wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 01:16 AM EDT

PDB ID	:	2Q7M
Title	:	Crystal structure of human FLAP with MK-591
Authors	:	Ferguson, A.D.
Deposited on	:	2007-06-07
Resolution	:	4.25 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 (i)) were used in the production of this report:

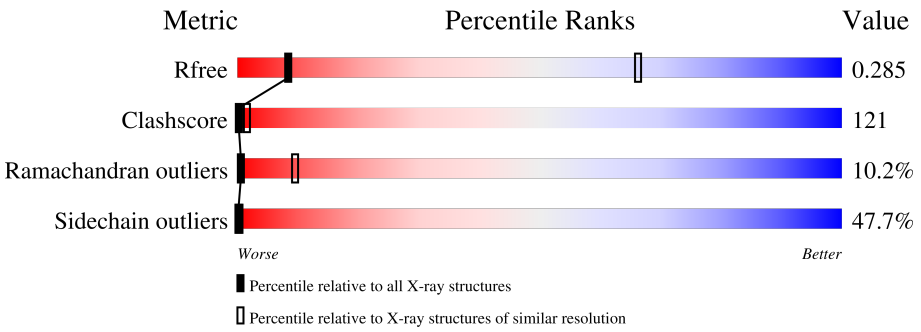
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 4.25 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	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)

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%

Mol	Chain	Length	Quality of chain
1	A	161	10% 40% 35% • 14%
1	B	161	7% 45% 36% • 8%
1	C	161	10% 41% 39% • 7%
1	D	161	7% 48% 34% • 9%
1	E	161	7% 45% 31% • 13%
1	F	161	11% 43% 33% 5% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2CS	A	502	-	-	X	-
2	2CS	A	503	-	X	X	-
2	2CS	C	501	-	-	X	-
2	2CS	D	504	-	-	X	-
2	2CS	E	505	-	-	X	-
2	2CS	E	506	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7233 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.

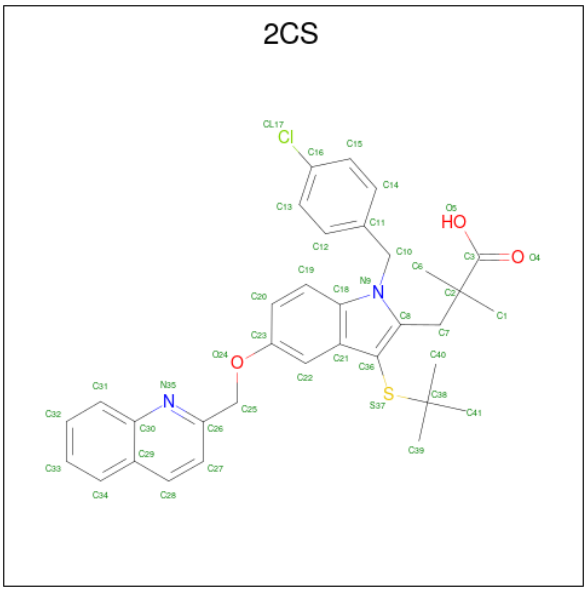
- Molecule 1 is a protein called Arachidonate 5-lipoxygenase-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	139	1115	737	182	191	5	0	0	0
1	B	148	1186	782	192	207	5	0	0	0
1	C	149	1193	786	193	209	5	0	0	0
1	D	147	1181	779	191	206	5	0	0	0
1	E	140	1119	739	183	192	5	0	0	0
1	F	149	1193	786	193	209	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	ALA	LYS	engineered mutation	UNP P20292
B	148	ALA	LYS	engineered mutation	UNP P20292
C	148	ALA	LYS	engineered mutation	UNP P20292
D	148	ALA	LYS	engineered mutation	UNP P20292
E	148	ALA	LYS	engineered mutation	UNP P20292
F	148	ALA	LYS	engineered mutation	UNP P20292

- Molecule 2 is 3-[3-(TERT-BUTYLTHIO)-1-(4-CHLOROBENZYL)-5-(QUINOLIN-2-YL METHOXY)-1H-INDOL-2-YL]-2,2-DIMETHYLPROPANOIC ACID (three-letter code: 2CS) (formula: $C_{34}H_{35}ClN_2O_3S$).



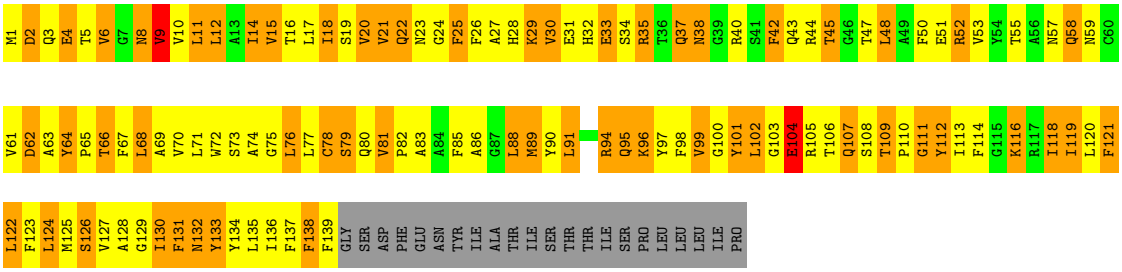
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			41	34	1	2	3	1		
2	A	1	Total	C	Cl	N	O	S	0	0
			41	34	1	2	3	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			41	34	1	2	3	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			41	34	1	2	3	1		
2	E	1	Total	C	Cl	N	O	S	0	0
			41	34	1	2	3	1		
2	E	1	Total	C	Cl	N	O	S	0	0
			41	34	1	2	3	1		

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. 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. 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.

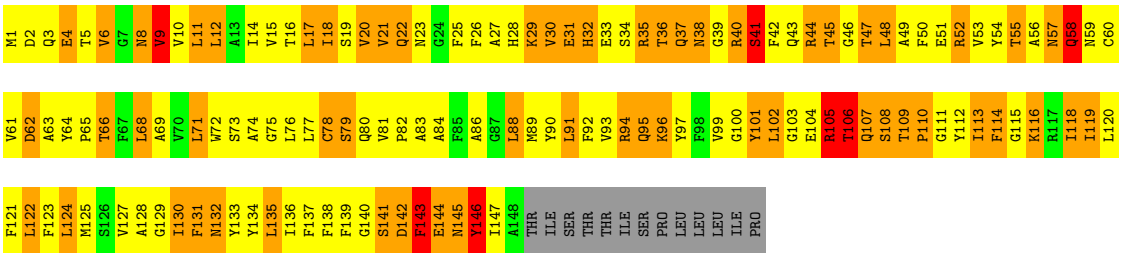
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein

Chain A: 10% 40% 35% • 14%



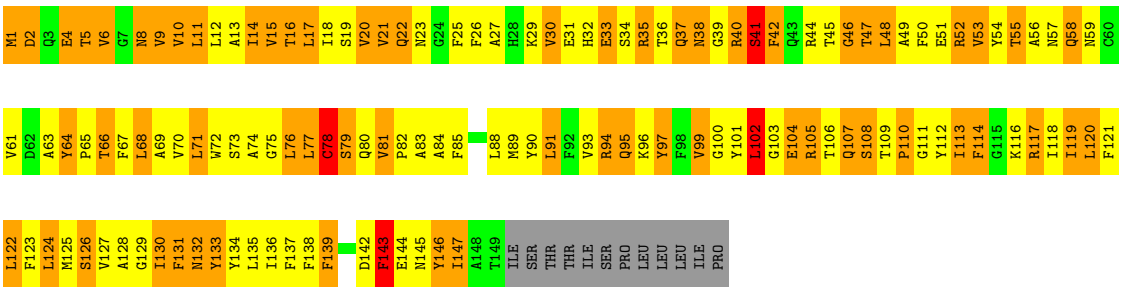
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein

Chain B: 7% 45% 36% • 8%



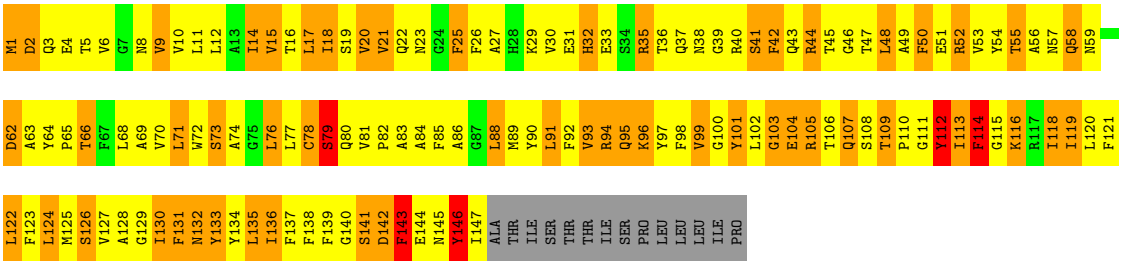
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein

Chain C: 10% 41% 39% • 7%



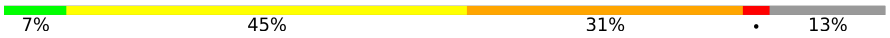
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein

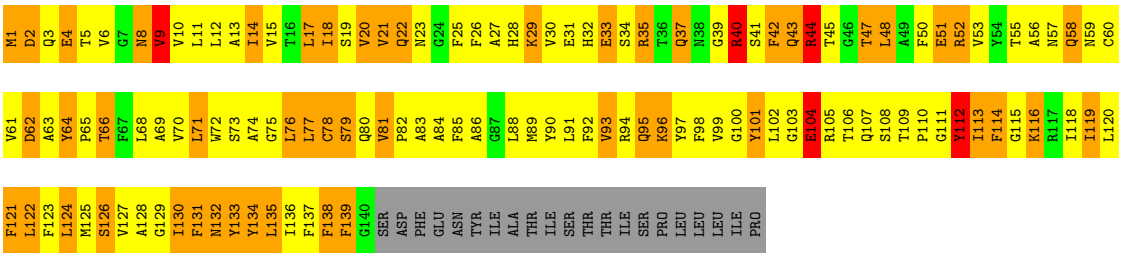
Chain D: 7% 48% 34% • 9%



- Molecule 1: Arachidonate 5-lipoxygenase-activating protein

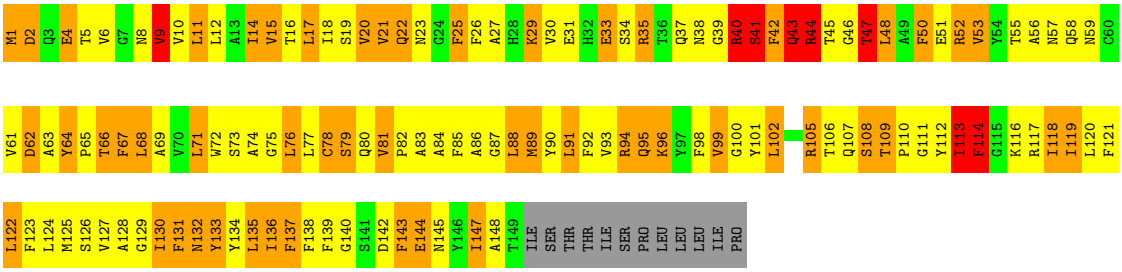
Chain E:





- Molecule 1: Arachidonate 5-lipoxygenase-activating protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	180.60Å 180.60Å 140.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.25 38.81 – 4.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-4.25) 99.3 (38.81-4.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.99 (at 4.28Å)	Xtriage
Refinement program	BUSTER-TNT 1.9.3	Depositor
R, R_{free}	0.242 , 0.283 0.257 , 0.285	Depositor DCC
R_{free} test set	849 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	193.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 194.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å^2)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.08% 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: 2CS

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	0.40	0/1144	0.61	1/1551 (0.1%)
1	B	0.41	0/1217	0.61	0/1650
1	C	0.44	0/1224	0.63	0/1660
1	D	0.43	0/1212	0.61	0/1643
1	E	0.40	0/1148	0.60	0/1556
1	F	0.43	0/1224	0.61	0/1660
All	All	0.42	0/7169	0.61	1/9720 (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	109	THR	C-N-CD	-7.20	104.76	120.60

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	1115	0	1113	292	0
1	B	1186	0	1171	334	0
1	C	1193	0	1178	292	0
1	D	1181	0	1166	328	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1119	0	1116	317	0
1	F	1193	0	1178	308	0
2	A	82	0	68	58	0
2	C	41	0	34	21	0
2	D	41	0	34	29	0
2	E	82	0	68	66	0
All	All	7233	0	7126	1731	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 121.

The worst 5 of 1731 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:E:120:LEU:HD23	2:E:506:2CS:H412	1.23	1.14
1:F:81:VAL:HG13	1:F:82:PRO:HD3	1.30	1.13
1:E:81:VAL:HG13	1:E:82:PRO:HD3	1.28	1.13
1:D:53:VAL:HG23	1:D:102:LEU:HD21	1.23	1.12
2:E:505:2CS:H61	2:E:505:2CS:H102	1.30	1.12

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	137/161 (85%)	108 (79%)	19 (14%)	10 (7%)	1 16
1	B	146/161 (91%)	104 (71%)	23 (16%)	19 (13%)	0 5
1	C	147/161 (91%)	112 (76%)	17 (12%)	18 (12%)	0 5
1	D	145/161 (90%)	104 (72%)	27 (19%)	14 (10%)	0 11
1	E	138/161 (86%)	103 (75%)	23 (17%)	12 (9%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	147/161 (91%)	108 (74%)	24 (16%)	15 (10%)	0 9
All	All	860/966 (89%)	639 (74%)	133 (16%)	88 (10%)	0 9

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	79	SER
1	A	111	GLY
1	B	36	THR
1	B	41	SER

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	117/137 (85%)	59 (50%)	58 (50%)	0 0
1	B	124/137 (90%)	68 (55%)	56 (45%)	0 0
1	C	125/137 (91%)	63 (50%)	62 (50%)	0 0
1	D	124/137 (90%)	68 (55%)	56 (45%)	0 0
1	E	117/137 (85%)	60 (51%)	57 (49%)	0 0
1	F	125/137 (91%)	65 (52%)	60 (48%)	0 0
All	All	732/822 (89%)	383 (52%)	349 (48%)	0 0

5 of 349 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	146	TYR
1	E	137	PHE
1	E	14	ILE
1	E	66	THR
1	F	22	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	80	GLN
1	D	38	ASN
1	F	57	ASN
1	D	28	HIS
1	D	58	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)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	2CS	D	504	-	40,45,45	2.03	17 (42%)	55,67,67	2.44	23 (41%)
2	2CS	A	502	-	40,45,45	2.04	14 (35%)	55,67,67	2.14	24 (43%)
2	2CS	A	503	-	40,45,45	2.19	18 (45%)	55,67,67	2.53	27 (49%)
2	2CS	C	501	-	40,45,45	2.09	10 (25%)	55,67,67	2.62	24 (43%)
2	2CS	E	505	-	40,45,45	2.43	18 (45%)	55,67,67	2.53	26 (47%)
2	2CS	E	506	-	40,45,45	2.18	21 (52%)	55,67,67	2.12	20 (36%)

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
2	2CS	D	504	-	-	12/17/25/25	0/5/5/5
2	2CS	A	502	-	-	9/17/25/25	0/5/5/5
2	2CS	A	503	-	-	12/17/25/25	0/5/5/5
2	2CS	C	501	-	-	11/17/25/25	0/5/5/5
2	2CS	E	505	-	-	11/17/25/25	0/5/5/5
2	2CS	E	506	-	-	9/17/25/25	0/5/5/5

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	505	2CS	O24-C23	-5.94	1.23	1.37
2	A	502	2CS	O24-C23	-5.59	1.24	1.37
2	C	501	2CS	C10-N9	-5.40	1.38	1.48
2	E	506	2CS	C22-C23	5.01	1.46	1.37
2	A	503	2CS	O24-C23	-4.82	1.26	1.37

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	503	2CS	C8-C36-S37	-8.35	117.42	126.77
2	C	501	2CS	C11-C10-N9	-7.23	101.39	112.63
2	E	505	2CS	C31-C30-C29	7.11	126.52	119.04
2	E	505	2CS	C11-C10-N9	-6.64	102.31	112.63
2	D	504	2CS	C7-C8-C36	-6.41	119.40	130.34

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	2CS	C11-C10-N9-C8
2	A	503	2CS	C1-C2-C7-C8
2	A	503	2CS	C3-C2-C7-C8
2	A	503	2CS	C6-C2-C7-C8
2	A	503	2CS	C2-C7-C8-N9

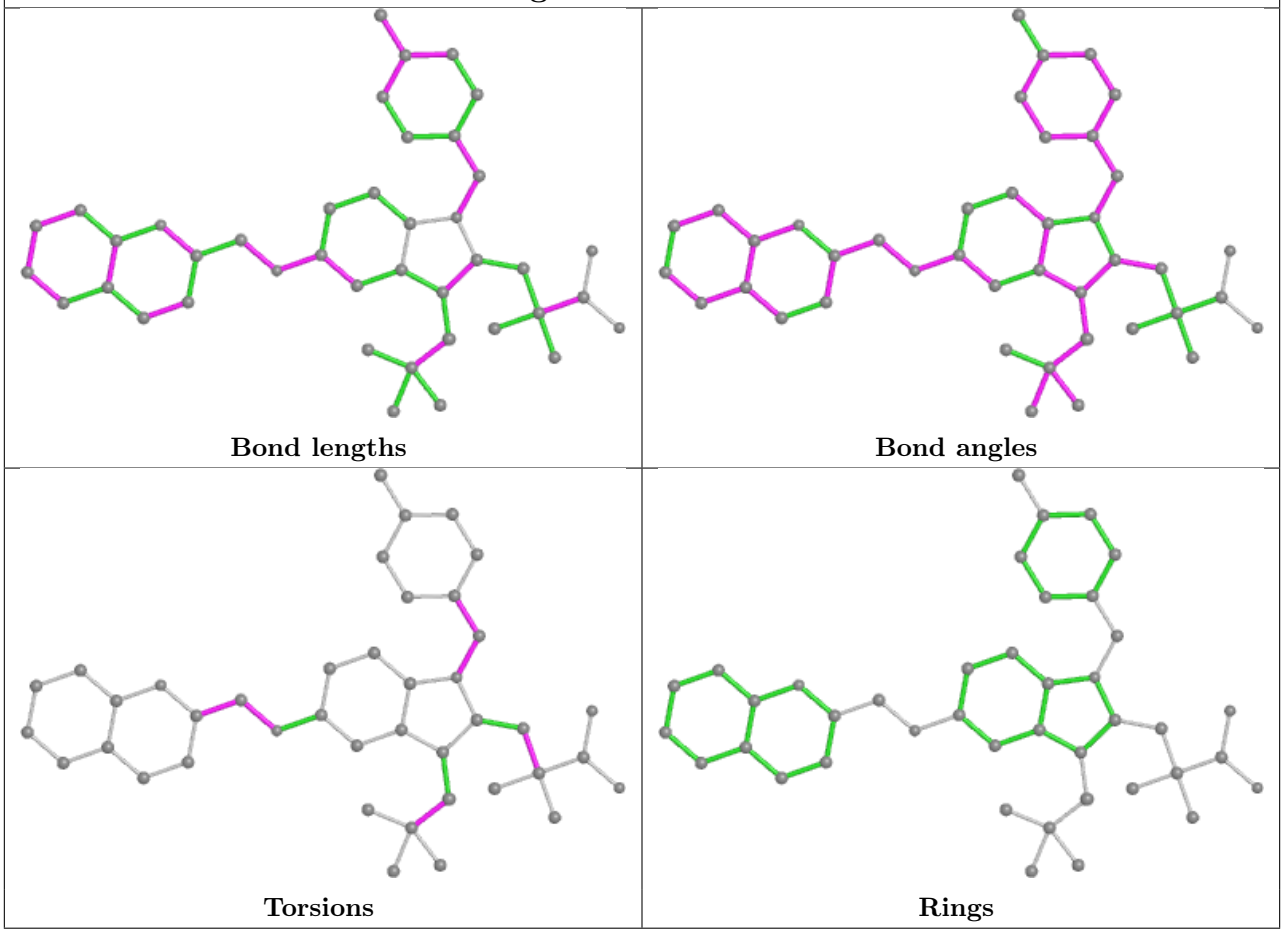
There are no ring outliers.

6 monomers are involved in 174 short contacts:

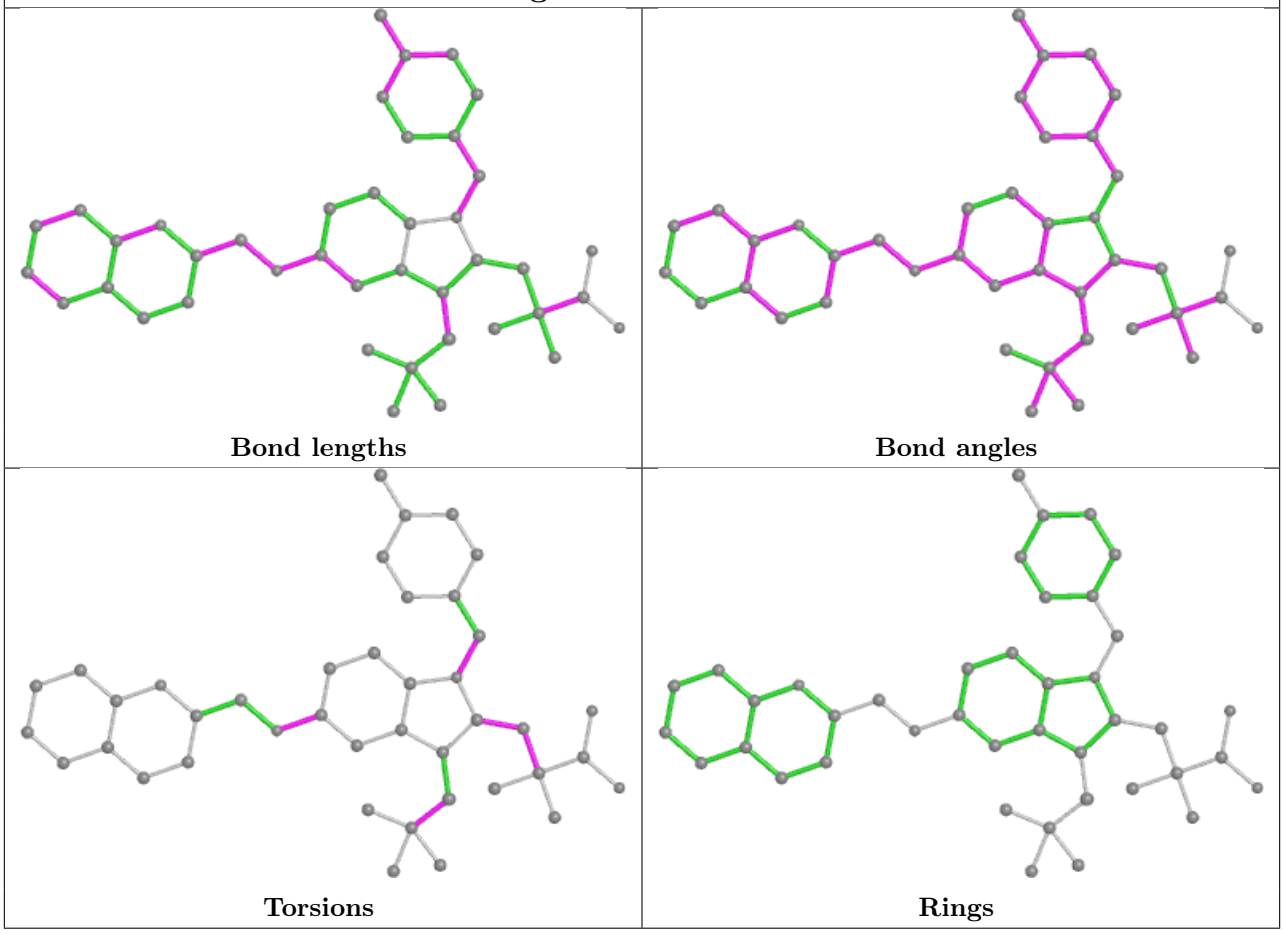
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	504	2CS	29	0
2	A	502	2CS	24	0
2	A	503	2CS	34	0
2	C	501	2CS	21	0
2	E	505	2CS	38	0
2	E	506	2CS	28	0

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.

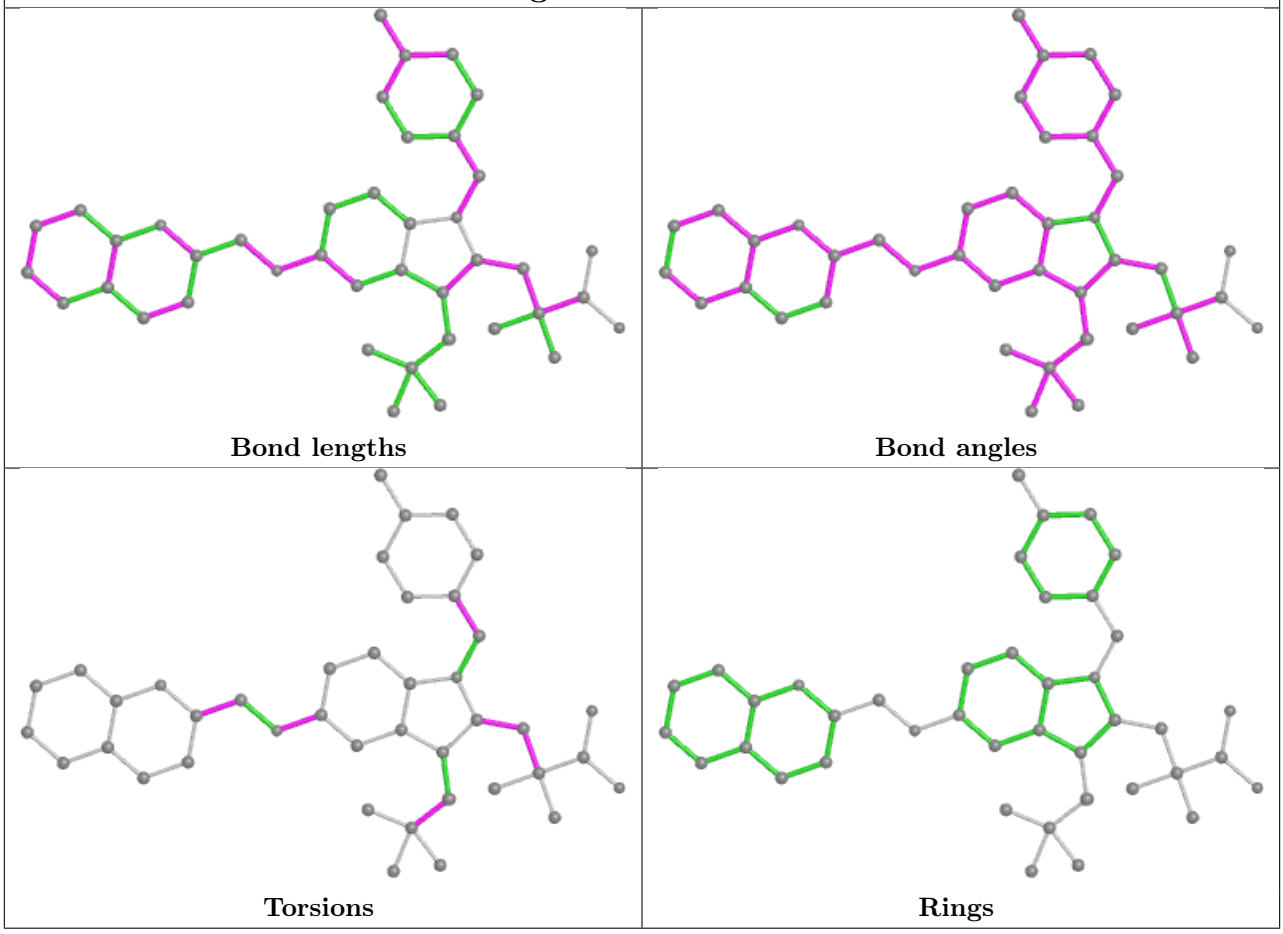
Ligand 2CS D 504



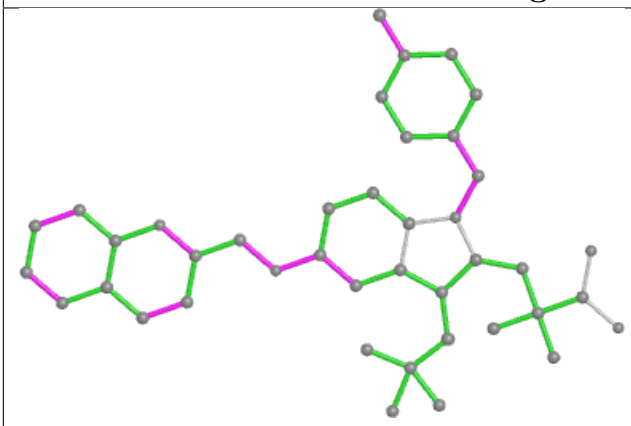
Ligand 2CS A 502



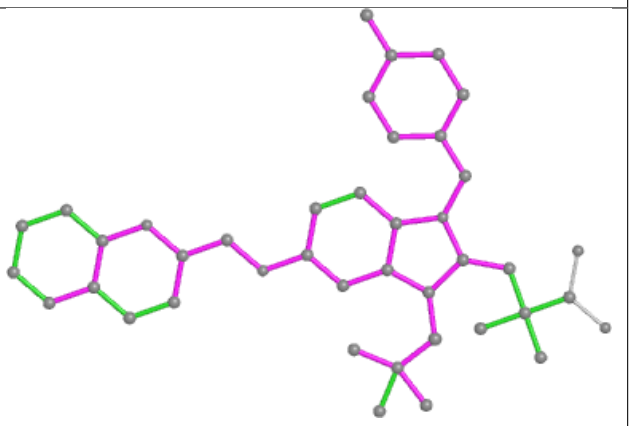
Ligand 2CS A 503



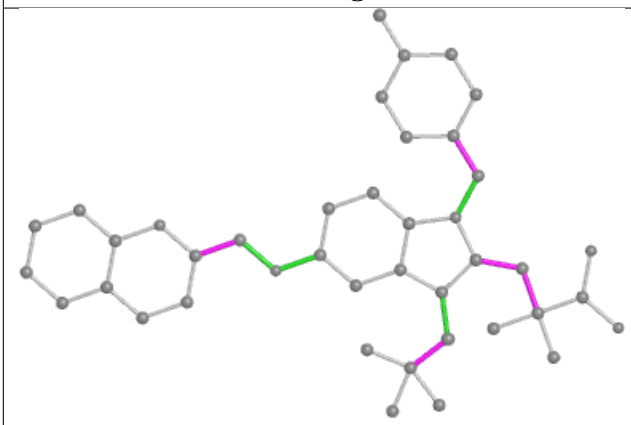
Ligand 2CS C 501



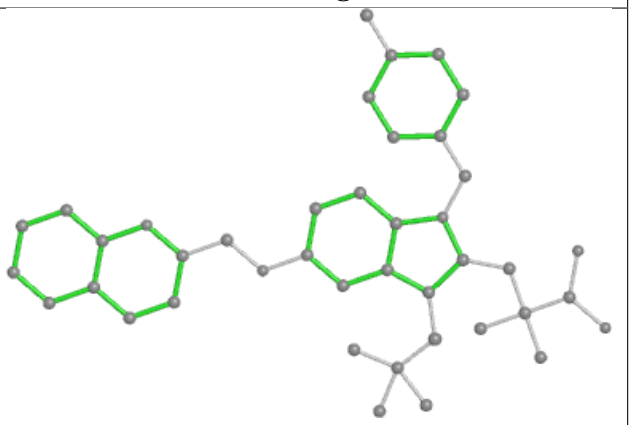
Bond lengths



Bond angles

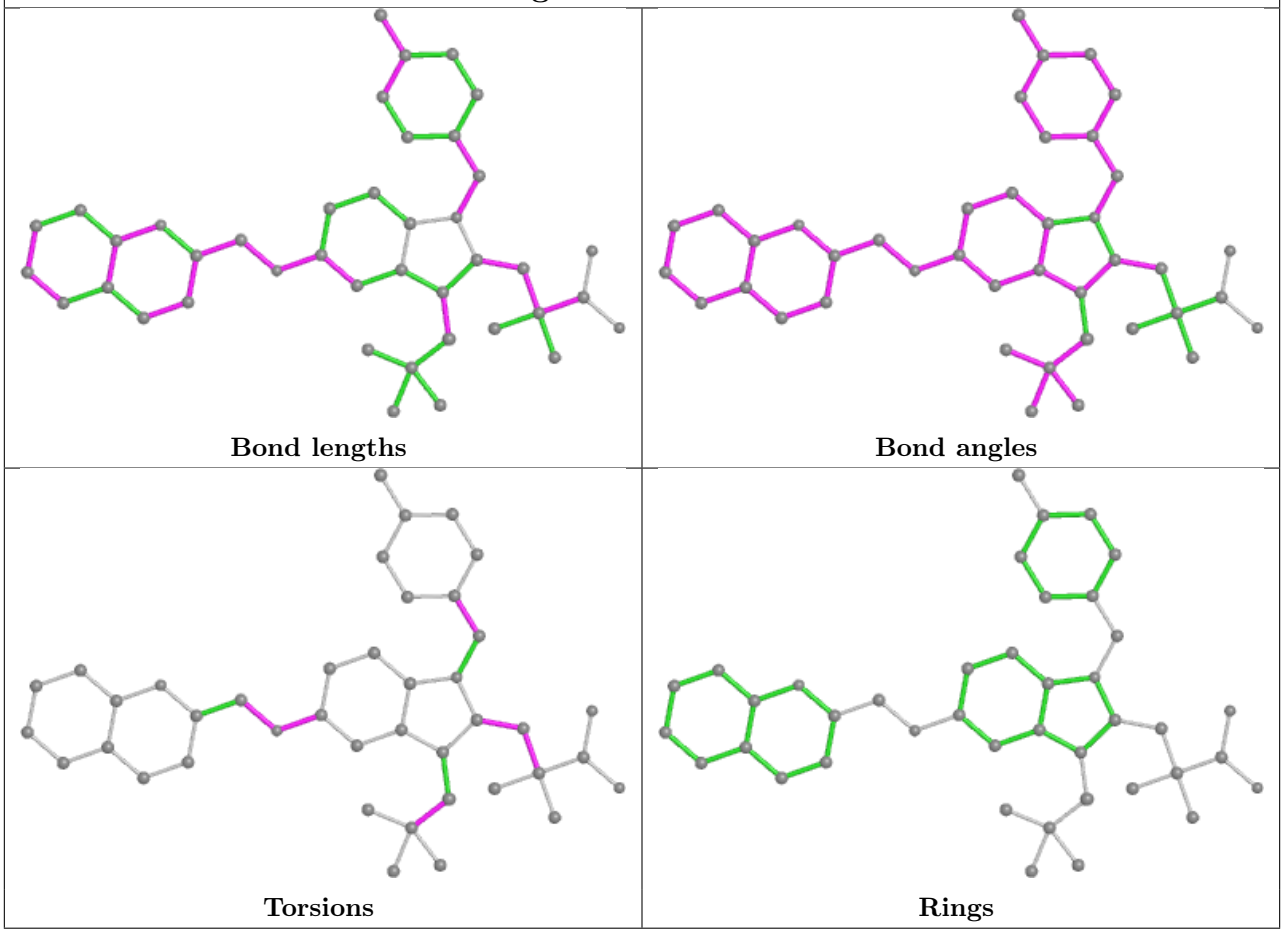


Torsions

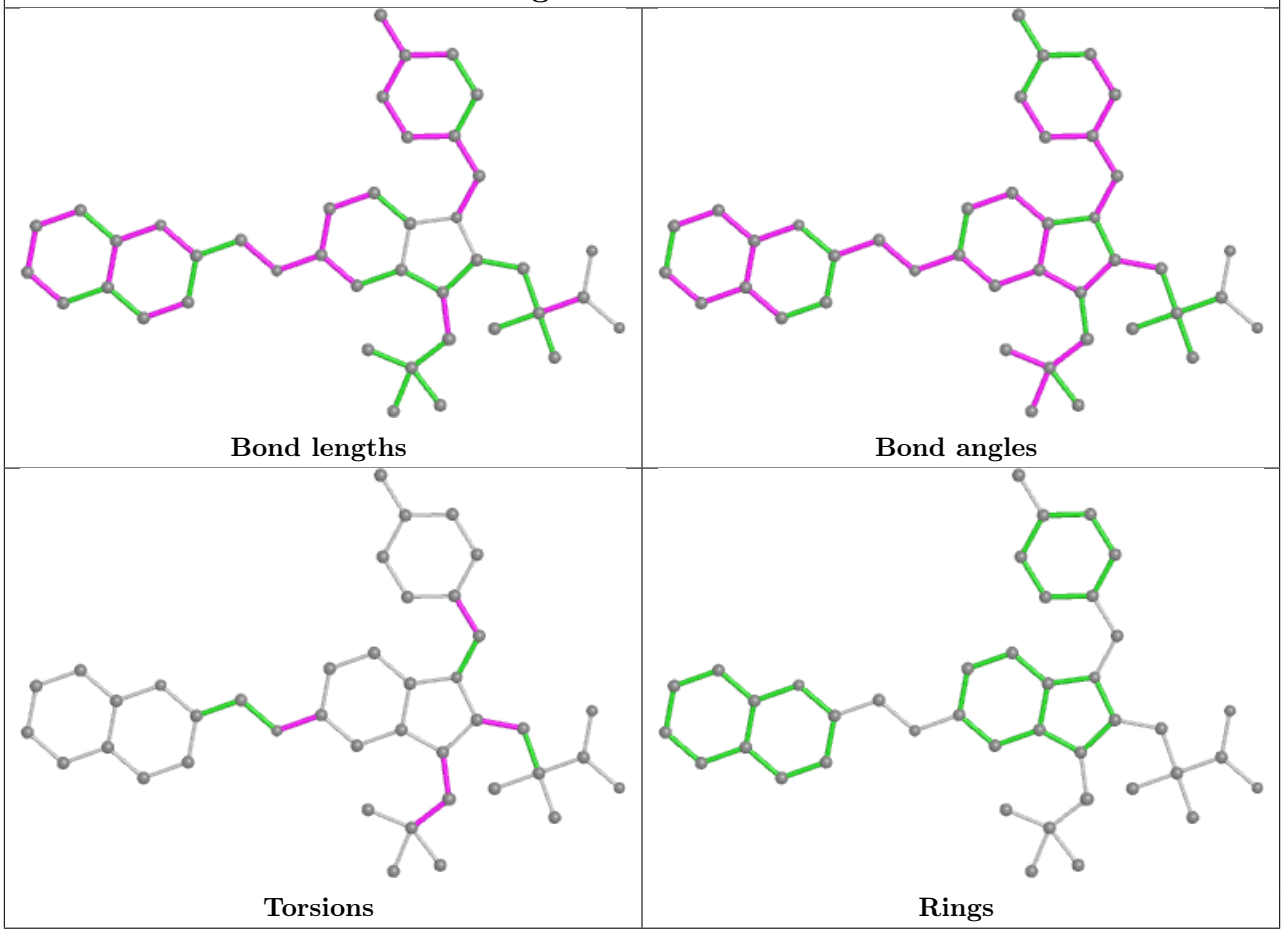


Rings

Ligand 2CS E 505



Ligand 2CS E 506



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

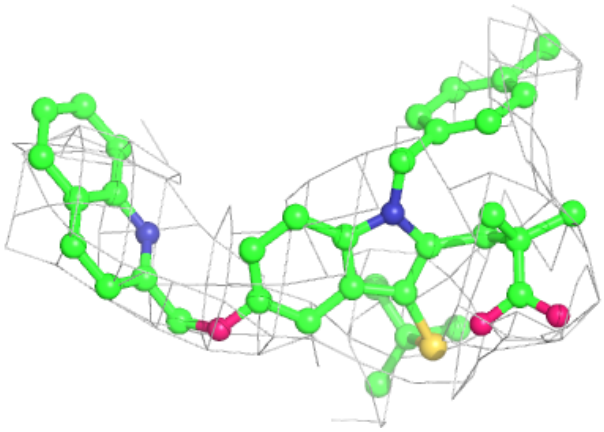
6.4 Ligands (i)

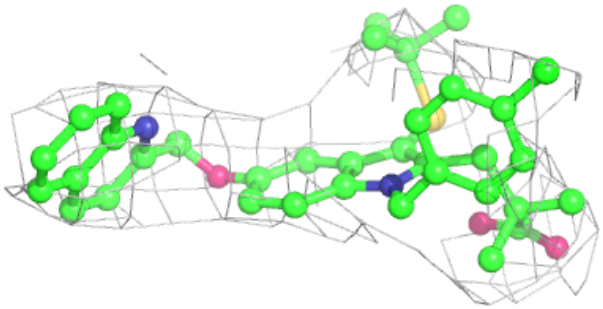
Unable to reproduce the depositors R factor - this section is therefore empty.

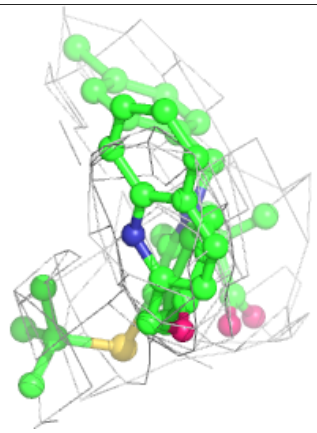
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CS A 502:

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

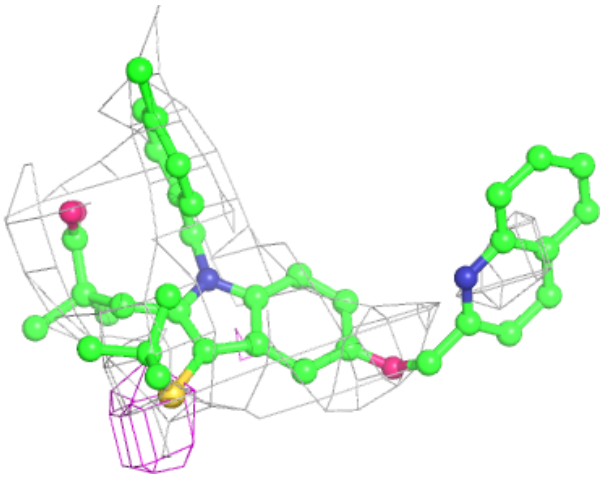


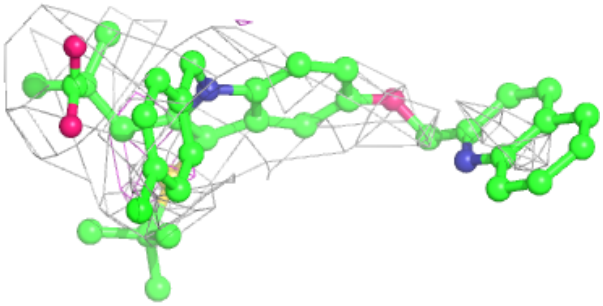


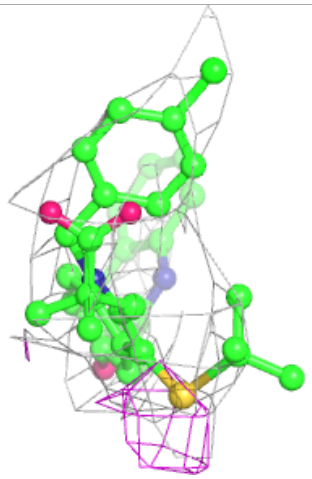


Electron density around 2CS A 503:

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

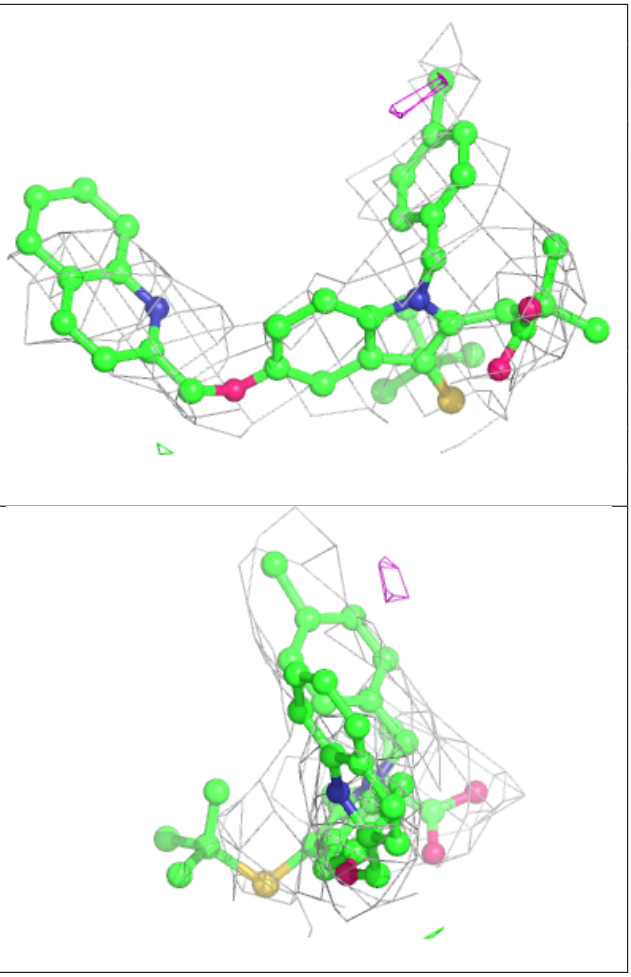






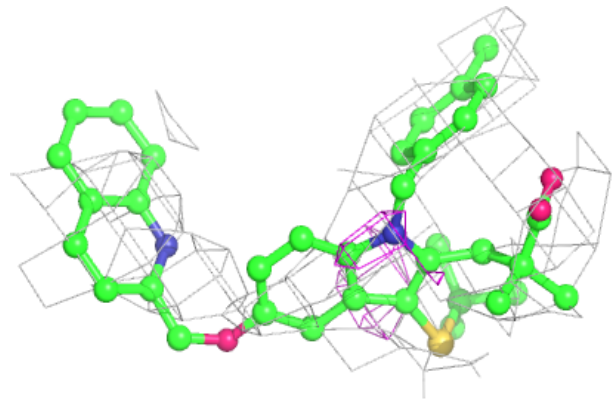
Electron density around 2CS C 501:

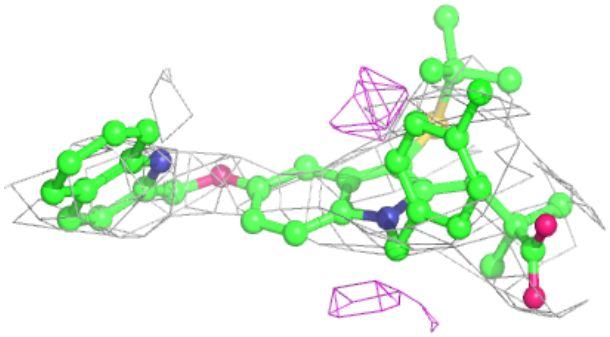
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

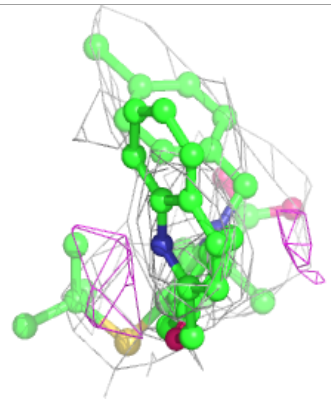


Electron density around 2CS D 504:

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

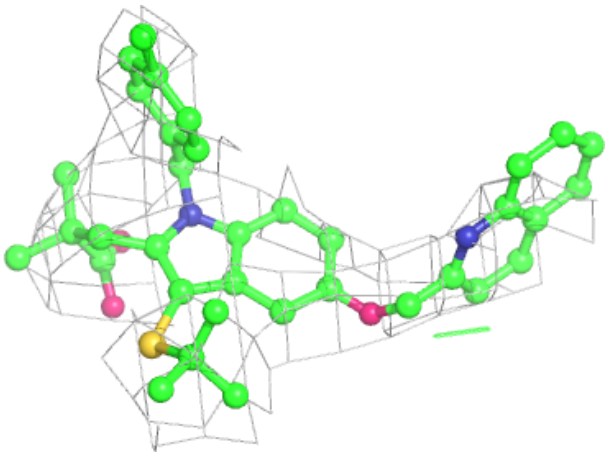


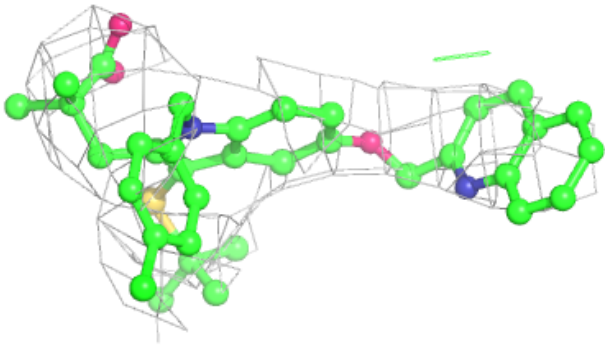


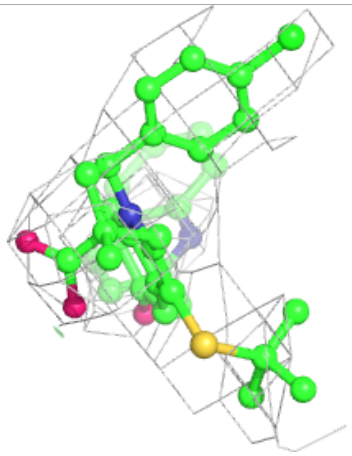


Electron density around 2CS E 505:

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

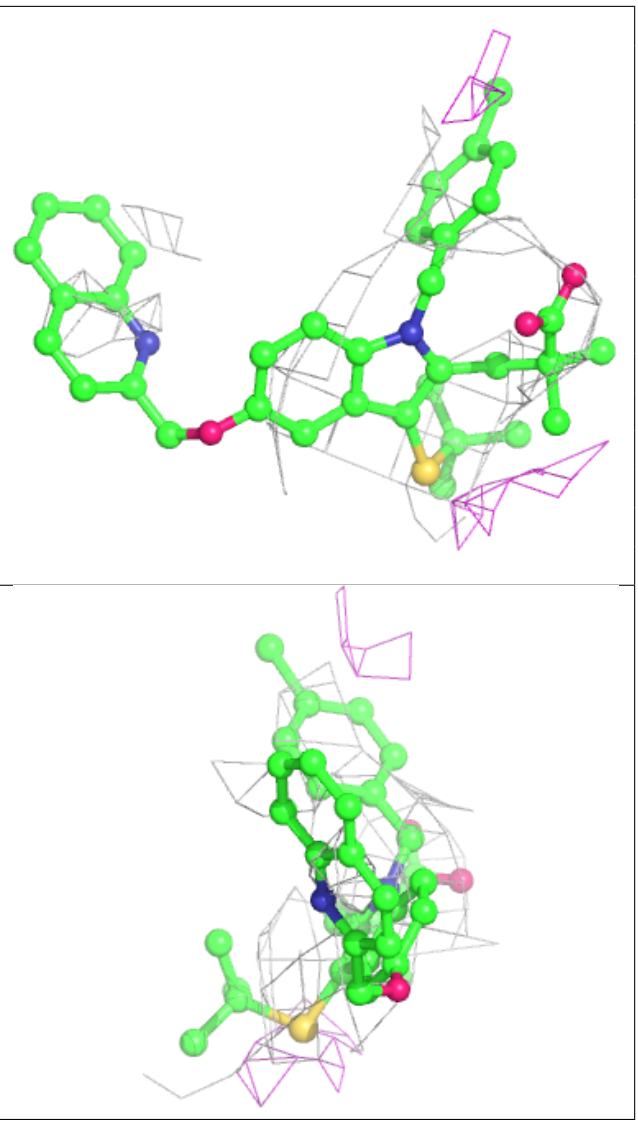






Electron density around 2CS E 506:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.