



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:08 am BST

PDB ID : 6H7M  
Title : ACTIVATED TURKEY BETA1 ADRENOCEPTOR WITH BOUND PARTIAL AGONIST SALBUTAMOL AND NANOBODY Nb6B9  
Authors : Warne, T.; Edwards, P.C.; Dore, A.S.; Leslie, A.G.W.; Tate, C.G.  
Deposited on : 2018-07-31  
Resolution : 2.76 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

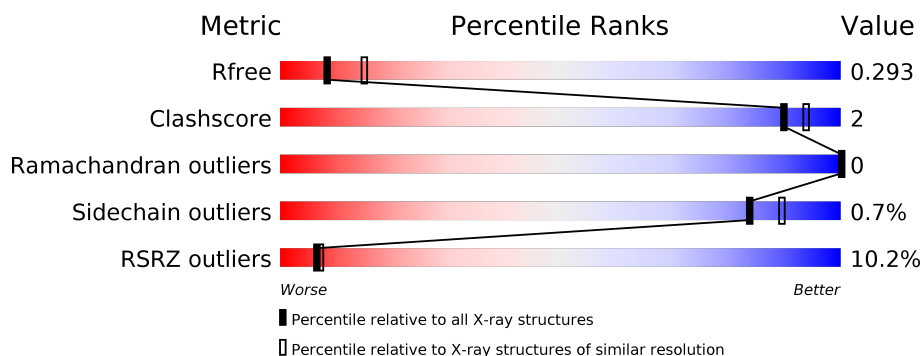
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	E	109	<div> <div>36%</div> <div>94%</div> <div>• •</div> </div>
1	F	109	<div> <div>22%</div> <div>98%</div> <div>•</div> </div>
2	A	307	<div> <div>4%</div> <div>87%</div> <div>8% 5%</div> </div>
2	B	307	<div> <div>7%</div> <div>87%</div> <div>6% 7%</div> </div>
3	C	121	<div> <div>2%</div> <div>97%</div> <div>• •</div> </div>
3	D	121	<div> <div>6%</div> <div>97%</div> <div>• •</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8230 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 Thioredoxin 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	E	107	Total	C	N	O	0	0	0
			805	518	129	158			
1	F	107	Total	C	N	O	0	0	0
			812	523	131	158			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	32	SER	CYS	engineered mutation	UNP P0AA25
E	35	SER	CYS	engineered mutation	UNP P0AA25
E	109	GLU	-	expression tag	UNP P0AA25
F	32	SER	CYS	engineered mutation	UNP P0AA25
F	35	SER	CYS	engineered mutation	UNP P0AA25
F	109	GLU	-	expression tag	UNP P0AA25

- Molecule 2 is a protein called Beta-1 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	291	Total	C	N	O	S	0	0	0
			2313	1526	385	382	20			
2	B	285	Total	C	N	O	S	0	0	0
			2264	1499	371	374	20			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ALA	-	expression tag	UNP P07700
A	40	ALA	-	expression tag	UNP P07700
A	41	ALA	-	expression tag	UNP P07700
A	42	LYS	-	expression tag	UNP P07700
A	43	VAL	-	expression tag	UNP P07700
A	68	SER	ARG	engineered mutation	UNP P07700

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Chain	Residue	Modelled	Actual	Comment	Reference
A	90	VAL	MET	engineered mutation	UNP P07700
A	116	LEU	CYS	engineered mutation	UNP P07700
A	?	-	ARG	deletion	UNP P07700
A	?	-	CYS	deletion	UNP P07700
A	?	-	GLU	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	?	-	ARG	deletion	UNP P07700
A	?	-	PHE	deletion	UNP P07700
A	?	-	TYR	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	?	-	SER	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	GLU	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	LEU	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	HIS	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	ILE	deletion	UNP P07700
A	?	-	LEU	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	?	-	ASN	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	284	LYS	ARG	conflict	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
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
B	39	ALA	-	expression tag	UNP P07700
B	40	ALA	-	expression tag	UNP P07700
B	41	ALA	-	expression tag	UNP P07700

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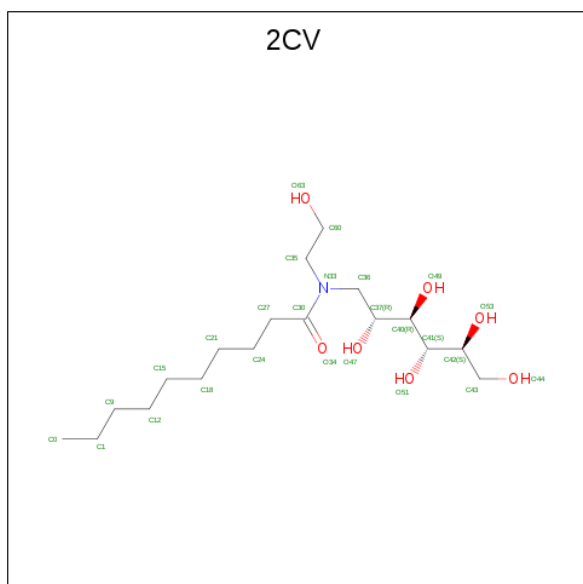
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Chain	Residue	Modelled	Actual	Comment	Reference
B	42	LYS	-	expression tag	UNP P07700
B	43	VAL	-	expression tag	UNP P07700
B	68	SER	ARG	engineered mutation	UNP P07700
B	90	VAL	MET	engineered mutation	UNP P07700
B	116	LEU	CYS	engineered mutation	UNP P07700
B	?	-	ARG	deletion	UNP P07700
B	?	-	CYS	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	ARG	deletion	UNP P07700
B	?	-	PHE	deletion	UNP P07700
B	?	-	TYR	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	SER	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	LEU	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	HIS	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	ILE	deletion	UNP P07700
B	?	-	LEU	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	ASN	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	284	LYS	ARG	conflict	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
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

- Molecule 3 is a protein called Camelid antibody fragment Nb6B9.

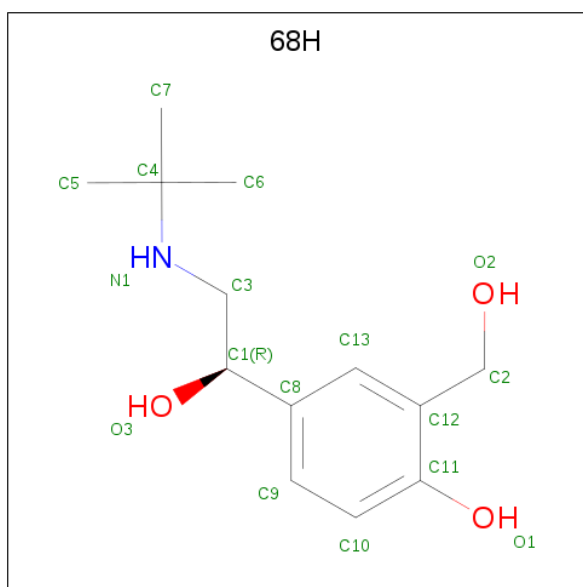
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	S	0	0	0
			910	569	159	178	4			
3	D	120	Total	C	N	O	S	0	0	0
			910	569	159	178	4			

- Molecule 4 is HEGA-10 (three-letter code: 2CV) (formula: C<sub>18</sub>H<sub>37</sub>NO<sub>7</sub>).



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

- Molecule 5 is SALBUTAMOL (three-letter code: 68H) (formula: C<sub>13</sub>H<sub>21</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	13	1	3		
5	B	1	Total	C	N	O	0	0
			17	13	1	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

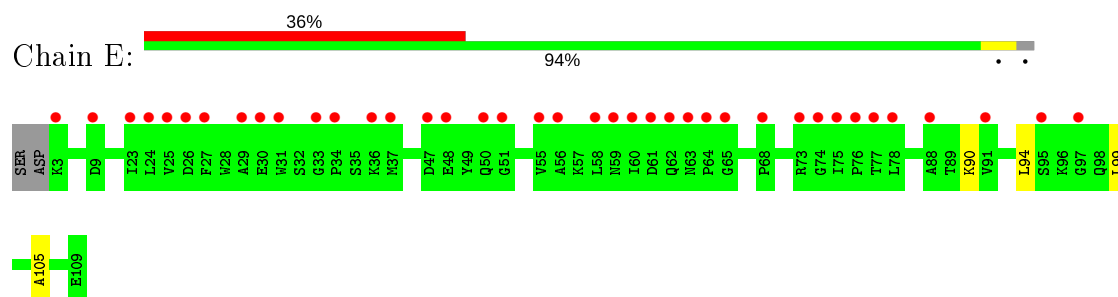
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	C	3	Total	O	0	0
			3	3		
7	B	4	Total	O	0	0
			4	4		

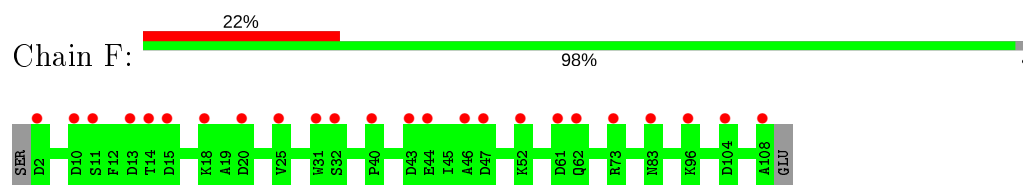
### 3 Residue-property plots [i](#)

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.

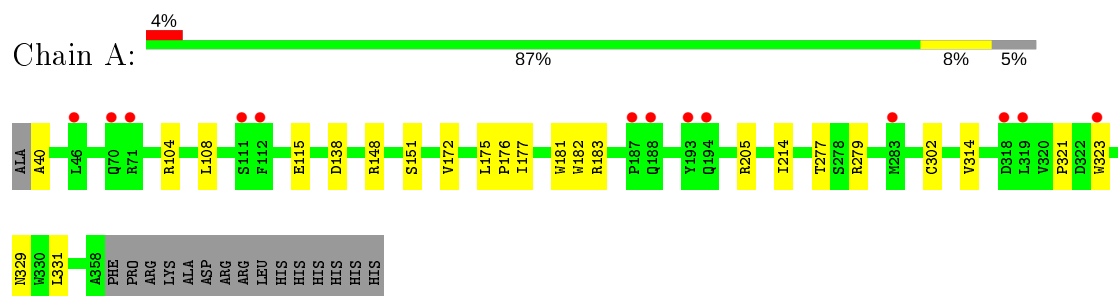
- Molecule 1: Thioredoxin 1



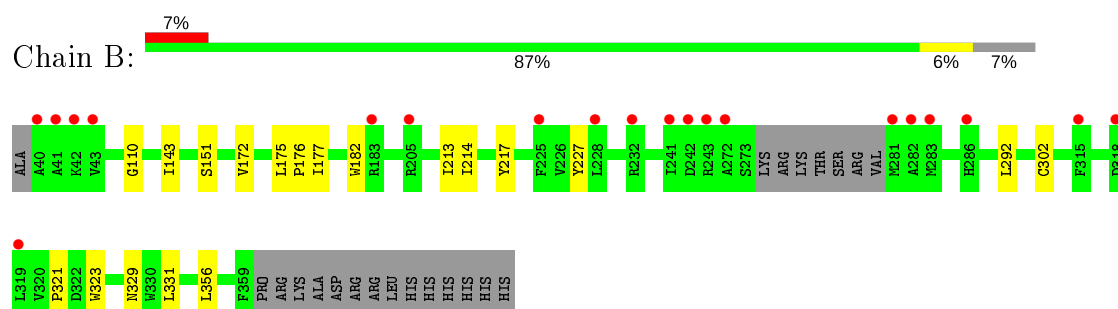
- Molecule 1: Thioredoxin 1



- Molecule 2: Beta-1 adrenergic receptor



- Molecule 2: Beta-1 adrenergic receptor





- Molecule 3: Camelid antibody fragment Nb6B9

Chain C:  2% 97% ..



- Molecule 3: Camelid antibody fragment Nb6B9

Chain D:  6% 97% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.64Å 121.50Å 130.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.77 – 2.76 25.77 – 2.76	Depositor EDS
% Data completeness (in resolution range)	66.8 (25.77-2.76) 66.9 (25.77-2.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0166	Depositor
R, $R_{free}$	0.265 , 0.285 0.271 , 0.293	Depositor DCC
$R_{free}$ test set	1590 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.2	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	8230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 68H

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	E	0.46	0/820	0.60	0/1116
1	F	0.47	0/827	0.60	0/1123
2	A	0.43	0/2367	0.68	1/3222 (0.0%)
2	B	0.43	0/2318	0.65	0/3157
3	C	0.42	0/927	0.61	0/1256
3	D	0.43	0/927	0.60	0/1256
All	All	0.44	0/8186	0.64	1/11130 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	138	ASP	CB-CG-OD1	-5.06	113.75	118.30

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	E	805	0	798	4	0
1	F	812	0	818	0	0
2	A	2313	0	2423	11	0
2	B	2264	0	2358	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	910	0	878	3	0
3	D	910	0	878	3	0
4	A	63	0	90	1	0
4	B	104	0	148	2	0
5	A	17	0	20	0	0
5	B	17	0	21	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	6	0	0	0	0
7	B	4	0	0	0	0
7	C	3	0	0	0	0
All	All	8230	0	8432	30	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 2.

All (30) 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)
3:C:11:LEU:HD23	3:C:117:THR:HB	1.75	0.67
3:D:11:LEU:HD23	3:D:117:THR:HB	1.77	0.65
2:A:115:GLU:OE2	2:A:183:ARG:NH2	2.29	0.58
2:B:302:CYS:HA	2:B:331:LEU:HG	1.86	0.57
3:C:11:LEU:CD2	3:C:117:THR:HB	2.35	0.56
2:A:302:CYS:HA	2:A:331:LEU:HG	1.88	0.56
3:D:11:LEU:CD2	3:D:117:THR:HB	2.37	0.55
2:A:177:ILE:HA	2:A:182:TRP:CD1	2.45	0.52
2:B:177:ILE:HA	2:B:182:TRP:CD1	2.45	0.51
4:B:404:2CV:H37	4:B:404:2CV:O63	2.11	0.51
2:B:175:LEU:HB3	2:B:176:PRO:HD3	1.95	0.48
1:E:90:LYS:NZ	1:E:99:LEU:HA	2.29	0.47
2:A:321:PRO:HB2	2:A:323:TRP:CD1	2.49	0.47
2:B:321:PRO:HB2	2:B:323:TRP:CD1	2.50	0.47
4:A:503:2CV:O47	4:A:503:2CV:H352	2.16	0.46
1:E:90:LYS:NZ	1:E:94:LEU:HD13	2.30	0.46
2:A:205:ARG:HG3	2:A:314:VAL:HG13	1.98	0.45
2:B:143:ILE:CG2	3:D:31:LEU:HD13	2.47	0.45
2:B:172:VAL:HG21	2:B:214:ILE:HG21	1.98	0.45
2:A:181:TRP:CD1	2:B:356:LEU:HD22	2.52	0.45
1:E:105:ALA:HA	2:A:40:ALA:HB2	1.98	0.45
2:A:104:ARG:HG3	2:A:108:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:402:2CV:O47	4:B:402:2CV:O34	2.30	0.44
2:B:227:TYR:HB3	2:B:292:LEU:HD11	2.00	0.43
2:A:175:LEU:HB3	2:A:176:PRO:HD3	2.00	0.43
2:A:148:ARG:HH22	2:B:110:GLY:CA	2.32	0.43
2:B:213:ILE:HA	2:B:217:TYR:HB2	2.01	0.42
3:C:90:THR:HG23	3:C:117:THR:HA	2.01	0.42
1:E:90:LYS:NZ	1:E:94:LEU:CD1	2.82	0.42
2:A:172:VAL:HG21	2:A:214:ILE:HG21	2.02	0.42

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	E	105/109 (96%)	102 (97%)	3 (3%)	0	100	100
1	F	105/109 (96%)	103 (98%)	2 (2%)	0	100	100
2	A	289/307 (94%)	280 (97%)	9 (3%)	0	100	100
2	B	281/307 (92%)	272 (97%)	9 (3%)	0	100	100
3	C	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
3	D	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
All	All	1016/1074 (95%)	989 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	83/88 (94%)	83 (100%)	0	100	100
1	F	85/88 (97%)	85 (100%)	0	100	100
2	A	252/266 (95%)	248 (98%)	4 (2%)	62	77
2	B	246/266 (92%)	244 (99%)	2 (1%)	81	88
3	C	94/95 (99%)	94 (100%)	0	100	100
3	D	94/95 (99%)	94 (100%)	0	100	100
All	All	854/898 (95%)	848 (99%)	6 (1%)	84	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	151	SER
2	A	277	THR
2	A	279	ARG
2	A	329	ASN
2	B	151	SER
2	B	329	ASN

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	2CV	B	404	-	25,25,25	0.40	0	29,30,30	1.16	4 (13%)
5	68H	A	504	-	17,17,17	1.61	1 (5%)	23,24,24	1.28	1 (4%)
4	2CV	A	502	-	15,15,25	0.63	0	16,16,30	0.83	0
4	2CV	B	401	-	25,25,25	0.81	1 (4%)	29,30,30	1.19	3 (10%)
4	2CV	A	501	-	25,25,25	0.36	0	29,30,30	1.25	3 (10%)
4	2CV	B	402	-	25,25,25	0.51	0	29,30,30	1.83	3 (10%)
4	2CV	A	503	-	20,20,25	0.83	2 (10%)	22,23,30	1.40	3 (13%)
5	68H	B	405	-	17,17,17	1.79	1 (5%)	23,24,24	1.28	1 (4%)
4	2CV	B	403	-	25,25,25	0.44	0	29,30,30	0.97	1 (3%)

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	2CV	B	404	-	-	17/34/34/34	-
5	68H	A	504	-	-	0/12/12/12	0/1/1/1
4	2CV	A	502	-	-	0/17/17/34	-
4	2CV	B	401	-	-	13/34/34/34	-
4	2CV	A	501	-	-	11/34/34/34	-
4	2CV	B	402	-	-	13/34/34/34	-
4	2CV	A	503	-	-	2/24/24/34	-
5	68H	B	405	-	-	0/12/12/12	0/1/1/1
4	2CV	B	403	-	-	8/34/34/34	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	405	68H	C11-C12	6.78	1.50	1.40
5	A	504	68H	C11-C12	5.77	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	2CV	C36-C37	2.44	1.56	1.52
4	A	503	2CV	C37-C40	2.21	1.56	1.53
4	A	503	2CV	C36-C37	2.18	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	2CV	C35-N33-C36	-7.45	107.54	116.41
5	B	405	68H	C3-N1-C4	5.10	121.98	116.54
5	A	504	68H	C3-N1-C4	4.80	121.65	116.54
4	A	503	2CV	C27-C30-N33	4.58	125.17	118.01
4	B	401	2CV	C42-C41-C40	3.45	117.86	112.47
4	A	501	2CV	C27-C30-N33	3.29	123.14	118.01
4	B	402	2CV	C37-C40-C41	3.17	117.42	112.47
4	B	404	2CV	C27-C30-N33	2.72	122.26	118.01
4	A	503	2CV	O34-C30-C27	-2.70	113.62	121.31
4	A	501	2CV	O34-C30-C27	-2.62	113.85	121.31
4	A	501	2CV	C35-N33-C36	-2.54	113.38	116.41
4	B	402	2CV	O34-C30-C27	-2.40	114.47	121.31
4	B	401	2CV	C27-C30-N33	2.36	121.70	118.01
4	B	404	2CV	C35-N33-C36	2.34	119.19	116.41
4	A	503	2CV	C60-C35-N33	-2.34	106.49	112.55
4	B	404	2CV	C43-C42-C41	2.27	117.32	112.41
4	B	403	2CV	C27-C30-N33	2.25	121.52	118.01
4	B	401	2CV	C37-C40-C41	2.08	115.71	112.47
4	B	404	2CV	C24-C27-C30	-2.01	107.23	112.67

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	2CV	C36-C37-C40-C41
4	B	404	2CV	C36-C37-C40-O49
4	B	404	2CV	O47-C37-C40-O49
4	B	404	2CV	C40-C41-C42-C43
4	B	404	2CV	O51-C41-C42-C43
4	B	401	2CV	C40-C41-C42-O53
4	B	401	2CV	O51-C41-C42-C43
4	B	401	2CV	O51-C41-C42-O53
4	B	401	2CV	C41-C42-C43-O44
4	B	401	2CV	O53-C42-C43-O44
4	A	501	2CV	N33-C36-C37-C40

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Mol	Chain	Res	Type	Atoms
4	A	501	2CV	O53-C42-C43-O44
4	B	402	2CV	C37-C36-N33-C30
4	B	402	2CV	C37-C36-N33-C35
4	B	403	2CV	N33-C35-C60-O63
4	A	501	2CV	N33-C35-C60-O63
4	A	501	2CV	C41-C42-C43-O44
4	B	404	2CV	O51-C41-C42-O53
4	B	404	2CV	O47-C37-C40-C41
4	B	404	2CV	C40-C41-C42-O53
4	B	401	2CV	C40-C41-C42-C43
4	B	402	2CV	O53-C42-C43-O44
4	B	402	2CV	C41-C42-C43-O44
4	B	404	2CV	N33-C35-C60-O63
4	A	501	2CV	C12-C15-C18-C21
4	B	402	2CV	C21-C24-C27-C30
4	B	403	2CV	C18-C21-C24-C27
4	B	404	2CV	C15-C18-C21-C24
4	A	503	2CV	C18-C21-C24-C27
4	A	501	2CV	C21-C24-C27-C30
4	B	404	2CV	C60-C35-N33-C36
4	B	402	2CV	C40-C41-C42-O53
4	B	404	2CV	C9-C12-C15-C18
4	B	401	2CV	C15-C12-C9-C1
4	B	402	2CV	O51-C41-C42-O53
4	B	403	2CV	C12-C15-C18-C21
4	B	402	2CV	N33-C35-C60-O63
4	B	401	2CV	O49-C40-C41-O51
4	A	501	2CV	O49-C40-C41-O51
4	B	402	2CV	O51-C41-C42-C43
4	B	402	2CV	C40-C41-C42-C43
4	B	404	2CV	C37-C36-N33-C35
4	B	403	2CV	C15-C12-C9-C1
4	A	501	2CV	C15-C12-C9-C1
4	A	503	2CV	C15-C12-C9-C1
4	B	401	2CV	C12-C15-C18-C21
4	B	402	2CV	N33-C36-C37-O47
4	B	402	2CV	C12-C15-C18-C21
4	B	404	2CV	C60-C35-N33-C30
4	B	402	2CV	C0-C1-C9-C12
4	B	404	2CV	C41-C42-C43-O44
4	B	403	2CV	O49-C40-C41-C42
4	B	404	2CV	O53-C42-C43-O44

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Mol	Chain	Res	Type	Atoms
4	B	401	2CV	C18-C21-C24-C27
4	B	404	2CV	C21-C24-C27-C30
4	B	401	2CV	C9-C12-C15-C18
4	A	501	2CV	O49-C40-C41-C42
4	B	403	2CV	C15-C18-C21-C24
4	B	403	2CV	O49-C40-C41-O51
4	A	501	2CV	O47-C37-C40-O49
4	B	401	2CV	C37-C36-N33-C35
4	B	403	2CV	C0-C1-C9-C12
4	A	501	2CV	C36-C37-C40-O49
4	B	401	2CV	N33-C35-C60-O63

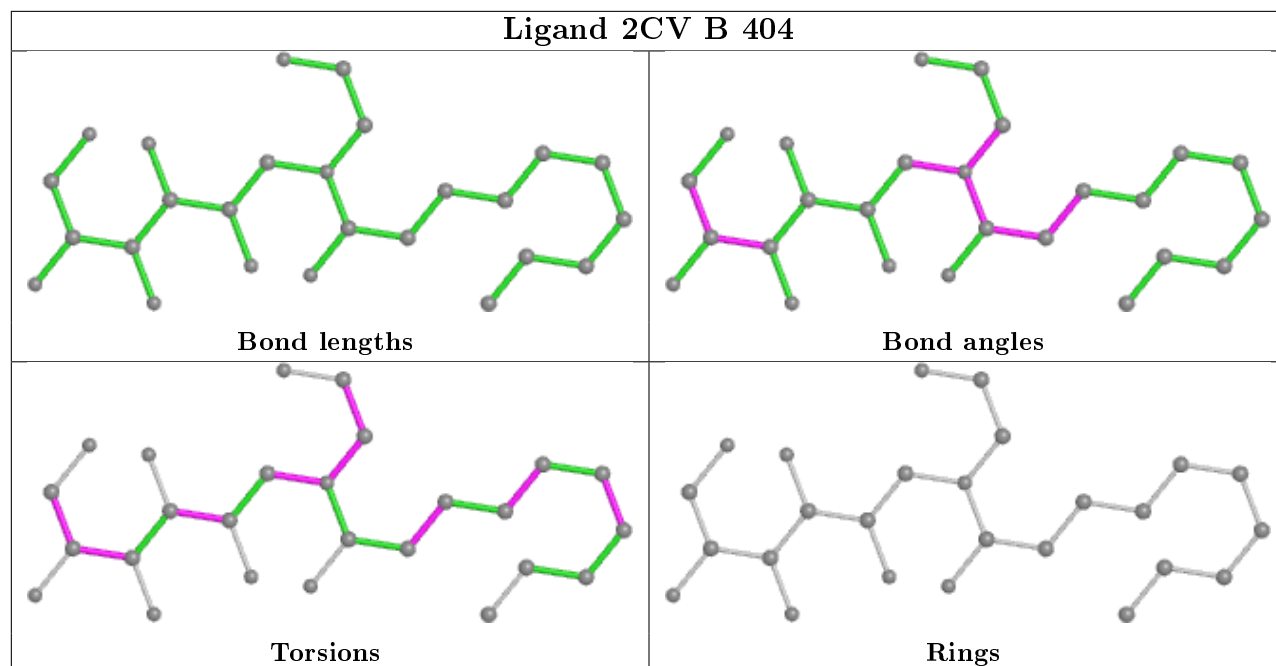
There are no ring outliers.

3 monomers are involved in 3 short contacts:

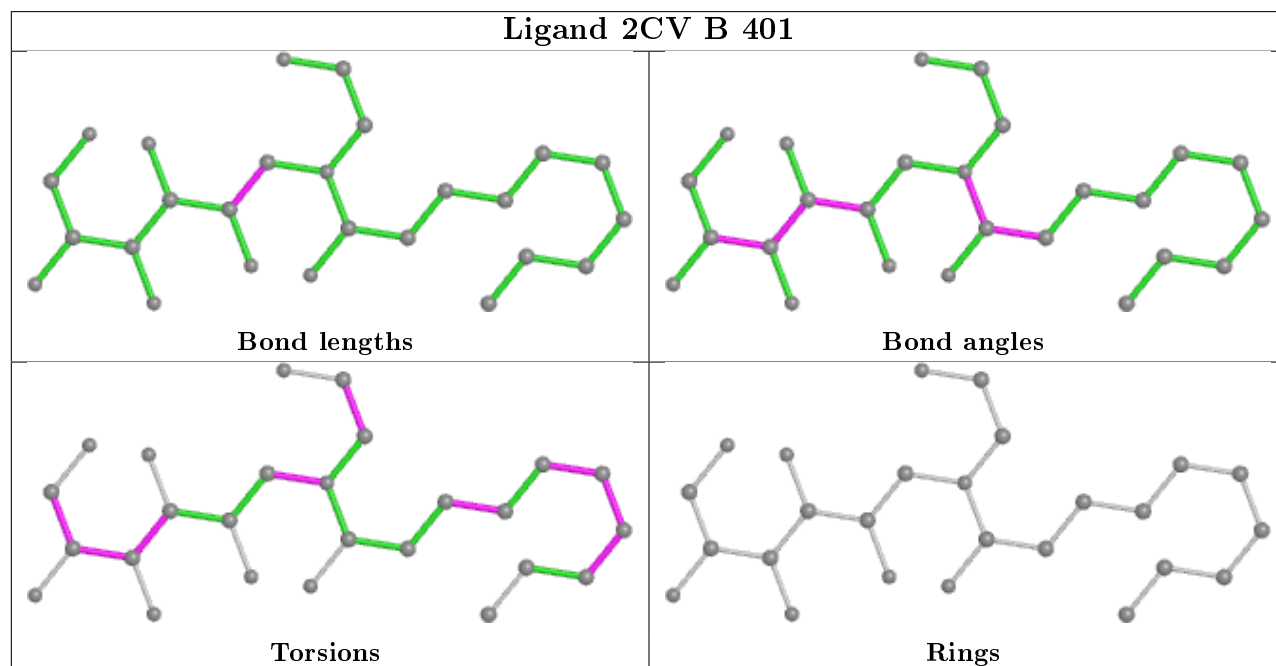
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	2CV	1	0
4	B	402	2CV	1	0
4	A	503	2CV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

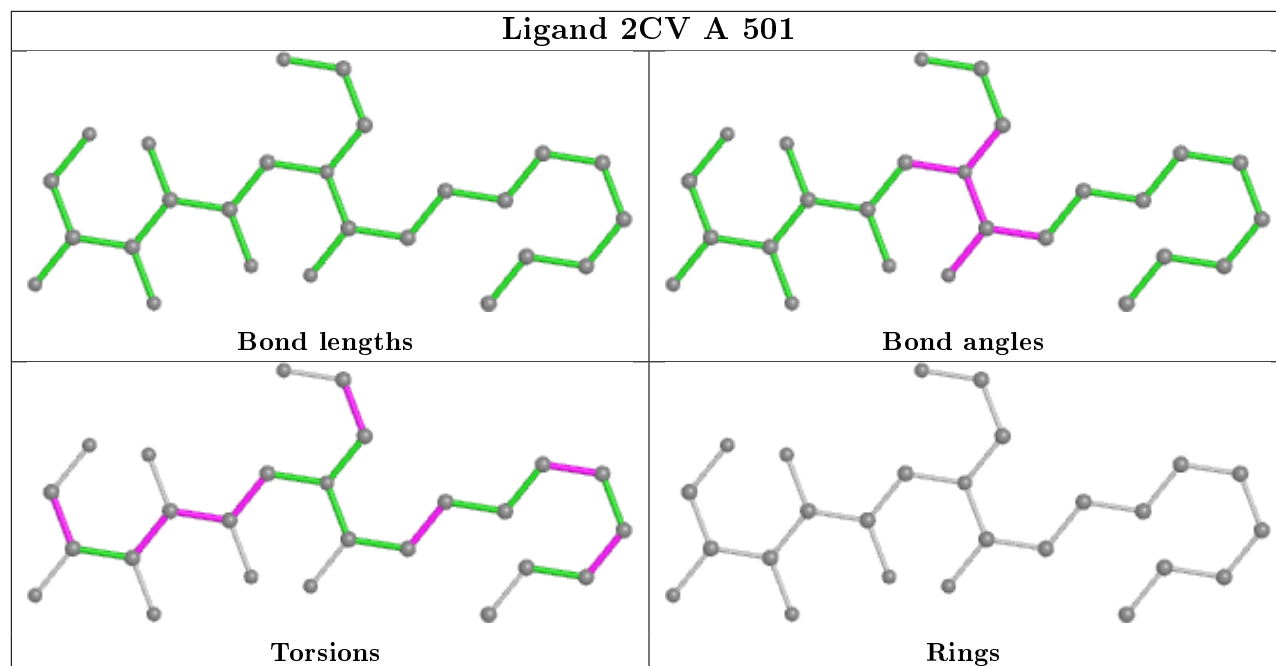
## Ligand 2CV B 404



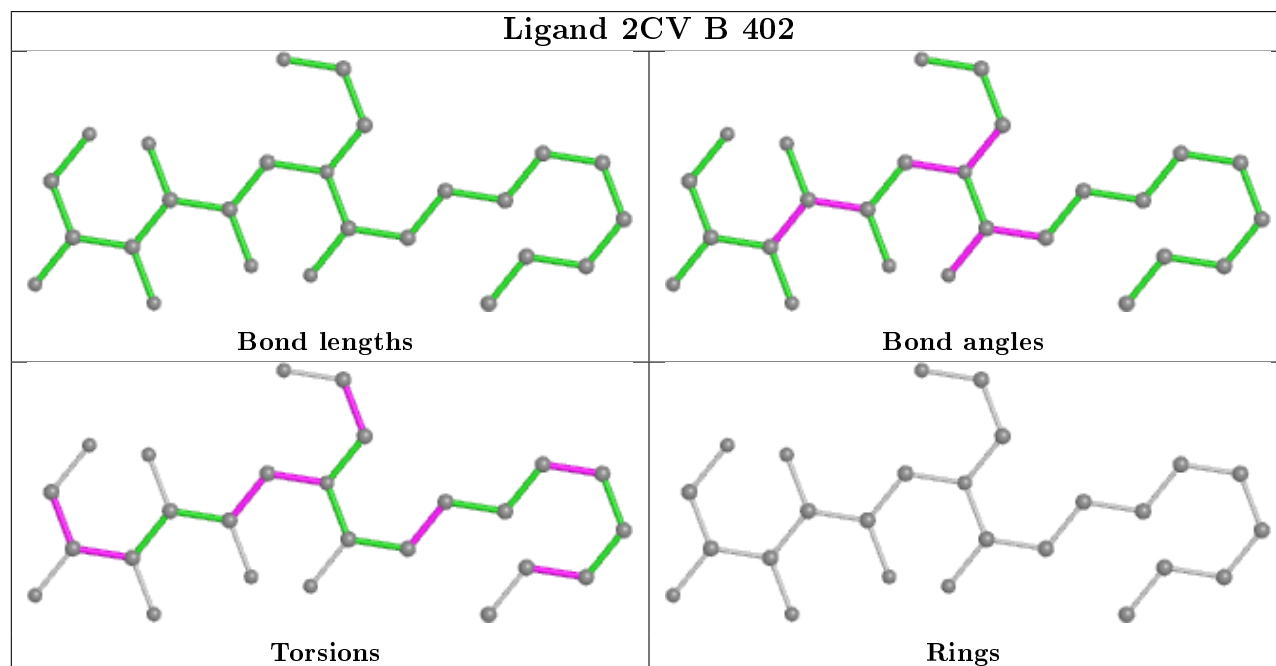
## Ligand 2CV B 401

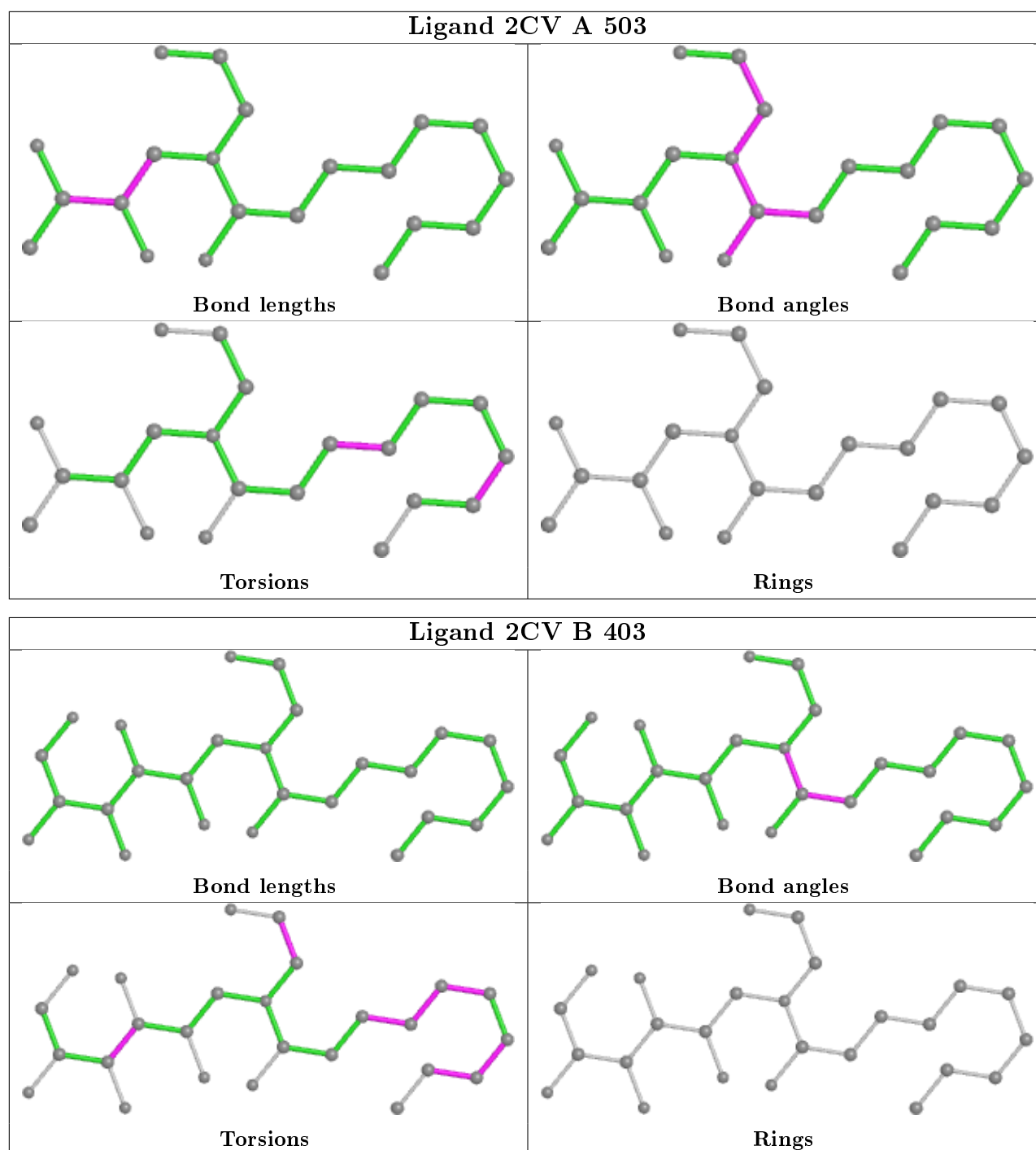


## Ligand 2CV A 501



## Ligand 2CV B 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	E	107/109 (98%)	1.71	39 (36%) 0 0	86, 130, 170, 206	0
1	F	107/109 (98%)	1.15	24 (22%) 0 0	80, 109, 141, 154	0
2	A	291/307 (94%)	0.14	13 (4%) 33 39	38, 63, 108, 123	0
2	B	285/307 (92%)	0.37	20 (7%) 16 19	44, 79, 130, 156	0
3	C	120/121 (99%)	-0.03	2 (1%) 70 78	41, 58, 92, 122	0
3	D	120/121 (99%)	0.50	7 (5%) 23 28	55, 74, 105, 121	0
All	All	1030/1074 (95%)	0.49	105 (10%) 6 7	38, 79, 138, 206	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	91	VAL	9.4
1	F	14	THR	9.1
1	E	76	PRO	8.7
3	D	120	SER	8.5
2	B	272	ALA	7.4
2	B	232	ARG	6.9
1	E	77	THR	6.6
1	F	15	ASP	6.4
1	E	31	TRP	6.4
1	E	50	GLN	6.1
1	F	10	ASP	5.9
3	C	1	GLN	5.8
3	D	13	GLN	5.7
1	F	108	ALA	5.7
2	B	281	MET	5.3
3	D	44	GLN	5.1
1	F	43	ASP	4.9
1	E	34	PRO	4.7
1	F	18	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	43	VAL	4.6
2	B	243	ARG	4.5
2	B	205	ARG	4.4
2	B	40	ALA	4.4
1	E	27	PHE	4.3
1	F	40	PRO	4.2
1	E	68	PRO	4.2
2	A	46	LEU	4.0
1	F	52	LYS	4.0
1	E	62	GLN	4.0
1	E	25	VAL	3.9
1	F	31	TRP	3.9
1	F	104	ASP	3.8
1	E	47	ASP	3.7
1	E	56	ALA	3.6
1	E	51	GLY	3.6
1	E	48	GLU	3.5
1	E	63	ASN	3.5
3	D	112	GLN	3.5
2	A	71	ARG	3.5
1	E	65	GLY	3.4
1	E	61	ASP	3.3
1	F	46	ALA	3.3
1	E	73	ARG	3.3
1	F	13	ASP	3.2
1	E	64	PRO	3.2
2	B	183	ARG	3.1
1	F	62	GLN	3.1
2	A	283	MET	3.1
1	E	74	GLY	3.0
1	E	3	LYS	2.9
2	A	111	SER	2.9
2	A	323	TRP	2.9
1	E	36	LYS	2.9
1	F	44	GLU	2.8
1	E	37	MET	2.8
1	F	11	SER	2.8
1	E	60	ILE	2.7
2	B	319	LEU	2.7
1	E	26	ASP	2.7
2	A	112	PHE	2.7
2	B	315	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	95	SER	2.7
1	E	59	ASN	2.7
1	E	88	ALA	2.7
2	A	188	GLN	2.7
2	A	193	TYR	2.7
1	E	55	VAL	2.6
2	B	242	ASP	2.6
2	B	42	LYS	2.6
1	F	61	ASP	2.6
1	F	96	LYS	2.5
1	E	9	ASP	2.5
3	D	74	ALA	2.5
1	E	23	ILE	2.5
2	A	194	GLN	2.4
2	B	225	PHE	2.4
1	F	2	ASP	2.4
2	A	70	GLN	2.4
2	B	286	HIS	2.4
3	D	119	SER	2.4
3	D	14	ALA	2.3
1	F	73	ARG	2.3
1	E	33	GLY	2.3
1	F	32	SER	2.2
2	B	41	ALA	2.2
2	B	282	ALA	2.2
2	B	283	MET	2.2
1	E	30	GLU	2.2
1	E	58	LEU	2.2
1	F	47	ASP	2.2
1	F	83	ASN	2.2
2	A	318	ASP	2.2
2	B	318	ASP	2.2
2	A	187	PRO	2.2
1	E	24	LEU	2.1
2	B	228	LEU	2.1
1	E	29	ALA	2.1
1	E	75	ILE	2.1
2	B	241	ILE	2.1
1	E	97	GLY	2.1
3	C	3	GLN	2.0
1	F	20	ASP	2.0
1	E	78	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	A	319	LEU	2.0
1	F	25	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

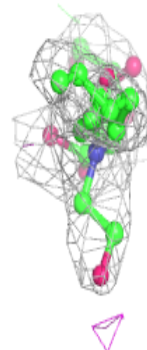
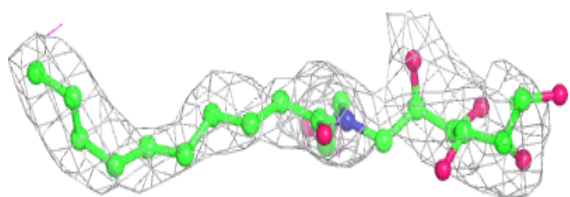
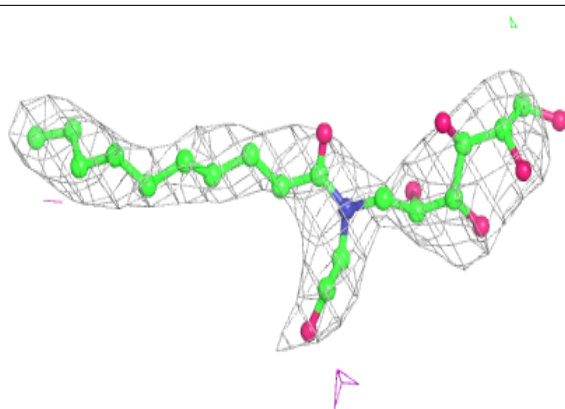
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	A	505	1/1	0.62	0.32	45,45,45,45	0
4	2CV	B	401	26/26	0.80	0.32	61,94,109,117	0
4	2CV	A	503	21/26	0.80	0.25	43,63,78,83	0
4	2CV	B	403	26/26	0.81	0.33	79,99,132,145	0
4	2CV	A	502	16/26	0.83	0.21	60,64,72,72	0
4	2CV	B	404	26/26	0.87	0.24	53,72,92,96	0
4	2CV	B	402	26/26	0.88	0.26	54,63,91,120	0
4	2CV	A	501	26/26	0.91	0.23	51,72,85,87	0
5	68H	B	405	17/17	0.93	0.22	66,70,72,72	0
5	68H	A	504	17/17	0.93	0.24	51,53,69,71	0
6	NA	B	406	1/1	0.94	0.10	56,56,56,56	0

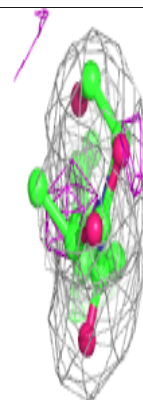
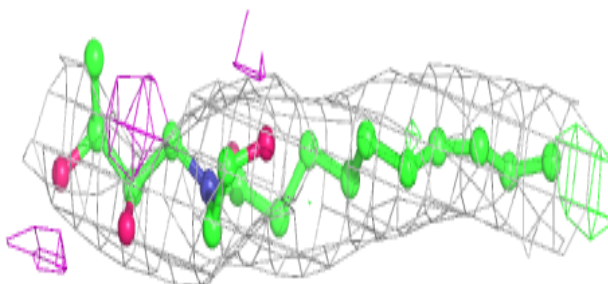
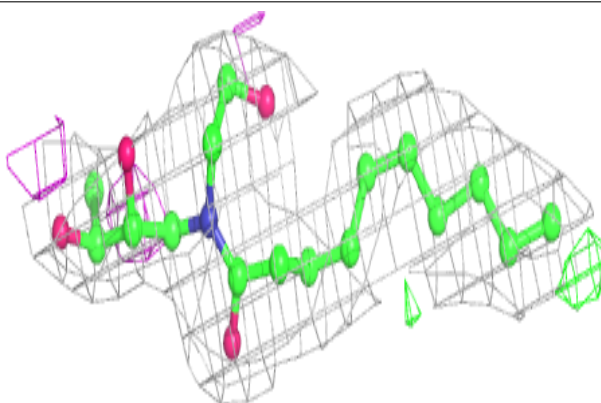
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2CV B 401:**

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

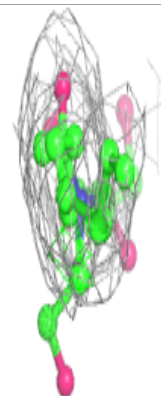
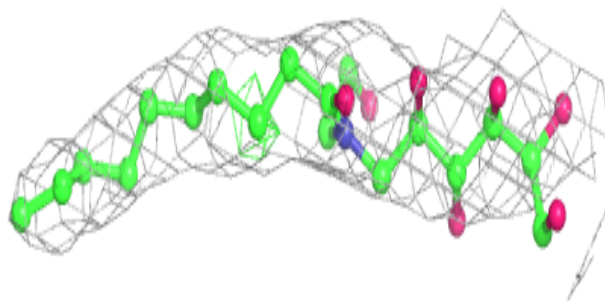
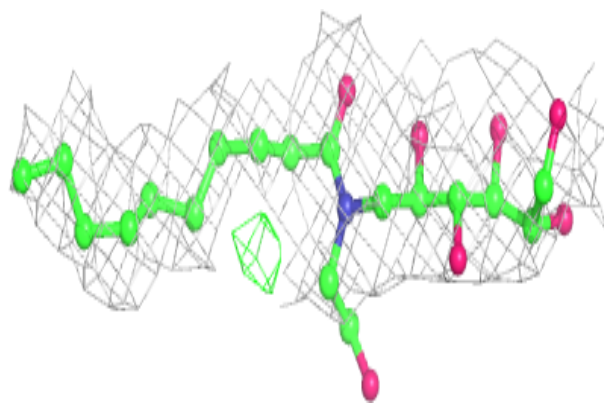
**Electron density around 2CV A 503:**

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

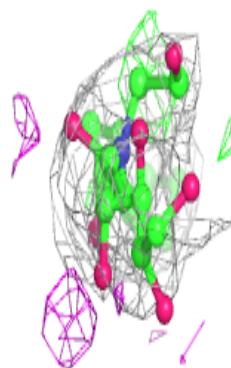
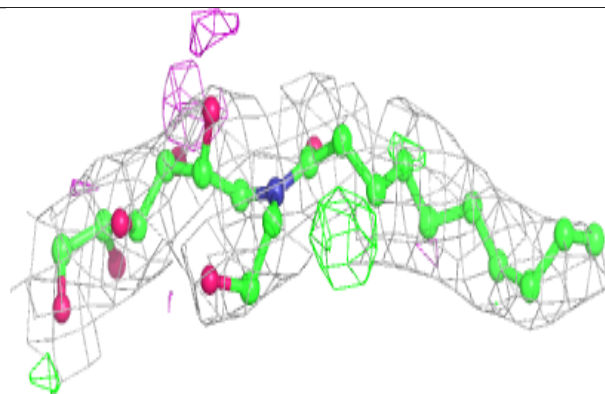
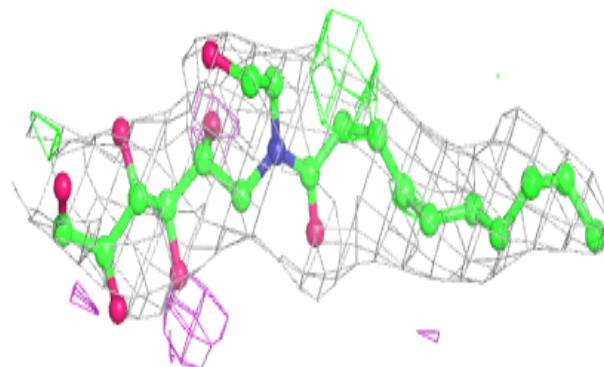


**Electron density around 2CV B 403:**

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

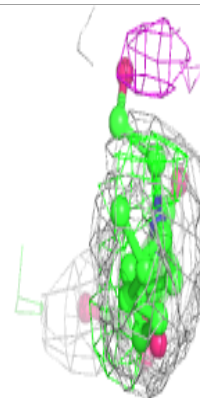
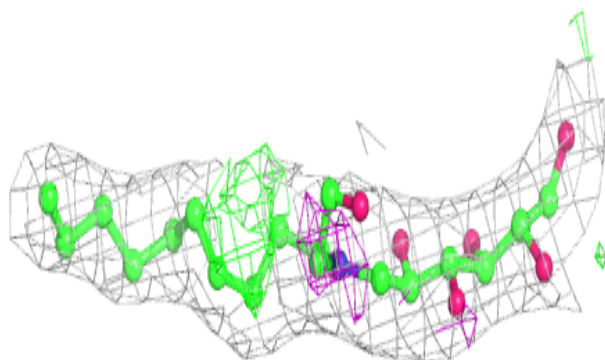
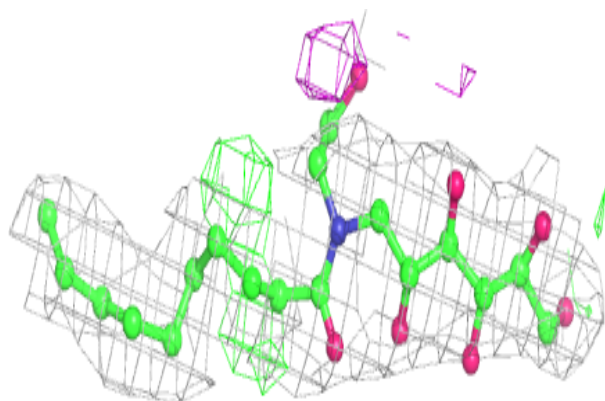
**Electron density around 2CV B 404:**

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

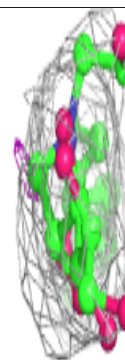
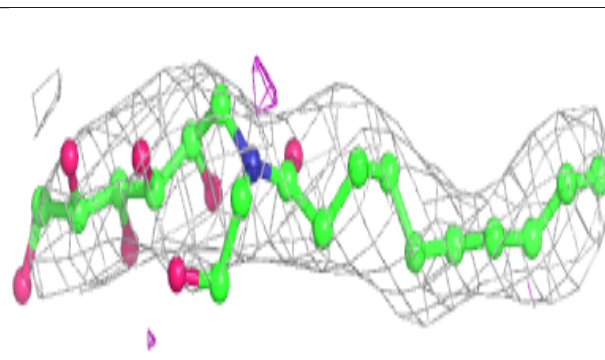
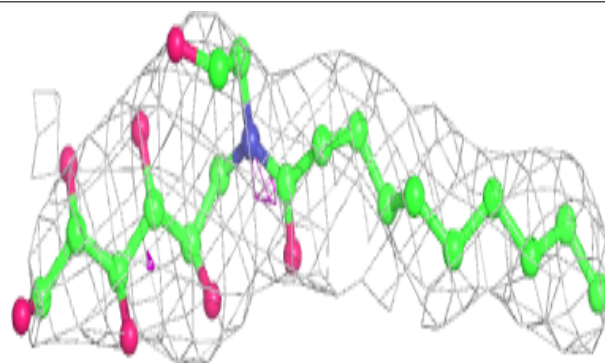


**Electron density around 2CV B 402:**

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

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

$2mF_o-DF_c$  (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.