



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:02 AM BST

PDB ID : 6WJC  
Title : Muscarinic acetylcholine receptor 1 - muscarinic toxin 7 complex  
Authors : Maeda, S.; Kobilka, B.K.  
Deposited on : 2020-04-13  
Resolution : 2.55 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 : 2.13.1  
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

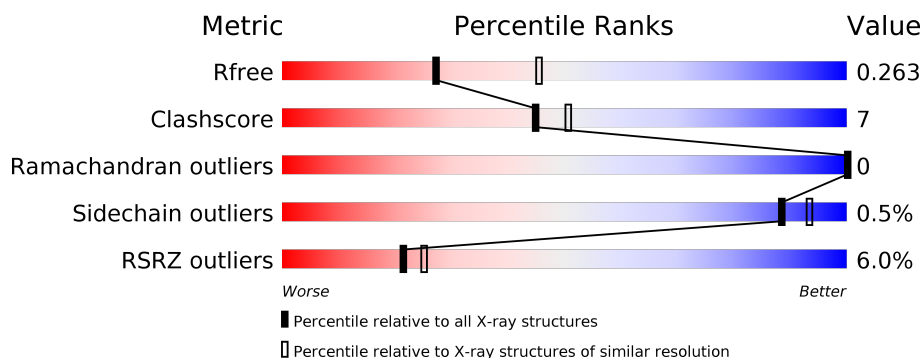
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	499	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>11%</div> </div> </div>
2	C	69	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>16%</div> </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
4	Y01	A	504	-	-	-	X
4	Y01	A	505	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4213 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 Muscarinic acetylcholine receptor M1,Endolysin fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3501	2281	586	612	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P11229
A	-7	TYR	-	expression tag	UNP P11229
A	-6	LYS	-	expression tag	UNP P11229
A	-5	ASP	-	expression tag	UNP P11229
A	-4	ASP	-	expression tag	UNP P11229
A	-3	ASP	-	expression tag	UNP P11229
A	-2	ASP	-	expression tag	UNP P11229
A	-1	ALA	-	expression tag	UNP P11229
A	0	ALA	-	expression tag	UNP P11229
A	1	ALA	-	expression tag	UNP P11229
A	2	GLN	ASN	conflict	UNP P11229
A	12	GLN	ASN	conflict	UNP P11229
A	110	GLN	ASN	conflict	UNP P11229
A	112	ARG	SER	conflict	UNP P11229
A	1053	THR	CYS	conflict	UNP D9IEF7
A	1096	ALA	CYS	conflict	UNP D9IEF7
A	461	HIS	-	expression tag	UNP P11229
A	462	HIS	-	expression tag	UNP P11229
A	463	HIS	-	expression tag	UNP P11229
A	464	HIS	-	expression tag	UNP P11229
A	465	HIS	-	expression tag	UNP P11229
A	466	HIS	-	expression tag	UNP P11229

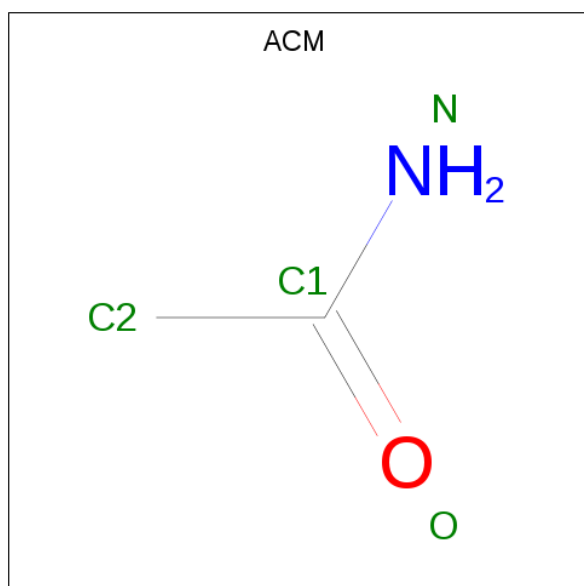
- Molecule 2 is a protein called Muscarinic toxin 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	69	Total	C	N	O	S	0	0	0
			540	334	94	103	9			

There are 4 discrepancies between the modelled and reference sequences:

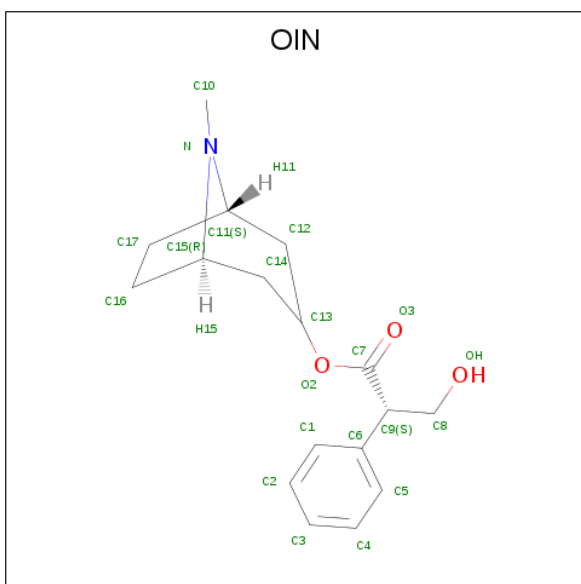
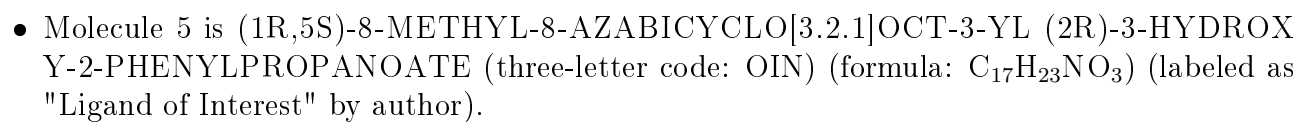
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q8QGR0
C	-2	PRO	-	expression tag	UNP Q8QGR0
C	-1	GLY	-	expression tag	UNP Q8QGR0
C	0	SER	-	expression tag	UNP Q8QGR0

- Molecule 3 is ACETAMIDE (three-letter code: ACM) (formula:  $C_2H_5NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ) (labeled as "Ligand of Interest" by author).



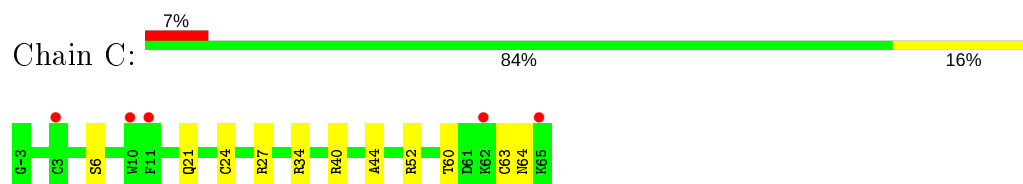
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	17	1	3		

- Molecule 6 is water.

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



- Molecule 1: Muscarinic acetylcholine receptor M1,Endolysin fusion





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.15Å 150.43Å 76.93Å 90.00° 98.77° 90.00°	Depositor
Resolution (Å)	44.11 – 2.55 44.11 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.11-2.55) 99.3 (44.11-2.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, $R_{free}$	0.244 , 0.263 0.244 , 0.263	Depositor DCC
$R_{free}$ test set	1997 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.3	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 88.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OIN, Y01, ACM

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	0.24	0/3583	0.41	0/4887
2	C	0.27	0/554	0.46	0/748
All	All	0.25	0/4137	0.42	0/5635

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	3501	0	3510	46	0
2	C	540	0	504	6	0
3	A	4	0	3	0	0
4	A	140	0	196	5	0
5	A	21	0	23	1	0
6	A	6	0	0	0	0
6	C	1	0	0	0	0
All	All	4213	0	4236	55	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 7.

All (55) 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:71:ASP:OD1	1:A:112:ARG:NH2	2.14	0.81
1:A:123:ARG:HG3	1:A:367:LEU:HD22	1.68	0.75
1:A:1086:VAL:HG12	1:A:1121:GLN:HB2	1.70	0.72
1:A:1125:TRP:HB3	1:A:1153:ARG:HA	1.82	0.61
1:A:397:GLU:OE2	2:C:52:ARG:NH1	2.33	0.60
1:A:32:THR:HG23	1:A:79:MET:HG2	1.85	0.59
1:A:47:LEU:HD13	1:A:65:LEU:HD11	1.84	0.59
2:C:60:THR:HB	2:C:63:CYS:HB3	1.83	0.59
1:A:63:PHE:HB3	1:A:119:ILE:HD11	1.89	0.54
1:A:382:ASN:HA	1:A:385:VAL:HG12	1.90	0.54
1:A:404:TYR:CE1	5:A:506:OIN:H15	2.43	0.54
1:A:24:GLN:O	1:A:28:ILE:HG12	2.09	0.52
1:A:1080:ASN:HD21	1:A:1111:ALA:HB2	1.75	0.52
1:A:1102:VAL:HG22	1:A:1110:VAL:HG21	1.93	0.51
1:A:165:GLN:OE1	1:A:171:ARG:NH2	2.36	0.51
1:A:59:VAL:HA	1:A:62:TYR:HD2	1.77	0.50
2:C:21:GLN:HA	2:C:44:ALA:HA	1.93	0.50
1:A:1024:TYR:CZ	1:A:1038:LEU:HB3	2.47	0.50
4:A:504:Y01:HAA1	4:A:505:Y01:HAP2	1.95	0.49
1:A:28:ILE:HD11	1:A:402:LEU:HD23	1.94	0.49
1:A:210:ARG:NH2	1:A:214:GLU:OE2	2.46	0.48
1:A:1010:GLU:OE2	1:A:1144:ARG:NH2	2.41	0.48
1:A:1008:ILE:HD11	1:A:1160:TYR:CE1	2.48	0.48
1:A:1124:ARG:NH2	1:A:1127:GLU:OE1	2.48	0.47
1:A:85:TYR:HE2	2:C:34:ARG:HD2	1.80	0.47
1:A:43:ASN:O	1:A:47:LEU:HD23	2.15	0.46
1:A:1145:ALA:O	1:A:1149:ILE:HG12	2.15	0.46
1:A:138:THR:HG23	1:A:141:ARG:H	1.79	0.46
2:C:6:SER:HB3	2:C:40:ARG:HB2	1.97	0.46
4:A:503:Y01:HAO1	4:A:503:Y01:HAP1	1.69	0.45
1:A:1084:LYS:HB3	1:A:1085:PRO:HD3	1.98	0.45
1:A:44:LEU:O	1:A:48:ILE:HG12	2.17	0.45
1:A:82:TYR:OH	1:A:401:GLU:OE1	2.22	0.45
1:A:395:VAL:HG13	1:A:400:TRP:HE1	1.82	0.45
4:A:504:Y01:HAA1	4:A:505:Y01:HAO1	2.00	0.44
1:A:172:THR:H	1:A:181:GLN:NE2	2.16	0.44
1:A:1093:VAL:HG11	1:A:1155:GLY:O	2.18	0.44
1:A:115:ASN:O	1:A:119:ILE:HD12	2.17	0.44
1:A:28:ILE:HD12	1:A:405:TRP:CD2	2.53	0.44
1:A:112:ARG:NH2	1:A:411:SER:OG	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ASP:OD1	1:A:1023:TYR:N	2.47	0.43
4:A:504:Y01:HAJ2	4:A:505:Y01:HAP2	2.01	0.43
1:A:127:VAL:HG13	1:A:218:ARG:HB2	1.99	0.43
1:A:173:VAL:HG23	1:A:179:TYR:CZ	2.53	0.43
1:A:199:LEU:HB3	1:A:200:PRO:HD3	2.00	0.43
1:A:362:LYS:HB3	1:A:362:LYS:HE2	1.89	0.42
1:A:132:SER:N	1:A:1063:GLU:OE2	2.44	0.42
1:A:1150:THR:HA	1:A:1153:ARG:HG2	2.02	0.42
2:C:24:CYS:HB3	2:C:64:ASN:ND2	2.35	0.42
1:A:194:MET:HA	1:A:198:TYR:HB2	2.00	0.41
1:A:211:ILE:O	1:A:215:THR:HG23	2.20	0.41
4:A:504:Y01:HAO1	4:A:504:Y01:HAP1	1.49	0.41
1:A:66:SER:HB2	1:A:150:TRP:HE1	1.86	0.41
1:A:1150:THR:HG22	1:A:1153:ARG:HH21	1.86	0.40
1:A:380:PRO:O	1:A:384:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/499 (89%)	436 (98%)	7 (2%)	0	100	100
2	C	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
All	All	510/568 (90%)	500 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	363/427 (85%)	362 (100%)	1 (0%)	92	96
2	C	61/61 (100%)	60 (98%)	1 (2%)	62	77
All	All	424/488 (87%)	422 (100%)	2 (0%)	88	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1118	ARG
2	C	27	ARG

Some 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 ⓘ

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 ⓘ

6 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
5	OIN	A	506	-	23,23,23	4.00	6 (26%)	32,32,32	2.48	4 (12%)
4	Y01	A	504	-	35,38,38	1.27	4 (11%)	54,57,57	1.62	9 (16%)
4	Y01	A	503	-	35,38,38	1.28	4 (11%)	54,57,57	1.58	12 (22%)
4	Y01	A	502	-	35,38,38	1.31	5 (14%)	54,57,57	1.34	8 (14%)
4	Y01	A	505	-	35,38,38	1.32	4 (11%)	54,57,57	1.44	10 (18%)
3	ACM	A	501	1	3,3,3	2.64	2 (66%)	3,3,3	0.91	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
5	OIN	A	506	-	-	2/14/35/35	0/4/3/3
4	Y01	A	502	-	-	5/17/77/77	0/4/4/4
4	Y01	A	503	-	-	4/17/77/77	0/4/4/4
4	Y01	A	504	-	-	4/17/77/77	0/4/4/4
4	Y01	A	505	-	-	5/17/77/77	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	506	OIN	C15-N	-9.85	1.33	1.48
5	A	506	OIN	C11-N	-9.37	1.34	1.48
5	A	506	OIN	O2-C13	-8.32	1.25	1.46
5	A	506	OIN	C12-C13	8.05	1.72	1.52
5	A	506	OIN	C14-C13	4.86	1.64	1.52
3	A	501	ACM	C1-N	3.59	1.45	1.32
5	A	506	OIN	O2-C7	3.44	1.42	1.34
4	A	503	Y01	OAW-CAY	3.37	1.43	1.34
4	A	505	Y01	OAW-CAY	3.23	1.43	1.34
4	A	504	Y01	OAW-CAY	3.10	1.43	1.34
4	A	502	Y01	OAW-CAY	3.06	1.42	1.34
4	A	505	Y01	CAS-CBF	-2.95	1.48	1.53
4	A	502	Y01	CBI-CBE	-2.87	1.49	1.55
4	A	502	Y01	CAS-CBF	-2.86	1.49	1.53
4	A	505	Y01	CBI-CBE	-2.81	1.49	1.55
4	A	502	Y01	CAQ-CAP	2.78	1.61	1.54
4	A	505	Y01	CAQ-CAP	2.78	1.61	1.54
4	A	504	Y01	CBI-CBE	-2.74	1.49	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	Y01	CAQ-CAP	2.72	1.61	1.54
4	A	503	Y01	CAS-CBF	-2.64	1.49	1.53
4	A	503	Y01	CBI-CBE	-2.63	1.50	1.55
4	A	504	Y01	CAQ-CAP	2.63	1.61	1.54
3	A	501	ACM	O-C1	-2.61	1.18	1.24
4	A	504	Y01	CAS-CBF	-2.45	1.49	1.53
4	A	502	Y01	OAW-CBC	-2.12	1.41	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	506	OIN	C15-N-C11	9.16	111.90	100.80
5	A	506	OIN	O2-C7-C9	7.88	119.44	111.16
4	A	504	Y01	CAP-CAQ-CBG	-3.95	97.31	105.13
5	A	506	OIN	C14-C15-N	3.79	112.95	107.53
4	A	504	Y01	OAW-CAY-CAM	3.76	119.60	111.50
4	A	505	Y01	OAW-CAY-CAM	3.68	119.44	111.50
4	A	503	Y01	OAW-CAY-CAM	3.38	118.80	111.50
4	A	503	Y01	CAP-CAQ-CBG	-3.35	98.50	105.13
4	A	503	Y01	CBI-CBG-CBD	-3.35	109.43	114.38
4	A	503	Y01	CAP-CBE-CBB	-3.21	107.17	112.15
4	A	504	Y01	CBI-CBG-CBD	-3.10	109.78	114.38
4	A	502	Y01	CAP-CAQ-CBG	-3.08	99.03	105.13
4	A	502	Y01	OAW-CAY-CAM	3.07	118.11	111.50
4	A	502	Y01	CBI-CBE-CBB	-3.03	114.74	119.49
4	A	505	Y01	CAP-CAQ-CBG	-3.02	99.14	105.13
4	A	504	Y01	CBI-CBE-CBB	-2.94	114.88	119.49
4	A	504	Y01	CBF-CBD-CBG	-2.94	105.16	109.09
4	A	504	Y01	CAP-CBE-CBB	-2.83	107.77	112.15
4	A	505	Y01	CAS-CBF-CBH	-2.77	109.44	113.08
4	A	503	Y01	CBG-CBI-CBE	2.73	103.31	100.07
4	A	505	Y01	CBI-CBG-CBD	-2.63	110.49	114.38
5	A	506	OIN	C12-C11-N	2.58	111.22	107.53
4	A	502	Y01	CAQ-CBG-CBD	-2.57	114.85	119.08
4	A	502	Y01	CAL-CAM-CAY	-2.49	106.91	113.82
4	A	503	Y01	CBH-CBF-CBD	-2.47	109.03	112.73
4	A	505	Y01	CBC-CAV-CAZ	2.46	115.34	111.52
4	A	502	Y01	CAS-CBF-CBH	-2.43	109.88	113.08
4	A	503	Y01	CAS-CBF-CBH	-2.40	109.92	113.08
4	A	503	Y01	CAQ-CBG-CBD	-2.39	115.14	119.08
4	A	504	Y01	CAU-CAS-CBF	2.39	117.25	113.11
4	A	503	Y01	CBI-CBE-CBB	-2.37	115.77	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	Y01	CBH-CBF-CBD	-2.32	109.25	112.73
4	A	503	Y01	CAD-CBH-CBF	-2.30	108.94	111.68
4	A	504	Y01	CAQ-CBG-CBD	-2.29	115.30	119.08
4	A	502	Y01	CAK-CBD-CBG	-2.28	107.60	110.91
4	A	505	Y01	CBF-CBD-CBG	-2.26	106.06	109.09
4	A	505	Y01	CAP-CBE-CBB	-2.24	108.69	112.15
4	A	505	Y01	CBI-CBE-CBB	-2.23	116.00	119.49
4	A	505	Y01	CAV-CAZ-CBH	2.19	119.32	116.42
4	A	503	Y01	CBF-CBD-CBG	-2.16	106.20	109.09
4	A	505	Y01	CAQ-CBG-CBD	-2.15	115.55	119.08
4	A	504	Y01	CBG-CBI-CBE	2.06	102.52	100.07
4	A	503	Y01	OAW-CBC-CAV	2.04	112.30	108.12

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	Y01	CAV-CBC-OAW-CAY
5	A	506	OIN	C9-C7-O2-C13
5	A	506	OIN	O3-C7-O2-C13
4	A	502	Y01	CAJ-CAN-CBA-CAB
4	A	502	Y01	CAJ-CAN-CBA-CAA
4	A	504	Y01	CAC-CBB-CBE-CBI
4	A	504	Y01	CAC-CBB-CBE-CAP
4	A	502	Y01	CAC-CBB-CBE-CBI
4	A	504	Y01	CAO-CBB-CBE-CBI
4	A	502	Y01	CAL-CAM-CAY-OAW
4	A	504	Y01	CAO-CBB-CBE-CAP
4	A	502	Y01	CAO-CBB-CBE-CBI
4	A	503	Y01	CAO-CAJ-CAN-CBA
4	A	505	Y01	OAG-CAY-OAW-CBC
4	A	503	Y01	CAC-CBB-CBE-CBI
4	A	505	Y01	CAJ-CAO-CBB-CAC
4	A	505	Y01	CAM-CAY-OAW-CBC
4	A	503	Y01	CAL-CAM-CAY-OAW
4	A	505	Y01	CAL-CAM-CAY-OAW
4	A	505	Y01	CAL-CAM-CAY-OAG

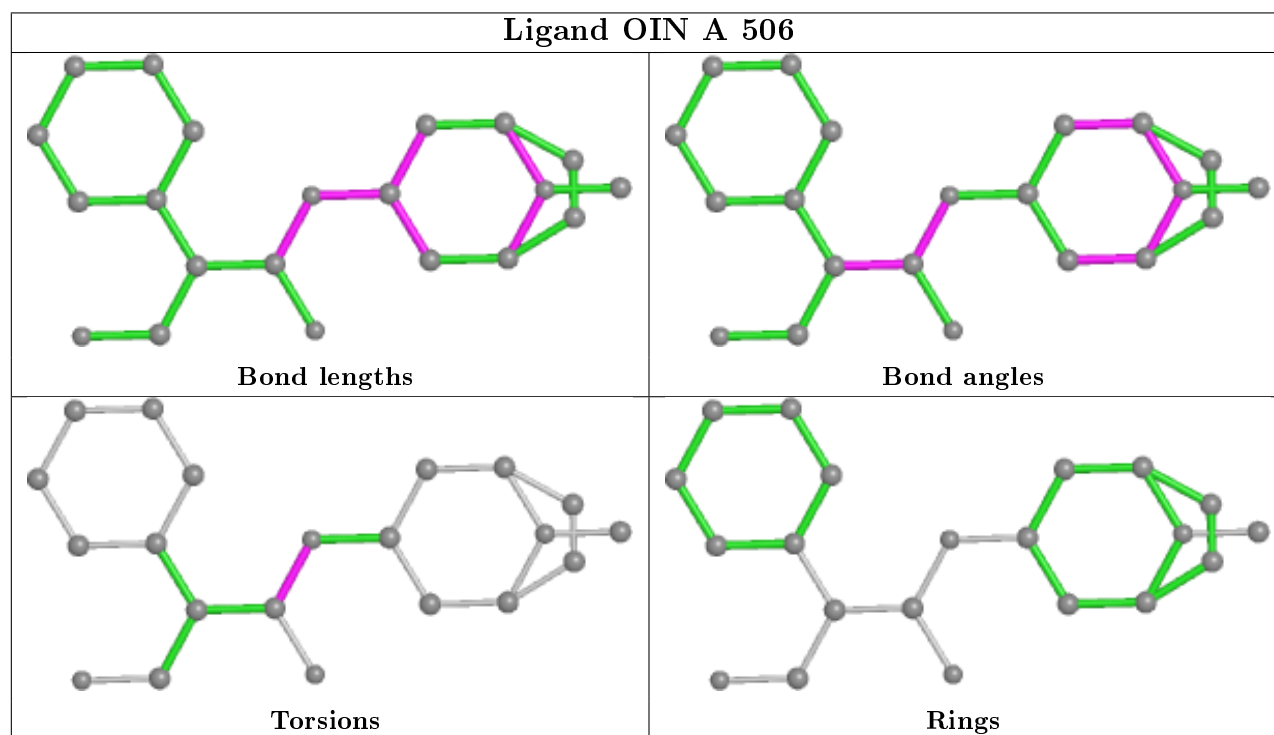
There are no ring outliers.

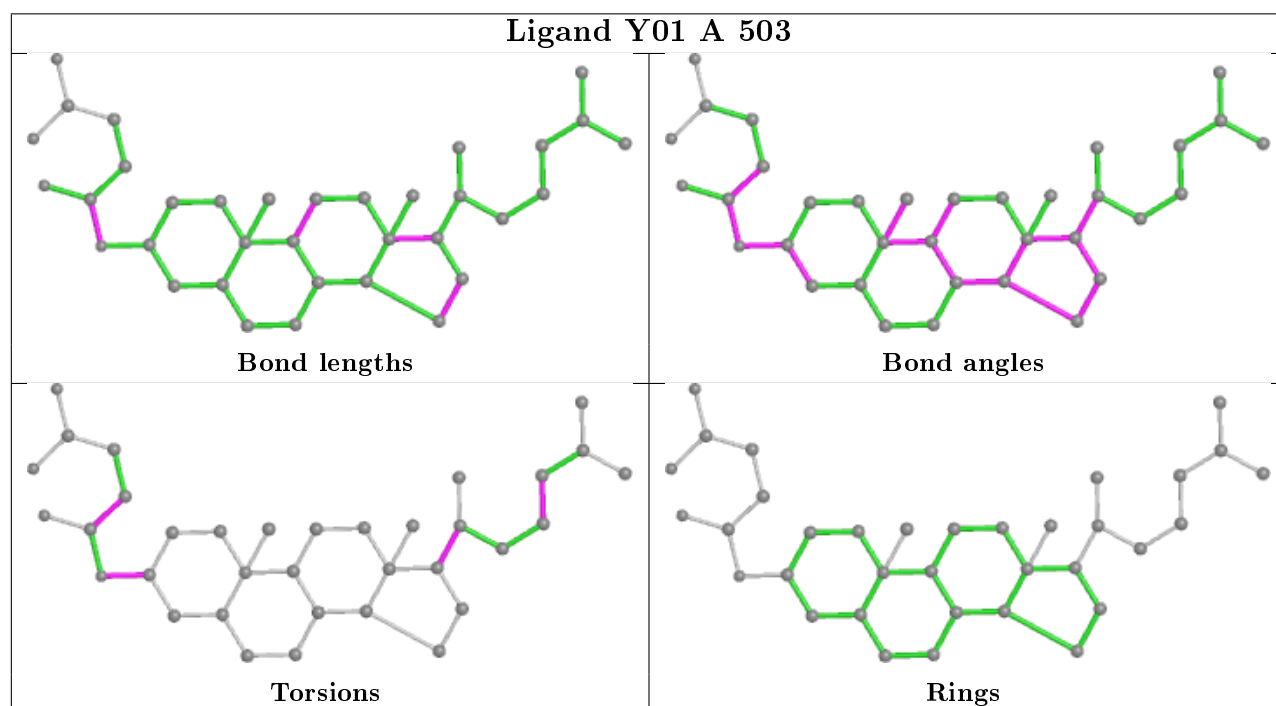
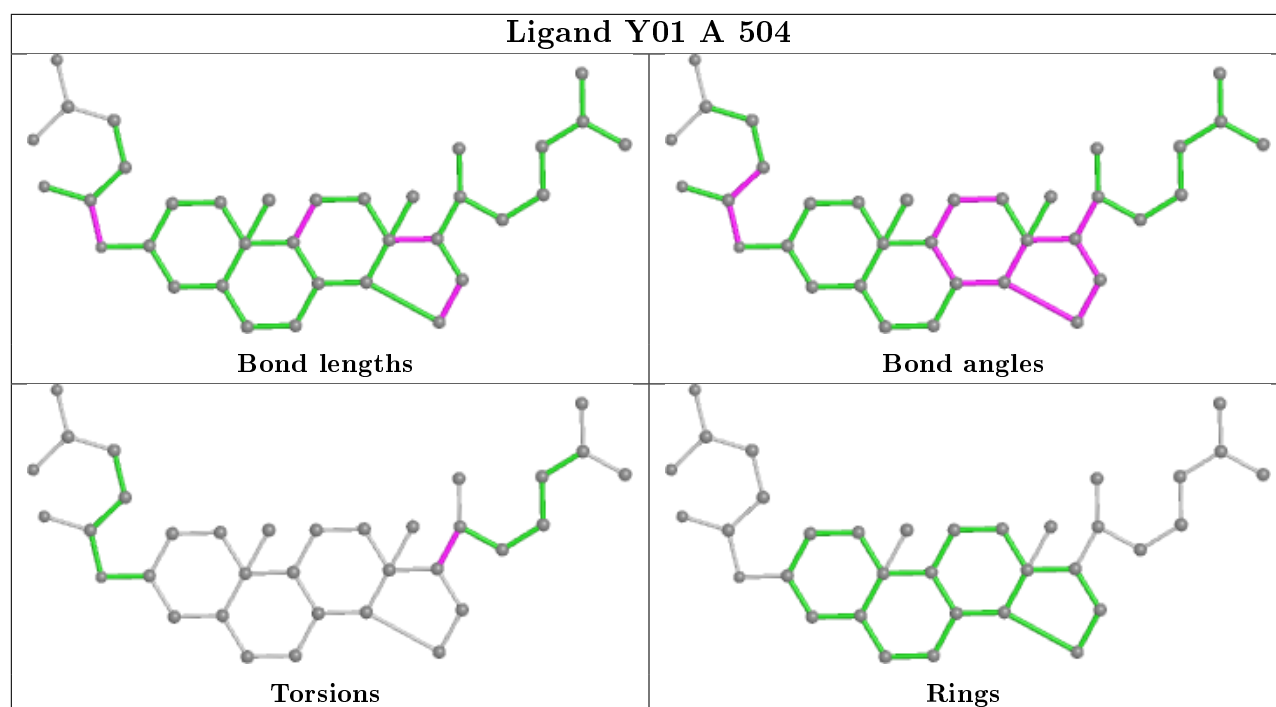
4 monomers are involved in 6 short contacts:

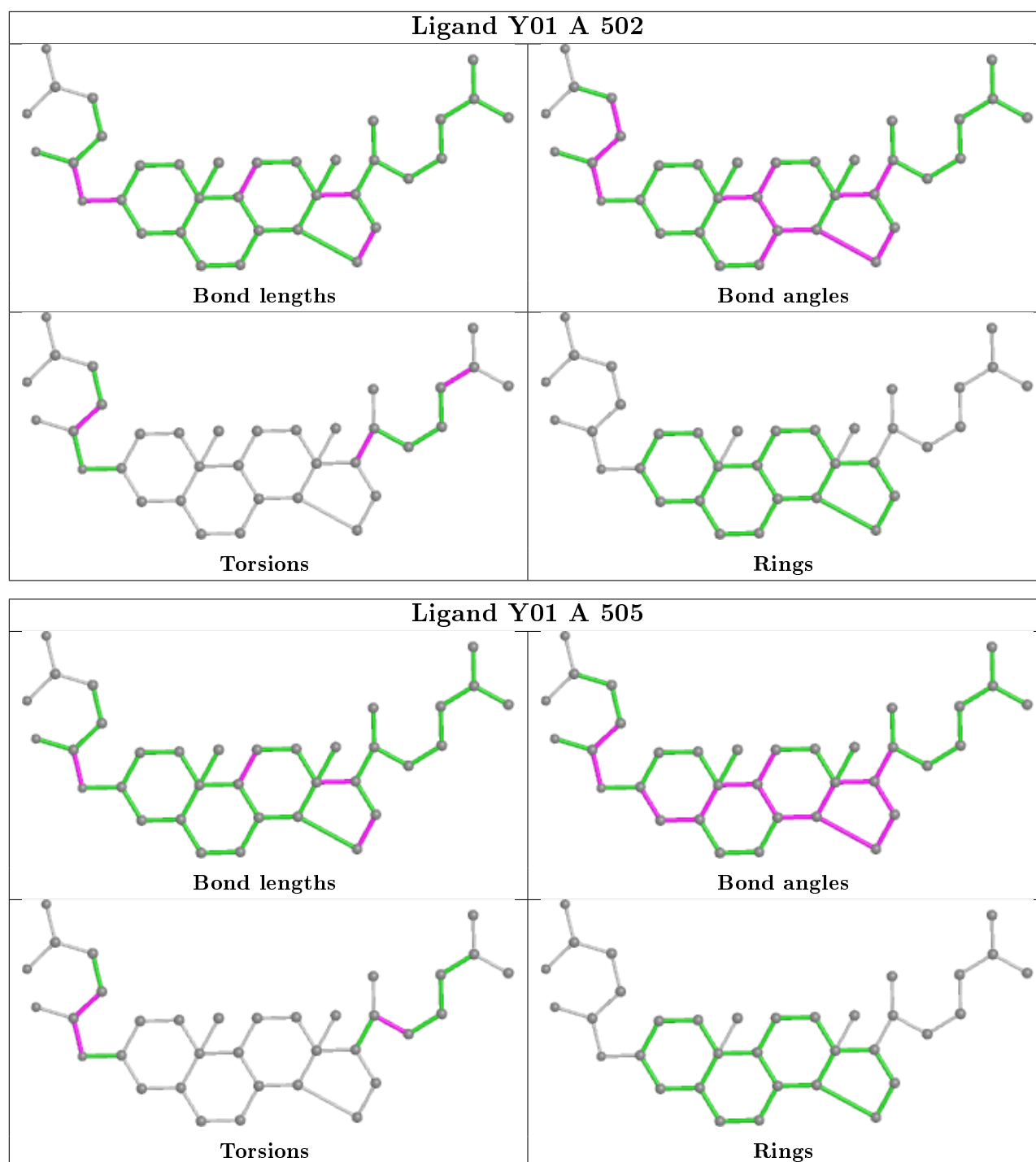


Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	506	OIN	1	0
4	A	504	Y01	4	0
4	A	503	Y01	1	0
4	A	505	Y01	3	0

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.







## 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	445/499 (89%)	0.55	26 (5%) 23 27	80, 117, 171, 214	0
2	C	69/69 (100%)	0.52	5 (7%) 15 18	102, 129, 165, 173	0
All	All	514/568 (90%)	0.54	31 (6%) 21 25	80, 120, 170, 214	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	TRP	5.2
2	C	11	PHE	4.0
2	C	10	TRP	3.9
2	C	62	LYS	3.8
1	A	431	LEU	3.7
1	A	1132	LEU	3.7
1	A	1012	LEU	3.5
1	A	1130	VAL	3.3
1	A	1134	LYS	3.3
1	A	433	LEU	3.2
1	A	18	PRO	2.9
1	A	1125	TRP	2.9
2	C	65	LYS	2.8
1	A	79	MET	2.8
1	A	1138	TYR	2.7
1	A	1142	PRO	2.6
1	A	1128	ALA	2.6
1	A	80	ASN	2.6
1	A	184	SER	2.6
1	A	1129	ALA	2.5
1	A	1028	ILE	2.5
1	A	1126	ASP	2.5
1	A	1113	PHE	2.5
1	A	167	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	436	ARG	2.4
1	A	1051	ARG	2.3
1	A	131	LEU	2.3
1	A	86	LEU	2.2
1	A	392	LYS	2.1
1	A	1117	LEU	2.1
2	C	3	CYS	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](#)

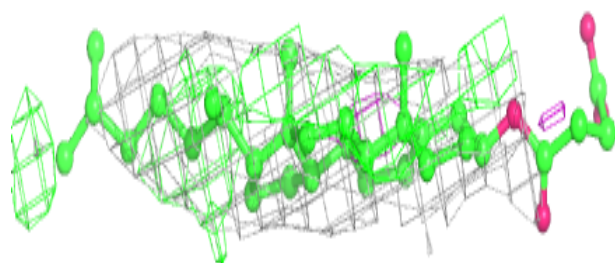
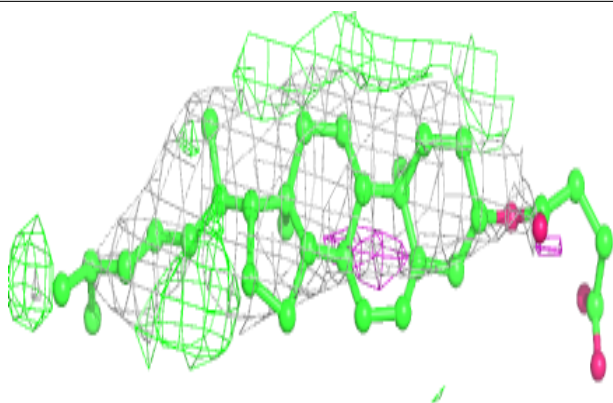
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	Y01	A	504	35/35	0.71	0.42	90,138,204,206	0
4	Y01	A	505	35/35	0.76	0.73	127,179,211,216	0
4	Y01	A	503	35/35	0.87	0.52	107,142,169,175	0
4	Y01	A	502	35/35	0.89	0.23	92,117,140,145	0
5	OIN	A	506	21/21	0.93	0.23	85,102,115,133	0
3	ACM	A	501	4/4	0.95	0.18	134,159,164,182	0

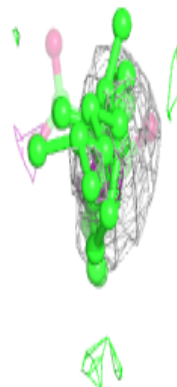
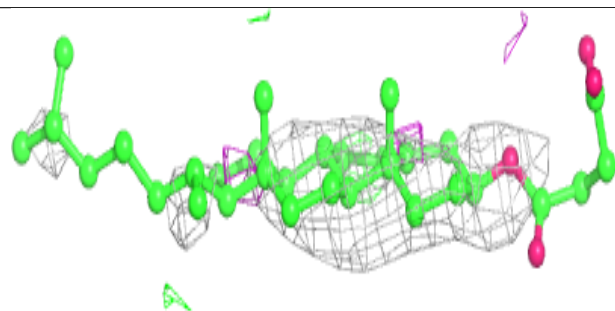
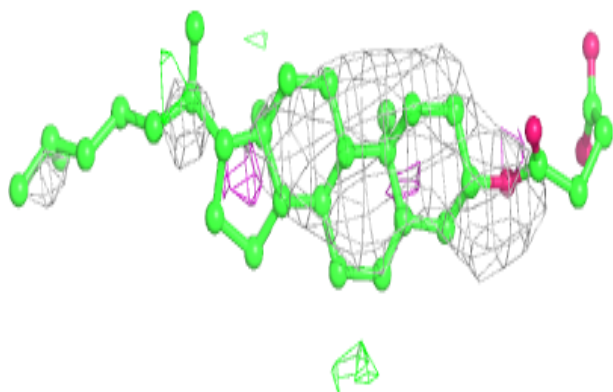
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around Y01 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)

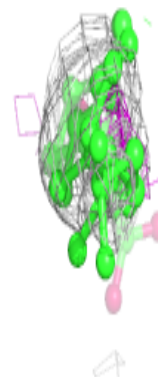
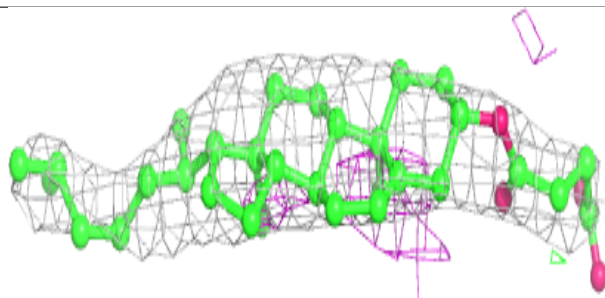
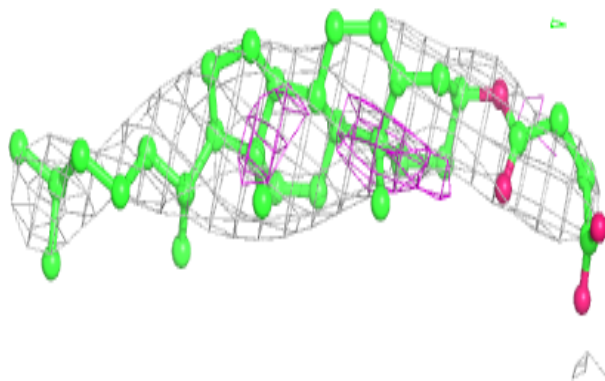
**Electron density around Y01 A 505:**

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

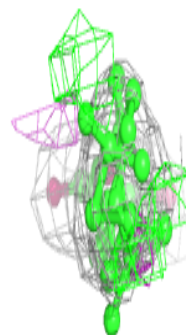
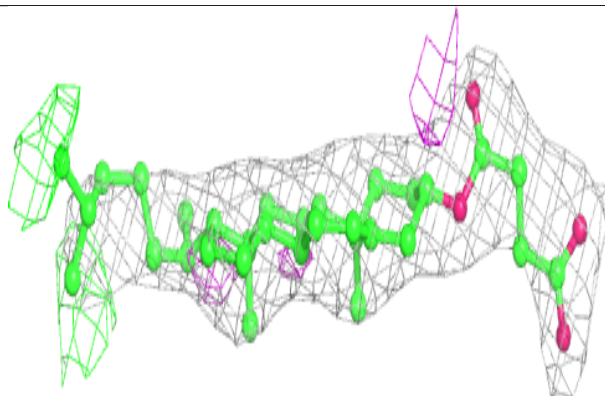
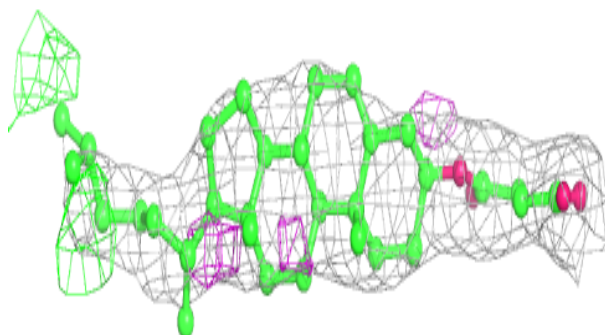


**Electron density around Y01 A 503:**

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

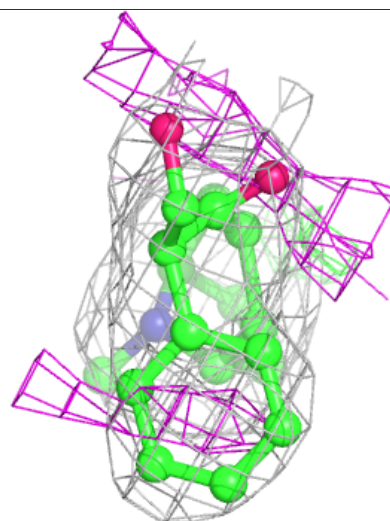
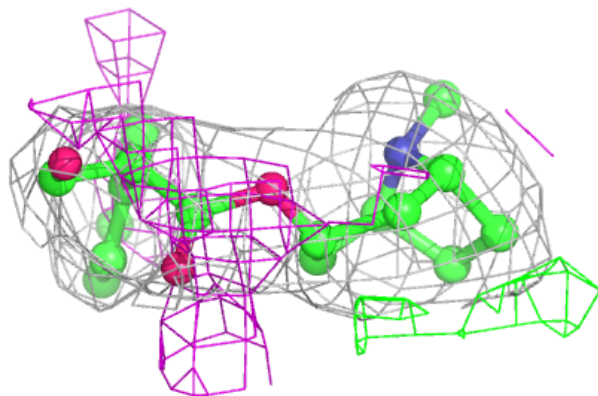
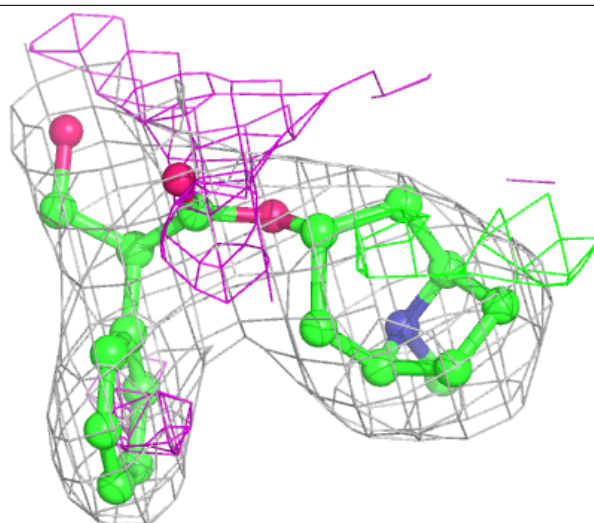
**Electron density around Y01 A 502:**

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



**Electron density around OIN A 506:**

$2mF_o-DF_c$  (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.