



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2025 – 01:04 PM EDT

PDB ID : 9DTY / pdb\_00009dtY  
Title : Crystal structure of PRT3789 in complex with the bromodomain of human BRM (SMARCA2) and pVHL:ElonginC:ElonginB  
Authors : Dou, Y.; Wang, M.; Xu, C.  
Deposited on : 2024-10-02  
Resolution : 3.19 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.

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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

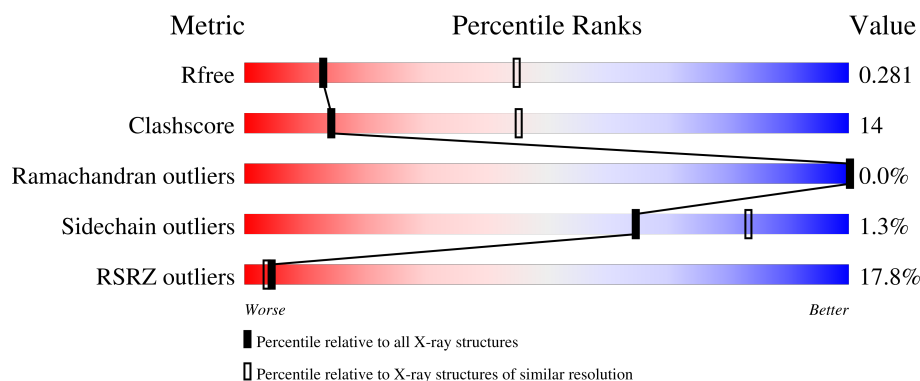
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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))
$R_{free}$	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	120	<div> <div>24%</div> <div> <div>70%</div> <div>19%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	120	<div> <div>53%</div> <div> <div>72%</div> <div>7%</div> <div>•</div> <div>20%</div> </div> </div>
1	I	120	<div> <div>49%</div> <div> <div>60%</div> <div>19%</div> <div>•</div> <div>18%</div> </div> </div>
1	M	120	<div> <div>37%</div> <div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
1	Q	120	<div> <div>46%</div> <div> <div>54%</div> <div>17%</div> <div>•</div> <div>28%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	U	120	
1	Y	120	
1	c	120	
1	g	120	
1	k	120	
2	B	161	
2	F	161	
2	J	161	
2	N	161	
2	R	161	
2	V	161	
2	Z	161	
2	d	161	
2	h	161	
2	l	161	
3	C	96	
3	G	96	
3	K	96	
3	O	96	
3	S	96	
3	W	96	
3	a	96	
3	e	96	
3	i	96	
3	m	96	

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Mol	Chain	Length	Quality of chain
4	D	104	
4	H	104	
4	L	104	
4	P	104	
4	T	104	
4	X	104	
4	b	104	
4	f	104	
4	j	104	
4	n	104	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36947 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 Isoform Short of Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			901	572	158	168	3			
1	E	96	Total	C	N	O	S	0	0	0
			798	505	141	149	3			
1	I	99	Total	C	N	O	S	0	0	0
			825	526	145	151	3			
1	M	109	Total	C	N	O	S	0	0	0
			901	572	158	168	3			
1	Q	86	Total	C	N	O	S	0	0	0
			706	447	128	128	3			
1	U	109	Total	C	N	O	S	0	0	0
			901	572	158	168	3			
1	Y	109	Total	C	N	O	S	0	0	0
			901	572	158	168	3			
1	c	109	Total	C	N	O	S	0	0	0
			901	572	158	168	3			
1	g	109	Total	C	N	O	S	0	0	0
			901	572	158	168	3			
1	k	109	Total	C	N	O	S	0	0	0
			901	572	158	168	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P51531
E	1	SER	-	expression tag	UNP P51531
I	1	SER	-	expression tag	UNP P51531
M	1	SER	-	expression tag	UNP P51531
Q	1	SER	-	expression tag	UNP P51531
U	1	SER	-	expression tag	UNP P51531
Y	1	SER	-	expression tag	UNP P51531
c	1	SER	-	expression tag	UNP P51531

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Chain	Residue	Modelled	Actual	Comment	Reference
g	1	SER	-	expression tag	UNP P51531
k	1	SER	-	expression tag	UNP P51531

- Molecule 2 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	1	0
			1224	776	227	219	2			
2	F	151	Total	C	N	O	S	0	0	0
			1240	786	230	221	3			
2	J	149	Total	C	N	O	S	0	0	0
			1221	775	225	219	2			
2	N	150	Total	C	N	O	S	0	0	0
			1232	781	229	220	2			
2	R	148	Total	C	N	O	S	0	0	0
			1214	770	224	218	2			
2	V	149	Total	C	N	O	S	0	0	0
			1221	775	225	219	2			
2	Z	150	Total	C	N	O	S	0	0	0
			1232	781	229	220	2			
2	d	148	Total	C	N	O	S	0	0	0
			1214	770	224	218	2			
2	h	149	Total	C	N	O	S	0	0	0
			1221	775	225	219	2			
2	l	146	Total	C	N	O	S	0	0	0
			1197	761	219	215	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P40337
F	1	GLY	-	expression tag	UNP P40337
J	1	GLY	-	expression tag	UNP P40337
N	1	GLY	-	expression tag	UNP P40337
R	1	GLY	-	expression tag	UNP P40337
V	1	GLY	-	expression tag	UNP P40337
Z	1	GLY	-	expression tag	UNP P40337
d	1	GLY	-	expression tag	UNP P40337
h	1	GLY	-	expression tag	UNP P40337
l	1	GLY	-	expression tag	UNP P40337

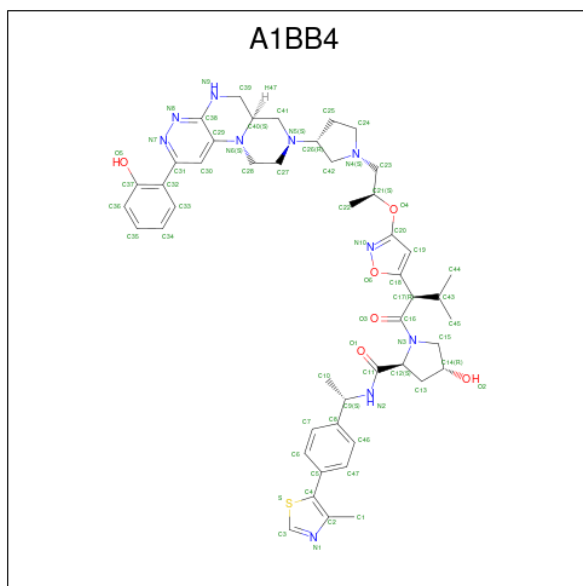
- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	87	Total	C	N	O	S	0	0	0
			693	447	111	129	6			
3	G	89	Total	C	N	O	S	0	0	0
			710	456	114	134	6			
3	K	92	Total	C	N	O	S	0	0	0
			735	473	117	139	6			
3	O	89	Total	C	N	O	S	0	0	0
			705	454	113	133	5			
3	S	91	Total	C	N	O	S	0	0	0
			717	461	116	134	6			
3	W	88	Total	C	N	O	S	0	0	0
			702	452	112	132	6			
3	a	93	Total	C	N	O	S	0	0	0
			734	470	119	139	6			
3	e	92	Total	C	N	O	S	0	0	0
			730	468	117	139	6			
3	i	89	Total	C	N	O	S	0	0	0
			704	454	113	131	6			
3	m	88	Total	C	N	O	S	0	0	0
			697	449	112	130	6			

- Molecule 4 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	104	Total	C	N	O	S	0	0	0
			822	520	138	159	5			
4	H	104	Total	C	N	O	S	0	0	0
			822	520	138	159	5			
4	L	103	Total	C	N	O	S	0	0	0
			814	515	137	158	4			
4	P	104	Total	C	N	O	S	0	0	0
			822	520	138	159	5			
4	T	104	Total	C	N	O	S	0	0	0
			822	520	138	159	5			
4	X	104	Total	C	N	O	S	0	0	0
			822	520	138	159	5			
4	b	104	Total	C	N	O	S	0	0	0
			822	520	138	159	5			
4	f	103	Total	C	N	O	S	0	0	0
			813	514	136	158	5			
4	j	103	Total	C	N	O	S	0	0	0
			814	515	137	158	4			
4	n	102	Total	C	N	O	S	0	0	0
			810	512	136	157	5			

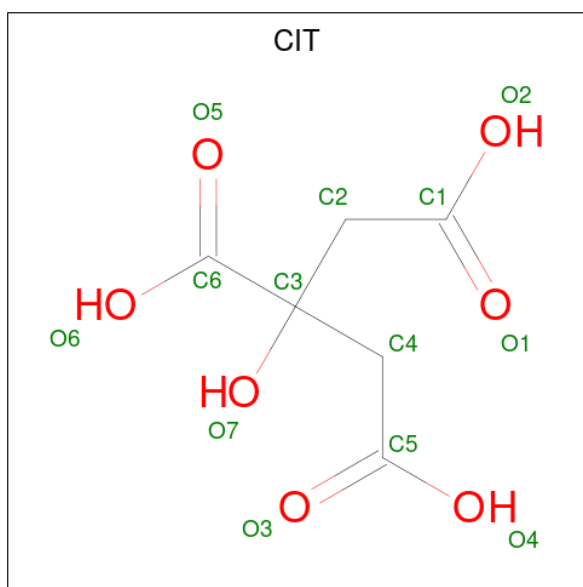
- Molecule 5 is (4R)-4-hydroxy-1-[(2R)-2-(3-{[(2S)-1-{(3R)-3-[(2M,6aS,11S)-2-(2-hydroxyphenyl)-5,6,6a,7,9,10-hexahydro-8H-pyrazino[1',2':4,5]pyrazino[2,3-c]pyridazin-8-yl]pyrrolidin-1-yl}propan-2-yl]oxy}-1,2-oxazol-5-yl)-3-methylbutanoyl]-N-{(1S)-1-[4-(4-methyl-1,3-thiazol-5-yl)phenyl]ethyl}-L-prolinamide (CCD ID: A1BB4) (formula: C<sub>47</sub>H<sub>58</sub>N<sub>10</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	F	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	J	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	N	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	R	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	V	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	Z	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	d	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	h	1	Total	C	N	O	S	0	0
			64	47	10	6	1		
5	k	1	Total	C	N	O	S	0	0
			64	47	10	6	1		

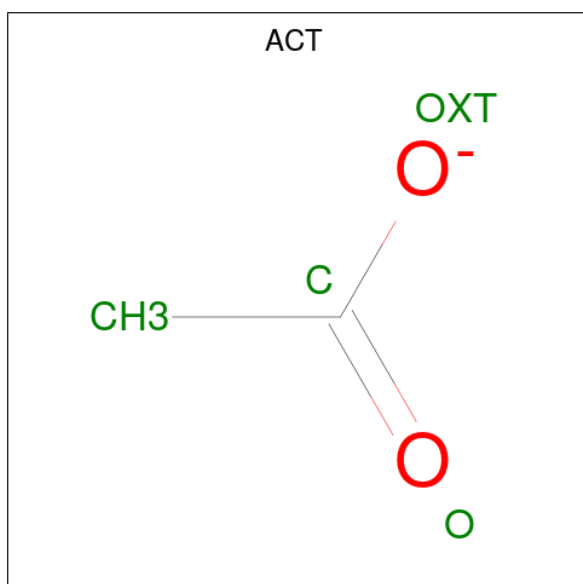
- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	6	7		
6	S	1	Total	C	O	0	0
			13	6	7		
6	W	1	Total	C	O	0	0
			13	6	7		
6	a	1	Total	C	O	0	0
			13	6	7		
6	e	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	10	Total	O		0	0
			10	10			
8	C	1	Total	O		0	0
			1	1			
8	E	1	Total	O		0	0
			1	1			
8	F	6	Total	O		0	0
			6	6			
8	G	3	Total	O		0	0
			3	3			
8	J	6	Total	O		0	0
			6	6			
8	L	1	Total	O		0	0
			1	1			
8	N	8	Total	O		0	0
			8	8			
8	O	2	Total	O		0	0
			2	2			
8	P	1	Total	O		0	0
			1	1			
8	R	5	Total	O		0	0
			5	5			
8	V	10	Total	O		0	0
			10	10			
8	W	3	Total	O		0	0
			3	3			
8	Y	1	Total	O		0	0
			1	1			
8	Z	6	Total	O		0	0
			6	6			
8	a	1	Total	O		0	0
			1	1			
8	c	1	Total	O		0	0
			1	1			
8	d	2	Total	O		0	0
			2	2			
8	h	4	Total	O		0	0
			4	4			

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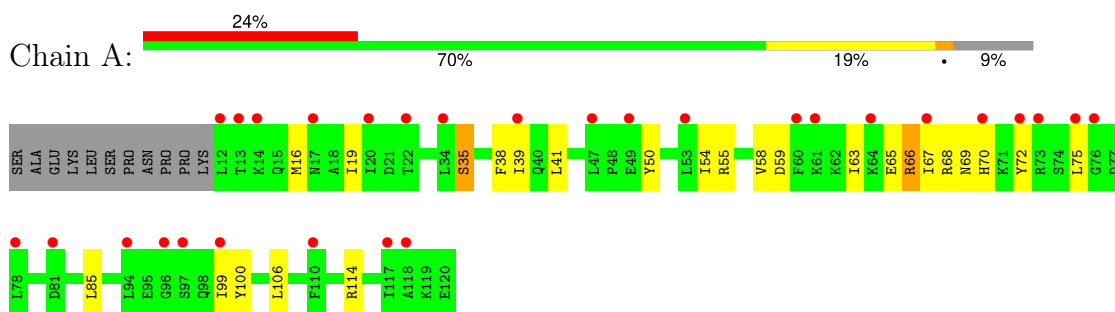
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	l	2	Total	O	0	0
			2	2		
8	m	2	Total	O	0	0
			2	2		

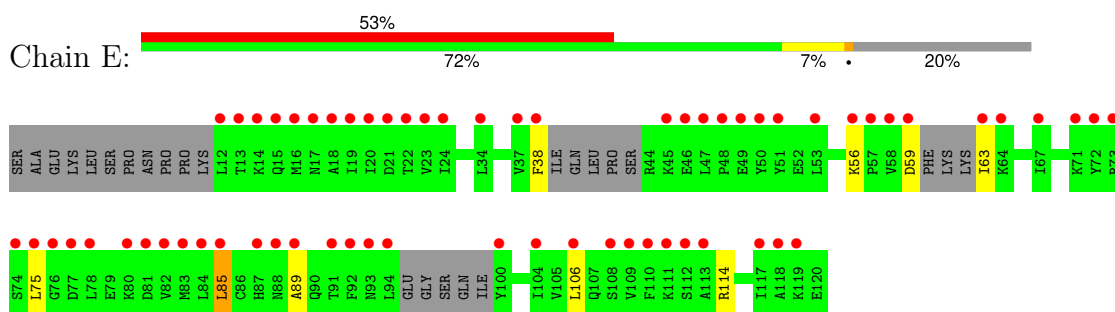
### 3 Residue-property plots [i](#)

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.

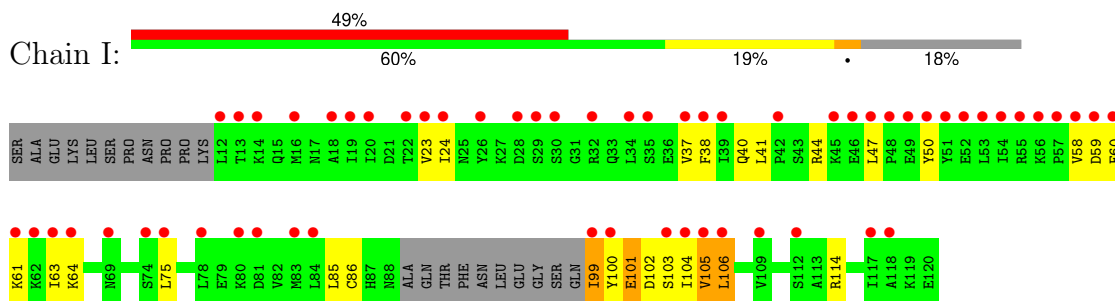
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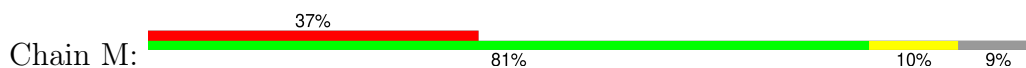
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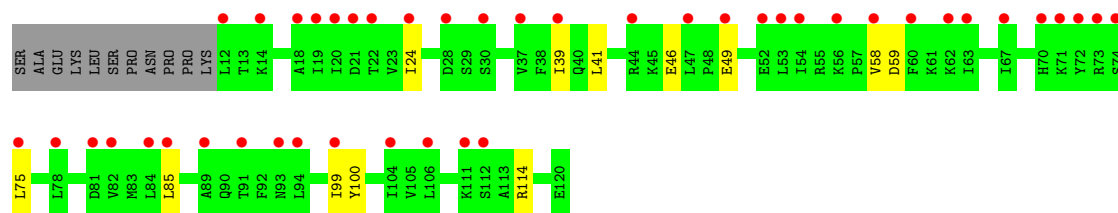


- Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

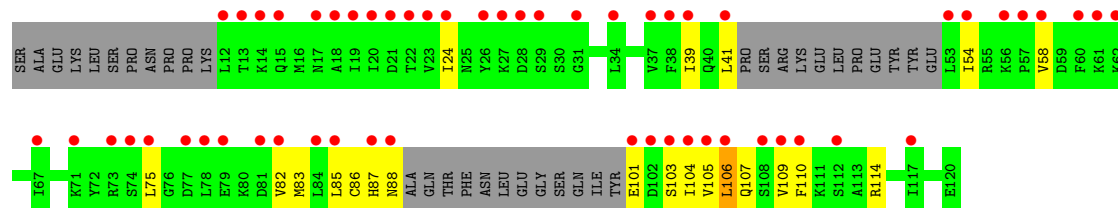


- Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

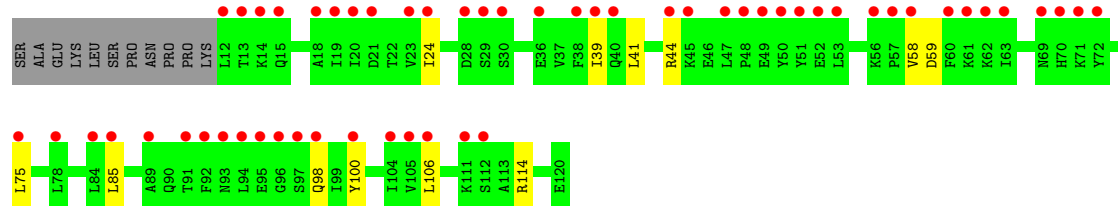
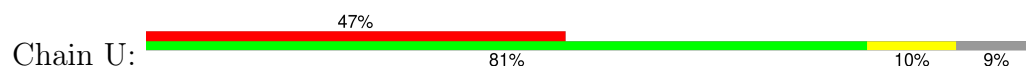




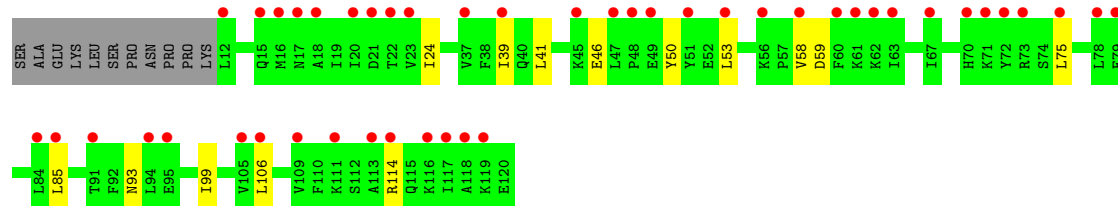
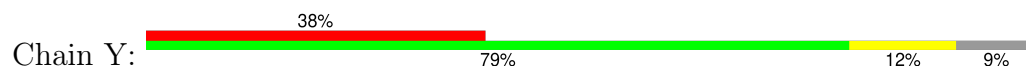
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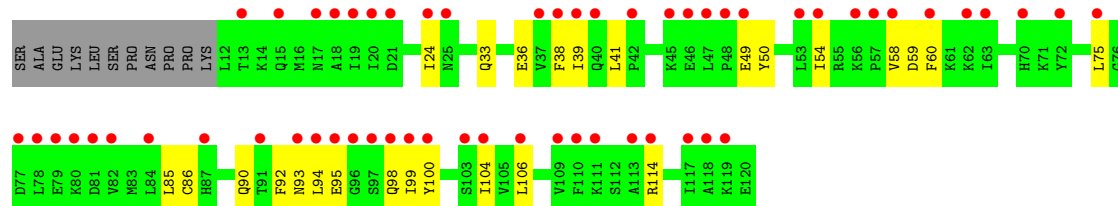
- Molecule 1: Isoform Short of Probable global transcription activator SNF2L2



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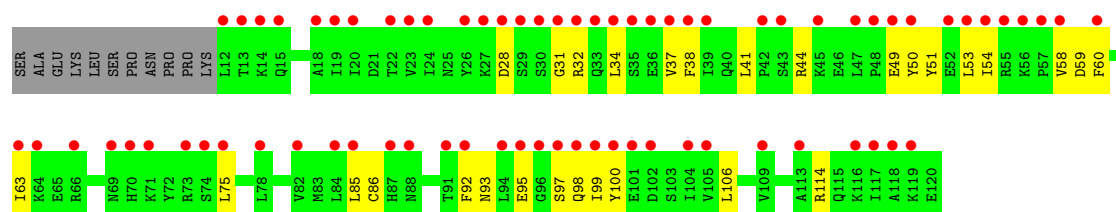


- Molecule 1: Isoform Short of Probable global transcription activator SNF2L2




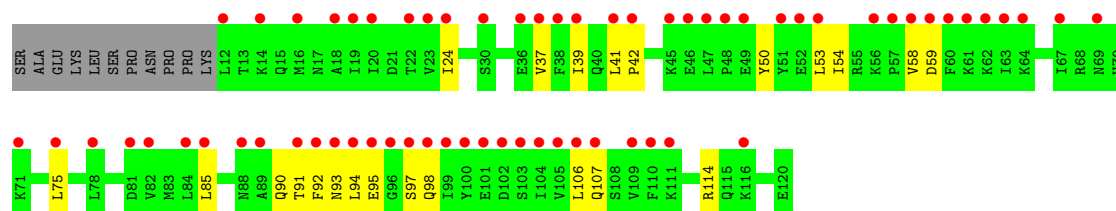
- Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain g: 




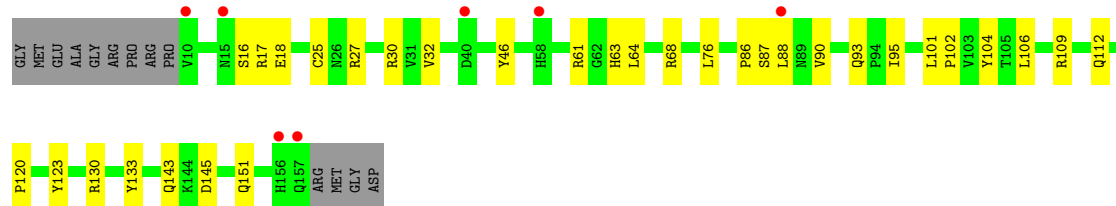
- Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain k: 



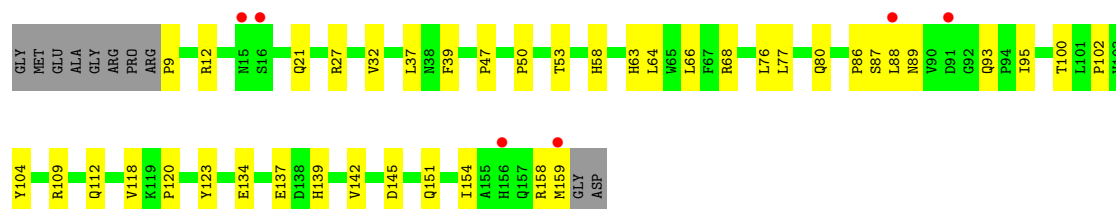
- Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain B: 



- Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain F: 



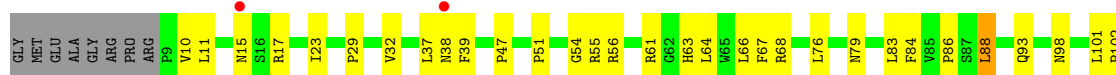
- Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain J: 





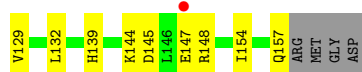
- Molecule 2: von Hippel-Lindau disease tumor suppressor



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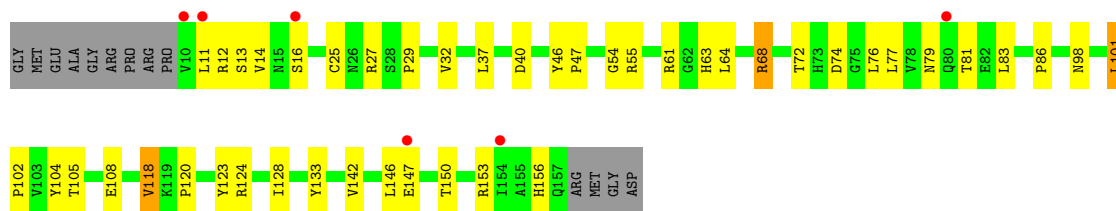


- Molecule 2: von Hippel-Lindau disease tumor suppressor

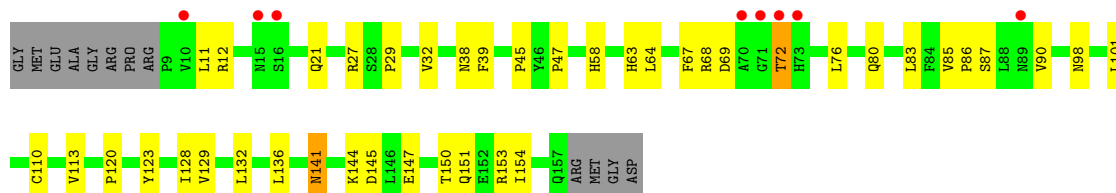


- Molecule 2: von Hippel-Lindau disease tumor suppressor

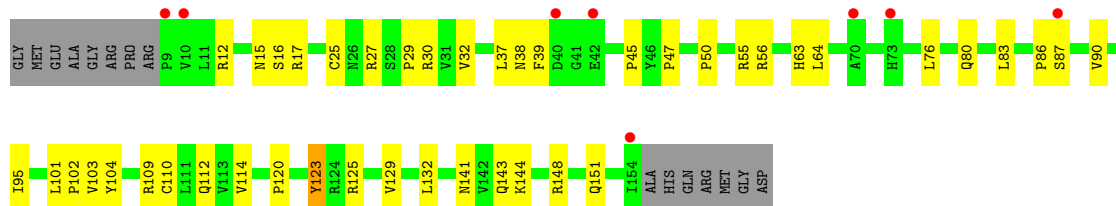




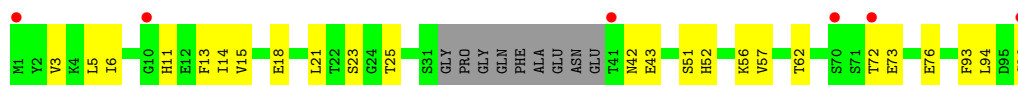
- Molecule 2: von Hippel-Lindau disease tumor suppressor



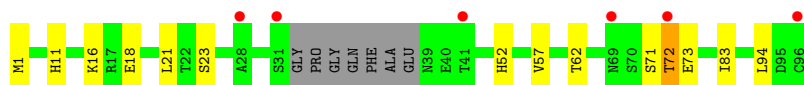
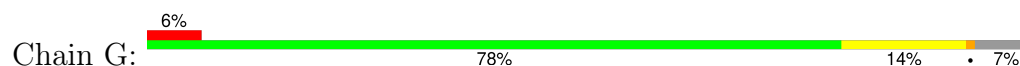
- Molecule 2: von Hippel-Lindau disease tumor suppressor



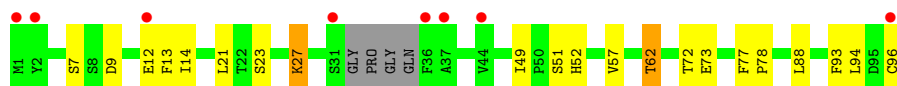
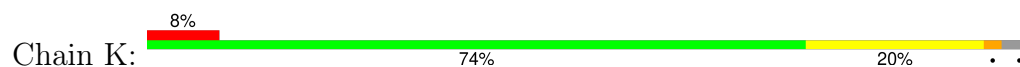
- Molecule 3: Elongin-C



- Molecule 3: Elongin-C

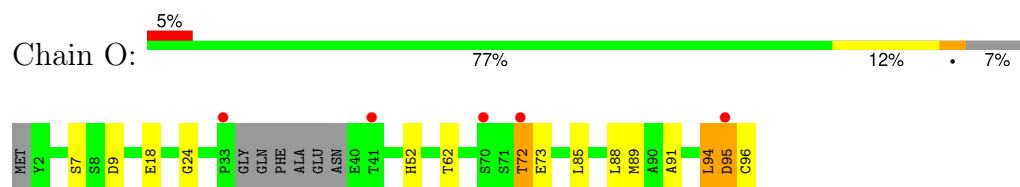


- Molecule 3: Elongin-C

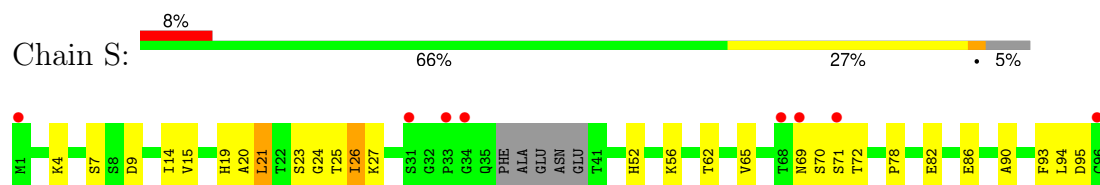




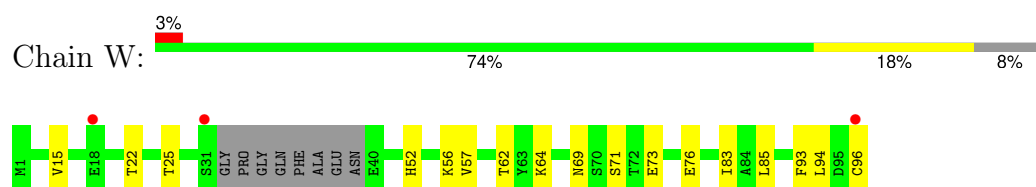
- Molecule 3: Elongin-C



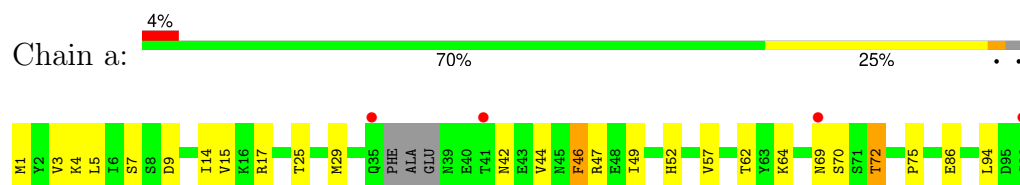
- Molecule 3: Elongin-C



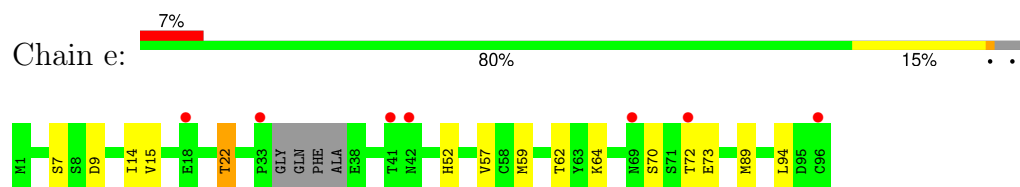
- Molecule 3: Elongin-C



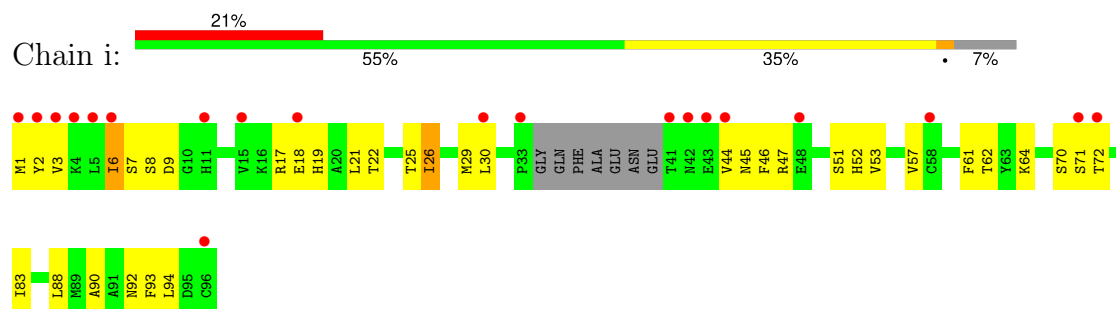
- Molecule 3: Elongin-C



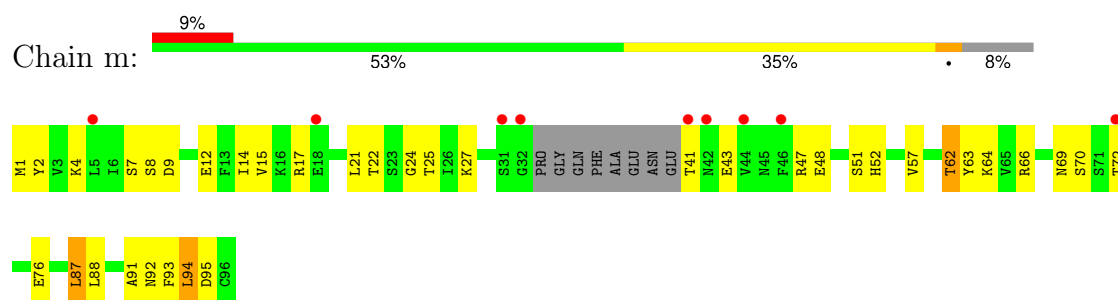
- Molecule 3: Elongin-C



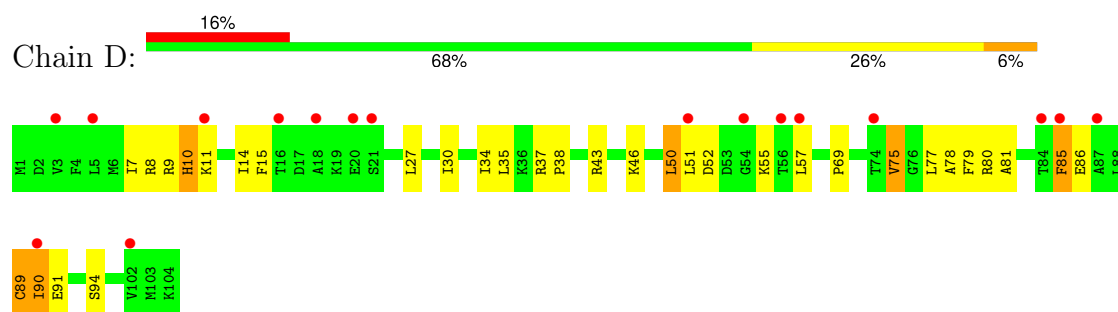
- Molecule 3: Elongin-C



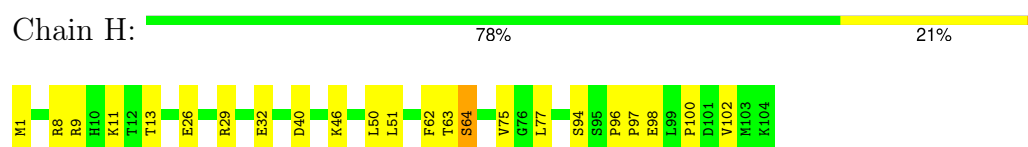
- Molecule 3: Elongin-C



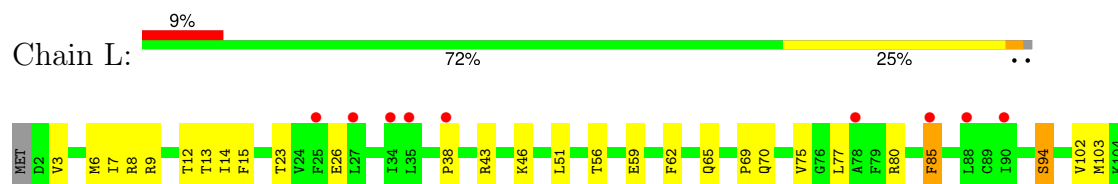
- Molecule 4: Elongin-B



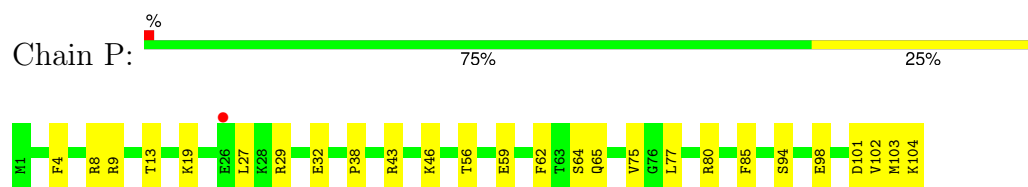
- Molecule 4: Elongin-B



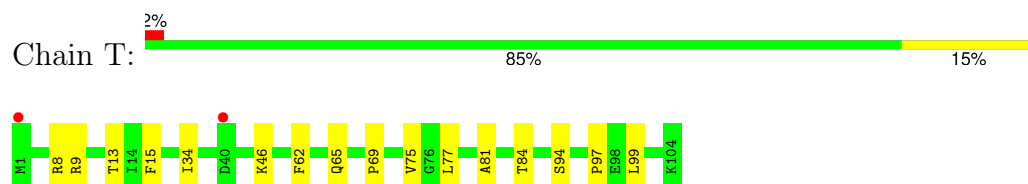
- Molecule 4: Elongin-B



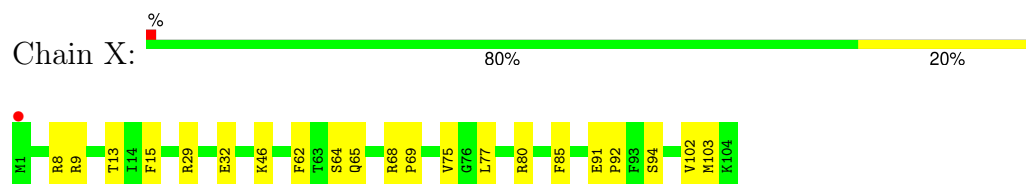
- Molecule 4: Elongin-B



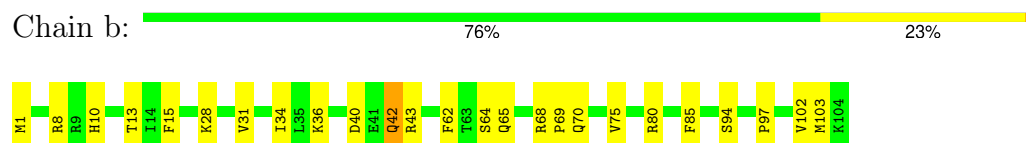
- Molecule 4: Elongin-B



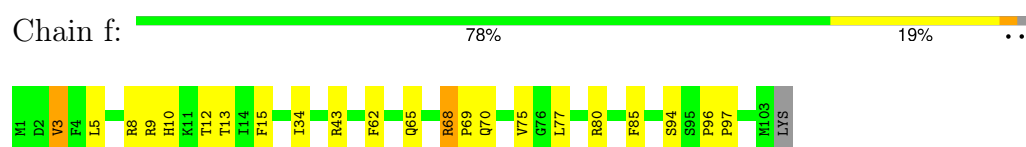
- Molecule 4: Elongin-B



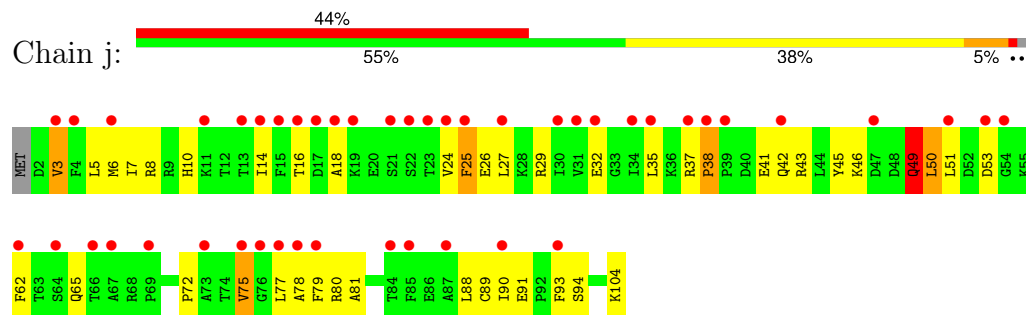
- Molecule 4: Elongin-B



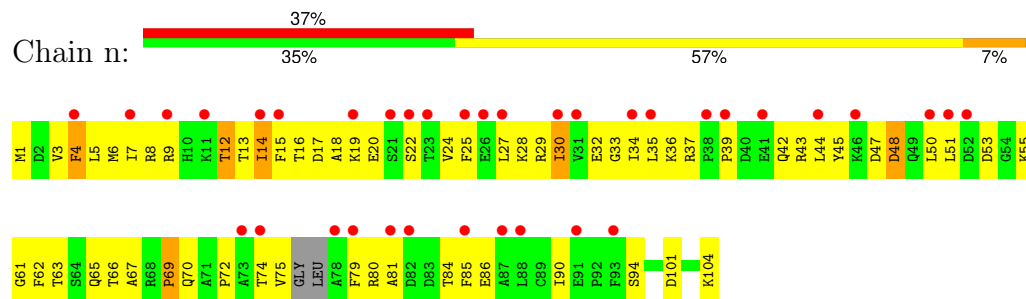
- Molecule 4: Elongin-B



- Molecule 4: Elongin-B



- Molecule 4: Elongin-B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.96Å 203.63Å 206.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.19 49.48 – 3.19	Depositor EDS
% Data completeness (in resolution range)	82.3 (49.48-3.19) 82.5 (49.48-3.19)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.05 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.256 , 0.285 0.255 , 0.281	Depositor DCC
$R_{free}$ test set	5456 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	36947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	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 34.21 % 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 7.0751e-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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, ACT, A1BB4

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	1.14	0/914	1.48	8/1224 (0.7%)
1	E	1.16	1/806 (0.1%)	1.53	3/1075 (0.3%)
1	I	1.10	1/836 (0.1%)	1.49	3/1117 (0.3%)
1	M	1.10	0/914	1.42	0/1224
1	Q	1.11	0/711	1.47	1/945 (0.1%)
1	U	1.09	0/914	1.45	0/1224
1	Y	1.05	0/914	1.49	1/1224 (0.1%)
1	c	1.04	0/914	1.47	0/1224
1	g	1.05	0/914	1.53	4/1224 (0.3%)
1	k	1.05	0/914	1.47	0/1224
2	B	0.94	0/1256	1.25	0/1713
2	F	0.98	0/1272	1.30	1/1733 (0.1%)
2	J	0.97	0/1253	1.28	2/1709 (0.1%)
2	N	1.05	0/1264	1.29	0/1723
2	R	0.96	0/1245	1.28	2/1698 (0.1%)
2	V	0.93	0/1253	1.26	1/1709 (0.1%)
2	Z	0.96	1/1264 (0.1%)	1.22	0/1723
2	d	0.93	0/1245	1.26	1/1698 (0.1%)
2	h	0.95	0/1253	1.27	3/1709 (0.2%)
2	l	0.93	0/1228	1.29	4/1675 (0.2%)
3	C	1.03	1/707 (0.1%)	1.36	0/955
3	G	0.98	0/724	1.36	2/978 (0.2%)
3	K	1.01	1/750 (0.1%)	1.39	2/1013 (0.2%)
3	O	0.99	0/720	1.42	4/974 (0.4%)
3	S	1.03	0/732	1.43	2/989 (0.2%)
3	W	1.01	0/716	1.37	0/967
3	a	0.96	0/749	1.40	3/1012 (0.3%)
3	e	0.96	0/745	1.36	0/1007
3	i	0.96	0/719	1.40	2/972 (0.2%)
3	m	1.01	0/711	1.41	3/960 (0.3%)
4	D	1.11	1/838 (0.1%)	1.47	7/1132 (0.6%)
4	H	0.94	1/838 (0.1%)	1.33	5/1132 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	L	1.02	0/830	1.40	3/1122 (0.3%)
4	P	0.96	0/838	1.31	4/1132 (0.4%)
4	T	0.94	0/838	1.30	1/1132 (0.1%)
4	X	0.89	0/838	1.27	1/1132 (0.1%)
4	b	0.91	0/838	1.29	2/1132 (0.2%)
4	f	0.91	0/829	1.27	1/1121 (0.1%)
4	j	1.13	1/830 (0.1%)	1.52	4/1122 (0.4%)
4	n	1.17	1/825 (0.1%)	1.54	7/1113 (0.6%)
All	All	1.01	9/36899 (0.0%)	1.37	87/49892 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	85	LEU	C-O	-6.01	1.17	1.24
2	Z	94	PRO	C-O	-5.85	1.17	1.23
4	n	33	GLY	C-O	5.71	1.31	1.23
4	H	100	PRO	C-O	-5.70	1.16	1.23
4	D	89	CYS	C-O	-5.46	1.17	1.24

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	61	LYS	N-CA-C	-9.15	101.21	111.82
2	R	57	ILE	N-CA-C	8.42	121.97	113.47
4	D	81	ALA	N-CA-C	-8.28	98.23	110.48
2	J	138	ASP	N-CA-C	-8.22	97.71	109.96
1	g	32	ARG	CA-C-O	-8.09	111.51	120.81

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	901	0	929	16	0
1	E	798	0	816	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	825	0	860	25	0
1	M	901	0	929	10	0
1	Q	706	0	747	13	0
1	U	901	0	929	9	0
1	Y	901	0	929	9	0
1	c	901	0	929	27	0
1	g	901	0	929	34	0
1	k	901	0	929	34	0
2	B	1224	0	1218	31	0
2	F	1240	0	1242	38	0
2	J	1221	0	1220	41	1
2	N	1232	0	1233	39	0
2	R	1214	0	1212	46	0
2	V	1221	0	1220	32	0
2	Z	1232	0	1233	27	1
2	d	1214	0	1212	52	0
2	h	1221	0	1220	33	0
2	l	1197	0	1200	46	1
3	C	693	0	698	25	0
3	G	710	0	710	12	0
3	K	735	0	730	22	0
3	O	705	0	702	15	0
3	S	717	0	719	33	0
3	W	702	0	704	16	0
3	a	734	0	731	25	0
3	e	730	0	726	15	0
3	i	704	0	708	44	0
3	m	697	0	701	48	0
4	D	822	0	824	36	0
4	H	822	0	824	17	0
4	L	814	0	812	26	0
4	P	822	0	824	19	0
4	T	822	0	824	12	0
4	X	822	0	824	12	1
4	b	822	0	824	22	1
4	f	813	0	811	20	0
4	j	814	0	812	86	0
4	n	810	0	809	112	0
5	B	64	0	0	3	0
5	F	64	0	0	3	0
5	J	64	0	0	3	0
5	N	64	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	64	0	0	2	0
5	V	64	0	0	1	0
5	Z	64	0	0	1	0
5	d	64	0	0	4	0
5	h	64	0	0	1	0
5	k	64	0	0	4	0
6	C	13	0	5	4	0
6	S	13	0	5	3	0
6	W	13	0	5	1	1
6	a	13	0	5	2	0
6	e	13	0	5	1	0
7	F	4	0	3	0	0
8	B	10	0	0	0	0
8	C	1	0	0	1	0
8	E	1	0	0	0	0
8	F	6	0	0	0	0
8	G	3	0	0	0	0
8	J	6	0	0	0	0
8	L	1	0	0	0	0
8	N	8	0	0	0	0
8	O	2	0	0	0	0
8	P	1	0	0	0	0
8	R	5	0	0	0	0
8	V	10	0	0	0	0
8	W	3	0	0	0	0
8	Y	1	0	0	0	0
8	Z	6	0	0	0	0
8	a	1	0	0	0	0
8	c	1	0	0	0	0
8	d	2	0	0	0	0
8	h	4	0	0	0	0
8	l	2	0	0	0	0
8	m	2	0	0	0	0
All	All	36947	0	36481	1017	3

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 14.

The worst 5 of 1017 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)
4:b:68:ARG:CZ	4:b:70:GLN:HE22	1.56	1.17
1:I:86:CYS:SG	1:I:106:LEU:HD22	1.87	1.15
4:j:37:ARG:CZ	4:j:79:PHE:HD1	1.62	1.12
1:g:37:VAL:HG11	1:g:99:ILE:HD12	1.29	1.11
4:j:45:TYR:CD1	4:j:88:LEU:HD11	1.86	1.10

All (3) 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:X:85:PHE:O	2:l:125:ARG:NH1[4_454]	2.10	0.10
2:Z:54:GLY:O	6:W:101:CIT:O6[1_556]	2.16	0.04
2:J:127:ASP:OD2	4:b:80:ARG:NH1[4_554]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	107/120 (89%)	103 (96%)	4 (4%)	0	100	100
1	E	88/120 (73%)	84 (96%)	4 (4%)	0	100	100
1	I	95/120 (79%)	88 (93%)	7 (7%)	0	100	100
1	M	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
1	Q	80/120 (67%)	76 (95%)	4 (5%)	0	100	100
1	U	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
1	Y	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
1	c	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
1	g	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
1	k	107/120 (89%)	104 (97%)	3 (3%)	0	100	100
2	B	147/161 (91%)	143 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	149/161 (92%)	143 (96%)	6 (4%)	0	100	100
2	J	147/161 (91%)	140 (95%)	7 (5%)	0	100	100
2	N	148/161 (92%)	142 (96%)	5 (3%)	1 (1%)	19	54
2	R	146/161 (91%)	141 (97%)	5 (3%)	0	100	100
2	V	147/161 (91%)	140 (95%)	7 (5%)	0	100	100
2	Z	148/161 (92%)	141 (95%)	7 (5%)	0	100	100
2	d	146/161 (91%)	141 (97%)	5 (3%)	0	100	100
2	h	147/161 (91%)	141 (96%)	6 (4%)	0	100	100
2	l	144/161 (89%)	140 (97%)	4 (3%)	0	100	100
3	C	83/96 (86%)	80 (96%)	3 (4%)	0	100	100
3	G	85/96 (88%)	84 (99%)	1 (1%)	0	100	100
3	K	88/96 (92%)	86 (98%)	2 (2%)	0	100	100
3	O	85/96 (88%)	83 (98%)	1 (1%)	1 (1%)	11	43
3	S	87/96 (91%)	86 (99%)	1 (1%)	0	100	100
3	W	84/96 (88%)	83 (99%)	1 (1%)	0	100	100
3	a	89/96 (93%)	88 (99%)	1 (1%)	0	100	100
3	e	88/96 (92%)	86 (98%)	2 (2%)	0	100	100
3	i	85/96 (88%)	84 (99%)	1 (1%)	0	100	100
3	m	84/96 (88%)	84 (100%)	0	0	100	100
4	D	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
4	H	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
4	L	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
4	P	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
4	T	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
4	X	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
4	b	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
4	f	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
4	j	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
4	n	98/104 (94%)	94 (96%)	4 (4%)	0	100	100
All	All	4352/4810 (90%)	4210 (97%)	140 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	15	ASN
3	O	72	THR

### 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	102/112 (91%)	101 (99%)	1 (1%)	73	87
1	E	90/112 (80%)	89 (99%)	1 (1%)	70	86
1	I	94/112 (84%)	93 (99%)	1 (1%)	70	86
1	M	102/112 (91%)	102 (100%)	0	100	100
1	Q	81/112 (72%)	81 (100%)	0	100	100
1	U	102/112 (91%)	101 (99%)	1 (1%)	73	87
1	Y	102/112 (91%)	101 (99%)	1 (1%)	73	87
1	c	102/112 (91%)	101 (99%)	1 (1%)	73	87
1	g	102/112 (91%)	101 (99%)	1 (1%)	73	87
1	k	102/112 (91%)	101 (99%)	1 (1%)	73	87
2	B	139/147 (95%)	138 (99%)	1 (1%)	81	92
2	F	141/147 (96%)	141 (100%)	0	100	100
2	J	139/147 (95%)	137 (99%)	2 (1%)	62	82
2	N	140/147 (95%)	137 (98%)	3 (2%)	48	74
2	R	138/147 (94%)	137 (99%)	1 (1%)	81	92
2	V	139/147 (95%)	137 (99%)	2 (1%)	62	82
2	Z	140/147 (95%)	137 (98%)	3 (2%)	48	74
2	d	138/147 (94%)	136 (99%)	2 (1%)	62	82
2	h	139/147 (95%)	138 (99%)	1 (1%)	81	92
2	l	137/147 (93%)	136 (99%)	1 (1%)	81	92
3	C	79/85 (93%)	79 (100%)	0	100	100
3	G	81/85 (95%)	80 (99%)	1 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	83/85 (98%)	82 (99%)	1 (1%)	67	85
3	O	80/85 (94%)	80 (100%)	0	100	100
3	S	81/85 (95%)	79 (98%)	2 (2%)	42	71
3	W	80/85 (94%)	80 (100%)	0	100	100
3	a	83/85 (98%)	81 (98%)	2 (2%)	44	71
3	e	83/85 (98%)	82 (99%)	1 (1%)	67	85
3	i	80/85 (94%)	78 (98%)	2 (2%)	42	71
3	m	79/85 (93%)	78 (99%)	1 (1%)	65	83
4	D	92/92 (100%)	90 (98%)	2 (2%)	47	73
4	H	92/92 (100%)	91 (99%)	1 (1%)	70	86
4	L	91/92 (99%)	88 (97%)	3 (3%)	33	64
4	P	92/92 (100%)	91 (99%)	1 (1%)	70	86
4	T	92/92 (100%)	92 (100%)	0	100	100
4	X	92/92 (100%)	91 (99%)	1 (1%)	70	86
4	b	92/92 (100%)	90 (98%)	2 (2%)	47	73
4	f	91/92 (99%)	88 (97%)	3 (3%)	33	64
4	j	91/92 (99%)	88 (97%)	3 (3%)	33	64
4	n	91/92 (99%)	88 (97%)	3 (3%)	33	64
All	All	4094/4360 (94%)	4041 (99%)	53 (1%)	65	83

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Z	101	LEU
2	d	118	VAL
3	m	87	LEU
3	a	42	ASN
4	b	42	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
4	b	65	GLN
4	j	10	HIS
1	c	87	HIS

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Mol	Chain	Res	Type
4	f	70	GLN
1	k	90	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

16 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	A1BB4	d	201	-	62,72,72	0.77	2 (3%)	73,105,105	1.63	10 (13%)
5	A1BB4	N	201	-	62,72,72	0.84	1 (1%)	73,105,105	1.99	15 (20%)
5	A1BB4	h	201	-	62,72,72	0.84	3 (4%)	73,105,105	1.82	16 (21%)
6	CIT	e	101	-	12,12,12	1.32	1 (8%)	17,17,17	1.02	0
5	A1BB4	B	201	-	62,72,72	0.91	2 (3%)	73,105,105	1.72	18 (24%)
6	CIT	C	101	-	12,12,12	1.27	1 (8%)	17,17,17	1.23	2 (11%)
5	A1BB4	F	201	-	62,72,72	0.89	3 (4%)	73,105,105	1.72	16 (21%)
6	CIT	S	101	-	12,12,12	1.18	1 (8%)	17,17,17	1.30	2 (11%)
5	A1BB4	R	201	-	62,72,72	0.79	1 (1%)	73,105,105	1.82	14 (19%)
7	ACT	F	202	-	3,3,3	1.02	0	3,3,3	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	A1BB4	Z	201	-	62,72,72	0.83	1 (1%)	73,105,105	1.46	12 (16%)
5	A1BB4	k	201	-	62,72,72	1.04	5 (8%)	73,105,105	1.65	12 (16%)
6	CIT	W	101	-	12,12,12	1.36	1 (8%)	17,17,17	1.16	2 (11%)
6	CIT	a	101	-	12,12,12	1.30	1 (8%)	17,17,17	1.21	3 (17%)
5	A1BB4	V	201	-	62,72,72	0.94	4 (6%)	73,105,105	1.55	11 (15%)
5	A1BB4	J	201	-	62,72,72	0.90	3 (4%)	73,105,105	1.70	16 (21%)

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	A1BB4	d	201	-	-	8/42/91/91	0/9/9/9
5	A1BB4	N	201	-	-	11/42/91/91	0/9/9/9
5	A1BB4	h	201	-	-	5/42/91/91	0/9/9/9
6	CIT	e	101	-	-	0/16/16/16	-
5	A1BB4	B	201	-	-	5/42/91/91	0/9/9/9
6	CIT	C	101	-	-	3/16/16/16	-
5	A1BB4	F	201	-	-	8/42/91/91	0/9/9/9
6	CIT	S	101	-	-	0/16/16/16	-
5	A1BB4	R	201	-	-	6/42/91/91	0/9/9/9
5	A1BB4	Z	201	-	-	9/42/91/91	0/9/9/9
5	A1BB4	k	201	-	-	5/42/91/91	0/9/9/9
6	CIT	W	101	-	-	9/16/16/16	-
6	CIT	a	101	-	-	9/16/16/16	-
5	A1BB4	V	201	-	-	3/42/91/91	0/9/9/9
5	A1BB4	J	201	-	-	8/42/91/91	0/9/9/9

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	A1BB4	C19-C18	-3.57	1.34	1.39
5	V	201	A1BB4	C19-C18	-3.44	1.35	1.39
6	W	101	CIT	C3-C6	3.40	1.57	1.53
6	a	101	CIT	C3-C6	3.19	1.56	1.53
5	Z	201	A1BB4	C19-C18	-3.11	1.35	1.39

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	201	A1BB4	C27-N5-C41	7.42	115.47	108.17
5	N	201	A1BB4	O4-C21-C23	6.69	113.90	105.97
5	h	201	A1BB4	C27-N5-C41	6.65	114.71	108.17
5	h	201	A1BB4	C14-C15-N3	6.02	108.80	103.00
5	d	201	A1BB4	C28-N6-C40	-5.70	107.69	115.20

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	201	A1BB4	C18-C17-C43-C45
5	B	201	A1BB4	C22-C21-O4-C20
5	B	201	A1BB4	C22-C21-C23-N4
5	B	201	A1BB4	O4-C21-C23-N4
5	B	201	A1BB4	C21-C23-N4-C42

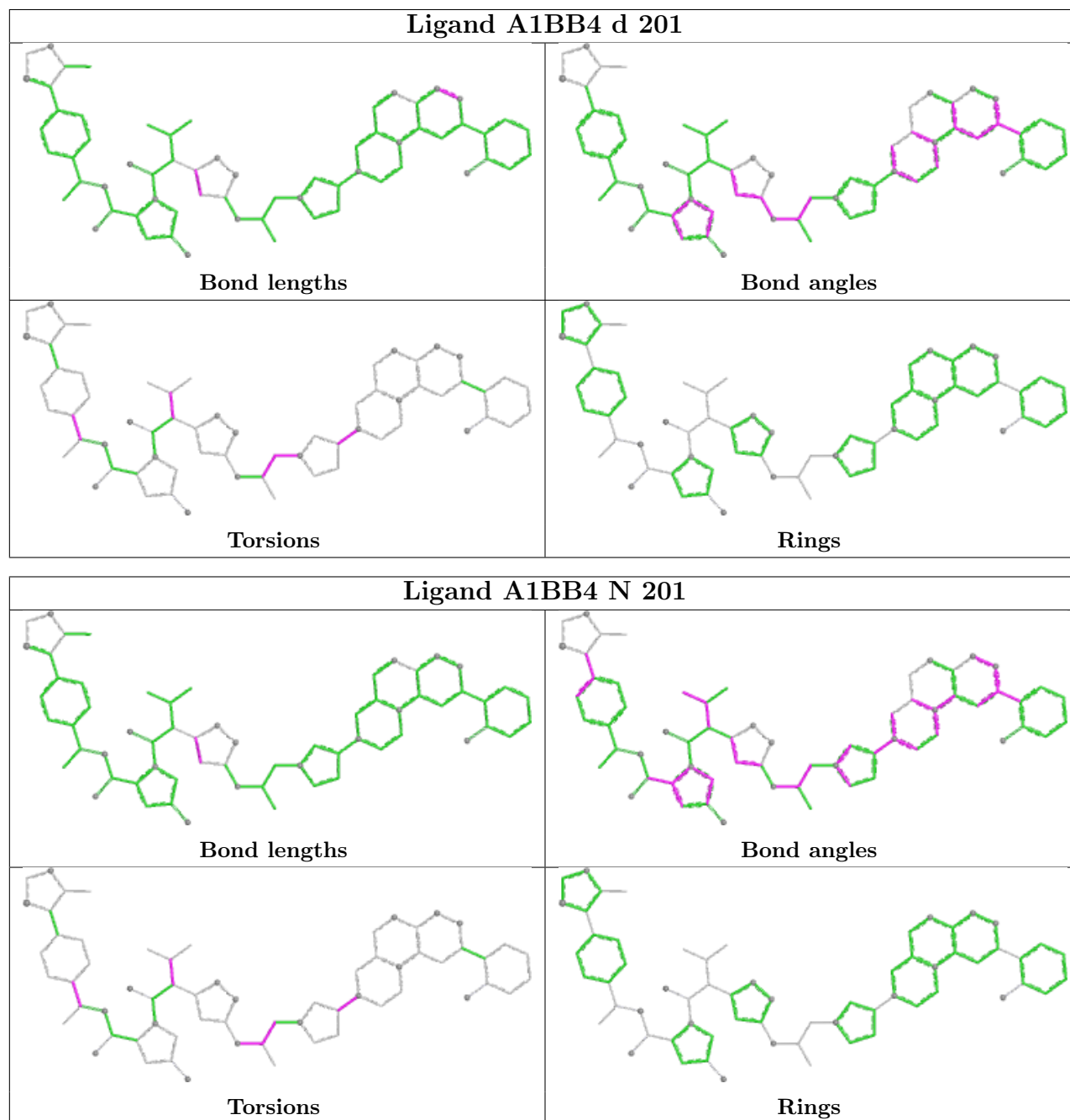
There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	d	201	A1BB4	4	0
5	N	201	A1BB4	2	0
5	h	201	A1BB4	1	0
6	e	101	CIT	1	0
5	B	201	A1BB4	3	0
6	C	101	CIT	4	0
5	F	201	A1BB4	3	0
6	S	101	CIT	3	0
5	R	201	A1BB4	2	0
5	Z	201	A1BB4	1	0
5	k	201	A1BB4	4	0
6	W	101	CIT	1	1
6	a	101	CIT	2	0
5	V	201	A1BB4	1	0
5	J	201	A1BB4	3	0

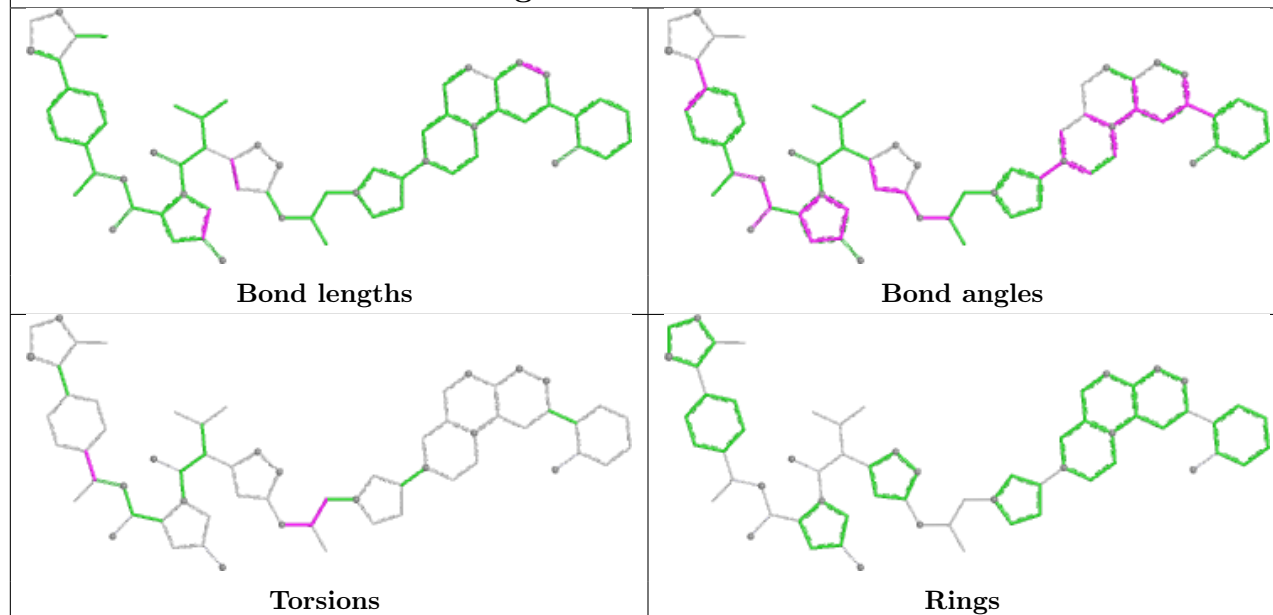
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

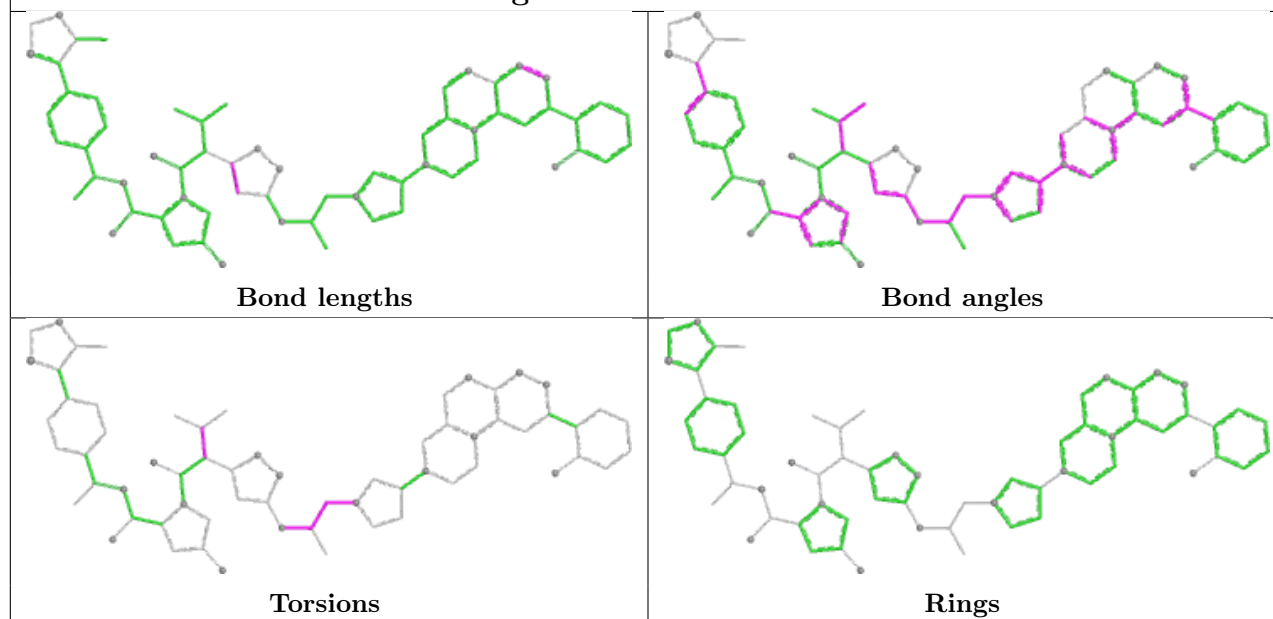




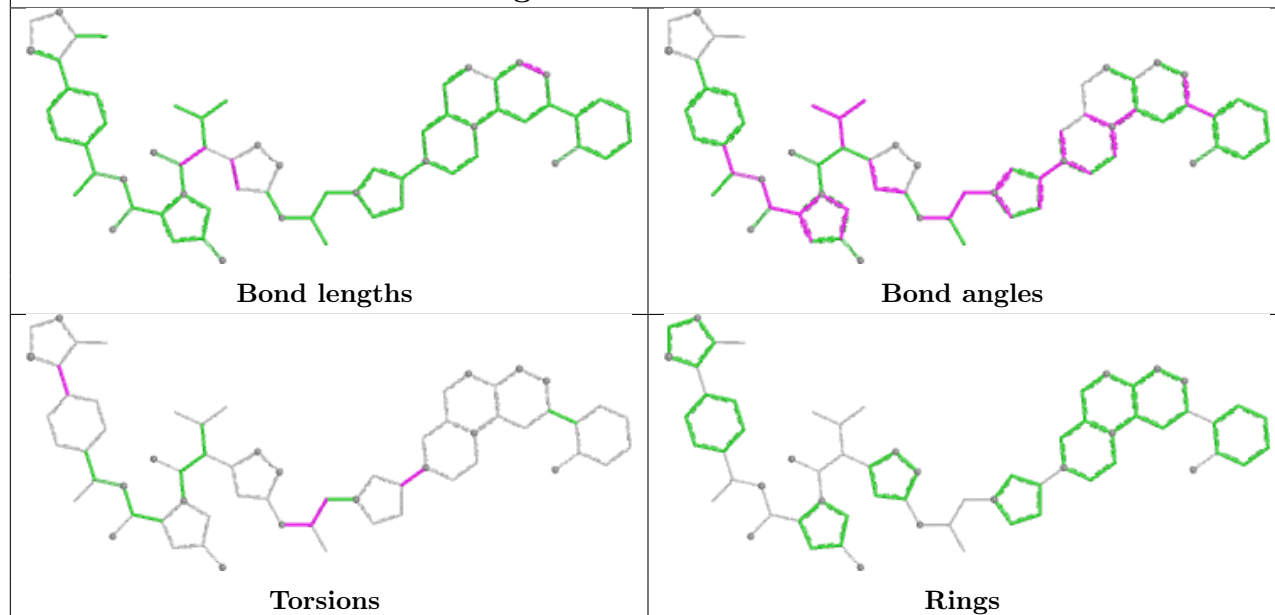
## Ligand A1BB4 h 201



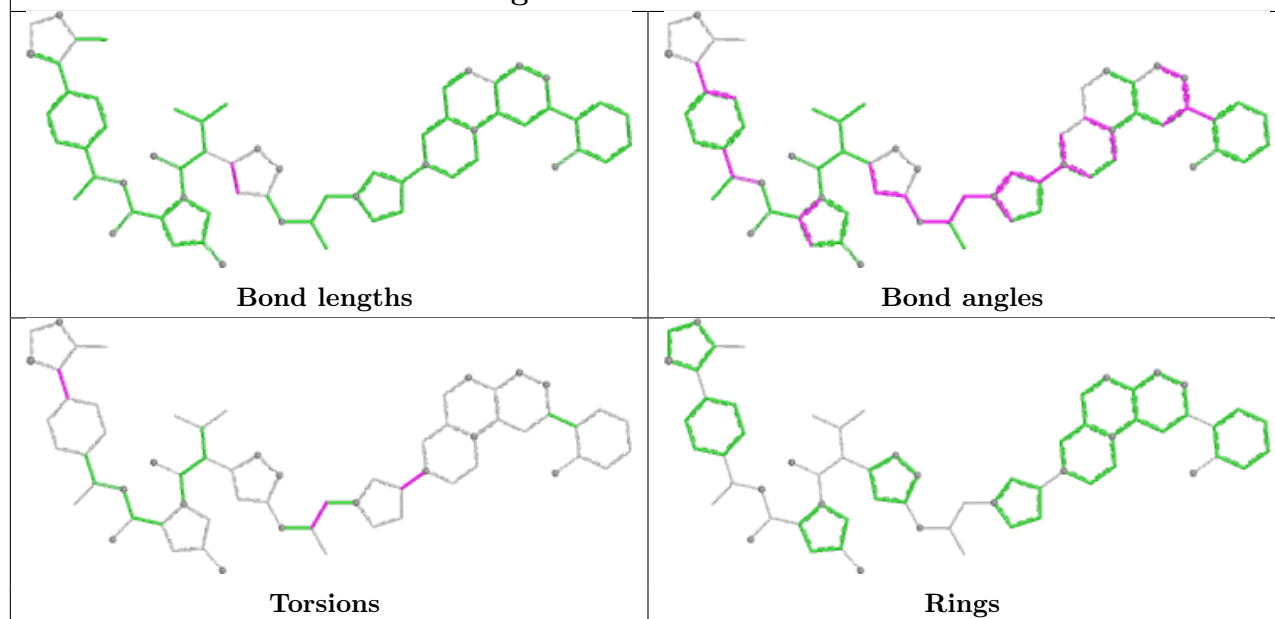
## Ligand A1BB4 B 201



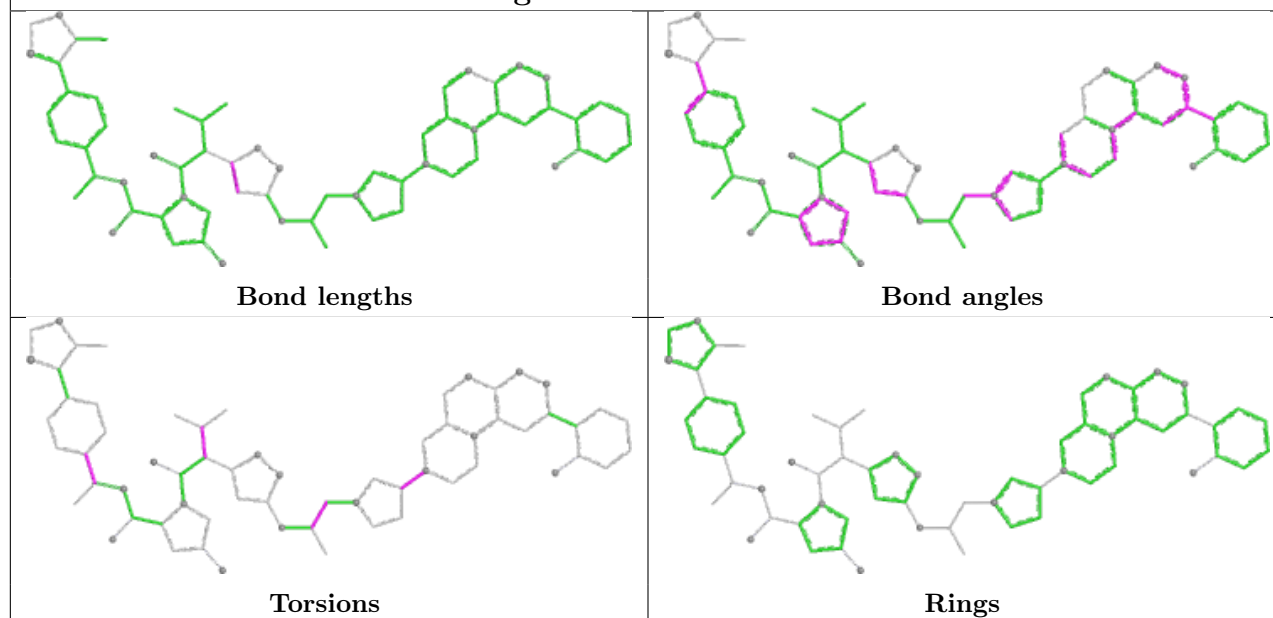
## Ligand A1BB4 F 201



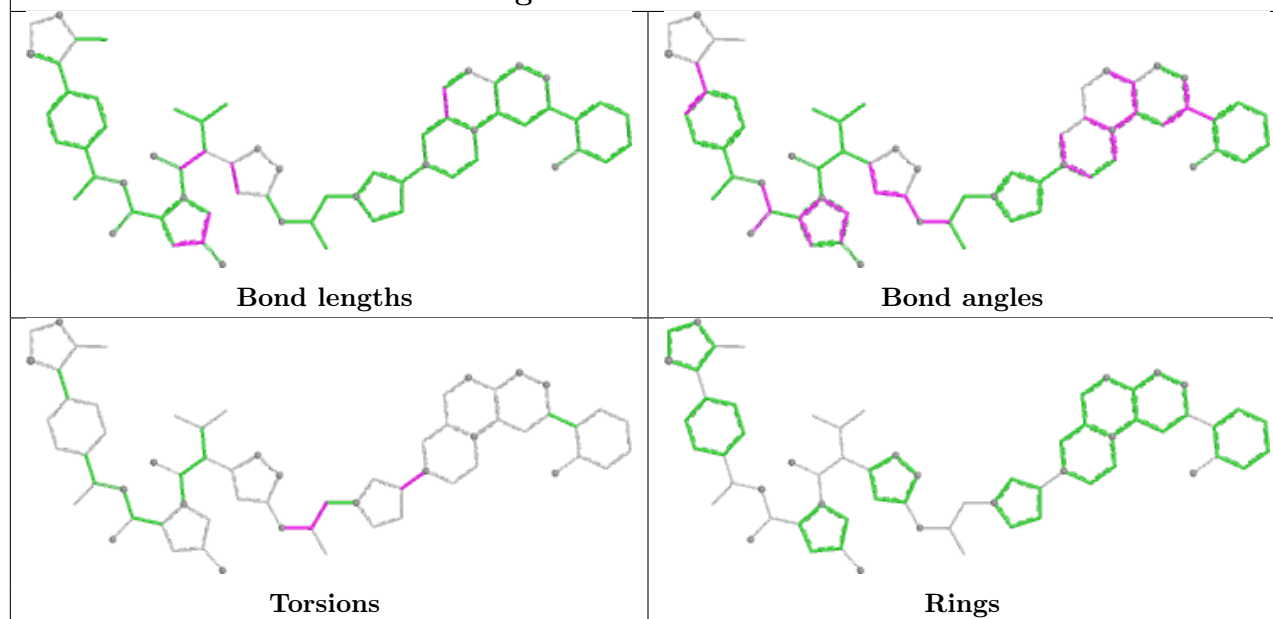
## Ligand A1BB4 R 201

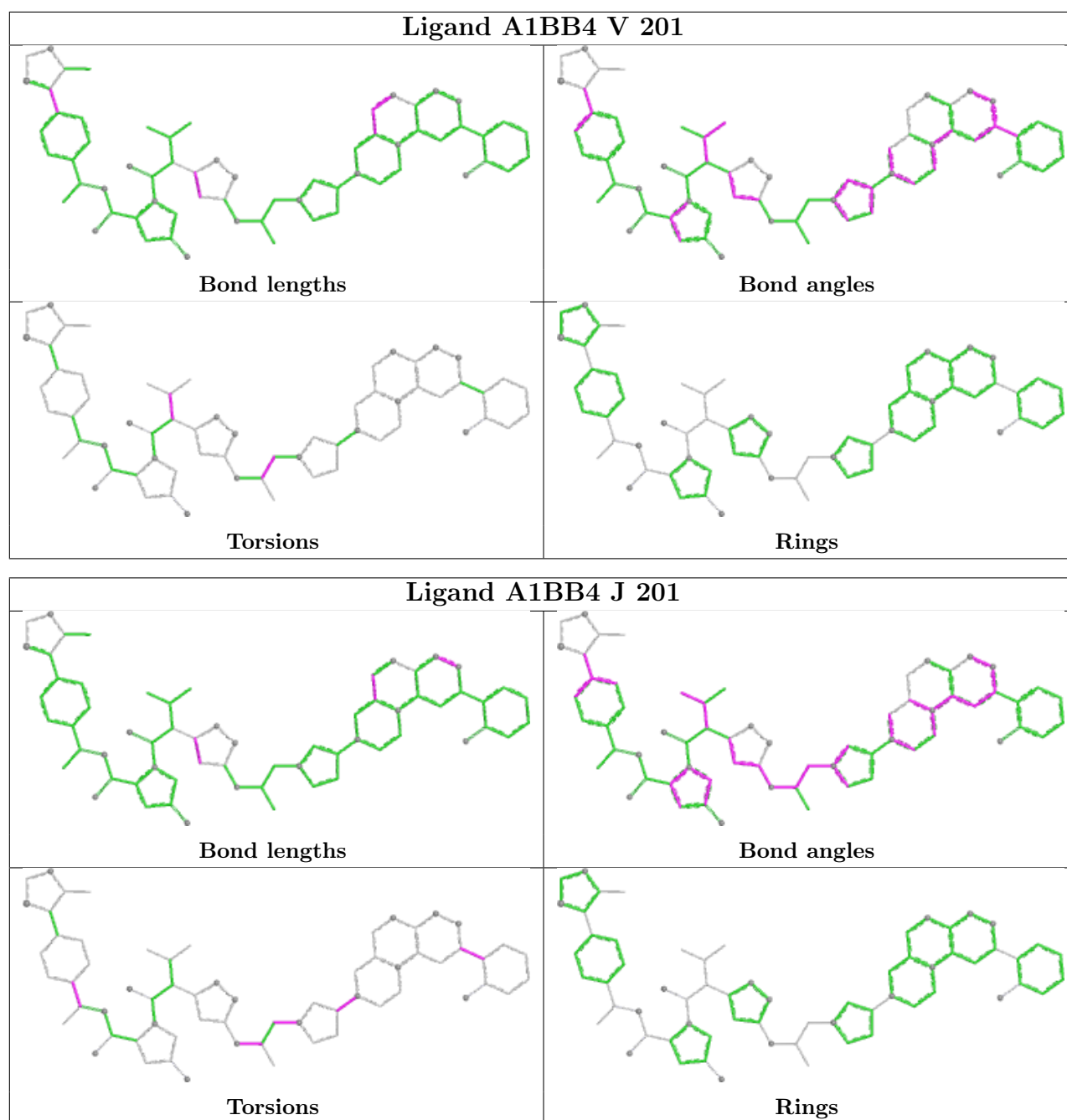


## Ligand A1BB4 Z 201



## Ligand A1BB4 k 201





## 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	109/120 (90%)	1.54	29 (26%) 2 2	86, 129, 169, 182	0
1	E	96/120 (80%)	2.61	64 (66%) 0 1	145, 213, 291, 339	0
1	I	99/120 (82%)	2.52	59 (59%) 0 1	160, 233, 308, 331	0
1	M	109/120 (90%)	1.74	44 (40%) 1 1	109, 144, 185, 213	0
1	Q	86/120 (71%)	2.63	55 (63%) 0 1	114, 211, 303, 346	0
1	U	109/120 (90%)	2.19	56 (51%) 0 1	122, 179, 251, 281	0
1	Y	109/120 (90%)	1.96	46 (42%) 1 1	112, 147, 195, 212	0
1	c	109/120 (90%)	2.02	58 (53%) 0 1	124, 179, 211, 239	0
1	g	109/120 (90%)	2.53	73 (66%) 0 1	152, 237, 325, 368	0
1	k	109/120 (90%)	2.42	65 (59%) 0 1	164, 230, 297, 354	0
2	B	148/161 (91%)	0.20	7 (4%) 37 25	16, 34, 82, 115	1 (0%)
2	F	151/161 (93%)	0.35	6 (3%) 43 29	12, 35, 97, 142	0
2	J	149/161 (92%)	0.18	3 (2%) 64 49	17, 32, 83, 148	0
2	N	150/161 (93%)	0.04	7 (4%) 37 25	8, 22, 69, 145	0
2	R	148/161 (91%)	0.30	5 (3%) 48 34	16, 38, 90, 116	0
2	V	149/161 (92%)	0.01	4 (2%) 56 40	6, 21, 76, 135	0
2	Z	150/161 (93%)	0.28	3 (2%) 64 49	12, 33, 97, 133	0
2	d	148/161 (91%)	0.41	6 (4%) 42 28	19, 42, 99, 128	0
2	h	149/161 (92%)	0.56	8 (5%) 32 22	23, 48, 100, 164	0
2	l	146/161 (90%)	0.49	8 (5%) 32 21	27, 46, 90, 117	0
3	C	87/96 (90%)	0.46	6 (6%) 24 17	28, 50, 98, 110	0
3	G	89/96 (92%)	0.21	6 (6%) 25 17	19, 43, 86, 121	0
3	K	92/96 (95%)	0.72	8 (8%) 17 12	28, 57, 116, 155	0
3	O	89/96 (92%)	0.16	5 (5%) 31 20	12, 27, 77, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	S	91/96 (94%)	0.35	8 (8%) 17 12	25, 49, 114, 155	0
3	W	88/96 (91%)	0.03	3 (3%) 48 34	12, 30, 71, 128	0
3	a	93/96 (96%)	0.40	4 (4%) 40 27	20, 42, 116, 120	0
3	e	92/96 (95%)	0.46	7 (7%) 21 15	25, 49, 117, 147	0
3	i	89/96 (92%)	1.24	20 (22%) 3 2	40, 80, 137, 145	0
3	m	88/96 (91%)	0.90	9 (10%) 13 9	40, 75, 117, 138	0
4	D	104/104 (100%)	1.20	17 (16%) 5 4	45, 98, 140, 167	0
4	H	104/104 (100%)	-0.20	0 100 100	19, 33, 70, 89	0
4	L	103/104 (99%)	0.85	9 (8%) 17 12	51, 79, 114, 141	0
4	P	104/104 (100%)	-0.15	1 (0%) 79 66	16, 35, 53, 70	0
4	T	104/104 (100%)	-0.05	2 (1%) 66 50	25, 44, 70, 87	0
4	X	104/104 (100%)	-0.12	1 (0%) 79 66	19, 35, 50, 77	0
4	b	104/104 (100%)	-0.10	0 100 100	15, 30, 65, 86	0
4	f	103/104 (99%)	-0.12	0 100 100	17, 29, 63, 83	0
4	j	103/104 (99%)	1.83	46 (44%) 1 1	67, 136, 170, 198	0
4	n	102/104 (98%)	1.76	38 (37%) 1 1	67, 120, 160, 182	0
All	All	4465/4810 (92%)	0.82	796 (17%) 4 4	6, 58, 233, 368	1 (0%)

The worst 5 of 796 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	72	TYR	7.0
1	k	99	ILE	6.7
1	E	94	LEU	6.6
1	U	94	LEU	6.4
1	I	60	PHE	6.2

## 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

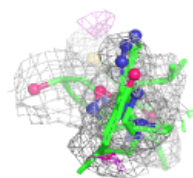
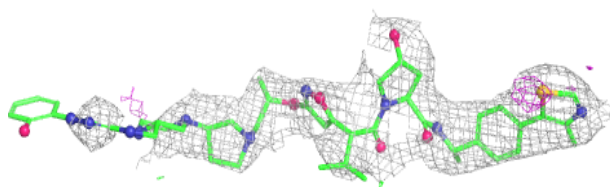
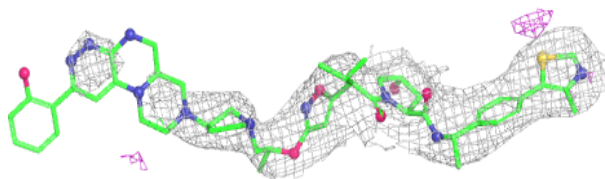
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	CIT	C	101	13/13	0.80	0.12	61,62,65,65	0
6	CIT	S	101	13/13	0.82	0.14	42,44,47,48	0
6	CIT	e	101	13/13	0.83	0.15	37,42,47,48	0
6	CIT	a	101	13/13	0.88	0.11	32,33,34,34	0
6	CIT	W	101	13/13	0.88	0.12	33,37,43,44	0
7	ACT	F	202	4/4	0.88	0.20	75,76,77,78	0
5	A1BB4	h	201	64/64	0.92	0.16	24,78,195,204	0
5	A1BB4	k	201	64/64	0.92	0.15	22,70,159,170	0
5	A1BB4	F	201	64/64	0.92	0.15	23,57,159,168	0
5	A1BB4	d	201	64/64	0.92	0.16	21,54,188,192	0
5	A1BB4	Z	201	64/64	0.94	0.14	19,47,160,163	0
5	A1BB4	B	201	64/64	0.94	0.12	14,42,105,111	0
5	A1BB4	J	201	64/64	0.94	0.15	16,54,193,202	0
5	A1BB4	N	201	64/64	0.94	0.16	11,48,161,170	0
5	A1BB4	R	201	64/64	0.94	0.13	22,46,166,169	0
5	A1BB4	V	201	64/64	0.96	0.14	9,35,184,187	0

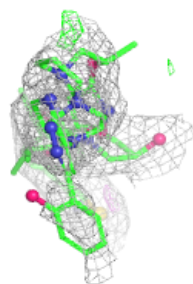
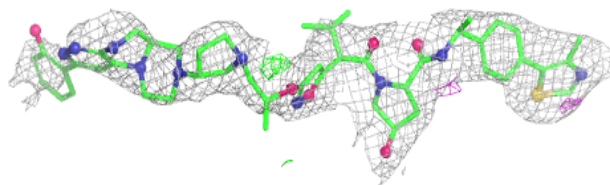
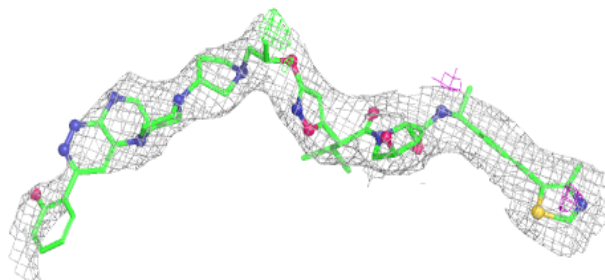
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around A1BB4 h 201:**

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

**Electron density around A1BB4 k 201:**

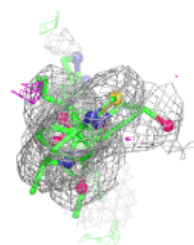
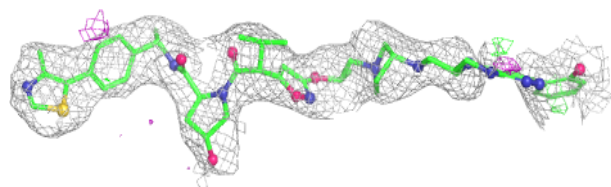
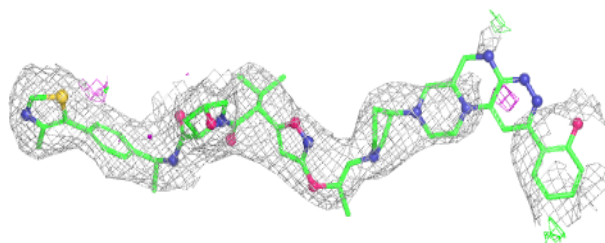
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



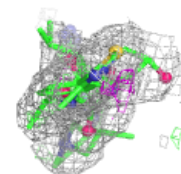
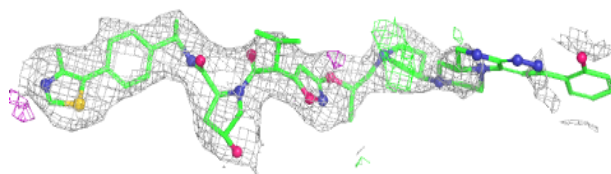
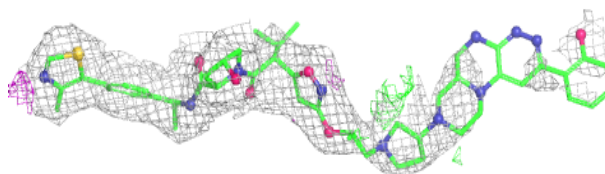


**Electron density around A1BB4 F 201:**

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

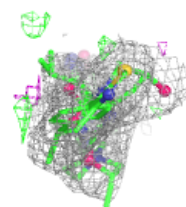
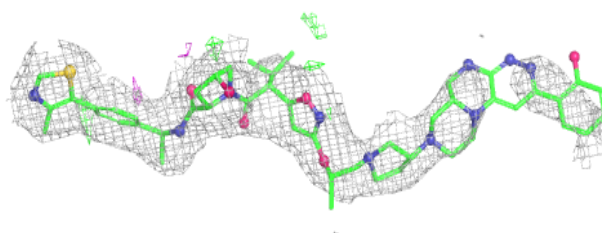
**Electron density around A1BB4 d 201:**

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and green (positive)

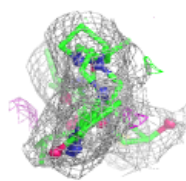
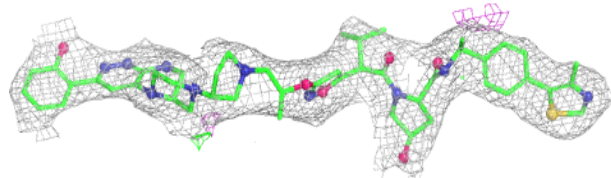
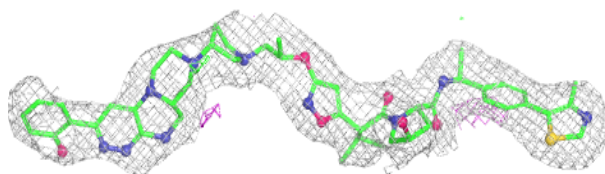


**Electron density around A1BB4 Z 201:**

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

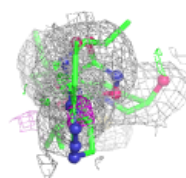
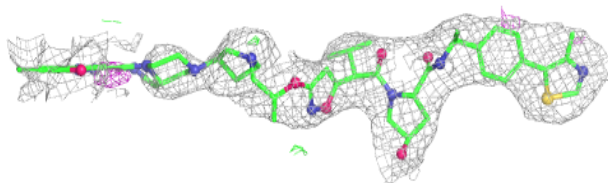
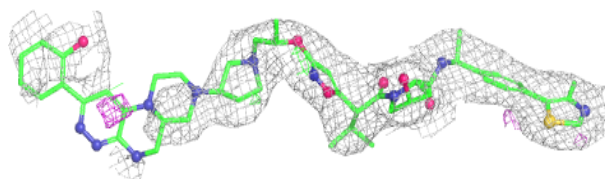
**Electron density around A1BB4 B 201:**

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

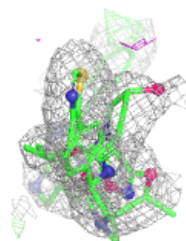
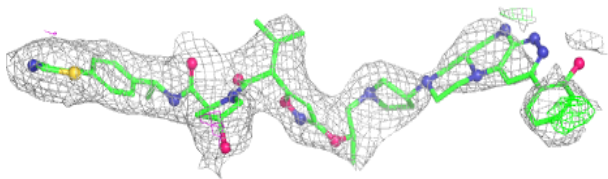
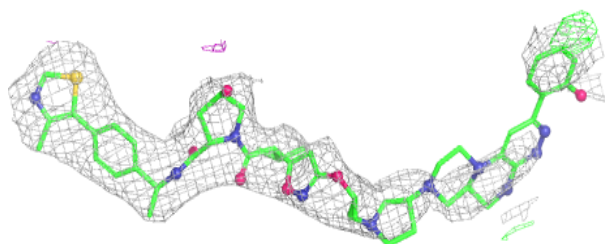


**Electron density around A1BB4 J 201:**

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

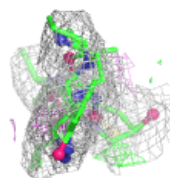
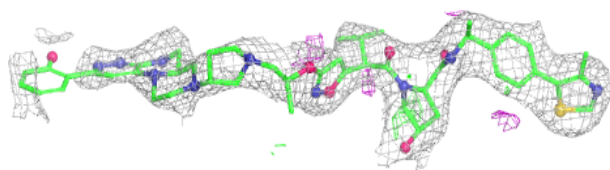
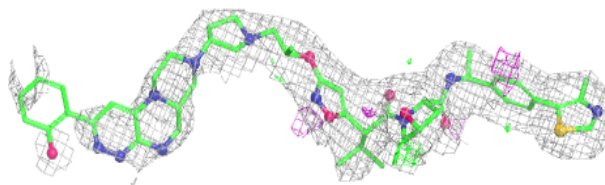
**Electron density around A1BB4 N 201:**

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

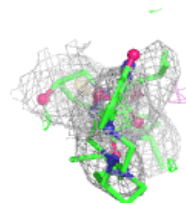
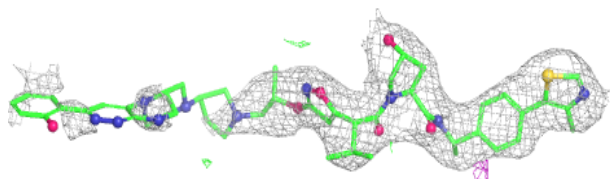
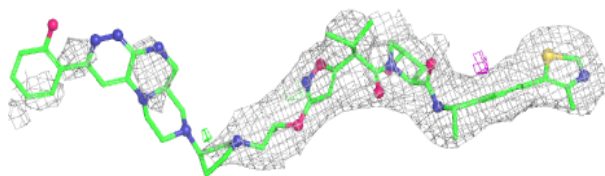


**Electron density around A1BB4 R 201:**

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

**Electron density around A1BB4 V 201:**

$2mF_o-DF_c$  (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.