



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2022 – 10:52 AM EDT

PDB ID : 7T61
Title : P. aeruginosa LpxA in complex with ligand L15
Authors : Sacco, M.; Chen, Y.
Deposited on : 2021-12-13
Resolution : 2.10 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:

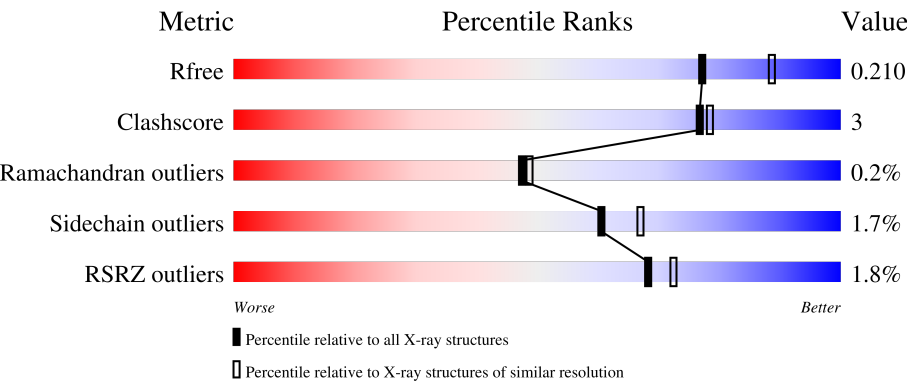
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.10 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.



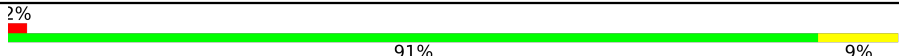
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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>92%7%</div></div>
1	B	258	<div><div>95%5%</div></div>
1	C	258	<div><div>93%6%</div></div>
1	D	258	<div><div>91%8%</div></div>
1	E	258	<div><div>92%7%</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
4	ACT	E	302	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12543 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.

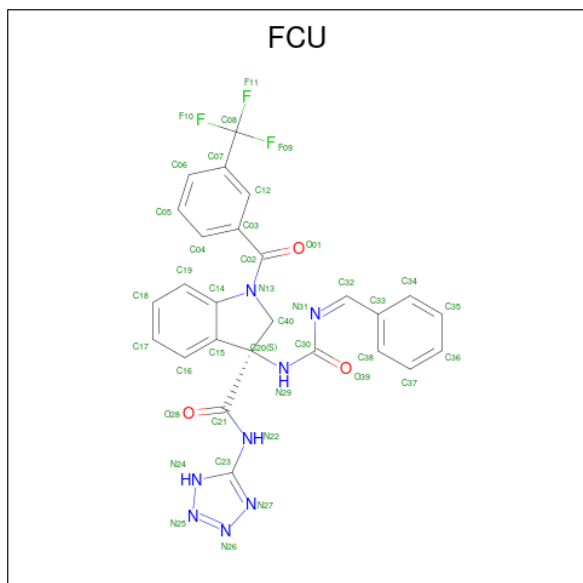
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			1984	1241	367	369	7			
1	B	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	C	256	Total	C	N	O	S	0	0	0
			1960	1227	362	365	6			
1	D	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	E	257	Total	C	N	O	S	0	1	0
			1971	1233	364	368	6			
1	F	257	Total	C	N	O	S	0	1	0
			1970	1233	363	368	6			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is (3S)-3-({[(Z)-phenylmethylidene]carbamoyl}amino)-N-(1H-tetrazol-5-yl)-1-[3-(trifluoromethyl)benzoyl]-2,3-dihydro-1H-indole-3-carboxamide (three-letter code: FCU) (formula: C₂₆H₁₉F₃N₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			40	26	3	8	3		
3	C	1	Total	C	F	N	O	0	0
			40	26	3	8	3		
3	C	1	Total	C	F	N	O	0	0
			40	26	3	8	3		
3	D	1	Total	C	F	N	O	0	0
			40	26	3	8	3		
3	E	1	Total	C	F	N	O	0	0
			40	26	3	8	3		
3	F	1	Total	C	F	N	O	0	0
			40	26	3	8	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

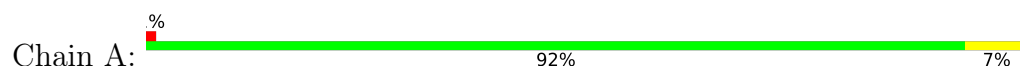
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total	O	0	0
			98	98		
5	B	87	Total	O	0	0
			87	87		
5	C	55	Total	O	0	0
			55	55		
5	D	86	Total	O	0	0
			86	86		
5	E	63	Total	O	0	0
			63	63		
5	F	77	Total	O	0	0
			77	77		

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



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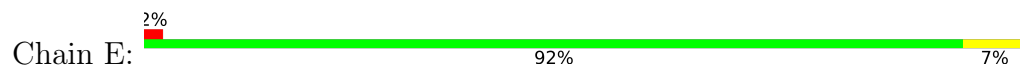
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



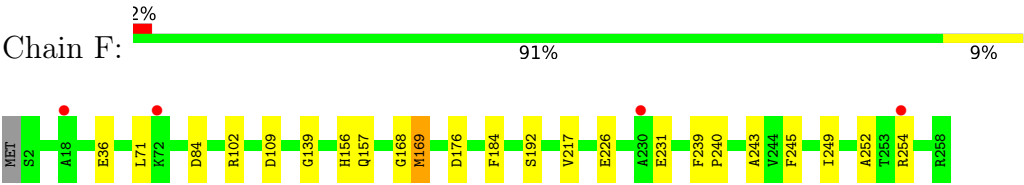
- Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase



- 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	79.48Å 82.29Å 220.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.87 – 2.10 45.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (45.87-2.10) 96.2 (45.83-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.214 0.195 , 0.210	Depositor DCC
R_{free} test set	4828 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12543	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: ACT, FCU, GOL

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	0.68	0/2027	0.81	0/2749
1	B	0.68	0/2008	0.78	0/2724
1	C	0.68	0/2002	0.79	0/2716
1	D	0.70	0/2008	0.82	0/2724
1	E	0.71	0/2013	0.77	0/2731
1	F	0.70	0/2013	0.80	0/2732
All	All	0.69	0/12071	0.80	0/16376

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	1984	0	1949	16	0
1	B	1966	0	1935	11	0
1	C	1960	0	1930	11	0
1	D	1966	0	1935	16	0
1	E	1971	0	1936	11	0
1	F	1970	0	1930	12	0
2	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	1	0
3	B	40	0	0	0	0
3	C	80	0	0	2	0
3	D	40	0	0	4	0
3	E	40	0	0	0	0
3	F	40	0	0	5	0
4	B	4	0	3	0	0
4	E	4	0	3	2	0
5	A	98	0	0	1	0
5	B	87	0	0	0	0
5	C	55	0	0	0	0
5	D	86	0	0	1	0
5	E	63	0	0	0	0
5	F	77	0	0	0	0
All	All	12543	0	11637	70	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 (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169[B]:MET:SD	1:B:156:HIS:CE1	2.80	0.74
1:B:182:THR:HG22	1:B:184:PHE:CE1	2.22	0.74
1:D:197:GLY:O	1:D:201:ARG:HD3	1.92	0.69
1:B:182:THR:CG2	1:B:184:PHE:CE1	2.85	0.60
1:D:70:ASP:HA	3:D:301:FCU:C34	2.31	0.60
1:D:76:GLU:CD	1:D:77:PRO:HA	2.22	0.59
1:D:70:ASP:HA	3:D:301:FCU:C35	2.33	0.58
1:F:217:VAL:HG11	1:F:231:GLU:HB3	1.85	0.57
1:F:245:PHE:CZ	1:F:249:ILE:HD11	2.39	0.57
1:C:228:ALA:O	1:C:232:LEU:HG	2.06	0.56
1:A:15:ARG:NH2	1:A:33:GLU:OE2	2.39	0.56
1:A:101:ASP:OD2	1:A:140[A]:HIS:HD2	1.90	0.55
1:A:218:VAL:HG21	1:A:249:ILE:HD13	1.87	0.55
1:A:74:LYS:HD2	1:A:76:GLU:HG2	1.88	0.55
1:D:175:LYS:HE2	1:D:256:ILE:O	2.07	0.54
1:C:201:ARG:NE	1:C:201:ARG:HA	2.22	0.54
1:F:176:ASP:OD2	1:F:252:ALA:HA	2.07	0.54
1:A:121:HIS:HE1	1:A:140[A]:HIS:CE1	2.26	0.53
1:C:139:GLY:O	1:C:157:GLN:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLY:O	1:A:157:GLN:HA	2.09	0.52
1:A:101:ASP:OD2	1:A:140[B]:HIS:ND1	2.40	0.52
1:A:101:ASP:OD2	1:A:140[A]:HIS:CD2	2.63	0.52
1:A:68:THR:HG23	5:A:851:HOH:O	2.09	0.51
1:F:157:GLN:HB2	3:F:301:FCU:O28	2.10	0.51
1:A:245:PHE:CZ	1:A:249:ILE:HD11	2.46	0.51
1:E:200[A]:ARG:NH2	4:E:302:ACT:O	2.39	0.50
1:D:156:HIS:NE2	1:E:169:MET:HE2	2.27	0.50
1:B:176:ASP:OD2	1:B:252:ALA:HA	2.12	0.49
1:B:182:THR:HG22	1:B:184:PHE:HE1	1.71	0.49
1:B:139:GLY:O	1:B:157:GLN:HA	2.13	0.49
1:B:182:THR:CG2	1:B:184:PHE:HE1	2.24	0.47
1:D:235:SER:HB3	1:D:242:VAL:HG11	1.96	0.47
1:C:132:VAL:HG11	3:C:601:FCU:C03	2.44	0.47
1:F:156[B]:HIS:HE1	3:F:301:FCU:C18	2.28	0.47
1:D:157:GLN:NE2	3:D:301:FCU:C38	2.78	0.47
1:D:74:LYS:O	1:D:74:LYS:HG3	2.16	0.46
1:B:36:GLU:O	1:B:54:LYS:HA	2.15	0.46
1:A:43:HIS:ND1	1:C:43:HIS:CE1	2.83	0.46
1:D:121:HIS:HE1	1:D:140:HIS:NE2	2.13	0.46
1:D:42:PRO:O	1:D:60:GLN:HA	2.17	0.45
1:C:197:GLY:O	1:C:201:ARG:HG2	2.17	0.45
1:F:156[A]:HIS:NE2	3:F:301:FCU:N24	2.65	0.45
1:F:84:ASP:O	1:F:109:ASP:HA	2.17	0.45
1:C:148:ILE:O	1:C:166:PHE:HA	2.18	0.44
1:A:121:HIS:CE1	1:A:140[A]:HIS:CE1	3.06	0.44
1:B:237:ALA:HB1	1:E:200[A]:ARG:HG3	2.00	0.44
1:D:76:GLU:OE1	1:D:77:PRO:HA	2.17	0.44
1:E:196:GLU:HB2	4:E:302:ACT:H3	1.99	0.44
1:D:132:VAL:HG11	3:F:301:FCU:C03	2.48	0.43
1:F:240:PRO:O	1:F:243:ALA:HB3	2.17	0.43
1:F:168:GLY:HA3	1:F:184:PHE:CD2	2.54	0.43
1:B:258:ARG:OXT	2:B:603:GOL:H32	2.19	0.43
1:F:139:GLY:O	1:F:157:GLN:HA	2.19	0.43
1:E:13:SER:HB2	1:E:30:ALA:HA	2.00	0.43
1:E:146:TRP:CZ3	1:E:201:ARG:CZ	3.02	0.42
1:E:101:ASP:OD2	1:E:140:HIS:ND1	2.47	0.42
1:C:98:THR:O	1:C:103:ALA:HA	2.19	0.42
1:D:70:ASP:CA	3:D:301:FCU:C35	2.98	0.42
1:F:156[B]:HIS:HE1	3:F:301:FCU:C19	2.32	0.41
1:E:3:LEU:O	1:E:21:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLY:O	1:D:157:GLN:HG2	2.20	0.41
1:C:42:PRO:O	1:C:60:GLN:HA	2.20	0.41
1:A:68:THR:HG22	1:A:70:ASP:H	1.86	0.41
1:A:69:PRO:HB2	1:C:112:LEU:HD11	2.03	0.41
1:B:233:ALA:HB1	1:E:199:ARG:HD3	2.03	0.41
1:D:219:TYR:O	5:D:401:HOH:O	2.22	0.41
1:E:119:ILE:HD12	1:E:125:ILE:HD11	2.03	0.40
1:C:169:MET:HE2	3:C:601:FCU:C12	2.51	0.40
1:E:154:LEU:HD13	1:F:169:MET:HG2	2.04	0.40
1:A:68:THR:HG21	1:A:121:HIS:CD2	2.57	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	257/258 (100%)	247 (96%)	10 (4%)	0	100	100
1	B	255/258 (99%)	243 (95%)	11 (4%)	1 (0%)	34	32
1	C	254/258 (98%)	237 (93%)	17 (7%)	0	100	100
1	D	255/258 (99%)	240 (94%)	14 (6%)	1 (0%)	34	32
1	E	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
1	F	256/258 (99%)	244 (95%)	11 (4%)	1 (0%)	34	32
All	All	1533/1548 (99%)	1453 (95%)	77 (5%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	SER
1	F	192	SER
1	D	70	ASP

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	207/206 (100%)	204 (99%)	3 (1%)	67	73
1	B	205/206 (100%)	205 (100%)	0	100	100
1	C	204/206 (99%)	202 (99%)	2 (1%)	76	82
1	D	205/206 (100%)	200 (98%)	5 (2%)	49	53
1	E	205/206 (100%)	201 (98%)	4 (2%)	55	60
1	F	205/206 (100%)	198 (97%)	7 (3%)	37	39
All	All	1231/1236 (100%)	1210 (98%)	21 (2%)	60	67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	74	LYS
1	A	254	ARG
1	C	25	TRP
1	C	201	ARG
1	D	71	LEU
1	D	72	LYS
1	D	169	MET
1	D	201	ARG
1	D	254	ARG
1	E	15	ARG
1	E	102	ARG
1	E	213	ARG
1	E	226	GLU
1	F	36	GLU
1	F	71	LEU
1	F	102	ARG
1	F	169	MET
1	F	226	GLU
1	F	239	PHE
1	F	254	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	157	GLN

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 ⓘ

10 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
3	FCU	D	301	-	41,44,44	3.26	11 (26%)	49,64,64	1.71	10 (20%)
3	FCU	C	601	-	41,44,44	3.46	13 (31%)	49,64,64	2.21	11 (22%)
4	ACT	B	602	-	3,3,3	1.06	0	3,3,3	0.74	0
2	GOL	A	701	-	5,5,5	0.15	0	5,5,5	0.29	0
3	FCU	E	301	-	41,44,44	3.15	11 (26%)	49,64,64	1.83	12 (24%)
4	ACT	E	302	-	3,3,3	1.05	0	3,3,3	0.80	0
3	FCU	C	602	-	41,44,44	3.21	10 (24%)	49,64,64	1.78	7 (14%)
2	GOL	B	603	-	5,5,5	0.27	0	5,5,5	0.53	0
3	FCU	B	601	-	41,44,44	3.40	10 (24%)	49,64,64	1.91	9 (18%)
3	FCU	F	301	-	41,44,44	3.19	11 (26%)	49,64,64	2.16	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FCU	D	301	-	-	6/30/49/49	0/5/5/5
3	FCU	C	601	-	-	8/30/49/49	0/5/5/5
2	GOL	A	701	-	-	2/4/4/4	-
3	FCU	E	301	-	-	4/30/49/49	0/5/5/5
3	FCU	C	602	-	-	4/30/49/49	0/5/5/5
2	GOL	B	603	-	-	2/4/4/4	-
3	FCU	B	601	-	-	6/30/49/49	0/5/5/5
3	FCU	F	301	-	-	6/30/49/49	0/5/5/5

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	FCU	C32-N31	15.52	1.47	1.28
3	B	601	FCU	C32-N31	15.27	1.47	1.28
3	E	301	FCU	C32-N31	14.29	1.46	1.28
3	C	602	FCU	C32-N31	14.26	1.46	1.28
3	D	301	FCU	C32-N31	14.12	1.45	1.28
3	F	301	FCU	C32-N31	14.03	1.45	1.28
3	C	601	FCU	C30-N29	9.03	1.47	1.34
3	C	602	FCU	C30-N29	8.74	1.46	1.34
3	E	301	FCU	C30-N29	8.37	1.46	1.34
3	D	301	FCU	C30-N29	8.32	1.46	1.34
3	F	301	FCU	C30-N29	8.12	1.45	1.34
3	B	601	FCU	C30-N29	7.87	1.45	1.34
3	B	601	FCU	C14-N13	6.10	1.51	1.39
3	D	301	FCU	C14-N13	5.63	1.50	1.39
3	C	602	FCU	C14-N13	5.36	1.50	1.39
3	E	301	FCU	C14-N13	5.34	1.50	1.39
3	D	301	FCU	C02-N13	5.34	1.45	1.36
3	C	601	FCU	C30-N31	5.31	1.48	1.38
3	B	601	FCU	C23-N22	5.27	1.45	1.38
3	F	301	FCU	C14-N13	5.13	1.49	1.39
3	F	301	FCU	C23-N22	5.11	1.45	1.38
3	D	301	FCU	C23-N22	5.02	1.45	1.38
3	C	601	FCU	C02-N13	4.88	1.44	1.36
3	C	601	FCU	C14-N13	4.83	1.49	1.39
3	B	601	FCU	C02-N13	4.81	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	FCU	C23-N22	4.71	1.45	1.38
3	B	601	FCU	C21-N22	4.38	1.46	1.35
3	B	601	FCU	C30-N31	4.30	1.46	1.38
3	F	301	FCU	C21-N22	4.23	1.45	1.35
3	E	301	FCU	C02-N13	4.16	1.43	1.36
3	C	601	FCU	C21-N22	4.11	1.45	1.35
3	D	301	FCU	C21-N22	4.08	1.45	1.35
3	E	301	FCU	C21-N22	4.06	1.45	1.35
3	C	601	FCU	C23-N22	4.06	1.44	1.38
3	D	301	FCU	C30-N31	4.03	1.46	1.38
3	C	602	FCU	C02-N13	3.96	1.42	1.36
3	C	602	FCU	C21-N22	3.67	1.44	1.35
3	F	301	FCU	C02-N13	3.61	1.42	1.36
3	E	301	FCU	C23-N22	3.56	1.43	1.38
3	F	301	FCU	C30-N31	3.44	1.45	1.38
3	F	301	FCU	O39-C30	-3.40	1.18	1.24
3	C	602	FCU	C30-N31	3.31	1.45	1.38
3	F	301	FCU	C33-C32	3.31	1.54	1.47
3	C	602	FCU	C33-C32	3.25	1.54	1.47
3	C	601	FCU	C33-C32	3.13	1.53	1.47
3	E	301	FCU	C30-N31	2.99	1.44	1.38
3	E	301	FCU	C33-C32	2.86	1.53	1.47
3	D	301	FCU	C33-C32	2.63	1.52	1.47
3	C	601	FCU	O39-C30	-2.56	1.19	1.24
3	D	301	FCU	O39-C30	-2.48	1.19	1.24
3	C	601	FCU	O01-C02	-2.46	1.17	1.22
3	B	601	FCU	C33-C32	2.45	1.52	1.47
3	E	301	FCU	O01-C02	-2.41	1.17	1.22
3	D	301	FCU	O28-C21	-2.37	1.18	1.22
3	C	602	FCU	O28-C21	-2.31	1.18	1.22
3	C	601	FCU	C20-C15	2.20	1.54	1.51
3	C	602	FCU	O39-C30	-2.20	1.20	1.24
3	D	301	FCU	O01-C02	-2.16	1.18	1.22
3	C	601	FCU	C16-C15	2.15	1.42	1.39
3	F	301	FCU	C40-N13	-2.08	1.45	1.47
3	C	601	FCU	O28-C21	-2.08	1.19	1.22
3	B	601	FCU	C19-C14	2.07	1.43	1.39
3	E	301	FCU	O39-C30	-2.05	1.20	1.24
3	E	301	FCU	O28-C21	-2.05	1.19	1.22
3	B	601	FCU	C06-C07	2.04	1.42	1.39
3	F	301	FCU	O28-C21	-2.03	1.19	1.22

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	FCU	N29-C30-N31	8.87	126.33	111.05
3	C	601	FCU	C15-C14-N13	-7.63	104.82	109.76
3	F	301	FCU	N29-C30-N31	6.83	122.81	111.05
3	B	601	FCU	C15-C14-N13	-6.74	105.39	109.76
3	E	301	FCU	C15-C14-N13	-6.60	105.48	109.76
3	C	602	FCU	C15-C14-N13	-6.51	105.54	109.76
3	F	301	FCU	C33-C32-N31	-5.89	113.46	122.08
3	F	301	FCU	C15-C14-N13	-5.52	106.18	109.76
3	D	301	FCU	C15-C14-N13	-4.91	106.58	109.76
3	C	602	FCU	N29-C30-N31	4.83	119.37	111.05
3	B	601	FCU	C33-C32-N31	-4.53	115.44	122.08
3	B	601	FCU	N29-C30-N31	4.44	118.70	111.05
3	D	301	FCU	C33-C32-N31	-4.43	115.59	122.08
3	F	301	FCU	N24-N25-N26	-4.29	106.73	109.53
3	C	601	FCU	O39-C30-N29	-4.28	113.38	123.62
3	E	301	FCU	C33-C32-N31	-4.07	116.11	122.08
3	C	602	FCU	C33-C32-N31	-3.94	116.31	122.08
3	B	601	FCU	N27-N26-N25	-3.77	107.07	109.53
3	F	301	FCU	F11-C08-C07	-3.75	104.69	112.93
3	E	301	FCU	N29-C30-N31	3.62	117.28	111.05
3	F	301	FCU	C20-C15-C14	-3.52	106.95	108.90
3	C	601	FCU	C33-C32-N31	-3.36	117.16	122.08
3	F	301	FCU	O39-C30-N31	-3.27	118.29	125.62
3	D	301	FCU	N29-C30-N31	3.16	116.49	111.05
3	C	601	FCU	C15-C20-C21	-3.10	102.01	110.39
3	D	301	FCU	C20-C15-C14	-3.08	107.19	108.90
3	E	301	FCU	C05-C06-C07	-3.06	117.54	120.76
3	B	601	FCU	F09-C08-C07	-2.95	106.45	112.93
3	C	602	FCU	O39-C30-N31	-2.94	119.03	125.62
3	E	301	FCU	N24-N25-N26	-2.93	107.62	109.53
3	C	601	FCU	F09-C08-C07	-2.92	106.52	112.93
3	C	602	FCU	N24-N25-N26	-2.90	107.64	109.53
3	B	601	FCU	F10-C08-C07	-2.88	106.60	112.93
3	C	602	FCU	F11-C08-C07	-2.85	106.67	112.93
3	E	301	FCU	F09-C08-C07	-2.83	106.72	112.93
3	D	301	FCU	N24-N25-N26	-2.69	107.77	109.53
3	D	301	FCU	F09-C08-C07	-2.68	107.04	112.93
3	E	301	FCU	C38-C33-C34	2.58	121.46	117.64
3	E	301	FCU	C06-C07-C12	2.58	122.73	117.76
3	D	301	FCU	N27-N26-N25	-2.56	107.86	109.53
3	B	601	FCU	C20-C15-C14	-2.53	107.50	108.90
3	D	301	FCU	C03-C12-C07	-2.46	117.73	121.07
3	E	301	FCU	O01-C02-N13	-2.43	118.47	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	FCU	O39-C30-N31	-2.38	120.27	125.62
3	C	601	FCU	C12-C07-C08	-2.36	116.39	119.58
3	E	301	FCU	C20-C15-C14	-2.35	107.60	108.90
3	D	301	FCU	C04-C03-C12	2.31	121.97	119.24
3	F	301	FCU	C12-C07-C08	-2.30	116.47	119.58
3	D	301	FCU	C06-C07-C12	2.26	122.11	117.76
3	E	301	FCU	C12-C07-C08	-2.24	116.56	119.58
3	C	601	FCU	C04-C03-C12	2.23	121.88	119.24
3	F	301	FCU	C05-C06-C07	-2.23	118.42	120.76
3	C	601	FCU	N27-N26-N25	-2.22	108.09	109.53
3	B	601	FCU	C12-C07-C08	-2.22	116.58	119.58
3	C	602	FCU	N27-N26-N25	-2.17	108.12	109.53
3	B	601	FCU	O39-C30-N31	-2.10	120.91	125.62
3	F	301	FCU	C04-C03-C12	2.10	121.72	119.24
3	C	601	FCU	F10-C08-C07	-2.07	108.39	112.93
3	F	301	FCU	C06-C07-C12	2.06	121.74	117.76
3	E	301	FCU	O39-C30-N31	-2.03	121.06	125.62
3	F	301	FCU	F09-C08-C07	-2.03	108.47	112.93
3	F	301	FCU	C12-C03-C02	-2.02	115.64	120.14

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	603	GOL	C1-C2-C3-O3
2	B	603	GOL	O2-C2-C3-O3
3	B	601	FCU	C33-C32-N31-C30
3	C	601	FCU	C15-C20-N29-C30
3	C	601	FCU	C21-C20-N29-C30
3	C	601	FCU	C40-C20-N29-C30
3	C	601	FCU	O39-C30-N29-C20
3	C	601	FCU	C33-C32-N31-C30
3	C	602	FCU	C33-C32-N31-C30
3	D	301	FCU	C33-C32-N31-C30
3	E	301	FCU	C33-C32-N31-C30
3	F	301	FCU	C33-C32-N31-C30
3	D	301	FCU	N31-C32-C33-C38
3	B	601	FCU	N31-C32-C33-C38
3	C	601	FCU	N31-C32-C33-C38
3	C	602	FCU	N31-C32-C33-C38
3	D	301	FCU	N31-C32-C33-C34
3	E	301	FCU	N31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
3	F	301	FCU	N31-C32-C33-C34
3	F	301	FCU	N31-C32-C33-C38
3	B	601	FCU	N31-C32-C33-C34
3	C	601	FCU	N31-C32-C33-C34
3	C	602	FCU	N31-C32-C33-C34
3	E	301	FCU	N31-C32-C33-C38
2	A	701	GOL	C1-C2-C3-O3
3	B	601	FCU	C15-C20-N29-C30
3	C	602	FCU	C15-C20-N29-C30
3	D	301	FCU	C15-C20-N29-C30
3	E	301	FCU	C15-C20-N29-C30
3	F	301	FCU	C15-C20-N29-C30
2	A	701	GOL	O2-C2-C3-O3
3	B	601	FCU	O01-C02-N13-C40
3	C	601	FCU	O01-C02-N13-C40
3	D	301	FCU	O01-C02-N13-C40
3	F	301	FCU	O01-C02-N13-C40
3	B	601	FCU	C03-C02-N13-C40
3	D	301	FCU	C03-C02-N13-C40
3	F	301	FCU	C03-C02-N13-C40

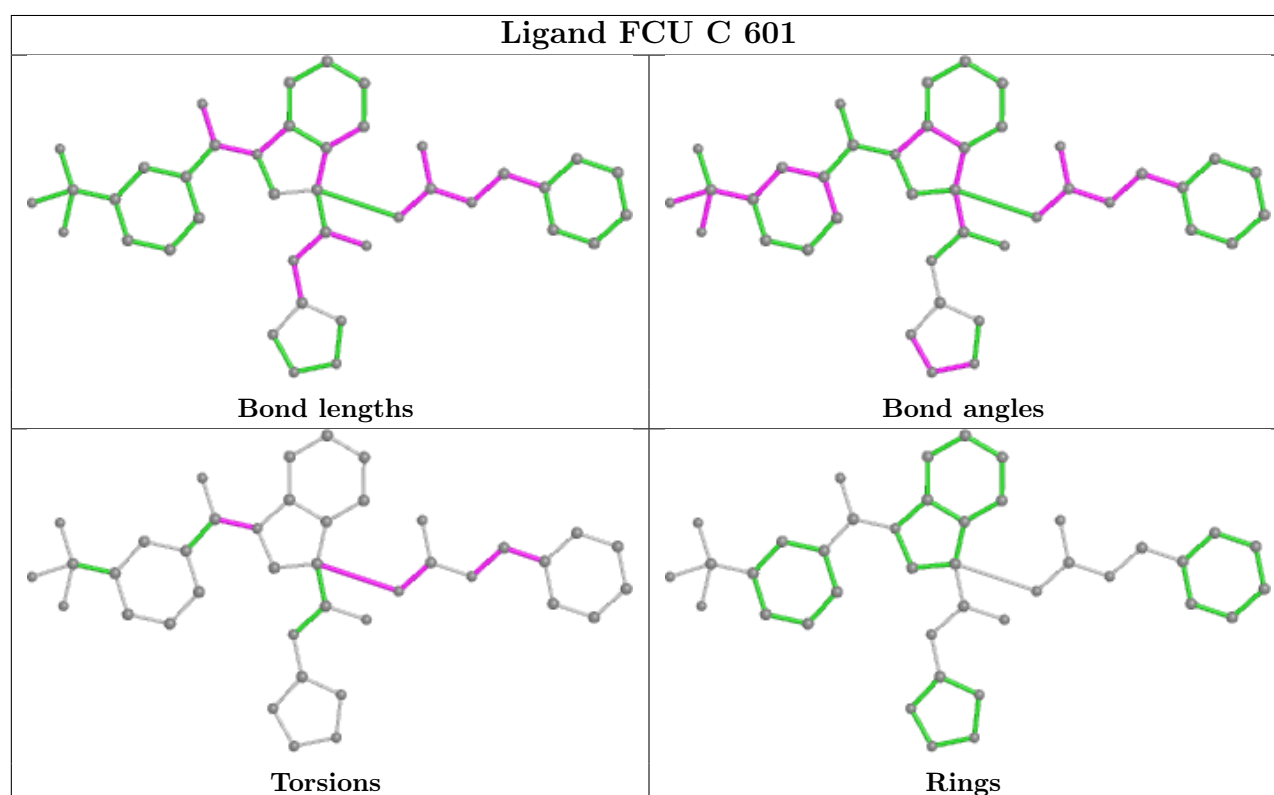
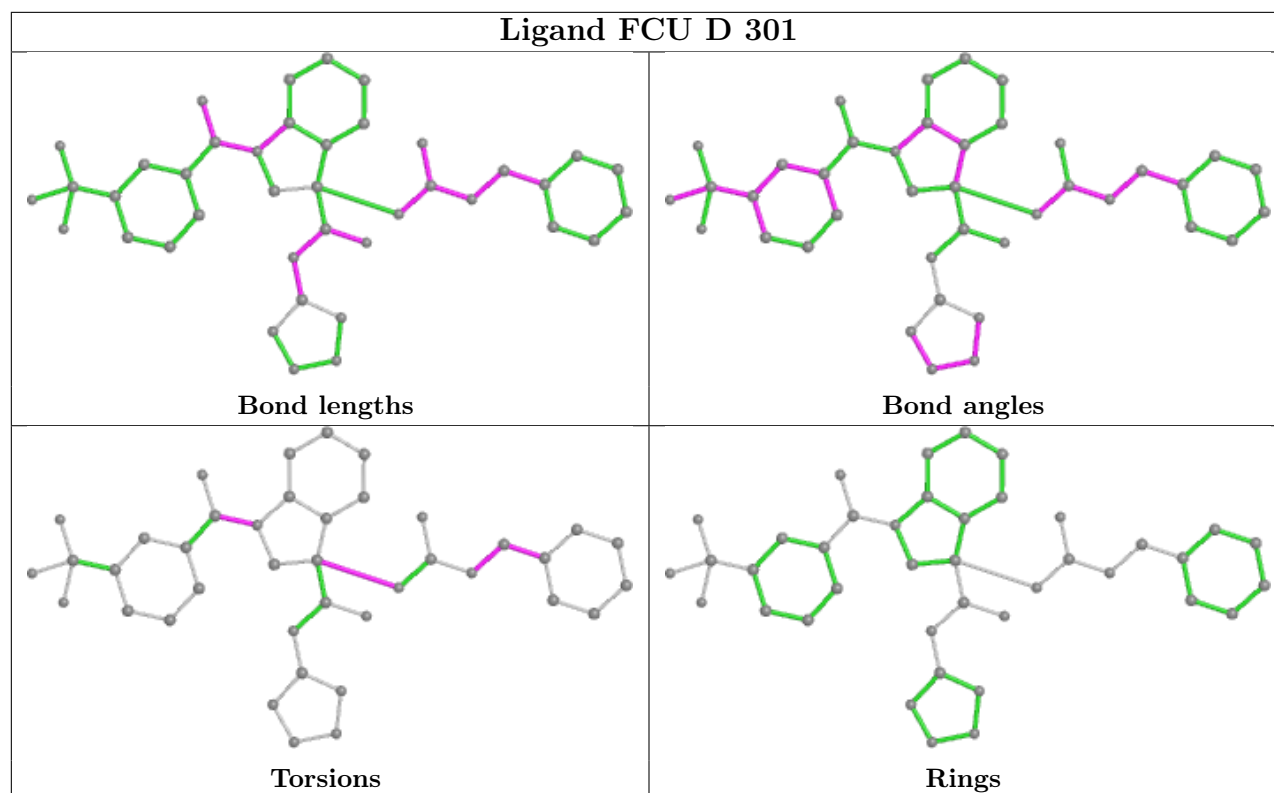
There are no ring outliers.

5 monomers are involved in 14 short contacts:

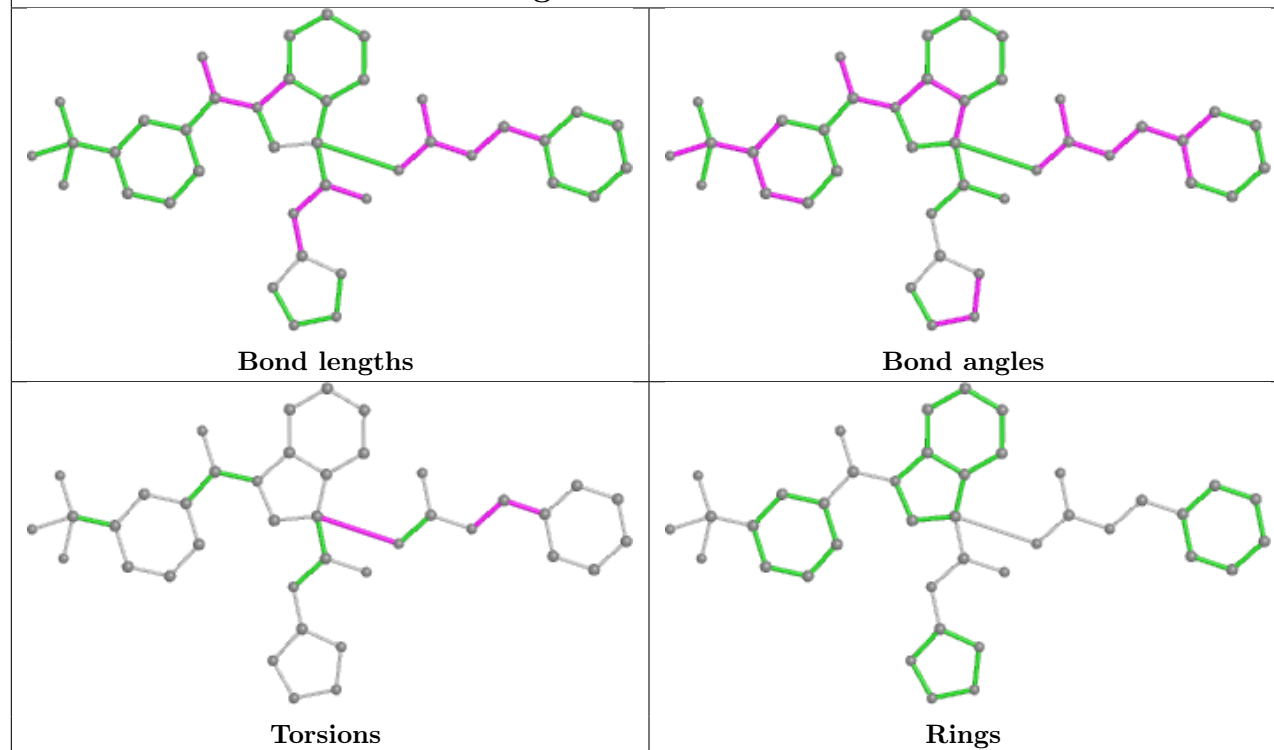
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	FCU	4	0
3	C	601	FCU	2	0
4	E	302	ACT	2	0
2	B	603	GOL	1	0
3	F	301	FCU	5	0

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

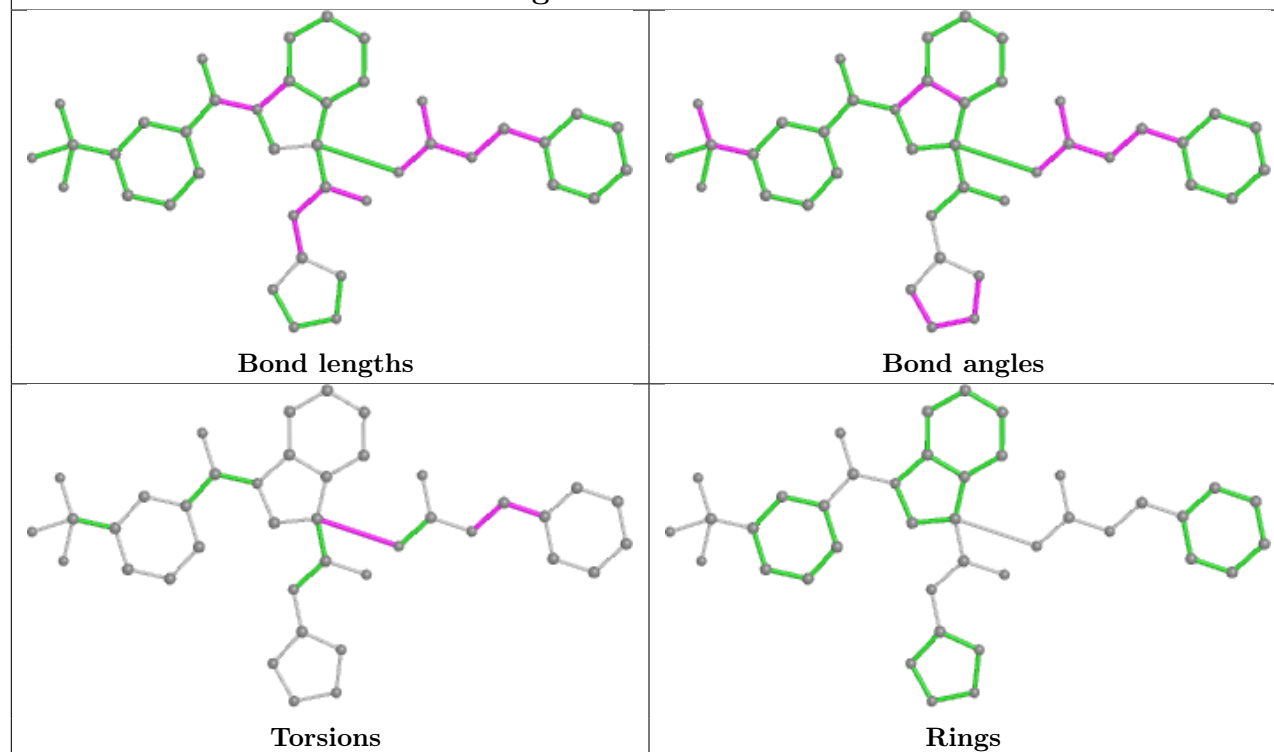
equivalents in the CSD to analyse the geometry.

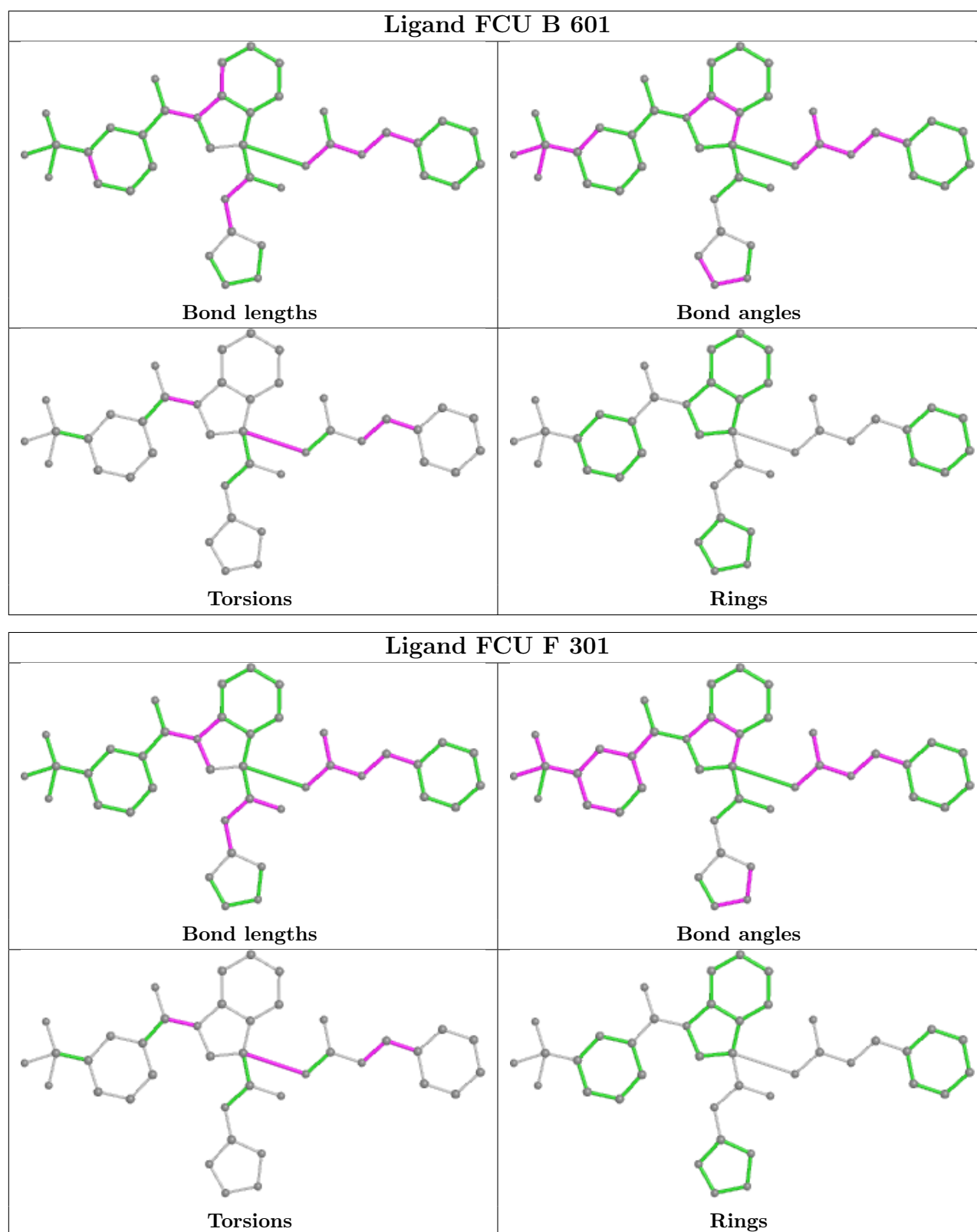


Ligand FCU E 301



Ligand FCU C 602





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	257/258 (99%)	-0.24	2 (0%) 86 88	22, 32, 63, 103	0
1	B	257/258 (99%)	-0.17	2 (0%) 86 88	21, 34, 63, 78	0
1	C	256/258 (99%)	0.03	7 (2%) 54 60	23, 41, 72, 85	0
1	D	257/258 (99%)	-0.05	9 (3%) 44 50	21, 34, 69, 118	0
1	E	257/258 (99%)	-0.08	4 (1%) 72 75	23, 40, 65, 84	0
1	F	257/258 (99%)	-0.13	4 (1%) 72 75	20, 35, 66, 93	0
All	All	1541/1548 (99%)	-0.11	28 (1%) 68 72	20, 37, 68, 118	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	TYR	6.0
1	A	73	TYR	5.7
1	F	18	ALA	4.8
1	D	72	LYS	4.4
1	C	233	ALA	3.8
1	E	230	ALA	3.7
1	C	237	ALA	3.7
1	D	250	GLN	3.3
1	F	72	LYS	3.3
1	D	2	SER	3.0
1	E	232	LEU	2.9
1	C	253	THR	2.7
1	F	230	ALA	2.6
1	B	224	THR	2.6
1	D	230	ALA	2.6
1	D	71	LEU	2.6
1	C	99	VAL	2.6
1	F	254	ARG	2.6
1	D	225	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	225	VAL	2.4
1	B	18	ALA	2.4
1	D	209	HIS	2.3
1	C	229	LEU	2.2
1	C	102	ARG	2.2
1	E	253	THR	2.2
1	D	222	GLY	2.2
1	A	70	ASP	2.1
1	E	209	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

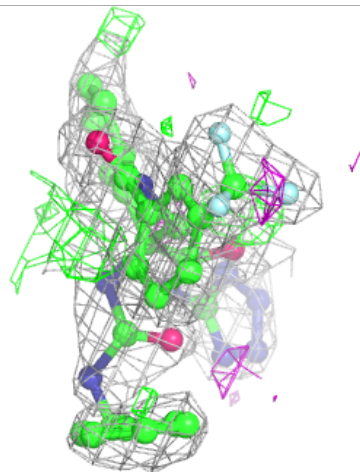
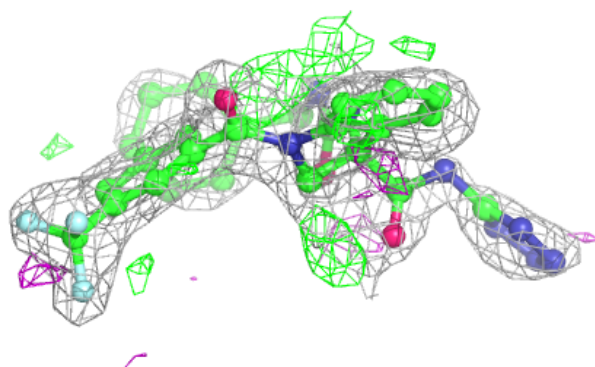
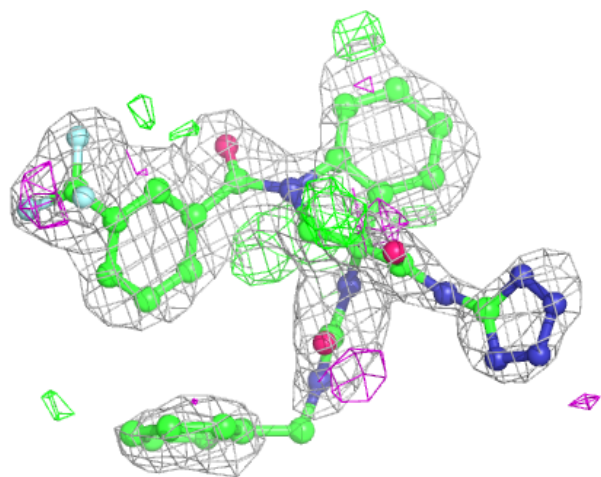
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FCU	F	301	40/40	0.80	0.19	42,52,64,66	0
3	FCU	C	601	40/40	0.82	0.22	45,63,89,90	0
4	ACT	B	602	4/4	0.84	0.17	55,55,61,62	0
4	ACT	E	302	4/4	0.84	0.12	52,58,63,63	0
2	GOL	B	603	6/6	0.86	0.16	36,42,47,52	0
2	GOL	A	701	6/6	0.87	0.19	53,57,60,62	0
3	FCU	D	301	40/40	0.89	0.22	46,76,95,96	0
3	FCU	E	301	40/40	0.90	0.15	32,43,66,70	0
3	FCU	B	601	40/40	0.90	0.13	34,41,51,54	0
3	FCU	C	602	40/40	0.92	0.14	36,43,53,55	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.

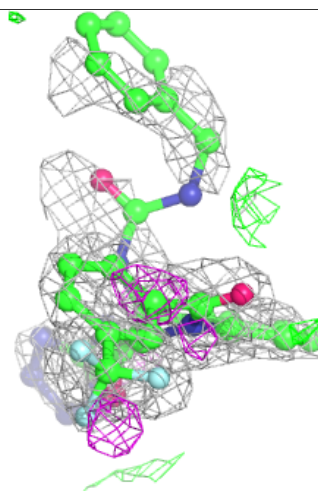
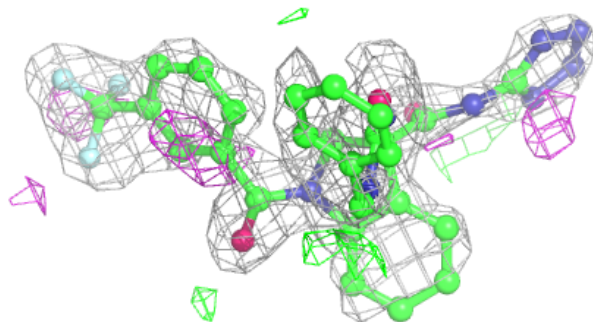
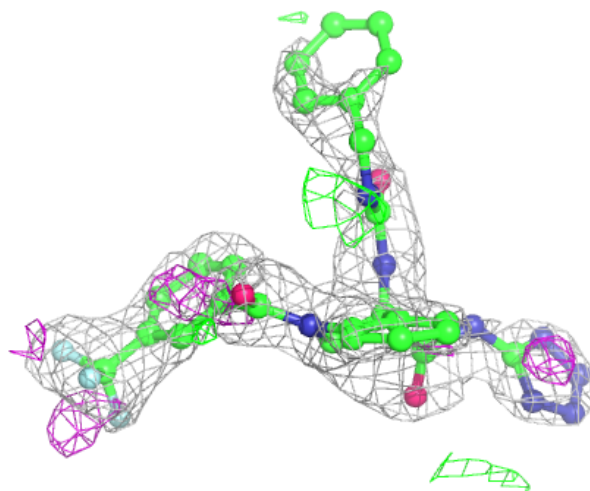
Electron density around FCU F 301:

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



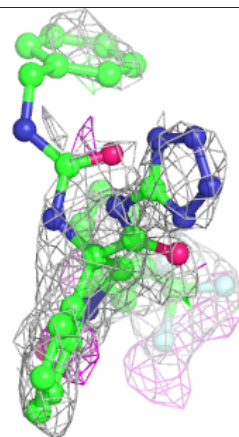
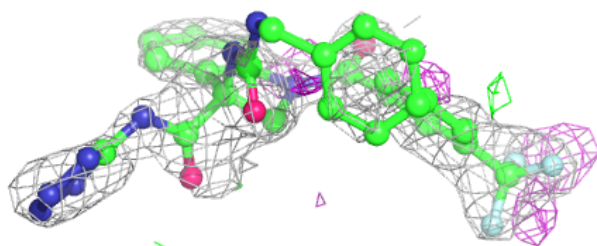
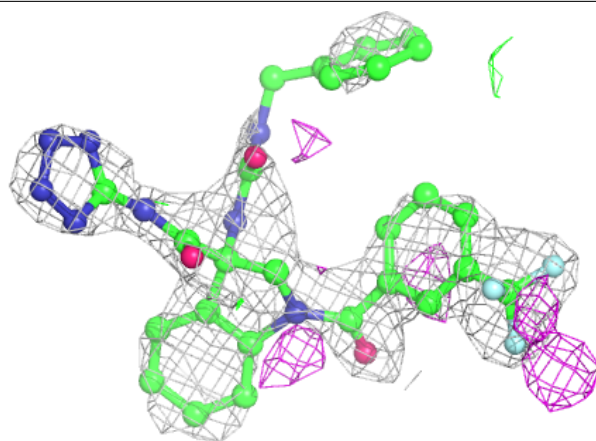
Electron density around FCU C 601:

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



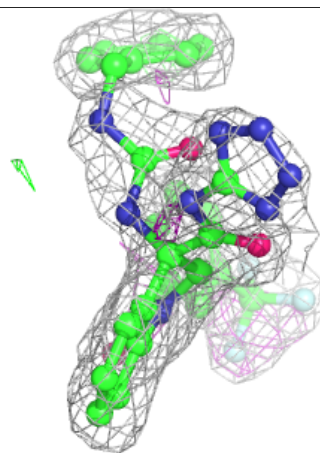
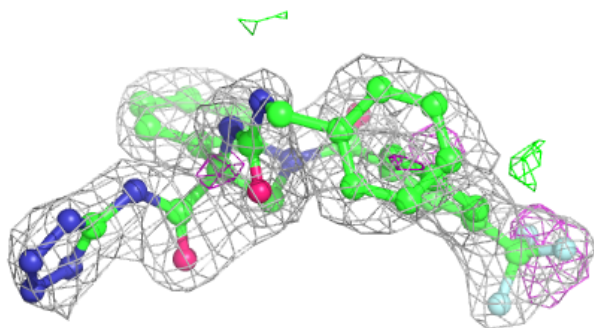
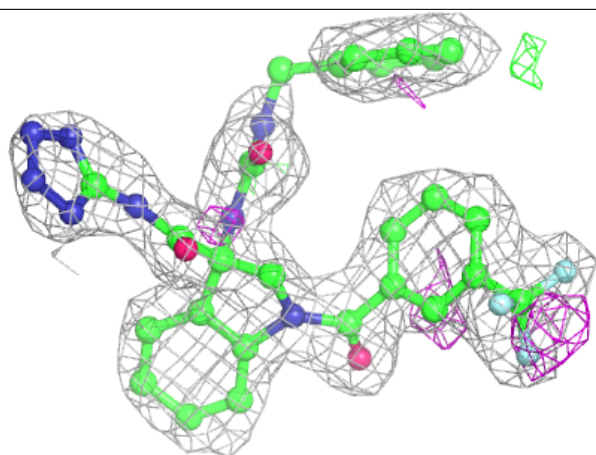
Electron density around FCU D 301:

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



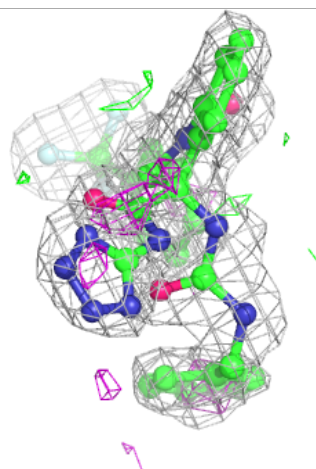
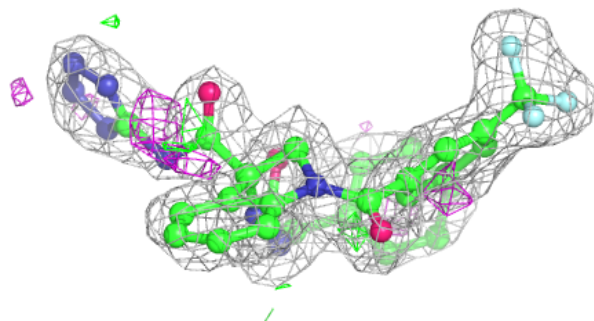
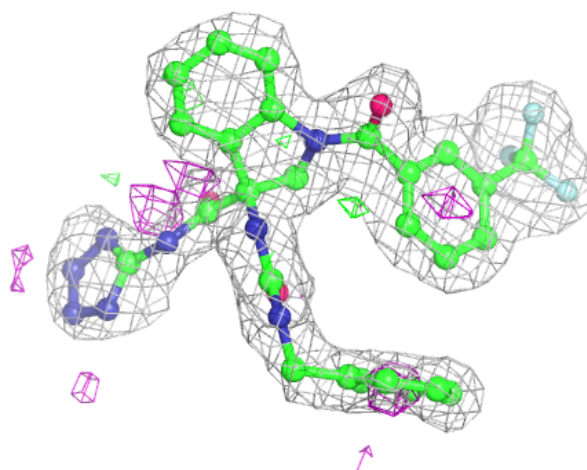
Electron density around FCU E 301:

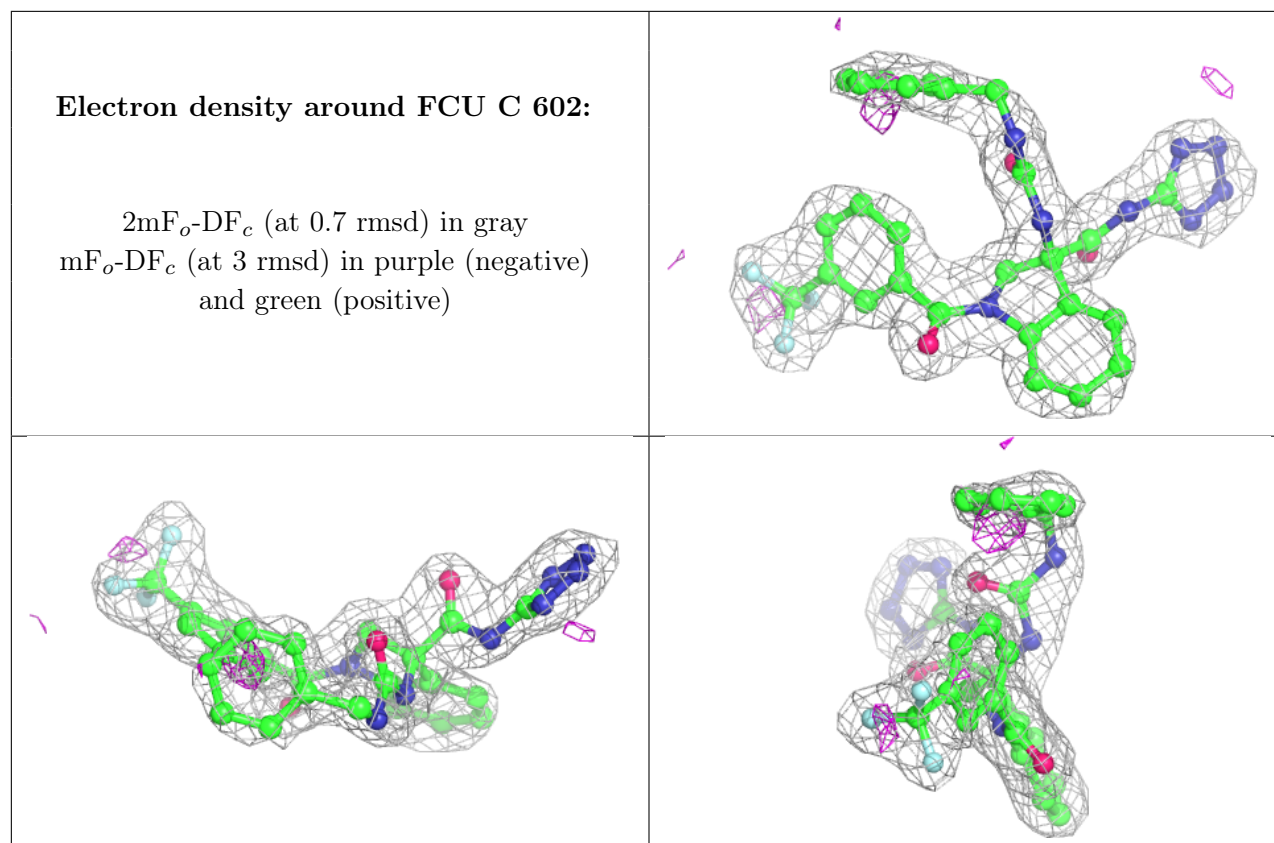
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FCU B 601:

$2mF_o-DF_c$ (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.