



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2020 – 02:10 PM EST

PDB ID : 6VGI
Title : Crystal Structures of FLAP bound to MK-866
Authors : Ho, J.D.; Lee, M.R.; Rauch, C.T.; Aznavour, K.; Park, J.S.; Luz, J.G.;
Antonyamy, S.; Condon, B.; Maletic, M.; Zhang, A.; Hickey, M.J.; Hughes,
N.E.; Chandrasekhar, S.; Sloan, A.V.; Gooding, K.; Harvey, A.; Yu, X.P.;
Kahl, S.D.; Norman, B.H.
Deposited on : 2020-01-08
Resolution : 2.61 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

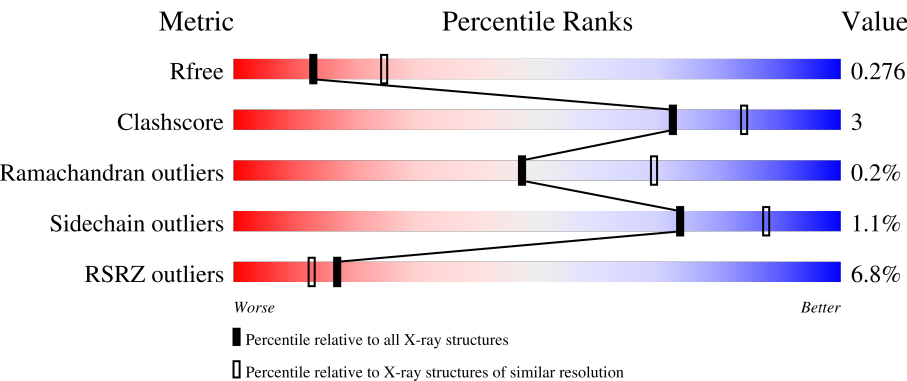
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 on 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	171	<div><div>5%</div><div><div></div><div>75%</div><div>6%</div><div>•</div><div>19%</div></div></div>
1	B	171	<div><div>9%</div><div><div></div><div>77%</div><div>5%</div><div>•</div><div>18%</div></div></div>
1	C	171	<div><div>2%</div><div><div></div><div>77%</div><div>6%</div><div>•</div><div>16%</div></div></div>
1	D	171	<div><div>5%</div><div><div></div><div>79%</div><div>8%</div><div>•</div><div>12%</div></div></div>
1	E	171	<div><div>7%</div><div><div></div><div>77%</div><div>6%</div><div>•</div><div>16%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	171	<div><div></div><div>6%</div><div>82%</div><div>8%</div><div>10%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7147 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 5-lipoxygenase-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1104	738	170	192	4			
1	B	140	Total	C	N	O	S	0	0	0
			1099	734	168	193	4			
1	C	143	Total	C	N	O	S	0	0	0
			1129	755	171	199	4			
1	D	150	Total	C	N	O	S	0	0	0
			1197	797	187	209	4			
1	E	144	Total	C	N	O	S	0	0	0
			1145	764	176	201	4			
1	F	154	Total	C	N	O	S	0	0	0
			1226	814	194	214	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P20292
A	0	SER	-	expression tag	UNP P20292
A	1	LEU	-	expression tag	UNP P20292
A	148	ALA	LYS	conflict	UNP P20292
A	162	GLU	-	expression tag	UNP P20292
A	163	GLY	-	expression tag	UNP P20292
A	164	HIS	-	expression tag	UNP P20292
A	165	HIS	-	expression tag	UNP P20292
A	166	HIS	-	expression tag	UNP P20292
A	167	HIS	-	expression tag	UNP P20292
A	168	HIS	-	expression tag	UNP P20292
A	169	HIS	-	expression tag	UNP P20292
B	-1	MET	-	initiating methionine	UNP P20292
B	0	SER	-	expression tag	UNP P20292
B	1	LEU	-	expression tag	UNP P20292
B	148	ALA	LYS	conflict	UNP P20292
B	162	GLU	-	expression tag	UNP P20292

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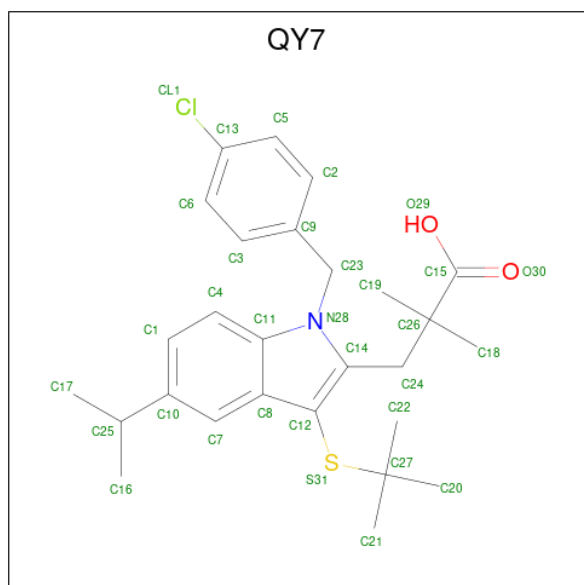
Chain	Residue	Modelled	Actual	Comment	Reference
B	163	GLY	-	expression tag	UNP P20292
B	164	HIS	-	expression tag	UNP P20292
B	165	HIS	-	expression tag	UNP P20292
B	166	HIS	-	expression tag	UNP P20292
B	167	HIS	-	expression tag	UNP P20292
B	168	HIS	-	expression tag	UNP P20292
B	169	HIS	-	expression tag	UNP P20292
C	-1	MET	-	initiating methionine	UNP P20292
C	0	SER	-	expression tag	UNP P20292
C	1	LEU	-	expression tag	UNP P20292
C	148	ALA	LYS	conflict	UNP P20292
C	162	GLU	-	expression tag	UNP P20292
C	163	GLY	-	expression tag	UNP P20292
C	164	HIS	-	expression tag	UNP P20292
C	165	HIS	-	expression tag	UNP P20292
C	166	HIS	-	expression tag	UNP P20292
C	167	HIS	-	expression tag	UNP P20292
C	168	HIS	-	expression tag	UNP P20292
C	169	HIS	-	expression tag	UNP P20292
D	-1	MET	-	initiating methionine	UNP P20292
D	0	SER	-	expression tag	UNP P20292
D	1	LEU	-	expression tag	UNP P20292
D	148	ALA	LYS	conflict	UNP P20292
D	162	GLU	-	expression tag	UNP P20292
D	163	GLY	-	expression tag	UNP P20292
D	164	HIS	-	expression tag	UNP P20292
D	165	HIS	-	expression tag	UNP P20292
D	166	HIS	-	expression tag	UNP P20292
D	167	HIS	-	expression tag	UNP P20292
D	168	HIS	-	expression tag	UNP P20292
D	169	HIS	-	expression tag	UNP P20292
E	-1	MET	-	initiating methionine	UNP P20292
E	0	SER	-	expression tag	UNP P20292
E	1	LEU	-	expression tag	UNP P20292
E	148	ALA	LYS	conflict	UNP P20292
E	162	GLU	-	expression tag	UNP P20292
E	163	GLY	-	expression tag	UNP P20292
E	164	HIS	-	expression tag	UNP P20292
E	165	HIS	-	expression tag	UNP P20292
E	166	HIS	-	expression tag	UNP P20292
E	167	HIS	-	expression tag	UNP P20292
E	168	HIS	-	expression tag	UNP P20292

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Chain	Residue	Modelled	Actual	Comment	Reference
E	169	HIS	-	expression tag	UNP P20292
F	-1	MET	-	initiating methionine	UNP P20292
F	0	SER	-	expression tag	UNP P20292
F	1	LEU	-	expression tag	UNP P20292
F	148	ALA	LYS	conflict	UNP P20292
F	162	GLU	-	expression tag	UNP P20292
F	163	GLY	-	expression tag	UNP P20292
F	164	HIS	-	expression tag	UNP P20292
F	165	HIS	-	expression tag	UNP P20292
F	166	HIS	-	expression tag	UNP P20292
F	167	HIS	-	expression tag	UNP P20292
F	168	HIS	-	expression tag	UNP P20292
F	169	HIS	-	expression tag	UNP P20292

- Molecule 2 is 3-[3-(tert-butylsulfanyl)-1-[(4-chlorophenyl)methyl]-5-(propan-2-yl)-1H-indol-2-yl]-2,2-dimethylpropanoic acid (three-letter code: QY7) (formula: C₂₇H₃₄ClNO₂S) (labeled as "Ligand of Interest" by author).



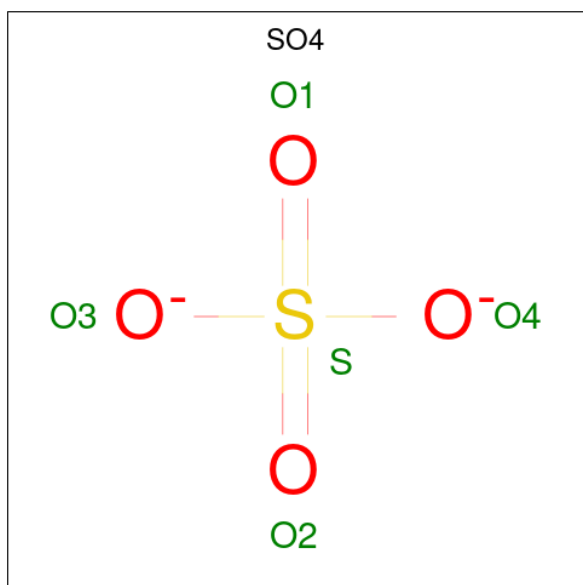
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 32	C 27	Cl 1	N 1	O 2	S 1	0	0
2	B	1	Total 32	C 27	Cl 1	N 1	O 2	S 1	0	0
2	B	1	Total 32	C 27	Cl 1	N 1	O 2	S 1	0	0
2	C	1	Total 32	C 27	Cl 1	N 1	O 2	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	Cl	N	O	S	0	0
			32	27	1	1	2	1		
2	F	1	Total	C	Cl	N	O	S	0	0
			32	27	1	1	2	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	5	Total	O	0	0
			5	5		

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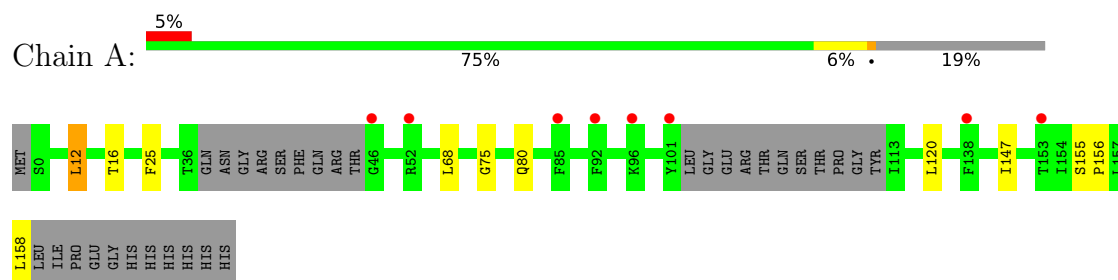
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	4	Total 4	O 4	0	0
4	D	5	Total 5	O 5	0	0
4	E	7	Total 7	O 7	0	0
4	F	3	Total 4	O 4	0	1

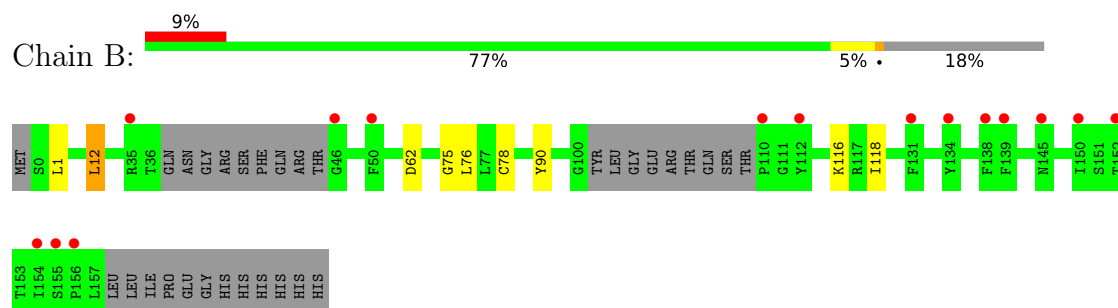
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

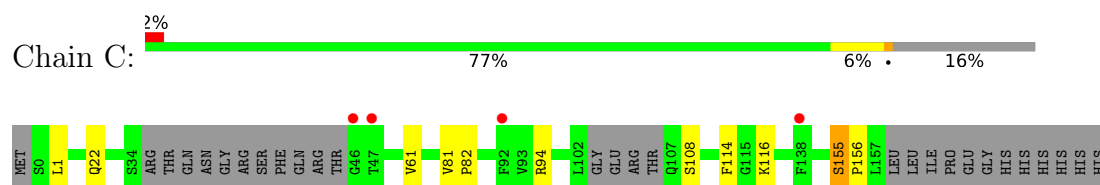
- Molecule 1: 5-lipoxygenase-activating protein



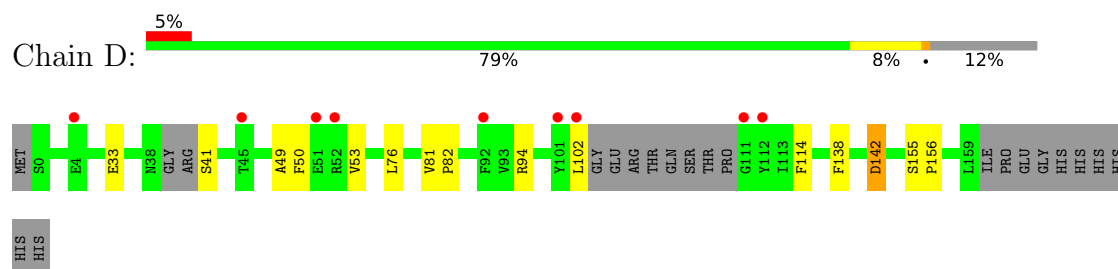
- Molecule 1: 5-lipoxygenase-activating protein



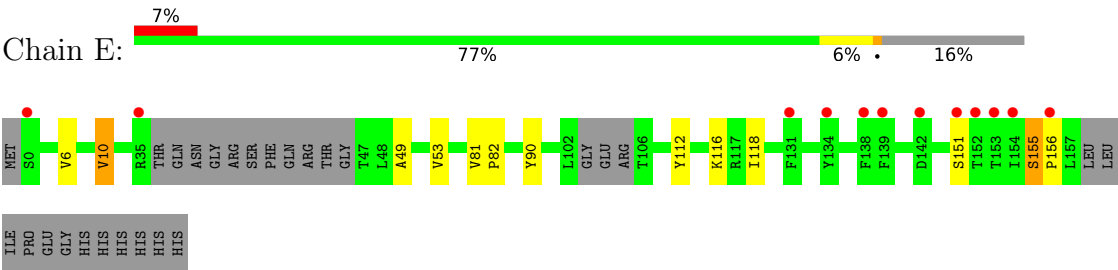
- Molecule 1: 5-lipoxygenase-activating protein



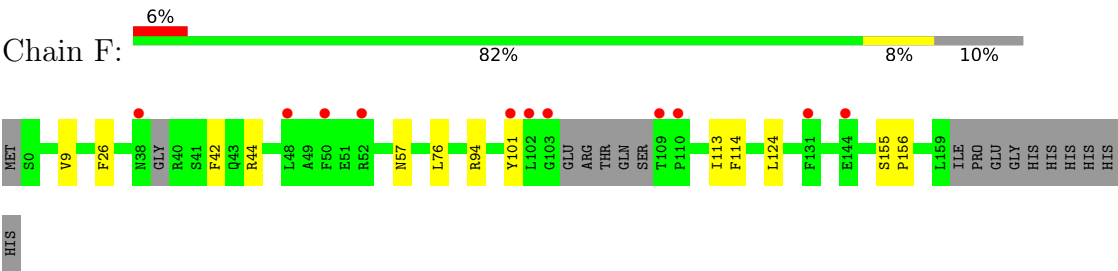
- Molecule 1: 5-lipoxygenase-activating protein



• Molecule 1: 5-lipoxygenase-activating protein



• Molecule 1: 5-lipoxygenase-activating protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.42Å 66.30Å 109.43Å 90.00° 101.53° 90.00°	Depositor
Resolution (Å)	30.00 – 2.61 53.61 – 2.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.61) 99.4 (53.61-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.259 , 0.276 0.257 , 0.276	Depositor DCC
R_{free} test set	2328 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QY7, SO4

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	0.37	0/1131	0.43	0/1536
1	B	0.37	0/1127	0.42	0/1531
1	C	0.36	0/1158	0.43	0/1575
1	D	0.36	0/1226	0.43	0/1664
1	E	0.37	0/1174	0.43	0/1596
1	F	0.37	0/1256	0.42	0/1705
All	All	0.37	0/7072	0.43	0/9607

There are no bond length outliers.

There are no bond angle outliers.

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	1104	0	1107	7	0
1	B	1099	0	1089	9	0
1	C	1129	0	1119	8	0
1	D	1197	0	1197	10	0
1	E	1145	0	1143	8	0
1	F	1226	0	1227	7	0
2	A	32	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	64	0	0	5	0
2	C	32	0	0	2	0
2	E	32	0	0	2	0
2	F	32	0	0	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
4	E	7	0	0	0	0
4	F	4	0	0	0	0
All	All	7147	0	6882	48	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 3.

All (48) 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:116:LYS:HE3	2:B:201:QY7:O30	1.54	1.06
1:F:94:ARG:HG2	1:F:114:PHE:CE1	2.23	0.74
1:D:94:ARG:HG2	1:D:114:PHE:CE1	2.29	0.68
1:B:116:LYS:HG2	2:B:201:QY7:C18	2.24	0.68
1:B:116:LYS:CE	2:B:201:QY7:O30	2.39	0.66
1:D:94:ARG:HG2	1:D:114:PHE:HE1	1.64	0.63
1:C:155:SER:HB3	1:C:156:PRO:HD3	1.81	0.62
1:B:12:LEU:HD21	1:B:75:GLY:HA3	1.85	0.57
1:F:155:SER:HB3	1:F:156:PRO:HD3	1.88	0.54
1:E:116:LYS:NZ	2:F:201:QY7:O30	2.37	0.53
1:D:138:PHE:O	1:D:142:ASP:HB2	2.09	0.53
1:D:33:GLU:HG2	1:D:50:PHE:HA	1.92	0.52
1:A:12:LEU:HD21	1:A:75:GLY:HA3	1.93	0.50
2:A:201:QY7:C17	1:F:113:ILE:HG23	2.42	0.50
1:F:94:ARG:HG2	1:F:114:PHE:HE1	1.71	0.50
2:B:201:QY7:C14	2:B:201:QY7:C3	2.91	0.47
1:C:22:GLN:OE1	1:C:94:ARG:HD3	2.14	0.47
1:D:155:SER:HB3	1:D:156:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:HB	1:C:82:PRO:HD3	1.98	0.46
1:B:1:LEU:HD11	1:D:76:LEU:HD22	1.98	0.45
1:E:151:SER:O	1:E:155:SER:HB2	2.17	0.45
1:E:49:ALA:O	1:E:53:VAL:HG23	2.16	0.45
1:B:62:ASP:HA	1:C:61:VAL:HG11	1.99	0.45
1:E:112:TYR:HB2	1:F:42:PHE:CE2	2.52	0.45
1:A:120:LEU:HD12	2:E:201:QY7:C22	2.48	0.44
1:E:90:TYR:HB2	1:E:118:ILE:HG21	1.99	0.44
1:F:26:PHE:HB3	1:F:57:ASN:HD22	1.81	0.44
1:D:49:ALA:O	1:D:53:VAL:HG23	2.18	0.43
1:D:81:VAL:HB	1:D:82:PRO:HD3	1.98	0.43
1:D:53:VAL:HG22	1:D:102:LEU:HD22	2.00	0.43
2:E:201:QY7:C14	2:E:201:QY7:C3	2.94	0.43
1:B:76:LEU:HD22	1:C:1:LEU:HD11	2.00	0.43
1:A:25:PHE:HD1	2:A:201:QY7:CL1	2.39	0.42
1:E:155:SER:H	1:E:156:PRO:CD	2.32	0.42
1:E:6:VAL:O	1:E:10:VAL:HG22	2.19	0.42
1:A:16:THR:HG23	1:A:68:LEU:HD11	2.01	0.42
1:F:9:VAL:HG12	1:F:76:LEU:HD21	2.00	0.42
1:A:12:LEU:HD13	1:A:80:GLN:HG3	2.01	0.41
1:C:94:ARG:HG3	1:C:114:PHE:CE1	2.55	0.41
1:E:81:VAL:HB	1:E:82:PRO:HD3	2.02	0.41
2:A:201:QY7:C14	2:A:201:QY7:C3	2.97	0.41
1:A:155:SER:OG	1:A:156:PRO:HD3	2.21	0.41
1:B:90:TYR:HB2	1:B:118:ILE:HG21	2.02	0.41
2:B:202:QY7:C24	2:B:202:QY7:C21	2.99	0.41
2:C:201:QY7:C3	2:C:201:QY7:C14	2.97	0.41
1:A:147:ILE:HG12	1:B:78:CYS:SG	2.61	0.40
1:C:108:SER:HA	1:D:41:SER:HB3	2.04	0.40
1:C:116:LYS:HG3	2:C:201:QY7:C8	2.52	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	133/171 (78%)	132 (99%)	1 (1%)	0	100	100
1	B	134/171 (78%)	132 (98%)	2 (2%)	0	100	100
1	C	137/171 (80%)	133 (97%)	3 (2%)	1 (1%)	22	41
1	D	144/171 (84%)	142 (99%)	2 (1%)	0	100	100
1	E	138/171 (81%)	133 (96%)	4 (3%)	1 (1%)	22	41
1	F	148/171 (86%)	147 (99%)	1 (1%)	0	100	100
All	All	834/1026 (81%)	819 (98%)	13 (2%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	C	155	SER

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	118/146 (81%)	116 (98%)	2 (2%)	60	80
1	B	116/146 (80%)	115 (99%)	1 (1%)	78	90
1	C	120/146 (82%)	120 (100%)	0	100	100
1	D	128/146 (88%)	127 (99%)	1 (1%)	81	92
1	E	123/146 (84%)	122 (99%)	1 (1%)	81	92
1	F	131/146 (90%)	128 (98%)	3 (2%)	50	73
All	All	736/876 (84%)	728 (99%)	8 (1%)	73	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	158	LEU
1	B	12	LEU
1	D	142	ASP
1	E	10	VAL
1	F	44	ARG
1	F	101	TYR
1	F	124	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	F	8	ASN
1	F	58	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	QY7	C	201	-	29,34,34	1.22	3 (10%)	40,52,52	1.37	5 (12%)
3	SO4	F	202	-	4,4,4	0.14	0	6,6,6	0.06	0
2	QY7	E	201	-	29,34,34	1.18	3 (10%)	40,52,52	1.42	4 (10%)
2	QY7	F	201	-	29,34,34	1.22	4 (13%)	40,52,52	1.33	4 (10%)
2	QY7	A	201	-	29,34,34	1.18	4 (13%)	40,52,52	1.35	4 (10%)
2	QY7	B	201	-	29,34,34	1.21	4 (13%)	40,52,52	1.56	4 (10%)
3	SO4	C	202	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	A	202	-	4,4,4	0.14	0	6,6,6	0.07	0
2	QY7	B	202	-	29,34,34	1.17	2 (6%)	40,52,52	1.27	5 (12%)
3	SO4	E	202	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	B	203	-	4,4,4	0.14	0	6,6,6	0.08	0

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	QY7	C	201	-	-	5/16/24/24	0/3/3/3
2	QY7	E	201	-	-	2/16/24/24	0/3/3/3
2	QY7	F	201	-	-	2/16/24/24	0/3/3/3
2	QY7	A	201	-	-	5/16/24/24	0/3/3/3
2	QY7	B	201	-	-	5/16/24/24	0/3/3/3
2	QY7	B	202	-	-	2/16/24/24	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201	QY7	C12-S31	-3.28	1.74	1.78
2	C	201	QY7	C12-S31	-3.19	1.74	1.78
2	B	201	QY7	C12-S31	-3.16	1.74	1.78
2	E	201	QY7	C12-S31	-3.09	1.75	1.78
2	A	201	QY7	C12-S31	-3.05	1.75	1.78
2	B	202	QY7	C12-S31	-3.02	1.75	1.78
2	C	201	QY7	C27-S31	-2.81	1.81	1.85
2	B	201	QY7	C27-S31	-2.64	1.82	1.85
2	E	201	QY7	C27-S31	-2.60	1.82	1.85
2	F	201	QY7	C27-S31	-2.58	1.82	1.85
2	B	202	QY7	C27-S31	-2.56	1.82	1.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	QY7	C27-S31	-2.53	1.82	1.85
2	C	201	QY7	C26-C15	2.22	1.54	1.50
2	A	201	QY7	C26-C15	2.09	1.54	1.50
2	E	201	QY7	C26-C15	2.08	1.54	1.50
2	B	201	QY7	C26-C15	2.07	1.54	1.50
2	A	201	QY7	C23-N28	-2.07	1.44	1.48
2	F	201	QY7	C26-C15	2.06	1.54	1.50
2	B	201	QY7	C23-N28	-2.02	1.44	1.48
2	F	201	QY7	C23-N28	-2.02	1.44	1.48

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	QY7	C9-C23-N28	-5.94	103.41	112.63
2	E	201	QY7	C9-C23-N28	-5.21	104.53	112.63
2	B	201	QY7	C10-C7-C8	-4.28	119.15	122.00
2	C	201	QY7	C10-C7-C8	-4.23	119.18	122.00
2	A	201	QY7	C10-C7-C8	-4.20	119.20	122.00
2	F	201	QY7	C9-C23-N28	-4.19	106.12	112.63
2	F	201	QY7	C10-C7-C8	-4.14	119.24	122.00
2	B	202	QY7	C10-C7-C8	-4.09	119.27	122.00
2	E	201	QY7	C10-C7-C8	-4.06	119.30	122.00
2	A	201	QY7	C9-C23-N28	-3.90	106.57	112.63
2	C	201	QY7	C9-C23-N28	-3.89	106.59	112.63
2	C	201	QY7	C27-S31-C12	-3.23	98.76	104.81
2	B	202	QY7	C9-C23-N28	-3.18	107.68	112.63
2	A	201	QY7	C27-S31-C12	-2.87	99.44	104.81
2	B	202	QY7	C27-S31-C12	-2.66	99.84	104.81
2	B	201	QY7	C12-C8-C11	-2.62	107.07	114.39
2	A	201	QY7	C12-C8-C11	-2.60	107.14	114.39
2	F	201	QY7	C12-C8-C11	-2.56	107.24	114.39
2	E	201	QY7	C12-C8-C11	-2.55	107.28	114.39
2	B	202	QY7	C12-C8-C11	-2.53	107.34	114.39
2	C	201	QY7	C12-C8-C11	-2.48	107.46	114.39
2	B	201	QY7	C27-S31-C12	-2.25	100.60	104.81
2	C	201	QY7	C7-C10-C25	-2.24	118.69	121.67
2	B	202	QY7	C7-C10-C25	-2.14	118.82	121.67
2	F	201	QY7	C7-C10-C25	-2.11	118.86	121.67
2	E	201	QY7	C7-C10-C25	-2.02	118.98	121.67

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	QY7	C14-C24-C26-C15
2	B	201	QY7	C14-C24-C26-C15
2	A	201	QY7	C14-C24-C26-C18
2	A	201	QY7	C14-C24-C26-C19
2	B	201	QY7	C14-C24-C26-C18
2	B	201	QY7	C14-C24-C26-C19
2	C	201	QY7	C14-C24-C26-C19
2	C	201	QY7	N28-C23-C9-C3
2	C	201	QY7	N28-C23-C9-C2
2	A	201	QY7	N28-C23-C9-C3
2	B	202	QY7	N28-C23-C9-C3
2	E	201	QY7	N28-C23-C9-C3
2	A	201	QY7	N28-C23-C9-C2
2	B	201	QY7	N28-C23-C9-C3
2	E	201	QY7	N28-C23-C9-C2
2	B	202	QY7	N28-C23-C9-C2
2	B	201	QY7	N28-C23-C9-C2
2	F	201	QY7	N28-C23-C9-C3
2	F	201	QY7	N28-C23-C9-C2
2	C	201	QY7	C14-C24-C26-C15
2	C	201	QY7	C14-C24-C26-C18

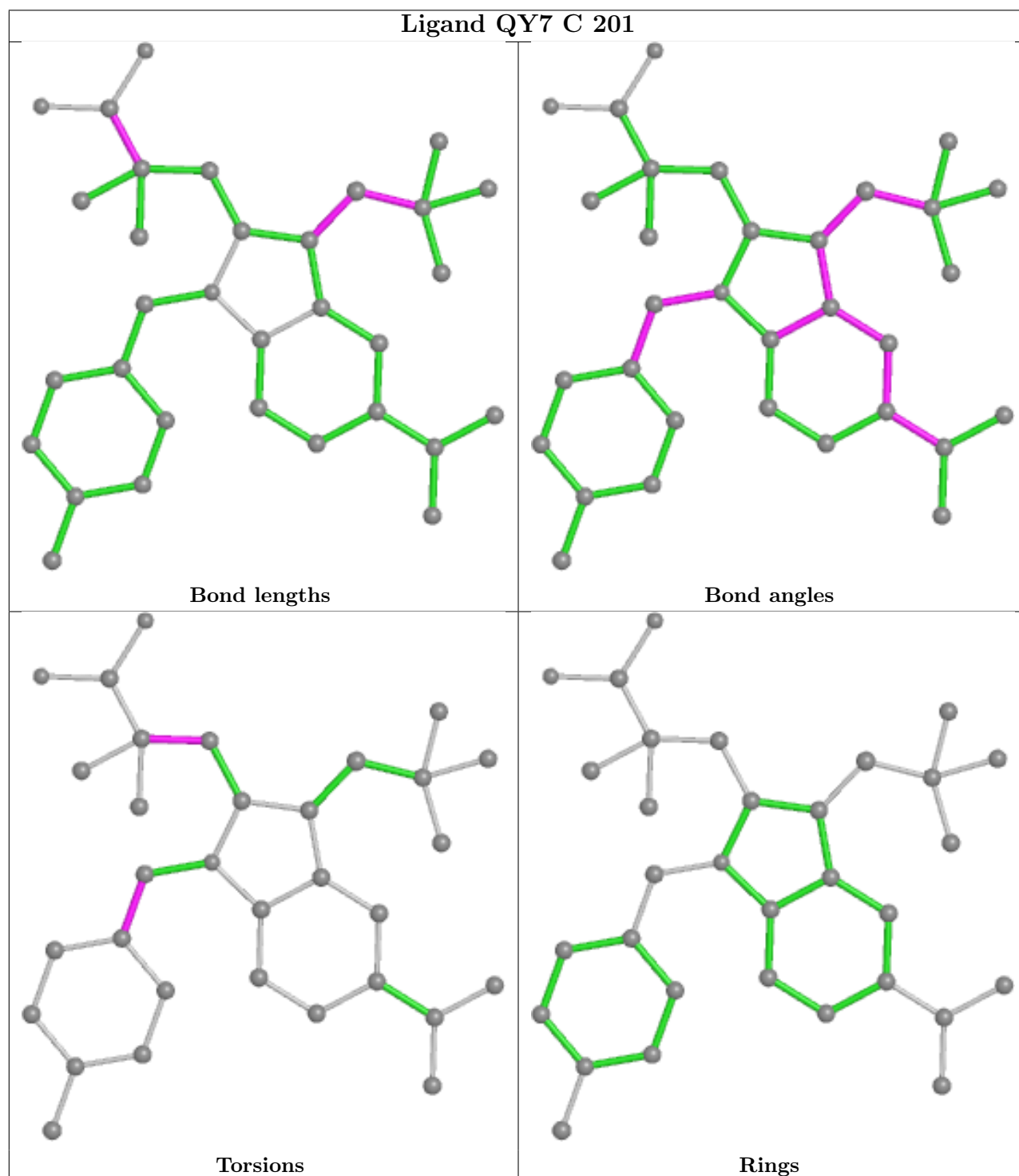
There are no ring outliers.

6 monomers are involved in 13 short contacts:

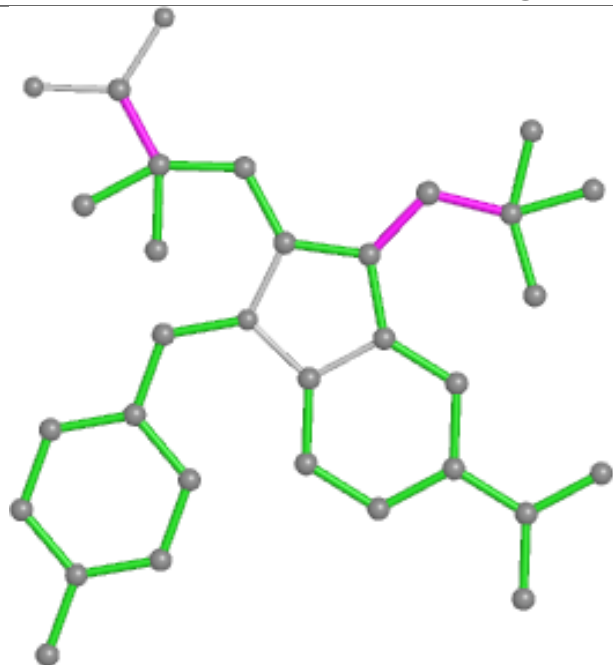
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	QY7	2	0
2	E	201	QY7	2	0
2	F	201	QY7	1	0
2	A	201	QY7	3	0
2	B	201	QY7	4	0
2	B	202	QY7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

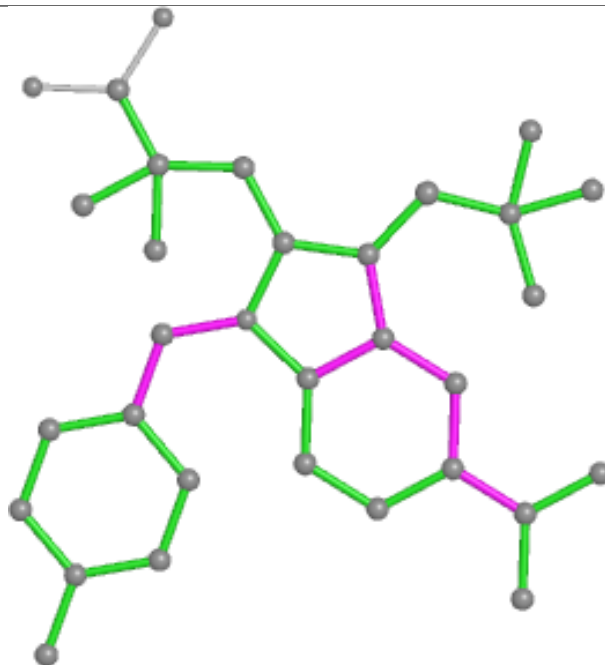
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



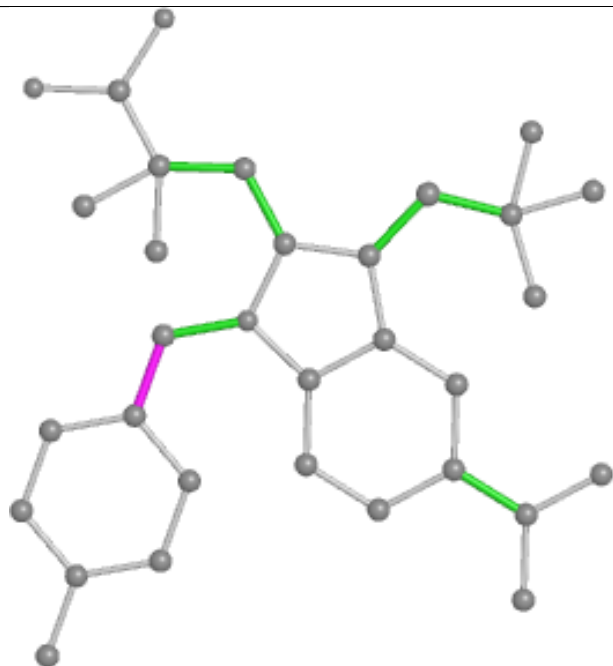
Ligand QY7 E 201



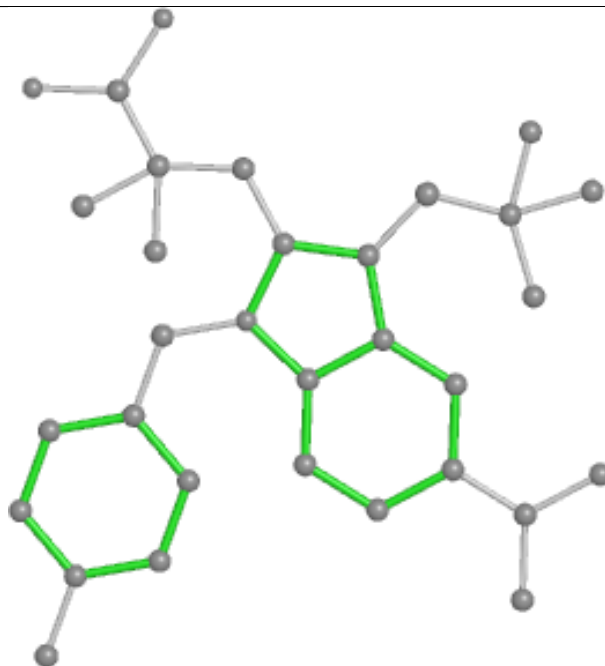
Bond lengths



Bond angles

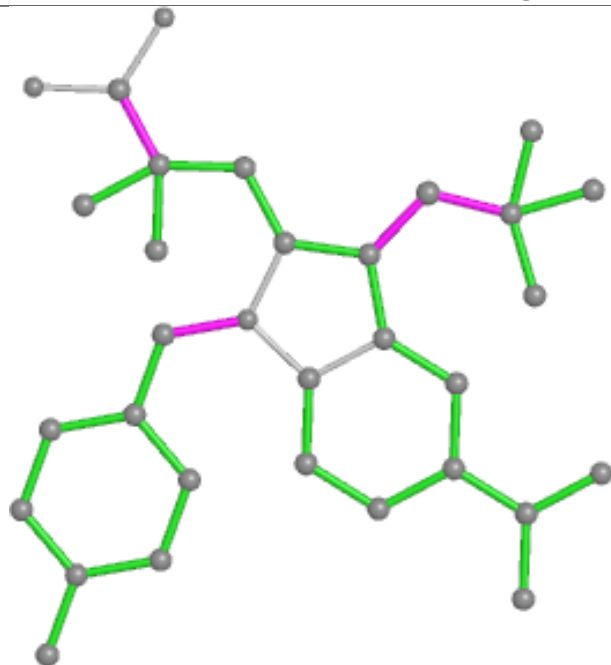


Torsions

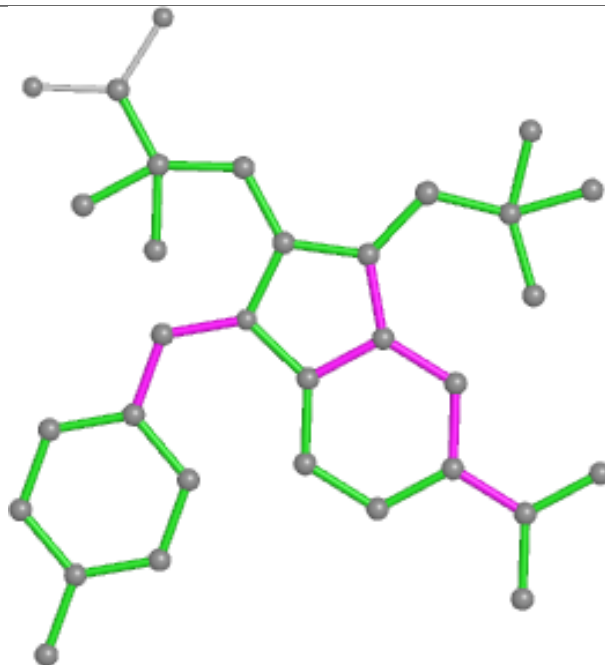


Rings

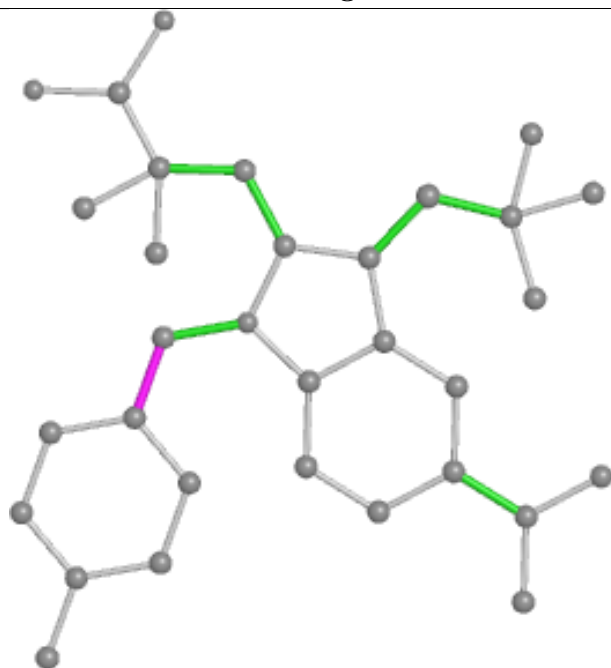
Ligand QY7 F 201



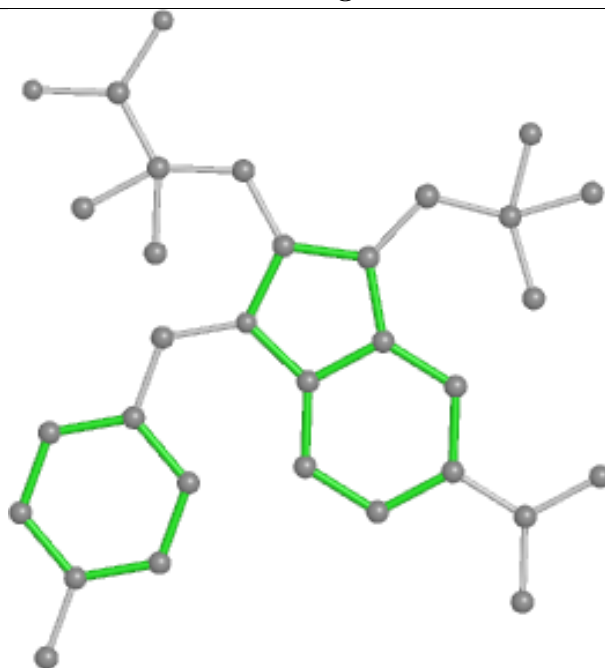
Bond lengths



Bond angles

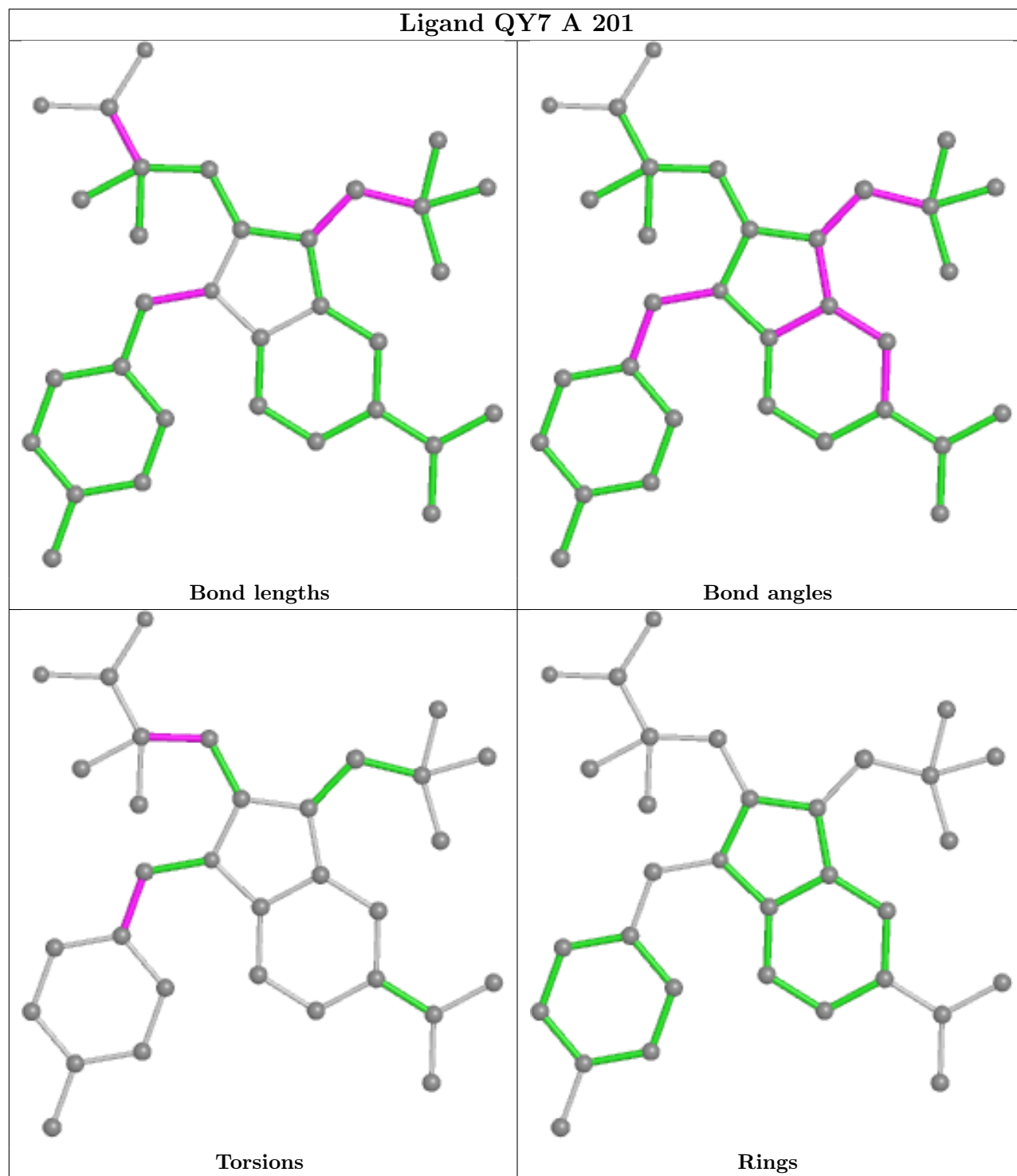


Torsions

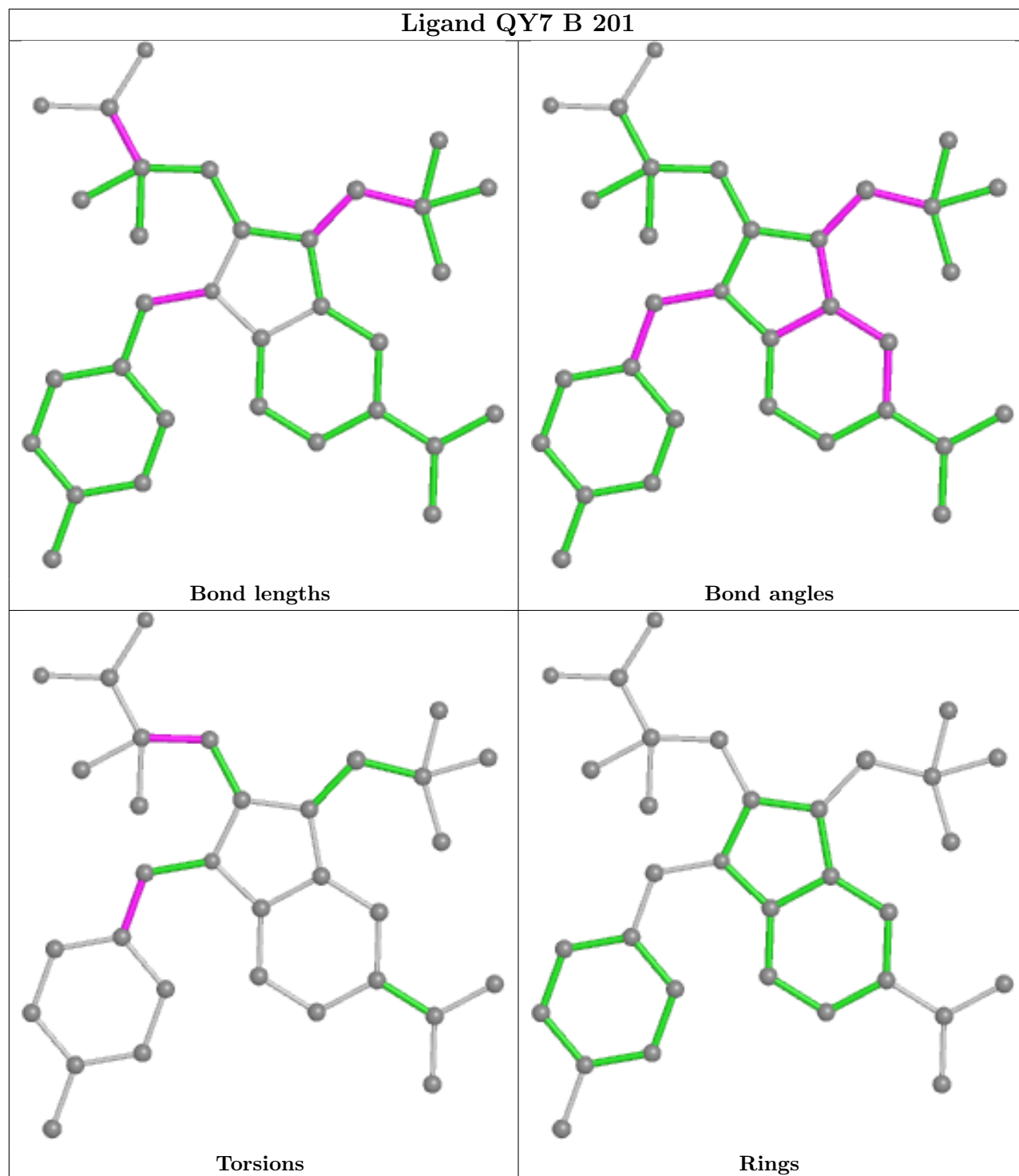


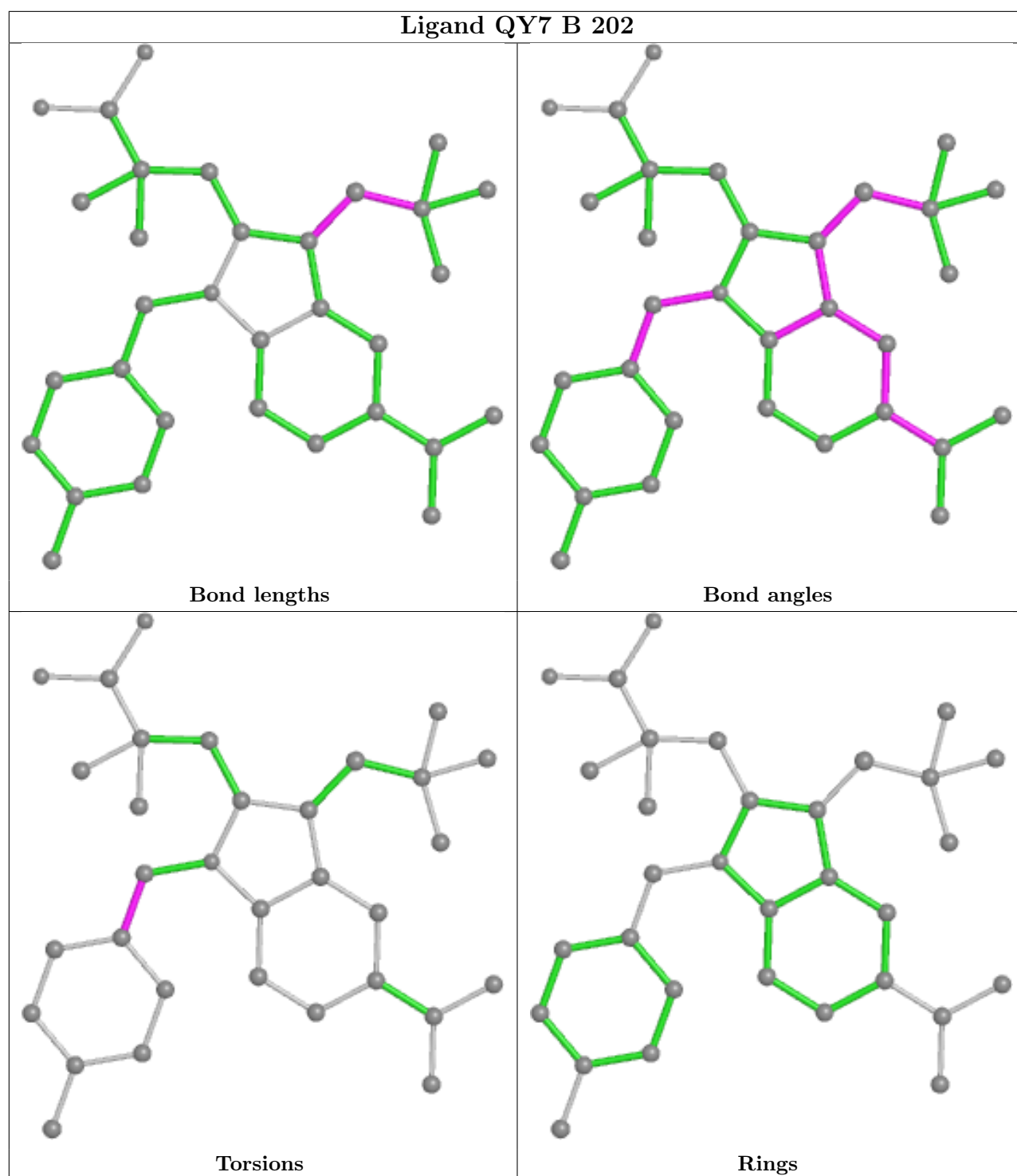
Rings

Ligand QY7 A 201



Ligand QY7 B 201





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	139/171 (81%)	0.41	8 (5%) 23 18	36, 53, 87, 98	0
1	B	140/171 (81%)	0.59	15 (10%) 6 4	29, 49, 88, 102	0
1	C	143/171 (83%)	0.37	4 (2%) 53 47	30, 47, 70, 88	0
1	D	150/171 (87%)	0.49	9 (6%) 21 17	31, 50, 78, 96	0
1	E	144/171 (84%)	0.38	12 (8%) 11 8	27, 42, 82, 88	0
1	F	154/171 (90%)	0.68	11 (7%) 16 11	33, 52, 79, 94	0
All	All	870/1026 (84%)	0.49	59 (6%) 17 13	27, 50, 84, 102	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	7.2
1	E	138	PHE	5.0
1	F	110	PRO	4.8
1	F	103	GLY	4.5
1	F	109	THR	4.3
1	B	138	PHE	4.0
1	A	46	GLY	4.0
1	E	153	THR	3.9
1	E	154	ILE	3.9
1	E	152	THR	3.8
1	B	110	PRO	3.5
1	D	52	ARG	3.5
1	B	152	THR	3.5
1	F	48	LEU	3.4
1	E	131	PHE	3.3
1	E	139	PHE	3.3
1	B	155	SER	3.2
1	D	111	GLY	3.1
1	D	92	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	131	PHE	3.0
1	D	102	LEU	3.0
1	C	46	GLY	3.0
1	B	139	PHE	2.8
1	F	101	TYR	2.7
1	C	47	THR	2.7
1	B	150	ILE	2.6
1	B	131	PHE	2.6
1	F	52	ARG	2.6
1	D	51	GLU	2.5
1	F	38	ASN	2.5
1	C	138	PHE	2.5
1	F	102	LEU	2.5
1	B	50	PHE	2.5
1	D	112	TYR	2.5
1	B	35	ARG	2.4
1	A	138	PHE	2.4
1	E	151	SER	2.4
1	A	92	PHE	2.3
1	A	153	THR	2.3
1	E	35	ARG	2.3
1	B	112	TYR	2.2
1	E	0	SER	2.2
1	A	85	PHE	2.2
1	A	101	TYR	2.2
1	E	142	ASP	2.1
1	F	144	GLU	2.1
1	D	4	GLU	2.1
1	A	52	ARG	2.1
1	B	154	ILE	2.1
1	B	156	PRO	2.1
1	B	145	ASN	2.1
1	B	134	TYR	2.1
1	F	50	PHE	2.1
1	D	45	THR	2.0
1	D	101	TYR	2.0
1	C	92	PHE	2.0
1	A	96	LYS	2.0
1	E	134	TYR	2.0
1	E	156	PRO	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](#)

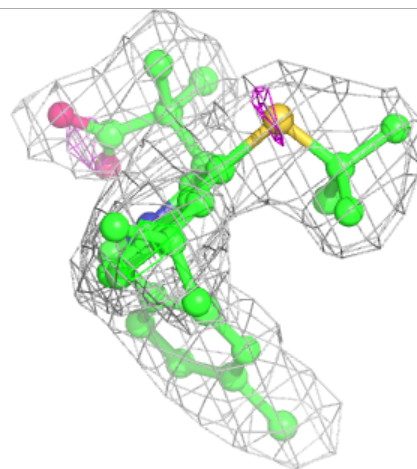
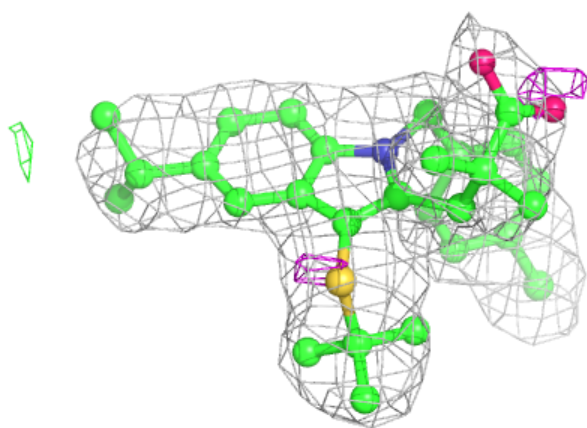
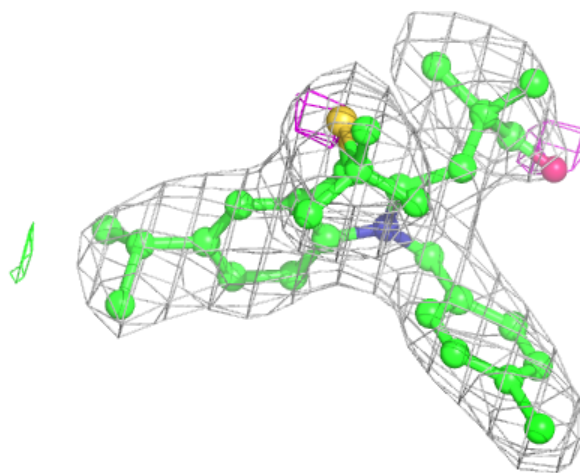
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	202	5/5	0.87	0.34	92,93,94,96	0
2	QY7	B	201	32/32	0.90	0.25	42,50,58,70	0
2	QY7	E	201	32/32	0.90	0.29	48,54,64,72	0
3	SO4	B	203	5/5	0.91	0.18	78,79,81,82	0
3	SO4	F	202	5/5	0.92	0.15	75,75,78,79	0
2	QY7	C	201	32/32	0.92	0.30	48,58,66,76	0
2	QY7	B	202	32/32	0.92	0.30	53,61,68,77	0
3	SO4	E	202	5/5	0.92	0.25	75,77,79,80	0
2	QY7	A	201	32/32	0.92	0.22	53,65,70,73	0
2	QY7	F	201	32/32	0.94	0.22	37,49,66,74	0
3	SO4	C	202	5/5	0.94	0.17	66,67,69,72	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.

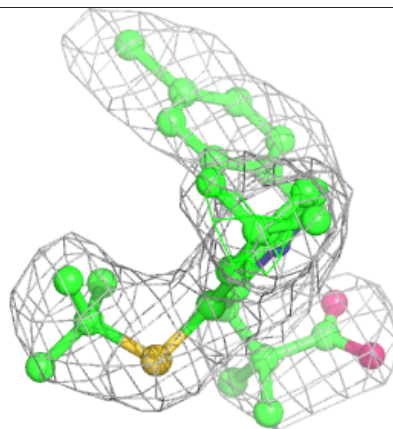
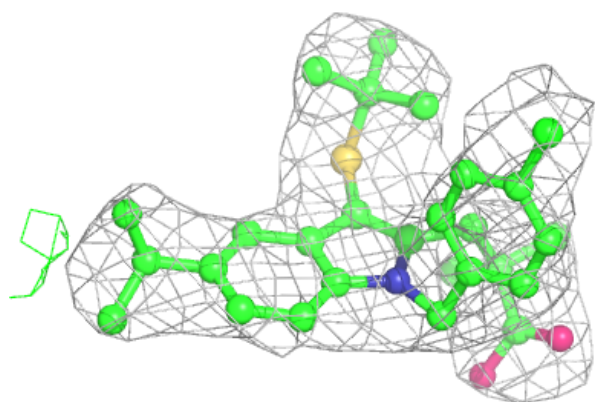
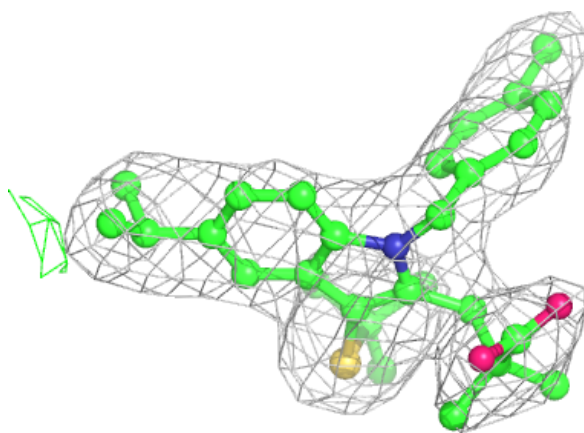
Electron density around QY7 B 201:

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



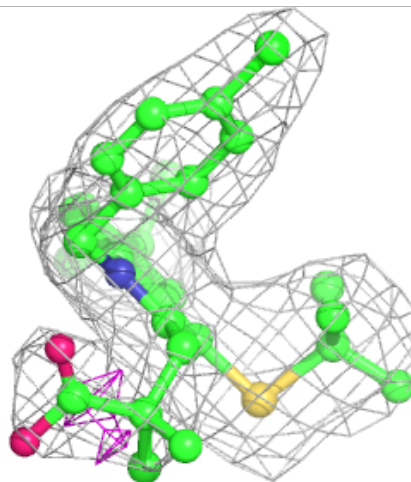
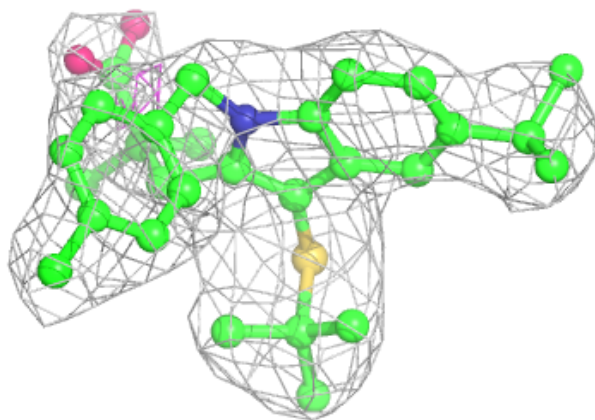
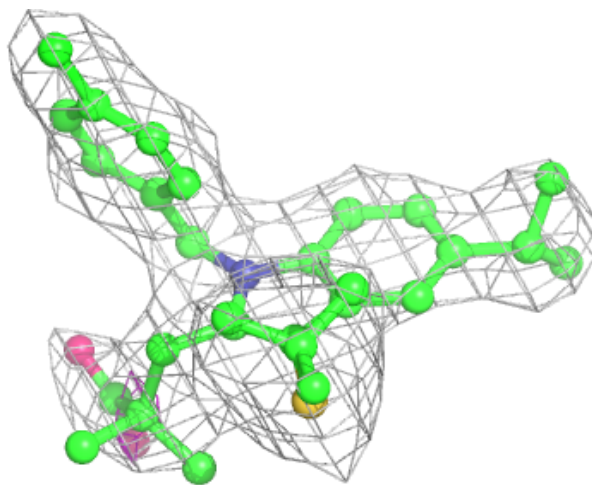
Electron density around QY7 E 201:

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



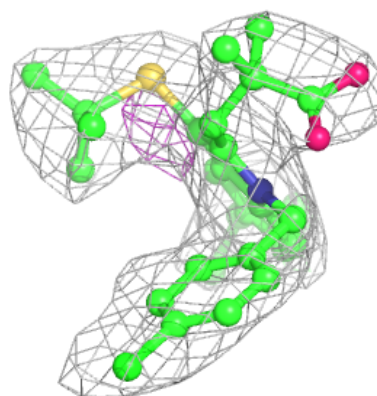
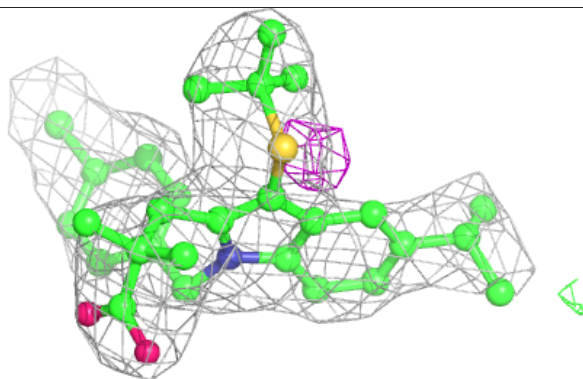
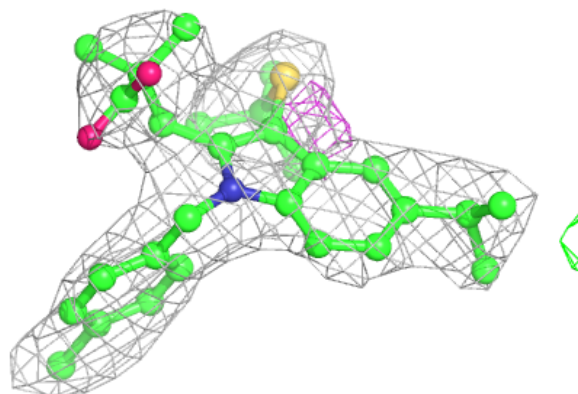
Electron density around QY7 C 201:

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



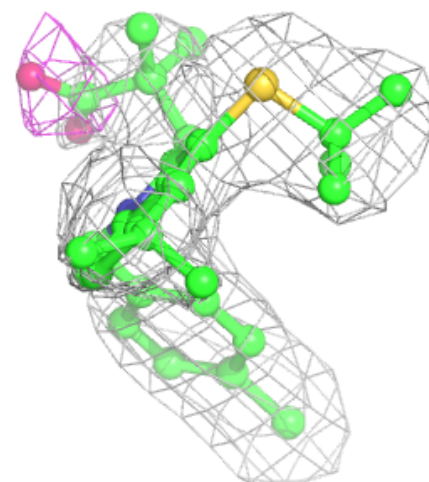
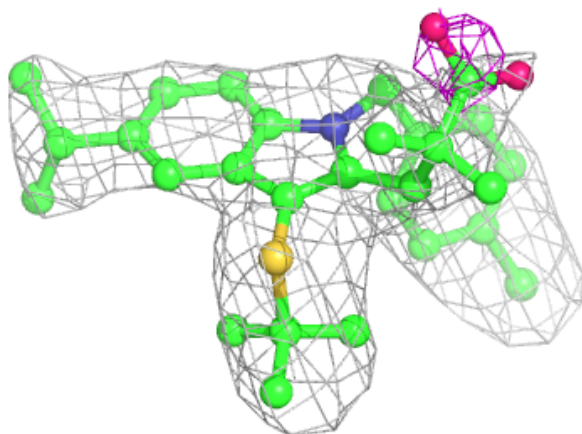
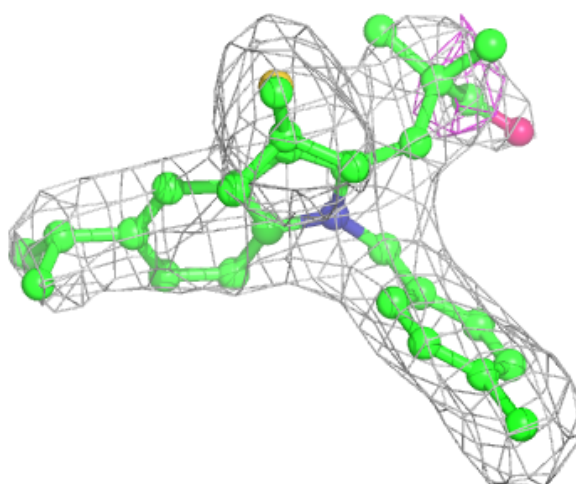
Electron density around QY7 B 202:

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



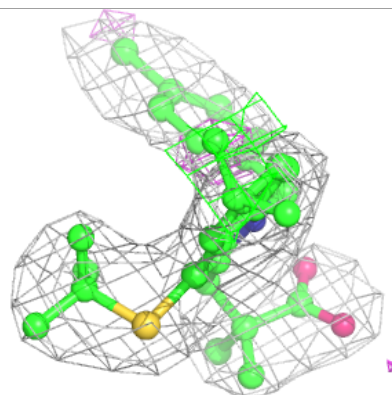
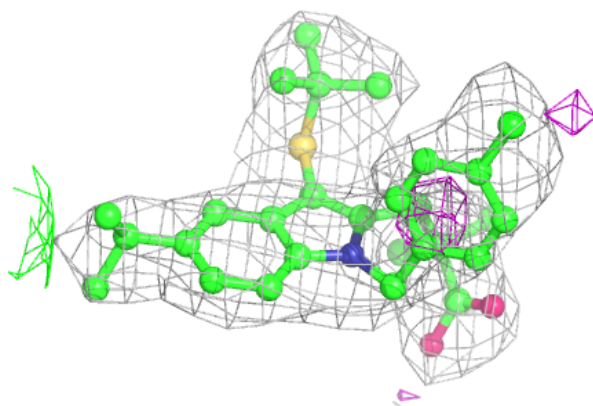
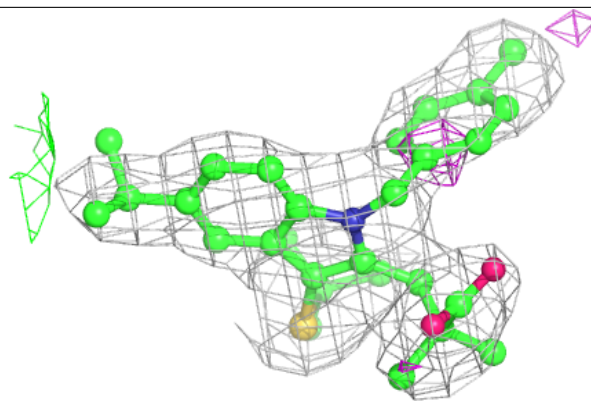
Electron density around QY7 A 201:

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



Electron density around QY7 F 201:

$2mF_o - DF_c$ (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.