



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2024 – 07:35 PM EDT

PDB ID : 4GL9  
Title : Crystal structure of inhibitory protein SOCS3 in complex with JAK2 kinase domain and fragment of GP130 intracellular domain  
Authors : Kershaw, N.J.; Murphy, J.M.; Laktyushin, A.; Nicola, N.A.; Babon, J.J.  
Deposited on : 2012-08-14  
Resolution : 3.90 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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

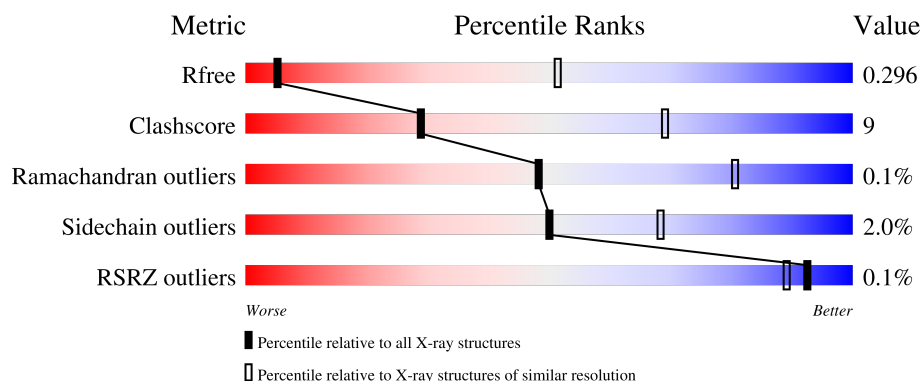
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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	1157 (4.10-3.70)
Clashscore	180529	1219 (4.10-3.70)
Ramachandran outliers	177936	1177 (4.10-3.70)
Sidechain outliers	177891	1169 (4.10-3.70)
RSRZ outliers	164620	1157 (4.10-3.70)

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	297	<div> <div>70%</div> <div>24%</div> <div>• •</div> </div>
1	B	297	<div> <div>72%</div> <div>23%</div> <div>5%</div> </div>
1	C	297	<div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	D	297	<div> <div>72%</div> <div>21%</div> <div>• •</div> </div>
2	I	15	<div> <div>47%</div> <div>7%</div> <div>47%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	15	<div><div></div><div>47%7%7%40%</div></div>
2	K	15	<div><div></div><div>40%7%7%47%</div></div>
2	L	15	<div><div></div><div>40%7%7%47%</div></div>
3	E	143	<div><div></div><div>%66%20%13%</div></div>
3	F	143	<div><div></div><div>69%20%12%</div></div>
3	G	143	<div><div></div><div>75%12%13%</div></div>
3	H	143	<div><div></div><div>75%13%13%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13682 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 Tyrosine-protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	P	S	0	0	0
			2355	1497	405	439	2	12			
1	B	282	Total	C	N	O	P	S	0	0	0
			2326	1477	400	435	2	12			
1	C	284	Total	C	N	O	P	S	0	0	0
			2350	1494	403	439	2	12			
1	D	284	Total	C	N	O	P	S	0	0	0
			2351	1494	404	439	2	12			

- Molecule 2 is a protein called Interleukin-6 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	8	Total	C	N	O	P	0	0	0
			69	42	10	16	1			
2	K	8	Total	C	N	O	P	0	0	0
			69	42	10	16	1			
2	J	9	Total	C	N	O	P	0	0	0
			76	46	11	18	1			
2	L	8	Total	C	N	O	P	0	0	0
			69	42	10	16	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	756	GLU	GLN	conflict	UNP Q00560
K	756	GLU	GLN	conflict	UNP Q00560
J	756	GLU	GLN	conflict	UNP Q00560
L	756	GLU	GLN	conflict	UNP Q00560

- Molecule 3 is a protein called Suppressor of cytokine signaling 3,Suppressor of cytokine signaling 3,Suppressor of cytokine signaling 3,Suppressor of cytokine signaling 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			976	623	169	181	3			
3	F	126	Total	C	N	O	S	0	0	0
			984	627	171	183	3			
3	G	125	Total	C	N	O	S	0	0	0
			980	625	170	182	3			
3	H	125	Total	C	N	O	S	0	0	0
			980	625	170	182	3			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	17	GLN	-	expression tag	UNP O35718
E	18	GLY	-	expression tag	UNP O35718
E	19	ALA	-	expression tag	UNP O35718
E	20	HIS	-	expression tag	UNP O35718
E	21	ASP	-	expression tag	UNP O35718
E	22	LEU	-	expression tag	UNP O35718
E	23	LYS	-	expression tag	UNP O35718
E	24	THR	-	expression tag	UNP O35718
E	25	PHE	-	expression tag	UNP O35718
E	26	SER	-	expression tag	UNP O35718
E	27	SER	-	expression tag	UNP O35718
E	28	LYS	-	expression tag	UNP O35718
E	29	SER	-	expression tag	UNP O35718
E	30	GLU	-	expression tag	UNP O35718
E	31	TYR	-	expression tag	UNP O35718
E	32	GLN	-	expression tag	UNP O35718
E	33	LEU	-	expression tag	UNP O35718
E	34	VAL	-	expression tag	UNP O35718
E	35	VAL	-	expression tag	UNP O35718
E	36	ASN	-	expression tag	UNP O35718
E	37	ALA	-	expression tag	UNP O35718
E	132	GLY	-	linker	UNP O35718
E	133	SER	-	linker	UNP O35718
E	134	GLY	-	linker	UNP O35718
E	135	SER	-	linker	UNP O35718
E	136	GLY	-	linker	UNP O35718
E	137	SER	-	linker	UNP O35718
E	138	GLY	-	linker	UNP O35718
E	139	SER	-	linker	UNP O35718
E	140	ARG	-	linker	UNP O35718
E	141	ALA	-	linker	UNP O35718

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	142	TYR	-	linker	UNP O35718
E	143	TYR	-	linker	UNP O35718
E	144	ILE	-	linker	UNP O35718
E	145	TYR	-	linker	UNP O35718
E	146	SER	-	linker	UNP O35718
E	147	GLY	-	linker	UNP O35718
E	148	GLY	-	linker	UNP O35718
E	149	GLU	-	linker	UNP O35718
E	150	LYS	-	linker	UNP O35718
E	151	ILE	-	linker	UNP O35718
E	152	PRO	-	linker	UNP O35718
E	153	LEU	-	linker	UNP O35718
E	154	VAL	-	linker	UNP O35718
E	155	LEU	-	linker	UNP O35718
E	156	SER	-	linker	UNP O35718
E	157	ARG	-	linker	UNP O35718
E	158	PRO	-	linker	UNP O35718
F	17	GLN	-	expression tag	UNP O35718
F	18	GLY	-	expression tag	UNP O35718
F	19	ALA	-	expression tag	UNP O35718
F	20	HIS	-	expression tag	UNP O35718
F	21	ASP	-	expression tag	UNP O35718
F	22	LEU	-	expression tag	UNP O35718
F	23	LYS	-	expression tag	UNP O35718
F	24	THR	-	expression tag	UNP O35718
F	25	PHE	-	expression tag	UNP O35718
F	26	SER	-	expression tag	UNP O35718
F	27	SER	-	expression tag	UNP O35718
F	28	LYS	-	expression tag	UNP O35718
F	29	SER	-	expression tag	UNP O35718
F	30	GLU	-	expression tag	UNP O35718
F	31	TYR	-	expression tag	UNP O35718
F	32	GLN	-	expression tag	UNP O35718
F	33	LEU	-	expression tag	UNP O35718
F	34	VAL	-	expression tag	UNP O35718
F	35	VAL	-	expression tag	UNP O35718
F	36	ASN	-	expression tag	UNP O35718
F	37	ALA	-	expression tag	UNP O35718
F	132	GLY	-	linker	UNP O35718
F	133	SER	-	linker	UNP O35718
F	134	GLY	-	linker	UNP O35718
F	135	SER	-	linker	UNP O35718

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	136	GLY	-	linker	UNP O35718
F	137	SER	-	linker	UNP O35718
F	138	GLY	-	linker	UNP O35718
F	139	SER	-	linker	UNP O35718
F	140	ARG	-	linker	UNP O35718
F	141	ALA	-	linker	UNP O35718
F	142	TYR	-	linker	UNP O35718
F	143	TYR	-	linker	UNP O35718
F	144	ILE	-	linker	UNP O35718
F	145	TYR	-	linker	UNP O35718
F	146	SER	-	linker	UNP O35718
F	147	GLY	-	linker	UNP O35718
F	148	GLY	-	linker	UNP O35718
F	149	GLU	-	linker	UNP O35718
F	150	LYS	-	linker	UNP O35718
F	151	ILE	-	linker	UNP O35718
F	152	PRO	-	linker	UNP O35718
F	153	LEU	-	linker	UNP O35718
F	154	VAL	-	linker	UNP O35718
F	155	LEU	-	linker	UNP O35718
F	156	SER	-	linker	UNP O35718
F	157	ARG	-	linker	UNP O35718
F	158	PRO	-	linker	UNP O35718
G	17	GLN	-	expression tag	UNP O35718
G	18	GLY	-	expression tag	UNP O35718
G	19	ALA	-	expression tag	UNP O35718
G	20	HIS	-	expression tag	UNP O35718
G	21	ASP	-	expression tag	UNP O35718
G	22	LEU	-	expression tag	UNP O35718
G	23	LYS	-	expression tag	UNP O35718
G	24	THR	-	expression tag	UNP O35718
G	25	PHE	-	expression tag	UNP O35718
G	26	SER	-	expression tag	UNP O35718
G	27	SER	-	expression tag	UNP O35718
G	28	LYS	-	expression tag	UNP O35718
G	29	SER	-	expression tag	UNP O35718
G	30	GLU	-	expression tag	UNP O35718
G	31	TYR	-	expression tag	UNP O35718
G	32	GLN	-	expression tag	UNP O35718
G	33	LEU	-	expression tag	UNP O35718
G	34	VAL	-	expression tag	UNP O35718
G	35	VAL	-	expression tag	UNP O35718

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	36	ASN	-	expression tag	UNP O35718
G	37	ALA	-	expression tag	UNP O35718
G	129	GLY	-	linker	UNP O35718
G	133	SER	-	linker	UNP O35718
G	134	GLY	-	linker	UNP O35718
G	135	SER	-	linker	UNP O35718
G	136	GLY	-	linker	UNP O35718
G	137	SER	-	linker	UNP O35718
G	138	GLY	-	linker	UNP O35718
G	139	SER	-	linker	UNP O35718
G	140	ARG	-	linker	UNP O35718
G	141	ALA	-	linker	UNP O35718
G	142	TYR	-	linker	UNP O35718
G	143	TYR	-	linker	UNP O35718
G	144	ILE	-	linker	UNP O35718
G	145	TYR	-	linker	UNP O35718
G	146	SER	-	linker	UNP O35718
G	147	GLY	-	linker	UNP O35718
G	148	GLY	-	linker	UNP O35718
G	149	GLU	-	linker	UNP O35718
G	150	LYS	-	linker	UNP O35718
G	151	ILE	-	linker	UNP O35718
G	152	PRO	-	linker	UNP O35718
G	153	LEU	-	linker	UNP O35718
G	154	VAL	-	linker	UNP O35718
G	155	LEU	-	linker	UNP O35718
G	156	SER	-	linker	UNP O35718
G	157	ARG	-	linker	UNP O35718
G	158	PRO	-	linker	UNP O35718
H	17	GLN	-	expression tag	UNP O35718
H	18	GLY	-	expression tag	UNP O35718
H	19	ALA	-	expression tag	UNP O35718
H	20	HIS	-	expression tag	UNP O35718
H	21	ASP	-	expression tag	UNP O35718
H	22	LEU	-	expression tag	UNP O35718
H	23	LYS	-	expression tag	UNP O35718
H	24	THR	-	expression tag	UNP O35718
H	25	PHE	-	expression tag	UNP O35718
H	26	SER	-	expression tag	UNP O35718
H	27	SER	-	expression tag	UNP O35718
H	28	LYS	-	expression tag	UNP O35718
H	29	SER	-	expression tag	UNP O35718

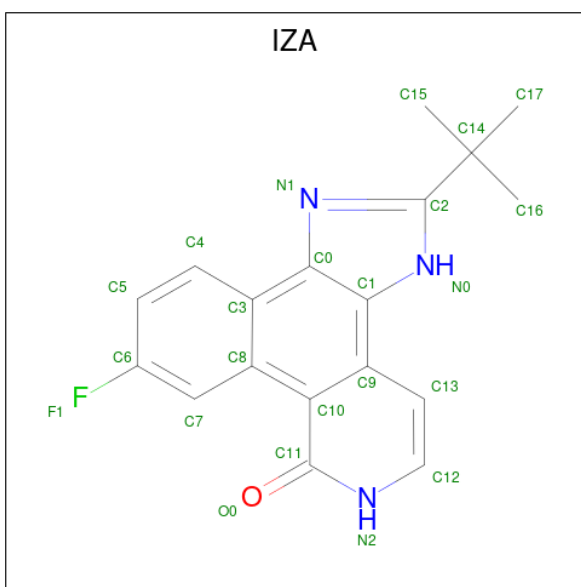
*Continued on next page...*



*Continued from previous page...*

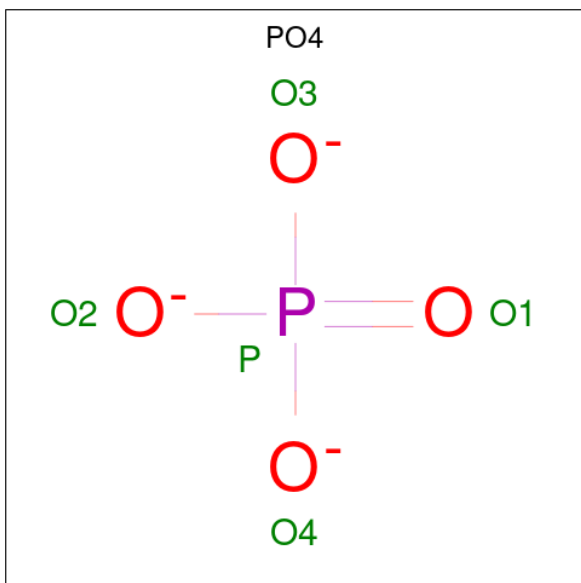
Chain	Residue	Modelled	Actual	Comment	Reference
H	30	GLU	-	expression tag	UNP O35718
H	31	TYR	-	expression tag	UNP O35718
H	32	GLN	-	expression tag	UNP O35718
H	33	LEU	-	expression tag	UNP O35718
H	34	VAL	-	expression tag	UNP O35718
H	35	VAL	-	expression tag	UNP O35718
H	36	ASN	-	expression tag	UNP O35718
H	37	ALA	-	expression tag	UNP O35718
H	129	GLY	-	linker	UNP O35718
H	133	SER	-	linker	UNP O35718
H	134	GLY	-	linker	UNP O35718
H	135	SER	-	linker	UNP O35718
H	136	GLY	-	linker	UNP O35718
H	137	SER	-	linker	UNP O35718
H	138	GLY	-	linker	UNP O35718
H	139	SER	-	linker	UNP O35718
H	140	ARG	-	linker	UNP O35718
H	141	ALA	-	linker	UNP O35718
H	142	TYR	-	linker	UNP O35718
H	143	TYR	-	linker	UNP O35718
H	144	ILE	-	linker	UNP O35718
H	145	TYR	-	linker	UNP O35718
H	146	SER	-	linker	UNP O35718
H	147	GLY	-	linker	UNP O35718
H	148	GLY	-	linker	UNP O35718
H	149	GLU	-	linker	UNP O35718
H	150	LYS	-	linker	UNP O35718
H	151	ILE	-	linker	UNP O35718
H	152	PRO	-	linker	UNP O35718
H	153	LEU	-	linker	UNP O35718
H	154	VAL	-	linker	UNP O35718
H	155	LEU	-	linker	UNP O35718
H	156	SER	-	linker	UNP O35718
H	157	ARG	-	linker	UNP O35718
H	158	PRO	-	linker	UNP O35718

- Molecule 4 is 2-TERT-BUTYL-9-FLUORO-3,6-DIHYDRO-7H-BENZ[H]-IMIDAZ[4,5-F]IS OQUINOLINE-7-ONE (three-letter code: IZA) (formula: C<sub>18</sub>H<sub>16</sub>FN<sub>3</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
4	B	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
4	C	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
4	D	1	Total	C	F	N	O	0	0
			23	18	1	3	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

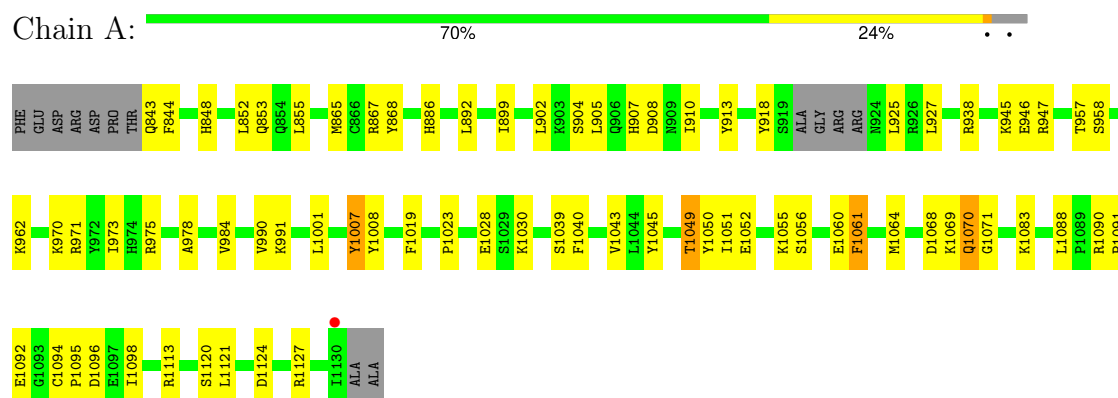


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

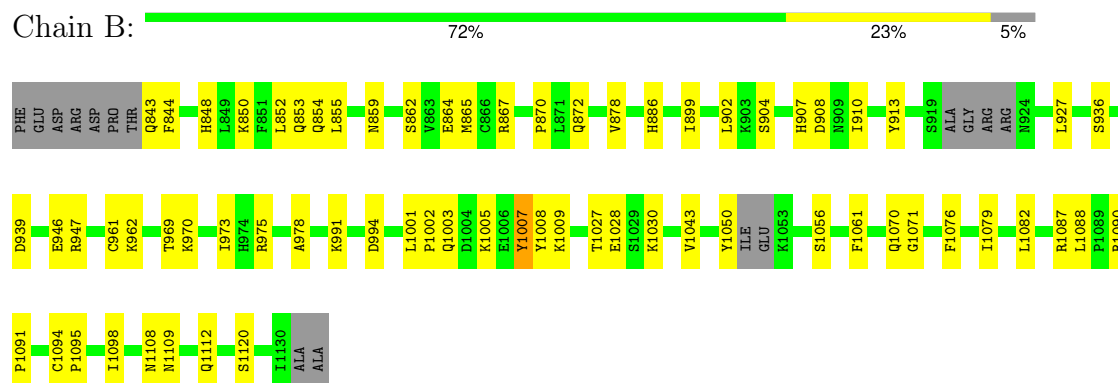
### 3 Residue-property plots

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.

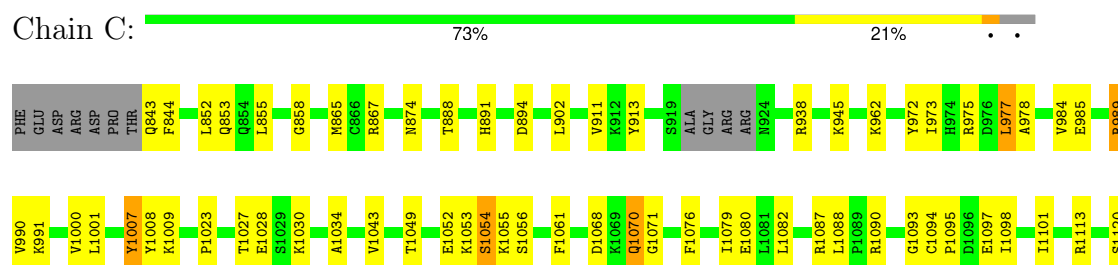
#### • Molecule 1: Tyrosine-protein kinase



#### • Molecule 1: Tyrosine-protein kinase



#### • Molecule 1: Tyrosine-protein kinase





- Molecule 1: Tyrosine-protein kinase

Chain D: 72% 21% . .



- Molecule 2: Interleukin-6 receptor subunit beta

Chain I: 47% 7% 47%



- Molecule 2: Interleukin-6 receptor subunit beta

Chain K: 40% 7% 7% 47%



- Molecule 2: Interleukin-6 receptor subunit beta

Chain J: 47% 7% 7% 40%



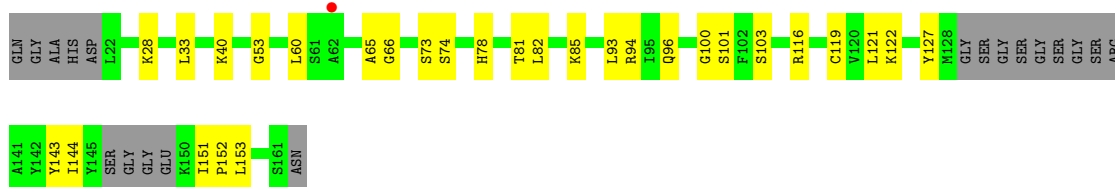
- Molecule 2: Interleukin-6 receptor subunit beta

Chain L: 40% 7% 7% 47%



- Molecule 3: Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3

Chain E: 66% 20% 13%



- Molecule 3: Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3

Chain F: 69% 20% 12%



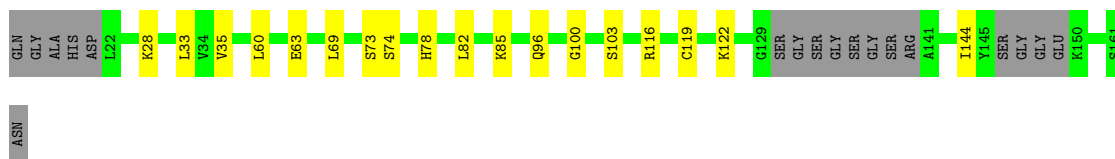
- Molecule 3: Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3

Chain G: 75% 12% 13%



- Molecule 3: Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3, Suppressor of cytokine signaling 3

Chain H: 75% 13% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.26Å 139.26Å 316.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.58 – 3.90 45.58 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.58-3.90) 99.9 (45.58-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.249 , 0.281 0.258 , 0.296	Depositor DCC
$R_{free}$ test set	1587 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 182.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.186 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: IZA, PO4, PTR

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	0.22	0/2371	0.40	0/3190
1	B	0.22	0/2341	0.39	0/3152
1	C	0.22	0/2366	0.39	0/3185
1	D	0.22	0/2367	0.39	0/3186
2	I	0.18	0/52	0.40	0/69
2	J	0.19	0/59	0.46	0/79
2	K	0.17	0/52	0.39	0/69
2	L	0.19	0/52	0.38	0/69
3	E	0.22	0/996	0.37	0/1344
3	F	0.23	0/1004	0.40	0/1354
3	G	0.22	0/1000	0.37	0/1349
3	H	0.22	0/1000	0.36	0/1349
All	All	0.22	0/13660	0.39	0/18395

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2355	0	2327	52	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2326	0	2276	44	0
1	C	2350	0	2311	44	1
1	D	2351	0	2316	47	0
2	I	69	0	58	2	0
2	J	76	0	65	2	0
2	K	69	0	58	4	0
2	L	69	0	58	2	0
3	E	976	0	976	21	0
3	F	984	0	980	18	0
3	G	980	0	979	12	0
3	H	980	0	979	11	1
4	A	23	0	16	1	0
4	B	23	0	16	1	0
4	C	23	0	16	2	0
4	D	23	0	16	2	0
5	B	5	0	0	0	0
All	All	13682	0	13447	232	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 232 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:LEU:HG	1:B:913:TYR:HB2	1.66	0.77
1:A:904:SER:O	1:A:970:LYS:NZ	2.21	0.72
1:D:908:ASP:O	1:D:991:LYS:NZ	2.25	0.69
3:E:101:SER:O	3:E:116:ARG:NH1	2.26	0.68
1:B:904:SER:O	1:B:970:LYS:NZ	2.26	0.68

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1056:SER:OG	3:H:63:GLU:OE1[5_455]	2.19	0.01

## 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	278/297 (94%)	262 (94%)	16 (6%)	0	100	100
1	B	274/297 (92%)	262 (96%)	12 (4%)	0	100	100
1	C	278/297 (94%)	263 (95%)	14 (5%)	1 (0%)	30	65
1	D	278/297 (94%)	263 (95%)	15 (5%)	0	100	100
2	I	5/15 (33%)	5 (100%)	0	0	100	100
2	J	6/15 (40%)	5 (83%)	1 (17%)	0	100	100
2	K	5/15 (33%)	5 (100%)	0	0	100	100
2	L	5/15 (33%)	5 (100%)	0	0	100	100
3	E	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
3	F	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
3	G	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
3	H	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
All	All	1605/1820 (88%)	1540 (96%)	64 (4%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1053	LYS

### 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	260/271 (96%)	253 (97%)	7 (3%)	40	60
1	B	255/271 (94%)	249 (98%)	6 (2%)	44	63
1	C	258/271 (95%)	251 (97%)	7 (3%)	40	60
1	D	259/271 (96%)	250 (96%)	9 (4%)	31	54
2	I	7/12 (58%)	7 (100%)	0	100	100
2	J	8/12 (67%)	8 (100%)	0	100	100
2	K	7/12 (58%)	7 (100%)	0	100	100
2	L	7/12 (58%)	7 (100%)	0	100	100
3	E	110/122 (90%)	110 (100%)	0	100	100
3	F	110/122 (90%)	110 (100%)	0	100	100
3	G	110/122 (90%)	109 (99%)	1 (1%)	75	83
3	H	110/122 (90%)	110 (100%)	0	100	100
All	All	1501/1620 (93%)	1471 (98%)	30 (2%)	50	68

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	977	LEU
1	D	1097	GLU
1	C	1061	PHE
3	G	150	LYS
1	D	1056	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	874	ASN
1	B	1109	ASN
1	C	1125	GLN
1	D	986	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	PTR	L	757	2	15,16,17	1.24	1 (6%)	17,22,24	0.63	0
1	PTR	A	1007	1	15,16,17	1.23	1 (6%)	17,22,24	0.57	0
2	PTR	I	757	2	15,16,17	1.24	1 (6%)	17,22,24	0.63	0
1	PTR	A	1008	1	15,16,17	1.23	1 (6%)	17,22,24	0.59	0
2	PTR	K	757	2	15,16,17	1.28	1 (6%)	17,22,24	0.67	0
1	PTR	B	1008	1	15,16,17	1.24	1 (6%)	17,22,24	0.59	0
1	PTR	C	1007	1	15,16,17	1.23	1 (6%)	17,22,24	0.60	0
1	PTR	D	1007	1	15,16,17	1.21	1 (6%)	17,22,24	0.56	0
2	PTR	J	757	2	15,16,17	1.22	1 (6%)	17,22,24	0.60	0
1	PTR	C	1008	1	15,16,17	1.23	1 (6%)	17,22,24	0.58	0
1	PTR	B	1007	1	15,16,17	1.21	1 (6%)	17,22,24	0.59	0
1	PTR	D	1008	1	15,16,17	1.21	1 (6%)	17,22,24	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	L	757	2	-	2/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1
2	PTR	I	757	2	-	2/10/11/13	0/1/1/1
1	PTR	A	1008	1	-	1/10/11/13	0/1/1/1
2	PTR	K	757	2	-	0/10/11/13	0/1/1/1
1	PTR	B	1008	1	-	1/10/11/13	0/1/1/1
1	PTR	C	1007	1	-	1/10/11/13	0/1/1/1
1	PTR	D	1007	1	-	0/10/11/13	0/1/1/1
2	PTR	J	757	2	-	0/10/11/13	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	2/10/11/13	0/1/1/1
1	PTR	D	1008	1	-	0/10/11/13	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	757	PTR	OH-CZ	-4.71	1.30	1.40
2	I	757	PTR	OH-CZ	-4.54	1.30	1.40
1	B	1008	PTR	OH-CZ	-4.51	1.30	1.40
2	L	757	PTR	OH-CZ	-4.50	1.30	1.40
1	C	1008	PTR	OH-CZ	-4.42	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1007	PTR	O-C-CA-CB
2	I	757	PTR	C-CA-CB-CG
2	I	757	PTR	N-CA-CB-CG
1	A	1008	PTR	CZ-OH-P-O1P
1	C	1007	PTR	CZ-OH-P-O1P

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	757	PTR	1	0
1	A	1007	PTR	1	0
2	I	757	PTR	2	0
2	K	757	PTR	3	0
1	C	1007	PTR	2	0
1	D	1007	PTR	1	0
2	J	757	PTR	1	0
1	B	1007	PTR	1	0
1	D	1008	PTR	1	0

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

5 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
4	IZA	C	1201	-	21,26,26	2.99	8 (38%)	27,41,41	1.78	8 (29%)
4	IZA	A	2001	-	21,26,26	2.98	8 (38%)	27,41,41	1.74	8 (29%)
5	PO4	B	1202	-	4,4,4	0.96	0	6,6,6	0.45	0
4	IZA	B	1201	-	21,26,26	3.00	8 (38%)	27,41,41	1.76	8 (29%)
4	IZA	D	1201	-	21,26,26	3.01	8 (38%)	27,41,41	1.77	8 (29%)

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
4	IZA	B	1201	-	-	3/6/6/6	0/4/4/4
4	IZA	D	1201	-	-	0/6/6/6	0/4/4/4
4	IZA	C	1201	-	-	3/6/6/6	0/4/4/4
4	IZA	A	2001	-	-	0/6/6/6	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1201	IZA	C13-C12	8.17	1.48	1.36
4	D	1201	IZA	C13-C12	8.16	1.48	1.36
4	B	1201	IZA	C13-C12	8.15	1.48	1.36
4	A	2001	IZA	C13-C12	8.11	1.48	1.36
4	D	1201	IZA	C11-N2	6.74	1.44	1.33

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1201	IZA	C13-C12-N2	-4.86	119.06	123.83
4	D	1201	IZA	C13-C12-N2	-4.77	119.16	123.83
4	A	2001	IZA	C13-C12-N2	-4.75	119.18	123.83
4	B	1201	IZA	C13-C12-N2	-4.70	119.22	123.83
4	D	1201	IZA	C13-C9-C1	-3.05	118.03	122.47

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

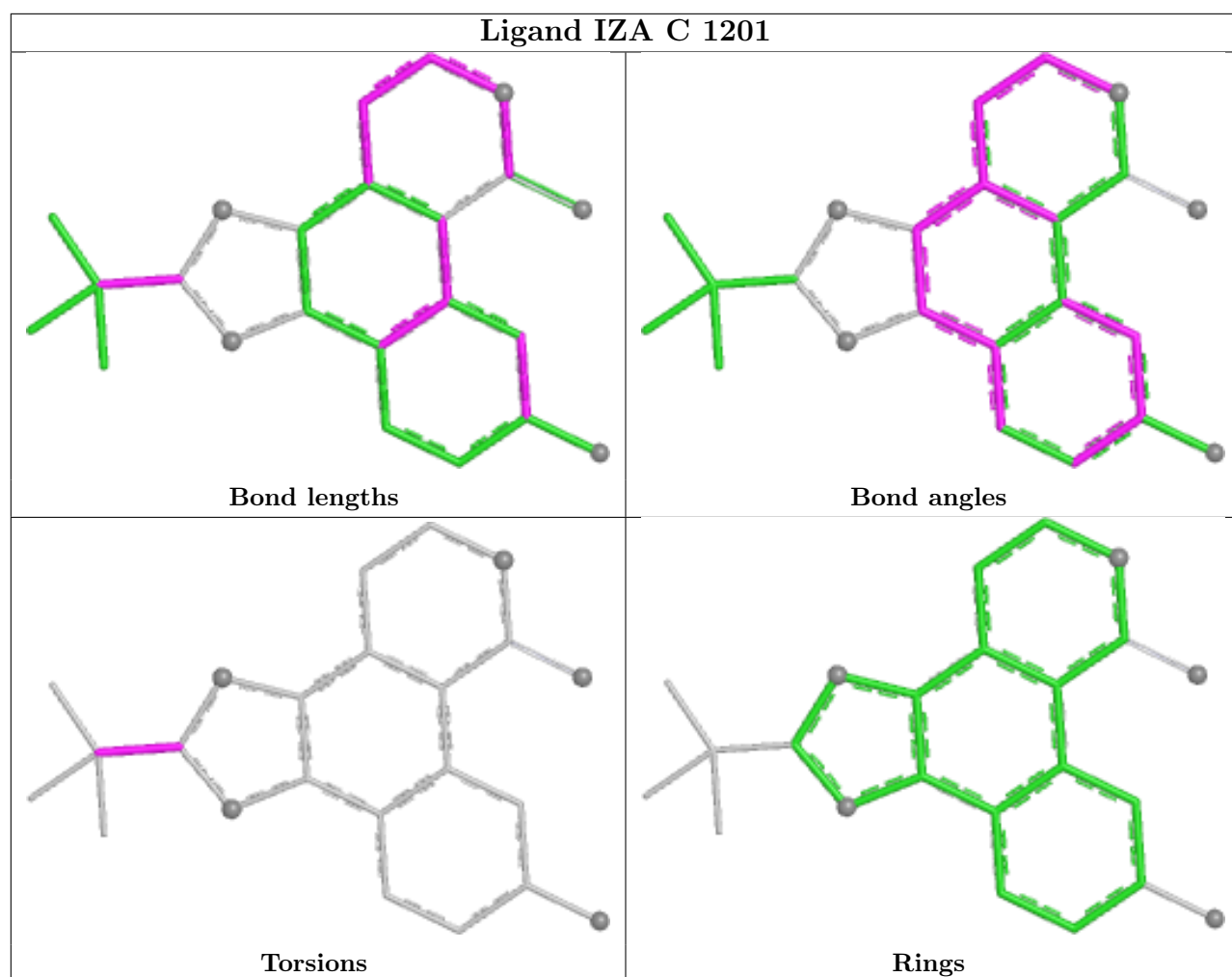
Mol	Chain	Res	Type	Atoms
4	B	1201	IZA	C17-C14-C2-N0
4	B	1201	IZA	C15-C14-C2-N0
4	C	1201	IZA	C17-C14-C2-N0
4	C	1201	IZA	C15-C14-C2-N0
4	B	1201	IZA	C16-C14-C2-N0

There are no ring outliers.

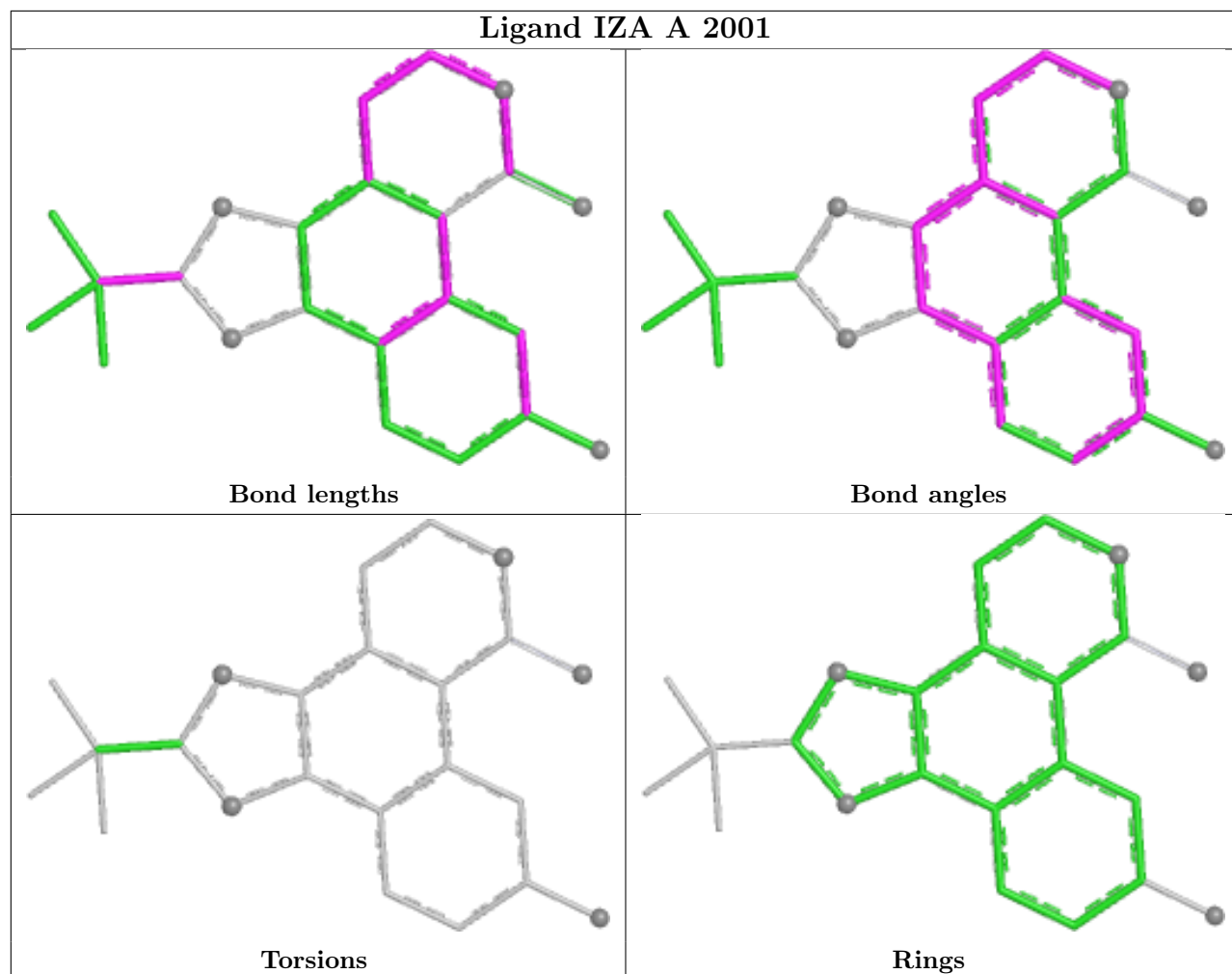
4 monomers are involved in 6 short contacts:

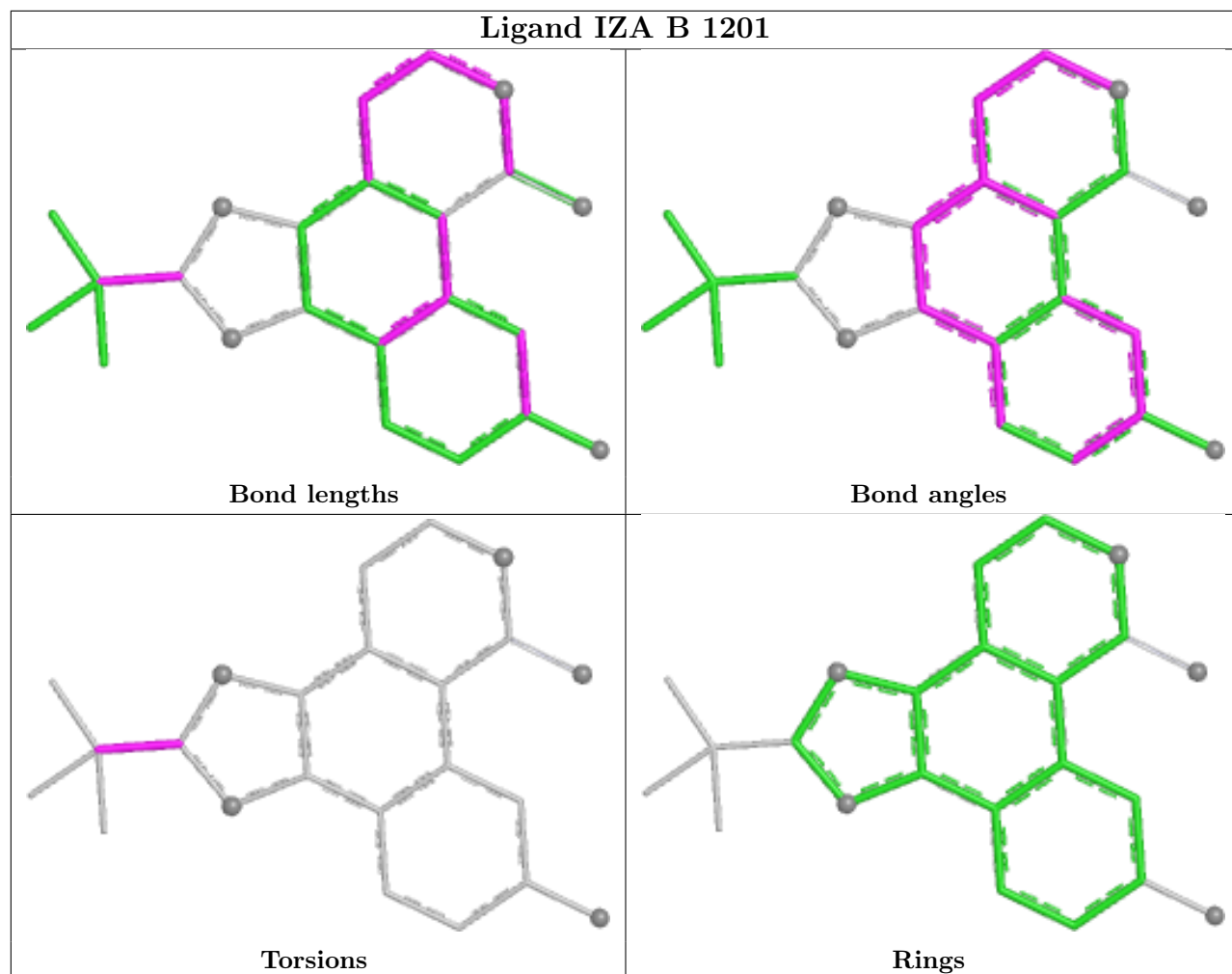
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1201	IZA	2	0
4	A	2001	IZA	1	0
4	B	1201	IZA	1	0
4	D	1201	IZA	2	0

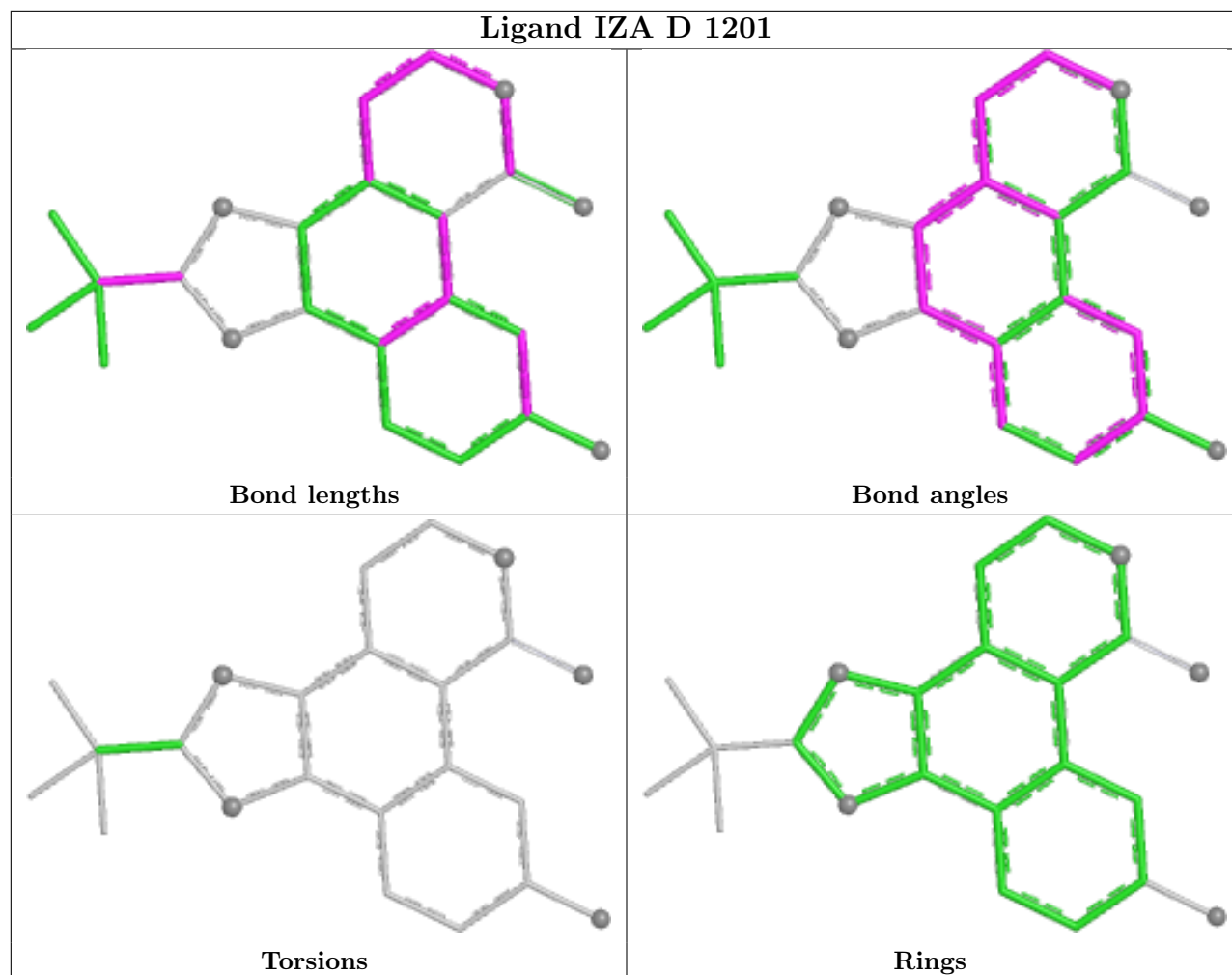
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	282/297 (94%)	-0.45	1 (0%) 89 78	125, 186, 246, 261	0
1	B	280/297 (94%)	-0.55	0 100 100	144, 189, 249, 262	0
1	C	282/297 (94%)	-0.55	0 100 100	122, 183, 254, 269	0
1	D	282/297 (94%)	-0.51	0 100 100	139, 190, 254, 278	0
2	I	7/15 (46%)	-0.65	0 100 100	176, 215, 231, 232	0
2	J	8/15 (53%)	-0.16	0 100 100	189, 216, 244, 247	0
2	K	7/15 (46%)	-0.19	0 100 100	178, 214, 241, 241	0
2	L	7/15 (46%)	-0.40	0 100 100	206, 215, 237, 239	0
3	E	124/143 (86%)	-0.55	1 (0%) 82 69	124, 157, 238, 250	0
3	F	126/143 (88%)	-0.51	0 100 100	135, 187, 247, 263	0
3	G	125/143 (87%)	-0.53	0 100 100	135, 165, 229, 259	0
3	H	125/143 (87%)	-0.54	0 100 100	144, 191, 246, 266	0
All	All	1655/1820 (90%)	-0.52	2 (0%) 92 89	122, 185, 249, 278	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1130	ILE	2.1
3	E	62	ALA	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	B	1008	16/17	0.85	0.09	201,219,238,238	4
1	PTR	D	1008	16/17	0.86	0.09	205,213,222,225	4
1	PTR	B	1007	16/17	0.89	0.11	205,228,253,260	0
1	PTR	D	1007	16/17	0.90	0.09	210,227,238,241	0
1	PTR	A	1008	16/17	0.91	0.11	197,214,223,225	4
2	PTR	J	757	16/17	0.91	0.07	176,184,214,215	0
2	PTR	K	757	16/17	0.92	0.07	146,164,202,217	0
2	PTR	I	757	16/17	0.92	0.07	145,165,210,218	0
1	PTR	C	1007	16/17	0.92	0.06	175,199,216,220	0
1	PTR	C	1008	16/17	0.92	0.08	175,205,218,223	4
1	PTR	A	1007	16/17	0.94	0.06	194,217,232,239	0
2	PTR	L	757	16/17	0.95	0.05	176,182,211,215	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

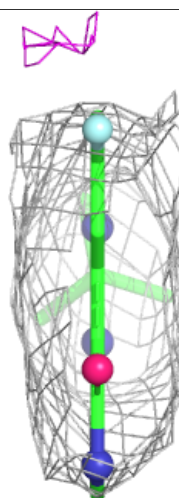
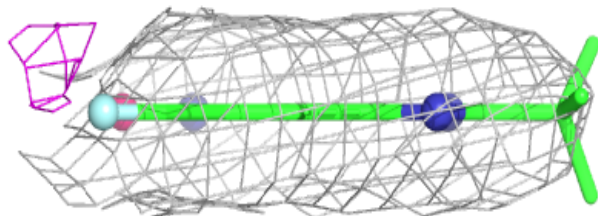
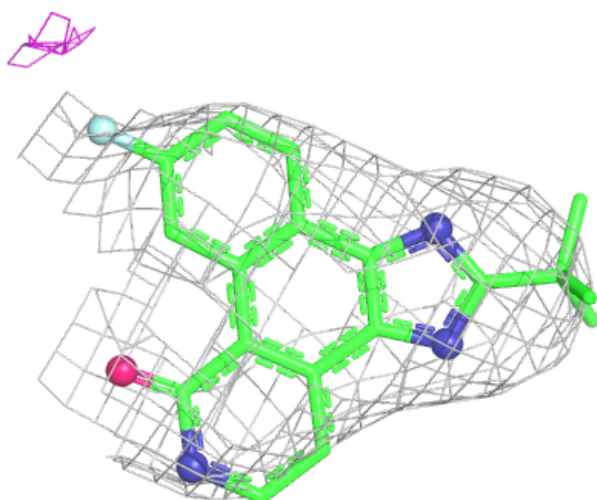
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	PO4	B	1202	5/5	0.80	0.09	197,203,214,216	0
4	IZA	A	2001	23/23	0.93	0.11	158,177,185,188	0
4	IZA	B	1201	23/23	0.94	0.10	183,196,206,209	0
4	IZA	D	1201	23/23	0.96	0.09	182,189,196,201	0
4	IZA	C	1201	23/23	0.96	0.12	183,192,202,204	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.

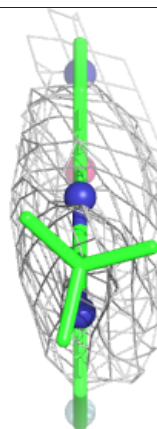
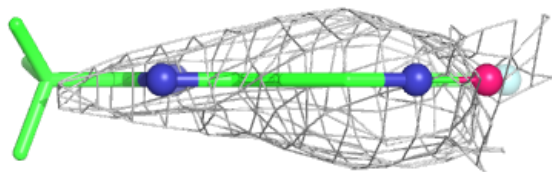
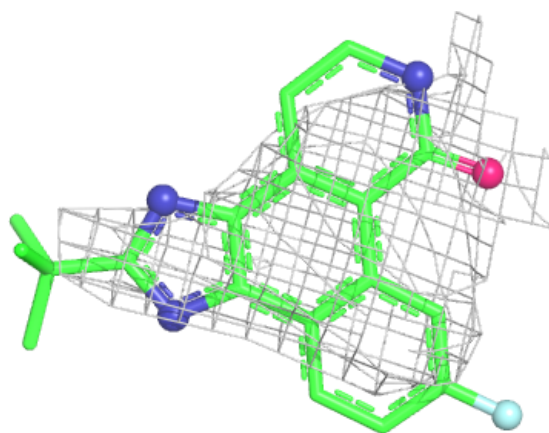
**Electron density around IZA A 2001:**

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

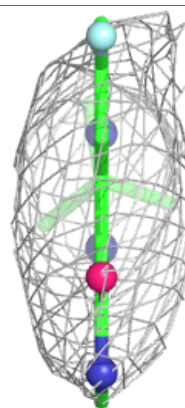
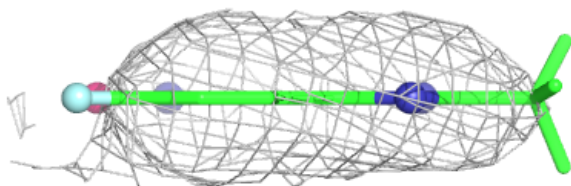
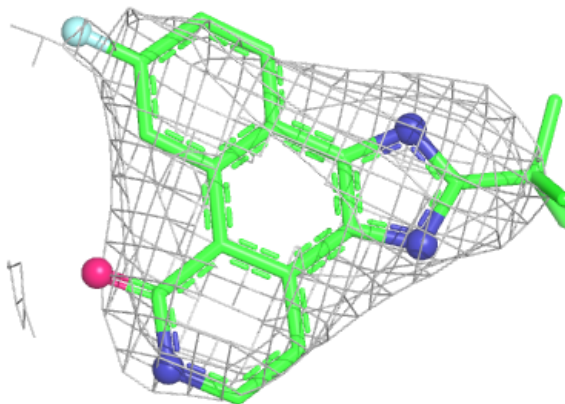


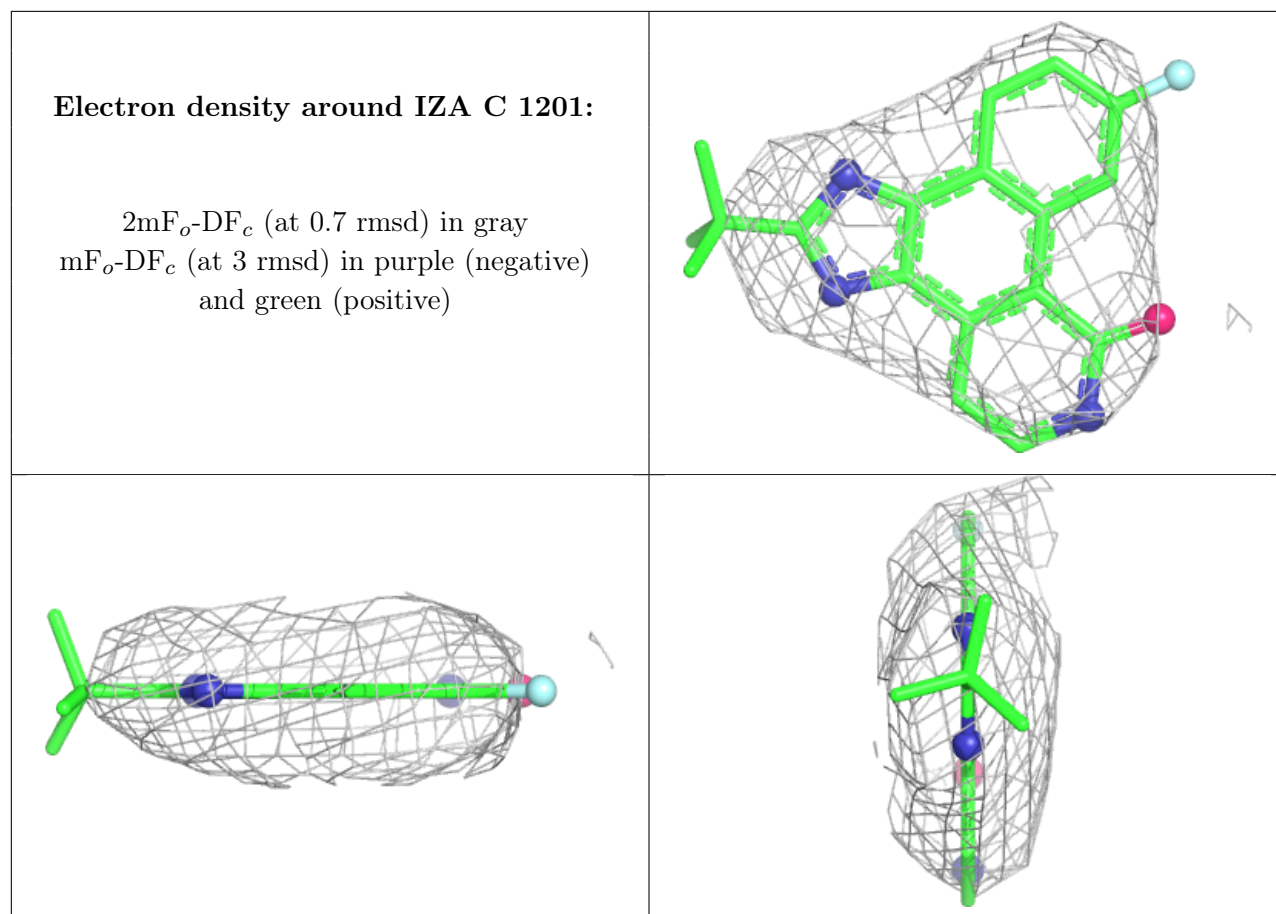
**Electron density around IZA B 1201:**

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

**Electron density around IZA D 1201:**

$2mF_o-DF_c$  (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.