



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 09:35 PM BST

PDB ID : 2GMH
Title : Structure of Porcine Electron Transfer Flavoprotein-Ubiquinone Oxidoreductase in Complexed with Ubiquinone
Authors : Zhang, J.; Frerman, F.E.; Kim, J.-J.P.
Deposited on : 2006-04-06
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

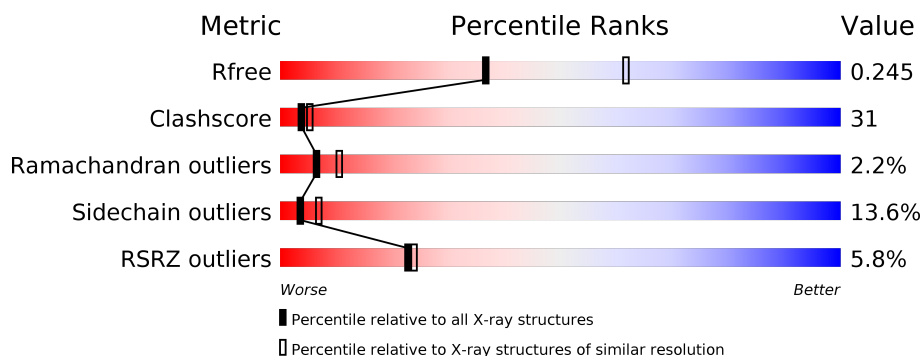
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	584	<div> <div>2%</div> <div>64%</div> <div>29%</div> <div>5% ..</div> </div>
1	B	584	<div> <div>10%</div> <div>41%</div> <div>47%</div> <div>11% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BHG	A	616	X	-	-	-
2	BHG	A	617	X	-	-	X
2	BHG	B	618	X	-	-	-
7	EDO	A	623	-	-	X	-

2 Entry composition [i](#)

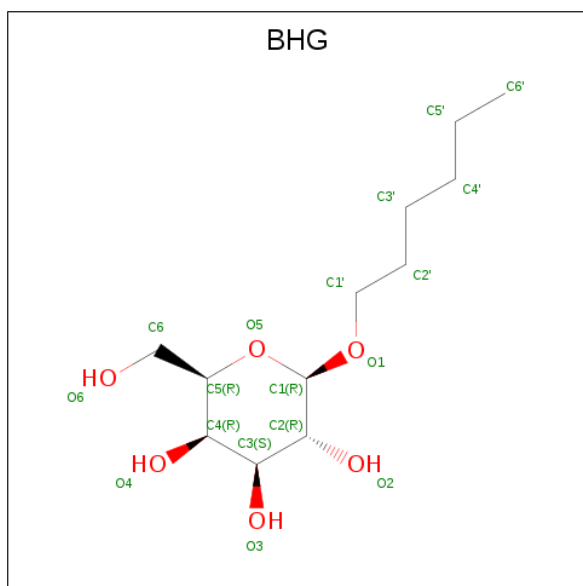
There are 8 unique types of molecules in this entry. The entry contains 9751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Electron transfer flavoprotein-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4558	2910	792	836	20			
1	B	578	Total	C	N	O	S	0	0	0
			4531	2893	787	832	19			

- Molecule 2 is hexyl beta-D-galactopyranoside (three-letter code: BHG) (formula: C₁₂H₂₄O₆).

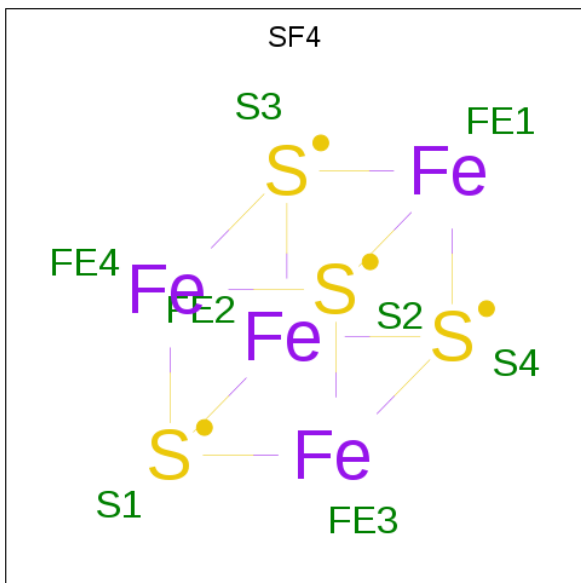


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



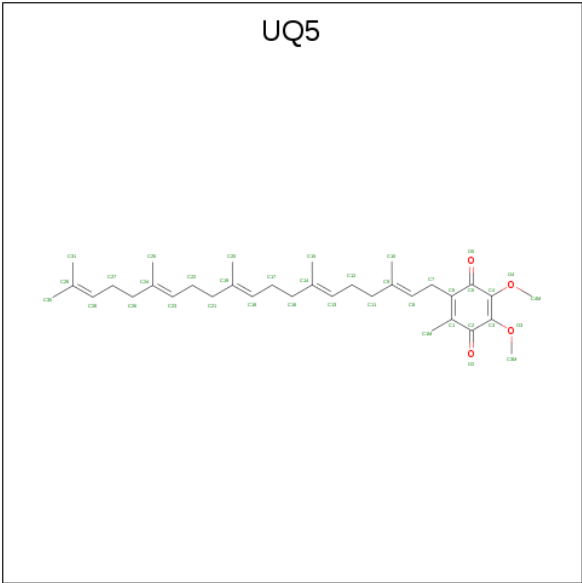
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: C₃₄H₅₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			38	34	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			38	34	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	301	Total 301	O 301	0	0
8	B	68	Total 68	O 68	0	0

D621	G522	P523	E524	Q525	H526	F527	V532	F535	V536	P537	L538	E539	Q540	G541	D542	G543	F544	R545	L546	Q547	I548	N549	A550	Q551	N552	H555	C556	K557	I561	K562	S565	Q566	N569	W570	V571	V572	P573	E574	G575	G578	P579	M584										
R446	G447	M448	E449	P450	H451	T452	K456	G457	S458	D459	S460	D461	Q462	L463	K467	P471	Y474	E475	K476	I481	S482	F483	D484	L485	L486	S487	S488	V489	T494	N495	H496	E497	H498	D499	Q500	P501	A502	H503	L504	T505	R506	S507	D508	E509	S510	P511	P512	V513	L514	N515	N516	L517
L204	H205	A206	F207	V208	T209	I210	F211	A212	E213	G214	H218	L219	Q222	L223	Y224	K225	K226	F227	D228	L229	R230	Q236	T237	Y238	G239	L242	K243	E244	L245	I248	D249	E250	K251	W253	K254	P255	G256	R257	V258	H260	T261	V262	G263	W264	P265	L266	D267	R268	G272	F275		

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.32Å 154.32Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.50 29.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.67-2.50) 98.8 (29.66-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.94 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.254 0.214 , 0.245	Depositor DCC
R_{free} test set	4358 reflections (8.14%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9751	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SF4, EDO, BHG, UQ5, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/4687	0.96	18/6363 (0.3%)
1	B	0.50	0/4660	0.88	10/6326 (0.2%)
All	All	0.55	0/9347	0.92	28/12689 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	VAL	C-N-CD	-15.72	86.01	120.60
1	A	542	ASP	N-CA-C	9.67	137.11	111.00
1	A	5	LYS	N-CA-C	8.39	133.65	111.00
1	A	6	VAL	C-N-CA	8.38	157.20	122.00
1	A	8	ARG	NE-CZ-NH1	-8.31	116.15	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	A	4558	0	4457	204	0
1	B	4531	0	4424	365	0
2	A	36	0	48	6	0
2	B	18	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	53	0	31	2	0
5	B	53	0	31	4	0
6	A	38	0	50	17	0
6	B	38	0	50	13	0
7	A	36	0	54	18	0
7	B	4	0	6	0	0
8	A	301	0	0	8	0
8	B	68	0	0	5	0
All	All	9751	0	9175	576	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 31.

The worst 5 of 576 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:B:38:VAL:HG12	1:B:67:VAL:HG12	1.26	1.13
1:B:55:LYS:HB2	1:B:157:LEU:HD12	1.30	1.08
1:B:351:LEU:HB3	1:B:356:PRO:HG3	1.43	1.00
1:B:510:SER:O	1:B:514:ASN:HB2	1.62	0.99
1:B:203:GLU:HG2	1:B:205:HIS:CE1	1.97	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	579/584 (99%)	544 (94%)	31 (5%)	4 (1%)	22 39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	576/584 (99%)	493 (86%)	62 (11%)	21 (4%)	3	4
All	All	1155/1168 (99%)	1037 (90%)	93 (8%)	25 (2%)	6	10

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ARG
1	B	74	ALA
1	B	84	ALA
1	B	99	LYS
1	B	391	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/486 (99%)	428 (89%)	55 (11%)	5	11
1	B	479/486 (99%)	403 (84%)	76 (16%)	2	4
All	All	962/972 (99%)	831 (86%)	131 (14%)	3	7

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	VAL
1	B	112	ASP
1	B	500	GLN
1	B	31	ARG
1	B	71	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	551	GLN
1	B	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	498	HIS
1	A	525	GLN
1	B	516	ASN

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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z > 2$
7	EDO	A	621	-	3,3,3	0.62	0	2,2,2	0.42	0
4	SF4	A	610	1	0,12,12	0.00	-	-		
5	FAD	B	614	-	51,58,58	2.59	17 (33%)	60,89,89	3.10	17 (28%)
7	EDO	A	625	-	3,3,3	0.72	0	2,2,2	0.45	0
6	UQ5	B	615	-	38,38,38	2.65	17 (44%)	46,49,49	2.35	21 (45%)
2	BHG	B	618	-	18,18,18	1.04	1 (5%)	23,23,23	2.87	3 (13%)
7	EDO	A	622	-	3,3,3	0.73	0	2,2,2	0.06	0
6	UQ5	A	612	-	38,38,38	2.61	15 (39%)	46,49,49	2.49	16 (34%)
7	EDO	A	623	-	3,3,3	0.52	0	2,2,2	0.61	0
7	EDO	A	626	-	3,3,3	0.78	0	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	628	-	3,3,3	0.85	0	2,2,2	0.32	0
7	EDO	A	627	-	3,3,3	0.84	0	2,2,2	0.44	0
2	BHG	A	616	-	18,18,18	1.08	2 (11%)	23,23,23	3.64	4 (17%)
7	EDO	B	620	-	3,3,3	0.64	0	2,2,2	0.56	0
7	EDO	A	619	-	3,3,3	0.61	0	2,2,2	0.42	0
5	FAD	A	611	-	51,58,58	2.78	22 (43%)	60,89,89	2.80	15 (25%)
4	SF4	B	613	1	0,12,12	0.00	-	-	-	-
2	BHG	A	617	-	18,18,18	1.39	4 (22%)	23,23,23	2.38	5 (21%)
7	EDO	A	624	-	3,3,3	0.65	0	2,2,2	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	621	-	-	1/1/1/1	-
4	SF4	A	610	1	-	-	0/6/5/5
5	FAD	B	614	-	-	6/30/50/50	0/6/6/6
7	EDO	A	625	-	-	1/1/1/1	-
6	UQ5	B	615	-	-	18/33/57/57	0/1/1/1
2	BHG	B	618	-	1/1/5/5	5/9/29/29	0/1/1/1
7	EDO	A	622	-	-	1/1/1/1	-
6	UQ5	A	612	-	-	19/33/57/57	0/1/1/1
7	EDO	A	623	-	-	1/1/1/1	-
7	EDO	A	626	-	-	0/1/1/1	-
7	EDO	A	628	-	-	0/1/1/1	-
7	EDO	A	627	-	-	0/1/1/1	-
2	BHG	A	616	-	1/1/5/5	7/9/29/29	0/1/1/1
7	EDO	B	620	-	-	0/1/1/1	-
7	EDO	A	619	-	-	1/1/1/1	-
5	FAD	A	611	-	-	2/30/50/50	0/6/6/6
7	EDO	A	624	-	-	1/1/1/1	-
2	BHG	A	617	-	1/1/5/5	5/9/29/29	0/1/1/1
4	SF4	B	613	1	-	-	0/6/5/5

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	FAD	C1'-N10	-9.86	1.38	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	615	UQ5	C28-C29	7.69	1.54	1.32
6	A	612	UQ5	C28-C29	7.37	1.53	1.32
5	B	614	FAD	C4X-C10	7.18	1.46	1.38
5	B	614	FAD	C4X-N5	6.39	1.42	1.33

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	614	FAD	C4-N3-C2	13.64	126.66	115.14
5	A	611	FAD	C4-N3-C2	13.25	126.33	115.14
2	B	618	BHG	O1-C1'-C2'	11.74	150.73	109.56
2	A	616	BHG	C1'-O1-C1	11.42	132.78	113.84
2	A	616	BHG	O1-C1'-C2'	10.04	144.74	109.56

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	618	BHG	C4
2	A	616	BHG	C4
2	A	617	BHG	C4

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	614	FAD	C5'-O5'-P-O2P
6	B	615	UQ5	C1-C6-C7-C8
6	B	615	UQ5	C5-C6-C7-C8
6	B	615	UQ5	C14-C16-C17-C18
6	B	615	UQ5	C16-C17-C18-C19

There are no ring outliers.

11 monomers are involved in 60 short contacts:

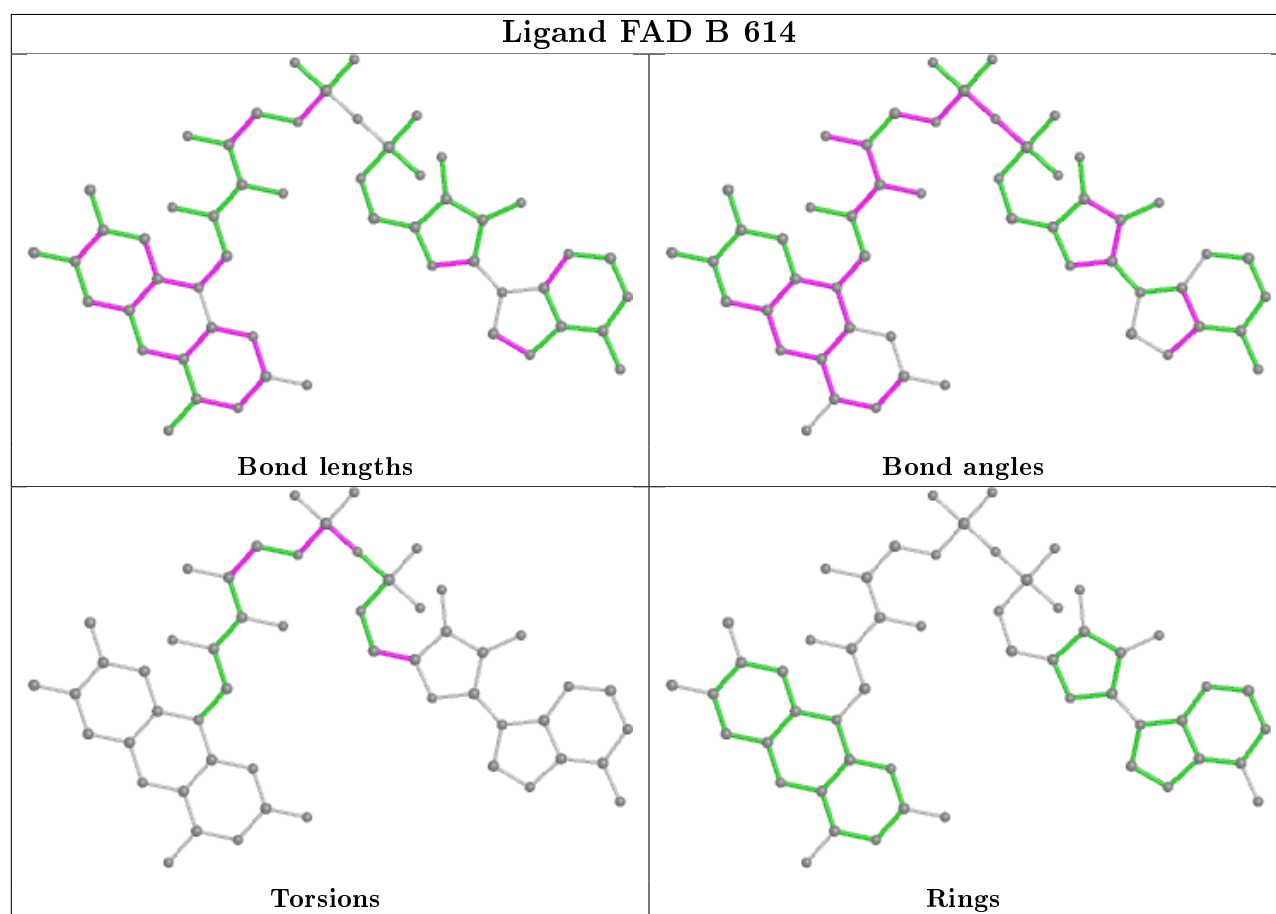
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	621	EDO	3	0
5	B	614	FAD	4	0
6	B	615	UQ5	13	0
7	A	622	EDO	3	0
6	A	612	UQ5	17	0
7	A	623	EDO	7	0
7	A	628	EDO	1	0

Continued on next page...

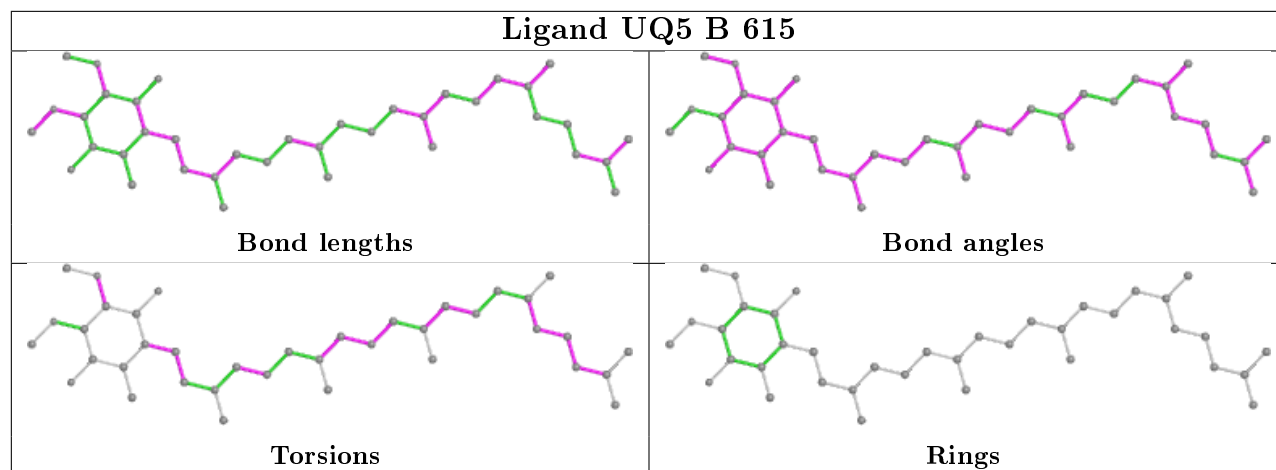
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	627	EDO	1	0
7	A	619	EDO	3	0
5	A	611	FAD	2	0
2	A	617	BHG	6	0

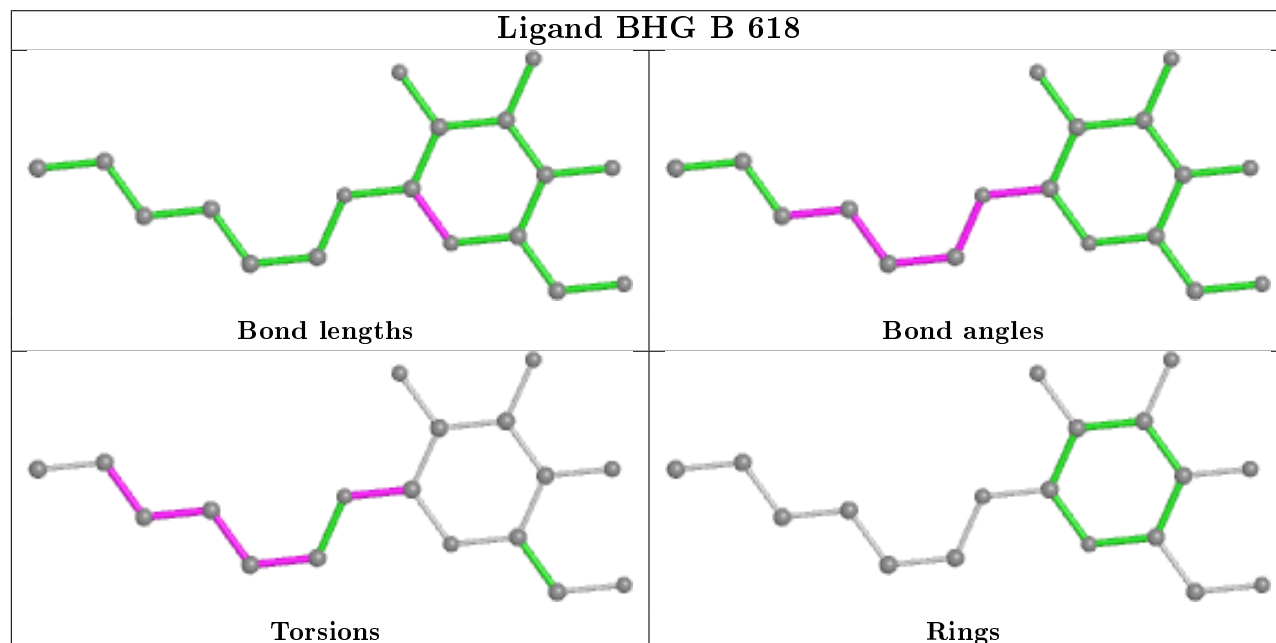
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



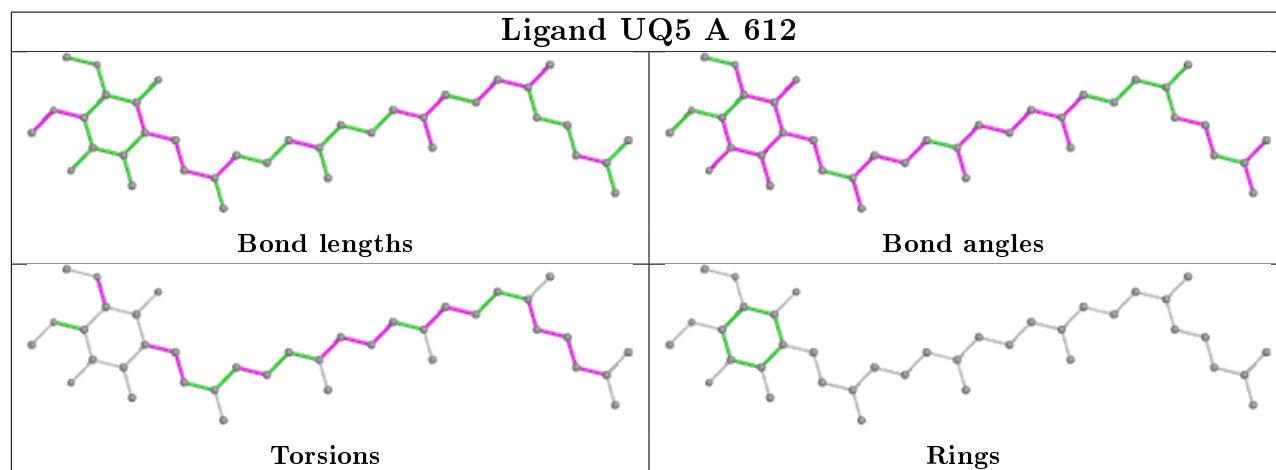
Ligand UQ5 B 615

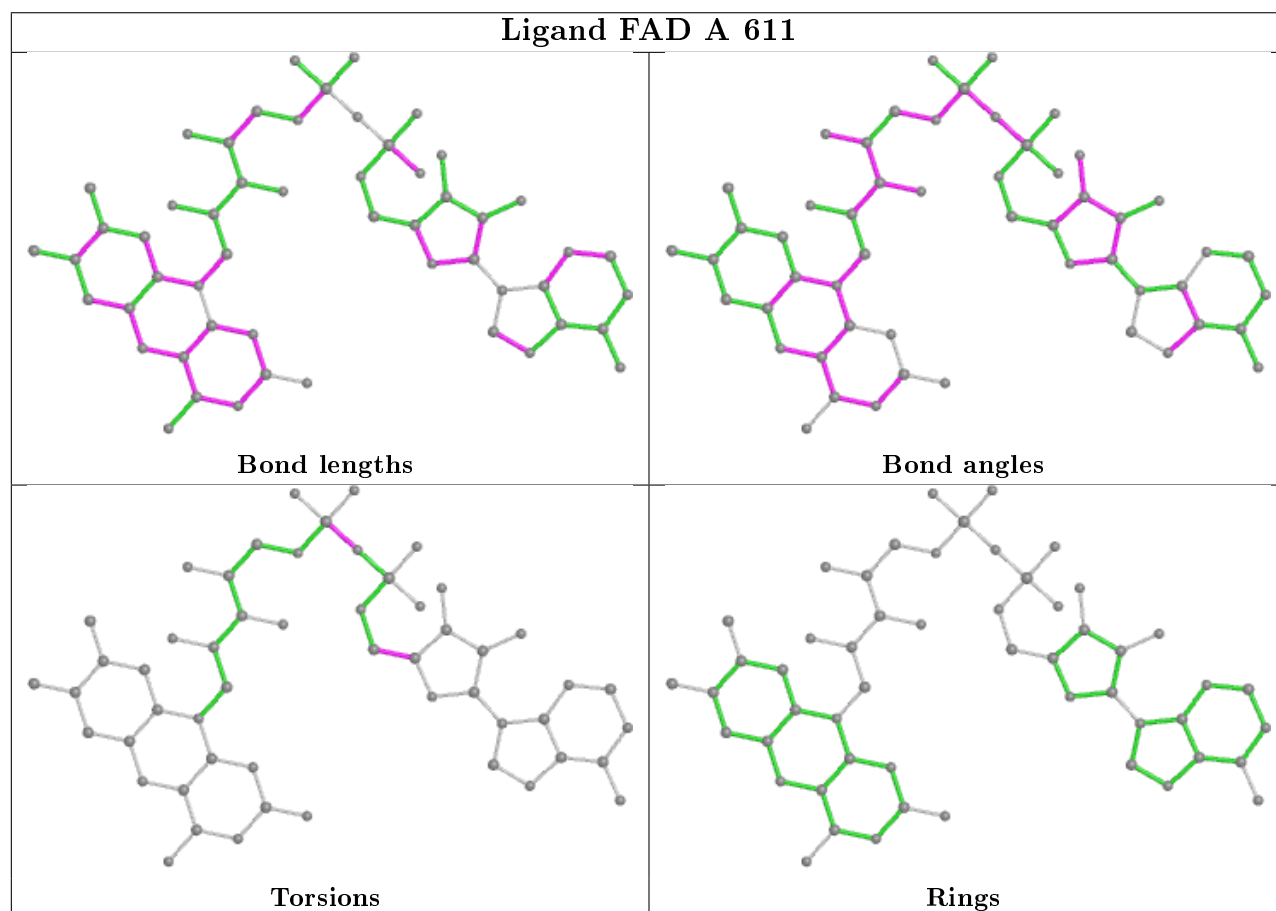
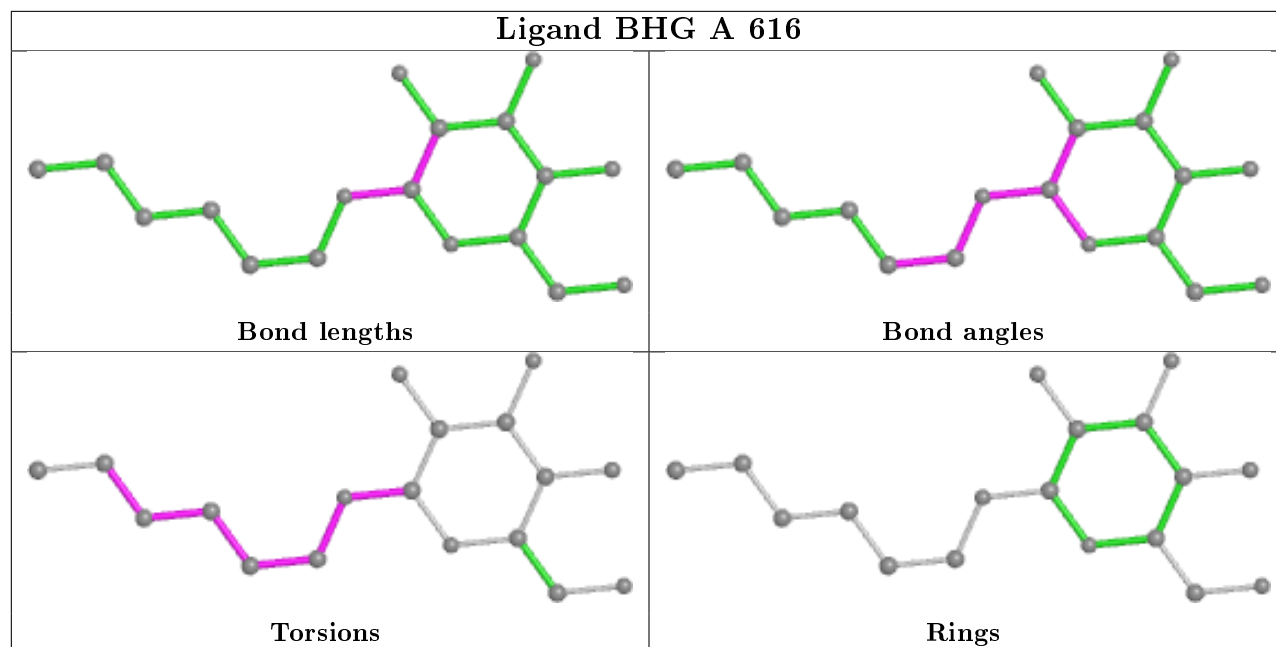


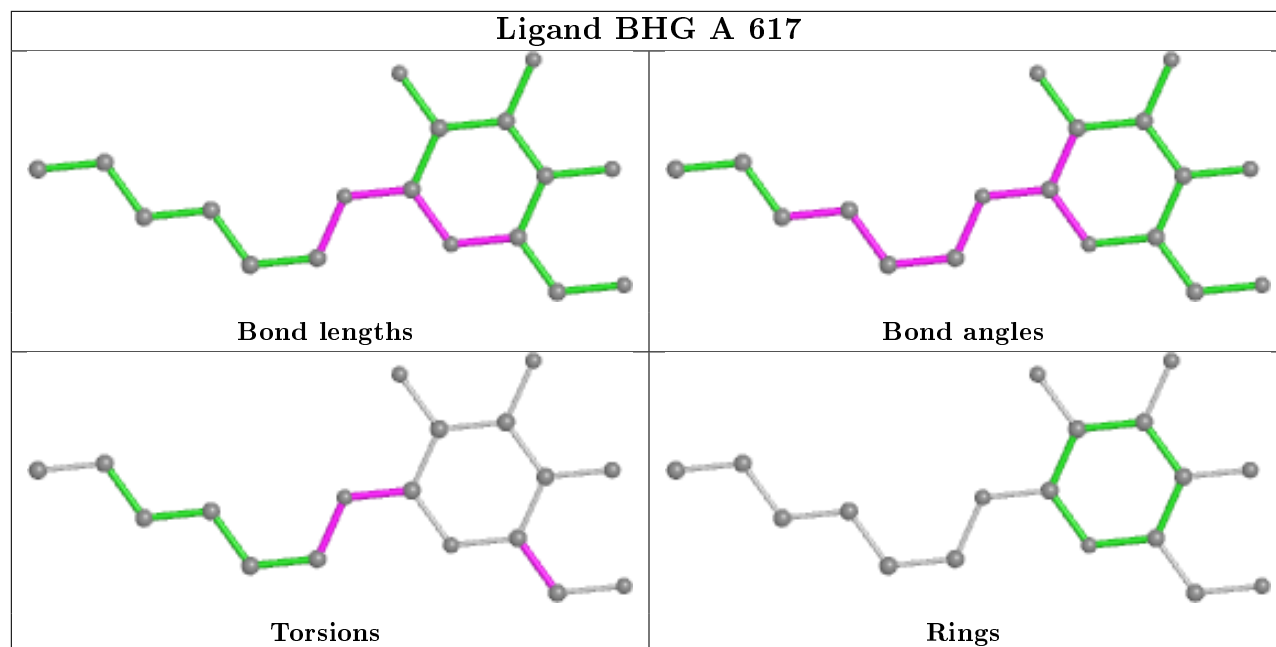
Ligand BHG B 618



Ligand UQ5 A 612







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/584 (99%)	-0.25	10 (1%) 70 72	13, 30, 57, 84	0
1	B	578/584 (98%)	0.62	57 (9%) 7 7	38, 64, 79, 86	0
All	All	1159/1168 (99%)	0.18	67 (5%) 23 24	13, 49, 77, 86	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	CYS	7.9
1	B	176	GLY	5.6
1	B	540	GLN	5.4
1	A	540	GLN	5.4
1	B	390	LEU	5.1

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](#)

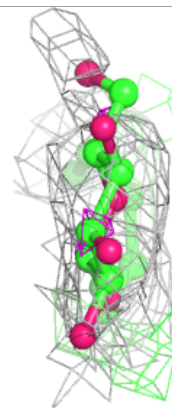
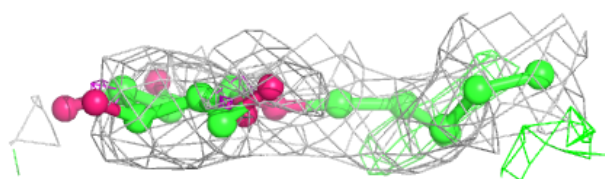
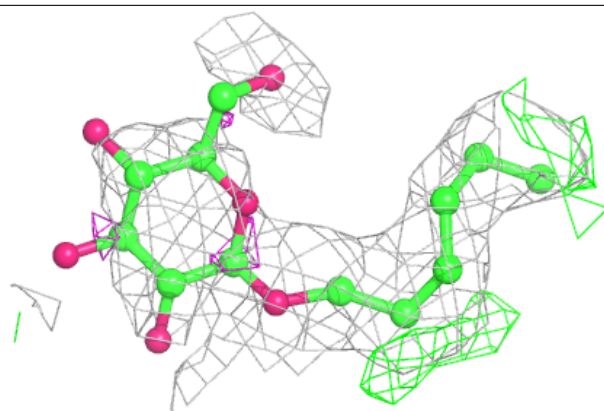
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BHG	B	618	18/18	0.53	0.37	61,76,78,78	0
2	BHG	A	616	18/18	0.58	0.39	52,76,78,79	0
2	BHG	A	617	18/18	0.59	0.58	55,75,78,79	0
7	EDO	A	628	4/4	0.77	0.33	53,54,55,55	0
7	EDO	A	627	4/4	0.81	0.52	57,58,58,58	0
7	EDO	A	622	4/4	0.82	0.40	51,55,55,57	0
6	UQ5	B	615	38/38	0.86	0.26	51,56,68,71	0
7	EDO	B	620	4/4	0.88	0.16	49,53,54,56	0
6	UQ5	A	612	38/38	0.88	0.26	39,48,62,63	0
7	EDO	A	626	4/4	0.89	0.14	43,45,45,46	0
7	EDO	A	619	4/4	0.90	0.21	37,37,38,43	0
7	EDO	A	625	4/4	0.90	0.15	49,55,55,57	0
7	EDO	A	623	4/4	0.92	0.49	48,49,49,53	0
5	FAD	B	614	53/53	0.93	0.19	44,60,68,69	0
7	EDO	A	621	4/4	0.94	0.26	45,47,48,49	0
3	NA	A	1070	1/1	0.95	0.08	37,37,37,37	0
7	EDO	A	624	4/4	0.95	0.31	35,41,42,42	0
5	FAD	A	611	53/53	0.98	0.17	16,20,24,26	0
4	SF4	B	613	8/8	0.98	0.09	55,58,59,59	0
4	SF4	A	610	8/8	0.99	0.12	16,19,22,22	0

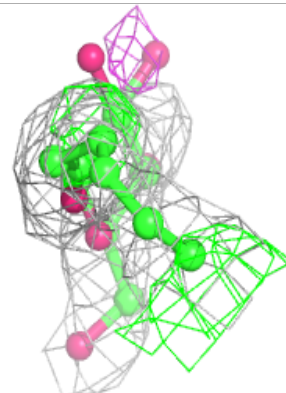
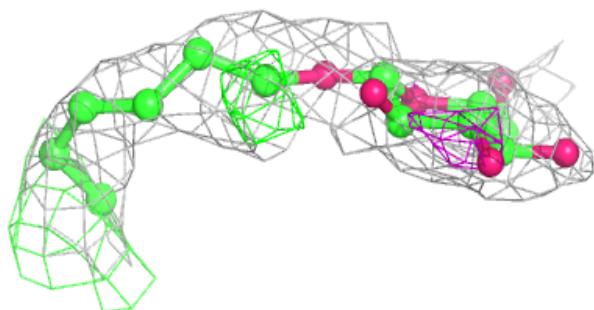
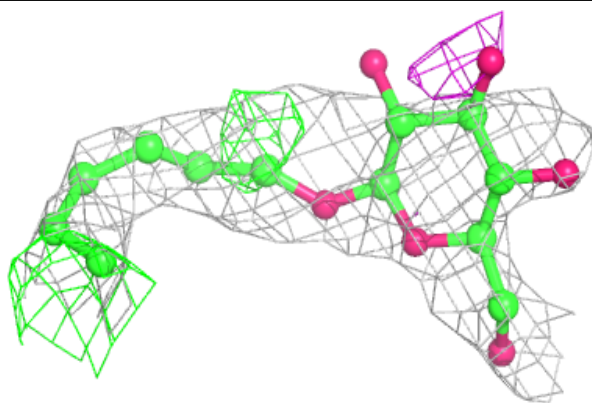
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BHG B 618:

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

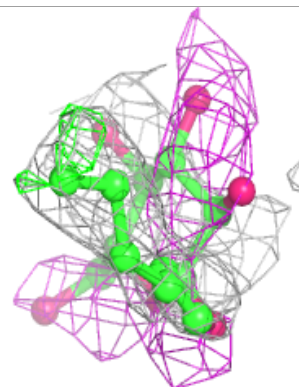
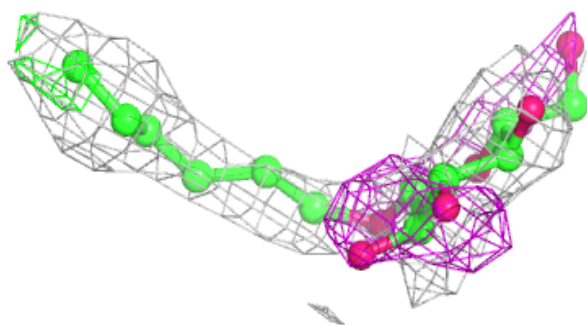
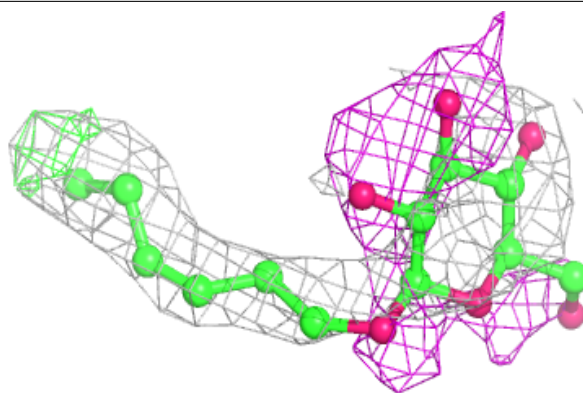
**Electron density around BHG A 616:**

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

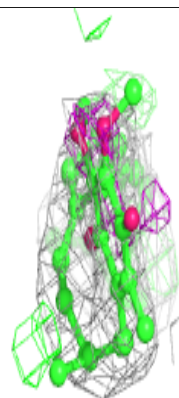
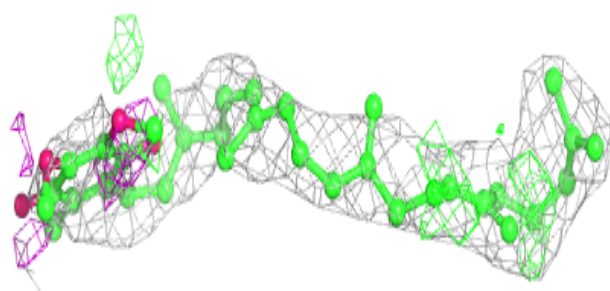
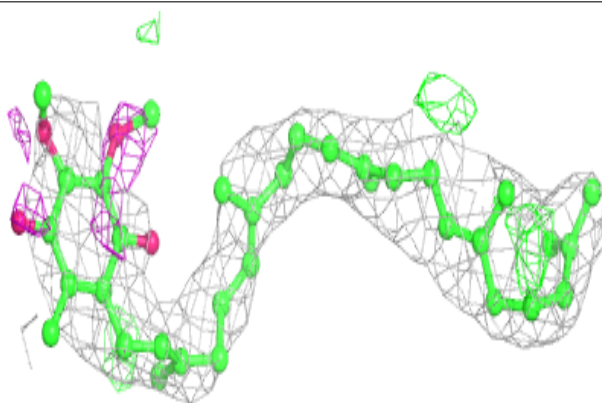


Electron density around BHG A 617:

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

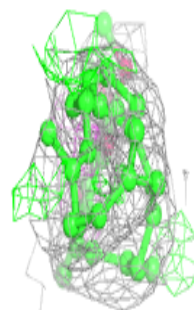
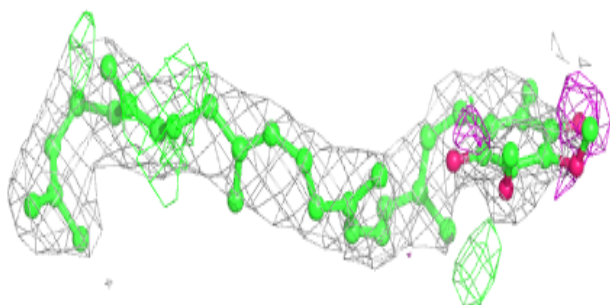
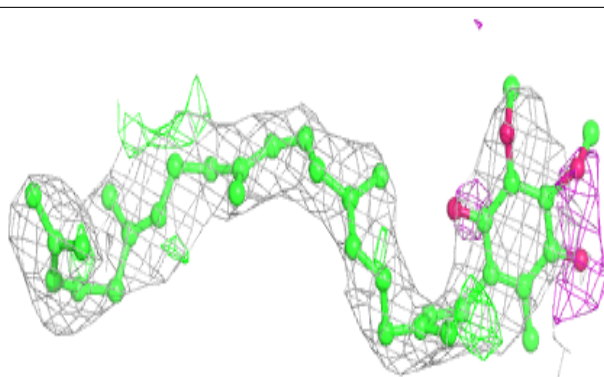
**Electron density around UQ5 B 615:**

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

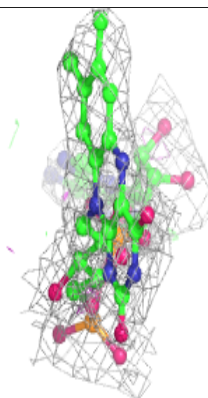
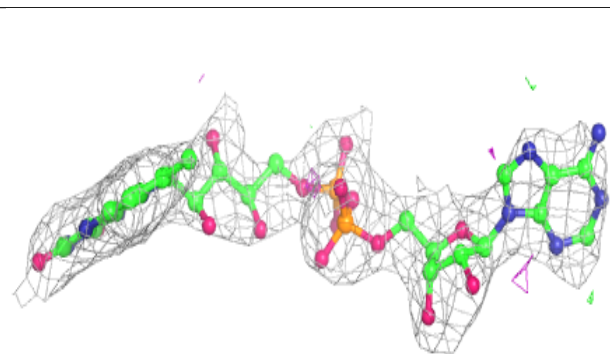
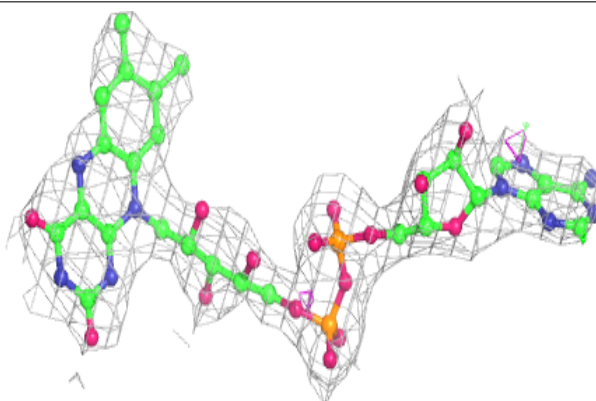


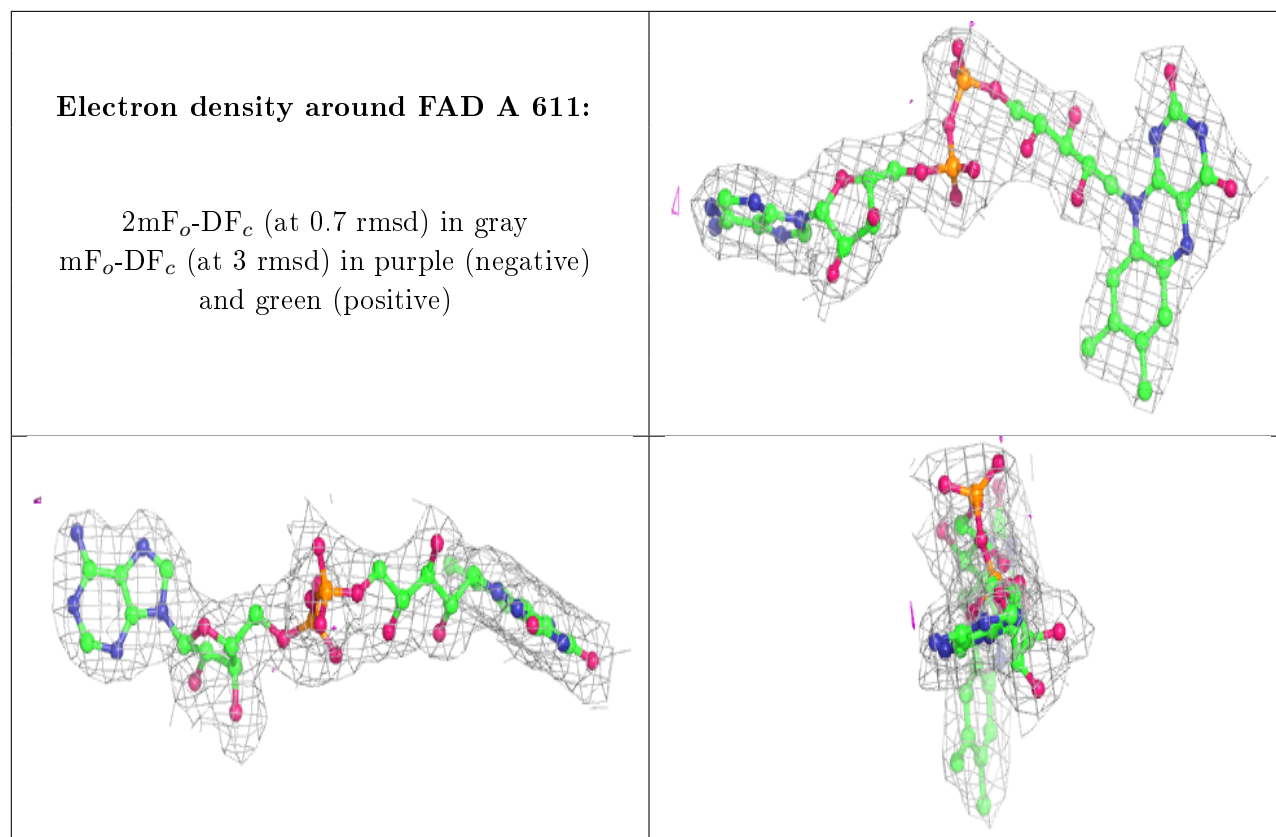
Electron density around UQ5 A 612:

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

**Electron density around FAD B 614:**

$2mF_o-DF_c$ (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.