



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:27 am BST

PDB ID : 3ZPR  
Title : Thermostabilised turkey beta1 adrenergic receptor with 4-methyl-2-(piperazin-1-yl) quinoline bound  
Authors : Christopher, J.A.; Congreve, M.; Dore, A.S.; Marshall, F.H.; Myszka, D.G.; Brown, J.; Koglin, M.; Tehan, B.; Errey, J.C.; Tate, C.G.; Warne, T.  
Deposited on : 2013-03-01  
Resolution : 2.70 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 : 2.11  
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) : 2.11

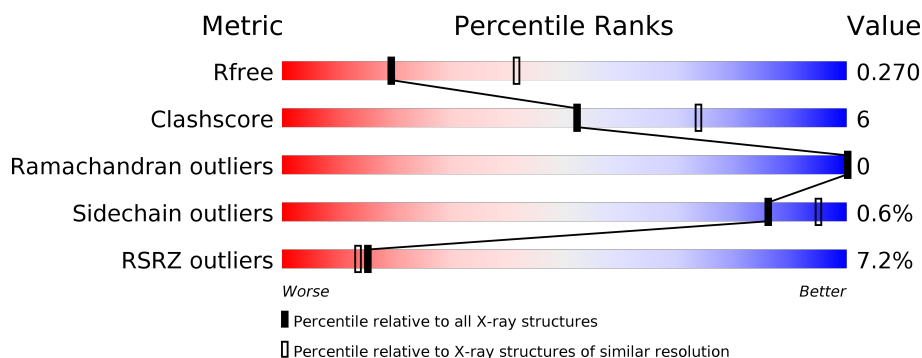
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	315	
1	B	315	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4952 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 BETA-1 ADRENERGIC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2244	1483	366	375	20			
1	B	298	Total	C	N	O	S	0	0	0
			2370	1559	396	395	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	expression tag	UNP P07700
A	32	GLY	-	expression tag	UNP P07700
A	369	HIS	-	expression tag	UNP P07700
A	370	HIS	-	expression tag	UNP P07700
A	371	HIS	-	expression tag	UNP P07700
A	372	HIS	-	expression tag	UNP P07700
A	373	HIS	-	expression tag	UNP P07700
A	68	SER	ARG	engineered mutation	UNP P07700
A	90	VAL	MET	engineered mutation	UNP P07700
A	116	LEU	CYS	engineered mutation	UNP P07700
A	227	ALA	TYR	engineered mutation	UNP P07700
A	282	LEU	ALA	engineered mutation	UNP P07700
A	327	ALA	PHE	engineered mutation	UNP P07700
A	338	MET	PHE	engineered mutation	UNP P07700
A	358	ALA	CYS	engineered mutation	UNP P07700
B	31	MET	-	expression tag	UNP P07700
B	32	GLY	-	expression tag	UNP P07700
B	369	HIS	-	expression tag	UNP P07700
B	370	HIS	-	expression tag	UNP P07700
B	371	HIS	-	expression tag	UNP P07700
B	372	HIS	-	expression tag	UNP P07700
B	373	HIS	-	expression tag	UNP P07700
B	68	SER	ARG	engineered mutation	UNP P07700
B	90	VAL	MET	engineered mutation	UNP P07700
B	116	LEU	CYS	engineered mutation	UNP P07700

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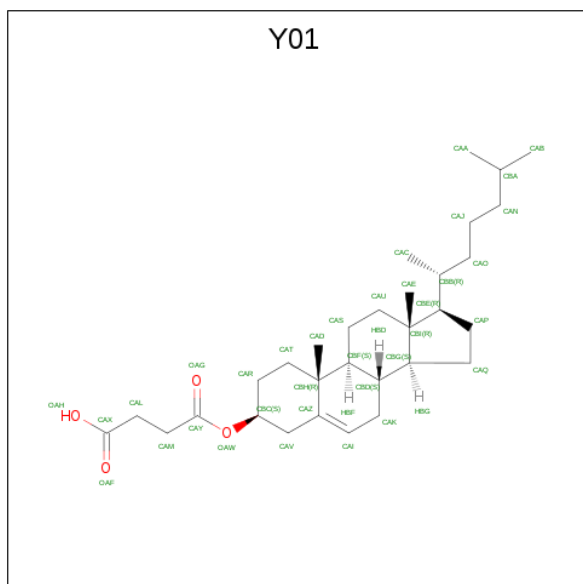
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Chain	Residue	Modelled	Actual	Comment	Reference
B	227	ALA	TYR	engineered mutation	UNP P07700
B	282	LEU	ALA	engineered mutation	UNP P07700
B	327	ALA	PHE	engineered mutation	UNP P07700
B	338	MET	PHE	engineered mutation	UNP P07700
B	358	ALA	CYS	engineered mutation	UNP P07700

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

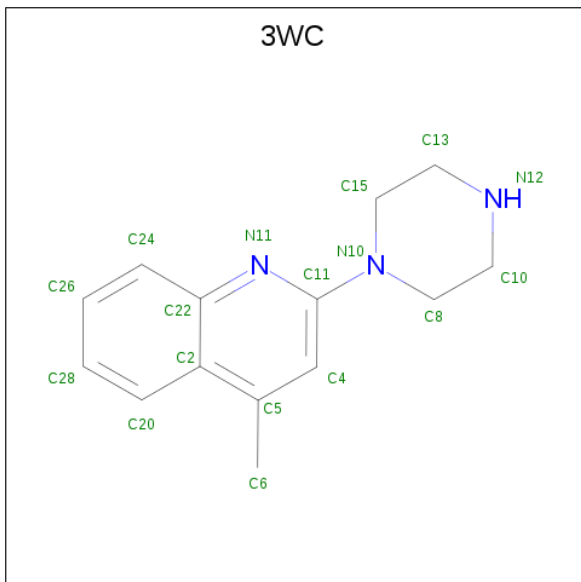
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Na 2 2	0	0
2	A	2	Total Na 2 2	0	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



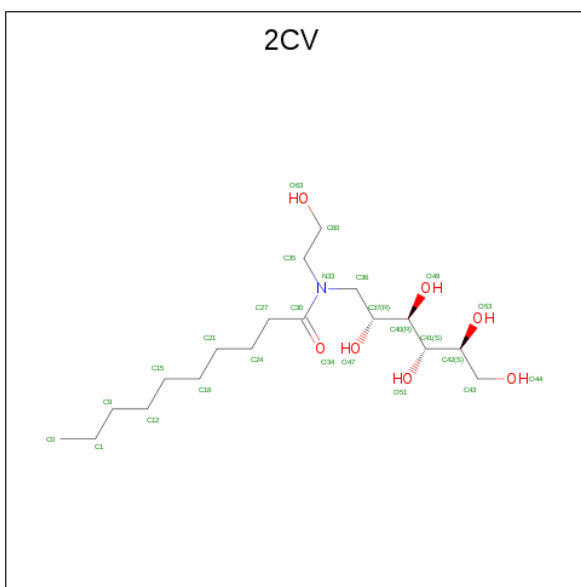
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 35	C 31	O 4	0	0
3	A	1	Total 35	C 31	O 4	0	0
3	B	1	Total 35	C 31	O 4	0	0
3	B	1	Total 35	C 31	O 4	0	0

- Molecule 4 is 4-METHYL-2-(PIPERAZIN-1-YL) QUINOLINE (three-letter code: 3WC) (formula:  $C_{14}H_{17}N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			17	14	3		
4	B	1	Total	C	N	0	0
			17	14	3		

- Molecule 5 is HEGA-10 (three-letter code: 2CV) (formula:  $C_{18}H_{37}NO_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 12 1 1	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C N O 21 16 1 4	0	0
5	B	1	Total C N O 26 18 1 7	0	0
5	B	1	Total C N O 14 12 1 1	0	0
5	B	1	Total C N O 12 10 1 1	0	0
5	B	1	Total C N O 17 14 1 2	0	0
5	B	1	Total C N O 14 12 1 1	0	0

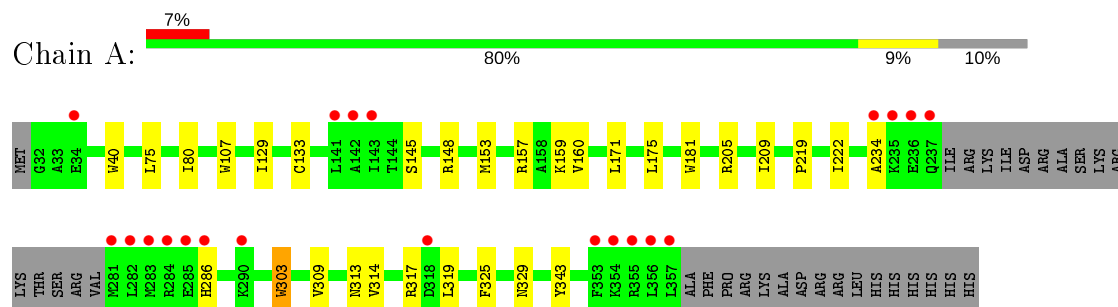
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	18	Total O 18 18	0	0
6	B	17	Total O 17 17	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: BETA-1 ADRENERGIC RECEPTOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.97Å 60.81Å 101.18Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	95.55 – 2.70 49.45 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (95.55-2.70) 95.8 (49.45-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.224 , 0.266 0.220 , 0.270	Depositor DCC
$R_{free}$ test set	1416 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: NA, 2CV, Y01, 3WC

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	0.64	4/2298 (0.2%)	0.66	0/3133
1	B	0.61	1/2425 (0.0%)	0.66	0/3301
All	All	0.62	5/4723 (0.1%)	0.66	0/6434

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	TRP	CD2-CE2	6.45	1.49	1.41
1	A	40	TRP	CD2-CE2	6.31	1.49	1.41
1	A	181	TRP	CD2-CE2	5.29	1.47	1.41
1	A	107	TRP	CD2-CE2	5.17	1.47	1.41
1	A	303	TRP	CD2-CE2	5.09	1.47	1.41

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	2244	0	2319	25	0
1	B	2370	0	2468	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	70	0	98	6	0
3	B	70	0	98	6	0
4	A	17	0	17	2	0
4	B	17	0	17	1	0
5	A	42	0	59	2	0
5	B	83	0	117	13	0
6	A	18	0	0	0	0
6	B	17	0	0	0	0
All	All	4952	0	5193	56	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 (56) 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)
5:B:501:2CV:H601	5:B:501:2CV:C27	1.84	1.08
1:A:159:LYS:HE2	3:A:402:Y01:HAL2	1.36	1.08
3:B:402:Y01:HAC1	3:B:402:Y01:HAE2	1.18	1.07
1:A:205:ARG:NH1	5:B:505:2CV:H361	1.72	1.04
1:A:175:LEU:HD13	1:B:175:LEU:HD22	1.50	0.93
5:B:501:2CV:H271	5:B:501:2CV:H601	1.53	0.88
5:B:501:2CV:H272	5:B:501:2CV:H601	1.53	0.88
1:A:171:LEU:HD12	1:B:175:LEU:HD23	1.59	0.83
1:A:205:ARG:HH12	5:B:505:2CV:H361	1.44	0.78
1:A:175:LEU:CD1	1:B:175:LEU:HD22	2.14	0.78
1:A:175:LEU:HD22	1:B:171:LEU:HD12	1.66	0.77
1:A:175:LEU:HD22	1:B:171:LEU:CD1	2.16	0.76
5:B:501:2CV:C60	5:B:501:2CV:H271	2.16	0.75
3:B:402:Y01:HAC1	3:B:402:Y01:CAE	2.03	0.75
3:B:402:Y01:CAC	3:B:402:Y01:HAE2	2.08	0.73
5:A:503:2CV:H602	5:A:503:2CV:H271	1.73	0.71
5:A:503:2CV:C60	5:A:503:2CV:H271	2.24	0.68
1:A:205:ARG:HH11	5:B:505:2CV:H361	1.57	0.67
1:A:319:LEU:O	1:A:319:LEU:HD12	1.96	0.66
1:A:171:LEU:CD1	1:B:175:LEU:HD23	2.30	0.61
3:A:402:Y01:OAG	3:A:402:Y01:HAV1	2.02	0.59
1:B:234:ALA:HB1	1:B:286:HIS:CE1	2.38	0.59
1:A:234:ALA:HB1	1:A:286:HIS:CE1	2.39	0.57
1:A:75:LEU:HD13	1:A:153:MET:HG3	1.88	0.56
3:A:402:Y01:HAC1	3:A:402:Y01:HAE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HG13	1:B:219:PRO:HB2	1.88	0.55
3:A:401:Y01:HAL2	5:B:505:2CV:H212	1.89	0.55
1:B:139:ARG:NH1	5:B:503:2CV:H151	2.21	0.54
1:B:209:ILE:HD11	1:B:314:VAL:HG11	1.89	0.54
3:A:401:Y01:OAG	3:A:401:Y01:CAV	2.52	0.54
1:B:75:LEU:HD13	1:B:153:MET:HG3	1.92	0.51
1:A:133:CYS:SG	1:A:222:ILE:HG22	2.51	0.50
1:A:157:ARG:HG2	3:B:401:Y01:HAL2	1.94	0.49
1:A:209:ILE:HD11	1:A:314:VAL:HG11	1.95	0.49
1:B:142:ALA:HB1	5:B:503:2CV:H242	1.94	0.49
1:B:80:ILE:HD12	1:B:343:TYR:OH	2.13	0.48
1:A:303:TRP:CH2	4:A:500:3WC:H132	2.50	0.47
4:A:500:3WC:H20	4:A:500:3WC:H61C	1.80	0.47
3:A:402:Y01:OAG	3:A:402:Y01:CAV	2.63	0.46
1:A:129:ILE:HG13	1:A:219:PRO:HB2	1.98	0.45
1:B:185:GLU:HG3	5:B:501:2CV:O47	2.17	0.45
1:A:80:ILE:HD12	1:A:343:TYR:OH	2.16	0.45
1:A:309:VAL:CG1	1:A:325:PHE:CD1	3.00	0.45
3:B:402:Y01:HAJ1	3:B:402:Y01:CAP	2.47	0.44
1:B:234:ALA:HB1	1:B:286:HIS:HE1	1.82	0.44
1:A:133:CYS:SG	1:A:222:ILE:CG2	3.05	0.44
4:B:500:3WC:H20	4:B:500:3WC:H61C	1.79	0.44
1:A:205:ARG:HG2	1:A:314:VAL:HG13	2.00	0.42
5:B:502:2CV:H121	5:B:502:2CV:H212	1.81	0.42
1:B:139:ARG:NE	1:B:139:ARG:HA	2.34	0.42
1:A:313:ASN:O	1:A:317:ARG:HD3	2.20	0.41
1:B:241:ILE:HG23	1:B:279:ARG:NH1	2.35	0.41
1:A:160:VAL:HG11	3:B:401:Y01:HAM2	2.02	0.41
1:B:231:TYR:HD1	5:B:502:2CV:H181	1.85	0.41
1:A:145:SER:OG	1:A:148:ARG:HB2	2.21	0.40
1:B:241:ILE:HD13	1:B:282:LEU:HD22	2.03	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	279/315 (89%)	272 (98%)	7 (2%)	0	100	100
1	B	296/315 (94%)	288 (97%)	8 (3%)	0	100	100
All	All	575/630 (91%)	560 (97%)	15 (3%)	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	244/273 (89%)	243 (100%)	1 (0%)	91	97
1	B	258/273 (94%)	256 (99%)	2 (1%)	81	93
All	All	502/546 (92%)	499 (99%)	3 (1%)	86	95

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

Mol	Chain	Res	Type
1	A	329	ASN
1	B	241	ILE
1	B	329	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	A	329	ASN
1	B	286	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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$
5	2CV	B	502	-	13,13,25	0.67	0	14,14,30	0.64	0
5	2CV	B	505	-	16,16,25	0.89	1 (6%)	17,18,30	0.54	0
3	Y01	A	401	-	35,38,38	1.24	3 (8%)	54,57,57	2.46	13 (24%)
3	Y01	B	401	-	35,38,38	1.14	2 (5%)	54,57,57	1.99	12 (22%)
5	2CV	B	501	-	25,25,25	0.55	0	29,30,30	1.11	3 (10%)
3	Y01	B	402	-	35,38,38	1.15	2 (5%)	54,57,57	1.45	7 (12%)
4	3WC	A	500	-	19,19,19	1.87	4 (21%)	24,26,26	1.63	5 (20%)
5	2CV	B	506	-	13,13,25	0.73	0	14,14,30	0.75	1 (7%)
5	2CV	A	503	-	20,20,25	0.69	0	22,23,30	0.86	1 (4%)
5	2CV	B	503	-	11,11,25	0.65	0	11,11,30	0.41	0
5	2CV	A	501	-	13,13,25	0.79	1 (7%)	14,14,30	0.62	0
4	3WC	B	500	-	19,19,19	1.78	4 (21%)	24,26,26	1.89	6 (25%)
3	Y01	A	402	-	35,38,38	1.27	2 (5%)	54,57,57	1.43	7 (12%)
5	2CV	A	502	-	6,6,25	0.51	0	5,5,30	0.26	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	2CV	B	502	-	-	3/13/13/34	-
5	2CV	B	505	-	-	7/17/17/34	-
3	Y01	A	401	-	-	9/17/77/77	0/4/4/4
3	Y01	B	401	-	-	12/17/77/77	0/4/4/4
5	2CV	B	501	-	-	19/34/34/34	-
3	Y01	B	402	-	-	14/17/77/77	0/4/4/4
4	3WC	A	500	-	-	0/4/12/12	0/3/3/3
5	2CV	B	506	-	-	3/13/13/34	-
5	2CV	A	503	-	-	10/24/24/34	-
5	2CV	B	503	-	-	4/9/9/34	-
5	2CV	A	501	-	-	3/13/13/34	-
4	3WC	B	500	-	-	0/4/12/12	0/3/3/3
3	Y01	A	402	-	-	10/17/77/77	0/4/4/4
5	2CV	A	502	-	-	2/4/4/34	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	3WC	C6-C5	-5.64	1.40	1.51
3	B	402	Y01	CAK-CAI	-4.99	1.39	1.50
3	A	402	Y01	CAK-CAI	-4.56	1.40	1.50
4	B	500	3WC	C6-C5	-4.46	1.42	1.51
3	B	401	Y01	CAK-CAI	-4.43	1.40	1.50
3	A	401	Y01	CAK-CAI	-4.29	1.40	1.50
3	A	402	Y01	CAI-CAZ	3.57	1.40	1.33
3	A	401	Y01	CAI-CAZ	3.25	1.40	1.33
4	B	500	3WC	C8-N10	3.14	1.51	1.46
3	B	402	Y01	CAI-CAZ	3.04	1.39	1.33
3	B	401	Y01	CAI-CAZ	2.87	1.39	1.33
4	A	500	3WC	C22-N11	-2.61	1.33	1.37
4	A	500	3WC	C11-N11	2.31	1.35	1.32
4	B	500	3WC	C11-N11	2.16	1.35	1.32
4	B	500	3WC	C22-N11	-2.16	1.34	1.37
3	A	401	Y01	CAK-CBD	2.15	1.56	1.53
5	B	505	2CV	C36-N33	2.07	1.48	1.46
4	A	500	3WC	C28-C20	2.06	1.41	1.36
5	A	501	2CV	C27-C30	2.05	1.55	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	Y01	OAW-CBC-CAV	10.82	130.26	108.12
3	B	401	Y01	OAW-CBC-CAV	8.55	125.61	108.12
3	A	401	Y01	CAR-CBC-CAV	-7.96	99.12	110.99
4	B	500	3WC	C11-N11-C22	5.65	123.76	117.49
3	A	401	Y01	CBC-CAV-CAZ	-5.10	103.59	111.52
3	B	401	Y01	CAR-CBC-CAV	-4.62	104.11	110.99
3	A	402	Y01	OAW-CBC-CAV	4.49	117.32	108.12
3	B	402	Y01	CAR-CBC-CAV	-4.32	104.54	110.99
3	A	401	Y01	OAW-CAY-CAM	3.86	119.81	111.50
3	A	402	Y01	OAW-CAY-CAM	3.85	119.80	111.50
4	A	500	3WC	C5-C2-C22	3.67	120.00	118.01
3	B	402	Y01	OAW-CAY-CAM	3.67	119.41	111.50
3	A	401	Y01	CBI-CBE-CBB	-3.56	113.91	119.49
3	B	401	Y01	OAW-CAY-CAM	3.54	119.13	111.50
3	B	402	Y01	OAW-CBC-CAV	3.47	115.22	108.12
4	A	500	3WC	C15-N10-C8	3.37	118.95	111.52
3	B	401	Y01	CAV-CAZ-CBH	3.13	120.57	116.42
3	B	401	Y01	CBH-CAZ-CAI	-3.06	118.22	122.90
3	B	401	Y01	CBC-CAV-CAZ	-3.02	106.83	111.52
4	A	500	3WC	C11-N11-C22	2.96	120.77	117.49
3	A	402	Y01	CAK-CBD-CBF	2.95	113.29	109.71
3	B	401	Y01	CAQ-CBG-CBI	-2.94	100.30	103.84
3	A	402	Y01	CAR-CBC-CAV	-2.94	106.60	110.99
3	A	401	Y01	CAQ-CBG-CBD	-2.93	114.26	119.08
4	B	500	3WC	C15-N10-C8	2.89	117.89	111.52
4	B	500	3WC	C2-C22-N11	-2.88	119.76	122.81
3	B	401	Y01	CAO-CBB-CBE	2.71	115.89	110.28
3	A	401	Y01	CBH-CAZ-CAI	-2.62	118.90	122.90
4	B	500	3WC	C15-C13-N12	-2.61	104.35	111.12
3	A	401	Y01	CBH-CBF-CBD	-2.55	108.91	112.73
4	A	500	3WC	C10-C8-N10	-2.55	104.97	110.48
5	A	503	2CV	C27-C30-N33	-2.54	114.05	118.01
3	A	402	Y01	CAQ-CBG-CBD	-2.48	115.00	119.08
5	B	501	2CV	O49-C40-C41	2.47	115.23	109.47
3	A	401	Y01	OAW-CAY-OAG	-2.45	117.77	123.70
3	B	402	Y01	CAO-CBB-CBE	2.45	115.35	110.28
5	B	501	2CV	C37-C40-C41	-2.45	108.63	112.47
4	B	500	3WC	C24-C22-C2	2.44	121.93	119.13
4	A	500	3WC	C2-C22-N11	-2.43	120.23	122.81
3	B	401	Y01	CAC-CBB-CBE	-2.43	109.21	112.92
3	B	402	Y01	CBI-CBE-CBB	-2.40	115.72	119.49
3	A	401	Y01	CAQ-CBG-CBI	-2.38	100.98	103.84
3	B	402	Y01	CAV-CAZ-CBH	2.35	119.55	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	Y01	CAQ-CBG-CBI	-2.31	101.06	103.84
3	A	402	Y01	CAV-CAZ-CBH	2.30	119.48	116.42
3	B	401	Y01	CAT-CAR-CBC	-2.26	106.48	110.33
3	B	402	Y01	CAQ-CBG-CBD	-2.24	115.39	119.08
3	A	401	Y01	CBI-CBG-CBD	-2.19	111.14	114.38
3	B	401	Y01	OAW-CAY-OAG	-2.17	118.45	123.70
5	B	501	2CV	C60-C35-N33	2.17	118.17	112.55
4	B	500	3WC	C28-C20-C2	-2.12	117.95	120.89
3	A	401	Y01	CAO-CBB-CBE	2.06	114.55	110.28
3	A	401	Y01	CAT-CAR-CBC	-2.06	106.82	110.33
3	B	401	Y01	CBG-CBI-CBE	-2.02	97.69	100.07
5	B	506	2CV	C27-C30-N33	-2.01	115.10	118.11

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	505	2CV	N33-C36-C37-C40
5	B	505	2CV	N33-C36-C37-O47
3	A	401	Y01	CAV-CBC-OAW-CAY
3	B	402	Y01	CAC-CBB-CBE-CBI
3	B	402	Y01	CAR-CBC-OAW-CAY
5	A	503	2CV	N33-C36-C37-O47
5	A	503	2CV	C36-C37-C40-C41
5	A	503	2CV	C36-C37-C40-O49
5	A	503	2CV	O47-C37-C40-C41
3	B	401	Y01	CAX-CAL-CAM-CAY
3	A	402	Y01	CAV-CBC-OAW-CAY
5	B	501	2CV	C60-C35-N33-C30
5	B	501	2CV	N33-C35-C60-O63
5	B	501	2CV	N33-C36-C37-C40
5	B	501	2CV	N33-C36-C37-O47
5	B	501	2CV	C36-C37-C40-C41
5	B	501	2CV	C36-C37-C40-O49
5	B	501	2CV	O47-C37-C40-O49
5	B	501	2CV	C37-C40-C41-C42
5	B	501	2CV	C37-C40-C41-O51
5	B	501	2CV	O49-C40-C41-C42
5	B	501	2CV	O49-C40-C41-O51
5	B	501	2CV	O53-C42-C43-O44
3	B	402	Y01	CAO-CBB-CBE-CAP
3	A	401	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
3	B	402	Y01	CAC-CBB-CBE-CAP
5	B	501	2CV	C41-C42-C43-O44
5	B	505	2CV	C21-C24-C27-C30
5	B	506	2CV	C21-C24-C27-C30
5	A	501	2CV	C21-C24-C27-C30
3	A	401	Y01	CAO-CBB-CBE-CAP
5	B	501	2CV	O47-C37-C40-C41
3	A	401	Y01	CAO-CBB-CBE-CBI
3	B	401	Y01	CAO-CBB-CBE-CBI
3	B	401	Y01	CAR-CBC-OAW-CAY
3	A	401	Y01	CAN-CAJ-CAO-CBB
3	A	401	Y01	CAC-CBB-CBE-CBI
3	A	401	Y01	CAX-CAL-CAM-CAY
5	B	501	2CV	C60-C35-N33-C36
3	B	401	Y01	CAC-CBB-CBE-CAP
3	B	401	Y01	CAC-CBB-CBE-CBI
3	B	401	Y01	CAN-CAJ-CAO-CBB
5	A	503	2CV	N33-C35-C60-O63
3	B	402	Y01	CAN-CAJ-CAO-CBB
5	B	501	2CV	C37-C36-N33-C35
5	B	505	2CV	C9-C12-C15-C18
5	A	501	2CV	C12-C15-C18-C21
3	A	401	Y01	CAJ-CAN-CBA-CAA
3	A	402	Y01	CAO-CBB-CBE-CAP
5	A	502	2CV	C15-C18-C21-C24
5	B	503	2CV	C15-C12-C9-C1
3	B	402	Y01	OAG-CAY-OAW-CBC
3	B	402	Y01	CAM-CAY-OAW-CBC
5	B	506	2CV	C12-C15-C18-C21
5	A	501	2CV	C15-C18-C21-C24
5	B	505	2CV	C18-C21-C24-C27
3	A	401	Y01	CAJ-CAN-CBA-CAB
3	B	402	Y01	CAJ-CAN-CBA-CAB
5	A	503	2CV	O47-C37-C40-O49
5	B	501	2CV	C37-C36-N33-C30
5	B	502	2CV	C12-C15-C18-C21
3	B	402	Y01	CAO-CBB-CBE-CBI
5	A	502	2CV	C12-C15-C18-C21
3	A	402	Y01	CAX-CAL-CAM-CAY
5	B	506	2CV	C15-C18-C21-C24
3	B	402	Y01	CAJ-CAN-CBA-CAA
5	B	505	2CV	C15-C12-C9-C1

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Mol	Chain	Res	Type	Atoms
3	B	402	Y01	CAJ-CAO-CBB-CBE
5	B	501	2CV	C18-C21-C24-C27
3	B	401	Y01	OAG-CAY-OAW-CBC
3	A	402	Y01	CAC-CBB-CBE-CAP
3	B	401	Y01	CAJ-CAN-CBA-CAB
3	A	402	Y01	CAJ-CAN-CBA-CAA
3	B	401	Y01	CAJ-CAN-CBA-CAA
3	B	401	Y01	CAM-CAY-OAW-CBC
5	B	503	2CV	C0-C1-C9-C12
3	B	402	Y01	CAO-CAJ-CAN-CBA
3	A	402	Y01	CAJ-CAN-CBA-CAB
5	B	502	2CV	C0-C1-C9-C12
5	A	503	2CV	N33-C36-C37-C40
5	B	503	2CV	C18-C21-C24-C27
3	B	401	Y01	CAO-CBB-CBE-CAP
3	A	402	Y01	CAC-CBB-CBE-CBI
5	A	503	2CV	C18-C21-C24-C27
3	B	402	Y01	CAV-CBC-OAW-CAY
5	B	505	2CV	C15-C18-C21-C24
3	A	402	Y01	CAJ-CAO-CBB-CBE
3	A	402	Y01	OAG-CAY-OAW-CBC
3	B	402	Y01	CAJ-CAO-CBB-CAC
5	A	503	2CV	C15-C18-C21-C24
5	A	503	2CV	C37-C36-N33-C35
5	B	501	2CV	C15-C12-C9-C1
3	A	402	Y01	CAM-CAY-OAW-CBC
5	B	502	2CV	C9-C12-C15-C18
5	B	503	2CV	C9-C12-C15-C18
3	B	401	Y01	CAL-CAM-CAY-OAW

There are no ring outliers.

11 monomers are involved in 29 short contacts:

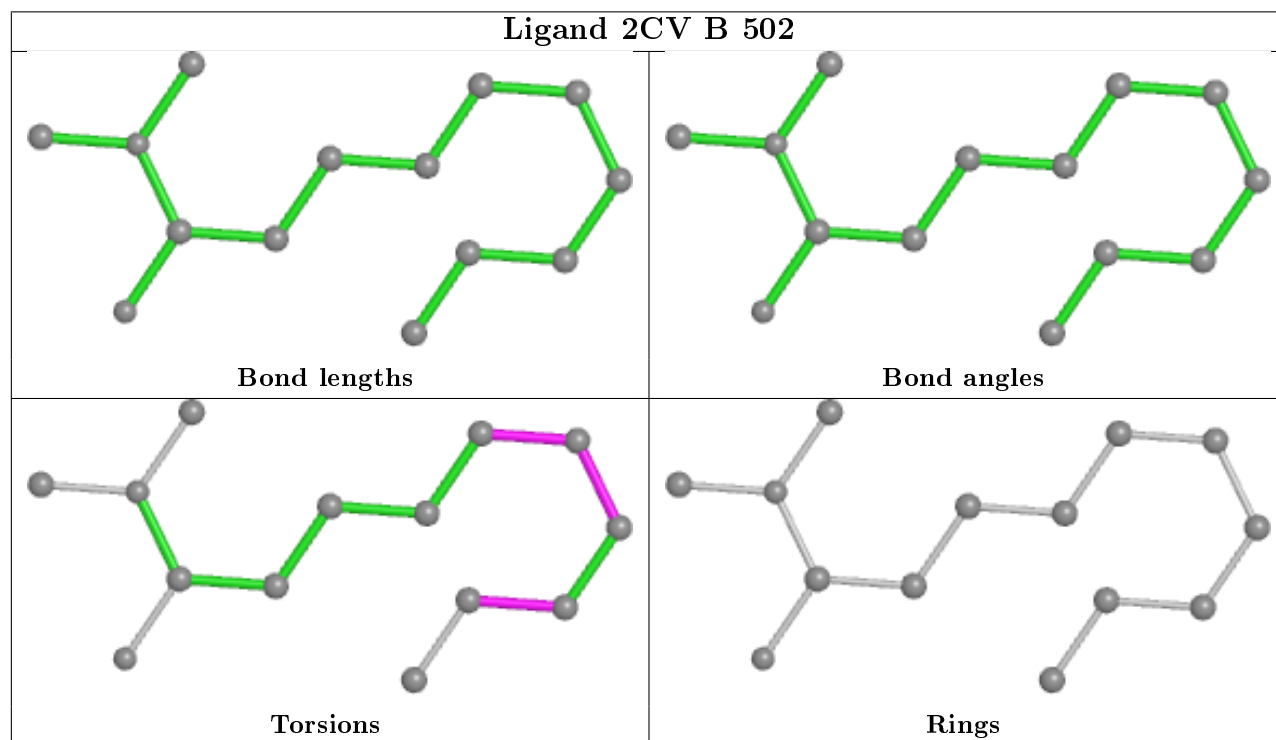
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	2CV	2	0
5	B	505	2CV	4	0
3	A	401	Y01	2	0
3	B	401	Y01	2	0
5	B	501	2CV	5	0
3	B	402	Y01	4	0
4	A	500	3WC	2	0
5	A	503	2CV	2	0

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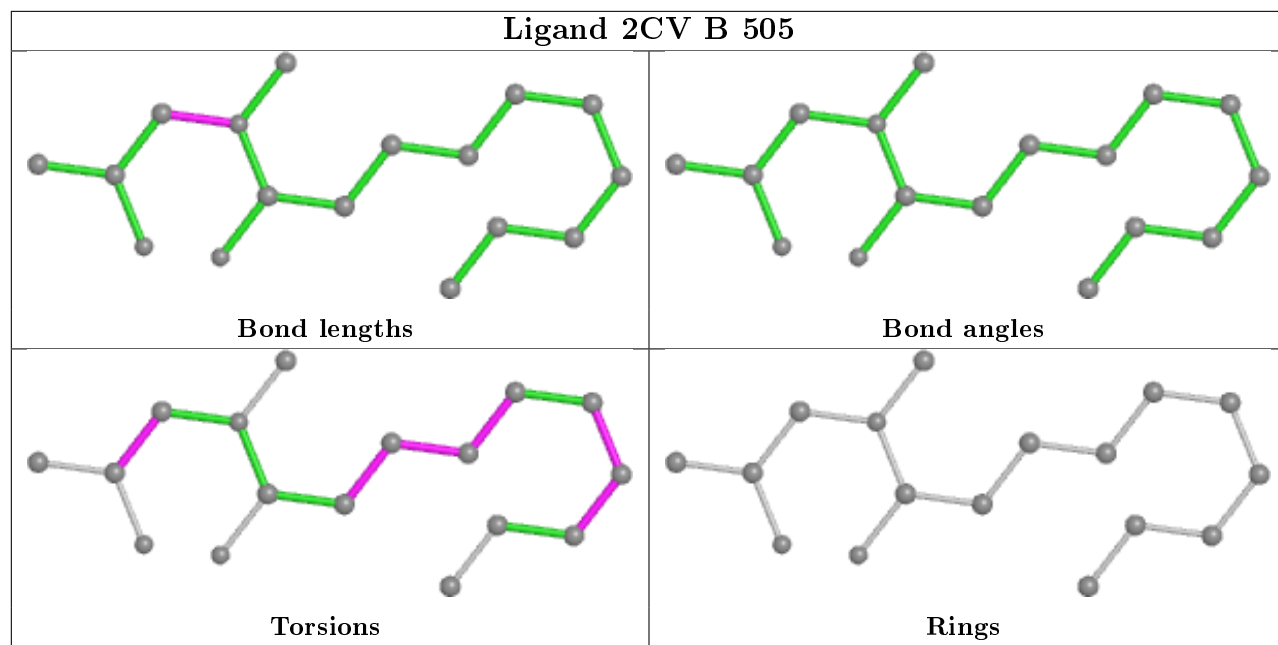
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	2CV	2	0
4	B	500	3WC	1	0
3	A	402	Y01	4	0

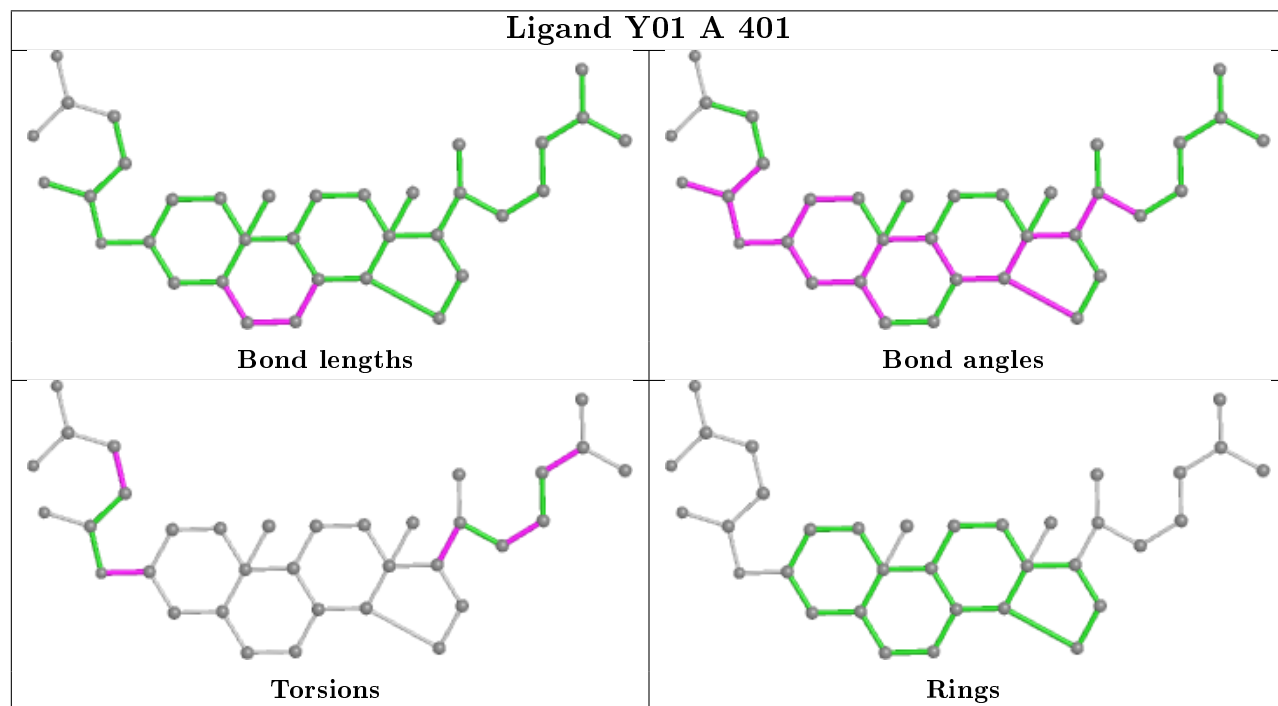
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



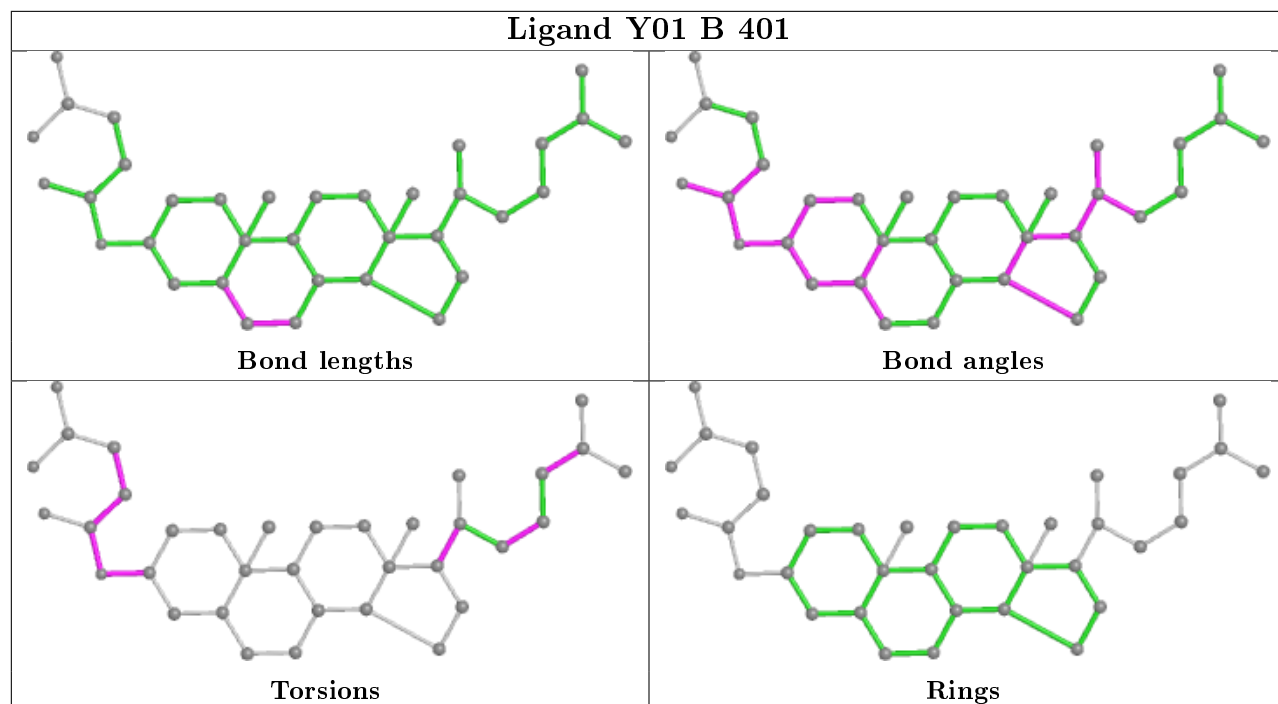
## Ligand 2CV B 505



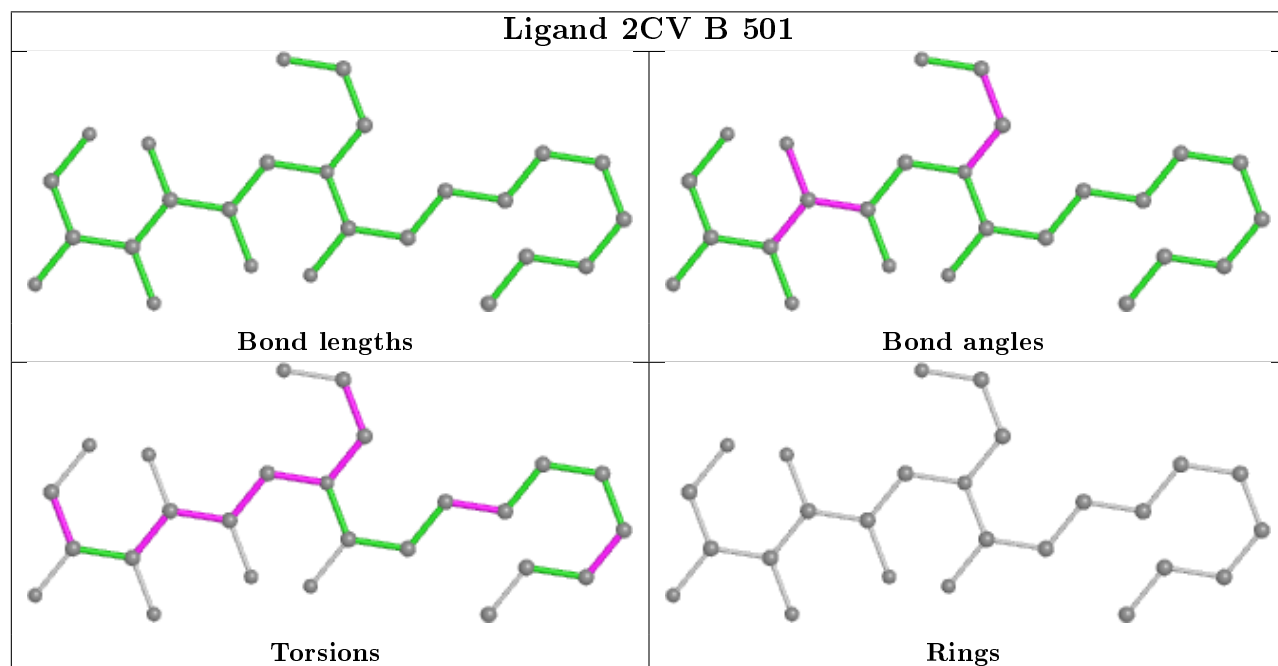
## Ligand Y01 A 401

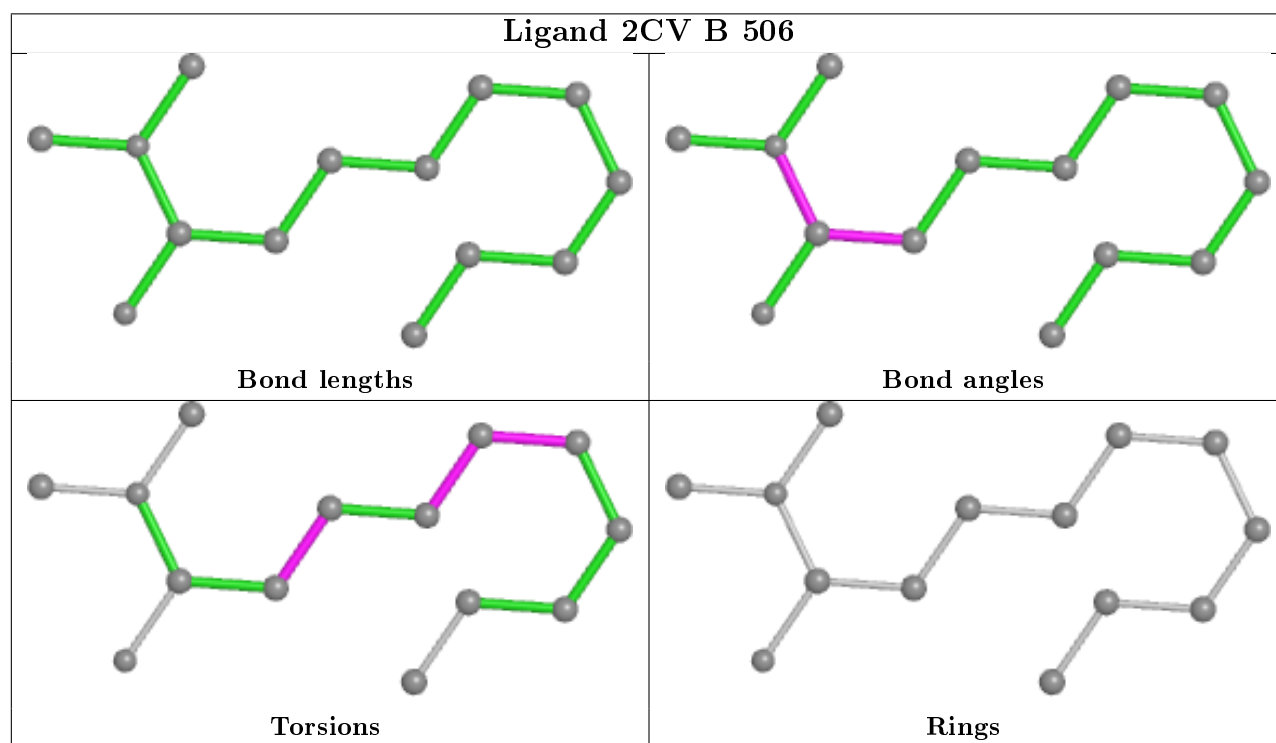
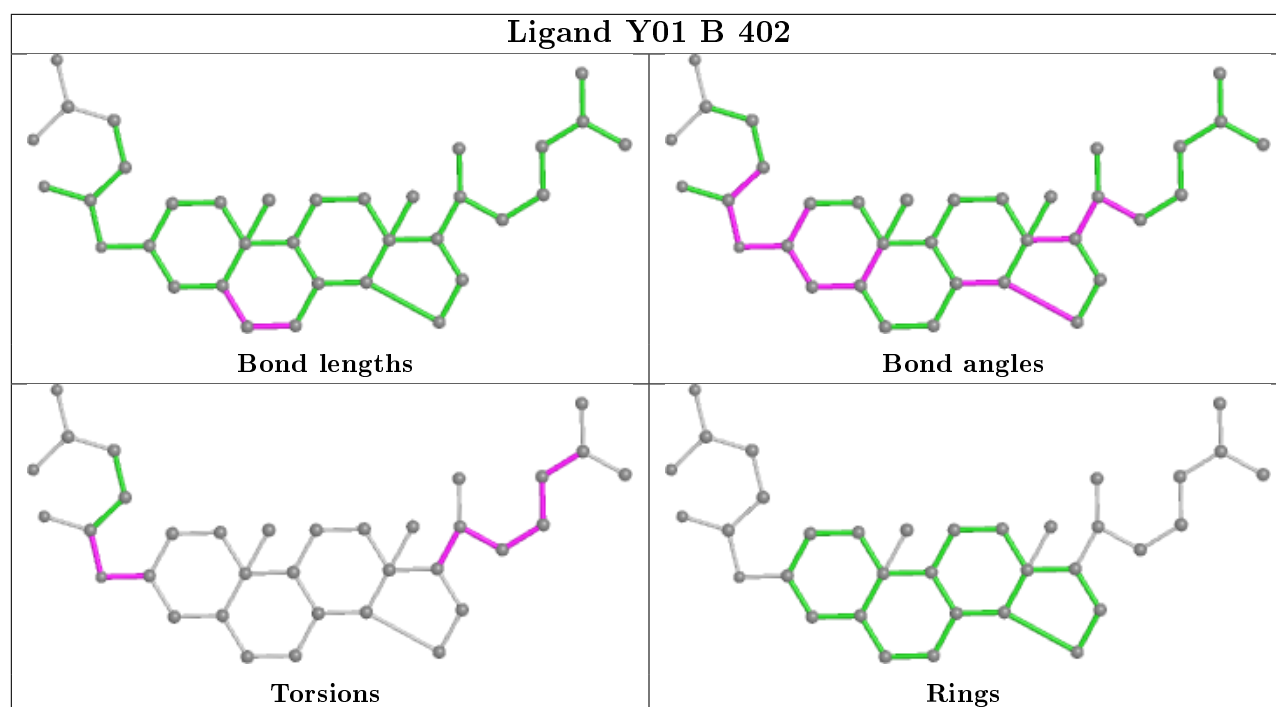


## Ligand Y01 B 401

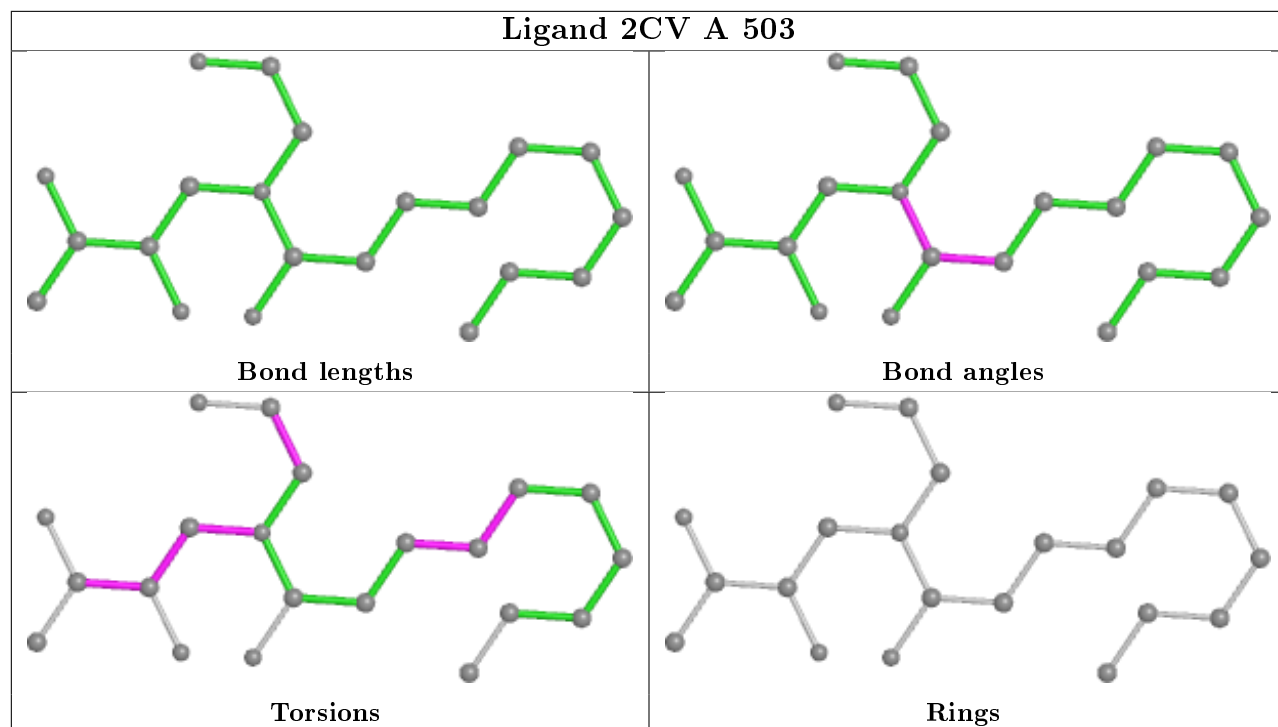


## Ligand 2CV B 501

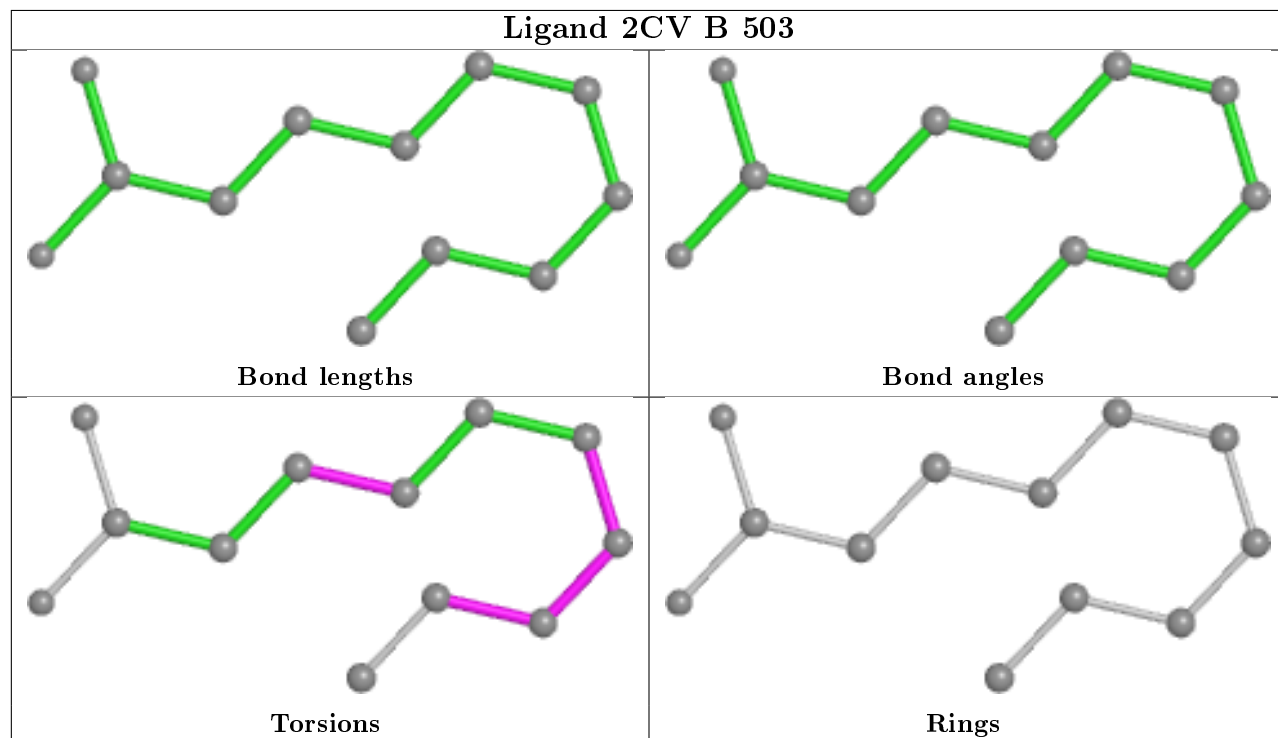




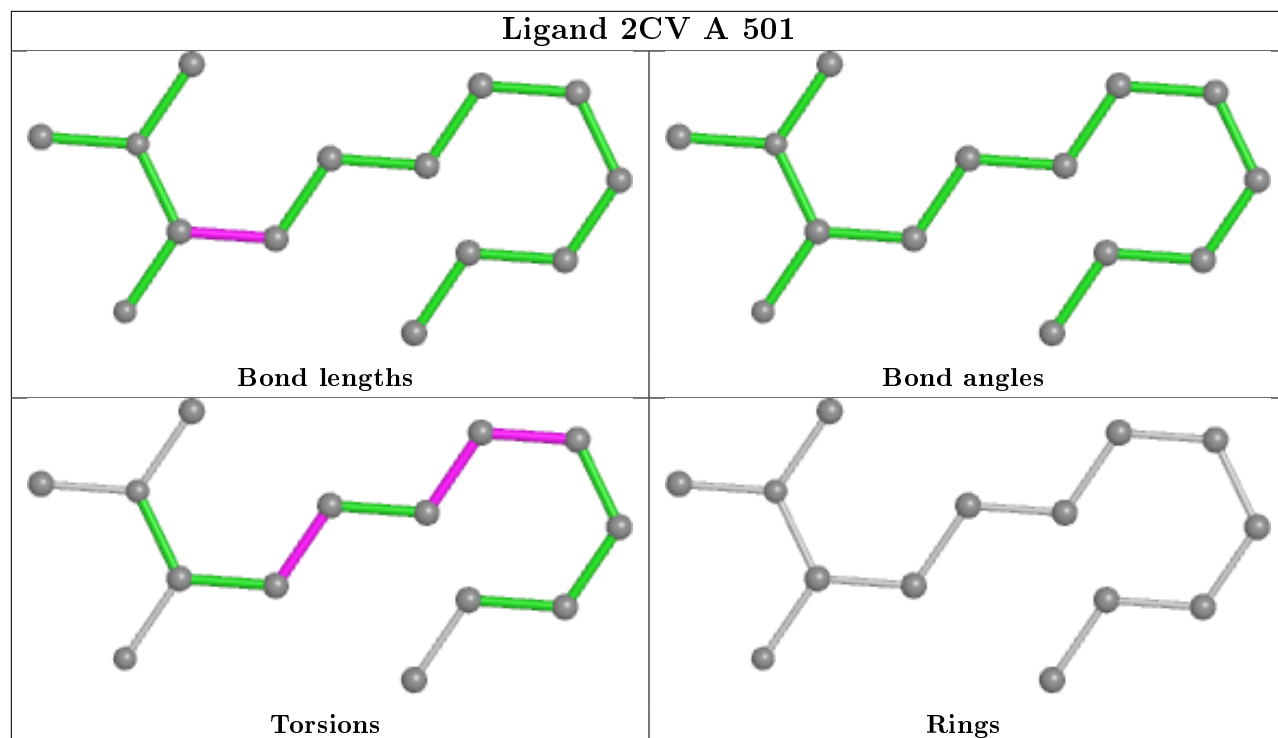
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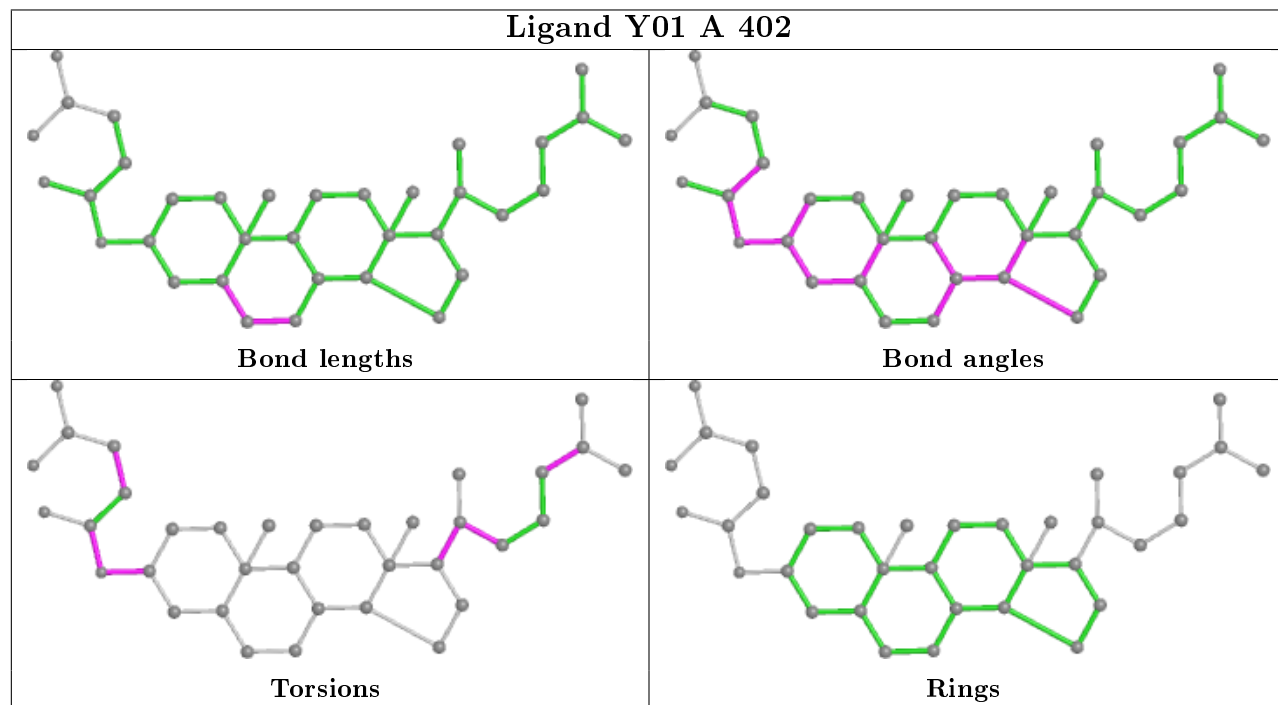
## Ligand 2CV B 503



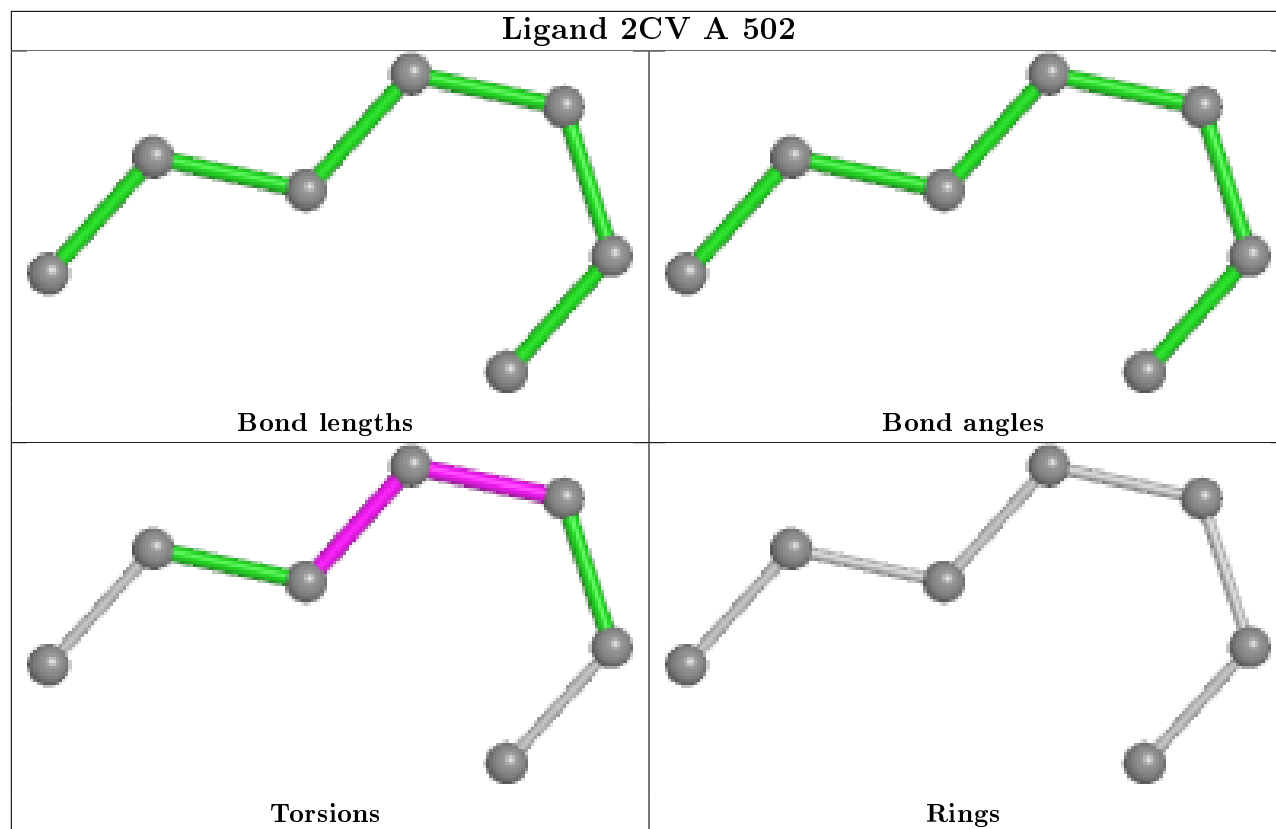
## Ligand 2CV A 501



## Ligand Y01 A 402







## 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	283/315 (89%)	0.33	21 (7%) 14 12	33, 53, 96, 144	0
1	B	298/315 (94%)	0.32	21 (7%) 16 14	33, 52, 84, 105	0
All	All	581/630 (92%)	0.32	42 (7%) 15 13	33, 53, 90, 144	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	MET	9.7
1	A	282	LEU	9.7
1	A	286	HIS	7.3
1	A	281	MET	6.7
1	B	277	THR	5.5
1	B	351	LYS	5.4
1	B	357	LEU	4.6
1	B	280	VAL	4.3
1	B	353	PHE	3.8
1	B	284	ARG	3.7
1	B	349	PHE	3.7
1	B	281	MET	3.7
1	B	347	PRO	3.4
1	B	348	ASP	3.4
1	B	276	LYS	3.3
1	A	234	ALA	3.2
1	A	284	ARG	3.1
1	A	285	GLU	3.1
1	A	236	GLU	2.9
1	B	311	ILE	2.9
1	A	235	LYS	2.8
1	B	238	ILE	2.8
1	B	282	LEU	2.8
1	A	141	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLU	2.7
1	A	354	LYS	2.7
1	A	318	ASP	2.6
1	A	353	PHE	2.5
1	A	142	ALA	2.5
1	A	355	ARG	2.5
1	A	357	LEU	2.5
1	B	322	ASP	2.4
1	B	283	MET	2.4
1	A	356	LEU	2.4
1	B	236	GLU	2.3
1	B	152	LEU	2.3
1	B	239	ARG	2.2
1	A	143	ILE	2.2
1	B	61	LEU	2.2
1	A	290	LYS	2.1
1	B	232	ARG	2.0
1	A	237	GLN	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 carbohydrates 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
2	NA	B	2	1/1	0.39	0.14	57,57,57,57	0
5	2CV	A	501	14/26	0.70	0.13	90,102,117,120	0
5	2CV	B	505	17/26	0.76	0.28	67,79,102,103	0
5	2CV	B	501	26/26	0.81	0.24	47,69,87,92	0
5	2CV	B	506	14/26	0.82	0.22	51,72,84,86	0

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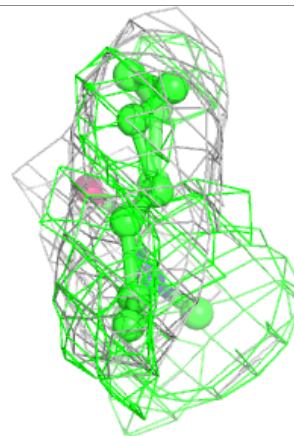
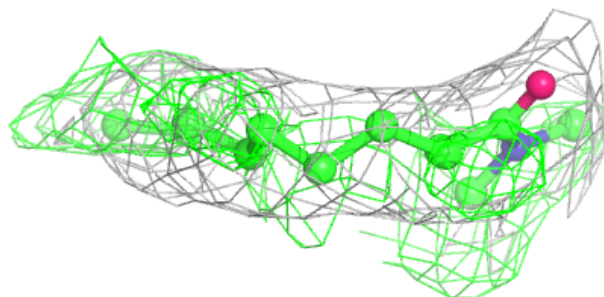
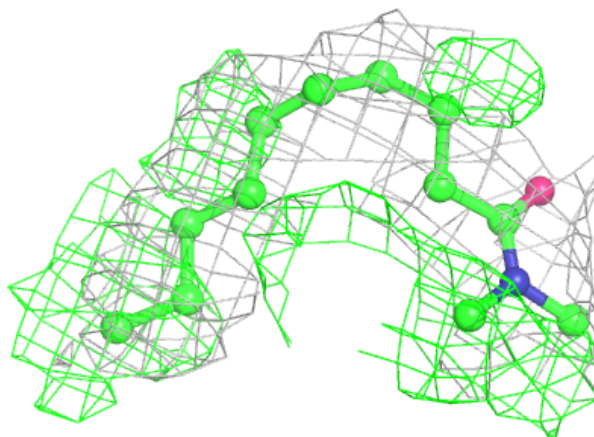
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	A	2	1/1	0.82	0.09	57,57,57,57	0
5	2CV	B	503	12/26	0.83	0.29	59,72,90,95	0
5	2CV	B	502	14/26	0.87	0.34	52,79,95,101	0
3	Y01	A	402	35/35	0.88	0.29	67,85,107,108	0
5	2CV	A	503	21/26	0.90	0.25	35,60,69,72	0
3	Y01	B	402	35/35	0.91	0.37	65,71,114,121	0
5	2CV	A	502	7/26	0.92	0.45	57,64,76,76	0
3	Y01	B	401	35/35	0.95	0.28	45,52,83,89	0
4	3WC	B	500	17/17	0.96	0.17	35,38,40,41	0
2	NA	B	1	1/1	0.96	0.10	52,52,52,52	0
3	Y01	A	401	35/35	0.96	0.21	43,50,63,70	0
2	NA	A	1	1/1	0.98	0.06	53,53,53,53	0
4	3WC	A	500	17/17	0.98	0.16	43,47,50,52	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.

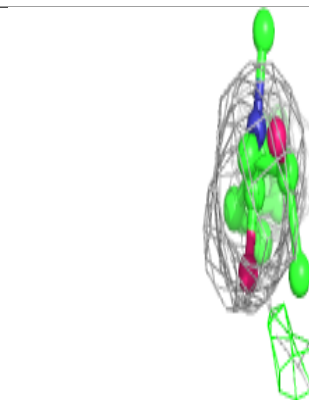
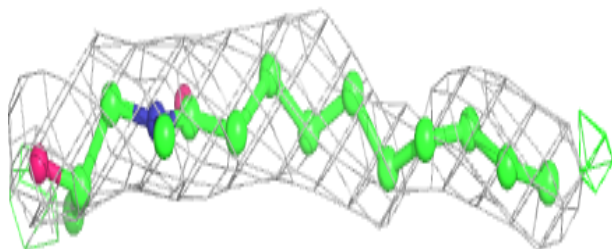
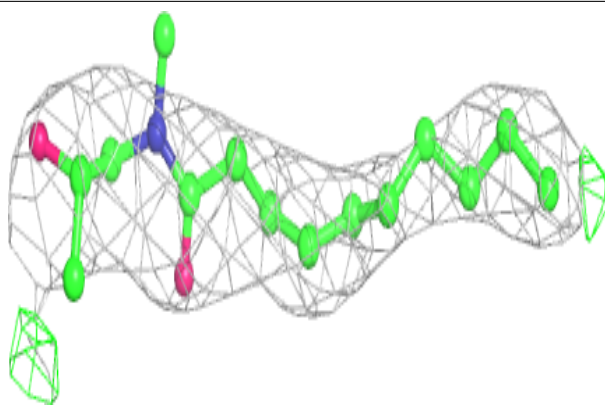
**Electron density around 2CV A 501:**

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)

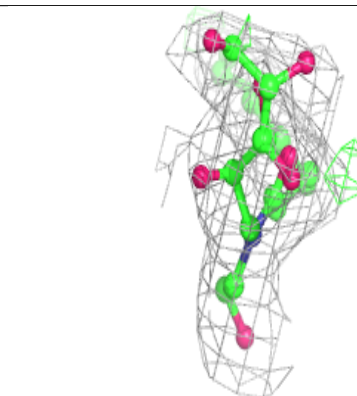
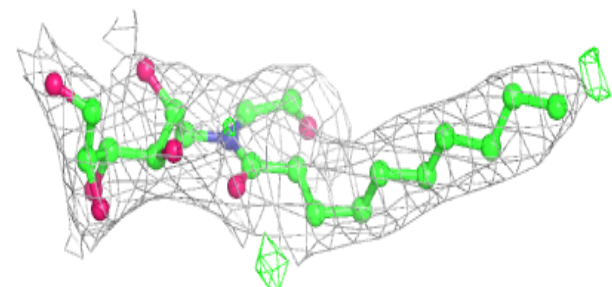
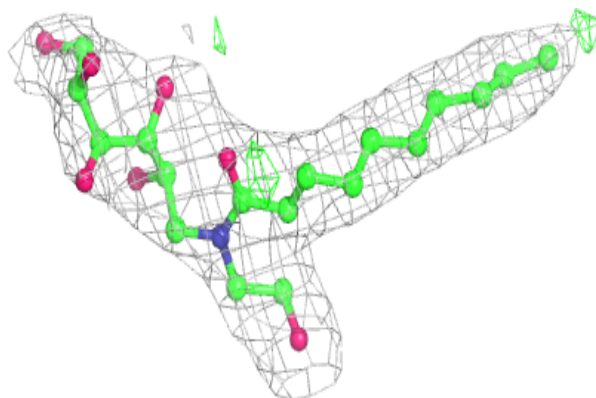


**Electron density around 2CV B 505:**

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

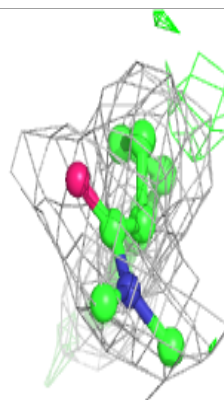
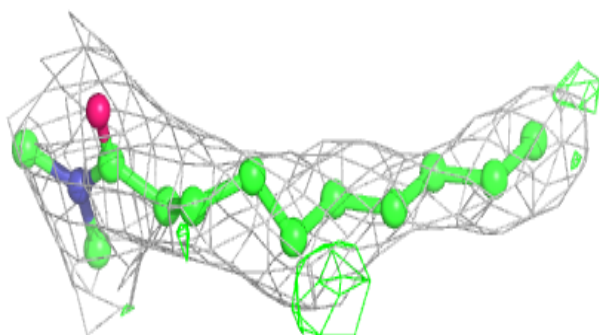
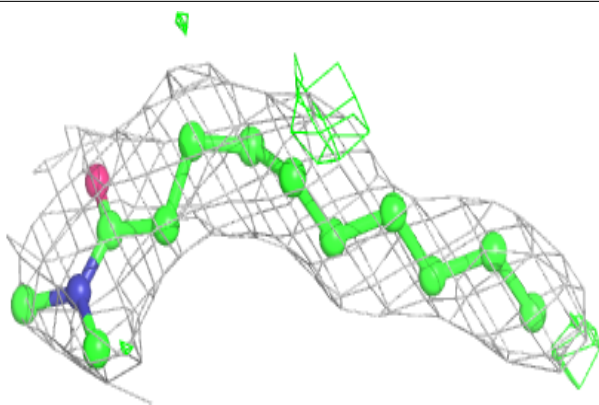
**Electron density around 2CV B 501:**

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

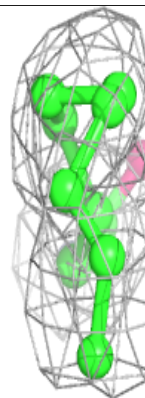
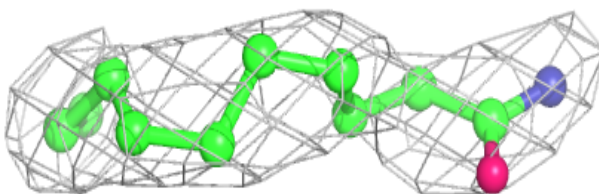
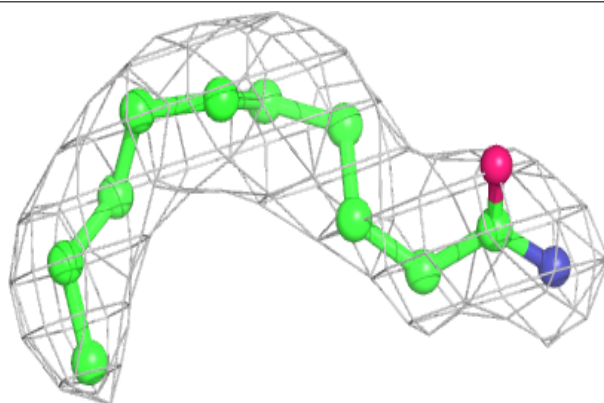


**Electron density around 2CV B 506:**

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

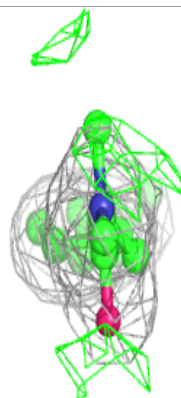
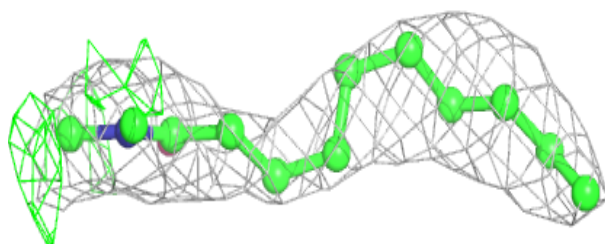
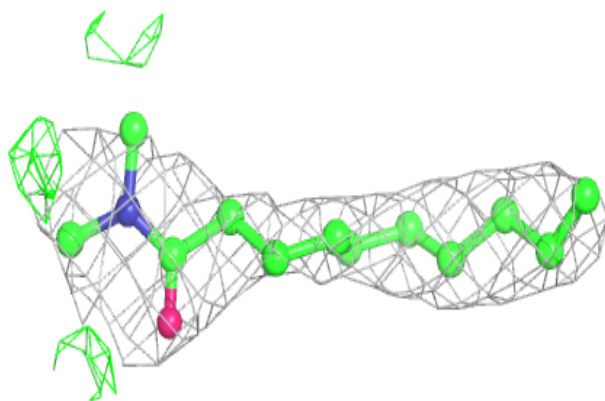
**Electron density around 2CV B 503:**

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

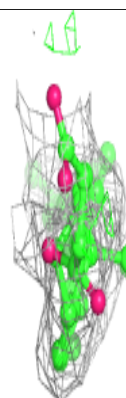
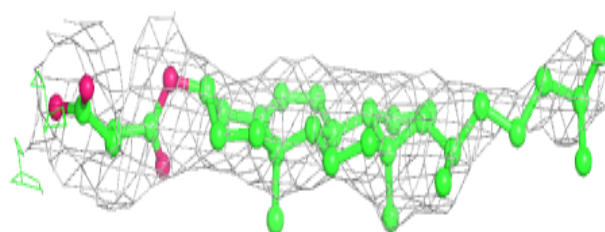
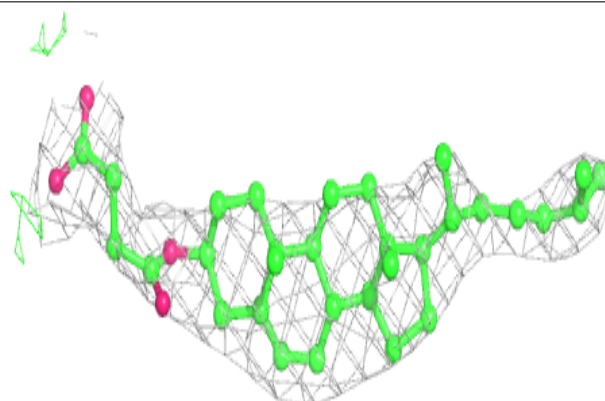


**Electron density around 2CV B 502:**

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

**Electron density around Y01 A 402:**

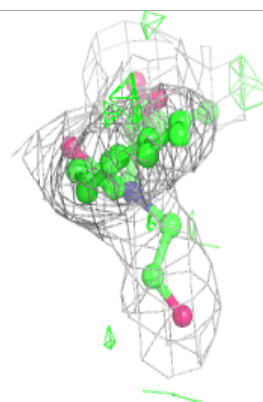
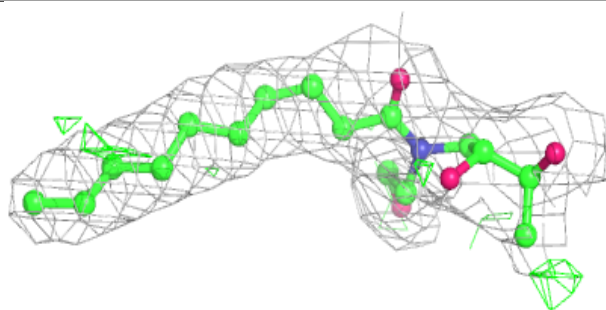
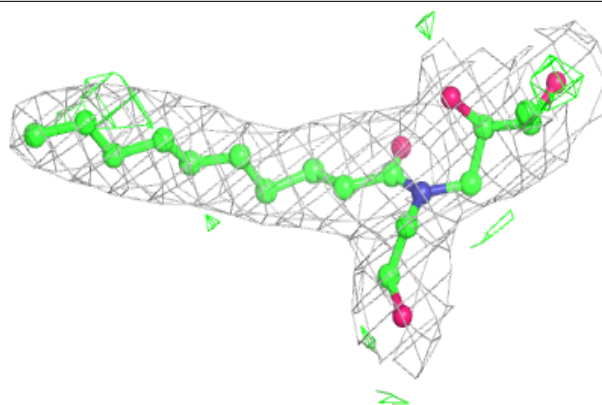
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



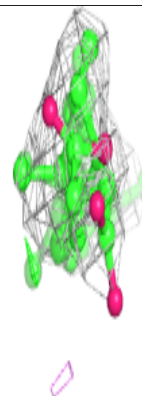
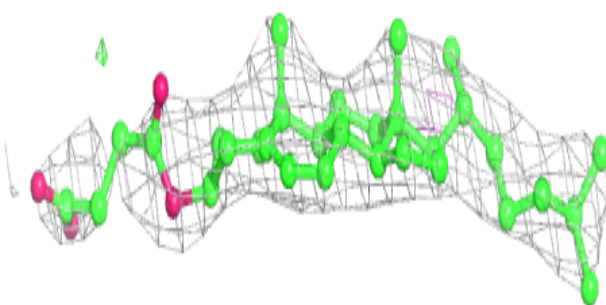
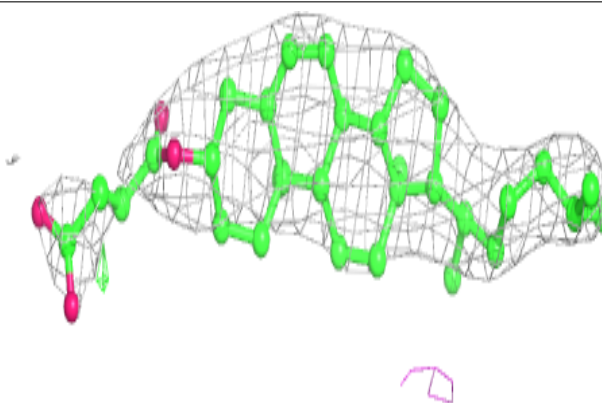


**Electron density around 2CV A 503:**

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

**Electron density around Y01 B 402:**

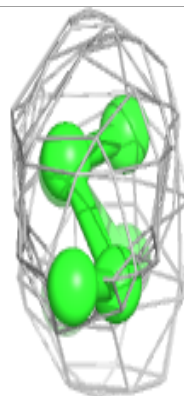
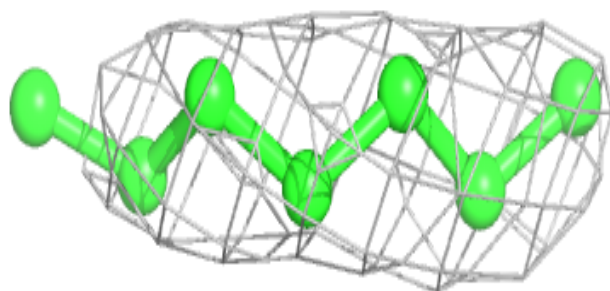
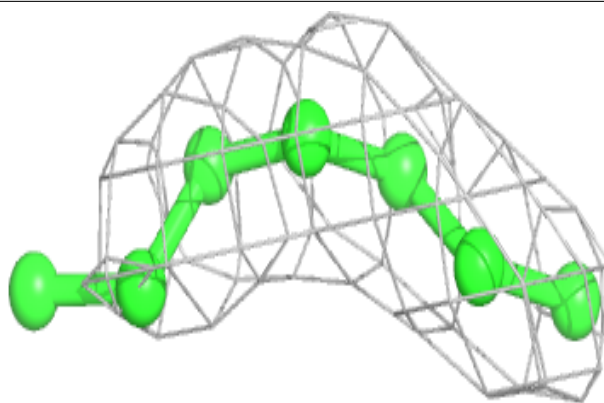
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



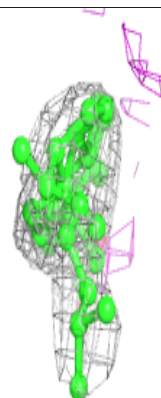
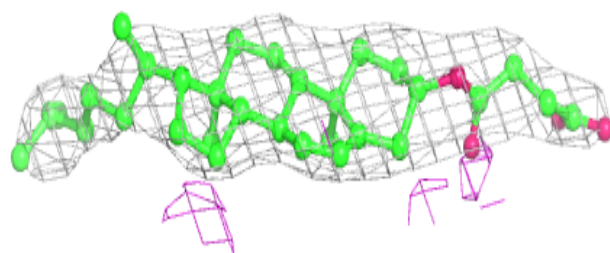
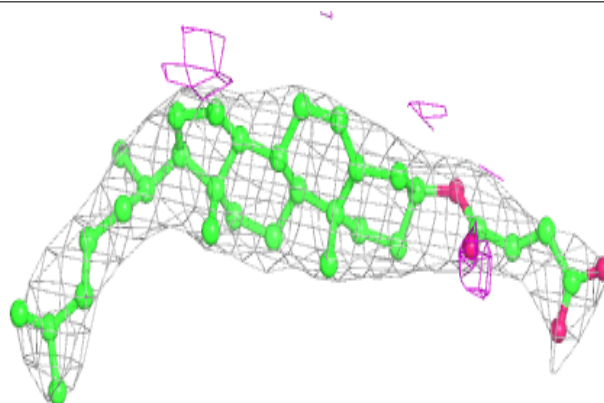


**Electron density around 2CV A 502:**

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

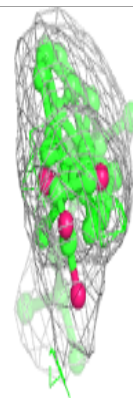
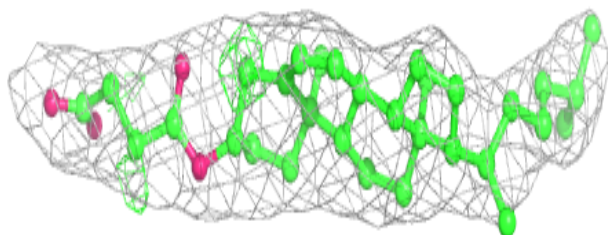
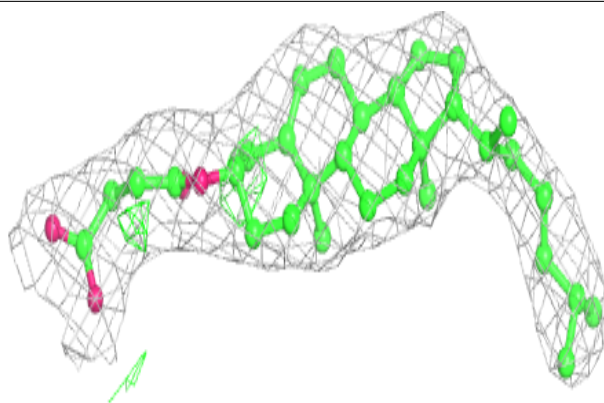
**Electron density around Y01 B 401:**

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



**Electron density around Y01 A 401:**

$2mF_o-DF_c$  (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.