



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 01:08 PM EDT

PDB ID : 6OI6  
Title : Crystal structure of human Sulfide Quinone Oxidoreductase in complex with coenzyme Q (sulfide soaked)  
Authors : Banerjee, R.; Cho, U.S.; Kim, H.; Moon, S.  
Deposited on : 2019-04-08  
Resolution : 2.56 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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

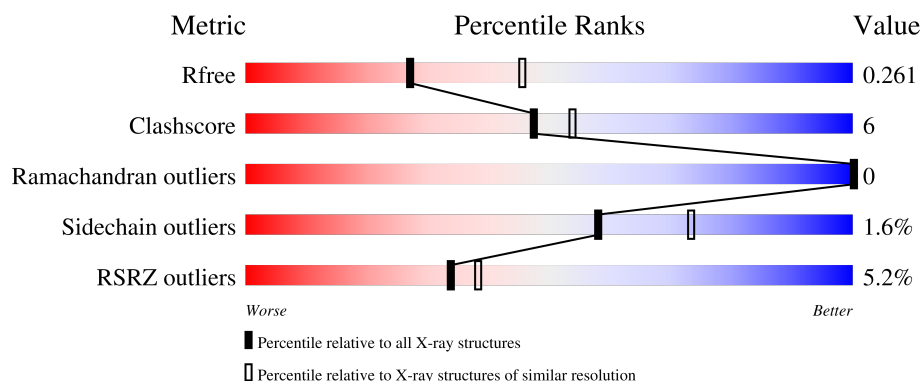
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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))
$R_{free}$	164625	1685 (2.58-2.54)
Clashscore	180529	1779 (2.58-2.54)
Ramachandran outliers	177936	1766 (2.58-2.54)
Sidechain outliers	177891	1766 (2.58-2.54)
RSRZ outliers	164620	1685 (2.58-2.54)

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	A	418	<div> <div>4%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	B	418	<div> <div>6%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6574 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 Sulfide:quinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3210	2060	543	590	17			
1	B	404	Total	C	N	O	S	0	0	0
			3184	2043	538	587	16			

There are 18 discrepancies between the modelled and reference sequences:

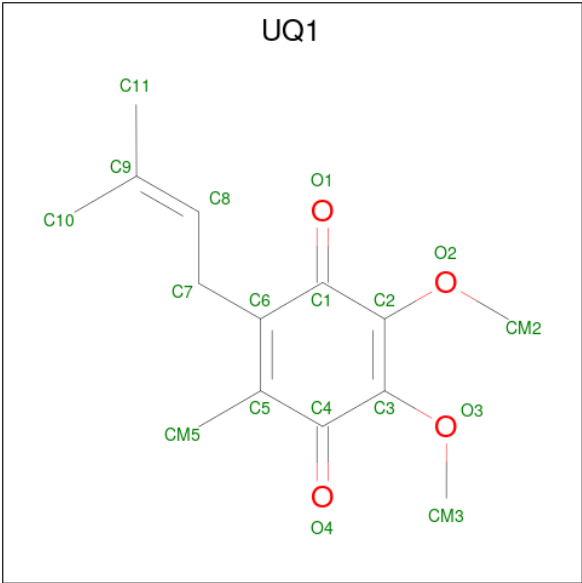
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP Q9Y6N5
A	451	LEU	-	expression tag	UNP Q9Y6N5
A	452	GLU	-	expression tag	UNP Q9Y6N5
A	453	HIS	-	expression tag	UNP Q9Y6N5
A	454	HIS	-	expression tag	UNP Q9Y6N5
A	455	HIS	-	expression tag	UNP Q9Y6N5
A	456	HIS	-	expression tag	UNP Q9Y6N5
A	457	HIS	-	expression tag	UNP Q9Y6N5
A	458	HIS	-	expression tag	UNP Q9Y6N5
B	41	MET	-	initiating methionine	UNP Q9Y6N5
B	451	LEU	-	expression tag	UNP Q9Y6N5
B	452	GLU	-	expression tag	UNP Q9Y6N5
B	453	HIS	-	expression tag	UNP Q9Y6N5
B	454	HIS	-	expression tag	UNP Q9Y6N5
B	455	HIS	-	expression tag	UNP Q9Y6N5
B	456	HIS	-	expression tag	UNP Q9Y6N5
B	457	HIS	-	expression tag	UNP Q9Y6N5
B	458	HIS	-	expression tag	UNP Q9Y6N5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 3 is UBIQUINONE-1 (three-letter code: UQ1) (formula: C<sub>14</sub>H<sub>18</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			18	14 4		
3	A	1	Total	C O	0	0
			18	14 4		

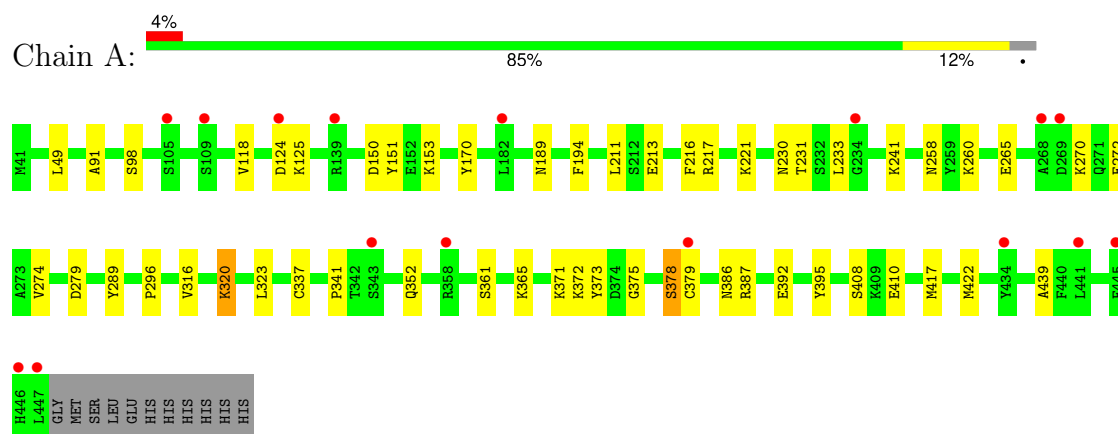
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	17	Total 17	O 17	0	0

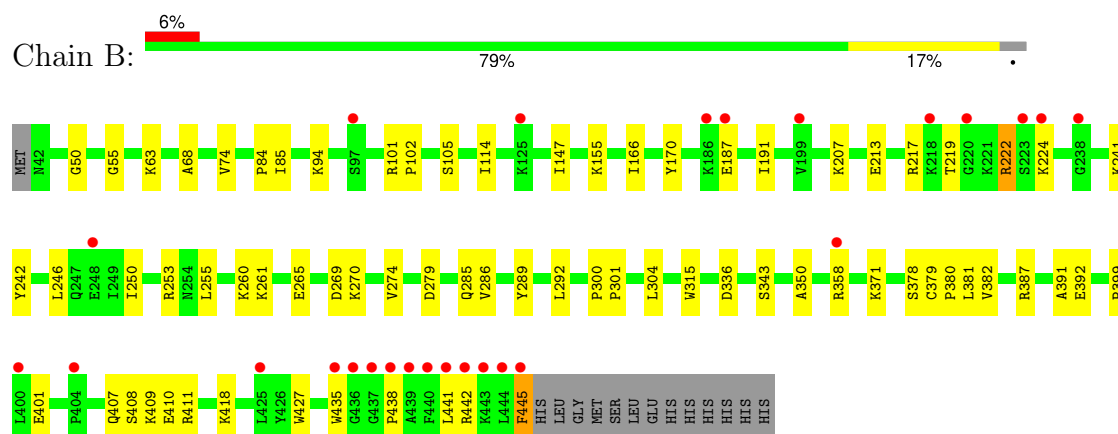
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sulfide:quinone oxidoreductase, mitochondrial



- Molecule 1: Sulfide:quinone oxidoreductase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.53Å 111.96Å 136.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.93 – 2.56 50.93 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.93-2.56) 88.3 (50.93-2.56)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.92 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, $R_{free}$	0.205 , 0.265 0.205 , 0.261	Depositor DCC
$R_{free}$ test set	36498 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: CSS, UQ1, 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	0.47	0/3279	0.58	0/4440
1	B	0.45	0/3252	0.61	0/4404
All	All	0.46	0/6531	0.59	0/8844

There are no bond length outliers.

There are no bond angle outliers.

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	A	3210	0	3229	30	0
1	B	3184	0	3202	41	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
3	A	36	0	36	2	0
4	A	21	0	0	0	0
4	B	17	0	0	0	0
All	All	6574	0	6529	72	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 6.



All (72) 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:A:231:THR:HG22	1:A:233:LEU:H	1.54	0.70
1:B:387:ARG:HB3	1:B:410:GLU:HB3	1.80	0.64
1:B:63:LYS:HG3	1:B:68:ALA:HB2	1.81	0.63
1:A:439:ALA:HB3	3:A:502:UQ1:H111	1.83	0.61
1:B:350:ALA:HB1	1:B:435:TRP:CD1	2.36	0.59
1:A:213:GLU:OE1	1:A:217:ARG:NH1	2.36	0.58
1:B:350:ALA:HB1	1:B:435:TRP:HD1	1.69	0.58
1:B:187:GLU:HG3	1:B:224:LYS:HB3	1.85	0.57
1:A:371:LYS:HD2	1:A:372:LYS:H	1.70	0.57
1:B:85:ILE:HD11	1:B:94:LYS:HE3	1.86	0.57
1:A:361:SER:O	1:A:365:LYS:HG3	2.05	0.57
1:A:320:LYS:HG2	1:A:341:PRO:HD3	1.87	0.56
1:B:300:PRO:HD3	1:B:315:TRP:CZ2	2.40	0.56
1:B:222:ARG:NH2	1:B:253:ARG:O	2.37	0.55
1:B:246:LEU:HD11	1:B:381:LEU:HD13	1.88	0.55
1:B:261:LYS:NZ	1:B:285:GLN:OE1	2.40	0.54
1:B:241:LYS:HE2	1:B:408:SER:HB3	1.90	0.54
1:A:387:ARG:HB3	1:A:410:GLU:HB3	1.88	0.54
1:B:250:ILE:HG23	1:B:255:LEU:HB2	1.90	0.54
1:B:265:GLU:HB3	1:B:274:VAL:HB	1.92	0.52
1:A:49:LEU:HD22	1:A:118:VAL:HG21	1.92	0.52
1:A:194:PHE:HB3	1:A:231:THR:HG23	1.91	0.52
1:B:358:ARG:HH11	1:B:371:LYS:HG2	1.75	0.51
1:A:150:ASP:HB3	1:A:153:LYS:HG2	1.92	0.51
1:B:217:ARG:HG2	1:B:222:ARG:HG3	1.93	0.50
1:A:241:LYS:HE2	1:A:408:SER:HB2	1.94	0.50
1:B:435:TRP:HZ2	1:B:438:PRO:HG3	1.77	0.50
1:A:170:TYR:CD2	2:A:501:FAD:HM83	2.48	0.49
1:B:191:ILE:HD12	1:B:289:TYR:HB3	1.94	0.49
1:A:316:VAL:HG23	1:A:337:CYS:O	2.15	0.47
1:B:50:GLY:O	1:B:55:GLY:HA3	2.15	0.47
1:A:151:TYR:CD1	1:A:296:PRO:HB3	2.50	0.47
1:B:442:ARG:HA	1:B:445:PHE:CE1	2.50	0.47
1:A:323:LEU:HD21	1:A:352:GLN:HB3	1.97	0.46
1:B:378:SER:HB2	1:B:392:GLU:HG2	1.97	0.46
1:B:170:TYR:CD2	2:B:501:FAD:HM83	2.51	0.45
1:A:373:TYR:CE2	1:A:375:GLY:HA2	2.51	0.45
1:A:91:ALA:HB2	1:A:211:LEU:HD13	1.99	0.45
3:A:502:UQ1:H72	3:A:502:UQ1:HM51	1.40	0.45
1:B:358:ARG:NH1	1:B:371:LYS:HE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LYS:HB2	1:A:272:GLU:HG3	1.98	0.44
1:B:166:ILE:HD12	1:B:292:LEU:HD23	2.00	0.44
1:B:260:LYS:HD2	1:B:279:ASP:OD1	2.17	0.44
1:B:401:GLU:HB3	1:B:407:GLN:OE1	2.18	0.44
1:B:213:GLU:HG3	1:B:255:LEU:HD21	2.00	0.44
1:A:151:TYR:CE1	1:A:296:PRO:HB3	2.53	0.43
1:B:274:VAL:HG22	1:B:286:VAL:HG22	1.99	0.43
1:A:265:GLU:HB3	1:A:274:VAL:HB	1.99	0.43
1:B:102:PRO:HG2	1:B:105:SER:OG	2.19	0.43
1:B:207:LYS:HD3	1:B:382:VAL:H	1.82	0.43
1:B:74:VAL:HA	1:B:114:ILE:O	2.19	0.43
1:A:260:LYS:HD2	1:A:279:ASP:OD1	2.19	0.43
1:A:230:ASN:OD1	1:A:258:ASN:HB2	2.19	0.43
1:B:442:ARG:HA	1:B:445:PHE:HE1	1.84	0.43
1:B:155:LYS:HB3	1:B:265:GLU:HG3	2.00	0.42
1:A:124:ASP:O	1:A:125:LYS:HD3	2.20	0.42
1:A:417:MET:O	1:A:422:MET:HG2	2.20	0.41
1:B:241:LYS:HG2	1:B:399:PRO:HG3	2.02	0.41
1:B:380:PRO:HB2	1:B:418:LYS:HG3	2.02	0.41
1:A:189:ASN:HB2	1:A:289:TYR:HA	2.02	0.41
1:A:378:SER:HB2	1:A:392:GLU:HG2	2.02	0.41
1:A:194:PHE:HB3	1:A:231:THR:HA	2.03	0.41
1:B:147:ILE:HB	1:B:336:ASP:HB3	2.03	0.41
1:B:301:PRO:HD2	1:B:304:LEU:HD12	2.03	0.41
1:A:371:LYS:HD2	1:A:372:LYS:N	2.35	0.41
1:B:242:TYR:CZ	1:B:391:ALA:HA	2.56	0.41
1:A:216:PHE:HD1	1:A:221:LYS:HE3	1.85	0.41
1:B:269:ASP:OD1	1:B:270:LYS:N	2.54	0.41
1:B:409:LYS:O	1:B:411:ARG:HG3	2.20	0.41
1:B:101:ARG:HD2	1:B:427:TRP:CE3	2.55	0.40
1:A:386:ASN:N	1:A:386:ASN:OD1	2.54	0.40
1:B:84:PRO:HA	2:B:501:FAD:C5X	2.51	0.40

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	404/418 (97%)	389 (96%)	15 (4%)	0	100	100
1	B	401/418 (96%)	385 (96%)	16 (4%)	0	100	100
All	All	805/836 (96%)	774 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/354 (97%)	339 (98%)	5 (2%)	60	75
1	B	341/354 (96%)	335 (98%)	6 (2%)	54	70
All	All	685/708 (97%)	674 (98%)	11 (2%)	58	73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	320	LYS
1	A	378	SER
1	A	379	CYS
1	A	395	TYR
1	B	219	THR
1	B	222	ARG
1	B	343	SER
1	B	379	CYS
1	B	441	LEU
1	B	445	PHE

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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSS	B	201	1	4,6,7	0.83	0	2,6,8	0.47	0
1	CSS	A	201	1	4,6,7	1.15	0	2,6,8	0.56	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
1	CSS	B	201	1	-	1/1/5/7	-
1	CSS	A	201	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	201	CSS	N-CA-CB-SG
1	B	201	CSS	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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$
3	UQ1	A	502	-	18,18,18	2.93	4 (22%)	24,25,25	2.74	7 (29%)
2	FAD	A	501	-	54,58,58	0.72	1 (1%)	71,89,89	0.66	2 (2%)
3	UQ1	A	503	-	18,18,18	2.87	7 (38%)	24,25,25	1.97	5 (20%)
2	FAD	B	501	-	54,58,58	0.51	0	71,89,89	0.78	2 (2%)

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	UQ1	A	502	-	-	1/9/33/33	0/1/1/1
2	FAD	A	501	-	-	11/30/50/50	0/6/6/6
3	UQ1	A	503	-	-	1/9/33/33	0/1/1/1
2	FAD	B	501	-	-	5/30/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	UQ1	C6-C5	9.30	1.51	1.35
3	A	502	UQ1	C6-C5	9.20	1.51	1.35
3	A	502	UQ1	C3-C2	5.14	1.54	1.36
3	A	503	UQ1	C3-C2	4.21	1.51	1.36
2	A	501	FAD	P-O2P	-3.03	1.41	1.55
3	A	502	UQ1	C6-C1	2.58	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	UQ1	O1-C1	-2.34	1.18	1.23
3	A	503	UQ1	O3-CM3	-2.33	1.40	1.45
3	A	503	UQ1	C6-C1	2.18	1.52	1.46
3	A	502	UQ1	O3-CM3	-2.11	1.40	1.45
3	A	503	UQ1	C5-C4	2.09	1.54	1.47
3	A	503	UQ1	O2-C2	2.08	1.41	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	UQ1	C7-C6-C1	6.84	126.46	118.52
3	A	502	UQ1	CM5-C5-C6	-6.07	114.47	124.45
3	A	502	UQ1	C6-C5-C4	5.81	123.75	119.17
3	A	502	UQ1	C7-C6-C5	-5.57	115.34	124.89
3	A	503	UQ1	CM5-C5-C6	-4.32	117.34	124.45
3	A	503	UQ1	C7-C8-C9	-4.31	115.06	127.25
3	A	503	UQ1	C7-C6-C5	-3.92	118.17	124.89
2	B	501	FAD	C4B-O4B-C1B	-3.15	107.04	109.92
3	A	502	UQ1	C7-C8-C9	-3.07	118.57	127.25
3	A	502	UQ1	C8-C7-C6	2.70	118.72	112.08
2	A	501	FAD	C4B-O4B-C1B	-2.60	107.54	109.92
2	B	501	FAD	C5A-C6A-N6A	2.43	124.01	120.31
2	A	501	FAD	C5A-C6A-N6A	2.42	124.00	120.31
3	A	503	UQ1	CM5-C5-C4	2.34	124.92	116.93
3	A	502	UQ1	C11-C9-C10	2.30	119.87	114.59
3	A	503	UQ1	O1-C1-C6	-2.03	117.86	121.79

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	O4'-C4'-C5'-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	A	501	FAD	O2'-C2'-C3'-O3'
2	B	501	FAD	C3'-C4'-C5'-O5'
2	A	501	FAD	O2'-C2'-C3'-C4'
2	A	501	FAD	P-O3P-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	B	501	FAD	C5B-O5B-PA-O3P
3	A	503	UQ1	C4-C3-O3-CM3
3	A	502	UQ1	C5-C6-C7-C8
2	A	501	FAD	C1'-C2'-C3'-O3'
2	A	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	P-O3P-PA-O2A

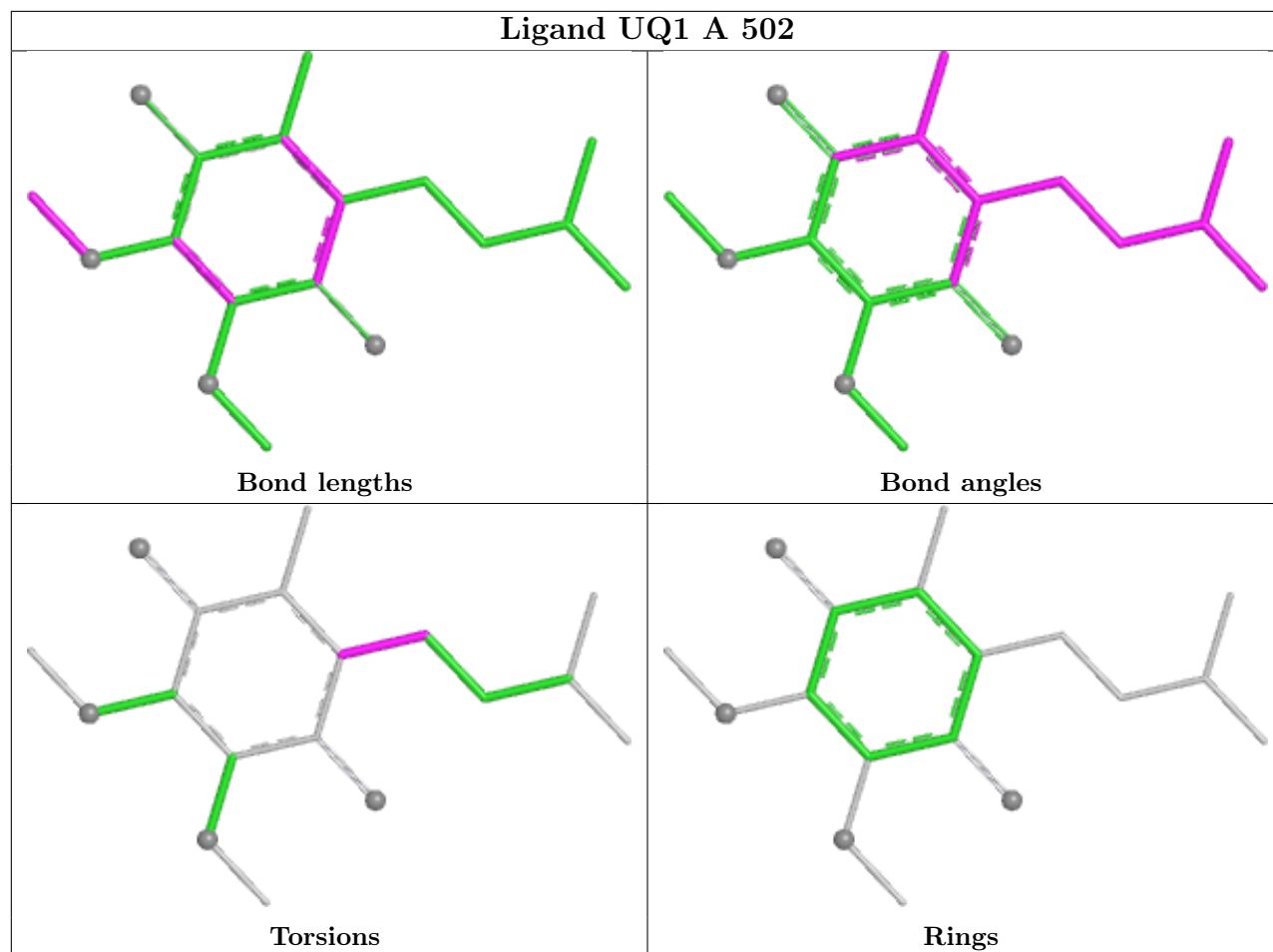
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	UQ1	2	0
2	A	501	FAD	1	0
2	B	501	FAD	2	0

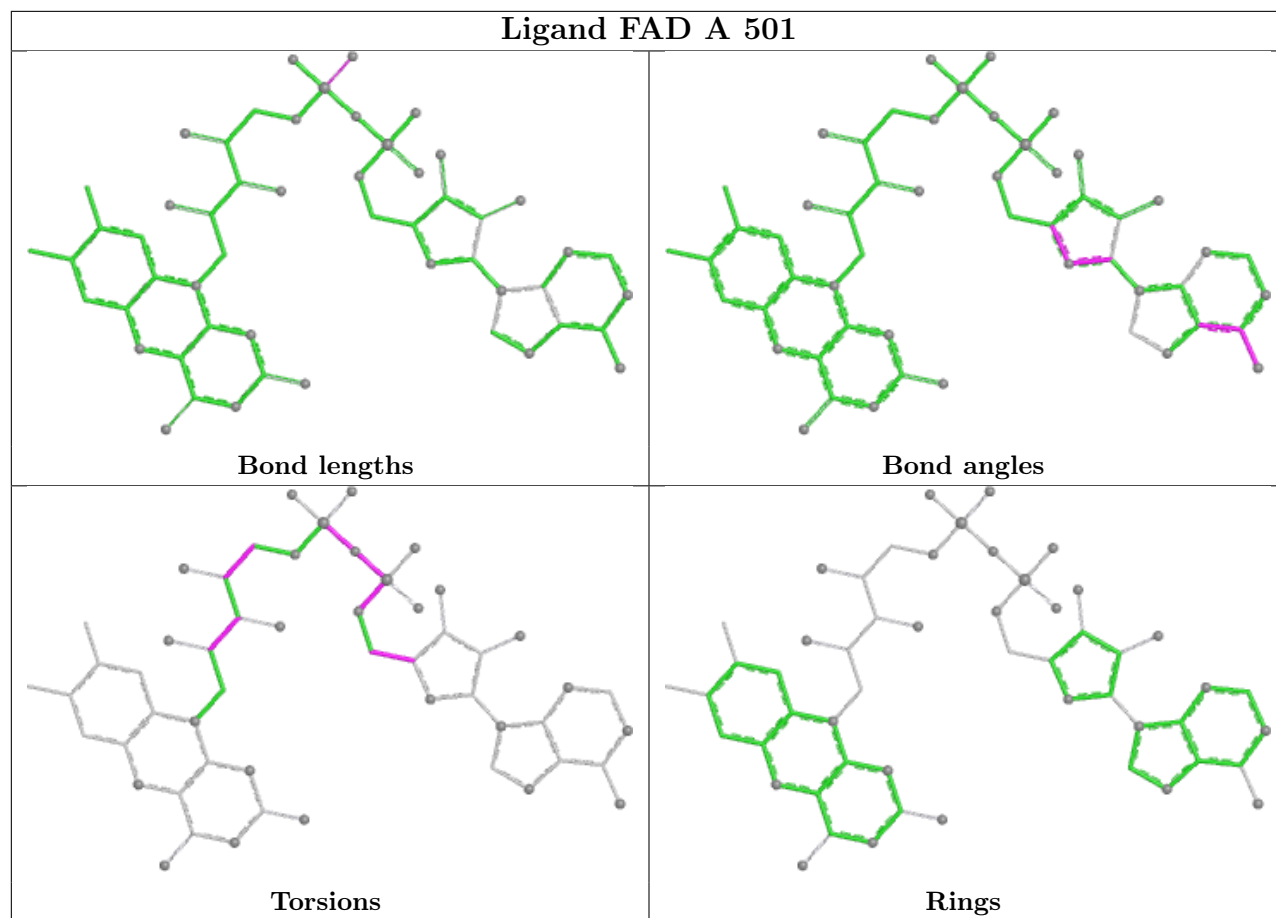
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand UQ1 A 502

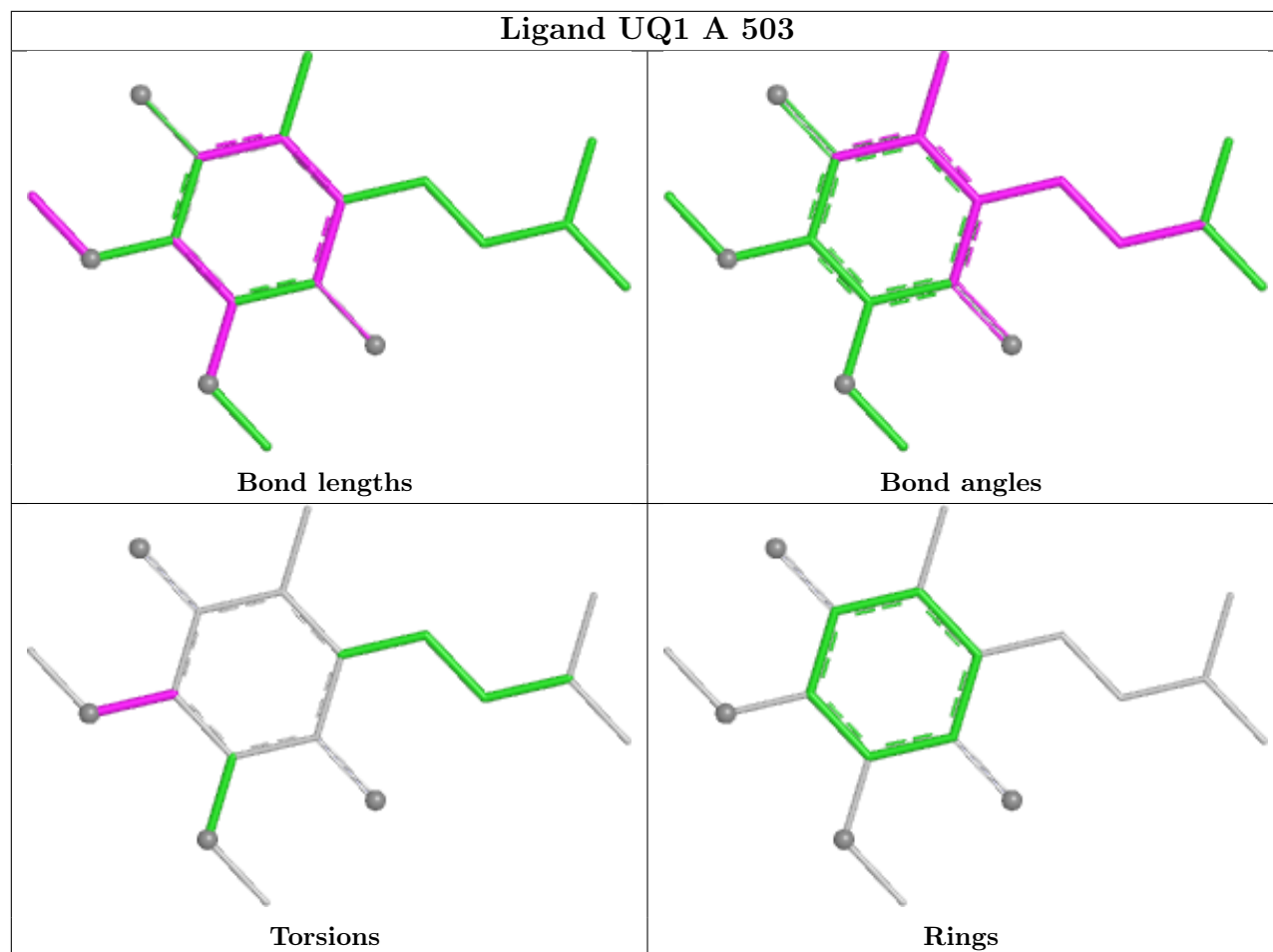


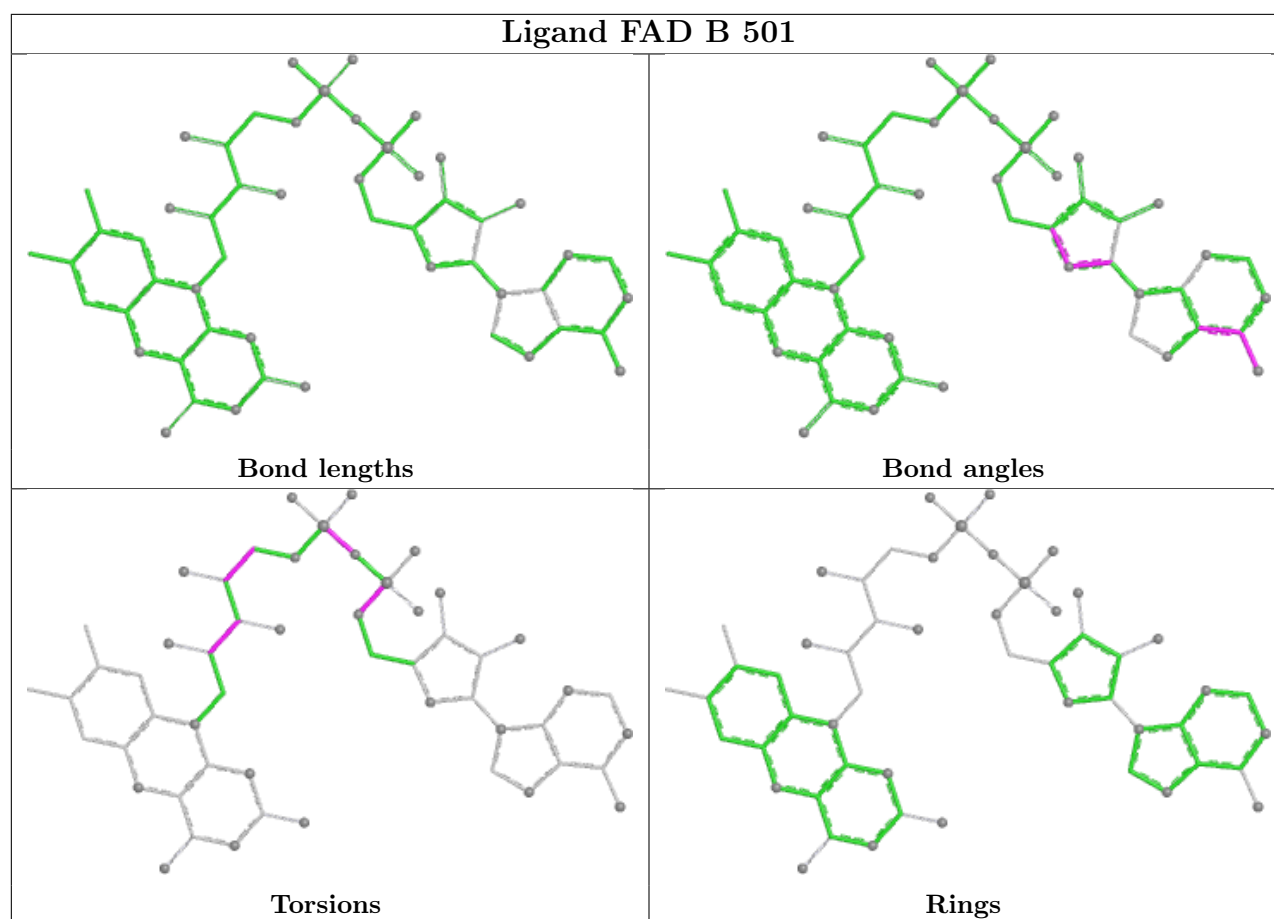


## Ligand FAD A 501



## Ligand UQ1 A 503





## 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<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	A	406/418 (97%)	0.42	16 (3%) 44 49	26, 43, 64, 83	0
1	B	403/418 (96%)	0.57	26 (6%) 26 30	28, 45, 70, 89	0
All	All	809/836 (96%)	0.49	42 (5%) 34 38	26, 44, 66, 89	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	PHE	7.8
1	B	436	GLY	6.3
1	B	439	ALA	5.5
1	A	447	LEU	5.4
1	B	441	LEU	4.6
1	B	437	GLY	3.4
1	B	224	LYS	3.3
1	A	269	ASP	3.3
1	B	186	LYS	3.2
1	B	400	LEU	3.2
1	B	404	PRO	3.1
1	A	105	SER	3.1
1	B	442	ARG	3.1
1	B	435	TRP	3.1
1	A	139	ARG	3.0
1	A	124	ASP	2.9
1	A	234	GLY	2.8
1	B	445	PHE	2.8
1	A	441	LEU	2.7
1	A	358	ARG	2.6
1	A	109	SER	2.6
1	B	444	LEU	2.5
1	B	199	VAL	2.5
1	B	125	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	187	GLU	2.5
1	A	446	HIS	2.4
1	B	223	SER	2.3
1	B	443	LYS	2.3
1	A	268	ALA	2.3
1	B	425	LEU	2.2
1	A	445	PHE	2.2
1	B	358	ARG	2.2
1	B	238	GLY	2.2
1	B	97	SER	2.2
1	A	182	LEU	2.2
1	A	379	CYS	2.2
1	B	218	LYS	2.2
1	B	220	GLY	2.1
1	A	434	TYR	2.1
1	B	248	GLU	2.0
1	A	343	SER	2.0
1	B	438	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSS	B	201	7/8	0.94	0.12	38,41,59,81	0
1	CSS	A	201	7/8	0.96	0.13	29,35,54,78	0

## 6.3 Carbohydrates [i](#)

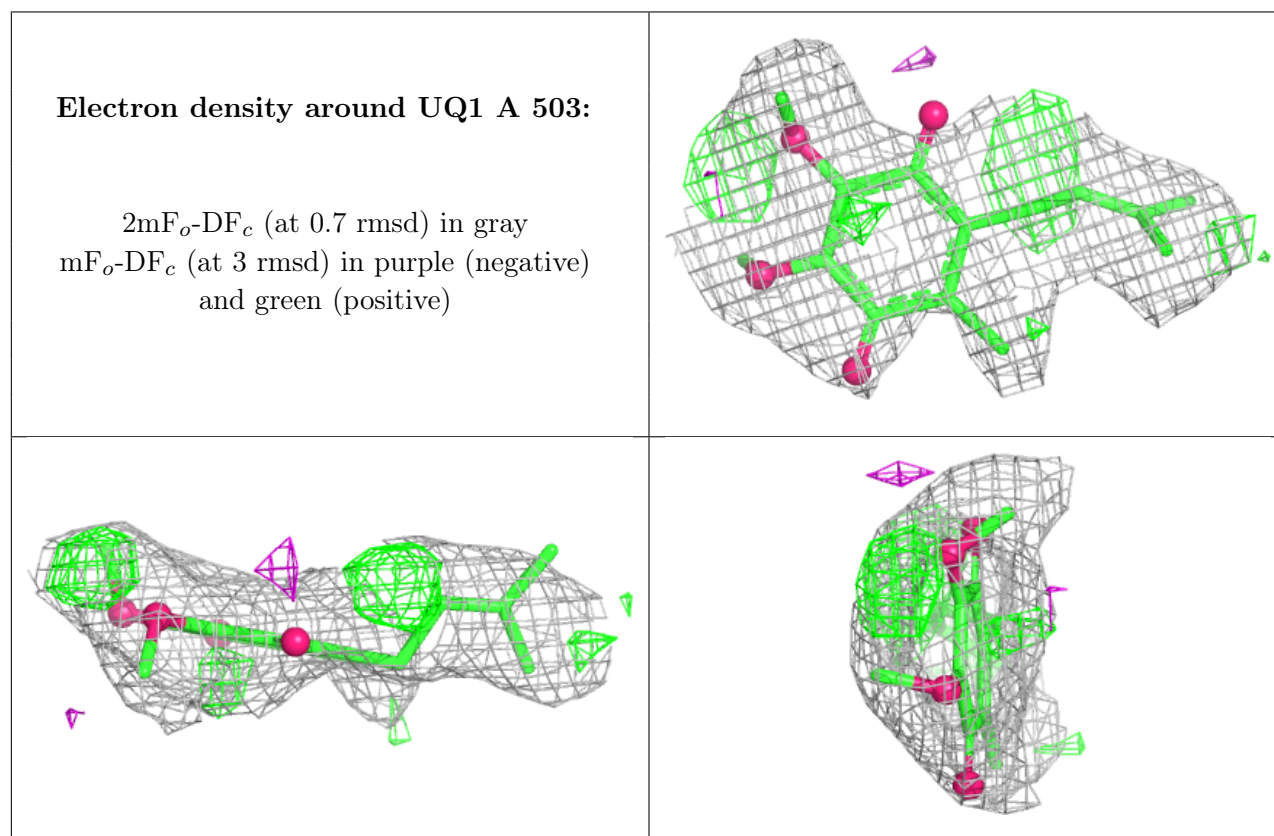
There are no monosaccharides in this entry.

## 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.

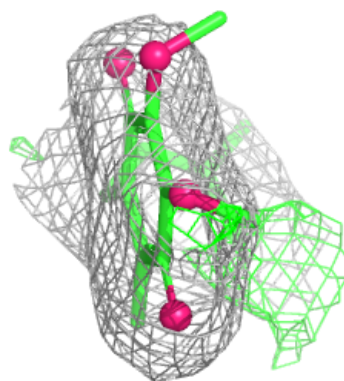
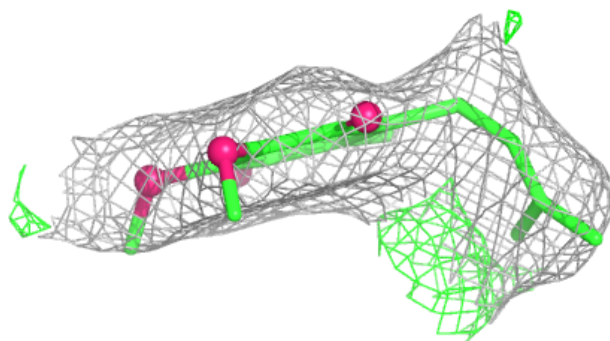
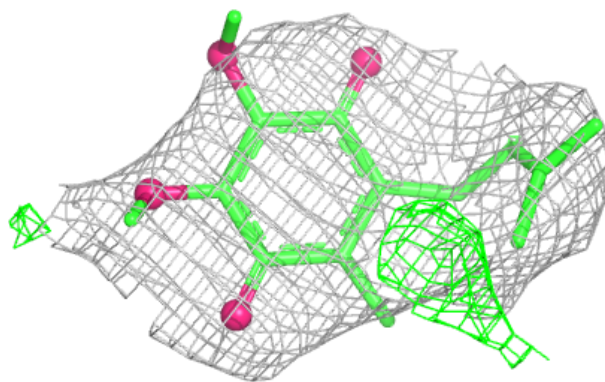
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UQ1	A	503	18/18	0.64	0.25	50,59,78,90	0
3	UQ1	A	502	18/18	0.77	0.21	50,70,81,84	0
2	FAD	B	501	53/53	0.95	0.09	24,40,49,51	0
2	FAD	A	501	53/53	0.96	0.09	19,35,40,45	0

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.

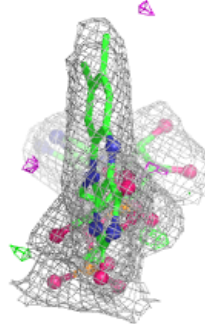
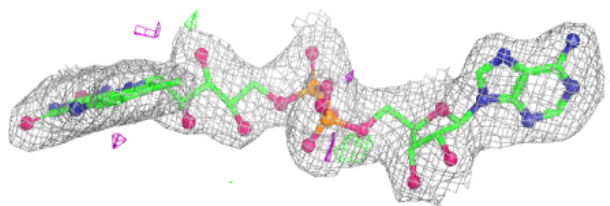
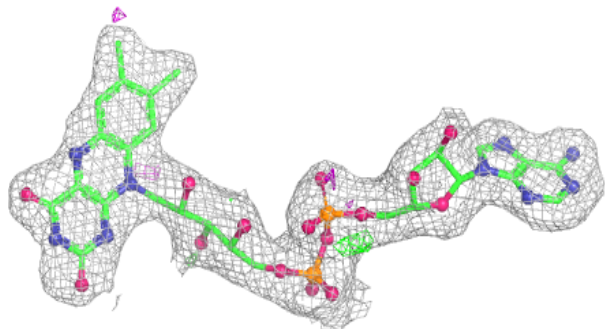


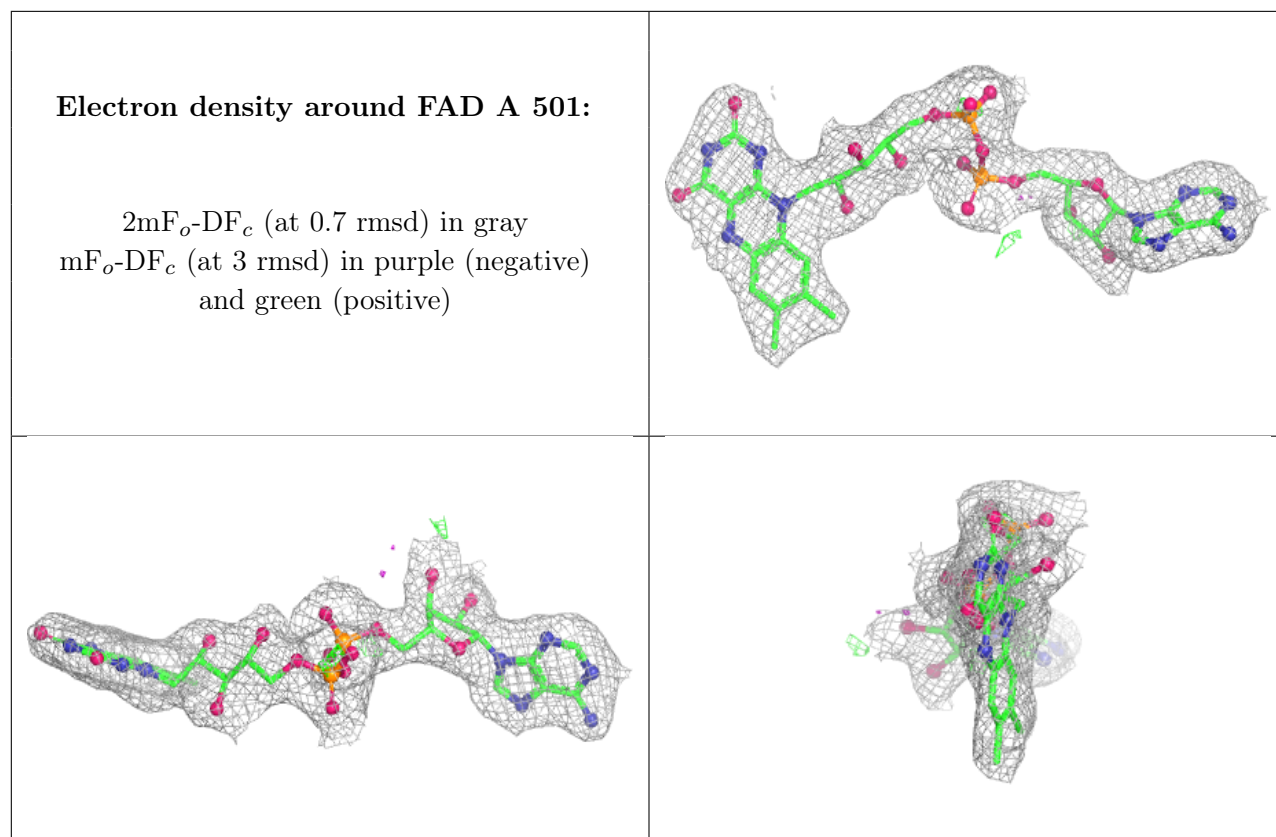
**Electron density around UQ1 A 502:**

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

**Electron density around FAD B 501:**

$2mF_o - DF_c$  (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.