



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2022 – 04:07 PM EDT

PDB ID : 7UJO  
Title : Estrogen Receptor Alpha Ligand Binding Domain in Complex with RU39411  
Authors : Hosfield, D.J.; Greene, G.L.; Fanning, S.W.  
Deposited on : 2022-03-31  
Resolution : 1.45 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
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) : 2.28.1



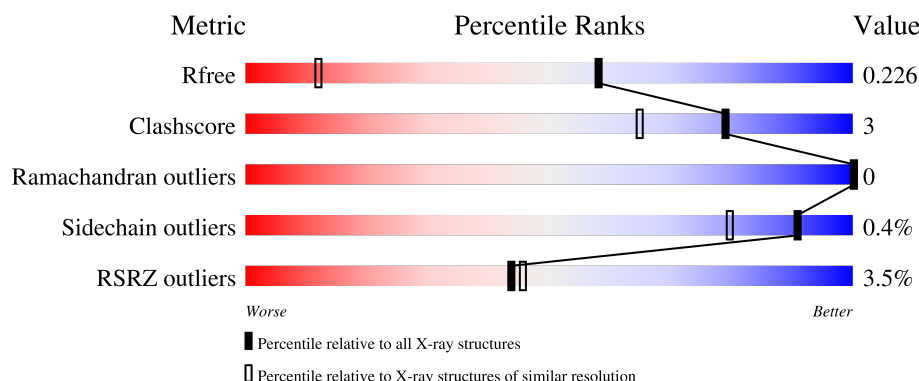
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	263	<div> <div>3%</div> <div>81% 6% 12%</div> </div>
1	B	263	<div> <div>3%</div> <div>84% 5% 11%</div> </div>
1	C	263	<div> <div>5%</div> <div>80% 8% 11%</div> </div>
1	D	263	<div> <div>2%</div> <div>86% 5% 9%</div> </div>



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8178 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	234	Total	C	N	O	S	0	3	0
			1853	1193	312	332	16			
1	D	240	Total	C	N	O	S	0	3	0
			1905	1220	323	346	16			
1	C	233	Total	C	N	O	S	0	3	0
			1860	1194	311	338	17			
1	A	231	Total	C	N	O	S	0	3	0
			1839	1181	310	332	16			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	292	HIS	-	expression tag	UNP P03372
B	293	HIS	-	expression tag	UNP P03372
B	294	HIS	-	expression tag	UNP P03372
B	295	HIS	-	expression tag	UNP P03372
B	296	HIS	-	expression tag	UNP P03372
B	297	HIS	-	expression tag	UNP P03372
B	298	GLU	-	expression tag	UNP P03372
B	299	ASN	-	expression tag	UNP P03372
B	300	LEU	-	expression tag	UNP P03372
B	301	TYR	-	expression tag	UNP P03372
B	302	GLN	-	expression tag	UNP P03372
B	303	PHE	-	expression tag	UNP P03372
B	304	SER	-	expression tag	UNP P03372
B	305	MET	-	expression tag	UNP P03372
B	381	SER	CYS	conflict	UNP P03372
B	417	SER	CYS	conflict	UNP P03372
B	530	SER	CYS	conflict	UNP P03372
B	536	SER	LEU	conflict	UNP P03372
D	292	HIS	-	expression tag	UNP P03372
D	293	HIS	-	expression tag	UNP P03372
D	294	HIS	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
D	295	HIS	-	expression tag	UNP P03372
D	296	HIS	-	expression tag	UNP P03372
D	297	HIS	-	expression tag	UNP P03372
D	298	GLU	-	expression tag	UNP P03372
D	299	ASN	-	expression tag	UNP P03372
D	300	LEU	-	expression tag	UNP P03372
D	301	TYR	-	expression tag	UNP P03372
D	302	GLN	-	expression tag	UNP P03372
D	303	PHE	-	expression tag	UNP P03372
D	304	SER	-	expression tag	UNP P03372
D	305	MET	-	expression tag	UNP P03372
D	381	SER	CYS	conflict	UNP P03372
D	417	SER	CYS	conflict	UNP P03372
D	530	SER	CYS	conflict	UNP P03372
D	536	SER	LEU	conflict	UNP P03372
C	292	HIS	-	expression tag	UNP P03372
C	293	HIS	-	expression tag	UNP P03372
C	294	HIS	-	expression tag	UNP P03372
C	295	HIS	-	expression tag	UNP P03372
C	296	HIS	-	expression tag	UNP P03372
C	297	HIS	-	expression tag	UNP P03372
C	298	GLU	-	expression tag	UNP P03372
C	299	ASN	-	expression tag	UNP P03372
C	300	LEU	-	expression tag	UNP P03372
C	301	TYR	-	expression tag	UNP P03372
C	302	GLN	-	expression tag	UNP P03372
C	303	PHE	-	expression tag	UNP P03372
C	304	SER	-	expression tag	UNP P03372
C	305	MET	-	expression tag	UNP P03372
C	381	SER	CYS	conflict	UNP P03372
C	417	SER	CYS	conflict	UNP P03372
C	530	SER	CYS	conflict	UNP P03372
C	536	SER	LEU	conflict	UNP P03372
A	292	HIS	-	expression tag	UNP P03372
A	293	HIS	-	expression tag	UNP P03372
A	294	HIS	-	expression tag	UNP P03372
A	295	HIS	-	expression tag	UNP P03372
A	296	HIS	-	expression tag	UNP P03372
A	297	HIS	-	expression tag	UNP P03372
A	298	GLU	-	expression tag	UNP P03372
A	299	ASN	-	expression tag	UNP P03372
A	300	LEU	-	expression tag	UNP P03372

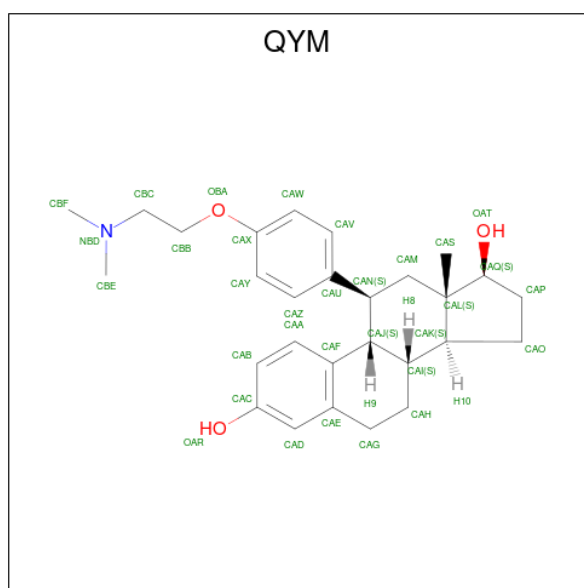
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Chain	Residue	Modelled	Actual	Comment	Reference
A	301	TYR	-	expression tag	UNP P03372
A	302	GLN	-	expression tag	UNP P03372
A	303	PHE	-	expression tag	UNP P03372
A	304	SER	-	expression tag	UNP P03372
A	305	MET	-	expression tag	UNP P03372
A	381	SER	CYS	conflict	UNP P03372
A	417	SER	CYS	conflict	UNP P03372
A	530	SER	CYS	conflict	UNP P03372
A	536	SER	LEU	conflict	UNP P03372

- Molecule 2 is (9beta,11beta,17beta)-11-{4-[2-(dimethylamino)ethoxy]phenyl}estra-1,3,5(10)-triene-3,17-diol (three-letter code: QYM) (formula: C<sub>28</sub>H<sub>37</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			32	28	1	3		
2	D	1	Total	C	N	O	0	0
			32	28	1	3		
2	C	1	Total	C	N	O	0	0
			32	28	1	3		
2	A	1	Total	C	N	O	0	0
			32	28	1	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	148	Total 148	O 148	0	0
4	D	151	Total 151	O 151	0	0
4	C	138	Total 138	O 138	0	0
4	A	155	Total 155	O 155	0	0



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- Molecule 1: Estrogen receptor





L509	N519	H524	K529	S530	K531	ASN	V533	L539	M543	A546	HIS	ARG	LEU	HIS	ALA	PRO	THR	SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.23Å 58.23Å 275.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.45 49.61 – 1.45	Depositor EDS
% Data completeness (in resolution range)	77.7 (50.00-1.45) 77.7 (49.61-1.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.82	Depositor
R, $R_{free}$	0.206 , 0.228 0.208 , 0.226	Depositor DCC
$R_{free}$ test set	7100 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.469 for -h,-k,l 0.477 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: QYM, MG

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	0.67	0/1880	0.61	0/2537
1	B	0.26	0/1897	0.44	0/2567
1	C	0.25	0/1900	0.44	0/2568
1	D	0.25	0/1946	0.43	0/2631
All	All	0.40	0/7623	0.49	0/10303

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	1839	0	1880	12	0
1	B	1853	0	1890	8	0
1	C	1860	0	1895	16	0
1	D	1905	0	1940	8	0
2	A	32	0	0	0	0
2	B	32	0	0	1	0
2	C	32	0	0	1	0
2	D	32	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	155	0	0	2	0
4	B	148	0	0	1	0
4	C	138	0	0	2	0
4	D	151	0	0	0	0
All	All	8178	0	7605	42	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 3.

All (42) 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:D:321:ASP:OD2	1:D:363:ARG:NH2	2.31	0.63
1:A:436:ARG:NH1	4:A:702:HOH:O	2.32	0.62
1:C:419:GLU:HG3	1:C:524:HIS:CE1	2.36	0.60
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.83	0.59
1:B:321:ASP:OD2	1:B:363:ARG:NH2	2.36	0.58
1:C:419:GLU:HG3	1:C:524:HIS:HE1	1.69	0.58
1:A:539:LEU:O	1:A:543:MET:HG3	2.06	0.55
1:B:477:ARG:NH1	4:B:702:HOH:O	2.40	0.55
1:B:516:HIS:CE1	1:A:519:ASN:HD21	2.25	0.54
1:A:416:LYS:CD	1:A:416:LYS:N	2.72	0.53
1:C:477:ARG:NH1	4:C:705:HOH:O	2.41	0.52
1:C:422:VAL:HG13	1:C:423:GLU:HG3	1.90	0.52
1:C:379:LEU:HD12	1:C:544:LEU:HD11	1.93	0.51
1:D:358:ILE:HD13	1:D:543:MET:HB3	1.92	0.49
1:B:498:GLN:HA	1:B:501[A]:HIS:CE1	2.48	0.49
1:A:419:GLU:HG3	1:A:524:HIS:HE2	1.80	0.47
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.98	0.44
1:A:416:LYS:N	1:A:416:LYS:HD3	2.33	0.44
1:A:498:GLN:HA	1:A:501:HIS:CE1	2.53	0.43
1:D:338:SER:O	1:D:341:SER:OG	2.36	0.43
1:D:509:LEU:HD23	1:D:509:LEU:HA	1.92	0.43
1:D:325:PRO:HB3	1:C:325:PRO:HB3	2.00	0.43
1:D:392:VAL:HG11	1:D:431:THR:HG22	2.01	0.43
1:B:351:ASP:OD1	2:B:601:QYM:NBD	2.51	0.43
1:C:488:HIS:CE1	1:C:492:LYS:HD2	2.54	0.42
1:C:456:SER:HB3	1:C:515:ARG:NH1	2.35	0.42
1:C:310:LEU:O	1:C:481:LYS:NZ	2.43	0.42
1:A:355:VAL:HG22	1:A:543:MET:HE1	2.02	0.42
1:C:351:ASP:OD1	2:C:601:QYM:NBD	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:MET:HE1	1:D:410:LEU:HD11	2.01	0.41
1:C:358:ILE:HD13	1:C:543:MET:HB3	2.02	0.41
1:C:413:ASN:ND2	4:C:715:HOH:O	2.52	0.41
1:B:372:LEU:O	1:B:376:VAL:HG23	2.20	0.41
1:D:525:LEU:HD22	1:D:533:VAL:HG22	2.03	0.41
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.85	0.41
1:B:420:GLY:O	1:B:424:ILE:HD12	2.21	0.41
1:A:411:ASP:HB2	4:A:804:HOH:O	2.21	0.41
1:C:509:LEU:HD23	1:C:509:LEU:HA	1.87	0.40
1:B:330:GLU:HG3	1:B:352:ARG:NH2	2.37	0.40
1:C:481:LYS:HA	1:C:481:LYS:HD2	1.95	0.40
1:C:396:MET:HE3	1:C:396:MET:HB2	1.95	0.40
1:C:520:LYS:HA	1:C:520:LYS:HD2	1.91	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	226/263 (86%)	225 (100%)	1 (0%)	0	100	100
1	B	233/263 (89%)	232 (100%)	1 (0%)	0	100	100
1	C	232/263 (88%)	231 (100%)	1 (0%)	0	100	100
1	D	239/263 (91%)	237 (99%)	2 (1%)	0	100	100
All	All	930/1052 (88%)	925 (100%)	5 (0%)	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	206/238 (87%)	204 (99%)	2 (1%)	76	50
1	B	207/238 (87%)	207 (100%)	0	100	100
1	C	209/238 (88%)	208 (100%)	1 (0%)	88	74
1	D	213/238 (90%)	213 (100%)	0	100	100
All	All	835/952 (88%)	832 (100%)	3 (0%)	91	80

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

Mol	Chain	Res	Type
1	C	309	SER
1	A	416	LYS
1	A	529	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	488	HIS
1	B	519	ASN
1	D	398	HIS
1	D	516	HIS
1	C	524	HIS
1	A	516	HIS
1	A	519	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
2	QYM	D	601	-	36,36,36	4.17	21 (58%)	48,54,54	2.01	15 (31%)
2	QYM	B	601	-	36,36,36	4.16	21 (58%)	48,54,54	2.05	14 (29%)
2	QYM	A	601	-	36,36,36	4.17	21 (58%)	48,54,54	2.03	15 (31%)
2	QYM	C	601	-	36,36,36	4.15	21 (58%)	48,54,54	2.04	16 (33%)

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
2	QYM	D	601	-	-	3/10/53/53	0/5/5/5
2	QYM	B	601	-	-	3/10/53/53	0/5/5/5
2	QYM	A	601	-	-	3/10/53/53	0/5/5/5
2	QYM	C	601	-	-	3/10/53/53	0/5/5/5

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	QYM	CAA-CAF	10.23	1.53	1.39
2	D	601	QYM	CAA-CAF	10.21	1.53	1.39
2	C	601	QYM	CAA-CAF	10.17	1.53	1.39
2	A	601	QYM	CAA-CAF	10.13	1.53	1.39
2	A	601	QYM	CAD-CAE	8.70	1.54	1.39
2	D	601	QYM	CAD-CAE	8.62	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	QYM	CAD-CAE	8.56	1.54	1.39
2	C	601	QYM	CAD-CAE	8.47	1.54	1.39
2	C	601	QYM	CAM-CAL	-8.00	1.41	1.54
2	D	601	QYM	CAM-CAL	-7.67	1.42	1.54
2	A	601	QYM	CAM-CAL	-7.65	1.42	1.54
2	B	601	QYM	CAM-CAL	-7.57	1.42	1.54
2	A	601	QYM	CAI-CAK	-7.17	1.39	1.53
2	D	601	QYM	CAI-CAK	-7.16	1.39	1.53
2	B	601	QYM	CAI-CAK	-7.12	1.40	1.53
2	A	601	QYM	CAG-CAE	-7.09	1.39	1.51
2	C	601	QYM	CAI-CAK	-7.07	1.40	1.53
2	B	601	QYM	CAG-CAE	-7.03	1.39	1.51
2	D	601	QYM	CAG-CAE	-6.98	1.39	1.51
2	C	601	QYM	CAG-CAE	-6.92	1.39	1.51
2	A	601	QYM	CAB-CAC	6.15	1.50	1.38
2	B	601	QYM	CAB-CAC	6.04	1.50	1.38
2	D	601	QYM	CAB-CAC	6.01	1.50	1.38
2	C	601	QYM	CAB-CAC	5.97	1.50	1.38
2	B	601	QYM	CAH-CAG	-5.71	1.40	1.52
2	D	601	QYM	CAE-CAF	-5.71	1.30	1.40
2	A	601	QYM	CAE-CAF	-5.71	1.30	1.40
2	B	601	QYM	CAE-CAF	-5.63	1.30	1.40
2	D	601	QYM	CAH-CAG	-5.61	1.41	1.52
2	C	601	QYM	CAH-CAG	-5.57	1.41	1.52
2	A	601	QYM	CAH-CAG	-5.57	1.41	1.52
2	C	601	QYM	CAE-CAF	-5.57	1.30	1.40
2	B	601	QYM	CAJ-CAI	5.26	1.68	1.54
2	D	601	QYM	CAJ-CAI	5.21	1.68	1.54
2	A	601	QYM	CAJ-CAI	5.20	1.68	1.54
2	C	601	QYM	CAJ-CAI	5.17	1.67	1.54
2	D	601	QYM	OAT-CAQ	-4.96	1.35	1.43
2	A	601	QYM	OAT-CAQ	-4.78	1.35	1.43
2	D	601	QYM	CAP-CAO	4.76	1.67	1.54
2	B	601	QYM	CAP-CAO	4.74	1.67	1.54
2	A	601	QYM	CAP-CAO	4.72	1.66	1.54
2	C	601	QYM	CAP-CAO	4.66	1.66	1.54
2	B	601	QYM	OAT-CAQ	-4.64	1.35	1.43
2	C	601	QYM	OAT-CAQ	-4.61	1.35	1.43
2	B	601	QYM	CAN-CAJ	4.40	1.59	1.54
2	A	601	QYM	CAF-CAJ	-4.35	1.44	1.51
2	C	601	QYM	CAF-CAJ	-4.30	1.44	1.51
2	D	601	QYM	CAF-CAJ	-4.27	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	QYM	CAN-CAJ	4.25	1.59	1.54
2	D	601	QYM	CAN-CAJ	4.21	1.59	1.54
2	C	601	QYM	CAN-CAJ	4.17	1.59	1.54
2	B	601	QYM	CAF-CAJ	-4.16	1.44	1.51
2	D	601	QYM	CAL-CAK	-3.90	1.47	1.55
2	C	601	QYM	CAL-CAK	-3.89	1.47	1.55
2	B	601	QYM	CAL-CAK	-3.77	1.47	1.55
2	A	601	QYM	CAL-CAK	-3.73	1.47	1.55
2	B	601	QYM	CAO-CAK	3.68	1.62	1.54
2	C	601	QYM	CAO-CAK	3.64	1.61	1.54
2	D	601	QYM	CAO-CAK	3.62	1.61	1.54
2	A	601	QYM	CAO-CAK	3.60	1.61	1.54
2	D	601	QYM	CAU-CAN	-3.22	1.47	1.51
2	A	601	QYM	OAR-CAC	3.15	1.44	1.37
2	C	601	QYM	CAU-CAN	-3.13	1.47	1.51
2	D	601	QYM	OAR-CAC	3.10	1.44	1.37
2	C	601	QYM	OAR-CAC	3.08	1.44	1.37
2	B	601	QYM	CAU-CAN	-3.07	1.47	1.51
2	B	601	QYM	OAR-CAC	3.04	1.44	1.37
2	A	601	QYM	CAU-CAN	-2.98	1.47	1.51
2	C	601	QYM	CAD-CAC	-2.58	1.35	1.39
2	A	601	QYM	CAD-CAC	-2.50	1.35	1.39
2	B	601	QYM	CAD-CAC	-2.46	1.35	1.39
2	D	601	QYM	CAD-CAC	-2.44	1.35	1.39
2	A	601	QYM	CAP-CAQ	2.24	1.58	1.53
2	B	601	QYM	CAP-CAQ	2.23	1.58	1.53
2	A	601	QYM	CAM-CAN	2.17	1.57	1.53
2	D	601	QYM	CAP-CAQ	2.16	1.57	1.53
2	C	601	QYM	CAP-CAQ	2.11	1.57	1.53
2	B	601	QYM	OBA-CAX	2.10	1.42	1.37
2	B	601	QYM	CAM-CAN	2.10	1.57	1.53
2	A	601	QYM	OBA-CAX	2.06	1.42	1.37
2	C	601	QYM	CAM-CAN	2.03	1.57	1.53
2	D	601	QYM	OBA-CAX	2.02	1.42	1.37
2	D	601	QYM	CAM-CAN	2.01	1.57	1.53
2	C	601	QYM	OBA-CAX	2.01	1.42	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	QYM	CAO-CAK-CAI	-5.42	110.16	119.08
2	B	601	QYM	CAO-CAK-CAI	-5.17	110.57	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	QYM	CAO-CAK-CAI	-5.11	110.67	119.08
2	C	601	QYM	CAO-CAK-CAI	-5.08	110.72	119.08
2	A	601	QYM	CAH-CAI-CAJ	-4.98	104.00	109.63
2	D	601	QYM	CAH-CAI-CAJ	-4.91	104.08	109.63
2	C	601	QYM	CAH-CAI-CAJ	-4.77	104.23	109.63
2	B	601	QYM	CAH-CAI-CAJ	-4.64	104.38	109.63
2	B	601	QYM	CAM-CAL-CAK	4.58	112.21	106.94
2	A	601	QYM	CAM-CAL-CAK	4.37	111.97	106.94
2	D	601	QYM	CAM-CAL-CAK	4.31	111.90	106.94
2	C	601	QYM	CAM-CAL-CAK	4.11	111.68	106.94
2	B	601	QYM	CAK-CAL-CAQ	4.08	103.59	99.27
2	C	601	QYM	CAK-CAL-CAQ	4.06	103.56	99.27
2	A	601	QYM	CAK-CAL-CAQ	4.00	103.50	99.27
2	B	601	QYM	CAS-CAL-CAQ	-3.82	103.47	109.54
2	D	601	QYM	CAH-CAI-CAK	3.76	118.52	112.08
2	D	601	QYM	CAK-CAL-CAQ	3.75	103.24	99.27
2	C	601	QYM	CAH-CAI-CAK	3.74	118.48	112.08
2	A	601	QYM	CAH-CAI-CAK	3.68	118.38	112.08
2	C	601	QYM	CAS-CAL-CAQ	-3.68	103.70	109.54
2	B	601	QYM	CAH-CAI-CAK	3.63	118.28	112.08
2	A	601	QYM	CAS-CAL-CAQ	-3.63	103.78	109.54
2	D	601	QYM	CAS-CAL-CAQ	-3.62	103.79	109.54
2	B	601	QYM	CAG-CAE-CAD	-3.09	113.73	119.91
2	B	601	QYM	CAH-CAG-CAE	-2.96	107.25	112.87
2	D	601	QYM	CAG-CAE-CAD	-2.89	114.12	119.91
2	A	601	QYM	CAH-CAG-CAE	-2.88	107.41	112.87
2	A	601	QYM	CAG-CAE-CAD	-2.87	114.16	119.91
2	C	601	QYM	CAY-CAZ-CAU	-2.83	118.35	121.20
2	C	601	QYM	CAH-CAG-CAE	-2.83	107.51	112.87
2	C	601	QYM	CAG-CAE-CAD	-2.79	114.32	119.91
2	D	601	QYM	CAH-CAG-CAE	-2.72	107.71	112.87
2	B	601	QYM	CAY-CAZ-CAU	-2.67	118.51	121.20
2	D	601	QYM	CAC-CAD-CAE	-2.65	117.89	120.83
2	B	601	QYM	CAG-CAE-CAF	2.63	125.06	121.13
2	A	601	QYM	CAC-CAD-CAE	-2.63	117.91	120.83
2	B	601	QYM	CAW-CAV-CAU	2.54	123.76	121.20
2	C	601	QYM	CAW-CAV-CAU	2.52	123.73	121.20
2	D	601	QYM	CAY-CAZ-CAU	-2.46	118.72	121.20
2	C	601	QYM	CAG-CAE-CAF	2.43	124.77	121.13
2	B	601	QYM	CAC-CAD-CAE	-2.37	118.20	120.83
2	C	601	QYM	CAC-CAD-CAE	-2.37	118.20	120.83
2	D	601	QYM	CAG-CAE-CAF	2.36	124.66	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	QYM	CAF-CAJ-CAI	2.29	115.36	110.59
2	A	601	QYM	CAY-CAZ-CAU	-2.27	118.92	121.20
2	A	601	QYM	CAW-CAV-CAU	2.24	123.45	121.20
2	C	601	QYM	CAF-CAJ-CAI	2.24	115.24	110.59
2	C	601	QYM	CAV-CAW-CAX	-2.22	117.02	119.73
2	C	601	QYM	CAV-CAU-CAN	-2.21	116.89	121.08
2	C	601	QYM	CAO-CAP-CAQ	-2.17	103.47	105.75
2	D	601	QYM	CAW-CAV-CAU	2.17	123.38	121.20
2	A	601	QYM	CAG-CAE-CAF	2.14	124.34	121.13
2	A	601	QYM	CAF-CAJ-CAI	2.14	115.04	110.59
2	A	601	QYM	CAV-CAU-CAN	-2.14	117.02	121.08
2	B	601	QYM	CAV-CAU-CAN	-2.09	117.11	121.08
2	D	601	QYM	CAV-CAU-CAN	-2.09	117.12	121.08
2	A	601	QYM	CAP-CAO-CAK	-2.07	101.03	105.13
2	D	601	QYM	CAO-CAP-CAQ	-2.05	103.59	105.75
2	B	601	QYM	CAF-CAJ-CAI	2.04	114.82	110.59

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	QYM	CAJ-CAN-CAU-CAV
2	B	601	QYM	CAJ-CAN-CAU-CAZ
2	D	601	QYM	CAJ-CAN-CAU-CAV
2	D	601	QYM	CAJ-CAN-CAU-CAZ
2	C	601	QYM	CAJ-CAN-CAU-CAV
2	C	601	QYM	CAJ-CAN-CAU-CAZ
2	A	601	QYM	CAJ-CAN-CAU-CAV
2	A	601	QYM	CAJ-CAN-CAU-CAZ
2	C	601	QYM	OBA-CBB-CBC-NBD
2	A	601	QYM	OBA-CBB-CBC-NBD
2	B	601	QYM	OBA-CBB-CBC-NBD
2	D	601	QYM	OBA-CBB-CBC-NBD

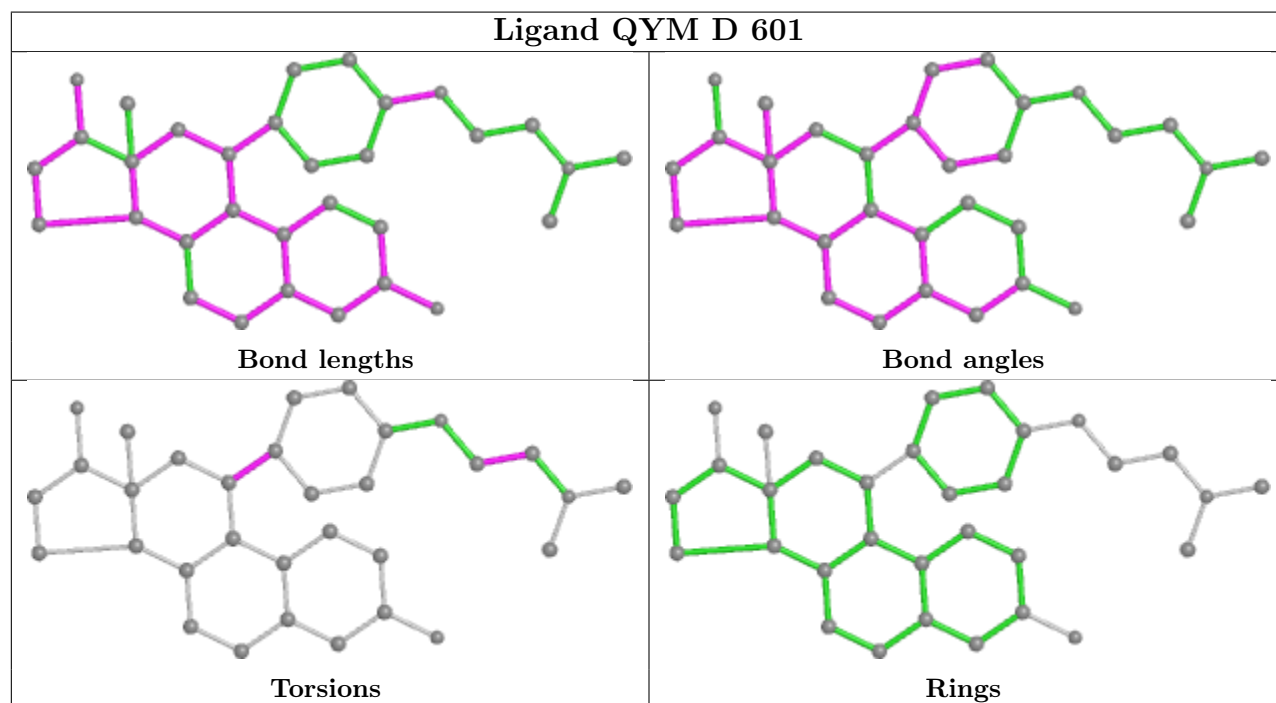
There are no ring outliers.

2 monomers are involved in 2 short contacts:

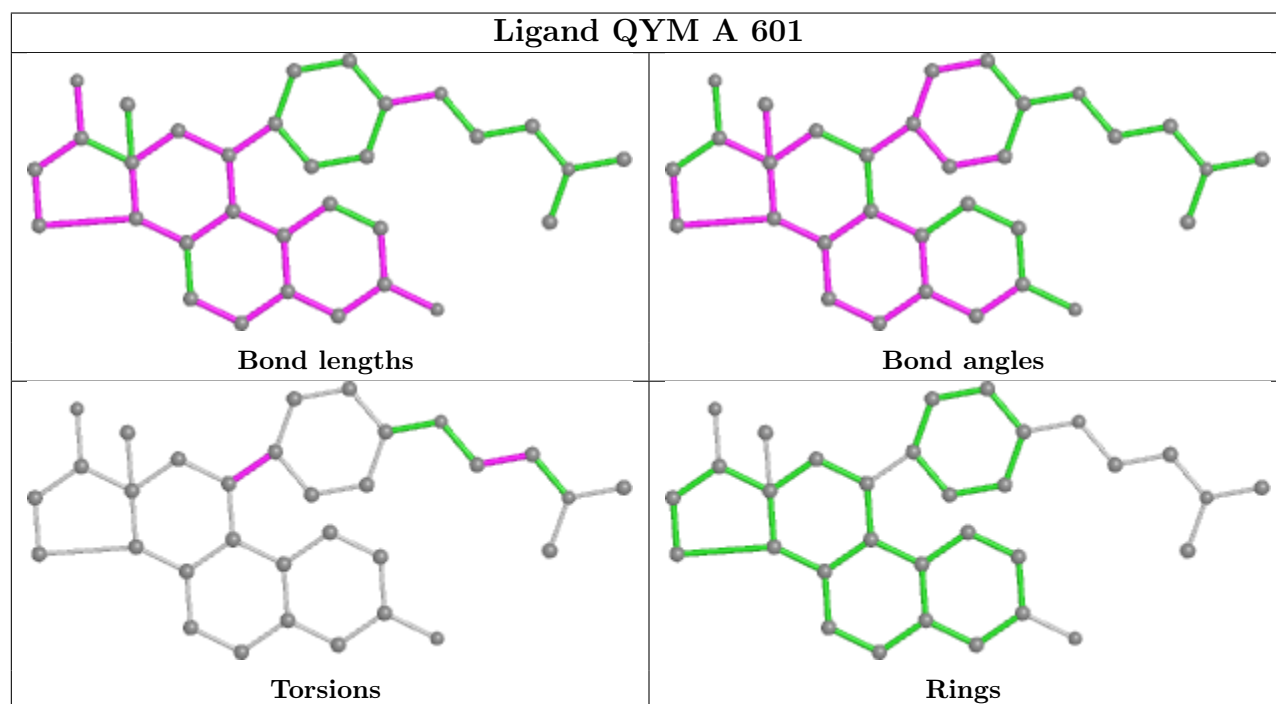
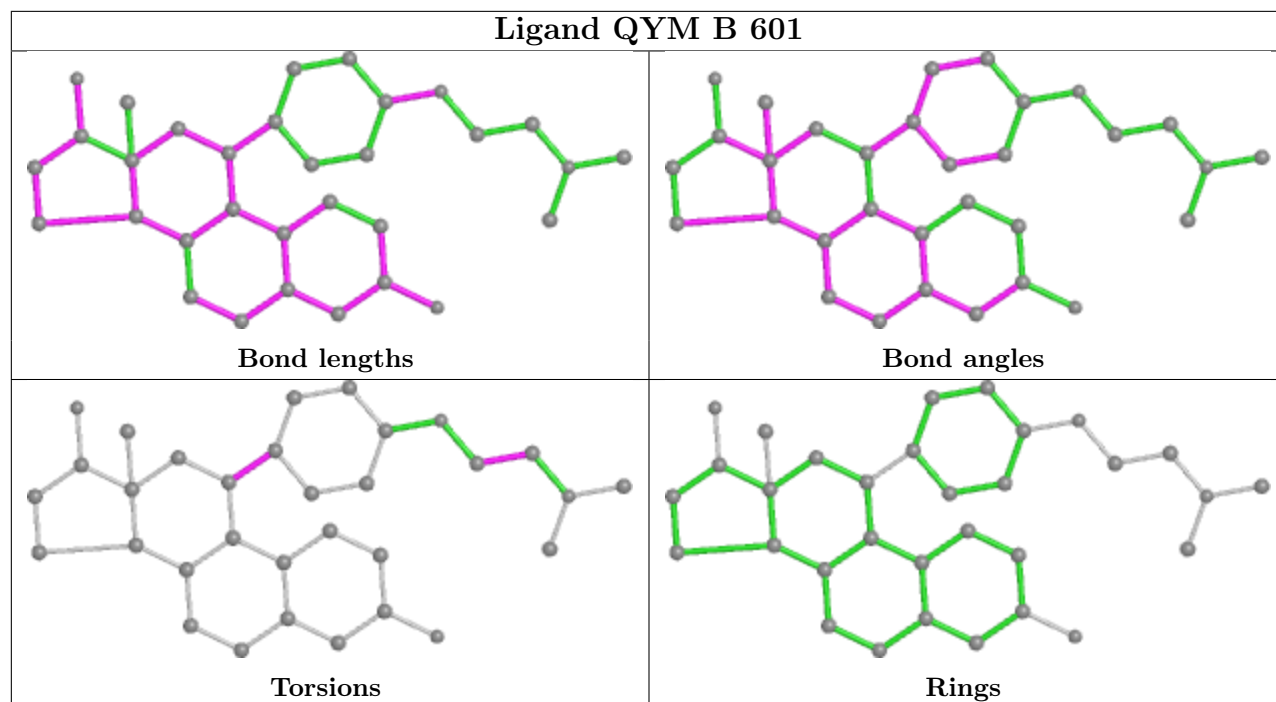
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	QYM	1	0
2	C	601	QYM	1	0



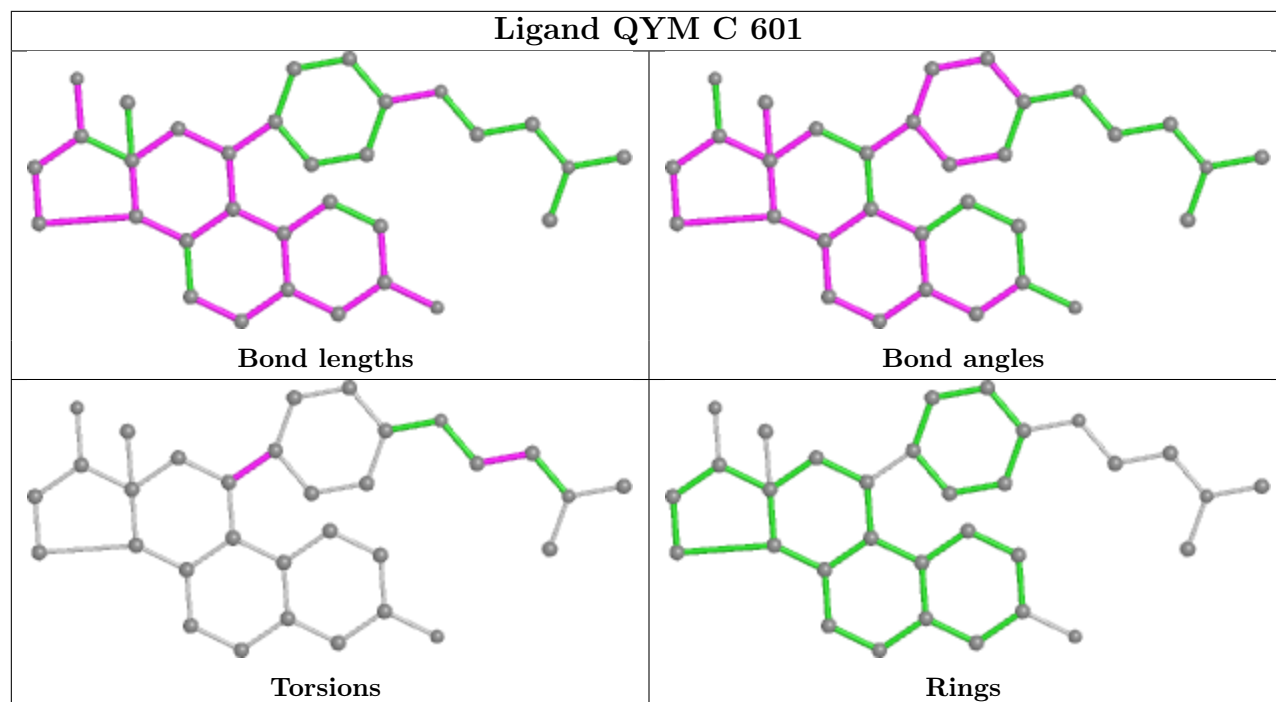
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

### 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	231/263 (87%)	0.19	8 (3%)	44	46	11, 21, 37, 45	1 (0%)
1	B	234/263 (88%)	0.23	7 (2%)	50	51	10, 21, 35, 45	0
1	C	233/263 (88%)	0.23	13 (5%)	24	24	11, 21, 37, 49	1 (0%)
1	D	240/263 (91%)	0.24	5 (2%)	63	64	11, 22, 40, 52	1 (0%)
All	All	938/1052 (89%)	0.22	33 (3%)	44	46	10, 21, 37, 52	3 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	TYR	5.2
1	C	459	TYR	5.2
1	A	459	TYR	5.1
1	C	461	PHE	4.9
1	B	459	TYR	4.8
1	D	459	TYR	4.4
1	C	331	TYR	4.0
1	A	331	TYR	4.0
1	A	336	PRO	3.7
1	B	422	VAL	3.7
1	C	422	VAL	3.5
1	D	331	TYR	3.3
1	C	463	SER	3.1
1	B	462	LEU	3.0
1	A	462	LEU	2.9
1	B	420	GLY	2.9
1	A	420	GLY	2.8
1	C	464	SER	2.7
1	D	307	ALA	2.6
1	C	334	THR	2.6
1	D	461	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	422	VAL	2.6
1	B	417	SER	2.6
1	D	464	SER	2.5
1	C	462	LEU	2.5
1	A	469	LEU	2.4
1	C	546	ALA	2.3
1	C	437[A]	MET	2.3
1	A	460	THR	2.2
1	C	419	GLU	2.1
1	C	337	PHE	2.1
1	B	418	VAL	2.0
1	C	458	VAL	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 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.

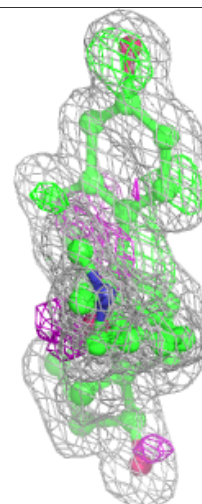
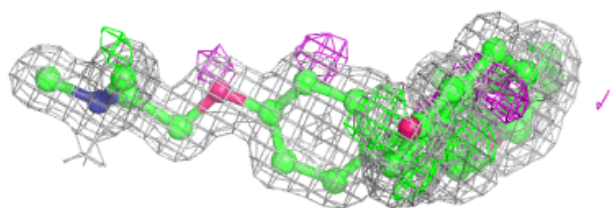
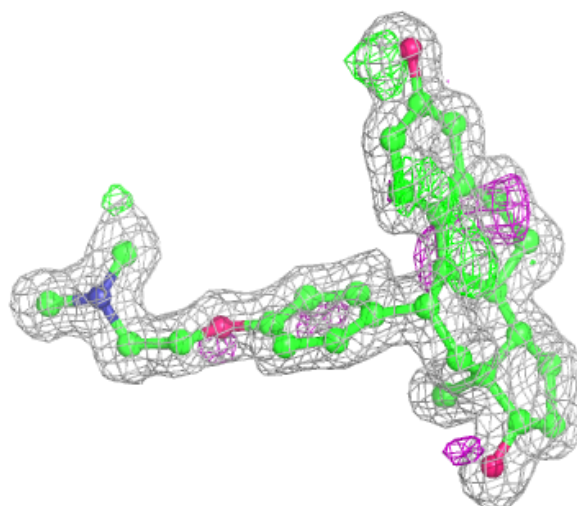
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	QYM	C	601	32/32	0.88	0.14	12,15,20,29	0
2	QYM	D	601	32/32	0.89	0.13	12,15,19,28	0
2	QYM	B	601	32/32	0.90	0.13	11,15,20,28	0
2	QYM	A	601	32/32	0.90	0.13	12,15,18,28	0
3	MG	A	602	1/1	0.96	0.13	41,41,41,41	0

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 QYM C 601:**

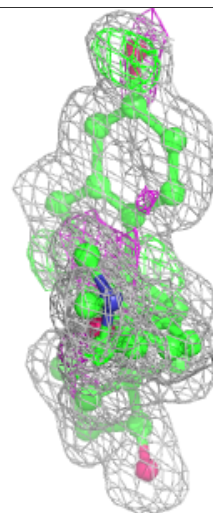
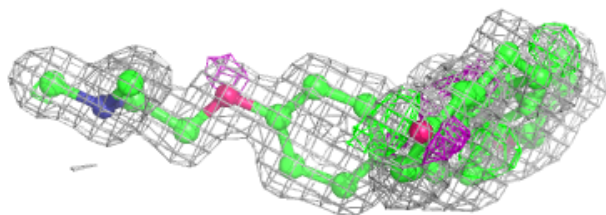
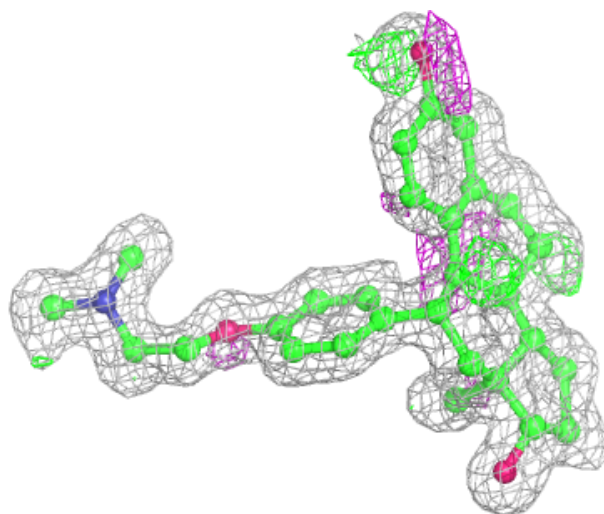
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around QYM D 601:**

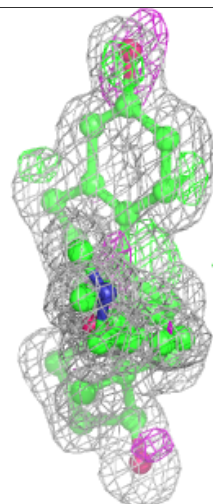
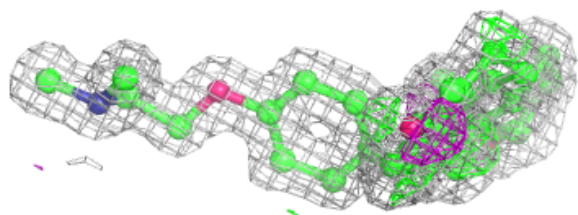
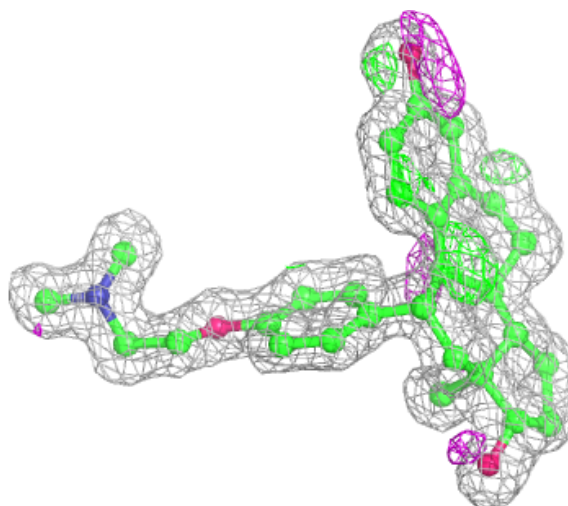
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around QYM B 601:**

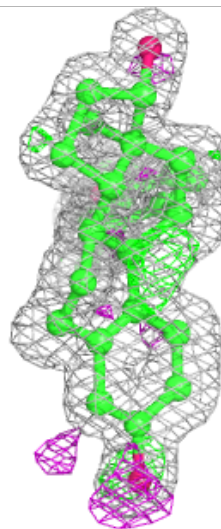
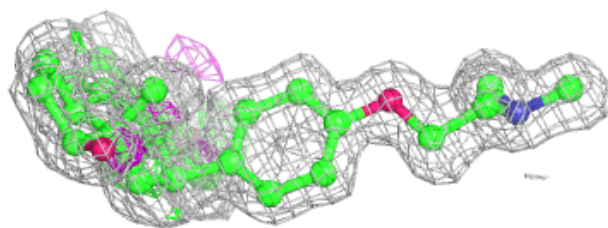
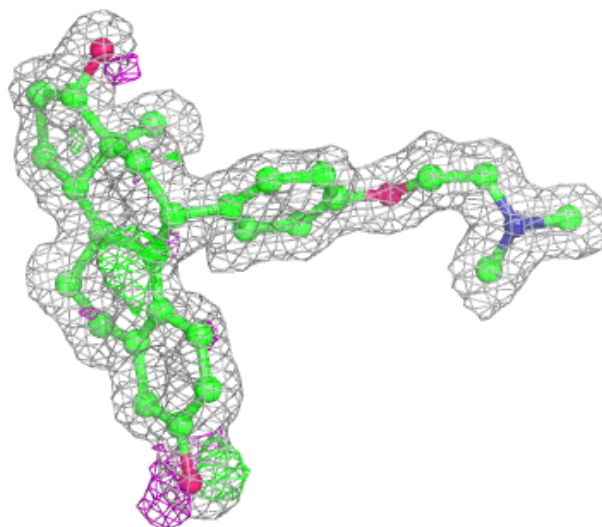
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around QYM A 601:**

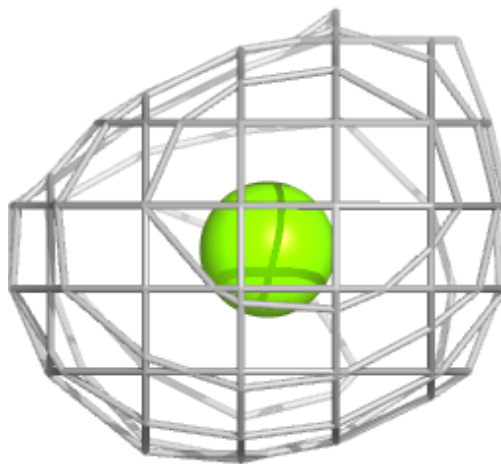
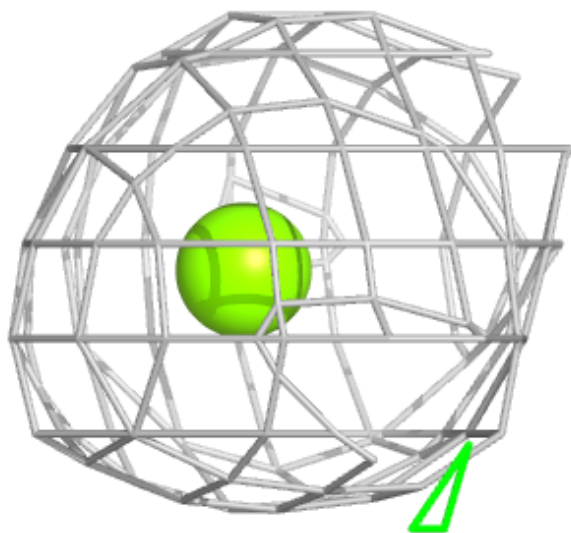
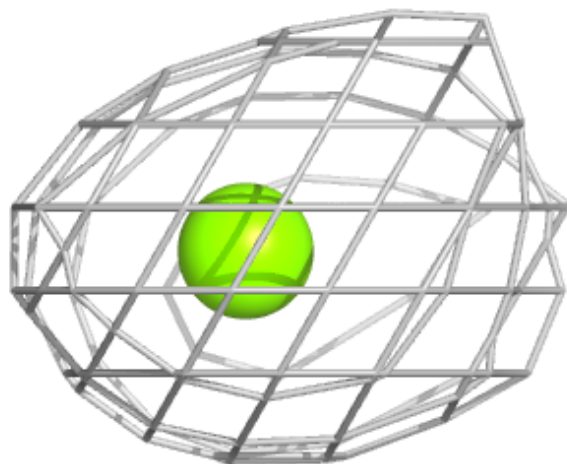
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG A 602:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.