Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 12:29 PM JST

PDB ID	:	5ZLA
Title	:	Crystal structure of mutant C387A of DFA-IIIase from Arthrobacter chlorophenolicus A6 in complex with DFA-III
Authors	:	Yu, S.H.; Shen, H.; Li, X.; Mu, W.M.
Deposited on	:	2018-03-27
Resolution	:	1.70 Å(reported)

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

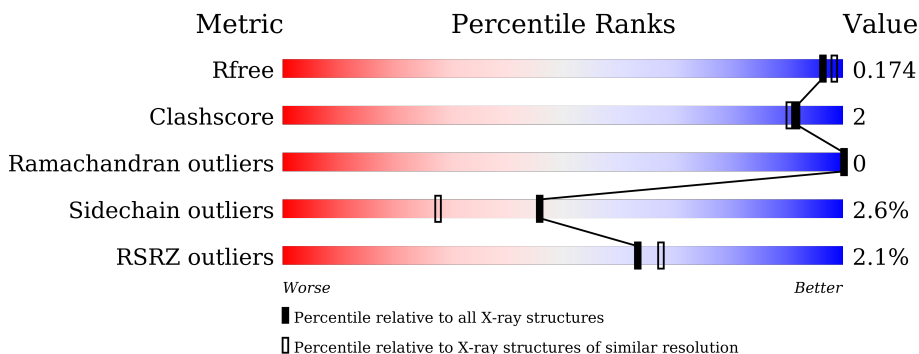|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.174
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		2.6%
RSRZ outliers		2.1%

Worse　　　　　*Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	.% ... 94% ... 5% ·
1	B	445	2% ... 94% ... · ··
1	C	445	3% ... 92% ... 6% ··
1	D	445	.% ... 94% ... · ·
1	E	445	2% ... 91% ... 7% ·
1	F	445	3% ... 93% ... · ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21791 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.
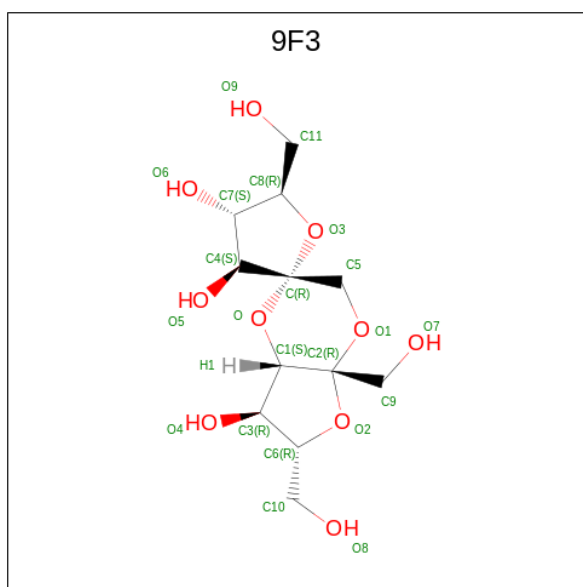
- Molecule 1 is a protein called DFA-IIIase C387A mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3283	2042	586	649	6			
1	B	441	Total	C	N	O	S	0	0	0
			3291	2046	588	651	6			
1	C	438	Total	C	N	O	S	0	0	0
			3281	2042	585	648	6			
1	D	437	Total	C	N	O	S	0	0	0
			3279	2043	584	646	6			
1	E	436	Total	C	N	O	S	0	0	0
			3272	2036	583	647	6			
1	F	436	Total	C	N	O	S	0	0	0
			3272	2036	583	647	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ALA	CYS	engineered mutation	UNP B8HDZ1
B	387	ALA	CYS	engineered mutation	UNP B8HDZ1
C	387	ALA	CYS	engineered mutation	UNP B8HDZ1
D	387	ALA	CYS	engineered mutation	UNP B8HDZ1
E	387	ALA	CYS	engineered mutation	UNP B8HDZ1
F	387	ALA	CYS	engineered mutation	UNP B8HDZ1

- Molecule 2 is (2R,3'S,4'S,4aR,5'R,6R,7R,7aS)-4a,5',6-tris(hydroxymethyl)spiro[3,6,7,7a-tetrahydrofuro[2,3-b][1,4]dioxine-2,2'-oxolane]-3',4',7-triol (three-letter code: 9F3) (formula: $C_{12}H_{20}O_{10}$) (labeled as "Ligand of Interest" by depositor).

9F3

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 22	C 12	O 10	0	0
2	B	1	Total 22	C 12	O 10	0	0
2	C	1	Total 22	C 12	O 10	0	0
2	D	1	Total 22	C 12	O 10	0	0
2	E	1	Total 22	C 12	O 10	0	0
2	F	1	Total 22	C 12	O 10	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	371	Total 371	O 371	0	0
3	B	358	Total 358	O 358	0	0
3	C	330	Total 330	O 330	0	0
3	D	321	Total 321	O 321	0	0
3	E	323	Total 323	O 323	0	0
3	F	278	Total 278	O 278	0	0

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.
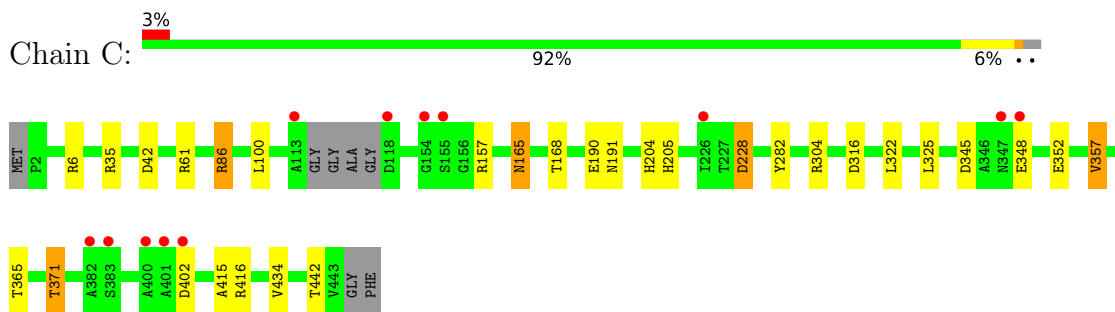
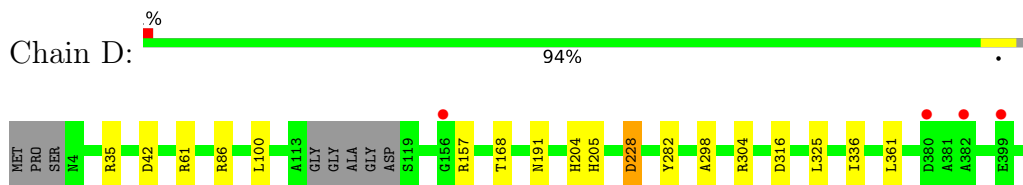• Molecule 1: DFA-IIIase C387A mutant
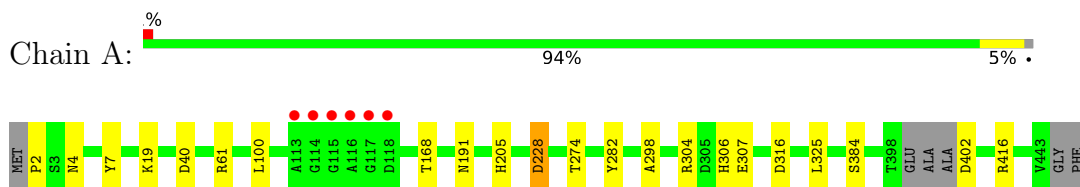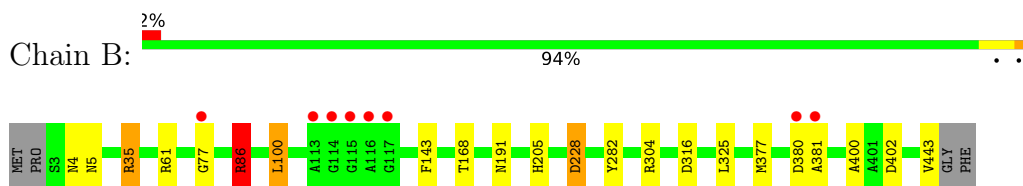
Chain A:

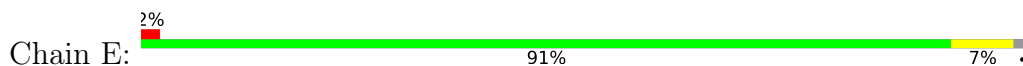• Molecule 1: DFA-IIIase C387A mutant

Chain B:

• Molecule 1: DFA-IIIase C387A mutant

Chain C:

• Molecule 1: DFA-IIIase C387A mutant

Chain D:

• Molecule 1: DFA-IIIase C387A mutant

Chain E:

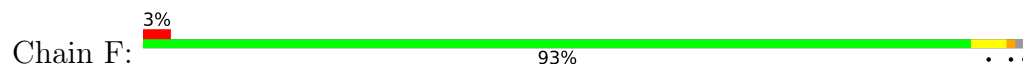• Molecule 1: DFA-IIIase C387A mutant

Chain F:
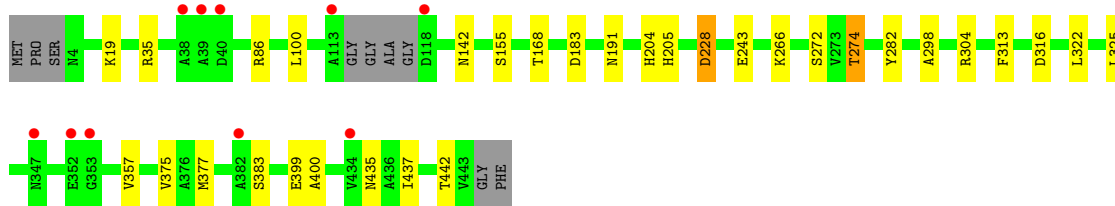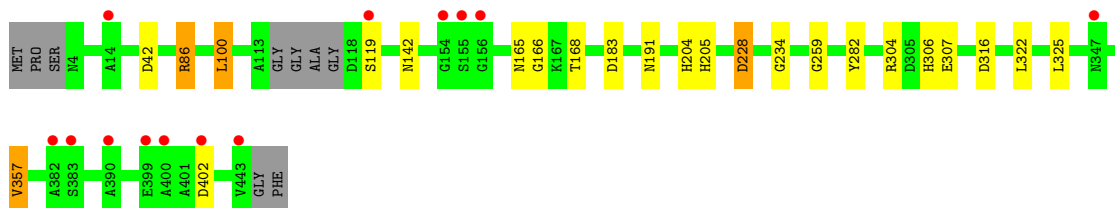
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	116.41Å　79.44Å　141.01Å 90.00°　100.62°　90.00°	Depositor
Resolution (Å)	50.00 – 1.70 45.19 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-1.70) 94.4 (45.19-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.131 , 0.174 0.133 , 0.174	Depositor DCC
R_{free} test set	13158 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	14.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21791	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 9F3

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	0.43	0/3355	0.71	0/4574
1	B	0.44	0/3363	0.77	5/4587 (0.1%)
1	C	0.43	0/3353	0.74	5/4573 (0.1%)
1	D	0.42	0/3351	0.74	5/4569 (0.1%)
1	E	0.42	0/3343	0.75	4/4559 (0.1%)
1	F	0.40	0/3343	0.71	2/4559 (0.0%)
All	All	0.42	0/20108	0.74	21/27421 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	165	ASN	CB-CA-C	11.28	132.95	110.40
1	B	86	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	D	35	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	C	86	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	C	86	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	E	86	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	E	86	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	E	35	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	B	35	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	D	35	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	35	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	E	35	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	86	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	D	86	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	B	86	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	C	35	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	C	35	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	157	ARG	NE-CZ-NH1	6.02	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	61	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	F	166	GLY	N-CA-C	-5.44	99.49	113.10
1	C	157	ARG	NE-CZ-NH1	5.17	122.88	120.30

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	3283	0	3135	8	0
1	B	3291	0	3140	13	0
1	C	3281	0	3133	16	0
1	D	3279	0	3132	7	0
1	E	3272	0	3124	12	0
1	F	3272	0	3124	9	0
2	A	22	0	0	0	0
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
2	E	22	0	0	0	0
2	F	22	0	0	0	0
3	A	371	0	0	1	0
3	B	358	0	0	2	0
3	C	330	0	0	6	0
3	D	321	0	0	1	0
3	E	323	0	0	0	0
3	F	278	0	0	1	0
All	All	21791	0	18788	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ASP:OD2	1:C:434:VAL:HG21	1.77	0.84
1:C:204:HIS:NE2	3:C:601:HOH:O	2.18	0.76
3:C:601:HOH:O	1:F:204:HIS:NE2	2.18	0.75
3:C:601:HOH:O	1:E:204:HIS:NE2	2.20	0.73
1:B:380:ASP:OD2	1:C:434:VAL:CG2	2.38	0.72
3:B:601:HOH:O	1:D:204:HIS:NE2	2.22	0.71
1:E:272:SER:OG	1:E:274:THR:HG23	1.98	0.63
1:B:377:MET:HG2	1:B:400:ALA:HB3	1.87	0.56
1:C:6:ARG:HG3	3:C:623:HOH:O	2.06	0.56
1:A:306:HIS:HD2	1:A:307:GLU:O	1.90	0.54
1:A:61:ARG:NH2	3:A:601:HOH:O	2.41	0.53
1:F:168:THR:HA	1:F:191:ASN:O	2.09	0.53
1:A:168:THR:HA	1:A:191:ASN:O	2.09	0.52
1:B:168:THR:HA	1:B:191:ASN:O	2.10	0.51
1:E:168:THR:HA	1:E:191:ASN:O	2.12	0.50
1:E:435:ASN:HB2	1:E:437:ILE:HD11	1.92	0.50
1:E:274:THR:HB	1:E:298:ALA:O	2.12	0.49
1:D:168:THR:HA	1:D:191:ASN:O	2.12	0.49
1:C:165:ASN:HD21	1:C:190:GLU:H	1.61	0.49
1:C:371:THR:HB	3:F:666:HOH:O	2.15	0.47
1:E:377:MET:HG2	1:E:400:ALA:HB3	1.96	0.47
1:A:2:PRO:HD3	1:A:7:TYR:CE2	2.50	0.47
1:C:282:TYR:CE1	1:C:316:ASP:HA	2.48	0.47
1:D:282:TYR:CE1	1:D:316:ASP:HA	2.50	0.46
1:F:322:LEU:HA	1:F:357:VAL:HG13	1.97	0.46
1:C:61:ARG:NH2	3:C:602:HOH:O	2.48	0.46
1:A:282:TYR:CE1	1:A:316:ASP:HA	2.52	0.45
1:B:380:ASP:OD1	1:B:381:ALA:N	2.41	0.45
1:B:77:GLY:O	1:B:143:PHE:HA	2.16	0.45
1:C:168:THR:HA	1:C:191:ASN:O	2.17	0.45
1:F:282:TYR:CE1	1:F:316:ASP:HA	2.51	0.45
1:C:205:HIS:HA	1:C:228:ASP:O	2.17	0.45
1:F:306:HIS:HD2	1:F:307:GLU:O	2.00	0.45
1:B:380:ASP:OD2	1:C:415:ALA:HB1	2.17	0.44
1:D:61:ARG:NH2	3:D:602:HOH:O	2.51	0.44
1:E:322:LEU:HA	1:E:357:VAL:HG13	2.00	0.44
1:F:205:HIS:HA	1:F:228:ASP:O	2.16	0.44
1:C:6:ARG:CG	3:C:623:HOH:O	2.66	0.44
1:C:322:LEU:HA	1:C:357:VAL:HG13	1.99	0.43
1:D:361:LEU:HD12	1:D:361:LEU:N	2.33	0.43
1:E:243:GLU:HA	1:E:266:LYS:O	2.19	0.43
1:B:5:ASN:OD1	1:B:35:ARG:NH2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:HIS:HA	1:E:228:ASP:O	2.20	0.42
1:B:380:ASP:OD2	1:C:434:VAL:CB	2.67	0.42
1:E:313:PHE:CD1	1:E:383:SER:HB3	2.55	0.42
1:C:345:ASP:HB3	1:C:348:GLU:HB2	2.02	0.42
1:B:282:TYR:CE1	1:B:316:ASP:HA	2.55	0.42
1:D:298:ALA:HA	1:D:336:ILE:O	2.21	0.41
1:E:142:ASN:HA	1:E:183:ASP:O	2.20	0.41
1:F:86:ARG:HD2	1:F:100:LEU:O	2.20	0.41
1:B:86:ARG:HD3	3:B:706:HOH:O	2.20	0.41
1:D:205:HIS:HA	1:D:228:ASP:O	2.21	0.41
1:E:282:TYR:CE1	1:E:316:ASP:HA	2.56	0.41
1:A:40:ASP:HB2	1:B:100:LEU:HD23	2.03	0.41
1:A:205:HIS:HA	1:A:228:ASP:O	2.21	0.41
1:B:205:HIS:HA	1:B:228:ASP:O	2.20	0.41
1:F:142:ASN:HA	1:F:183:ASP:O	2.21	0.41
1:F:234:GLY:O	1:F:259:GLY:HA2	2.21	0.41
1:C:365:THR:HA	1:C:415:ALA:O	2.21	0.41
1:A:274:THR:HA	1:A:298:ALA:O	2.22	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	435/445 (98%)	415 (95%)	20 (5%)	0	100	100
1	B	439/445 (99%)	421 (96%)	18 (4%)	0	100	100
1	C	434/445 (98%)	416 (96%)	18 (4%)	0	100	100
1	D	433/445 (97%)	415 (96%)	18 (4%)	0	100	100
1	E	432/445 (97%)	415 (96%)	17 (4%)	0	100	100
1	F	432/445 (97%)	411 (95%)	21 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2605/2670 (98%)	2493 (96%)	112 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	349/352 (99%)	340 (97%)	9 (3%)	46	28
1	B	348/352 (99%)	340 (98%)	8 (2%)	50	33
1	C	349/352 (99%)	336 (96%)	13 (4%)	34	15
1	D	348/352 (99%)	342 (98%)	6 (2%)	60	46
1	E	348/352 (99%)	338 (97%)	10 (3%)	42	23
1	F	348/352 (99%)	339 (97%)	9 (3%)	46	28
All	All	2090/2112 (99%)	2035 (97%)	55 (3%)	46	28

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	19	LYS
1	A	100	LEU
1	A	228	ASP
1	A	304	ARG
1	A	325	LEU
1	A	384	SER
1	A	402	ASP
1	A	416	ARG
1	B	4	ASN
1	B	86	ARG
1	B	100	LEU
1	B	228	ASP
1	B	304	ARG

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Mol	Chain	Res	Type
1	B	325	LEU
1	B	402	ASP
1	B	443	VAL
1	C	42	ASP
1	C	86	ARG
1	C	100	LEU
1	C	165	ASN
1	C	228	ASP
1	C	304	ARG
1	C	325	LEU
1	C	352	GLU
1	C	357	VAL
1	C	371	THR
1	C	402	ASP
1	C	416	ARG
1	C	442	THR
1	D	42	ASP
1	D	100	LEU
1	D	228	ASP
1	D	304	ARG
1	D	325	LEU
1	D	416	ARG
1	E	19	LYS
1	E	100	LEU
1	E	155	SER
1	E	228	ASP
1	E	274	THR
1	E	304	ARG
1	E	325	LEU
1	E	375	VAL
1	E	399	GLU
1	E	442	THR
1	F	42	ASP
1	F	86	ARG
1	F	100	LEU
1	F	119	SER
1	F	228	ASP
1	F	304	ARG
1	F	325	LEU
1	F	357	VAL
1	F	402	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	176	ASN
1	A	306	HIS
1	B	4	ASN
1	B	176	ASN
1	B	347	ASN
1	C	165	ASN
1	C	176	ASN
1	C	291	ASN
1	D	176	ASN
1	E	176	ASN
1	E	291	ASN
1	F	176	ASN
1	F	306	HIS

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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	9F3	C	501	-	24,24,24	1.39	4 (16%)	33,38,38	1.56	7 (21%)
2	9F3	D	501	-	24,24,24	1.25	3 (12%)	33,38,38	1.24	3 (9%)
2	9F3	A	501	-	24,24,24	1.37	4 (16%)	33,38,38	1.31	4 (12%)
2	9F3	B	501	-	24,24,24	1.03	1 (4%)	33,38,38	1.21	4 (12%)
2	9F3	F	501	-	24,24,24	1.34	4 (16%)	33,38,38	1.36	4 (12%)
2	9F3	E	501	-	24,24,24	1.23	3 (12%)	33,38,38	1.13	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9F3	C	501	-	-	0/7/57/57	0/3/3/3
2	9F3	D	501	-	-	0/7/57/57	0/3/3/3
2	9F3	A	501	-	-	0/7/57/57	0/3/3/3
2	9F3	B	501	-	-	1/7/57/57	0/3/3/3
2	9F3	F	501	-	-	1/7/57/57	0/3/3/3
2	9F3	E	501	-	-	0/7/57/57	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	9F3	O-C	3.60	1.50	1.42
2	C	501	9F3	O-C	3.33	1.49	1.42
2	D	501	9F3	O-C	3.28	1.49	1.42
2	E	501	9F3	O-C	3.23	1.49	1.42
2	F	501	9F3	O-C	3.06	1.49	1.42
2	C	501	9F3	O-C1	2.74	1.48	1.43
2	C	501	9F3	O2-C6	2.66	1.49	1.43
2	B	501	9F3	O-C	2.60	1.48	1.42
2	D	501	9F3	O3-C	2.54	1.48	1.42
2	E	501	9F3	O1-C5	-2.45	1.40	1.43
2	F	501	9F3	O-C1	2.44	1.48	1.43
2	A	501	9F3	O-C1	2.37	1.47	1.43
2	C	501	9F3	O3-C	2.29	1.47	1.42
2	A	501	9F3	O1-C2	2.18	1.45	1.42
2	F	501	9F3	O3-C	2.15	1.47	1.42
2	D	501	9F3	O1-C5	-2.15	1.40	1.43
2	F	501	9F3	O2-C6	2.13	1.48	1.43
2	E	501	9F3	C2-C1	2.12	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	9F3	O3-C	2.09	1.47	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	9F3	O1-C2-O2	-3.20	102.73	109.48
2	F	501	9F3	O-C-C5	-3.16	106.56	110.09
2	F	501	9F3	O1-C5-C	-2.93	107.06	111.70
2	C	501	9F3	C10-C6-C3	-2.90	108.09	115.09
2	C	501	9F3	O-C1-C2	2.87	115.33	110.53
2	D	501	9F3	O1-C5-C	-2.70	107.42	111.70
2	A	501	9F3	O-C-C5	-2.53	107.27	110.09
2	B	501	9F3	O1-C2-O2	-2.51	104.19	109.48
2	A	501	9F3	O-C1-C2	2.50	114.73	110.53
2	F	501	9F3	O3-C8-C11	2.50	115.81	108.85
2	C	501	9F3	O1-C5-C	-2.45	107.81	111.70
2	F	501	9F3	O-C1-C2	2.42	114.59	110.53
2	D	501	9F3	O-C1-C2	2.40	114.56	110.53
2	B	501	9F3	O-C1-C2	2.40	114.55	110.53
2	A	501	9F3	O1-C5-C	-2.32	108.02	111.70
2	C	501	9F3	O-C-C5	-2.29	107.54	110.09
2	B	501	9F3	O1-C2-C9	2.25	109.29	103.65
2	C	501	9F3	O1-C2-C9	2.23	109.23	103.65
2	B	501	9F3	O1-C5-C	-2.22	108.18	111.70
2	D	501	9F3	O1-C2-C9	2.21	109.18	103.65
2	E	501	9F3	O-C1-C2	2.09	114.03	110.53
2	C	501	9F3	O2-C6-C10	2.06	114.58	108.85
2	A	501	9F3	O3-C8-C7	-2.05	100.39	105.49
2	E	501	9F3	C5-O1-C2	2.03	117.12	113.63
2	E	501	9F3	C10-C6-C3	-2.02	110.20	115.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

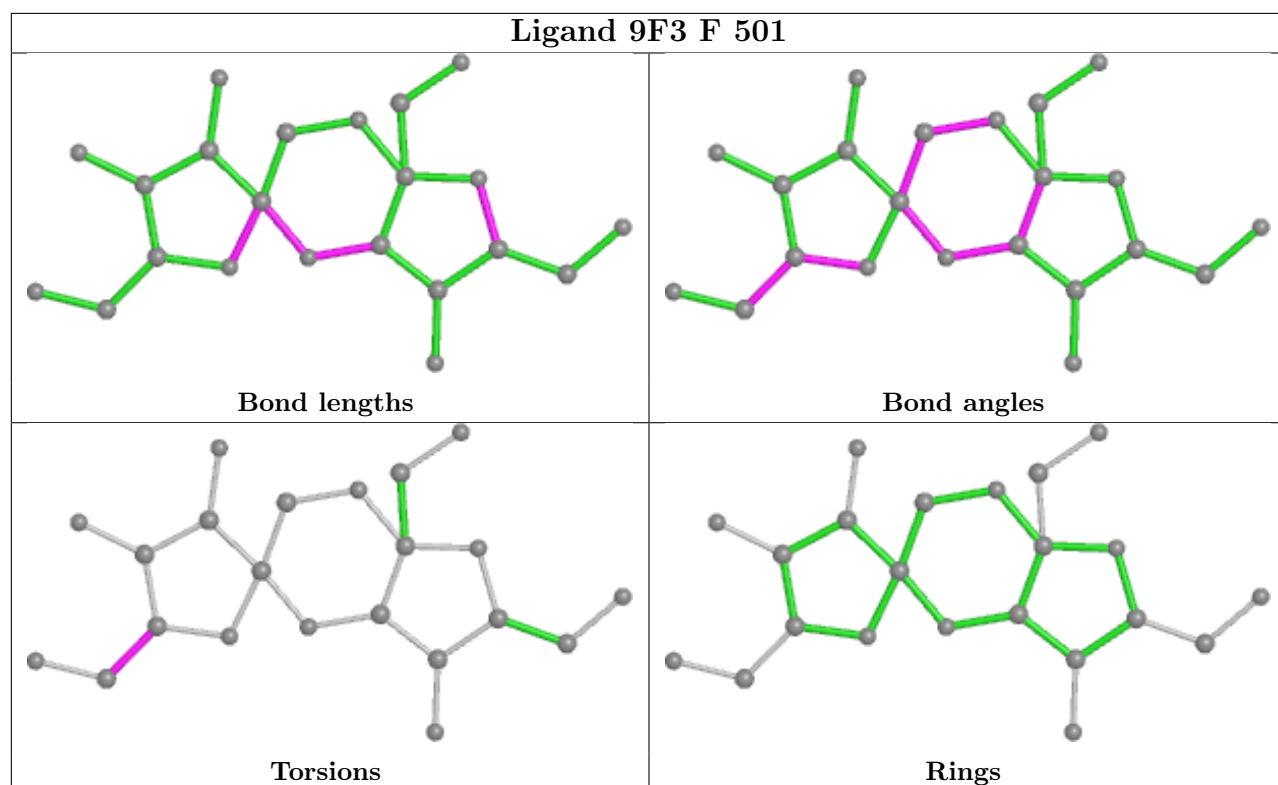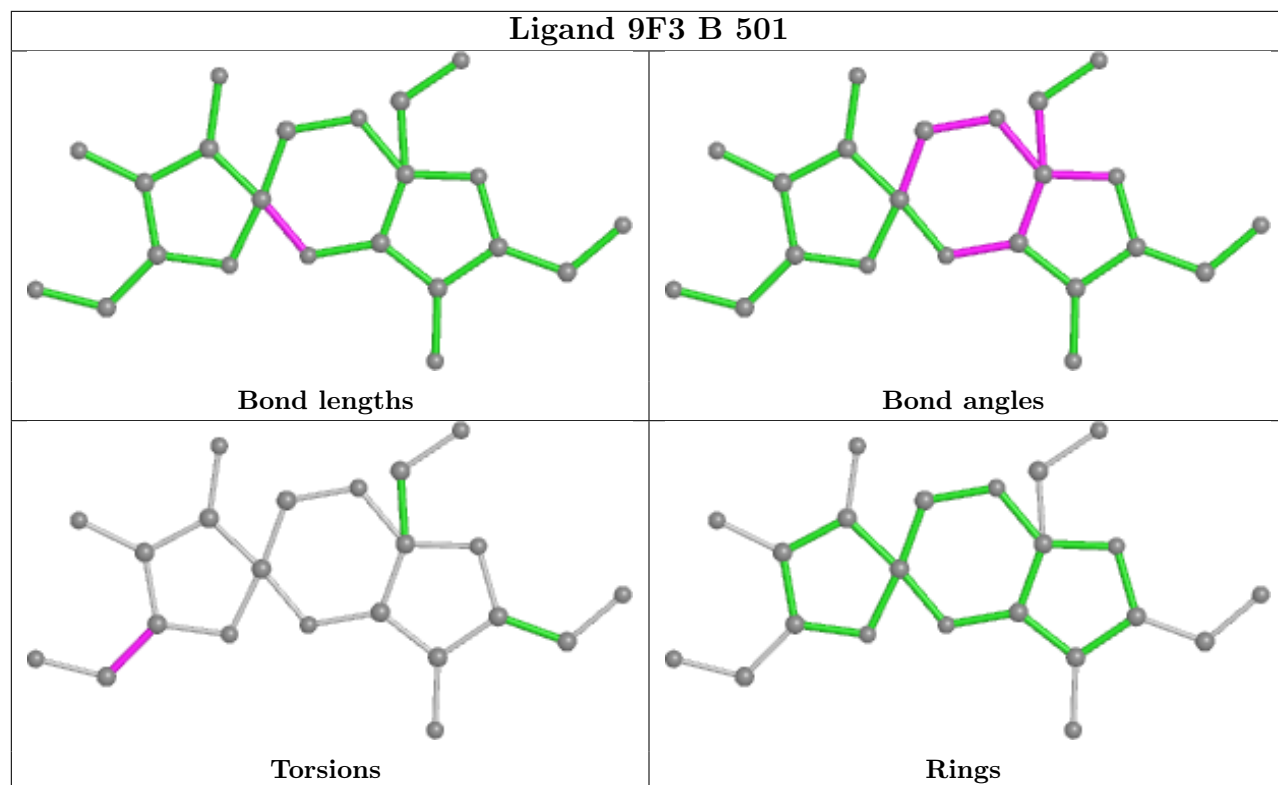| Mol	Chain	Res	Type	Atoms
2	F	501	9F3	O9-C11-C8-O3
2	B	501	9F3	O9-C11-C8-O3

There are no ring outliers.

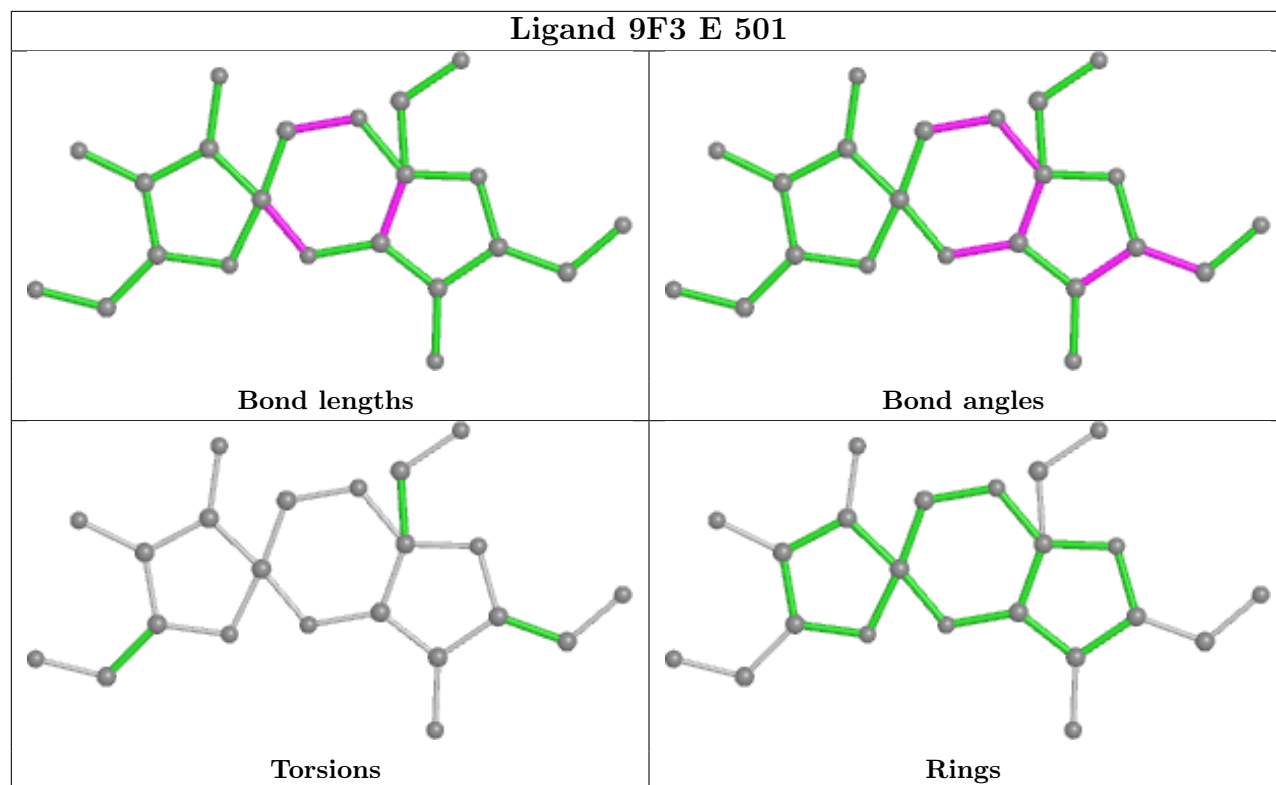No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

Ligand 9F3 C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 9F3 D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 9F3 A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 9F3 B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 9F3 F 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 9F3 E 501
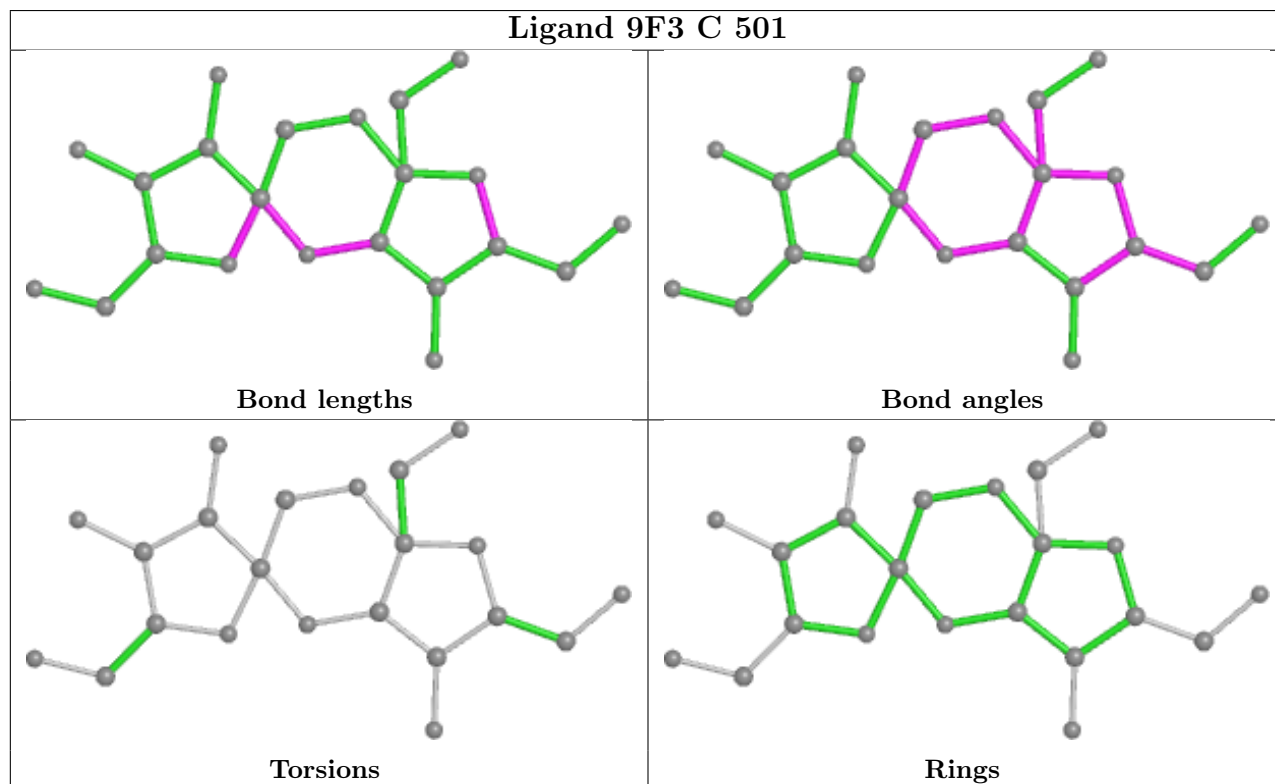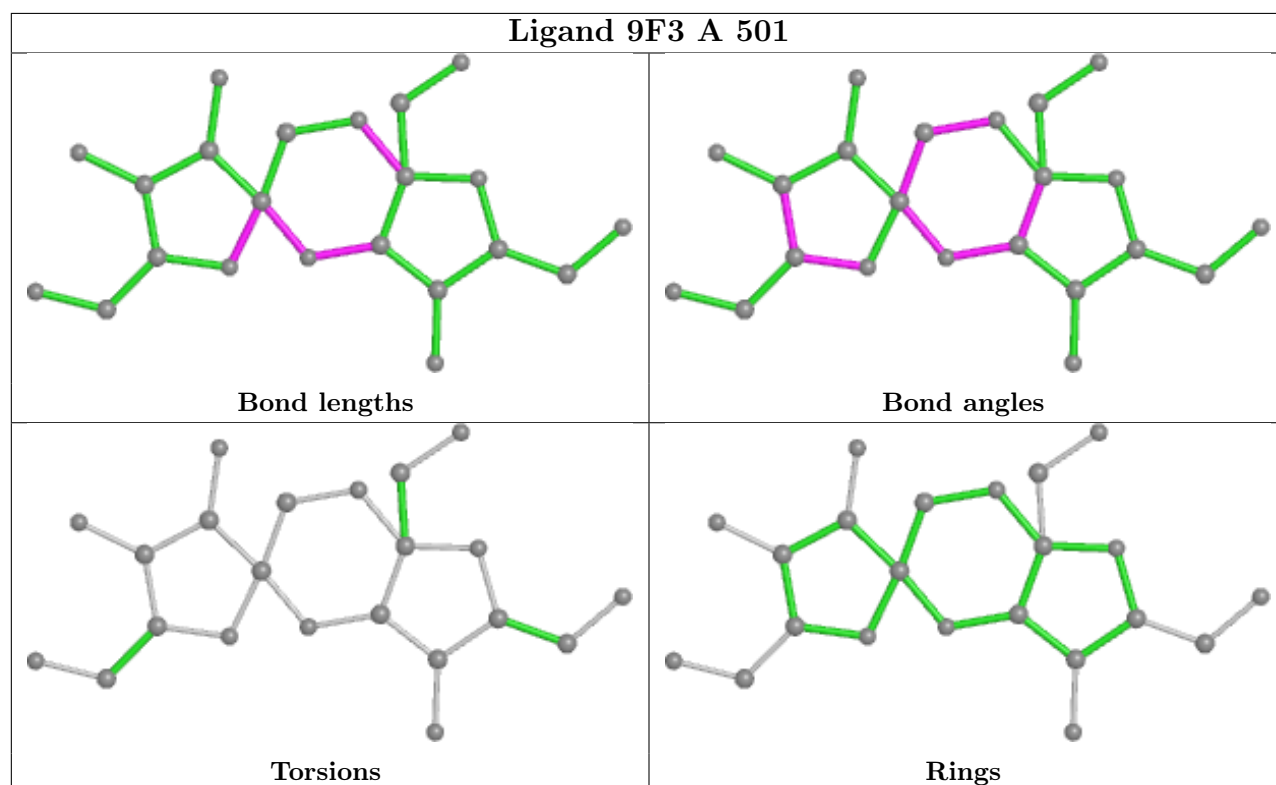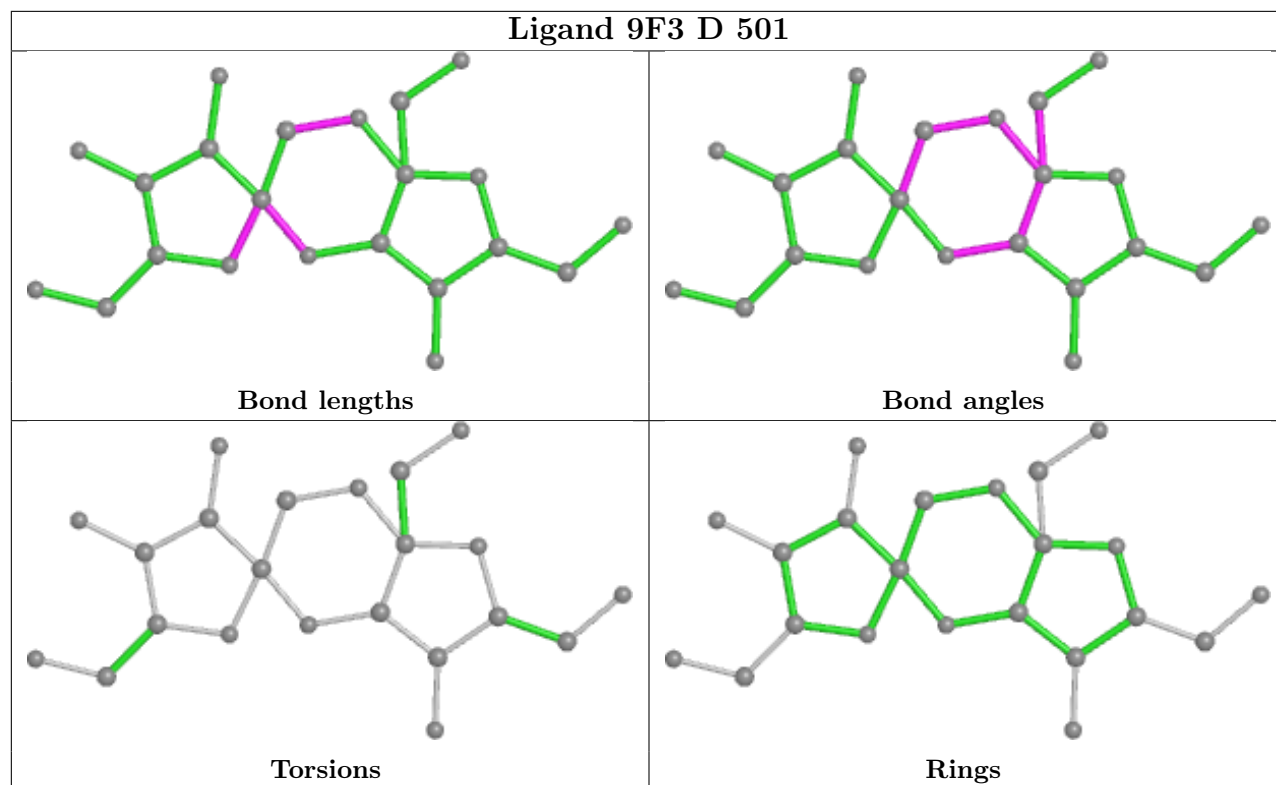
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	439/445 (98%)	-0.47	6 (1%)	75	79	8, 13, 28, 48	0
1	B	441/445 (99%)	-0.46	8 (1%)	68	72	9, 13, 30, 43	0
1	C	438/445 (98%)	-0.32	12 (2%)	54	58	10, 14, 31, 54	0
1	D	437/445 (98%)	-0.38	5 (1%)	80	83	9, 15, 32, 68	0
1	E	436/445 (97%)	-0.29	10 (2%)	60	65	11, 17, 36, 50	0
1	F	436/445 (97%)	-0.24	13 (2%)	50	54	11, 18, 40, 77	0
All	All	2627/2670 (98%)	-0.36	54 (2%)	63	67	8, 15, 33, 77	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	382	ALA	6.6
1	A	117	GLY	6.0
1	A	116	ALA	6.0
1	B	116	ALA	5.6
1	F	399	GLU	5.1
1	A	115	GLY	4.6
1	C	400	ALA	4.1
1	C	401	ALA	4.0
1	C	113	ALA	4.0
1	F	382	ALA	4.0
1	D	399	GLU	3.9
1	F	156	GLY	3.7
1	E	38	ALA	3.5
1	E	347	ASN	3.4
1	F	400	ALA	3.4
1	E	39	ALA	3.4
1	B	115	GLY	3.3
1	F	119	SER	3.3
1	B	77	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	443	VAL	3.1
1	F	154	GLY	3.1
1	E	118	ASP	3.0
1	B	381	ALA	3.0
1	F	383	SER	2.9
1	B	117	GLY	2.9
1	D	156	GLY	2.9
1	A	114	GLY	2.8
1	B	113	ALA	2.8
1	C	118	ASP	2.8
1	C	347	ASN	2.7
1	E	352	GLU	2.6
1	E	434	VAL	2.5
1	F	14	ALA	2.5
1	D	382	ALA	2.4
1	C	154	GLY	2.4
1	E	353	GLY	2.4
1	E	113	ALA	2.4
1	F	155	SER	2.4
1	D	445	PHE	2.3
1	C	348	GLU	2.3
1	C	383	SER	2.3
1	A	118	ASP	2.3
1	C	402	ASP	2.3
1	D	380	ASP	2.2
1	F	390	ALA	2.2
1	B	380	ASP	2.2
1	E	40	ASP	2.2
1	F	347	ASN	2.1
1	C	155	SER	2.1
1	F	402	ASP	2.1
1	A	113	ALA	2.1
1	E	382	ALA	2.1
1	B	114	GLY	2.0
1	C	226	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	9F3	F	501	22/22	0.93	0.09	20,23,26,30	0
2	9F3	D	501	22/22	0.94	0.08	16,20,24,25	0
2	9F3	A	501	22/22	0.95	0.08	14,18,20,21	0
2	9F3	E	501	22/22	0.95	0.07	15,17,19,21	0
2	9F3	C	501	22/22	0.95	0.08	15,20,22,25	0
2	9F3	B	501	22/22	0.97	0.06	12,14,16,16	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.
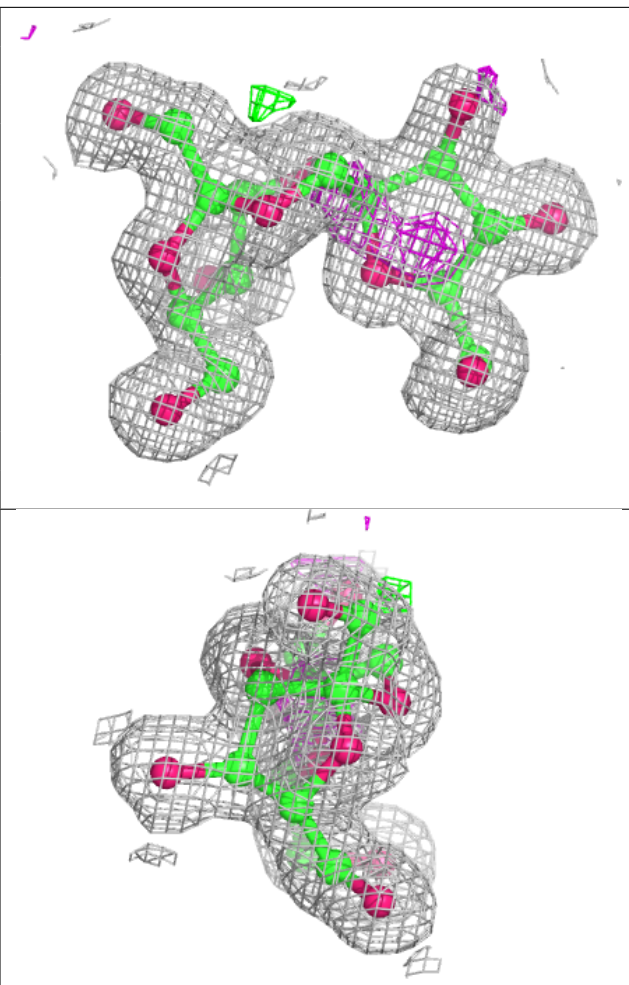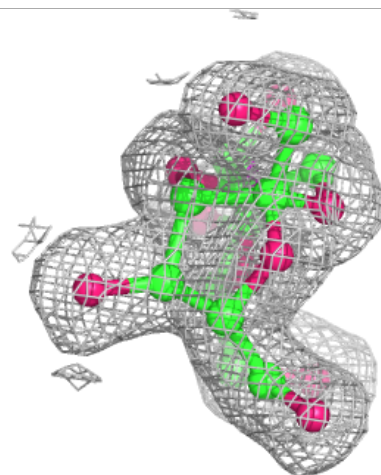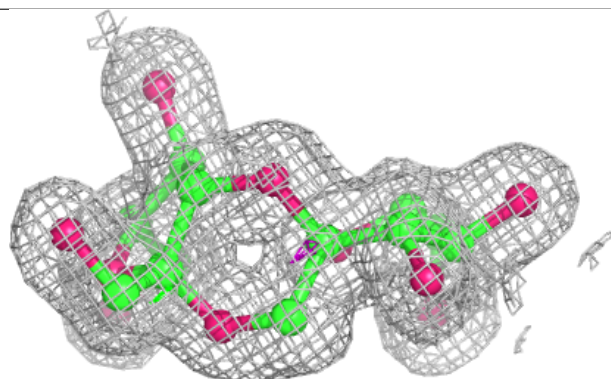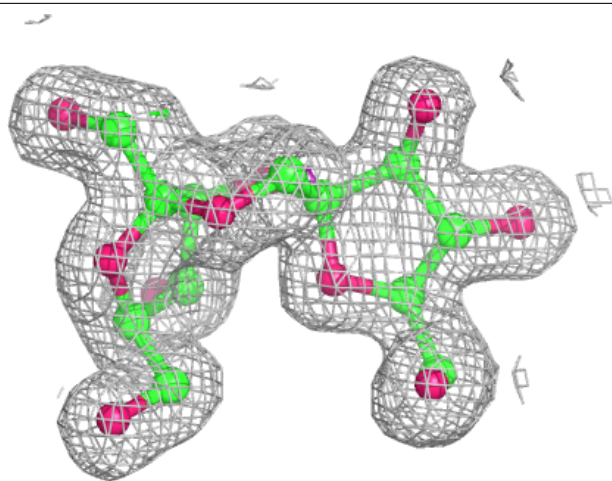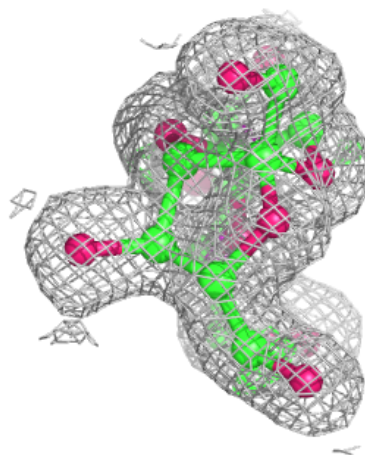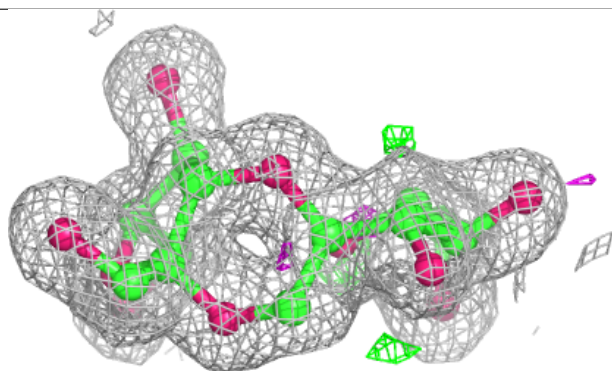
Electron density around 9F3 F 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
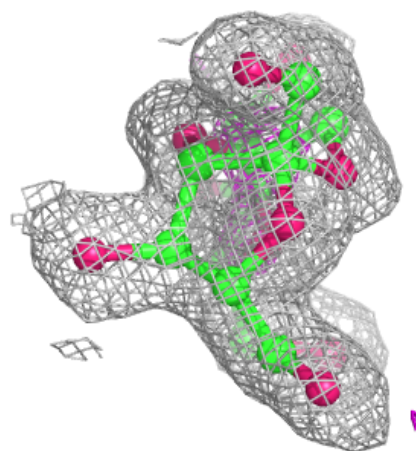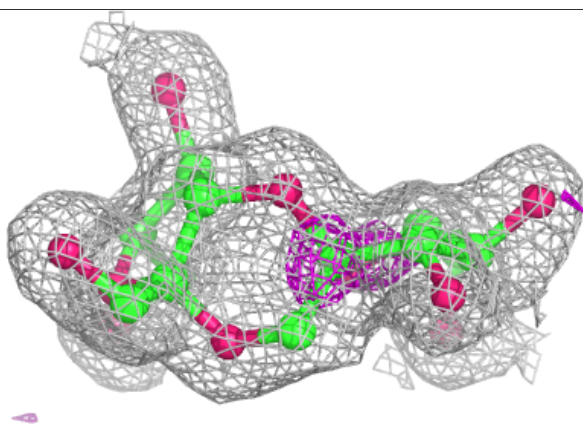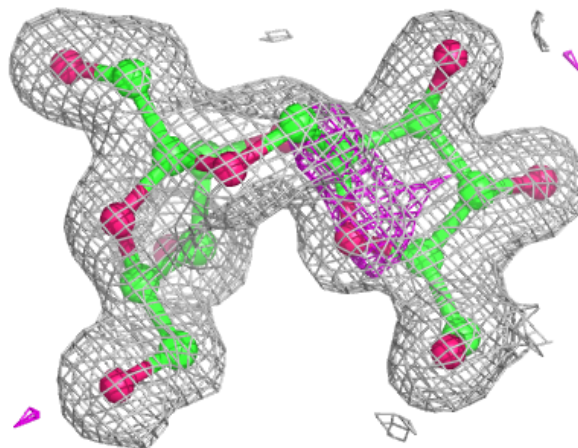
Electron density around 9F3 D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
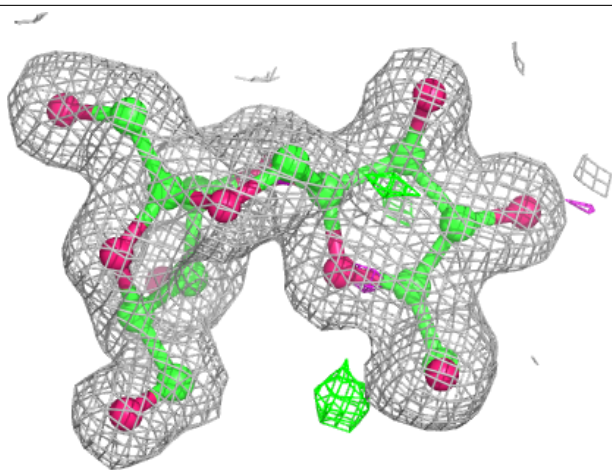and green (positive)
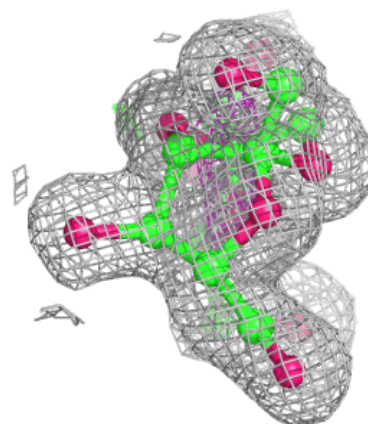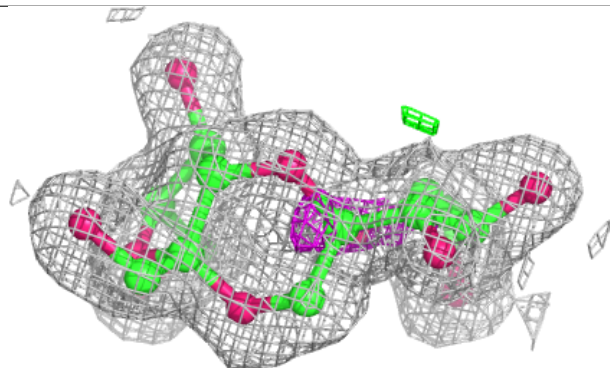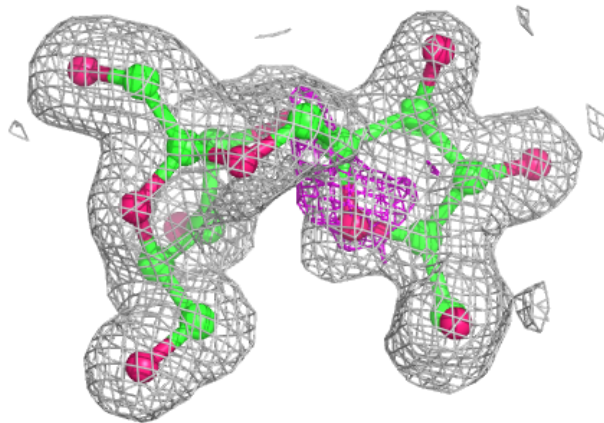
Electron density around 9F3 A 501:

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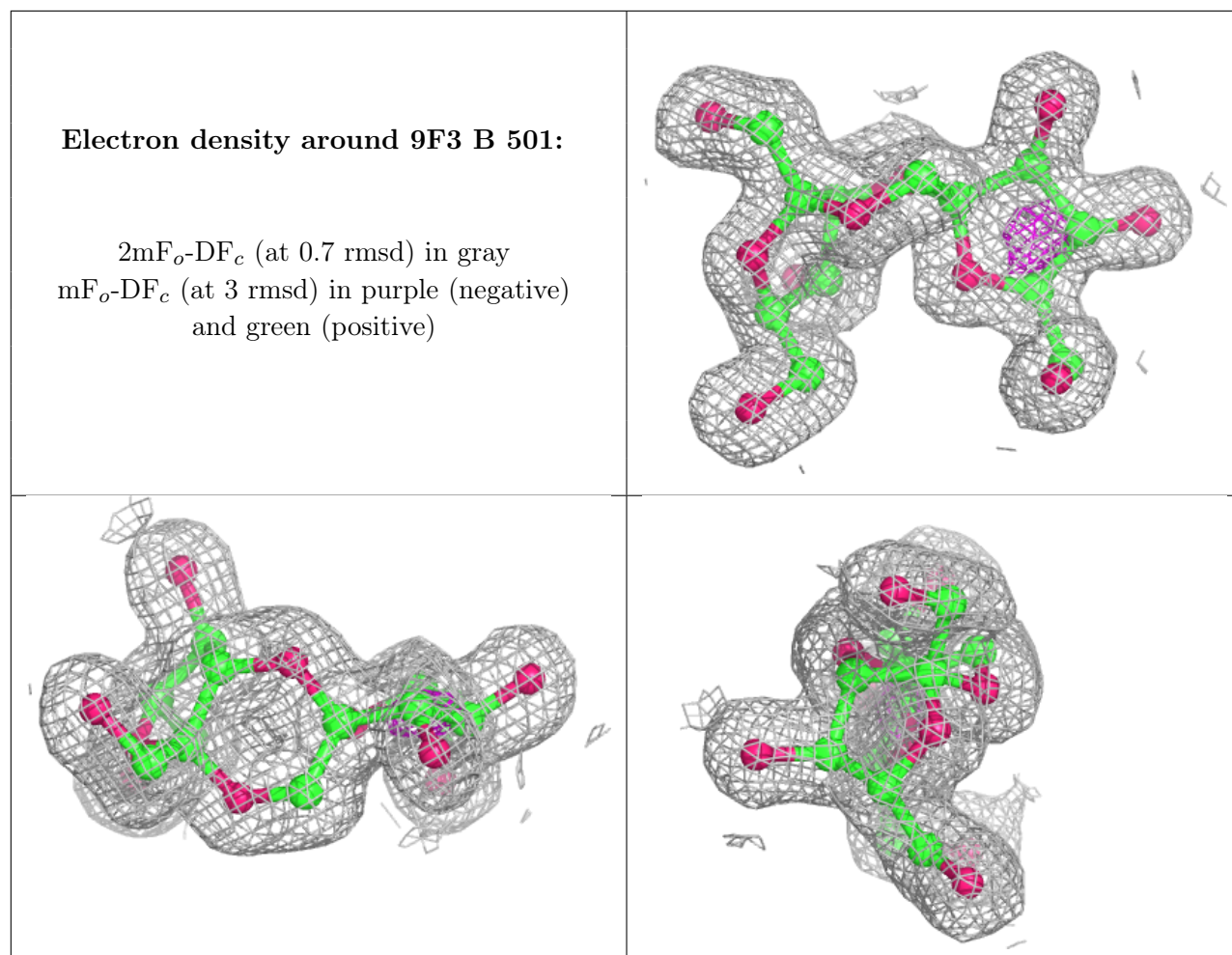and green (positive)

Electron density around 9F3 E 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 9F3 C 501:

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

Electron density around 9F3 B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.