



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 03:46 AM EDT

PDB ID : 2GH6  
Title : Crystal structure of a HDAC-like protein with 9,9,9-trifluoro-8-oxo-N-phenyl nonan amide bound  
Authors : Nielsen, T.K.; Hildmann, C.; Riester, D.; Wegener, D.; Schwienhorst, A.; Ficner, R.  
Deposited on : 2006-03-26  
Resolution : 2.20 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

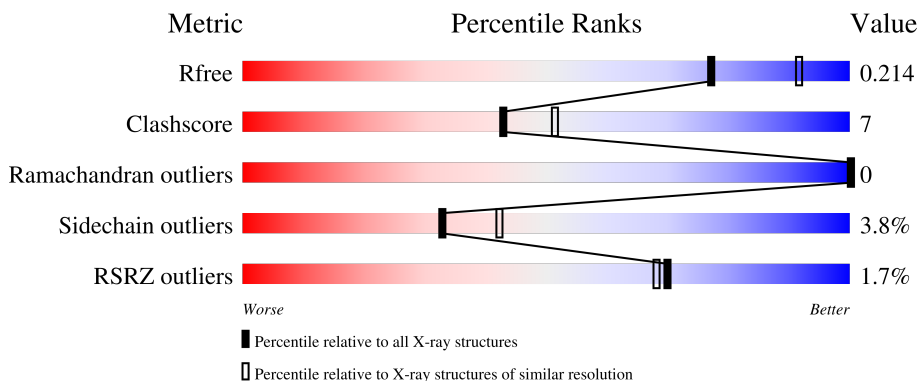
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	369	 84% 15% .
1	B	369	 2% 86% 14% .
1	C	369	 % 85% 13% ..
1	D	369	 4% 83% 15% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11879 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 Histone deacetylase-like amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	367	2747	1724	494	511	18	0	0	0
1	B	367	2747	1724	494	511	18	0	0	0
1	C	367	2747	1724	494	511	18	0	0	0
1	D	367	2747	1724	494	511	18	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	insertion	UNP Q70I53
A	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
B	1	MET	-	insertion	UNP Q70I53
B	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
C	1	MET	-	insertion	UNP Q70I53
C	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
D	1	MET	-	insertion	UNP Q70I53
D	251	PRO	HIS	SEE REMARK 999	UNP Q70I53

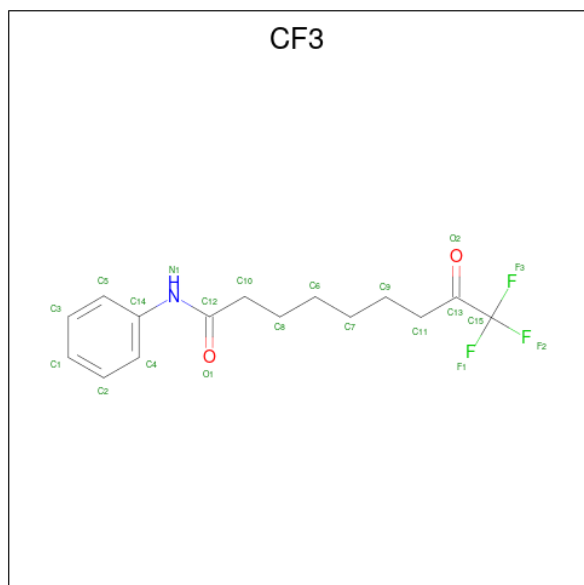
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is 9,9,9-TRIFLUORO-8-OXO-N-PHENYLNONANAMIDE (three-letter code: CF3) (formula: C<sub>15</sub>H<sub>18</sub>F<sub>3</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O 24 17 3 1 3	0	1
4	B	1	Total C F N O 24 17 3 1 3	0	1
4	C	1	Total C F N O 24 17 3 1 3	0	1
4	D	1	Total C F N O 24 17 3 1 3	0	1

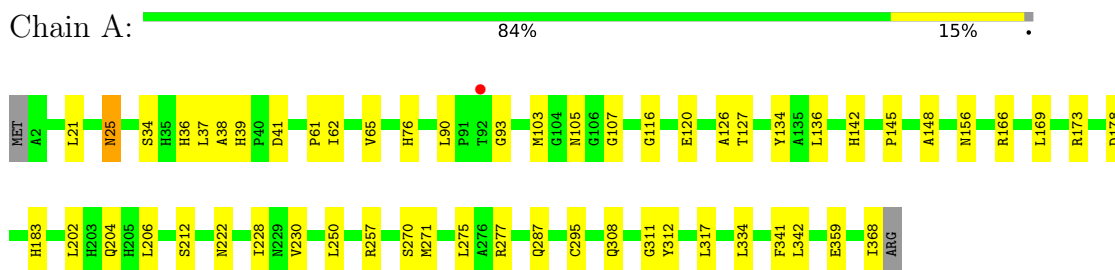
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total 214	O 214	0	0
5	B	220	Total 220	O 220	0	0
5	C	187	Total 187	O 187	0	0
5	D	162	Total 162	O 162	0	0

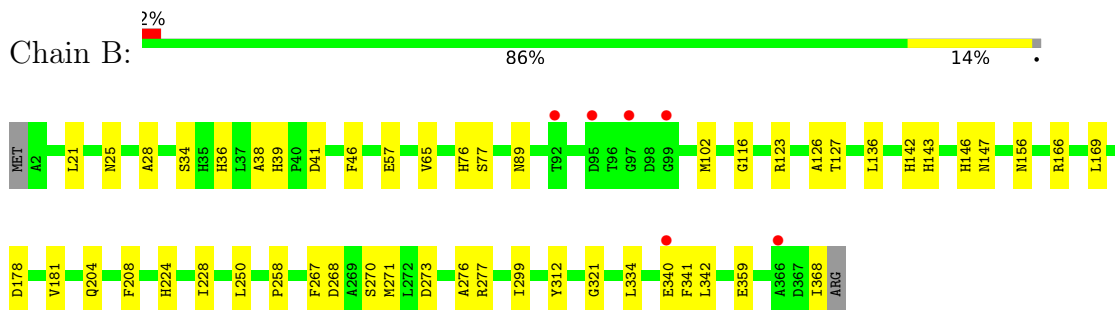
### 3 Residue-property plots [i](#)

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.

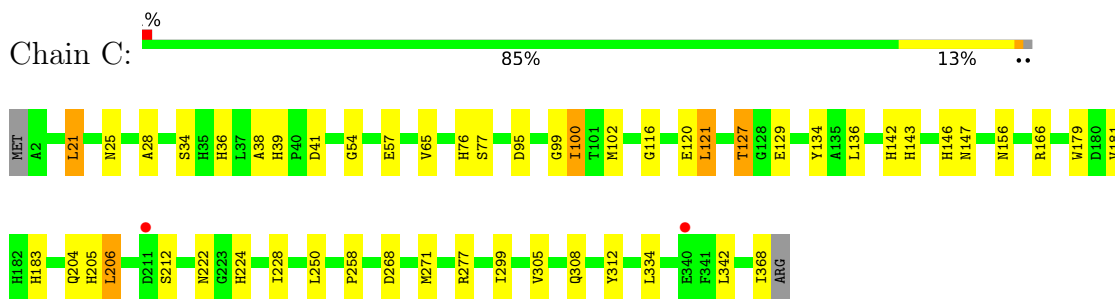
- Molecule 1: Histone deacetylase-like amidohydrolase



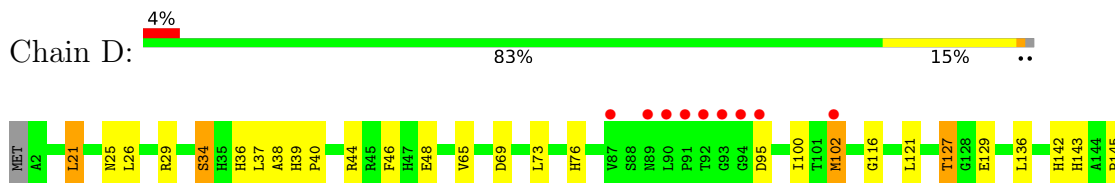
- Molecule 1: Histone deacetylase-like amidohydrolase

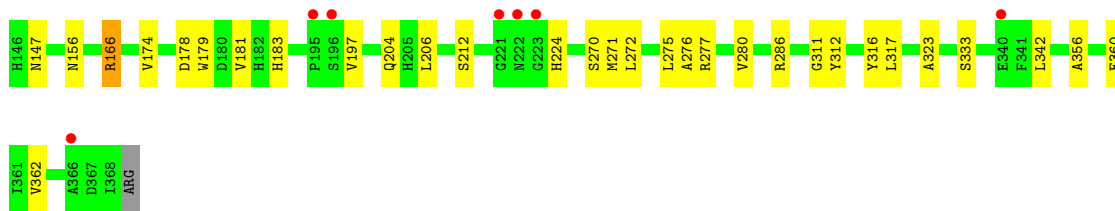


- Molecule 1: Histone deacetylase-like amidohydrolase



- Molecule 1: Histone deacetylase-like amidohydrolase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.51Å 94.90Å 123.30Å 90.00° 104.28° 90.00°	Depositor
Resolution (Å)	39.84 – 2.20 39.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.84-2.20) 98.9 (39.83-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.158 , 0.214 0.158 , 0.214	Depositor DCC
$R_{free}$ test set	3863 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CF3, K, ZN

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	0.71	0/2815	0.76	3/3840 (0.1%)
1	B	0.74	0/2815	0.75	4/3840 (0.1%)
1	C	0.72	0/2815	0.73	2/3840 (0.1%)
1	D	0.71	0/2815	0.74	2/3840 (0.1%)
All	All	0.72	0/11260	0.75	11/15360 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	166	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	B	166	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	166	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	166	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	178	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	334	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	166	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	178	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	178	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	166	ARG	NE-CZ-NH2	-5.07	117.77	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	2747	0	2662	40	0
1	B	2747	0	2662	35	0
1	C	2747	0	2662	37	0
1	D	2747	0	2662	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	24	0	8	1	0
4	B	24	0	8	3	0
4	C	24	0	8	3	0
4	D	24	0	8	3	0
5	A	214	0	0	7	0
5	B	220	0	0	6	0
5	C	187	0	0	4	0
5	D	162	0	0	3	0
All	All	11879	0	10680	149	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 7.

All (149) 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:A:287:GLN:HG2	5:A:9618:HOH:O	1.67	0.95
1:A:36:HIS:HD2	1:A:38:ALA:H	1.15	0.95
1:B:204:GLN:HE22	1:B:277:ARG:H	1.16	0.94
1:D:204:GLN:HE22	1:D:277:ARG:H	1.15	0.92
1:C:36:HIS:HD2	1:C:38:ALA:H	1.13	0.88
1:A:204:GLN:HE22	1:A:277:ARG:H	1.21	0.88
1:C:204:GLN:HE22	1:C:277:ARG:H	1.22	0.86
1:D:76:HIS:HE1	1:D:156:ASN:H	1.22	0.85
1:D:36:HIS:HD2	1:D:38:ALA:H	1.26	0.84
1:B:36:HIS:HD2	1:B:38:ALA:H	1.25	0.81
1:D:36:HIS:CD2	1:D:38:ALA:H	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:CD2	1:A:38:ALA:H	1.99	0.79
1:C:76:HIS:HE1	1:C:156:ASN:H	1.29	0.79
1:A:76:HIS:HE1	1:A:156:ASN:H	1.27	0.79
1:B:25:ASN:HD22	1:B:28:ALA:H	1.32	0.78
1:B:143:HIS:CD2	4:B:9552[A]:CF3:H112	2.19	0.78
1:B:123:ARG:O	1:B:127:THR:HG23	1.84	0.77
1:D:224:HIS:HE1	5:D:9853:HOH:O	1.66	0.77
1:C:100:ILE:O	1:C:100:ILE:HG12	1.82	0.77
1:C:76:HIS:CE1	1:C:156:ASN:H	2.04	0.76
1:D:76:HIS:CE1	1:D:156:ASN:H	2.06	0.74
1:C:36:HIS:CD2	1:C:38:ALA:H	2.03	0.74
1:C:127:THR:HG22	1:C:129:GLU:H	1.54	0.73
1:D:204:GLN:NE2	1:D:277:ARG:H	1.87	0.72
1:B:143:HIS:NE2	4:B:9552[A]:CF3:H112	2.04	0.72
1:C:143:HIS:CD2	4:C:9652[A]:CF3:H112	2.25	0.72
1:B:76:HIS:HE1	1:B:156:ASN:H	1.37	0.71
1:D:143:HIS:CD2	4:D:9752[A]:CF3:H112	2.25	0.71
1:B:76:HIS:CE1	1:B:156:ASN:H	2.09	0.71
1:A:76:HIS:CE1	1:A:156:ASN:H	2.08	0.70
1:B:36:HIS:CD2	1:B:38:ALA:H	2.07	0.70
1:C:121:LEU:HD13	1:C:305:VAL:HG13	1.72	0.69
1:B:127:THR:HG22	5:B:9679:HOH:O	1.91	0.69
1:A:287:GLN:NE2	5:A:9618:HOH:O	2.26	0.67
1:B:204:GLN:NE2	1:B:277:ARG:H	1.90	0.67
1:C:228:ILE:HD11	1:C:368:ILE:HD11	1.76	0.66
1:C:127:THR:HG21	5:C:9691:HOH:O	1.96	0.65
1:A:204:GLN:NE2	1:A:277:ARG:H	1.93	0.65
1:B:39:HIS:HD2	1:B:41:ASP:H	1.45	0.64
1:D:204:GLN:HE22	1:D:277:ARG:N	1.92	0.64
1:A:312:TYR:OH	4:A:9452[B]:CF3:H111	1.97	0.64
1:A:37:LEU:HD13	1:A:275:LEU:HD21	1.81	0.62
1:A:359:GLU:HG3	5:A:9605:HOH:O	2.00	0.61
1:A:39:HIS:HD2	1:A:41:ASP:H	1.48	0.61
1:C:127:THR:CG2	1:C:129:GLU:H	2.12	0.61
1:C:205:HIS:CE1	1:C:206:LEU:HD13	2.37	0.59
1:B:25:ASN:ND2	1:B:28:ALA:H	1.99	0.59
1:D:37:LEU:HD13	1:D:275:LEU:HD21	1.84	0.59
1:C:25:ASN:HD22	1:C:28:ALA:H	1.50	0.57
1:C:77:SER:OG	1:C:147:ASN:ND2	2.31	0.57
1:A:34:SER:HB2	1:C:34:SER:HB2	1.85	0.57
1:D:36:HIS:HD2	1:D:38:ALA:N	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:GLU:HG2	5:B:9639:HOH:O	2.05	0.57
1:C:143:HIS:NE2	4:C:9652[A]:CF3:H112	2.20	0.56
1:A:65:VAL:O	1:A:116:GLY:HA3	2.05	0.56
1:C:65:VAL:O	1:C:116:GLY:HA3	2.05	0.56
1:D:127:THR:HG22	1:D:129:GLU:H	1.70	0.56
1:D:143:HIS:O	1:D:145:PRO:HD3	2.06	0.56
1:A:36:HIS:HD2	1:A:38:ALA:N	1.94	0.56
1:B:146:HIS:HE1	5:B:9712:HOH:O	1.89	0.56
1:C:258:PRO:HD2	1:C:299:ILE:HD12	1.89	0.55
1:A:228:ILE:HD11	1:A:368:ILE:HD11	1.87	0.54
1:C:204:GLN:NE2	1:C:277:ARG:H	1.99	0.54
1:C:271:MET:HG2	1:C:342:LEU:HD22	1.89	0.54
1:A:173:ARG:HD2	5:A:9462:HOH:O	2.05	0.54
1:B:258:PRO:HD2	1:B:299:ILE:HD12	1.91	0.53
1:B:65:VAL:O	1:B:116:GLY:HA3	2.08	0.53
1:A:271:MET:HG2	1:A:342:LEU:HD22	1.89	0.53
1:A:103:MET:HG2	1:A:107:GLY:HA3	1.91	0.52
1:A:183:HIS:HD2	1:A:212:SER:OG	1.93	0.52
1:A:204:GLN:HE22	1:A:277:ARG:N	2.00	0.52
1:B:34:SER:HB2	1:D:34:SER:HB2	1.92	0.51
1:C:224:HIS:HD2	5:C:9806:HOH:O	1.93	0.51
1:D:312:TYR:OH	4:D:9752[B]:CF3:H111	2.10	0.50
1:D:311:GLY:HA3	1:D:317:LEU:HD12	1.93	0.50
1:B:77:SER:OG	1:B:147:ASN:ND2	2.40	0.50
1:D:311:GLY:HA3	1:D:317:LEU:CD1	2.43	0.49
1:B:312:TYR:OH	4:B:9552[B]:CF3:H111	2.12	0.49
1:C:39:HIS:HD2	1:C:41:ASP:H	1.61	0.49
1:A:105:ASN:ND2	5:A:9571:HOH:O	2.46	0.49
1:A:311:GLY:HA3	1:A:317:LEU:HD12	1.93	0.49
1:D:143:HIS:NE2	4:D:9752[A]:CF3:H112	2.27	0.48
1:A:287:GLN:CG	5:A:9618:HOH:O	2.43	0.48
1:D:39:HIS:CG	1:D:40:PRO:HD2	2.48	0.48
1:A:65:VAL:HG23	1:A:120:GLU:HG3	1.95	0.48
1:A:127:THR:HG21	5:A:9499:HOH:O	2.13	0.48
1:A:39:HIS:CD2	1:A:41:ASP:H	2.31	0.47
1:B:228:ILE:HD11	1:B:368:ILE:HD11	1.97	0.47
1:C:334:LEU:HD21	1:D:29:ARG:HB2	1.96	0.47
1:C:54:GLY:O	1:C:57:GLU:HG2	2.14	0.46
1:D:69:ASP:O	1:D:73:LEU:HG	2.15	0.46
1:C:146:HIS:HE1	5:C:9705:HOH:O	1.98	0.46
1:B:271:MET:HG2	1:B:342:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:HIS:HD2	1:D:212:SER:OG	1.98	0.46
1:B:181:VAL:HG12	1:B:268:ASP:CG	2.36	0.46
1:B:39:HIS:HE1	5:B:9710:HOH:O	1.98	0.46
1:B:126:ALA:CB	1:B:169:LEU:HD13	2.45	0.46
1:C:65:VAL:HG23	1:C:120:GLU:HG3	1.99	0.45
1:A:126:ALA:CB	1:A:169:LEU:HD13	2.46	0.45
1:A:134:TYR:OH	1:A:308:GLN:NE2	2.50	0.45
1:B:204:GLN:HE22	1:B:277:ARG:N	1.98	0.45
1:B:39:HIS:CD2	1:B:41:ASP:H	2.29	0.44
1:D:181:VAL:HG11	1:D:276:ALA:HB2	1.98	0.44
1:D:272:LEU:HD12	1:D:316:TYR:HB2	1.98	0.44
1:B:39:HIS:CE1	5:B:9710:HOH:O	2.70	0.44
1:C:312:TYR:OH	4:C:9652[B]:CF3:H111	2.17	0.44
1:D:271:MET:HG2	1:D:342:LEU:HD22	1.99	0.44
1:A:90:LEU:HB2	1:A:93:GLY:HA2	1.99	0.44
1:D:21:LEU:HD22	1:D:100:ILE:HD12	1.98	0.44
1:D:65:VAL:O	1:D:116:GLY:HA3	2.17	0.44
1:C:134:TYR:OH	1:C:308:GLN:NE2	2.51	0.44
1:A:61:PRO:O	1:A:62:ILE:HD13	2.18	0.43
1:D:270:SER:HA	1:D:280:VAL:O	2.18	0.43
1:A:311:GLY:HA3	1:A:317:LEU:CD1	2.47	0.43
1:A:145:PRO:HD2	1:A:148:ALA:O	2.18	0.43
1:B:224:HIS:HE1	5:B:9747:HOH:O	2.00	0.43
1:D:356:ALA:O	1:D:360:GLU:HG3	2.19	0.42
1:B:181:VAL:HG11	1:B:276:ALA:HB2	2.01	0.42
1:D:174:VAL:O	1:D:197:VAL:HA	2.18	0.42
1:C:222:ASN:HD22	1:C:222:ASN:HA	1.72	0.42
1:D:127:THR:HG22	1:D:129:GLU:N	2.33	0.42
1:C:95:ASP:OD1	1:C:99:GLY:HA2	2.20	0.42
1:C:181:VAL:HG12	1:C:268:ASP:CG	2.40	0.42
1:D:44:ARG:NH1	1:D:48:GLU:OE2	2.48	0.42
1:D:95:ASP:HA	1:D:102:MET:SD	2.60	0.41
1:A:250:LEU:HD22	1:A:295:CYS:HB2	2.01	0.41
1:D:36:HIS:CD2	1:D:38:ALA:HB3	2.55	0.41
1:C:36:HIS:HD2	1:C:38:ALA:N	1.97	0.41
1:A:25:ASN:C	1:A:25:ASN:HD22	2.23	0.41
1:C:39:HIS:CD2	1:C:41:ASP:H	2.39	0.41
1:A:183:HIS:CD2	1:A:212:SER:OG	2.73	0.41
1:A:222:ASN:HD22	1:A:222:ASN:HA	1.68	0.41
1:A:202:LEU:HD23	1:A:230:VAL:HB	2.03	0.41
1:C:183:HIS:HD2	1:C:212:SER:OG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PHE:CZ	1:B:321:GLY:HA2	2.56	0.40
1:D:147:ASN:CG	1:D:147:ASN:O	2.60	0.40
1:D:286:ARG:HB2	1:D:323:ALA:HB1	2.03	0.40
1:D:333:SER:HB3	5:D:9876:HOH:O	2.20	0.40
1:C:76:HIS:HE1	1:C:156:ASN:N	2.08	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	365/369 (99%)	354 (97%)	11 (3%)	0	100	100
1	B	365/369 (99%)	354 (97%)	11 (3%)	0	100	100
1	C	365/369 (99%)	352 (96%)	13 (4%)	0	100	100
1	D	365/369 (99%)	355 (97%)	10 (3%)	0	100	100
All	All	1460/1476 (99%)	1415 (97%)	45 (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	280/282 (99%)	273 (98%)	7 (2%)	47	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	280/282 (99%)	269 (96%)	11 (4%)	32	41
1	C	280/282 (99%)	270 (96%)	10 (4%)	35	45
1	D	280/282 (99%)	266 (95%)	14 (5%)	24	30
All	All	1120/1128 (99%)	1078 (96%)	42 (4%)	33	42

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	136	LEU
1	A	142	HIS
1	A	206	LEU
1	A	257	ARG
1	A	270	SER
1	A	334	LEU
1	B	21	LEU
1	B	46	PHE
1	B	57	GLU
1	B	89	ASN
1	B	102	MET
1	B	136	LEU
1	B	142	HIS
1	B	250	LEU
1	B	270	SER
1	B	273	ASP
1	B	340	GLU
1	C	21	LEU
1	C	100	ILE
1	C	102	MET
1	C	121	LEU
1	C	127	THR
1	C	136	LEU
1	C	142	HIS
1	C	179	TRP
1	C	206	LEU
1	C	250	LEU
1	D	21	LEU
1	D	25	ASN
1	D	26	LEU
1	D	34	SER
1	D	46	PHE

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Mol	Chain	Res	Type
1	D	102	MET
1	D	121	LEU
1	D	127	THR
1	D	136	LEU
1	D	142	HIS
1	D	166	ARG
1	D	179	TRP
1	D	206	LEU
1	D	362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	36	HIS
1	A	39	HIS
1	A	76	HIS
1	A	89	ASN
1	A	105	ASN
1	A	147	ASN
1	A	183	HIS
1	A	204	GLN
1	A	222	ASN
1	A	224	HIS
1	A	227	ASN
1	A	229	ASN
1	A	308	GLN
1	B	25	ASN
1	B	36	HIS
1	B	39	HIS
1	B	76	HIS
1	B	147	ASN
1	B	204	GLN
1	B	224	HIS
1	B	227	ASN
1	B	229	ASN
1	B	308	GLN
1	C	25	ASN
1	C	31	GLN
1	C	36	HIS
1	C	39	HIS
1	C	76	HIS

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Mol	Chain	Res	Type
1	C	105	ASN
1	C	146	HIS
1	C	147	ASN
1	C	183	HIS
1	C	204	GLN
1	C	222	ASN
1	C	224	HIS
1	C	227	ASN
1	C	229	ASN
1	C	308	GLN
1	D	25	ASN
1	D	31	GLN
1	D	36	HIS
1	D	76	HIS
1	D	105	ASN
1	D	147	ASN
1	D	183	HIS
1	D	204	GLN
1	D	227	ASN
1	D	229	ASN
1	D	308	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 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	CF3	B	9552[A]	2	21,21,21	0.96	1 (4%)	26,27,27	1.22	2 (7%)
4	CF3	A	9452[A]	2	21,21,21	1.07	2 (9%)	26,27,27	1.25	5 (19%)
4	CF3	B	9552[B]	2	21,21,21	1.09	2 (9%)	26,27,27	1.05	2 (7%)
4	CF3	A	9452[B]	2	21,21,21	1.18	2 (9%)	26,27,27	1.11	3 (11%)
4	CF3	C	9652[A]	2	21,21,21	1.20	2 (9%)	26,27,27	1.16	3 (11%)
4	CF3	C	9652[B]	2	21,21,21	1.27	2 (9%)	26,27,27	1.12	3 (11%)
4	CF3	D	9752[A]	2	21,21,21	1.27	3 (14%)	26,27,27	1.24	3 (11%)
4	CF3	D	9752[B]	2	21,21,21	1.31	4 (19%)	26,27,27	1.04	3 (11%)

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	CF3	B	9552[A]	2	-	7/19/19/19	0/1/1/1
4	CF3	A	9452[A]	2	-	5/19/19/19	0/1/1/1
4	CF3	B	9552[B]	2	-	5/19/19/19	0/1/1/1
4	CF3	A	9452[B]	2	-	6/19/19/19	0/1/1/1
4	CF3	C	9652[A]	2	-	3/19/19/19	0/1/1/1
4	CF3	C	9652[B]	2	-	4/19/19/19	0/1/1/1
4	CF3	D	9752[A]	2	-	4/19/19/19	0/1/1/1
4	CF3	D	9752[B]	2	-	4/19/19/19	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	9752[A]	CF3	C10-C12	3.26	1.57	1.51
4	D	9752[B]	CF3	C10-C12	3.26	1.57	1.51
4	C	9652[A]	CF3	C10-C12	2.98	1.57	1.51
4	C	9652[B]	CF3	C10-C12	2.98	1.57	1.51
4	C	9652[B]	CF3	C11-C13	2.93	1.56	1.51
4	D	9752[A]	CF3	C14-N1	-2.50	1.36	1.41
4	D	9752[B]	CF3	C14-N1	-2.50	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	9452[A]	CF3	C10-C12	2.44	1.56	1.51
4	A	9452[B]	CF3	C10-C12	2.44	1.56	1.51
4	C	9652[A]	CF3	C11-C13	2.32	1.55	1.51
4	A	9452[B]	CF3	C11-C13	2.32	1.55	1.51
4	A	9452[A]	CF3	C11-C13	2.20	1.55	1.51
4	D	9752[A]	CF3	C11-C13	2.19	1.55	1.51
4	B	9552[B]	CF3	O2-C13	2.15	1.24	1.21
4	D	9752[B]	CF3	O2-C13	2.15	1.24	1.21
4	D	9752[B]	CF3	C11-C13	2.14	1.55	1.51
4	B	9552[A]	CF3	C14-N1	-2.10	1.37	1.41
4	B	9552[B]	CF3	C14-N1	-2.10	1.37	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	9752[A]	CF3	C9-C11-C13	3.37	119.35	113.62
4	B	9552[A]	CF3	C14-N1-C12	-2.96	122.32	127.50
4	B	9552[B]	CF3	C14-N1-C12	-2.96	122.32	127.50
4	D	9752[A]	CF3	F1-C15-C13	-2.88	98.16	112.62
4	C	9652[B]	CF3	C9-C11-C13	2.77	118.33	113.62
4	C	9652[A]	CF3	C9-C11-C13	2.70	118.22	113.62
4	B	9552[A]	CF3	F1-C15-C13	-2.48	100.18	112.62
4	C	9652[A]	CF3	F1-C15-C13	-2.40	100.61	112.62
4	D	9752[B]	CF3	F3-C15-C13	-2.36	100.78	112.62
4	A	9452[A]	CF3	O1-C12-C10	-2.35	117.72	122.02
4	A	9452[B]	CF3	O1-C12-C10	-2.35	117.72	122.02
4	A	9452[A]	CF3	F1-C15-C13	-2.30	101.08	112.62
4	D	9752[B]	CF3	O2-C13-C15	2.19	121.89	116.37
4	A	9452[A]	CF3	C7-C9-C11	-2.18	105.35	113.19
4	B	9552[B]	CF3	O2-C13-C15	2.18	121.87	116.37
4	A	9452[A]	CF3	C10-C12-N1	2.15	118.38	114.59
4	A	9452[B]	CF3	C10-C12-N1	2.15	118.38	114.59
4	C	9652[B]	CF3	F3-C15-C13	-2.08	102.17	112.62
4	D	9752[A]	CF3	C14-N1-C12	2.06	131.10	127.50
4	D	9752[B]	CF3	C14-N1-C12	2.06	131.10	127.50
4	C	9652[A]	CF3	C14-N1-C12	2.06	131.10	127.50
4	C	9652[B]	CF3	C14-N1-C12	2.06	131.10	127.50
4	A	9452[B]	CF3	O2-C13-C15	2.06	121.55	116.37
4	A	9452[A]	CF3	C9-C11-C13	2.00	117.03	113.62

There are no chirality outliers.

All (38) torsion outliers are listed below:

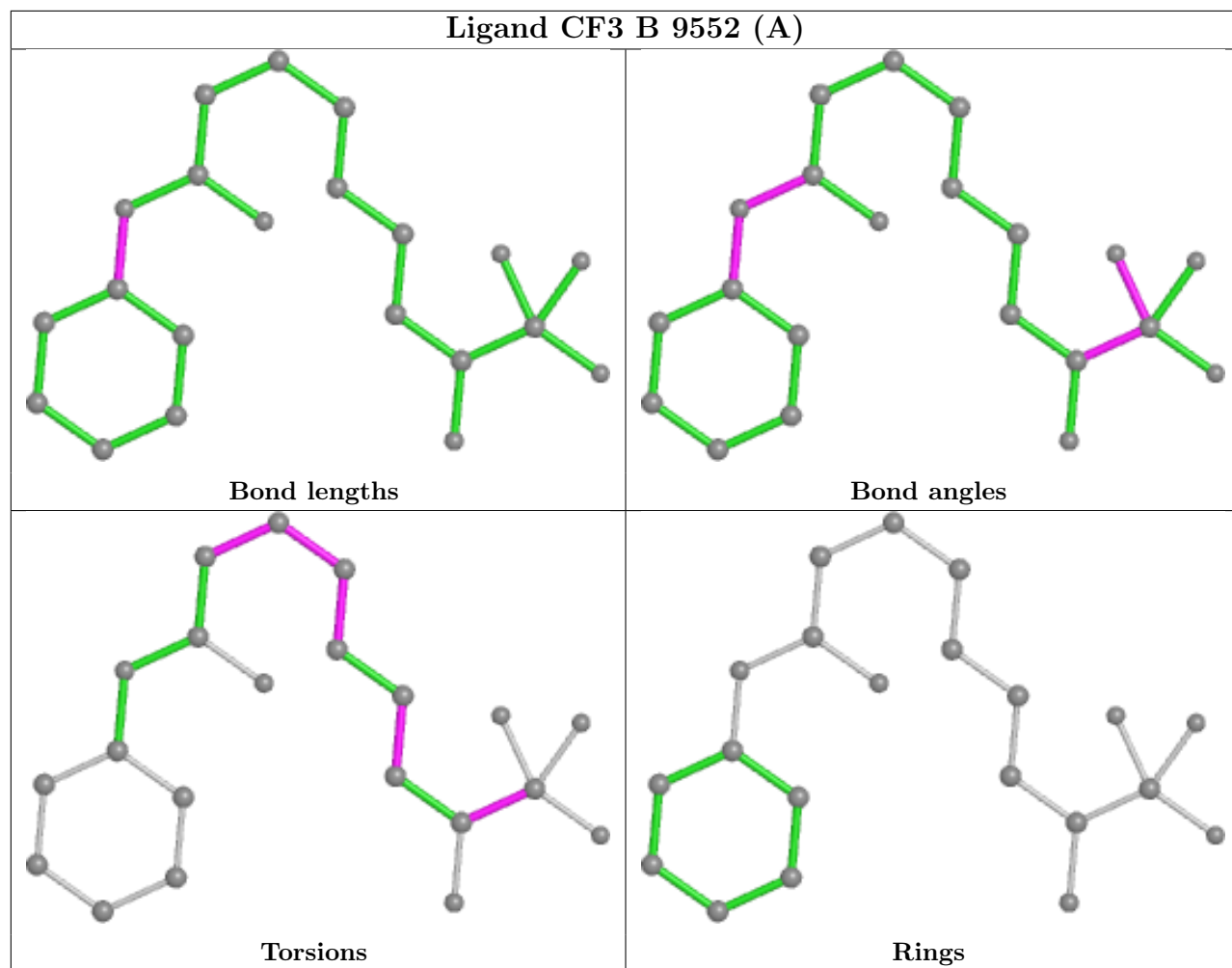
Mol	Chain	Res	Type	Atoms
4	A	9452[A]	CF3	C12-C10-C8-C6
4	A	9452[B]	CF3	C12-C10-C8-C6
4	B	9552[A]	CF3	C12-C10-C8-C6
4	B	9552[B]	CF3	C12-C10-C8-C6
4	B	9552[A]	CF3	C13-C11-C9-C7
4	B	9552[B]	CF3	C13-C11-C9-C7
4	C	9652[B]	CF3	C13-C11-C9-C7
4	D	9752[B]	CF3	C13-C11-C9-C7
4	B	9552[A]	CF3	C7-C6-C8-C10
4	B	9552[B]	CF3	C7-C6-C8-C10
4	A	9452[A]	CF3	C7-C6-C8-C10
4	A	9452[B]	CF3	C7-C6-C8-C10
4	C	9652[A]	CF3	O2-C13-C15-F3
4	C	9652[A]	CF3	O2-C13-C15-F1
4	A	9452[B]	CF3	C13-C11-C9-C7
4	B	9552[B]	CF3	C6-C7-C9-C11
4	A	9452[A]	CF3	C8-C6-C7-C9
4	A	9452[B]	CF3	C8-C6-C7-C9
4	A	9452[B]	CF3	C6-C7-C9-C11
4	B	9552[A]	CF3	C8-C6-C7-C9
4	B	9552[B]	CF3	C8-C6-C7-C9
4	D	9752[A]	CF3	C7-C6-C8-C10
4	D	9752[B]	CF3	C7-C6-C8-C10
4	A	9452[A]	CF3	O2-C13-C15-F3
4	A	9452[A]	CF3	O2-C13-C15-F1
4	A	9452[B]	CF3	O2-C13-C15-F3
4	B	9552[A]	CF3	O2-C13-C15-F3
4	B	9552[A]	CF3	O2-C13-C15-F1
4	B	9552[A]	CF3	O2-C13-C15-F2
4	C	9652[A]	CF3	O2-C13-C15-F2
4	C	9652[B]	CF3	O2-C13-C15-F3
4	C	9652[B]	CF3	O2-C13-C15-F1
4	C	9652[B]	CF3	O2-C13-C15-F2
4	D	9752[A]	CF3	O2-C13-C15-F3
4	D	9752[A]	CF3	O2-C13-C15-F1
4	D	9752[A]	CF3	O2-C13-C15-F2
4	D	9752[B]	CF3	O2-C13-C15-F3
4	D	9752[B]	CF3	O2-C13-C15-F2

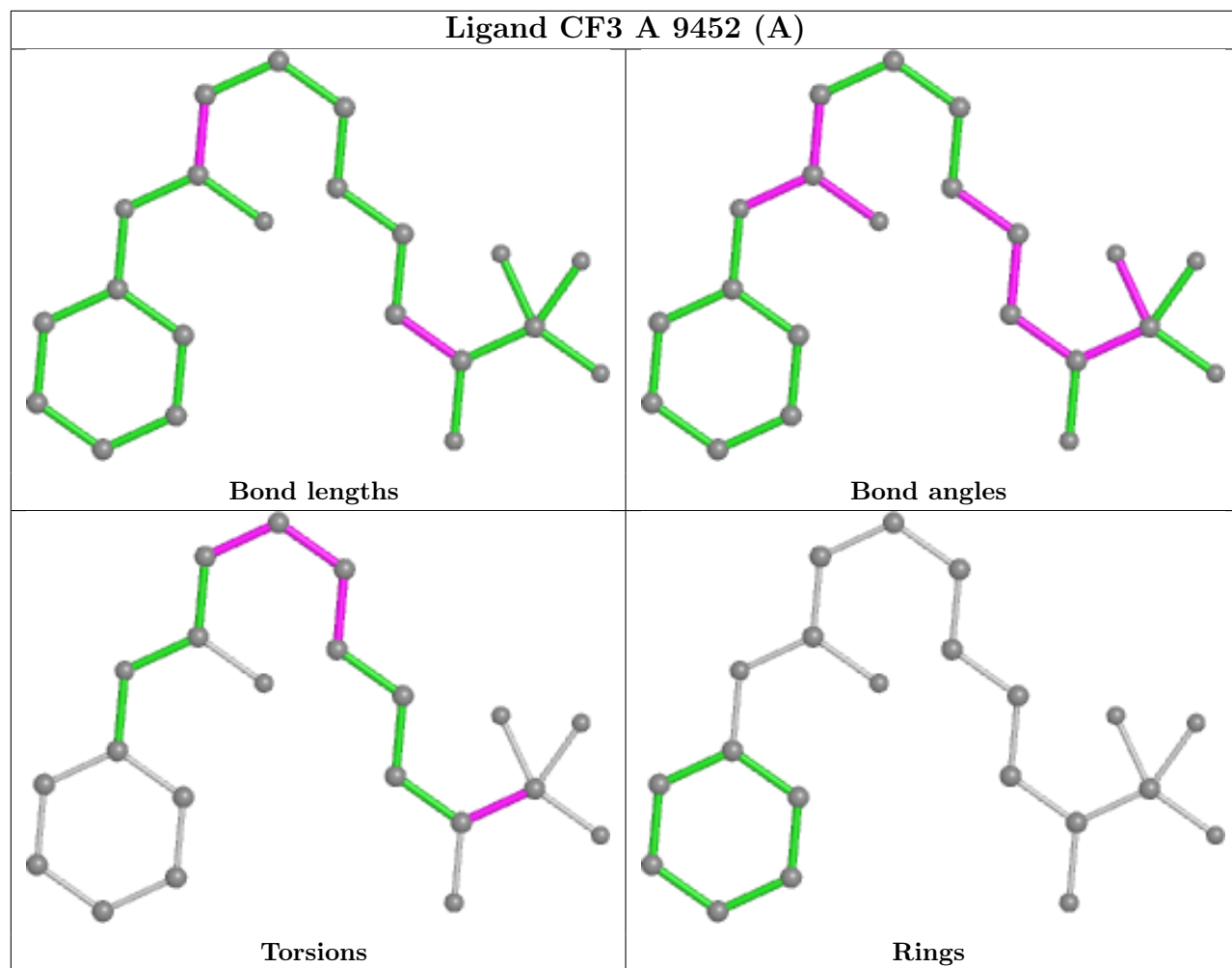
There are no ring outliers.

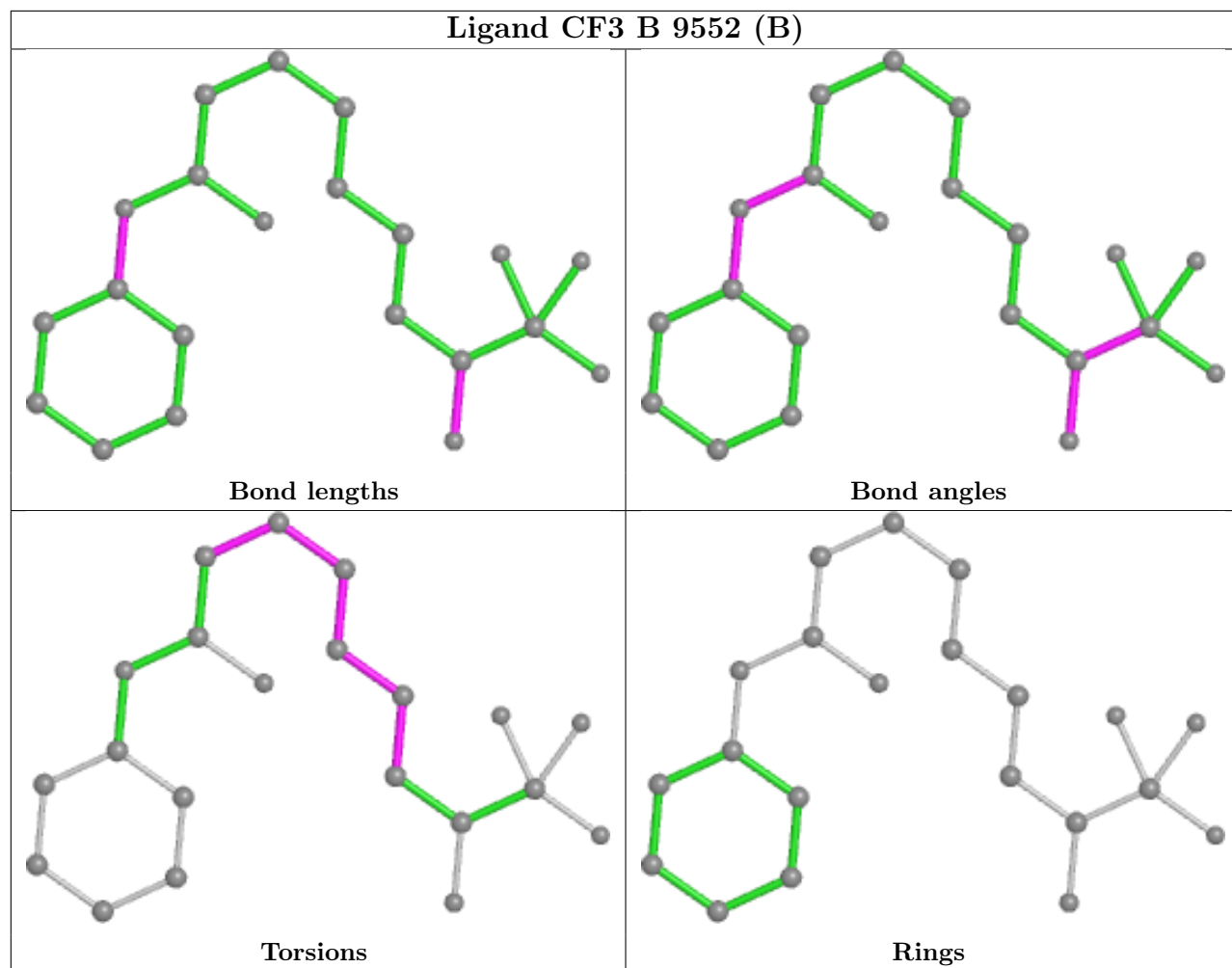
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	9552[A]	CF3	2	0
4	B	9552[B]	CF3	1	0
4	A	9452[B]	CF3	1	0
4	C	9652[A]	CF3	2	0
4	C	9652[B]	CF3	1	0
4	D	9752[A]	CF3	2	0
4	D	9752[B]	CF3	1	0

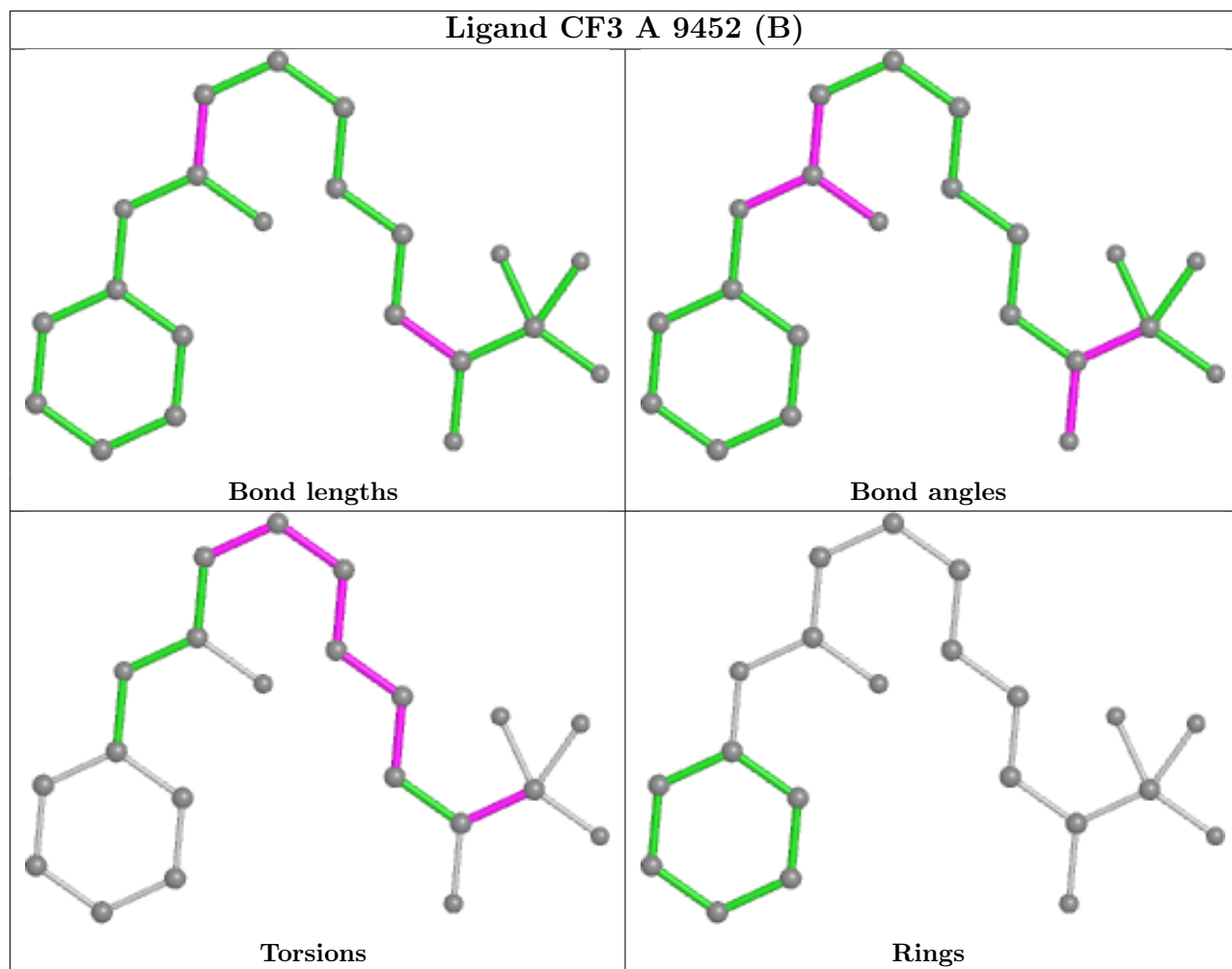
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

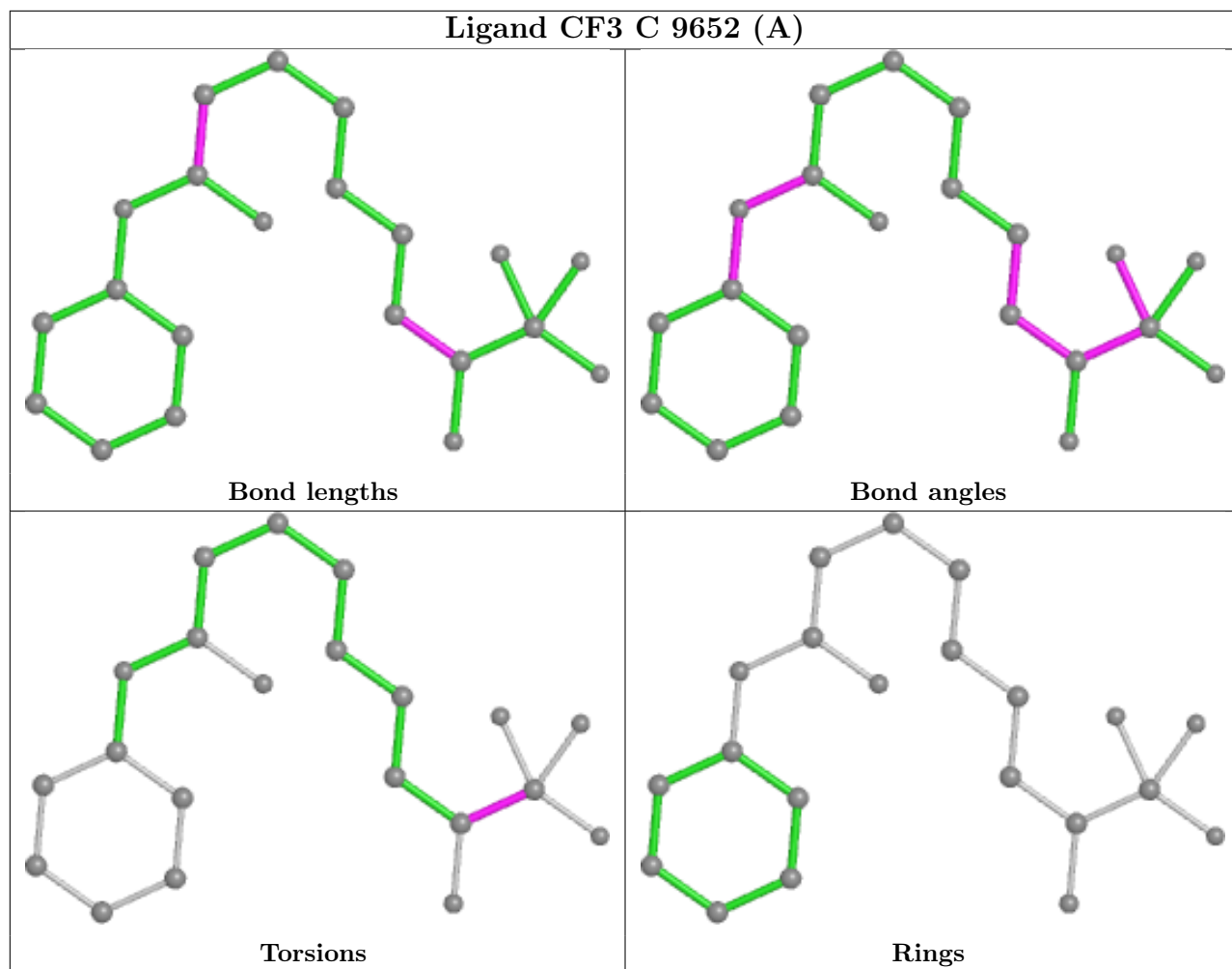


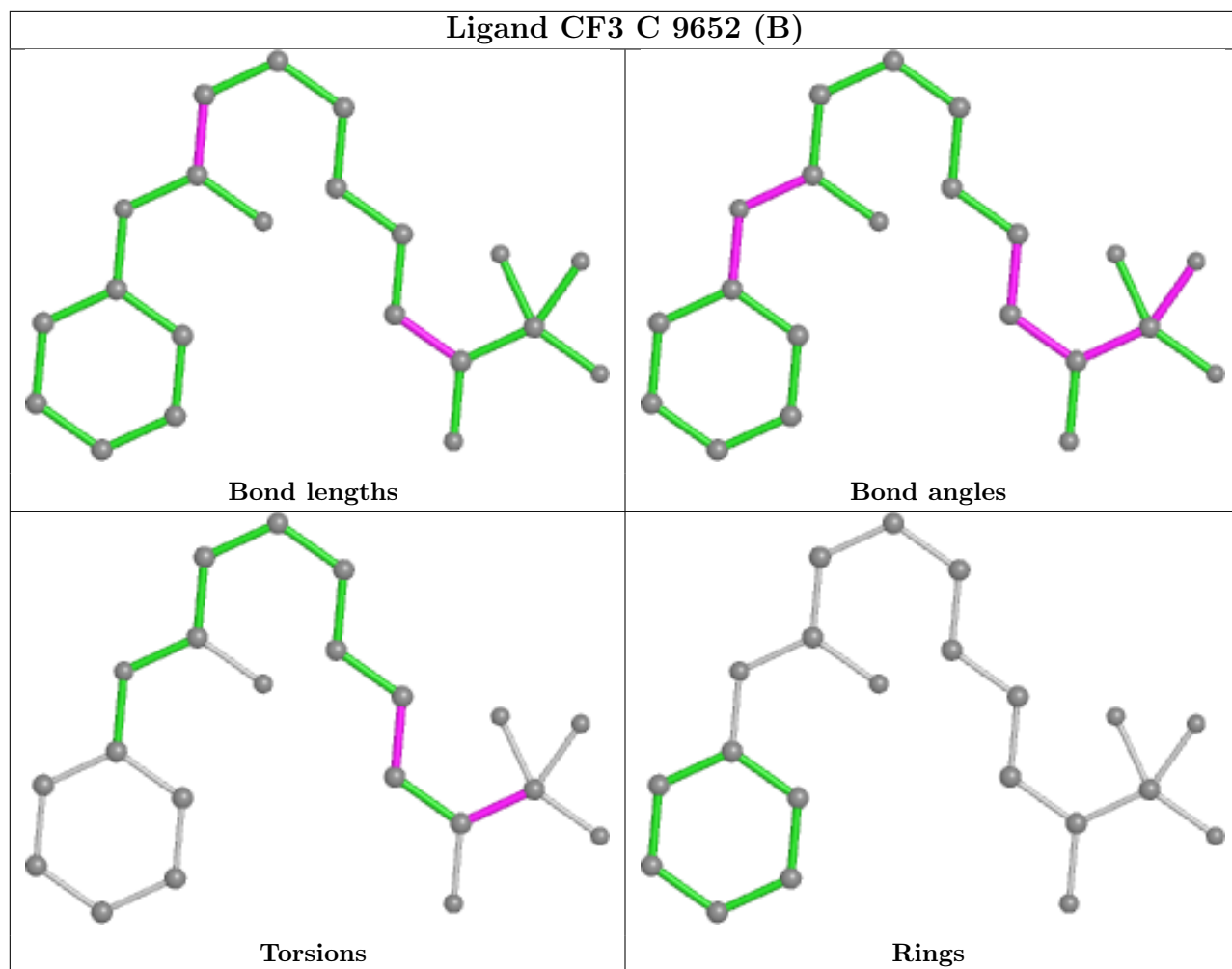


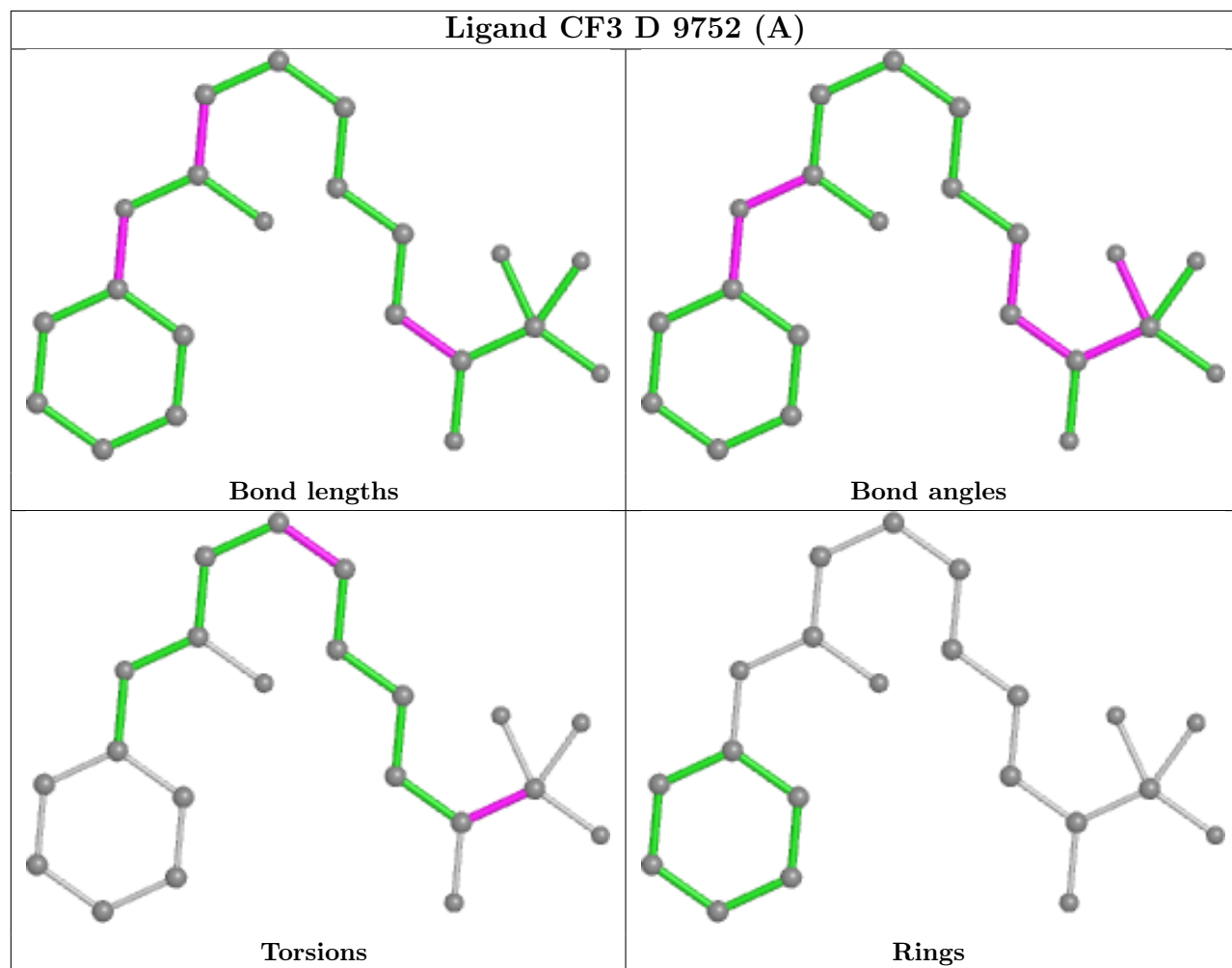


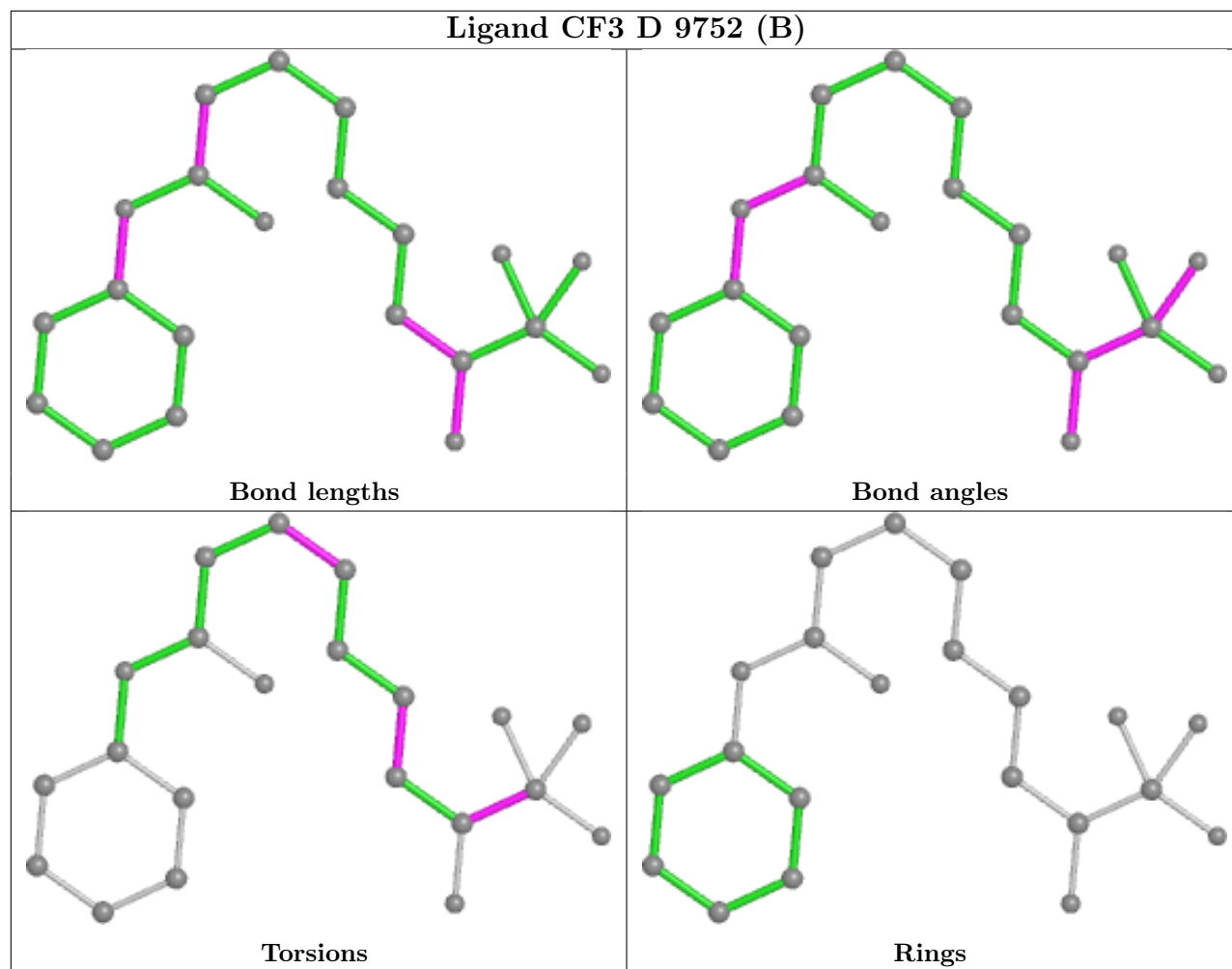












## 5.7 Other polymers [\(i\)](#)

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	367/369 (99%)	-0.31	1 (0%) 94 93	15, 22, 36, 45	0
1	B	367/369 (99%)	-0.29	6 (1%) 72 70	15, 22, 37, 44	0
1	C	367/369 (99%)	-0.39	2 (0%) 91 90	16, 23, 37, 45	0
1	D	367/369 (99%)	-0.15	16 (4%) 34 32	16, 25, 38, 46	0
All	All	1468/1476 (99%)	-0.29	25 (1%) 70 68	15, 23, 37, 46	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91	PRO	3.5
1	D	366	ALA	2.9
1	D	222	ASN	2.9
1	D	92	THR	2.9
1	D	90	LEU	2.9
1	D	195	PRO	2.9
1	D	94	GLY	2.7
1	D	93	GLY	2.6
1	D	221	GLY	2.6
1	D	89	ASN	2.6
1	B	340	GLU	2.6
1	B	95	ASP	2.5
1	B	97	GLY	2.5
1	D	223	GLY	2.5
1	D	196	SER	2.4
1	B	92	THR	2.4
1	D	340	GLU	2.2
1	B	99	GLY	2.2
1	C	211	ASP	2.2
1	A	92	THR	2.1
1	D	87	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	102	MET	2.1
1	C	340	GLU	2.1
1	B	366	ALA	2.1
1	D	95	ASP	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, 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(Å <sup>2</sup> )	Q<0.9
4	CF3	D	9752[A]	21/21	0.83	0.30	15,44,74,75	3
4	CF3	D	9752[B]	21/21	0.83	0.30	16,44,74,75	3
4	CF3	A	9452[A]	21/21	0.84	0.26	17,41,70,70	3
4	CF3	A	9452[B]	21/21	0.84	0.26	14,41,70,70	3
4	CF3	C	9652[A]	21/21	0.86	0.24	16,41,69,69	3
4	CF3	C	9652[B]	21/21	0.86	0.24	11,41,69,69	3
4	CF3	B	9552[A]	21/21	0.86	0.24	5,37,67,68	3
4	CF3	B	9552[B]	21/21	0.86	0.24	6,37,67,68	3
2	ZN	C	9651	1/1	0.94	0.10	31,31,31,31	1
3	K	D	9749	1/1	0.94	0.17	55,55,55,55	0
3	K	B	9549	1/1	0.95	0.13	42,42,42,42	0
3	K	A	9449	1/1	0.97	0.06	34,34,34,34	0
2	ZN	D	9751	1/1	0.97	0.08	29,29,29,29	1
3	K	C	9649	1/1	0.97	0.07	46,46,46,46	0
2	ZN	B	9551	1/1	0.98	0.09	26,26,26,26	1
3	K	D	9750	1/1	0.99	0.06	22,22,22,22	0
2	ZN	A	9451	1/1	0.99	0.07	31,31,31,31	1
3	K	C	9650	1/1	1.00	0.06	22,22,22,22	0
3	K	B	9550	1/1	1.00	0.10	20,20,20,20	0

*Continued on next page...*

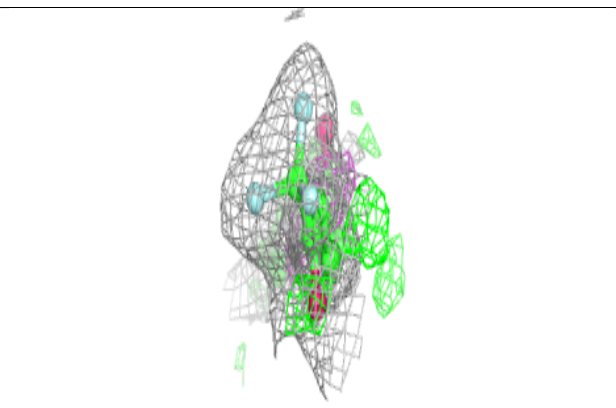
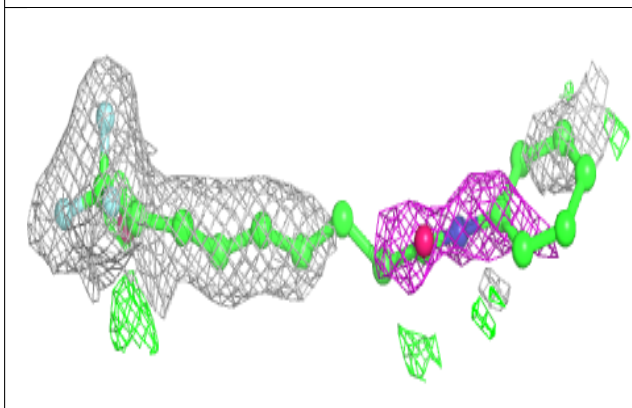
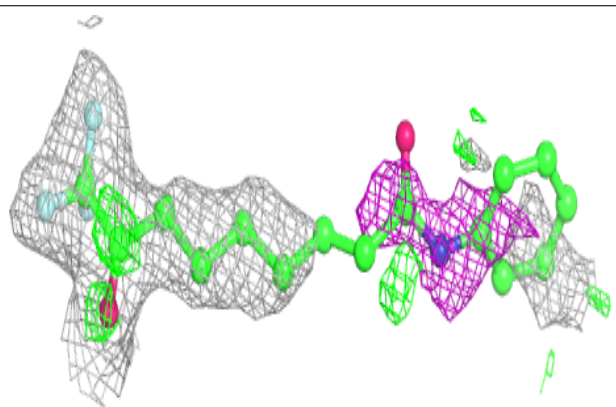
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	K	A	9450	1/1	1.00	0.08	23,23,23,23	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 CF3 D 9752 (A):**

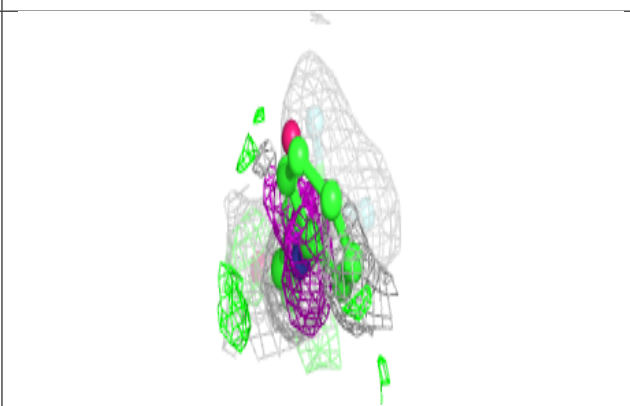
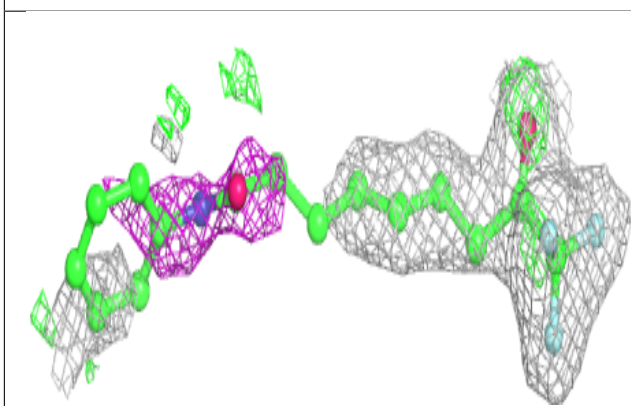
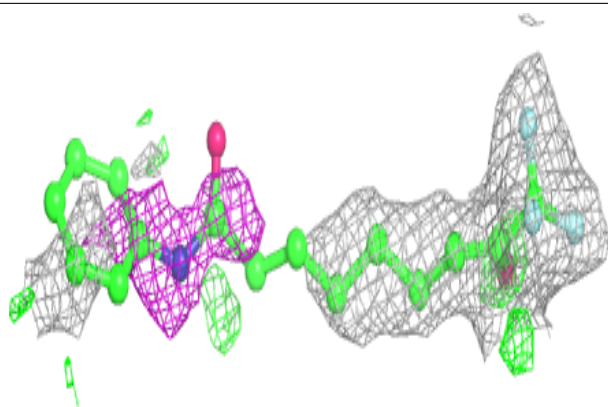
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)



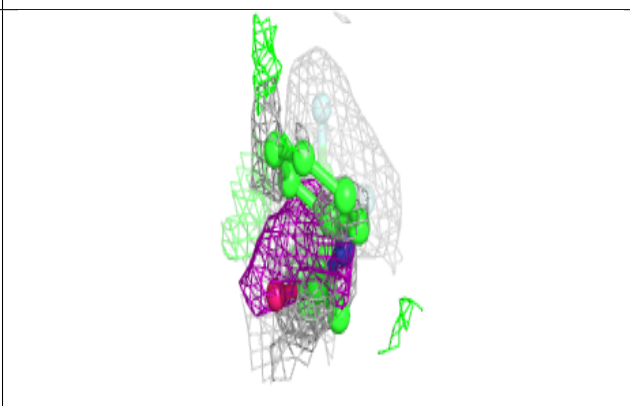
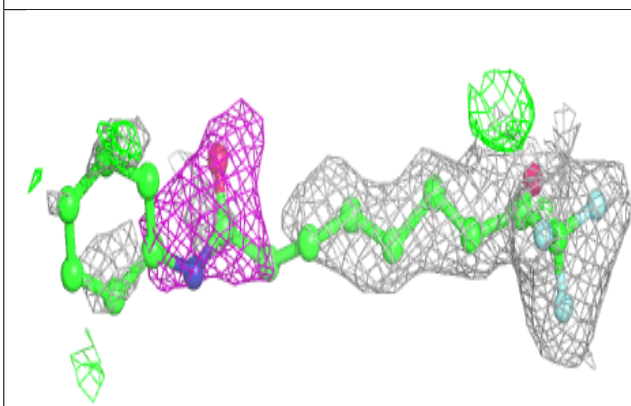
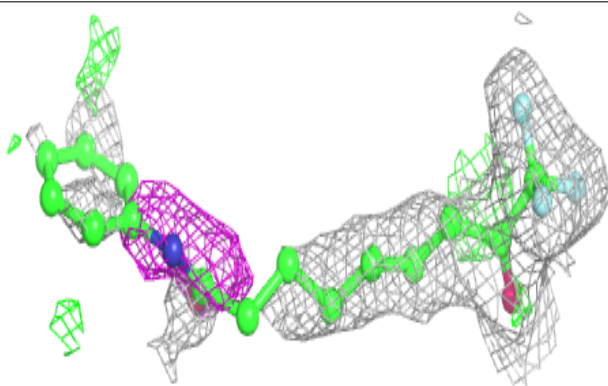


**Electron density around CF3 D 9752 (B):**

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

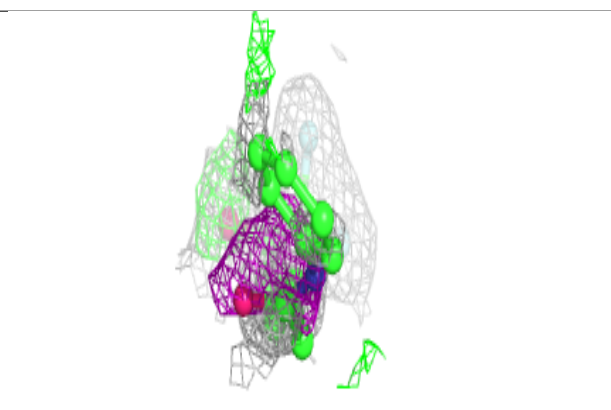
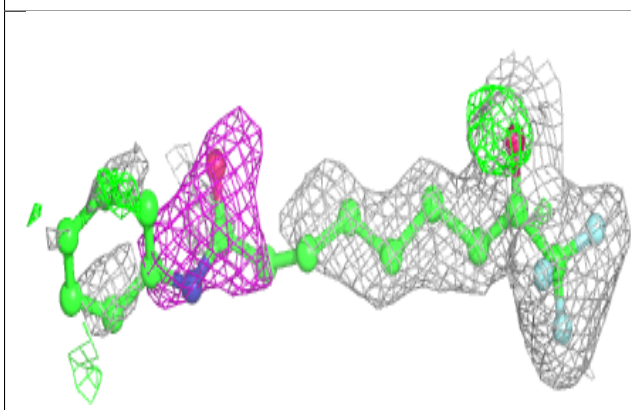
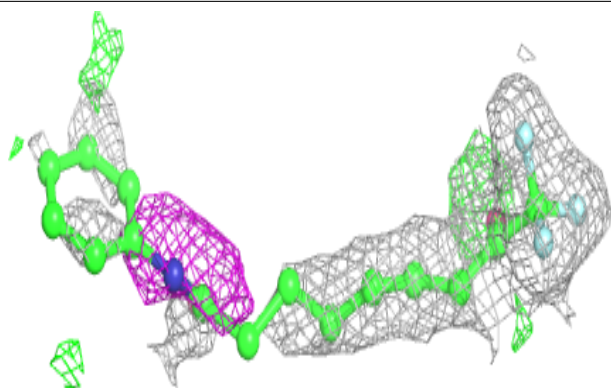
**Electron density around CF3 A 9452 (A):**

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and green (positive)

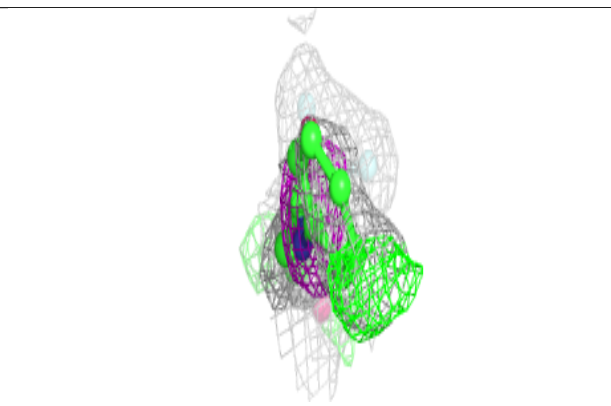
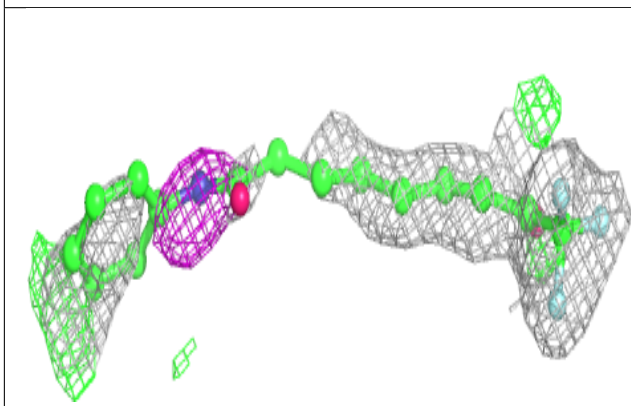
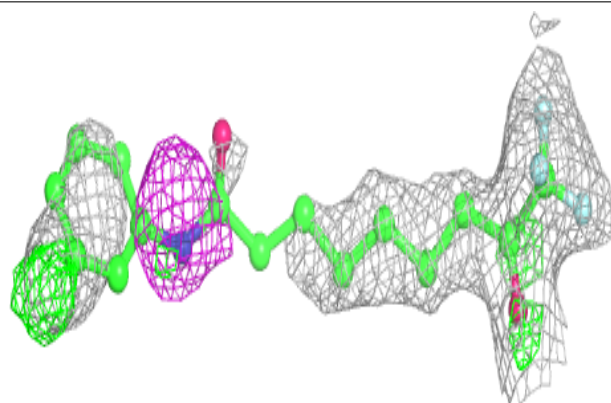


**Electron density around CF3 A 9452 (B):**

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

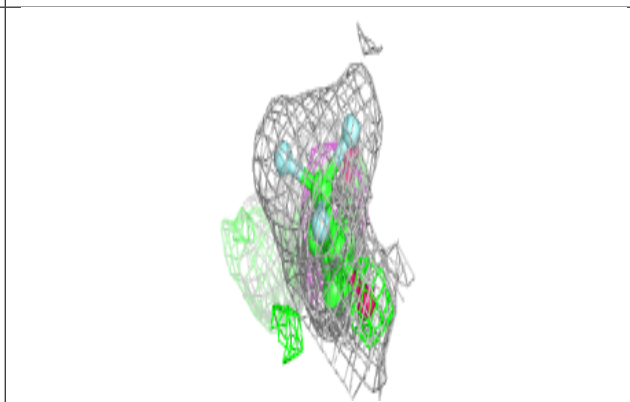
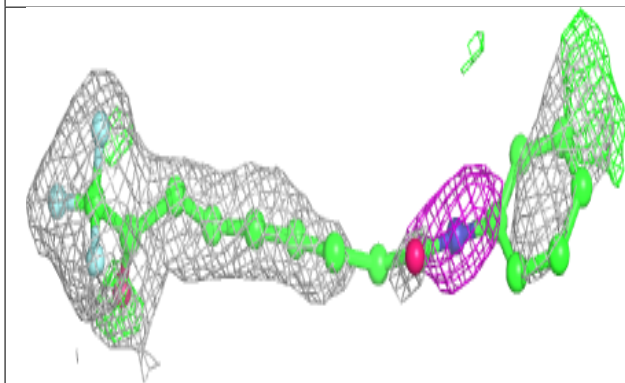
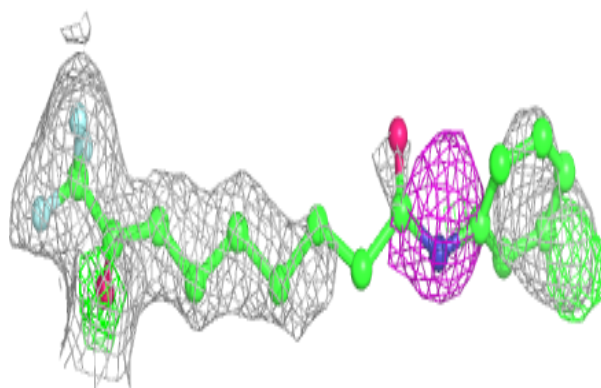
**Electron density around CF3 C 9652 (A):**

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

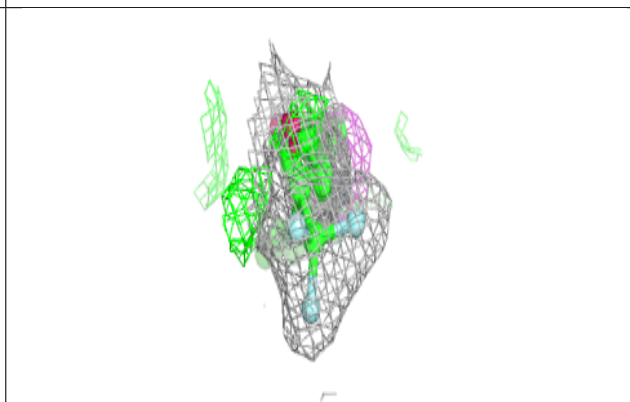
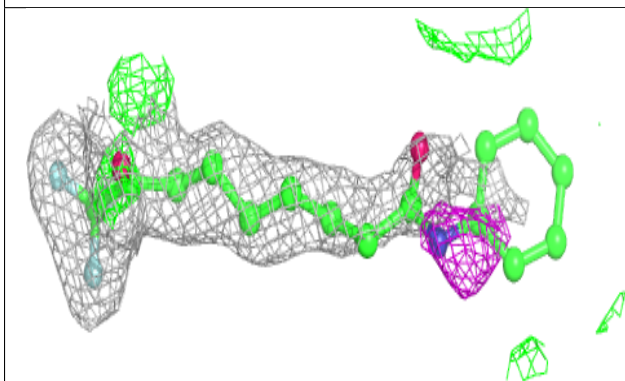
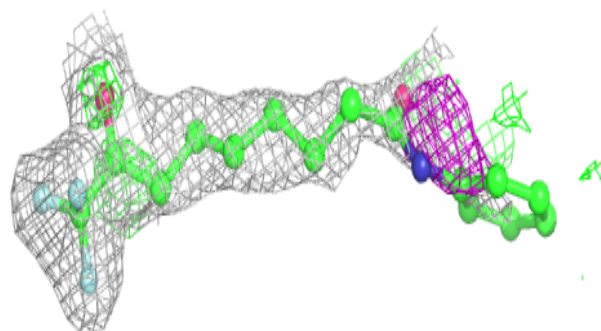


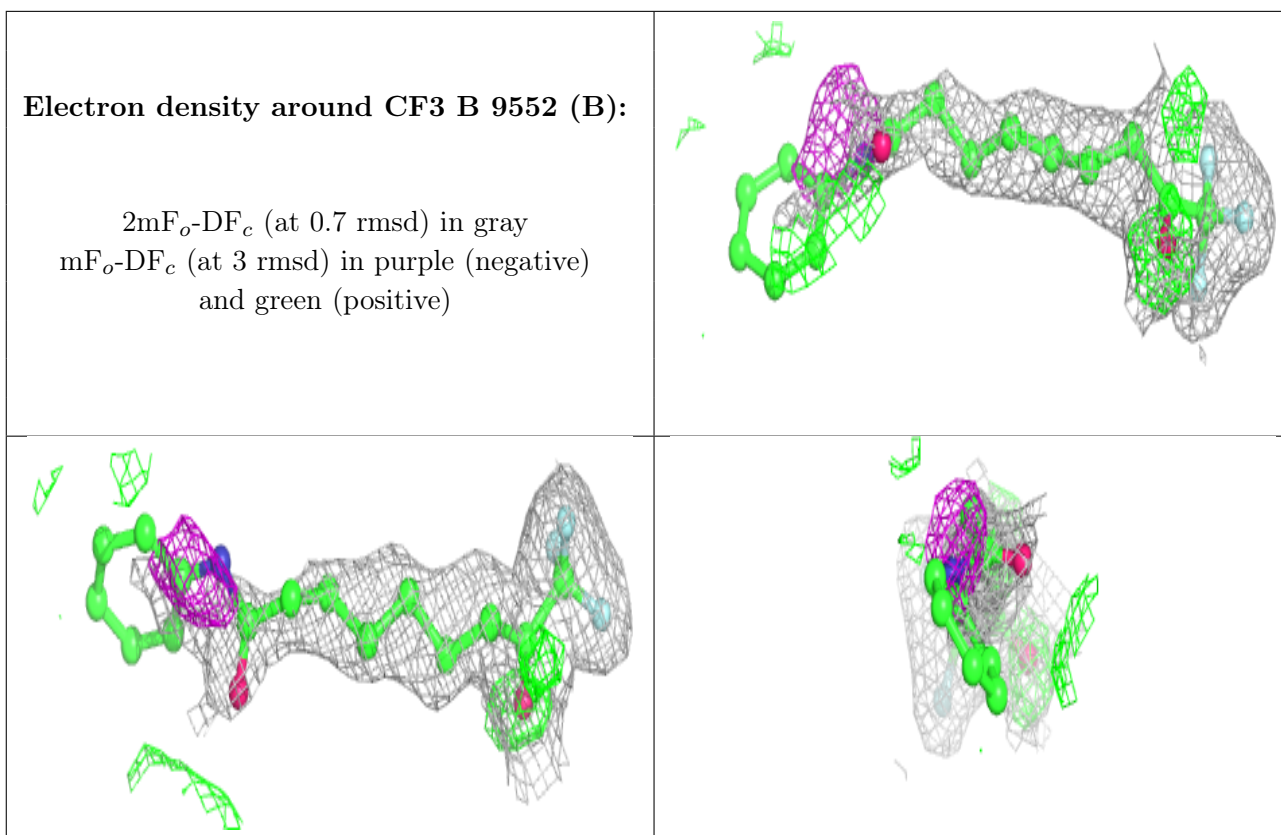
**Electron density around CF3 C 9652 (B):**

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

**Electron density around CF3 B 9552 (A):**

$2mF_o-DF_c$  (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.