



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 3, 2021 – 10:14 pm BST

PDB ID : 2V97  
Title : Structure of the unphotolysed complex of TcAChE with 1-(2- nitrophenyl)-2,2,2-trifluoroethyl-arsenocholine after a 9 seconds annealing to room temperature  
Authors : Colletier, J.-P.; Sanson, B.; Royant, A.; Specht, A.; Nachon, F.; Masson, P.; Zaccai, G.; Sussman, J.L.; Goeldner, M.; Silman, I.; Bourgeois, D.; Weik, M.  
Deposited on : 2007-08-22  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

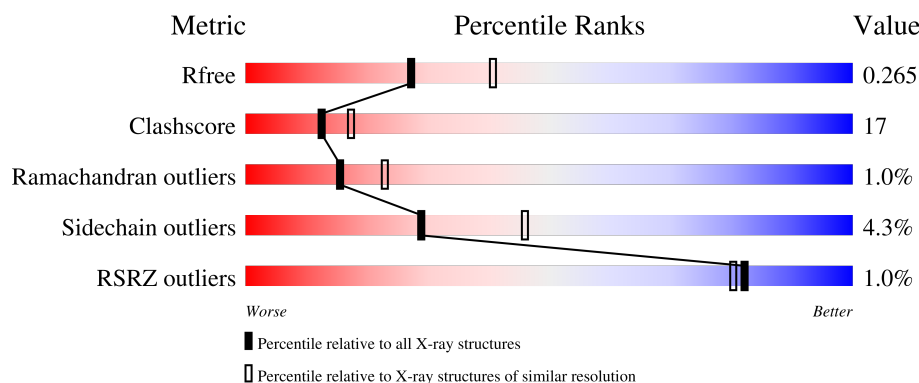
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	537	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>54%</span> <span>42%</span> <span>..</span> </div> </div>
1	B	537	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>54%</span> <span>42%</span> <span>..</span> </div> </div>

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	CL	A	1536[A]	-	-	X	-
2	CL	A	1536[B]	-	-	X	-
3	CFQ	A	1538[A]	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18979 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.

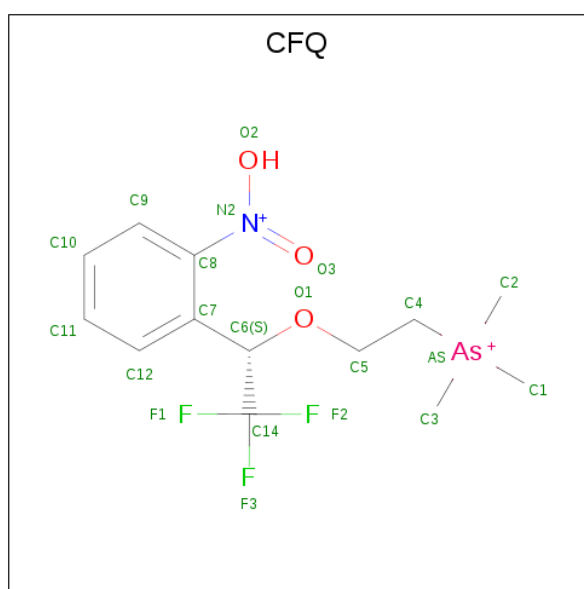
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	527	0
			8356	5379	1405	1528	44			
1	B	532	Total	C	N	O	S	0	532	0
			8398	5406	1410	1538	44			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	1
			2	2		

- Molecule 3 is 1-(2-nitrophenyl)-2,2,2-trifluoroethyl]-arsenocholine (three-letter code: CFQ) (formula: C<sub>13</sub>H<sub>19</sub>AsF<sub>3</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		
3	B	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		
3	B	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			28	16	2	10		
4	A	1	Total	C	N	O	0	1
			28	16	2	10		
4	B	1	Total	C	N	O	0	1
			28	16	2	10		
4	B	1	Total	C	N	O	0	1
			28	16	2	10		

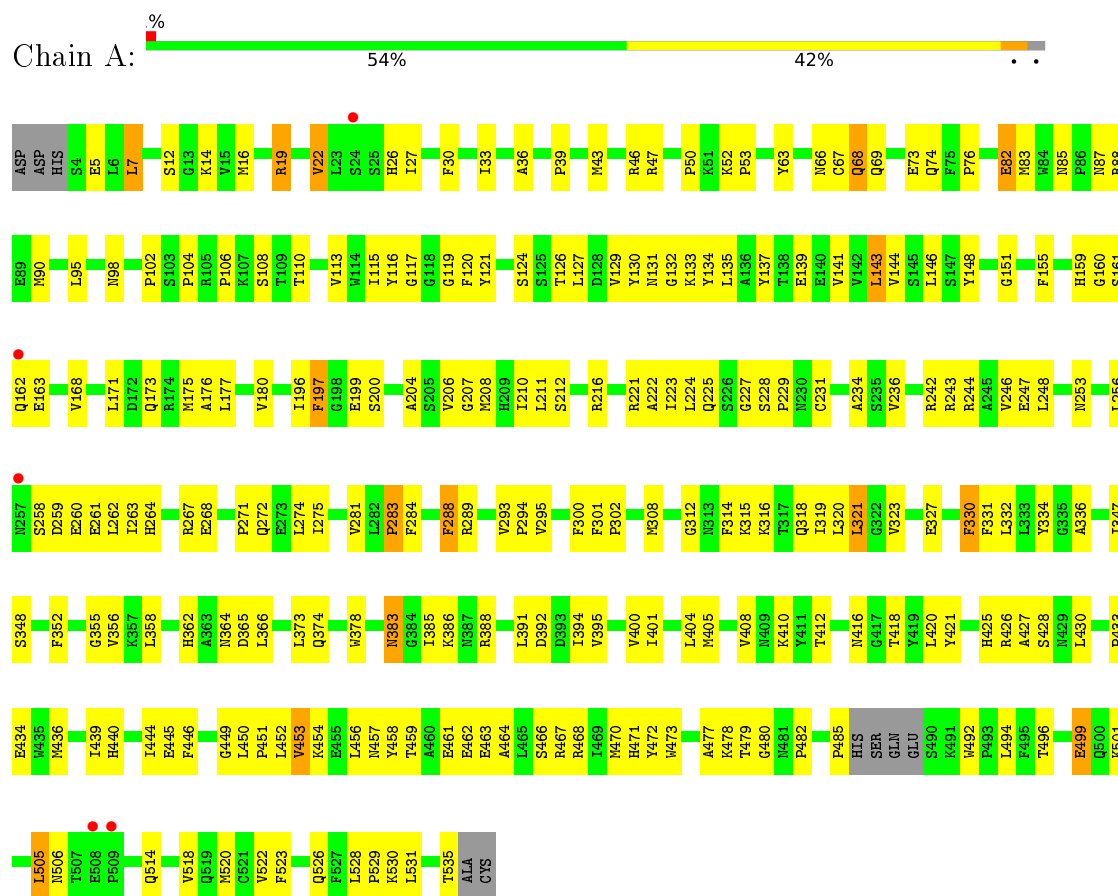
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	926	Total	O	0	832
			926	926		
5	B	1017	Total	O	0	929
			1017	1017		

### 3 Residue-property plots

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: ACETYLCHOLINESTERASE



R515	I439	F352	P271	W179
V518	T444	G355	Q272	V180
Q519	E445	V356	E273	H181
M520		K357	L274	
G521	G449	L358	I275	V194
V522	L450	S359	L282	T195
F523	P451	V360	P283	I196
W524	L452	P361		F197
N525	V453	H362	S286	G198
	K454		I287	E199
L528	P455	D365	F288	S200
P529	L456	L366	R289	A201
K530	H457		G202	G203
L531	Y458	L373	V293	A204
T535	T459	Q374	V295	S205
ALA	E461	Y375		V206
CYS	E462	T376	F300	G207
	E463	D377	F301	M208
	A464	W378	P302	H209
	L465	R379	T303	I210
	S466	D380	T304	L211
	R467	D381	S304	S212
	R468			P213
		G384	M308	
		I385		R216
	H471		N313	
	Y472	R388	F314	F219
	W473	D389	K315	R220
		G390	K316	R221
	A477	L391	T317	A223
	T478		Q318	I223
	G480	I394	F319	L224
		V400	L321	Q225
	M483	I401	G322	S226
E484	P485	C402	V323	G227
P486	H486	P403	N324	S228
S487			K325	P229
		V408	D326	
		N409	E327	V238
	K491			A239
	W492	T418	F330	
	L493	Y419	F331	
	L494	L420		R242
	T496	Y421	Y334	A245
	T497	F422		
K498	E499	F423	F339	N253
		N424	S340	
		H425	K341	R257
		R426	B342	S258
	R501		S343	D259
F502		L430	E344	E260
I503	D504	V431	S345	
		W432	K346	I263
L505		P433	I347	H264
N506		E434	S348	
		G437	R349	R267
		V438	E350	E268
			D351	K270

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.20Å 104.46Å 148.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.40 19.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.81-2.40) 100.0 (19.81-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.272 0.206 , 0.265	Depositor DCC
$R_{free}$ test set	6041 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2793e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CFQ, CL

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	0.60	0/8598	0.74	0/11678
1	B	0.63	0/8642	0.74	2/11738 (0.0%)
All	All	0.62	0/17240	0.74	2/23416 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358[A]	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	358[B]	LEU	CA-CB-CG	5.55	128.06	115.30

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	8356	0	8032	268	0
1	B	8398	0	8068	251	0
2	A	2	0	0	4	0
3	A	84	0	32	27	0
3	B	84	0	32	26	0
4	A	56	0	52	1	0
4	B	56	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	926	0	0	63	0
5	B	1017	0	0	51	0
All	All	18979	0	16268	561	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 17.

The worst 5 of 561 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1537[A]:CFQ:C4	3:B:1537[A]:CFQ:AS	2.20	1.49
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C2	2.21	1.48
3:A:1538[A]:CFQ:C4	3:A:1538[A]:CFQ:AS	2.22	1.47
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C1	2.22	1.47
3:A:1538[A]:CFQ:AS	3:A:1538[A]:CFQ:C2	2.22	1.47

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	1048/537 (195%)	932 (89%)	108 (10%)	8 (1%)	19	29
1	B	1060/537 (197%)	970 (92%)	76 (7%)	14 (1%)	12	17
All	All	2108/1074 (196%)	1902 (90%)	184 (9%)	22 (1%)	15	23

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283[A]	PRO
1	A	283[B]	PRO

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Mol	Chain	Res	Type
1	B	486[A]	HIS
1	B	486[B]	HIS
1	A	22[A]	VAL

### 5.3.2 Protein sidechains ⓘ

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	899/469 (192%)	861 (96%)	38 (4%)	30	47
1	B	902/469 (192%)	862 (96%)	40 (4%)	28	45
All	All	1801/938 (192%)	1723 (96%)	78 (4%)	29	46

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	358[B]	LEU
1	B	497[B]	THR
1	B	365[B]	ASP
1	B	455[B]	GLU
1	B	505[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	NAG	A	1539[B]	-	14,14,15	0.51	0	17,19,21	0.65	0
3	CFQ	B	1536[B]	-	16,21,21	2.68	5 (31%)	20,31,31	1.63	5 (25%)
3	CFQ	B	1537[A]	-	16,21,21	2.55	5 (31%)	20,31,31	1.83	3 (15%)
4	NAG	A	1540[B]	-	14,14,15	0.52	0	17,19,21	0.62	0
4	NAG	B	1539[B]	-	14,14,15	0.50	0	17,19,21	0.62	0
4	NAG	B	1538[A]	-	14,14,15	0.80	0	17,19,21	0.87	1 (5%)
3	CFQ	A	1538[A]	-	16,21,21	2.31	4 (25%)	20,31,31	1.72	5 (25%)
4	NAG	A	1539[A]	-	14,14,15	0.66	0	17,19,21	0.80	1 (5%)
3	CFQ	B	1536[A]	-	16,21,21	2.20	5 (31%)	20,31,31	1.72	6 (30%)
3	CFQ	A	1537[A]	-	16,21,21	2.32	5 (31%)	20,31,31	1.79	7 (35%)
3	CFQ	B	1537[B]	-	16,21,21	2.96	5 (31%)	20,31,31	1.82	7 (35%)
4	NAG	B	1539[A]	-	14,14,15	0.71	0	17,19,21	0.64	0
4	NAG	A	1540[A]	-	14,14,15	0.78	0	17,19,21	0.80	1 (5%)
3	CFQ	A	1538[B]	-	16,21,21	2.91	5 (31%)	20,31,31	1.78	7 (35%)
3	CFQ	A	1537[B]	-	16,21,21	2.75	5 (31%)	20,31,31	1.68	5 (25%)
4	NAG	B	1538[B]	-	14,14,15	0.51	0	17,19,21	0.67	1 (5%)

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	NAG	A	1539[B]	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CFQ	B	1536[B]	-	-	1/18/21/21	0/1/1/1
3	CFQ	B	1537[A]	-	-	8/18/21/21	0/1/1/1
4	NAG	A	1540[B]	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1539[B]	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1538[A]	-	-	4/6/23/26	0/1/1/1
3	CFQ	A	1538[A]	-	-	7/18/21/21	0/1/1/1
4	NAG	A	1539[A]	-	-	3/6/23/26	0/1/1/1
3	CFQ	B	1536[A]	-	-	1/18/21/21	0/1/1/1
3	CFQ	A	1537[A]	-	-	1/18/21/21	0/1/1/1
3	CFQ	B	1537[B]	-	-	2/18/21/21	0/1/1/1
4	NAG	B	1539[A]	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1540[A]	-	-	0/6/23/26	0/1/1/1
3	CFQ	A	1538[B]	-	-	2/18/21/21	0/1/1/1
3	CFQ	A	1537[B]	-	-	3/18/21/21	0/1/1/1
4	NAG	B	1538[B]	-	-	3/6/23/26	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1537[B]	CFQ	C8-C7	6.67	1.48	1.39
3	B	1537[B]	CFQ	C7-C6	6.61	1.59	1.51
3	A	1538[B]	CFQ	C8-C7	6.57	1.48	1.39
3	A	1538[B]	CFQ	C7-C6	6.45	1.58	1.51
3	A	1538[A]	CFQ	C7-C6	6.06	1.58	1.51

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1537[A]	CFQ	C5-O1-C6	4.32	119.89	114.01
3	A	1538[A]	CFQ	C9-C8-C7	-3.98	117.44	121.35
3	B	1537[A]	CFQ	C9-C8-C7	-3.97	117.45	121.35
3	A	1537[A]	CFQ	C9-C8-C7	-3.76	117.66	121.35
3	B	1536[A]	CFQ	O1-C6-C7	-3.76	105.55	110.93

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1538[A]	CFQ	F1-C14-C6-O1

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Mol	Chain	Res	Type	Atoms
3	A	1538[A]	CFQ	F2-C14-C6-O1
3	A	1538[A]	CFQ	F3-C14-C6-O1
3	A	1538[A]	CFQ	F1-C14-C6-C7
3	A	1538[A]	CFQ	F2-C14-C6-C7

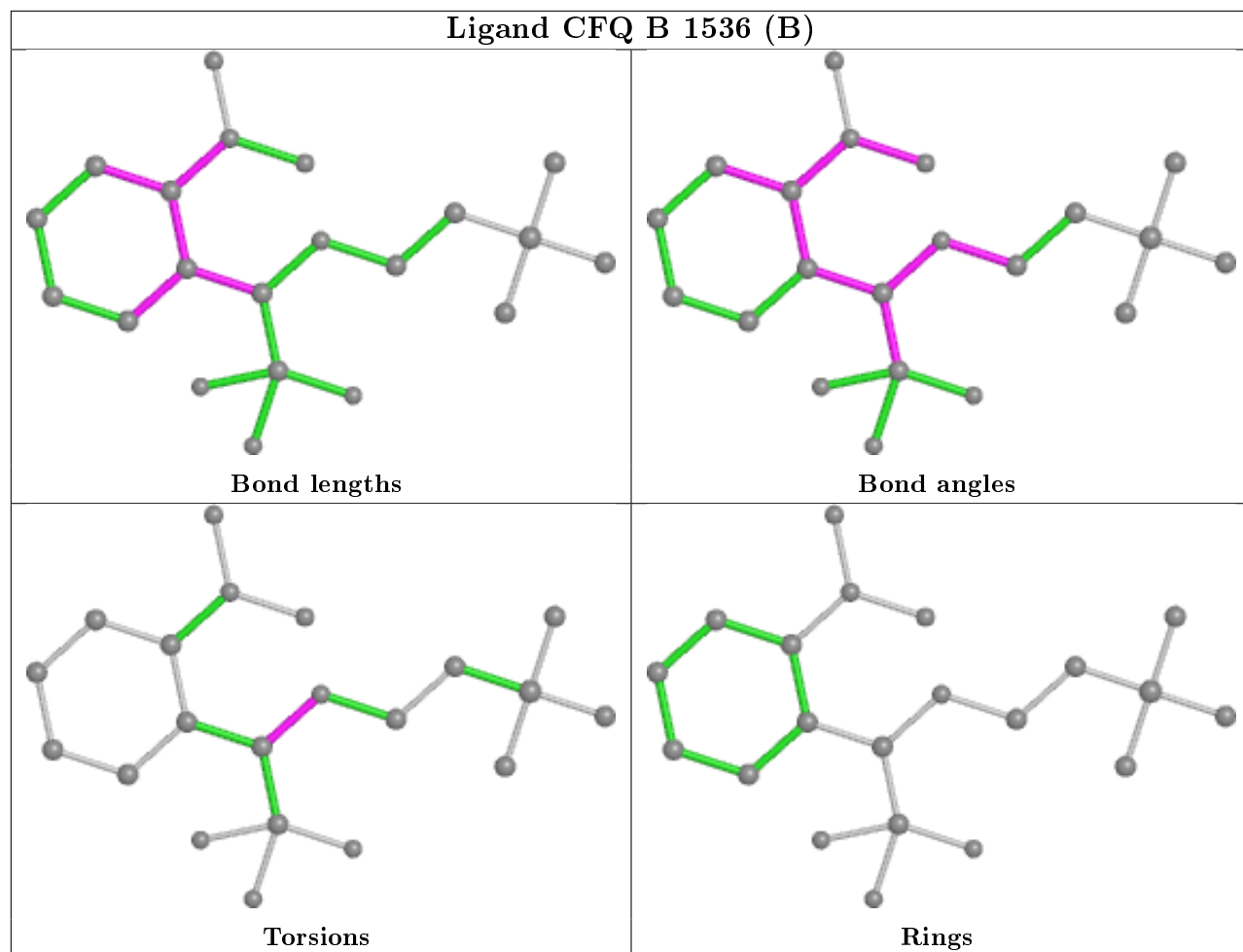
There are no ring outliers.

10 monomers are involved in 55 short contacts:

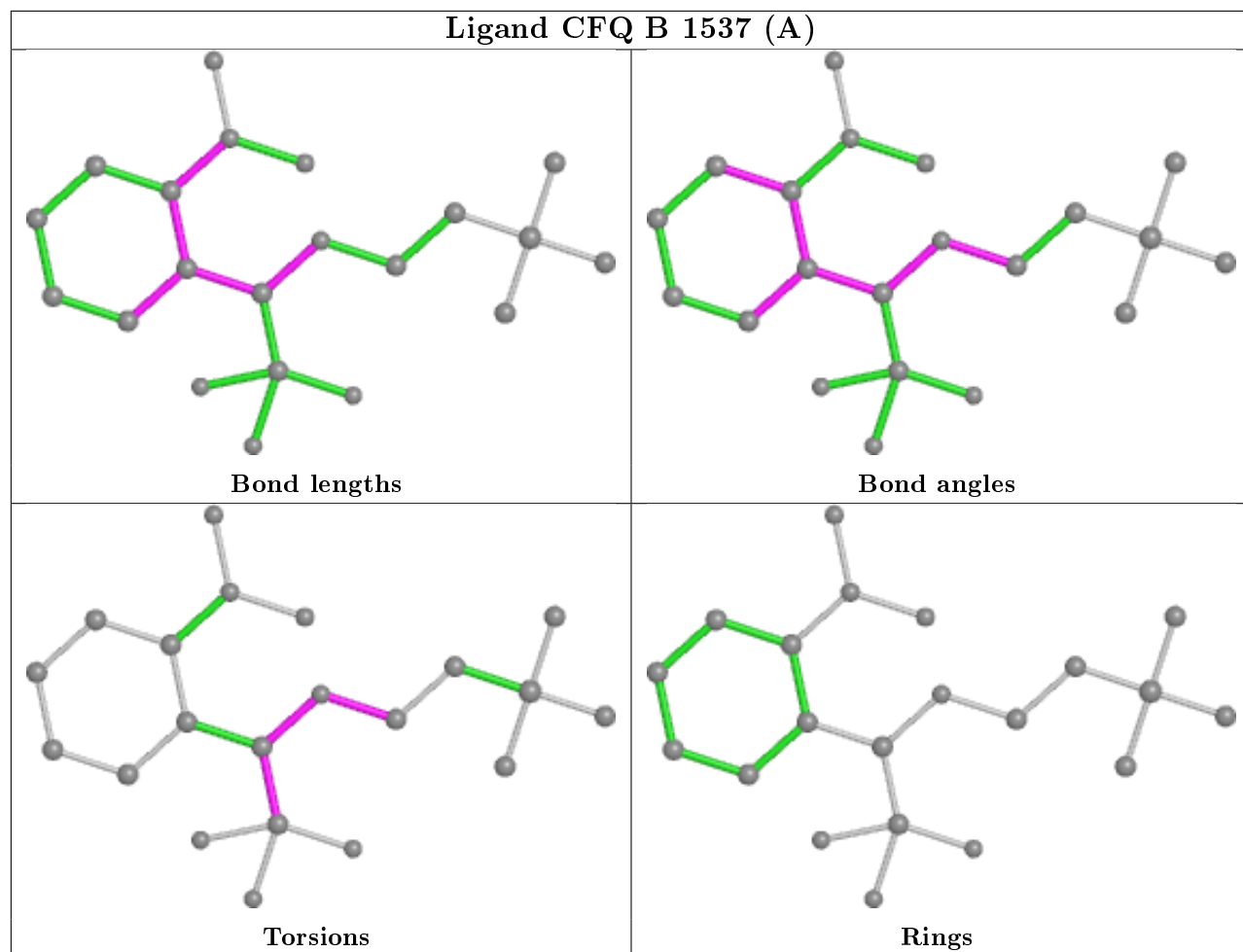
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1536[B]	CFQ	6	0
3	B	1537[A]	CFQ	8	0
4	A	1540[B]	NAG	1	0
3	A	1538[A]	CFQ	9	0
3	B	1536[A]	CFQ	7	0
3	A	1537[A]	CFQ	7	0
3	B	1537[B]	CFQ	5	0
3	A	1538[B]	CFQ	5	0
3	A	1537[B]	CFQ	6	0
4	B	1538[B]	NAG	1	0

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

## Ligand CFQ B 1536 (B)

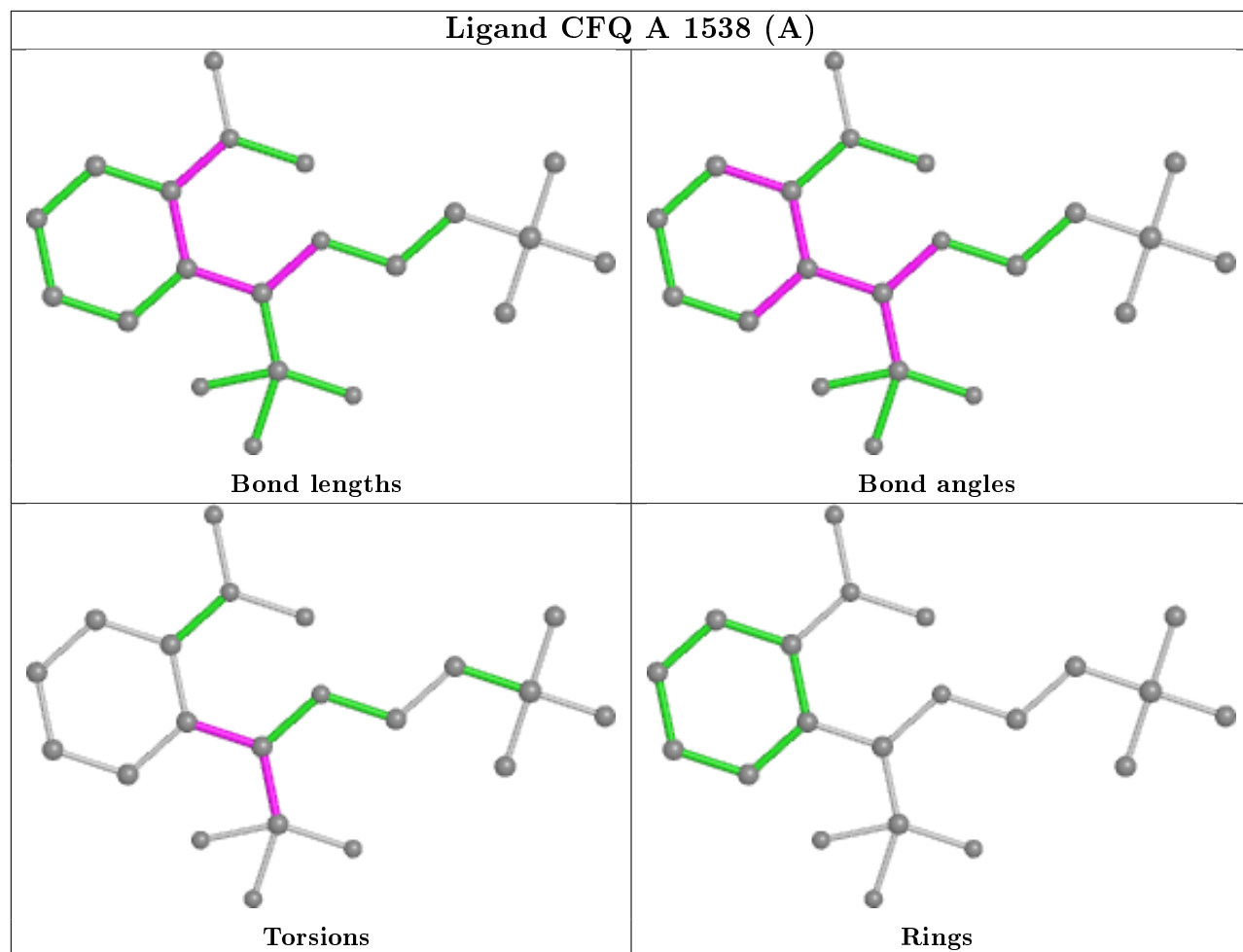


## Ligand CFQ B 1537 (A)

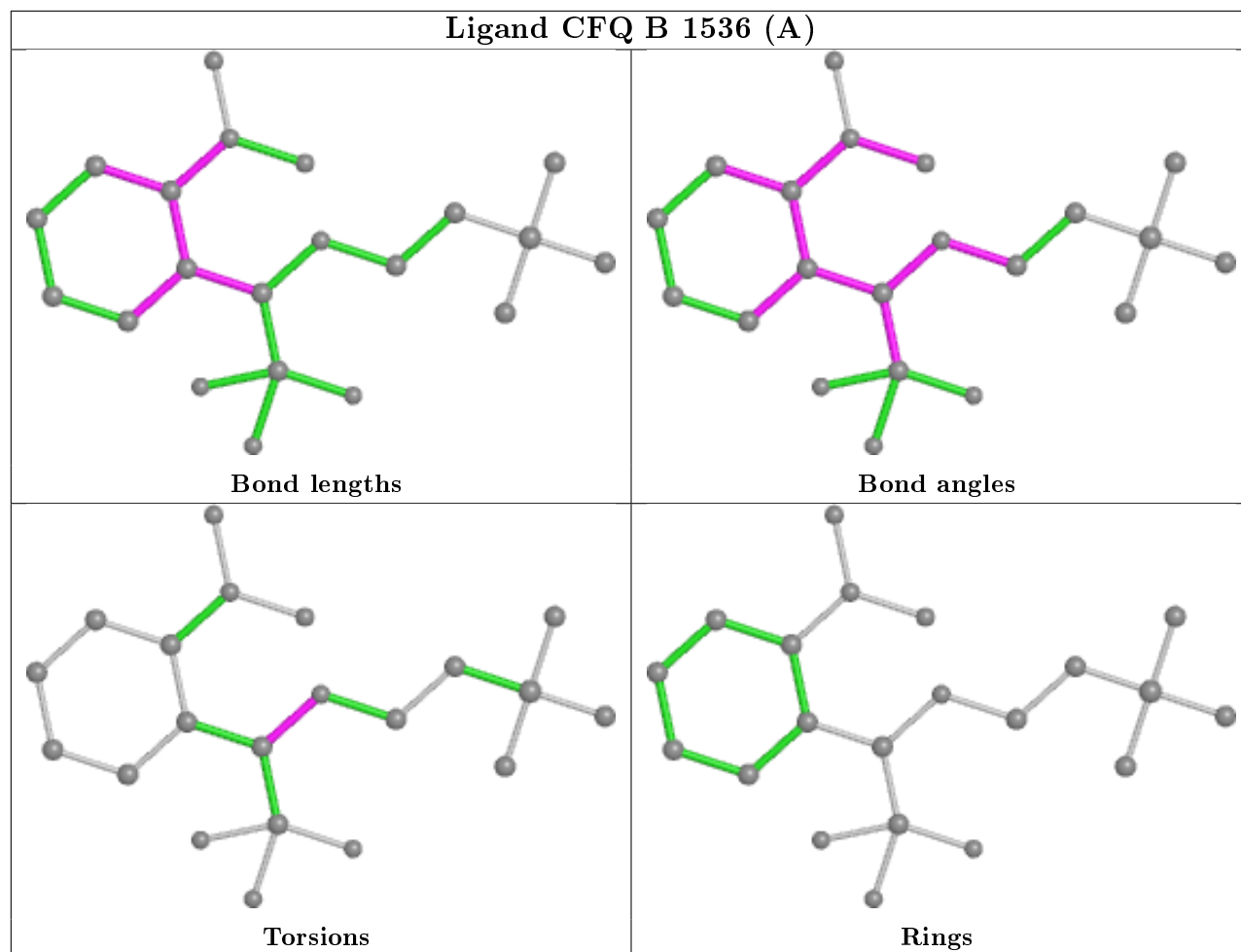




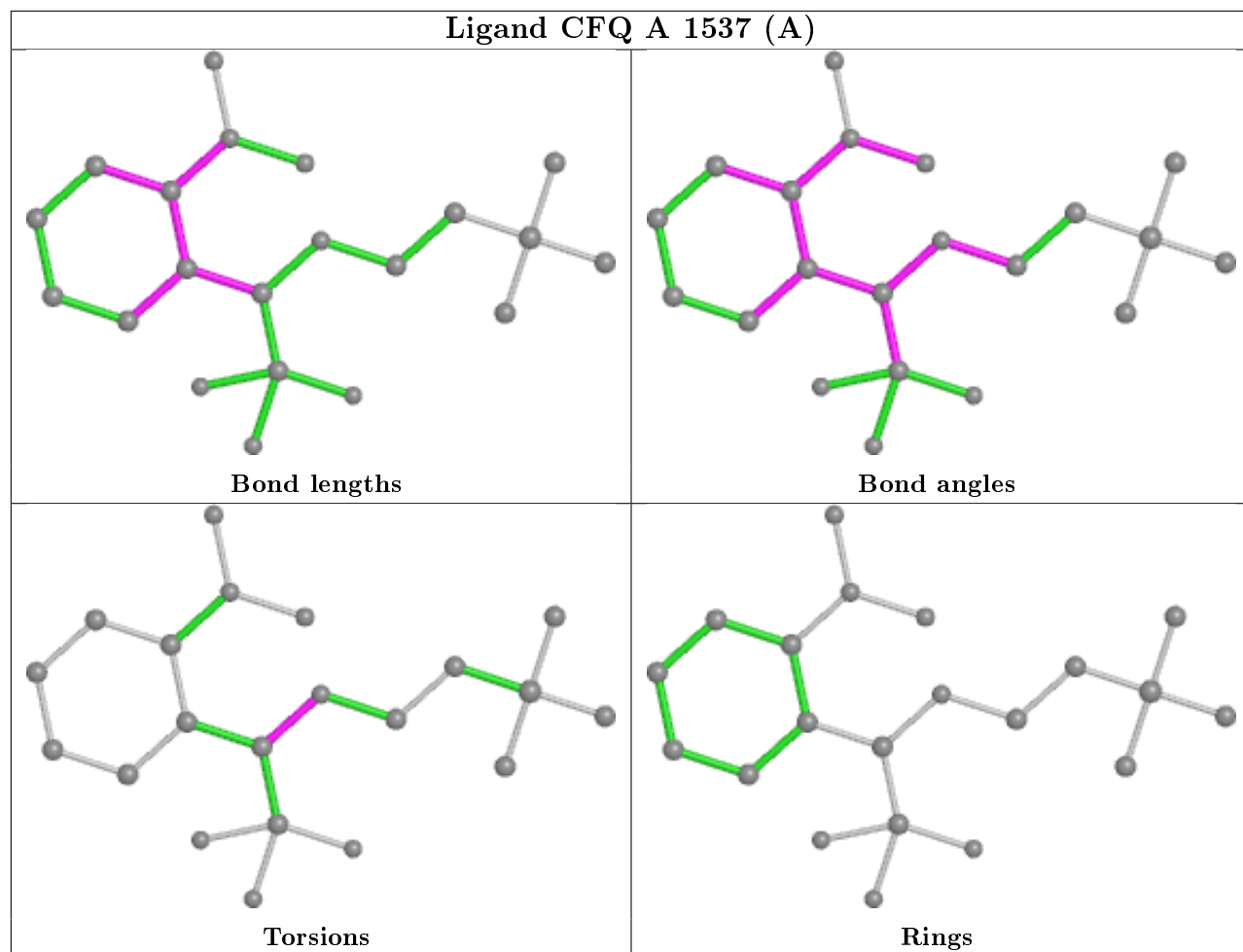
## Ligand CFQ A 1538 (A)



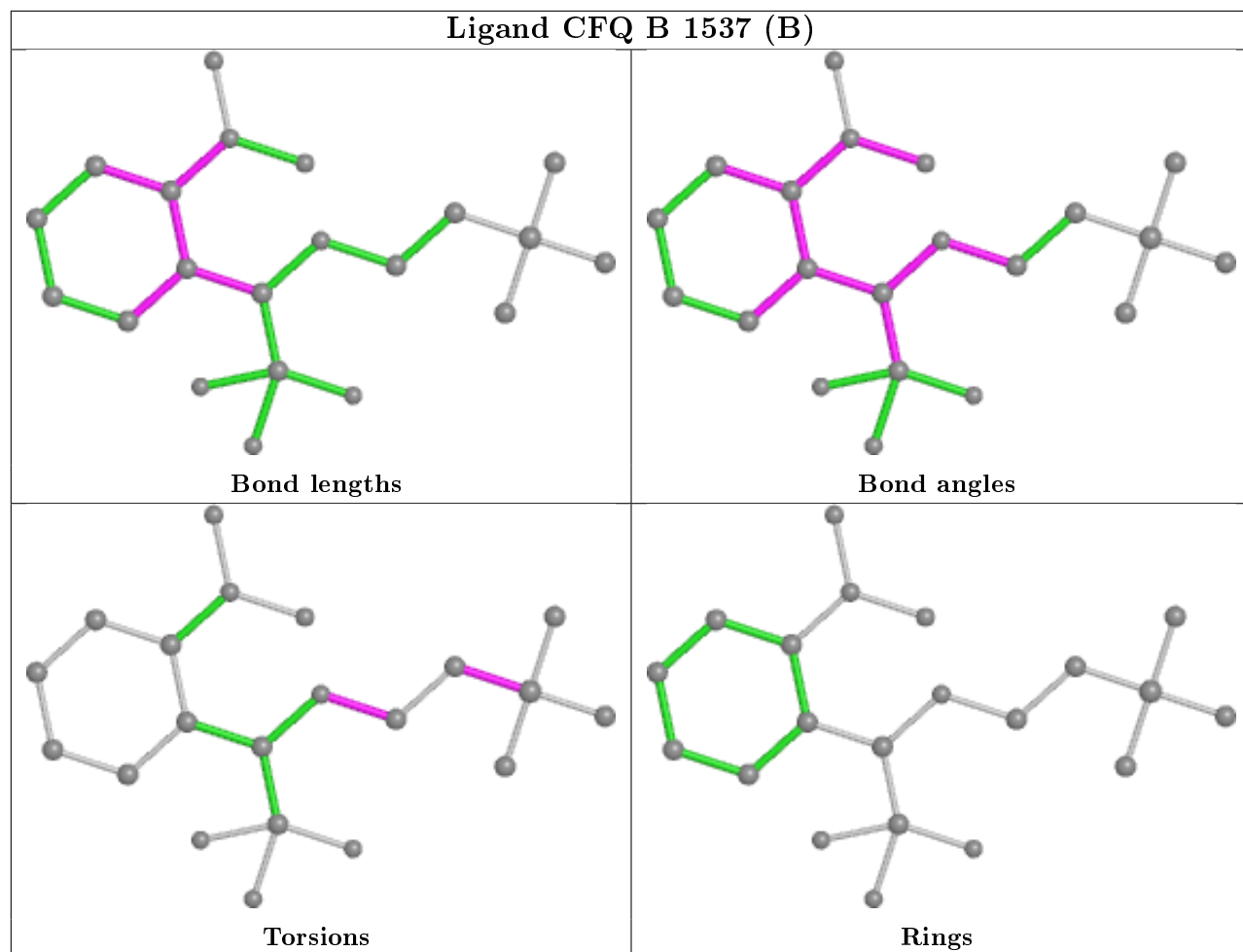
## Ligand CFQ B 1536 (A)



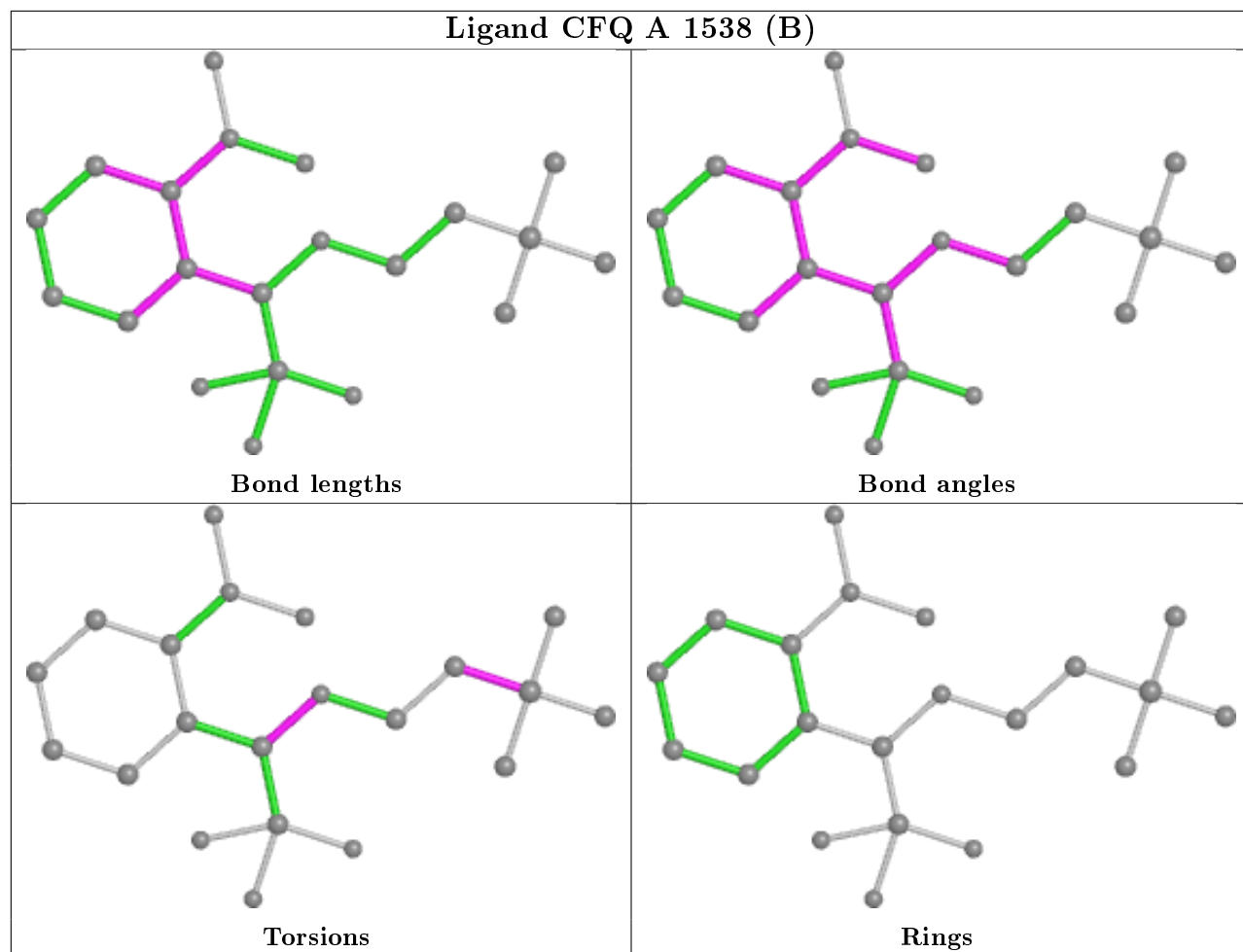
## Ligand CFQ A 1537 (A)

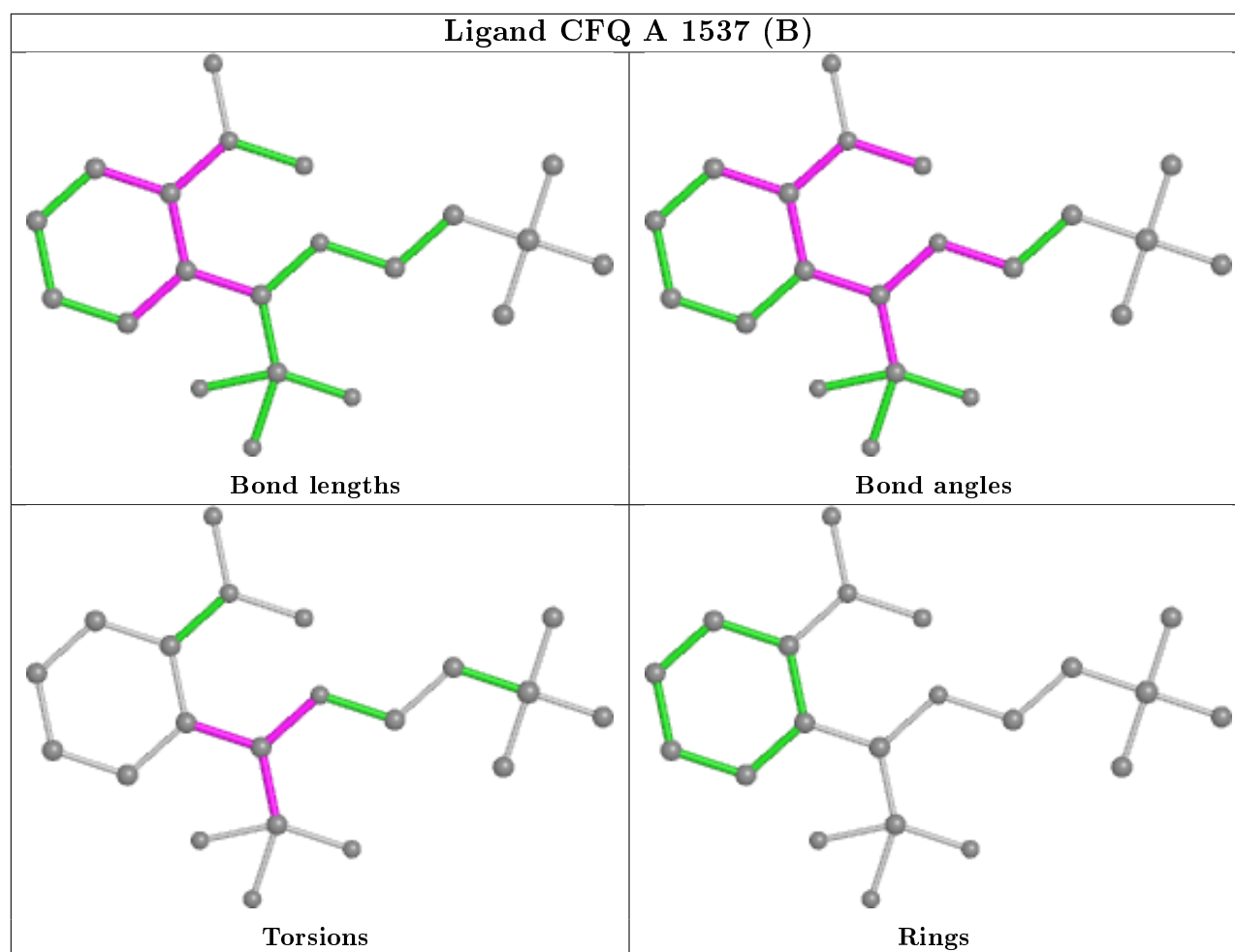


## Ligand CFQ B 1537 (B)



## Ligand CFQ A 1538 (B)





## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	528/537 (98%)	-0.49	5 (0%) 84 82	20, 35, 51, 65	1 (0%)
1	B	532/537 (99%)	-0.51	6 (1%) 80 79	20, 35, 52, 74	0
All	All	1060/1074 (98%)	-0.50	11 (1%) 82 80	20, 35, 52, 74	1 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	535[A]	THR	4.7
1	B	257[A]	ASN	2.9
1	B	253[A]	ASN	2.7
1	A	508[A]	GLU	2.6
1	A	509[A]	PRO	2.6

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

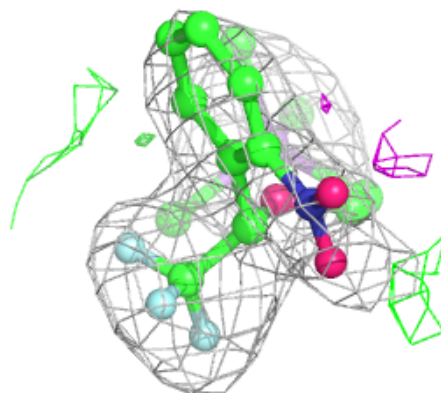
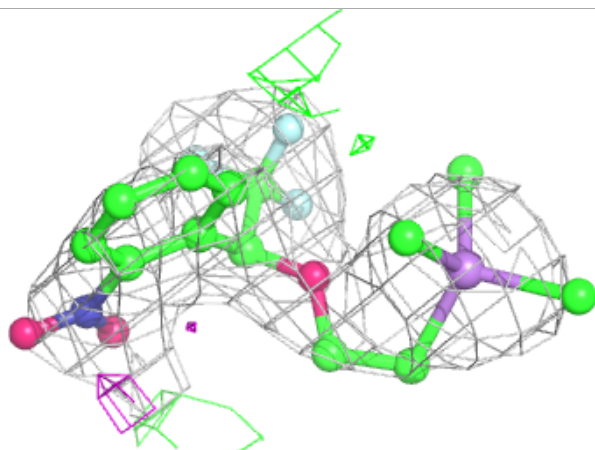
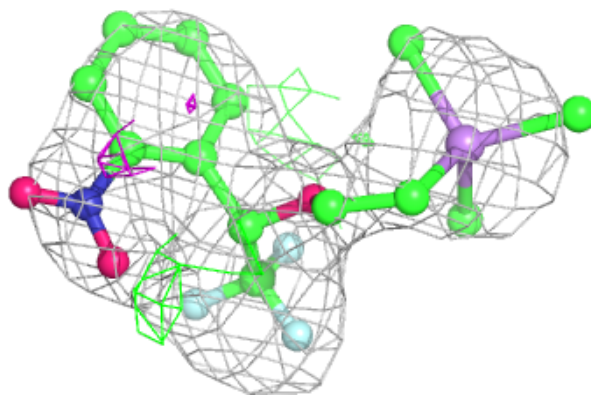
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1539[A]	14/15	0.82	0.35	65,70,72,73	14
4	NAG	A	1539[B]	14/15	0.82	0.35	67,70,71,72	14
4	NAG	B	1538[A]	14/15	0.90	0.23	64,66,68,68	14
4	NAG	B	1538[B]	14/15	0.90	0.23	64,66,66,67	14
4	NAG	A	1540[A]	14/15	0.92	0.30	47,52,55,57	14
4	NAG	A	1540[B]	14/15	0.92	0.30	49,51,52,52	14
4	NAG	B	1539[A]	14/15	0.94	0.22	34,49,52,55	14
4	NAG	B	1539[B]	14/15	0.94	0.22	44,46,48,50	14
2	CL	A	1536[A]	1/1	0.95	0.13	49,49,49,49	1
2	CL	A	1536[B]	1/1	0.95	0.13	49,49,49,49	1
3	CFQ	A	1537[A]	21/21	0.96	0.17	50,57,64,66	21
3	CFQ	A	1537[B]	21/21	0.96	0.17	55,61,64,64	21
3	CFQ	A	1538[A]	21/21	0.96	0.18	44,48,54,57	21
3	CFQ	A	1538[B]	21/21	0.96	0.18	48,51,56,56	21
3	CFQ	B	1536[A]	21/21	0.97	0.14	50,57,61,64	21
3	CFQ	B	1536[B]	21/21	0.97	0.14	54,58,61,62	21
3	CFQ	B	1537[A]	21/21	0.97	0.16	45,47,53,58	21
3	CFQ	B	1537[B]	21/21	0.97	0.16	47,49,53,54	21

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.



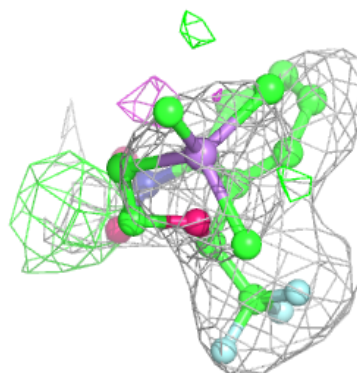
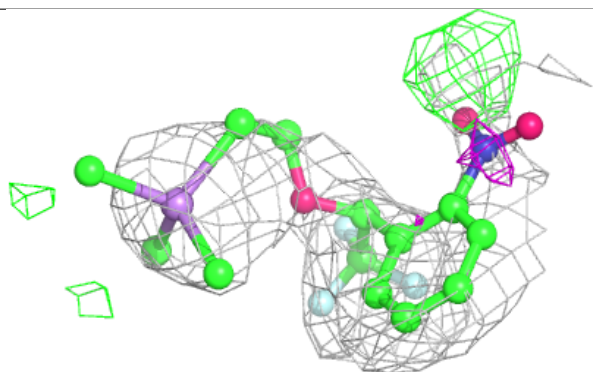
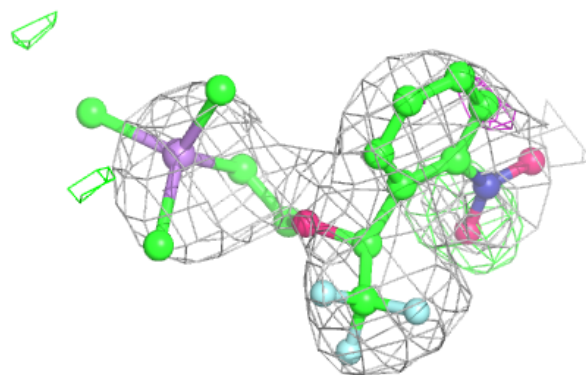
**Electron density around CFQ A 1537 (A):**

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

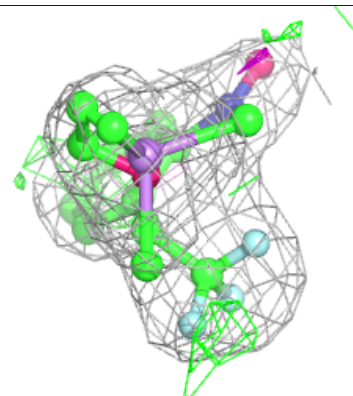
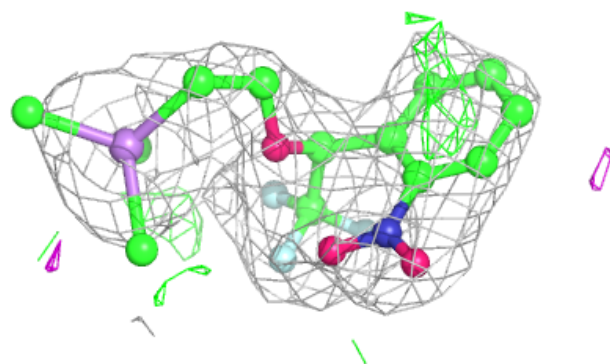
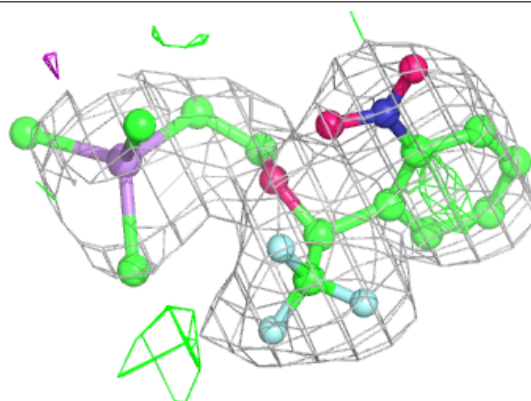


**Electron density around CFQ A 1537 (B):**

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

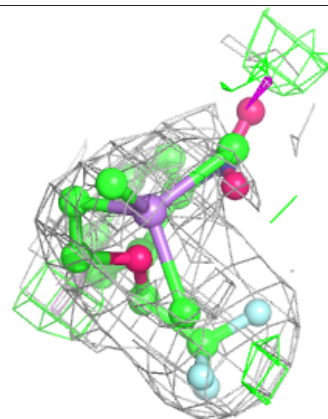
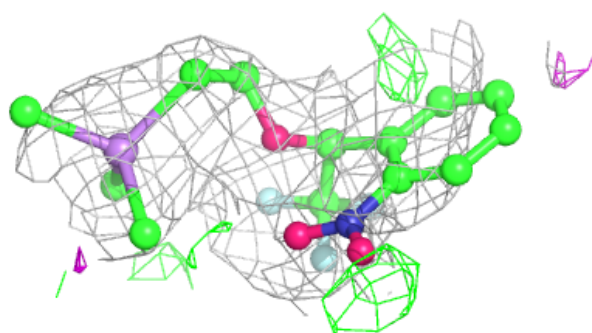
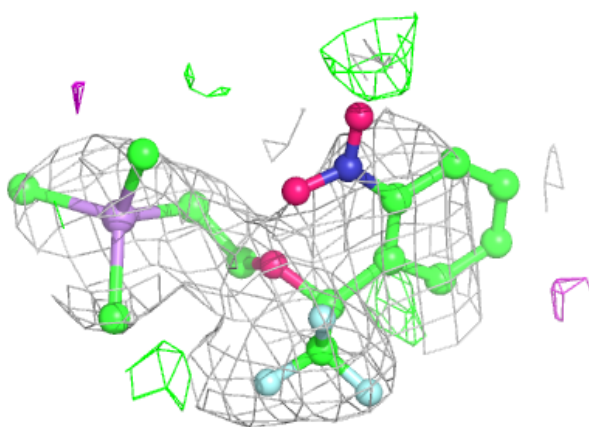
**Electron density around CFQ A 1538 (A):**

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

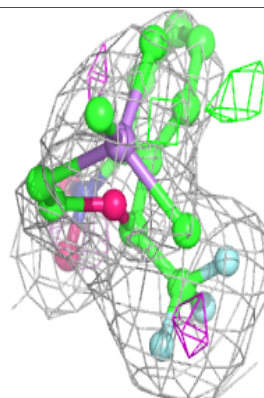
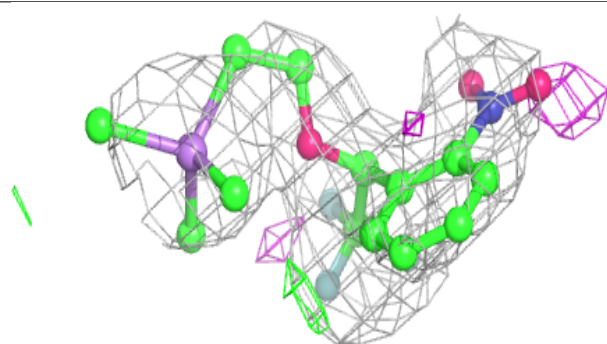
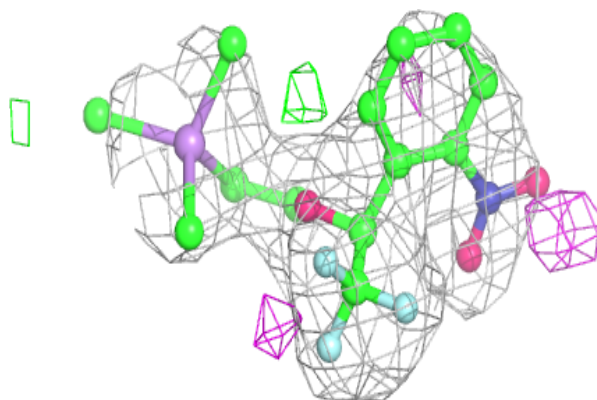


**Electron density around CFQ A 1538 (B):**

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

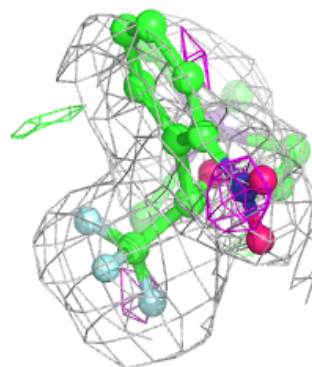
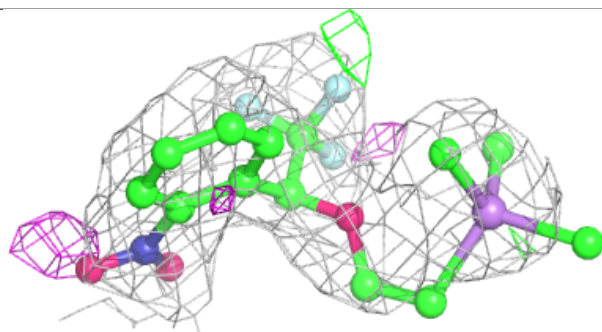
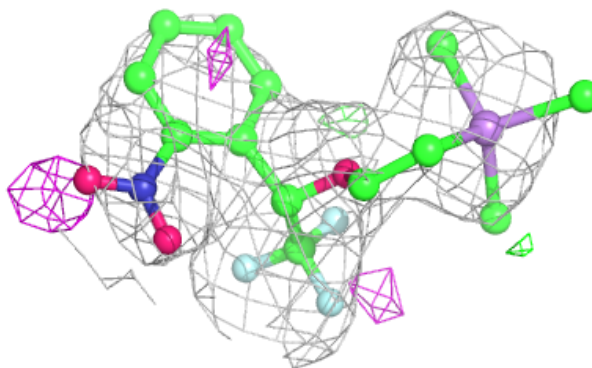
**Electron density around CFQ B 1536 (A):**

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

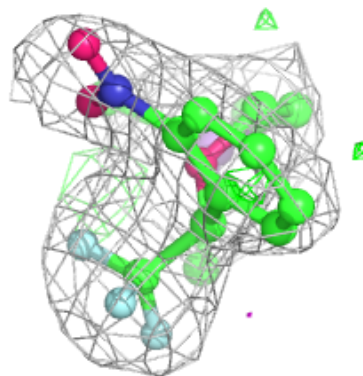
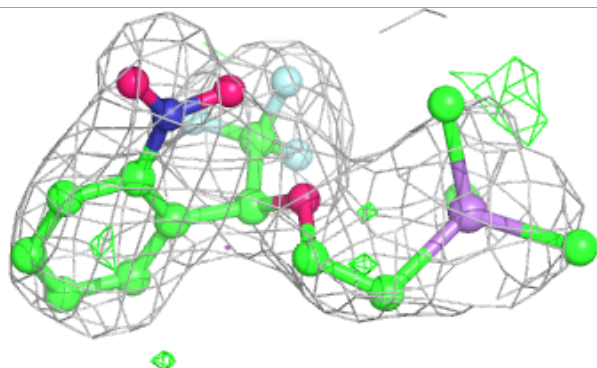
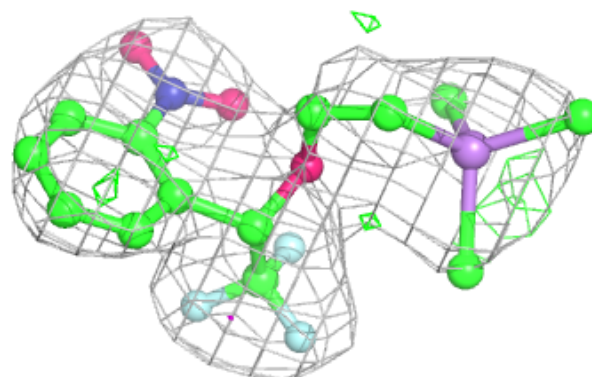


**Electron density around CFQ B 1536 (B):**

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

**Electron density around CFQ B 1537 (A):**

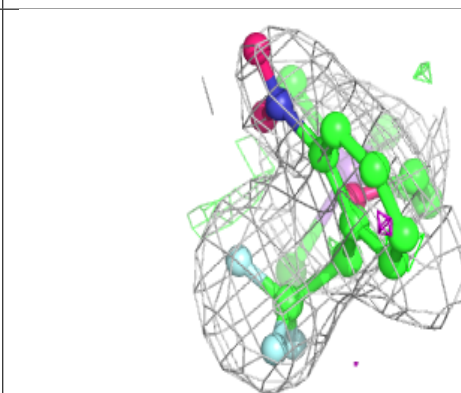
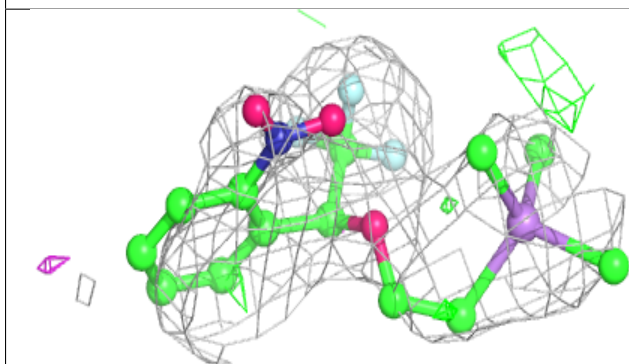
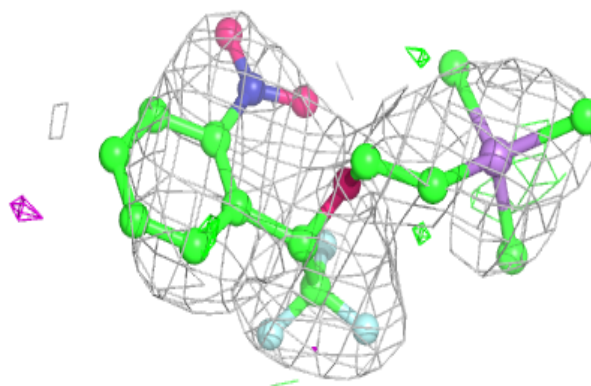
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CFQ B 1537 (B):**

$2mF_o - DF_c$  (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.