



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:26 PM BST

PDB ID : 3ZPQ  
Title : Thermostabilised turkey beta1 adrenergic receptor with 4-(piperazin-1-yl)-1H-indole bound (compound 19)  
Authors : Christopher, J.A.; Congreve, M.; Dore, A.S.; Marshall, F.H.; Myszkka, D.G.; Brown, J.; Koglin, M.; Tehan, B.; Errey, J.C.; Tate, C.G.; Warne, T.  
Deposited on : 2013-03-01  
Resolution : 2.80 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

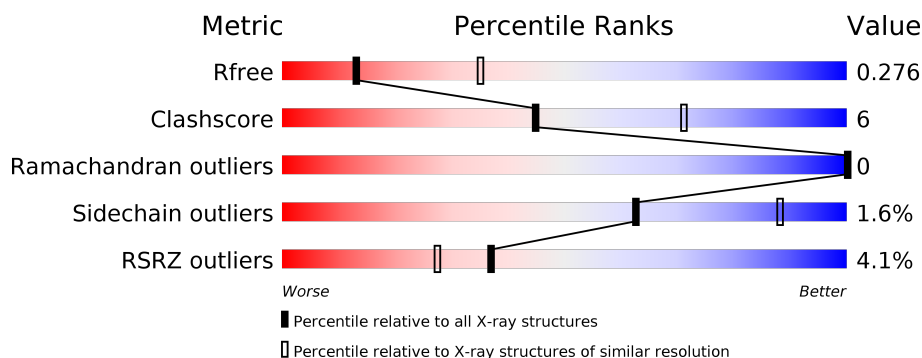
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	<div> <div>4%</div> <div>83%</div> <div>8%</div> <div>9%</div> </div>
1	B	315	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>5%</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
3	2CV	B	504	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4996 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	287	Total	C	N	O	S	0	0	0
			2273	1500	373	380	20			
1	B	299	Total	C	N	O	S	0	0	0
			2375	1562	397	396	20			

There are 30 discrepancies between the modelled and reference sequences:

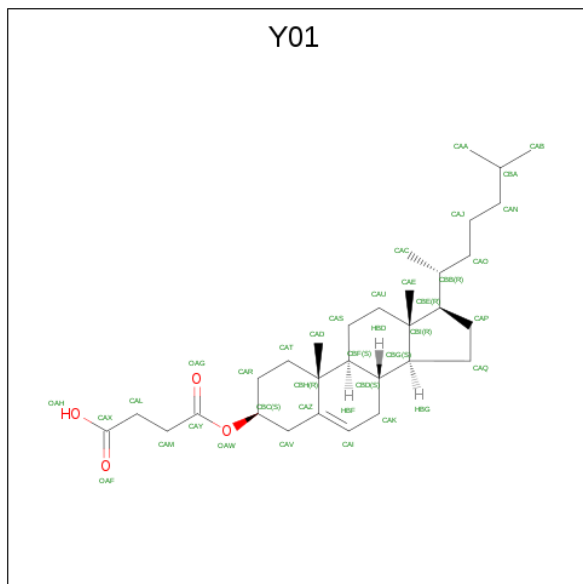
Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	expression tag	UNP P07700
A	32	GLY	-	expression tag	UNP P07700
A	369	HIS	-	expression tag	UNP P07700
A	370	HIS	-	expression tag	UNP P07700
A	371	HIS	-	expression tag	UNP P07700
A	372	HIS	-	expression tag	UNP P07700
A	373	HIS	-	expression tag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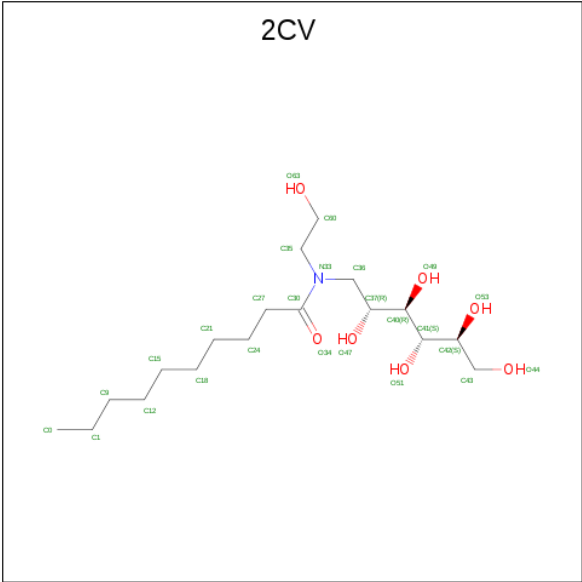
Chain	Residue	Modelled	Actual	Comment	Reference
B	227	ALA	TYR	engineered mutation	UNP P07700
B	282	LEU	ALA	engineered mutation	UNP P07700
B	327	ALA	PHE	engineered mutation	UNP P07700
B	338	MET	PHE	engineered mutation	UNP P07700
B	358	ALA	CYS	engineered mutation	UNP P07700

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



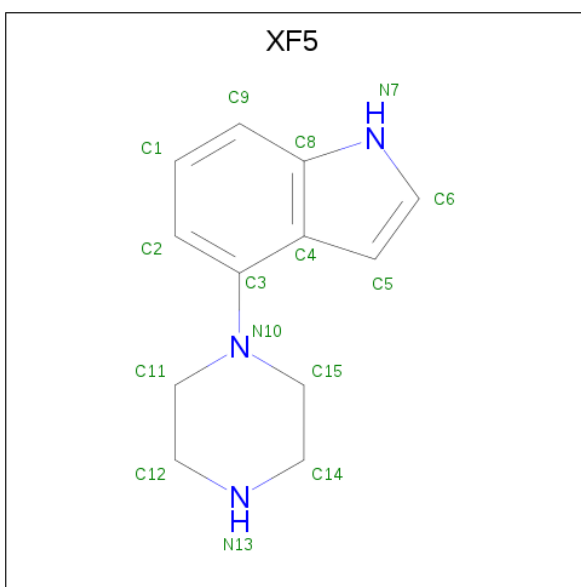
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 35	C 31	O 4	0	0
2	A	1	Total 35	C 31	O 4	0	0
2	B	1	Total 35	C 31	O 4	0	0
2	B	1	Total 35	C 31	O 4	0	0

- Molecule 3 is HEGA-10 (three-letter code: 2CV) (formula:  $\text{C}_{18}\text{H}_{37}\text{NO}_7$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C			0	0
			10	10				
3	A	1	Total	C	N	O	0	0
			21	16	1	4		
3	A	1	Total	C	N	O	0	0
			14	12	1	1		
3	A	1	Total	C	N	O	0	0
			12	10	1	1		
3	B	1	Total	C	N	O	0	0
			19	15	1	3		
3	B	1	Total	C	N	O	0	0
			12	10	1	1		
3	B	1	Total	C	N	O	0	0
			12	10	1	1		
3	B	1	Total	C	N	O	0	0
			21	16	1	4		
3	B	1	Total	C	N	O	0	0
			19	15	1	3		

- Molecule 4 is 4-(PIPERAZIN-1-YL)-1H-INDOLE (three-letter code: XF5) (formula: C<sub>12</sub>H<sub>15</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			15	12	3		
4	B	1	Total	C	N	0	0
			15	12	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	1	Total	Na	0	0
			1	1		

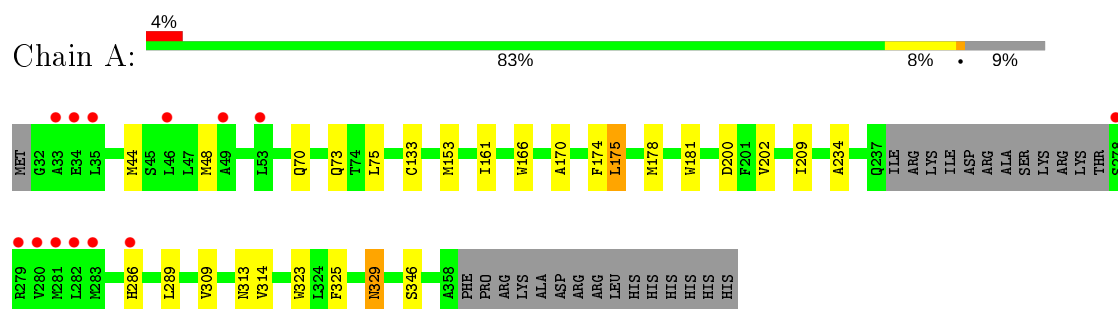
- Molecule 6 is water.

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

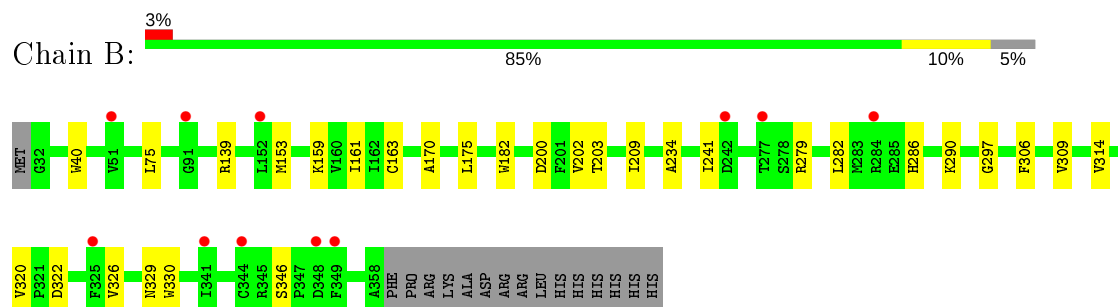
### 3 Residue-property plots

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

#### • Molecule 1: BETA-1 ADRENERGIC RECEPTOR



#### • 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, $\alpha$ , $\beta$ , $\gamma$	89.85Å 61.44Å 100.78Å 90.00° 108.89° 90.00°	Depositor
Resolution (Å)	95.36 – 2.80 55.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.7 (95.36-2.80) 91.9 (55.20-2.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.220 , 0.274 0.221 , 0.276	Depositor DCC
$R_{free}$ test set	1214 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.6	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	0.90	EDS
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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, XF5

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	0.56	1/2327 (0.0%)	0.61	0/3172
1	B	0.57	1/2430 (0.0%)	0.61	0/3308
All	All	0.56	2/4757 (0.0%)	0.61	0/6480

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	TRP	CD2-CE2	5.86	1.48	1.41
1	A	323	TRP	CD2-CE2	5.12	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	2273	0	2352	22	0
1	B	2375	0	2473	28	0
2	A	70	0	98	4	0
2	B	70	0	98	8	0
3	A	57	0	87	7	0
3	B	83	0	124	16	0
4	A	15	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	15	1	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	18	0	0	0	0
6	B	17	0	0	0	0
All	All	4996	0	5262	66	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 (66) 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:170:ALA:HB2	3:A:505:2CV:H03C	1.66	0.78
3:A:503:2CV:C60	3:A:503:2CV:H271	2.13	0.77
3:A:503:2CV:H601	3:A:503:2CV:H271	1.66	0.77
1:B:290:LYS:HG3	3:B:504:2CV:H272	1.72	0.71
1:A:175:LEU:HD22	1:B:175:LEU:HD22	1.73	0.70
1:B:163:CYS:CB	3:B:505:2CV:H602	2.22	0.70
1:B:163:CYS:HB2	3:B:505:2CV:H602	1.74	0.69
1:B:309:VAL:HG13	1:B:320:VAL:HG21	1.74	0.67
3:A:503:2CV:C60	3:A:503:2CV:C27	2.75	0.65
1:B:209:ILE:HD11	1:B:314:VAL:HG11	1.80	0.64
3:B:502:2CV:H601	3:B:502:2CV:H37	1.79	0.63
1:B:234:ALA:HB1	1:B:286:HIS:NE2	2.13	0.63
1:A:234:ALA:HB1	1:A:286:HIS:NE2	2.15	0.61
4:A:1359:XF5:H112	4:A:1359:XF5:H5	1.86	0.58
1:A:174:PHE:HB3	1:A:178:MET:HE1	1.86	0.58
1:A:175:LEU:CD2	1:B:175:LEU:HD22	2.33	0.57
1:A:174:PHE:HB3	1:A:178:MET:CE	2.35	0.56
3:B:502:2CV:C60	3:B:502:2CV:H37	2.34	0.55
1:A:44:MET:HE3	1:A:48:MET:CE	2.37	0.54
1:A:209:ILE:HD11	1:A:314:VAL:HG11	1.90	0.53
1:B:241:ILE:HD11	1:B:279:ARG:HA	1.90	0.53
1:B:290:LYS:HG3	3:B:504:2CV:C27	2.40	0.52
1:A:44:MET:HE3	1:A:48:MET:HE3	1.91	0.51
1:A:181:TRP:HB3	3:A:503:2CV:H181	1.92	0.51
3:B:502:2CV:H601	3:B:502:2CV:C37	2.39	0.51
1:A:75:LEU:HD13	1:A:153:MET:HG3	1.93	0.51
1:A:166:TRP:CE2	2:A:402:Y01:HAP1	2.46	0.51
1:B:309:VAL:CG1	1:B:320:VAL:HG11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:Y01:HAC1	2:B:402:Y01:HAE2	1.93	0.50
1:B:306:PHE:CE2	4:B:1360:XF5:H151	2.47	0.49
1:B:326:VAL:O	1:B:330:TRP:HD1	1.96	0.49
1:B:297:GLY:HA3	3:B:504:2CV:H91C	1.96	0.48
1:A:289:LEU:HB3	3:A:502:2CV:H151	1.96	0.47
1:B:159:LYS:HE2	2:B:402:Y01:CAY	2.44	0.47
3:B:505:2CV:O47	3:B:505:2CV:H352	2.14	0.47
1:B:75:LEU:HD13	1:B:153:MET:HG3	1.95	0.47
3:A:503:2CV:H361	3:B:505:2CV:H362	1.96	0.46
2:A:402:Y01:HAC1	2:A:402:Y01:HAE2	1.98	0.46
2:B:401:Y01:HAO1	2:B:401:Y01:HAE2	1.98	0.46
1:A:200:ASP:HB3	1:A:202:VAL:HG23	1.98	0.45
2:A:401:Y01:HBC	1:B:161:ILE:HG12	1.98	0.45
1:A:44:MET:CE	1:A:48:MET:HE3	2.46	0.45
1:A:44:MET:CE	1:A:48:MET:CE	2.95	0.45
2:B:401:Y01:HAC3	2:B:401:Y01:HAJ2	1.80	0.45
1:B:170:ALA:HB2	3:B:505:2CV:H02C	1.97	0.45
1:A:329:ASN:HD22	1:A:329:ASN:C	2.21	0.44
3:B:502:2CV:H272	3:B:502:2CV:H351	1.46	0.44
2:B:402:Y01:HAR1	2:B:402:Y01:OAG	2.16	0.44
1:A:175:LEU:CD2	1:B:175:LEU:HD13	2.47	0.44
1:B:182:TRP:O	1:B:203:THR:HA	2.17	0.44
1:B:139:ARG:NH1	3:B:503:2CV:H151	2.32	0.43
1:B:200:ASP:HB3	1:B:202:VAL:HG23	2.00	0.43
2:B:401:Y01:HAS2	2:B:401:Y01:HAD2	1.88	0.42
1:A:161:ILE:HG12	2:B:401:Y01:HBC	2.02	0.42
3:B:506:2CV:H351	3:B:506:2CV:H272	1.69	0.42
1:A:175:LEU:HD22	1:B:175:LEU:CD2	2.46	0.42
2:A:401:Y01:HAE1	2:A:401:Y01:HAS2	1.88	0.42
1:B:241:ILE:HD13	1:B:282:LEU:HD22	2.02	0.42
1:B:241:ILE:HG23	1:B:279:ARG:NH1	2.34	0.41
4:A:1359:XF5:C11	4:A:1359:XF5:C5	2.98	0.41
2:B:402:Y01:HAQ1	2:B:402:Y01:HAE3	1.86	0.41
1:A:70:GLN:HA	1:A:73:GLN:OE1	2.20	0.41
1:A:309:VAL:CG1	1:A:325:PHE:CD1	3.04	0.41
1:B:163:CYS:SG	3:B:505:2CV:H602	2.60	0.41
1:B:241:ILE:HA	1:B:241:ILE:HD12	1.96	0.41
1:B:290:LYS:HD2	3:B:502:2CV:H602	2.04	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	283/315 (90%)	276 (98%)	7 (2%)	0	100	100
1	B	297/315 (94%)	289 (97%)	8 (3%)	0	100	100
All	All	580/630 (92%)	565 (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	247/273 (90%)	242 (98%)	5 (2%)	55	84
1	B	258/273 (94%)	255 (99%)	3 (1%)	71	92
All	All	505/546 (92%)	497 (98%)	8 (2%)	62	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	CYS
1	A	175	LEU
1	A	313	ASN
1	A	329	ASN
1	A	346	SER
1	B	322	ASP
1	B	329	ASN
1	B	346	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	XF5	A	1359	-	15,17,17	1.96	5 (33%)	19,23,23	1.43	2 (10%)
4	XF5	B	1360	-	15,17,17	2.06	4 (26%)	19,23,23	1.62	5 (26%)
2	Y01	B	402	-	35,38,38	1.20	2 (5%)	54,57,57	1.49	10 (18%)
3	2CV	B	505	-	20,20,25	0.71	1 (5%)	22,23,30	0.86	1 (4%)
3	2CV	B	502	-	18,18,25	0.62	0	20,20,30	0.88	1 (5%)
3	2CV	B	506	-	18,18,25	0.67	0	20,20,30	0.94	2 (10%)
2	Y01	B	401	-	35,38,38	1.13	2 (5%)	54,57,57	2.17	15 (27%)
2	Y01	A	401	-	35,38,38	1.10	2 (5%)	54,57,57	2.10	11 (20%)
3	2CV	A	506	-	11,11,25	0.46	0	11,11,30	0.69	0
3	2CV	A	505	-	13,13,25	0.81	1 (7%)	14,14,30	0.46	0
2	Y01	A	402	-	35,38,38	1.30	2 (5%)	54,57,57	1.37	9 (16%)
3	2CV	B	504	-	11,11,25	0.51	0	11,11,30	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	2CV	A	502	-	9,9,25	0.48	0	8,8,30	0.36	0
3	2CV	B	503	-	11,11,25	0.57	0	11,11,30	0.37	0
3	2CV	A	503	-	20,20,25	0.59	0	22,23,30	1.01	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XF5	A	1359	-	-	2/4/12/12	0/3/3/3
4	XF5	B	1360	-	-	2/4/12/12	0/3/3/3
2	Y01	B	402	-	-	6/17/77/77	0/4/4/4
3	2CV	B	505	-	-	7/24/24/34	-
3	2CV	B	502	-	-	9/20/20/34	-
3	2CV	B	506	-	-	8/20/20/34	-
2	Y01	B	401	-	-	12/17/77/77	0/4/4/4
2	Y01	A	401	-	-	12/17/77/77	0/4/4/4
3	2CV	A	506	-	-	1/9/9/34	-
3	2CV	A	505	-	-	4/13/13/34	-
2	Y01	A	402	-	-	7/17/77/77	0/4/4/4
3	2CV	B	504	-	-	6/9/9/34	-
3	2CV	A	502	-	-	5/7/7/34	-
3	2CV	B	503	-	-	4/9/9/34	-
3	2CV	A	503	-	-	11/24/24/34	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	Y01	CAK-CAI	-4.99	1.39	1.50
2	A	402	Y01	CAK-CAI	-4.89	1.39	1.50
4	B	1360	XF5	C9-C8	-4.88	1.33	1.41
2	B	401	Y01	CAK-CAI	-4.84	1.39	1.50
2	A	401	Y01	CAK-CAI	-4.61	1.40	1.50
4	A	1359	XF5	C9-C8	-4.35	1.34	1.41
4	B	1360	XF5	C3-C4	-3.64	1.34	1.42
2	A	402	Y01	CAI-CAZ	3.28	1.40	1.33
2	A	401	Y01	CAI-CAZ	3.26	1.40	1.33
4	A	1359	XF5	C3-C4	-3.21	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1360	XF5	C4-C8	-3.05	1.34	1.42
2	B	402	Y01	CAI-CAZ	3.00	1.39	1.33
2	B	401	Y01	CAI-CAZ	2.75	1.39	1.33
4	A	1359	XF5	C4-C8	-2.65	1.35	1.42
4	A	1359	XF5	C11-N10	2.49	1.50	1.46
4	B	1360	XF5	C11-N10	2.27	1.50	1.46
3	A	505	2CV	C27-C30	2.20	1.56	1.51
3	B	505	2CV	C36-C37	2.11	1.55	1.52
4	A	1359	XF5	C15-N10	2.10	1.50	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	Y01	CAR-CBC-CAV	-8.47	98.36	110.99
2	B	401	Y01	CAR-CBC-CAV	-8.10	98.91	110.99
2	B	401	Y01	OAW-CBC-CAV	8.10	124.69	108.12
2	A	401	Y01	OAW-CBC-CAR	6.68	124.46	108.33
2	A	402	Y01	OAW-CAY-CAM	5.05	122.38	111.50
4	A	1359	XF5	C15-N10-C11	4.36	121.13	111.52
2	A	401	Y01	OAW-CAY-CAM	4.29	120.75	111.50
2	B	402	Y01	OAW-CAY-CAM	4.23	120.63	111.50
4	B	1360	XF5	C15-N10-C11	3.93	120.19	111.52
2	A	401	Y01	CBC-CAV-CAZ	-3.71	105.75	111.52
2	A	401	Y01	CBI-CBE-CBB	-3.55	113.93	119.49
2	B	401	Y01	OAW-CAY-CAM	3.52	119.10	111.50
2	A	401	Y01	CAS-CAU-CBI	-3.32	107.09	112.78
2	B	401	Y01	OAW-CBC-CAR	3.32	116.33	108.33
2	B	402	Y01	CAV-CAZ-CBH	3.20	120.67	116.42
2	B	402	Y01	CAR-CBC-CAV	-3.12	106.33	110.99
2	B	402	Y01	CAP-CBE-CBB	-3.07	107.40	112.15
3	A	503	2CV	C27-C30-N33	-3.05	113.25	118.01
2	A	401	Y01	OAW-CBC-CAV	3.00	114.26	108.12
2	B	401	Y01	CBI-CBG-CBD	-2.99	109.95	114.38
4	B	1360	XF5	C12-C11-N10	2.98	116.93	110.48
2	A	402	Y01	OAW-CBC-CAV	2.95	114.15	108.12
3	B	502	2CV	C35-N33-C36	2.94	119.90	116.41
2	B	402	Y01	CBG-CBI-CBE	-2.87	96.67	100.07
2	B	401	Y01	CBC-CAV-CAZ	-2.86	107.08	111.52
2	A	402	Y01	CAQ-CBG-CBD	-2.83	114.42	119.08
2	B	402	Y01	CAP-CAQ-CBG	-2.82	99.55	105.13
3	B	506	2CV	C37-C36-N33	-2.77	110.34	113.28
2	A	402	Y01	CAK-CBD-CBF	2.75	113.04	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	Y01	CAV-CAZ-CBH	2.74	120.06	116.42
2	B	401	Y01	CBI-CBE-CBB	-2.70	115.25	119.49
4	B	1360	XF5	C2-C3-N10	-2.56	118.69	122.18
2	B	402	Y01	CAQ-CBG-CBD	-2.52	114.93	119.08
2	B	401	Y01	CAV-CAZ-CBH	2.46	119.69	116.42
2	B	402	Y01	CBC-OAW-CAY	-2.46	111.74	117.79
4	B	1360	XF5	C14-C15-N10	-2.43	105.23	110.48
2	B	401	Y01	CAO-CBB-CBE	2.41	115.27	110.28
2	B	402	Y01	CAQ-CBG-CBI	-2.40	100.95	103.84
2	A	402	Y01	CAQ-CBG-CBI	-2.40	100.96	103.84
2	B	401	Y01	CAC-CBB-CBE	-2.37	109.29	112.92
3	B	506	2CV	C27-C30-N33	-2.33	114.37	118.01
2	B	401	Y01	CAQ-CBG-CBD	-2.32	115.26	119.08
2	A	402	Y01	OAW-CAY-OAG	-2.30	118.15	123.70
2	A	402	Y01	CAP-CBE-CBI	-2.29	101.08	103.84
2	A	401	Y01	CAO-CBB-CBE	2.23	114.90	110.28
2	A	402	Y01	CBC-OAW-CAY	-2.22	112.33	117.79
3	B	505	2CV	C35-N33-C36	2.17	118.99	116.41
2	B	402	Y01	OAW-CBC-CAR	2.12	113.46	108.33
2	A	401	Y01	OAW-CAY-OAG	-2.11	118.59	123.70
2	B	401	Y01	CAT-CBH-CBF	2.09	111.65	108.73
2	A	401	Y01	CAP-CBE-CBB	2.08	115.37	112.15
2	B	401	Y01	CBH-CAZ-CAI	-2.07	119.73	122.90
4	A	1359	XF5	C12-C11-N10	2.07	114.97	110.48
2	B	401	Y01	CBG-CBI-CBE	-2.07	97.62	100.07
4	B	1360	XF5	C15-N10-C3	2.04	122.40	116.46
2	B	401	Y01	CAT-CAR-CBC	-2.03	106.86	110.33
2	A	401	Y01	CAL-CAM-CAY	-2.01	108.24	113.82

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	2CV	C37-C36-N33-C35
3	B	502	2CV	N33-C36-C37-C40
3	B	502	2CV	N33-C36-C37-O47
3	B	506	2CV	N33-C36-C37-C40
3	B	506	2CV	N33-C36-C37-O47
2	B	401	Y01	CAR-CBC-OAW-CAY
2	B	401	Y01	CAX-CAL-CAM-CAY
2	A	401	Y01	CAR-CBC-OAW-CAY
2	A	401	Y01	CAX-CAL-CAM-CAY

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Mol	Chain	Res	Type	Atoms
2	A	402	Y01	OAG-CAY-OAW-CBC
3	A	503	2CV	N33-C36-C37-C40
3	A	503	2CV	N33-C36-C37-O47
3	B	505	2CV	C21-C24-C27-C30
3	B	502	2CV	C21-C24-C27-C30
2	A	402	Y01	CAM-CAY-OAW-CBC
2	A	401	Y01	CAC-CBB-CBE-CAP
3	B	506	2CV	C21-C24-C27-C30
3	A	503	2CV	N33-C35-C60-O63
2	A	401	Y01	CAO-CBB-CBE-CAP
2	A	401	Y01	CAO-CBB-CBE-CBI
3	B	505	2CV	N33-C35-C60-O63
2	A	401	Y01	CAC-CBB-CBE-CBI
2	B	401	Y01	CAO-CBB-CBE-CBI
4	A	1359	XF5	C4-C3-N10-C15
4	A	1359	XF5	C2-C3-N10-C15
2	B	401	Y01	CAN-CAJ-CAO-CBB
2	A	401	Y01	CAN-CAJ-CAO-CBB
2	B	401	Y01	CAC-CBB-CBE-CAP
3	B	502	2CV	C37-C36-N33-C30
2	B	401	Y01	CAC-CBB-CBE-CBI
2	B	402	Y01	CAM-CAY-OAW-CBC
3	B	504	2CV	C15-C18-C21-C24
3	A	502	2CV	C15-C18-C21-C24
3	B	506	2CV	C18-C21-C24-C27
2	B	402	Y01	OAG-CAY-OAW-CBC
3	B	502	2CV	C9-C12-C15-C18
2	A	401	Y01	CAJ-CAN-CBA-CAA
2	A	402	Y01	CAJ-CAN-CBA-CAB
2	A	402	Y01	CAO-CBB-CBE-CAP
3	B	506	2CV	C12-C15-C18-C21
2	B	401	Y01	CAJ-CAN-CBA-CAB
3	B	504	2CV	C18-C21-C24-C27
3	A	502	2CV	C9-C12-C15-C18
3	B	503	2CV	C15-C12-C9-C1
2	A	401	Y01	CAJ-CAN-CBA-CAB
3	B	505	2CV	C37-C36-N33-C35
3	A	503	2CV	C15-C18-C21-C24
3	B	504	2CV	C12-C15-C18-C21
2	A	401	Y01	CAM-CAY-OAW-CBC
3	B	506	2CV	C9-C12-C15-C18
3	A	502	2CV	C18-C21-C24-C27

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Mol	Chain	Res	Type	Atoms
2	A	401	Y01	OAG-CAY-OAW-CBC
2	B	401	Y01	CAJ-CAN-CBA-CAA
2	A	402	Y01	CAJ-CAN-CBA-CAA
3	A	503	2CV	O47-C37-C40-O49
3	A	505	2CV	C15-C18-C21-C24
3	B	502	2CV	C0-C1-C9-C12
3	B	505	2CV	C15-C12-C9-C1
2	A	402	Y01	CAC-CBB-CBE-CAP
4	B	1360	XF5	C4-C3-N10-C15
4	B	1360	XF5	C2-C3-N10-C15
3	B	503	2CV	C18-C21-C24-C27
3	B	506	2CV	C15-C12-C9-C1
3	A	505	2CV	C0-C1-C9-C12
3	A	506	2CV	C15-C12-C9-C1
3	A	502	2CV	C0-C1-C9-C12
3	B	504	2CV	C0-C1-C9-C12
3	A	503	2CV	C9-C12-C15-C18
2	B	401	Y01	CAO-CBB-CBE-CAP
3	B	506	2CV	N33-C35-C60-O63
3	B	505	2CV	C36-C37-C40-C41
2	B	401	Y01	OAG-CAY-OAW-CBC
3	A	503	2CV	C18-C21-C24-C27
3	A	502	2CV	C15-C12-C9-C1
3	B	502	2CV	C12-C15-C18-C21
2	A	402	Y01	CAC-CBB-CBE-CBI
3	B	502	2CV	C60-C35-N33-C36
3	B	503	2CV	C0-C1-C9-C12
3	A	503	2CV	O47-C37-C40-C41
3	A	503	2CV	C60-C35-N33-C30
3	B	504	2CV	C9-C12-C15-C18
3	B	503	2CV	C12-C15-C18-C21
3	A	505	2CV	C18-C21-C24-C27
3	B	505	2CV	C37-C36-N33-C30
3	B	505	2CV	C9-C12-C15-C18
2	B	402	Y01	CAJ-CAN-CBA-CAA
3	A	503	2CV	C37-C36-N33-C35
3	B	504	2CV	C15-C12-C9-C1
2	B	402	Y01	CAJ-CAN-CBA-CAB
3	A	503	2CV	C15-C12-C9-C1
2	B	401	Y01	CAM-CAY-OAW-CBC
2	B	402	Y01	CAL-CAM-CAY-OAW
3	A	505	2CV	C15-C12-C9-C1

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Mol	Chain	Res	Type	Atoms
2	B	402	Y01	CAL-CAM-CAY-OAG
2	B	401	Y01	CAV-CBC-OAW-CAY
2	A	401	Y01	CAL-CAM-CAY-OAW

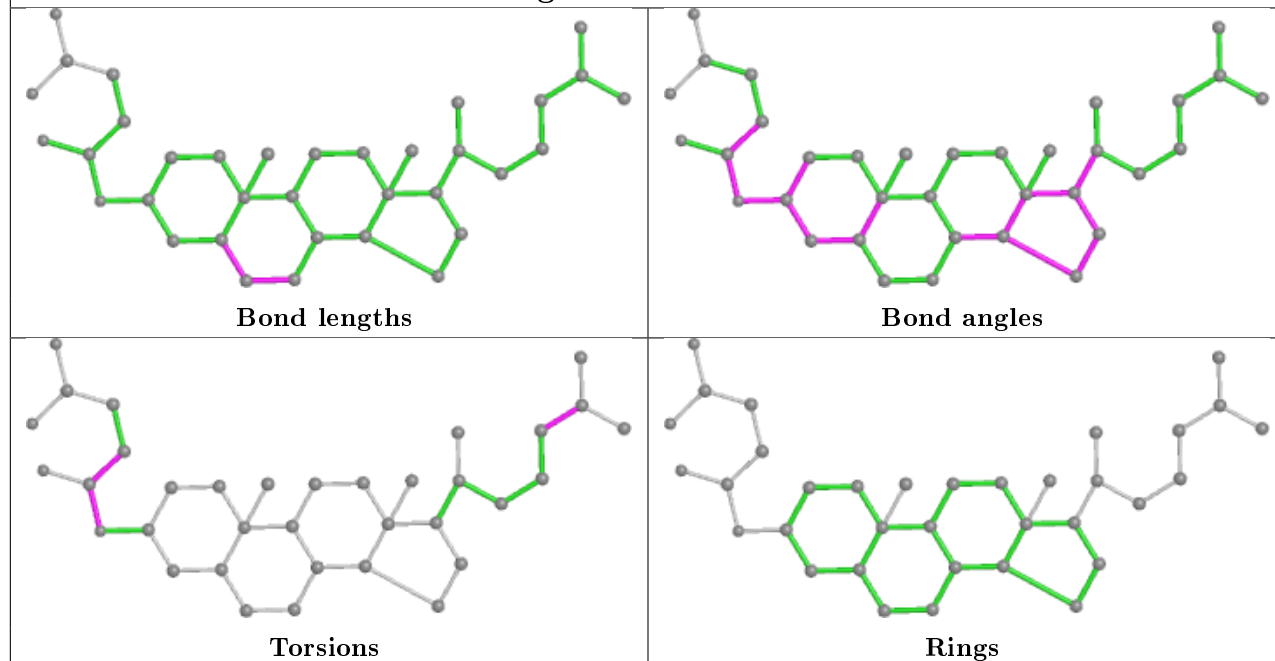
There are no ring outliers.

14 monomers are involved in 37 short contacts:

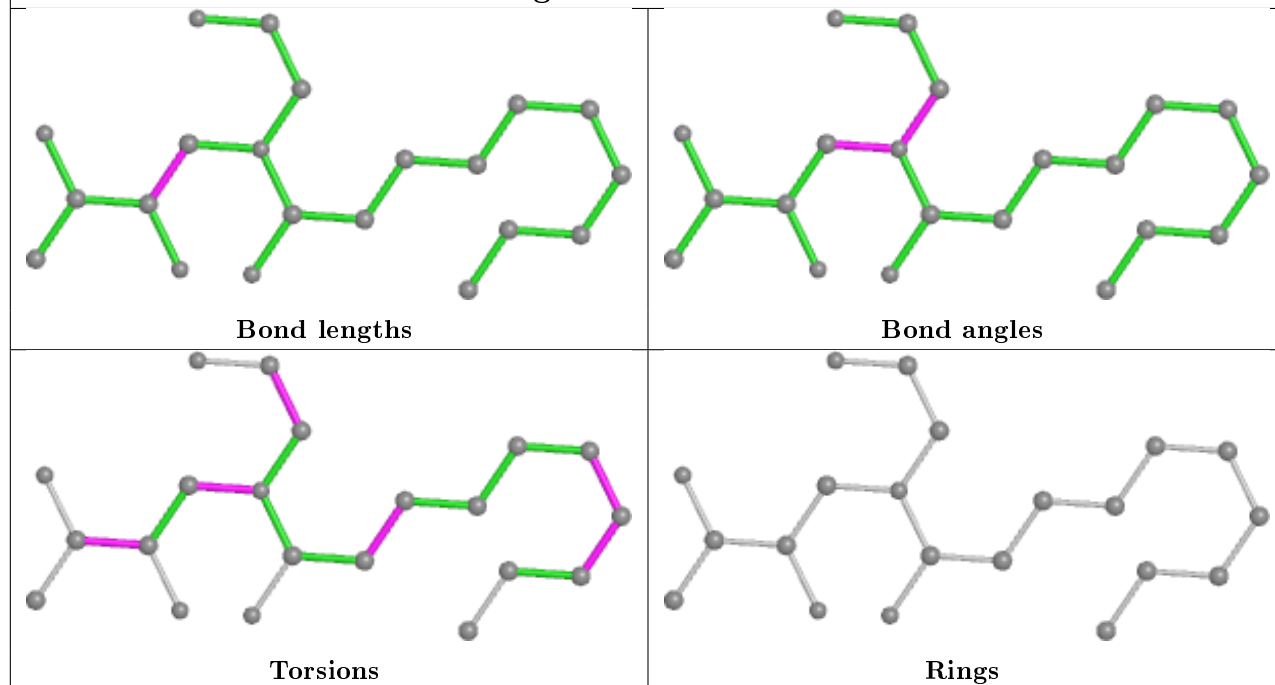
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1359	XF5	2	0
4	B	1360	XF5	1	0
2	B	402	Y01	4	0
3	B	505	2CV	6	0
3	B	502	2CV	5	0
3	B	506	2CV	1	0
2	B	401	Y01	4	0
2	A	401	Y01	2	0
3	A	505	2CV	1	0
2	A	402	Y01	2	0
3	B	504	2CV	3	0
3	A	502	2CV	1	0
3	B	503	2CV	1	0
3	A	503	2CV	5	0

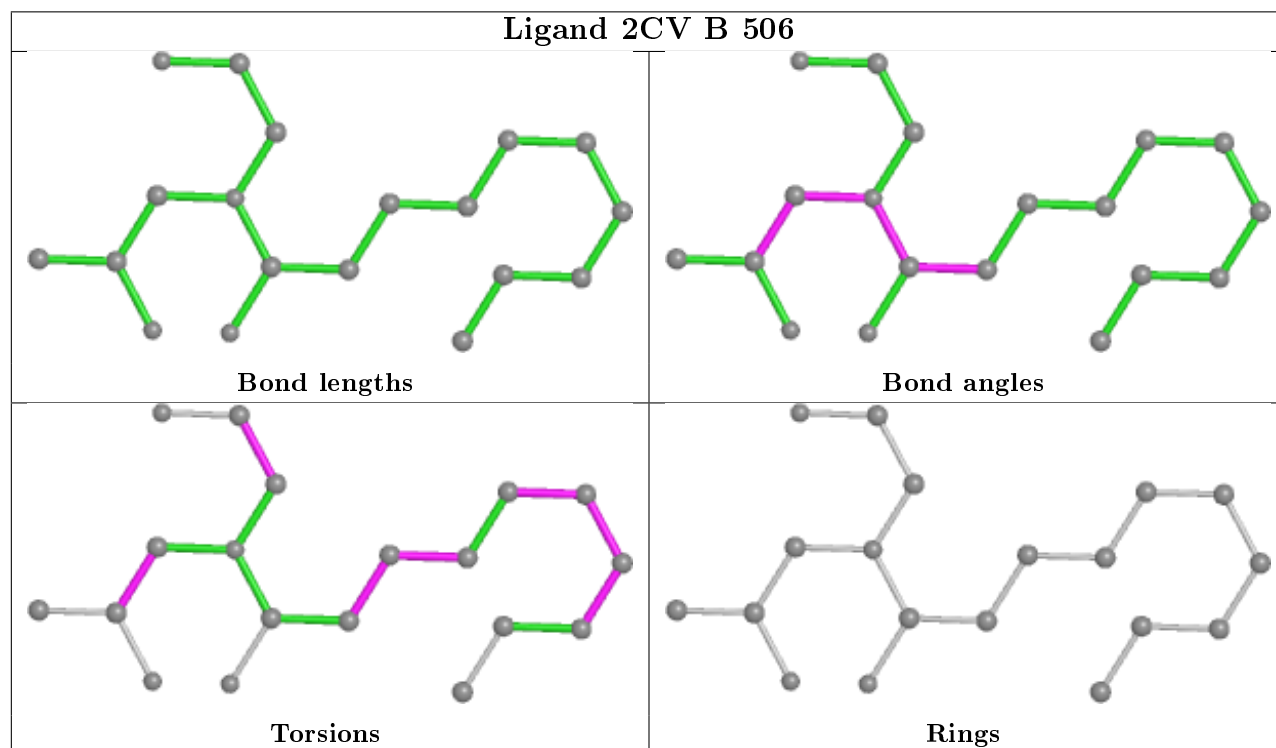
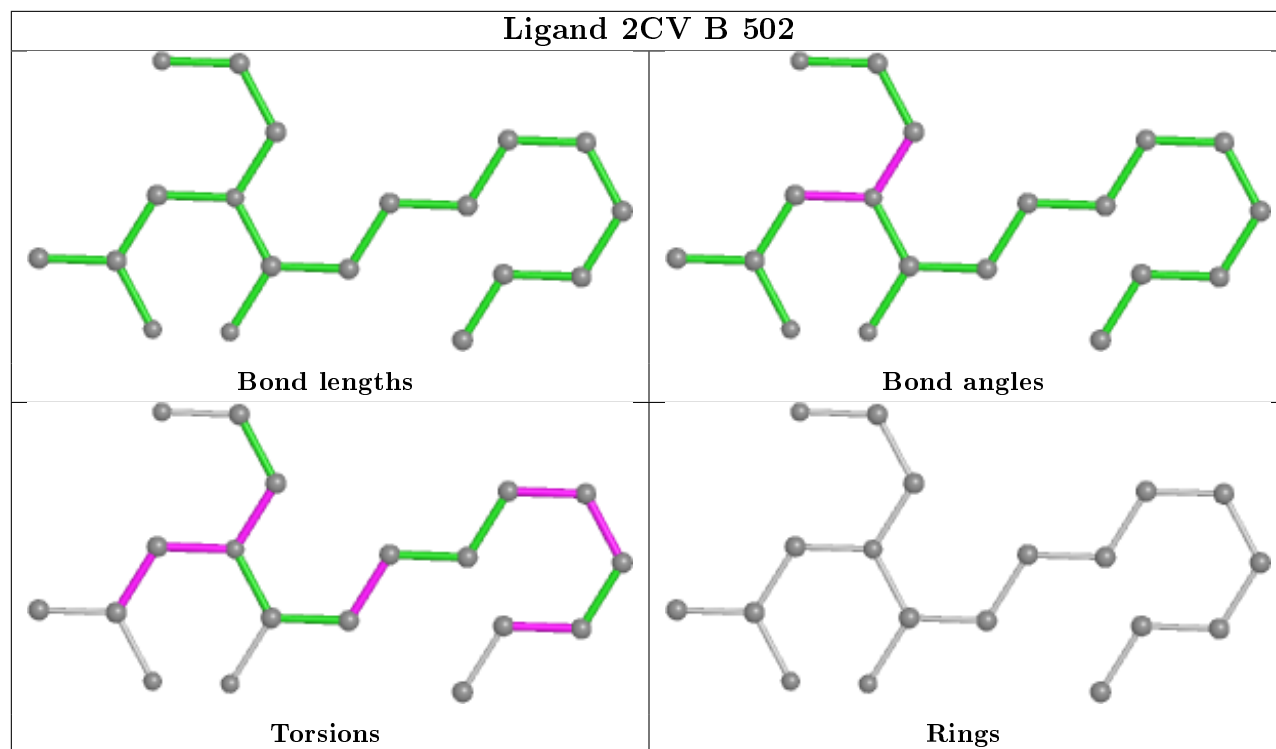
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 Y01 B 402

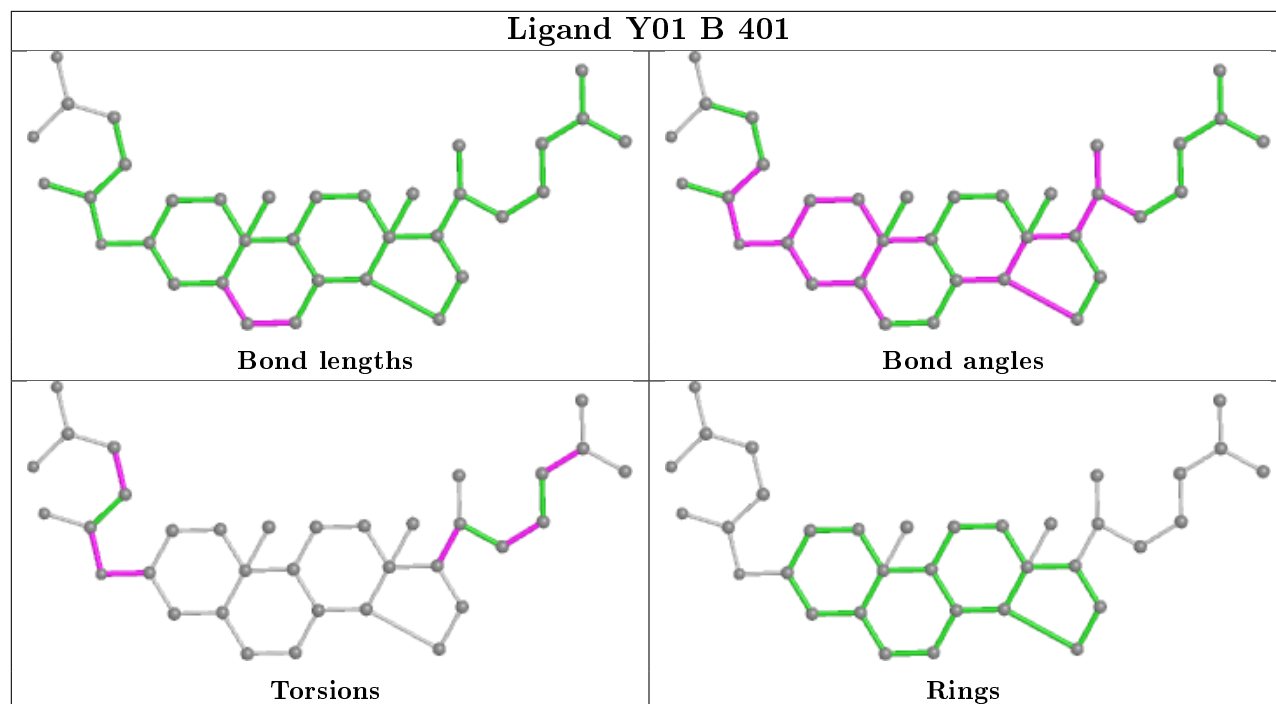


## Ligand 2CV B 505

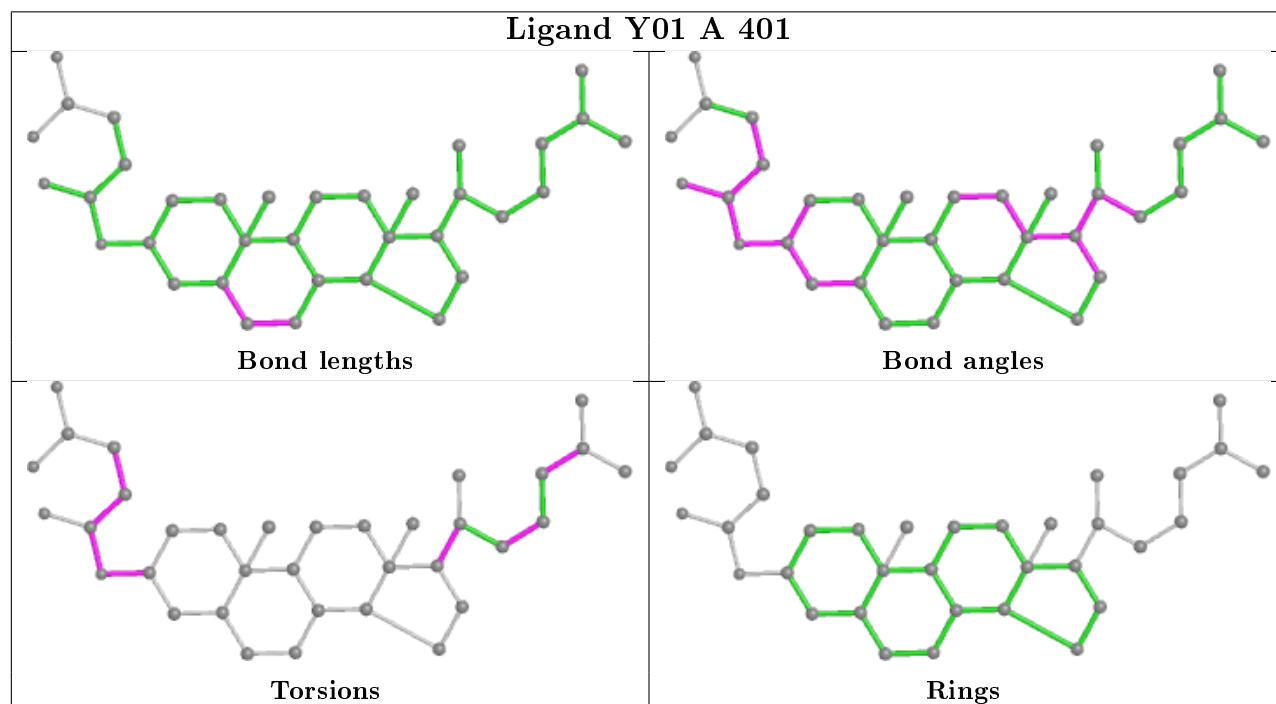


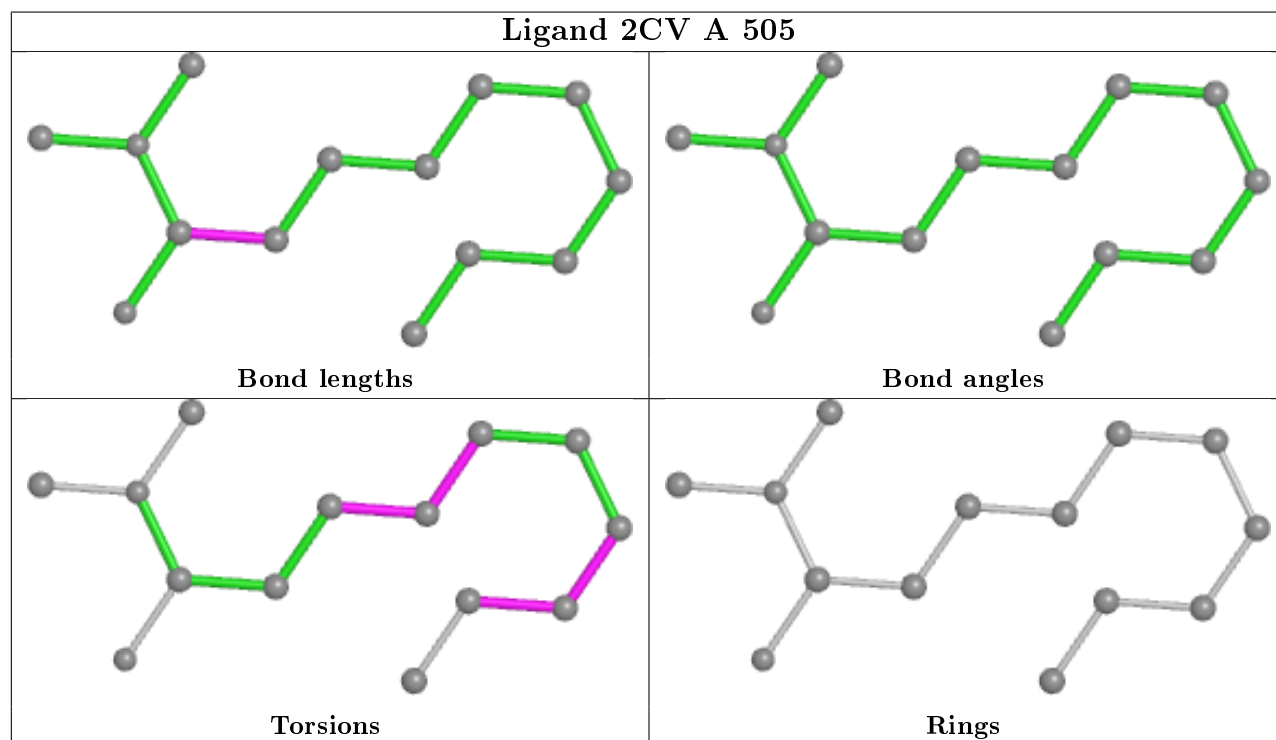
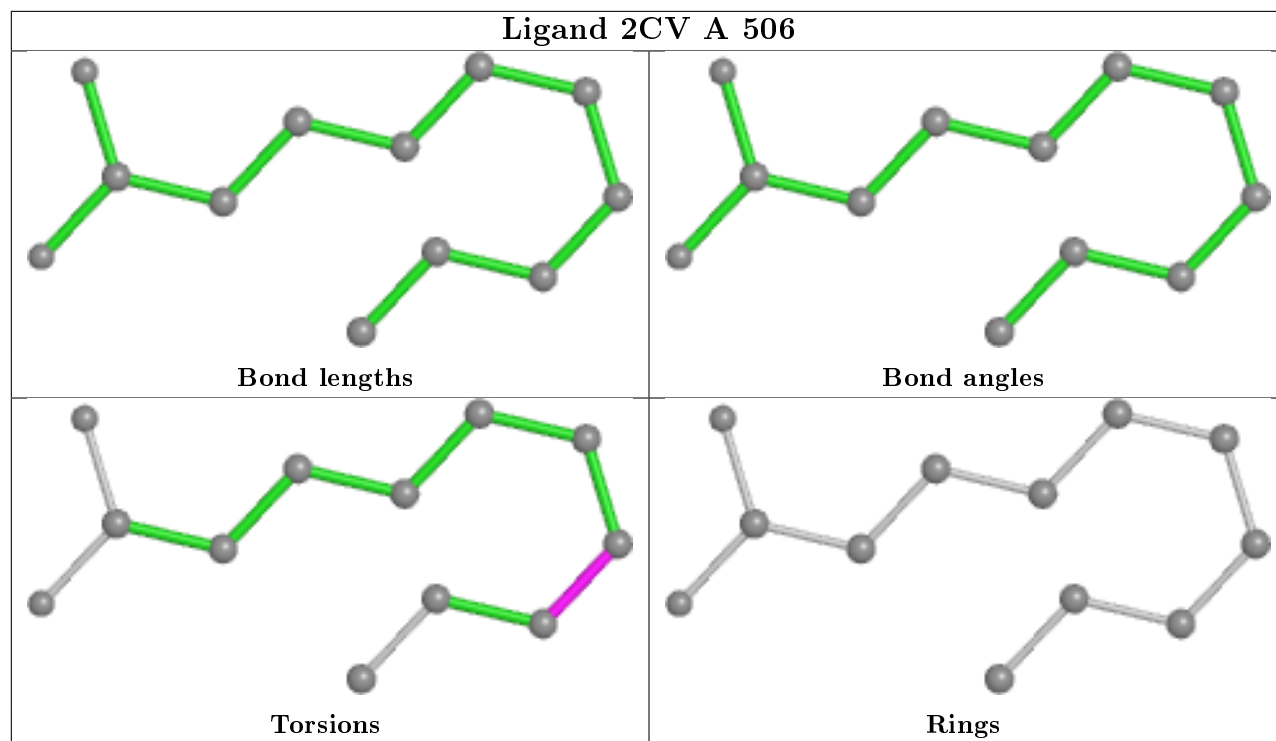


## Ligand Y01 B 401



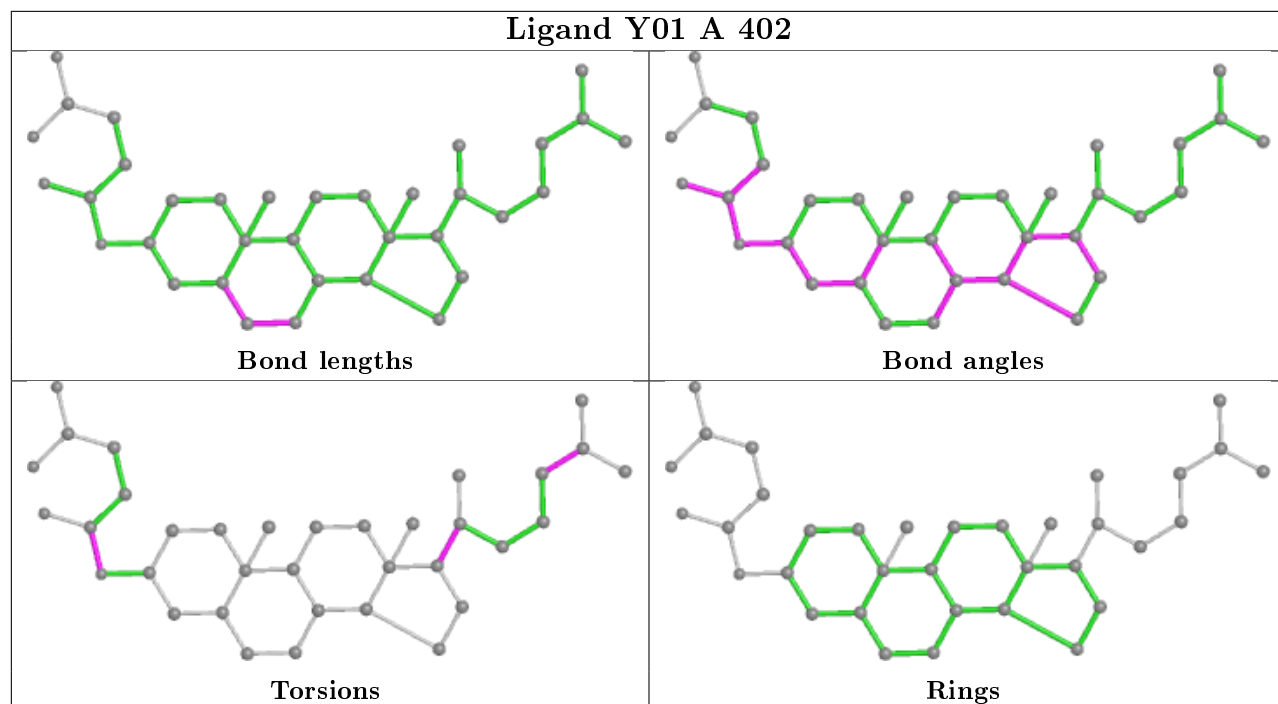
## Ligand Y01 A 401



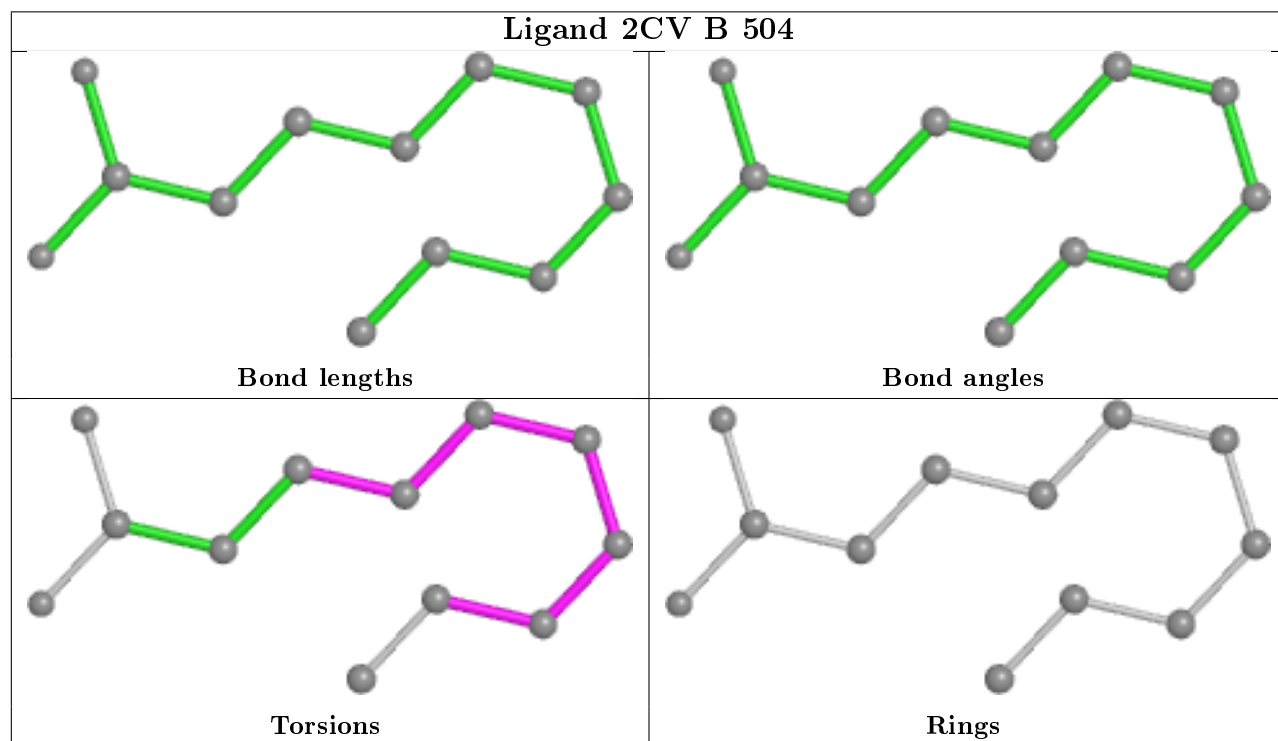


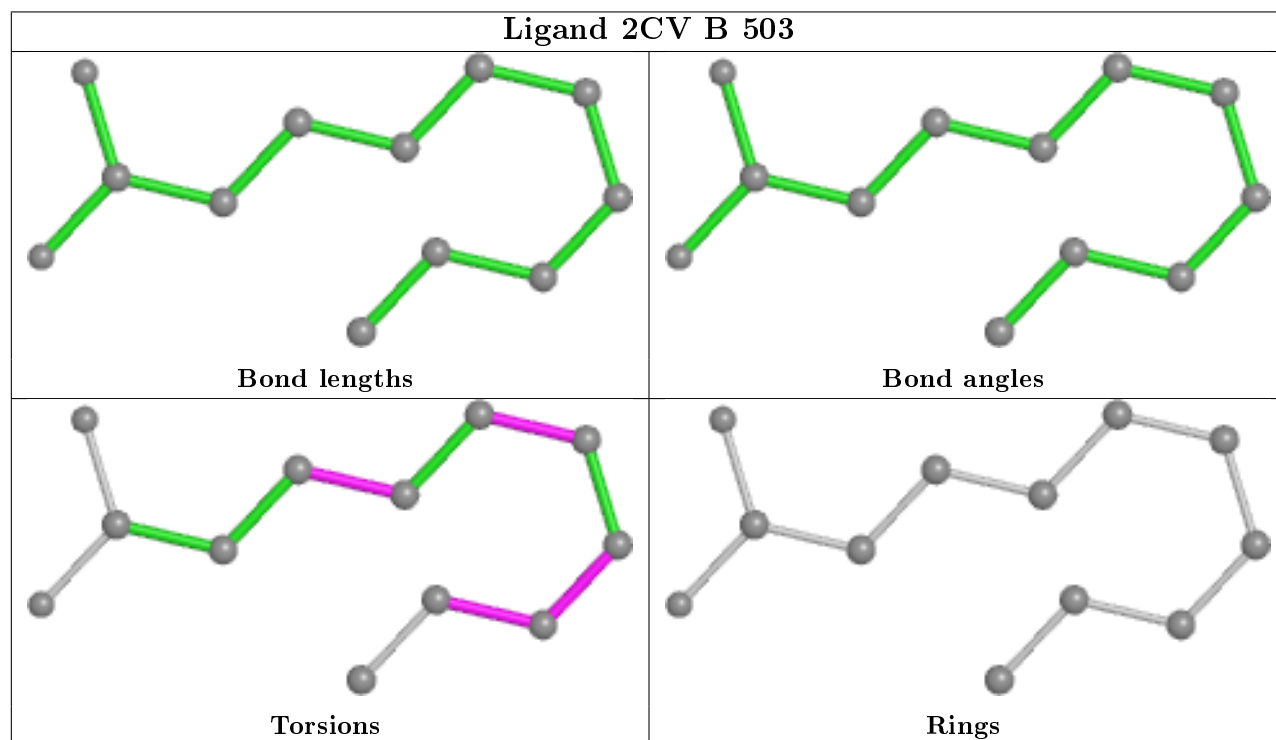
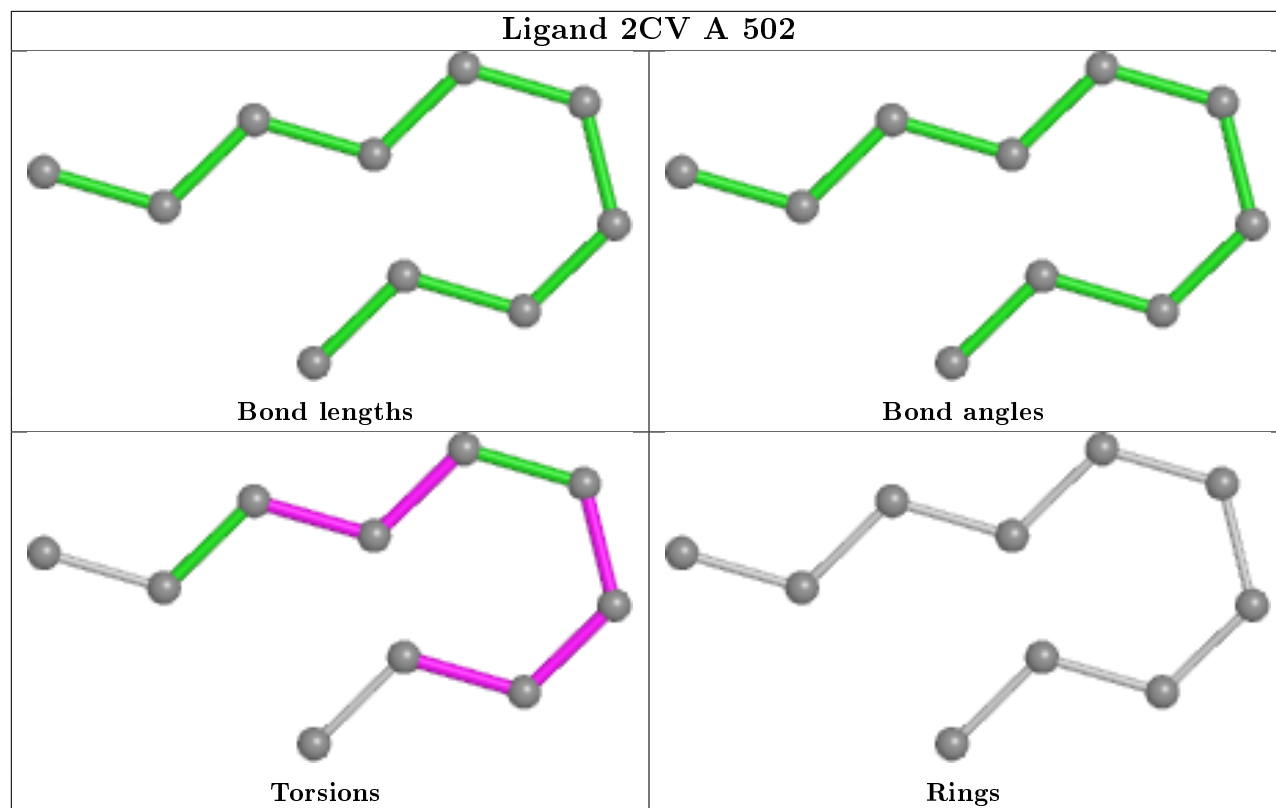


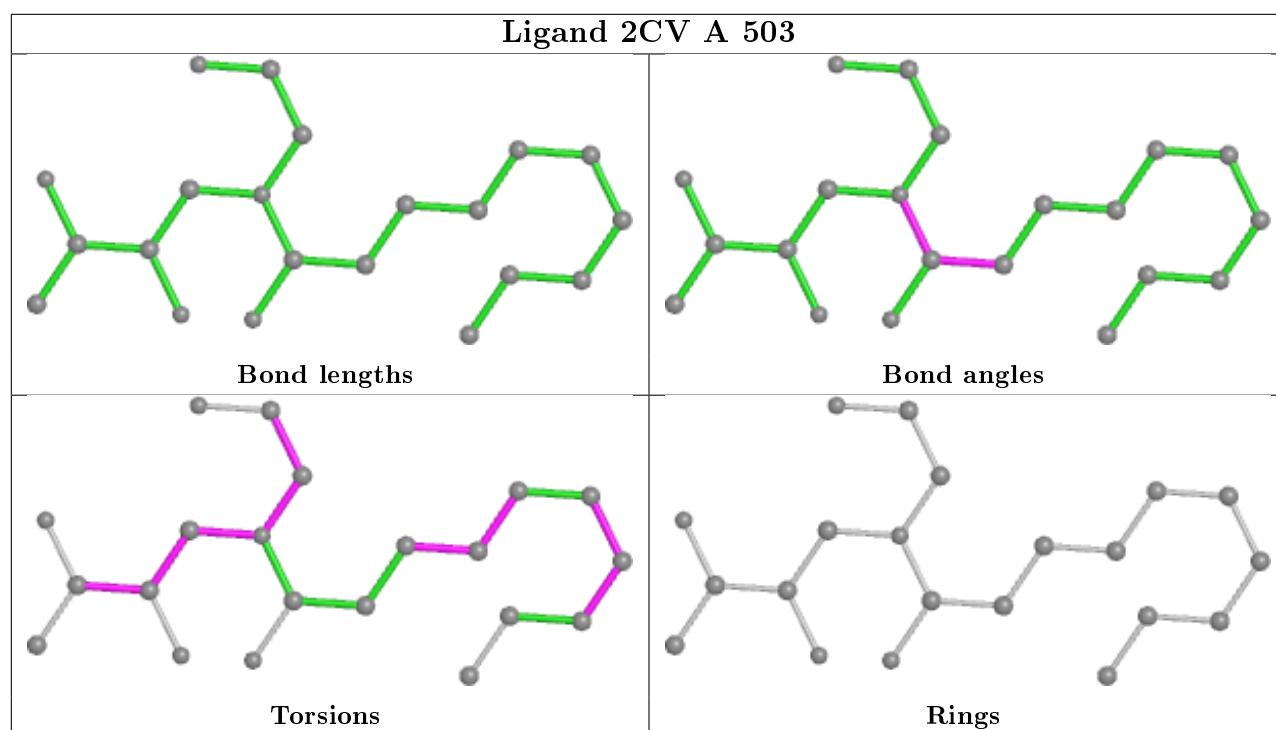
## Ligand Y01 A 402



## Ligand 2CV B 504







## 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	287/315 (91%)	0.34	13 (4%) 33 23	30, 49, 93, 146	0
1	B	299/315 (94%)	0.33	11 (3%) 41 31	27, 49, 80, 104	0
All	All	586/630 (93%)	0.34	24 (4%) 37 27	27, 49, 87, 146	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	ARG	6.7
1	A	282	LEU	4.3
1	A	286	HIS	4.2
1	A	46	LEU	3.6
1	A	278	SER	3.5
1	B	242	ASP	3.4
1	A	283	MET	3.3
1	A	280	VAL	3.3
1	A	35	LEU	3.3
1	B	325	PHE	3.2
1	B	349	PHE	3.2
1	A	53	LEU	3.0
1	B	277	THR	3.0
1	B	344	CYS	2.9
1	B	51	VAL	2.6
1	A	34	GLU	2.6
1	B	341	ILE	2.5
1	B	284	ARG	2.5
1	A	281	MET	2.5
1	B	91	GLY	2.4
1	A	49	ALA	2.4
1	A	33	ALA	2.3
1	B	348	ASP	2.3
1	B	152	LEU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

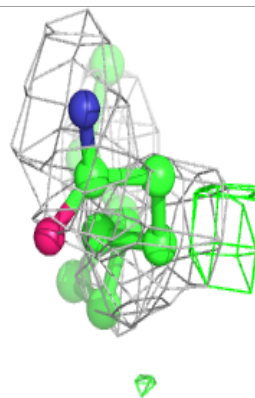
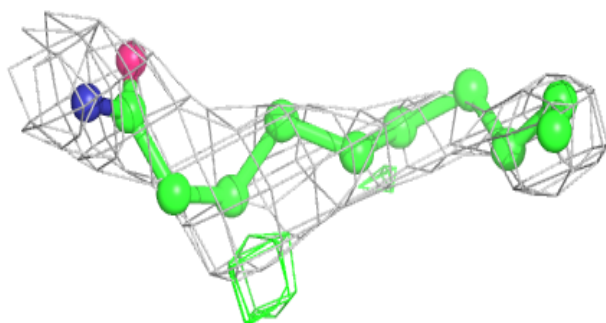
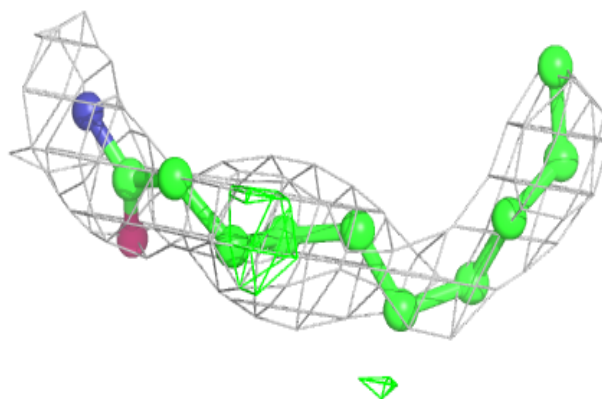
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	2CV	B	504	12/26	0.70	0.43	75,85,88,89	0
5	NA	B	1361	1/1	0.72	0.22	56,56,56,56	0
3	2CV	A	502	10/26	0.81	0.74	60,70,82,82	0
3	2CV	A	505	14/26	0.85	0.39	60,82,97,102	0
2	Y01	A	402	35/35	0.85	0.39	64,71,114,116	0
3	2CV	A	506	12/26	0.85	0.28	71,75,79,80	0
3	2CV	B	502	19/26	0.85	0.35	48,76,92,94	0
3	2CV	B	505	21/26	0.86	0.21	47,75,85,89	0
5	NA	A	1360	1/1	0.88	0.09	61,61,61,61	0
3	2CV	B	503	12/26	0.89	0.31	47,62,84,88	0
3	2CV	A	503	21/26	0.91	0.25	38,49,56,61	0
3	2CV	B	506	19/26	0.92	0.25	36,48,59,65	0
2	Y01	B	402	35/35	0.93	0.33	52,63,108,114	0
2	Y01	A	401	35/35	0.95	0.27	39,45,62,65	0
4	XF5	A	1359	15/15	0.96	0.16	39,41,41,42	0
5	NA	B	1359	1/1	0.96	0.12	47,47,47,47	0
2	Y01	B	401	35/35	0.96	0.41	44,48,74,85	0
4	XF5	B	1360	15/15	0.97	0.18	37,38,42,43	0

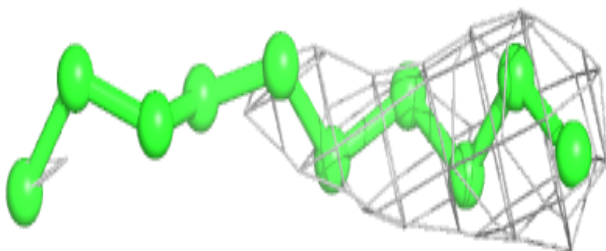
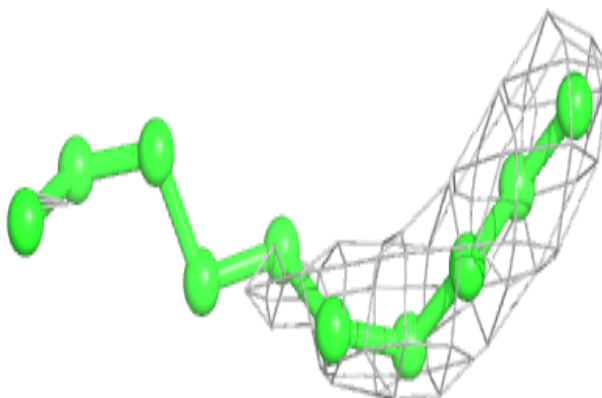
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2CV B 504:**

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

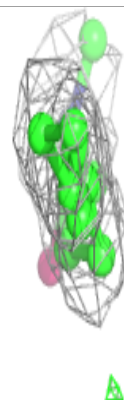
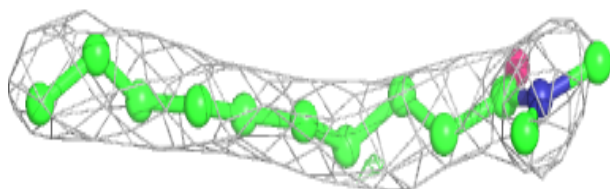
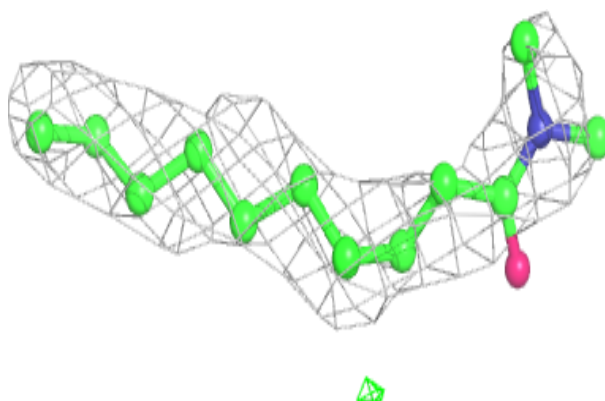
**Electron density around 2CV A 502:**

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

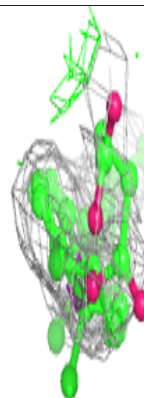
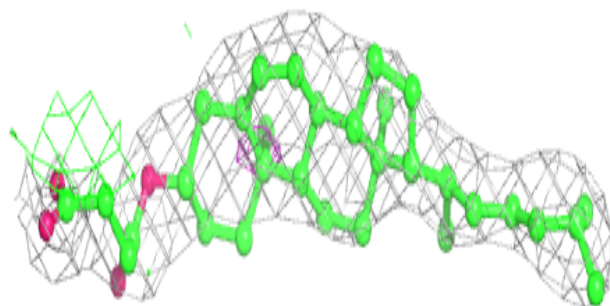
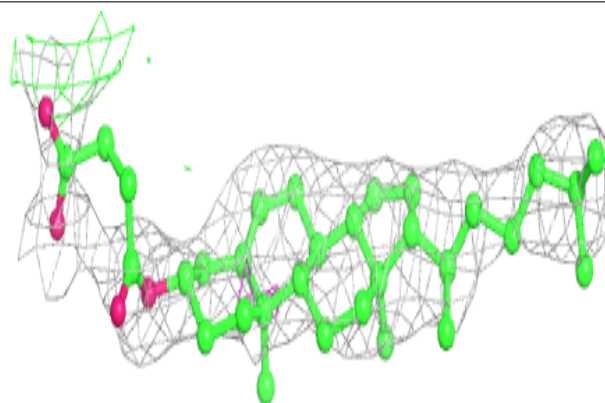


**Electron density around 2CV A 505:**

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

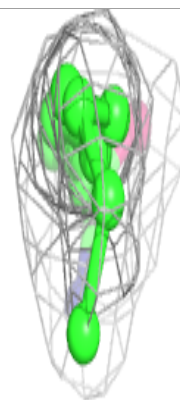
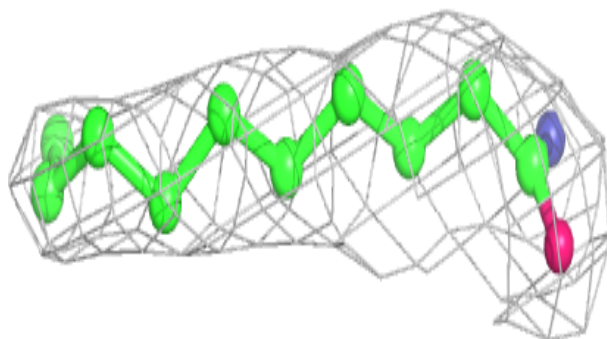
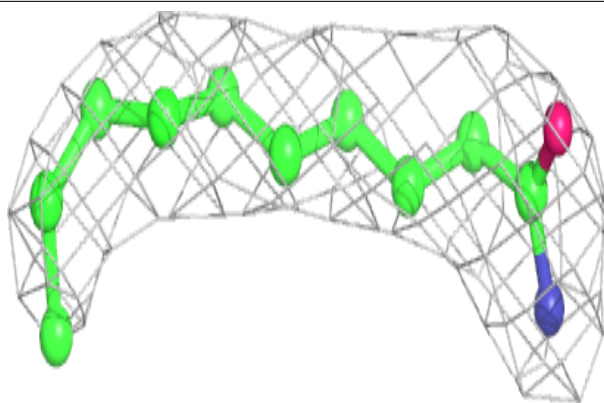
**Electron density around Y01 A 402:**

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

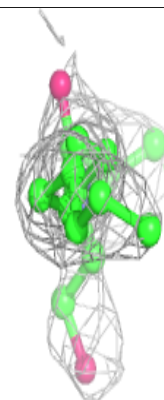
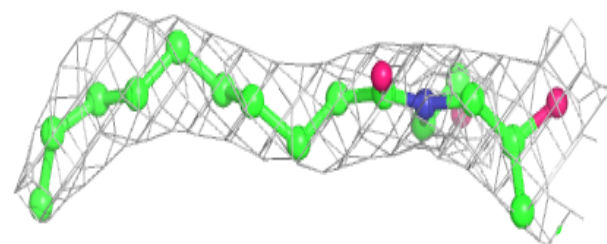
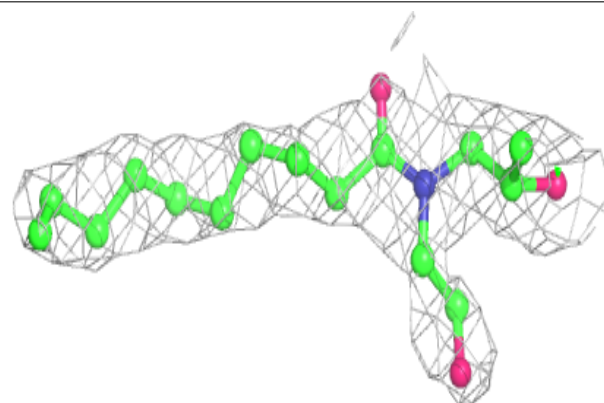


**Electron density around 2CV A 506:**

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

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

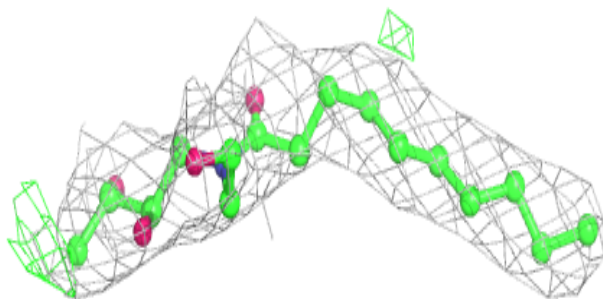
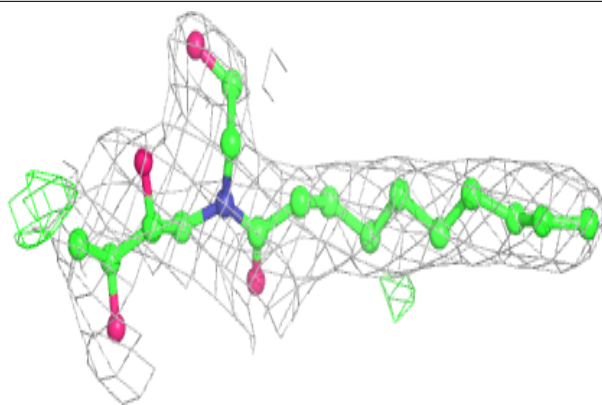
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



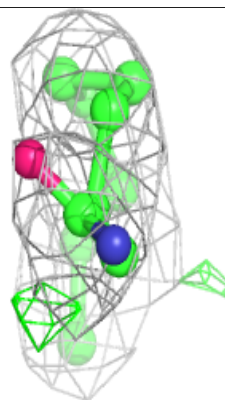
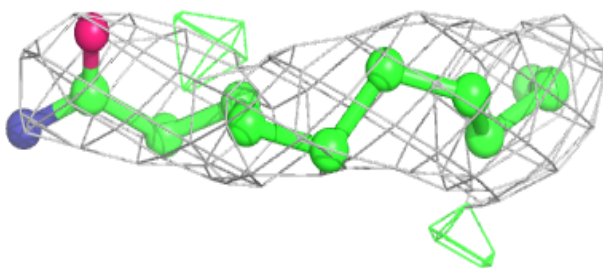
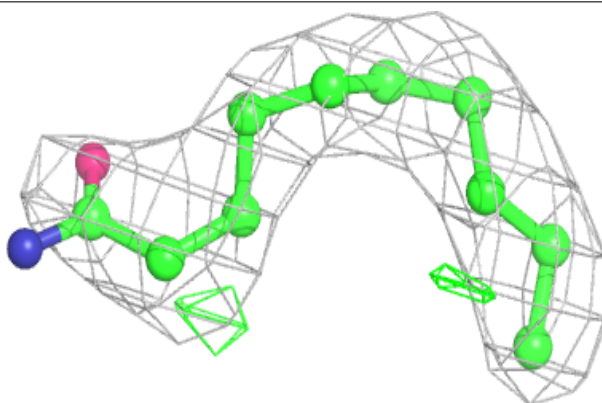


**Electron density around 2CV B 505:**

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

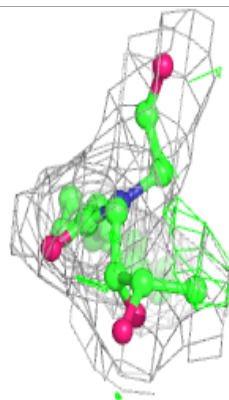
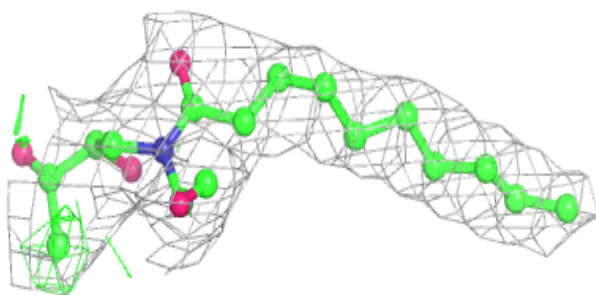
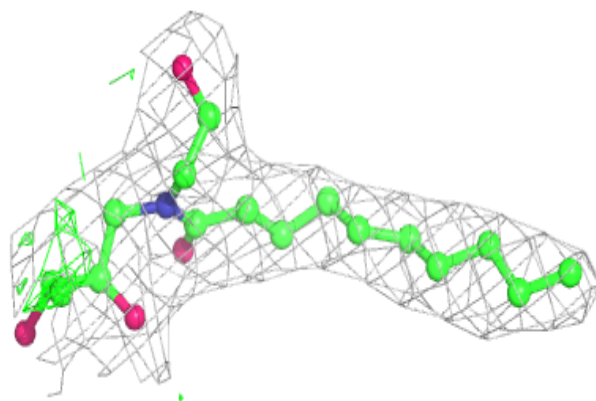
**Electron density around 2CV B 503:**

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

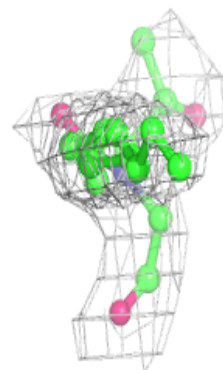
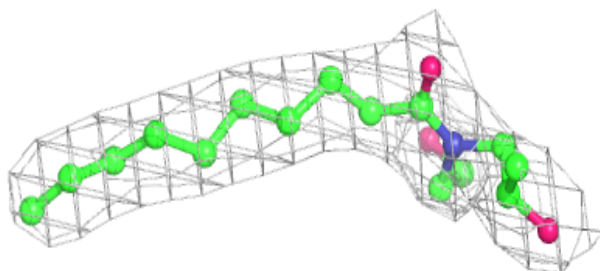
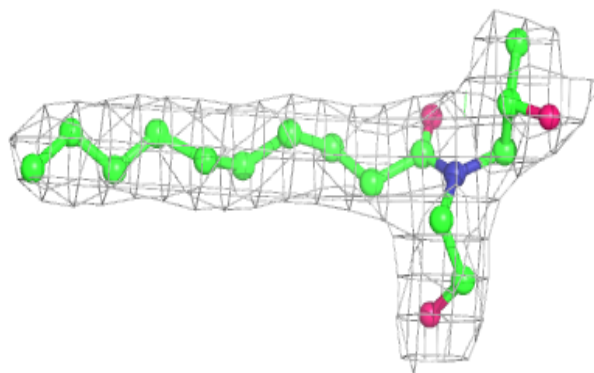


**Electron density around 2CV A 503:**

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

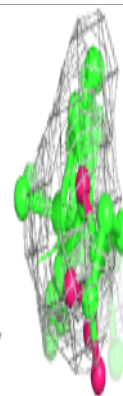
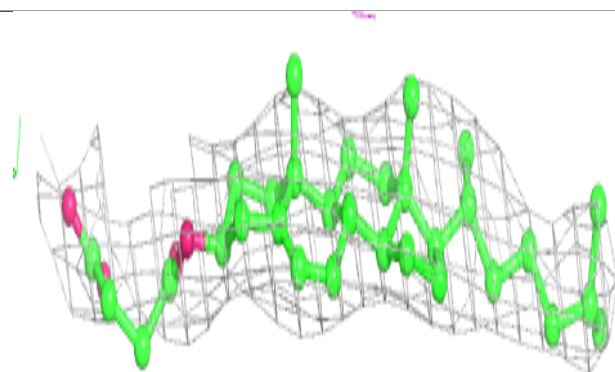
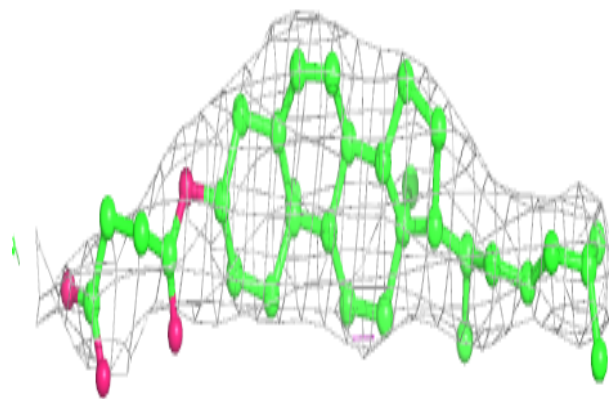
**Electron density around 2CV B 506:**

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

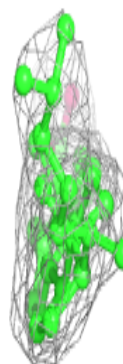
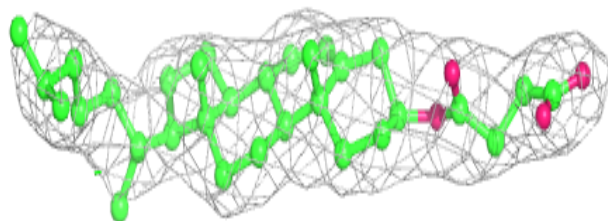
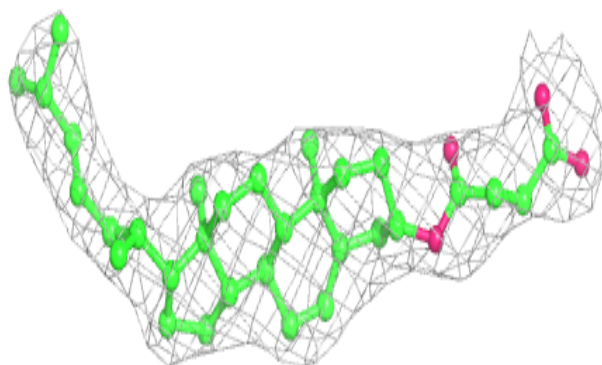


**Electron density around Y01 B 402:**

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

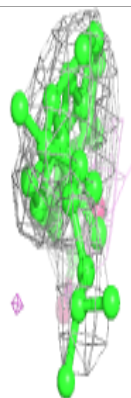
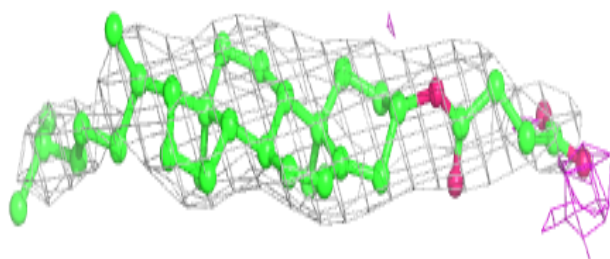
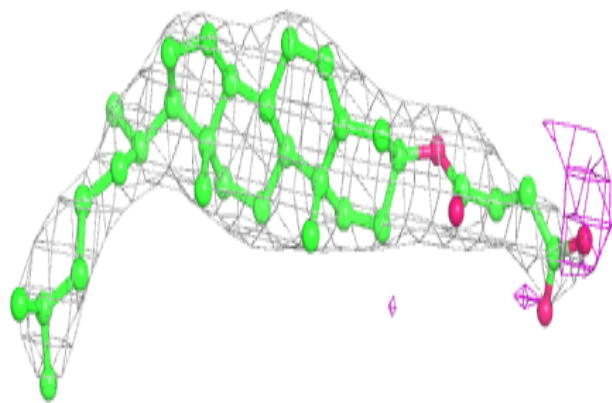
**Electron density around Y01 A 401:**

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



**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.