Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 02:42 PM EDT

PDB ID	:	6IBL
Title	:	ACTIVATED TURKEY BETA1 ADRENOCEPTOR WITH BOUND AGONIST FORMOTEROL AND NANOBODY Nb80
Authors	:	Warne, T.; Edwards, P.C.; Dore, A.S.; Leslie, A.G.W.; Tate, C.G.
Deposited on	:	2018-11-30
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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:

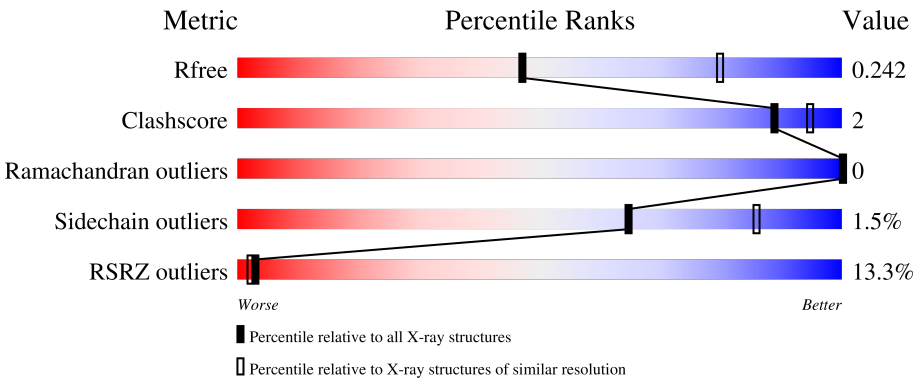
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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	416	14% 90% 6% 5%
1	B	416	16% 88% 6% 6%
2	C	121	7% 90% 8% •
2	D	121	6% 93% 7% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8271 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,Beta-1 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3105	2036	512	537	20	0	0	0
1	B	391	3068	2017	501	531	19	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1032	SER	CYS	engineered mutation	UNP P0AA25
A	1035	SER	CYS	engineered mutation	UNP P0AA25
A	1109	GLU	-	linker	UNP P0AA25
A	39	ALA	-	linker	UNP P0AA25
A	40	ALA	-	linker	UNP P0AA25
A	41	ALA	-	linker	UNP P0AA25
A	42	LYS	-	linker	UNP P0AA25
A	43	VAL	-	linker	UNP P0AA25
A	68	SER	ARG	conflict	UNP P07700
A	90	VAL	MET	conflict	UNP P07700
A	116	LEU	CYS	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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
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	1032	SER	CYS	engineered mutation	UNP P0AA25
B	1035	SER	CYS	engineered mutation	UNP P0AA25
B	1109	GLU	-	linker	UNP P0AA25
B	39	ALA	-	linker	UNP P0AA25
B	40	ALA	-	linker	UNP P0AA25
B	41	ALA	-	linker	UNP P0AA25
B	42	LYS	-	linker	UNP P0AA25
B	43	VAL	-	linker	UNP P0AA25
B	68	SER	ARG	conflict	UNP P07700
B	90	VAL	MET	conflict	UNP P07700
B	116	LEU	CYS	conflict	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

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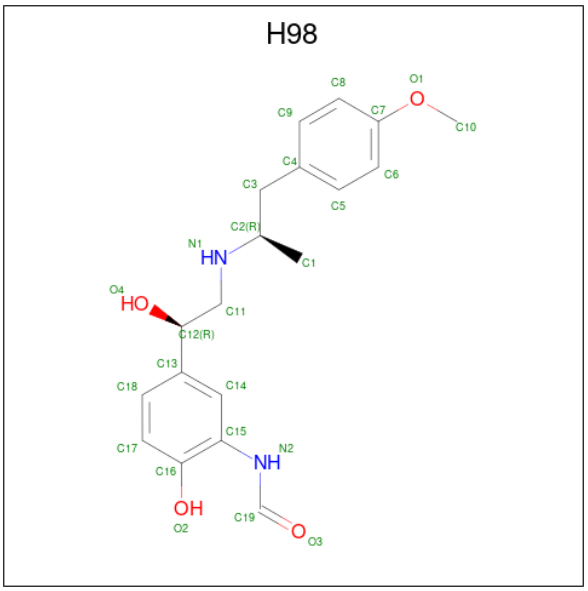
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	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	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
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 2 is a protein called Camelid antibody fragment Nb80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	119	901	561	157	179	4	0	0	0
			Total	C	N	O	S			
2	D	120	910	566	159	181	4	0	0	0

- Molecule 3 is {N}-[5-[(1 {R})-2-[[(2 {R})-1-(4-methoxyphenyl)propan-2-yl]amino]-1-oxidanyl-ethyl]-2-oxidanyl-phenyl]methanamide (three-letter code: H98) (formula: $C_{19}H_{24}N_2O_4$).

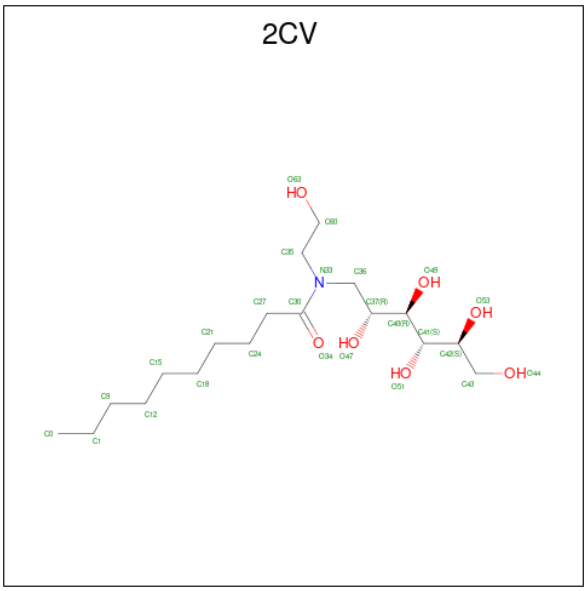


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	25	19	2	4	0	0
			Total	C	N	O		
3	B	1	25	19	2	4	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	26	18	1	7	0	0
			Total	C	N	O		
5	A	1	26	18	1	7	0	0
			Total	C	N	O		
5	A	1	24	16	1	7	0	0
			Total	C	N	O		
5	A	1	26	18	1	7	0	0
			Total	C	N	O		
5	A	1	26	18	1	7	0	0
			Total	C	N	O		
5	B	1	26	18	1	7	0	0
			Total	C	N	O		
5	B	1	26	18	1	7	0	0
			Total	C	N	O		
5	B	1	26	18	1	7	0	0

- Molecule 6 is water.

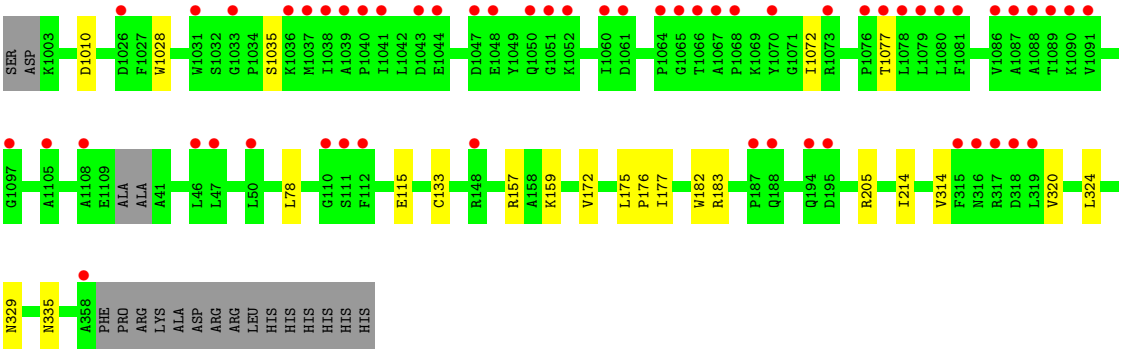
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	8	8	8	0	0
			Total	O		
6	C	6	6	6	0	0
			Total	O		
6	B	11	11	11	0	0
			Total	O		
6	D	4	4	4	0	0

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.

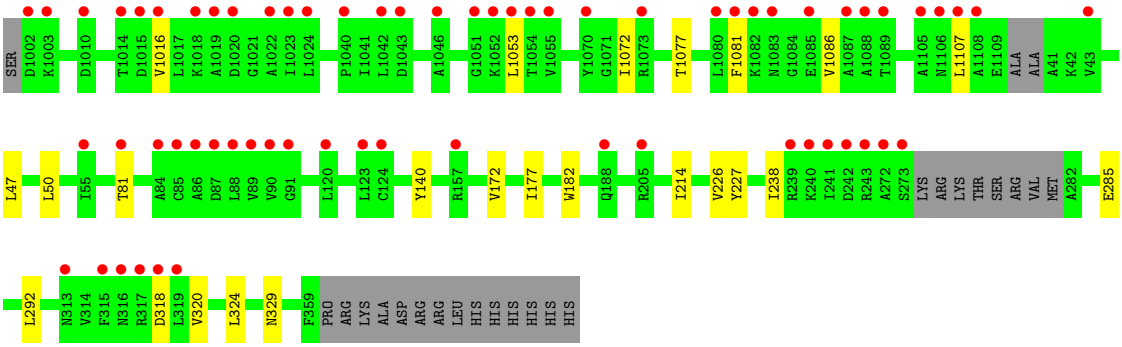
• Molecule 1: Thioredoxin 1,Beta-1 adrenergic receptor

Chain A:



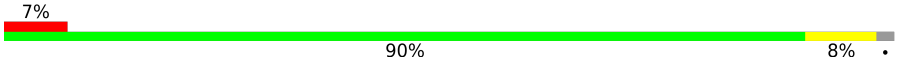
• Molecule 1: Thioredoxin 1,Beta-1 adrenergic receptor

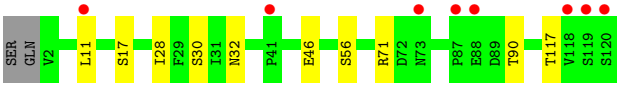
Chain B:



• Molecule 2: Camelid antibody fragment Nb80

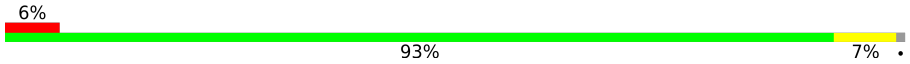
Chain C:

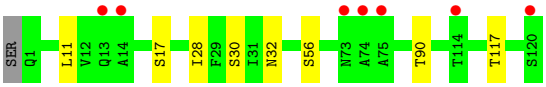




• Molecule 2: Camelid antibody fragment Nb80

Chain D:


6%
93%
7%


SER
Q1
L11
V12
Q13
A14
S17
I28
F29
S30
I31
N32
S56
N73
A74
A75
T90
T114
T117
S120

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.65Å 121.12Å 129.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 2.70 44.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	62.7 (44.32-2.70) 62.8 (44.28-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.35 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.240 , 0.277 0.244 , 0.242	Depositor DCC
R_{free} test set	1578 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.031 for k,h,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8271	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: 2CV, NA, H98

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	0.74	0/3174	0.88	1/4322 (0.0%)
1	B	0.72	0/3137	0.87	0/4270
2	C	0.70	0/918	0.89	0/1244
2	D	0.69	0/927	0.90	0/1256
All	All	0.72	0/8156	0.88	1/11092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	157	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	3105	0	3201	10	0
1	B	3068	0	3164	14	0
2	C	901	0	861	5	0
2	D	910	0	872	3	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	128	0	178	1	0
5	B	78	0	111	0	0
6	A	8	0	0	0	0
6	B	11	0	0	0	0
6	C	6	0	0	0	0
6	D	4	0	0	0	0
All	All	8271	0	8387	32	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 (32) 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:B:320:VAL:HG13	1:B:324:LEU:HD23	1.73	0.71
1:A:320:VAL:HG13	1:A:324:LEU:HD23	1.75	0.67
1:B:227:TYR:HB3	1:B:292:LEU:HD11	1.83	0.60
1:B:238:ILE:HD11	1:B:285:GLU:HG2	1.85	0.57
5:A:507:2CV:H431	1:B:81:THR:HG21	1.85	0.56
1:B:177:ILE:HA	1:B:182:TRP:CD1	2.41	0.55
1:B:1072:ILE:HD12	1:B:1077:THR:HG21	1.92	0.52
2:D:28:ILE:HG22	2:D:32:ASN:HD22	1.75	0.52
1:B:1081:PHE:CE1	1:B:1086:VAL:HG22	2.44	0.52
2:C:28:ILE:HG22	2:C:32:ASN:HD22	1.76	0.51
1:A:1072:ILE:HD12	1:A:1077:THR:HG21	1.94	0.49
1:B:1072:ILE:HG23	1:B:1077:THR:HG21	1.94	0.49
1:A:115:GLU:OE2	1:A:183:ARG:NH2	2.46	0.48
1:A:177:ILE:HA	1:A:182:TRP:CD1	2.48	0.48
1:B:47:LEU:HD12	1:B:50:LEU:HD21	1.95	0.47
1:A:1072:ILE:HG23	1:A:1077:THR:HG21	1.97	0.46
2:C:11:LEU:HD23	2:C:117:THR:HB	1.98	0.46
1:B:1053:LEU:HD23	1:B:1107:LEU:HD11	1.99	0.45
2:D:11:LEU:HD23	2:D:117:THR:HB	1.99	0.45
2:C:90:THR:HG23	2:C:117:THR:HA	1.99	0.44
1:B:172:VAL:HG21	1:B:214:ILE:HG21	1.99	0.43
1:A:172:VAL:HG21	1:A:214:ILE:HG21	2.00	0.43
1:A:175:LEU:HB3	1:A:176:PRO:HD3	2.01	0.42
2:D:90:THR:HG23	2:D:117:THR:HA	2.01	0.42
1:A:78:LEU:HD21	1:A:159:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:VAL:HG12	1:B:1081:PHE:HD2	1.84	0.41
1:A:1028:TRP:HB2	1:A:1035:SER:HB2	2.03	0.41
1:A:205:ARG:HG3	1:A:314:VAL:HG13	2.03	0.41
2:C:32:ASN:OD1	2:C:71:ARG:NH2	2.47	0.41
1:B:140:TYR:CB	1:B:226:VAL:HG13	2.52	0.40
1:B:140:TYR:HB2	1:B:226:VAL:HG13	2.04	0.40
2:C:28:ILE:CG2	2:C:32:ASN:HD22	2.35	0.40

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	393/416 (94%)	384 (98%)	9 (2%)	0	100	100
1	B	385/416 (92%)	374 (97%)	11 (3%)	0	100	100
2	C	117/121 (97%)	113 (97%)	4 (3%)	0	100	100
2	D	118/121 (98%)	113 (96%)	5 (4%)	0	100	100
All	All	1013/1074 (94%)	984 (97%)	29 (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	A	333/354 (94%)	329 (99%)	4 (1%)	71	88
1	B	330/354 (93%)	328 (99%)	2 (1%)	86	95
2	C	94/96 (98%)	90 (96%)	4 (4%)	29	57
2	D	95/96 (99%)	92 (97%)	3 (3%)	39	68
All	All	852/900 (95%)	839 (98%)	13 (2%)	65	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	ASP
1	A	133	CYS
1	A	329	ASN
1	A	335	ASN
2	C	17	SER
2	C	30	SER
2	C	46	GLU
2	C	56	SER
1	B	318	ASP
1	B	329	ASN
2	D	17	SER
2	D	30	SER
2	D	56	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	13	GLN
2	D	13	GLN

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	2CV	A	505	-	23,23,25	0.35	0	27,28,30	1.36	2 (7%)
5	2CV	A	506	-	25,25,25	0.35	0	29,30,30	1.17	3 (10%)
5	2CV	A	503	-	25,25,25	0.33	0	29,30,30	0.84	1 (3%)
3	H98	B	501	-	26,26,26	0.31	0	33,34,34	0.63	0
3	H98	A	501	-	26,26,26	0.38	0	33,34,34	0.61	0
5	2CV	A	507	-	25,25,25	0.42	0	29,30,30	0.95	2 (6%)
5	2CV	B	505	-	25,25,25	0.37	0	29,30,30	1.11	2 (6%)
5	2CV	B	503	-	25,25,25	0.32	0	29,30,30	0.84	1 (3%)
5	2CV	B	504	-	25,25,25	0.42	0	29,30,30	1.22	1 (3%)
5	2CV	A	504	-	25,25,25	0.36	0	29,30,30	1.04	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2CV	A	505	-	-	13/32/32/34	-
5	2CV	A	506	-	-	7/34/34/34	-
5	2CV	A	503	-	-	8/34/34/34	-
3	H98	B	501	-	-	4/18/18/18	0/2/2/2
3	H98	A	501	-	-	5/18/18/18	0/2/2/2
5	2CV	A	507	-	-	10/34/34/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2CV	B	505	-	-	7/34/34/34	-
5	2CV	B	503	-	-	9/34/34/34	-
5	2CV	B	504	-	-	11/34/34/34	-
5	2CV	A	504	-	-	9/34/34/34	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	504	2CV	C37-C40-C41	5.55	121.15	112.47
5	A	505	2CV	C37-C40-C41	5.27	120.72	112.47
5	B	505	2CV	C36-C37-C40	3.34	119.13	109.79
5	A	503	2CV	C36-C37-C40	3.18	118.69	109.79
5	A	506	2CV	C37-C40-C41	2.94	117.06	112.47
5	A	507	2CV	C35-N33-C36	2.93	119.89	116.41
5	B	505	2CV	C37-C40-C41	2.80	116.85	112.47
5	A	504	2CV	C36-C37-C40	2.69	117.30	109.79
5	A	504	2CV	C24-C27-C30	2.37	119.08	112.67
5	B	503	2CV	C37-C40-C41	2.37	116.18	112.47
5	A	505	2CV	C36-C37-C40	2.36	116.37	109.79
5	A	507	2CV	C37-C40-C41	2.36	116.15	112.47
5	A	504	2CV	C37-C40-C41	2.33	116.11	112.47
5	A	506	2CV	C27-C30-N33	2.16	121.39	118.01
5	A	506	2CV	C36-C37-C40	2.07	115.56	109.79

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	H98	C1-C2-C3-C4
3	A	501	H98	N1-C2-C3-C4
3	A	501	H98	O3-C19-N2-C15
3	B	501	H98	N1-C2-C3-C4
3	B	501	H98	O3-C19-N2-C15
5	A	503	2CV	C36-C37-C40-C41
5	A	503	2CV	C36-C37-C40-O49
5	A	504	2CV	C37-C36-N33-C35
5	A	505	2CV	N33-C36-C37-O47
5	A	505	2CV	C40-C41-C42-C43
5	A	505	2CV	O51-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
5	A	505	2CV	O51-C41-C42-O53
5	A	507	2CV	C60-C35-N33-C36
5	B	504	2CV	N33-C36-C37-C40
5	B	504	2CV	N33-C36-C37-O47
5	B	505	2CV	C41-C42-C43-O44
5	B	505	2CV	O53-C42-C43-O44
5	A	504	2CV	O34-C30-N33-C36
5	A	504	2CV	O53-C42-C43-O44
3	A	501	H98	C8-C7-O1-C10
3	A	501	H98	C6-C7-O1-C10
3	B	501	H98	C6-C7-O1-C10
3	B	501	H98	C8-C7-O1-C10
5	B	503	2CV	C24-C27-C30-O34
5	A	505	2CV	O34-C30-N33-C36
5	A	507	2CV	C60-C35-N33-C30
5	A	506	2CV	C60-C35-N33-C36
5	A	507	2CV	O34-C30-N33-C36
5	A	504	2CV	O34-C30-N33-C35
5	B	504	2CV	O34-C30-N33-C36
5	A	505	2CV	C24-C27-C30-O34
5	B	505	2CV	O51-C41-C42-O53
5	A	504	2CV	C41-C42-C43-O44
5	A	505	2CV	C24-C27-C30-N33
5	B	503	2CV	C24-C27-C30-N33
5	A	505	2CV	C40-C41-C42-O53
5	B	505	2CV	C40-C41-C42-O53
5	A	504	2CV	C27-C30-N33-C36
5	A	505	2CV	C27-C30-N33-C36
5	A	506	2CV	C15-C18-C21-C24
5	A	504	2CV	C37-C36-N33-C30
5	A	506	2CV	C12-C15-C18-C21
5	A	506	2CV	C60-C35-N33-C30
5	A	505	2CV	O34-C30-N33-C35
5	A	503	2CV	O47-C37-C40-O49
5	B	503	2CV	C60-C35-N33-C36
5	A	503	2CV	N33-C35-C60-O63
5	A	503	2CV	C27-C30-N33-C36
5	A	507	2CV	C27-C30-N33-C36
5	B	504	2CV	C27-C30-N33-C36
5	B	503	2CV	N33-C35-C60-O63
5	B	505	2CV	C40-C41-C42-C43
5	B	504	2CV	O53-C42-C43-O44

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Mol	Chain	Res	Type	Atoms
5	A	507	2CV	O34-C30-N33-C35
5	B	504	2CV	C15-C18-C21-C24
5	A	505	2CV	N33-C35-C60-O63
5	A	503	2CV	C12-C15-C18-C21
5	A	507	2CV	C15-C18-C21-C24
5	A	506	2CV	C15-C12-C9-C1
5	A	503	2CV	C15-C12-C9-C1
5	B	503	2CV	C18-C21-C24-C27
5	A	503	2CV	O47-C37-C40-C41
5	B	505	2CV	O51-C41-C42-C43
5	B	504	2CV	C40-C41-C42-O53
5	A	504	2CV	C27-C30-N33-C35
5	A	505	2CV	C27-C30-N33-C35
5	B	503	2CV	C15-C18-C21-C24
5	A	505	2CV	N33-C36-C37-C40
5	A	504	2CV	C0-C1-C9-C12
5	B	503	2CV	C15-C12-C9-C1
5	B	504	2CV	O34-C30-N33-C35
5	B	503	2CV	C12-C15-C18-C21
5	A	507	2CV	C27-C30-N33-C35
5	B	504	2CV	C27-C30-N33-C35
5	B	505	2CV	N33-C35-C60-O63
5	A	506	2CV	C9-C12-C15-C18
5	A	507	2CV	C15-C12-C9-C1
5	B	503	2CV	C60-C35-N33-C30
5	A	506	2CV	C21-C24-C27-C30
5	B	504	2CV	C0-C1-C9-C12
5	B	504	2CV	O51-C41-C42-O53
5	A	507	2CV	C12-C15-C18-C21
5	A	507	2CV	C9-C12-C15-C18

There are no ring outliers.

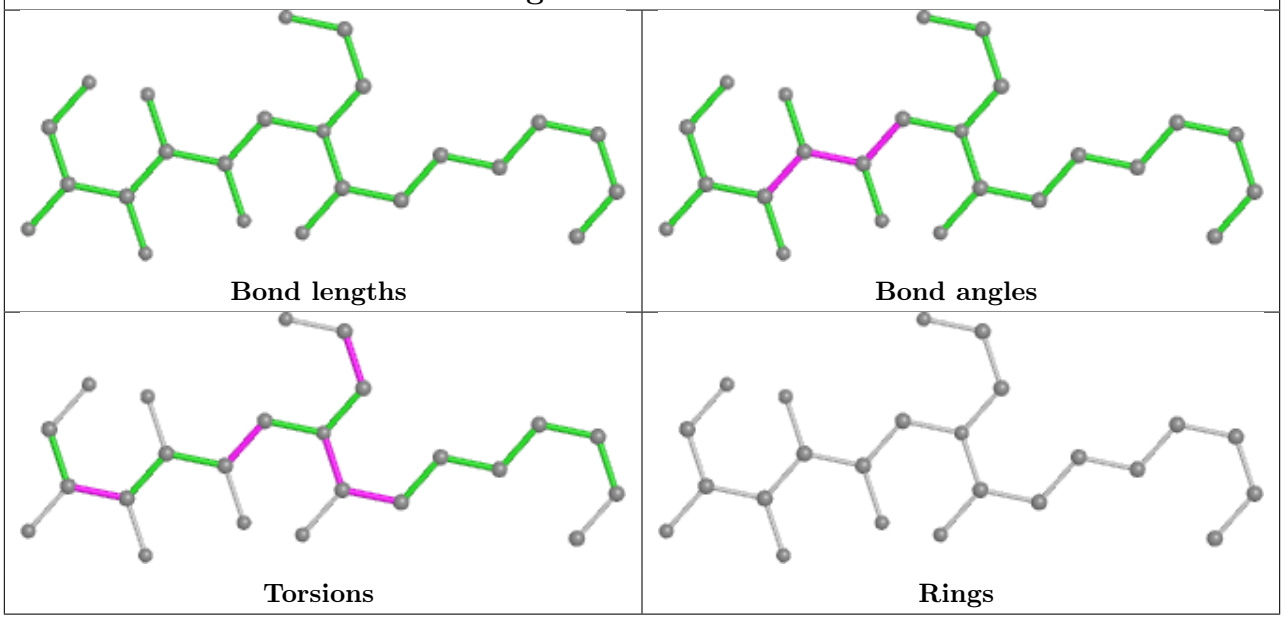
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	2CV	1	0

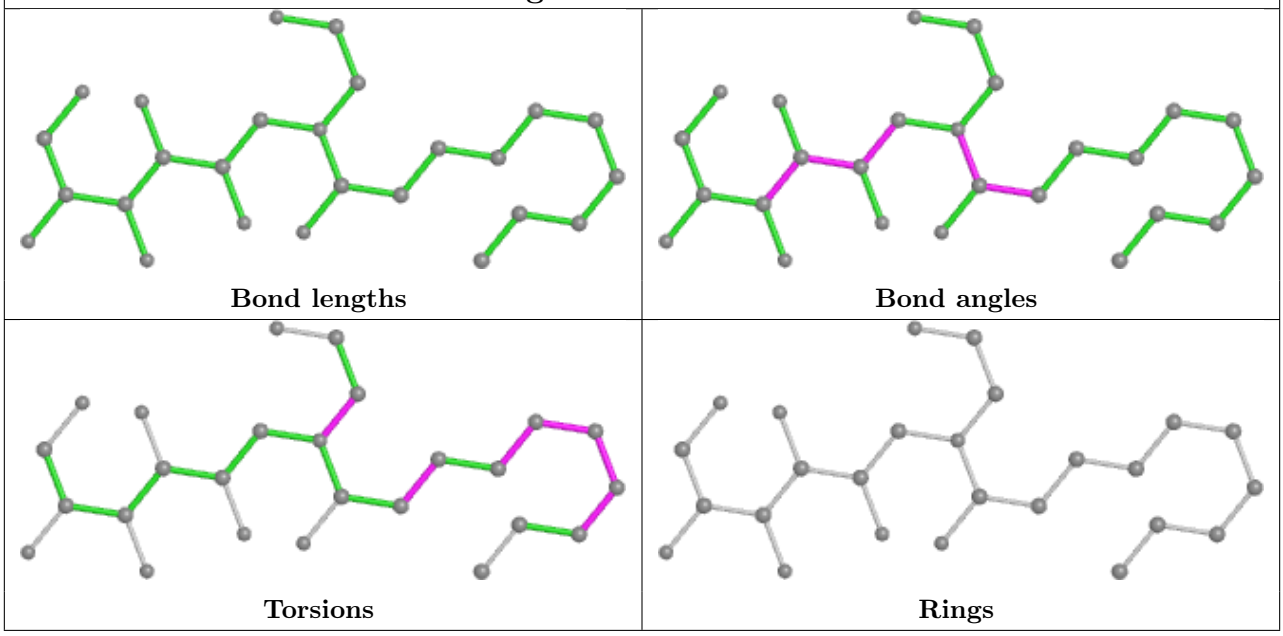
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

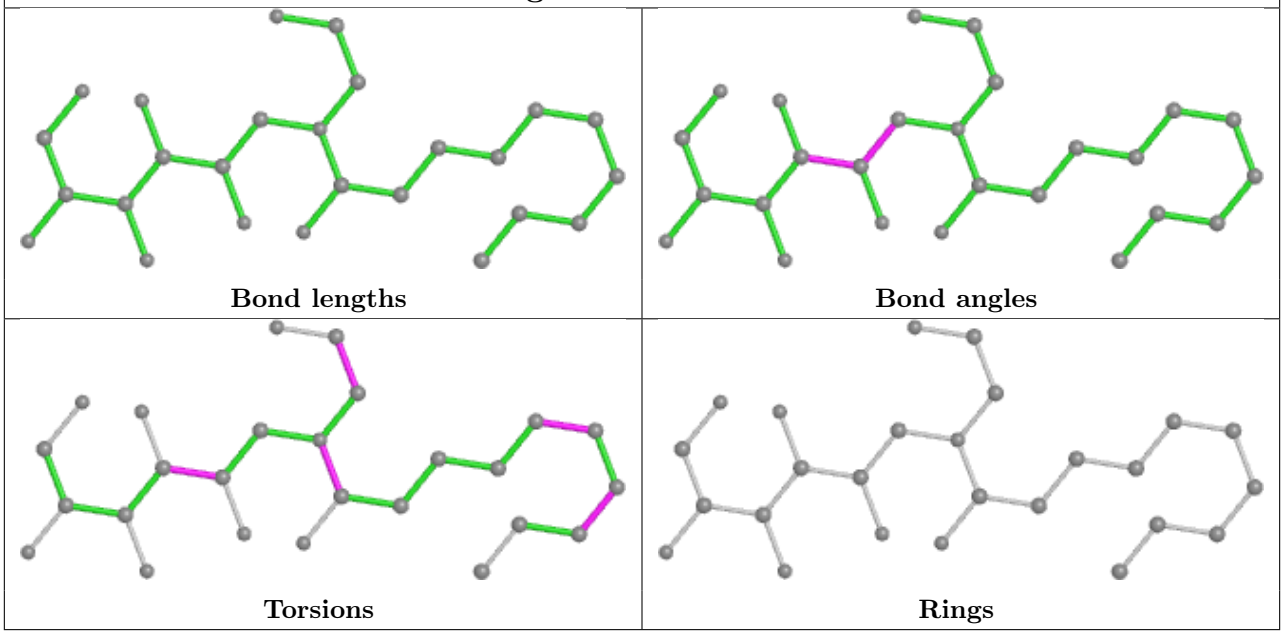
Ligand 2CV A 505



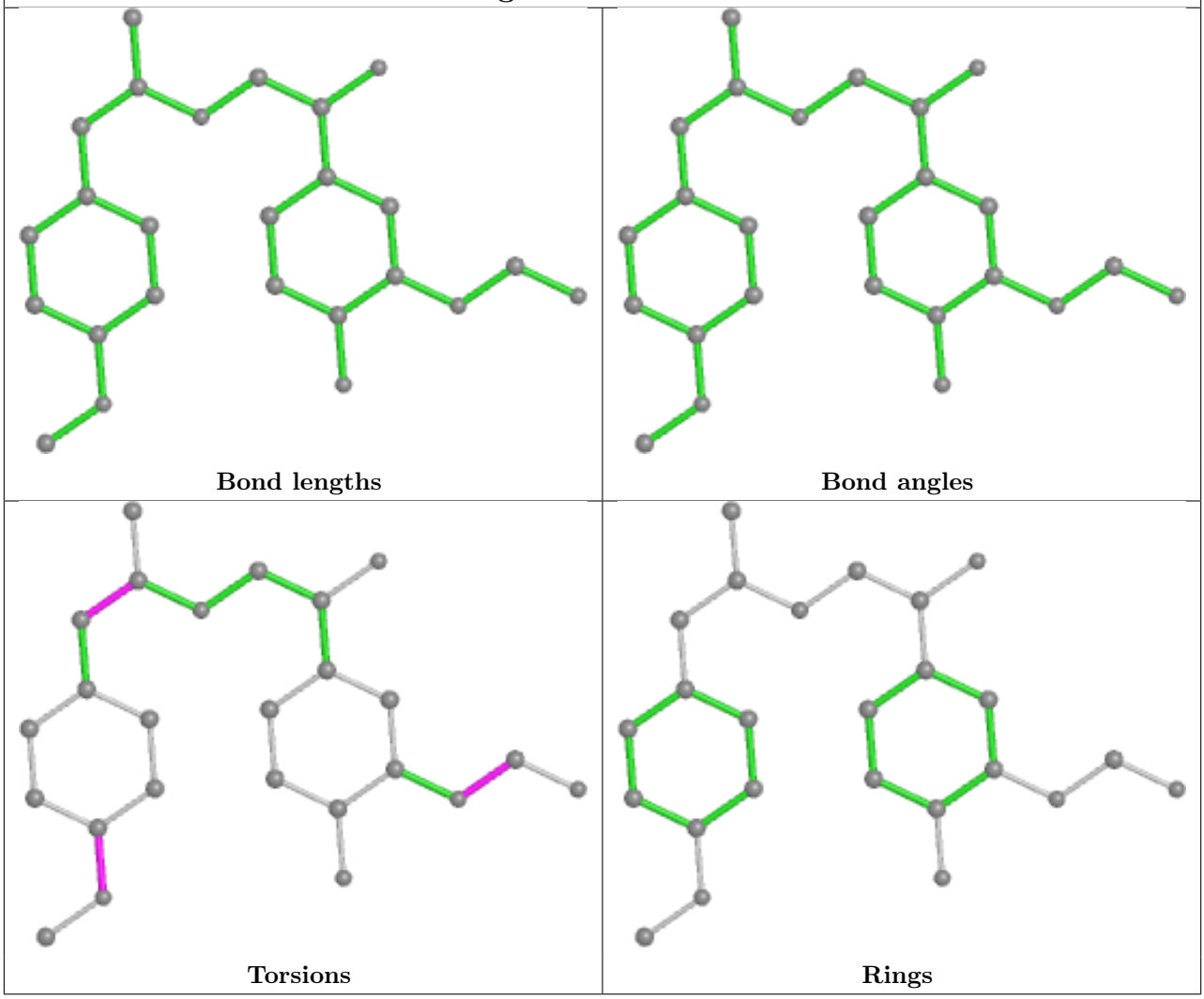
Ligand 2CV A 506



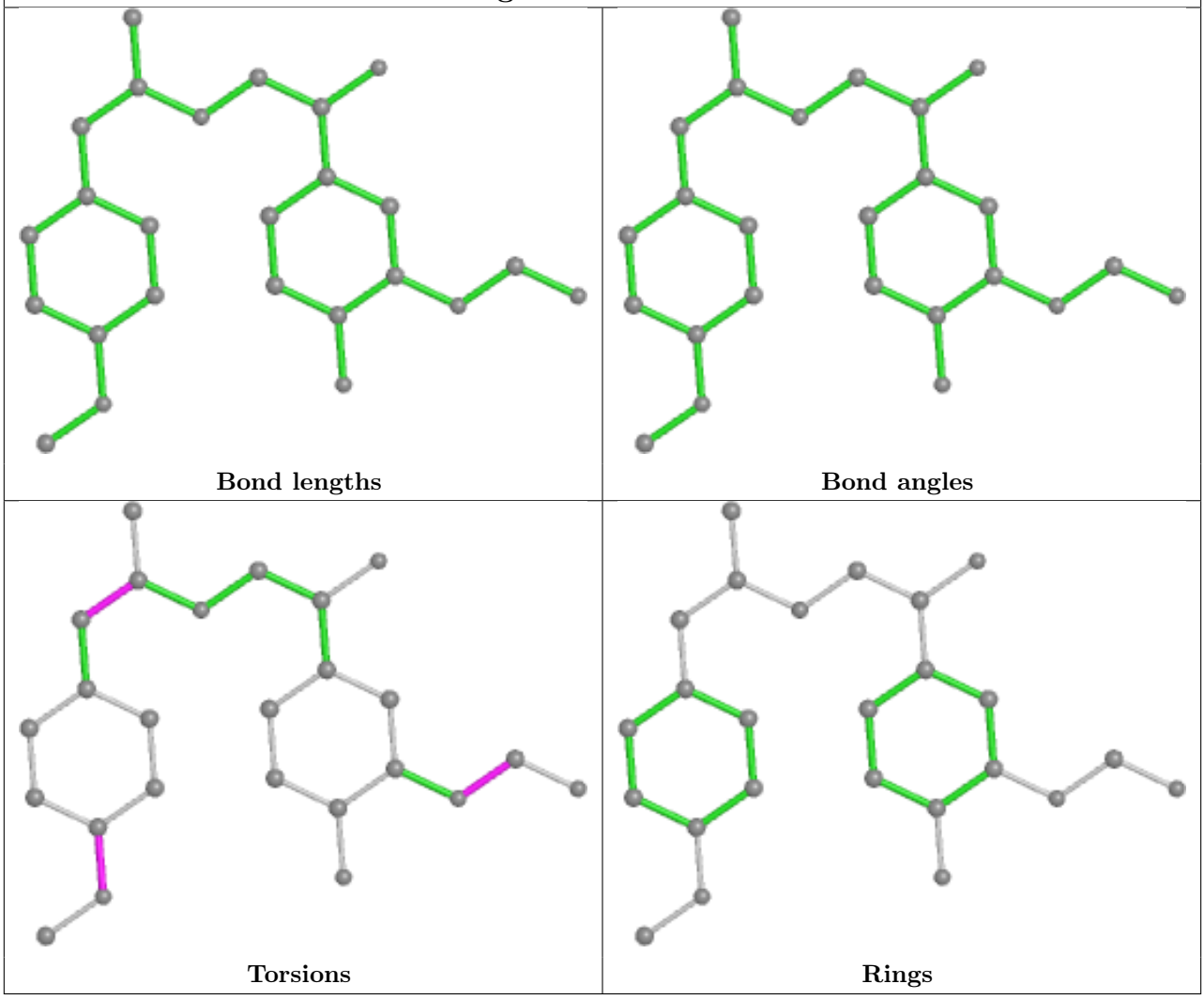
Ligand 2CV A 503



Ligand H98 B 501



Ligand H98 A 501



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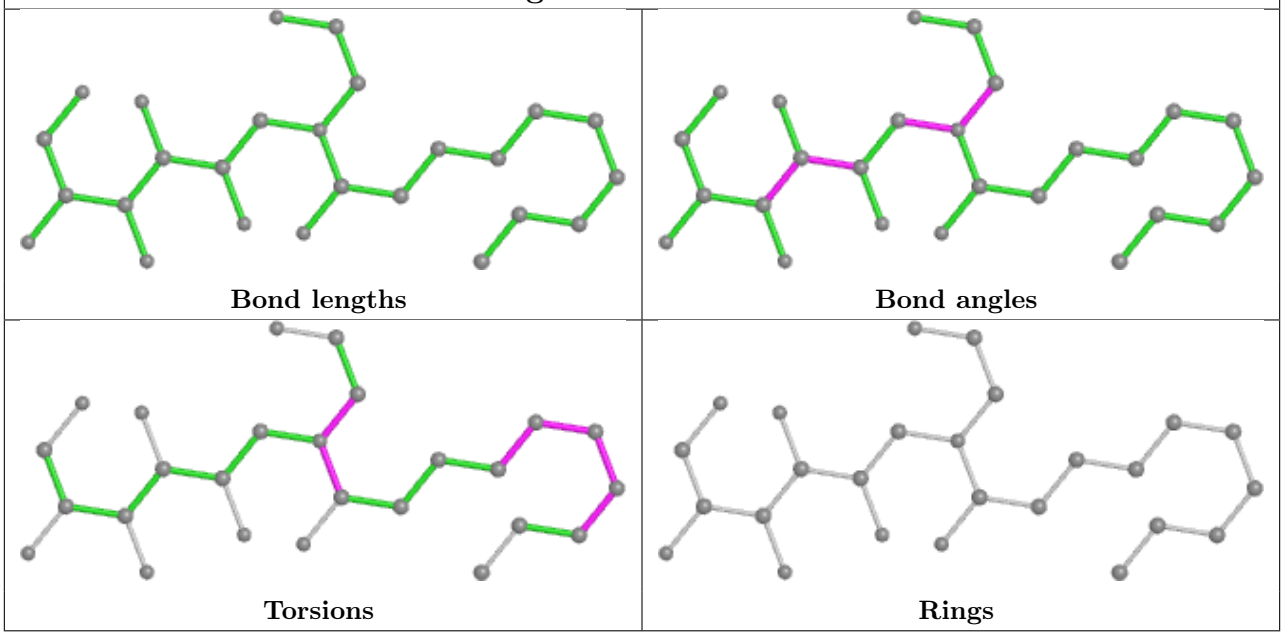

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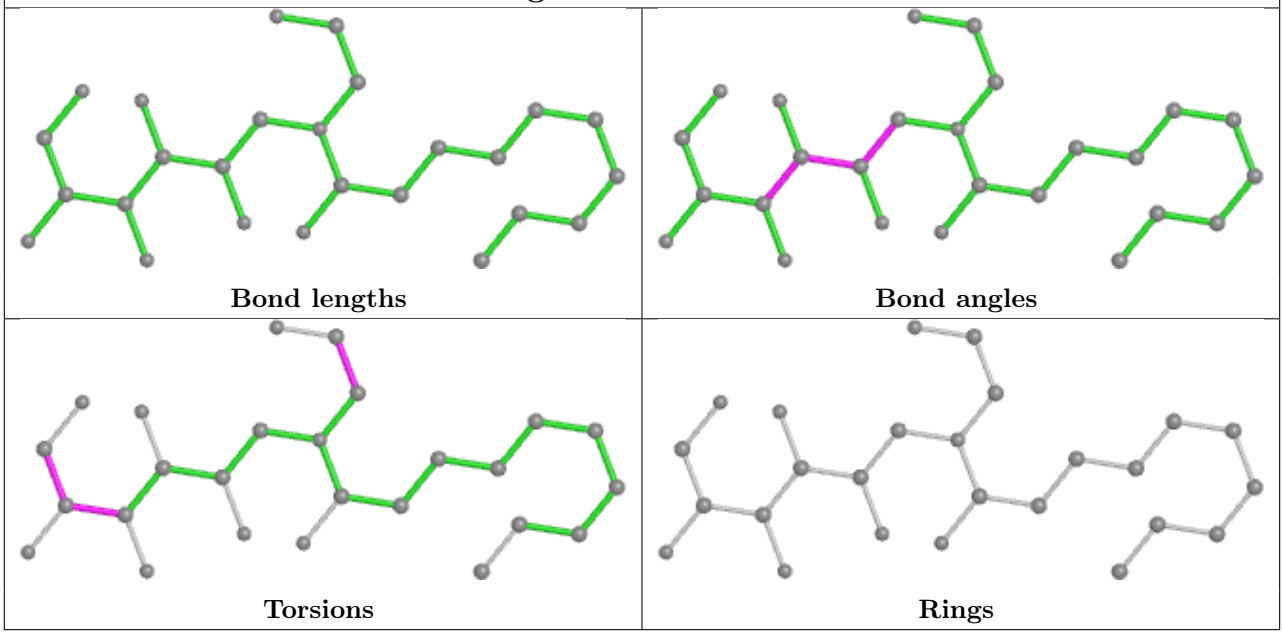

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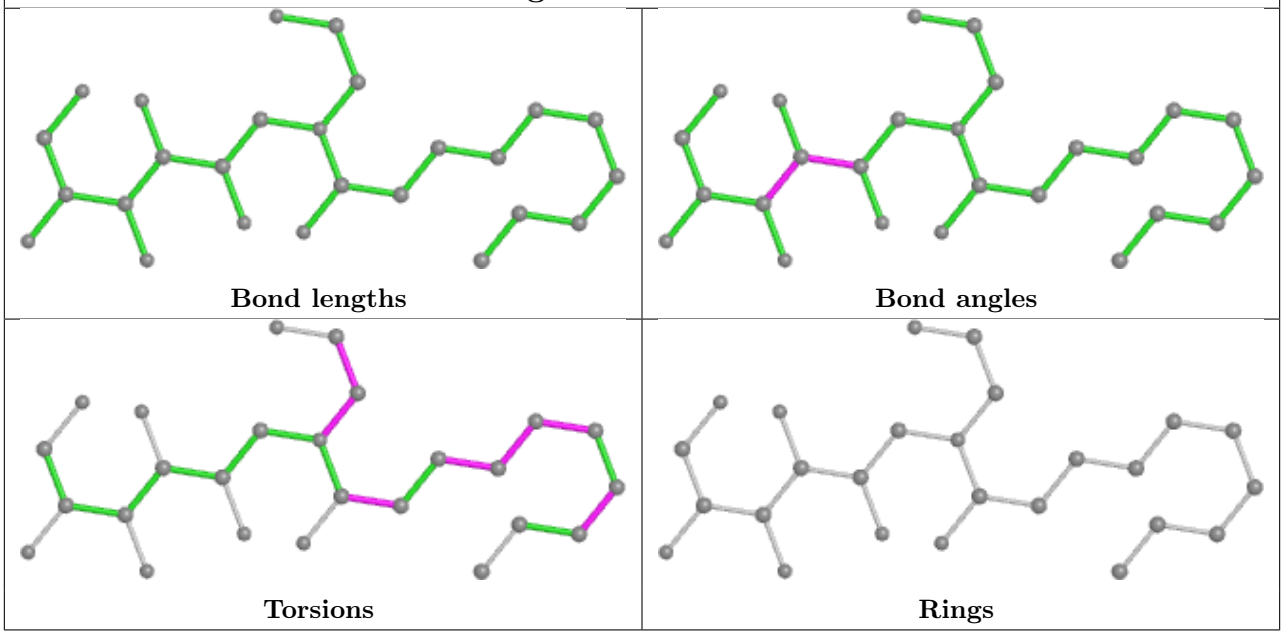

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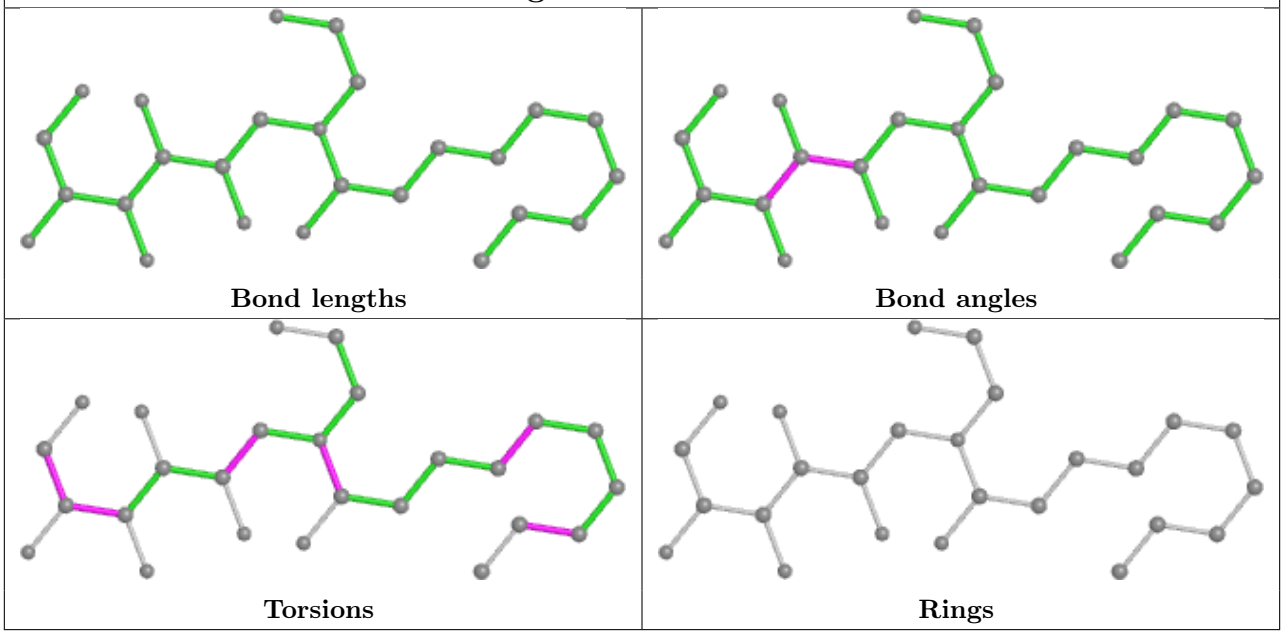
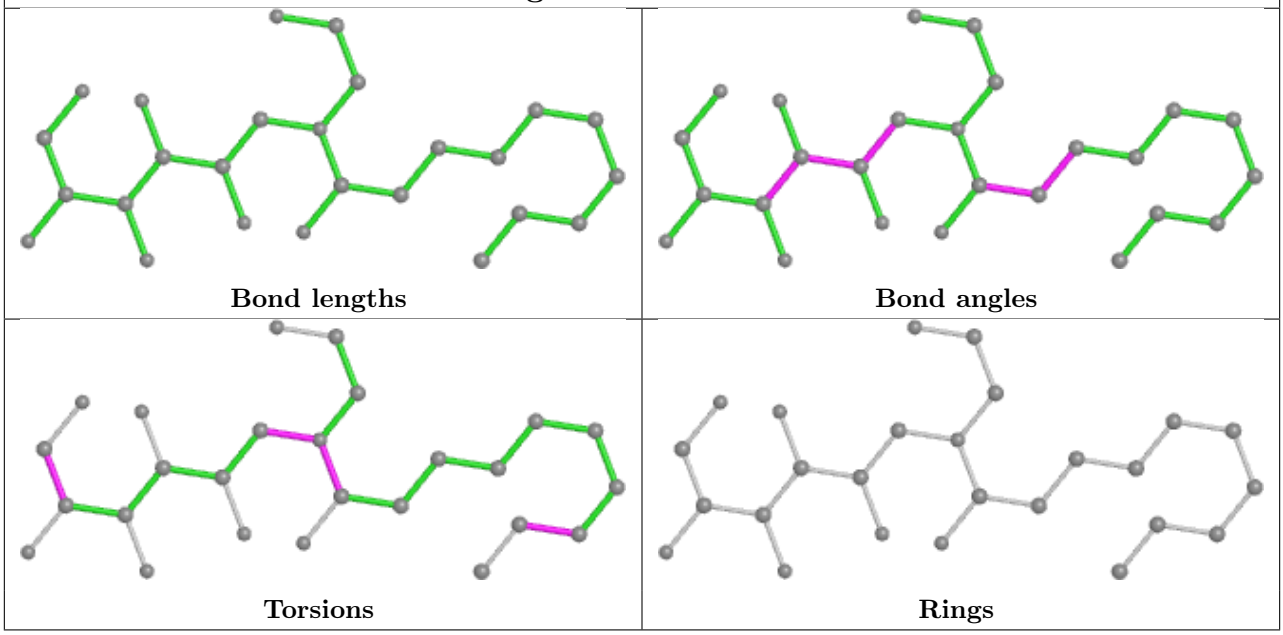


Ligand 2CV A 504



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	397/416 (95%)	0.60	57 (14%)	2	1	30, 72, 138, 182	0
1	B	391/416 (93%)	0.76	65 (16%)	1	1	35, 73, 117, 142	0
2	C	119/121 (98%)	-0.07	8 (6%)	17	16	30, 48, 82, 100	0
2	D	120/121 (99%)	0.05	7 (5%)	23	22	36, 60, 95, 112	0
All	All	1027/1074 (95%)	0.52	137 (13%)	3	2	30, 66, 122, 182	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ARG	11.2
1	B	315	PHE	7.6
1	B	272	ALA	7.0
1	A	1037	MET	7.0
1	A	1040	PRO	6.9
1	A	1088	ALA	6.7
1	A	1078	LEU	6.6
1	A	111	SER	6.6
1	B	1108	ALA	6.5
1	B	1106	ASN	6.4
1	A	1068	PRO	5.8
1	B	1016	VAL	5.5
1	A	194	GLN	5.5
1	A	1091	VAL	5.4
1	A	318	ASP	5.4
1	A	1077	THR	5.2
1	A	1076	PRO	5.2
1	B	1019	ALA	5.2
1	B	1022	ALA	5.0
1	B	1055	VAL	4.9
1	B	1015	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	1018	LYS	4.9
1	A	1067	ALA	4.8
2	D	75	ALA	4.7
1	B	1002	ASP	4.7
2	D	73	ASN	4.7
1	A	1089	THR	4.6
1	A	1073	ARG	4.6
1	B	1014	THR	4.5
1	A	1080	LEU	4.5
1	A	1050	GLN	4.5
1	B	188	GLN	4.4
1	A	1043	ASP	4.4
1	A	1036	LYS	4.4
1	B	1020	ASP	4.3
1	A	1079	LEU	4.3
1	A	1066	THR	4.2
1	A	1047	ASP	4.1
1	A	315	PHE	4.1
1	B	1046	ALA	4.1
1	A	1070	TYR	4.1
1	A	188	GLN	4.0
1	A	1033	GLY	3.9
1	B	1052	LYS	3.9
1	B	43	VAL	3.9
1	B	1080	LEU	3.9
2	D	13	GLN	3.9
1	B	1105	ALA	3.8
1	B	273	SER	3.8
1	B	239	ARG	3.8
1	B	1053	LEU	3.8
1	B	1054	THR	3.8
1	A	1031	TRP	3.8
1	A	1051	GLY	3.8
1	B	1070	TYR	3.7
1	B	241	ILE	3.7
1	A	1097	GLY	3.7
2	C	88	GLU	3.7
1	A	187	PRO	3.7
1	B	242	ASP	3.6
1	B	84	ALA	3.6
1	A	50	LEU	3.5
1	A	1090	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	3.5
1	B	205	ARG	3.4
2	C	120	SER	3.3
1	A	1038	ILE	3.3
1	B	90	VAL	3.3
1	A	1048	GLU	3.3
1	B	1042	LEU	3.3
1	A	319	LEU	3.3
1	A	112	PHE	3.2
1	B	1023	ILE	3.2
1	B	1087	ALA	3.1
1	B	1107	LEU	3.1
2	D	120	SER	3.1
1	B	1083	ASN	3.0
1	A	1044	GLU	3.0
1	A	1041	ILE	3.0
1	A	317	ARG	3.0
2	C	11	LEU	3.0
1	B	88	LEU	3.0
1	B	1051	GLY	3.0
2	C	41	PRO	2.9
1	A	46	LEU	2.9
1	B	1082	LYS	2.9
2	C	73	ASN	2.8
1	B	317	ARG	2.8
1	A	1061	ASP	2.8
1	B	1081	PHE	2.7
2	D	74	ALA	2.7
2	D	14	ALA	2.7
1	B	1043	ASP	2.7
1	A	47	LEU	2.7
2	C	87	PRO	2.7
1	A	1065	GLY	2.6
1	A	316	ASN	2.6
1	A	1052	LYS	2.6
1	B	319	LEU	2.6
1	A	148	ARG	2.6
1	B	1003	LYS	2.6
1	A	1039	ALA	2.6
1	B	85	CYS	2.6
1	A	195	ASP	2.5
1	A	1060	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	157	ARG	2.5
1	B	120	LEU	2.5
1	A	1108	ALA	2.5
1	B	1088	ALA	2.5
1	B	89	VAL	2.4
2	C	119	SER	2.4
1	A	110	GLY	2.4
1	B	1040	PRO	2.4
1	B	1085	GLU	2.4
1	A	1081	PHE	2.3
1	B	240	LYS	2.3
1	B	316	ASN	2.3
1	B	1073	ARG	2.3
1	B	1024	LEU	2.3
1	B	86	ALA	2.3
1	A	1105	ALA	2.2
1	B	318	ASP	2.2
1	B	91	GLY	2.2
1	B	1089	THR	2.2
1	A	1086	VAL	2.1
1	B	87	ASP	2.1
2	C	118	VAL	2.1
1	B	1010	ASP	2.1
1	B	124	CYS	2.1
1	A	1026	ASP	2.1
1	B	55	ILE	2.1
2	D	114	THR	2.1
1	B	81	THR	2.1
1	A	358	ALA	2.0
1	B	123	LEU	2.0
1	A	1064	PRO	2.0
1	B	313	ASN	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)

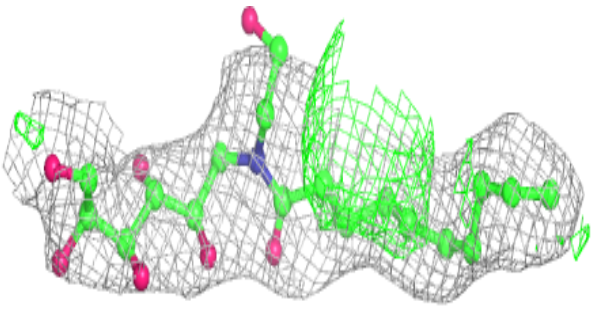
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

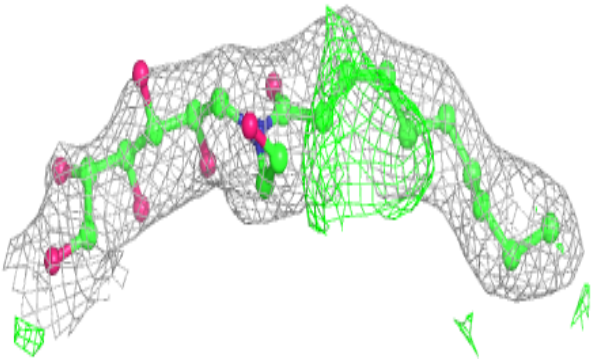
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	2CV	B	504	26/26	0.75	0.38	55,74,89,118	0
5	2CV	A	504	26/26	0.78	0.33	52,104,124,132	0
5	2CV	B	505	26/26	0.80	0.25	72,89,107,131	0
5	2CV	A	507	26/26	0.84	0.40	50,63,66,71	0
5	2CV	A	506	26/26	0.85	0.28	45,59,81,86	0
5	2CV	B	503	26/26	0.87	0.25	72,80,103,120	0
4	NA	A	502	1/1	0.88	0.09	79,79,79,79	0
5	2CV	A	505	24/26	0.91	0.52	64,91,97,99	0
5	2CV	A	503	26/26	0.91	0.32	48,68,78,80	0
3	H98	B	501	25/25	0.92	0.22	54,60,70,76	0
4	NA	B	502	1/1	0.92	0.09	68,68,68,68	0
3	H98	A	501	25/25	0.95	0.18	45,54,64,65	0

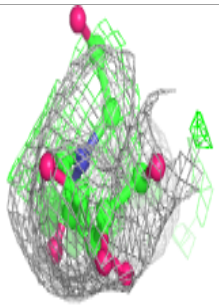
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CV B 504:

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

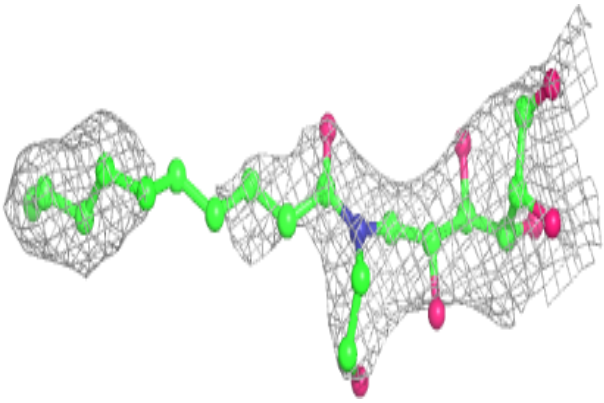


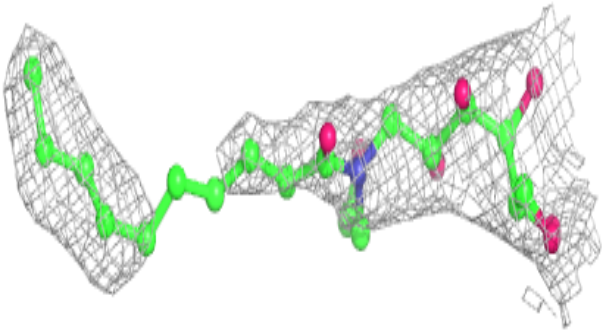


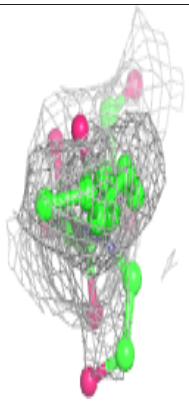


Electron density around 2CV A 504:

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

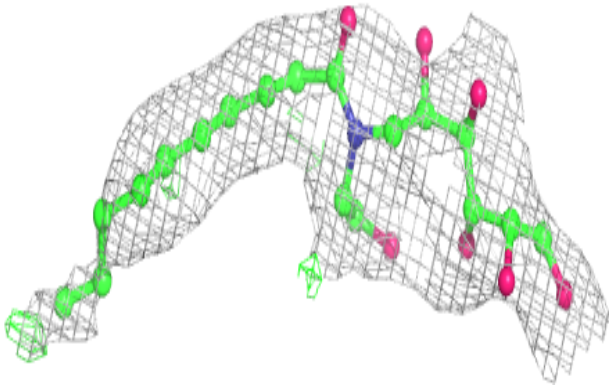


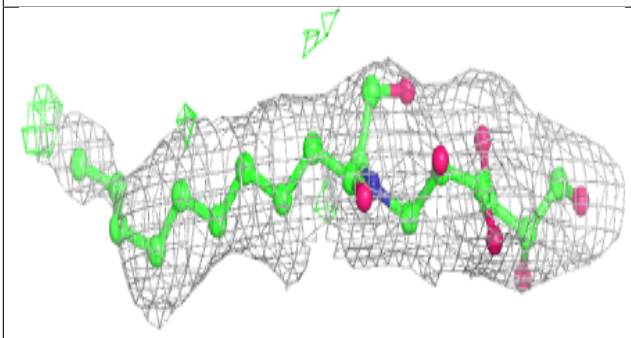


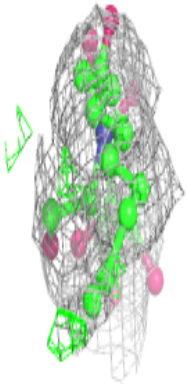


Electron density around 2CV B 505:

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

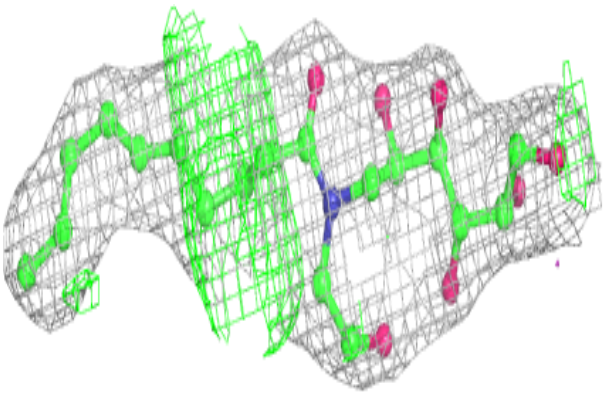


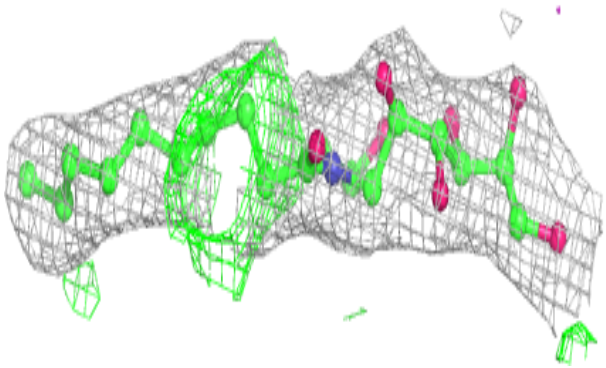


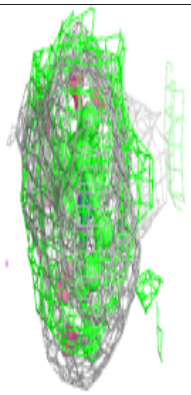


Electron density around 2CV A 507:

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

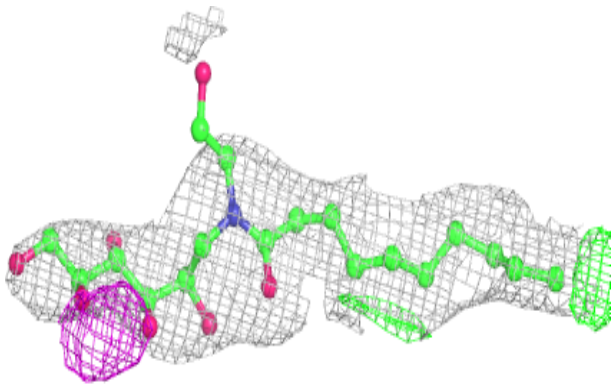


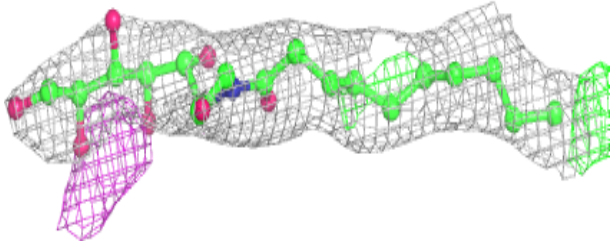


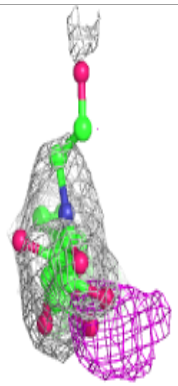


Electron density around 2CV A 506:

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

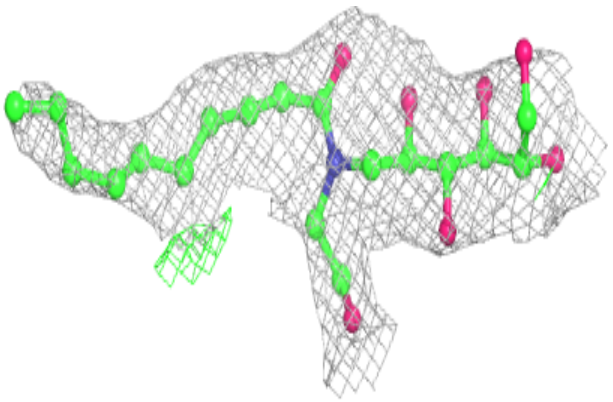


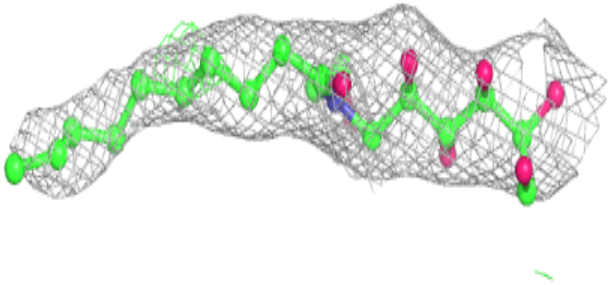




Electron density around 2CV B 503:

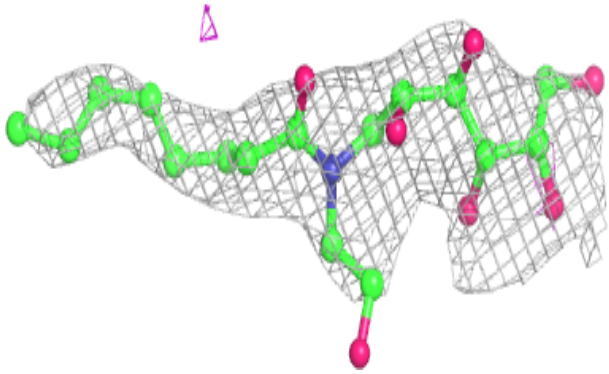
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

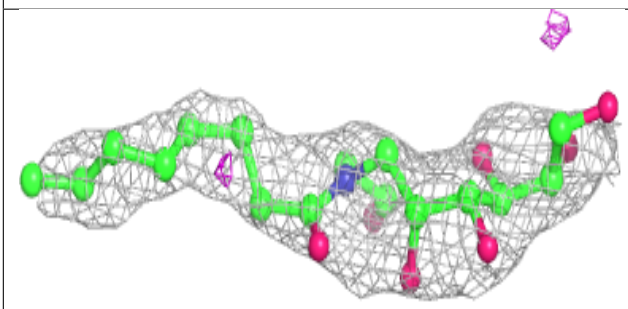


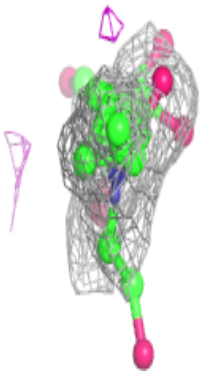


Electron density around 2CV A 505:

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

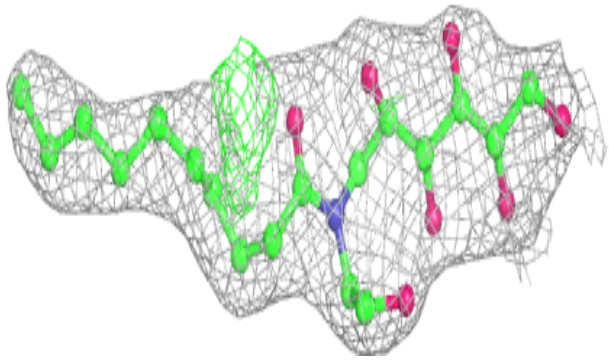


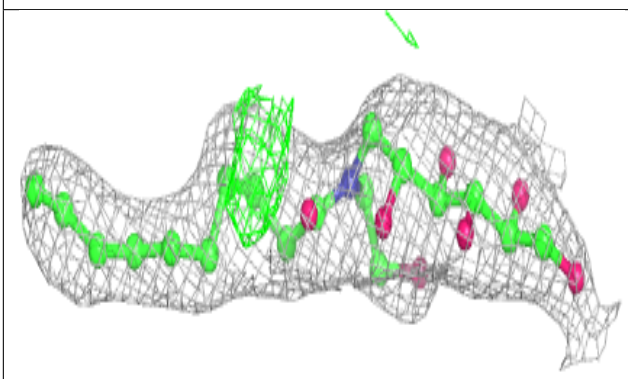


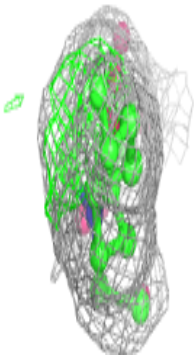


Electron density around 2CV A 503:

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

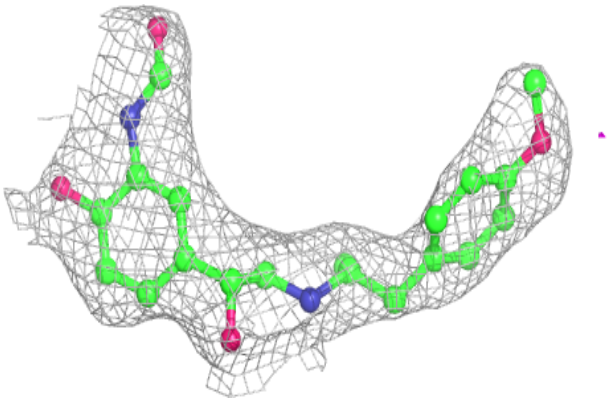


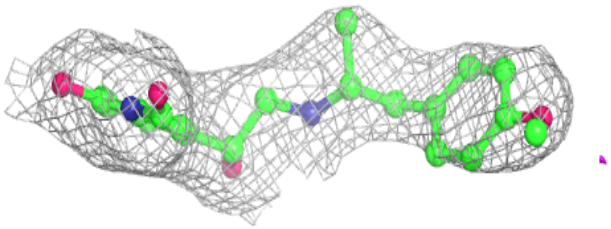


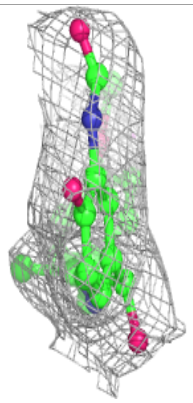


Electron density around H98 B 501:

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

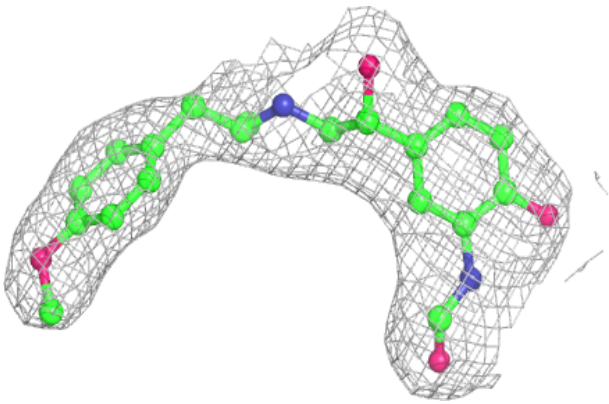


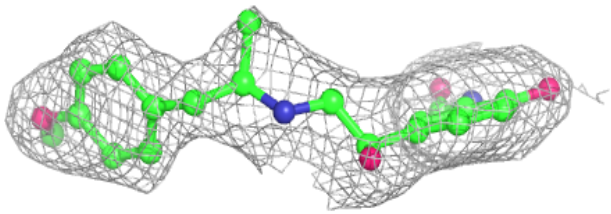


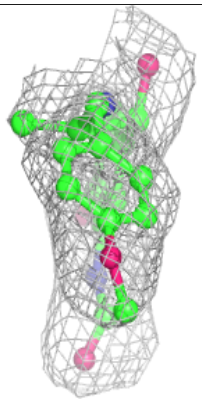


Electron density around H98 A 501:

$2mF_o$-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.