



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2024 – 03:27 pm GMT

PDB ID : 8AM8  
Title : Cyclohexanone dehydrogenase (CDH) from Alicyclophilus 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 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

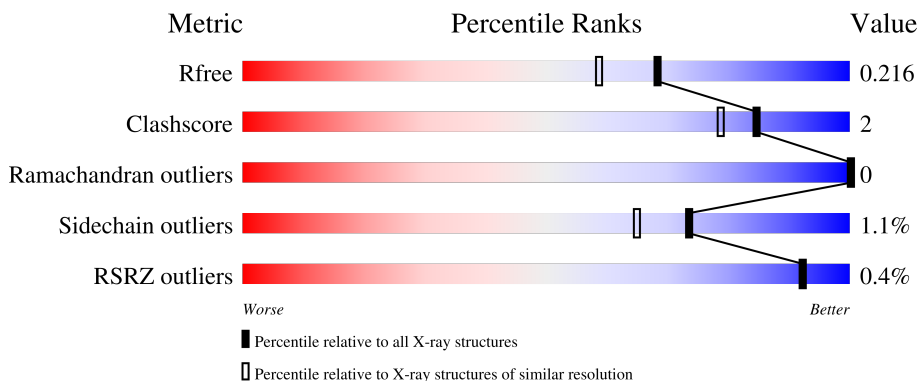
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	598	 84% 5% 10%
1	BBB	598	 85% 11%

## 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
			Total	C	N	O	S			
1	BBB	535	4115	2590	733	776	16	0	4	0
1	AAA	536	4107	2587	729	775	16	0	3	0

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

*Continued on next page...*

Continued from previous page...

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:  $C_3H_8O_3$ ).



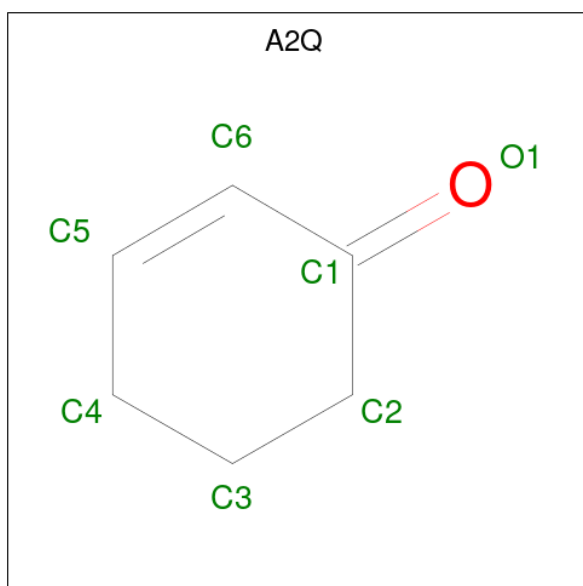
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0

- 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	0	0
			7	4	3		
4	AAA	1	Total	C	O	0	0
			7	4	3		

- 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	0	0
			7	6	1		

*Continued on next page...*

Continued from previous page...

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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


- Molecule 7 is water.

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

### 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:  85% 11%

MET  
GLY  
SER  
SER  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
SER  
SER  
GLY  
LEU  
VAL  
PRO  
ARG  
GLY  
SER  
HIS  
MET  
THR  
THR  
LYS  
PRO  
ASN  
ALA  
GLU  
THR  
VAL  
ALA  
SER  
ARG  
ARG  
GLY  
PHE  
LEU  
ARG  
ALA  
THR  
THR  
VAL  
ALA  
ALA  
ALA  
ALA  
SER  
SER  
SER  
SER  
LEU  
GLY  
VAL  
LEU  
THR  
THR  
MET  
THR  
ASP  
ALA  
GLN  
ALA

ALA  
SER  
ALA  
S64  
S110  
T187  
R228  
L261  
D267  
N288  
R274  
A275  
R276  
T287  
L292  
R293  
V299  
P300  
V301  
C305  
E385  
P394  
S400  
R445  
I453  
M456  
E695  
Y521  
A522  
K550  
Y570  
T576  
T598

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

Chain AAA:  84% 5% 10%

MET  
GLY  
SER  
SER  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
SER  
SER  
GLY  
LEU  
VAL  
PRO  
ARG  
GLY  
SER  
HIS  
MET  
THR  
THR  
LYS  
PRO  
ASN  
ALA  
GLU  
THR  
VAL  
ALA  
SER  
ARG  
ARG  
GLY  
PHE  
LEU  
ARG  
ALA  
THR  
THR  
VAL  
ALA  
ALA  
ALA  
ALA  
SER  
SER  
SER  
SER  
LEU  
GLY  
VAL  
LEU  
THR  
THR  
MET  
THR  
ASP  
ALA  
GLN  
ALA

ALA  
SER  
A63  
S64  
F65  
S66  
S110  
R143  
T193  
R228  
L252  
E257  
L261  
E262  
D267  
N268  
S269  
V270  
R274  
T287  
R293  
S294  
N295  
V299  
P300  
V301  
E385  
P394  
S400  
S417  
R445  
I453  
M456  
L495  
A522  
K550  
Y570

T576  
F583  
T598



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 1.84Å)	Xtrriage
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 <sup>2</sup> )	23.8	Xtrriage
Anisotropy	0.016	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	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

*Continued on next page...*

*Continued from previous page...*

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.

All (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
4:BBB:607:PEG:H21	1:AAA:295:ASN:HD21	1.68	0.58
1:BBB:400:SER:O	1:BBB:522:ALA:HA	2.04	0.58
1:AAA:400:SER:O	1:AAA:522:ALA:HA	2.06	0.55
1:AAA:143:ARG:NH2	3:AAA:603:GOL:H32	2.23	0.53
1:AAA:417:SER:HB2	7:AAA:742:HOH:O	2.09	0.52
1:AAA:583:PHE:CD2	3:AAA:602:GOL:H2	2.46	0.51
1:AAA:110:SER:HA	2:AAA:601:FAD:C6	2.42	0.49
1:AAA:193:THR:HB	1:AAA:495:LEU:HD13	1.93	0.49
1:BBB:157:THR:HG21	4:BBB:607:PEG:H41	1.95	0.48
1:AAA:287:THR:O	1:AAA:293:ARG:HD3	2.14	0.47
1:AAA:299:VAL:HG23	1:AAA:301:VAL:HG13	1.96	0.47
1:BBB:274:ARG:HH12	1:BBB:598:THR:HG22	1.80	0.47
1:BBB:385[B]:GLU:HG3	3:BBB:605:GOL:H2	1.97	0.47
1:BBB:299:VAL:HG23	1:BBB:301:VAL:HG13	1.96	0.47
1:BBB:261:ILE:C	1:BBB:261:ILE:HD12	2.38	0.44
1:BBB:287:THR:O	1:BBB:293:ARG:HD3	2.18	0.44
1:BBB:305:CYS:SG	2:BBB:601:FAD:C8	2.97	0.44
1:AAA:453:ILE:HB	1:AAA:456:MET:HE3	2.00	0.44
1:BBB:110:SER:HA	2:BBB:601:FAD:C6	2.47	0.43
1:BBB:267:ASP:O	1:BBB:268:ASN:HB2	2.19	0.43
1:BBB:305:CYS:SG	2:BBB:601:FAD:HM81	2.34	0.43
2:BBB:601:FAD:H9	2:BBB:601:FAD:H1'1	1.86	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:261:ILE:C	1:AAA:261:ILE:HD12	2.39	0.42
1:AAA:445:ARG:HD3	1:AAA:445:ARG:HA	1.87	0.42
1:BBB:292:LEU:HD21	4:AAA:605:PEG:C1	2.44	0.42
1:AAA:262:GLU:HG3	1:AAA:270:VAL:HG13	2.01	0.41
1:AAA:385:GLU:O	1:AAA:394:PRO:HD2	2.20	0.41
1:BBB:228:ARG:NH1	7:BBB:716:HOH:O	2.54	0.41
1:AAA:274:ARG:HH12	1:AAA:598:THR:CG2	2.33	0.41
1:AAA:267:ASP:O	1:AAA:268:ASN:HB2	2.19	0.41
1:BBB:521:TYR:HE2	3:BBB:604:GOL:H32	1.85	0.40
1:AAA:252:LEU:HA	1:AAA:257:GLU:O	2.22	0.40
1:BBB:453:ILE:HB	1:BBB:456:MET:HE3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	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

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	445	ARG
1	BBB	550	LYS
1	BBB	570	TYR
1	BBB	576	THR
1	AAA	66	SER
1	AAA	445	ARG
1	AAA	550	LYS
1	AAA	570	TYR
1	AAA	576	THR

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	-
5	A2Q	AAA	606	-	-	-	0/1/1/1
3	GOL	BBB	605	-	-	4/4/4/4	-
3	GOL	BBB	604	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	AAA	602	-	-	1/4/4/4	-
2	FAD	AAA	601	1	-	1/30/50/50	0/6/6/6

All (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
5	BBB	608	A2Q	C3-C2	-3.82	1.39	1.52
5	BBB	608	A2Q	C3-C4	-3.75	1.38	1.51
5	AAA	606	A2Q	C3-C4	-3.69	1.38	1.51
2	AAA	601	FAD	C1'-C2'	3.25	1.57	1.52
5	AAA	606	A2Q	C6-C1	-3.22	1.39	1.46
5	BBB	608	A2Q	C6-C1	-2.92	1.40	1.46
5	AAA	606	A2Q	C4-C5	-2.72	1.38	1.48
5	BBB	608	A2Q	C4-C5	-2.69	1.39	1.48
5	AAA	606	A2Q	C6-C5	2.57	1.40	1.33
2	BBB	601	FAD	C9-C8	-2.37	1.36	1.39
5	BBB	608	A2Q	C6-C5	2.37	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	BBB	601	FAD	C5A-C6A-N6A	2.53	124.20	120.35
2	AAA	601	FAD	C5A-C6A-N6A	2.45	124.07	120.35
5	BBB	608	A2Q	C3-C2-C1	2.44	120.02	113.93
2	AAA	601	FAD	O4-C4-C4X	-2.34	120.40	126.60
2	BBB	601	FAD	C4-N3-C2	-2.12	121.72	125.64
2	AAA	601	FAD	C4X-C4-N3	2.03	118.36	113.19

There are no chirality outliers.

All (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
3	AAA	604	GOL	O1-C1-C2-C3
3	AAA	604	GOL	C1-C2-C3-O3
3	BBB	605	GOL	O2-C2-C3-O3
4	AAA	605	PEG	O2-C3-C4-O4
3	BBB	603	GOL	O1-C1-C2-C3
3	BBB	604	GOL	C1-C2-C3-O3
3	BBB	605	GOL	O1-C1-C2-C3
3	AAA	602	GOL	O1-C1-C2-C3
3	AAA	603	GOL	O1-C1-C2-C3
3	BBB	606	GOL	O1-C1-C2-O2
3	AAA	603	GOL	O1-C1-C2-O2
3	AAA	604	GOL	O2-C2-C3-O3
3	BBB	604	GOL	O1-C1-C2-O2
3	BBB	604	GOL	O2-C2-C3-O3
3	AAA	603	GOL	O2-C2-C3-O3
2	BBB	601	FAD	PA-O3P-P-O5'
4	AAA	605	PEG	O1-C1-C2-O2
4	BBB	607	PEG	C1-C2-O2-C3
3	BBB	603	GOL	O2-C2-C3-O3
2	AAA	601	FAD	O4B-C4B-C5B-O5B
4	AAA	605	PEG	C1-C2-O2-C3
2	BBB	601	FAD	P-O3P-PA-O1A
3	BBB	606	GOL	O2-C2-C3-O3
2	BBB	601	FAD	P-O3P-PA-O2A
2	BBB	601	FAD	O4B-C4B-C5B-O5B

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
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

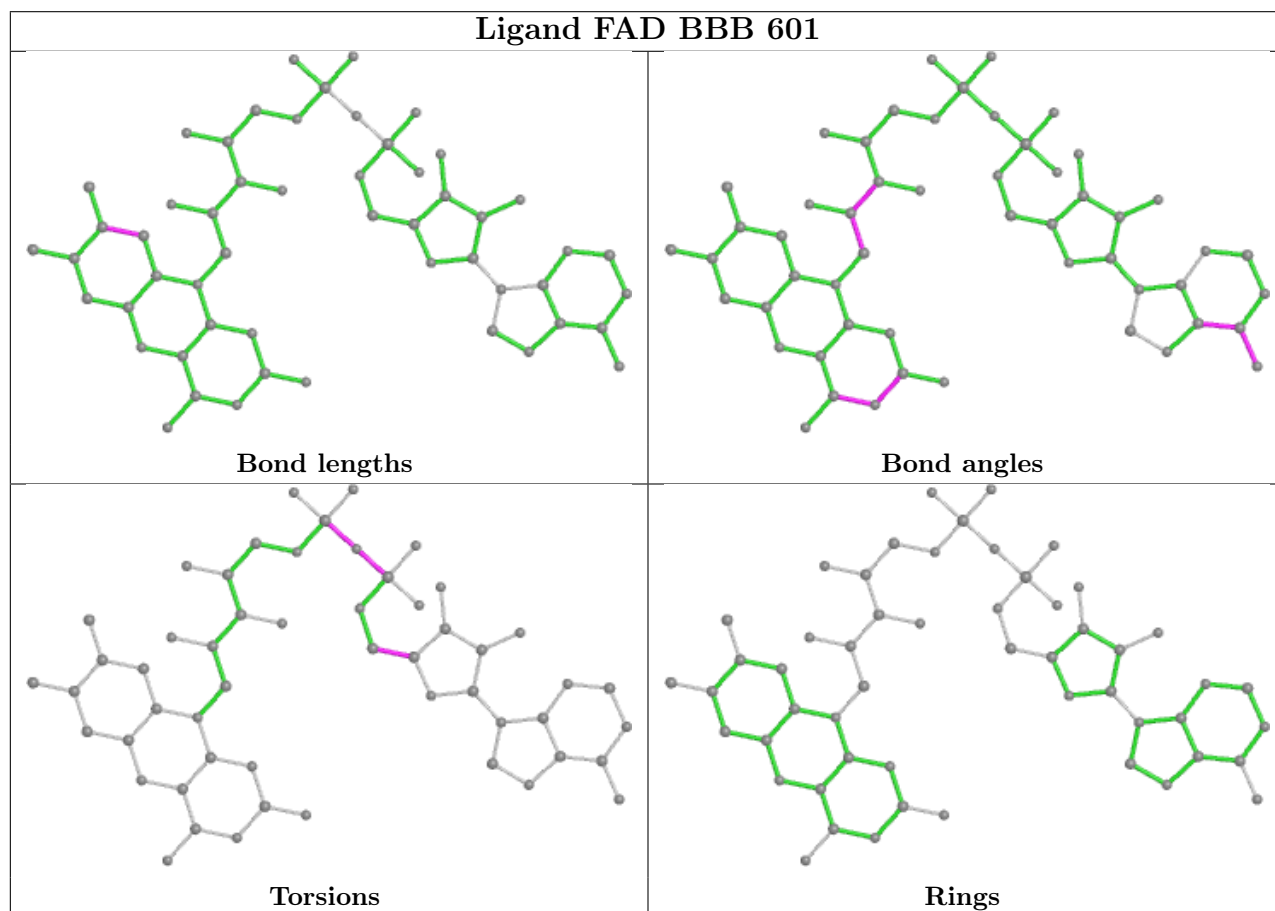
*Continued on next page...*

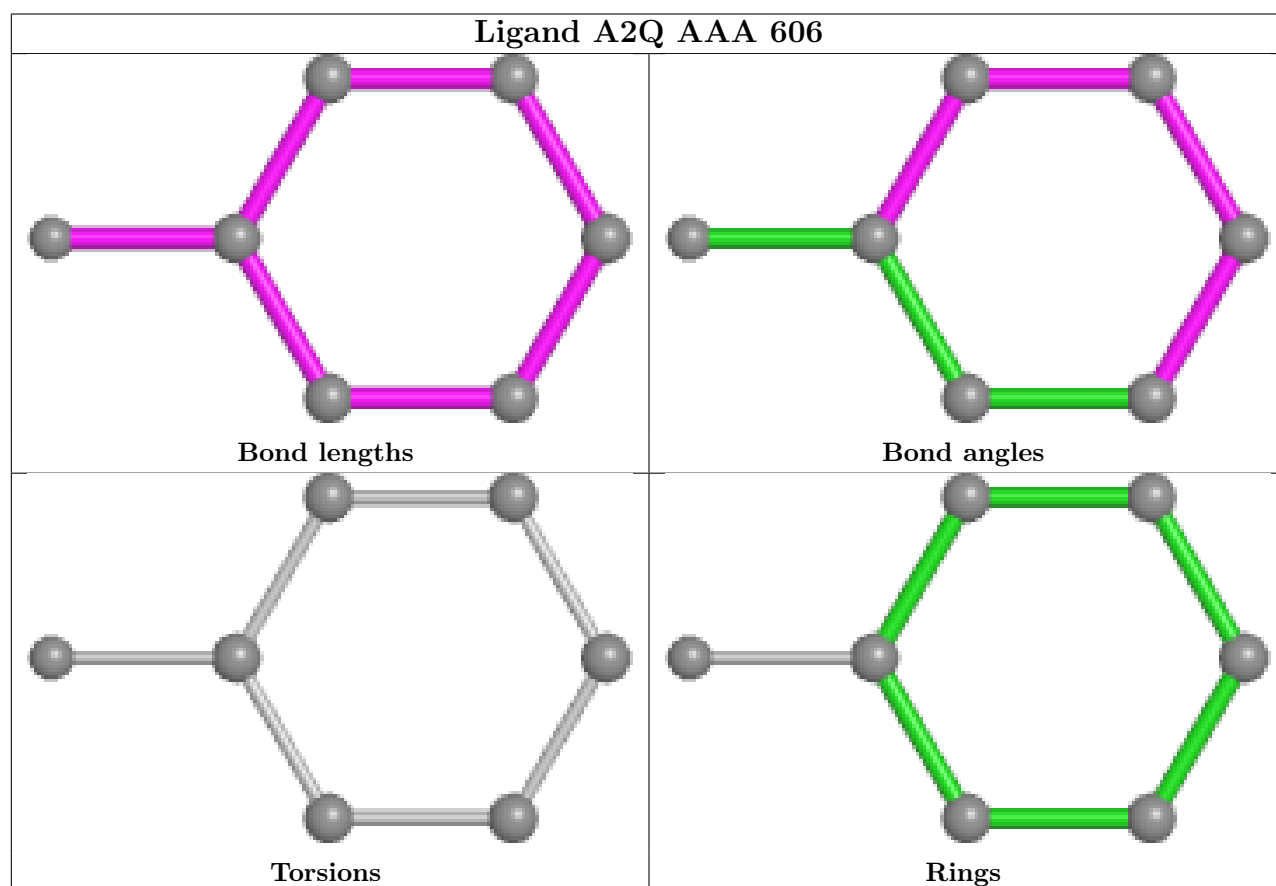
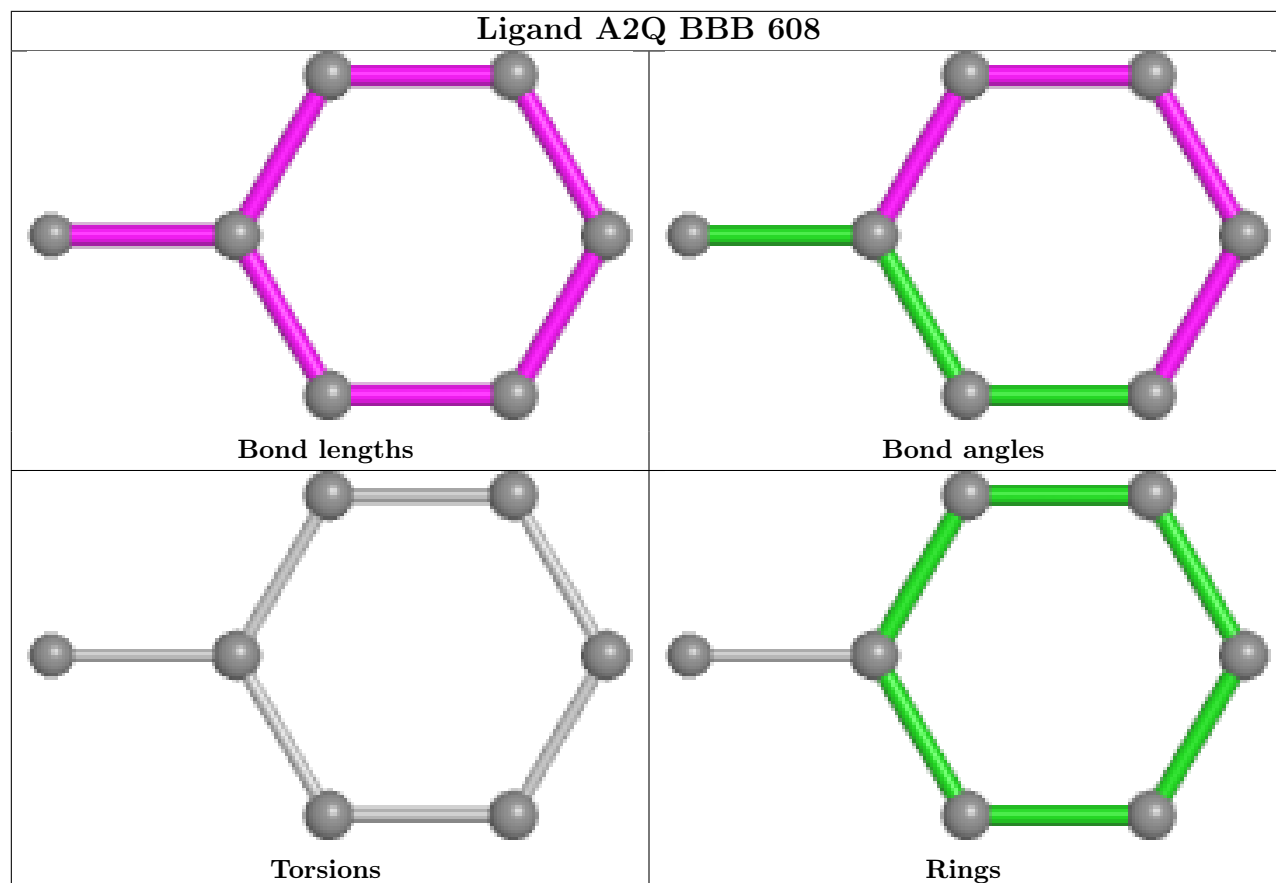


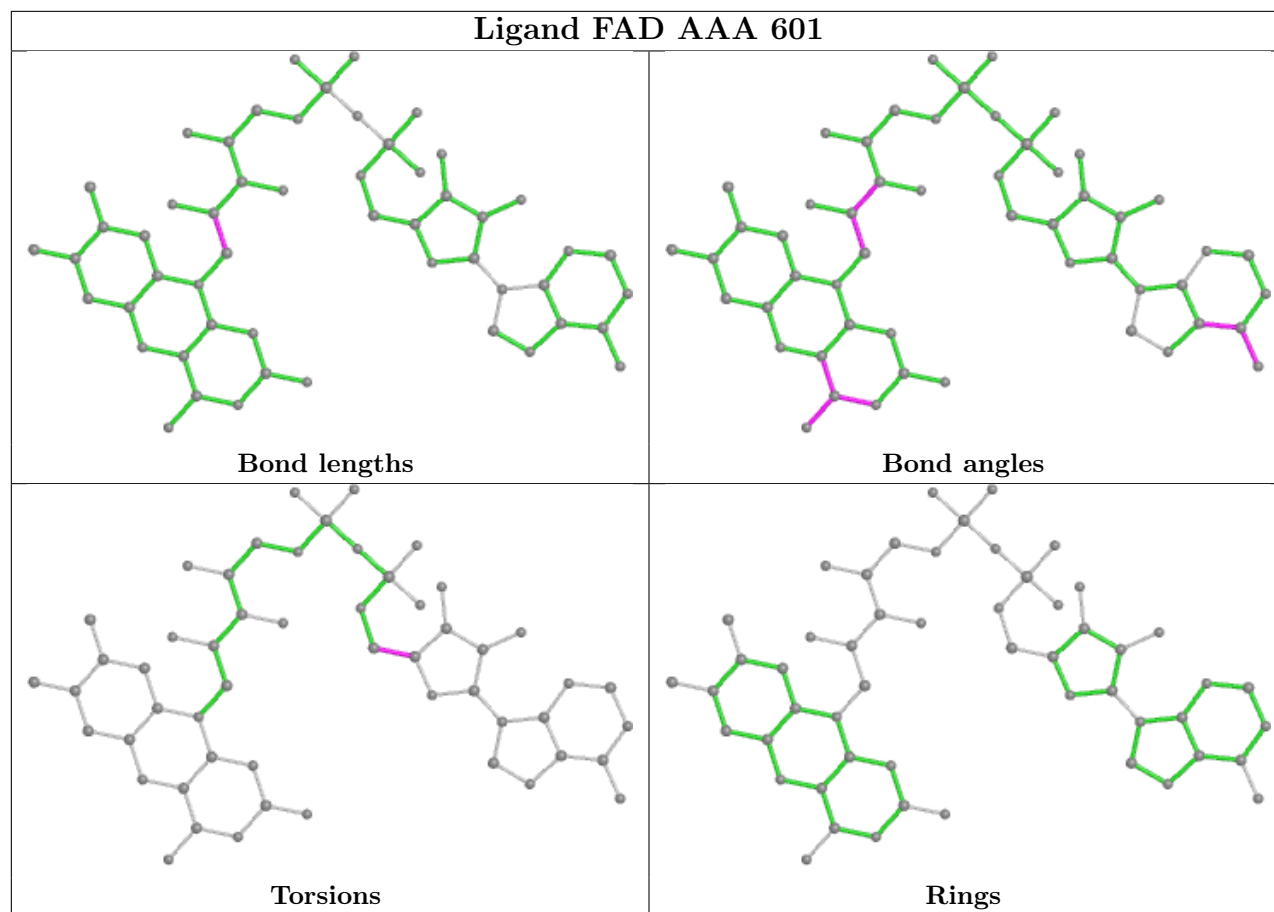
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 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.







## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	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 [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PEG	BBB	607	7/7	0.76	0.25	44,52,57,67	0

*Continued on next page...*

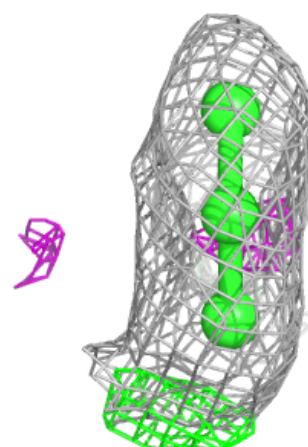
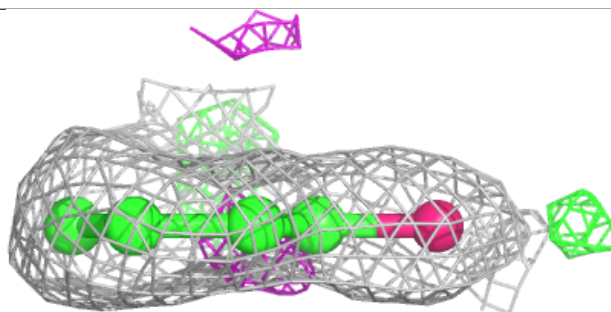
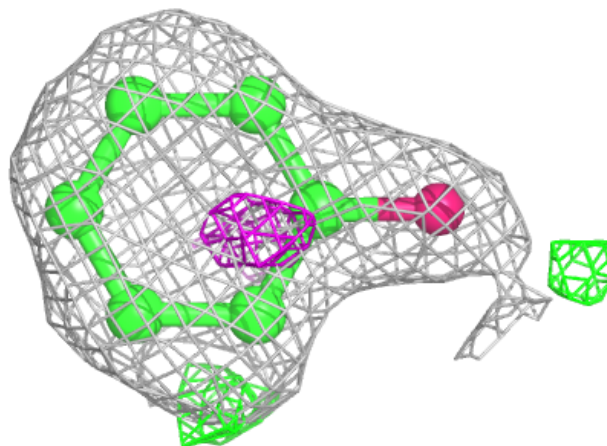
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	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.

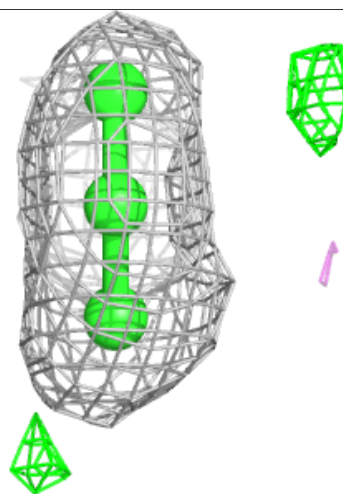
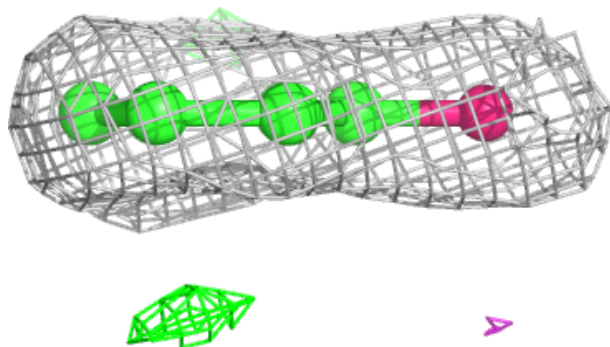
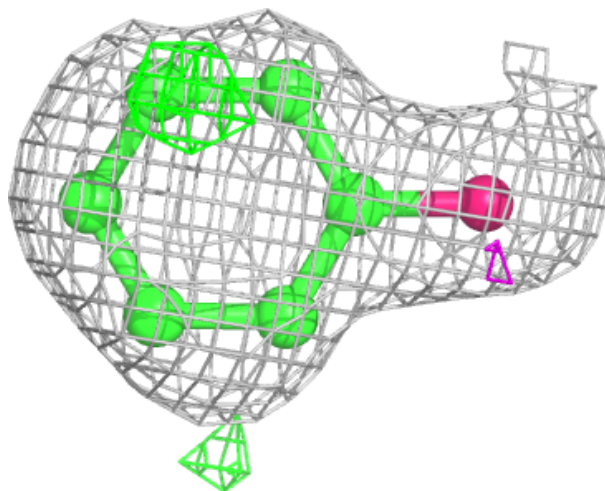
**Electron density around A2Q BBB 608:**

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



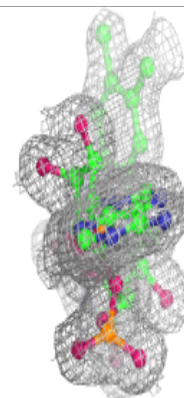
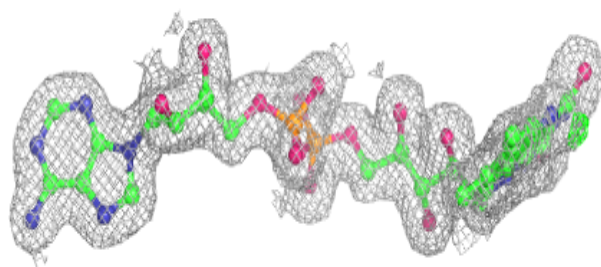
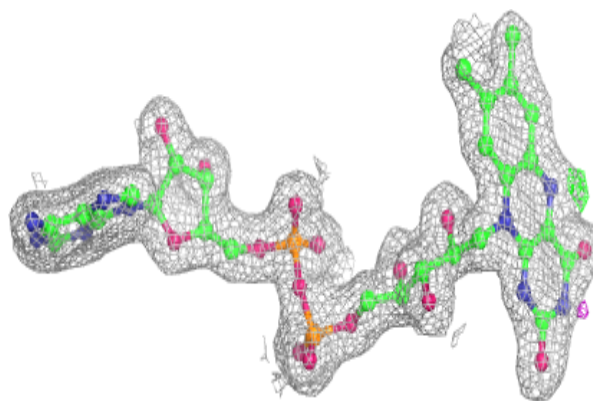
**Electron density around A2Q AAA 606:**

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

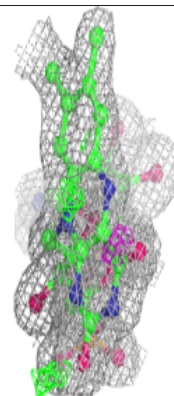
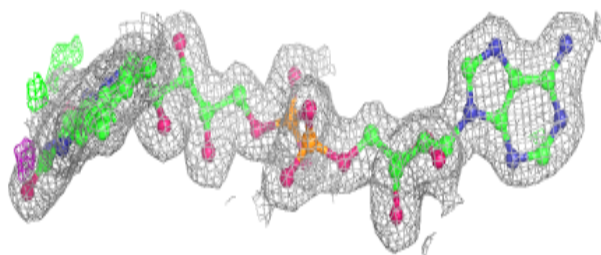
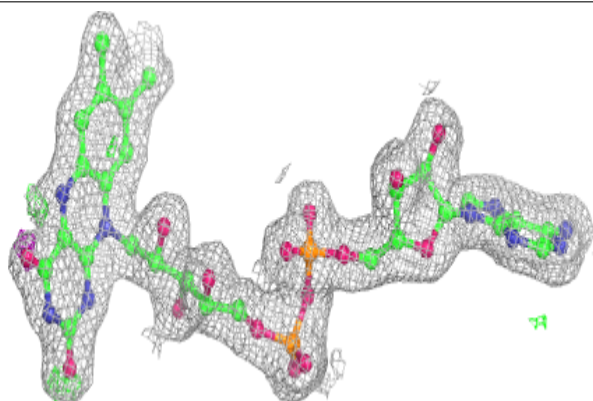


**Electron density around FAD AAA 601:**

$2mF_o-DF_c$  (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.