Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 04:13 am GMT

PDB ID	:	4AMJ
Title	:	Turkey beta1 adrenergic receptor with stabilising mutations and bound biased agonist carvedilol
Authors	:	Warne, T.; Edwards, P.C.; Leslie, A.G.; Tate, C.G.
Deposited on	:	2012-03-12
Resolution	:	2.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

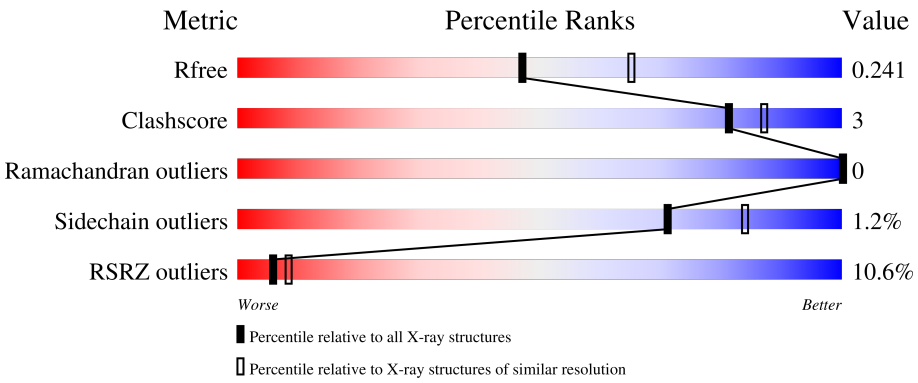
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	11% 86% 5% 9%
1	B	315	9% 89% 6% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4962 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
			Total	C	N	O	S			
1	A	287	2273	1500	373	380	20	0	0	0
1	B	299	2375	1562	397	396	20	0	0	0

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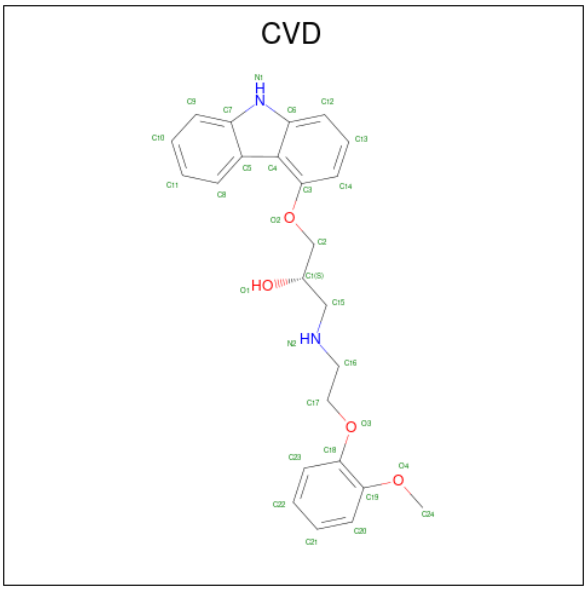
Chain	Residue	Modelled	Actual	Comment	Reference
B	227	ALA	TYR	engineered mutation	UNP P07700
B	282	LEU	ALA	engineered mutation	UNP P07700
B	327	ALA	PHE	engineered mutation	UNP P07700
B	338	MET	PHE	engineered mutation	UNP P07700
B	358	ALA	CYS	engineered mutation	UNP P07700

- Molecule 2 is (2S)-1-(8H-CARBAZOL-4-YLOXY)-3-[2-(2-METHOXYPHENOXY)ETHYL AMINO]PROPAN-2-OL (three-letter code: CVD) (formula: $C_{24}H_{26}N_2O_4$).

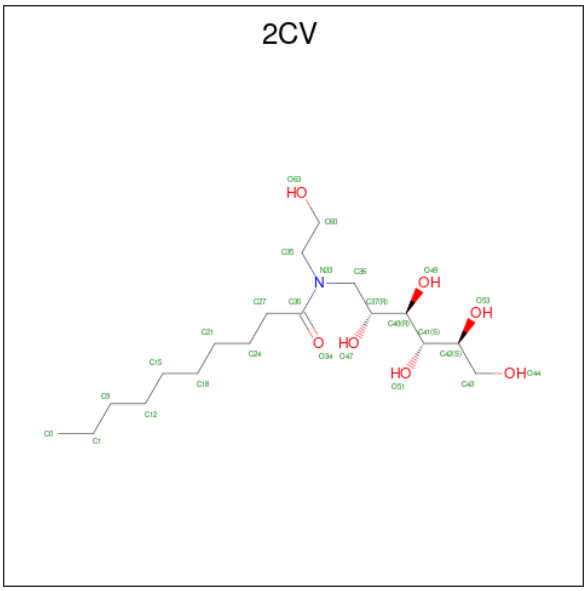


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	24	2	4	0	0
			Total	C	N	O		
2	B	1	30	24	2	4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is HEGA-10 (three-letter code: 2CV) (formula: $C_{18}H_{37}NO_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 16 13 1 2	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C N O 21 16 1 4	0	0
4	A	1	Total C N O 14 12 1 1	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C N O 12 10 1 1	0	0
4	A	1	Total C N O 16 13 1 2	0	0
4	B	1	Total C N O 20 15 1 4	0	0
4	B	1	Total C N O 12 10 1 1	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 10 10	0	0

- Molecule 5 is water.

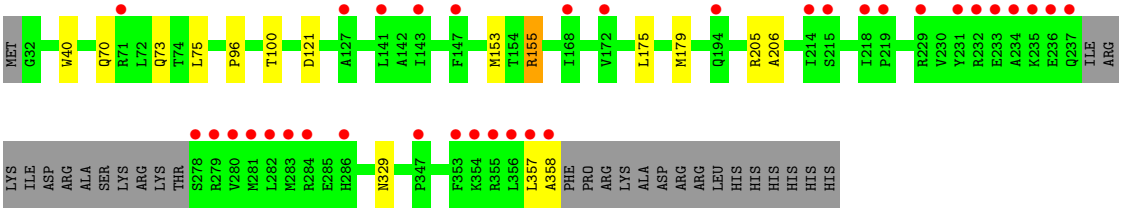
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	47	47	47	0	0
			Total	O		
5	B	54	54	54	0	0

3 Residue-property plots (i)

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.

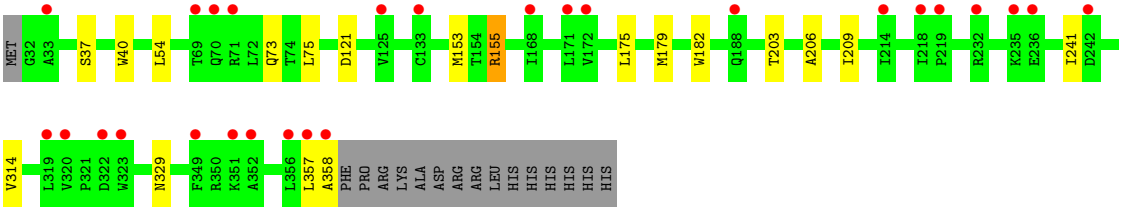
• Molecule 1: BETA-1 ADRENERGIC RECEPTOR

Chain A:



• Molecule 1: BETA-1 ADRENERGIC RECEPTOR

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.06Å 62.20Å 100.93Å 90.00° 109.17° 90.00°	Depositor
Resolution (Å)	95.33 – 2.30 44.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.33-2.30) 99.7 (44.68-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.240 0.203 , 0.241	Depositor DCC
R_{free} test set	2378 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4962	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CVD, 2CV, NA

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	0.66	1/2327 (0.0%)	0.67	1/3172 (0.0%)
1	B	0.67	1/2430 (0.0%)	0.69	1/3308 (0.0%)
All	All	0.67	2/4757 (0.0%)	0.68	2/6480 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	TRP	CD2-CE2	6.52	1.49	1.41
1	A	40	TRP	CD2-CE2	5.13	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	121	ASP	CB-CG-OD1	5.02	122.82	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	A	2273	0	2352	13	0
1	B	2375	0	2474	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	30	0	26	0	0
2	B	30	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	100	0	148	5	0
4	B	51	0	84	2	0
5	A	47	0	0	1	0
5	B	54	0	0	1	0
All	All	4962	0	5110	26	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (26) 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:73:GLN:O	1:A:155:ARG:NH2	1.96	0.98
1:A:205:ARG:NH1	4:A:1365:2CV:H272	2.09	0.67
1:A:175:LEU:CD1	1:B:175:LEU:HD12	2.25	0.67
1:B:73:GLN:O	1:B:155:ARG:NH2	2.28	0.66
1:A:205:ARG:CZ	4:A:1365:2CV:H272	2.26	0.64
1:A:175:LEU:HD12	1:B:175:LEU:CD1	2.29	0.62
1:A:70:GLN:HG2	5:A:2002:HOH:O	1.99	0.61
1:A:75:LEU:HD13	1:A:153:MET:HG3	1.81	0.61
1:B:75:LEU:HD13	1:B:153:MET:HG3	1.84	0.59
1:A:175:LEU:CD1	1:B:175:LEU:CD1	2.82	0.57
1:B:175:LEU:HB2	5:B:2029:HOH:O	2.10	0.52
1:A:175:LEU:HD12	1:B:175:LEU:HD12	1.90	0.51
4:B:1359:2CV:H602	4:B:1359:2CV:H272	1.93	0.50
1:B:357:LEU:O	1:B:358:ALA:C	2.52	0.48
1:A:357:LEU:O	1:A:358:ALA:C	2.53	0.47
1:B:175:LEU:HD23	1:B:179:MET:HG3	1.98	0.46
1:B:209:ILE:HD11	1:B:314:VAL:HG11	1.98	0.46
4:A:1361:2CV:H182	1:B:206:ALA:HA	1.98	0.45
1:A:206:ALA:HA	4:A:1367:2CV:H121	1.98	0.45
1:A:175:LEU:HD21	1:A:179:MET:SD	2.57	0.44
4:A:1368:2CV:H351	4:A:1368:2CV:H271	1.57	0.44
4:B:1364:2CV:H122	4:B:1364:2CV:H211	1.77	0.42
1:B:175:LEU:CD2	1:B:179:MET:HG3	2.50	0.42
1:B:182:TRP:O	1:B:203:THR:HA	2.20	0.41
1:B:241:ILE:HD12	1:B:241:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:O	1:A:100:THR:HG23	2.19	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/315 (90%)	278 (98%)	5 (2%)	0	100	100
1	B	297/315 (94%)	290 (98%)	7 (2%)	0	100	100
All	All	580/630 (92%)	568 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/273 (90%)	245 (99%)	2 (1%)	81	91
1	B	258/273 (94%)	254 (98%)	4 (2%)	62	78
All	All	505/546 (92%)	499 (99%)	6 (1%)	71	84

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

Mol	Chain	Res	Type
1	A	155	ARG
1	A	329	ASN
1	B	37	SER
1	B	54	LEU
1	B	155	ARG
1	B	329	ASN

Sometimes 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 16 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	2CV	A	1362	-	4,4,25	0.53	0	3,3,30	0.23	0
4	2CV	B	1359	-	19,19,25	0.71	1 (5%)	20,21,30	0.91	1 (5%)
2	CVD	B	1360	-	31,33,33	1.17	2 (6%)	41,44,44	1.40	7 (17%)
2	CVD	A	1359	-	31,33,33	1.11	1 (3%)	41,44,44	1.70	8 (19%)
4	2CV	B	1363	-	8,8,25	0.39	0	7,7,30	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	2CV	A	1364	-	20,20,25	0.47	0	22,23,30	0.95	1 (4%)
4	2CV	A	1368	-	15,15,25	0.69	0	15,16,30	0.63	0
4	2CV	B	1362	-	11,11,25	0.48	0	11,11,30	0.50	0
4	2CV	B	1364	-	9,9,25	0.54	0	8,8,30	0.36	0
4	2CV	A	1367	-	11,11,25	0.43	0	11,11,30	0.43	0
4	2CV	A	1361	-	14,15,25	0.69	0	13,16,30	0.83	0
4	2CV	A	1366	-	6,6,25	0.62	0	5,5,30	0.18	0
4	2CV	A	1365	-	13,13,25	0.62	0	14,14,30	0.53	0
4	2CV	A	1363	-	8,8,25	0.61	0	7,7,30	0.21	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
4	2CV	A	1362	-	-	1/2/2/34	-
4	2CV	B	1359	-	-	0/22/22/34	-
2	CVD	B	1360	-	-	6/15/15/15	0/4/4/4
2	CVD	A	1359	-	-	5/15/15/15	0/4/4/4
4	2CV	B	1363	-	-	5/6/6/34	-
4	2CV	A	1364	-	-	6/24/24/34	-
4	2CV	A	1368	-	-	7/16/16/34	-
4	2CV	B	1362	-	-	2/9/9/34	-
4	2CV	B	1364	-	-	2/7/7/34	-
4	2CV	A	1367	-	-	4/9/9/34	-
4	2CV	A	1361	-	-	3/14/14/34	-
4	2CV	A	1366	-	-	2/4/4/34	-
4	2CV	A	1365	-	-	5/13/13/34	-
4	2CV	A	1363	-	-	2/6/6/34	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1359	CVD	O4-C19	2.82	1.41	1.37
2	B	1360	CVD	C11-C8	2.77	1.43	1.36
2	B	1360	CVD	C12-C6	-2.76	1.37	1.41
4	B	1359	2CV	O49-C40	2.08	1.51	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1359	CVD	C24-O4-C19	5.30	125.53	117.53
2	A	1359	CVD	O4-C19-C18	4.46	121.63	115.41
4	A	1364	2CV	C35-N33-C36	2.77	119.70	116.41
2	A	1359	CVD	C4-C5-C7	2.68	108.98	106.09
2	B	1360	CVD	O4-C19-C20	-2.54	120.01	124.37
2	B	1360	CVD	O2-C3-C4	2.51	120.68	117.11
2	B	1360	CVD	O4-C19-C18	2.50	118.89	115.41
2	A	1359	CVD	O4-C19-C20	-2.42	120.23	124.37
2	B	1360	CVD	O2-C3-C14	-2.41	119.16	124.46
2	A	1359	CVD	O3-C18-C19	2.37	120.62	115.73
2	B	1360	CVD	O3-C18-C19	2.33	120.54	115.73
2	A	1359	CVD	C5-C4-C6	2.28	108.57	106.10
2	B	1360	CVD	C4-C5-C7	2.26	108.53	106.09
2	B	1360	CVD	C15-C1-C2	-2.22	106.91	110.42
4	B	1359	2CV	O47-C37-C36	-2.16	103.67	109.87
2	A	1359	CVD	O3-C18-C23	-2.15	119.32	123.97
2	A	1359	CVD	C8-C5-C7	2.09	120.94	118.17

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1360	CVD	C2-C1-C15-N2
4	A	1364	2CV	C36-C37-C40-C41
4	A	1364	2CV	O47-C37-C40-C41
4	A	1364	2CV	O47-C37-C40-O49
2	A	1359	CVD	C18-C19-O4-C24
4	A	1368	2CV	C21-C24-C27-C30
2	A	1359	CVD	C20-C19-O4-C24
4	A	1365	2CV	C21-C24-C27-C30
2	B	1360	CVD	O1-C1-C15-N2
4	B	1363	2CV	C15-C12-C9-C1
4	A	1364	2CV	C18-C21-C24-C27
4	B	1362	2CV	C21-C24-C27-C30
4	A	1368	2CV	C15-C18-C21-C24
4	A	1368	2CV	C12-C15-C18-C21
4	A	1366	2CV	C12-C15-C18-C21
4	A	1368	2CV	C18-C21-C24-C27
2	B	1360	CVD	C19-C18-O3-C17
4	A	1366	2CV	C9-C12-C15-C18
2	A	1359	CVD	N2-C16-C17-O3

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Mol	Chain	Res	Type	Atoms
4	B	1363	2CV	C15-C18-C21-C24
4	A	1368	2CV	C0-C1-C9-C12
4	A	1361	2CV	C18-C21-C24-C27
4	A	1367	2CV	C21-C24-C27-C30
4	A	1364	2CV	N33-C35-C60-O63
4	B	1364	2CV	C15-C12-C9-C1
4	A	1363	2CV	C0-C1-C9-C12
4	B	1364	2CV	C18-C21-C24-C27
4	A	1367	2CV	C18-C21-C24-C27
4	B	1363	2CV	C18-C21-C24-C27
4	A	1363	2CV	C15-C12-C9-C1
4	A	1365	2CV	C12-C15-C18-C21
2	B	1360	CVD	C23-C18-O3-C17
4	A	1368	2CV	C15-C12-C9-C1
2	A	1359	CVD	C23-C18-O3-C17
4	A	1368	2CV	C9-C12-C15-C18
4	B	1363	2CV	C0-C1-C9-C12
4	A	1362	2CV	C12-C15-C18-C21
4	A	1367	2CV	C15-C18-C21-C24
4	B	1363	2CV	C9-C12-C15-C18
4	A	1361	2CV	C15-C18-C21-C24
4	A	1365	2CV	C0-C1-C9-C12
4	B	1362	2CV	C18-C21-C24-C27
4	A	1367	2CV	C0-C1-C9-C12
2	A	1359	CVD	C19-C18-O3-C17
2	B	1360	CVD	C18-C19-O4-C24
4	A	1364	2CV	C36-C37-C40-O49
4	A	1365	2CV	C18-C21-C24-C27
2	B	1360	CVD	C20-C19-O4-C24
4	A	1361	2CV	C37-C36-N33-C30
4	A	1365	2CV	C15-C12-C9-C1

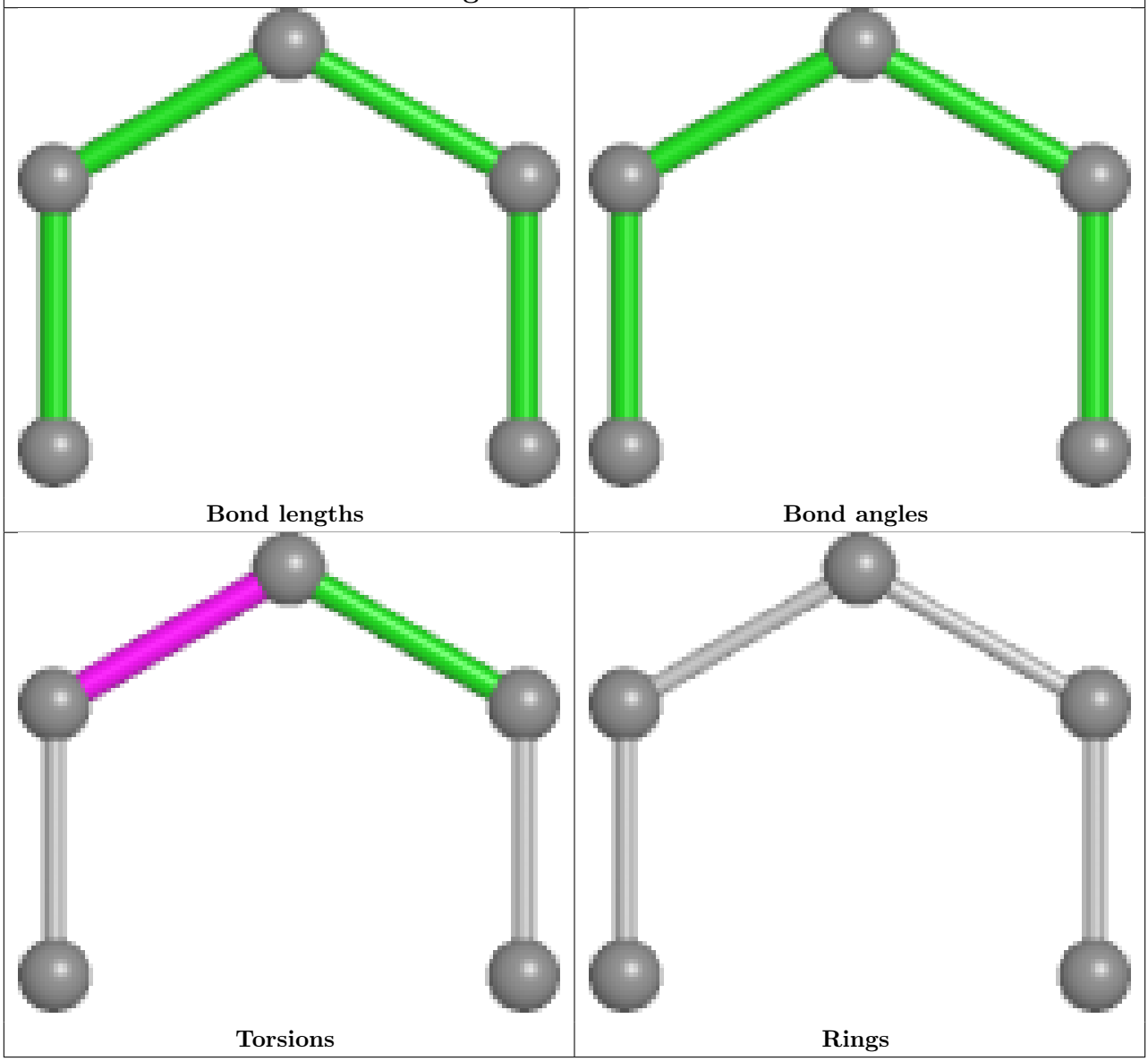
There are no ring outliers.

6 monomers are involved in 7 short contacts:

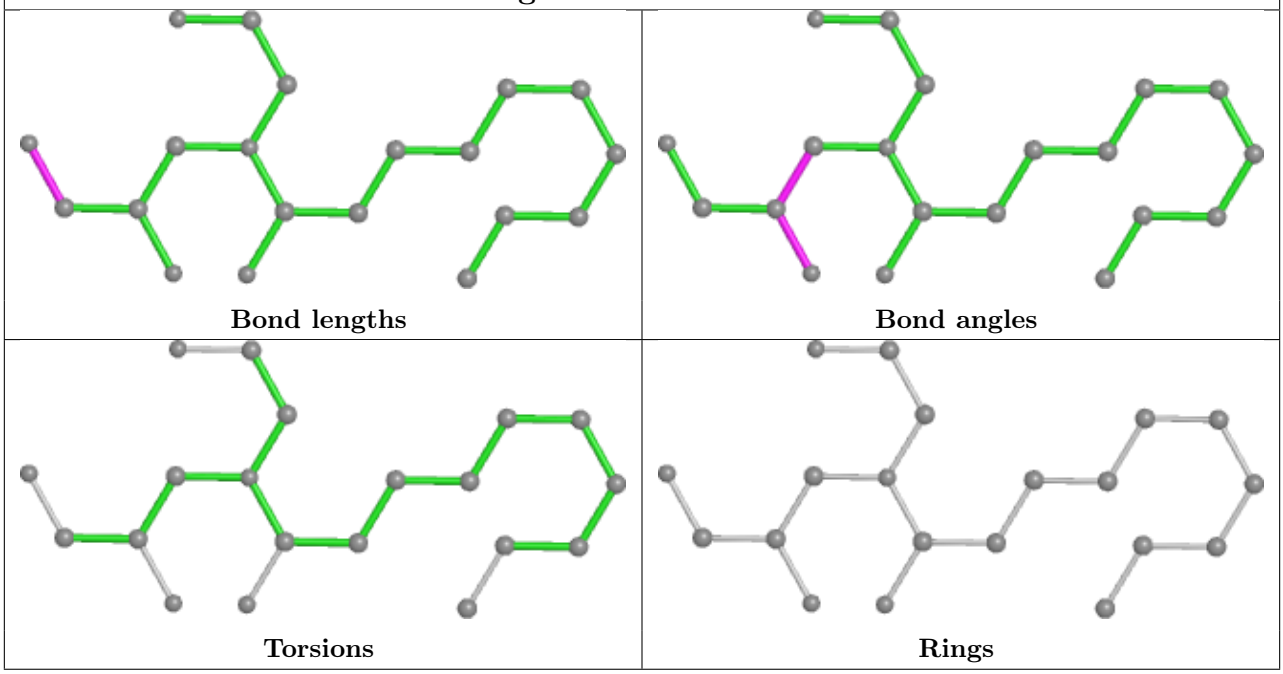
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1359	2CV	1	0
4	A	1368	2CV	1	0
4	B	1364	2CV	1	0
4	A	1367	2CV	1	0
4	A	1361	2CV	1	0
4	A	1365	2CV	2	0

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 then 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.

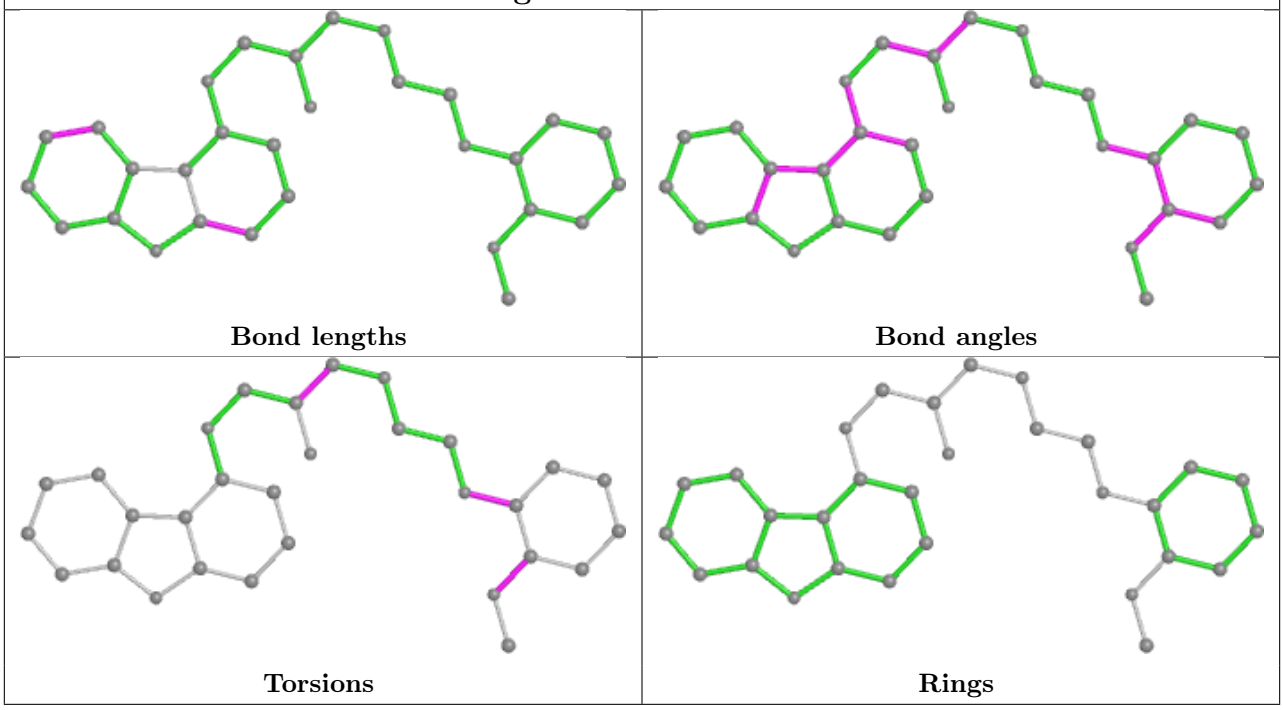
Ligand 2CV A 1362



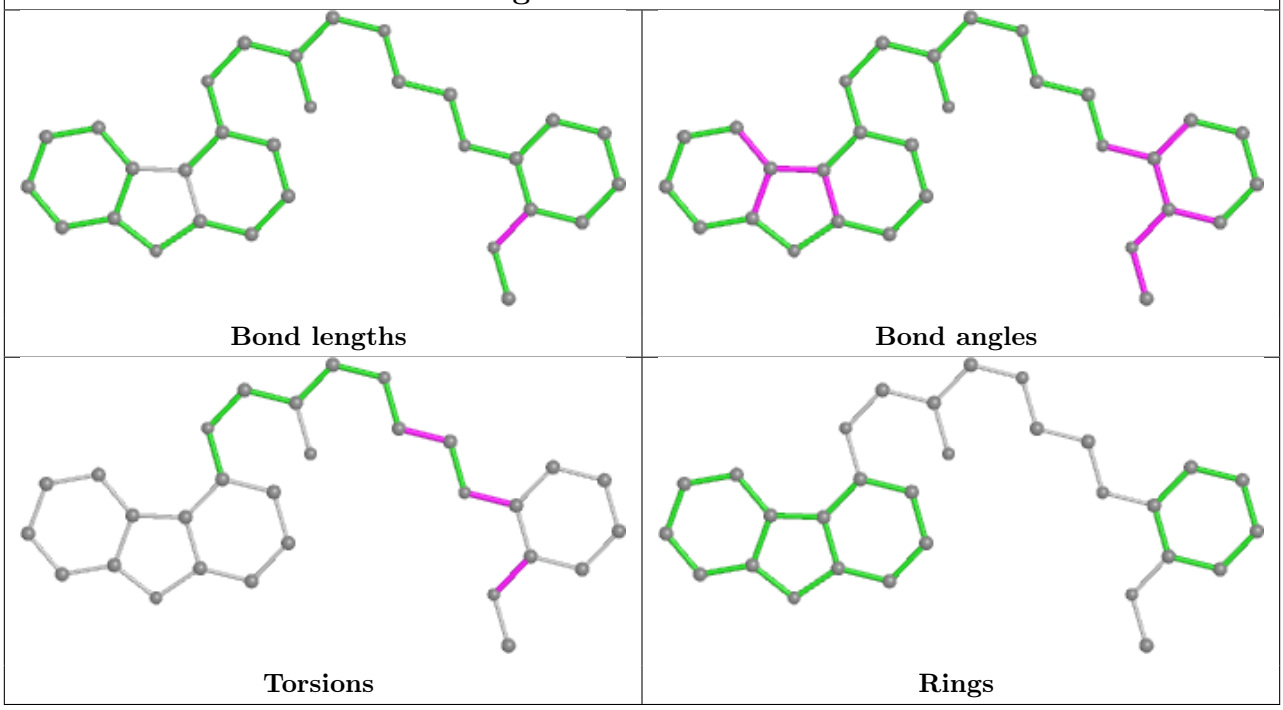
Ligand 2CV B 1359



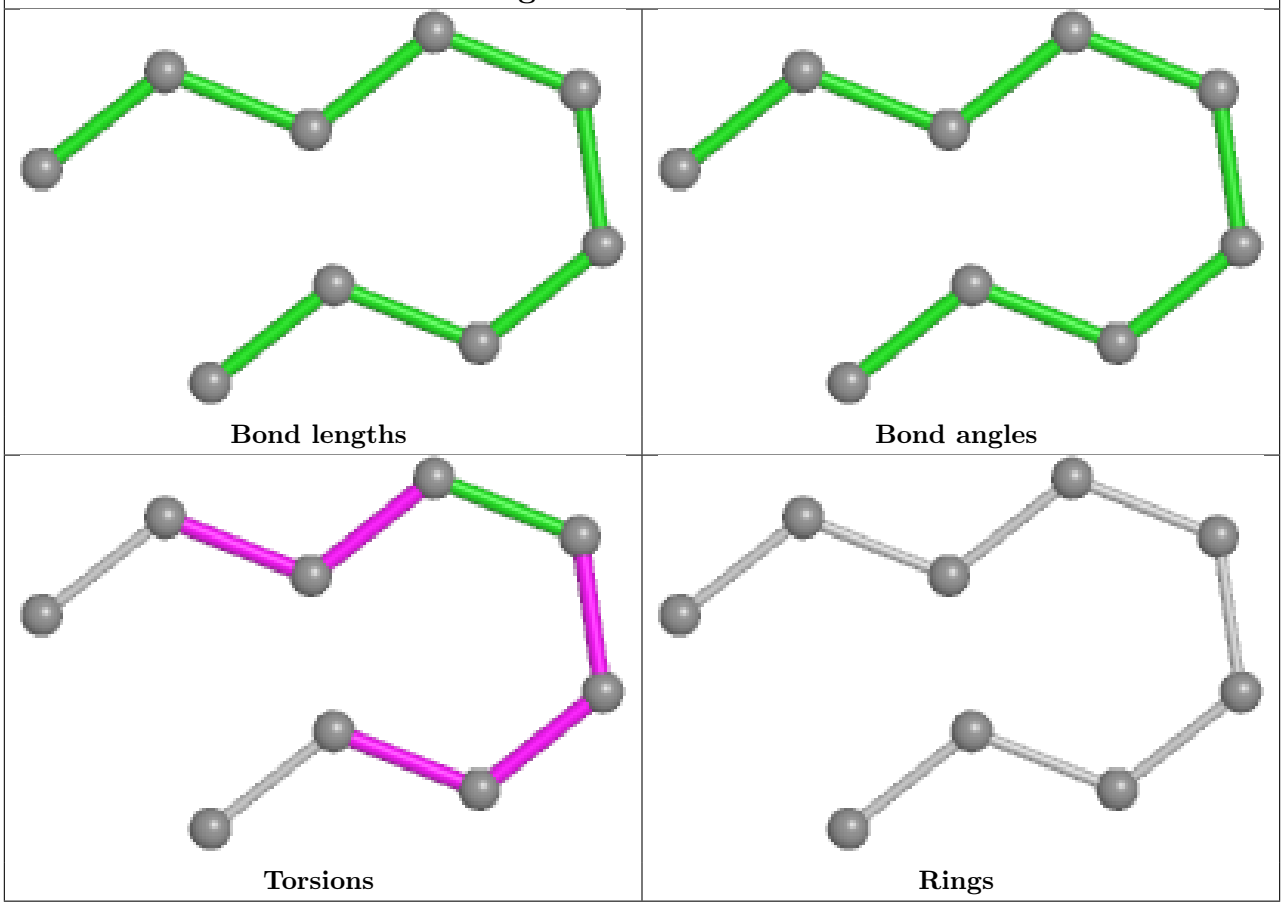
Ligand CVD B 1360



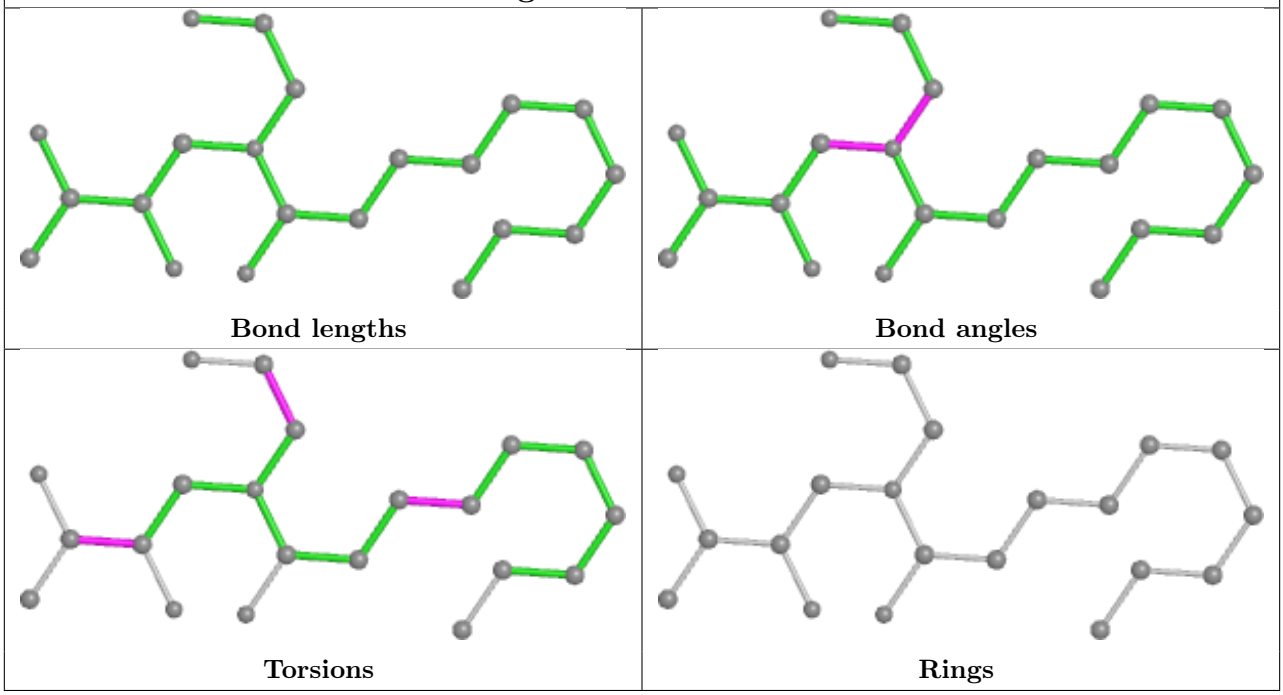
Ligand CVD A 1359



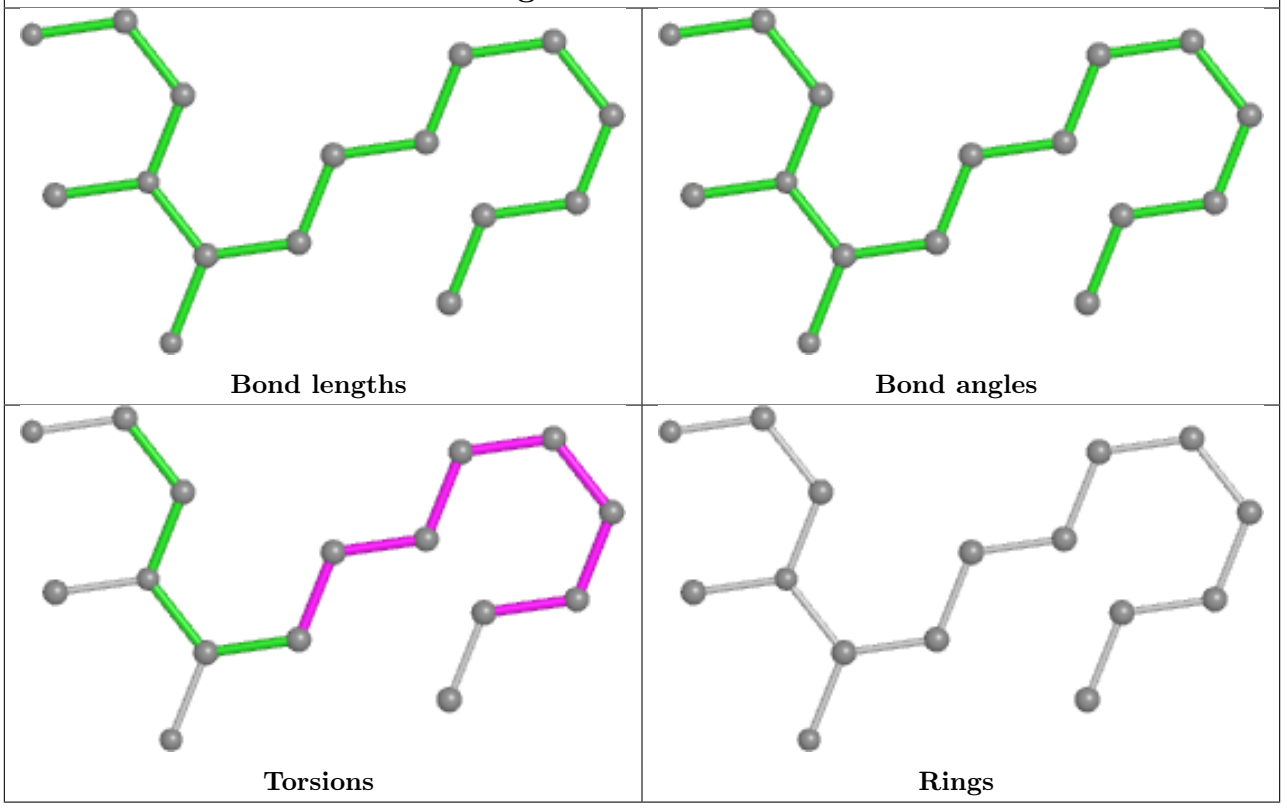
Ligand 2CV B 1363



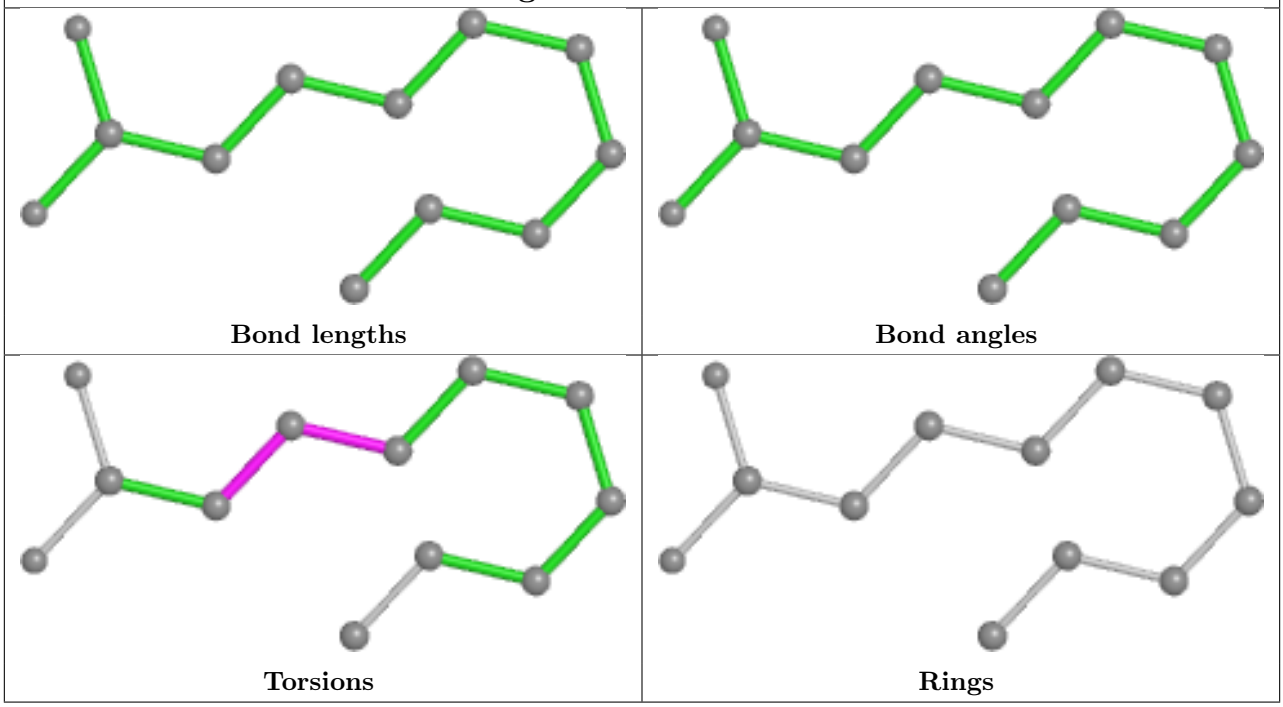
Ligand 2CV A 1364



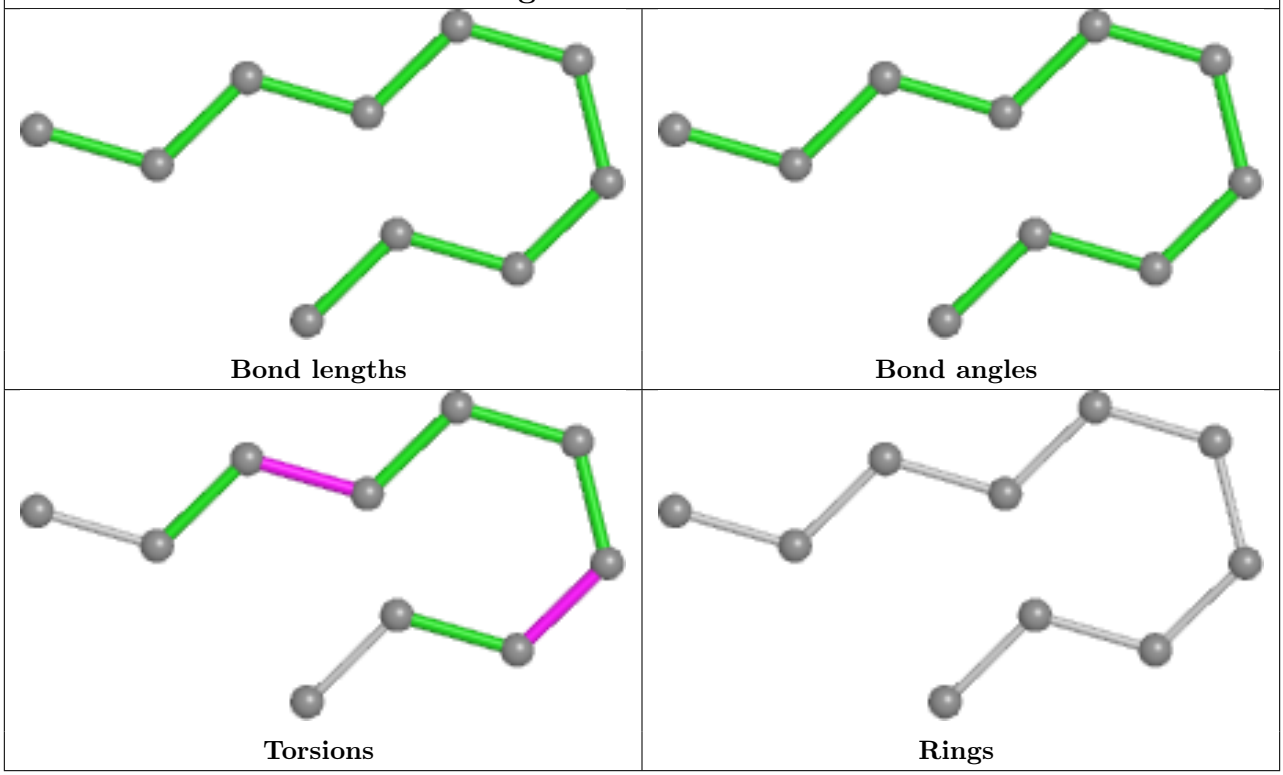
Ligand 2CV A 1368



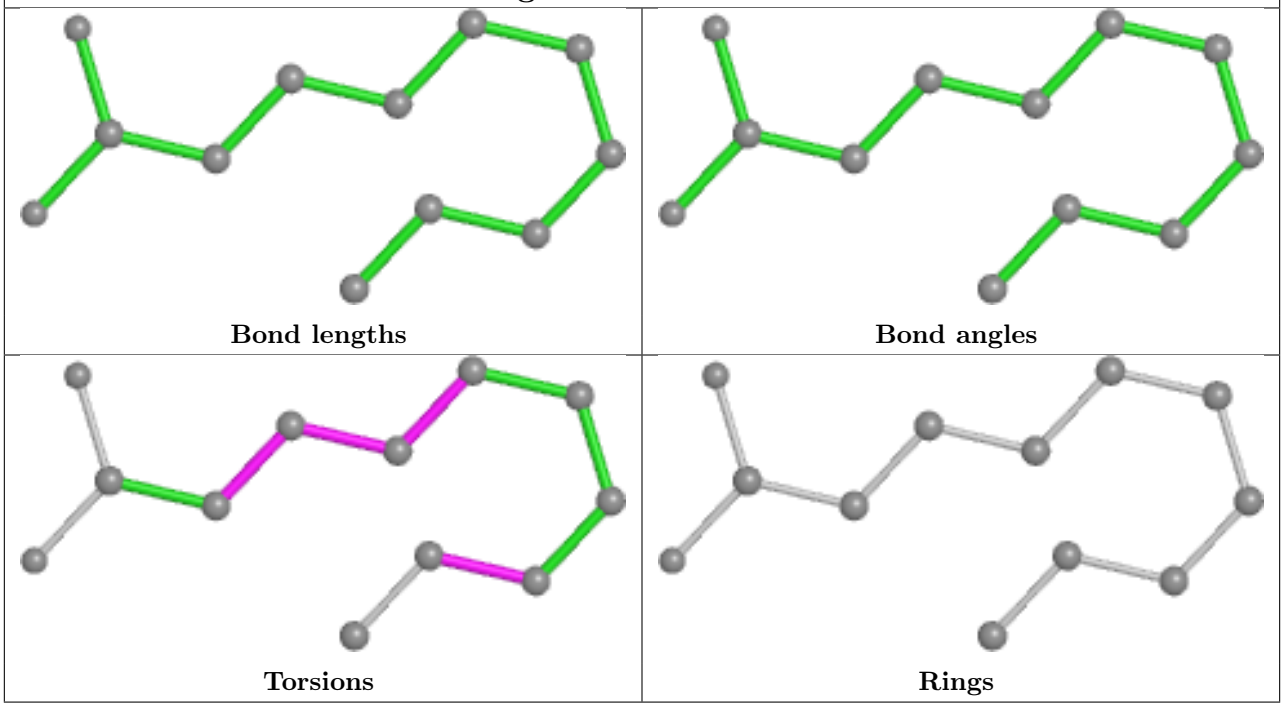
Ligand 2CV B 1362



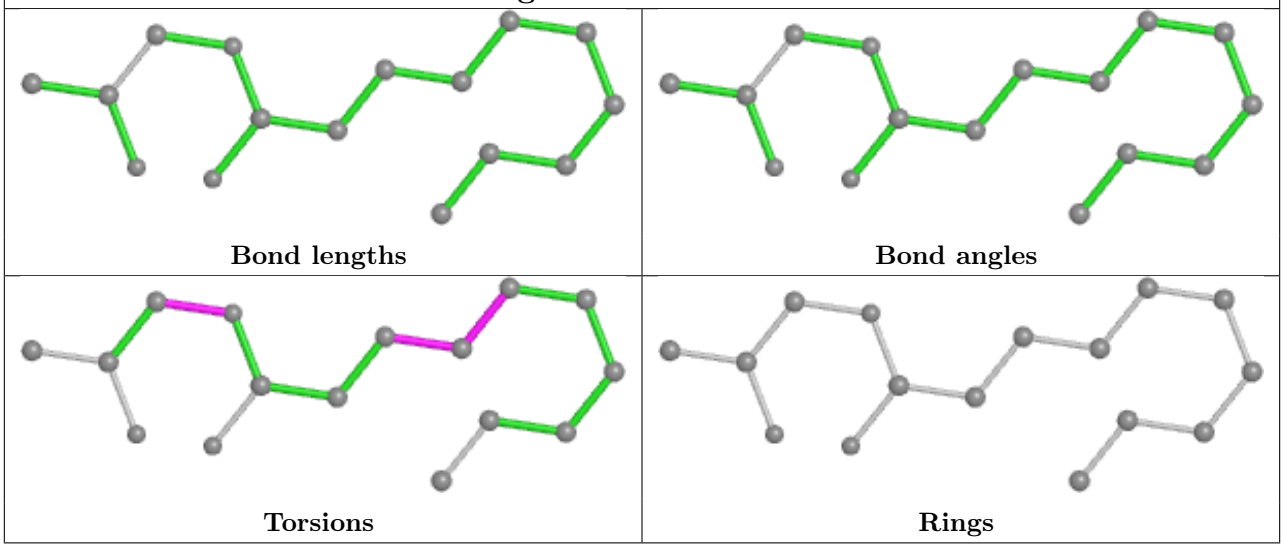
Ligand 2CV B 1364



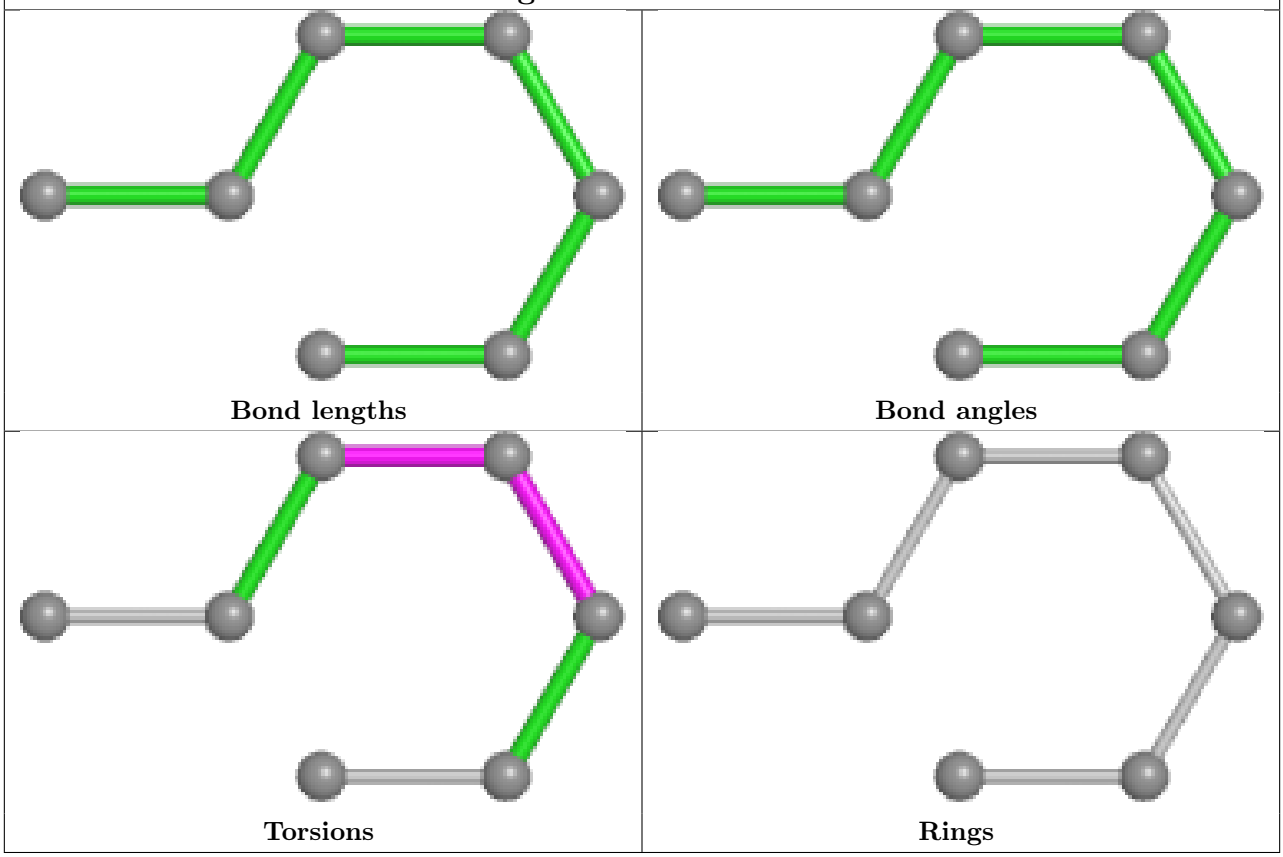
Ligand 2CV A 1367



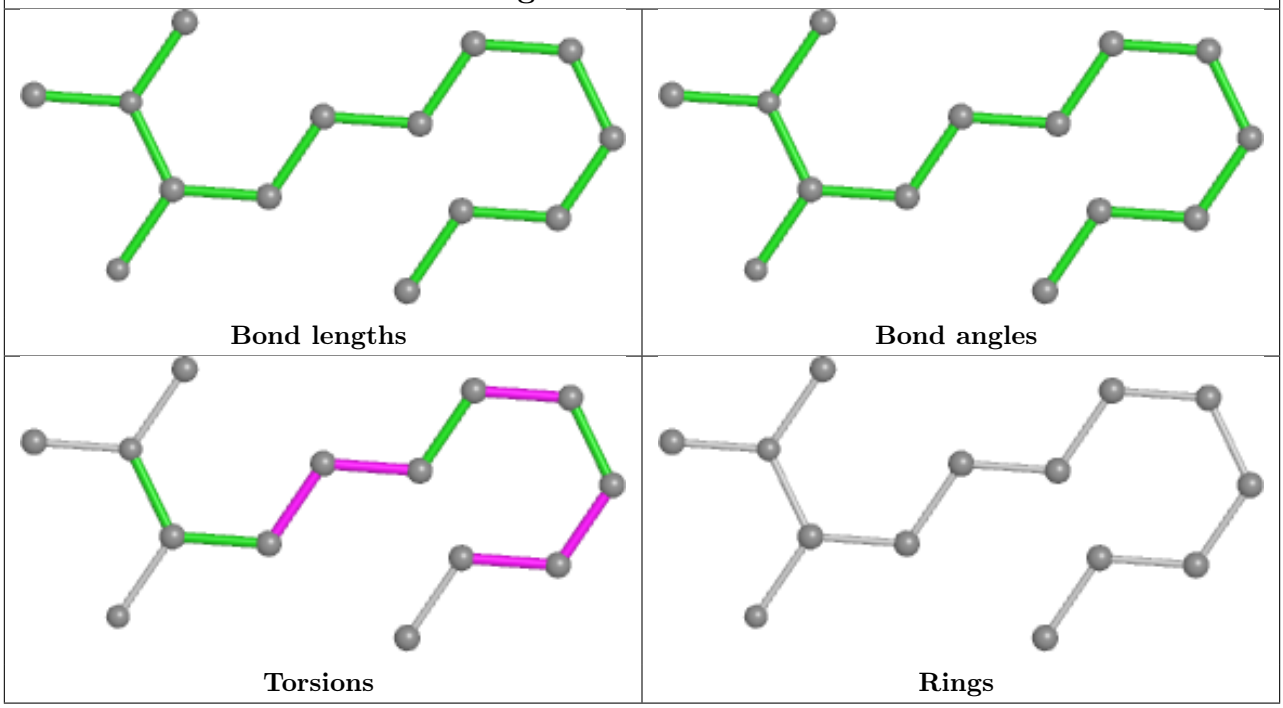
Ligand 2CV A 1361

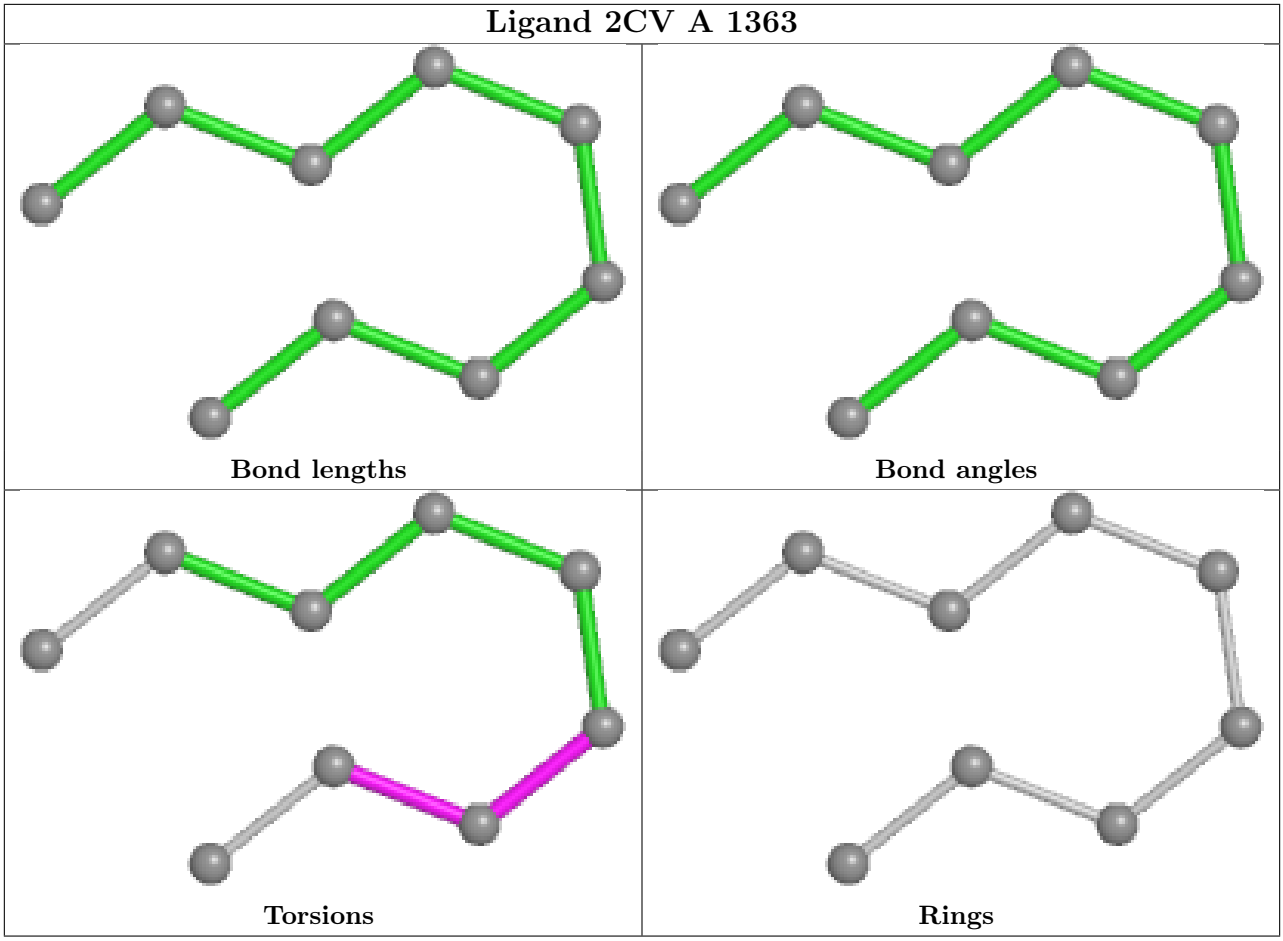


Ligand 2CV A 1366



Ligand 2CV A 1365





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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	287/315 (91%)	0.43	35 (12%)	4	6	24, 43, 85, 130	0
1	B	299/315 (94%)	0.33	27 (9%)	9	12	24, 41, 75, 107	0
All	All	586/630 (93%)	0.38	62 (10%)	6	8	24, 42, 79, 130	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	358	ALA	8.9
1	A	279	ARG	8.1
1	A	280	VAL	5.9
1	A	283	MET	5.5
1	A	357	LEU	5.0
1	A	236	GLU	4.9
1	A	281	MET	4.6
1	A	358	ALA	4.6
1	A	282	LEU	4.3
1	B	357	LEU	4.2
1	B	323	TRP	4.2
1	B	351	LYS	3.9
1	A	354	LYS	3.8
1	A	231	TYR	3.8
1	A	232	ARG	3.8
1	B	70	GLN	3.7
1	A	353	PHE	3.7
1	B	322	ASP	3.7
1	B	349	PHE	3.6
1	B	352	ALA	3.2
1	A	286	HIS	3.2
1	A	235	LYS	3.2
1	B	218	ILE	3.1
1	B	133	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	320	VAL	3.1
1	B	236	GLU	3.0
1	A	278	SER	3.0
1	B	71	ARG	3.0
1	A	233	GLU	3.0
1	A	234	ALA	3.0
1	B	319	LEU	2.9
1	A	214	ILE	2.8
1	B	356	LEU	2.8
1	B	125	VAL	2.8
1	A	347	PRO	2.8
1	A	356	LEU	2.6
1	A	71	ARG	2.5
1	A	229	ARG	2.5
1	B	214	ILE	2.5
1	A	237	GLN	2.5
1	A	147	PHE	2.5
1	A	141	LEU	2.3
1	B	219	PRO	2.3
1	B	232	ARG	2.3
1	B	242	ASP	2.3
1	A	219	PRO	2.3
1	A	143	ILE	2.3
1	B	69	THR	2.3
1	A	218	ILE	2.3
1	A	194	GLN	2.2
1	B	171	LEU	2.2
1	A	168	ILE	2.2
1	B	33	ALA	2.2
1	B	172	VAL	2.2
1	B	168	ILE	2.2
1	A	215	SER	2.1
1	B	235	LYS	2.1
1	A	355	ARG	2.1
1	A	284	ARG	2.1
1	B	188	GLN	2.1
1	A	172	VAL	2.1
1	A	127	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

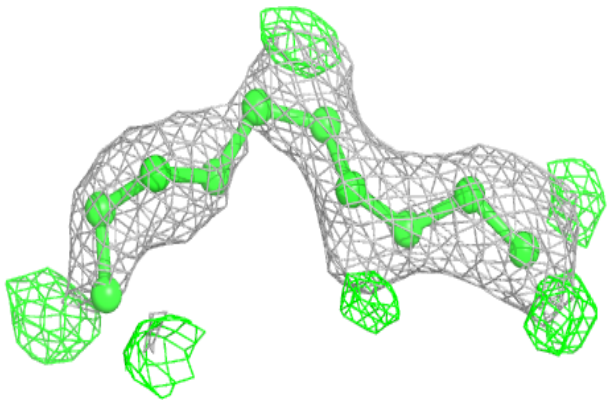
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

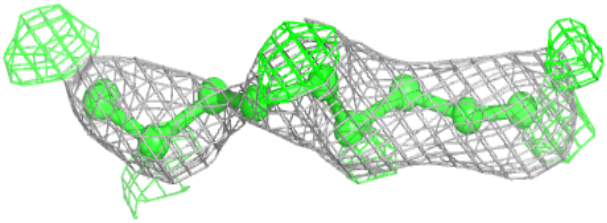
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	2CV	B	1364	10/26	0.49	0.32	65,77,82,83	0
4	2CV	A	1366	7/26	0.66	0.19	63,69,74,75	0
4	2CV	A	1361	16/26	0.70	0.29	48,61,82,91	0
4	2CV	B	1359	20/26	0.74	0.28	34,62,71,74	0
4	2CV	A	1367	12/26	0.76	0.28	45,51,62,75	0
4	2CV	A	1364	21/26	0.77	0.23	37,63,78,90	0
4	2CV	A	1368	16/26	0.77	0.25	71,86,103,107	0
4	2CV	A	1365	14/26	0.81	0.34	73,80,92,93	0
4	2CV	A	1363	9/26	0.84	0.19	57,66,73,74	0
4	2CV	B	1363	9/26	0.88	0.18	53,65,77,79	0
4	2CV	B	1362	12/26	0.90	0.30	42,52,66,75	0
4	2CV	A	1362	5/26	0.91	0.18	53,55,56,57	0
3	NA	A	1360	1/1	0.92	0.04	43,43,43,43	0
3	NA	B	1361	1/1	0.93	0.04	48,48,48,48	0
2	CVD	A	1359	30/30	0.94	0.14	21,24,48,53	0
2	CVD	B	1360	30/30	0.96	0.13	15,19,38,46	0

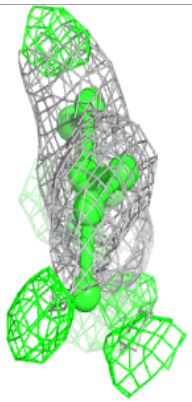
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CV B 1364:

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

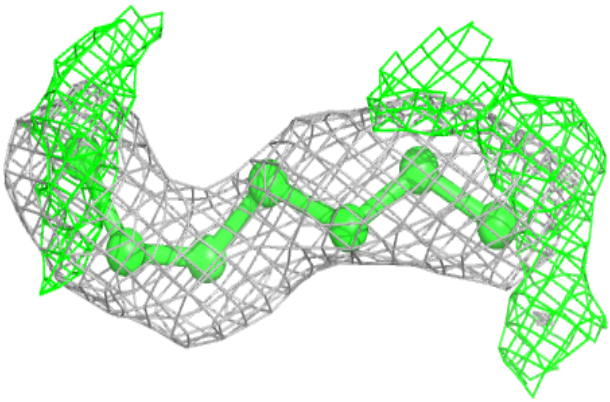


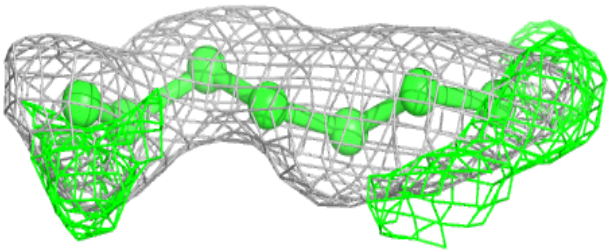


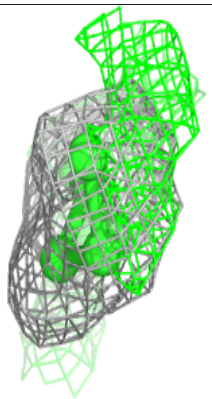


Electron density around 2CV A 1366:

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

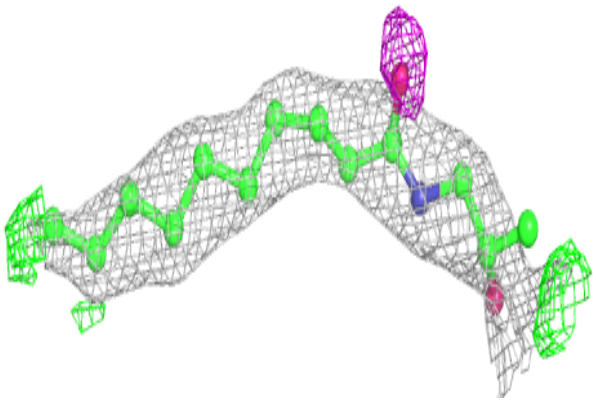


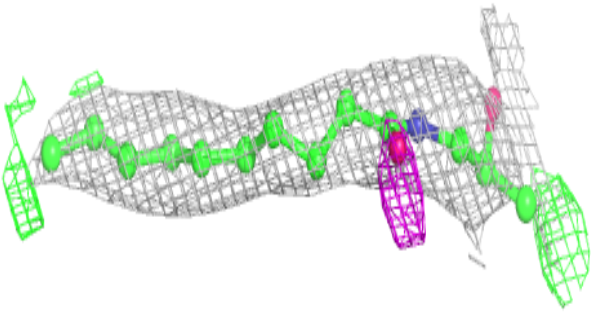


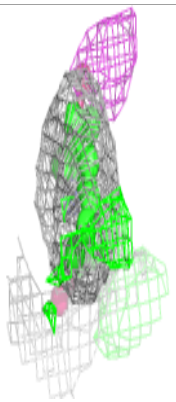


Electron density around 2CV A 1361:

$2mF_o$-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 1359:

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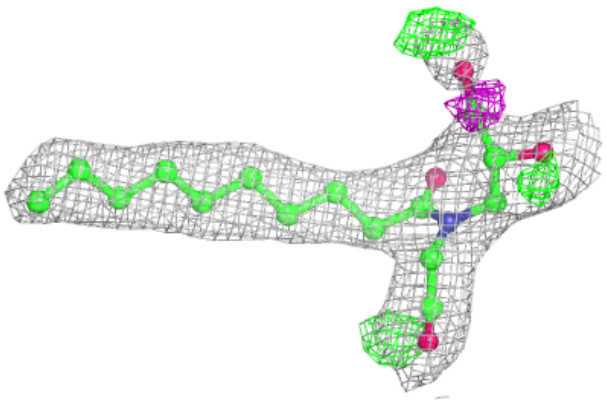
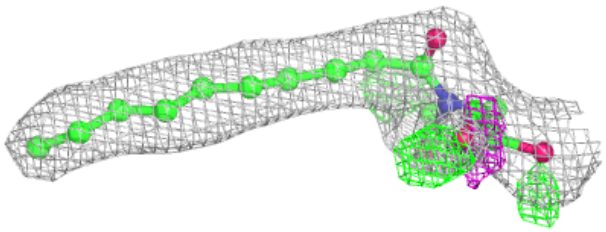
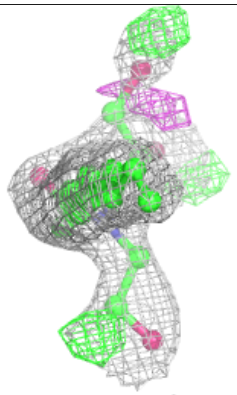
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

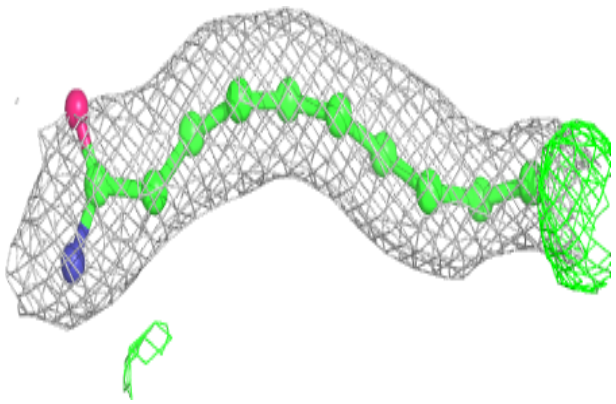


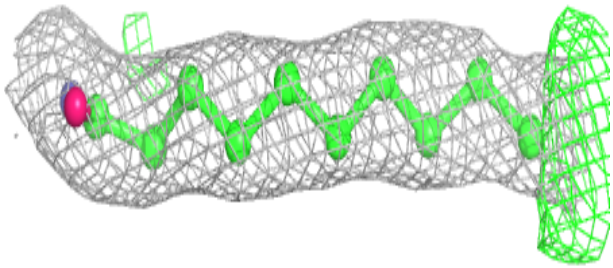


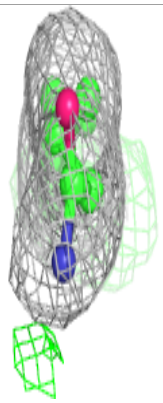


Electron density around 2CV A 1367:

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

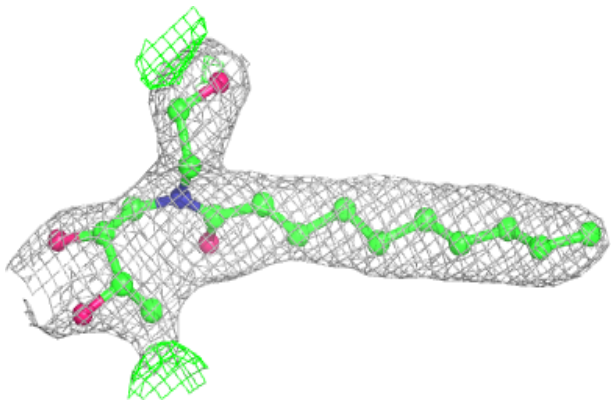


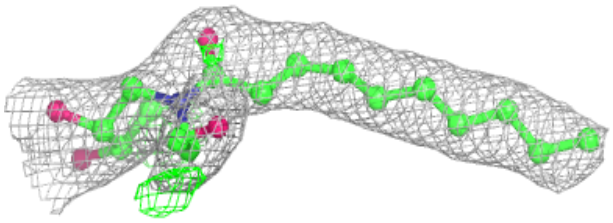


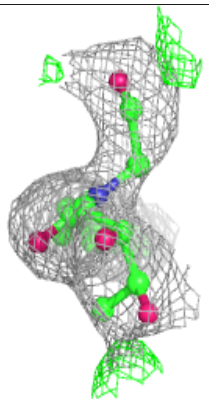


Electron density around 2CV A 1364:

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

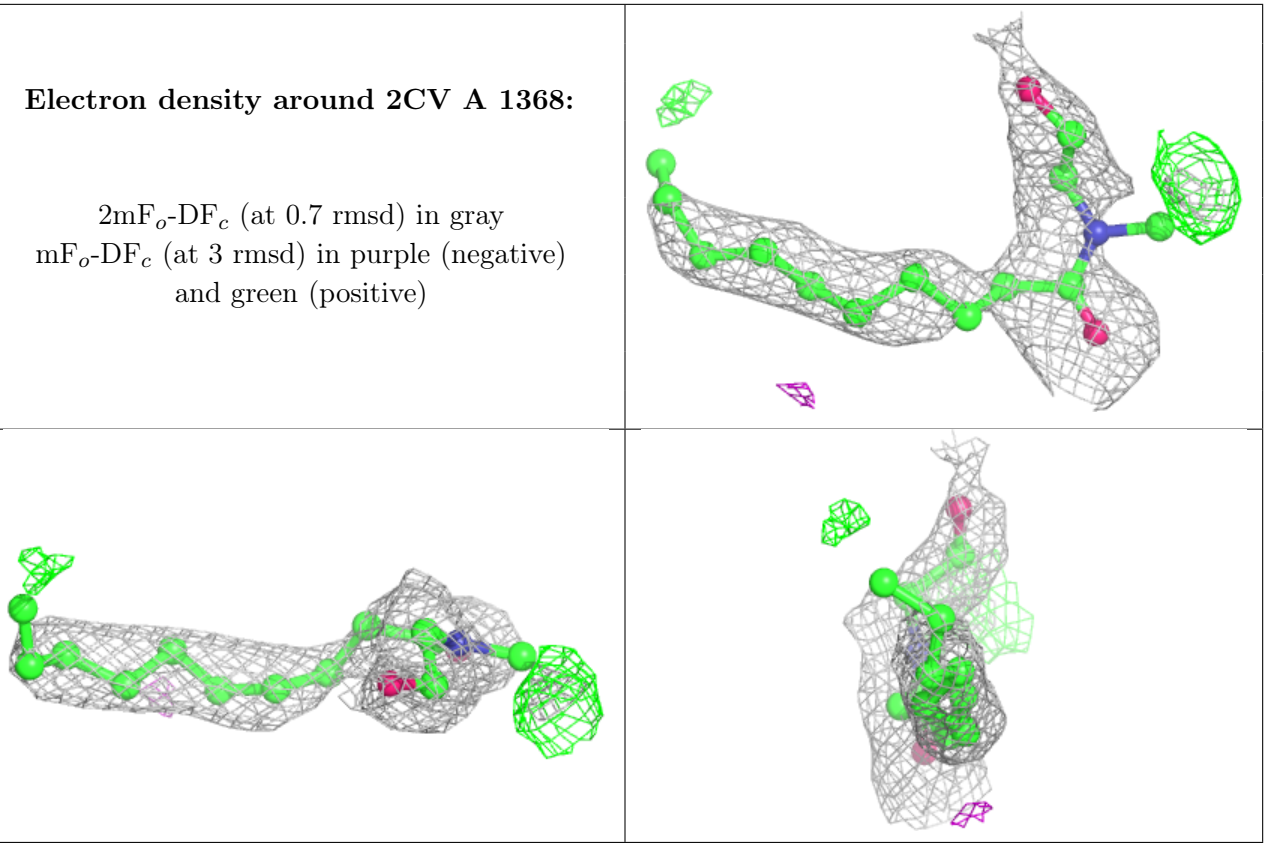






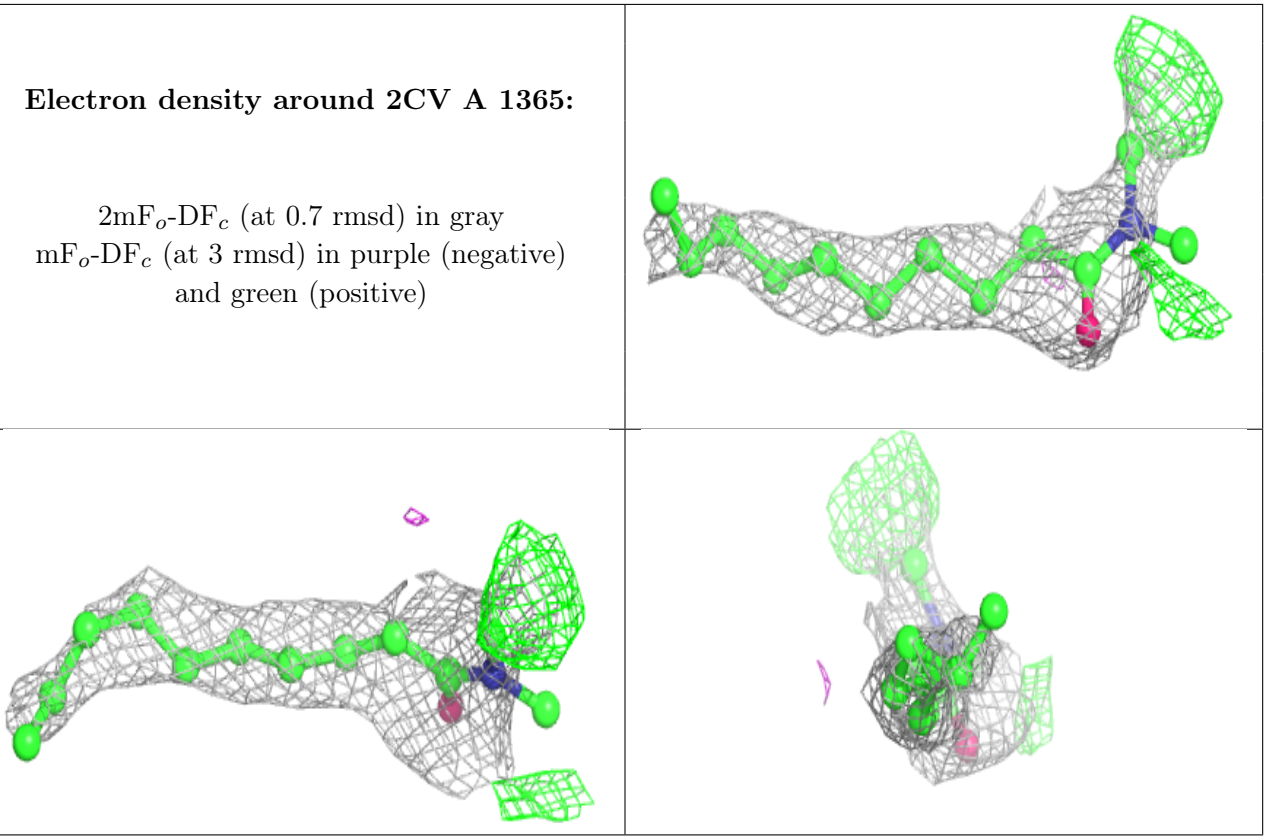
Electron density around 2CV A 1368:

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



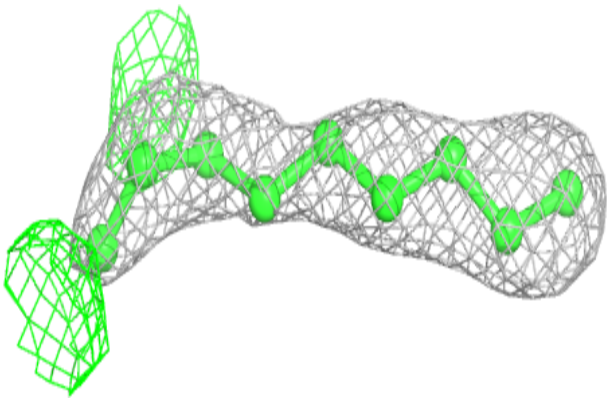
Electron density around 2CV A 1365:

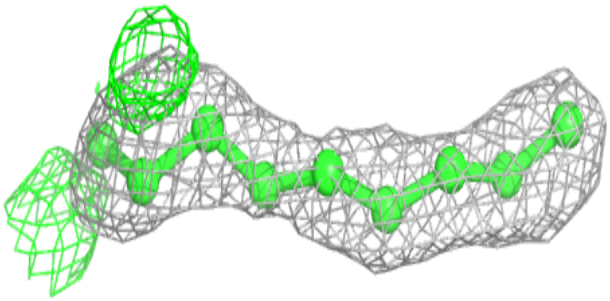
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

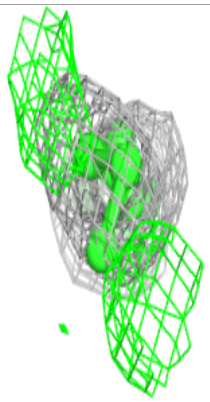


Electron density around 2CV A 1363:

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

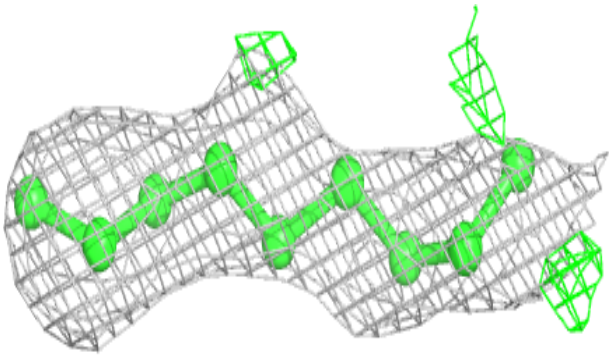


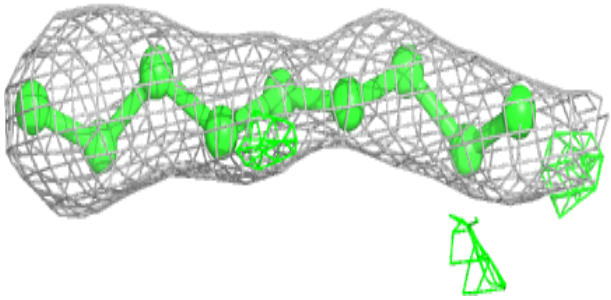


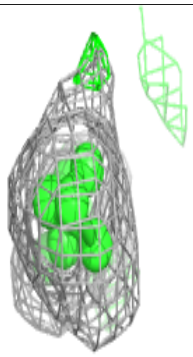


Electron density around 2CV B 1363:

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

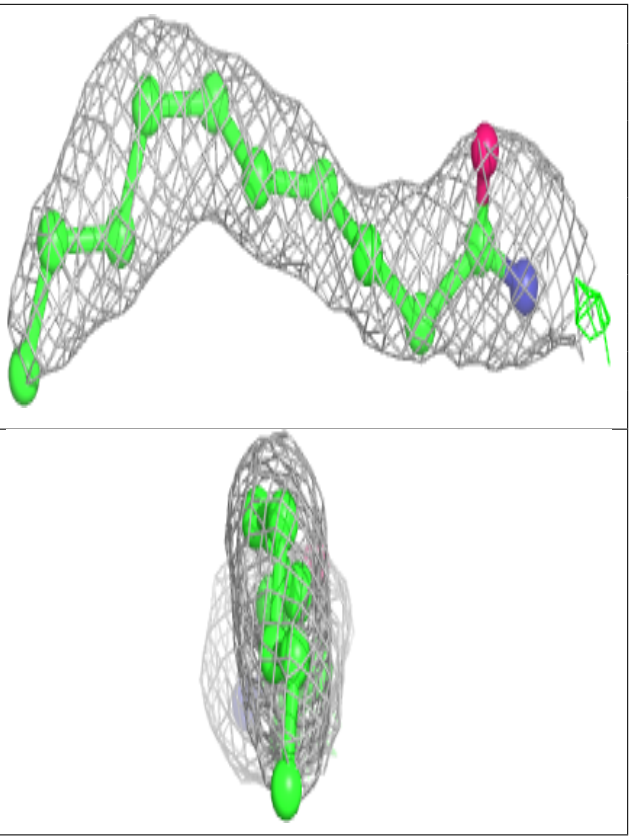






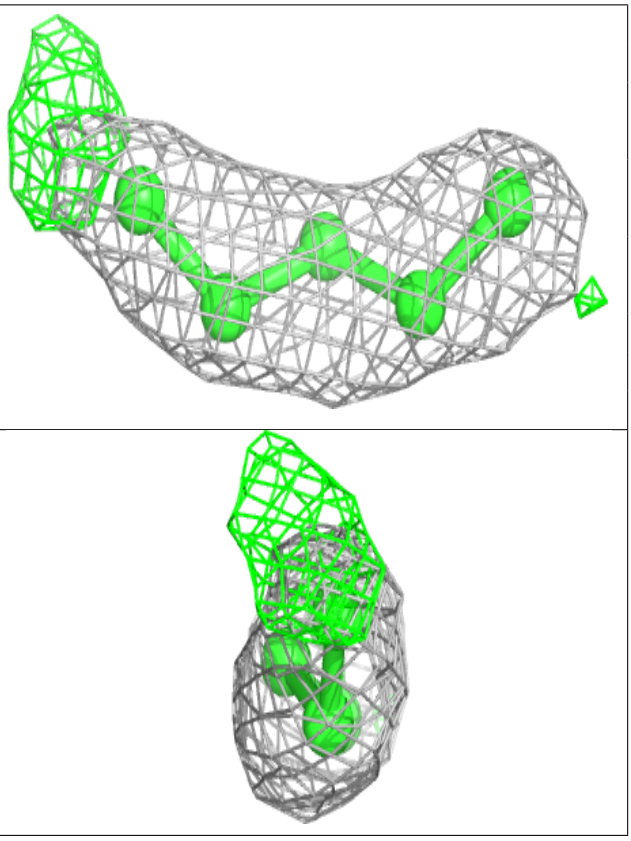
Electron density around 2CV B 1362:

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



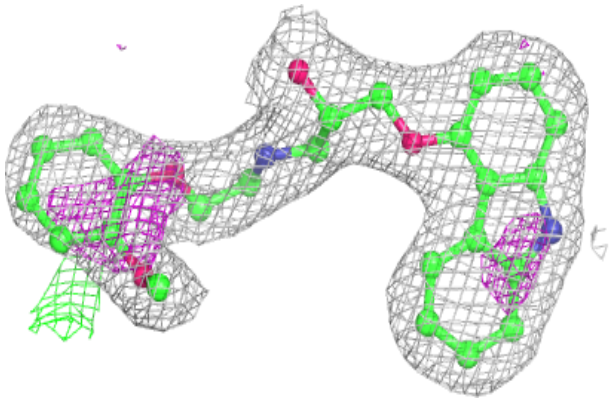
Electron density around 2CV A 1362:

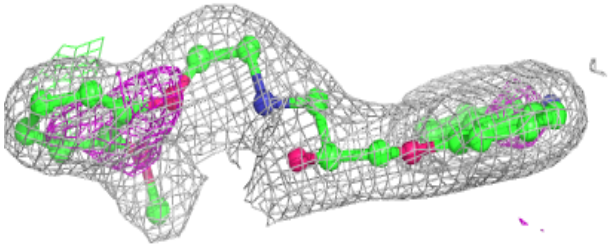
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

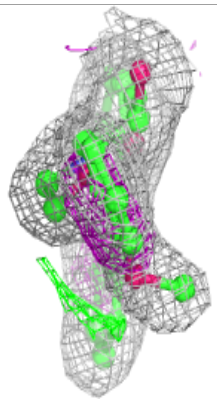


Electron density around CVD A 1359:

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

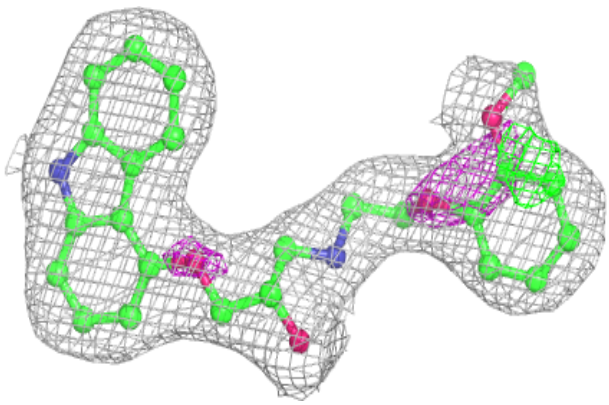


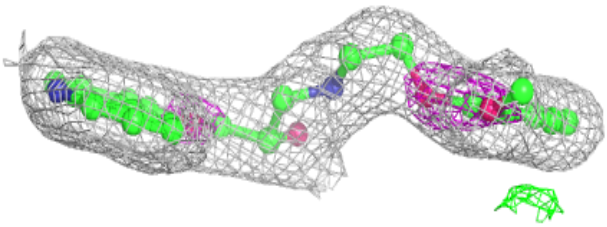


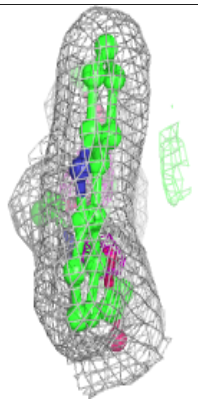


Electron density around CVD B 1360:

$2mF_o$-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.