



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:32 AM UTC

PDB ID : 6CUL / pdb\_00006cul  
Title : PvdF of pyoverdinin biosynthesis is a structurally unique N10-formyltetrahydrofolate-dependent formyltransferase  
Authors : Kenjic, N.; Hoag, M.R.; Moraski, G.C.; Caperelli, C.A.; Moran, G.R.; Lamb, A.L.  
Deposited on : 2018-03-26  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

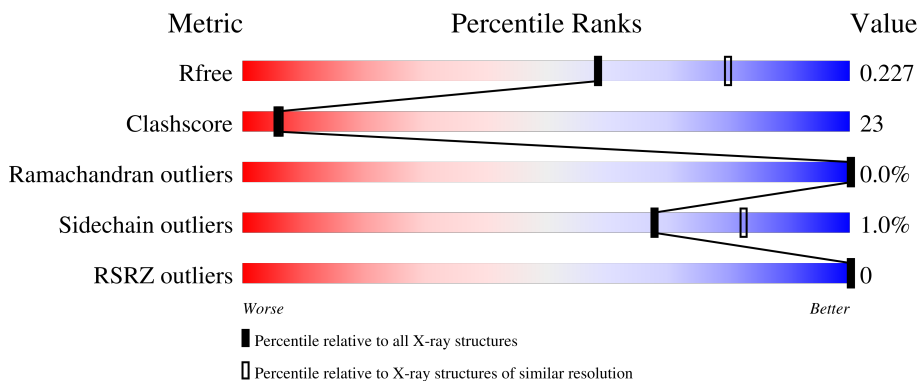
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



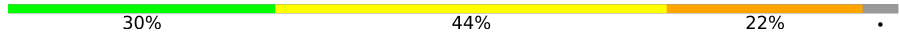
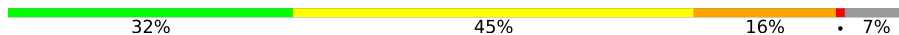
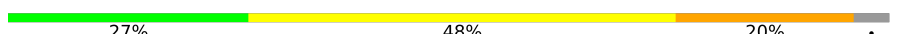
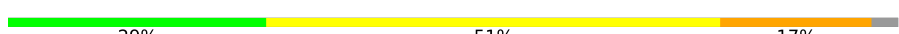
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	275	
1	B	275	
1	C	275	
1	D	275	

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Mol	Chain	Length	Quality of chain
1	E	275	
1	F	275	
1	G	275	
1	H	275	

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	FGD	C	301	-	X	-	-
2	FGD	E	301	-	X	X	-
3	CIT	F	302	-	X	-	-
3	CIT	G	302	-	-	X	-

## 2 Entry composition [i](#)

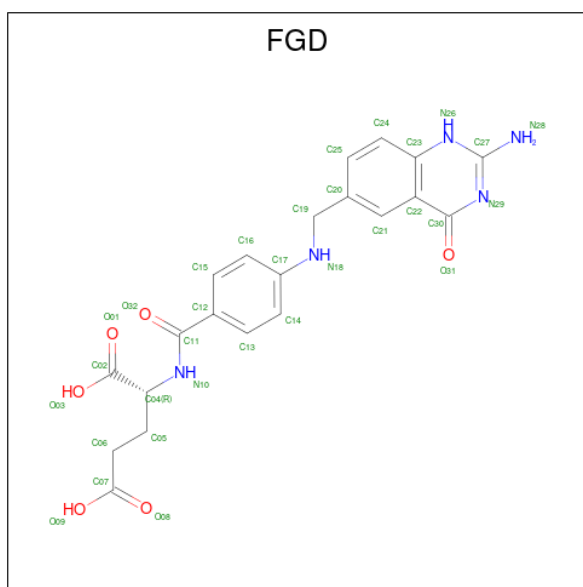
There are 4 unique types of molecules in this entry. The entry contains 34394 atoms, of which 16779 are hydrogens and 0 are deuteriums.

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 Pyoverdine synthetase F.

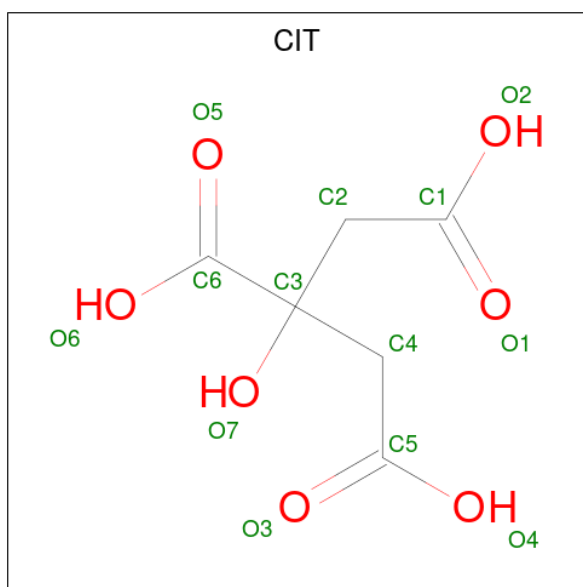
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				Se
1	A	267	4231	1368	2093	367	400	3	0	0	0
1	B	263	4167	1346	2059	362	397	3	0	0	0
1	C	267	4253	1374	2104	371	401	3	0	1	0
1	D	267	4239	1370	2098	367	401	3	0	0	0
1	E	264	4183	1353	2071	363	393	3	0	0	0
1	F	257	4075	1322	2016	351	383	3	0	0	0
1	G	265	4197	1358	2075	362	399	3	0	0	0
1	H	267	4224	1367	2090	363	401	3	0	0	0

- Molecule 2 is N-(4-{{(2-amino-4-oxo-1,4-dihydroquinazolin-6-yl)methyl}amino}benzene-1-carbonyl)-D-glutamic acid (CCD ID: FGD) (formula: C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			
2	A	1	Total	51	21	19	5	6	0	0
2	C	1	Total	51	21	19	5	6	0	0
2	D	1	Total	51	21	19	5	6	0	0
2	E	1	Total	51	21	19	5	6	0	0
2	F	1	Total	51	21	19	5	6	0	0
2	G	1	Total	51	21	19	5	6	0	0
2	H	1	Total	51	21	19	5	6	0	0

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
3	A	1	18	6	5	7	0	0
3	B	1	18	6	5	7	0	0
3	C	1	18	6	5	7	0	0
3	D	1	18	6	5	7	0	0
3	E	1	18	6	5	7	0	0
3	F	1	18	6	5	7	0	0
3	G	1	18	6	5	7	0	0
3	H	1	18	6	5	7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	51	Total	O	0	0
			51	51		
4	C	32	Total	O	0	0
			32	32		
4	D	37	Total	O	0	0
			37	37		

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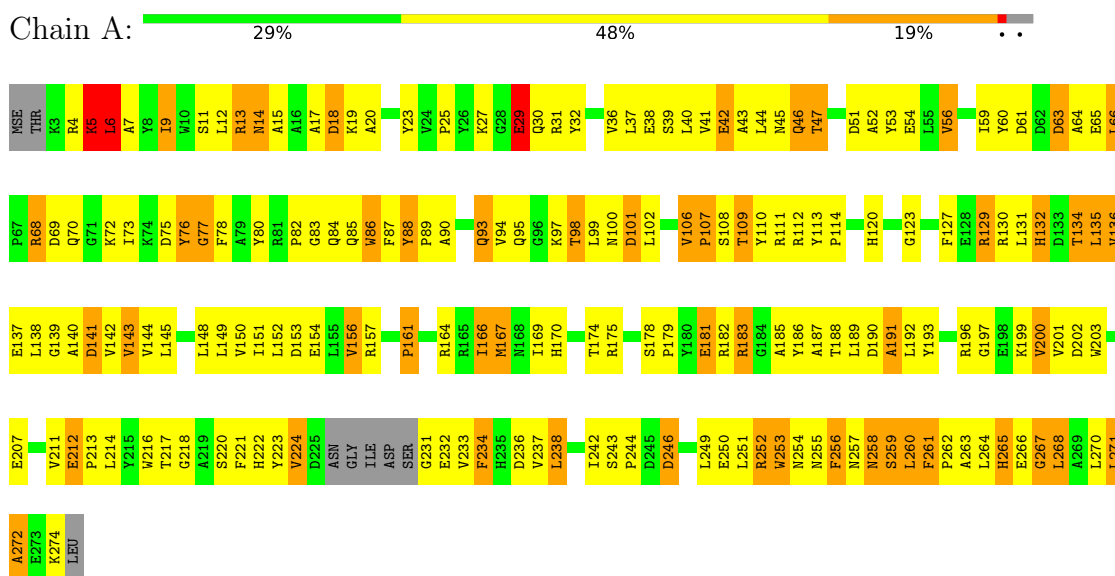
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	E	36	Total O 36 36	0	0
4	F	33	Total O 33 33	0	0
4	G	47	Total O 47 47	0	0
4	H	45	Total O 45 45	0	0

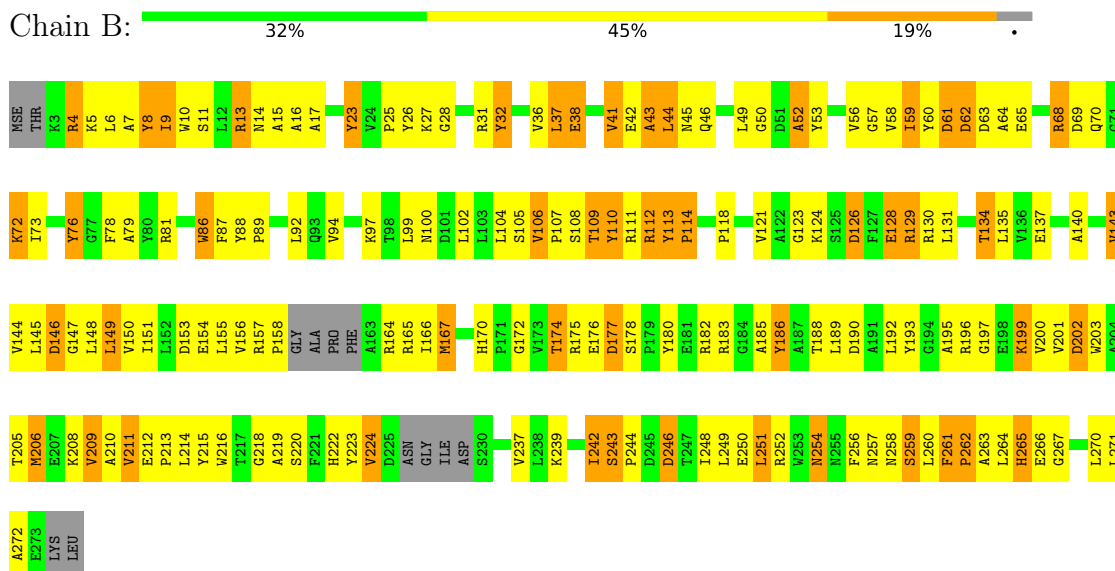
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

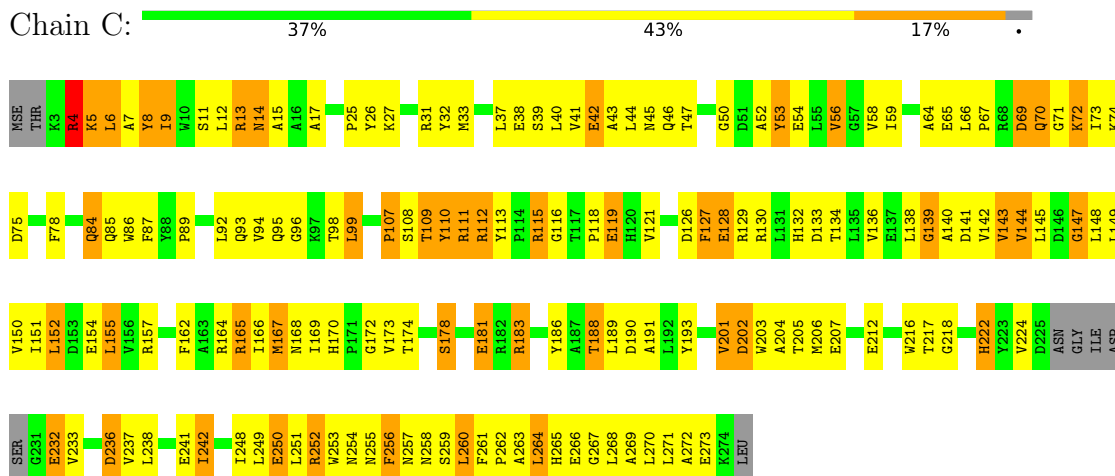
- Molecule 1: Pyoverdine synthetase F



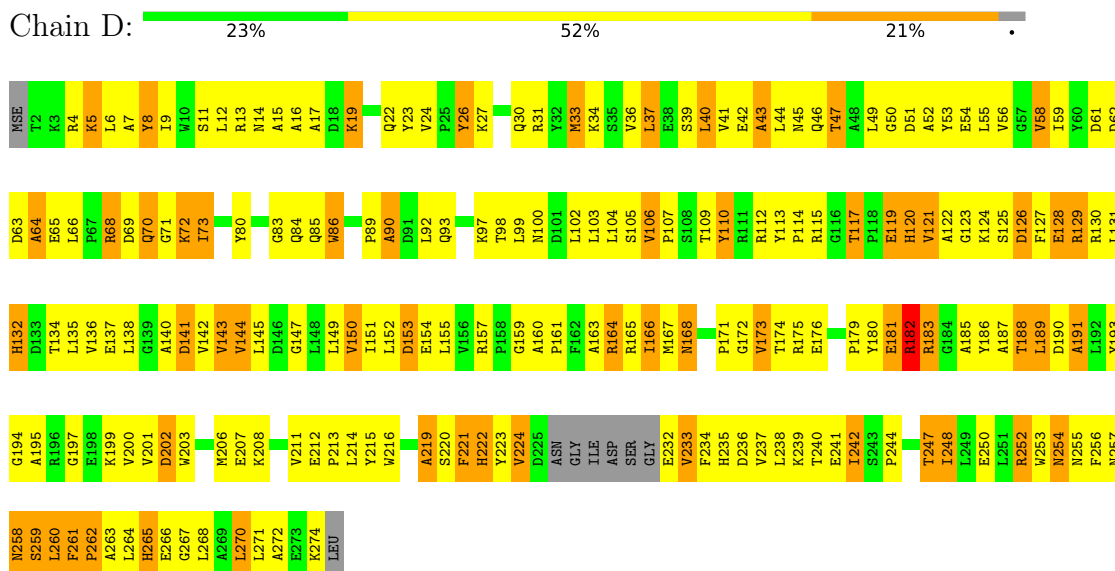
- Molecule 1: Pyoverdine synthetase F



- Molecule 1: Pyoverdine synthetase F

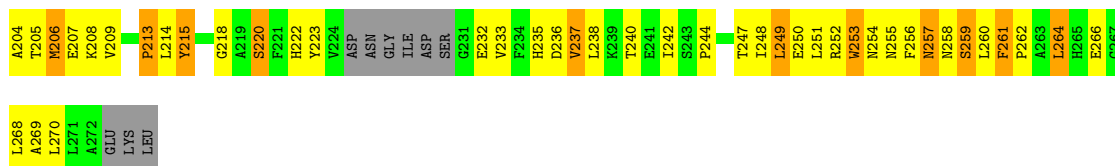


- Molecule 1: Pyoverdine synthetase F

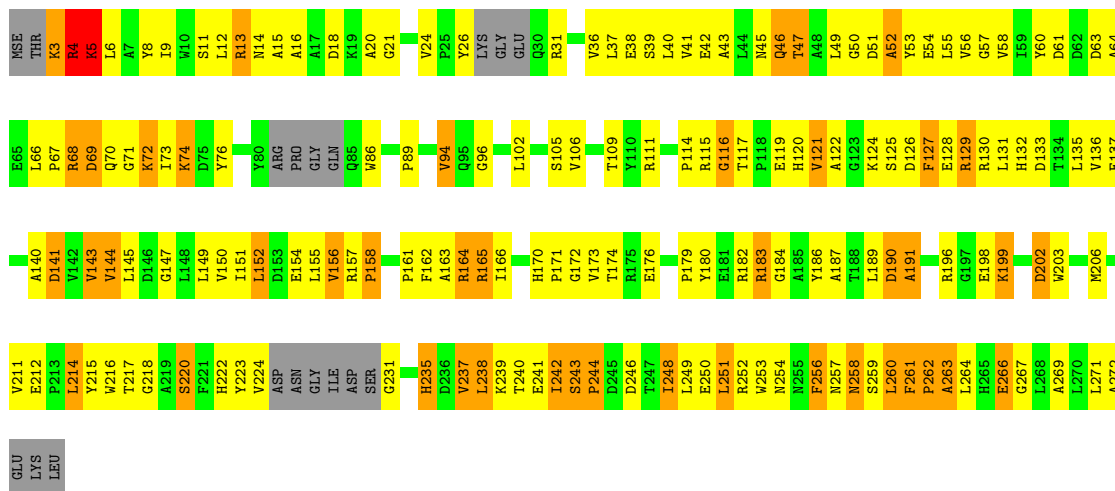


- Molecule 1: Pyoverdine synthetase F

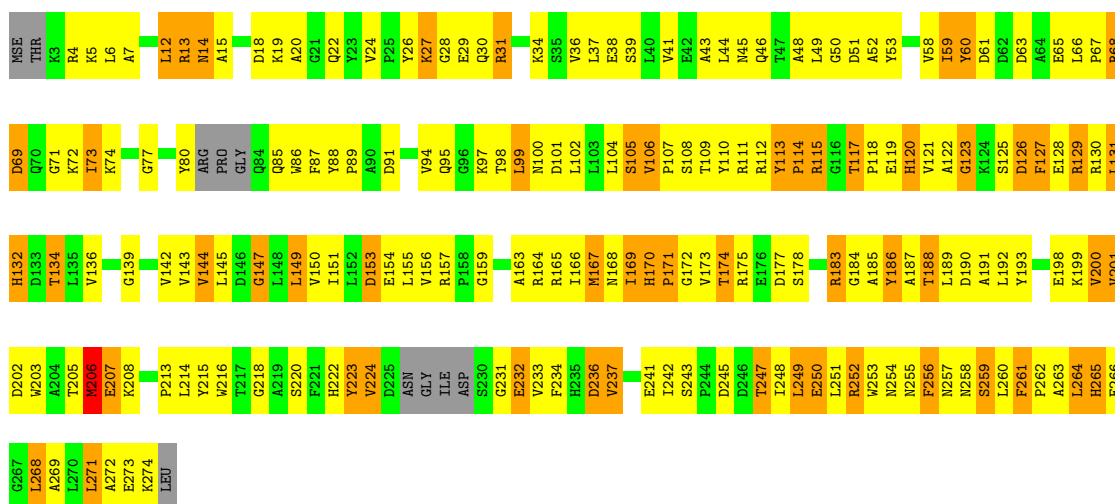




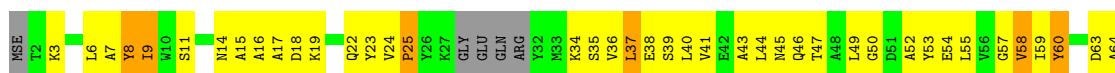
• Molecule 1: Pyoverdine synthetase F



• Molecule 1: Pyoverdine synthetase F



• Molecule 1: Pyoverdine synthetase F



E65	R129	G194	P262
L66	R130	A195	A263
P67	L131	R196	L264
R68	H132	G197	L268
D69	E133	E198	A269
Q70	T134	K199	L270
G71	L135	V200	L271
K72	V136	V201	L272
I73	E137	W202	E273
	L138	A204	K274
Y76	G139	T205	L275
G77	A140	M206	
F78	V143	E207	
A79	V144	K208	
Y80	L145	V209	
R81	D146		
P82	G147	P213	
G83	L148	L214	
Q84	L149	Y215	
Q85	V150	W216	
W86	I151	T217	
F87	L152	G218	
Y88	D153	A219	
P89	E154	S220	
A90	L155	F221	
D91	V156	H222	
L92	R157	Y223	
Q93		V224	
V94	F162	D225	
	L99	ASN	
	M100	GLY	
	D101	ILE	
	L102	D229	
	L103	S230	
	L104		
	S105	D236	
	V106	V237	
	P107	L238	
	S108		
	T109	E241	
	Y110	I242	
	R111	S243	
	R112	P244	
	Y113	E245	
	P114	D246	
	R115		
	G116	L249	
	T117	E250	
	P118	L251	
	E119	R252	
	H120	W253	
	V121	N254	
	A122	N255	
	G123	F256	
	K124	N257	
	S125	N258	
	D126	S259	
	F127	L260	
	E128	Y193	

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.99Å 92.77Å 127.58Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	38.76 – 2.30 38.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.8 (38.76-2.30) 91.0 (38.76-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.227 , 0.249 0.207 , 0.227	Depositor DCC
$R_{free}$ test set	6150 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 16.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.317 for -l,k,h 0.389 for -h,-k,l 0.299 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7216e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FGD, CIT

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	2.40	115/2187 (5.3%)	1.49	35/2967 (1.2%)
1	B	2.49	124/2154 (5.8%)	1.53	31/2921 (1.1%)
1	C	2.47	130/2198 (5.9%)	1.45	21/2981 (0.7%)
1	D	2.56	153/2190 (7.0%)	1.46	31/2972 (1.0%)
1	E	2.46	124/2161 (5.7%)	1.51	24/2933 (0.8%)
1	F	2.37	107/2105 (5.1%)	1.44	28/2856 (1.0%)
1	G	2.50	134/2169 (6.2%)	1.56	30/2941 (1.0%)
1	H	2.60	148/2182 (6.8%)	1.51	24/2961 (0.8%)
All	All	2.48	1035/17346 (6.0%)	1.49	224/23532 (1.0%)

The worst 5 of 1035 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	PRO	N-CD	-14.23	1.27	1.47
1	B	114	PRO	N-CD	-14.19	1.27	1.47
1	G	218	GLY	C-O	-11.97	1.15	1.23
1	H	67	PRO	N-CD	-11.83	1.31	1.47
1	B	158	PRO	N-CD	-11.47	1.31	1.47

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3	LYS	N-CA-C	11.92	127.99	109.52
1	D	224	VAL	N-CA-C	11.28	124.55	109.21
1	E	29	GLU	N-CA-C	11.10	134.45	110.80
1	B	106	VAL	N-CA-C	-10.91	96.75	107.55
1	E	30	GLN	N-CA-C	9.99	125.80	108.02

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	2138	2093	2093	124	0
1	B	2108	2059	2061	92	0
1	C	2149	2104	2102	81	0
1	D	2141	2098	2098	101	0
1	E	2112	2071	2071	123	0
1	F	2059	2016	2015	95	0
1	G	2122	2075	2075	111	0
1	H	2134	2090	2090	76	0
2	A	32	19	0	3	0
2	C	32	19	0	3	0
2	D	32	19	0	0	0
2	E	32	19	0	9	0
2	F	32	19	0	3	0
2	G	32	19	0	0	0
2	H	32	19	0	1	0
3	A	13	5	5	1	0
3	B	13	5	5	3	0
3	C	13	5	5	2	0
3	D	13	5	5	0	0
3	E	13	5	5	1	0
3	F	13	5	5	0	0
3	G	13	5	5	9	0
3	H	13	5	5	0	0
4	A	43	0	0	1	0
4	B	51	0	0	10	0
4	C	32	0	0	4	0
4	D	37	0	0	3	1
4	E	36	0	0	4	0
4	F	33	0	0	2	0
4	G	47	0	0	2	1
4	H	45	0	0	3	0
All	All	17615	16779	16645	786	1

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 23.

The worst 5 of 786 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:6:LEU:HD12	1:A:142:VAL:CG1	1.29	1.55
1:F:174:THR:O	1:F:183:ARG:NH2	1.60	1.35
1:A:196:ARG:NH1	1:A:244:PRO:O	1.64	1.29
1:B:154:GLU:O	1:B:157:ARG:CG	1.82	1.28
1:C:27:LYS:HD3	1:C:250:GLU:OE2	1.34	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:406:HOH:O	4:G:424:HOH:O[2_545]	2.14	0.06

## 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	263/275 (96%)	255 (97%)	8 (3%)	0	100	100
1	B	257/275 (94%)	248 (96%)	9 (4%)	0	100	100
1	C	264/275 (96%)	253 (96%)	11 (4%)	0	100	100
1	D	263/275 (96%)	254 (97%)	9 (3%)	0	100	100
1	E	260/275 (94%)	249 (96%)	11 (4%)	0	100	100
1	F	249/275 (90%)	243 (98%)	5 (2%)	1 (0%)	30	38
1	G	259/275 (94%)	249 (96%)	10 (4%)	0	100	100
1	H	261/275 (95%)	254 (97%)	7 (3%)	0	100	100
All	All	2076/2200 (94%)	2005 (97%)	70 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	5	LYS

### 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	222/225 (99%)	218 (98%)	4 (2%)	51	70
1	B	220/225 (98%)	219 (100%)	1 (0%)	81	90
1	C	223/225 (99%)	220 (99%)	3 (1%)	61	77
1	D	223/225 (99%)	221 (99%)	2 (1%)	70	84
1	E	219/225 (97%)	216 (99%)	3 (1%)	59	76
1	F	214/225 (95%)	212 (99%)	2 (1%)	70	84
1	G	221/225 (98%)	218 (99%)	3 (1%)	59	76
1	H	223/225 (99%)	223 (100%)	0	100	100
All	All	1765/1800 (98%)	1747 (99%)	18 (1%)	68	82

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	4	ARG
1	G	206	MSE
1	G	31	ARG
1	D	181	GLU
1	F	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	93	GLN
1	H	85	GLN
1	H	254	ASN
1	H	95	GLN
1	D	258	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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	CIT	E	302	-	12,12,12	1.16	1 (8%)	17,17,17	2.06	5 (29%)
3	CIT	A	302	-	12,12,12	0.99	0	17,17,17	2.11	6 (35%)
3	CIT	C	302	-	12,12,12	1.27	0	17,17,17	2.01	7 (41%)
3	CIT	D	302	-	12,12,12	1.05	0	17,17,17	1.81	4 (23%)
2	FGD	G	301	-	34,34,34	2.61	18 (52%)	46,47,47	1.95	14 (30%)
3	CIT	G	302	-	12,12,12	2.30	6 (50%)	17,17,17	2.63	9 (52%)
3	CIT	B	301	-	12,12,12	1.00	0	17,17,17	2.40	8 (47%)
3	CIT	F	302	-	12,12,12	1.65	2 (16%)	17,17,17	2.28	8 (47%)
2	FGD	E	301	-	34,34,34	2.34	13 (38%)	46,47,47	2.86	25 (54%)
2	FGD	H	301	-	34,34,34	2.12	15 (44%)	46,47,47	1.52	9 (19%)
3	CIT	H	302	-	12,12,12	1.09	0	17,17,17	1.67	3 (17%)
2	FGD	F	301	-	34,34,34	2.70	12 (35%)	46,47,47	2.52	16 (34%)
2	FGD	C	301	-	34,34,34	2.59	13 (38%)	46,47,47	3.14	28 (60%)
2	FGD	A	301	-	34,34,34	2.28	9 (26%)	46,47,47	0.91	1 (2%)
2	FGD	D	301	-	34,34,34	2.45	12 (35%)	46,47,47	1.64	12 (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	CIT	E	302	-	-	8/16/16/16	-
3	CIT	A	302	-	-	7/16/16/16	-
3	CIT	C	302	-	-	5/16/16/16	-
3	CIT	D	302	-	-	10/16/16/16	-
2	FGD	G	301	-	-	10/22/22/22	0/3/3/3
3	CIT	G	302	-	-	2/16/16/16	-
3	CIT	B	301	-	-	8/16/16/16	-
3	CIT	F	302	-	-	11/16/16/16	-
2	FGD	E	301	-	-	8/22/22/22	0/3/3/3
2	FGD	H	301	-	-	8/22/22/22	0/3/3/3
3	CIT	H	302	-	-	5/16/16/16	-
2	FGD	F	301	-	-	7/22/22/22	0/3/3/3
2	FGD	C	301	-	-	11/22/22/22	0/3/3/3
2	FGD	A	301	-	-	2/22/22/22	0/3/3/3
2	FGD	D	301	-	-	10/22/22/22	0/3/3/3

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	FGD	C23-N26	8.43	1.54	1.39
2	C	301	FGD	O31-C30	-6.25	1.13	1.23
2	G	301	FGD	O31-C30	-6.06	1.13	1.23
2	D	301	FGD	O32-C11	-6.02	1.09	1.23
2	F	301	FGD	C27-N29	5.93	1.47	1.33

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	FGD	C12-C11-N10	8.99	133.70	117.04
2	C	301	FGD	C05-C04-N10	-8.61	93.86	110.91
2	F	301	FGD	O03-C02-O01	-7.52	107.01	124.08
2	C	301	FGD	C02-C04-N10	6.80	126.34	110.57
3	E	302	CIT	O6-C6-C3	5.67	124.03	113.14

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

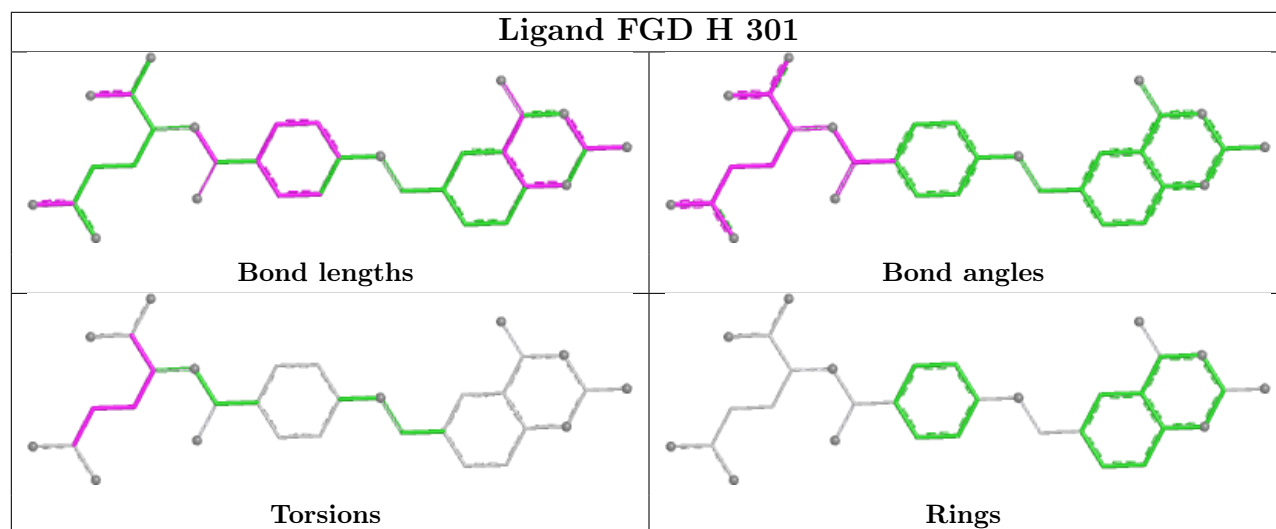
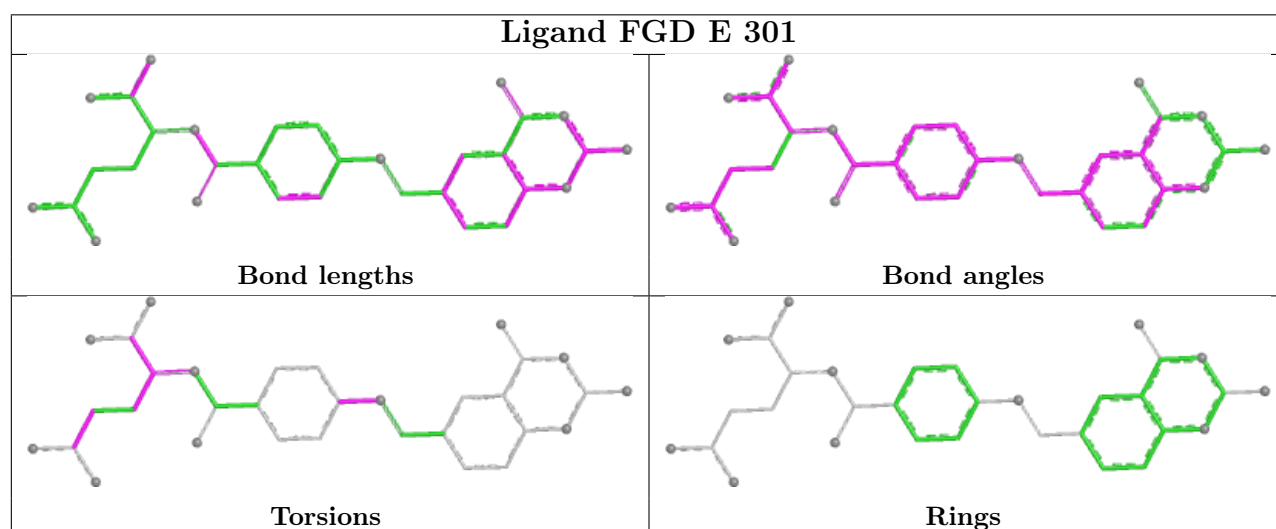
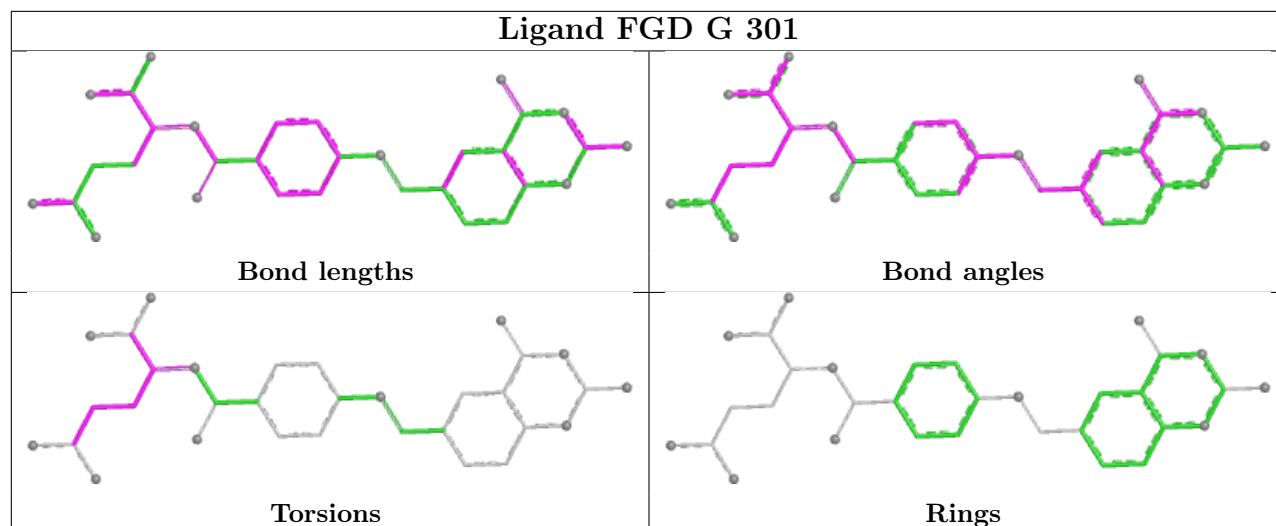
Mol	Chain	Res	Type	Atoms
2	C	301	FGD	C02-C04-C05-C06
3	A	302	CIT	C2-C3-C6-O5
3	A	302	CIT	C2-C3-C6-O6
3	A	302	CIT	O7-C3-C6-O5
3	A	302	CIT	O7-C3-C6-O6

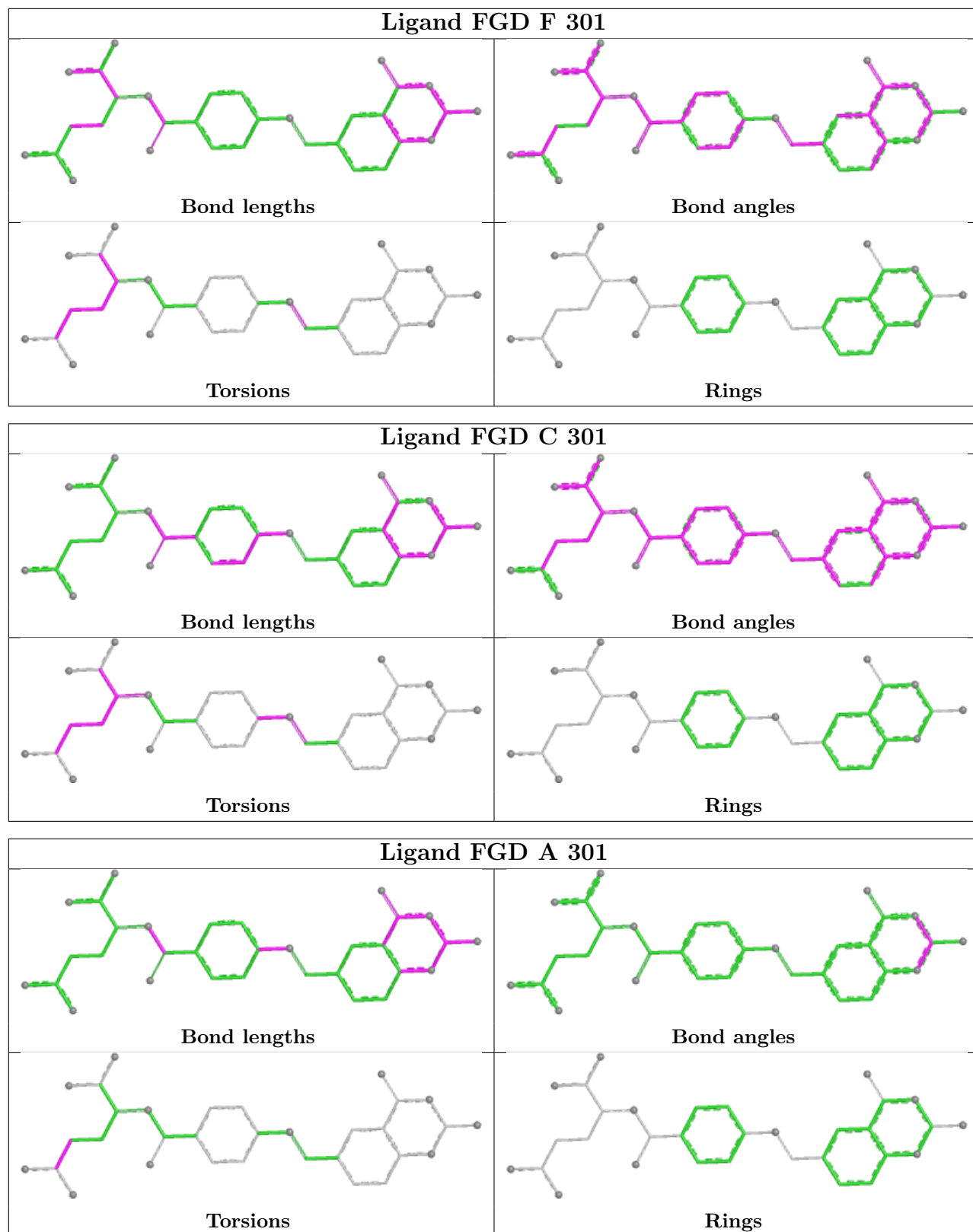
There are no ring outliers.

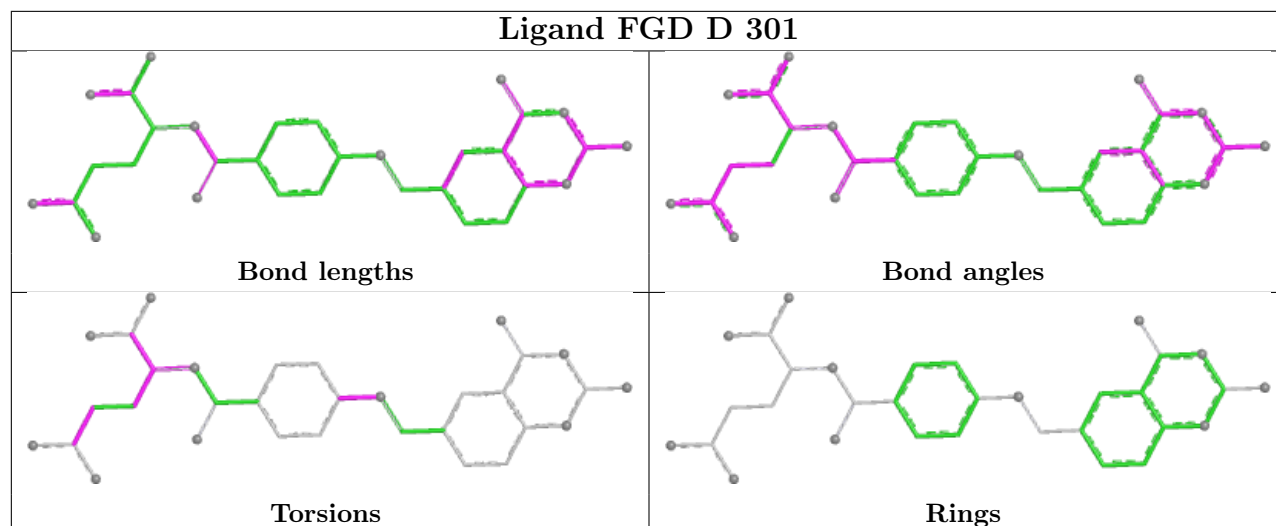
10 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	CIT	1	0
3	A	302	CIT	1	0
3	C	302	CIT	2	0
3	G	302	CIT	9	0
3	B	301	CIT	3	0
2	E	301	FGD	9	0
2	H	301	FGD	1	0
2	F	301	FGD	3	0
2	C	301	FGD	3	0
2	A	301	FGD	3	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.







## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/275 (96%)	-0.93	0 100 100	25, 42, 70, 89	0
1	B	260/275 (94%)	-0.99	0 100 100	24, 40, 64, 82	0
1	C	264/275 (96%)	-0.97	0 100 100	20, 43, 64, 90	1 (0%)
1	D	264/275 (96%)	-1.03	0 100 100	20, 40, 61, 76	0
1	E	261/275 (94%)	-0.95	0 100 100	29, 43, 66, 87	0
1	F	254/275 (92%)	-0.89	0 100 100	32, 48, 70, 90	0
1	G	262/275 (95%)	-1.04	0 100 100	19, 38, 57, 73	0
1	H	264/275 (96%)	-1.01	0 100 100	19, 37, 56, 74	0
All	All	2093/2200 (95%)	-0.98	0 100 100	19, 41, 65, 90	1 (0%)

There are no RSRZ outliers to report.

### 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](#)

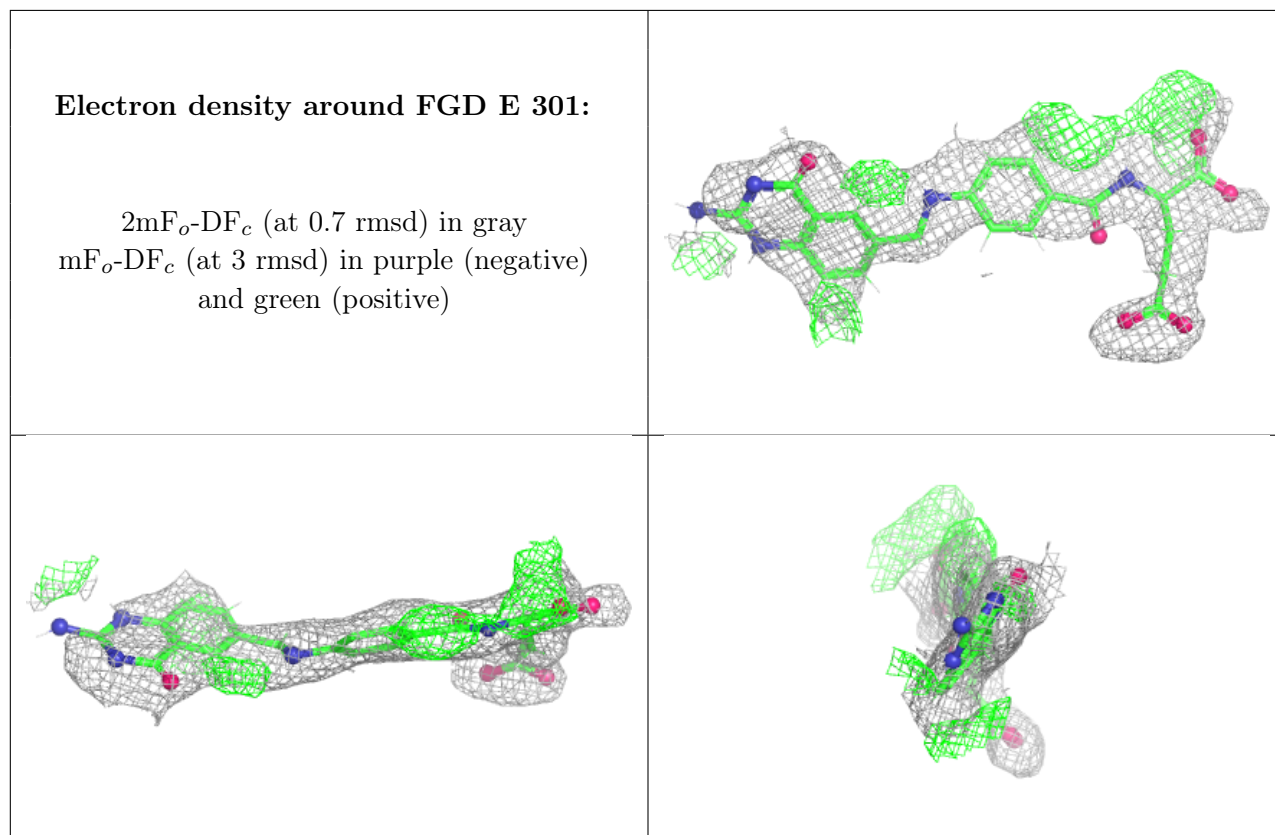
There are no oligosaccharides in this entry.

### 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<sup>th</sup> 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.

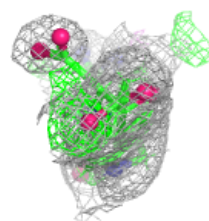
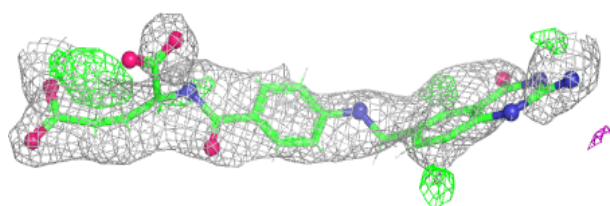
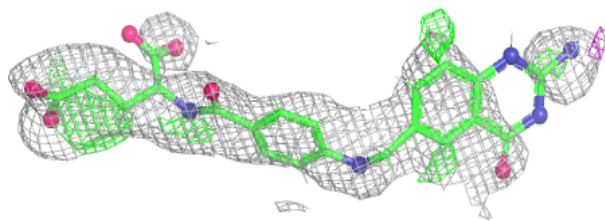
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FGD	E	301	32/32	0.97	0.08	20,25,30,31	51
2	FGD	F	301	32/32	0.97	0.09	18,25,29,30	51
3	CIT	D	302	13/13	0.97	0.05	17,34,49,49	0
2	FGD	A	301	32/32	0.98	0.04	15,26,44,59	0
2	FGD	C	301	32/32	0.98	0.06	20,25,30,32	51
2	FGD	G	301	32/32	0.98	0.04	19,20,24,24	0
2	FGD	H	301	32/32	0.98	0.05	13,25,45,54	0
3	CIT	A	302	13/13	0.98	0.04	18,29,39,39	0
3	CIT	B	301	13/13	0.98	0.06	25,33,49,49	0
2	FGD	D	301	32/32	0.98	0.05	21,29,43,51	0
3	CIT	E	302	13/13	0.98	0.05	24,34,53,53	0
3	CIT	F	302	13/13	0.98	0.06	27,44,53,54	0
3	CIT	G	302	13/13	0.98	0.05	27,33,41,41	0
3	CIT	H	302	13/13	0.98	0.05	18,32,47,50	0
3	CIT	C	302	13/13	0.99	0.05	22,37,45,48	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.

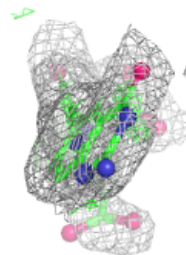
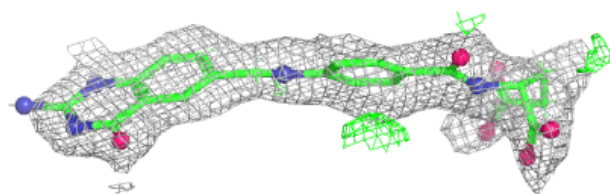
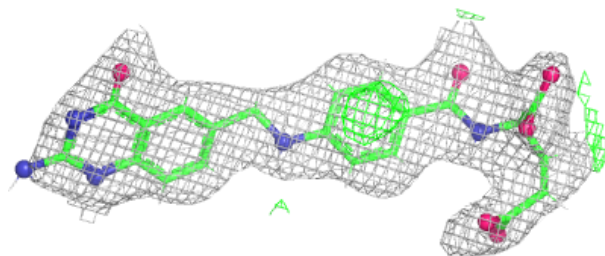


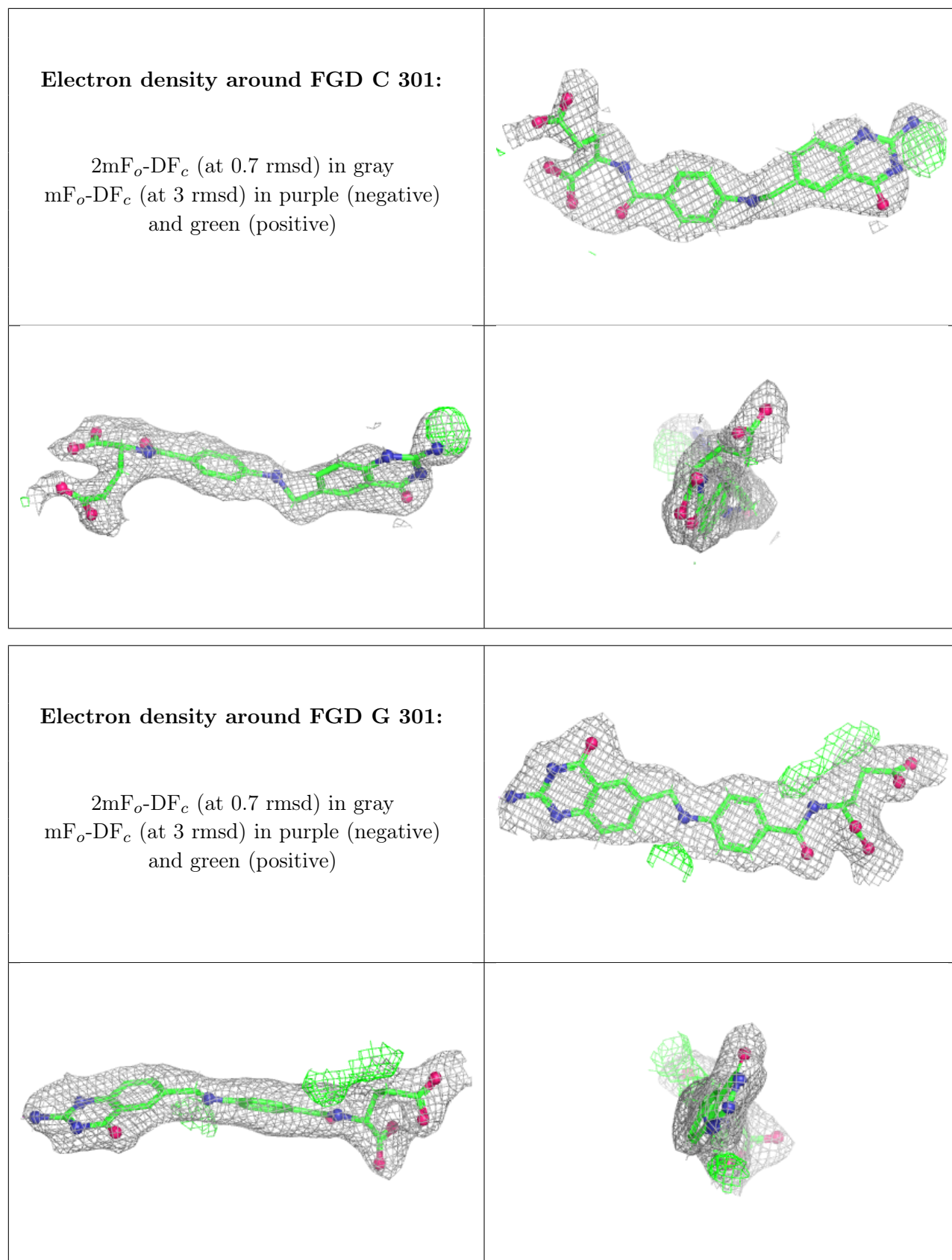
**Electron density around FGD F 301:**

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

**Electron density around FGD A 301:**

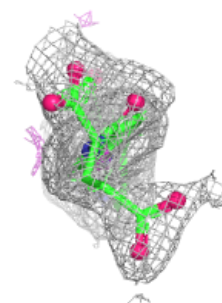
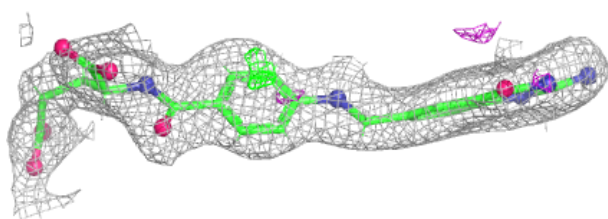
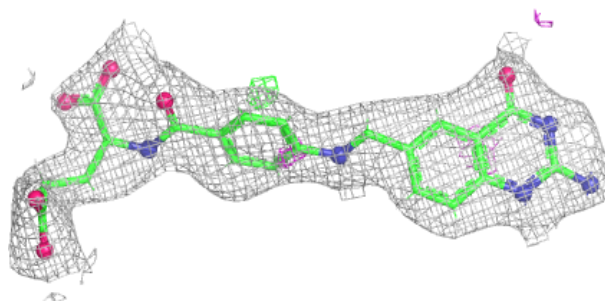
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



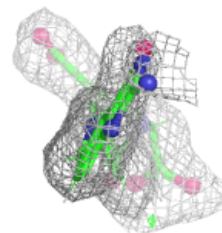
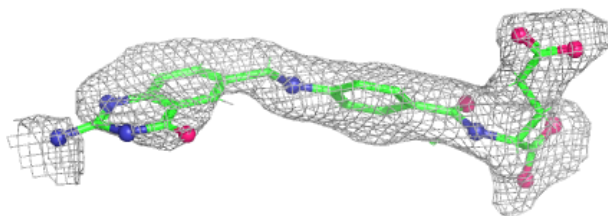
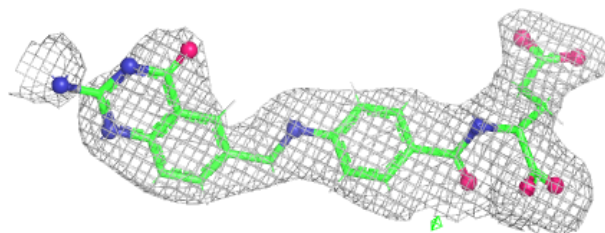


**Electron density around FGD H 301:**

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

**Electron density around FGD 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.