



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2026 – 01:03 AM UTC

PDB ID : 2V98 / pdb_00002v98
Title : Structure of the complex of TcAChE with 1-(2-nitrophenyl)-2,2,2- trifluoro ethyl-arsenocholine after a 9 seconds annealing to room temperature, during the first 5 seconds of which laser irradiation at 266nm took place
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Deposited on : 2007-08-22
Resolution : 3.00 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 ⓘ 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

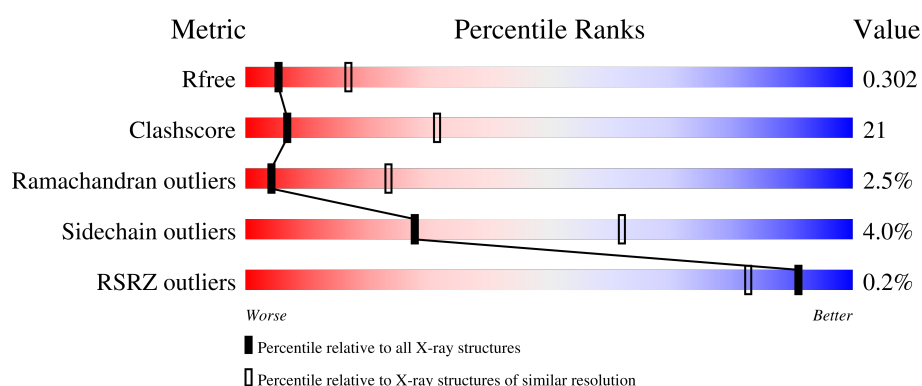
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	37% 56% 5% •
1	B	537	44% 49% 5% •

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	1537[A]	-	-	X	-
3	CFQ	A	1538[A]	-	-	X	-
3	CFQ	B	1537[A]	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18984 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.

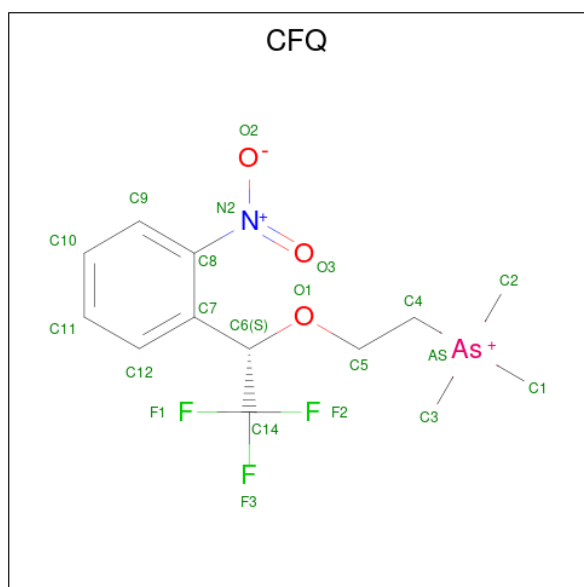
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	528	0
			8362	5382	1406	1530	44			
1	B	532	Total	C	N	O	S	0	532	0
			8398	5406	1410	1538	44			

- Molecule 2 is CHLORIDE ION (CCD ID: 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 (CCD ID: CFQ) (formula: C₁₃H₁₈AsF₃NO₃).



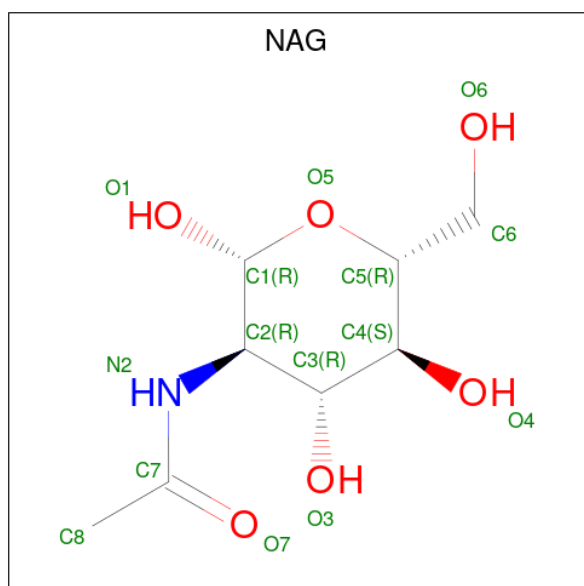
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	As	C	F	N	O	
			42	2	26	6	2	6	1

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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 (CCD ID: 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		

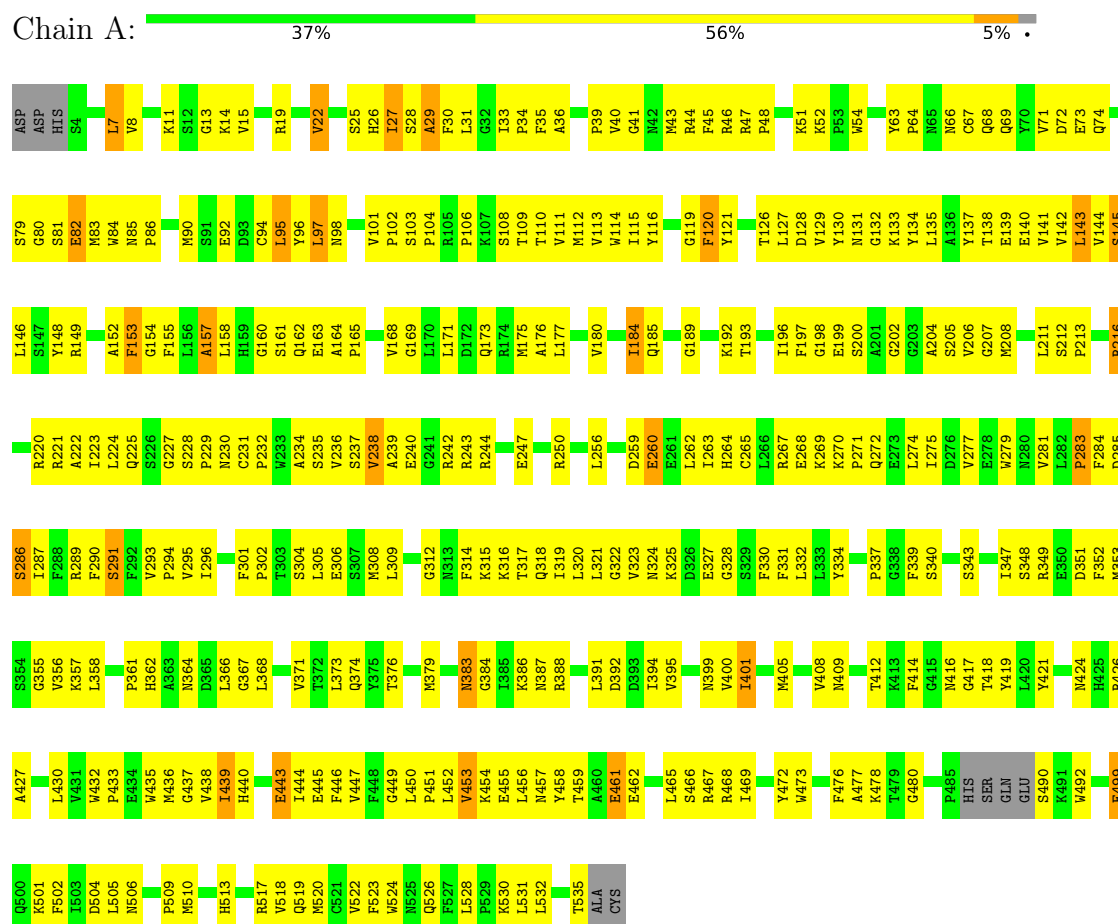
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	925	Total	O	0	814
			925	925		
5	B	1017	Total	O	0	919
			1017	1017		

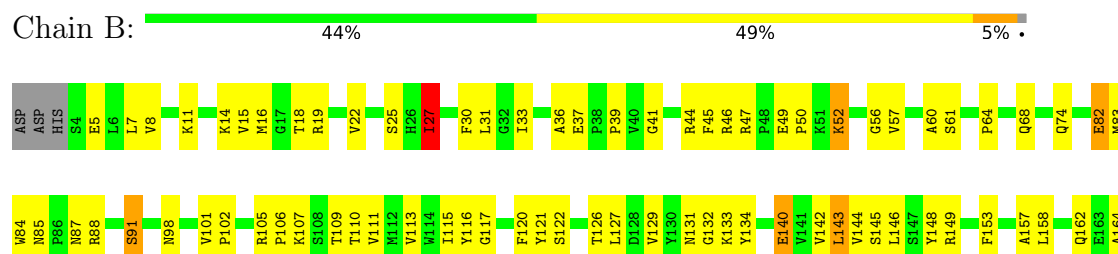
3 Residue-property plots

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



• Molecule 1: ACETYLCHOLINESTERASE



P165	S228	Q318	R388	E455	F523
V168	P229	I319	D389	L456	N524
G169	W233	L320	G390	N457	N525
L170	W236	L321	L391	Y458	Q526
L171		G322	D392	T459	F527
D172		V323	R393	A460	L528
Q173	E240	N324	I394	E461	P529
A174	G241	D326	R395	E462	K530
M175	R242	E327	G396	E463	L531
A176	R243		N399	A464	L532
L177		F331	V400	L465	N533
Q178	V246	L332	I401	S466	A534
W179	E247	L333	C402	S467	T535
V180	L248	Y334	L403	R468	ALA
H181	G249		L404	I469	CYS
D182	R250	G338	V408	N470	
N183	N251	F339	M409	A474	
I184	L252	S340	K410	K478	
Q185	L262	D342	Y411	T479	
F186	I263	S343	T412	G480	
F187		E344	K413	N481	
G188	R267	S345	F414	P482	
G189	E268	K346	G415	N483	
D190	K269	I347	M416	E484	
P191	R270	S348	G417	P485	
K192	P271	R349	T418	H486	
T193	Q272	D350	Y419	S487	
V194	E273	L420	L421	K491	
T195	L274	F352	Y421	L494	
I196		M353	F422	F495	
F197	V277	S354	F423	N496	
G198		G355	M424	T496	
E199	N280	V356	H425	T497	
S200	V281	K357	R426	K498	
A201	L282	L358	A427	E499	
G202	P283	S359		Q500	
G203	F284	V360	L430	K501	
V206	D285	P361	V431	F502	
G207		H362	W432	L503	
M208	V293	A363	P433	D504	
H209	P294	N364	M436	L505	
I210	V295	D365	G437	N506	
L211	G298	L366	V438		
S212	E299	G367	I439	P509	
P213	F300	A370	H440	N510	
R216	F301	V371	G441	K511	
D217	P302	T372	Y442	N512	
L218	S304	L373	E443	N513	
F219	S304	Q374		Q514	
R220			V447	R514	
R221	M308	V378	F448	L516	
A222	M379	M379	G449	R517	
I223			L450	V518	
L224	N313	N383	P451	Q519	
Q225	F314	K386	L452	N520	
S226	K315	V453	V453	C521	
G227	T317	N387	K454	V522	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.62Å 104.47Å 148.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (8.00-3.00) 93.6 (8.00-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.249 0.277 , 0.302	Depositor DCC
R_{free} test set	2672 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 87.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18984	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 42.68 % 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 1.9698e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.31	0/8604	0.81	22/11686 (0.2%)
1	B	0.31	0/8642	0.83	32/11738 (0.3%)
All	All	0.31	0/17246	0.82	54/23424 (0.2%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401[A]	ILE	N-CA-C	9.13	119.18	110.42
1	A	401[B]	ILE	N-CA-C	9.13	119.18	110.42
1	A	443[A]	GLU	N-CA-C	-7.74	103.96	113.41
1	A	443[B]	GLU	N-CA-C	-7.74	103.96	113.41
1	B	443[A]	GLU	N-CA-C	-6.94	104.94	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8362	0	8036	357	0
1	B	8398	0	8068	319	0
2	A	2	0	0	6	0
3	A	84	0	32	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	84	0	32	25	0
4	A	56	0	52	0	0
4	B	56	0	52	0	0
5	A	925	0	0	61	0
5	B	1017	0	0	57	0
All	All	18984	0	16272	711	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 21.

The worst 5 of 711 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	2.21	1.49
3:A:1538[A]:CFQ:C4	3:A:1538[A]:CFQ:AS	2.23	1.47
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C1	2.23	1.47
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C2	2.23	1.46
3:A:1537[A]:CFQ:AS	3:A:1537[A]:CFQ:C4	2.24	1.46

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%)	892 (85%)	128 (12%)	28 (3%)	4	22
1	B	1060/537 (197%)	910 (86%)	126 (12%)	24 (2%)	5	25
All	All	2108/1074 (196%)	1802 (86%)	254 (12%)	52 (2%)	4	23

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27[A]	ILE
1	A	27[B]	ILE
1	A	95[A]	LEU
1	A	95[B]	LEU
1	B	27[A]	ILE

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	900/469 (192%)	870 (97%)	30 (3%)	33	67
1	B	902/469 (192%)	860 (95%)	42 (5%)	23	58
All	All	1802/938 (192%)	1730 (96%)	72 (4%)	28	62

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	461[B]	GLU
1	B	535[B]	THR
1	B	494[B]	LEU
1	B	505[B]	LEU
1	A	453[A]	VAL

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	CFQ	B	1537[A]	-	17,21,21	3.10	7 (41%)	19,31,31	1.86	5 (26%)
4	NAG	A	1539[A]	-	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
3	CFQ	A	1537[B]	-	17,21,21	2.99	6 (35%)	19,31,31	1.57	4 (21%)
3	CFQ	A	1538[B]	-	17,21,21	3.28	6 (35%)	19,31,31	1.79	6 (31%)
4	NAG	A	1540[B]	-	14,14,15	0.64	0	17,19,21	0.68	1 (5%)
4	NAG	B	1538[A]	-	14,14,15	0.70	0	17,19,21	0.89	1 (5%)
4	NAG	B	1539[A]	-	14,14,15	0.80	0	17,19,21	0.63	0
3	CFQ	B	1537[B]	-	17,21,21	3.25	6 (35%)	19,31,31	1.78	7 (36%)
4	NAG	A	1539[B]	-	14,14,15	0.57	0	17,19,21	0.77	0
4	NAG	B	1538[B]	-	14,14,15	0.54	0	17,19,21	0.74	0
3	CFQ	B	1536[A]	-	17,21,21	3.33	6 (35%)	19,31,31	1.66	6 (31%)
4	NAG	A	1540[A]	-	14,14,15	0.60	0	17,19,21	0.54	0
3	CFQ	A	1537[A]	-	17,21,21	3.21	6 (35%)	19,31,31	1.54	5 (26%)
3	CFQ	A	1538[A]	-	17,21,21	2.95	5 (29%)	19,31,31	1.89	5 (26%)
4	NAG	B	1539[B]	-	14,14,15	0.54	0	17,19,21	0.68	1 (5%)
3	CFQ	B	1536[B]	-	17,21,21	3.11	5 (29%)	19,31,31	1.71	5 (26%)

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
3	CFQ	B	1537[A]	-	-	11/18/21/21	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1539[A]	-	-	2/6/23/26	0/1/1/1
3	CFQ	A	1537[B]	-	-	7/18/21/21	0/1/1/1
3	CFQ	A	1538[B]	-	-	7/18/21/21	0/1/1/1
4	NAG	A	1540[B]	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1538[A]	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1539[A]	-	-	0/6/23/26	0/1/1/1
3	CFQ	B	1537[B]	-	-	3/18/21/21	0/1/1/1
4	NAG	A	1539[B]	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1538[B]	-	-	2/6/23/26	0/1/1/1
3	CFQ	B	1536[A]	-	-	1/18/21/21	0/1/1/1
4	NAG	A	1540[A]	-	-	0/6/23/26	0/1/1/1
3	CFQ	A	1537[A]	-	-	5/18/21/21	0/1/1/1
3	CFQ	A	1538[A]	-	-	10/18/21/21	0/1/1/1
4	NAG	B	1539[B]	-	-	2/6/23/26	0/1/1/1
3	CFQ	B	1536[B]	-	-	1/18/21/21	0/1/1/1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1536[A]	CFQ	C7-C6	7.94	1.60	1.51
3	A	1538[B]	CFQ	C7-C6	7.78	1.60	1.51
3	A	1537[A]	CFQ	C7-C6	7.67	1.60	1.51
3	B	1537[A]	CFQ	C8-C7	7.43	1.49	1.39
3	B	1537[B]	CFQ	C8-C7	7.41	1.49	1.39

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1538[A]	CFQ	C9-C8-C7	-4.65	116.80	121.32
3	B	1537[A]	CFQ	C9-C8-C7	-4.53	116.92	121.32
3	B	1537[B]	CFQ	C9-C8-C7	-4.00	117.43	121.32
3	A	1537[A]	CFQ	C5-O1-C6	3.87	119.17	114.03
3	B	1536[A]	CFQ	C9-C8-C7	-3.69	117.74	121.32

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1537[A]	CFQ	O1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	1537[A]	CFQ	O1-C6-C7-C12
3	A	1537[A]	CFQ	C14-C6-C7-C8
3	A	1537[A]	CFQ	C14-C6-C7-C12
3	A	1537[B]	CFQ	F1-C14-C6-O1

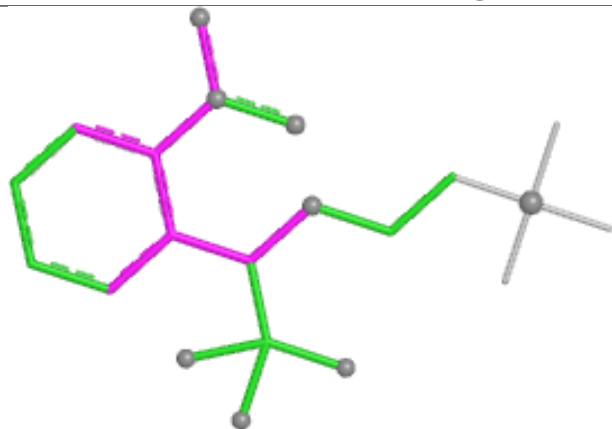
There are no ring outliers.

8 monomers are involved in 56 short contacts:

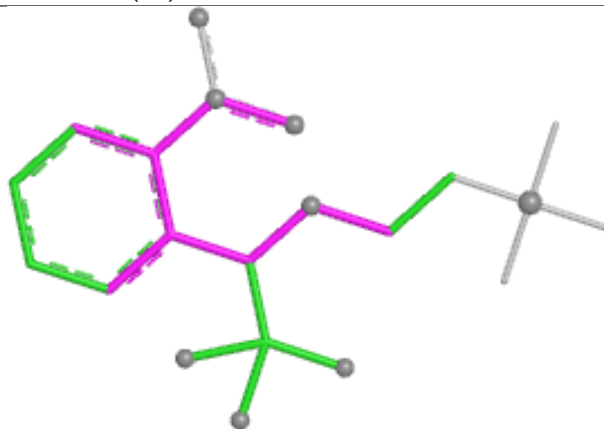
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1537[A]	CFQ	9	0
3	A	1537[B]	CFQ	5	0
3	A	1538[B]	CFQ	6	0
3	B	1537[B]	CFQ	5	0
3	B	1536[A]	CFQ	6	0
3	A	1537[A]	CFQ	8	0
3	A	1538[A]	CFQ	12	0
3	B	1536[B]	CFQ	5	0

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.

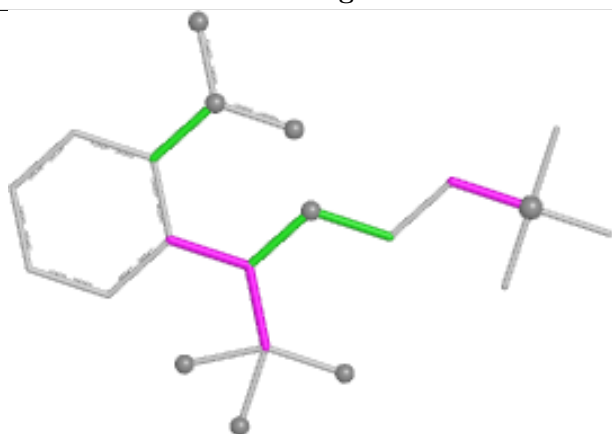
Ligand CFQ B 1537 (A)



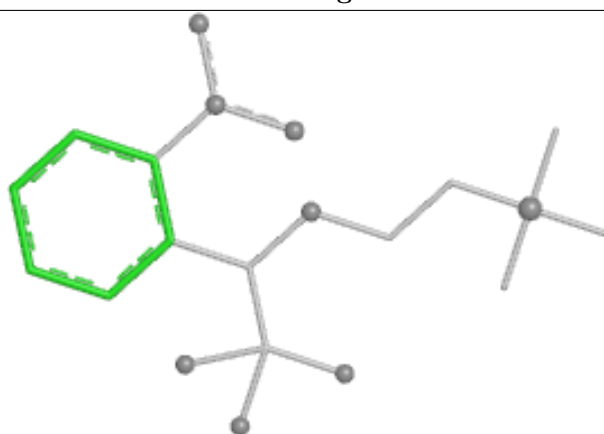
Bond lengths



Bond angles

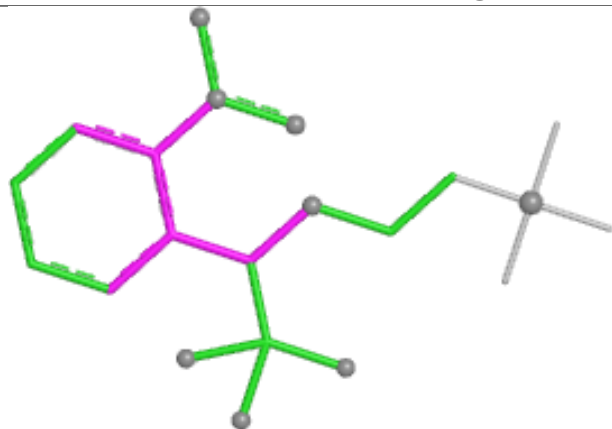


Torsions

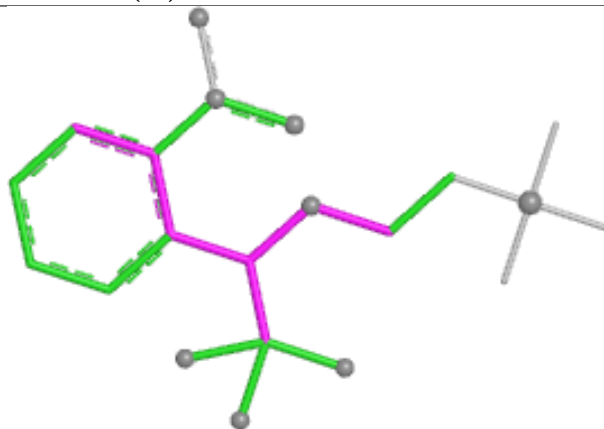


Rings

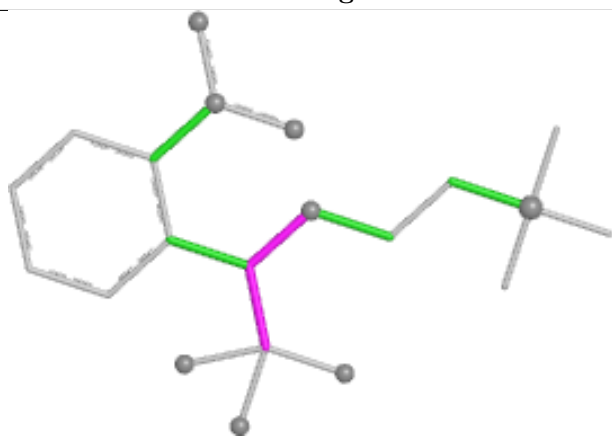
Ligand CFQ A 1537 (B)



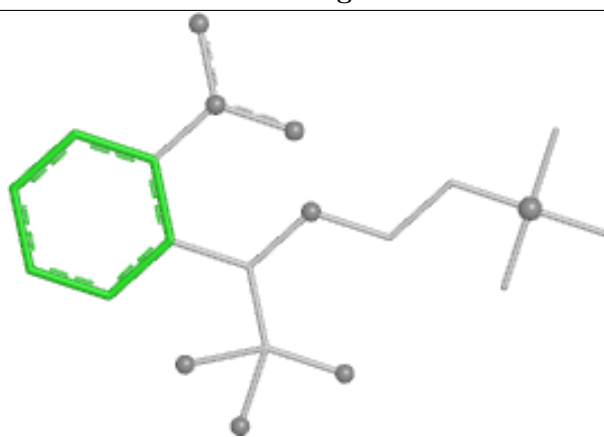
Bond lengths



Bond angles

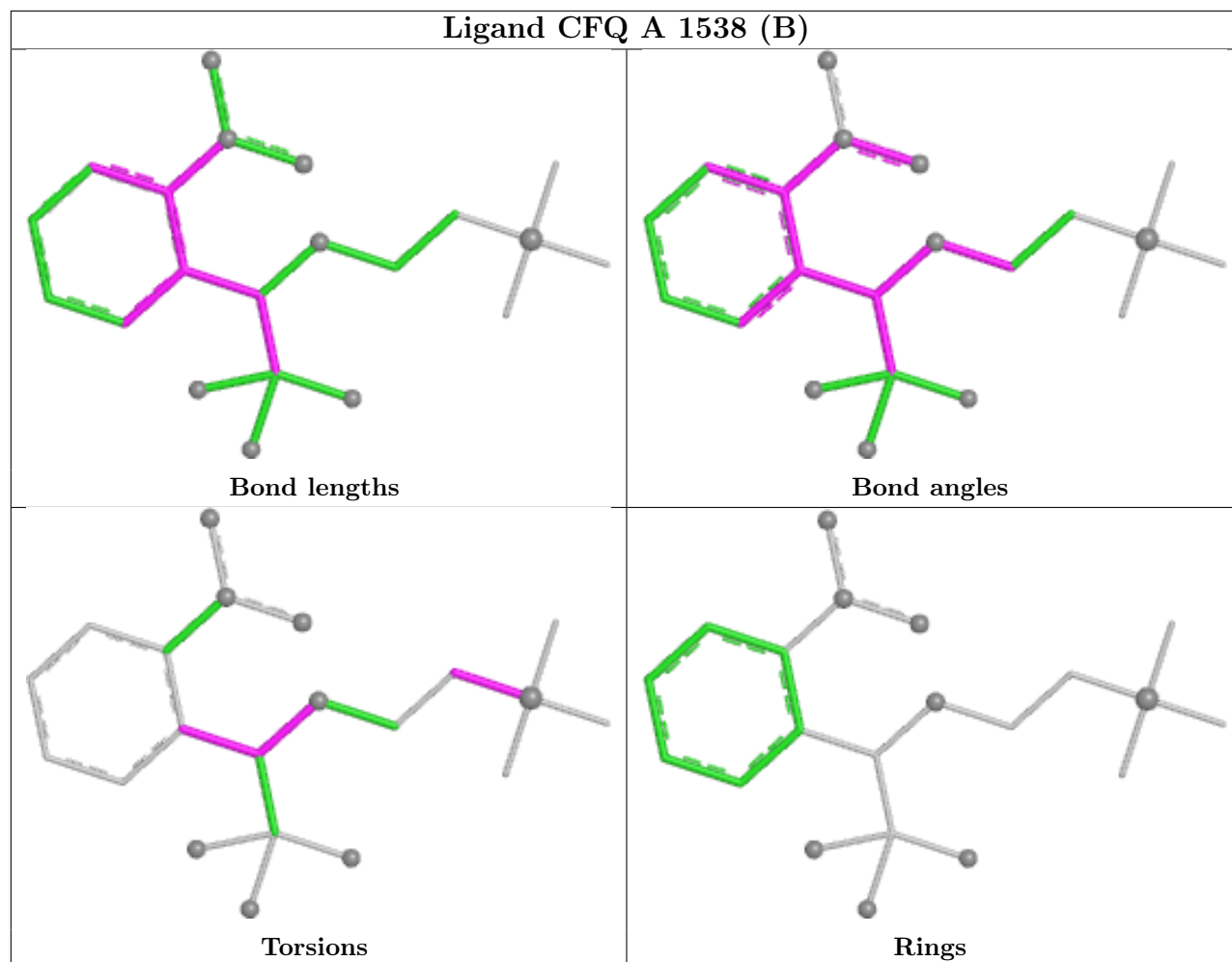


Torsions

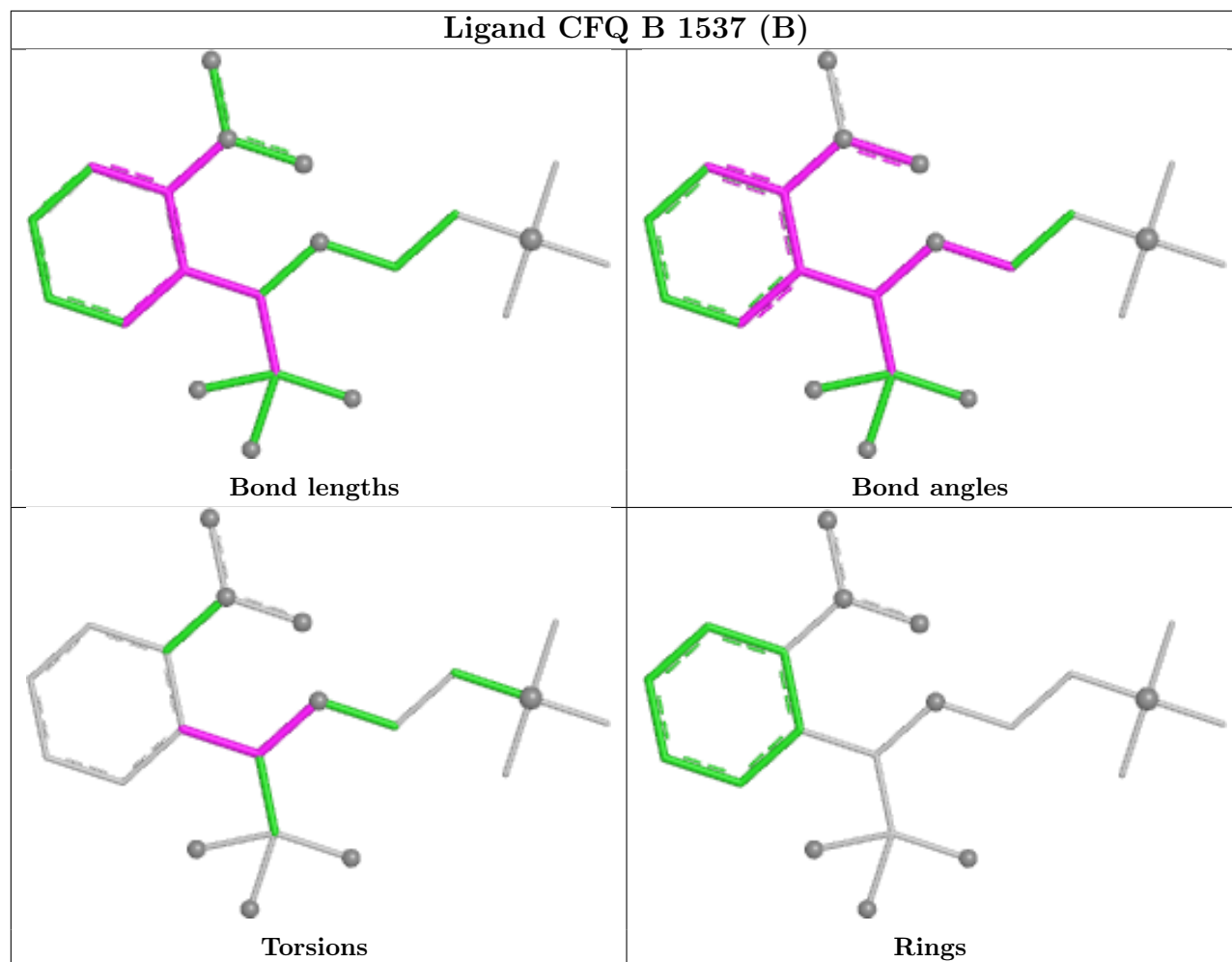


Rings

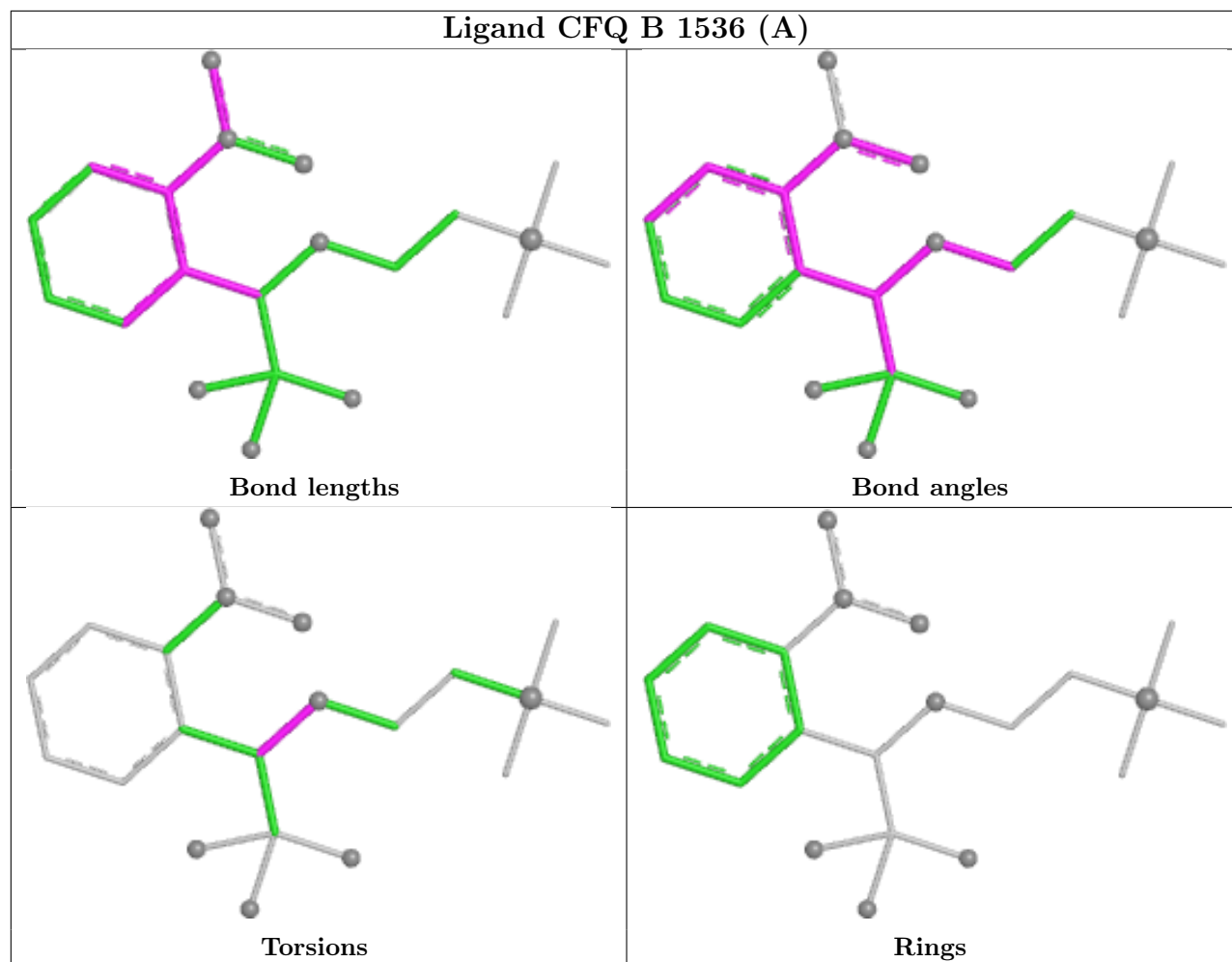
Ligand CFQ A 1538 (B)



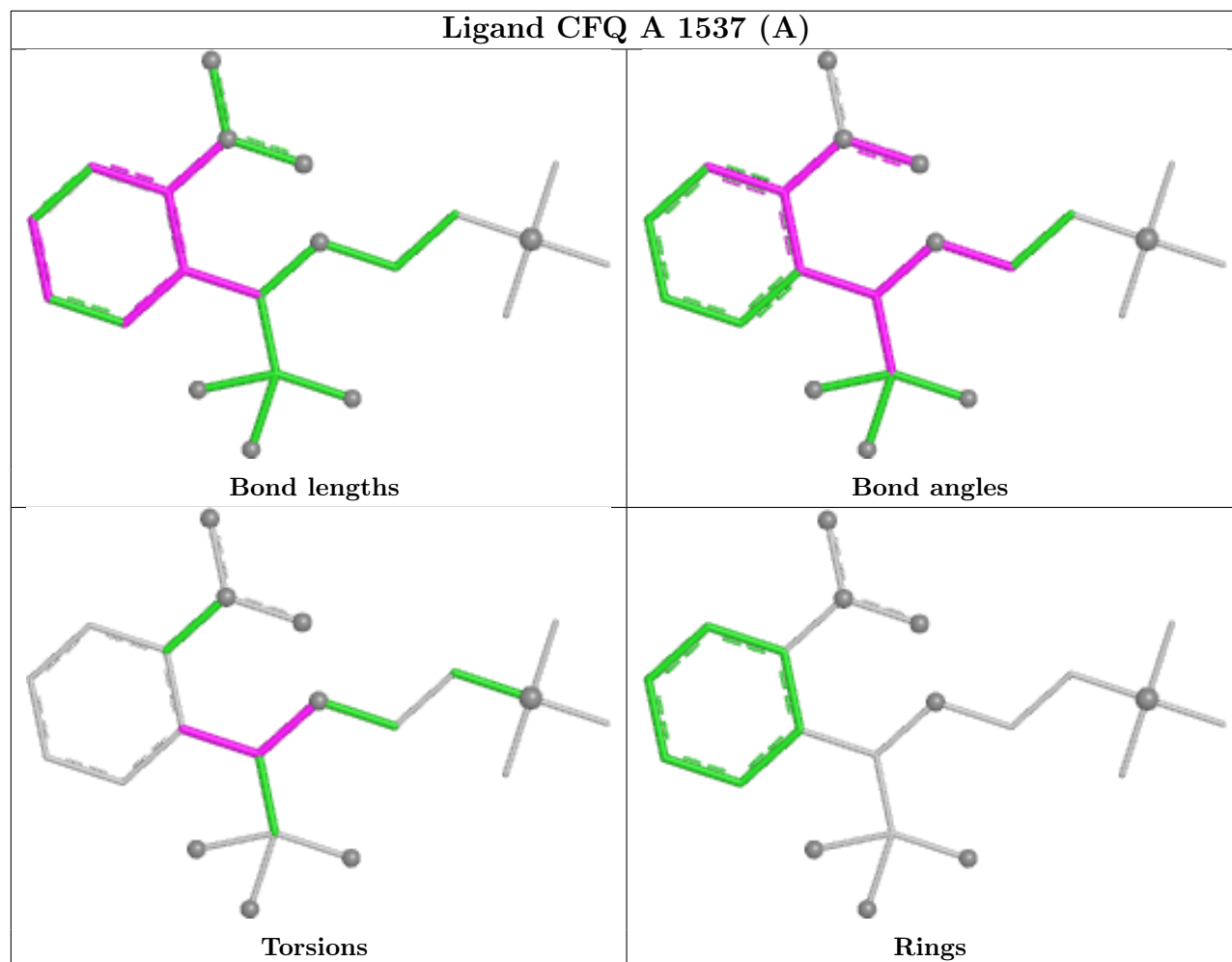
Ligand CFQ B 1537 (B)



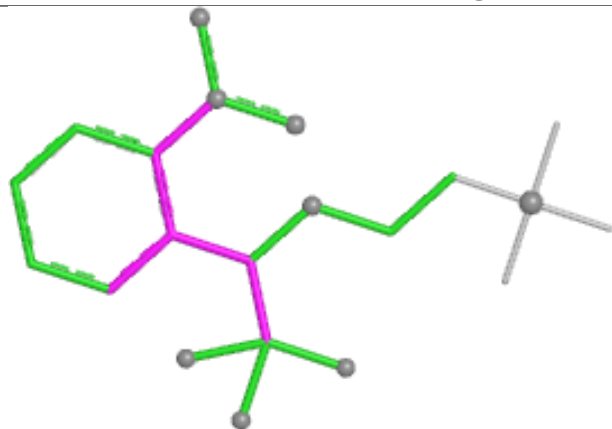
Ligand CFQ B 1536 (A)



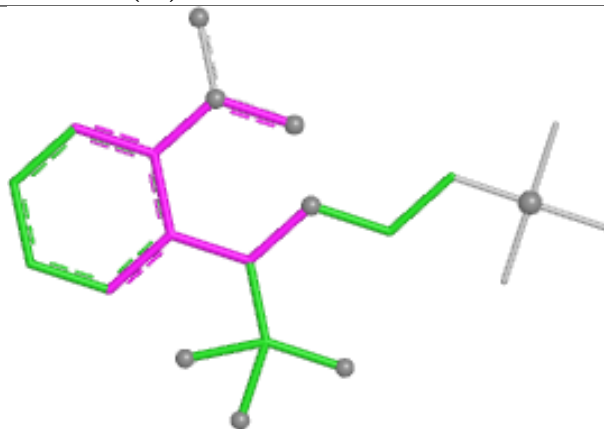
Ligand CFQ A 1537 (A)



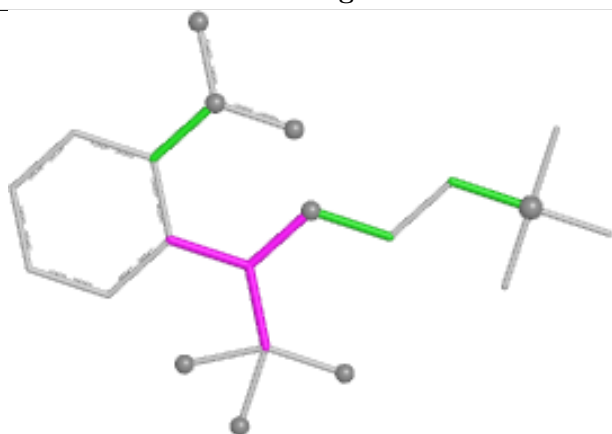
Ligand CFQ A 1538 (A)



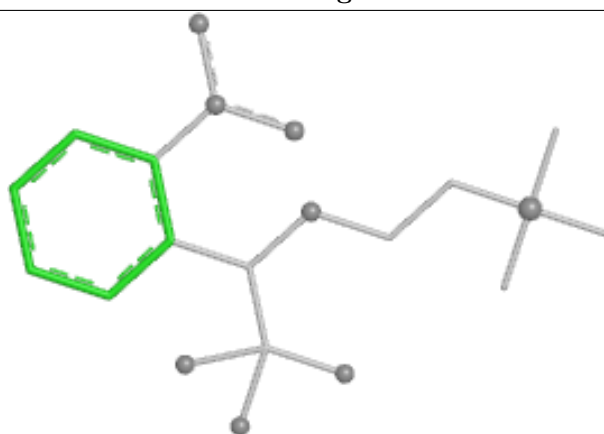
Bond lengths



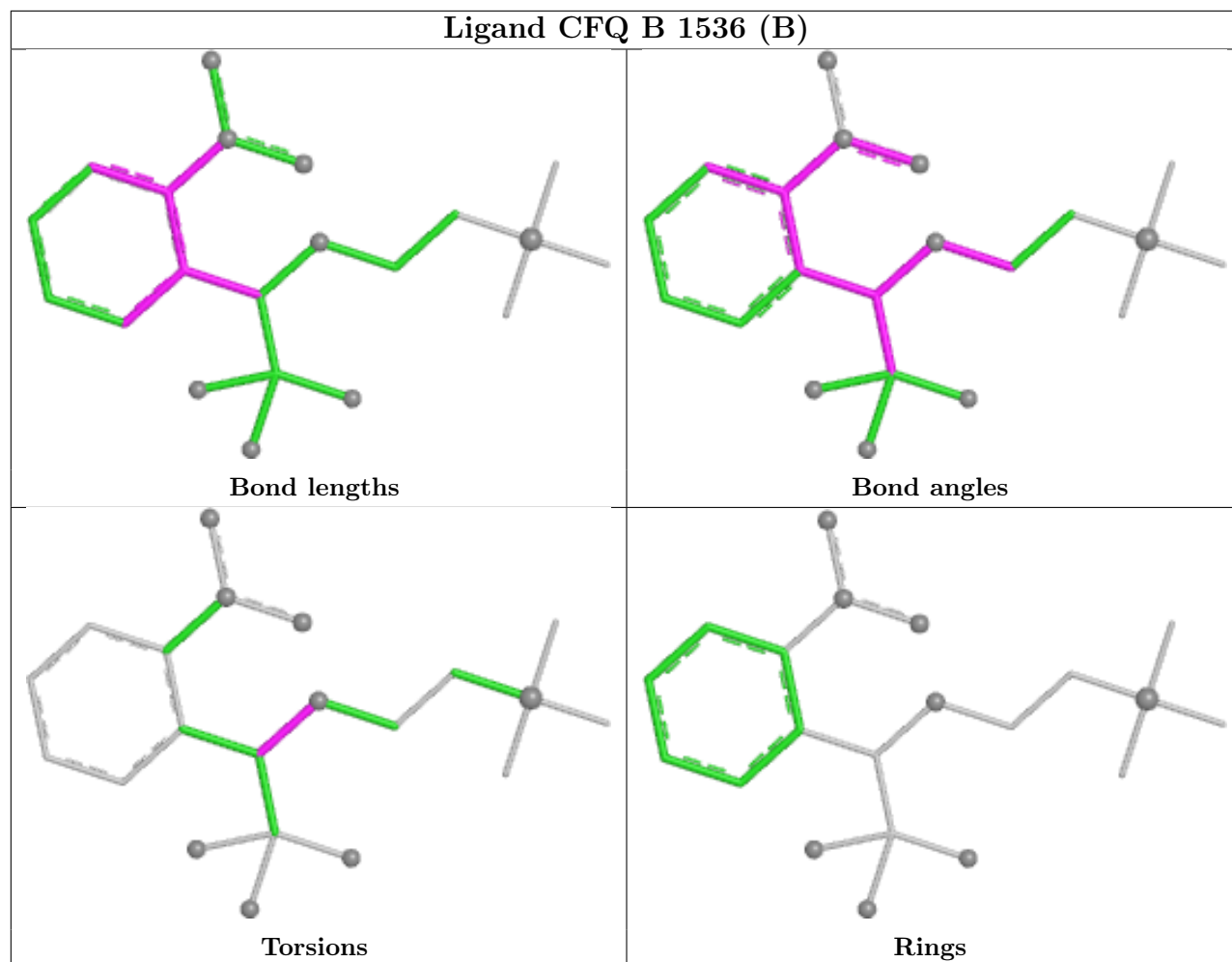
Bond angles



Torsions



Rings



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	528/537 (98%)	-0.16	0 100 100	9, 19, 26, 31	528 (100%)
1	B	532/537 (99%)	-0.14	2 (0%) 88 76	8, 19, 28, 32	532 (100%)
All	All	1060/1074 (98%)	-0.15	2 (0%) 91 83	8, 19, 27, 32	1060 (100%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183[A]	ASN	2.1
1	B	459[A]	THR	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1539[A]	14/15	0.40	0.14	63,66,68,70	14
4	NAG	A	1539[B]	14/15	0.40	0.14	61,63,63,63	14
4	NAG	B	1538[A]	14/15	0.61	0.12	59,61,64,64	14

Continued on next page...

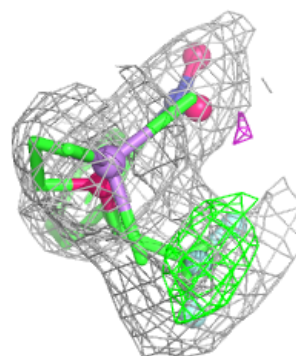
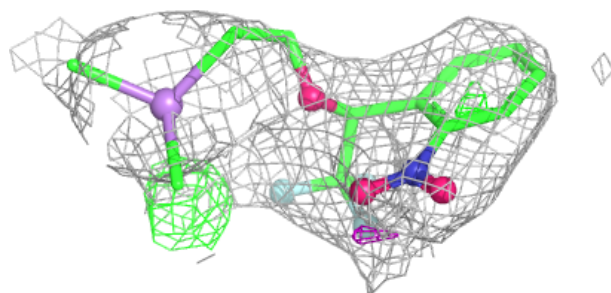
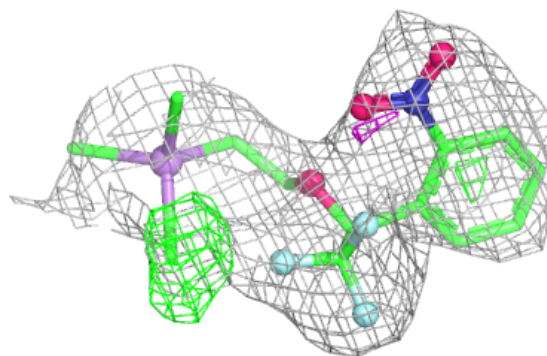
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1538[B]	14/15	0.61	0.12	57,59,60,60	14
4	NAG	B	1539[A]	14/15	0.70	0.11	40,44,46,48	14
4	NAG	B	1539[B]	14/15	0.70	0.11	42,43,44,45	14
4	NAG	A	1540[A]	14/15	0.71	0.12	50,52,54,55	14
4	NAG	A	1540[B]	14/15	0.71	0.12	44,46,48,48	14
2	CL	A	1536[A]	1/1	0.85	0.08	48,48,48,48	1
2	CL	A	1536[B]	1/1	0.85	0.08	50,50,50,50	1
3	CFQ	A	1538[A]	21/21	0.91	0.13	47,50,53,55	21
3	CFQ	A	1538[B]	21/21	0.91	0.13	47,47,49,50	21
3	CFQ	B	1536[A]	21/21	0.91	0.11	56,60,66,67	21
3	CFQ	B	1536[B]	21/21	0.91	0.11	53,53,57,57	21
3	CFQ	A	1537[A]	21/21	0.93	0.11	47,52,58,59	21
3	CFQ	A	1537[B]	21/21	0.93	0.11	38,40,48,50	21
3	CFQ	B	1537[A]	21/21	0.93	0.12	50,52,55,58	21
3	CFQ	B	1537[B]	21/21	0.93	0.12	49,50,51,51	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.

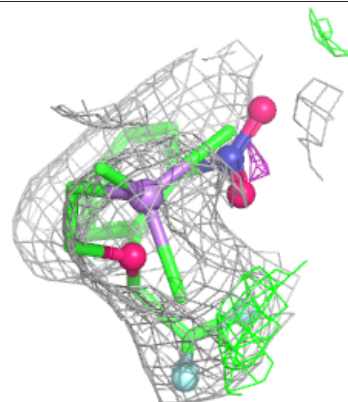
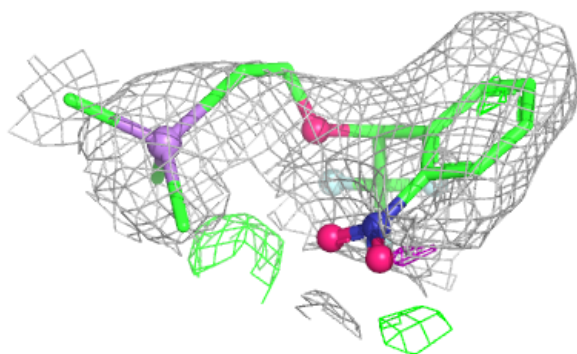
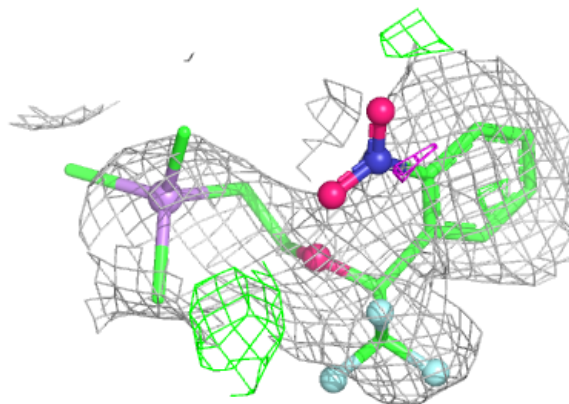
Electron density around CFQ A 1538 (A):

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



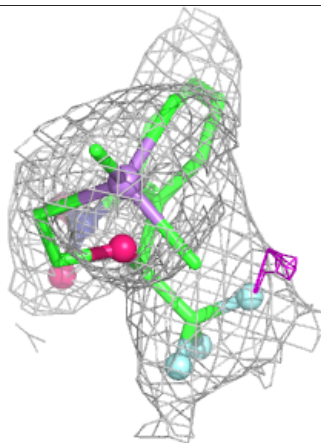
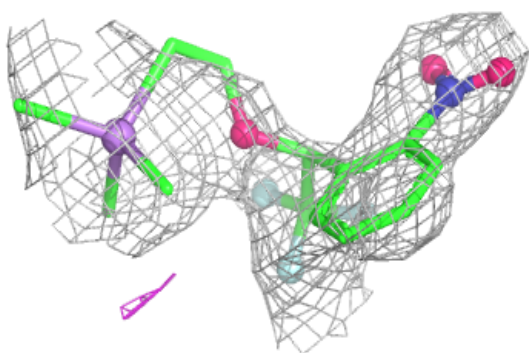
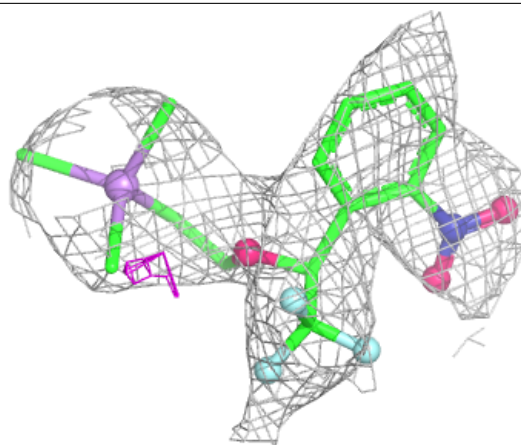
Electron density around CFQ A 1538 (B):

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



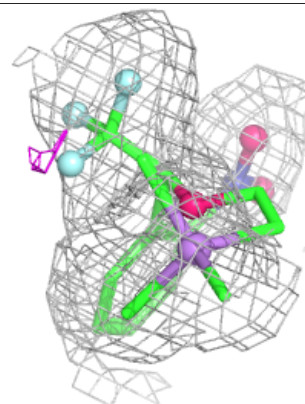
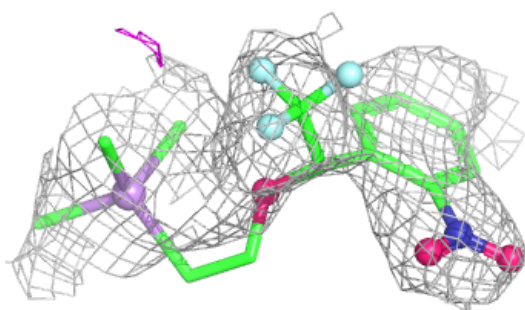
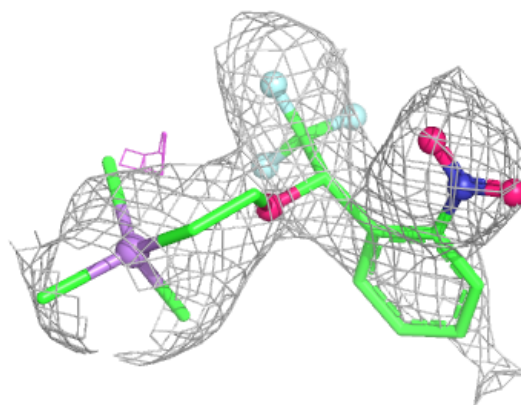
Electron density around CFQ B 1536 (A):

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

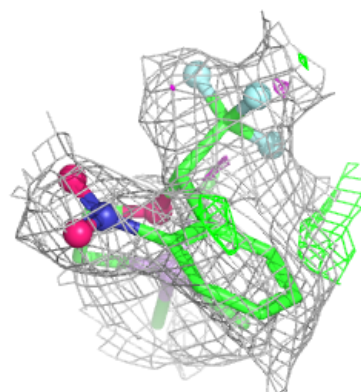
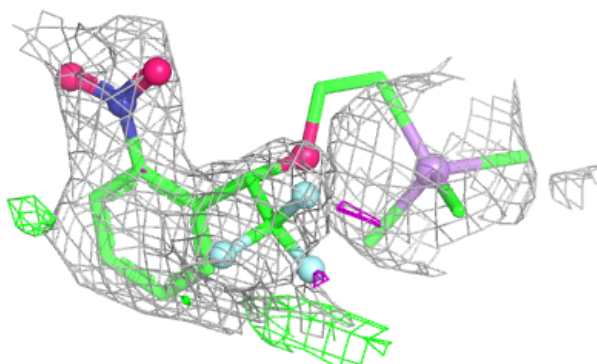
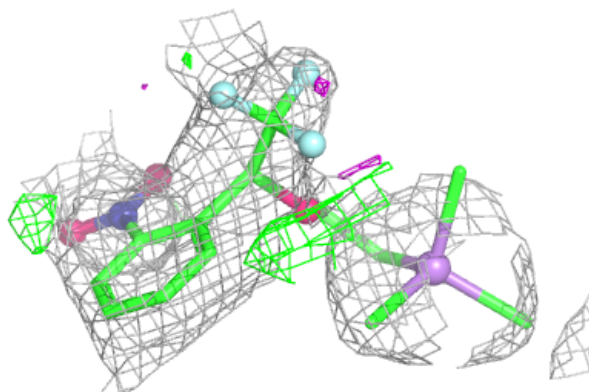


Electron density around CFQ B 1536 (B):

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

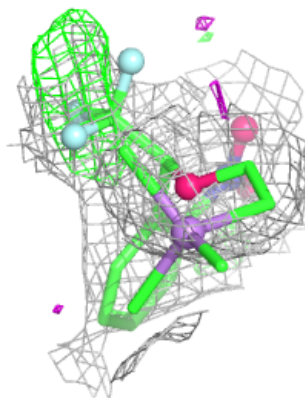
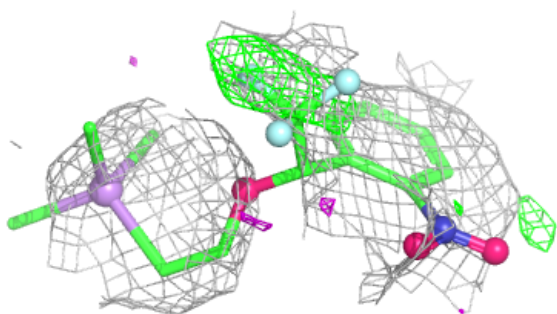
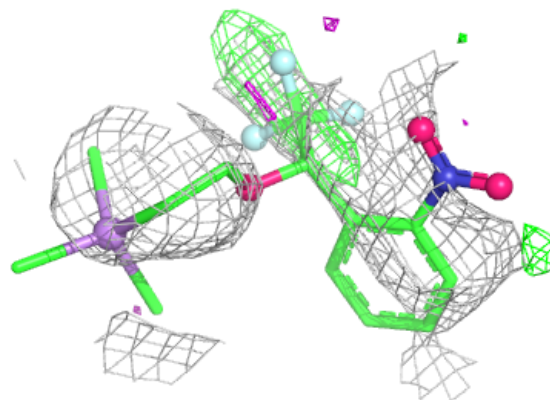
**Electron density around CFQ A 1537 (A):**

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

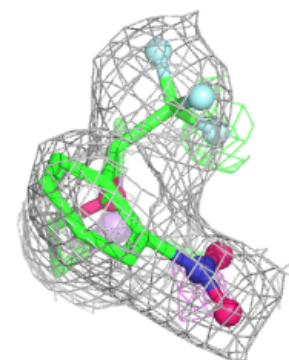
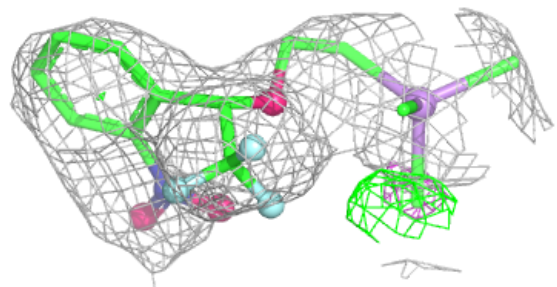
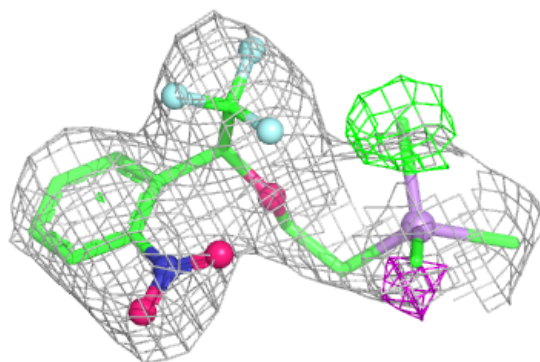


Electron density around CFQ A 1537 (B):

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

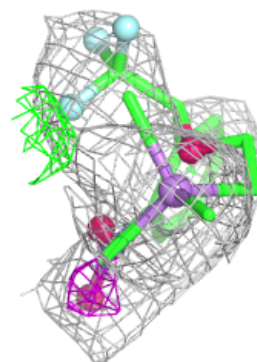
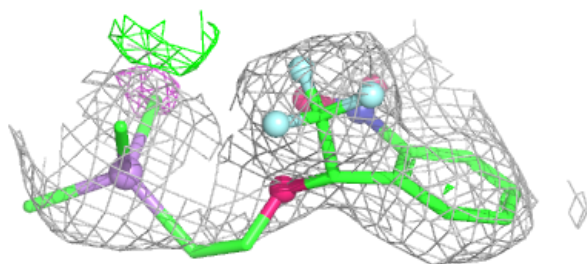
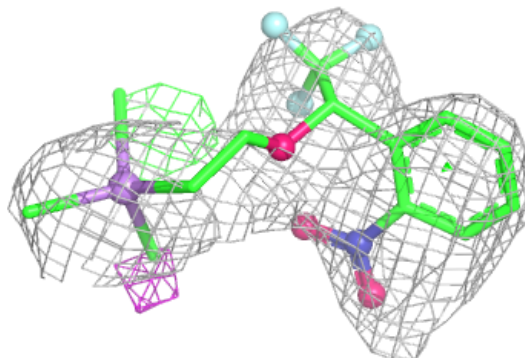
**Electron density around CFQ B 1537 (A):**

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.