



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:04 PM UTC

PDB ID : 6OIB / pdb_00006oib
Title : Crystal structure of human Sulfide Quinone Oxidoreductase in complex with coenzyme Q
Authors : Banerjee, R.; Cho, U.S.; Kim, H.; Moon, S.
Deposited on : 2019-04-09
Resolution : 2.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

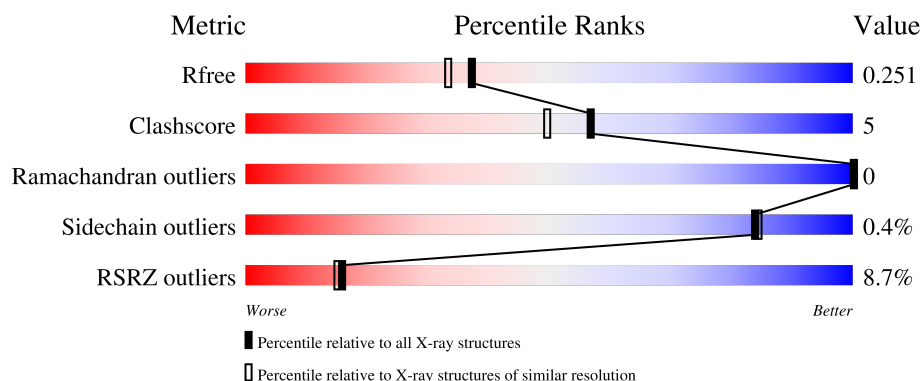
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 $\leq 5\%$. 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	8% 85% 13% .
1	B	418	9% 86% 11% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6770 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.

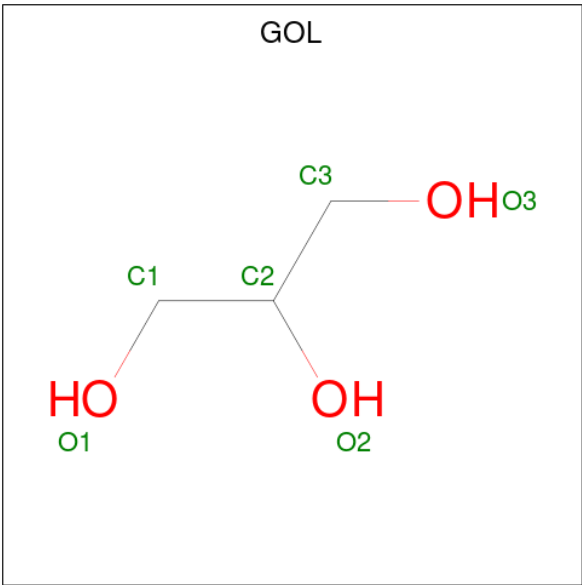
- Molecule 1 is a protein called Sulfide:quinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3209	2060	543	590	16			
1	B	406	Total	C	N	O	S	0	0	0
			3201	2054	542	589	16			

There are 18 discrepancies between the modelled and reference sequences:

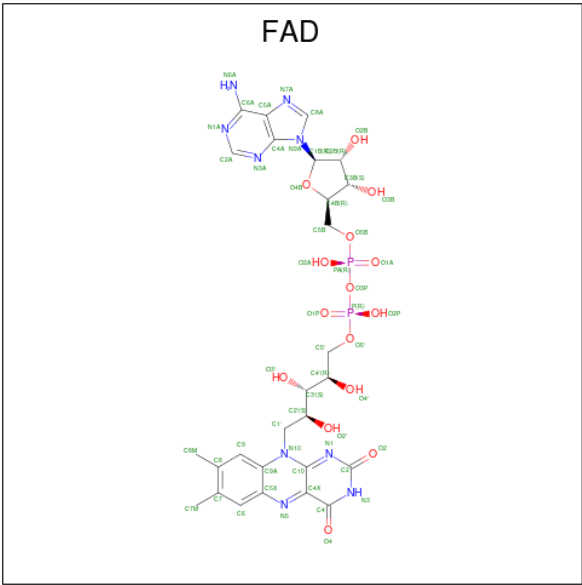
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP Q9Y6N5
A	451	LEU	-	expression tag	UNP Q9Y6N5
A	452	GLU	-	expression tag	UNP Q9Y6N5
A	453	HIS	-	expression tag	UNP Q9Y6N5
A	454	HIS	-	expression tag	UNP Q9Y6N5
A	455	HIS	-	expression tag	UNP Q9Y6N5
A	456	HIS	-	expression 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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



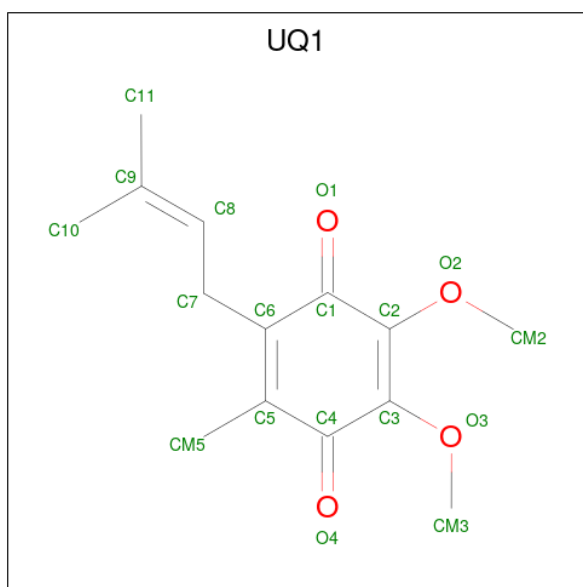
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



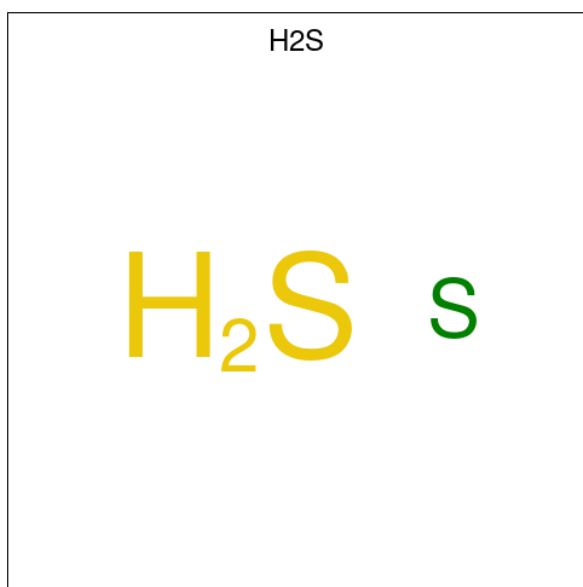
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



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

- Molecule 5 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	S	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 1 1	0	0
5	B	1	Total S 1 1	0	0
5	B	1	Total S 1 1	0	0

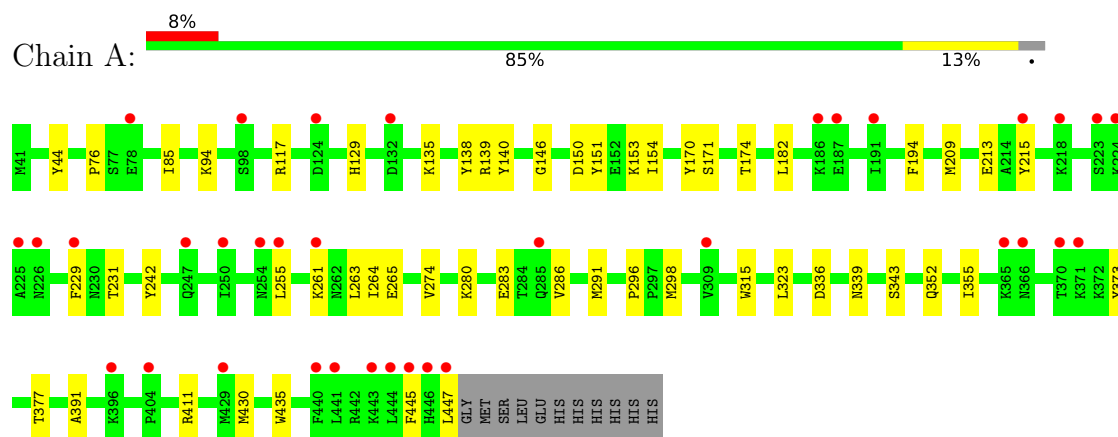
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	104	Total O 104 104	0	0
6	B	86	Total O 86 86	0	0

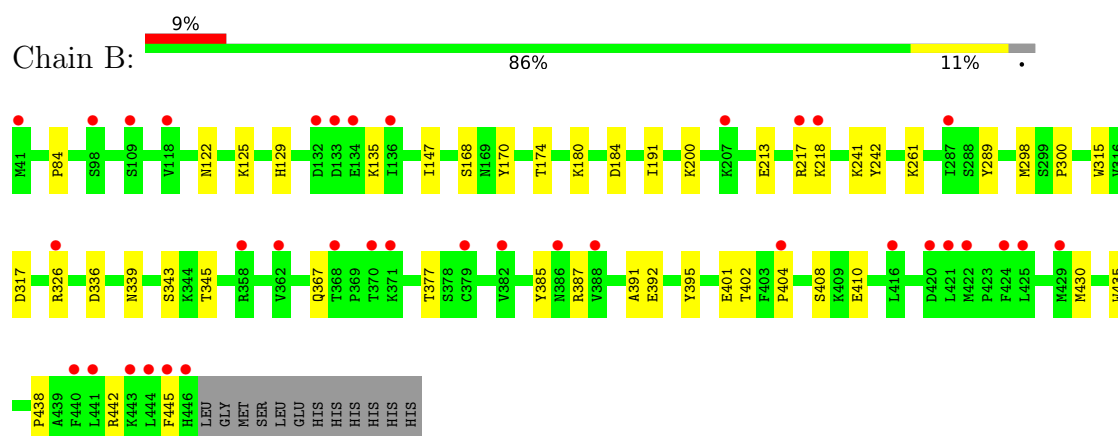
3 Residue-property plots [i](#)

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: 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, α , β , γ	78.52Å 111.51Å 133.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.37 – 2.03 41.37 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.2 (41.37-2.03) 86.7 (41.37-2.03)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.209 , 0.250 0.210 , 0.251	Depositor DCC
R_{free} test set	1987 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6770	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: H2S, UQ1, GOL, 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	0.34	0/3286	0.52	0/4451
1	B	0.33	0/3278	0.51	0/4440
All	All	0.34	0/6564	0.51	0/8891

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

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	3209	0	3230	30	0
1	B	3201	0	3219	29	0
2	A	6	0	8	1	0
3	A	53	0	31	0	0
3	B	53	0	31	3	0
4	A	36	0	36	4	0
4	B	18	0	18	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	104	0	0	1	0
6	B	86	0	0	3	0
All	All	6770	0	6573	60	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 5.

All (60) 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:274:VAL:HG22	1:A:286:VAL:HG22	1.69	0.74
1:A:264:ILE:HD12	1:B:326:ARG:HH12	1.53	0.74
1:B:129:HIS:NE2	1:B:135:LYS:HE2	2.14	0.62
4:A:504:UQ1:HM32	4:A:504:UQ1:HM23	1.82	0.60
1:B:392:GLU:OE1	1:B:402:THR:N	2.31	0.57
1:B:191:ILE:HD12	1:B:289:TYR:HB3	1.86	0.56
4:B:501:UQ1:HM23	4:B:501:UQ1:HM32	1.87	0.56
1:B:392:GLU:OE1	1:B:401:GLU:HA	2.06	0.56
1:A:343:SER:HB2	1:A:377:THR:HG21	1.89	0.54
1:A:411:ARG:HG2	2:A:501:GOL:H31	1.88	0.53
1:B:345:THR:HB	3:B:502:FAD:O2	2.08	0.52
1:A:430:MET:SD	4:A:504:UQ1:HM21	2.50	0.52
1:B:122:ASN:HD21	1:B:125:LYS:HG3	1.75	0.51
1:B:180:LYS:HE3	1:B:184:ASP:OD2	2.10	0.51
1:A:170:TYR:CE2	1:A:298:MET:HE1	2.47	0.50
1:B:180:LYS:NZ	6:B:602:HOH:O	2.44	0.49
1:A:44:TYR:O	1:A:138:TYR:HA	2.12	0.49
1:B:387:ARG:HB3	1:B:410:GLU:HB3	1.95	0.49
1:A:129:HIS:CD2	1:A:135:LYS:HG2	2.47	0.48
1:B:170:TYR:CE2	1:B:298:MET:HE1	2.48	0.48
1:A:150:ASP:HB3	1:A:153:LYS:HG2	1.94	0.48
1:A:76:PRO:HG3	1:A:117:ARG:HG2	1.97	0.47
1:A:146:GLY:HA2	1:A:336:ASP:HB2	1.97	0.47
1:A:154:ILE:HD13	1:A:263:LEU:HD23	1.97	0.47
1:B:438:PRO:HG3	4:B:501:UQ1:H112	1.96	0.47
1:B:343:SER:HB2	1:B:377:THR:HG21	1.97	0.47
1:B:404:PRO:HD3	1:B:445:PHE:HB3	1.95	0.47
1:B:84:PRO:HA	3:B:502:FAD:C5X	2.45	0.46
1:A:280:LYS:HD2	1:A:283:GLU:OE1	2.15	0.46
1:A:85:ILE:HD11	1:A:94:LYS:HG3	1.97	0.46
1:A:265:GLU:HB3	1:A:274:VAL:HB	1.97	0.46
1:A:445:PHE:O	1:A:447:LEU:N	2.49	0.45
1:A:315:TRP:HB2	1:A:339:ASN:HB3	1.97	0.45
1:B:147:ILE:HB	1:B:336:ASP:HB3	1.98	0.45
1:B:442:ARG:NH2	6:B:606:HOH:O	2.50	0.45
1:B:218:LYS:NZ	1:B:385:TYR:HB2	2.32	0.44
1:A:213:GLU:HG3	1:A:255:LEU:HD21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:HG13	1:A:373:TYR:HB2	1.99	0.44
1:B:317:ASP:O	1:B:326:ARG:HG2	2.18	0.44
1:A:151:TYR:CD1	1:A:296:PRO:HB3	2.53	0.43
1:B:213:GLU:OE2	1:B:217:ARG:HD2	2.18	0.43
1:B:200:LYS:HE3	3:B:502:FAD:HM81	2.00	0.43
1:A:261:LYS:HE2	6:A:611:HOH:O	2.17	0.43
1:B:367:GLN:NE2	6:B:604:HOH:O	2.46	0.42
1:A:194:PHE:HB3	1:A:231:THR:HA	2.01	0.42
1:A:139:ARG:HG3	1:A:140:TYR:CE2	2.55	0.42
1:A:242:TYR:CZ	1:A:391:ALA:HA	2.55	0.42
1:B:242:TYR:CZ	1:B:391:ALA:HA	2.55	0.42
4:A:503:UQ1:O4	4:A:503:UQ1:HM32	2.20	0.41
1:A:323:LEU:HD21	1:A:352:GLN:HB3	2.01	0.41
1:A:435:TRP:NE1	4:A:504:UQ1:O1	2.45	0.41
1:A:171:SER:HB3	1:A:174:THR:OG1	2.20	0.41
1:B:168:SER:HB3	1:B:174:THR:OG1	2.20	0.41
1:B:430:MET:HA	1:B:435:TRP:HB3	2.02	0.41
1:A:182:LEU:HG	1:A:215:TYR:CD2	2.56	0.41
1:A:209:MET:SD	1:A:229:PHE:HB2	2.61	0.40
1:B:315:TRP:HB2	1:B:339:ASN:HB3	2.03	0.40
1:A:264:ILE:HD12	1:B:326:ARG:NH1	2.31	0.40
1:B:241:LYS:HE2	1:B:408:SER:HB3	2.03	0.40
1:B:300:PRO:HG3	1:B:315:TRP:CD2	2.57	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	405/418 (97%)	390 (96%)	15 (4%)	0	100	100
1	B	404/418 (97%)	393 (97%)	11 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	809/836 (97%)	783 (97%)	26 (3%)	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	A	345/355 (97%)	344 (100%)	1 (0%)	86	86
1	B	344/355 (97%)	342 (99%)	2 (1%)	78	79
All	All	689/710 (97%)	686 (100%)	3 (0%)	84	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	MET
1	B	261	LYS
1	B	395	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	183	GLN
1	A	247	GLN
1	B	122	ASN
1	B	183	GLN
1	B	247	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are modelled with single atom - leaving 6 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
4	UQ1	B	501	-	18,18,18	3.08	5 (27%)	24,25,25	1.33	4 (16%)
2	GOL	A	501	-	5,5,5	0.81	0	5,5,5	1.05	0
3	FAD	B	502	-	58,58,58	0.33	0	85,89,89	0.39	0
4	UQ1	A	503	-	18,18,18	3.17	8 (44%)	24,25,25	2.11	7 (29%)
3	FAD	A	502	-	58,58,58	0.38	0	85,89,89	0.49	0
4	UQ1	A	504	-	18,18,18	3.02	5 (27%)	24,25,25	1.26	4 (16%)

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
4	UQ1	B	501	-	-	2/9/33/33	0/1/1/1
2	GOL	A	501	-	-	1/4/4/4	-
3	FAD	B	502	-	-	0/34/50/50	0/6/6/6
4	UQ1	A	503	-	-	0/9/33/33	0/1/1/1
3	FAD	A	502	-	-	1/34/50/50	0/6/6/6
4	UQ1	A	504	-	-	0/9/33/33	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	UQ1	C6-C5	10.42	1.53	1.35
4	B	501	UQ1	C6-C5	10.35	1.53	1.35
4	A	504	UQ1	C6-C5	10.09	1.53	1.35
4	B	501	UQ1	C3-C2	4.86	1.53	1.36
4	A	504	UQ1	C3-C2	4.56	1.52	1.36
4	A	503	UQ1	C3-C2	4.24	1.51	1.36
4	A	503	UQ1	C5-C4	3.09	1.57	1.47
4	A	503	UQ1	C6-C1	2.68	1.54	1.46
4	A	504	UQ1	C6-C1	2.50	1.53	1.46
4	B	501	UQ1	C6-C1	2.46	1.53	1.46
4	B	501	UQ1	O3-CM3	-2.35	1.40	1.45
4	A	503	UQ1	C7-C8	2.32	1.54	1.50
4	A	503	UQ1	O2-CM2	-2.30	1.40	1.45
4	A	503	UQ1	CM5-C5	2.23	1.55	1.50
4	A	504	UQ1	O3-CM3	-2.15	1.40	1.45
4	B	501	UQ1	O2-CM2	-2.12	1.40	1.45
4	A	503	UQ1	O3-CM3	-2.12	1.40	1.45
4	A	504	UQ1	O1-C1	-2.01	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	UQ1	CM5-C5-C6	-6.46	113.82	124.45
4	A	503	UQ1	C7-C8-C9	-3.70	116.78	127.25
4	B	501	UQ1	C7-C6-C5	-3.28	119.26	124.89
4	A	503	UQ1	CM5-C5-C4	3.04	127.33	116.93
4	A	503	UQ1	O4-C4-C3	-3.01	114.65	121.03
4	A	504	UQ1	C7-C6-C5	-2.85	120.00	124.89
4	B	501	UQ1	C7-C8-C9	-2.71	119.58	127.25
4	B	501	UQ1	CM5-C5-C6	-2.70	120.02	124.45
4	A	504	UQ1	C7-C8-C9	-2.59	119.94	127.25
4	A	504	UQ1	CM5-C5-C6	-2.57	120.22	124.45
4	A	503	UQ1	C7-C6-C5	-2.50	120.60	124.89
4	B	501	UQ1	C11-C9-C10	2.24	119.74	114.59
4	A	503	UQ1	C11-C9-C10	2.17	119.59	114.59
4	A	504	UQ1	C11-C9-C10	2.17	119.58	114.59
4	A	503	UQ1	O2-C2-C1	2.10	123.71	116.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O2-C2-C3-O3
4	B	501	UQ1	C4-C3-O3-CM3
3	A	502	FAD	O4B-C4B-C5B-O5B
4	B	501	UQ1	C2-C3-O3-CM3

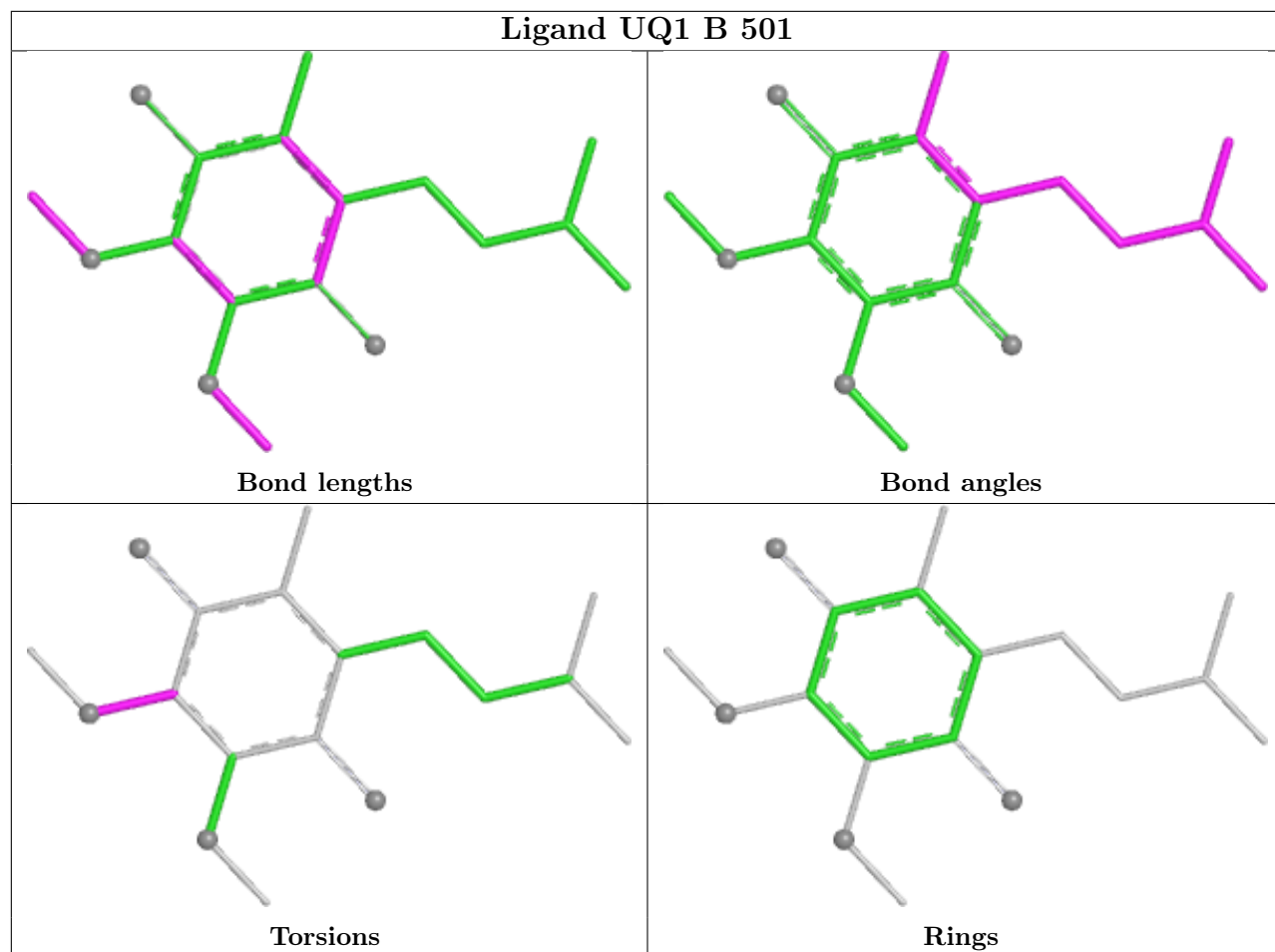
There are no ring outliers.

5 monomers are involved in 10 short contacts:

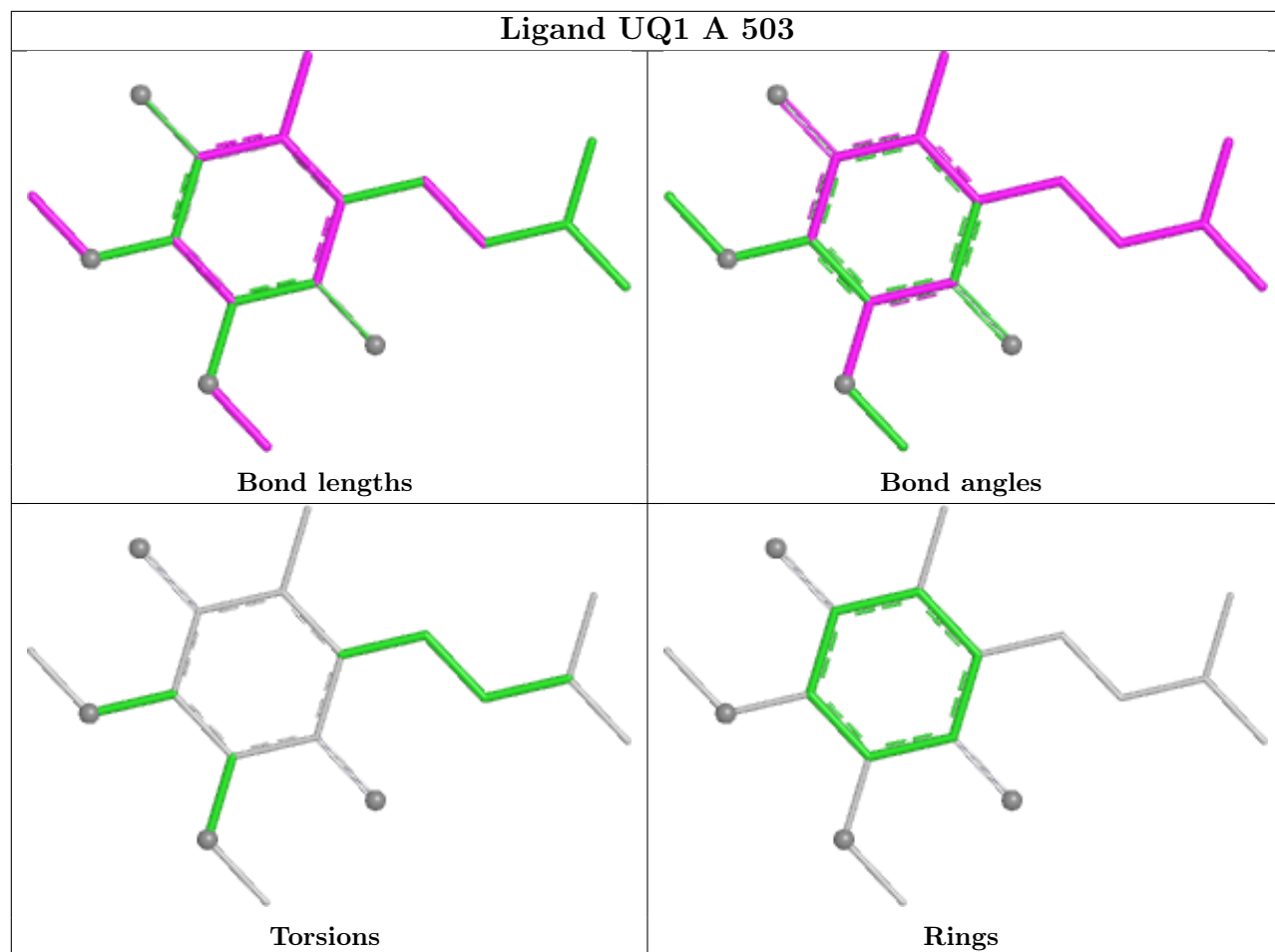
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	UQ1	2	0
2	A	501	GOL	1	0
3	B	502	FAD	3	0
4	A	503	UQ1	1	0
4	A	504	UQ1	3	0

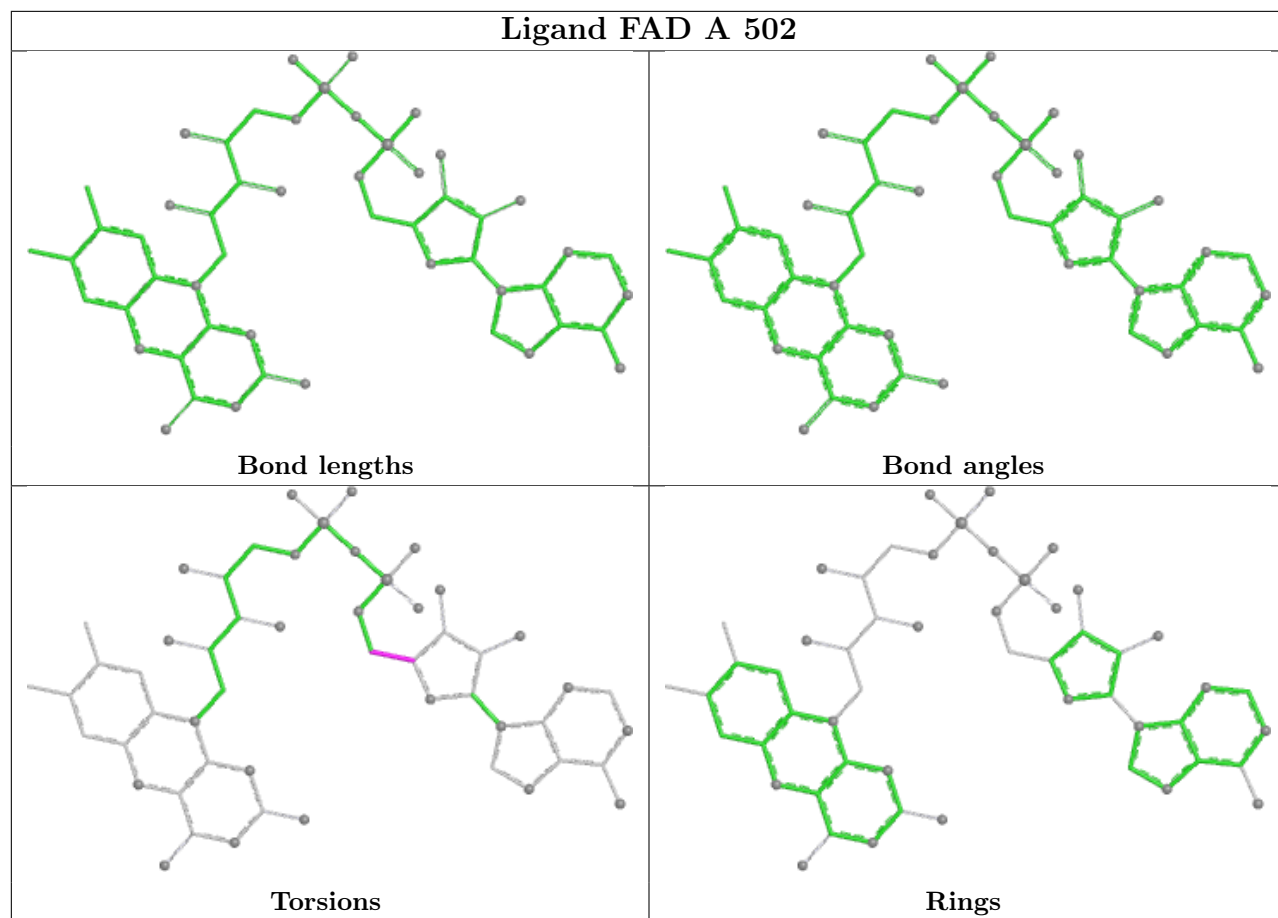
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

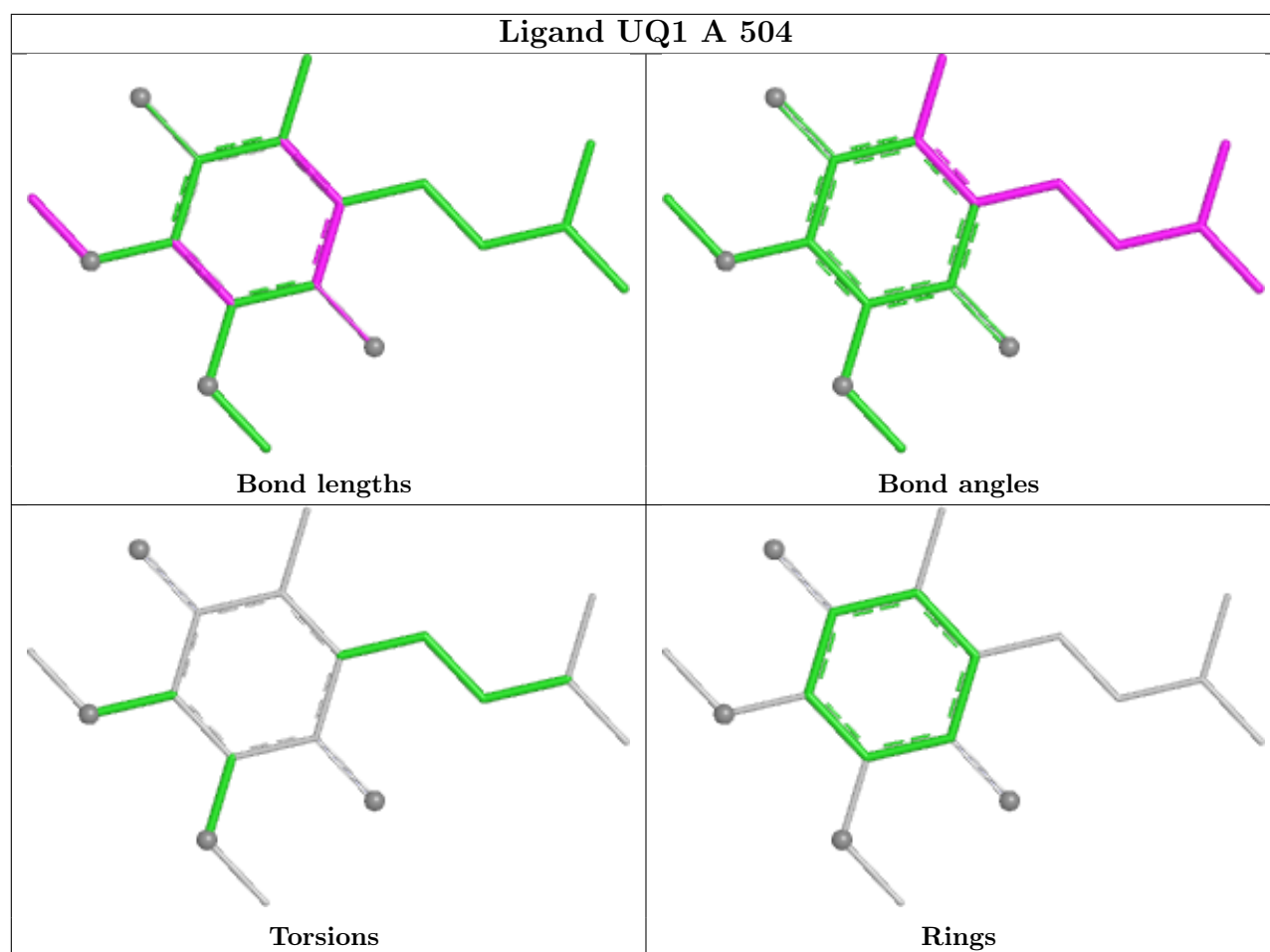
Ligand UQ1 B 501



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, 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	407/418 (97%)	0.87	35 (8%) 16 15	20, 34, 56, 80	0
1	B	406/418 (97%)	0.91	36 (8%) 15 14	22, 35, 56, 71	0
All	All	813/836 (97%)	0.89	71 (8%) 16 15	20, 35, 56, 80	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	GLU	5.2
1	A	447	LEU	4.9
1	B	445	PHE	4.8
1	B	41	MET	4.1
1	A	261	LYS	3.8
1	B	382	VAL	3.8
1	B	133	ASP	3.7
1	A	224	LYS	3.5
1	B	444	LEU	3.5
1	B	441	LEU	3.5
1	A	223	SER	3.5
1	A	370	THR	3.5
1	A	446	HIS	3.4
1	A	440	PHE	3.4
1	A	445	PHE	3.4
1	B	440	PHE	3.4
1	B	443	LYS	3.3
1	A	255	LEU	3.2
1	A	225	ALA	3.2
1	A	250	ILE	3.1
1	B	358	ARG	3.0
1	A	309	VAL	3.0
1	A	124	ASP	3.0
1	A	285	GLN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	218	LYS	2.9
1	A	98	SER	2.9
1	B	425	LEU	2.8
1	B	132	ASP	2.8
1	B	422	MET	2.8
1	B	429	MET	2.8
1	B	446	HIS	2.8
1	A	396	LYS	2.7
1	A	444	LEU	2.7
1	B	388	VAL	2.7
1	B	370	THR	2.6
1	B	362	VAL	2.6
1	A	366	ASN	2.6
1	A	229	PHE	2.6
1	B	136	ILE	2.6
1	A	371	LYS	2.5
1	A	226	ASN	2.5
1	B	420	ASP	2.5
1	B	109	SER	2.5
1	B	424	PHE	2.5
1	B	287	ILE	2.5
1	B	98	SER	2.4
1	B	371	LYS	2.4
1	B	207	LYS	2.4
1	B	217	ARG	2.4
1	A	365	LYS	2.4
1	B	404	PRO	2.4
1	A	247	GLN	2.3
1	B	368	THR	2.3
1	A	254	ASN	2.3
1	A	441	LEU	2.3
1	A	187	GLU	2.2
1	B	118	VAL	2.2
1	A	186	LYS	2.2
1	B	416	LEU	2.2
1	A	443	LYS	2.2
1	B	386	ASN	2.2
1	A	78	GLU	2.2
1	A	218	LYS	2.1
1	A	132	ASP	2.1
1	B	326	ARG	2.1
1	A	215	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	429	MET	2.0
1	B	421	LEU	2.0
1	B	379	CYS	2.0
1	A	404	PRO	2.0
1	A	191	ILE	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

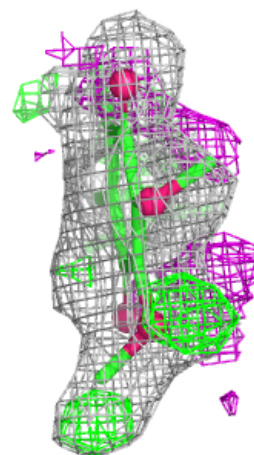
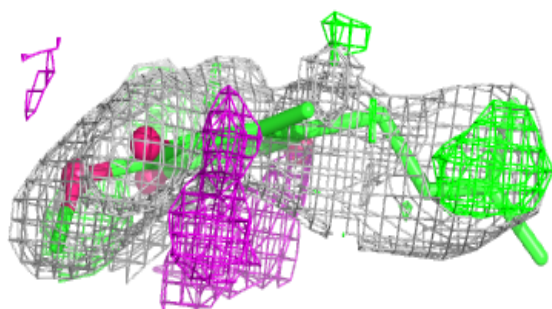
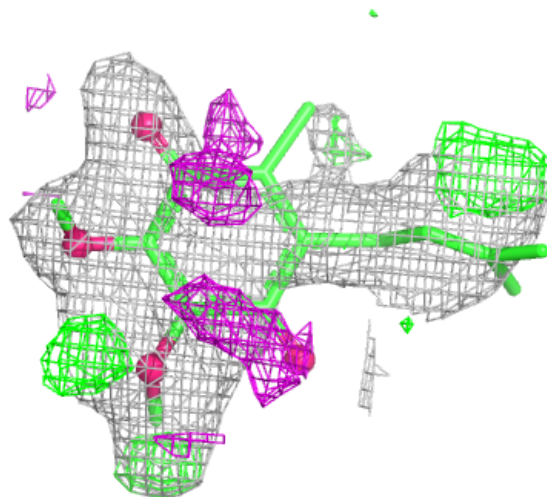
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	UQ1	A	503	18/18	0.71	0.35	48,61,75,88	0
2	GOL	A	501	6/6	0.78	0.17	45,50,54,56	0
5	H2S	A	506	1/1	0.82	0.16	70,70,70,70	0
5	H2S	B	504	1/1	0.85	0.20	57,57,57,57	0
4	UQ1	B	501	18/18	0.86	0.17	41,57,60,60	0
4	UQ1	A	504	18/18	0.87	0.18	50,52,63,66	0
3	FAD	B	502	53/53	0.95	0.10	20,28,37,41	0
5	H2S	B	503	1/1	0.95	0.14	40,40,40,40	0
3	FAD	A	502	53/53	0.95	0.08	17,24,30,32	0
5	H2S	A	505	1/1	0.97	0.05	34,34,34,34	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.

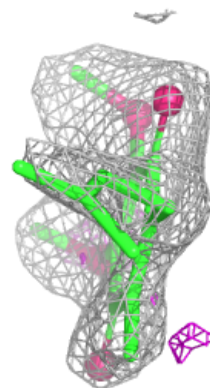
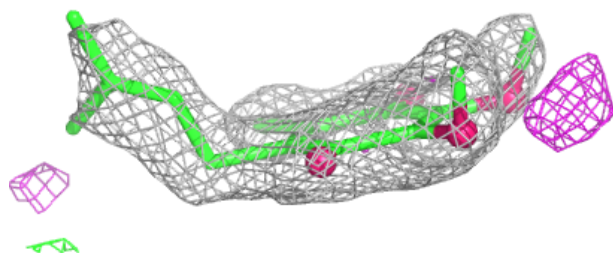
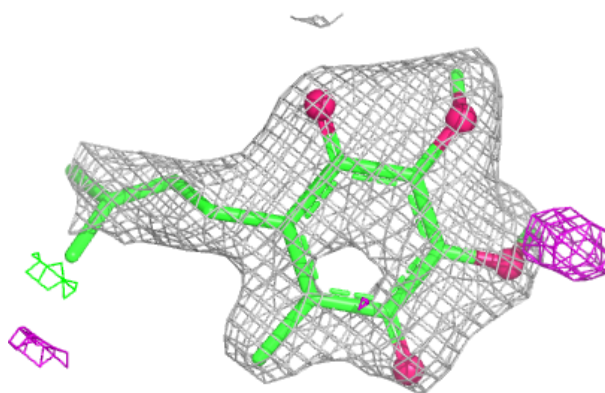
Electron density around UQ1 A 503:

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

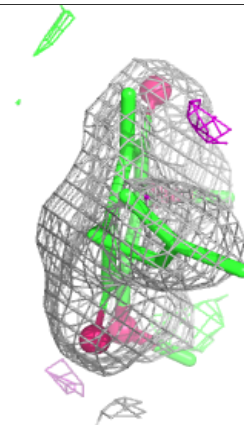
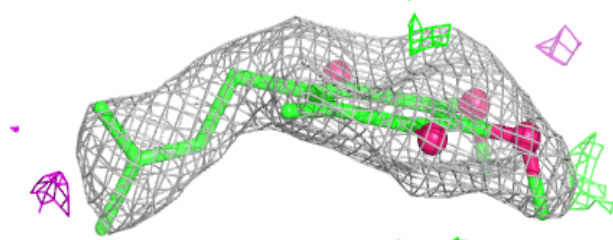
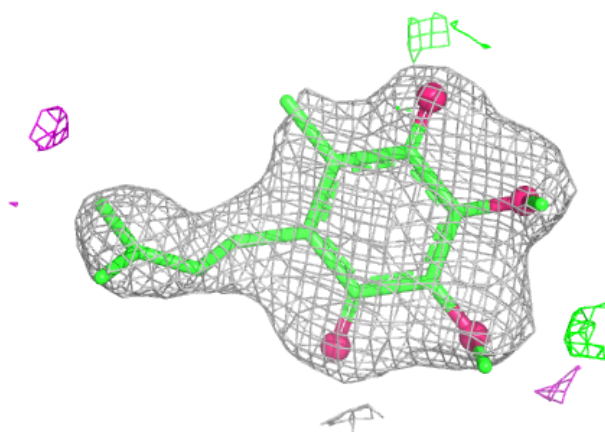


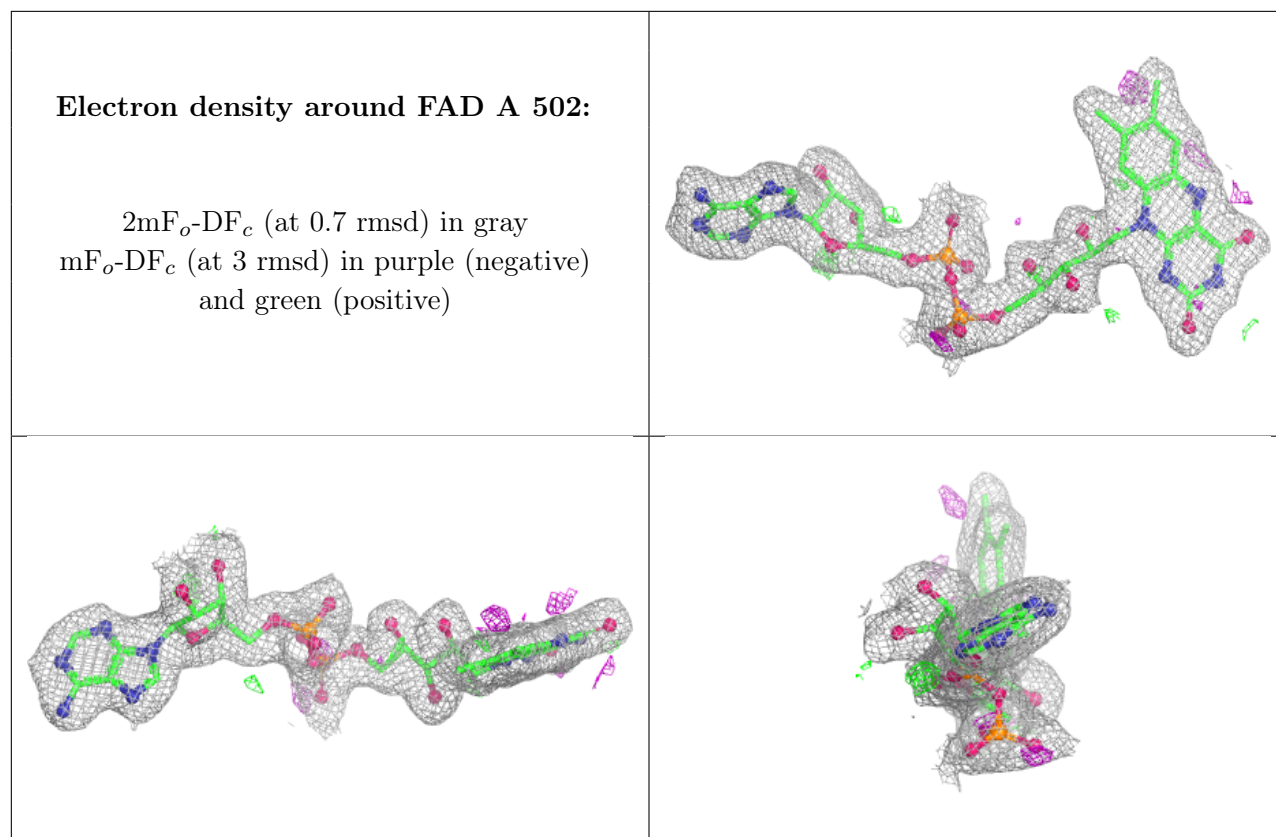
Electron density around UQ1 B 501:

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

**Electron density around UQ1 A 504:**

$2mF_o-DF_c$ (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.