wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 10:45 am BST

PDB ID	:	6H7L
Title	:	ACTIVATED TURKEY BETA1 ADRENOCEPTOR WITH BOUND PARTIAL AGONIST DOBUTAMINE 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	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

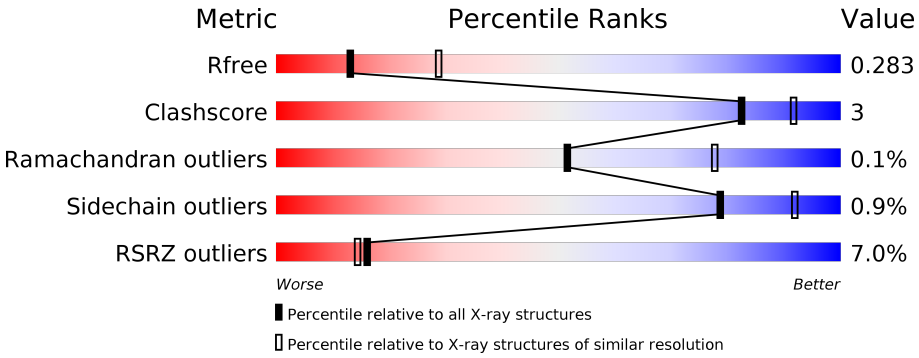
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	E	109	34% 94% 5%
1	F	109	17% 95%
2	A	307	% 86% 8% 5%
2	B	307	4% 82% 11% 7%
3	C	121	% 95%
3	D	121	2% 95%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8280 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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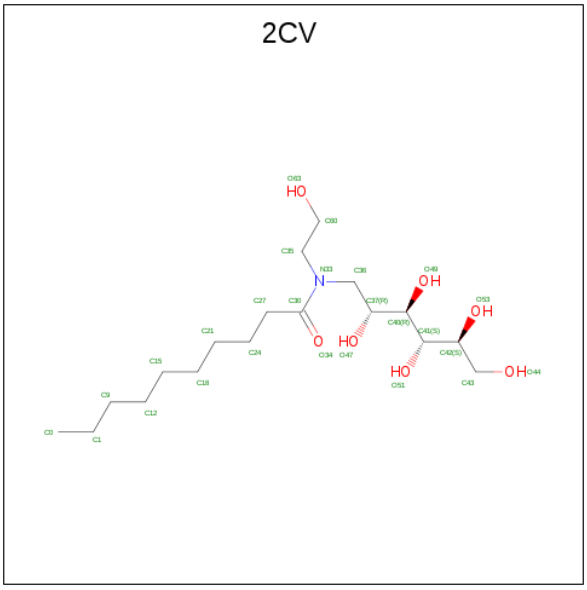
Chain	Residue	Modelled	Actual	Comment	Reference
B	42	LYS	-	expression tag	UNP P07700
B	43	VAL	-	expression tag	UNP P07700
B	68	SER	ARG	engineered mutation	UNP P07700
B	90	VAL	MET	engineered mutation	UNP P07700
B	116	LEU	CYS	engineered mutation	UNP P07700
B	?	-	ARG	deletion	UNP P07700
B	?	-	CYS	deletion	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: $C_{18}H_{37}NO_7$).

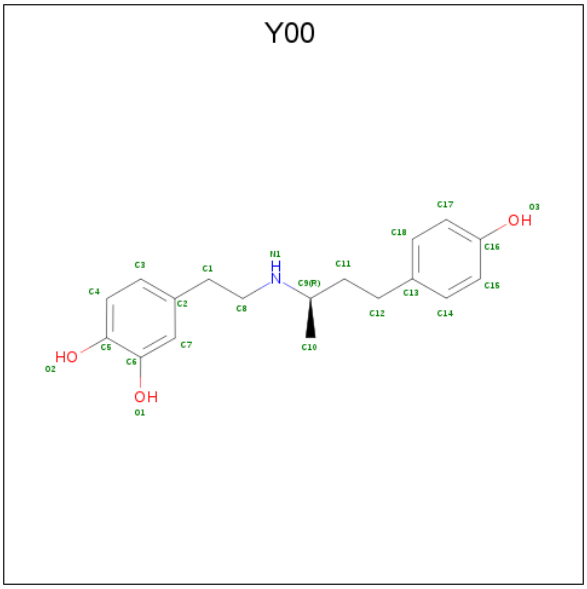


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			17	9	1	7		
4	A	1	Total	C	N	O	0	0
			26	18	1	7		
4	A	1	Total	C	N	O	0	0
			26	18	1	7		
4	A	1	Total	C	N	O	0	0
			26	18	1	7		
4	A	1	Total	C	N	O	0	0
			18	15	1	2		
4	A	1	Total	C	N	O	0	0
			26	18	1	7		
4	B	1	Total	C	N	O	0	0
			26	18	1	7		
4	B	1	Total	C	N	O	0	0
			15	10	1	4		
4	B	1	Total	C	N	O	0	0
			26	18	1	7		

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

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

- Molecule 6 is DOBUTAMINE (three-letter code: Y00) (formula: $C_{18}H_{23}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 22 18 1 3	0	0
6	B	1	Total C N O 22 18 1 3	0	0

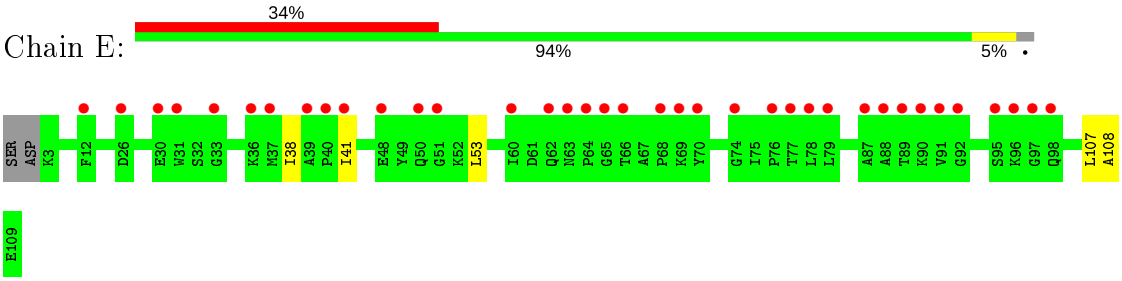
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	6	Total O 6 6	0	0
7	C	5	Total O 5 5	0	0
7	B	1	Total O 1 1	0	0
7	D	2	Total O 2 2	0	0

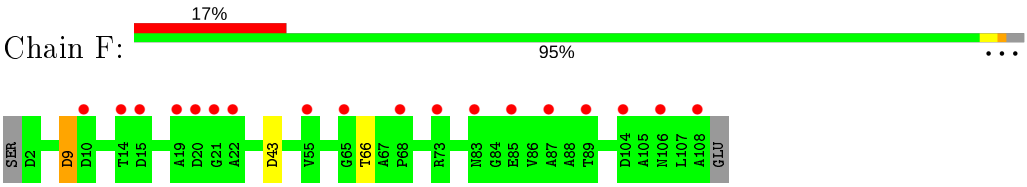
3 Residue-property plots (i)

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

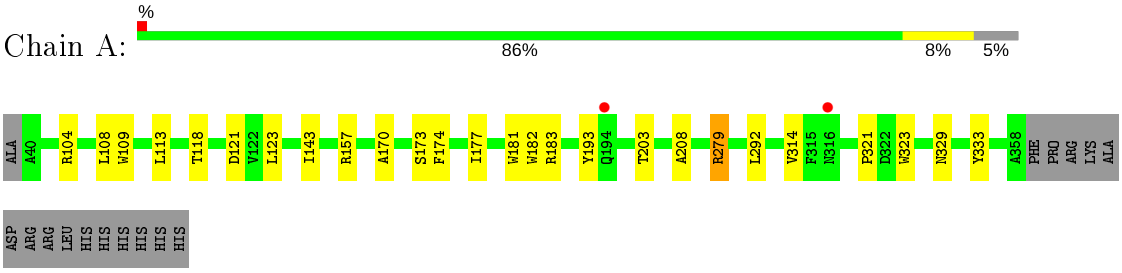
- Molecule 1: Thioredoxin 1



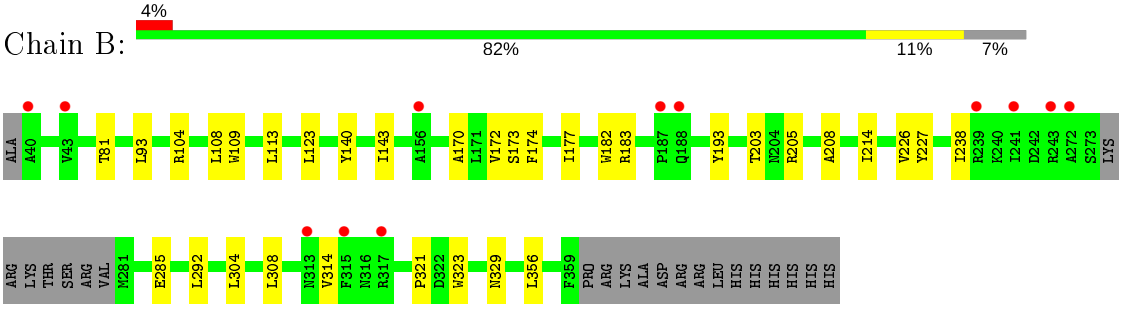
- Molecule 1: Thioredoxin 1



- Molecule 2: Beta-1 adrenergic receptor

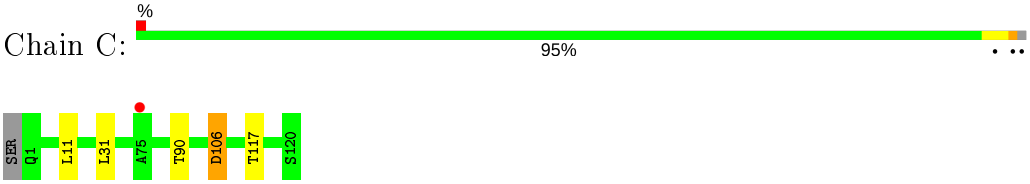


- Molecule 2: Beta-1 adrenergic receptor



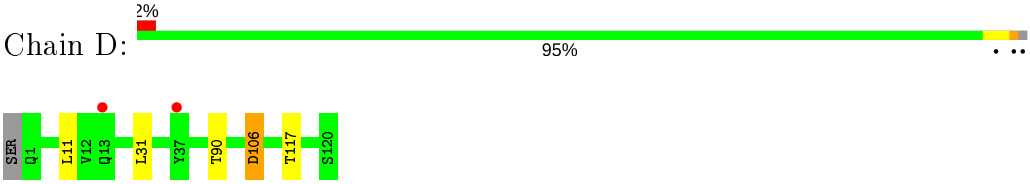
- Molecule 3: Camelid antibody fragment Nb6B9

Chain C:



- Molecule 3: Camelid antibody fragment Nb6B9

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.51Å 119.70Å 129.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.08 – 2.70 41.08 – 2.70	Depositor EDS
% Data completeness (in resolution range)	58.8 (41.08-2.70) 58.8 (41.08-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0174	Depositor
R, R_{free}	0.241 , 0.278 0.246 , 0.283	Depositor DCC
R_{free} test set	1416 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 7.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.043 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	8280	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, Y00, 2CV

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	0.44	0/820	0.56	0/1116
1	F	0.45	0/827	0.57	0/1123
2	A	0.45	0/2367	0.67	2/3222 (0.1%)
2	B	0.45	0/2318	0.63	0/3157
3	C	0.42	0/927	0.61	0/1256
3	D	0.43	0/927	0.61	0/1256
All	All	0.44	0/8186	0.62	2/11130 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	157	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	A	279	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	805	0	798	2	0
1	F	812	0	818	1	0
2	A	2313	0	2423	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2264	0	2358	20	0
3	C	910	0	878	4	0
3	D	910	0	878	4	0
4	A	122	0	173	2	0
4	B	67	0	90	2	0
4	E	17	0	18	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	22	0	20	0	0
6	B	22	0	21	0	0
7	A	6	0	0	0	0
7	B	1	0	0	0	0
7	C	5	0	0	0	0
7	D	2	0	0	0	0
All	All	8280	0	8475	42	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.

The worst 5 of 42 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)
2:B:81:THR:HG21	4:B:402:2CV:H431	1.74	0.69
2:A:104:ARG:HG3	2:A:108:LEU:HD11	1.85	0.57
3:D:106:ASP:OD1	3:D:106:ASP:N	2.39	0.56
3:C:106:ASP:N	3:C:106:ASP:OD1	2.38	0.54
2:B:104:ARG:HG3	2:B:108:LEU:HD11	1.90	0.53

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%)	2 (2%)	1 (1%)	15 37
1	F	105/109 (96%)	104 (99%)	1 (1%)	0	100 100
2	A	289/307 (94%)	283 (98%)	6 (2%)	0	100 100
2	B	281/307 (92%)	274 (98%)	7 (2%)	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%)	995 (98%)	20 (2%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	108	ALA

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%)	83 (98%)	2 (2%)	49 77
2	A	252/266 (95%)	249 (99%)	3 (1%)	71 88
2	B	246/266 (92%)	245 (100%)	1 (0%)	91 97
3	C	94/95 (99%)	93 (99%)	1 (1%)	73 90
3	D	94/95 (99%)	93 (99%)	1 (1%)	73 90
All	All	854/898 (95%)	846 (99%)	8 (1%)	78 92

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	106	ASP
3	D	106	ASP
1	F	43	ASP
2	A	329	ASN

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Mol	Chain	Res	Type
1	F	9	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	50	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	0.45	0	29,30,30	1.13	4 (13%)
4	2CV	A	402	-	25,25,25	0.28	0	29,30,30	1.03	1 (3%)
4	2CV	B	403	-	14,14,25	0.54	0	15,16,30	1.24	3 (20%)
4	2CV	A	403	-	25,25,25	0.59	0	29,30,30	1.02	2 (6%)
4	2CV	A	407	-	25,25,25	0.50	0	29,30,30	1.63	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	Y00	A	406	-	23,23,23	1.24	1 (4%)	29,30,30	1.12	1 (3%)
4	2CV	B	402	-	25,25,25	0.47	0	29,30,30	1.26	3 (10%)
4	2CV	A	404	-	25,25,25	0.50	0	29,30,30	1.70	9 (31%)
4	2CV	E	201	-	15,16,25	0.63	0	19,20,30	1.39	2 (10%)
6	Y00	B	405	-	23,23,23	1.21	1 (4%)	29,30,30	1.14	1 (3%)
4	2CV	A	405	-	17,17,25	0.50	0	19,19,30	1.57	4 (21%)

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	-	-	6/34/34/34	-
4	2CV	A	402	-	-	7/34/34/34	-
4	2CV	B	403	-	-	2/17/17/34	-
4	2CV	A	403	-	-	13/34/34/34	-
4	2CV	A	407	-	-	8/34/34/34	-
6	Y00	A	406	-	-	0/11/11/11	0/2/2/2
4	2CV	B	402	-	-	11/34/34/34	-
4	2CV	A	404	-	-	4/34/34/34	-
4	2CV	E	201	-	-	8/22/23/34	-
6	Y00	B	405	-	-	0/11/11/11	0/2/2/2
4	2CV	A	405	-	-	3/19/19/34	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	406	Y00	C5-C6	5.30	1.48	1.40
6	B	405	Y00	C5-C6	5.15	1.48	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	405	Y00	C8-N1-C9	4.71	121.17	114.05
4	A	407	2CV	C24-C27-C30	-4.48	100.57	112.67
4	A	404	2CV	C27-C30-N33	4.39	124.87	118.01
4	E	201	2CV	C42-C41-C40	4.33	119.23	112.47
6	A	406	Y00	C8-N1-C9	4.32	120.57	114.05

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	2CV	C40-C41-C42-O53
4	B	404	2CV	O51-C41-C42-C43
4	B	404	2CV	O51-C41-C42-O53
4	A	403	2CV	C36-C37-C40-C41
4	A	403	2CV	C36-C37-C40-O49

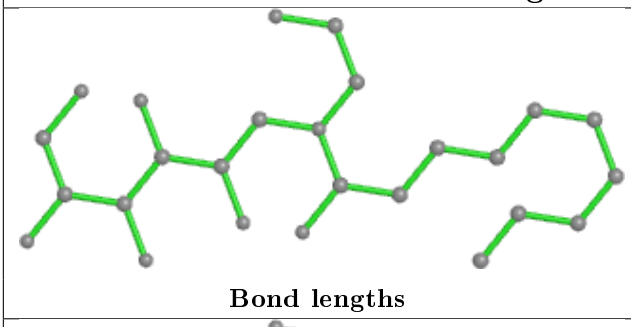
There are no ring outliers.

3 monomers are involved in 4 short contacts:

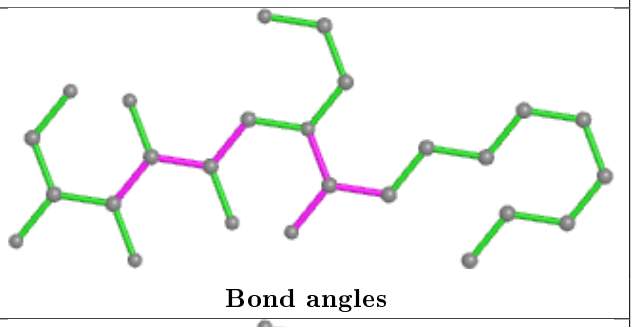
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	2CV	1	0
4	A	407	2CV	1	0
4	B	402	2CV	2	0

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.

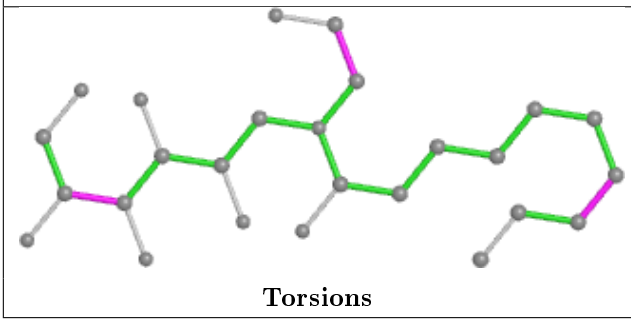
Ligand 2CV B 404



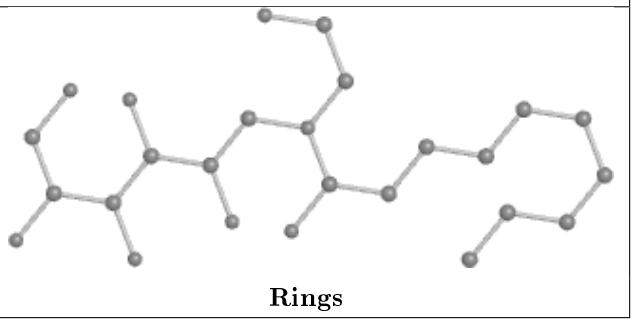
Bond lengths



Bond angles

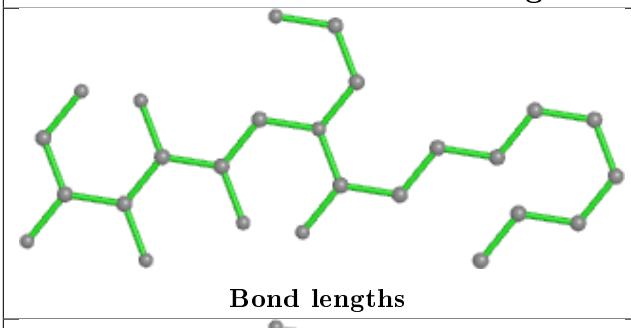


Torsions

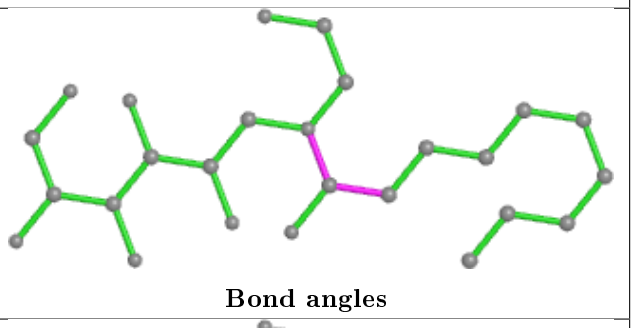


Rings

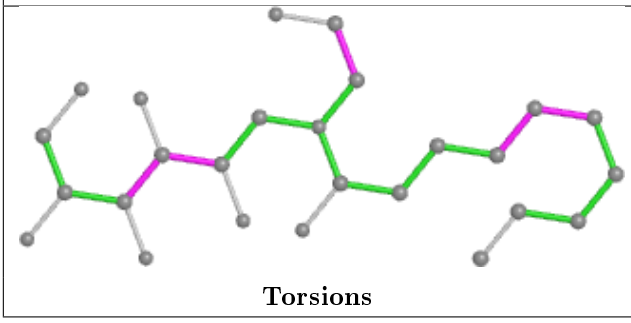
Ligand 2CV A 402



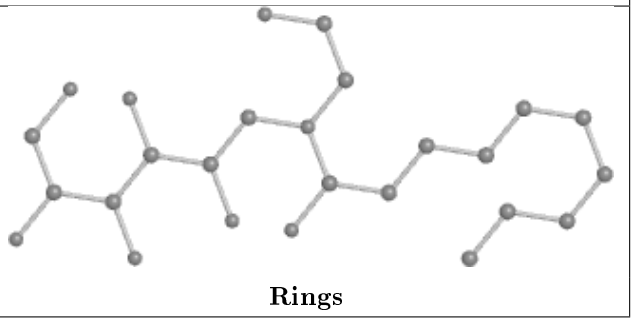
Bond lengths



Bond angles

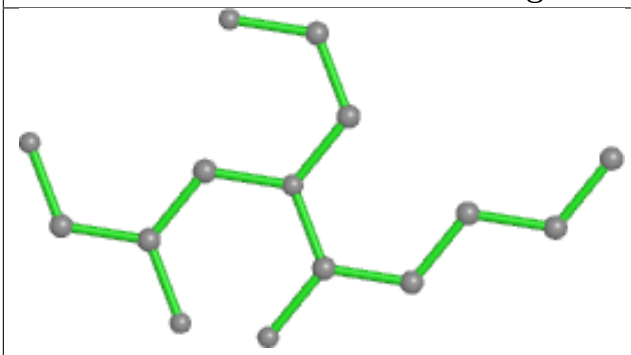


Torsions

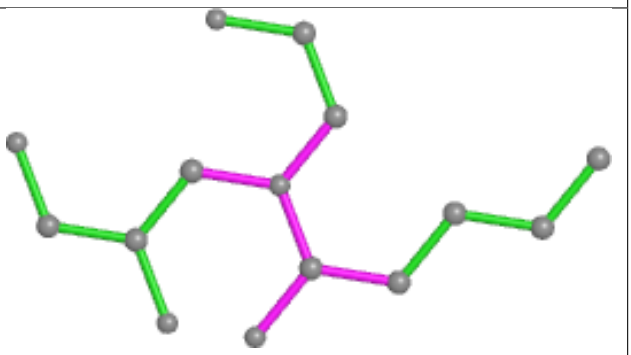


Rings

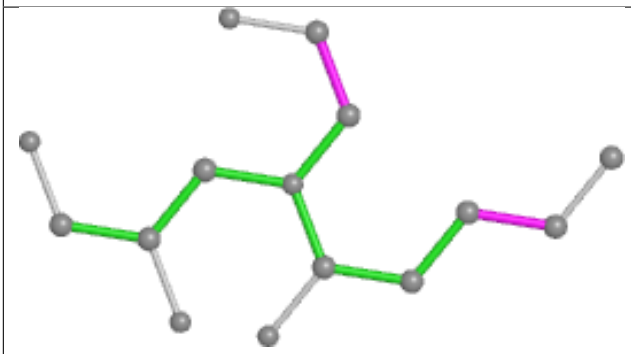
Ligand 2CV B 403



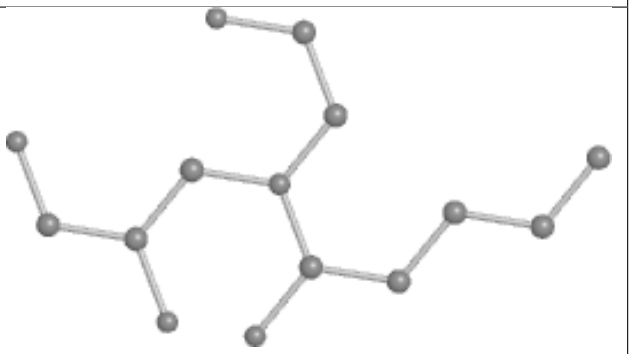
Bond lengths



Bond angles

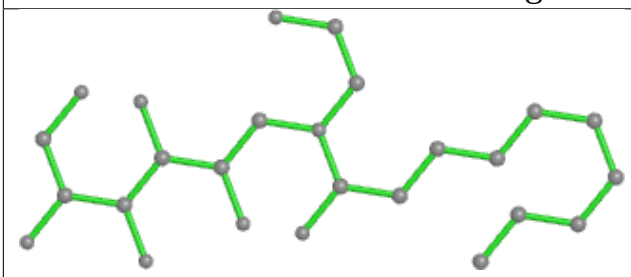


Torsions

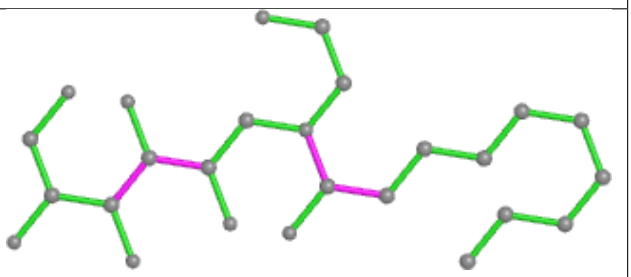


Rings

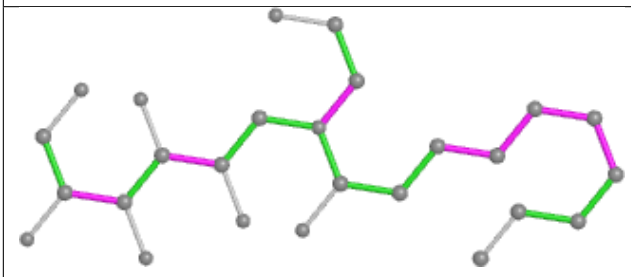
Ligand 2CV A 403



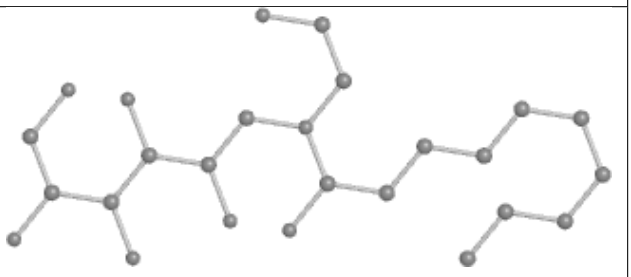
Bond lengths



Bond angles

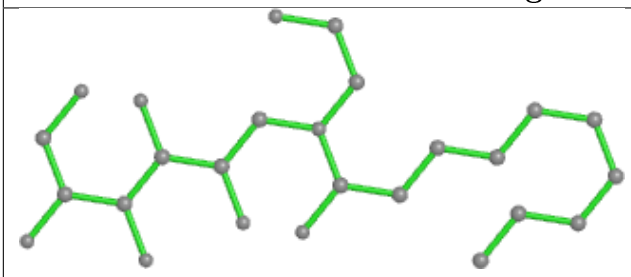


Torsions

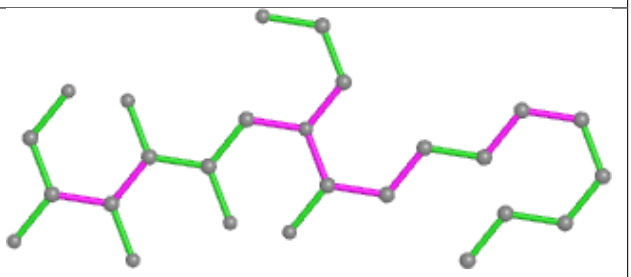


Rings

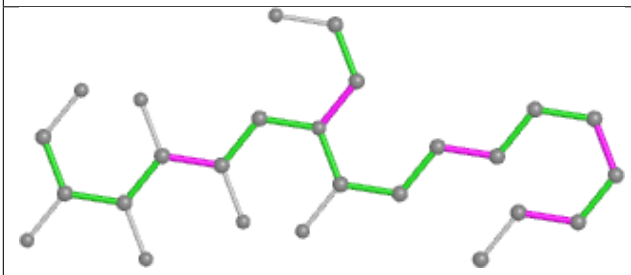
Ligand 2CV A 407



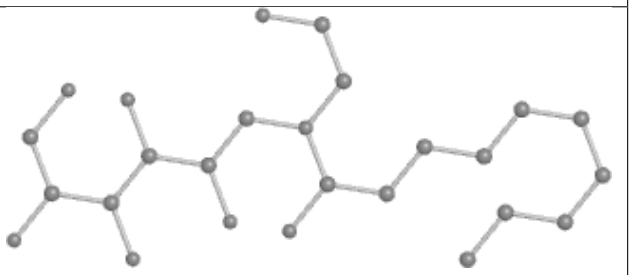
Bond lengths



Bond angles

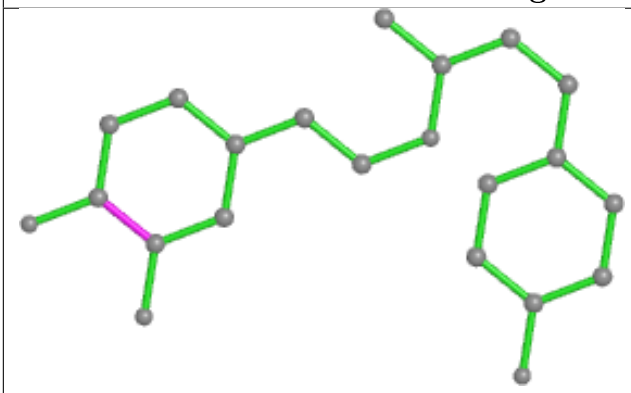


Torsions

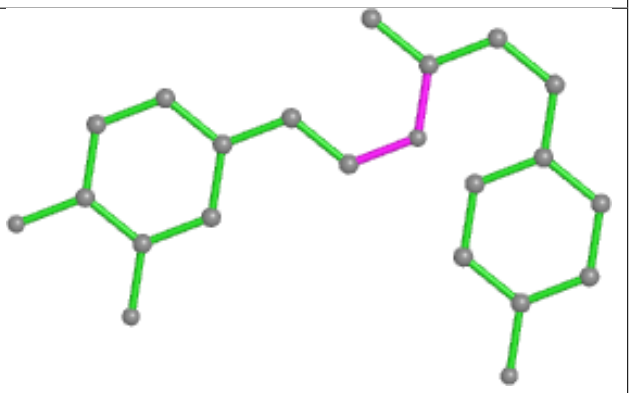


Rings

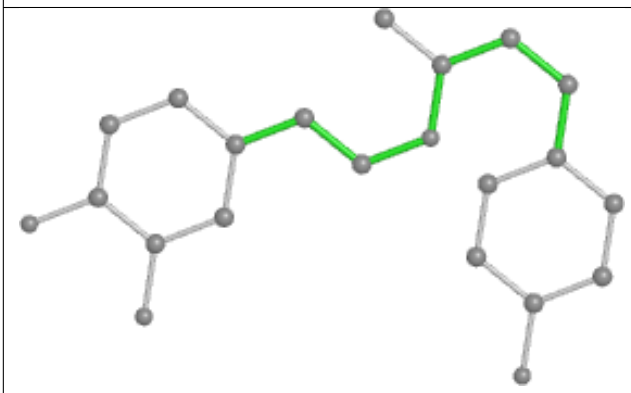
Ligand Y00 A 406



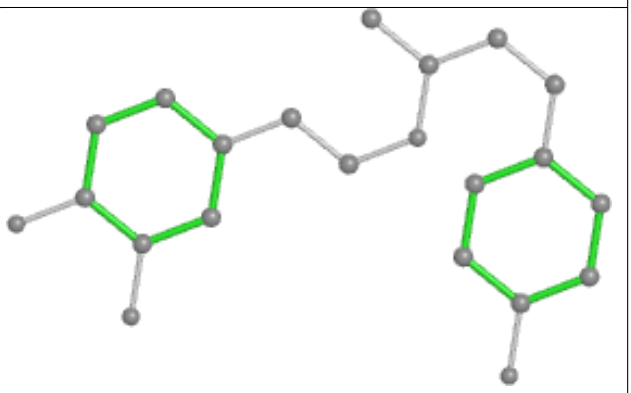
Bond lengths



Bond angles

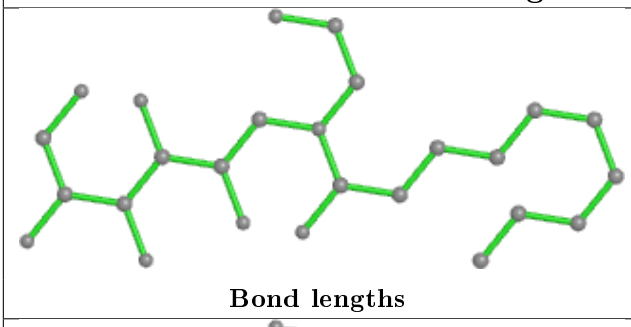


Torsions

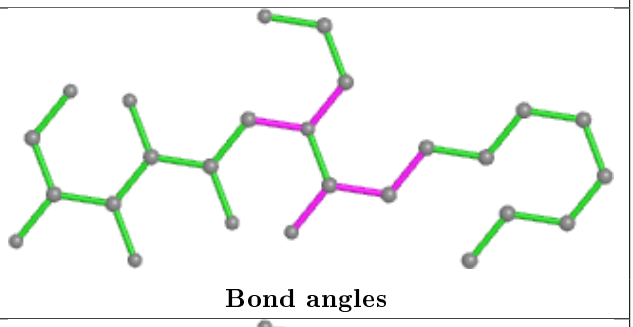


Rings

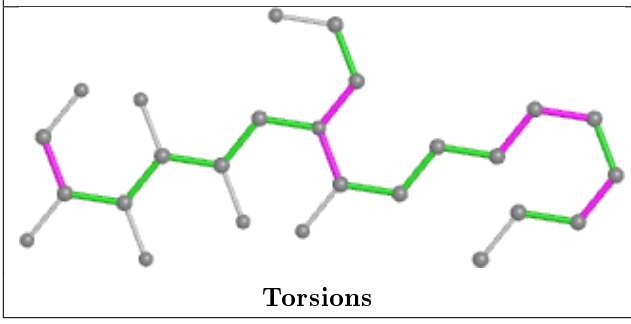
Ligand 2CV B 402



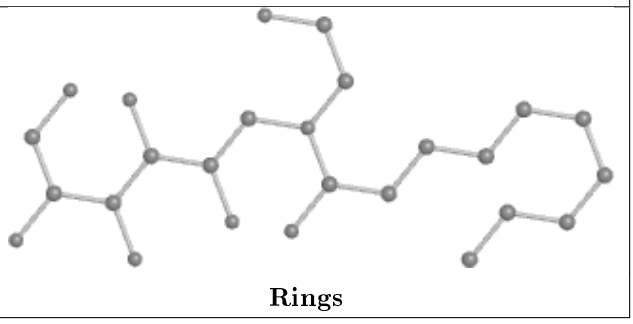
Bond lengths



Bond angles

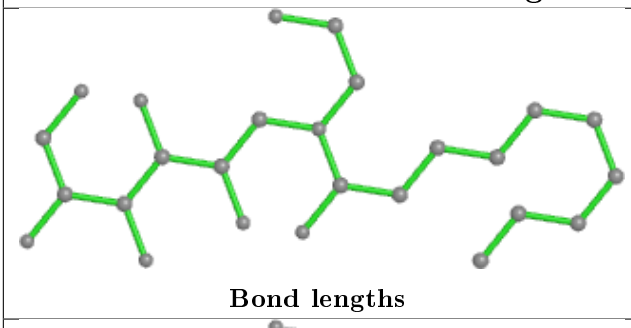


Torsions

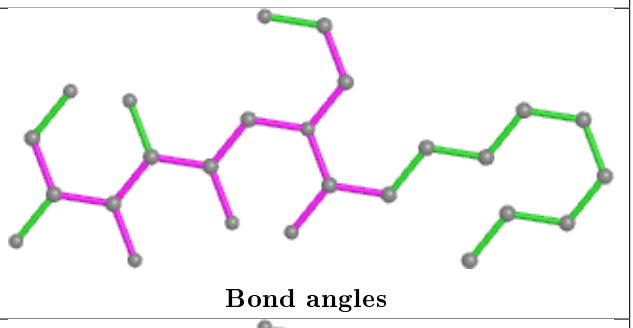


Rings

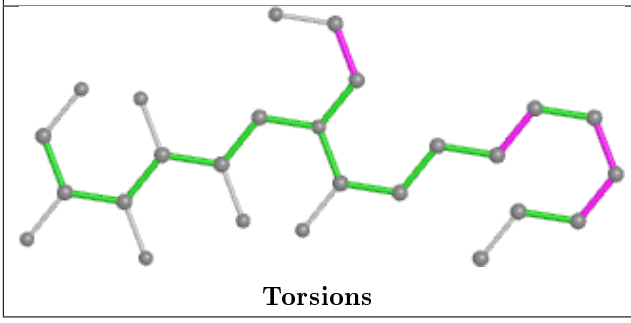
Ligand 2CV A 404



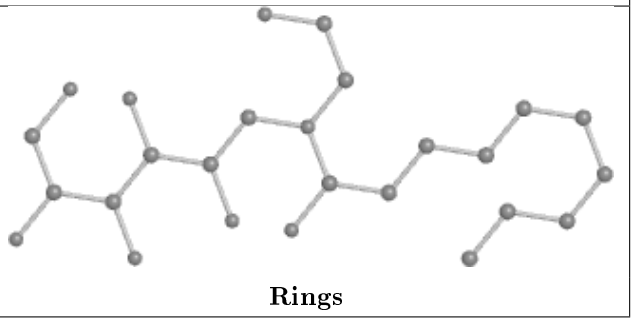
Bond lengths



Bond angles

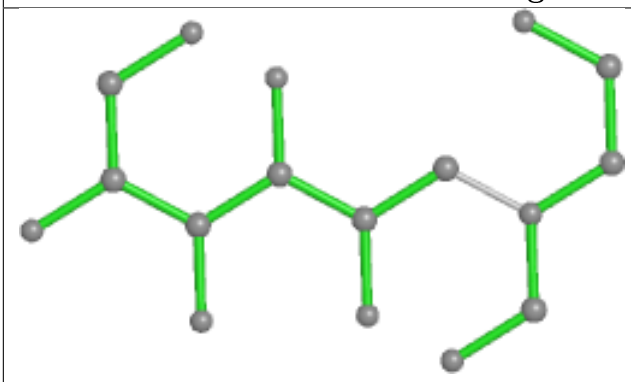


Torsions

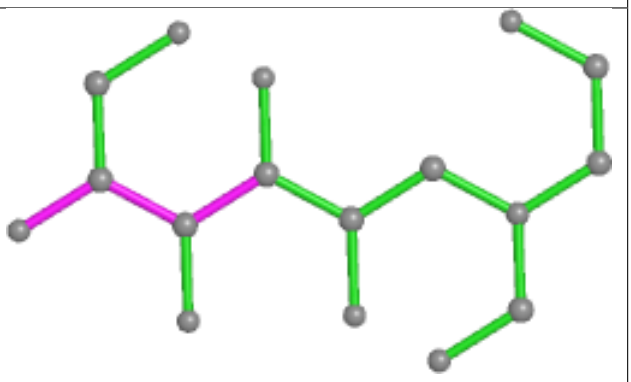


Rings

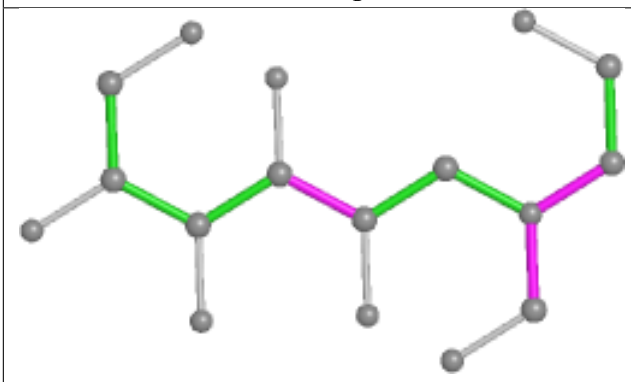
Ligand 2CV E 201



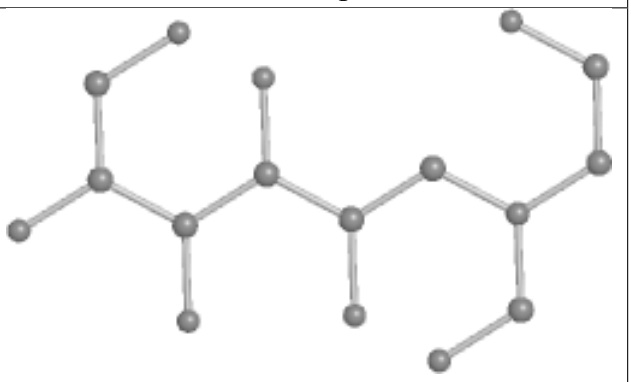
Bond lengths



Bond angles

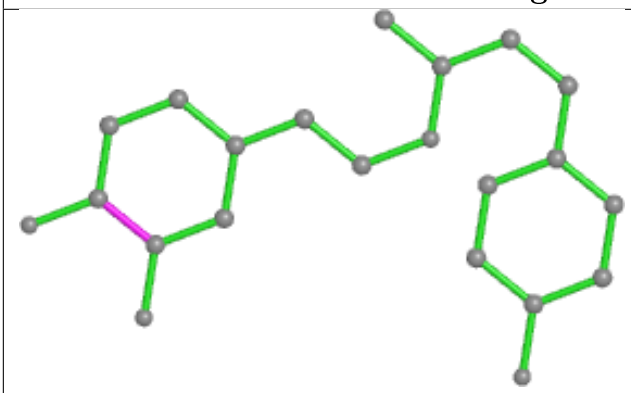


Torsions

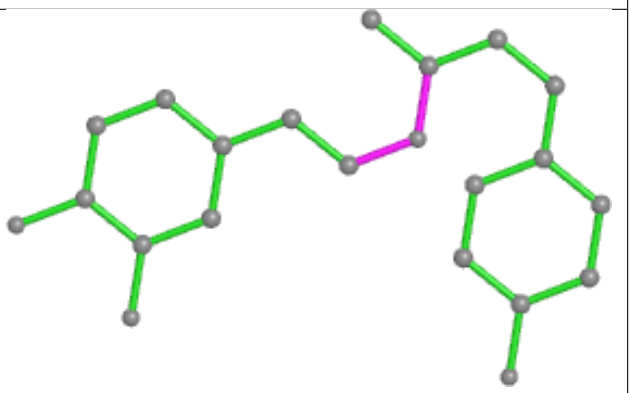


Rings

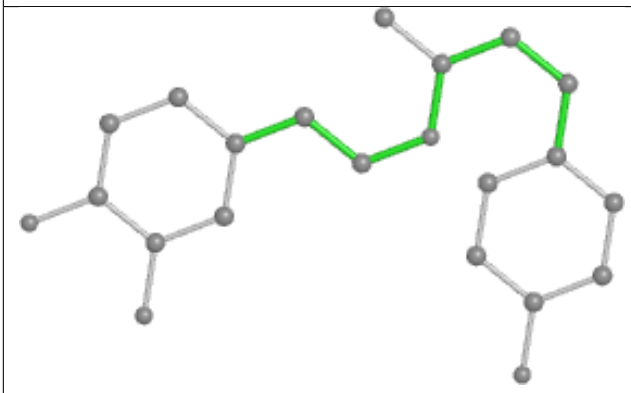
Ligand Y00 B 405



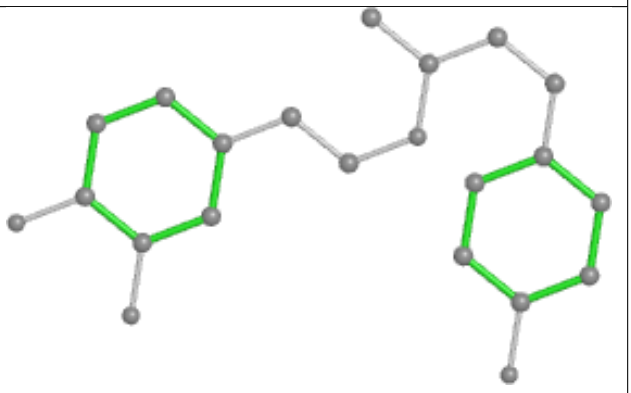
Bond lengths



Bond angles

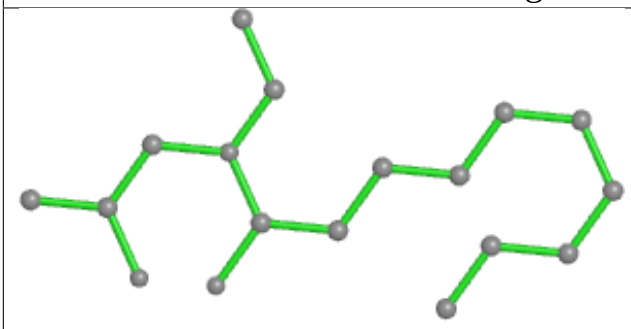


Torsions

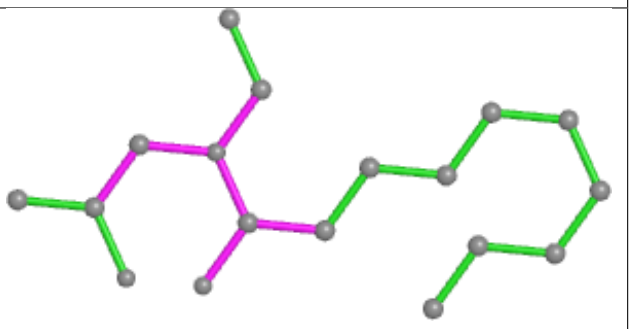


Rings

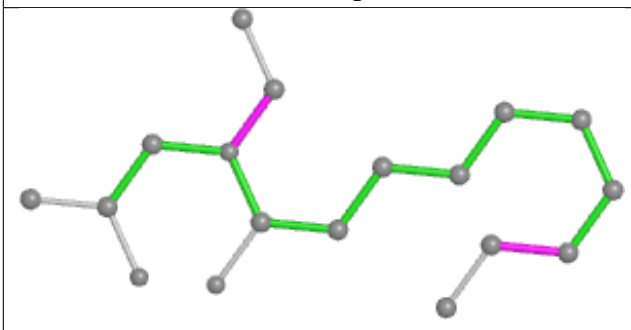
Ligand 2CV A 405



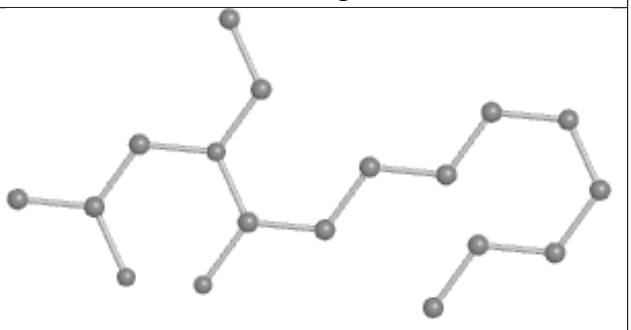
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	E	107/109 (98%)	1.45	37 (34%) 0 0	64, 115, 157, 173	0
1	F	107/109 (98%)	0.70	18 (16%) 1 1	55, 95, 128, 140	0
2	A	291/307 (94%)	-0.13	2 (0%) 87 89	19, 44, 86, 110	0
2	B	285/307 (92%)	0.06	12 (4%) 36 35	24, 57, 99, 122	0
3	C	120/121 (99%)	-0.24	1 (0%) 86 87	25, 42, 77, 99	0
3	D	120/121 (99%)	0.01	2 (1%) 70 72	36, 53, 86, 97	0
All	All	1030/1074 (95%)	0.18	72 (6%) 16 14	19, 57, 124, 173	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	40	PRO	6.7
1	E	91	VAL	6.6
1	F	10	ASP	6.6
1	E	76	PRO	6.2
2	B	243	ARG	6.1

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 carbohydrates in this entry.

6.4 Ligands (i)

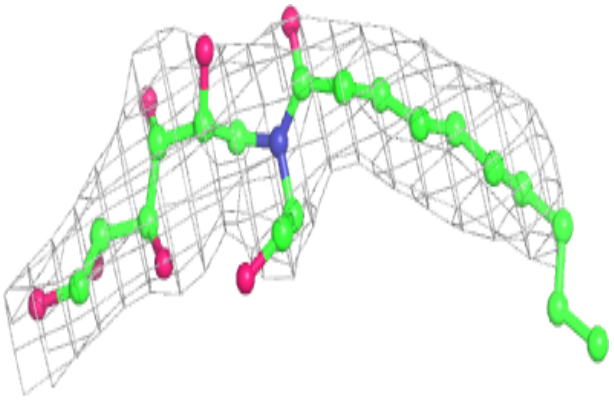
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

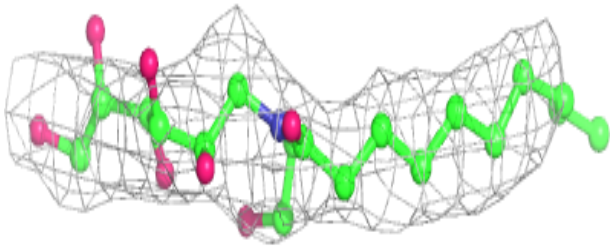
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	2CV	B	404	26/26	0.78	0.31	88,115,126,139	0
4	2CV	E	201	17/26	0.79	0.27	62,93,100,101	0
4	2CV	A	407	26/26	0.84	0.23	44,55,65,80	0
4	2CV	A	404	26/26	0.86	0.21	46,59,73,87	0
4	2CV	A	403	26/26	0.86	0.27	54,81,92,97	0
4	2CV	B	403	15/26	0.88	0.20	49,61,65,66	0
6	Y00	B	405	22/22	0.92	0.20	56,60,66,69	0
4	2CV	B	402	26/26	0.93	0.21	38,45,58,66	0
4	2CV	A	405	18/26	0.93	0.28	45,53,70,73	0
5	NA	A	401	1/1	0.93	0.07	42,42,42,42	0
4	2CV	A	402	26/26	0.94	0.15	40,50,57,61	0
6	Y00	A	406	22/22	0.96	0.21	36,52,66,67	0
5	NA	B	401	1/1	0.96	0.20	39,39,39,39	0

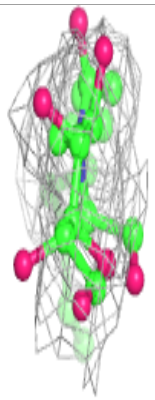
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CV B 404:

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

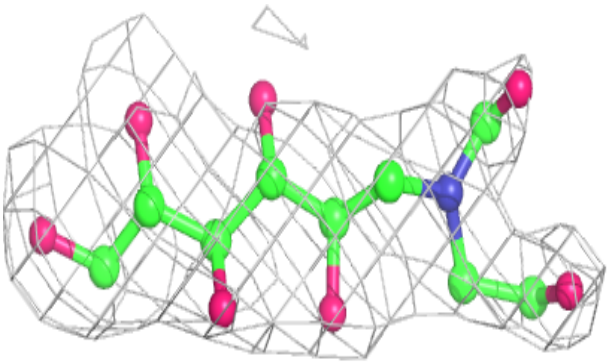


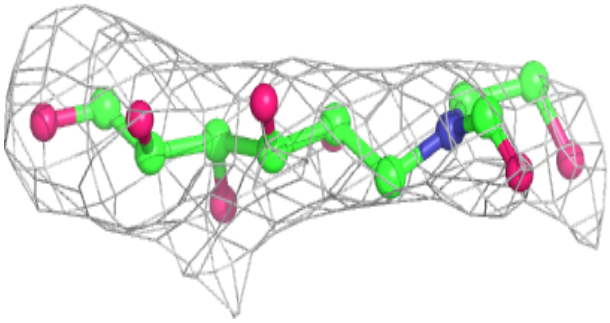


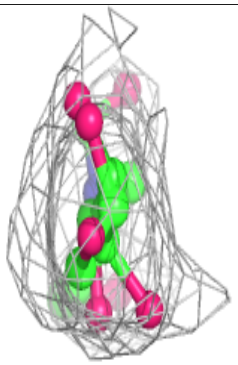


Electron density around 2CV E 201:

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

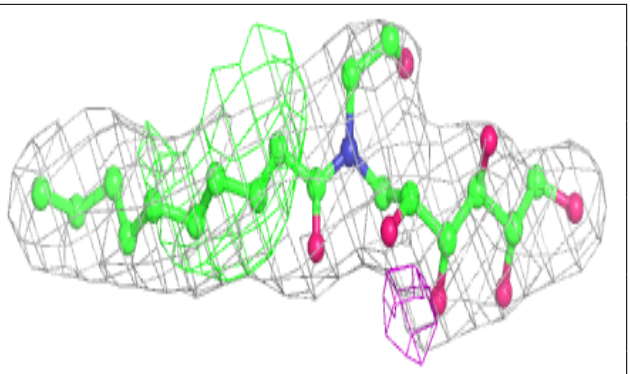


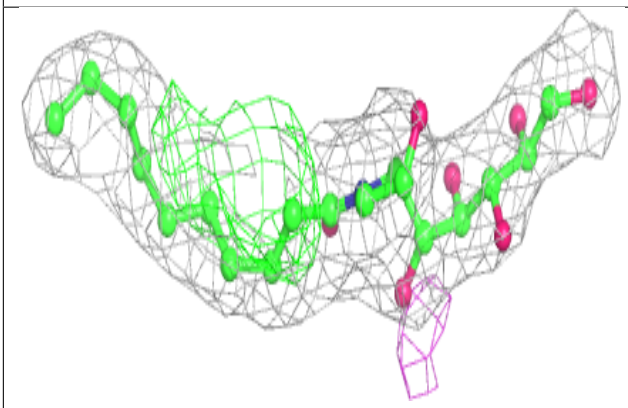


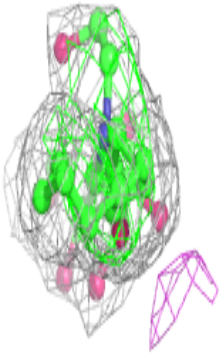


Electron density around 2CV A 407:

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

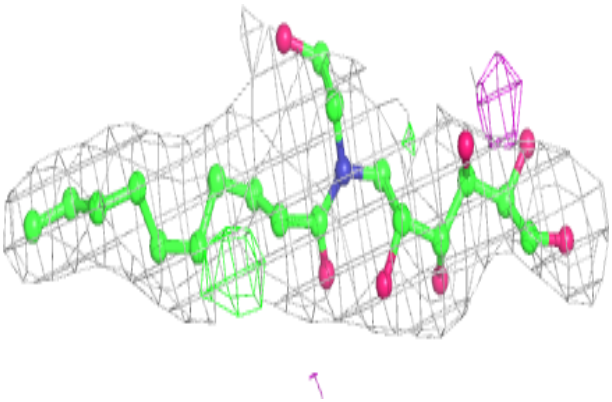


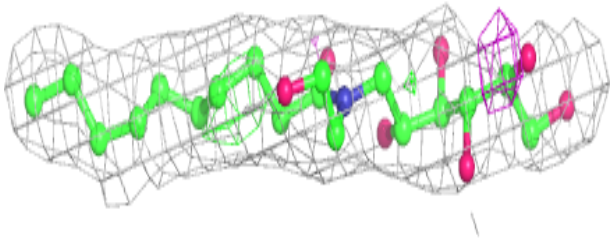




Electron density around 2CV A 404:

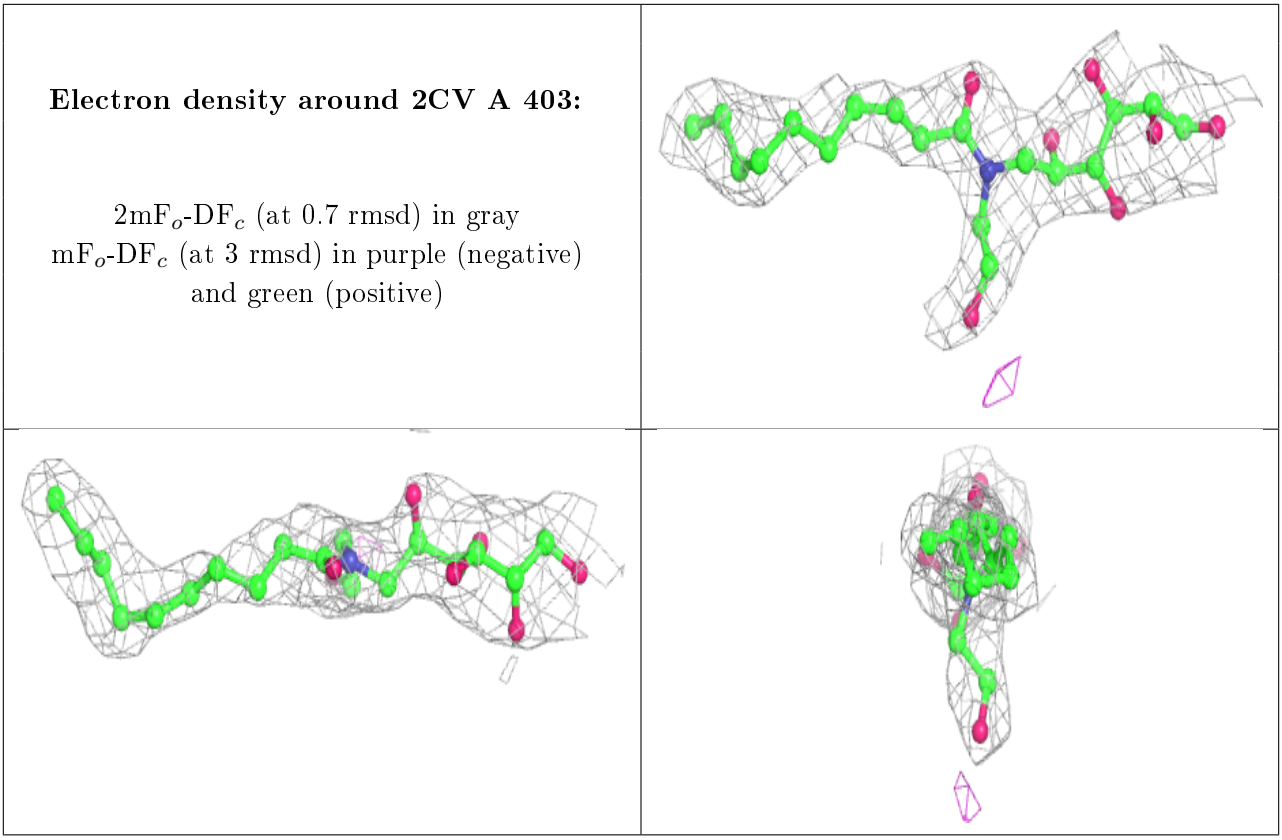
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





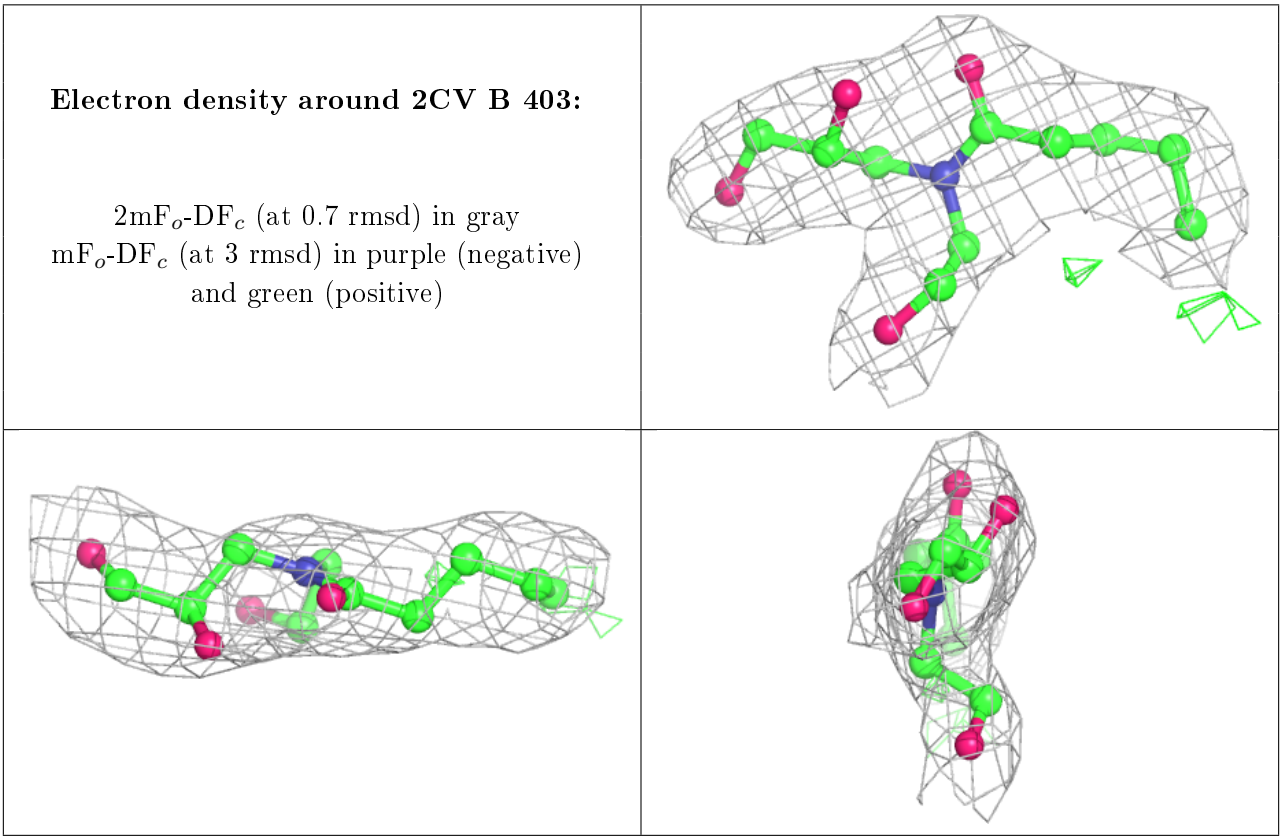
Electron density around 2CV A 403:

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



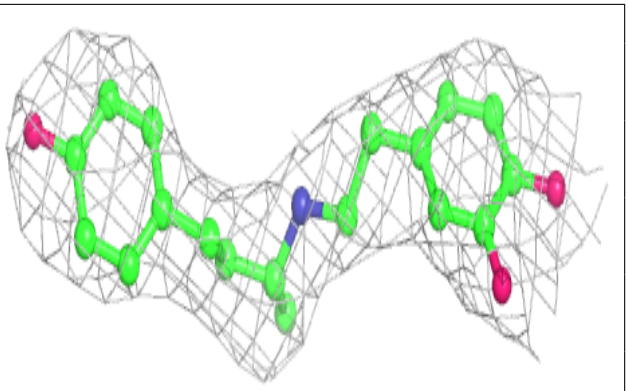
Electron density around 2CV B 403:

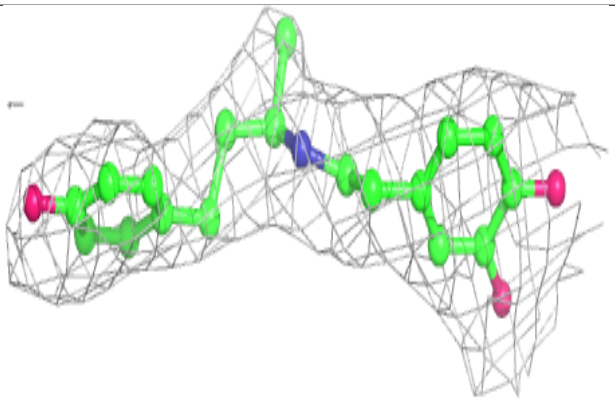
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

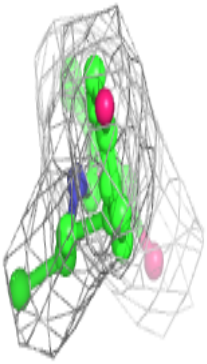


Electron density around Y00 B 405:

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

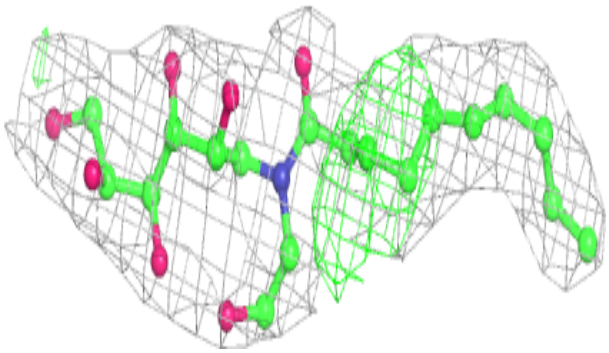


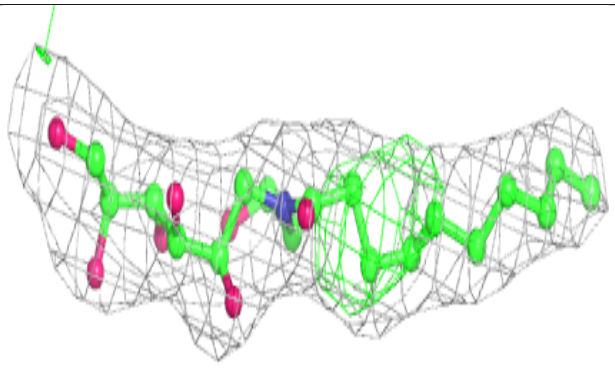


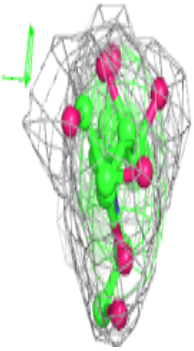


Electron density around 2CV B 402:

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

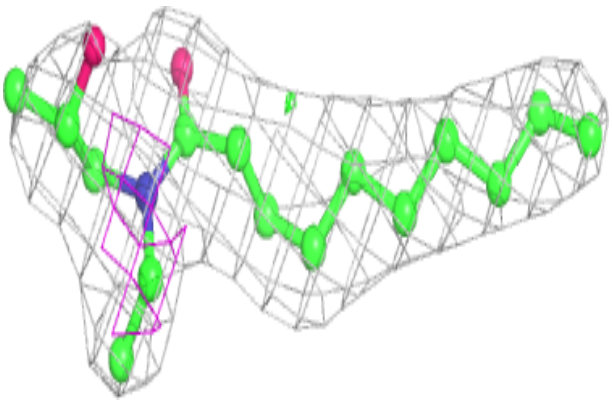


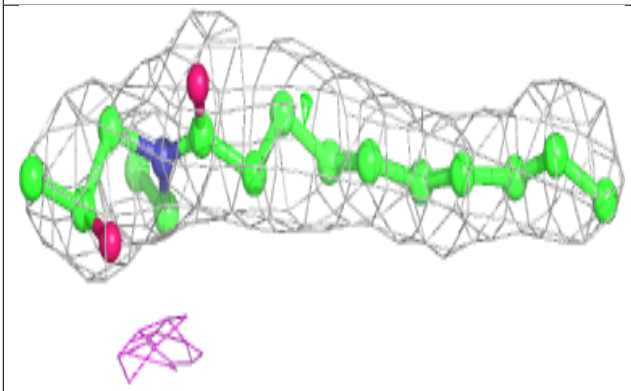


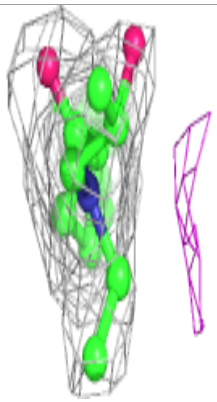


Electron density around 2CV A 405:

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

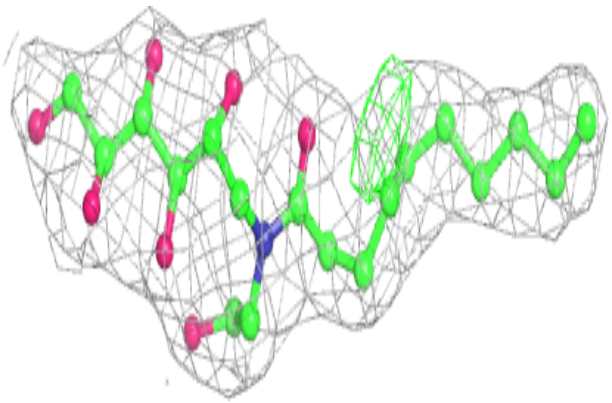


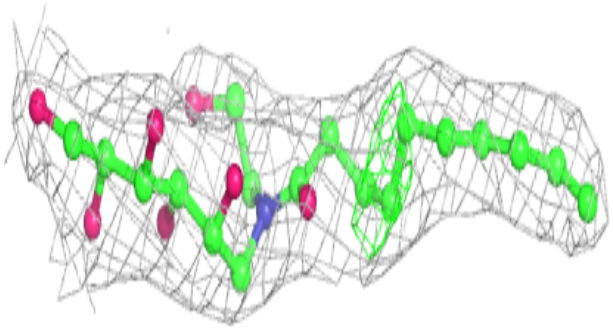


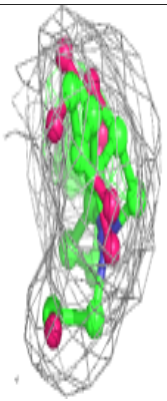


Electron density around 2CV A 402:

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

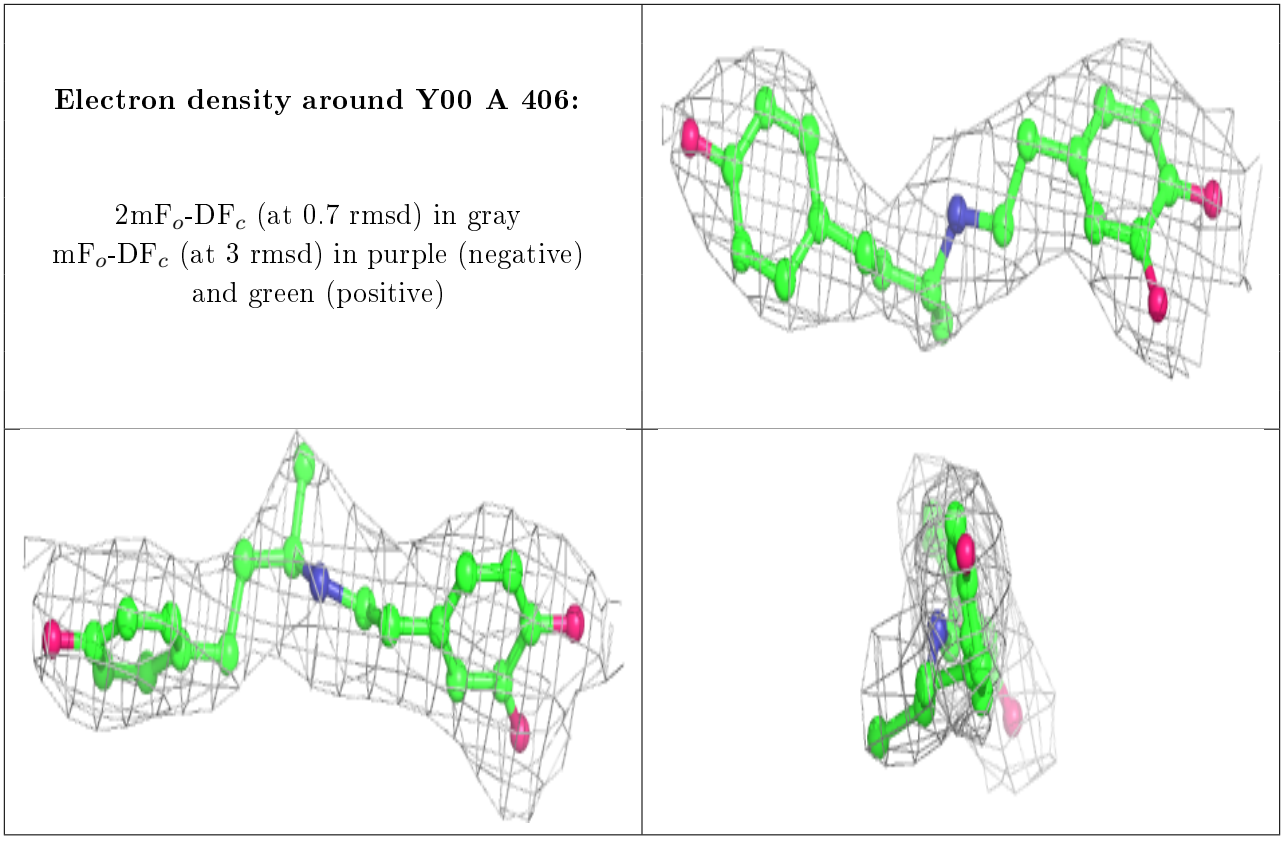






Electron density around Y00 A 406:

$2mF_o$-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.