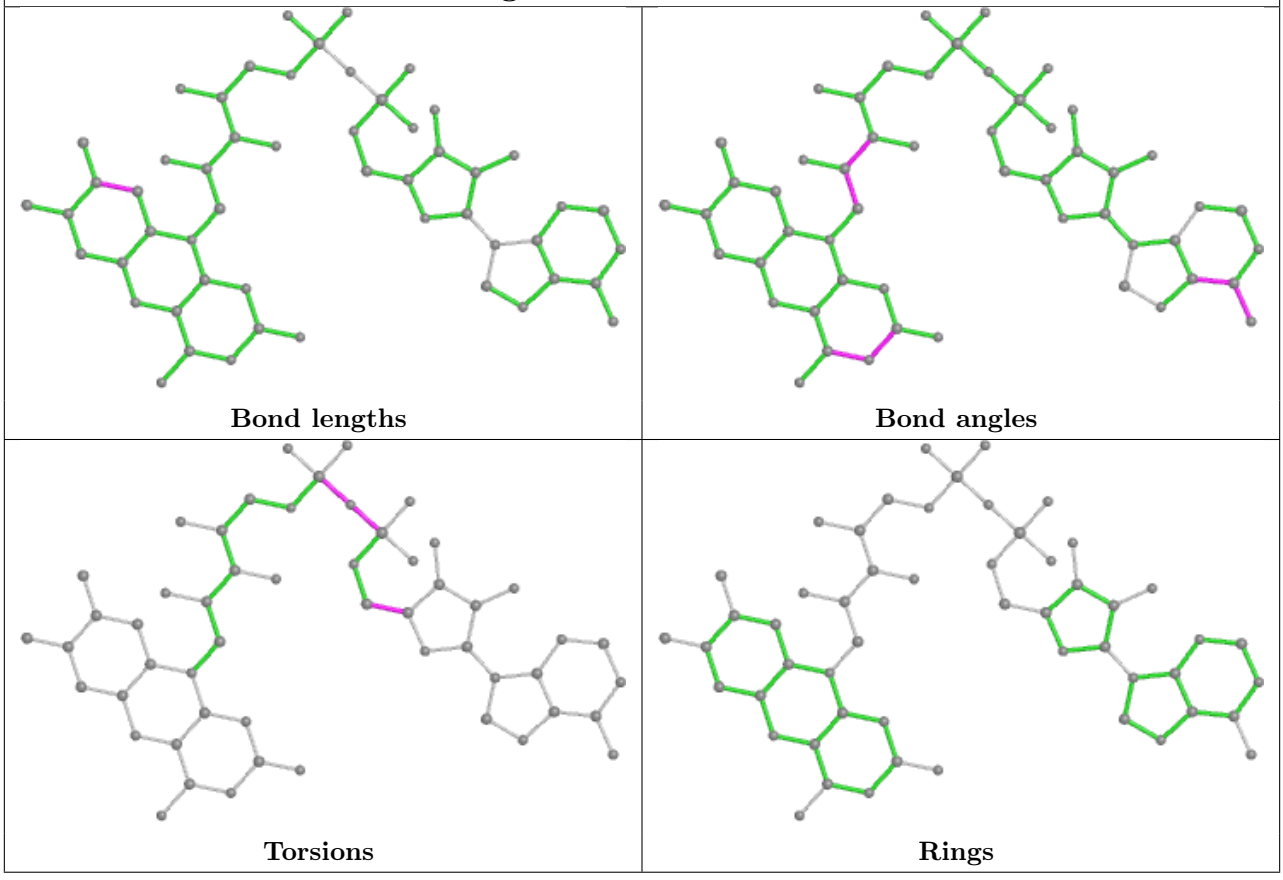
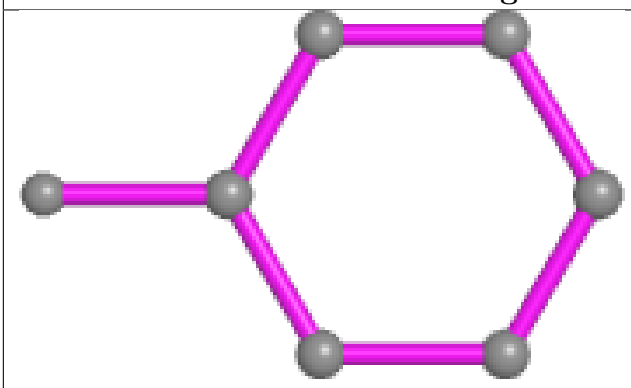
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	603	GOL	2	0
4	AAA	605	PEG	2	0
4	BBB	607	PEG	2	0
3	BBB	605	GOL	1	0
3	BBB	604	GOL	1	0
3	AAA	602	GOL	1	0
2	AAA	601	FAD	1	0

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.

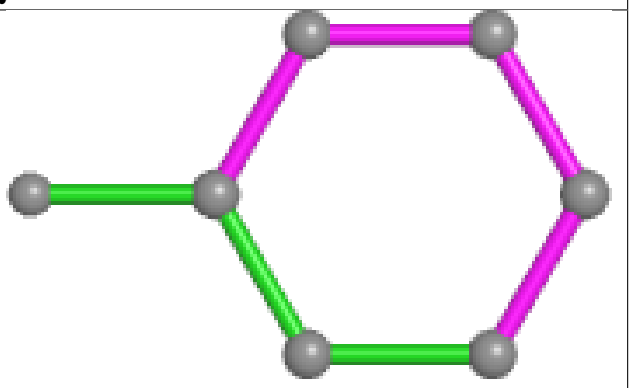
Ligand FAD BBB 601



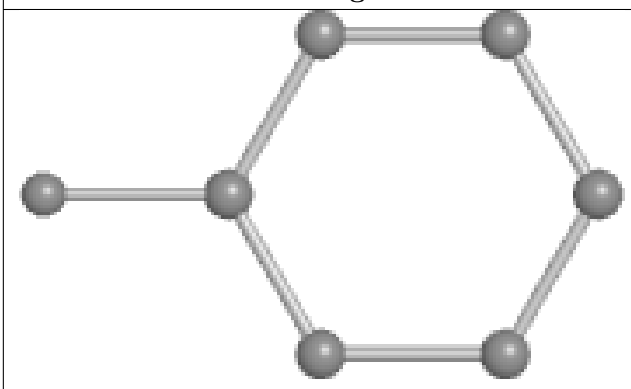
Ligand A2Q BBB 608



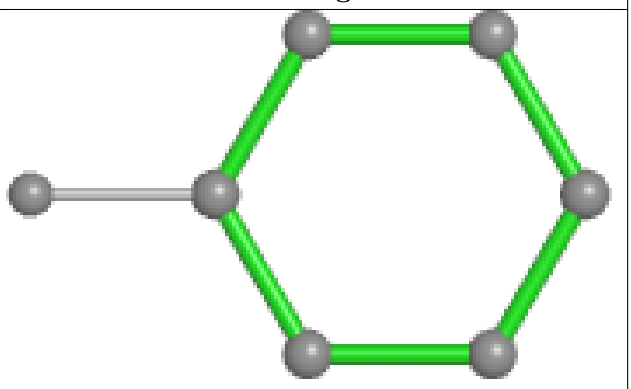
Bond lengths



Bond angles

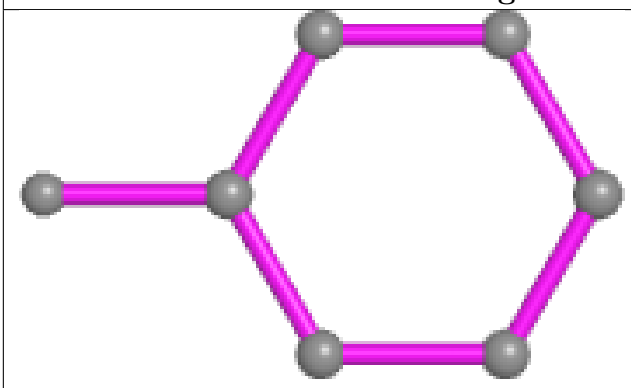


Torsions

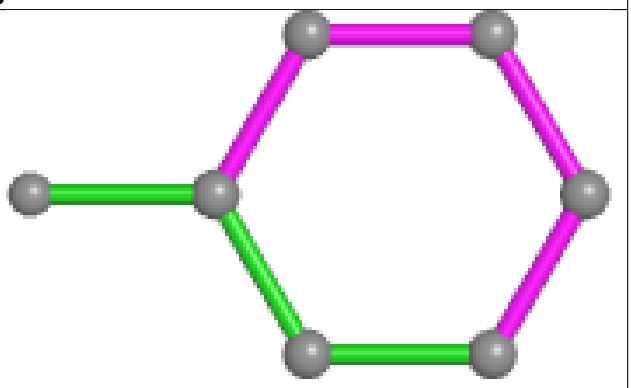


Rings

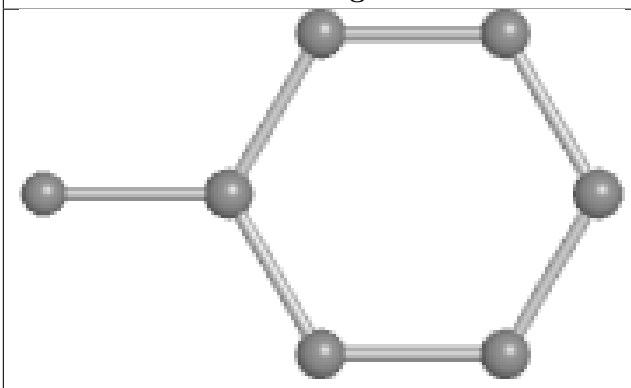
Ligand A2Q AAA 606



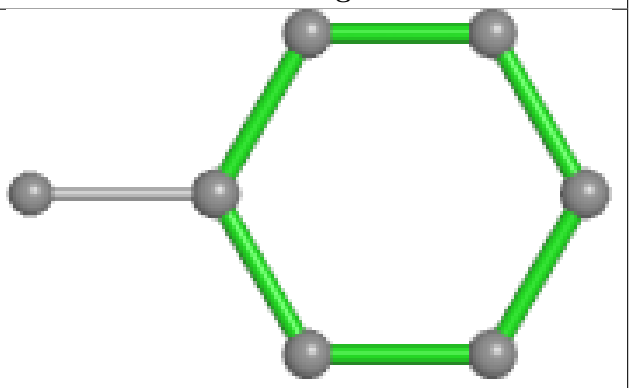
Bond lengths



Bond angles

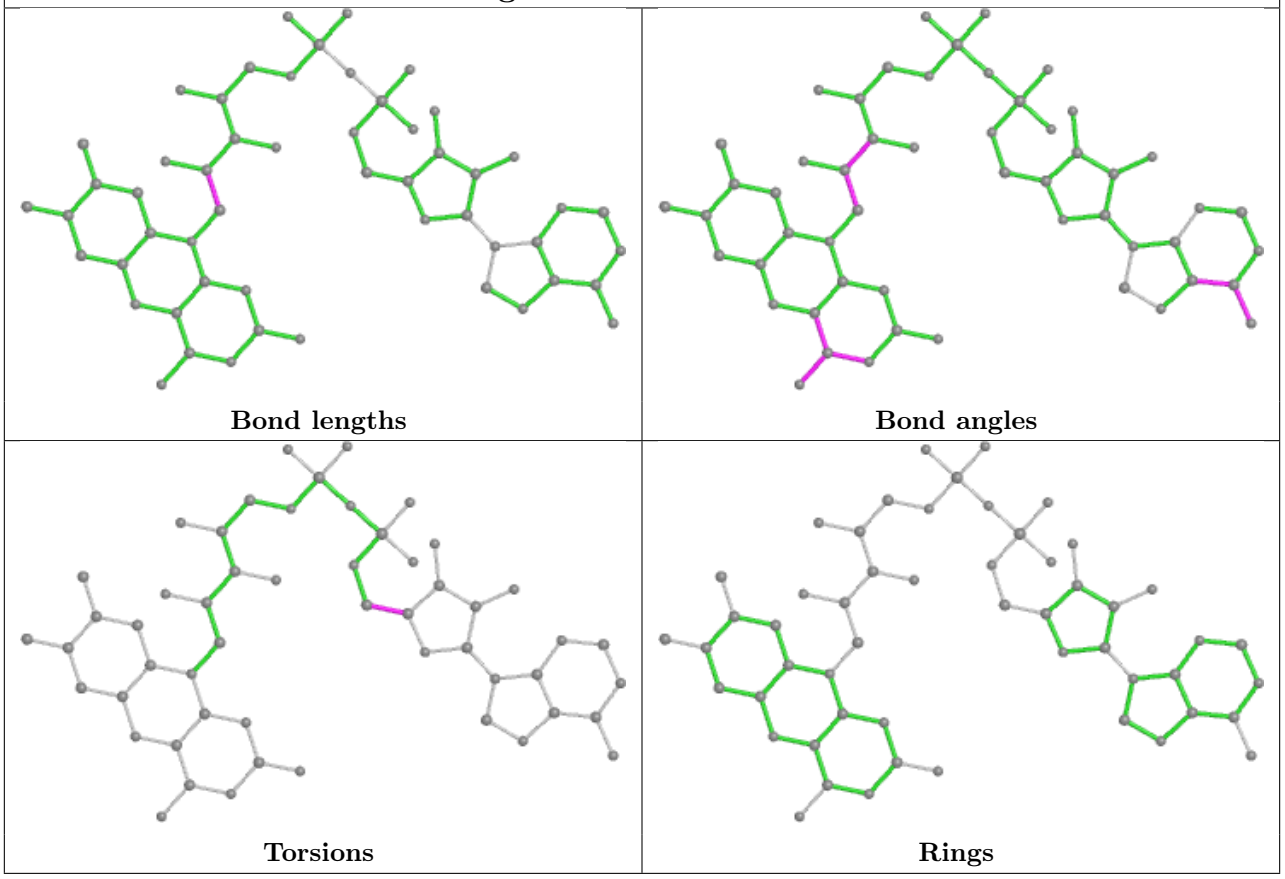


Torsions



Rings

Ligand FAD AAA 601



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	536/598 (89%)	-0.53	3 (0%)	89	89	17, 23, 38, 70	0
1	BBB	535/598 (89%)	-0.55	1 (0%)	95	94	17, 24, 39, 74	0
All	All	1071/1196 (89%)	-0.54	4 (0%)	92	92	17, 23, 38, 74	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	505	ASP	3.9
1	AAA	63	ALA	3.0
1	AAA	267	ASP	2.3
1	AAA	64	SER	2.1

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

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
4	PEG	BBB	607	7/7	0.76	0.25	44,52,57,67	0

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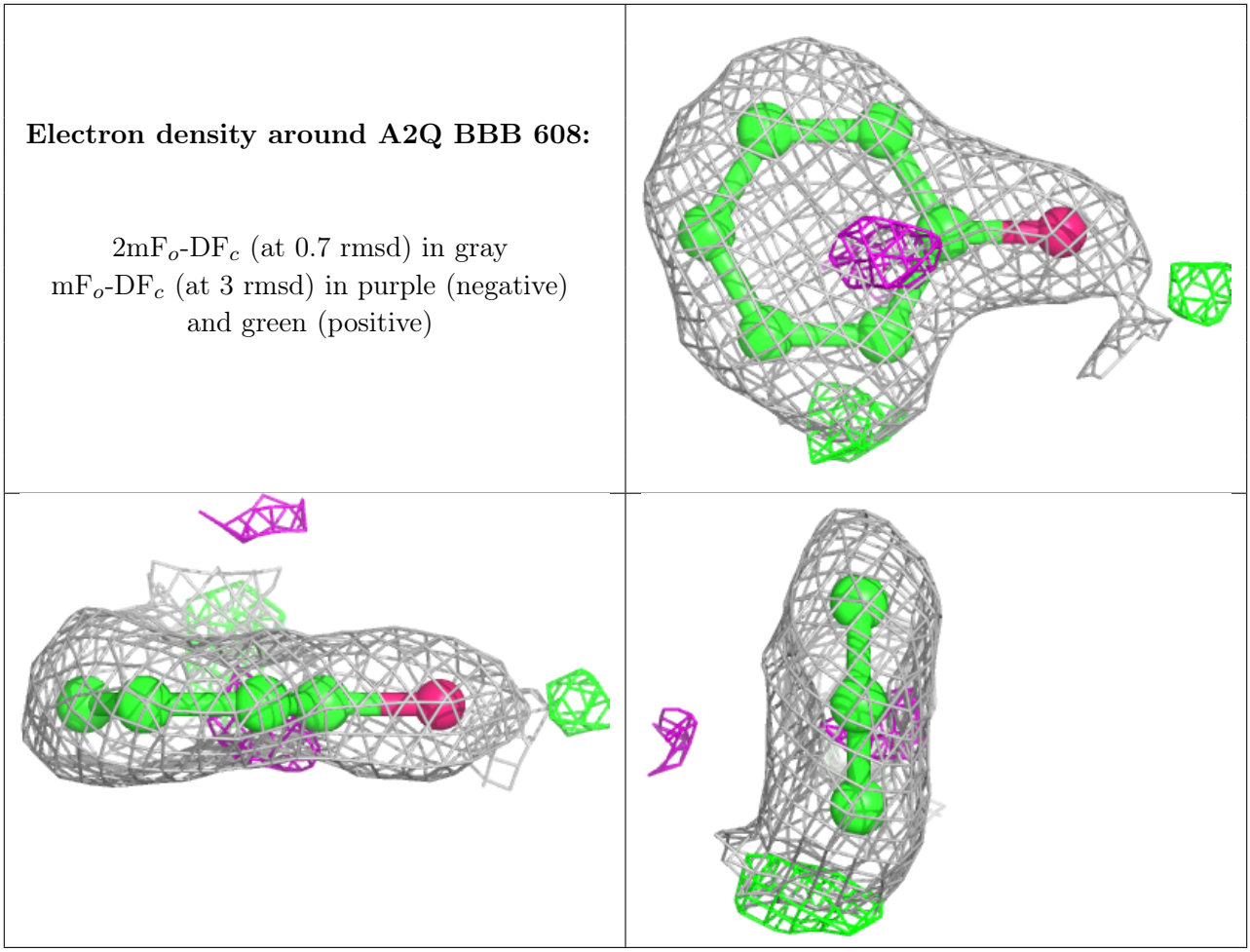
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	A2Q	BBB	608	7/7	0.82	0.19	38,38,41,42	0
6	SO4	AAA	607	5/5	0.85	0.17	74,78,85,87	0
3	GOL	BBB	606	6/6	0.89	0.12	49,57,62,62	0
3	GOL	BBB	605	6/6	0.90	0.20	29,36,46,56	0
6	SO4	BBB	609	5/5	0.91	0.17	54,65,69,73	0
3	GOL	AAA	603	6/6	0.92	0.15	27,34,35,38	0
5	A2Q	AAA	606	7/7	0.92	0.13	28,30,32,34	0
3	GOL	BBB	603	6/6	0.92	0.14	28,29,34,37	0
4	PEG	AAA	605	7/7	0.92	0.13	31,32,34,42	0
3	GOL	BBB	604	6/6	0.93	0.13	26,37,41,42	0
3	GOL	AAA	604	6/6	0.94	0.18	32,37,41,42	0
3	GOL	AAA	602	6/6	0.95	0.09	25,30,31,32	0
6	SO4	AAA	608	5/5	0.95	0.16	39,44,52,53	0
3	GOL	BBB	602	6/6	0.96	0.07	24,28,29,31	0
2	FAD	AAA	601	53/53	0.98	0.08	17,20,23,26	0
2	FAD	BBB	601	53/53	0.98	0.09	18,21,26,30	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.

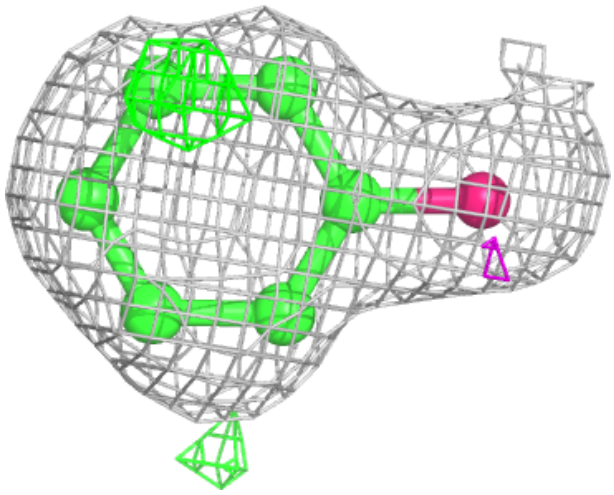
Electron density around A2Q BBB 608:

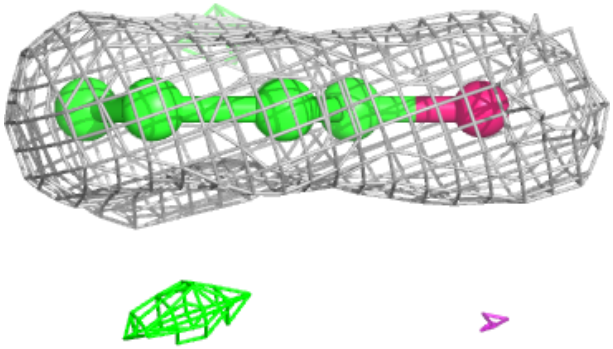
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

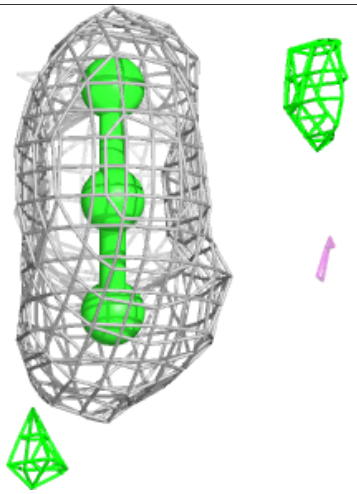


Electron density around A2Q AAA 606:

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

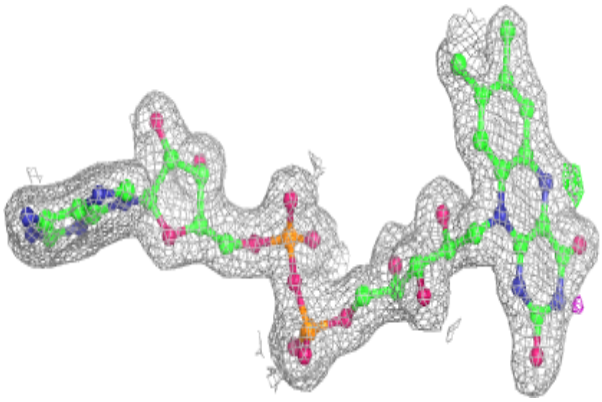


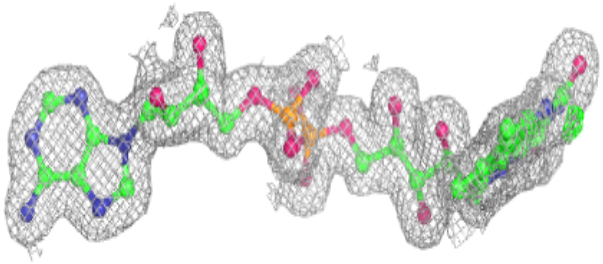


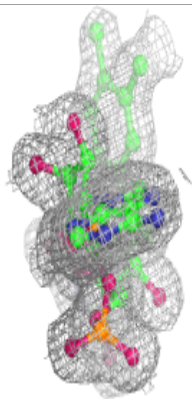


Electron density around FAD AAA 601:

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

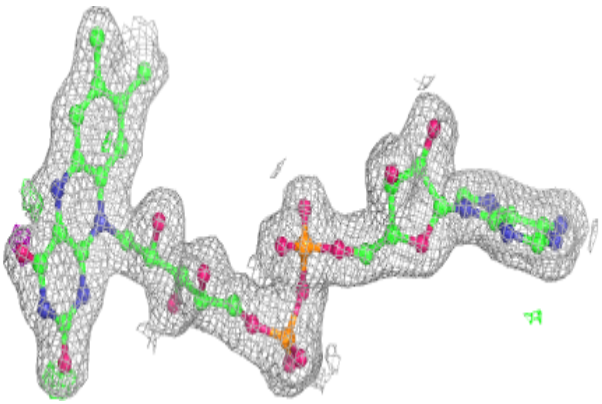


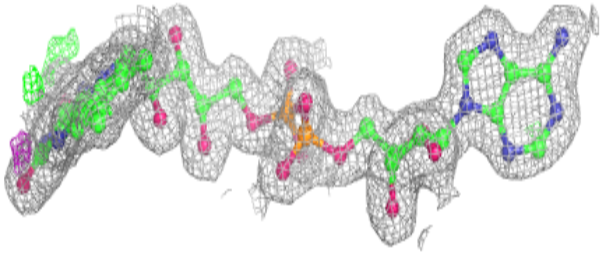


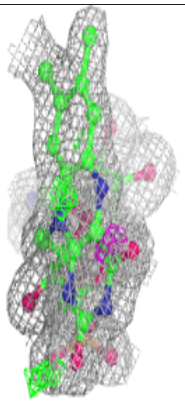


Electron density around FAD BBB 601:

$2mF_o$-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.