



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 11:01 AM EDT

PDB ID : 7T5Z
Title : P. aeruginosa LpxA in complex with ligand L8
Authors : Sacco, M.; Chen, Y.
Deposited on : 2021-12-13
Resolution : 2.25 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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.29
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) : 2.29

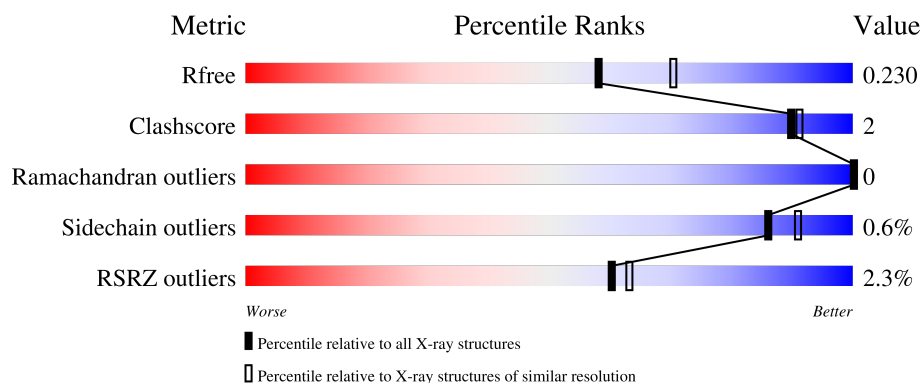
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



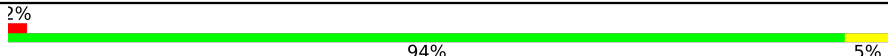
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	258	<div> <div>0%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	B	258	<div> <div>0%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	C	258	<div> <div>2%</div> <div> <div></div> <div>97%</div> <div>..</div> </div> </div>
1	D	258	<div> <div>4%</div> <div> <div></div> <div>97%</div> <div>.</div> </div> </div>
1	E	258	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	258	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	F6I	F	301	X	-	-	-
2	F6I	F	302	X	-	-	-
3	PEG	F	303	-	-	X	-

2 Entry composition [i](#)

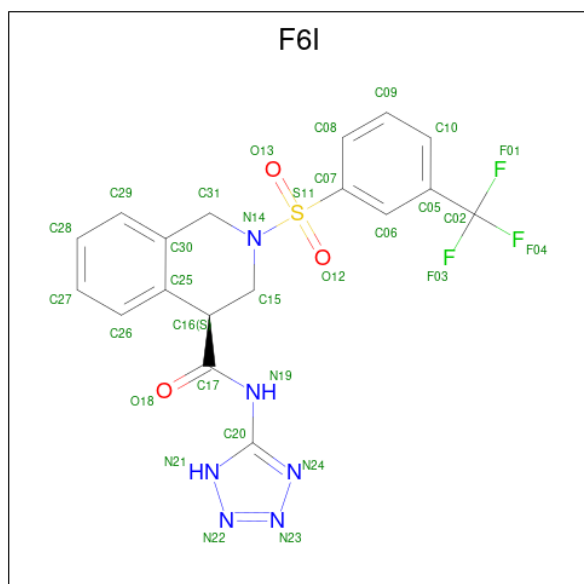
There are 4 unique types of molecules in this entry. The entry contains 12344 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase.

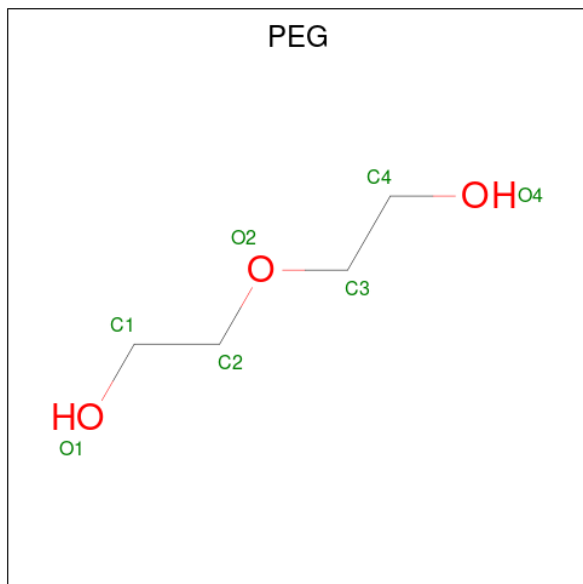
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	B	257	Total	C	N	O	S	0	1	0
			1976	1236	366	368	6			
1	C	256	Total	C	N	O	S	0	0	0
			1960	1227	362	365	6			
1	D	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	E	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	F	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			

- Molecule 2 is (4S)-N-(1H-tetrazol-5-yl)-2-[3-(trifluoromethyl)benzene-1-sulfonyl]-1,2,3,4-tetrahydroisoquinoline-4-carboxamide (three-letter code: F6I) (formula: C₁₈H₁₅F₃N₆O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	S	0	0
			31	18	3	6	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			31	18	3	6	3	1		
2	C	1	Total	C	F	N	O	S	0	0
			31	18	3	6	3	1		
2	E	1	Total	C	F	N	O	S	0	0
			31	18	3	6	3	1		
2	F	1	Total	C	F	N	O	S	0	0
			31	18	3	6	3	1		
2	F	1	Total	C	F	N	O	S	0	0
			31	18	3	6	3	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	53	Total	O	0	0
			53	53		
4	C	54	Total	O	0	0
			54	54		

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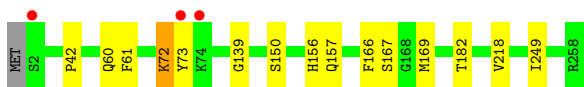
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	62	Total 62	O 62	0	0
4	E	38	Total 38	O 38	0	0
4	F	61	Total 61	O 61	0	0

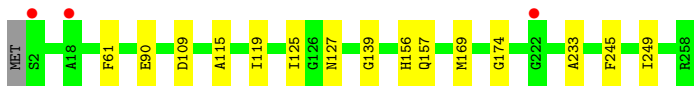
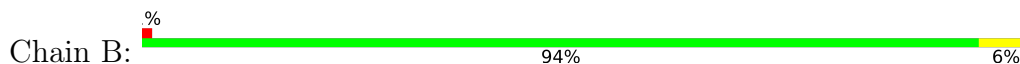
3 Residue-property plots [i](#)

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.

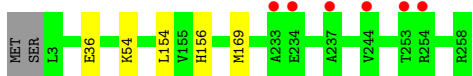
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



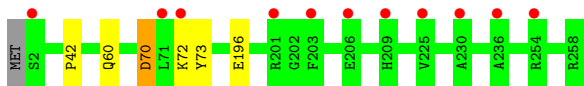
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



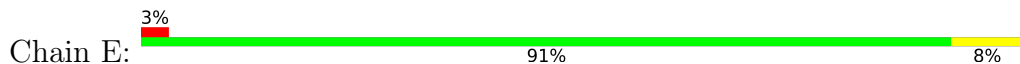
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



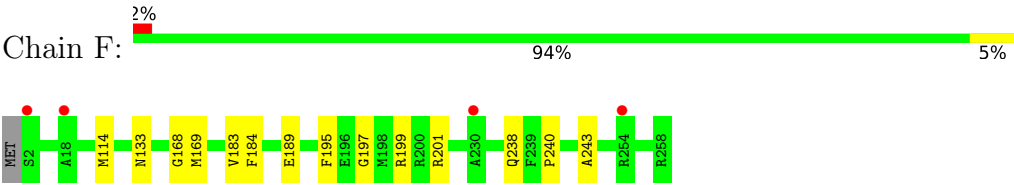
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.83Å 82.85Å 221.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.04 – 2.25 46.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	80.7 (46.04-2.25) 80.7 (46.00-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.227 0.196 , 0.230	Depositor DCC
R_{free} test set	2813 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.039 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12344	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: F6I, PEG

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	0/2008	0.80	0/2724
1	B	0.72	0/2019	0.78	0/2739
1	C	0.68	0/2002	0.79	0/2716
1	D	0.71	0/2008	0.79	0/2724
1	E	0.69	0/2008	0.78	0/2724
1	F	0.70	0/2008	0.78	0/2724
All	All	0.70	0/12053	0.79	0/16351

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	1966	0	1935	10	0
1	B	1976	0	1941	12	0
1	C	1960	0	1930	4	0
1	D	1966	0	1935	2	0
1	E	1966	0	1935	12	0
1	F	1966	0	1935	7	0
2	B	62	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	0	0	0
2	E	31	0	0	0	0
2	F	62	0	0	1	0
3	F	7	0	10	6	0
4	A	83	0	0	0	0
4	B	53	0	0	0	0
4	C	54	0	0	0	0
4	D	62	0	0	0	0
4	E	38	0	0	1	0
4	F	61	0	0	0	0
All	All	12344	0	11621	43	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 (43) 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:F:133:ASN:OD1	3:F:303:PEG:H32	1.95	0.66
1:E:69:PRO:HD2	3:F:303:PEG:H12	1.78	0.65
1:B:233:ALA:HB1	1:E:199:ARG:HD3	1.84	0.60
1:E:128:HIS:HB3	1:E:146:TRP:CZ3	2.41	0.56
1:B:156[A]:HIS:HE1	2:B:301:F6I:N22	2.05	0.54
1:B:169:MET:HE2	1:C:156:HIS:CE1	2.43	0.53
1:E:95:HIS:HE1	3:F:303:PEG:H42	1.74	0.52
1:E:100:GLN:OE1	1:E:100:GLN:N	2.39	0.50
1:F:197:GLY:O	1:F:201:ARG:HB2	2.11	0.50
1:A:156:HIS:CE1	1:C:169:MET:SD	3.06	0.49
1:C:36:GLU:HG2	1:C:54:LYS:HD2	1.93	0.49
1:A:169:MET:CE	1:B:156[A]:HIS:CD2	2.96	0.49
4:E:401:HOH:O	3:F:303:PEG:H11	2.13	0.49
1:D:70:ASP:HB3	1:D:73:TYR:CD2	2.48	0.49
1:B:169:MET:HG2	1:C:154:LEU:HD13	1.96	0.47
1:A:139:GLY:O	1:A:157:GLN:HA	2.15	0.47
1:E:73:TYR:OH	1:E:96:ARG:NH2	2.48	0.47
1:A:150:SER:HB2	1:A:167:SER:O	2.14	0.47
1:A:72:LYS:HA	1:A:72:LYS:HD3	1.79	0.46
1:E:166:PHE:O	1:E:182:THR:HA	2.16	0.46
1:F:195:PHE:O	1:F:199:ARG:HG3	2.16	0.46
1:A:218:VAL:HG21	1:A:249:ILE:HD13	1.97	0.46
1:D:42:PRO:O	1:D:60:GLN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:LEU:HD11	1:E:28:VAL:HG11	1.98	0.45
2:F:302:F6I:C09	3:F:303:PEG:H22	2.46	0.45
1:F:168:GLY:HA3	1:F:184:PHE:CD2	2.52	0.45
1:A:166:PHE:O	1:A:182:THR:HA	2.19	0.43
1:B:156[A]:HIS:CD2	1:B:174:GLY:HA2	2.54	0.43
1:E:14:ALA:O	1:E:15:ARG:NH1	2.51	0.43
1:E:119:ILE:HD12	1:E:125:ILE:HD11	1.99	0.42
1:B:139:GLY:O	1:B:157:GLN:HA	2.19	0.42
1:A:73:TYR:N	1:A:73:TYR:CD2	2.86	0.42
1:B:109:ASP:O	1:B:127:ASN:HA	2.20	0.42
1:B:119:ILE:HD13	1:B:125:ILE:HD12	2.00	0.42
1:B:90:GLU:O	1:B:115:ALA:HA	2.20	0.41
1:F:183:VAL:HA	1:F:189:GLU:O	2.20	0.41
1:F:240:PRO:O	1:F:243:ALA:HB3	2.20	0.41
1:F:114:MET:SD	3:F:303:PEG:H21	2.60	0.41
1:B:245:PHE:CZ	1:B:249:ILE:HD11	2.55	0.41
1:A:61:PHE:CZ	1:B:61:PHE:HA	2.56	0.41
1:E:139:GLY:O	1:E:157:GLN:HA	2.21	0.40
1:E:186:ASN:HA	1:E:187:PRO:HA	1.95	0.40
1:A:42:PRO:O	1:A:60:GLN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	255/258 (99%)	244 (96%)	11 (4%)	0	100	100
1	B	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
1	C	254/258 (98%)	244 (96%)	10 (4%)	0	100	100
1	D	255/258 (99%)	240 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	255/258 (99%)	241 (94%)	14 (6%)	0	100	100
1	F	255/258 (99%)	238 (93%)	17 (7%)	0	100	100
All	All	1530/1548 (99%)	1452 (95%)	78 (5%)	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	205/206 (100%)	204 (100%)	1 (0%)	88	92
1	B	206/206 (100%)	206 (100%)	0	100	100
1	C	204/206 (99%)	204 (100%)	0	100	100
1	D	205/206 (100%)	202 (98%)	3 (2%)	65	75
1	E	205/206 (100%)	204 (100%)	1 (0%)	88	92
1	F	205/206 (100%)	203 (99%)	2 (1%)	76	84
All	All	1230/1236 (100%)	1223 (99%)	7 (1%)	86	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	D	70	ASP
1	D	72	LYS
1	D	196	GLU
1	E	258	ARG
1	F	169	MET
1	F	238	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	B	157	GLN
1	B	238	GLN
1	C	250	GLN
1	E	164	HIS
1	F	157	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](#)

7 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	F6I	F	302	-	32,34,34	2.51	12 (37%)	43,51,51	3.49	15 (34%)
2	F6I	B	301	-	32,34,34	2.58	12 (37%)	43,51,51	3.06	20 (46%)
2	F6I	B	302	-	32,34,34	2.39	10 (31%)	43,51,51	2.24	11 (25%)
2	F6I	E	301	-	32,34,34	2.74	13 (40%)	43,51,51	2.19	12 (27%)
2	F6I	C	301	-	32,34,34	2.85	11 (34%)	43,51,51	1.90	9 (20%)
3	PEG	F	303	-	6,6,6	0.47	0	5,5,5	0.48	0
2	F6I	F	301	-	32,34,34	2.32	11 (34%)	43,51,51	2.76	17 (39%)

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	F6I	F	302	-	1/1/5/6	7/24/38/38	0/4/4/4
2	F6I	B	301	-	-	6/24/38/38	0/4/4/4
2	F6I	B	302	-	-	5/24/38/38	0/4/4/4
2	F6I	C	301	-	-	2/24/38/38	0/4/4/4
2	F6I	E	301	-	-	5/24/38/38	0/4/4/4
3	PEG	F	303	-	-	2/4/4/4	-
2	F6I	F	301	-	1/1/5/6	8/24/38/38	0/4/4/4

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	F6I	O13-S11	8.68	1.53	1.43
2	F	302	F6I	C20-N19	8.08	1.49	1.38
2	E	301	F6I	C20-N19	6.40	1.47	1.38
2	B	302	F6I	C20-N19	6.39	1.47	1.38
2	B	301	F6I	C25-C16	6.10	1.58	1.51
2	C	301	F6I	C25-C16	6.01	1.58	1.51
2	B	301	F6I	C20-N19	5.82	1.46	1.38
2	B	301	F6I	O12-S11	5.72	1.49	1.43
2	C	301	F6I	C17-N19	5.58	1.48	1.35
2	E	301	F6I	O13-S11	5.57	1.49	1.43
2	F	301	F6I	C25-C16	5.51	1.58	1.51
2	B	301	F6I	C17-N19	5.46	1.47	1.35
2	C	301	F6I	C20-N19	5.39	1.45	1.38
2	F	302	F6I	C17-N19	5.30	1.47	1.35
2	E	301	F6I	C25-C16	5.29	1.57	1.51
2	E	301	F6I	O12-S11	5.29	1.49	1.43
2	C	301	F6I	O12-S11	5.19	1.49	1.43
2	F	301	F6I	C20-N19	5.10	1.45	1.38
2	F	301	F6I	C17-N19	5.08	1.47	1.35
2	F	301	F6I	O13-S11	4.98	1.49	1.43
2	E	301	F6I	S11-N14	4.96	1.70	1.63
2	B	302	F6I	C17-N19	4.96	1.46	1.35
2	B	302	F6I	O13-S11	4.86	1.48	1.43
2	E	301	F6I	C17-N19	4.75	1.46	1.35
2	F	302	F6I	O13-S11	4.54	1.48	1.43
2	B	302	F6I	C25-C16	4.24	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	F6I	C07-S11	4.15	1.82	1.76
2	B	302	F6I	C07-S11	3.97	1.82	1.76
2	F	302	F6I	S11-N14	3.95	1.69	1.63
2	C	301	F6I	S11-N14	3.85	1.68	1.63
2	B	302	F6I	O12-S11	3.81	1.47	1.43
2	B	301	F6I	S11-N14	3.71	1.68	1.63
2	F	301	F6I	S11-N14	3.71	1.68	1.63
2	F	302	F6I	O12-S11	3.67	1.47	1.43
2	B	301	F6I	O13-S11	3.15	1.47	1.43
2	B	302	F6I	C30-C25	-3.14	1.34	1.40
2	C	301	F6I	C29-C30	3.01	1.44	1.39
2	B	301	F6I	C26-C25	2.86	1.43	1.39
2	B	301	F6I	C30-C25	-2.84	1.35	1.40
2	F	302	F6I	C07-S11	2.80	1.80	1.76
2	C	301	F6I	C07-S11	2.79	1.80	1.76
2	B	301	F6I	C16-C17	2.78	1.56	1.53
2	F	301	F6I	O18-C17	-2.72	1.18	1.23
2	B	302	F6I	S11-N14	2.72	1.67	1.63
2	F	301	F6I	C26-C25	2.71	1.43	1.39
2	E	301	F6I	C30-C25	-2.63	1.35	1.40
2	F	302	F6I	C26-C25	2.59	1.43	1.39
2	F	302	F6I	C25-C16	2.58	1.54	1.51
2	B	301	F6I	C29-C30	2.58	1.44	1.39
2	B	302	F6I	C31-N14	-2.51	1.43	1.47
2	E	301	F6I	O18-C17	-2.48	1.18	1.23
2	F	302	F6I	C30-C25	-2.44	1.36	1.40
2	E	301	F6I	C26-C25	2.44	1.42	1.39
2	E	301	F6I	C29-C30	2.38	1.43	1.39
2	F	301	F6I	C07-S11	2.37	1.79	1.76
2	F	302	F6I	O18-C17	-2.35	1.18	1.23
2	C	301	F6I	C26-C25	2.32	1.42	1.39
2	F	302	F6I	C15-N14	2.32	1.49	1.47
2	B	301	F6I	C07-S11	2.30	1.79	1.76
2	B	301	F6I	O18-C17	-2.23	1.18	1.23
2	E	301	F6I	C16-C17	2.22	1.55	1.53
2	F	301	F6I	O12-S11	2.20	1.46	1.43
2	C	301	F6I	N23-N22	2.19	1.36	1.32
2	F	302	F6I	N24-N23	2.14	1.38	1.34
2	E	301	F6I	C02-C05	2.14	1.54	1.49
2	B	302	F6I	N23-N22	2.12	1.35	1.32
2	C	301	F6I	C16-C17	2.12	1.55	1.53
2	F	301	F6I	N23-N22	2.07	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	F6I	N21-N22	2.00	1.37	1.34

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	302	F6I	C07-S11-N14	12.76	122.50	107.30
2	B	301	F6I	O12-S11-N14	10.89	116.62	106.69
2	F	302	F6I	O13-S11-O12	-10.00	103.31	119.52
2	B	301	F6I	O13-S11-O12	-9.82	103.60	119.52
2	F	301	F6I	O13-S11-N14	8.72	114.64	106.69
2	B	302	F6I	O13-S11-O12	-8.70	105.42	119.52
2	F	301	F6I	O13-S11-O12	-8.39	105.93	119.52
2	E	301	F6I	O13-S11-O12	-7.70	107.04	119.52
2	F	302	F6I	O18-C17-C16	-7.25	115.53	122.46
2	F	302	F6I	C31-N14-S11	6.77	127.74	116.94
2	B	301	F6I	C07-S11-N14	5.68	114.06	107.30
2	C	301	F6I	N21-N22-N23	-5.61	105.86	109.53
2	F	301	F6I	O18-C17-C16	-5.33	117.37	122.46
2	F	302	F6I	C20-N19-C17	-4.92	122.83	130.28
2	C	301	F6I	O13-S11-C07	4.87	114.20	108.05
2	F	302	F6I	C15-C16-C25	-4.82	103.34	110.60
2	B	302	F6I	O13-S11-C07	4.60	113.87	108.05
2	C	301	F6I	O13-S11-O12	-4.53	112.19	119.52
2	E	301	F6I	O13-S11-C07	4.47	113.70	108.05
2	F	302	F6I	N21-N22-N23	-4.37	106.68	109.53
2	B	301	F6I	O18-C17-C16	-4.15	118.49	122.46
2	E	301	F6I	N21-N22-N23	-4.15	106.82	109.53
2	F	301	F6I	C31-N14-S11	4.09	123.47	116.94
2	C	301	F6I	C31-N14-S11	4.04	123.39	116.94
2	B	301	F6I	C20-N19-C17	-3.96	124.29	130.28
2	E	301	F6I	O18-C17-N19	-3.92	115.49	123.93
2	B	301	F6I	O18-C17-N19	-3.88	115.58	123.93
2	B	302	F6I	N21-N22-N23	-3.75	107.09	109.53
2	E	301	F6I	C20-N19-C17	-3.71	124.67	130.28
2	B	302	F6I	C20-N19-C17	-3.50	124.97	130.28
2	B	302	F6I	O18-C17-C16	-3.49	119.12	122.46
2	F	301	F6I	C15-C16-C25	-3.46	105.38	110.60
2	E	301	F6I	O12-S11-N14	3.35	109.74	106.69
2	F	302	F6I	F03-C02-C05	-3.23	105.83	112.93
2	F	301	F6I	C20-N19-C17	-3.19	125.44	130.28
2	F	301	F6I	C30-C31-N14	3.18	115.34	110.58
2	B	301	F6I	C31-N14-S11	3.14	121.95	116.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	F6I	C15-N14-S11	3.09	122.85	117.26
2	B	301	F6I	C30-C31-N14	3.08	115.20	110.58
2	F	302	F6I	F04-C02-C05	-3.06	106.21	112.93
2	F	301	F6I	N21-N22-N23	-3.03	107.55	109.53
2	C	301	F6I	F01-C02-C05	-3.01	106.33	112.93
2	F	301	F6I	O12-S11-C07	2.99	111.83	108.05
2	B	301	F6I	O13-S11-N14	-2.95	104.00	106.69
2	F	301	F6I	C07-S11-N14	-2.92	103.82	107.30
2	B	302	F6I	O18-C17-N19	-2.91	117.67	123.93
2	B	301	F6I	F01-C02-C05	-2.90	106.55	112.93
2	E	301	F6I	O12-S11-C07	2.90	111.71	108.05
2	B	302	F6I	F01-C02-C05	-2.86	106.66	112.93
2	B	302	F6I	C29-C30-C25	2.85	121.85	118.76
2	B	302	F6I	O12-S11-N14	2.85	109.28	106.69
2	C	301	F6I	C29-C30-C25	2.83	121.82	118.76
2	F	301	F6I	C29-C30-C25	2.82	121.81	118.76
2	F	301	F6I	O12-S11-N14	2.81	109.25	106.69
2	F	301	F6I	O13-S11-C07	2.72	111.49	108.05
2	F	302	F6I	C26-C25-C30	2.70	122.05	118.74
2	E	301	F6I	O13-S11-N14	2.68	109.13	106.69
2	F	302	F6I	C09-C10-C05	-2.64	117.98	120.76
2	F	301	F6I	N24-N23-N22	-2.64	107.81	109.53
2	E	301	F6I	C31-N14-S11	2.64	121.15	116.94
2	C	301	F6I	O18-C17-C16	2.63	124.97	122.46
2	F	302	F6I	N24-N23-N22	-2.57	107.86	109.53
2	E	301	F6I	C29-C30-C25	2.56	121.53	118.76
2	F	302	F6I	C10-C05-C06	2.56	122.69	117.76
2	B	301	F6I	C10-C05-C06	2.53	122.64	117.76
2	F	301	F6I	C16-C15-N14	-2.52	105.13	110.96
2	F	302	F6I	C15-N14-S11	-2.49	112.75	117.26
2	B	301	F6I	F04-C02-F01	2.49	114.85	105.72
2	F	301	F6I	F03-C02-F01	2.47	114.79	105.72
2	B	302	F6I	O13-S11-N14	2.41	108.89	106.69
2	B	302	F6I	C07-S11-N14	2.29	110.03	107.30
2	C	301	F6I	C10-C05-C06	2.25	122.09	117.76
2	B	301	F6I	F04-C02-C05	-2.24	108.00	112.93
2	B	301	F6I	C09-C10-C05	-2.23	118.42	120.76
2	B	301	F6I	C29-C30-C25	2.20	121.14	118.76
2	B	301	F6I	N24-N23-N22	-2.19	108.10	109.53
2	F	302	F6I	C10-C05-C02	-2.18	116.49	119.97
2	B	301	F6I	N21-N22-N23	-2.17	108.11	109.53
2	C	301	F6I	C15-C16-C25	2.17	113.87	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	F6I	C15-N14-S11	2.16	121.18	117.26
2	F	301	F6I	C15-N14-S11	-2.15	113.38	117.26
2	B	301	F6I	F03-C02-C05	-2.14	108.23	112.93
2	E	301	F6I	O18-C17-C16	-2.06	120.49	122.46
2	B	301	F6I	C06-C05-C02	-2.03	116.83	119.58

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	301	F6I	C16
2	F	302	F6I	C16

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	F6I	C16-C17-N19-C20
2	B	301	F6I	O18-C17-N19-C20
2	B	302	F6I	C16-C17-N19-C20
2	B	302	F6I	O18-C17-N19-C20
2	E	301	F6I	C16-C17-N19-C20
2	E	301	F6I	O18-C17-N19-C20
2	F	301	F6I	C15-C16-C17-O18
2	F	301	F6I	C15-C16-C17-N19
2	F	302	F6I	C31-N14-S11-C07
2	F	301	F6I	C15-N14-S11-O13
2	F	301	F6I	C31-N14-S11-O12
2	F	302	F6I	C31-N14-S11-O13
2	F	301	F6I	C31-N14-S11-C07
2	F	302	F6I	C15-N14-S11-C07
2	B	301	F6I	C15-N14-S11-O12
2	F	301	F6I	C31-N14-S11-O13
2	E	301	F6I	C15-N14-S11-O13
2	F	301	F6I	C15-N14-S11-O12
2	F	301	F6I	C15-N14-S11-C07
3	F	303	PEG	O1-C1-C2-O2
2	F	302	F6I	C31-N14-S11-O12
3	F	303	PEG	O2-C3-C4-O4
2	B	301	F6I	C31-N14-S11-O13
2	B	301	F6I	C15-C16-C17-O18
2	B	301	F6I	C15-C16-C17-N19
2	B	302	F6I	C15-C16-C17-O18
2	B	302	F6I	C15-C16-C17-N19

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Mol	Chain	Res	Type	Atoms
2	C	301	F6I	C15-C16-C17-O18
2	C	301	F6I	C15-C16-C17-N19
2	E	301	F6I	C15-C16-C17-N19
2	F	302	F6I	C15-C16-C17-O18
2	F	302	F6I	C15-C16-C17-N19
2	B	302	F6I	C15-N14-S11-O13
2	E	301	F6I	C15-N14-S11-C07
2	F	302	F6I	C06-C07-S11-O13

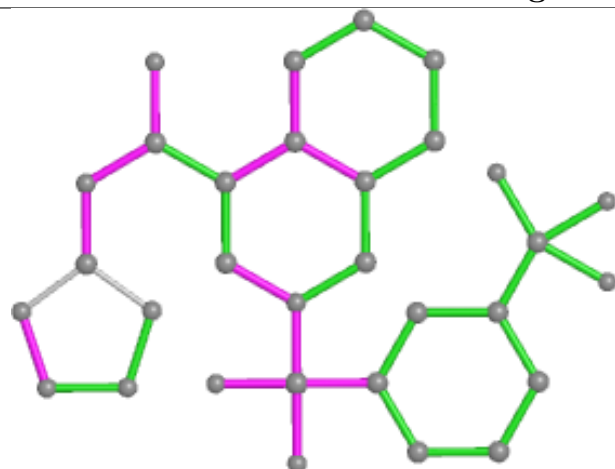
There are no ring outliers.

3 monomers are involved in 7 short contacts:

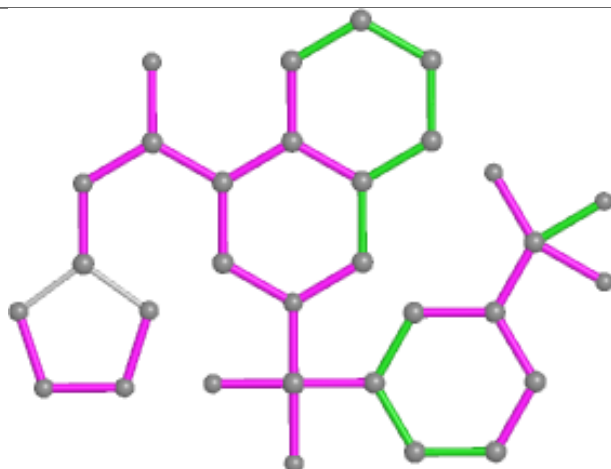
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	302	F6I	1	0
2	B	301	F6I	1	0
3	F	303	PEG	6	0

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.

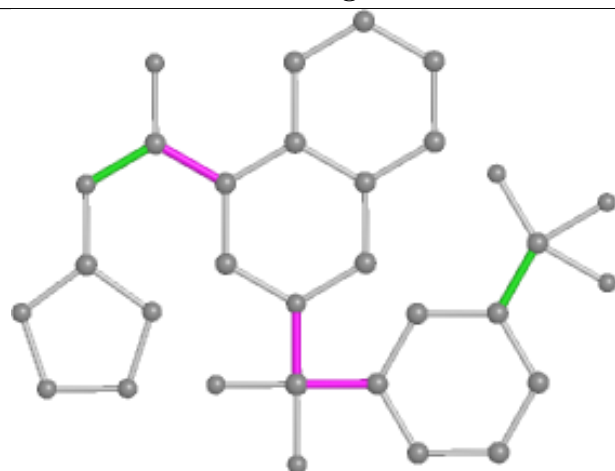
Ligand F6I F 302



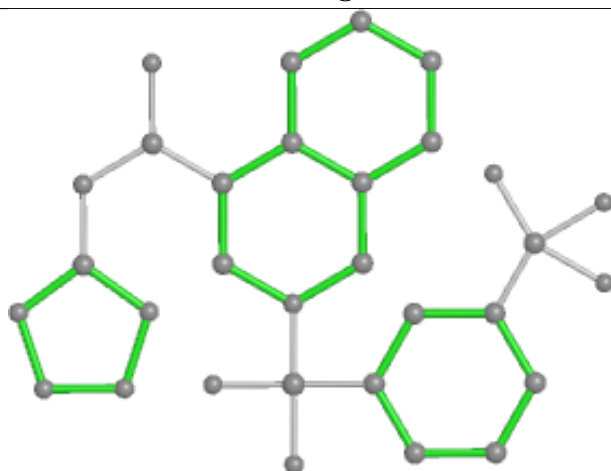
Bond lengths



Bond angles

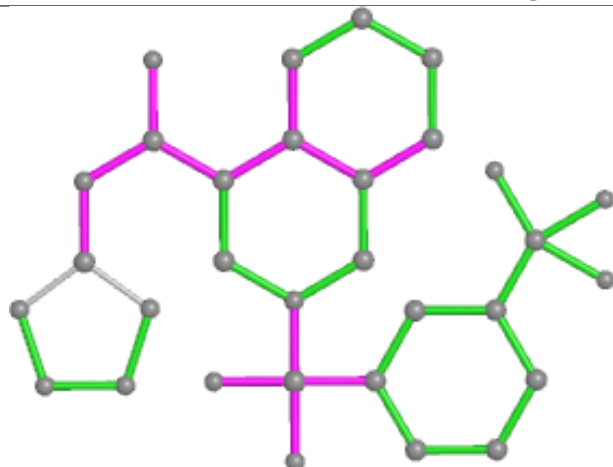


Torsions

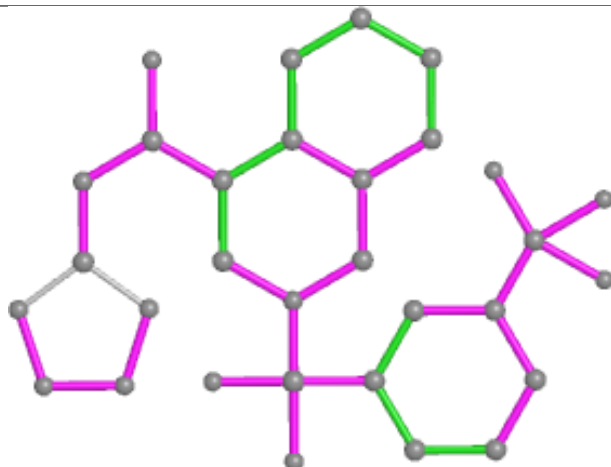


Rings

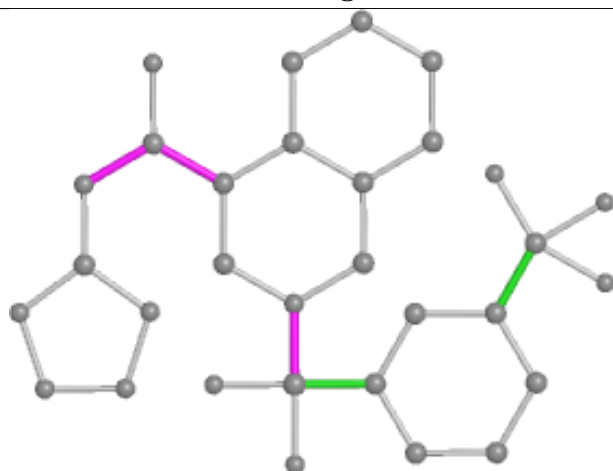
Ligand F6I B 301



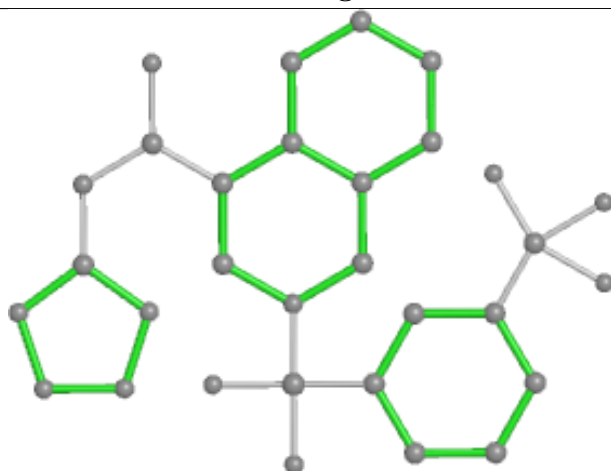
Bond lengths



Bond angles

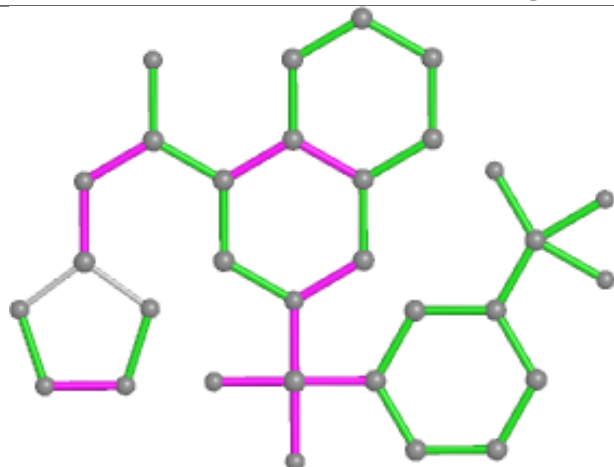


Torsions

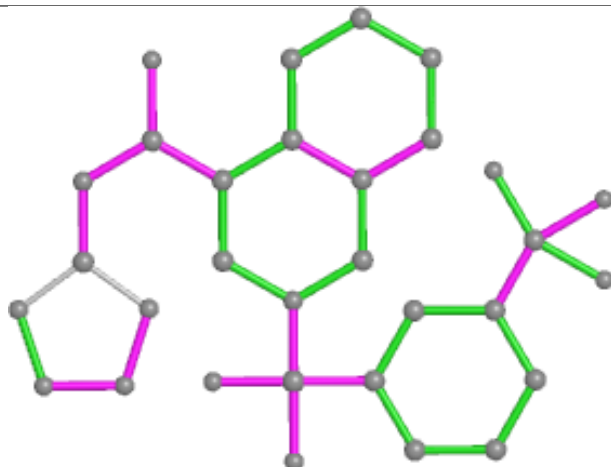


Rings

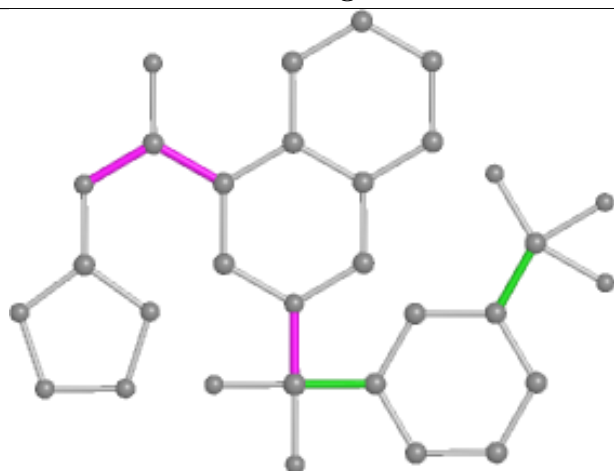
Ligand F6I B 302



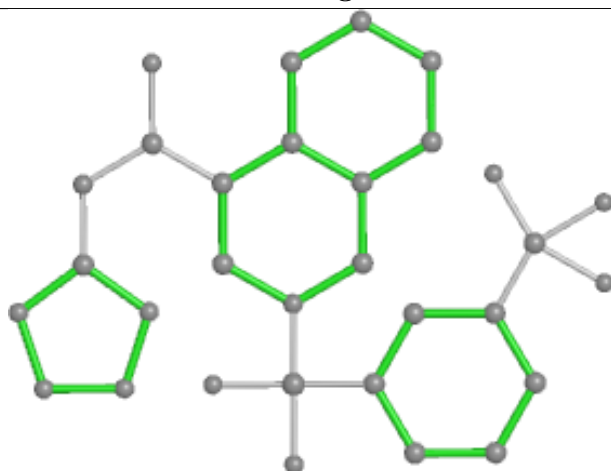
Bond lengths



Bond angles

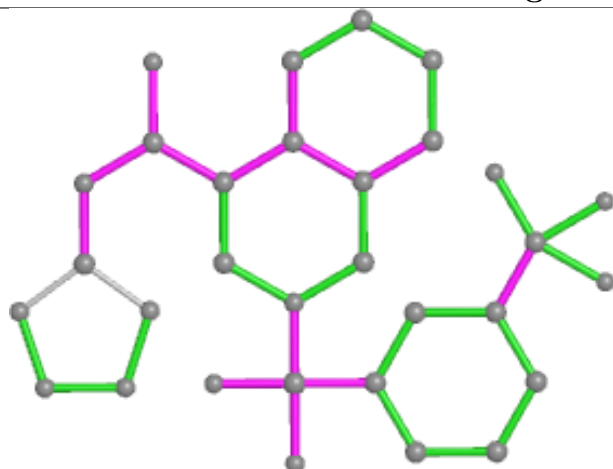


Torsions



Rings

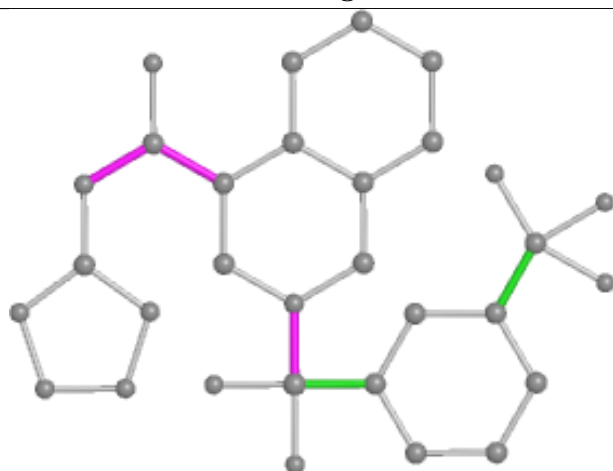
Ligand F6I E 301



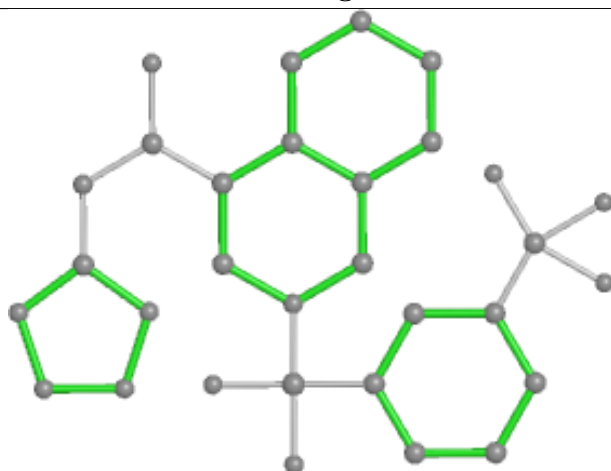
Bond lengths



Bond angles

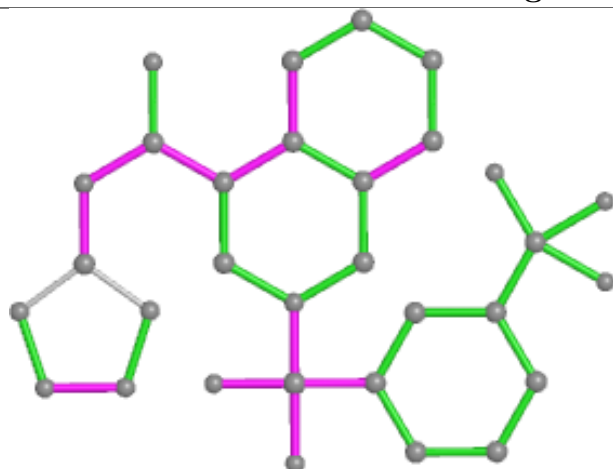


Torsions



Rings

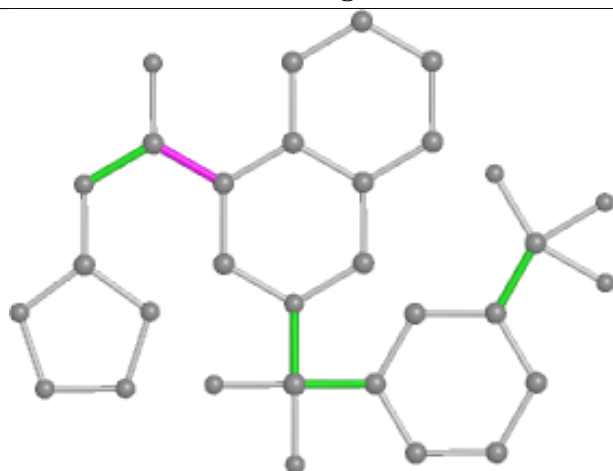
Ligand F6I C 301



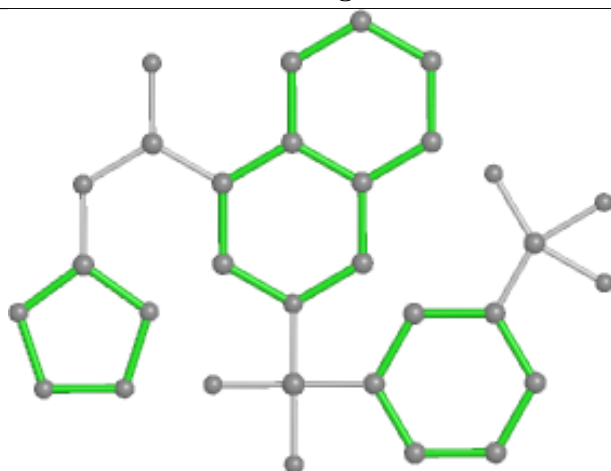
Bond lengths



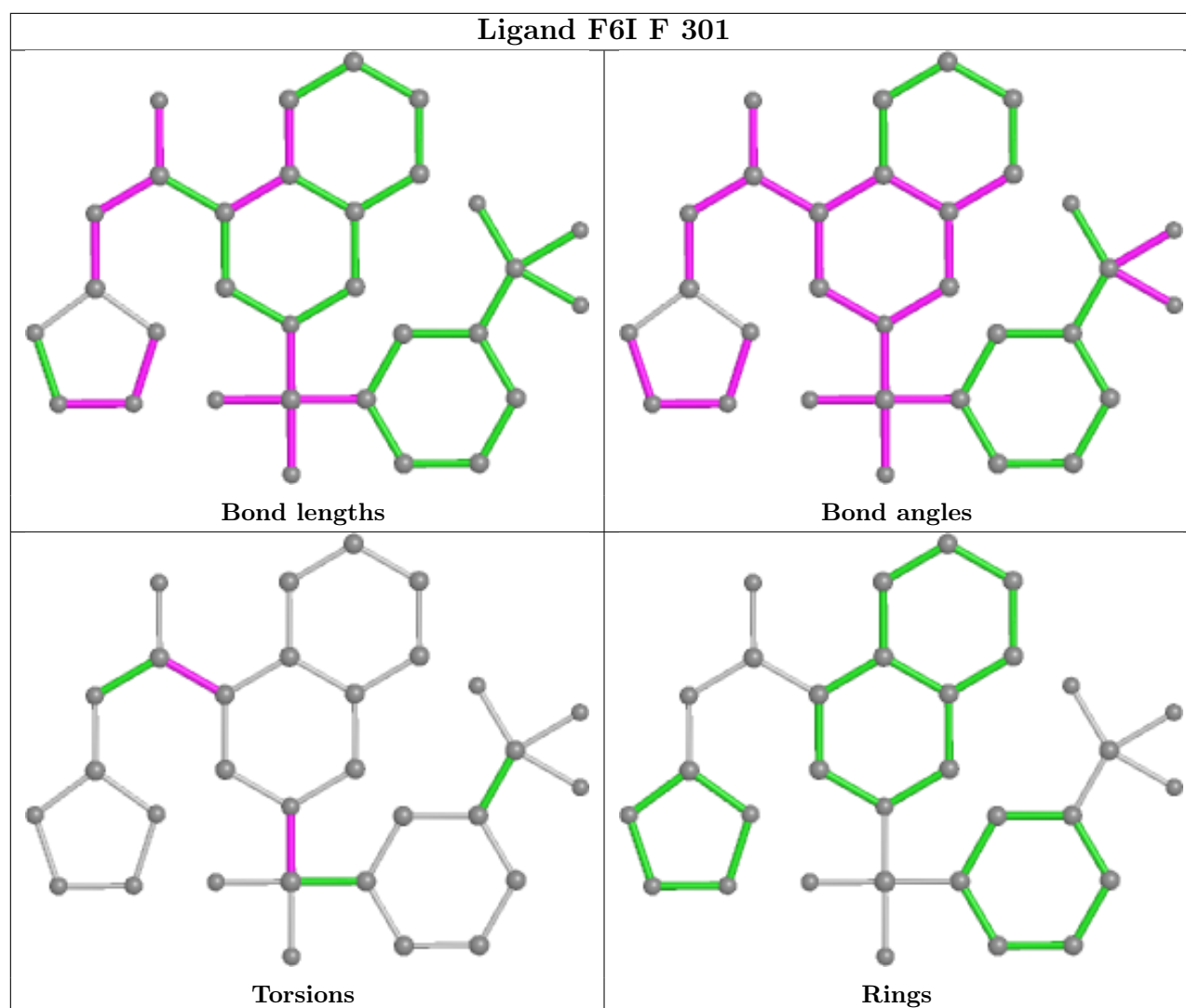
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	257/258 (99%)	-0.23	3 (1%) 79 81	17, 27, 58, 90	0
1	B	257/258 (99%)	-0.08	3 (1%) 79 81	18, 32, 65, 89	0
1	C	256/258 (99%)	-0.03	6 (2%) 60 63	19, 36, 69, 97	0
1	D	257/258 (99%)	-0.01	11 (4%) 35 37	17, 33, 74, 101	0
1	E	257/258 (99%)	0.15	9 (3%) 44 46	20, 42, 70, 94	0
1	F	257/258 (99%)	-0.09	4 (1%) 72 74	17, 31, 70, 110	0
All	All	1541/1548 (99%)	-0.05	36 (2%) 60 63	17, 33, 69, 110	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	TYR	8.2
1	C	253	THR	4.7
1	A	2	SER	4.3
1	E	3	LEU	4.0
1	F	254	ARG	3.9
1	F	18	ALA	3.6
1	D	71	LEU	3.3
1	F	230	ALA	3.2
1	D	201	ARG	3.1
1	B	222	GLY	3.0
1	D	225	VAL	2.8
1	E	210	ALA	2.8
1	B	2	SER	2.8
1	E	237	ALA	2.7
1	E	240	PRO	2.6
1	E	230	ALA	2.5
1	C	233	ALA	2.4
1	C	234	GLU	2.4
1	F	2	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	237	ALA	2.4
1	D	206	GLU	2.4
1	D	72	LYS	2.3
1	E	209	HIS	2.3
1	D	254	ARG	2.3
1	A	74	LYS	2.3
1	E	253	THR	2.2
1	D	203	PHE	2.2
1	E	15	ARG	2.2
1	D	236	ALA	2.1
1	E	232	LEU	2.1
1	D	230	ALA	2.1
1	C	244	VAL	2.1
1	D	2	SER	2.1
1	B	18	ALA	2.0
1	C	254	ARG	2.0
1	D	209	HIS	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(Å ²)	Q<0.9
3	PEG	F	303	7/7	0.84	0.21	35,37,41,46	0
2	F6I	C	301	31/31	0.88	0.17	37,53,63,67	0
2	F6I	F	301	31/31	0.90	0.15	32,45,52,55	0
2	F6I	E	301	31/31	0.91	0.15	48,57,61,62	0
2	F6I	F	302	31/31	0.94	0.14	31,44,61,62	0
2	F6I	B	301	31/31	0.94	0.16	34,46,52,53	0

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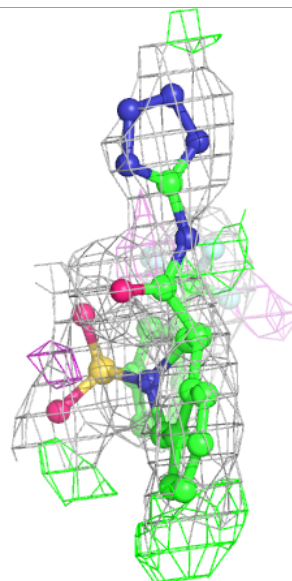
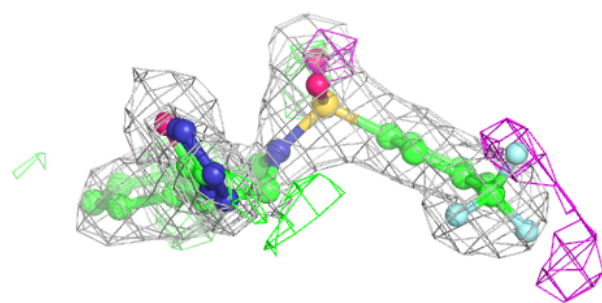
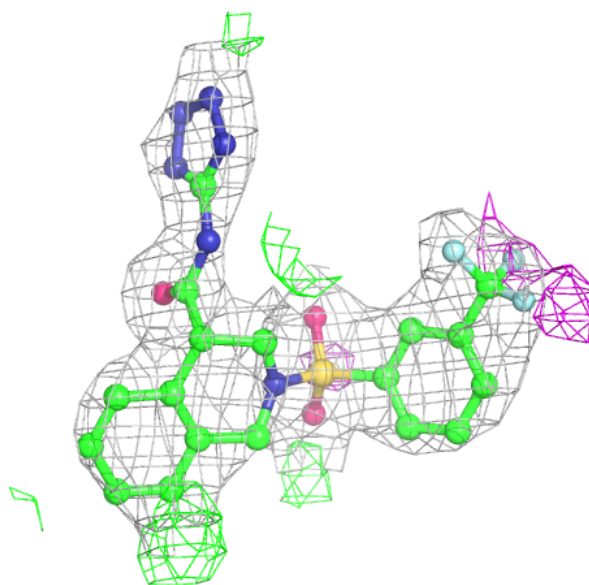
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	F6I	B	302	31/31	0.96	0.12	29,40,43,45	0

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.

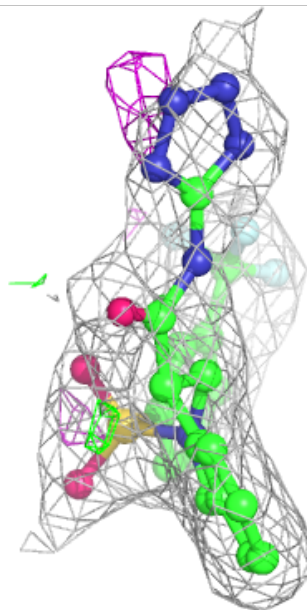
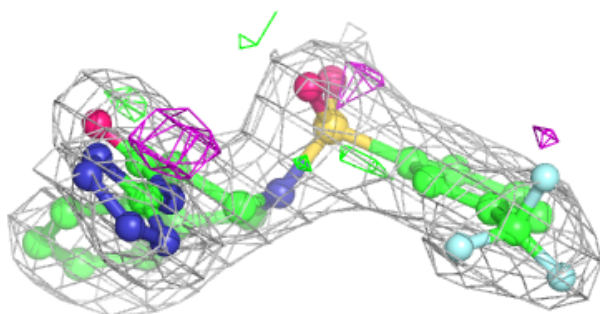
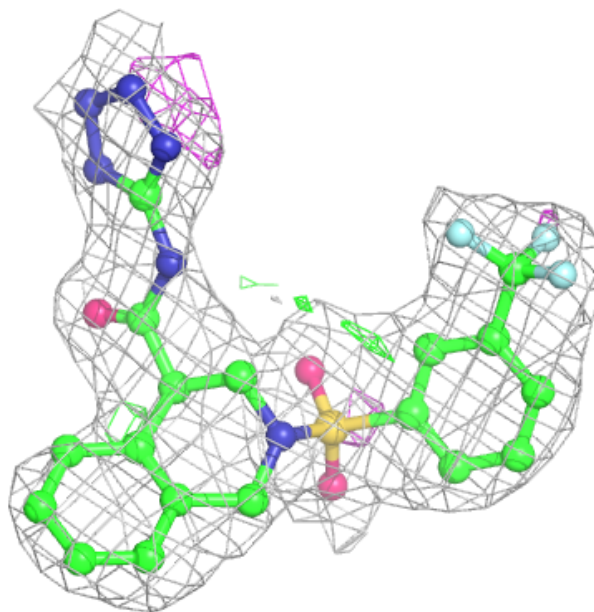
Electron density around F6I C 301:

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



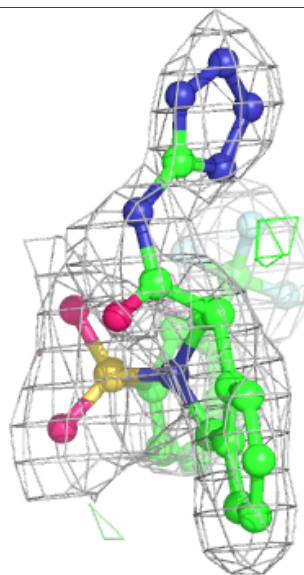
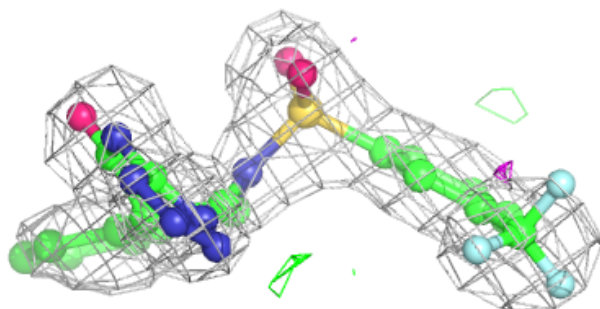
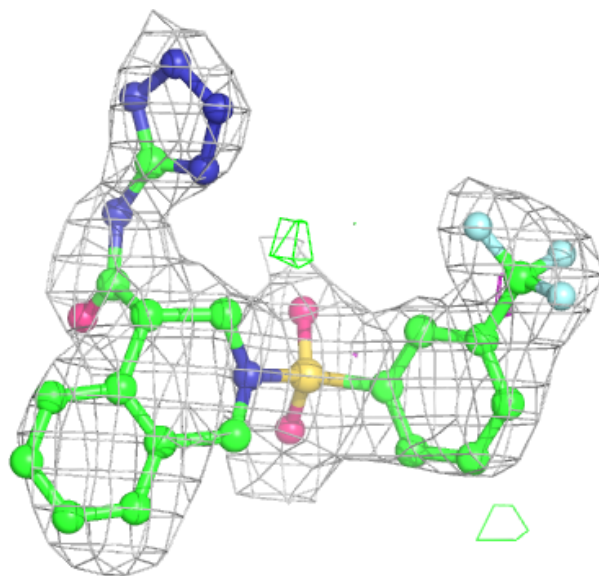
Electron density around F6I F 301:

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



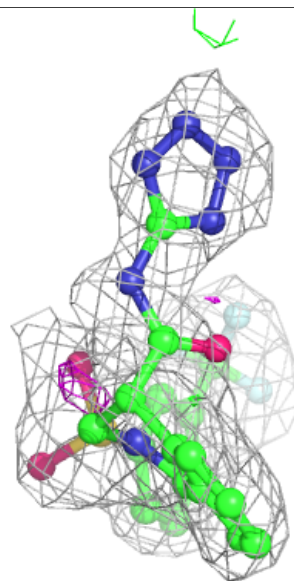
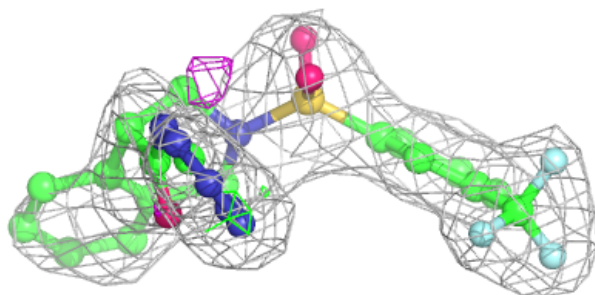
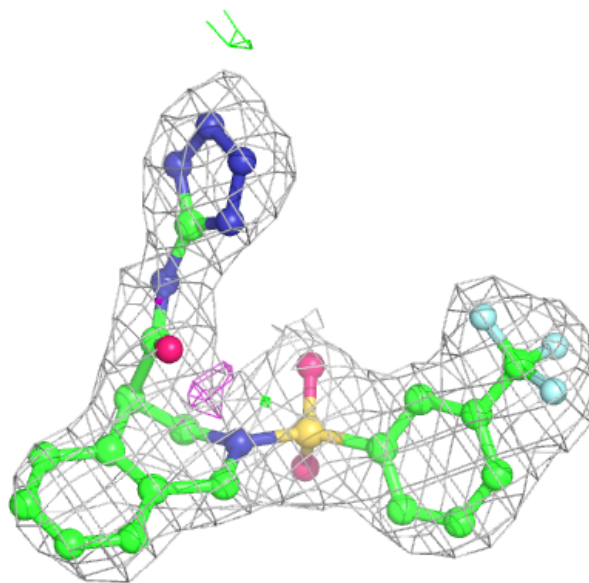
Electron density around F6I E 301:

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



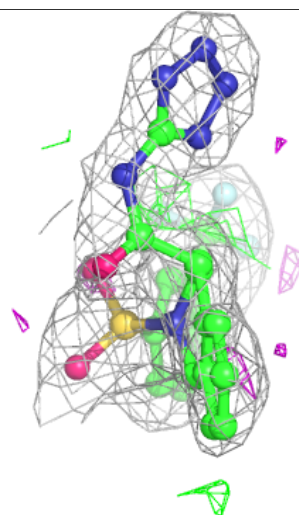
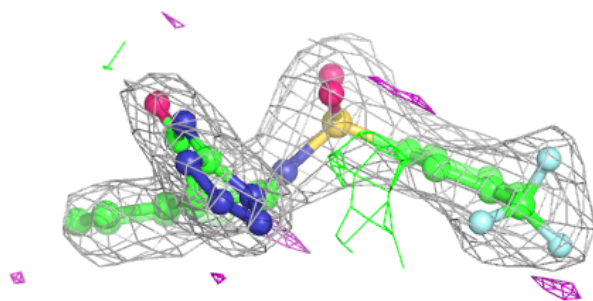
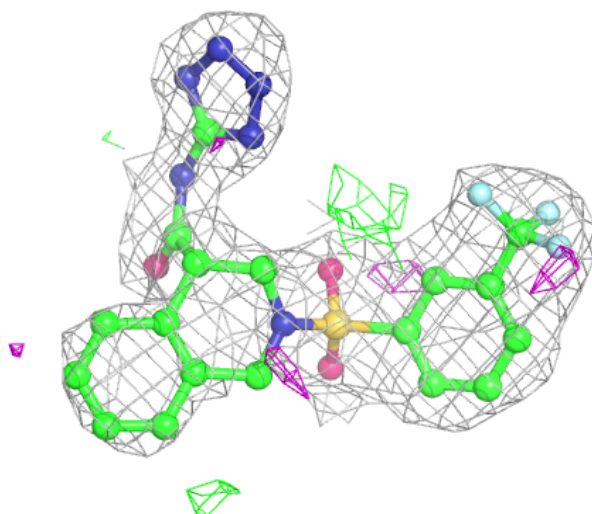
Electron density around F6I F 302:

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



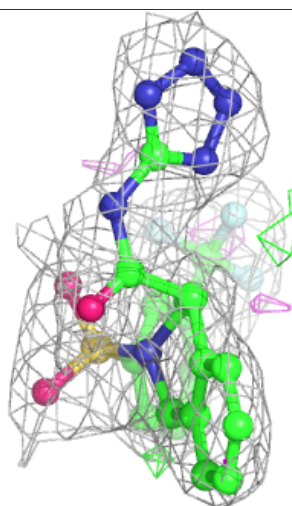
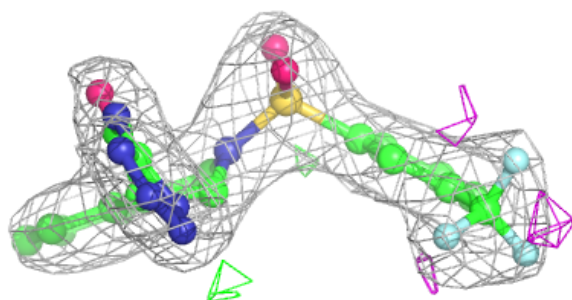
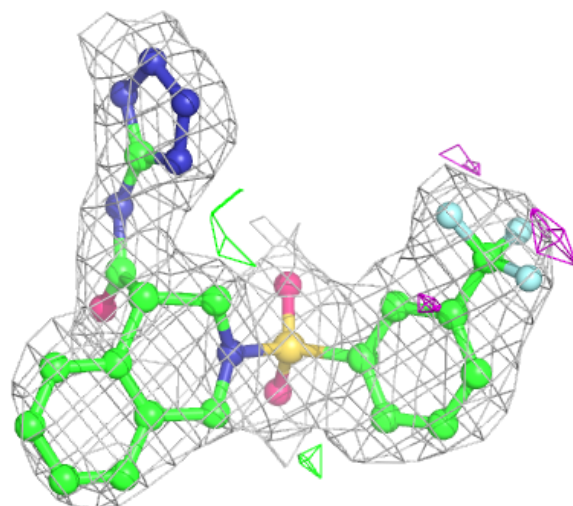
Electron density around F6I B 301:

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



Electron density around F6I B 302:

$2mF_o-DF_c$ (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.