



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:44 AM UTC

PDB ID : 9HYN / pdb\_00009hyn  
Title : CRYSTAL STRUCTURE OF THE SMARCA2-VCB-COMPLEX WITH  
PROTAC P1  
Authors : Bader, G.; Wolkerstorfer, B.  
Deposited on : 2025-01-10  
Resolution : 2.37 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](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.

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)  
Xtriage (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

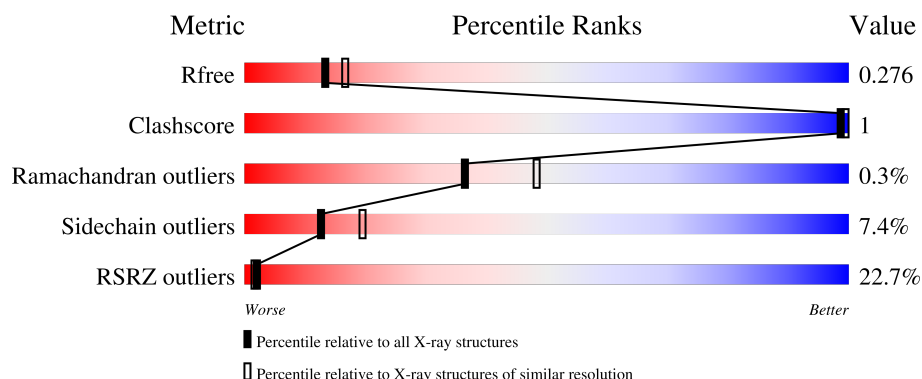
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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.



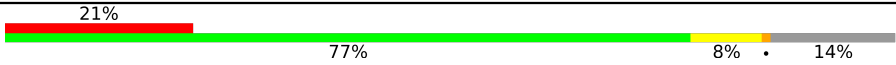


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	104	<div> <div>16%</div> <div>97%</div> </div>
1	D	104	<div> <div>13%</div> <div>94%</div> </div>
2	B	103	<div> <div>10%</div> <div>77%</div> <div>7%</div> <div>16%</div> </div>
2	E	103	<div> <div>21%</div> <div>75%</div> <div>8%</div> <div>16%</div> </div>
3	C	168	<div> <div>23%</div> <div>81%</div> <div>8%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	168	
4	G	129	
4	H	129	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15127 atoms, of which 7508 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 Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	104	Total	C	H	N	O	S	824	0	0
			1647	520	824	138	160	5			
1	D	104	Total	C	H	N	O	S	824	0	0
			1647	520	824	138	160	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	87	Total	C	H	N	O	S	697	0	0
			1391	448	697	111	128	7			
2	E	87	Total	C	H	N	O	S	697	0	0
			1391	448	697	111	128	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
B	113	LEU	-	expression tag	UNP Q15369
B	114	GLU	-	expression tag	UNP Q15369
B	115	LEU	-	expression tag	UNP Q15369
B	116	LEU	-	expression tag	UNP Q15369
B	117	MET	-	expression tag	UNP Q15369
B	118	ALA	-	expression tag	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369
E	113	LEU	-	expression tag	UNP Q15369
E	114	GLU	-	expression tag	UNP Q15369
E	115	LEU	-	expression tag	UNP Q15369
E	116	LEU	-	expression tag	UNP Q15369
E	117	MET	-	expression tag	UNP Q15369
E	118	ALA	-	expression tag	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	150	Total	C	H	N	O	S	1227	0	0
			2455	780	1227	226	220	2			
3	F	145	Total	C	H	N	O	S	1176	0	0
			2365	755	1176	218	214	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337
C	213	THR	-	expression tag	UNP P40337
C	214	GLN	-	expression tag	UNP P40337
C	215	GLU	-	expression tag	UNP P40337
C	216	ARG	-	expression tag	UNP P40337
C	217	ILE	-	expression tag	UNP P40337
C	218	ALA	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337
F	214	THR	-	expression tag	UNP P40337
F	215	GLN	-	expression tag	UNP P40337
F	216	GLU	-	expression tag	UNP P40337
F	217	ARG	-	expression tag	UNP P40337
F	218	ILE	-	expression tag	UNP P40337
F	219	ALA	-	expression tag	UNP P40337

- Molecule 4 is a protein called Isoform Short of Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	G	115	Total	C	H	N	O	S	979	0	0
			1923	601	979	166	174	3			
4	H	114	Total	C	H	N	O	S	968	0	0
			1904	595	968	165	173	3			

There are 16 discrepancies between the modelled and reference sequences:

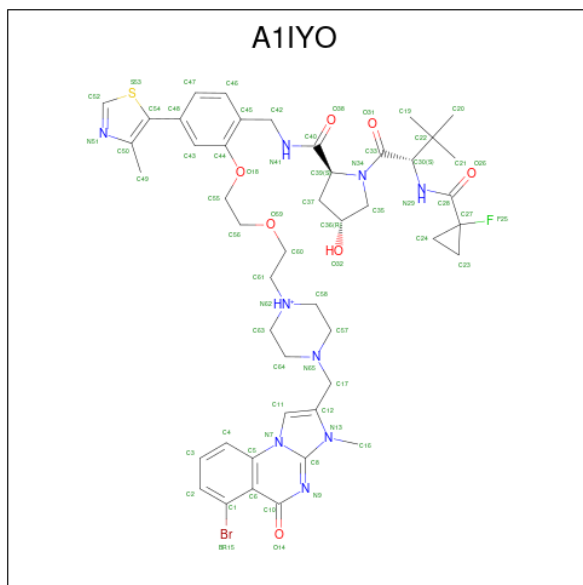
Chain	Residue	Modelled	Actual	Comment	Reference
G	1371	SER	-	expression tag	UNP P51531
G	1372	MET	-	expression tag	UNP P51531
G	1494	LYS	-	expression tag	UNP P51531
G	1495	SER	-	expression tag	UNP P51531
G	1496	ALA	-	expression tag	UNP P51531
G	1497	ARG	-	expression tag	UNP P51531

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1498	GLN	-	expression tag	UNP P51531
G	1499	LYS	-	expression tag	UNP P51531
H	1371	SER	-	expression tag	UNP P51531
H	1372	MET	-	expression tag	UNP P51531
H	1494	LYS	-	expression tag	UNP P51531
H	1495	SER	-	expression tag	UNP P51531
H	1496	ALA	-	expression tag	UNP P51531
H	1497	ARG	-	expression tag	UNP P51531
H	1498	GLN	-	expression tag	UNP P51531
H	1499	LYS	-	expression tag	UNP P51531

- Molecule 5 is (2 {S},4 {R})- {N}-[[2-[2-[2-[4-[(6-bromanyl-3-methyl-5-oxidanylidene-4 {H}-imidazo[1,2-a]quinazolin-2-yl)methyl]piperazin-1-yl]ethoxy]ethoxy]-4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-1-[(2 {S})-2-[(1-fluoranylcyclopropyl)carbonylamino]-3,3-dimethyl-butanoyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: A1IYO) (formula: C<sub>46</sub>H<sub>58</sub>BrFN<sub>9</sub>O<sub>7</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
			Total	Br	C	F	H	N	O	S		
5	C	1	123	1	46	1	58	9	7	1	58	0
5	F	1	123	1	46	1	58	9	7	1	58	0

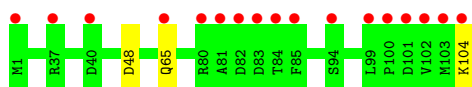
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total 21	O 21	0	0
6	B	11	Total 11	O 11	0	0
6	C	30	Total 30	O 30	0	0
6	D	29	Total 29	O 29	0	0
6	E	12	Total 12	O 12	0	0
6	F	24	Total 24	O 24	0	0
6	G	9	Total 9	O 9	0	0
6	H	22	Total 22	O 22	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.

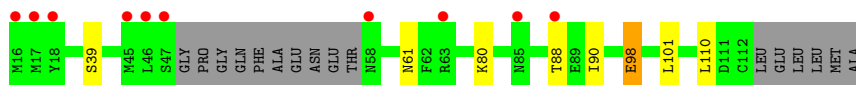
- Molecule 1: Elongin-B



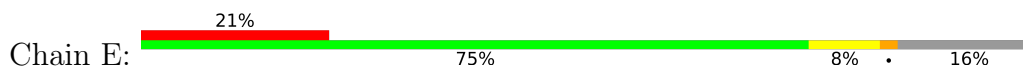
- Molecule 1: Elongin-B



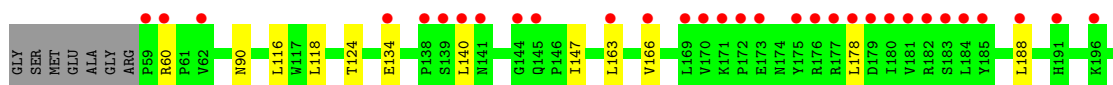
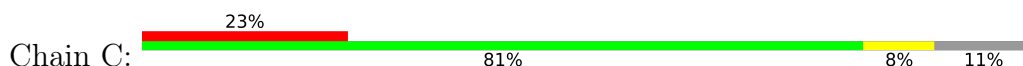
- Molecule 2: Elongin-C



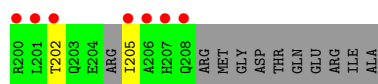
- Molecule 2: Elongin-C



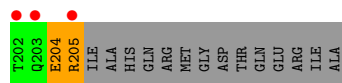
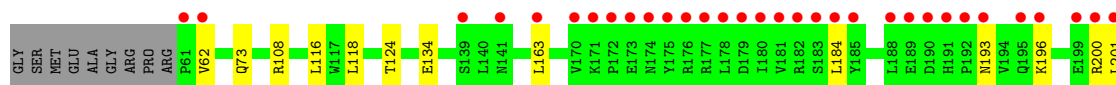
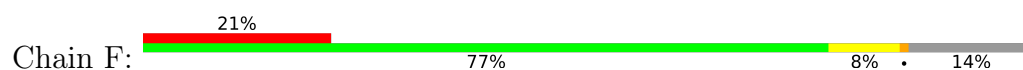
- Molecule 3: von Hippel-Lindau disease tumor suppressor



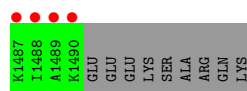
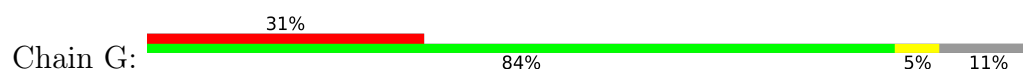




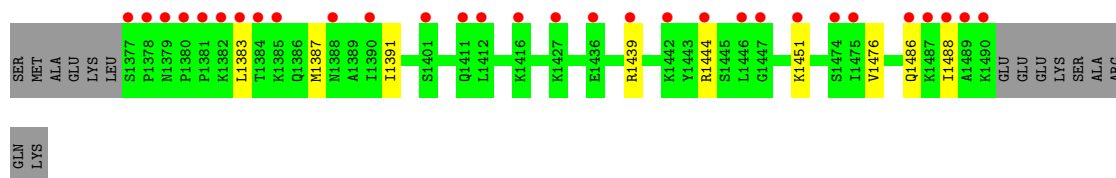
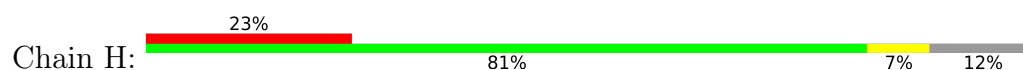
- Molecule 3: von Hippel-Lindau disease tumor suppressor



- Molecule 4: Isoform Short of Probable global transcription activator SNF2L2



- Molecule 4: Isoform Short of Probable global transcription activator SNF2L2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.94Å 118.23Å 122.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.01 – 2.37 45.01 – 2.37	Depositor EDS
% Data completeness (in resolution range)	84.8 (45.01-2.37) 85.2 (45.01-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.246 , 0.262 0.258 , 0.276	Depositor DCC
$R_{free}$ test set	1981 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.3	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 -h,l,k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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 22.03 % 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 6.2015e-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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IYO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.71	0/839	1.00	0/1132
1	D	0.71	0/839	1.00	1/1132 (0.1%)
2	B	0.79	0/708	1.10	2/955 (0.2%)
2	E	0.79	0/708	1.12	2/955 (0.2%)
3	C	0.74	0/1261	1.08	1/1721 (0.1%)
3	F	0.72	0/1220	1.04	0/1664
4	G	0.80	0/960	1.11	0/1289
4	H	0.79	1/952 (0.1%)	1.11	0/1278
All	All	0.75	1/7487 (0.0%)	1.07	6/10126 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1387	MET	SD-CE	-5.42	1.66	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	98	GLU	CB-CG-CD	8.81	127.57	112.60
2	B	98	GLU	CB-CG-CD	8.47	127.01	112.60
2	E	98	GLU	CA-CB-CG	5.95	126.00	114.10
2	B	98	GLU	CA-CB-CG	5.59	125.29	114.10
1	D	65	GLN	CB-CG-CD	5.12	121.30	112.60
3	C	90	ASN	CA-CB-CG	5.07	117.67	112.60

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	823	824	824	0	0
1	D	823	824	824	2	0
2	B	694	697	697	0	0
2	E	694	697	697	1	0
3	C	1228	1227	1227	1	0
3	F	1189	1176	1189	3	0
4	G	944	979	979	0	0
4	H	936	968	968	0	0
5	C	65	58	0	1	0
5	F	65	58	0	1	0
6	A	21	0	0	0	0
6	B	11	0	0	0	0
6	C	30	0	0	0	0
6	D	29	0	0	0	0
6	E	12	0	0	0	0
6	F	24	0	0	0	0
6	G	9	0	0	0	0
6	H	22	0	0	0	0
All	All	7619	7508	7405	8	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 1.

All (8) 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)
3:F:205:ARG:HG2	3:F:205:ARG:O	1.94	0.67
3:F:204:GLU:HG3	3:F:204:GLU:O	1.97	0.63
3:F:201:LEU:O	3:F:204:GLU:HG2	2.01	0.60
5:F:301:A1IYO:BR15	5:F:301:A1IYO:O14	2.80	0.53
5:C:301:A1IYO:O14	5:C:301:A1IYO:BR15	2.80	0.53
3:C:166:VAL:HG13	3:C:188:LEU:HD11	1.94	0.49
1:D:3:VAL:HG12	1:D:67:ALA:HB3	1.94	0.48
1:D:103:MET:SD	2:E:101:LEU:HD21	2.59	0.43

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	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
1	D	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
2	B	83/103 (81%)	82 (99%)	1 (1%)	0	100	100
2	E	83/103 (81%)	82 (99%)	0	1 (1%)	10	14
3	C	148/168 (88%)	142 (96%)	5 (3%)	1 (1%)	18	26
3	F	143/168 (85%)	134 (94%)	8 (6%)	1 (1%)	18	26
4	G	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
4	H	112/129 (87%)	109 (97%)	3 (3%)	0	100	100
All	All	886/1008 (88%)	855 (96%)	28 (3%)	3 (0%)	36	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	60	ARG
2	E	17	MET
3	F	62	VAL

### 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	92/92 (100%)	89 (97%)	3 (3%)	33	52
1	D	92/92 (100%)	88 (96%)	4 (4%)	26	41
2	B	79/91 (87%)	71 (90%)	8 (10%)	7	10
2	E	79/91 (87%)	70 (89%)	9 (11%)	5	7
3	C	140/153 (92%)	130 (93%)	10 (7%)	13	21
3	F	136/153 (89%)	123 (90%)	13 (10%)	8	11
4	G	108/120 (90%)	101 (94%)	7 (6%)	15	24
4	H	107/120 (89%)	99 (92%)	8 (8%)	12	19
All	All	833/912 (91%)	771 (93%)	62 (7%)	13	19

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	65	GLN
1	A	104	LYS
2	B	39	SER
2	B	61	ASN
2	B	80	LYS
2	B	88	THR
2	B	90	ILE
2	B	98	GLU
2	B	101	LEU
2	B	110	LEU
3	C	116	LEU
3	C	118	LEU
3	C	124	THR
3	C	134	GLU
3	C	140	LEU
3	C	147	ILE
3	C	163	LEU
3	C	178	LEU
3	C	202	THR
3	C	205	ILE
1	D	3	VAL
1	D	48	ASP
1	D	65	GLN
1	D	66	THR
2	E	34	GLU
2	E	37	LEU

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Mol	Chain	Res	Type
2	E	39	SER
2	E	61	ASN
2	E	80	LYS
2	E	88	THR
2	E	90	ILE
2	E	98	GLU
2	E	101	LEU
3	F	73	GLN
3	F	108	ARG
3	F	116	LEU
3	F	118	LEU
3	F	124	THR
3	F	134	GLU
3	F	163	LEU
3	F	184	LEU
3	F	193	ASN
3	F	196	LYS
3	F	200	ARG
3	F	204	GLU
3	F	205	ARG
4	G	1377	SER
4	G	1382	LYS
4	G	1412	LEU
4	G	1418	LEU
4	G	1435	LYS
4	G	1451	LYS
4	G	1476	VAL
4	H	1383	LEU
4	H	1391	ILE
4	H	1439	ARG
4	H	1444	ARG
4	H	1451	LYS
4	H	1476	VAL
4	H	1486	GLN
4	H	1488	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	HIS
2	B	108	ASN
3	C	67	ASN

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Mol	Chain	Res	Type
3	C	131	ASN
3	C	208	GLN
2	E	35	HIS
4	G	1388	ASN
4	H	1486	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
5	A1IYO	C	301	-	69,72,72	0.43	0	92,107,107	0.99	4 (4%)
5	A1IYO	F	301	-	69,72,72	0.42	0	92,107,107	1.11	4 (4%)

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
5	A1IYO	C	301	-	-	5/48/76/76	0/8/8/8
5	A1IYO	F	301	-	-	5/48/76/76	0/8/8/8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	301	A1IYO	C17-C12-N13	5.79	129.25	123.01
5	C	301	A1IYO	C17-C12-N13	4.81	128.19	123.01
5	F	301	A1IYO	C17-C12-C11	-4.67	123.26	130.75
5	F	301	A1IYO	C24-C27-C28	4.58	125.56	116.20
5	C	301	A1IYO	C17-C12-C11	-4.06	124.24	130.75
5	C	301	A1IYO	C24-C27-C28	3.40	123.13	116.20
5	C	301	A1IYO	C23-C27-C28	2.72	121.75	116.20
5	F	301	A1IYO	C60-C61-N62	2.28	119.80	113.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	A1IYO	C60-C61-N62-C58
5	F	301	A1IYO	C60-C61-N62-C58
5	F	301	A1IYO	O18-C55-C56-O59
5	C	301	A1IYO	C60-C61-N62-C63
5	F	301	A1IYO	C60-C61-N62-C63
5	C	301	A1IYO	C56-C55-O18-C44
5	C	301	A1IYO	O59-C60-C61-N62
5	C	301	A1IYO	C55-C56-O59-C60
5	F	301	A1IYO	C43-C44-O18-C55
5	F	301	A1IYO	C45-C44-O18-C55

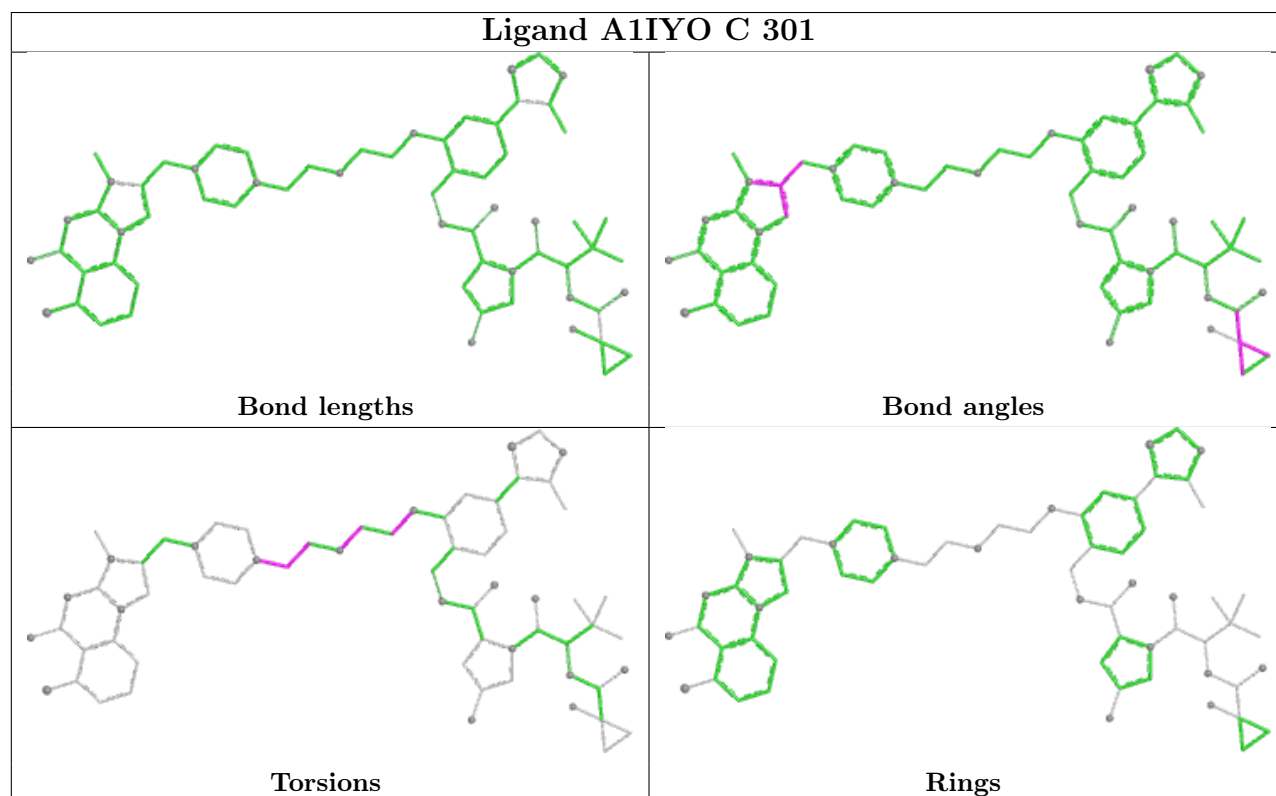
There are no ring outliers.

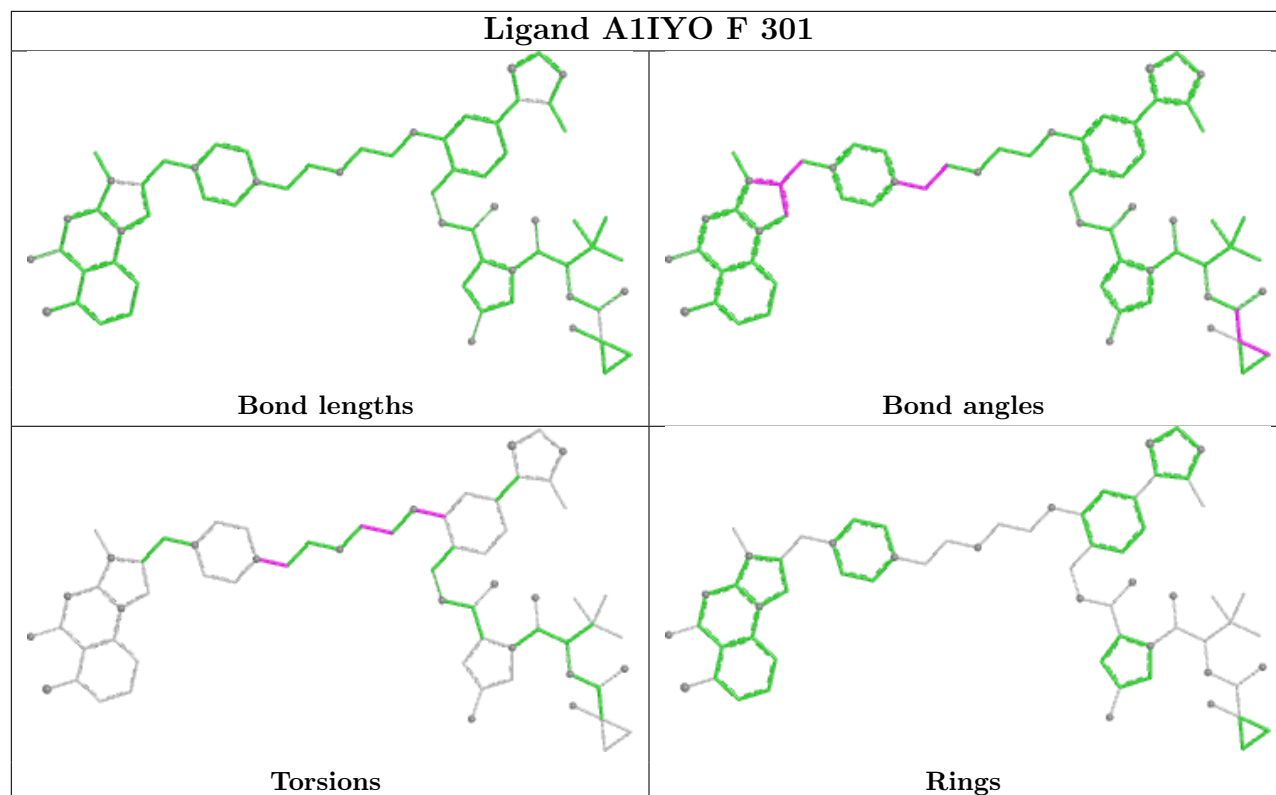
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	A1IYO	1	0
5	F	301	A1IYO	1	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

### 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<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	104/104 (100%)	1.05	17 (16%)	4 4	12, 24, 53, 78	0
1	D	104/104 (100%)	0.79	14 (13%)	7 6	10, 20, 43, 79	0
2	B	87/103 (84%)	0.93	10 (11%)	9 8	14, 23, 39, 61	0
2	E	87/103 (84%)	1.27	22 (25%)	1 1	15, 25, 41, 63	0
3	C	150/168 (89%)	1.22	38 (25%)	1 1	11, 23, 50, 69	0
3	F	145/168 (86%)	1.20	35 (24%)	2 1	10, 21, 58, 73	0
4	G	115/129 (89%)	1.80	40 (34%)	1 0	18, 33, 49, 56	0
4	H	114/129 (88%)	1.24	30 (26%)	1 1	11, 26, 42, 57	0
All	All	906/1008 (89%)	1.20	206 (22%)	2 2	10, 24, 50, 79	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ASP	8.4
3	F	181	VAL	6.7
1	D	81	ALA	6.3
3	C	140	LEU	5.9
3	C	59	PRO	5.3
3	F	175	TYR	5.2
3	F	182	ARG	5.2
1	A	81	ALA	5.2
3	C	180	ILE	5.2
3	F	180	ILE	5.2
3	F	176	ARG	5.1
2	B	88	THR	5.1
4	G	1488	ILE	5.0
3	F	184	LEU	5.0
3	C	141	ASN	5.0
4	H	1490	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	103	MET	4.9
3	F	178	LEU	4.9
3	C	205	ILE	4.7
2	E	47	SER	4.6
3	F	205	ARG	4.6
4	H	1488	ILE	4.6
2	E	37	LEU	4.5
1	A	99	LEU	4.5
2	B	16	MET	4.5
2	E	16	MET	4.5
1	D	102	VAL	4.4
4	G	1490	LYS	4.4
1	A	102	VAL	4.4
3	F	185	TYR	4.4
3	F	188	LEU	4.3
4	G	1381	PRO	4.3
3	C	181	VAL	4.3
4	G	1489	ALA	4.2
4	H	1377	SER	4.2
3	F	177	ARG	4.1
3	F	173	GLU	4.1
3	C	207	HIS	4.1
4	G	1376	LEU	4.0
4	G	1383	LEU	4.0
1	A	103	MET	4.0
3	C	175	TYR	4.0
2	B	47	SER	4.0
1	D	99	LEU	3.9
3	F	174	ASN	3.9
3	C	202	THR	3.9
4	G	1379	ASN	3.9
3	C	206	ALA	3.8
4	G	1387	MET	3.8
2	B	46	LEU	3.7
3	C	184	LEU	3.7
4	G	1426	ARG	3.7
3	C	183	SER	3.7
2	E	88	THR	3.6
3	F	183	SER	3.6
3	F	172	PRO	3.5
4	G	1382	LYS	3.5
4	G	1481	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	104	LYS	3.5
1	D	1	MET	3.4
3	C	172	PRO	3.4
4	H	1451	LYS	3.4
3	F	196	LYS	3.4
3	C	139	SER	3.4
4	G	1391	ILE	3.4
3	C	144	GLY	3.4
3	C	134	GLU	3.3
4	G	1441	HIS	3.3
3	C	166	VAL	3.3
4	H	1489	ALA	3.2
2	E	46	LEU	3.2
4	G	1435	LYS	3.2
4	G	1485	ARG	3.2
1	A	83	ASP	3.2
4	G	1451	LYS	3.2
3	C	176	ARG	3.1
4	G	1443	TYR	3.1
1	A	100	PRO	3.1
3	F	61	PRO	3.1
1	D	100	PRO	3.1
3	F	193	ASN	3.1
4	H	1487	LYS	3.0
4	G	1442	LYS	3.0
4	H	1379	ASN	3.0
3	C	178	LEU	3.0
4	H	1383	LEU	3.0
3	F	192	PRO	3.0
2	E	17	MET	2.9
4	G	1388	ASN	2.9
4	G	1487	LYS	2.9
4	H	1388	ASN	2.9
4	H	1382	LYS	2.9
3	C	179	ASP	2.9
4	H	1447	GLY	2.8
4	H	1380	PRO	2.8
4	H	1381	PRO	2.8
1	A	84	THR	2.8
4	G	1384	THR	2.8
3	F	191	HIS	2.8
4	G	1424	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	G	1385	LYS	2.8
3	C	177	ARG	2.8
4	H	1439	ARG	2.8
2	E	85	ASN	2.8
1	D	66	THR	2.7
3	F	62	VAL	2.7
1	D	101	ASP	2.7
1	A	104	LYS	2.7
3	C	201	LEU	2.7
2	B	58	ASN	2.7
4	H	1436	GLU	2.7
4	G	1380	PRO	2.7
3	C	145	GLN	2.6
4	G	1486	GLN	2.6
1	A	101	ASP	2.6
4	G	1448	ASP	2.6
3	C	171	LYS	2.6
3	F	141	ASN	2.6
3	F	179	ASP	2.6
2	E	43	LYS	2.6
4	H	1486	GLN	2.5
3	C	182	ARG	2.5
3	F	201	LEU	2.5
1	A	40	ASP	2.5
2	E	44	ALA	2.5
4	H	1385	LYS	2.5
3	C	208	GLN	2.5
4	G	1411	GLN	2.5
3	C	185	TYR	2.4
2	B	45	MET	2.4
2	B	63	ARG	2.4
1	D	97	PRO	2.4
3	F	139	SER	2.4
4	H	1401	SER	2.4
4	H	1474	SER	2.4
4	G	1395	ILE	2.4
3	C	188	LEU	2.4
3	F	190	ASP	2.4
1	A	85	PHE	2.4
2	E	105	MET	2.4
4	H	1446	LEU	2.4
4	H	1411	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	98	GLU	2.4
3	C	173	GLU	2.4
3	F	171	LYS	2.3
1	A	94	SER	2.3
3	C	62	VAL	2.3
3	F	170	VAL	2.3
4	G	1425	ILE	2.3
3	C	169	LEU	2.3
3	F	203	GLN	2.3
4	G	1418	LEU	2.3
2	E	58	ASN	2.3
3	F	200	ARG	2.3
4	H	1475	ILE	2.3
3	C	138	PRO	2.3
4	H	1378	PRO	2.3
4	H	1390	ILE	2.3
2	E	112	CYS	2.3
3	C	191	HIS	2.3
3	C	163	LEU	2.2
3	F	163	LEU	2.2
1	A	1	MET	2.2
4	H	1444	ARG	2.2
4	G	1445	SER	2.2
4	H	1427	LYS	2.2
2	E	101	LEU	2.2
2	B	17	MET	2.2
2	E	40	GLY	2.2
2	E	45	MET	2.2
4	G	1422	TYR	2.2
2	E	99	ILE	2.2
1	A	80	ARG	2.2
3	C	200	ARG	2.2
2	E	61	ASN	2.2
1	A	65	GLN	2.2
1	D	95	SER	2.2
2	E	42	ILE	2.1
4	G	1390	ILE	2.1
4	G	1446	LEU	2.1
4	G	1427	LYS	2.1
1	D	65	GLN	2.1
1	D	94	SER	2.1
1	A	37	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	196	LYS	2.1
4	G	1398	LYS	2.1
3	C	170	VAL	2.1
3	F	202	THR	2.1
3	F	199	GLU	2.1
4	H	1412	LEU	2.1
2	E	108	ASN	2.1
4	G	1439	ARG	2.1
4	H	1442	LYS	2.1
2	E	110	LEU	2.1
2	B	18	TYR	2.1
2	E	33	ARG	2.1
4	G	1444	ARG	2.1
2	E	59	GLU	2.0
4	G	1389	ALA	2.0
3	F	195	GLN	2.0
3	C	60	ARG	2.0
3	F	189	GLU	2.0
4	H	1384	THR	2.0
2	B	85	ASN	2.0
4	G	1438	ILE	2.0
4	H	1416	LYS	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 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.

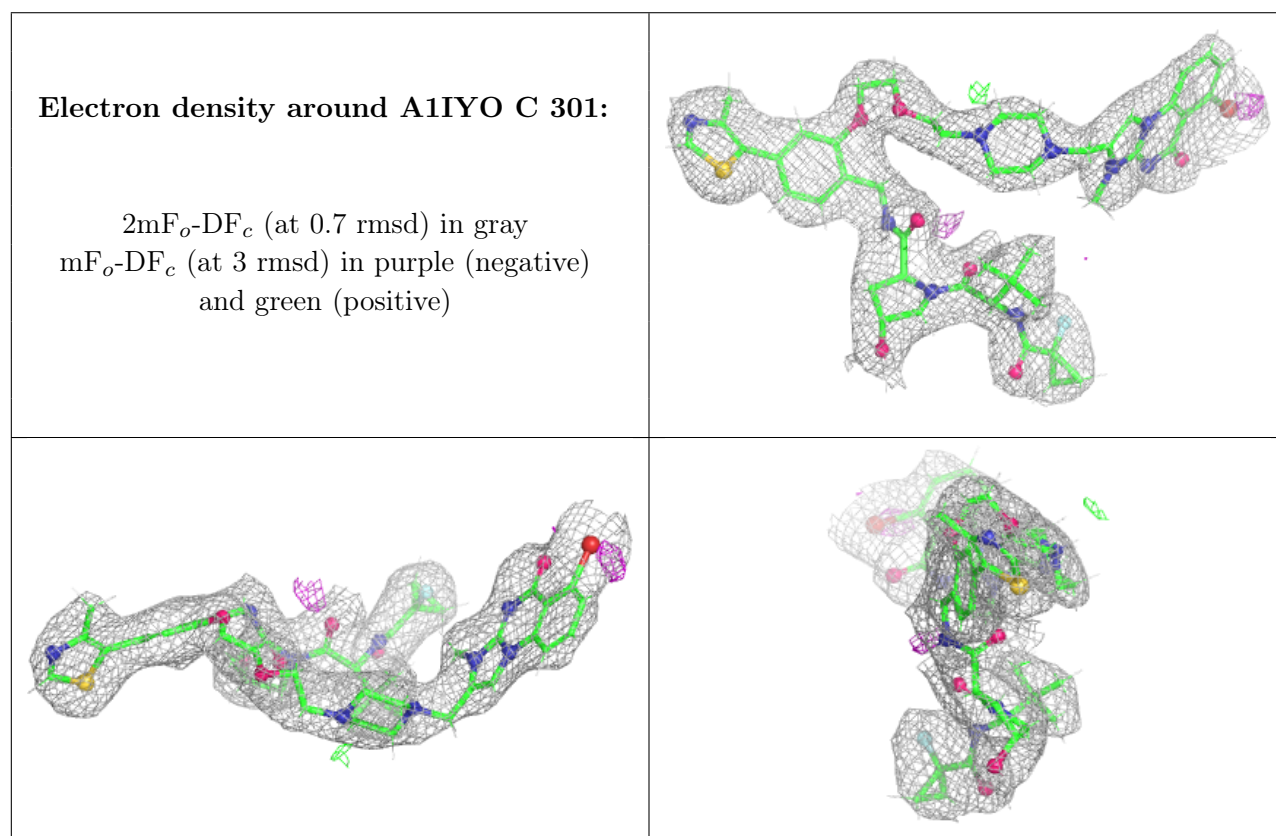
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	AIYO	C	301	65/65	0.96	0.08	27,34,53,55	58

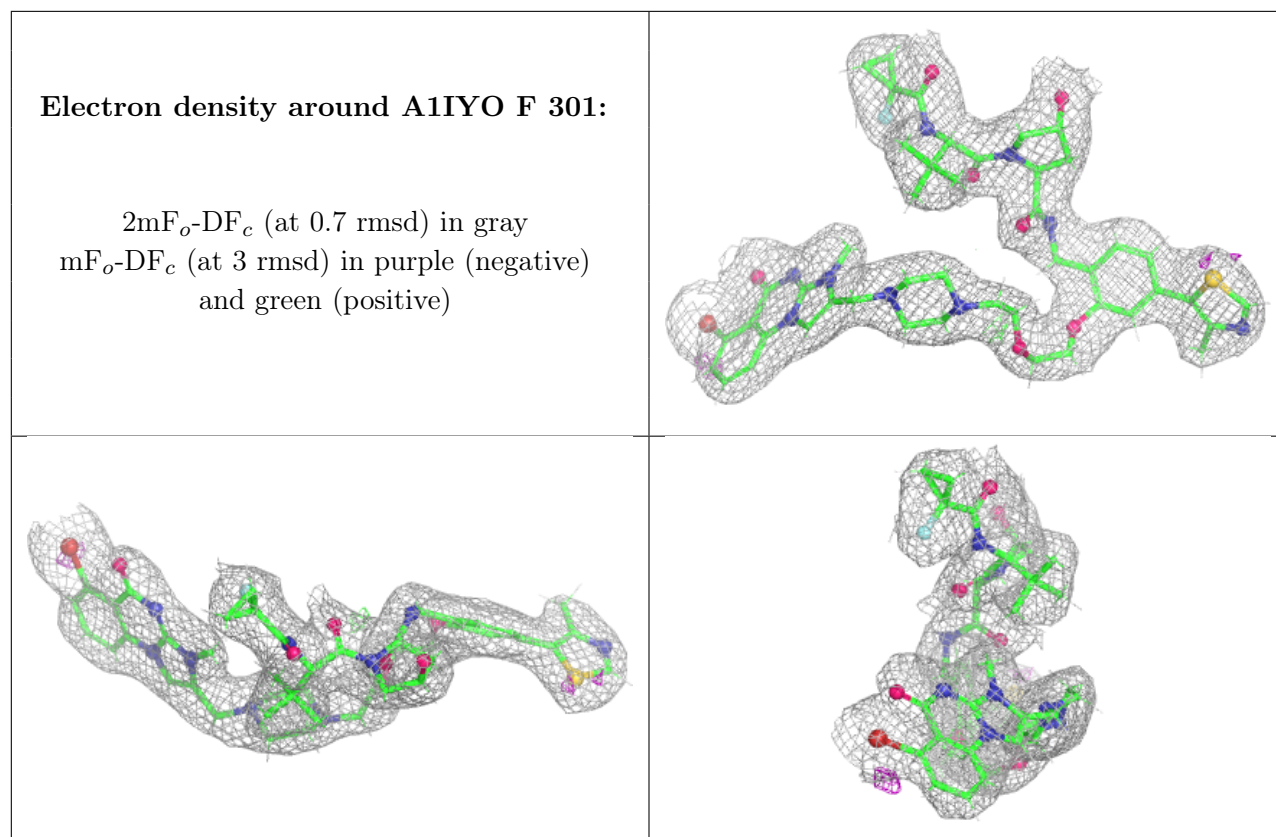
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	A1IYO	F	301	65/65	0.96	0.07	22,27,35,42	58

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.