



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2021 – 12:36 PM EDT

PDB ID : 7JXH  
Title : HER2 in complex with JBJ-08-178-01  
Authors : Beyett, T.S.; Eck, M.J.  
Deposited on : 2020-08-27  
Resolution : 3.27 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.23.1  
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) : 2.23.1

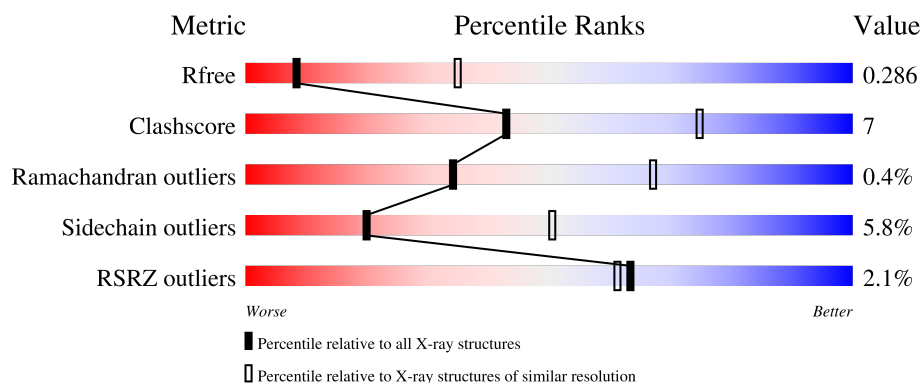
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.27 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	326	<div> <div>0%</div> <div>65% 18% 17%</div> </div>
1	B	326	<div> <div>2%</div> <div>69% 13% 15%</div> </div>
1	C	326	<div> <div>2%</div> <div>66% 17% 16%</div> </div>
1	D	326	<div> <div>3%</div> <div>69% 17% 13%</div> </div>
1	E	326	<div> <div>2%</div> <div>63% 18% 18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	326	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>63%</div><div>15%</div><div>•</div><div>20%</div></div></div>
1	G	326	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>63%</div><div>19%</div><div>•</div><div>16%</div></div></div>
1	H	326	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>69%</div><div>17%</div><div>•</div><div>13%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17908 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	276	Total	C	N	O	S	0	2	0
			2202	1406	388	391	17			
1	A	272	Total	C	N	O	S	0	2	0
			2181	1391	387	386	17			
1	C	274	Total	C	N	O	S	0	2	0
			2197	1402	390	388	17			
1	D	283	Total	C	N	O	S	0	2	0
			2277	1452	401	407	17			
1	E	268	Total	C	N	O	S	0	2	0
			2154	1374	382	381	17			
1	F	262	Total	C	N	O	S	0	2	0
			2109	1352	373	368	16			
1	G	273	Total	C	N	O	S	0	2	0
			2189	1397	388	387	17			
1	H	282	Total	C	N	O	S	0	2	0
			2263	1444	399	403	17			

There are 32 discrepancies between the modelled and reference sequences:

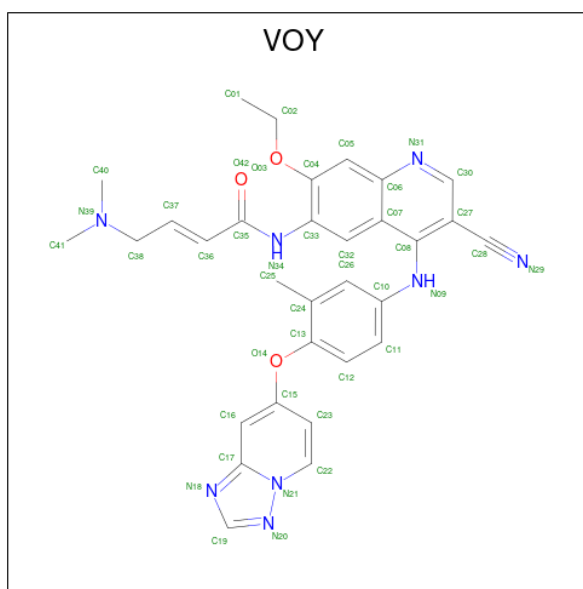
Chain	Residue	Modelled	Actual	Comment	Reference
B	699	GLY	-	expression tag	UNP P04626
B	700	SER	-	expression tag	UNP P04626
B	701	THR	-	expression tag	UNP P04626
B	702	SER	-	expression tag	UNP P04626
A	699	GLY	-	expression tag	UNP P04626
A	700	SER	-	expression tag	UNP P04626
A	701	THR	-	expression tag	UNP P04626
A	702	SER	-	expression tag	UNP P04626
C	699	GLY	-	expression tag	UNP P04626
C	700	SER	-	expression tag	UNP P04626
C	701	THR	-	expression tag	UNP P04626
C	702	SER	-	expression tag	UNP P04626
D	699	GLY	-	expression tag	UNP P04626

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Chain	Residue	Modelled	Actual	Comment	Reference
D	700	SER	-	expression tag	UNP P04626
D	701	THR	-	expression tag	UNP P04626
D	702	SER	-	expression tag	UNP P04626
E	699	GLY	-	expression tag	UNP P04626
E	700	SER	-	expression tag	UNP P04626
E	701	THR	-	expression tag	UNP P04626
E	702	SER	-	expression tag	UNP P04626
F	699	GLY	-	expression tag	UNP P04626
F	700	SER	-	expression tag	UNP P04626
F	701	THR	-	expression tag	UNP P04626
F	702	SER	-	expression tag	UNP P04626
G	699	GLY	-	expression tag	UNP P04626
G	700	SER	-	expression tag	UNP P04626
G	701	THR	-	expression tag	UNP P04626
G	702	SER	-	expression tag	UNP P04626
H	699	GLY	-	expression tag	UNP P04626
H	700	SER	-	expression tag	UNP P04626
H	701	THR	-	expression tag	UNP P04626
H	702	SER	-	expression tag	UNP P04626

- Molecule 2 is (2E)-N-[3-cyano-7-ethoxy-4-({3-methyl-4-[(1,2,4]triazolo[1,5-a]pyridin-7-yl)oxy]phenyl}amino)quinolin-6-yl]-4-(dimethylamino)but-2-enamide (three-letter code: VOY) (formula: C<sub>31</sub>H<sub>30</sub>N<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			42	31	8	3		

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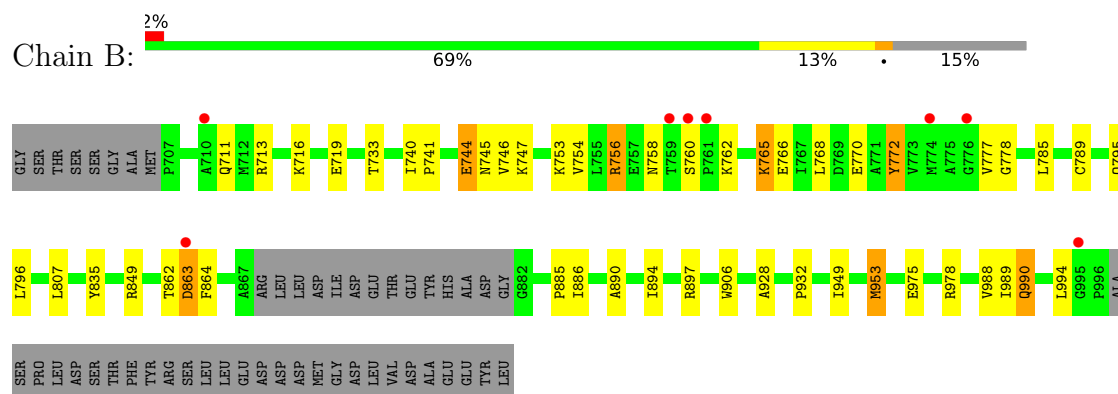
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	31	8	3		
2	C	1	Total	C	N	O	0	0
			42	31	8	3		
2	D	1	Total	C	N	O	0	0
			42	31	8	3		
2	E	1	Total	C	N	O	0	0
			42	31	8	3		
2	F	1	Total	C	N	O	0	0
			42	31	8	3		
2	G	1	Total	C	N	O	0	0
			42	31	8	3		
2	H	1	Total	C	N	O	0	0
			42	31	8	3		

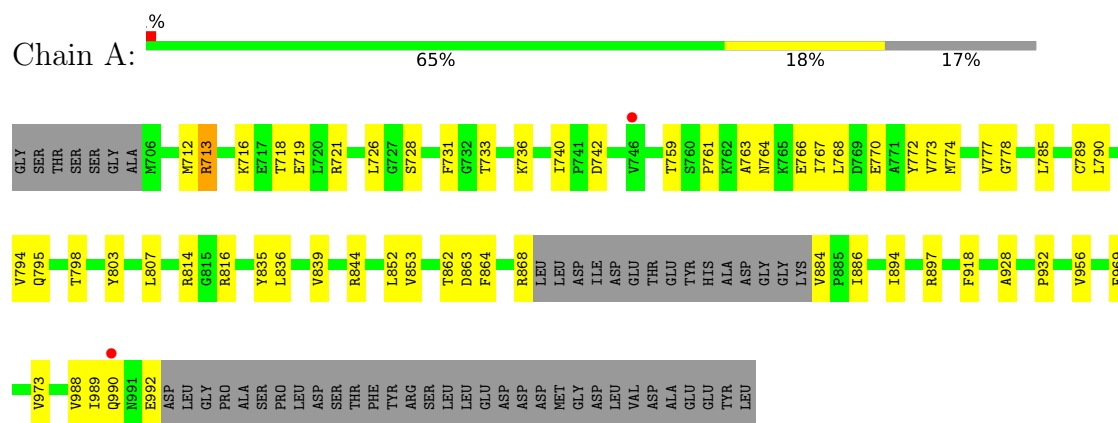
### 3 Residue-property plots [i](#)

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.

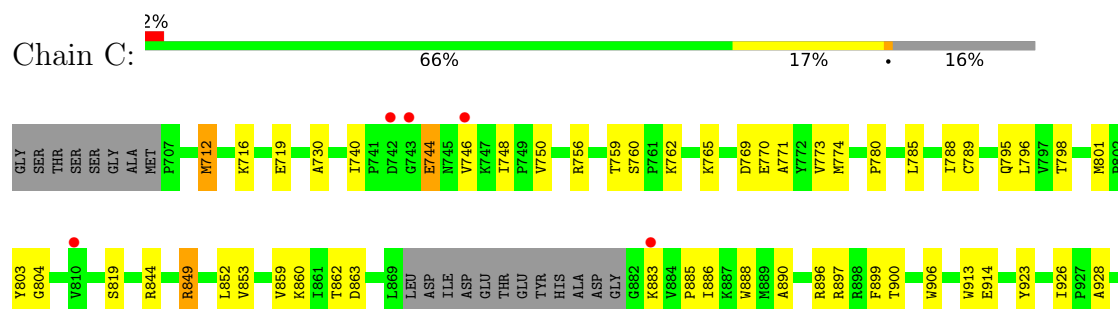
#### • Molecule 1: Receptor tyrosine-protein kinase erbB-2

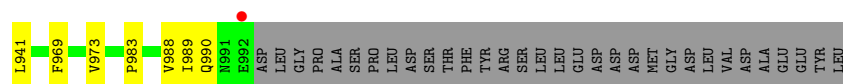


#### • Molecule 1: Receptor tyrosine-protein kinase erbB-2

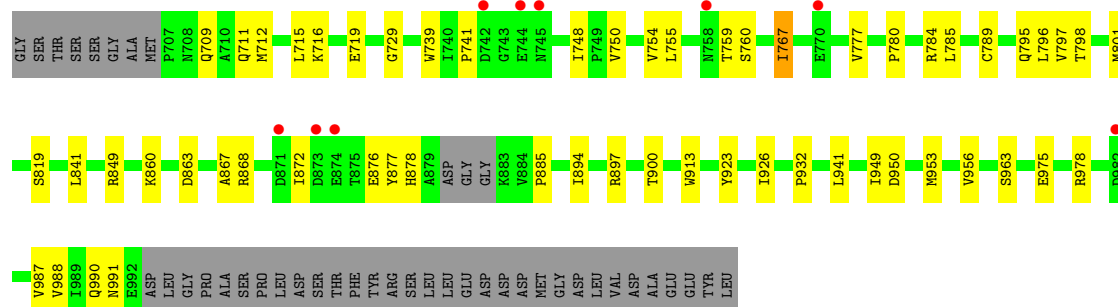


#### • Molecule 1: Receptor tyrosine-protein kinase erbB-2

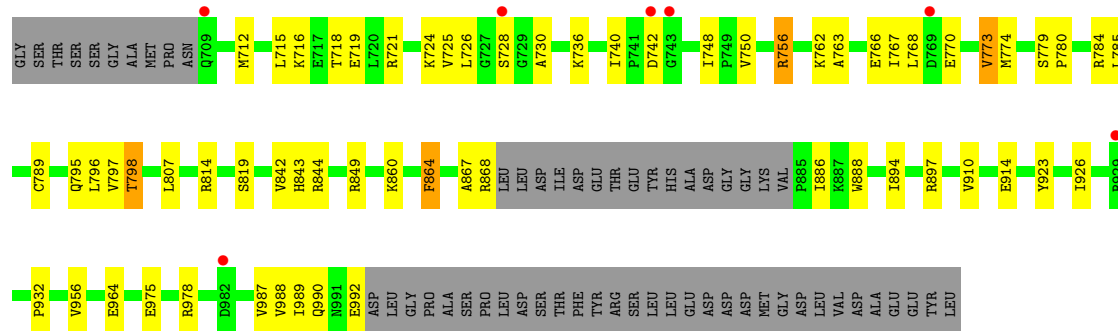




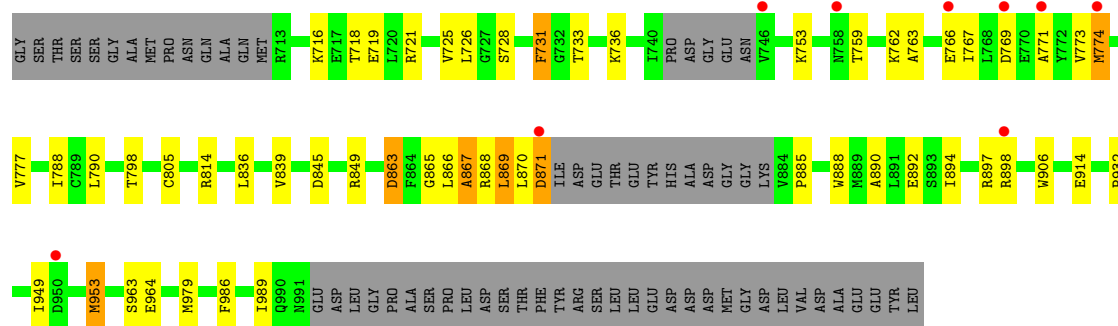
- Molecule 1: Receptor tyrosine-protein kinase erbB-2



- Molecule 1: Receptor tyrosine-protein kinase erbB-2



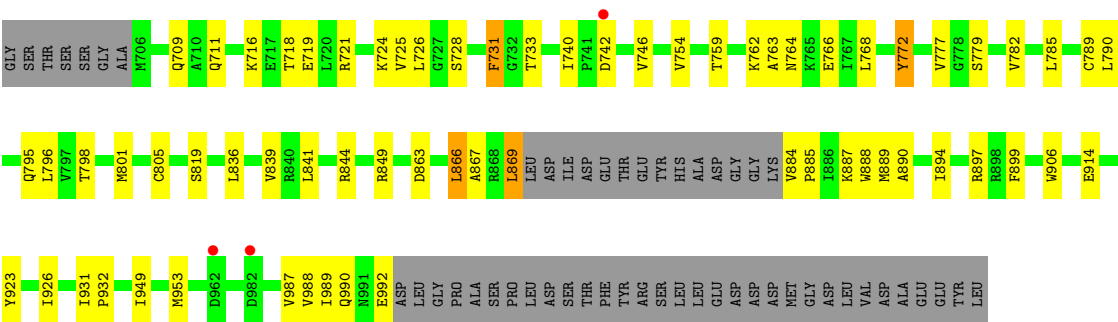
- Molecule 1: Receptor tyrosine-protein kinase erbB-2



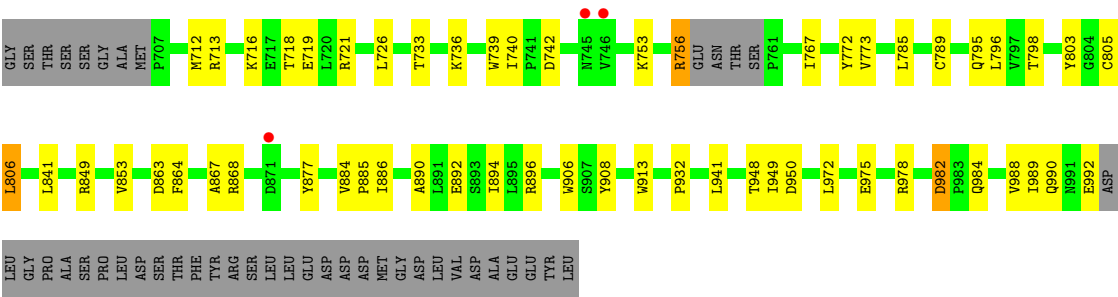
- Molecule 1: Receptor tyrosine-protein kinase erbB-2







● Molecule 1: Receptor tyrosine-protein kinase erbB-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.14Å 154.62Å 93.55Å 90.00° 102.47° 90.00°	Depositor
Resolution (Å)	91.34 – 3.27 91.34 – 3.27	Depositor EDS
% Data completeness (in resolution range)	98.4 (91.34-3.27) 83.6 (91.34-3.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.61 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.239 , 0.285 0.242 , 0.286	Depositor DCC
$R_{free}$ test set	36776 reflections (94.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	17908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.80 % 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 1.9345e-04. 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: VOY

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	0.31	0/2234	0.54	0/3023
1	B	0.31	0/2256	0.54	0/3052
1	C	0.27	0/2250	0.49	0/3042
1	D	0.32	0/2332	0.52	0/3155
1	E	0.31	0/2206	0.54	0/2982
1	F	0.31	0/2159	0.51	0/2919
1	G	0.29	0/2242	0.52	0/3034
1	H	0.35	0/2318	0.58	2/3134 (0.1%)
All	All	0.31	0/17997	0.53	2/24341 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	805	CYS	CB-CA-C	-8.20	94.00	110.40
1	H	864	PHE	CB-CA-C	5.95	122.31	110.40

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	2181	0	2232	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2202	0	2255	23	0
1	C	2197	0	2258	28	0
1	D	2277	0	2325	35	0
1	E	2154	0	2209	33	0
1	F	2109	0	2180	31	0
1	G	2189	0	2244	36	0
1	H	2263	0	2312	26	0
2	A	42	0	0	2	0
2	B	42	0	0	1	0
2	C	42	0	0	3	0
2	D	42	0	0	5	0
2	E	42	0	0	2	0
2	F	42	0	0	4	0
2	G	42	0	0	4	0
2	H	42	0	0	1	0
All	All	17908	0	18015	243	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 7.

The worst 5 of 243 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)
2:D:1101:VOY:C38	2:D:1101:VOY:N39	1.67	1.57
2:F:1101:VOY:C38	2:F:1101:VOY:N39	1.72	1.50
1:G:805:CYS:SG	2:G:1101:VOY:C37	2.08	1.40
1:D:988:VAL:HG12	1:D:990:GLN:HG2	1.15	1.12
1:D:988:VAL:CG1	1:D:990:GLN:HG2	2.00	0.92

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	270/326 (83%)	263 (97%)	7 (3%)	0	100	100
1	B	274/326 (84%)	260 (95%)	12 (4%)	2 (1%)	22	56
1	C	272/326 (83%)	264 (97%)	8 (3%)	0	100	100
1	D	281/326 (86%)	274 (98%)	6 (2%)	1 (0%)	34	67
1	E	266/326 (82%)	260 (98%)	4 (2%)	2 (1%)	19	52
1	F	258/326 (79%)	249 (96%)	6 (2%)	3 (1%)	13	44
1	G	271/326 (83%)	260 (96%)	10 (4%)	1 (0%)	34	67
1	H	280/326 (86%)	269 (96%)	11 (4%)	0	100	100
All	All	2172/2608 (83%)	2099 (97%)	64 (3%)	9 (0%)	34	67

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	773	VAL
1	F	867	ALA
1	E	867	ALA
1	G	863	ASP
1	B	863	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	242/285 (85%)	226 (93%)	16 (7%)	16	46
1	B	244/285 (86%)	224 (92%)	20 (8%)	11	36
1	C	244/285 (86%)	230 (94%)	14 (6%)	20	51
1	D	253/285 (89%)	243 (96%)	10 (4%)	31	61
1	E	239/285 (84%)	226 (95%)	13 (5%)	22	53
1	F	235/285 (82%)	222 (94%)	13 (6%)	21	52
1	G	243/285 (85%)	228 (94%)	15 (6%)	18	48
1	H	250/285 (88%)	238 (95%)	12 (5%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1950/2280 (86%)	1837 (94%)	113 (6%)	20	50

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	878	HIS
1	H	982	ASP
1	E	897	ARG
1	H	949	ILE
1	G	989	ILE

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

Mol	Chain	Res	Type
1	B	711	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	VOY	A	1101	1	40,46,46	3.42	22 (55%)	52,64,64	3.42	26 (50%)
2	VOY	G	1101	-	40,46,46	2.74	17 (42%)	52,64,64	3.66	26 (50%)
2	VOY	F	1101	1	40,46,46	3.31	14 (35%)	52,64,64	3.48	25 (48%)
2	VOY	D	1101	1	40,46,46	3.74	21 (52%)	52,64,64	3.32	27 (51%)
2	VOY	B	1101	1	40,46,46	3.03	18 (45%)	52,64,64	3.62	25 (48%)
2	VOY	E	1101	1	40,46,46	3.51	20 (50%)	52,64,64	3.71	27 (51%)
2	VOY	H	1101	1	40,46,46	3.01	14 (35%)	52,64,64	4.01	23 (44%)
2	VOY	C	1101	1	40,46,46	3.53	20 (50%)	52,64,64	3.86	25 (48%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VOY	A	1101	1	-	5/23/23/23	0/5/5/5
2	VOY	G	1101	-	-	7/23/23/23	0/5/5/5
2	VOY	F	1101	1	-	6/23/23/23	0/5/5/5
2	VOY	D	1101	1	-	5/23/23/23	0/5/5/5
2	VOY	B	1101	1	-	7/23/23/23	0/5/5/5
2	VOY	E	1101	1	-	8/23/23/23	0/5/5/5
2	VOY	H	1101	1	-	8/23/23/23	0/5/5/5
2	VOY	C	1101	1	-	5/23/23/23	0/5/5/5

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	VOY	C38-N39	16.12	1.72	1.47
2	D	1101	VOY	C38-N39	13.31	1.67	1.47
2	H	1101	VOY	C38-N39	12.77	1.67	1.47
2	C	1101	VOY	C38-N39	12.19	1.66	1.47
2	E	1101	VOY	C38-N39	11.80	1.65	1.47

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1101	VOY	C38-C37-C36	-15.94	99.02	124.67
2	C	1101	VOY	C38-C37-C36	-14.66	101.07	124.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1101	VOY	C38-C37-C36	-14.38	101.52	124.67
2	E	1101	VOY	C36-C35-N34	11.56	132.44	114.09
2	G	1101	VOY	C38-C37-C36	-11.41	106.31	124.67

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	VOY	C08-C27-C28-N29
2	A	1101	VOY	C30-C27-C28-N29
2	B	1101	VOY	O42-C35-C36-C37
2	B	1101	VOY	N34-C35-C36-C37
2	H	1101	VOY	N34-C35-C36-C37

There are no ring outliers.

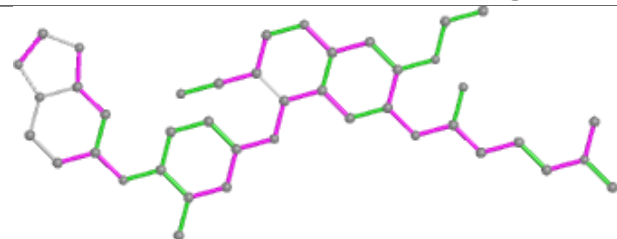
8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	VOY	2	0
2	G	1101	VOY	4	0
2	F	1101	VOY	4	0
2	D	1101	VOY	5	0
2	B	1101	VOY	1	0
2	E	1101	VOY	2	0
2	H	1101	VOY	1	0
2	C	1101	VOY	3	0

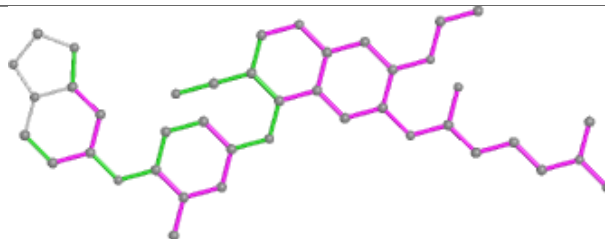
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



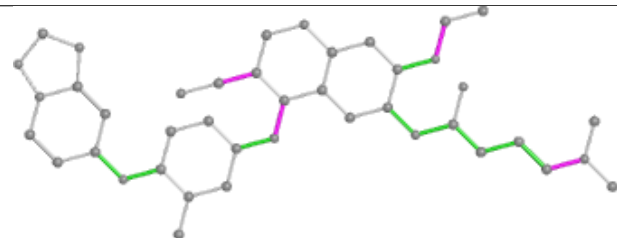
## Ligand VOY A 1101



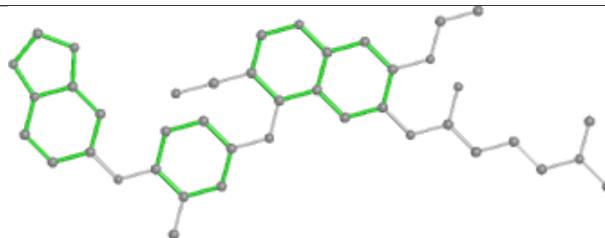
Bond lengths



Bond angles

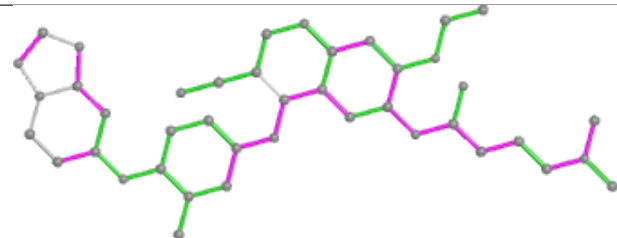


Torsions

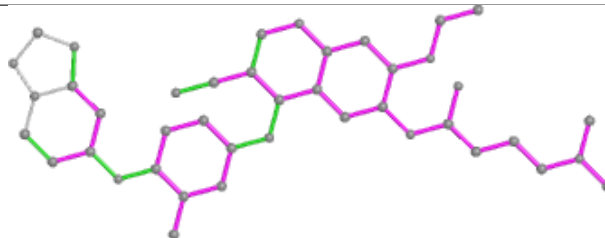


Rings

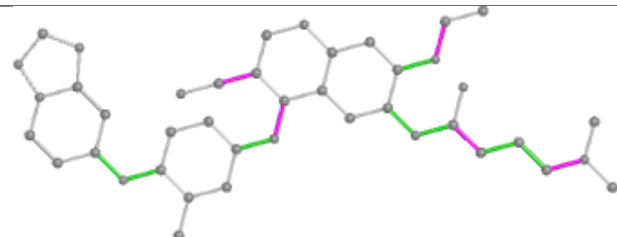
## Ligand VOY G 1101



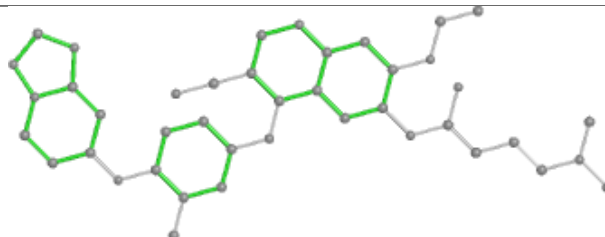
Bond lengths



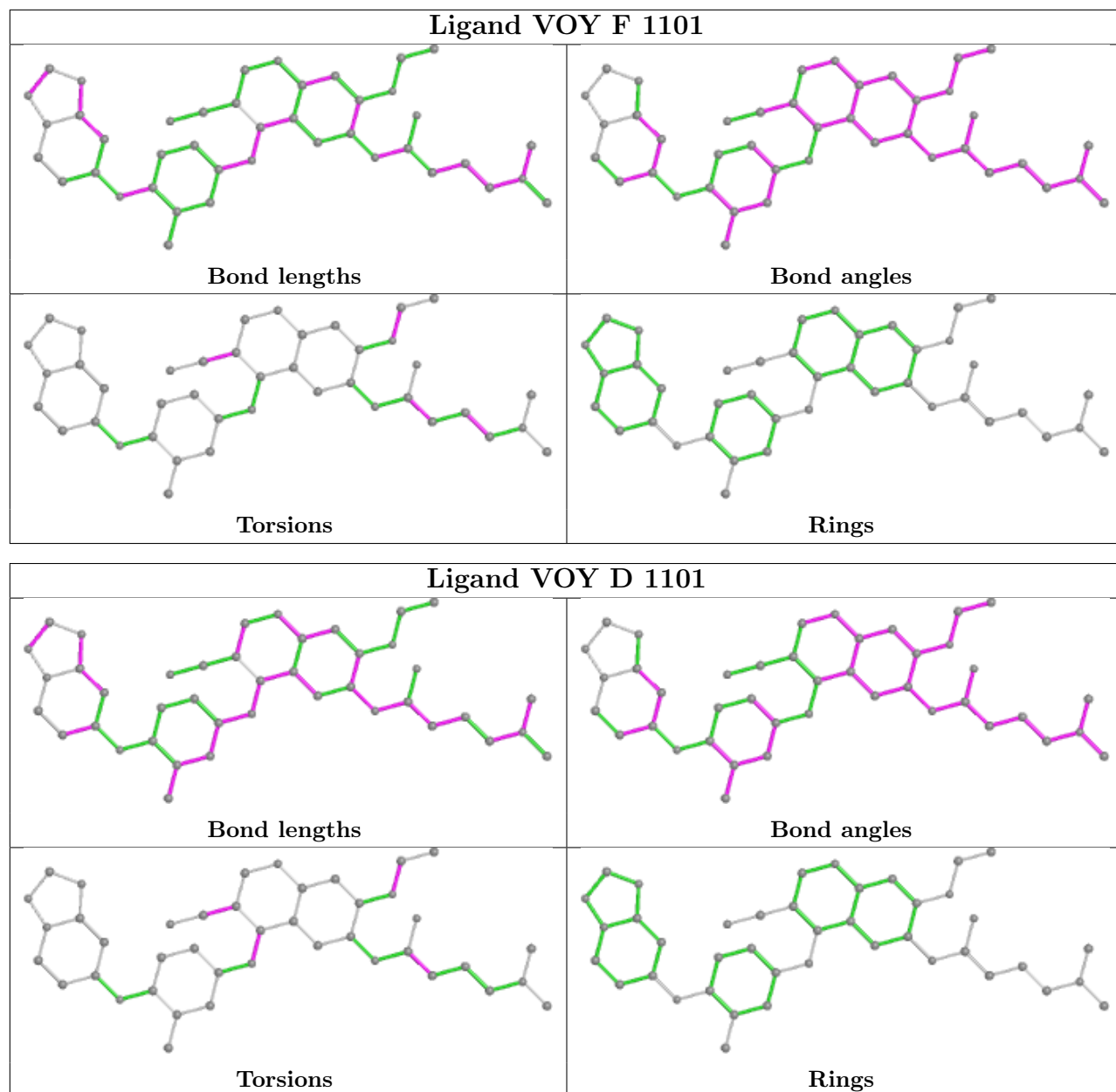
Bond angles



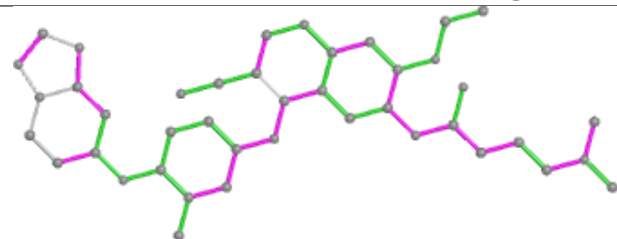
Torsions



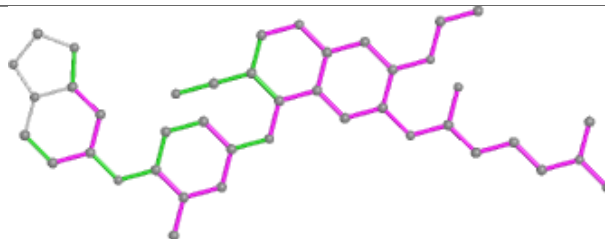
Rings



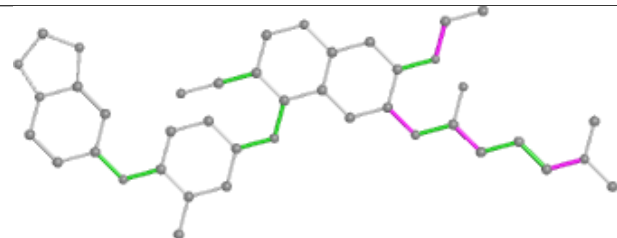
## Ligand VOY B 1101



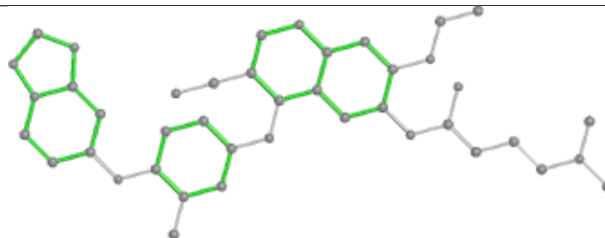
Bond lengths



Bond angles

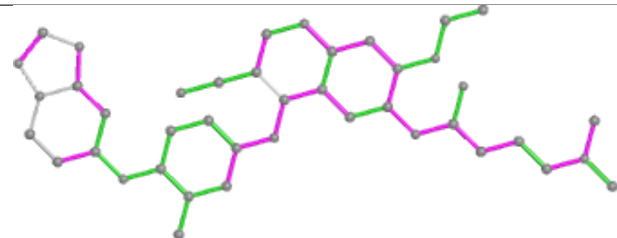


Torsions

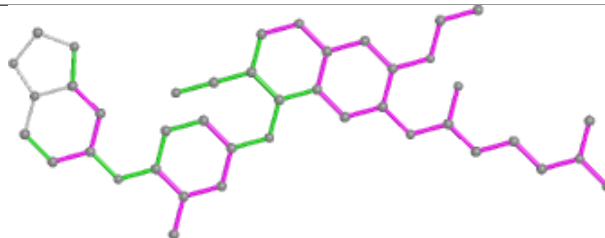


Rings

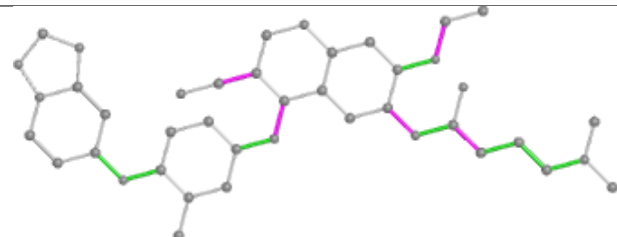
## Ligand VOY E 1101



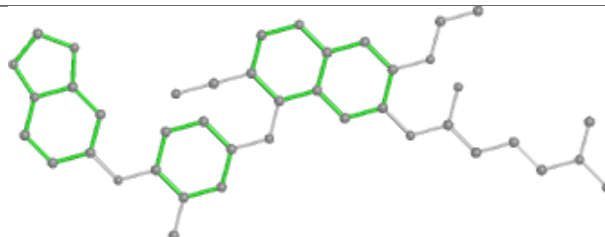
Bond lengths



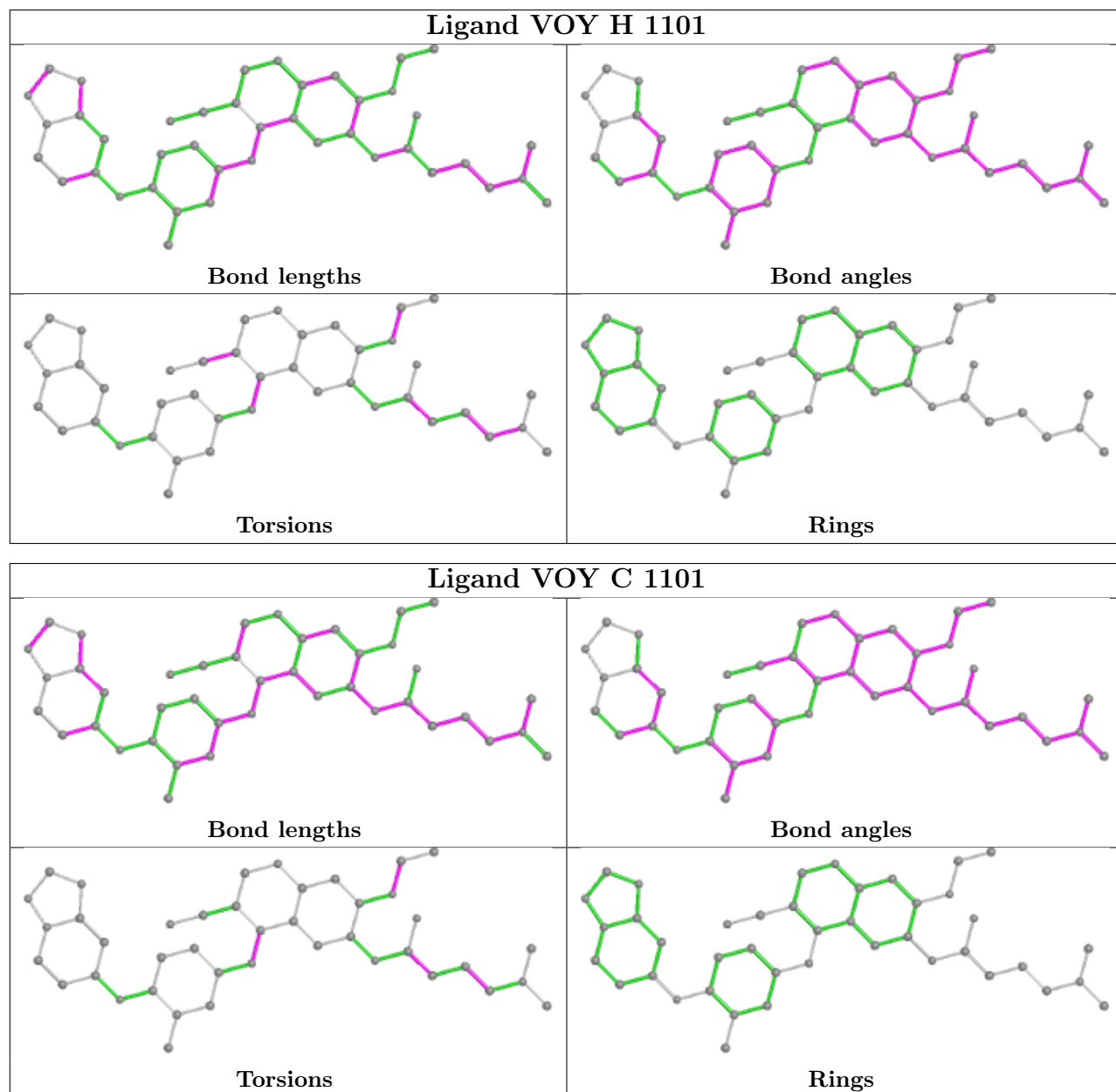
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	272/326 (83%)	0.18	2 (0%) 87 88	28, 59, 104, 147	0
1	B	276/326 (84%)	0.30	8 (2%) 51 50	34, 62, 117, 173	0
1	C	274/326 (84%)	0.16	6 (2%) 62 59	36, 62, 108, 140	0
1	D	283/326 (86%)	0.14	9 (3%) 47 46	26, 56, 110, 138	0
1	E	268/326 (82%)	0.20	7 (2%) 56 52	25, 58, 112, 155	0
1	F	262/326 (80%)	0.28	9 (3%) 45 43	33, 63, 110, 139	0
1	G	273/326 (83%)	0.17	3 (1%) 80 80	34, 61, 114, 173	0
1	H	282/326 (86%)	0.20	3 (1%) 80 80	30, 62, 109, 157	0
All	All	2190/2608 (83%)	0.20	47 (2%) 63 61	25, 60, 111, 173	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	742	ASP	4.4
1	H	745	ASN	4.3
1	B	776	GLY	4.1
1	F	758	ASN	3.7
1	E	982	ASP	3.5

### 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](#)

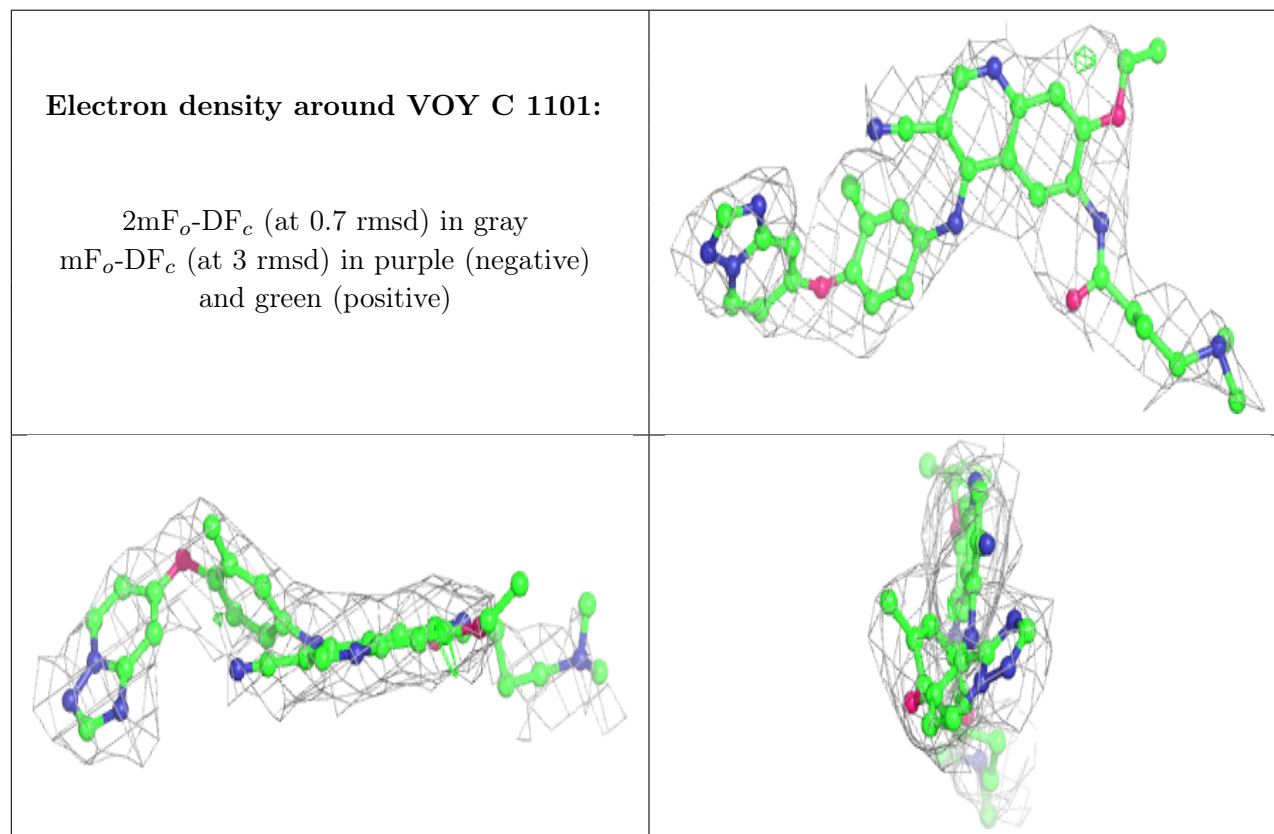
There are no monosaccharides in this entry.

## 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<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.

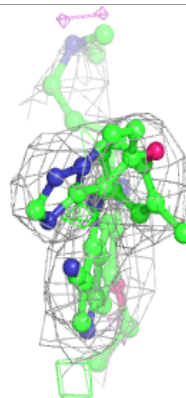
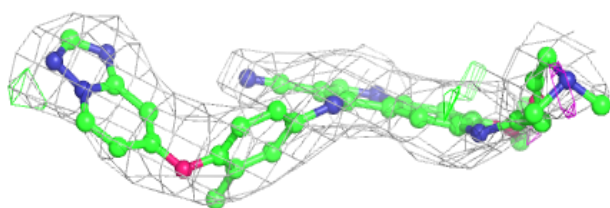
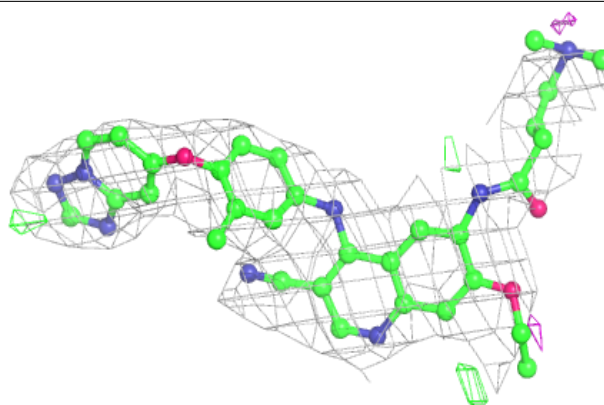
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	VOY	C	1101	42/42	0.88	0.26	39,52,63,68	0
2	VOY	E	1101	42/42	0.89	0.27	31,44,61,68	0
2	VOY	B	1101	42/42	0.90	0.28	33,51,74,82	0
2	VOY	D	1101	42/42	0.91	0.29	25,44,63,65	0
2	VOY	A	1101	42/42	0.91	0.26	25,35,52,56	0
2	VOY	F	1101	42/42	0.92	0.26	33,41,83,99	0
2	VOY	H	1101	42/42	0.92	0.27	23,39,56,59	0
2	VOY	G	1101	42/42	0.93	0.25	16,36,56,60	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.

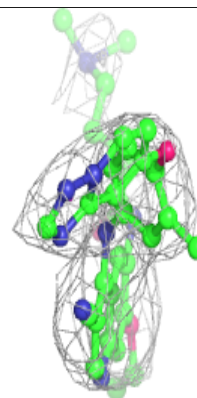
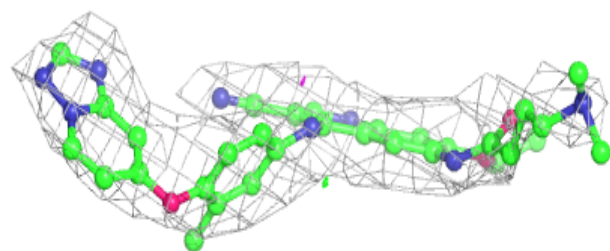
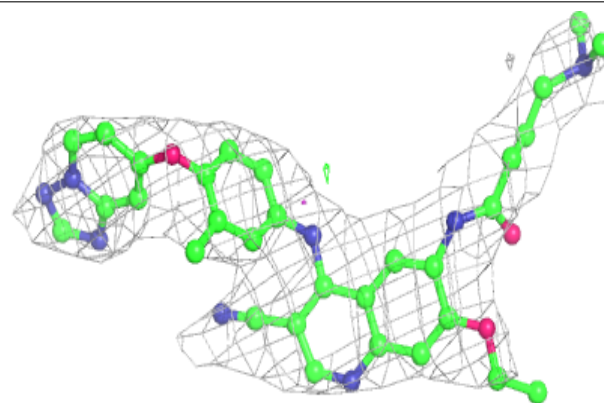


**Electron density around VOY E 1101:**

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

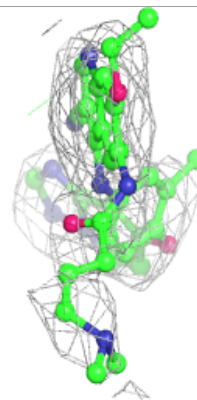
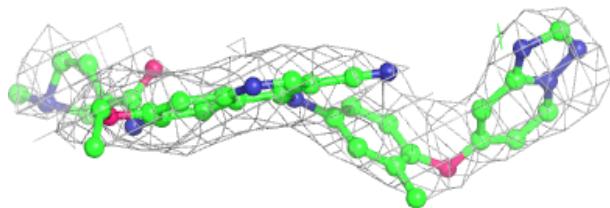
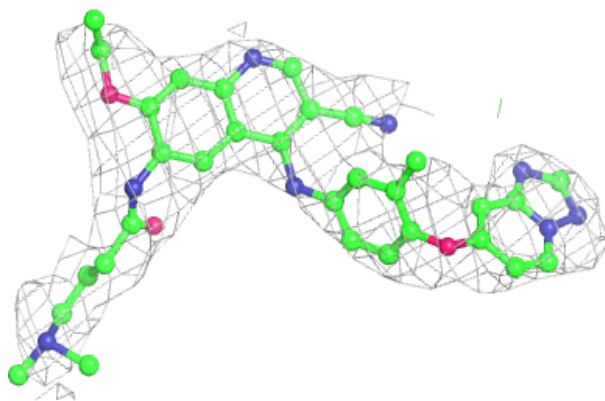
**Electron density around VOY B 1101:**

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

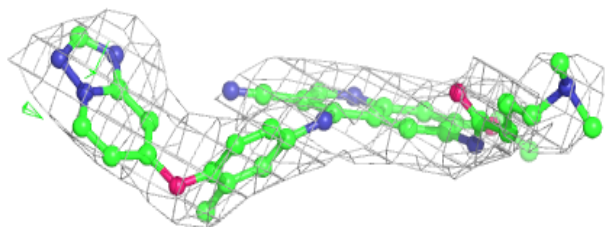
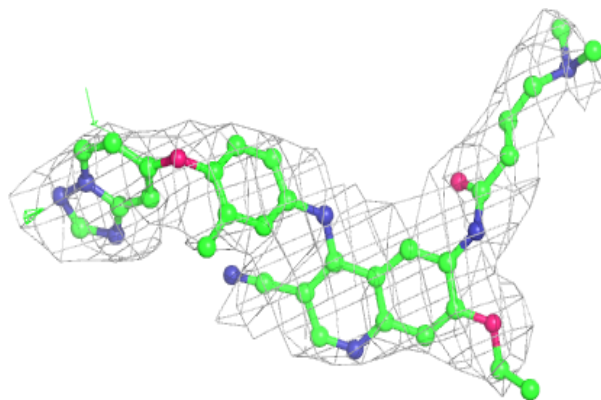


**Electron density around VOY D 1101:**

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

**Electron density around VOY A 1101:**

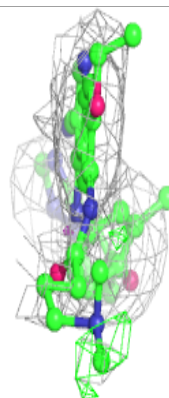
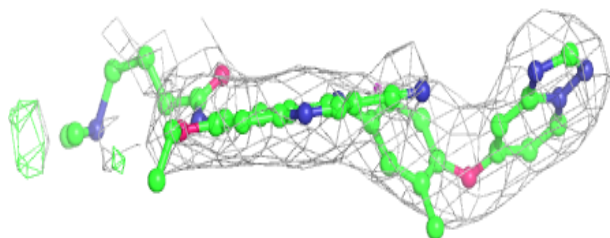
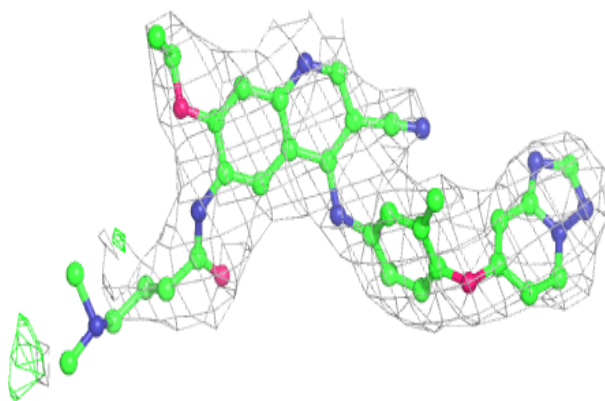
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



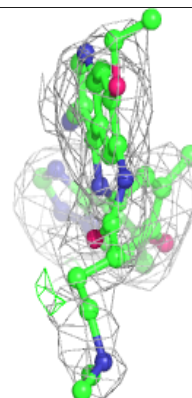
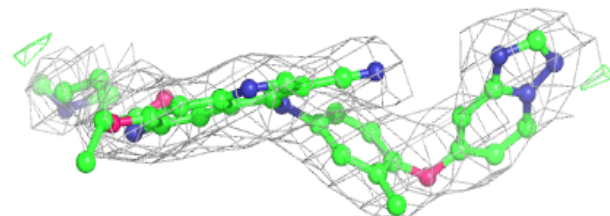
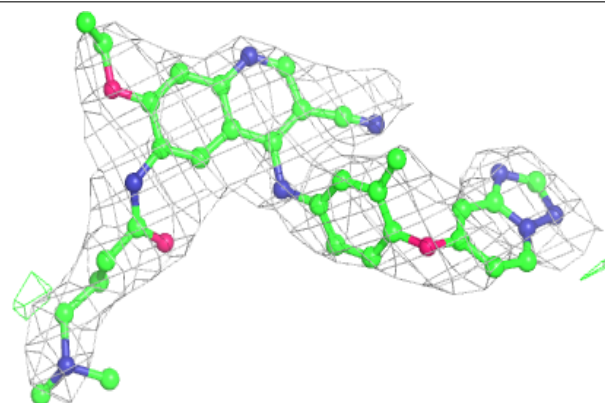


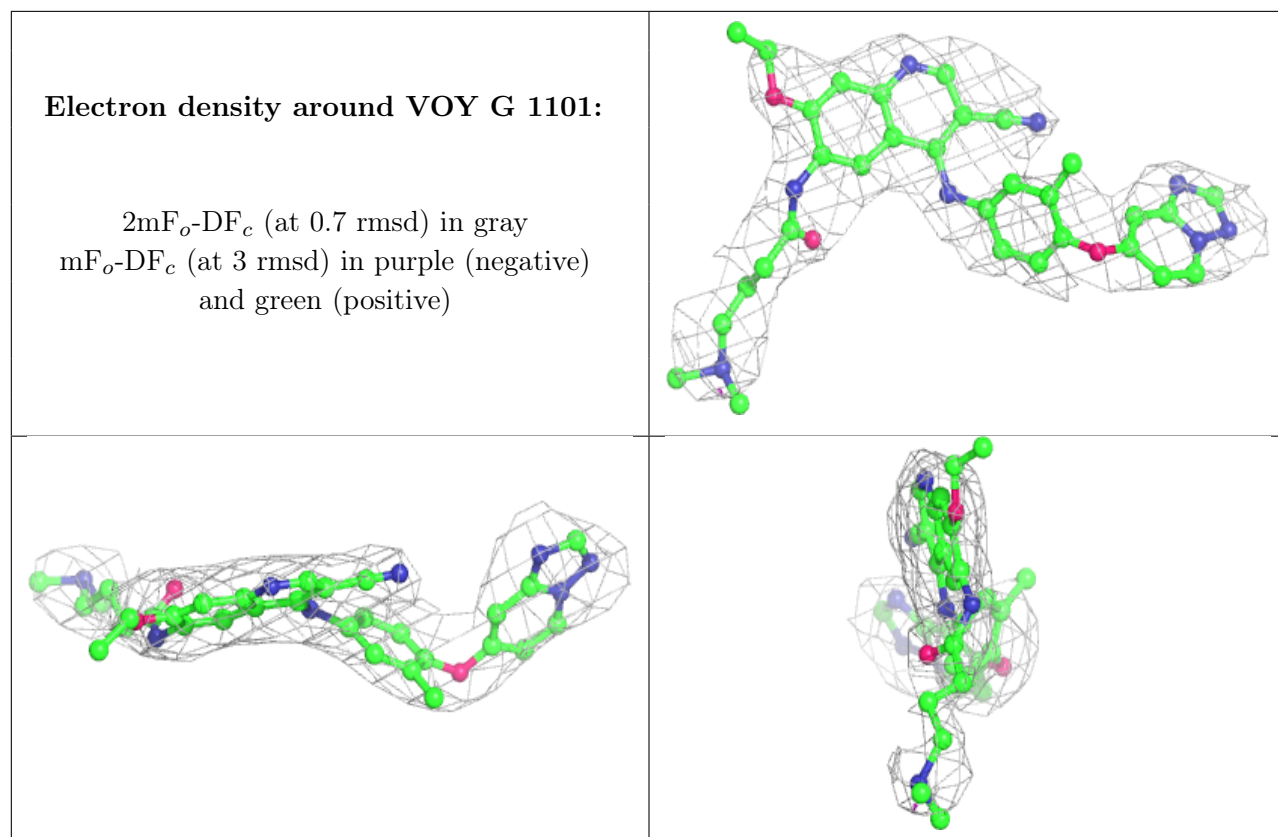
**Electron density around VOY F 1101:**

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

**Electron density around VOY H 1101:**

$2mF_o-DF_c$  (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.