Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 02:27 AM EDT

PDB ID	:	7T60
Title	:	P. aeruginosa LpxA in complex with ligand L13
Authors	:	Sacco, M.; Chen, Y.
Deposited on	:	2021-12-13
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

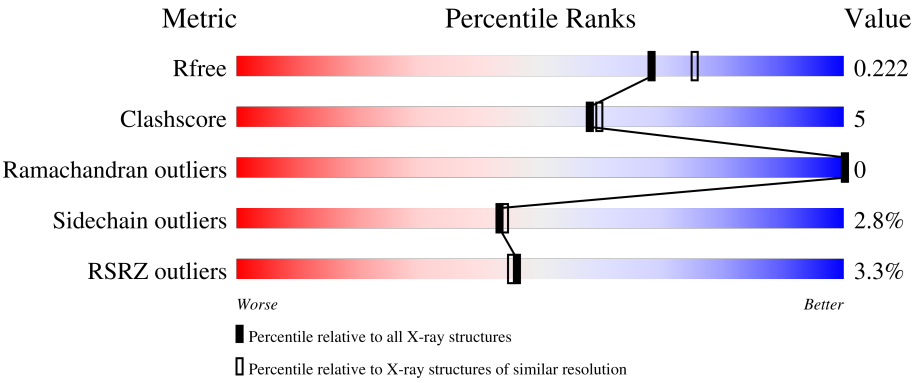
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	258	92% 7%
1	B	258	2% 87% 11%
1	C	258	3% 91% 8%
1	D	258	4% 90% 9%
1	E	258	8% 85% 13%

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Mol	Chain	Length	Quality of chain
1	F	258	2% 88% 12%

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	GOL	B	303	-	-	X	-

2 Entry composition (i)

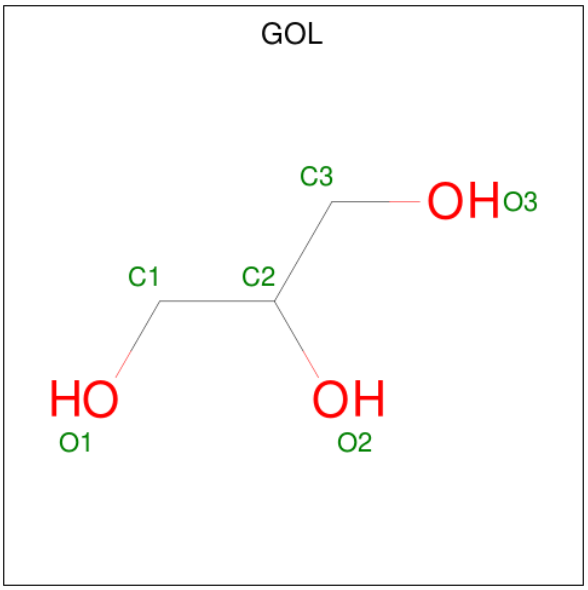
There are 5 unique types of molecules in this entry. The entry contains 12455 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

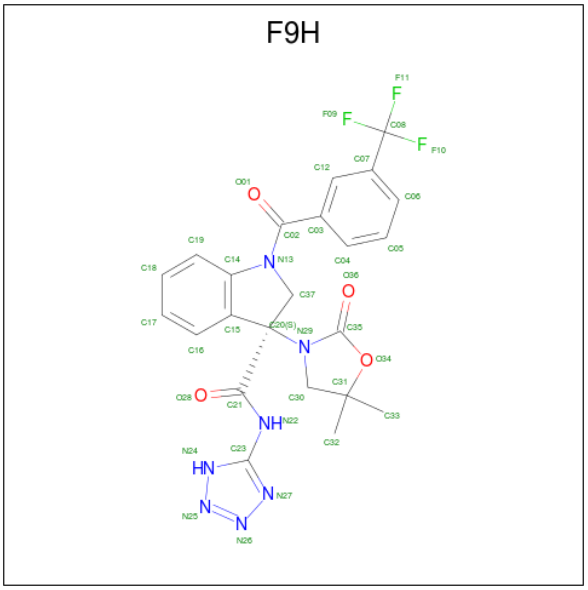
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			1983	1239	368	370	6			
1	B	257	Total	C	N	O	S	0	1	0
			1977	1236	367	368	6			
1	C	256	Total	C	N	O	S	0	1	0
			1970	1233	365	366	6			
1	D	257	Total	C	N	O	S	0	2	0
			1984	1241	367	369	7			
1	E	257	Total	C	N	O	S	0	0	0
			1966	1230	363	367	6			
1	F	257	Total	C	N	O	S	0	1	0
			1968	1232	361	368	7			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

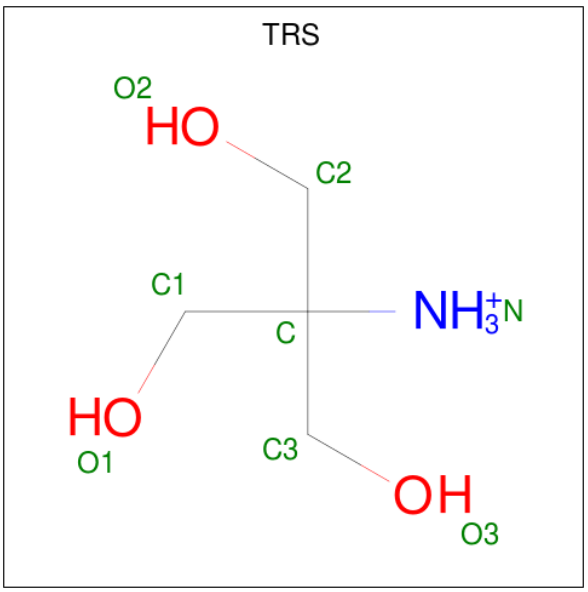
- Molecule 3 is (3S)-3-(5,5-dimethyl-2-oxo-1,3-oxazolidin-3-yl)-N-(1H-tetrazol-5-yl)-1-[3-(trifluoromethyl)benzoyl]-2,3-dihydro-1H-indole-3-carboxamide (three-letter code: F9H) (formula: $C_{23}H_{20}F_3N_7O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C F N O 37 23 3 7 4	0	0
3	C	1	Total C F N O 37 23 3 7 4	0	0
3	C	1	Total C F N O 37 23 3 7 4	0	0
3	C	1	Total C F N O 37 23 3 7 4	0	0
3	D	1	Total C F N O 37 23 3 7 4	0	0
3	E	1	Total C F N O 37 23 3 7 4	0	0
3	E	1	Total C F N O 37 23 3 7 4	0	0
3	F	1	Total C F N O 37 23 3 7 4	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

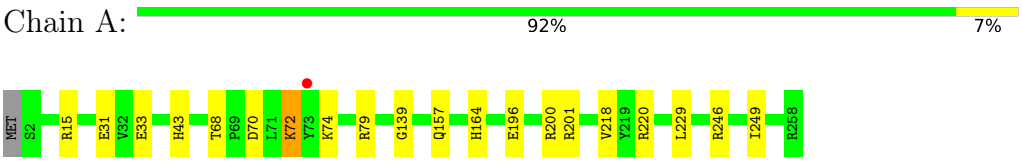
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	1
			75	75		
5	B	44	Total	O	0	0
			44	44		
5	C	42	Total	O	0	0
			42	42		
5	D	37	Total	O	0	0
			37	37		
5	E	33	Total	O	0	0
			33	33		
5	F	60	Total	O	0	0
			60	60		

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.

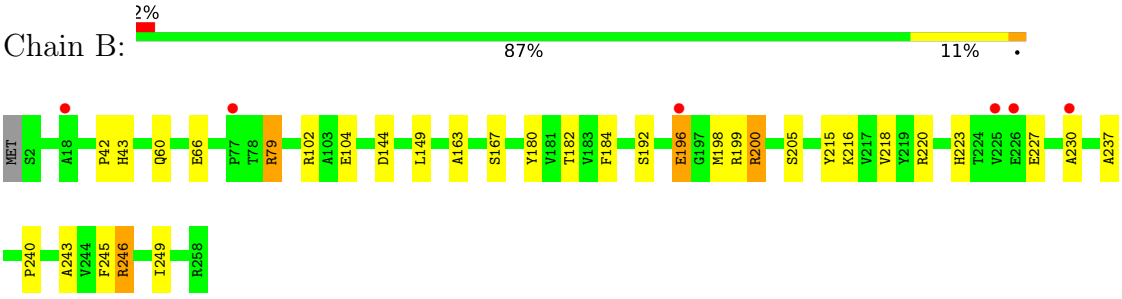
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain A:



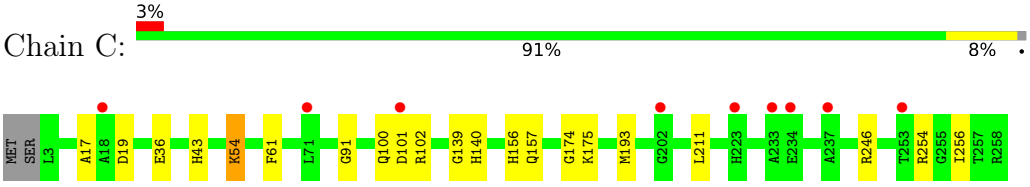
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain B:



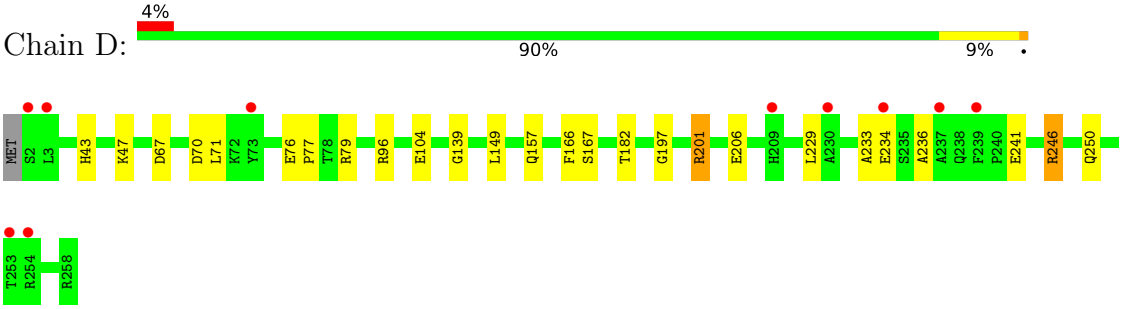
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain C:



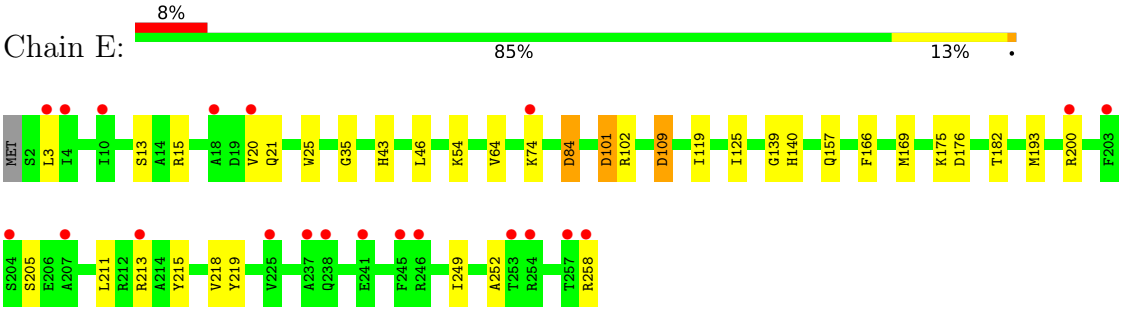
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain D:



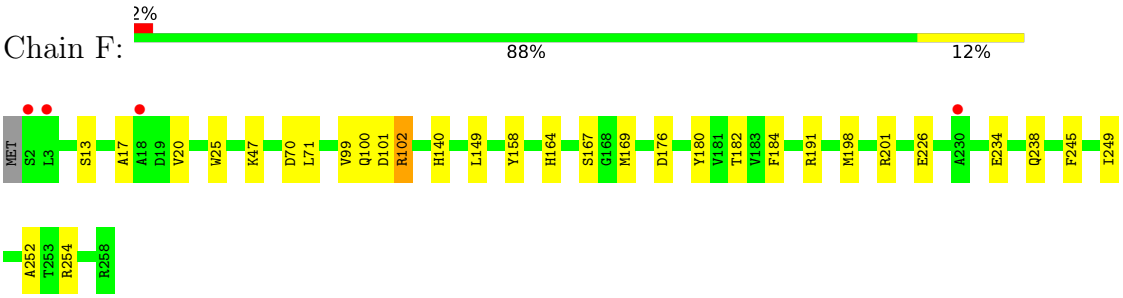
• Molecule 1: Acyl-[acyl-carrier-protein]--UDP-N-acetylglucosamine O-acyltransferase

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.10Å 82.22Å 222.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.04 – 2.00 46.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.04-2.00) 99.1 (46.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.218 0.199 , 0.222	Depositor DCC
R_{free} test set	5004 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.076 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12455	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, GOL, F9H

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	0.77	0/2025	0.91	0/2746
1	B	0.77	0/2019	0.88	0/2738
1	C	0.74	0/2013	0.89	0/2731
1	D	0.74	0/2027	0.92	0/2749
1	E	0.73	0/2008	0.90	0/2724
1	F	0.76	0/2010	0.90	0/2727
All	All	0.75	0/12102	0.90	0/16415

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

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	1983	0	1951	13	0
1	B	1977	0	1947	35	0
1	C	1970	0	1936	17	0
1	D	1984	0	1949	20	0
1	E	1966	0	1935	18	0
1	F	1968	0	1932	17	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	5	0
3	B	37	0	0	1	0
3	C	111	0	0	0	0
3	D	37	0	0	0	0
3	E	74	0	0	0	0
3	F	37	0	0	1	0
4	B	8	0	12	0	0
5	A	75	0	0	1	0
5	B	44	0	0	1	0
5	C	42	0	0	3	0
5	D	37	0	0	0	0
5	E	33	0	0	0	0
5	F	60	0	0	1	0
All	All	12455	0	11678	115	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 5.

All (115) 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:200:ARG:HB3	1:B:200:ARG:HH11	1.25	0.97
1:E:54:LYS:O	1:E:84:ASP:HB3	1.69	0.92
1:C:193:MET:HE1	1:C:211:LEU:HB3	1.55	0.87
1:B:196:GLU:O	1:B:200:ARG:HG2	1.80	0.81
1:B:79[A]:ARG:HG2	1:B:79[A]:ARG:HH11	1.46	0.80
1:B:200:ARG:HH11	1:B:200:ARG:CB	1.98	0.77
1:D:197:GLY:O	1:D:201:ARG:HD3	1.88	0.72
1:F:176:ASP:OD2	1:F:252:ALA:HA	1.89	0.72
1:C:156:HIS:NE2	5:C:401:HOH:O	2.22	0.71
1:E:84:ASP:O	1:E:109:ASP:HB3	1.93	0.69
1:B:240:PRO:O	1:B:243:ALA:HB3	1.92	0.69
1:C:36:GLU:O	1:C:54:LYS:HB3	1.94	0.67
1:D:67:ASP:OD1	1:D:96:ARG:NH2	2.26	0.67
1:F:100:GLN:OE1	1:F:100:GLN:N	2.25	0.66
1:D:79:ARG:NH2	1:D:104:GLU:OE1	2.28	0.64
1:A:15:ARG:NH2	1:A:33:GLU:OE2	2.29	0.64
1:C:102:ARG:O	1:C:102:ARG:HG2	1.98	0.63
1:C:100:GLN:OE1	1:C:100:GLN:N	2.24	0.62
1:C:19:ASP:OD1	1:C:19:ASP:N	2.32	0.62
1:D:229:LEU:HD22	1:D:250:GLN:CG	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:HB2	2:B:303:GOL:H32	1.81	0.62
1:A:68:THR:HG23	5:A:652:HOH:O	1.99	0.61
1:D:229:LEU:HD22	1:D:250:GLN:HG2	1.82	0.61
1:E:193:MET:CE	1:E:211:LEU:HB3	2.31	0.61
1:B:43:HIS:CE1	1:C:43:HIS:ND1	2.71	0.58
1:B:223:HIS:HB3	1:B:227:GLU:HB3	1.85	0.58
1:A:68:THR:HG22	1:A:70:ASP:H	1.70	0.57
1:B:79[A]:ARG:HG2	1:B:79[A]:ARG:NH1	2.20	0.56
1:F:182:THR:CG2	1:F:184:PHE:HE1	2.20	0.54
1:F:234:GLU:O	1:F:238:GLN:HG3	2.08	0.54
1:D:229:LEU:HD13	1:D:250:GLN:HG2	1.89	0.54
1:B:245:PHE:CZ	1:B:249:ILE:HD11	2.43	0.54
1:F:17:ALA:HB3	1:F:20:VAL:HG23	1.90	0.54
1:D:139:GLY:O	1:D:157:GLN:HA	2.08	0.53
1:C:17:ALA:HB1	1:C:36:GLU:HG3	1.89	0.53
1:A:43:HIS:ND1	1:C:43:HIS:CE1	2.77	0.52
1:B:200:ARG:HB3	1:B:200:ARG:NH1	2.09	0.51
1:D:229:LEU:CD2	1:D:250:GLN:HG2	2.39	0.51
1:B:220:ARG:NH2	2:B:303:GOL:O2	2.43	0.51
1:B:223:HIS:HA	1:B:227:GLU:OE2	2.11	0.51
1:F:245:PHE:CZ	1:F:249:ILE:HD11	2.46	0.51
1:A:164:HIS:ND1	1:A:201:ARG:NH2	2.59	0.51
1:B:200:ARG:HH11	1:B:200:ARG:CG	2.23	0.50
1:B:218:VAL:HG21	1:B:249:ILE:HD13	1.93	0.50
1:E:119:ILE:HD12	1:E:125:ILE:HD11	1.94	0.49
1:F:191:ARG:HH21	1:F:191:ARG:HG3	1.77	0.49
1:A:218:VAL:HG21	1:A:249:ILE:HD13	1.93	0.49
1:D:241:GLU:OE1	1:D:241:GLU:N	2.33	0.49
1:A:79:ARG:HG3	1:A:79:ARG:HH21	1.76	0.49
1:B:79[B]:ARG:CZ	1:D:250:GLN:OE1	2.60	0.49
1:C:246:ARG:HD3	5:C:405:HOH:O	2.13	0.49
1:A:164:HIS:CE1	1:A:201:ARG:HD3	2.49	0.48
1:B:66:GLU:OE1	5:B:401:HOH:O	2.20	0.48
1:B:182:THR:CG2	1:B:184:PHE:HE2	2.27	0.48
1:D:47:LYS:NZ	1:D:67:ASP:OD2	2.47	0.47
1:C:175:LYS:HE3	1:C:256:ILE:O	2.15	0.47
1:A:196:GLU:HG2	1:A:200:ARG:NH2	2.30	0.47
1:F:191:ARG:HG3	1:F:191:ARG:NH2	2.30	0.47
1:D:139:GLY:O	1:D:157:GLN:HG3	2.15	0.47
1:F:169:MET:HE2	3:F:301:F9H:F10	2.05	0.46
1:D:229:LEU:CD1	1:D:250:GLN:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ALA:HA	1:D:236:ALA:HB3	1.97	0.46
1:C:101:ASP:OD2	1:C:140:HIS:ND1	2.35	0.46
1:A:139:GLY:O	1:A:157:GLN:HA	2.15	0.46
1:C:174:GLY:O	1:C:254:ARG:NH2	2.48	0.46
1:B:237:ALA:HB2	1:E:200:ARG:HG2	1.98	0.46
1:B:220:ARG:NE	2:B:303:GOL:O2	2.46	0.46
1:A:229:LEU:O	1:A:246[A]:ARG:NH1	2.49	0.46
1:E:166:PHE:O	1:E:182:THR:HA	2.16	0.45
1:F:149:LEU:HA	1:F:167:SER:OG	2.16	0.45
1:D:246:ARG:CZ	1:D:246:ARG:HB3	2.46	0.45
1:C:102:ARG:HB3	5:C:402:HOH:O	2.17	0.45
1:B:216:LYS:HG2	2:B:303:GOL:O1	2.17	0.45
1:E:166:PHE:HB3	1:E:182:THR:HG22	1.98	0.45
1:B:149:LEU:HA	1:B:167:SER:OG	2.16	0.45
1:C:139:GLY:O	1:C:157:GLN:HA	2.17	0.45
1:F:102:ARG:H	1:F:102:ARG:HG3	1.69	0.45
1:B:180:TYR:HB3	1:B:198:MET:CE	2.46	0.44
1:B:215:TYR:HB3	2:B:303:GOL:H12	1.98	0.44
1:B:246:ARG:HH21	1:B:246:ARG:HG3	1.82	0.44
3:B:301:F9H:C37	3:B:301:F9H:C12	2.96	0.44
1:C:61:PHE:O	1:C:91:GLY:HA2	2.17	0.44
1:D:43:HIS:ND1	1:E:43:HIS:CE1	2.86	0.44
1:E:139:GLY:O	1:E:157:GLN:HA	2.18	0.44
1:B:144:ASP:HB3	1:B:163:ALA:N	2.33	0.44
1:A:79:ARG:HG3	1:A:79:ARG:NH2	2.33	0.44
1:C:100:GLN:H	1:C:100:GLN:CD	2.14	0.44
1:E:20:VAL:CG2	1:E:35:GLY:O	2.66	0.44
1:B:199:ARG:CG	1:B:199:ARG:HH21	2.31	0.43
1:D:76:GLU:CD	1:D:77:PRO:HA	2.39	0.43
1:F:180:TYR:HB3	1:F:198:MET:CE	2.48	0.43
1:D:166:PHE:HB3	1:D:182:THR:HG22	2.00	0.43
1:D:149:LEU:HA	1:D:167:SER:OG	2.18	0.43
1:A:72:LYS:HA	1:A:72:LYS:HD3	1.78	0.43
1:E:219:TYR:HE1	1:E:258:ARG:HA	1.84	0.43
1:D:76:GLU:OE2	1:D:76:GLU:HA	2.19	0.43
1:E:101:ASP:OD2	1:E:140:HIS:ND1	2.44	0.43
1:F:101:ASP:HB3	1:F:102:ARG:H	1.65	0.43
1:B:182:THR:CG2	1:B:184:PHE:CE2	3.02	0.43
1:B:42:PRO:O	1:B:60:GLN:HA	2.20	0.42
1:F:99:VAL:HG22	5:F:416:HOH:O	2.17	0.42
1:E:46:LEU:HD23	1:E:64:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ASP:OD2	1:E:252:ALA:HA	2.20	0.42
1:B:102:ARG:NH2	1:B:104:GLU:OE2	2.53	0.42
1:E:3:LEU:O	1:E:21:GLN:HA	2.20	0.42
1:E:25:TRP:HA	1:F:25:TRP:CZ2	2.55	0.41
1:B:79[A]:ARG:HH11	1:B:79[A]:ARG:CG	2.17	0.41
1:F:164:HIS:CE1	1:F:201:ARG:HD3	2.55	0.41
1:B:246:ARG:HG3	1:B:246:ARG:NH2	2.36	0.41
1:F:140:HIS:O	1:F:158:TYR:HA	2.21	0.41
1:B:79[A]:ARG:NH1	1:B:79[A]:ARG:CG	2.76	0.41
1:E:193:MET:HG2	1:E:215:TYR:CD1	2.56	0.41
1:B:180:TYR:HB3	1:B:198:MET:HE1	2.02	0.40
1:B:227:GLU:O	1:B:230:ALA:HB3	2.21	0.40
1:E:218:VAL:HG21	1:E:249:ILE:HD13	2.04	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%)	250 (97%)	7 (3%)	0	100	100
1	B	256/258 (99%)	243 (95%)	13 (5%)	0	100	100
1	C	255/258 (99%)	244 (96%)	11 (4%)	0	100	100
1	D	257/258 (100%)	246 (96%)	11 (4%)	0	100	100
1	E	255/258 (99%)	239 (94%)	16 (6%)	0	100	100
1	F	256/258 (99%)	245 (96%)	11 (4%)	0	100	100
All	All	1536/1548 (99%)	1467 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/206 (100%)	203 (98%)	4 (2%)	57	61
1	B	206/206 (100%)	200 (97%)	6 (3%)	42	43
1	C	205/206 (100%)	204 (100%)	1 (0%)	88	92
1	D	207/206 (100%)	201 (97%)	6 (3%)	42	43
1	E	205/206 (100%)	194 (95%)	11 (5%)	22	18
1	F	205/206 (100%)	198 (97%)	7 (3%)	37	36
All	All	1235/1236 (100%)	1200 (97%)	35 (3%)	43	44

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	72	LYS
1	A	74	LYS
1	A	220	ARG
1	B	79[A]	ARG
1	B	79[B]	ARG
1	B	196	GLU
1	B	200	ARG
1	B	205	SER
1	B	246	ARG
1	C	54	LYS
1	D	70	ASP
1	D	71	LEU
1	D	201	ARG
1	D	206	GLU
1	D	234	GLU
1	D	246	ARG
1	E	13	SER
1	E	15	ARG
1	E	74	LYS
1	E	84	ASP
1	E	101	ASP

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Mol	Chain	Res	Type
1	E	102	ARG
1	E	109	ASP
1	E	169	MET
1	E	175	LYS
1	E	205	SER
1	E	213	ARG
1	F	13	SER
1	F	47	LYS
1	F	70	ASP
1	F	71	LEU
1	F	102	ARG
1	F	226	GLU
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	A	140	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	F9H	E	301	-	35,41,41	3.07	11 (31%)	46,64,64	2.81	20 (43%)
4	TRS	B	302	-	7,7,7	0.43	0	9,9,9	0.92	0
3	F9H	B	301	-	35,41,41	2.60	12 (34%)	46,64,64	2.28	23 (50%)
3	F9H	C	303	-	35,41,41	2.99	12 (34%)	46,64,64	2.57	20 (43%)
3	F9H	D	301	-	35,41,41	3.24	11 (31%)	46,64,64	2.77	20 (43%)
3	F9H	C	302	-	35,41,41	3.26	10 (28%)	46,64,64	2.51	15 (32%)
3	F9H	F	301	-	35,41,41	3.02	11 (31%)	46,64,64	2.90	22 (47%)
2	GOL	A	501	-	5,5,5	0.12	0	5,5,5	0.30	0
3	F9H	E	302	-	35,41,41	3.50	12 (34%)	46,64,64	1.88	11 (23%)
3	F9H	C	301	-	35,41,41	3.04	14 (40%)	46,64,64	2.45	16 (34%)
2	GOL	B	303	-	5,5,5	0.13	0	5,5,5	0.40	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
3	F9H	E	301	-	-	2/26/59/59	0/5/5/5
4	TRS	B	302	-	-	3/9/9/9	-
3	F9H	B	301	-	-	3/26/59/59	0/5/5/5
3	F9H	C	303	-	-	2/26/59/59	0/5/5/5
3	F9H	D	301	-	-	3/26/59/59	0/5/5/5
3	F9H	C	302	-	-	3/26/59/59	0/5/5/5
3	F9H	F	301	-	-	2/26/59/59	0/5/5/5
2	GOL	A	501	-	-	0/4/4/4	-
3	F9H	E	302	-	-	2/26/59/59	0/5/5/5
3	F9H	C	301	-	-	2/26/59/59	0/5/5/5
2	GOL	B	303	-	-	2/4/4/4	-

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	F9H	C35-N29	14.37	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	F9H	C35-N29	11.51	1.48	1.35
3	C	303	F9H	C35-N29	11.43	1.48	1.35
3	F	301	F9H	C35-N29	10.80	1.47	1.35
3	C	302	F9H	C35-N29	10.72	1.47	1.35
3	C	301	F9H	C35-N29	10.37	1.47	1.35
3	E	301	F9H	C35-N29	8.74	1.45	1.35
3	B	301	F9H	C35-N29	8.58	1.45	1.35
3	D	301	F9H	O34-C35	7.31	1.47	1.35
3	C	302	F9H	O34-C35	7.16	1.47	1.35
3	F	301	F9H	O34-C35	6.91	1.46	1.35
3	E	301	F9H	O34-C35	6.91	1.46	1.35
3	C	303	F9H	O34-C35	6.39	1.45	1.35
3	E	302	F9H	O34-C35	6.37	1.45	1.35
3	E	302	F9H	C14-N13	6.29	1.52	1.39
3	C	302	F9H	C02-N13	6.29	1.46	1.36
3	C	302	F9H	C14-N13	6.18	1.51	1.39
3	D	301	F9H	C02-N13	6.10	1.46	1.36
3	E	302	F9H	C02-N13	6.08	1.46	1.36
3	E	301	F9H	C23-N22	5.99	1.46	1.38
3	C	303	F9H	C14-N13	5.56	1.50	1.39
3	C	301	F9H	C21-N22	5.49	1.48	1.35
3	C	301	F9H	C02-N13	5.30	1.45	1.36
3	F	301	F9H	C02-N13	5.14	1.44	1.36
3	F	301	F9H	C14-N13	5.09	1.49	1.39
3	D	301	F9H	C20-C15	-5.05	1.45	1.51
3	C	301	F9H	C14-N13	5.04	1.49	1.39
3	D	301	F9H	C23-N22	4.95	1.45	1.38
3	B	301	F9H	C37-N13	-4.91	1.41	1.47
3	E	301	F9H	C21-N22	4.87	1.47	1.35
3	E	301	F9H	C02-N13	4.85	1.44	1.36
3	D	301	F9H	C14-N13	4.74	1.49	1.39
3	E	301	F9H	C14-N13	4.73	1.48	1.39
3	C	301	F9H	C23-N22	4.71	1.45	1.38
3	C	302	F9H	C21-N22	4.66	1.46	1.35
3	C	301	F9H	O34-C35	4.62	1.43	1.35
3	C	302	F9H	C23-N22	4.47	1.44	1.38
3	B	301	F9H	O34-C35	4.30	1.42	1.35
3	E	301	F9H	C30-N29	-4.30	1.40	1.47
3	D	301	F9H	C37-N13	-4.26	1.42	1.47
3	E	302	F9H	C21-N22	4.15	1.45	1.35
3	B	301	F9H	C14-N13	4.10	1.47	1.39
3	F	301	F9H	C21-N22	4.05	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	F9H	C21-N22	4.02	1.45	1.35
3	F	301	F9H	C23-N22	4.00	1.44	1.38
3	C	302	F9H	C03-C02	3.99	1.56	1.50
3	C	301	F9H	C30-N29	-3.95	1.41	1.47
3	B	301	F9H	C21-N22	3.94	1.45	1.35
3	C	303	F9H	C02-N13	3.93	1.42	1.36
3	E	301	F9H	O34-C31	-3.81	1.41	1.50
3	C	302	F9H	C20-C15	-3.74	1.46	1.51
3	D	301	F9H	C21-N22	3.62	1.44	1.35
3	E	302	F9H	C23-N22	3.59	1.43	1.38
3	F	301	F9H	C20-C15	-3.44	1.47	1.51
3	B	301	F9H	C30-N29	-3.40	1.42	1.47
3	C	302	F9H	C08-C07	3.37	1.57	1.49
3	E	302	F9H	O34-C31	-3.36	1.42	1.50
3	F	301	F9H	C30-N29	-3.30	1.42	1.47
3	E	301	F9H	C16-C15	3.30	1.43	1.39
3	B	301	F9H	O34-C31	-3.30	1.43	1.50
3	C	301	F9H	C12-C03	3.28	1.44	1.39
3	E	301	F9H	C37-N13	-3.22	1.43	1.47
3	B	301	F9H	O36-C35	-3.20	1.16	1.21
3	B	301	F9H	C02-N13	3.14	1.41	1.36
3	C	301	F9H	C20-C15	-3.14	1.47	1.51
3	C	302	F9H	O34-C31	-3.03	1.43	1.50
3	B	301	F9H	C20-C15	-2.98	1.47	1.51
3	D	301	F9H	C30-N29	-2.93	1.43	1.47
3	C	303	F9H	C04-C03	-2.80	1.34	1.39
3	C	301	F9H	N27-N26	2.76	1.39	1.34
3	E	302	F9H	C20-C15	-2.72	1.48	1.51
3	C	301	F9H	O34-C31	-2.71	1.44	1.50
3	C	301	F9H	C37-N13	-2.71	1.44	1.47
3	F	301	F9H	O34-C31	-2.69	1.44	1.50
3	C	303	F9H	C23-N22	2.67	1.42	1.38
3	B	301	F9H	O01-C02	-2.66	1.17	1.22
3	E	302	F9H	C30-N29	-2.66	1.43	1.47
3	C	303	F9H	O34-C31	-2.65	1.44	1.50
3	E	302	F9H	C03-C02	2.60	1.54	1.50
3	B	301	F9H	N24-N25	2.54	1.38	1.34
3	E	302	F9H	C16-C15	2.54	1.42	1.39
3	F	301	F9H	C19-C14	2.49	1.43	1.39
3	C	303	F9H	C30-N29	-2.45	1.43	1.47
3	C	303	F9H	C16-C15	2.37	1.42	1.39
3	C	301	F9H	N24-N25	2.33	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	F9H	C12-C03	2.33	1.42	1.39
3	C	303	F9H	C12-C03	2.31	1.42	1.39
3	F	301	F9H	C16-C15	2.15	1.42	1.39
3	C	303	F9H	C37-N13	-2.14	1.45	1.47
3	E	302	F9H	C19-C14	2.12	1.43	1.39
3	C	301	F9H	C19-C14	2.10	1.43	1.39
3	D	301	F9H	C19-C14	2.07	1.43	1.39
3	E	301	F9H	C19-C14	2.02	1.43	1.39

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	301	F9H	O34-C35-N29	-8.41	103.92	109.82
3	C	301	F9H	O34-C35-N29	-7.57	104.52	109.82
3	D	301	F9H	O34-C35-N29	-6.40	105.33	109.82
3	C	302	F9H	C03-C02-N13	6.27	128.61	118.36
3	C	302	F9H	O34-C35-N29	-6.23	105.45	109.82
3	D	301	F9H	N27-N26-N25	-6.23	105.46	109.53
3	E	301	F9H	C15-C20-C21	-6.18	92.92	109.49
3	F	301	F9H	O34-C35-N29	-6.18	105.49	109.82
3	F	301	F9H	F09-C08-C07	-6.14	99.43	112.93
3	D	301	F9H	O34-C35-O36	6.14	129.55	122.46
3	F	301	F9H	C03-C02-N13	5.98	128.14	118.36
3	F	301	F9H	C15-C14-N13	-5.98	105.89	109.76
3	C	302	F9H	O01-C02-N13	-5.82	113.98	121.69
3	C	303	F9H	F10-C08-C07	-5.70	100.41	112.93
3	E	302	F9H	C16-C15-C20	5.62	139.56	130.13
3	B	301	F9H	C37-C20-C21	-5.54	92.01	110.00
3	C	303	F9H	N24-N25-N26	-5.45	105.97	109.53
3	F	301	F9H	C20-N29-C35	5.34	129.86	121.29
3	C	302	F9H	O34-C35-O36	5.25	128.51	122.46
3	E	301	F9H	O34-C35-O36	5.22	128.48	122.46
3	D	301	F9H	C03-C02-N13	5.21	126.88	118.36
3	C	301	F9H	O34-C35-O36	5.17	128.43	122.46
3	C	301	F9H	C15-C20-C21	-5.02	96.04	109.49
3	C	303	F9H	O34-C35-N29	-4.89	106.39	109.82
3	E	302	F9H	C15-C14-N13	-4.84	106.63	109.76
3	E	301	F9H	C37-C20-C21	-4.80	94.42	110.00
3	D	301	F9H	C19-C14-C15	-4.69	117.08	121.76
3	E	301	F9H	C19-C14-C15	-4.67	117.10	121.76
3	C	303	F9H	C15-C20-C21	-4.67	96.99	109.49
3	C	302	F9H	C15-C14-N13	-4.62	106.77	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	F9H	C16-C15-C20	4.62	137.88	130.13
3	C	301	F9H	C19-C14-C15	-4.59	117.18	121.76
3	D	301	F9H	C37-C20-C21	-4.58	95.14	110.00
3	C	303	F9H	C19-C14-C15	-4.54	117.23	121.76
3	C	303	F9H	C20-N29-C35	4.51	128.53	121.29
3	E	301	F9H	C20-N29-C35	4.51	128.52	121.29
3	C	303	F9H	C37-C20-C21	-4.25	96.21	110.00
3	E	301	F9H	C16-C15-C14	4.20	123.77	120.01
3	F	301	F9H	N24-N25-N26	-4.19	106.80	109.53
3	F	301	F9H	C12-C03-C02	-4.19	110.80	120.14
3	D	301	F9H	O01-C02-C03	-4.11	112.23	120.23
3	B	301	F9H	C03-C02-N13	4.02	124.94	118.36
3	B	301	F9H	C15-C20-C21	-4.02	98.72	109.49
3	F	301	F9H	C15-C20-C21	-4.00	98.77	109.49
3	C	303	F9H	C12-C07-C08	3.99	124.97	119.58
3	E	302	F9H	C20-N29-C35	3.94	127.62	121.29
3	C	301	F9H	C37-C20-C21	-3.91	97.30	110.00
3	F	301	F9H	C19-C14-C15	-3.89	117.88	121.76
3	C	303	F9H	C03-C02-N13	3.88	124.70	118.36
3	C	302	F9H	N27-N26-N25	-3.83	107.03	109.53
3	E	301	F9H	C12-C03-C02	-3.81	111.65	120.14
3	D	301	F9H	C12-C03-C02	-3.78	111.71	120.14
3	B	301	F9H	C19-C14-C15	-3.77	118.00	121.76
3	F	301	F9H	O01-C02-N13	-3.76	116.71	121.69
3	E	301	F9H	C04-C03-C02	3.66	129.55	120.29
3	D	301	F9H	C15-C20-C21	-3.57	99.92	109.49
3	C	301	F9H	C15-C20-N29	3.57	117.75	110.79
3	D	301	F9H	F10-C08-C07	-3.56	105.12	112.93
3	C	303	F9H	C12-C03-C02	-3.55	112.22	120.14
3	F	301	F9H	C33-C31-C30	-3.52	106.88	112.18
3	E	301	F9H	O01-C02-N13	-3.49	117.07	121.69
3	F	301	F9H	C15-C20-N29	3.31	117.25	110.79
3	C	303	F9H	C16-C15-C20	3.30	135.66	130.13
3	C	301	F9H	C12-C03-C02	-3.29	112.79	120.14
3	C	301	F9H	N24-N25-N26	-3.28	107.39	109.53
3	B	301	F9H	O34-C35-O36	3.24	126.20	122.46
3	B	301	F9H	O01-C02-N13	-3.24	117.41	121.69
3	E	302	F9H	N27-N26-N25	-3.24	107.42	109.53
3	C	301	F9H	O34-C31-C32	3.23	113.09	106.35
3	E	301	F9H	C15-C20-N29	3.22	117.08	110.79
3	B	301	F9H	C32-C31-C30	3.22	117.02	112.18
3	E	301	F9H	C32-C31-C30	-3.21	107.34	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	301	F9H	C05-C06-C07	-3.21	117.39	120.76
3	C	301	F9H	C12-C07-C08	3.21	123.91	119.58
3	D	301	F9H	C05-C04-C03	-3.19	116.57	120.34
3	D	301	F9H	C16-C15-C20	3.18	135.47	130.13
3	E	302	F9H	O01-C02-N13	-3.18	117.48	121.69
3	F	301	F9H	C04-C03-C02	3.16	128.28	120.29
3	C	303	F9H	O34-C35-O36	3.15	126.09	122.46
3	E	302	F9H	C15-C20-N29	-3.12	104.71	110.79
3	C	301	F9H	C03-C02-N13	3.11	123.44	118.36
3	D	301	F9H	C15-C20-N29	3.09	116.82	110.79
3	D	301	F9H	C06-C05-C04	3.06	124.59	120.25
3	D	301	F9H	O34-C31-C33	3.05	112.70	106.35
3	E	301	F9H	N27-N26-N25	-3.00	107.57	109.53
3	B	301	F9H	C12-C03-C02	-2.99	113.46	120.14
3	E	301	F9H	F10-C08-C07	-2.97	106.40	112.93
3	E	301	F9H	C16-C15-C20	2.96	135.09	130.13
3	F	301	F9H	O01-C02-C03	-2.96	114.48	120.23
3	C	302	F9H	O28-C21-N22	-2.95	116.05	123.23
3	D	301	F9H	C04-C03-C02	2.94	127.73	120.29
3	C	302	F9H	C30-N29-C20	2.93	129.12	119.71
3	C	301	F9H	C16-C15-C20	2.92	135.03	130.13
3	B	301	F9H	F10-C08-C07	-2.91	106.55	112.93
3	B	301	F9H	O36-C35-N29	-2.89	124.75	128.22
3	C	302	F9H	C16-C15-C14	2.89	122.60	120.01
3	C	302	F9H	C37-C20-C21	-2.88	100.65	110.00
3	E	301	F9H	C03-C02-N13	2.84	123.01	118.36
3	F	301	F9H	O34-C35-O36	2.84	125.73	122.46
3	E	302	F9H	C37-C20-C21	-2.83	100.82	110.00
3	C	303	F9H	C32-C31-C30	-2.82	107.94	112.18
3	B	301	F9H	N24-N25-N26	-2.81	107.70	109.53
3	E	302	F9H	C30-N29-C20	2.80	128.72	119.71
3	F	301	F9H	C16-C15-C20	2.80	134.82	130.13
3	C	302	F9H	O28-C21-C20	2.79	123.38	119.30
3	B	301	F9H	C05-C06-C07	-2.77	117.84	120.76
3	E	301	F9H	F11-C08-C07	-2.75	106.89	112.93
3	C	303	F9H	O01-C02-C03	-2.69	115.00	120.23
3	C	301	F9H	O01-C02-N13	-2.67	118.15	121.69
3	B	301	F9H	C04-C03-C02	2.63	126.94	120.29
3	D	301	F9H	C33-C31-C30	-2.62	108.23	112.18
3	B	301	F9H	C04-C03-C12	-2.62	116.14	119.24
3	B	301	F9H	N27-N26-N25	-2.59	107.84	109.53
3	D	301	F9H	O36-C35-N29	-2.58	125.12	128.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	301	F9H	F11-C08-C07	-2.57	107.29	112.93
3	B	301	F9H	O34-C31-C33	2.55	111.66	106.35
3	C	301	F9H	C20-N29-C35	2.55	125.38	121.29
3	C	303	F9H	C05-C04-C03	-2.53	117.35	120.34
3	C	303	F9H	C06-C07-C08	-2.49	116.00	119.97
3	B	301	F9H	C30-N29-C20	2.49	127.71	119.71
3	B	301	F9H	C33-C31-C32	-2.47	105.18	110.25
3	C	303	F9H	C15-C20-N29	2.45	115.58	110.79
3	D	301	F9H	C20-N29-C35	2.45	125.22	121.29
3	C	301	F9H	C04-C03-C02	2.43	126.45	120.29
3	E	302	F9H	C03-C02-N13	2.43	122.32	118.36
3	C	301	F9H	F10-C08-C07	-2.40	107.67	112.93
3	B	301	F9H	C12-C07-C08	2.39	122.81	119.58
3	E	301	F9H	C05-C06-C07	-2.37	118.27	120.76
3	C	302	F9H	C12-C07-C08	2.36	122.77	119.58
3	F	301	F9H	C16-C15-C14	2.35	122.12	120.01
3	B	301	F9H	C15-C20-N29	2.35	115.37	110.79
3	F	301	F9H	F11-C08-F09	2.33	114.25	105.72
3	F	301	F9H	O28-C21-C20	2.32	122.69	119.30
3	E	301	F9H	C06-C05-C04	2.30	123.51	120.25
3	D	301	F9H	C12-C07-C08	2.28	122.66	119.58
3	E	302	F9H	O28-C21-C20	2.27	122.62	119.30
3	C	302	F9H	C37-N13-C02	2.26	130.79	123.01
3	B	301	F9H	O01-C02-C03	-2.22	115.91	120.23
3	E	301	F9H	O34-C31-C32	2.21	110.95	106.35
3	C	303	F9H	O01-C02-N13	-2.17	118.82	121.69
3	B	301	F9H	C06-C05-C04	2.06	123.18	120.25
3	C	303	F9H	C15-C14-N13	-2.06	108.42	109.76
3	E	302	F9H	F10-C08-C07	-2.06	108.40	112.93
3	C	303	F9H	F09-C08-C07	2.06	117.45	112.93
3	C	302	F9H	C19-C14-C15	-2.04	119.73	121.76
3	F	301	F9H	C06-C05-C04	2.01	123.10	120.25
3	B	301	F9H	O28-C21-C20	2.00	122.23	119.30

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	F9H	C15-C20-N29-C30
3	B	301	F9H	C37-C20-N29-C35
3	C	301	F9H	C15-C20-N29-C30
3	C	302	F9H	C15-C20-N29-C30

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Mol	Chain	Res	Type	Atoms
3	C	302	F9H	C21-C20-N29-C35
3	C	303	F9H	C15-C20-N29-C30
3	C	303	F9H	C37-C20-N29-C35
3	D	301	F9H	C15-C20-N29-C30
3	E	301	F9H	C15-C20-N29-C30
3	F	301	F9H	C15-C20-N29-C30
4	B	302	TRS	C1-C-C3-O3
2	B	303	GOL	O1-C1-C2-O2
3	C	302	F9H	C15-C20-N29-C35
3	E	302	F9H	C15-C20-N29-C35
3	E	302	F9H	C15-C20-N29-C30
4	B	302	TRS	N-C-C3-O3
2	B	303	GOL	O1-C1-C2-C3
4	B	302	TRS	C2-C-C3-O3
3	C	301	F9H	C37-C20-N29-C35
3	D	301	F9H	C37-C20-N29-C35
3	E	301	F9H	C37-C20-N29-C35
3	F	301	F9H	C37-C20-N29-C35
3	B	301	F9H	O01-C02-N13-C37
3	D	301	F9H	O01-C02-N13-C37

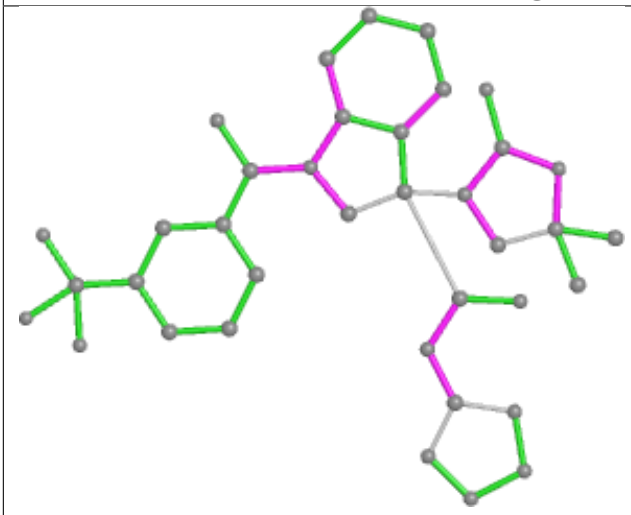
There are no ring outliers.

3 monomers are involved in 7 short contacts:

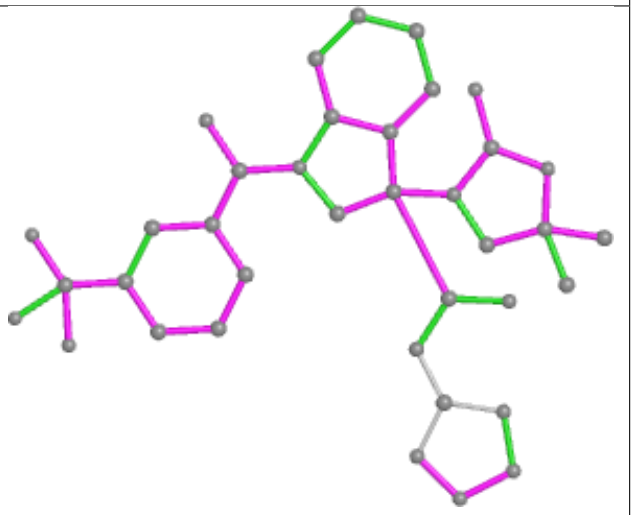
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	F9H	1	0
3	F	301	F9H	1	0
2	B	303	GOL	5	0

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

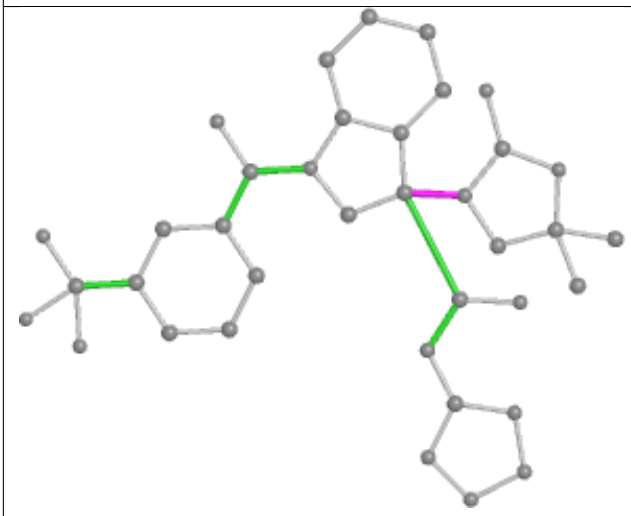
Ligand F9H E 301



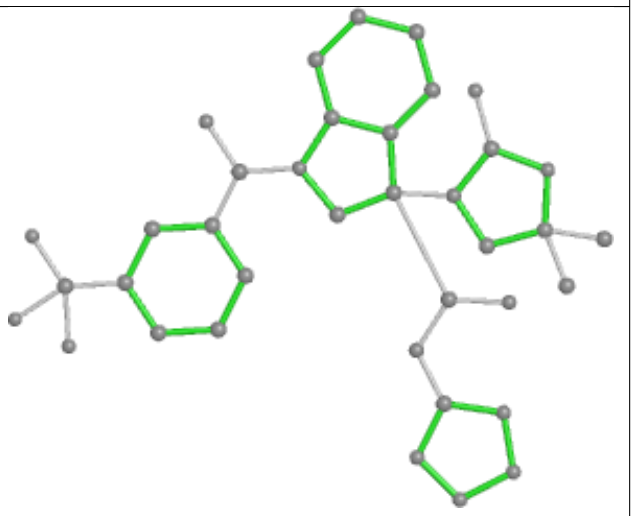
Bond lengths



Bond angles

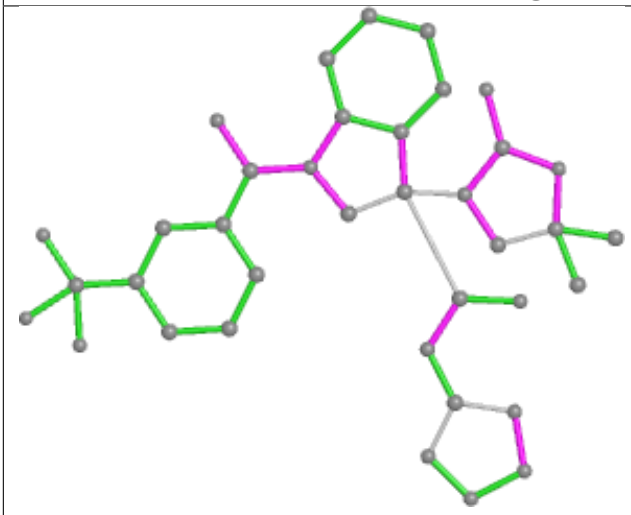


Torsions

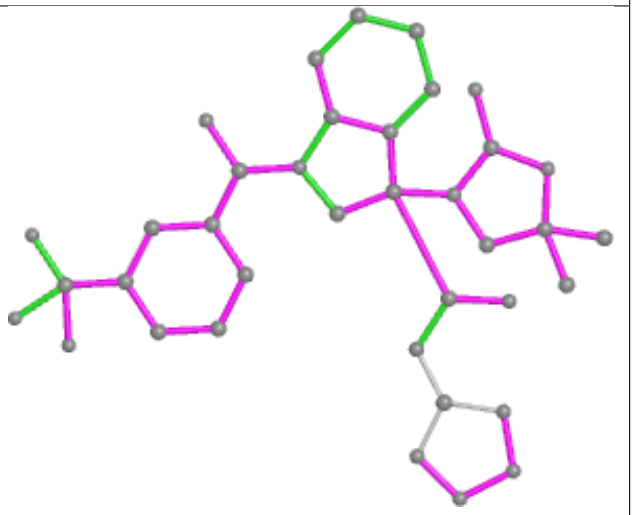


Rings

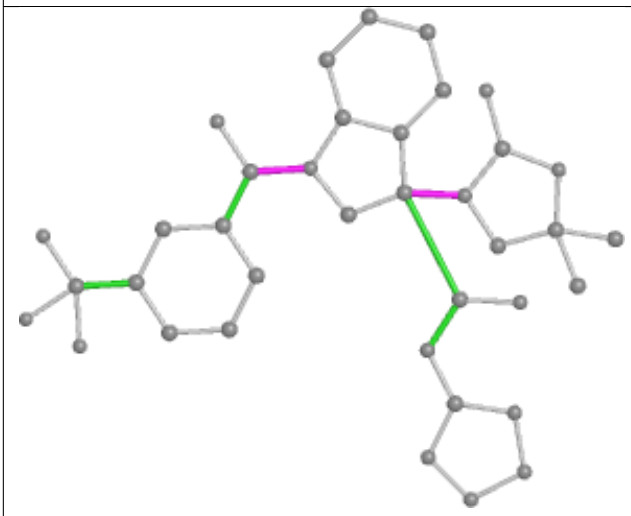
Ligand F9H B 301



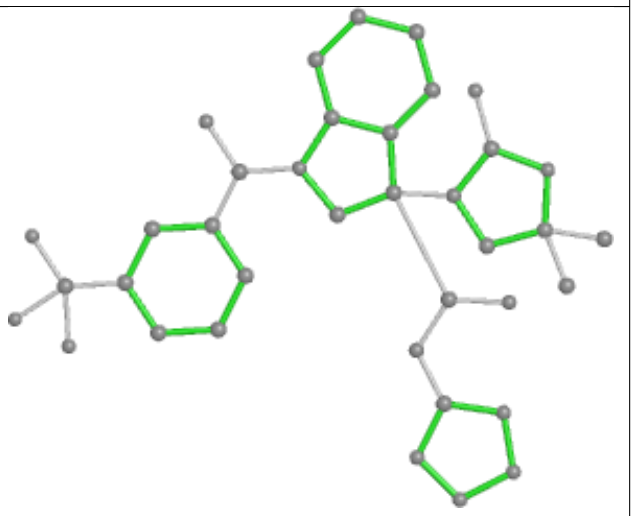
Bond lengths



Bond angles

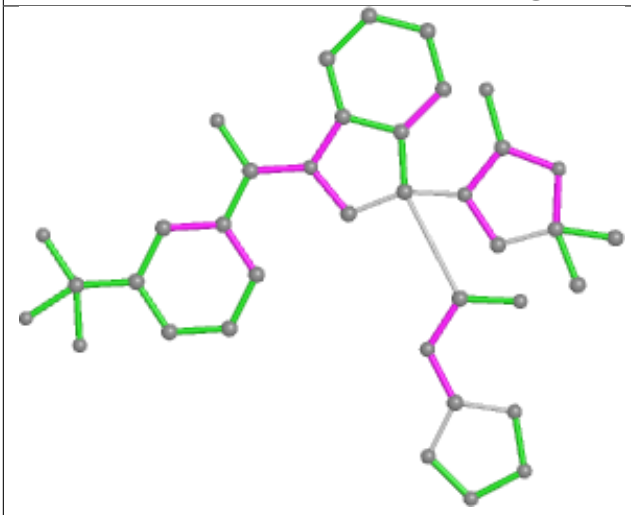


Torsions

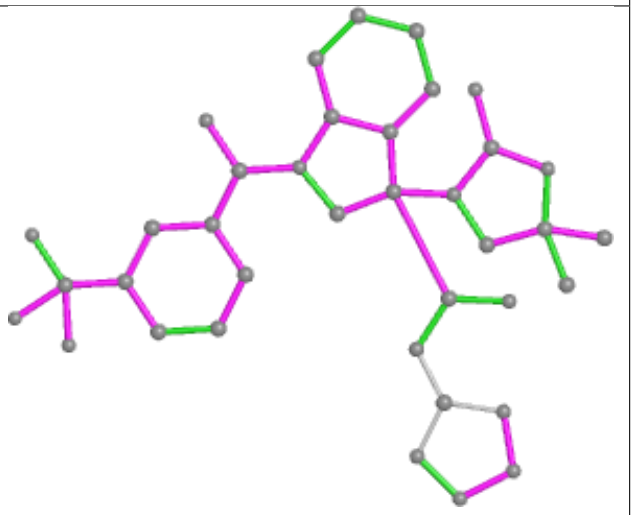


Rings

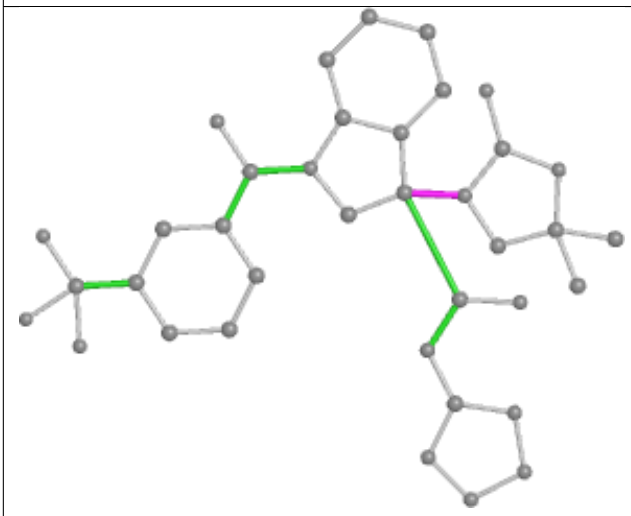
Ligand F9H C 303



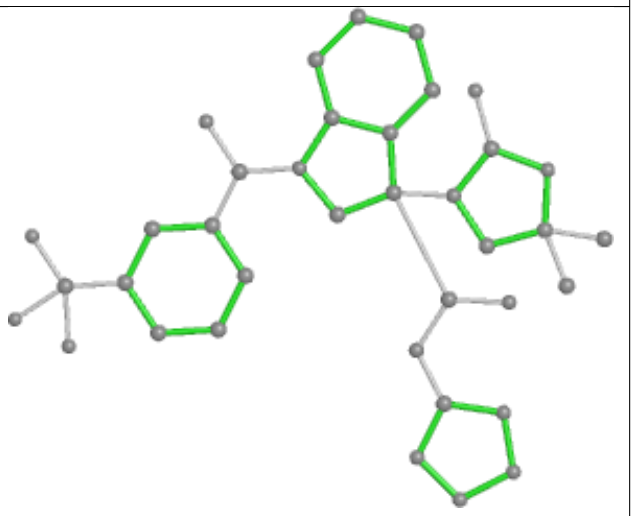
Bond lengths



Bond angles

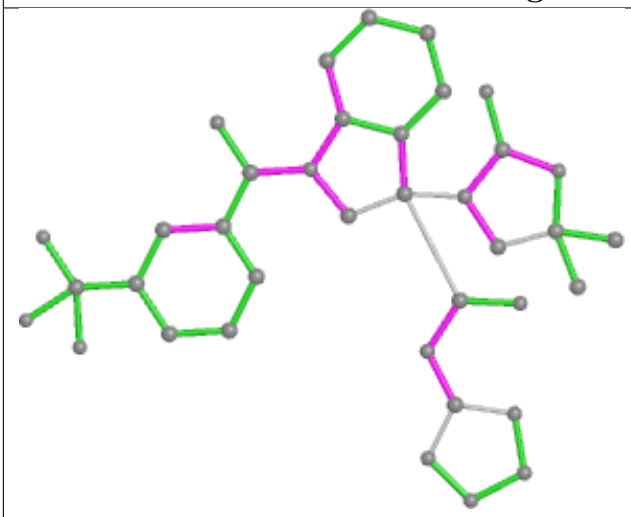


Torsions



Rings

Ligand F9H D 301



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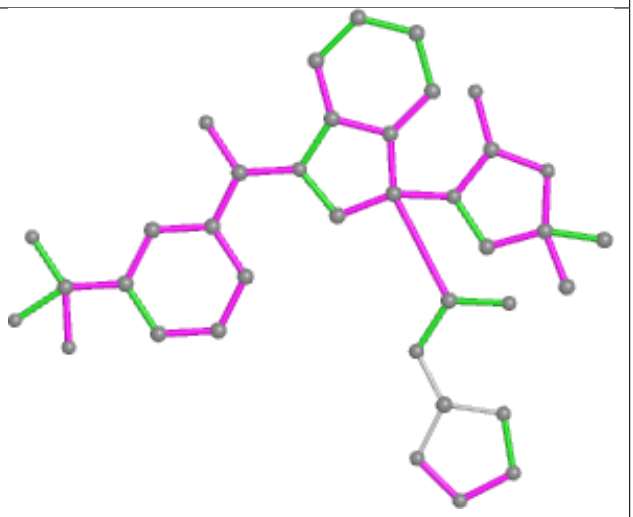
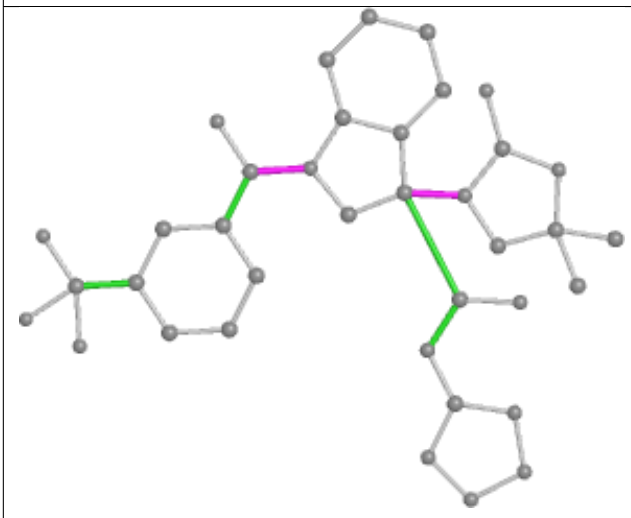


Bond angles



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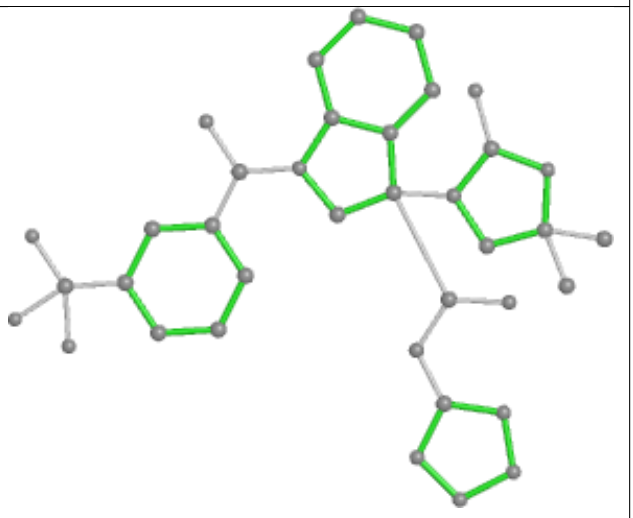
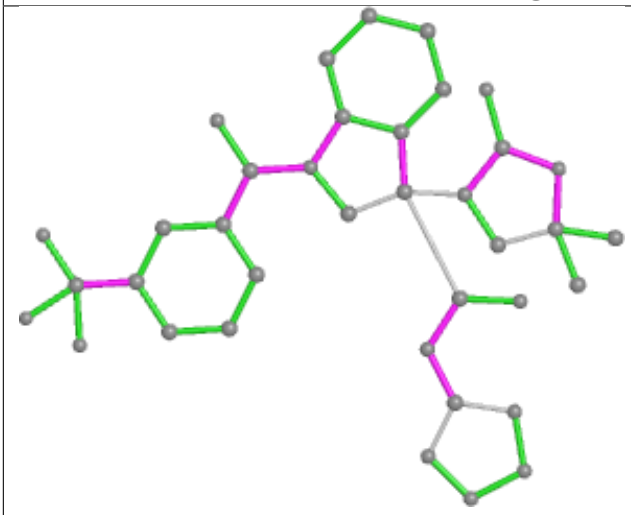


Rings

Ligand F9H C 302



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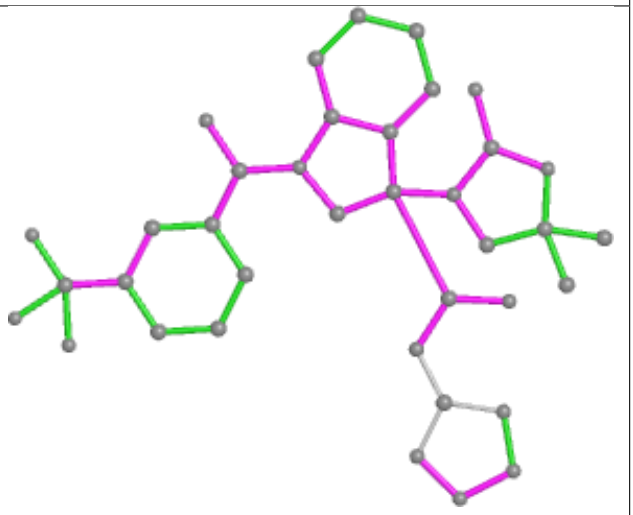
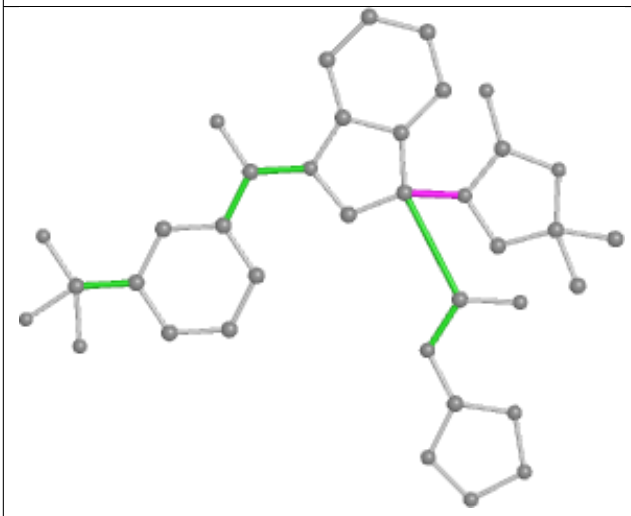
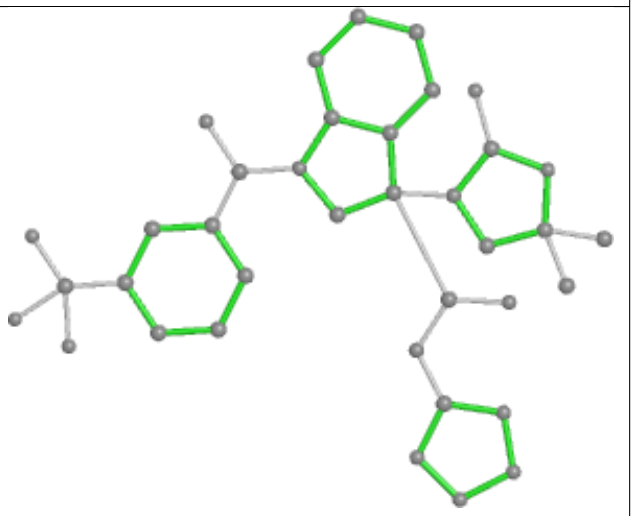


Bond angles

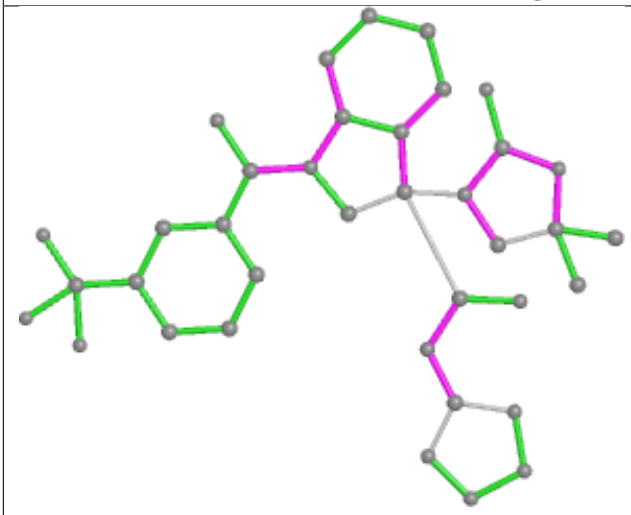


Torsions



Rings

Ligand F9H F 301



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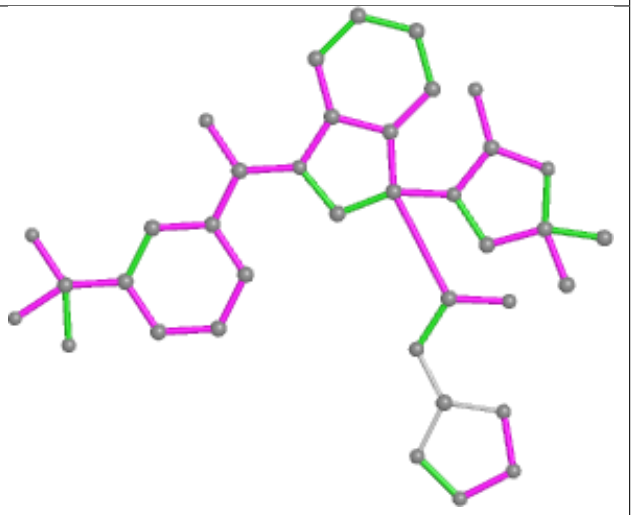
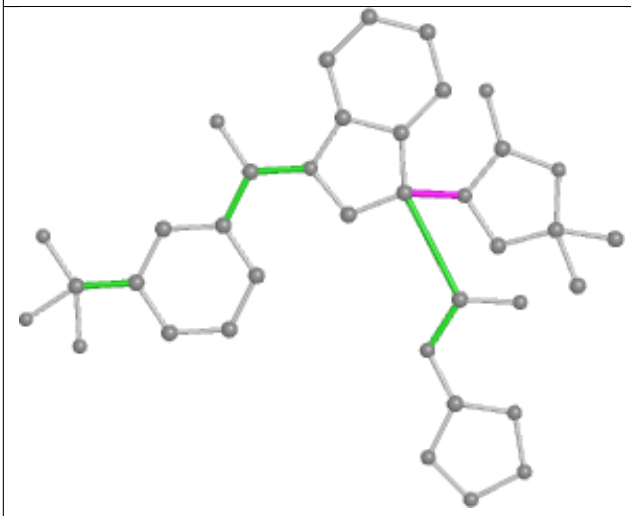


Bond angles



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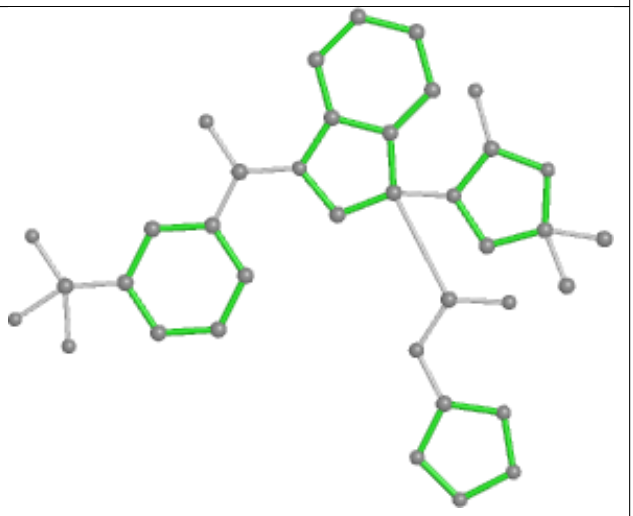
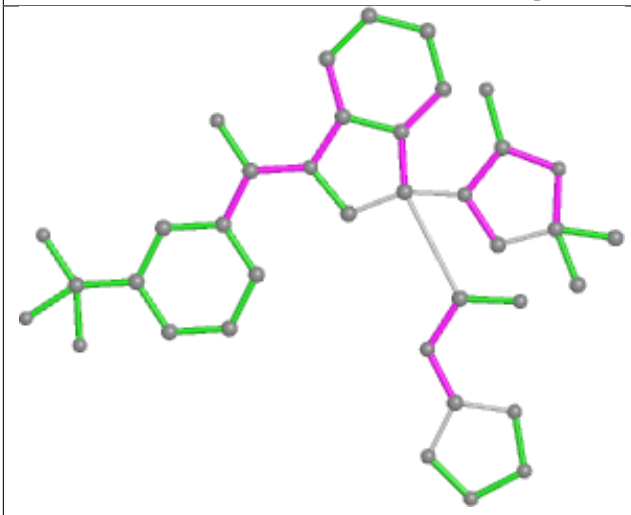
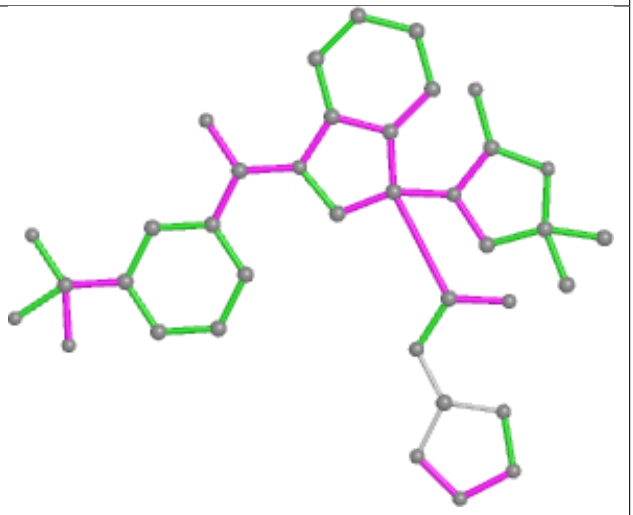


Rings

Ligand F9H E 302



Bond lengths



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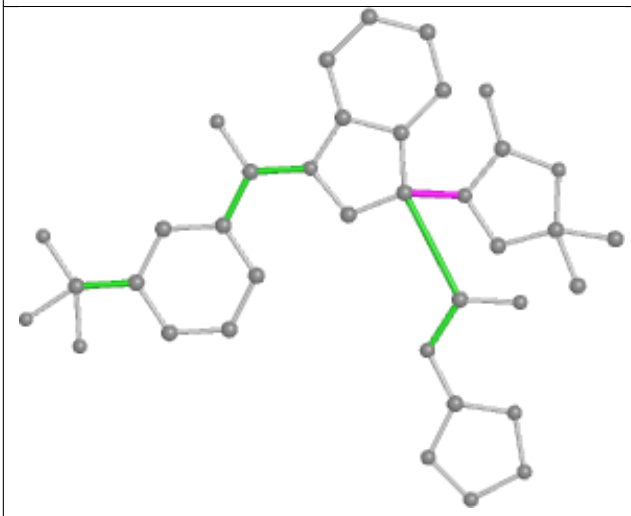

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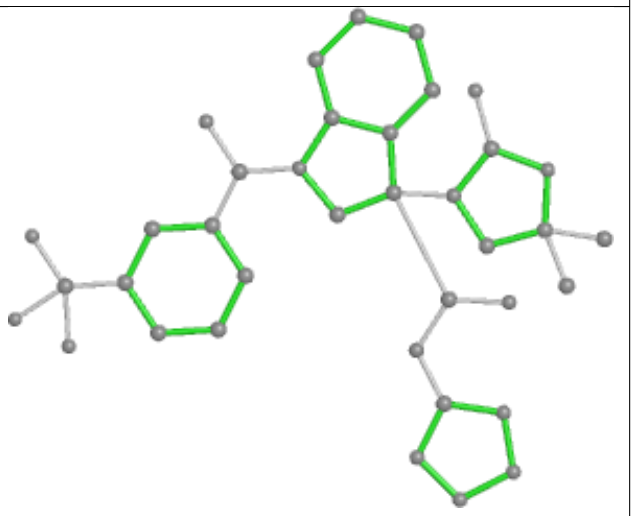
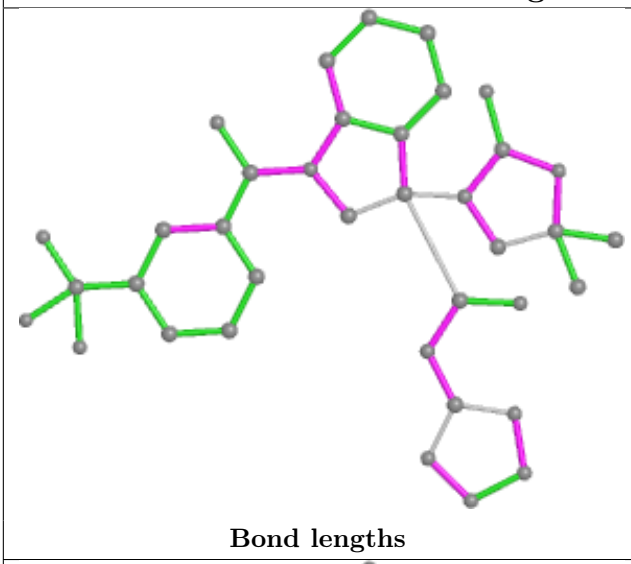


Rings

Ligand F9H C 301



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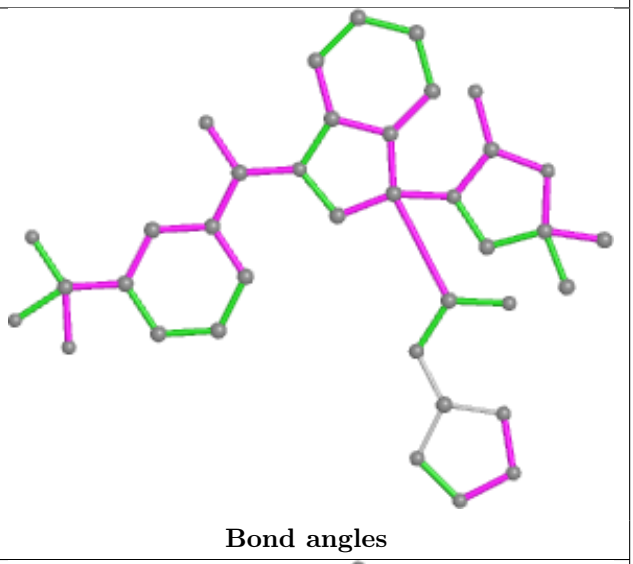

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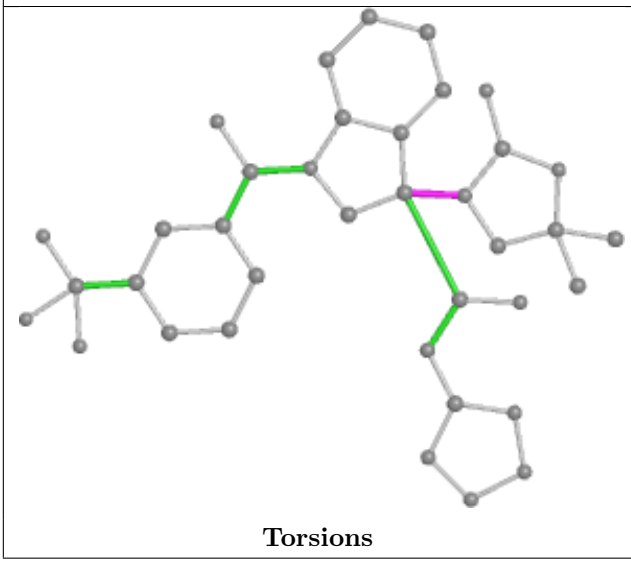
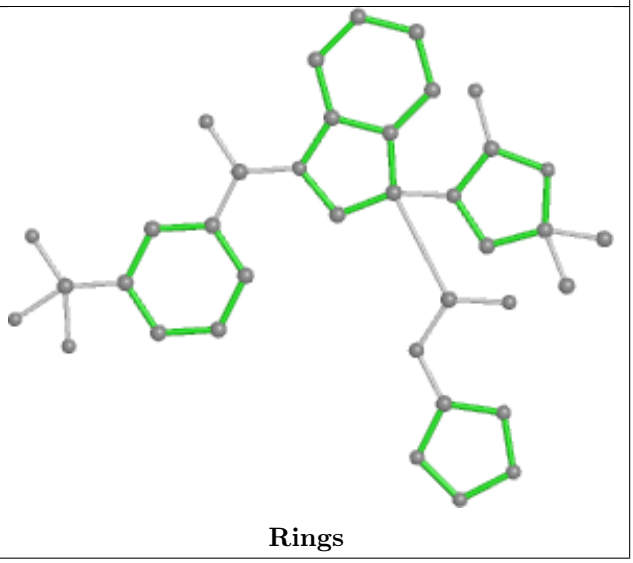


Torsions



Rings

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, 95^{th} 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%)	-0.07	1 (0%)	92	92	22, 35, 67, 87	0
1	B	257/258 (99%)	0.15	6 (2%)	60	59	25, 41, 70, 95	0
1	C	256/258 (99%)	0.24	9 (3%)	44	43	24, 44, 74, 97	0
1	D	257/258 (99%)	0.25	10 (3%)	39	38	22, 41, 82, 98	0
1	E	257/258 (99%)	0.55	21 (8%)	11	11	25, 52, 87, 114	0
1	F	257/258 (99%)	0.16	4 (1%)	72	70	22, 40, 69, 92	0
All	All	1541/1548 (99%)	0.21	51 (3%)	46	45	22, 42, 76, 114	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	18	ALA	6.3
1	D	253	THR	4.4
1	E	254	ARG	4.3
1	D	230	ALA	4.1
1	E	20	VAL	3.9
1	E	203	PHE	3.9
1	E	253	THR	3.9
1	D	209	HIS	3.6
1	E	200	ARG	3.4
1	C	253	THR	3.4
1	B	230	ALA	3.3
1	F	18	ALA	3.1
1	E	213	ARG	3.1
1	B	18	ALA	3.1
1	C	237	ALA	3.0
1	E	237	ALA	3.0
1	D	237	ALA	2.9
1	E	204	SER	2.6
1	C	71	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	230	ALA	2.6
1	D	3	LEU	2.6
1	D	239	PHE	2.5
1	E	246	ARG	2.5
1	E	257	THR	2.4
1	E	241	GLU	2.4
1	E	207	ALA	2.4
1	D	234	GLU	2.3
1	B	196	GLU	2.3
1	E	258	ARG	2.3
1	E	225	VAL	2.3
1	E	3	LEU	2.3
1	C	202	GLY	2.3
1	E	10	ILE	2.3
1	E	74	LYS	2.3
1	A	73	TYR	2.3
1	D	73	TYR	2.3
1	C	234	GLU	2.3
1	B	225	VAL	2.3
1	E	4	ILE	2.2
1	E	245	PHE	2.2
1	C	18	ALA	2.2
1	D	2	SER	2.2
1	D	254	ARG	2.2
1	F	3	LEU	2.1
1	B	77	PRO	2.1
1	C	101	ASP	2.1
1	B	226	GLU	2.0
1	C	223	HIS	2.0
1	E	238	GLN	2.0
1	F	2	SER	2.0
1	C	233	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

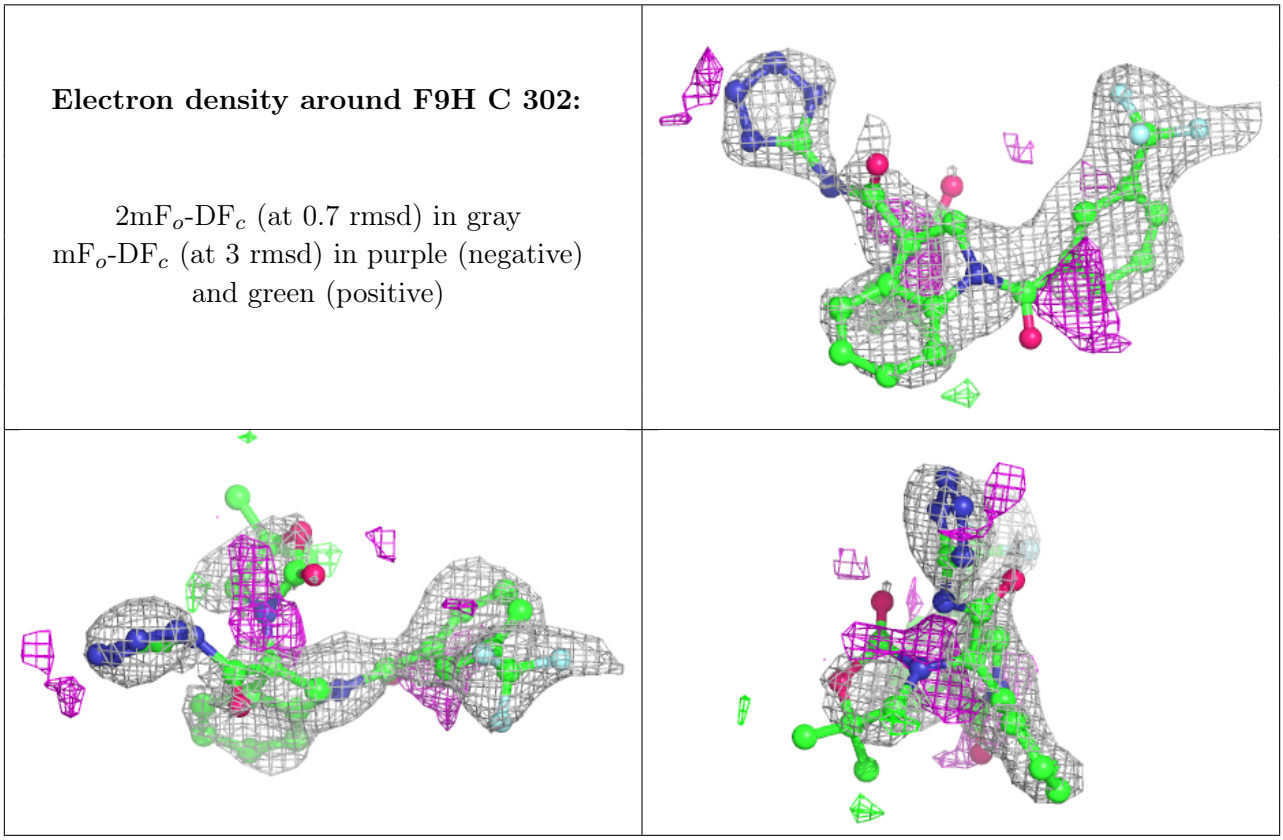
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	303	6/6	0.70	0.33	54,57,59,62	0
4	TRS	B	302	8/8	0.74	0.37	59,67,71,71	0
3	F9H	C	302	37/37	0.76	0.32	60,82,102,105	0
3	F9H	E	302	37/37	0.86	0.24	44,51,68,72	37
2	GOL	A	501	6/6	0.90	0.20	64,71,77,83	0
3	F9H	F	301	37/37	0.92	0.15	42,53,59,70	0
3	F9H	C	303	37/37	0.92	0.16	44,59,66,68	0
3	F9H	E	301	37/37	0.93	0.12	40,47,54,61	0
3	F9H	C	301	37/37	0.94	0.12	35,41,48,52	0
3	F9H	B	301	37/37	0.95	0.11	31,37,45,46	0
3	F9H	D	301	37/37	0.95	0.11	30,40,47,50	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.

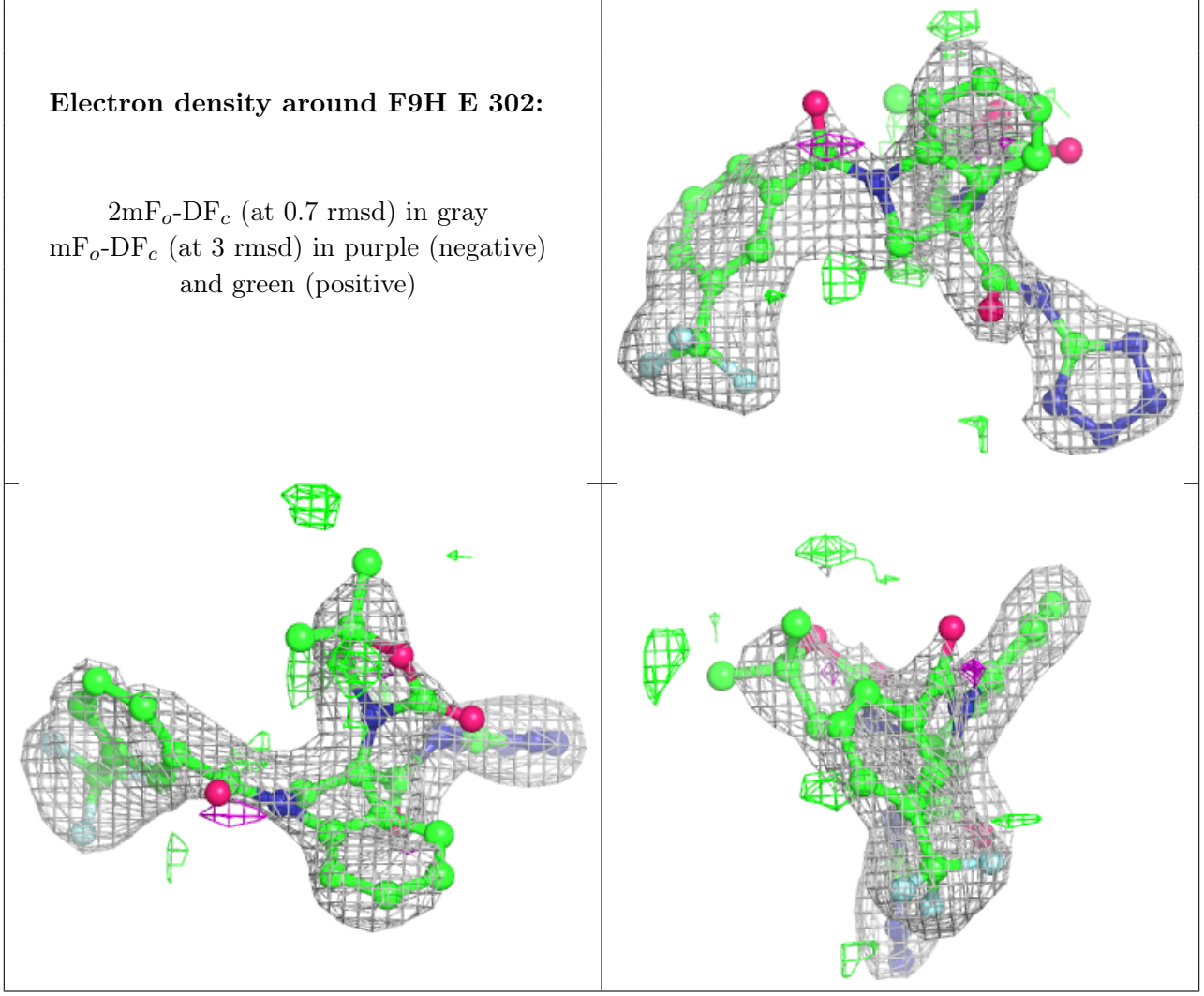
Electron density around F9H C 302:

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



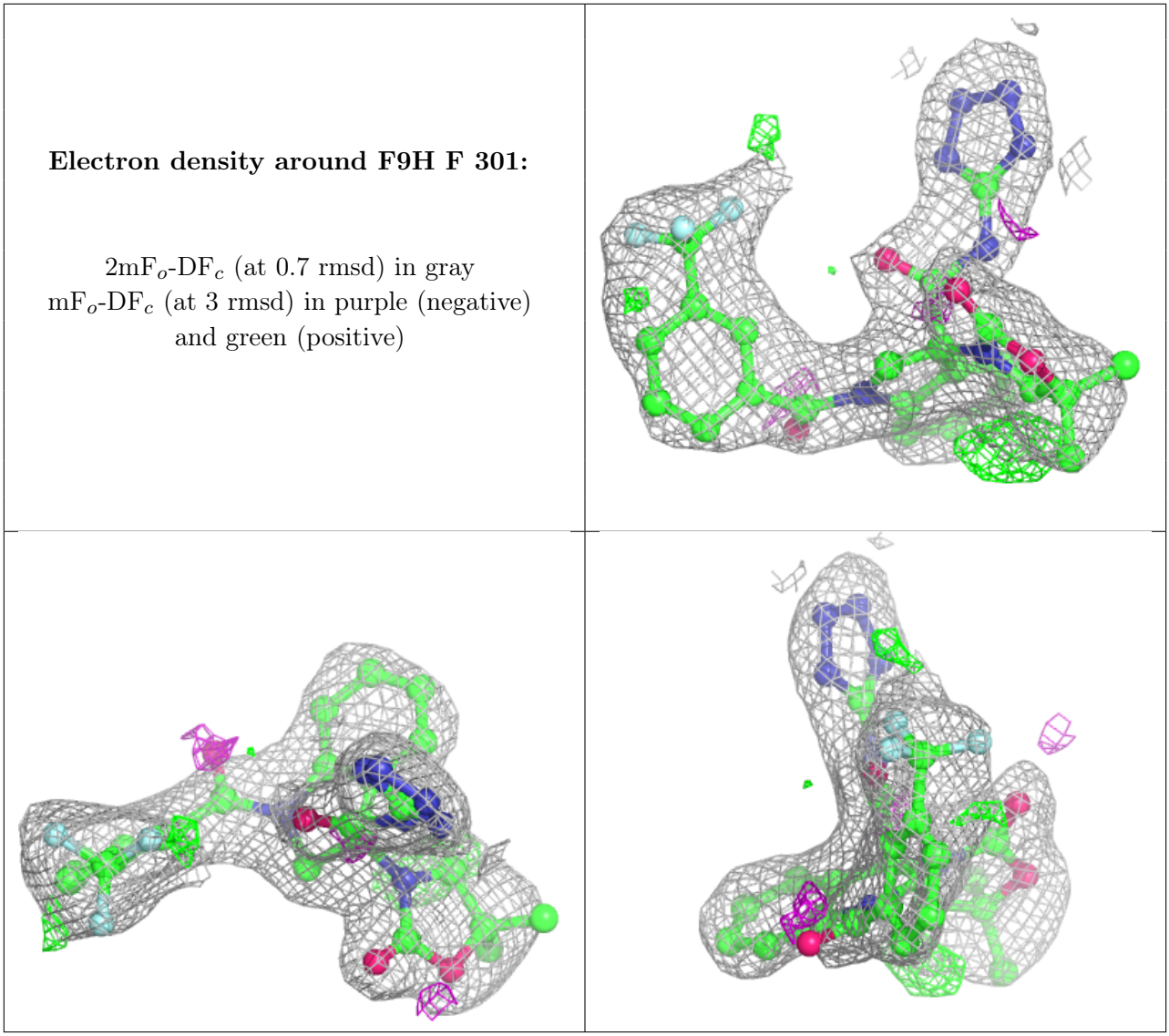
Electron density around F9H E 302:

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



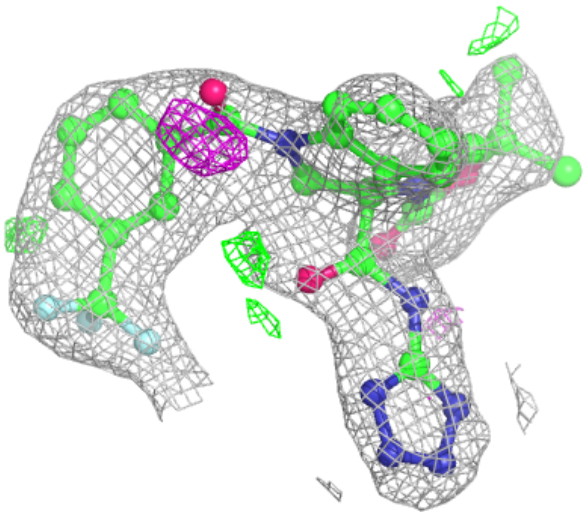
Electron density around F9H F 301:

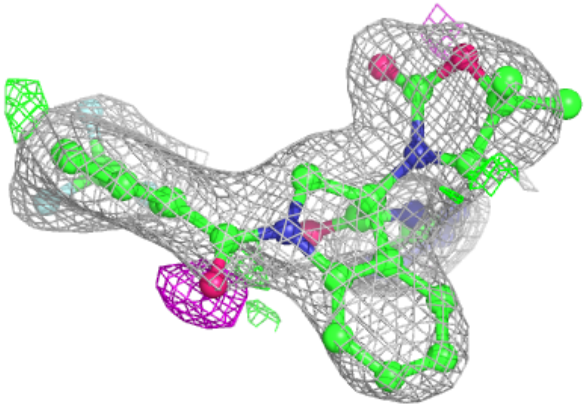
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

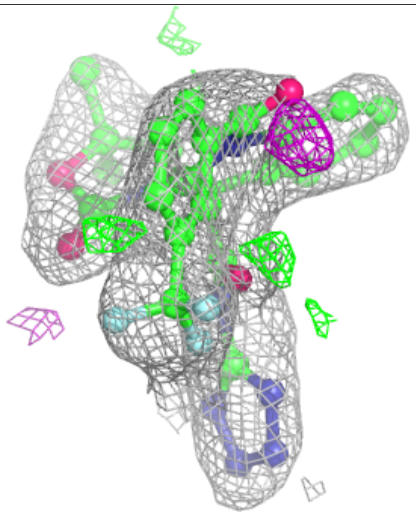


Electron density around F9H C 303:

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

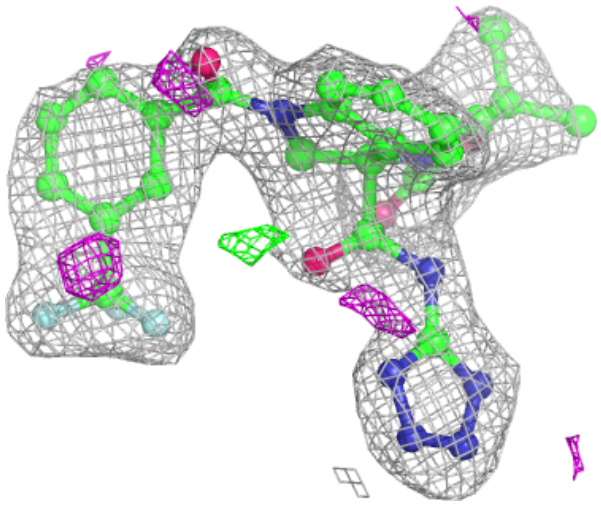


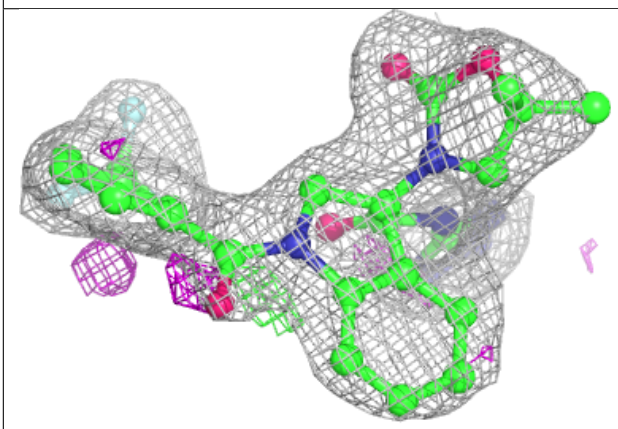


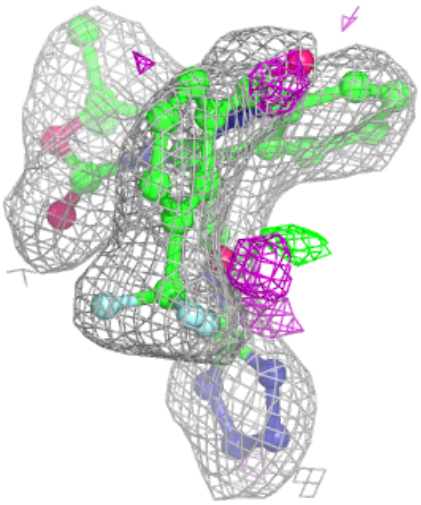


Electron density around F9H E 301:

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

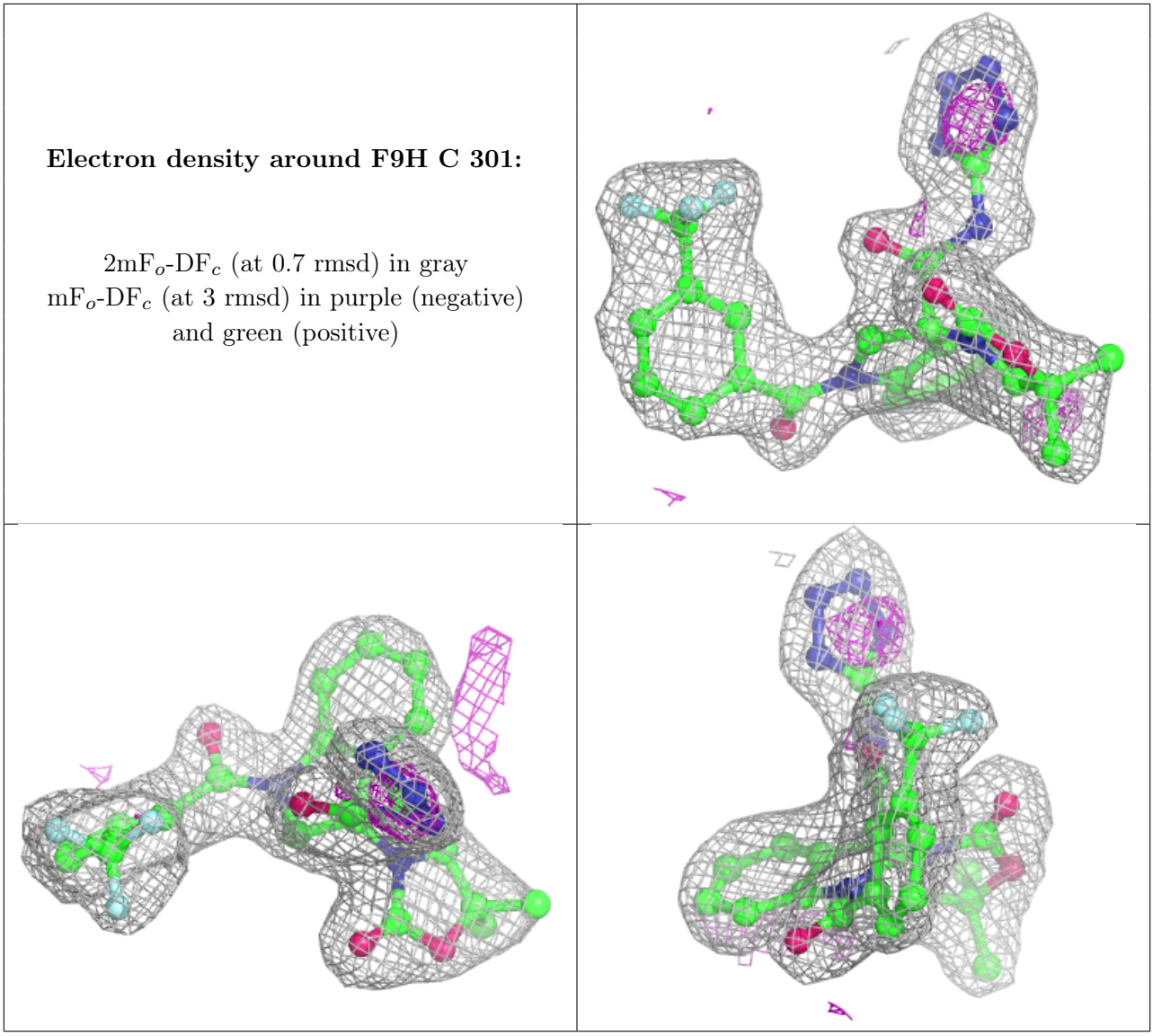






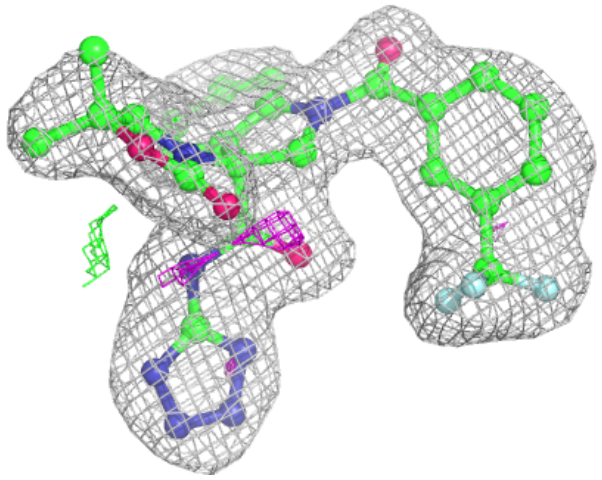
Electron density around F9H C 301:

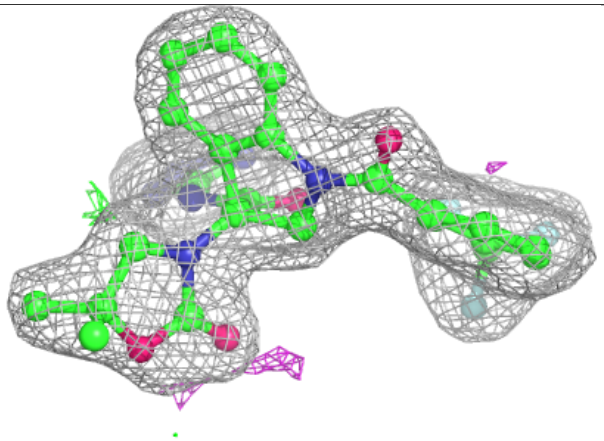
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

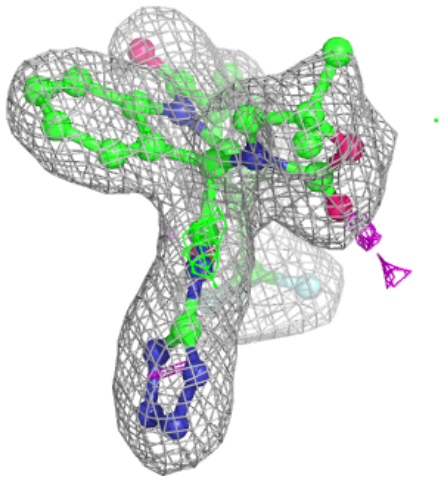


Electron density around F9H B 301:

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

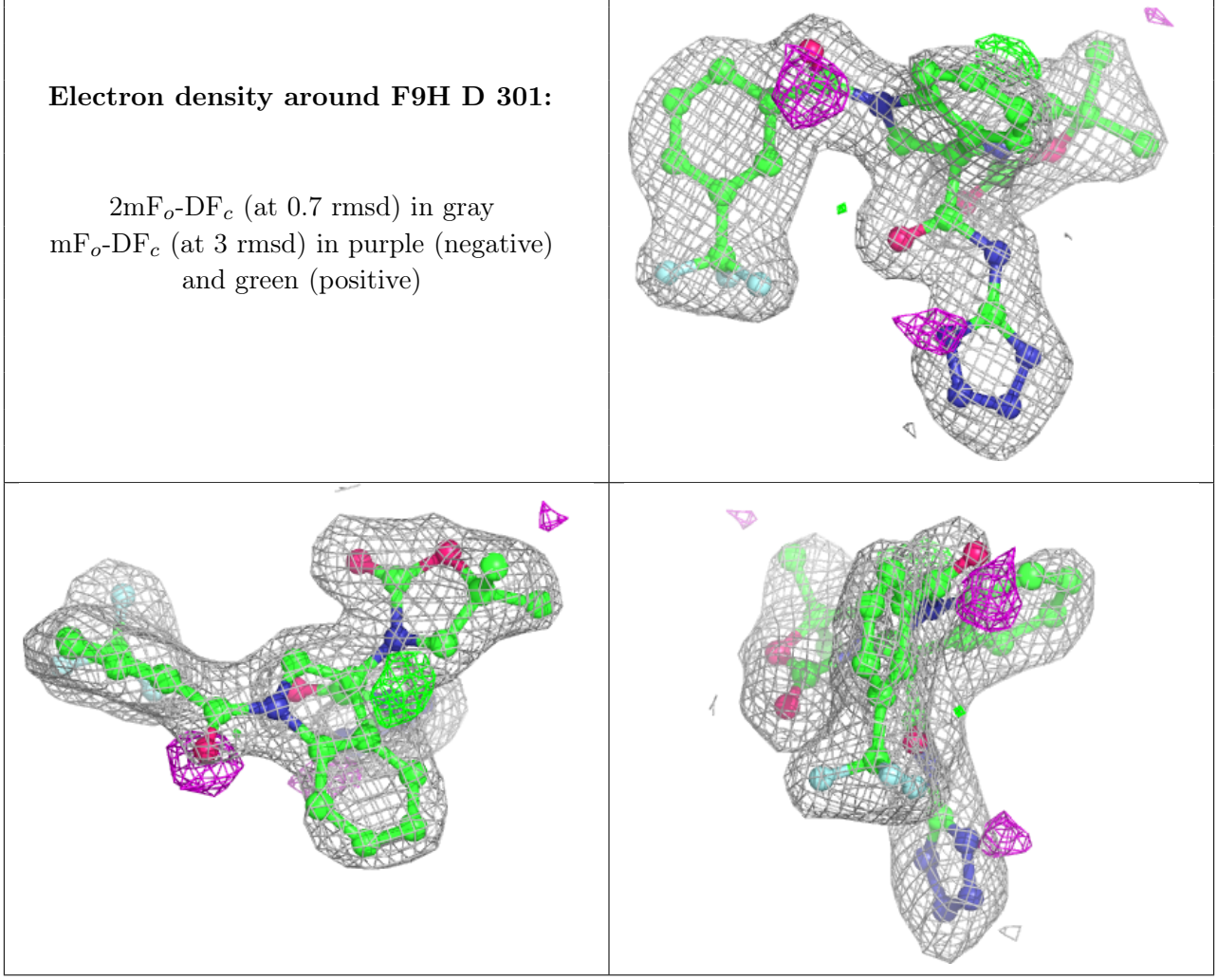






Electron density around F9H D 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.