



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 11:23 AM EDT

PDB ID : 6FQJ  
Title : GluA2(flop) G724C ligand binding core dimer bound to ZK200775 at 2.50 Angstrom resolution  
Authors : Coombs, I.D.; Soto, D.; Gold, M.G.; Farrant, M.F.; Cull-Candy, S.G.  
Deposited on : 2018-02-14  
Resolution : 2.50 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

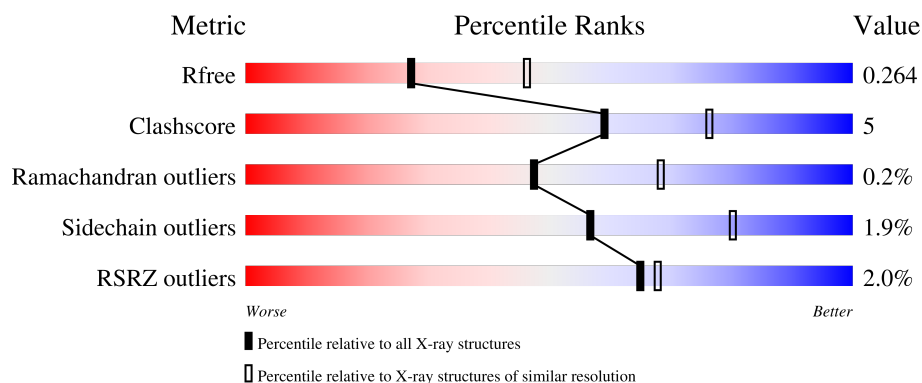
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

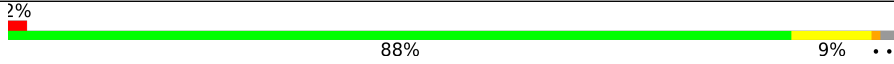


The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	264	
1	B	264	
1	C	264	
1	D	264	
1	E	264	

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Mol	Chain	Length	Quality of chain
1	F	264	<div><div></div><div>3%</div><div>83%</div><div>14%</div><div></div><div>.</div></div>
1	G	264	<div><div></div><div>2%</div><div>90%</div><div>8%</div><div></div><div>..</div></div>
1	H	264	<div><div></div><div>3%</div><div>91%</div><div>8%</div><div></div><div>.</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33622 atoms, of which 16422 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 Glutamate receptor 2,Glutamate receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	H	N	O	S	0	0	0
			4079	1291	2049	338	386	15			
1	B	258	Total	C	H	N	O	S	0	0	0
			4039	1280	2028	334	382	15			
1	C	259	Total	C	H	N	O	S	0	0	0
			4046	1282	2031	335	383	15			
1	D	259	Total	C	H	N	O	S	0	0	0
			4070	1288	2046	337	384	15			
1	E	258	Total	C	H	N	O	S	0	0	0
			4056	1284	2040	335	382	15			
1	F	258	Total	C	H	N	O	S	0	0	0
			4039	1280	2028	334	382	15			
1	G	260	Total	C	H	N	O	S	0	0	0
			4074	1289	2048	337	385	15			
1	H	260	Total	C	H	N	O	S	0	0	0
			4074	1289	2048	337	385	15			

There are 40 discrepancies between the modelled and reference sequences:

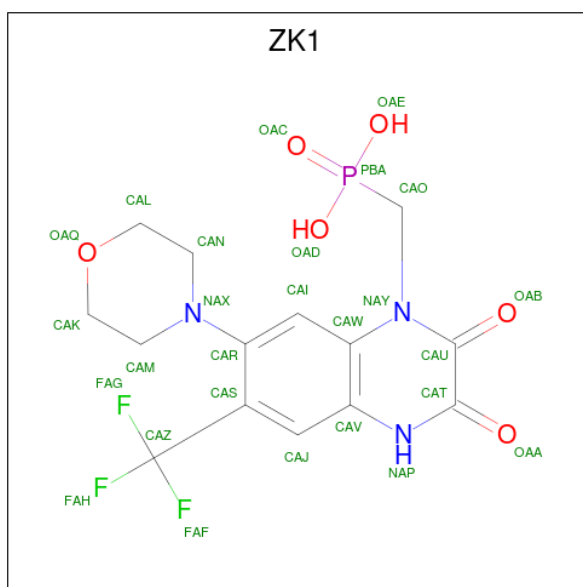
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P19491
A	2	ALA	-	expression tag	UNP P19491
A	118	GLY	-	linker	UNP P19491
A	119	THR	-	linker	UNP P19491
A	212	CYS	GLY	conflict	UNP P19491
B	1	GLY	-	expression tag	UNP P19491
B	2	ALA	-	expression tag	UNP P19491
B	118	GLY	-	linker	UNP P19491
B	119	THR	-	linker	UNP P19491
B	212	CYS	GLY	conflict	UNP P19491
C	1	GLY	-	expression tag	UNP P19491
C	2	ALA	-	expression tag	UNP P19491
C	118	GLY	-	linker	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	119	THR	-	linker	UNP P19491
C	212	CYS	GLY	conflict	UNP P19491
D	1	GLY	-	expression tag	UNP P19491
D	2	ALA	-	expression tag	UNP P19491
D	118	GLY	-	linker	UNP P19491
D	119	THR	-	linker	UNP P19491
D	212	CYS	GLY	conflict	UNP P19491
E	1	GLY	-	expression tag	UNP P19491
E	2	ALA	-	expression tag	UNP P19491
E	118	GLY	-	linker	UNP P19491
E	119	THR	-	linker	UNP P19491
E	212	CYS	GLY	conflict	UNP P19491
F	1	GLY	-	expression tag	UNP P19491
F	2	ALA	-	expression tag	UNP P19491
F	118	GLY	-	linker	UNP P19491
F	119	THR	-	linker	UNP P19491
F	212	CYS	GLY	conflict	UNP P19491
G	1	GLY	-	expression tag	UNP P19491
G	2	ALA	-	expression tag	UNP P19491
G	118	GLY	-	linker	UNP P19491
G	119	THR	-	linker	UNP P19491
G	212	CYS	GLY	conflict	UNP P19491
H	1	GLY	-	expression tag	UNP P19491
H	2	ALA	-	expression tag	UNP P19491
H	118	GLY	-	linker	UNP P19491
H	119	THR	-	linker	UNP P19491
H	212	CYS	GLY	conflict	UNP P19491

- Molecule 2 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C<sub>14</sub>H<sub>15</sub>F<sub>3</sub>N<sub>3</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		
2	B	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		
2	C	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		
2	D	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		
2	E	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		
2	F	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		
2	G	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		
2	H	1	Total	C	F	H	N	O	P	0	0
			40	14	3	13	3	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	97	Total	O	0	0
			97	97		
3	C	81	Total	O	0	0
			81	81		
3	D	101	Total	O	0	0
			101	101		

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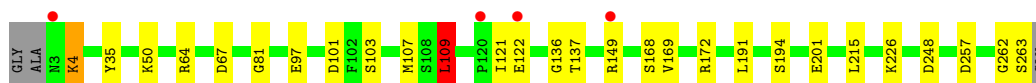
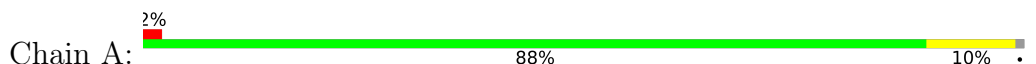
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	118	Total 118	O 118	0	0
3	F	89	Total 89	O 89	0	0
3	G	113	Total 113	O 113	0	0
3	H	129	Total 129	O 129	0	0

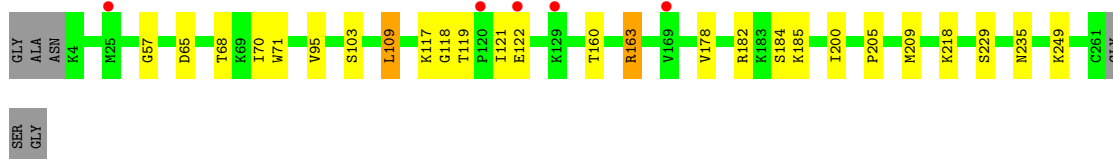
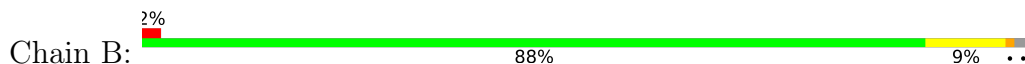
### 3 Residue-property plots

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

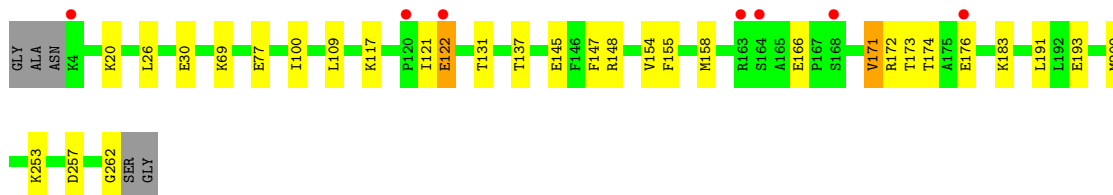
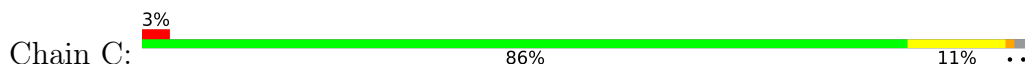
- Molecule 1: Glutamate receptor 2, Glutamate receptor 2



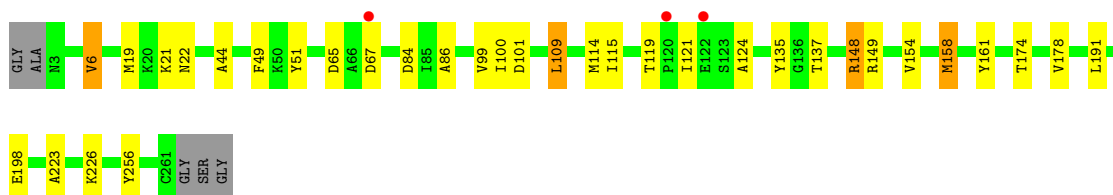
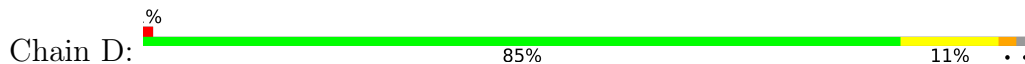
- Molecule 1: Glutamate receptor 2, Glutamate receptor 2



- Molecule 1: Glutamate receptor 2, Glutamate receptor 2

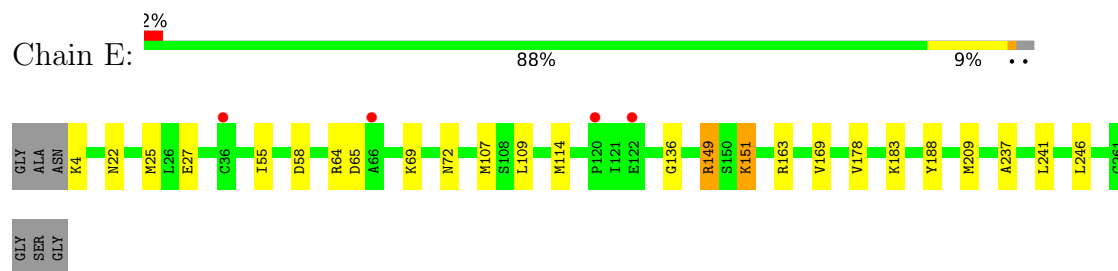


- Molecule 1: Glutamate receptor 2, Glutamate receptor 2

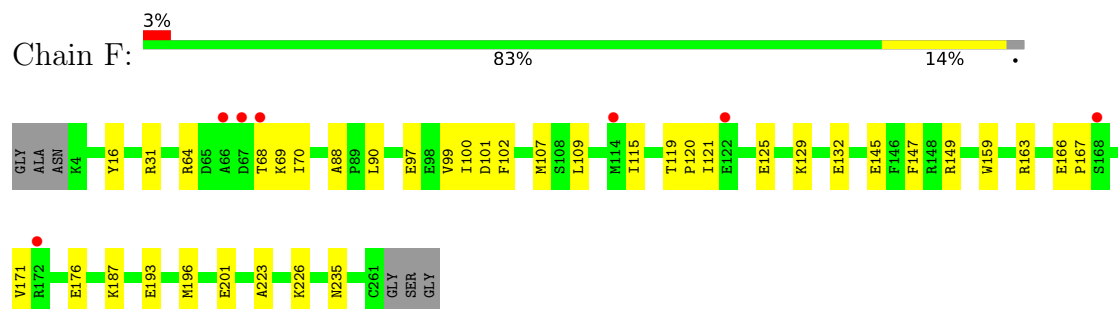




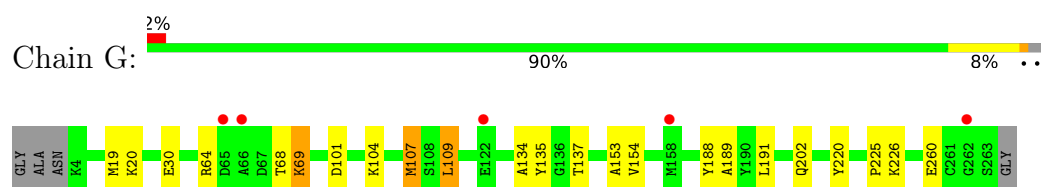
- Molecule 1: Glutamate receptor 2,Glutamate receptor 2



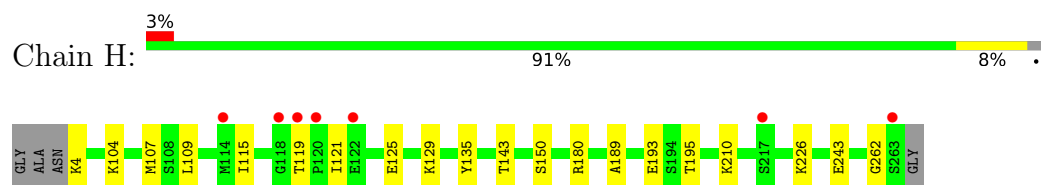
- Molecule 1: Glutamate receptor 2,Glutamate receptor 2



- Molecule 1: Glutamate receptor 2,Glutamate receptor 2



- Molecule 1: Glutamate receptor 2,Glutamate receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.01Å 144.29Å 199.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.83 – 2.50 81.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (81.83-2.50) 90.7 (81.96-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.198 , 0.265 0.199 , 0.264	Depositor DCC
$R_{free}$ test set	4273 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	33622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.44% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZK1

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	0.63	0/2066	0.71	1/2779 (0.0%)
1	B	0.59	0/2047	0.68	1/2755 (0.0%)
1	C	0.61	0/2051	0.71	0/2760
1	D	0.64	0/2060	0.74	2/2772 (0.1%)
1	E	0.63	0/2052	0.73	0/2761
1	F	0.60	0/2047	0.69	0/2755
1	G	0.61	0/2062	0.73	0/2774
1	H	0.62	0/2062	0.74	0/2774
All	All	0.62	0/16447	0.72	4/22130 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	LEU	CA-CB-CG	6.17	129.50	115.30
1	D	109	LEU	CA-CB-CG	5.94	128.97	115.30
1	B	109	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	158	MET	CG-SD-CE	-5.22	91.85	100.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2030	2049	2049	18	0
1	B	2011	2028	2028	20	0
1	C	2015	2031	2031	25	0
1	D	2024	2046	2046	22	0
1	E	2016	2040	2040	17	0
1	F	2011	2028	2028	28	0
1	G	2026	2048	2048	16	0
1	H	2026	2048	2048	11	0
2	A	27	13	13	0	0
2	B	27	13	13	0	0
2	C	27	13	13	1	0
2	D	27	13	13	0	0
2	E	27	13	13	0	0
2	F	27	13	13	1	0
2	G	27	13	13	1	0
2	H	27	13	13	1	0
3	A	97	0	0	6	0
3	B	97	0	0	7	0
3	C	81	0	0	6	0
3	D	101	0	0	5	0
3	E	118	0	0	8	2
3	F	89	0	0	7	0
3	G	113	0	0	8	2
3	H	129	0	0	5	0
All	All	17200	16422	16422	153	2

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 5.

The worst 5 of 153 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:C:172:ARG:N	1:C:176:GLU:OE2	1.90	1.05
1:E:114:MET:SD	3:E:486:HOH:O	2.13	1.05
1:C:147:PHE:O	3:C:401:HOH:O	1.85	0.94
1:F:193:GLU:OE2	3:F:401:HOH:O	1.87	0.93
1:E:4:LYS:O	3:E:401:HOH:O	1.88	0.88

All (2) 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)
3:E:496:HOH:O	3:G:411:HOH:O[1_455]	1.88	0.32
3:E:485:HOH:O	3:G:498:HOH:O[1_455]	1.93	0.27

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/264 (98%)	250 (96%)	8 (3%)	1 (0%)	34	54
1	B	256/264 (97%)	251 (98%)	5 (2%)	0	100	100
1	C	257/264 (97%)	254 (99%)	2 (1%)	1 (0%)	34	54
1	D	257/264 (97%)	252 (98%)	4 (2%)	1 (0%)	34	54
1	E	256/264 (97%)	252 (98%)	4 (2%)	0	100	100
1	F	256/264 (97%)	250 (98%)	6 (2%)	0	100	100
1	G	258/264 (98%)	256 (99%)	2 (1%)	0	100	100
1	H	258/264 (98%)	251 (97%)	6 (2%)	1 (0%)	34	54
All	All	2057/2112 (97%)	2016 (98%)	37 (2%)	4 (0%)	47	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	GLY
1	D	67	ASP
1	C	122	GLU
1	H	262	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/220 (99%)	213 (98%)	5 (2%)	50	76
1	B	216/220 (98%)	213 (99%)	3 (1%)	67	86
1	C	216/220 (98%)	212 (98%)	4 (2%)	57	80
1	D	218/220 (99%)	213 (98%)	5 (2%)	50	76
1	E	217/220 (99%)	210 (97%)	7 (3%)	39	65
1	F	216/220 (98%)	215 (100%)	1 (0%)	88	96
1	G	218/220 (99%)	214 (98%)	4 (2%)	59	81
1	H	218/220 (99%)	214 (98%)	4 (2%)	59	81
All	All	1737/1760 (99%)	1704 (98%)	33 (2%)	57	80

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	109	LEU
1	H	107	MET
1	H	226	LYS
1	D	6	VAL
1	C	183	LYS

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

Mol	Chain	Res	Type
1	D	244	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 monosaccharides in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ZK1	H	301	-	28,29,29	2.17	10 (35%)	42,45,45	1.71	12 (28%)
2	ZK1	A	301	-	28,29,29	2.36	11 (39%)	42,45,45	1.35	9 (21%)
2	ZK1	F	301	-	28,29,29	2.61	11 (39%)	42,45,45	1.58	10 (23%)
2	ZK1	D	301	-	28,29,29	2.07	9 (32%)	42,45,45	1.80	11 (26%)
2	ZK1	E	301	-	28,29,29	2.25	8 (28%)	42,45,45	1.48	8 (19%)
2	ZK1	G	301	-	28,29,29	2.04	10 (35%)	42,45,45	2.03	12 (28%)
2	ZK1	C	301	-	28,29,29	2.14	9 (32%)	42,45,45	1.69	10 (23%)
2	ZK1	B	301	-	28,29,29	2.30	12 (42%)	42,45,45	1.96	10 (23%)

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	ZK1	H	301	-	-	5/13/23/23	0/3/3/3
2	ZK1	A	301	-	-	6/13/23/23	0/3/3/3
2	ZK1	F	301	-	-	6/13/23/23	0/3/3/3
2	ZK1	D	301	-	-	6/13/23/23	0/3/3/3
2	ZK1	E	301	-	-	6/13/23/23	0/3/3/3
2	ZK1	G	301	-	-	2/13/23/23	0/3/3/3
2	ZK1	C	301	-	-	5/13/23/23	0/3/3/3
2	ZK1	B	301	-	-	7/13/23/23	0/3/3/3

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	ZK1	CAZ-CAS	6.15	1.63	1.50

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	ZK1	CAT-NAP	6.03	1.44	1.35
2	E	301	ZK1	CAZ-CAS	5.70	1.62	1.50
2	A	301	ZK1	CAZ-CAS	5.39	1.62	1.50
2	B	301	ZK1	CAZ-CAS	5.22	1.61	1.50

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	ZK1	FAH-CAZ-CAS	-5.23	103.59	112.70
2	D	301	ZK1	FAG-CAZ-CAS	-4.82	104.31	112.70
2	D	301	ZK1	CAV-NAP-CAT	-4.44	119.15	124.80
2	B	301	ZK1	CAO-NAY-CAU	4.43	120.83	116.51
2	B	301	ZK1	FAH-CAZ-CAS	-4.36	105.11	112.70

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ZK1	NAY-CAO-PBA-OAD
2	B	301	ZK1	NAY-CAO-PBA-OAD
2	D	301	ZK1	NAY-CAO-PBA-OAD
2	D	301	ZK1	NAY-CAO-PBA-OAE
2	E	301	ZK1	NAY-CAO-PBA-OAC

There are no ring outliers.

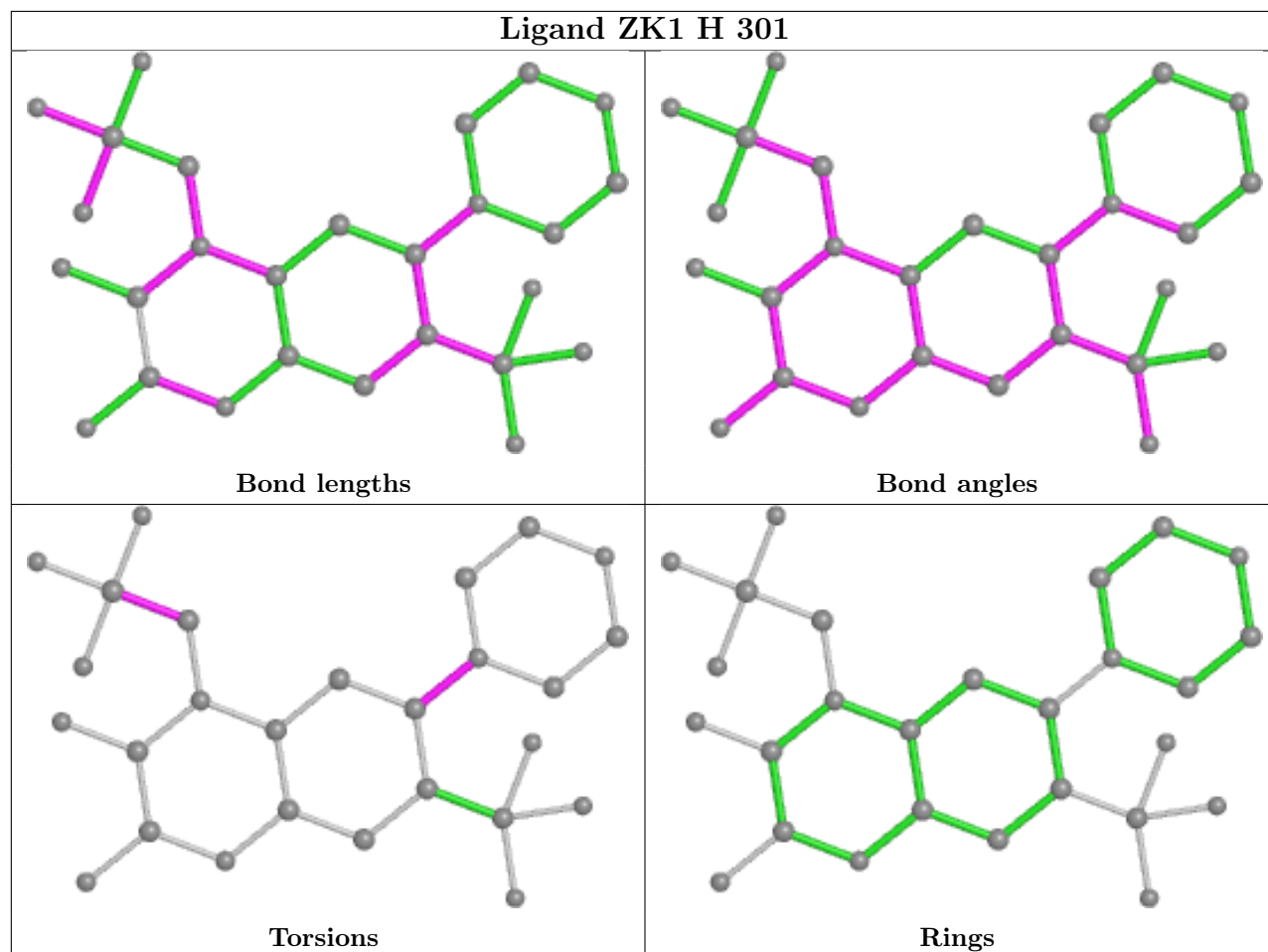
4 monomers are involved in 4 short contacts:

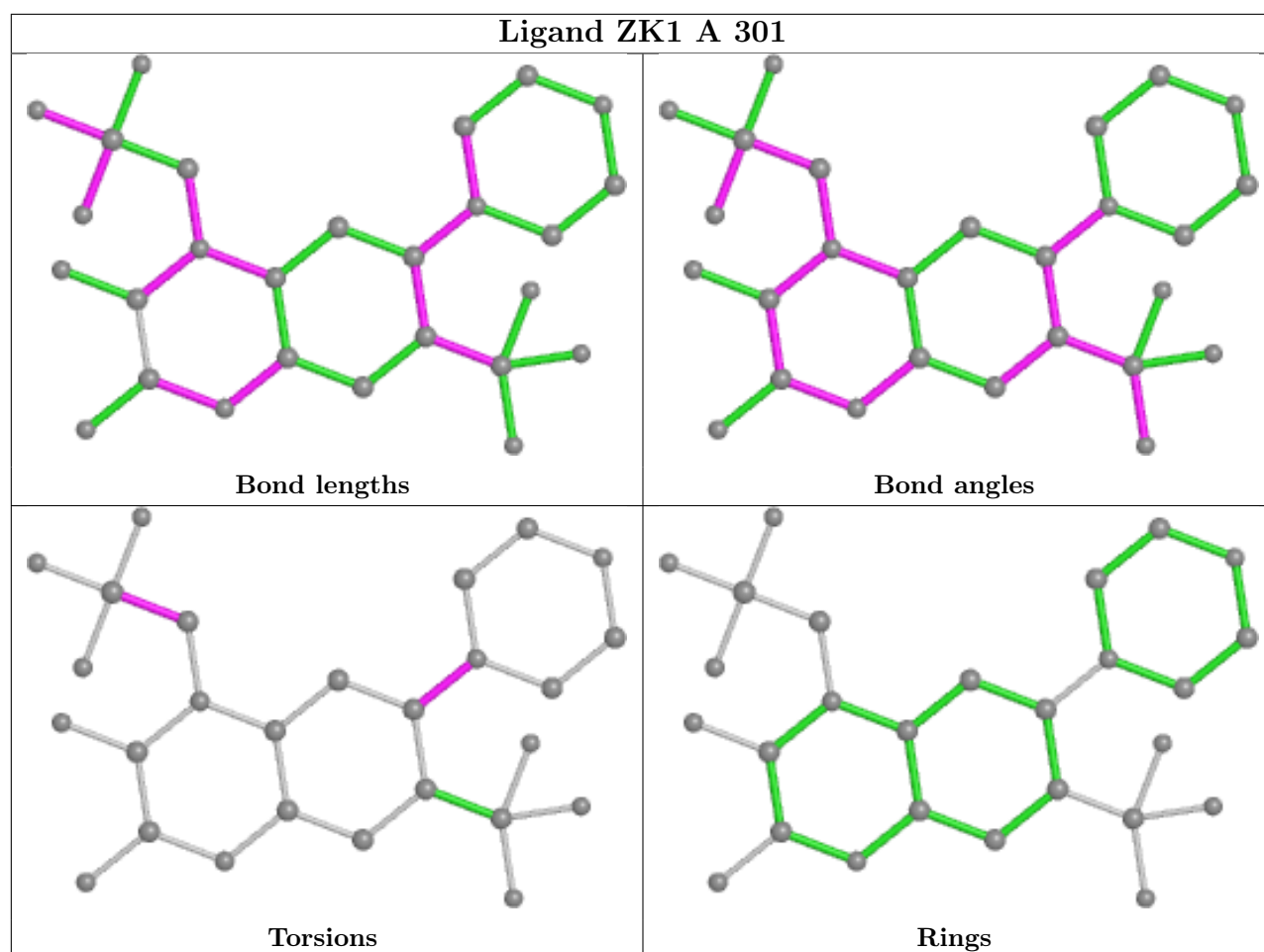
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	ZK1	1	0
2	F	301	ZK1	1	0
2	G	301	ZK1	1	0
2	C	301	ZK1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

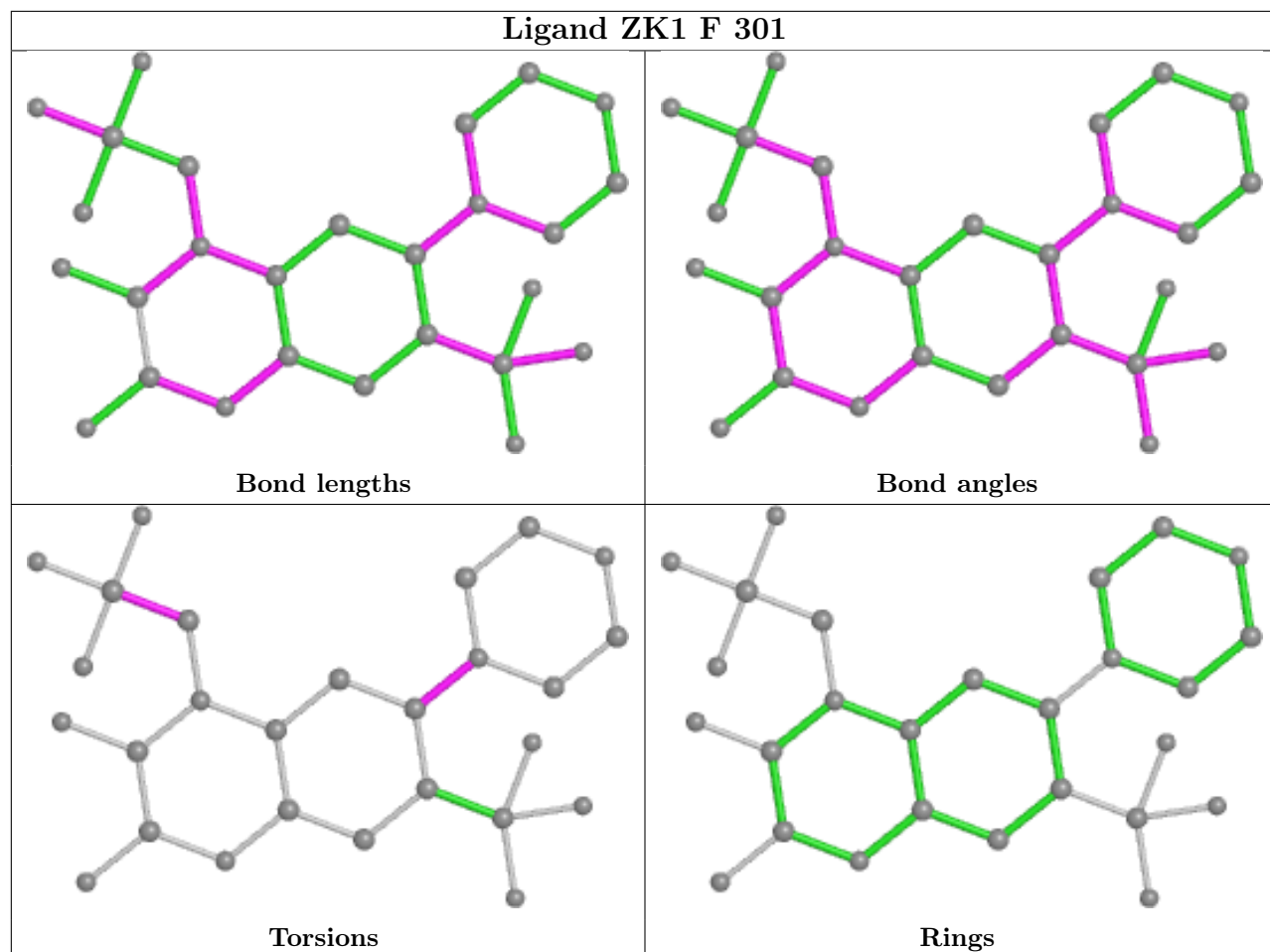


any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

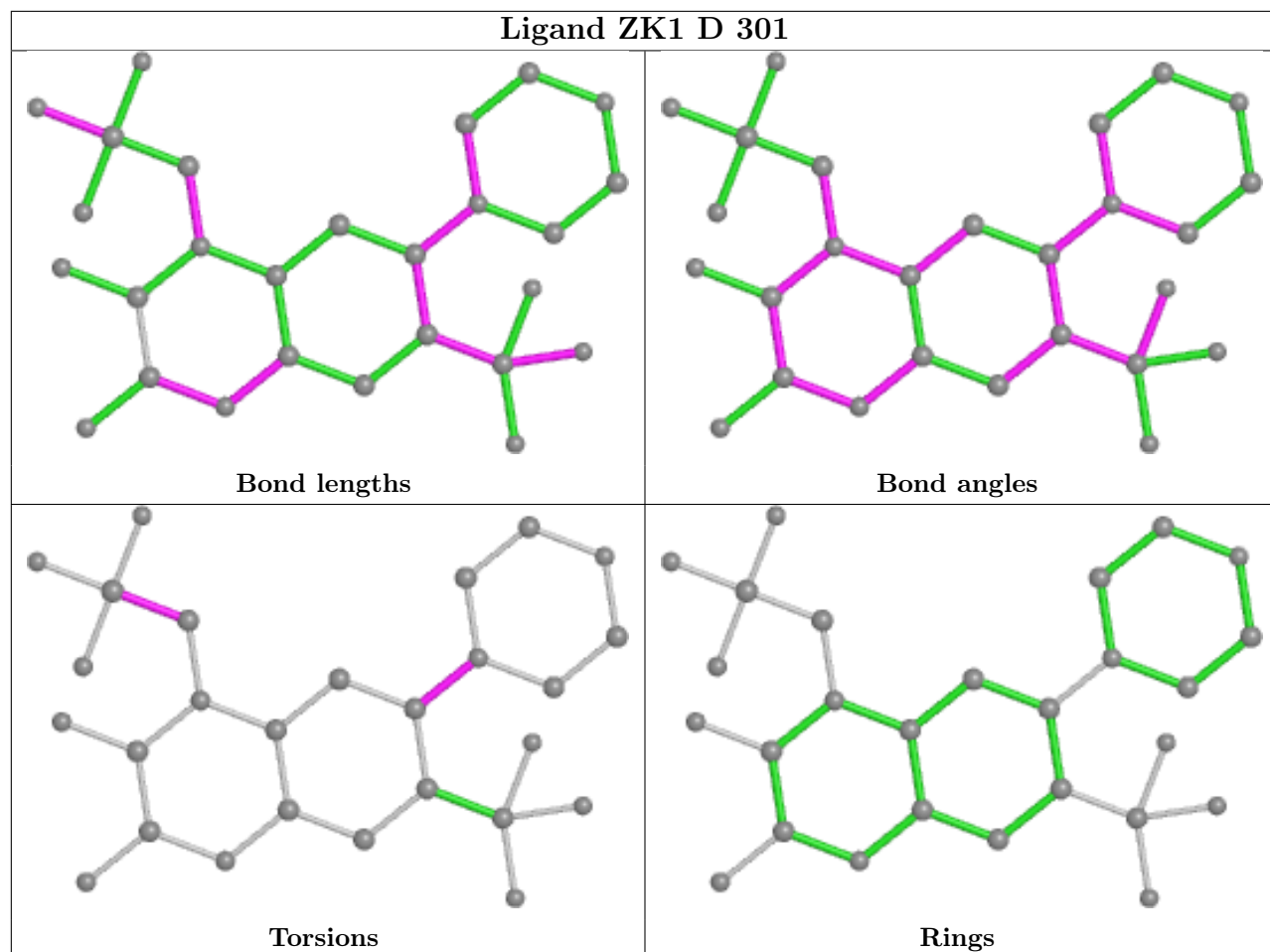


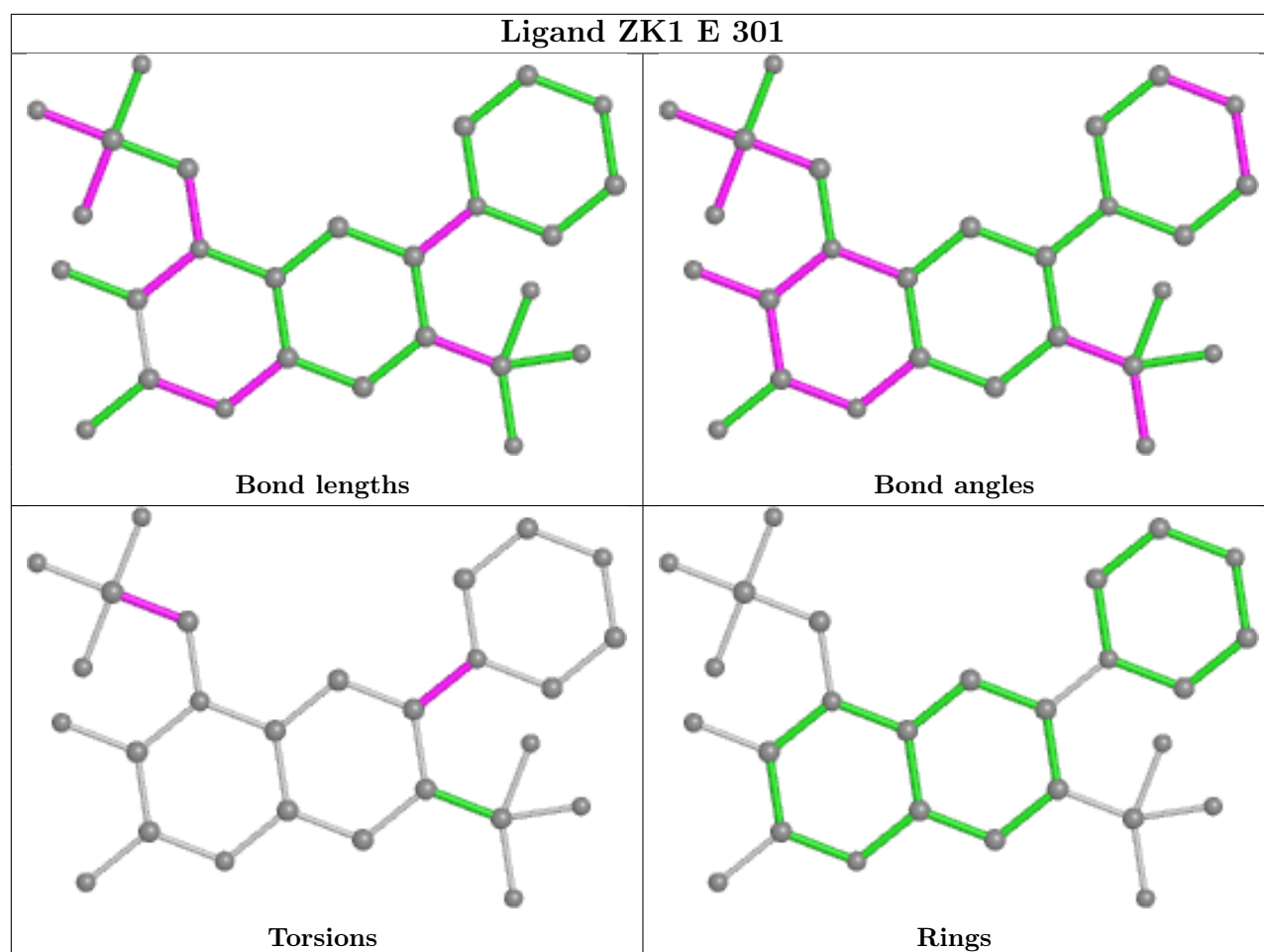


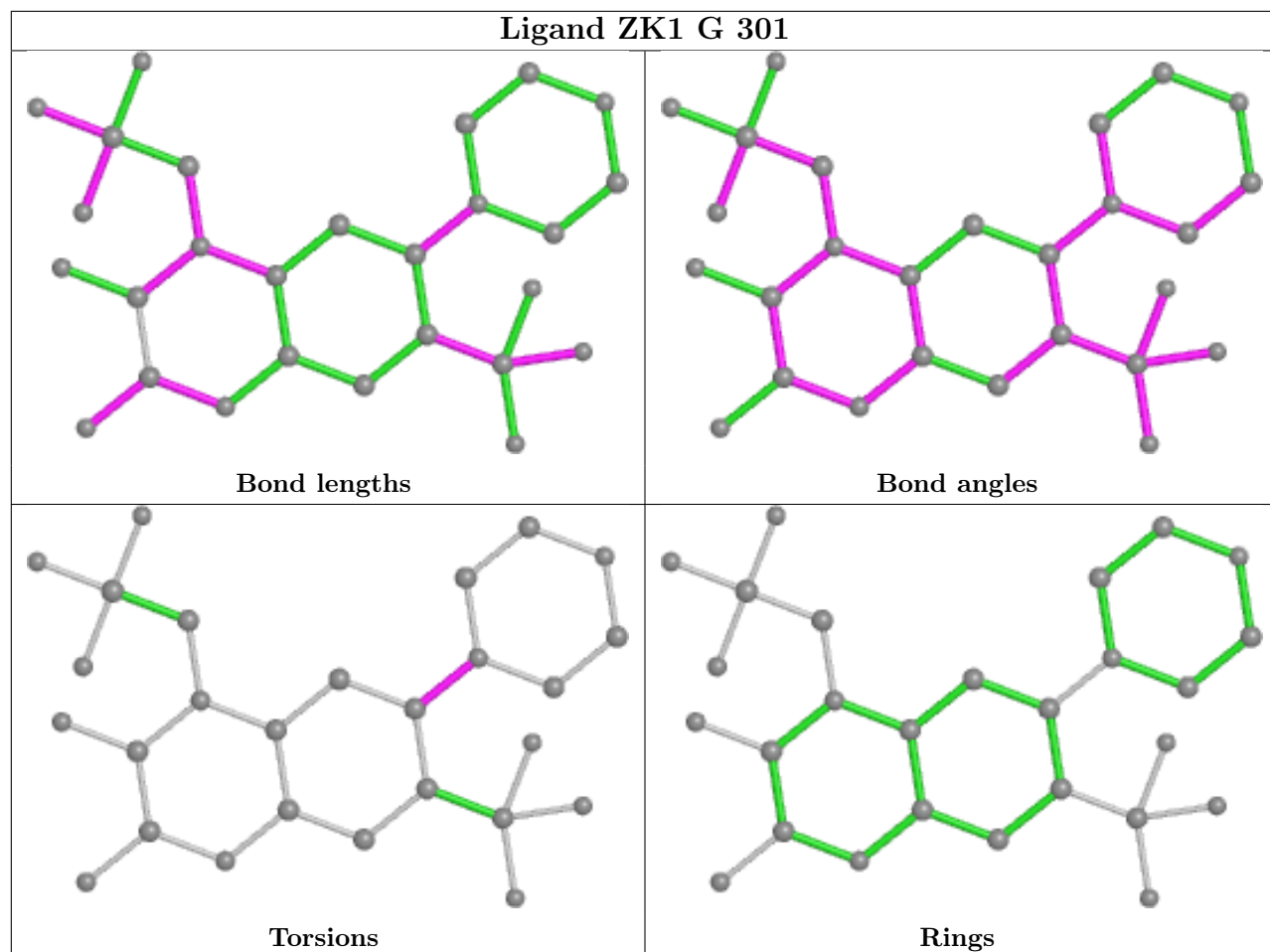
## Ligand ZK1 F 301

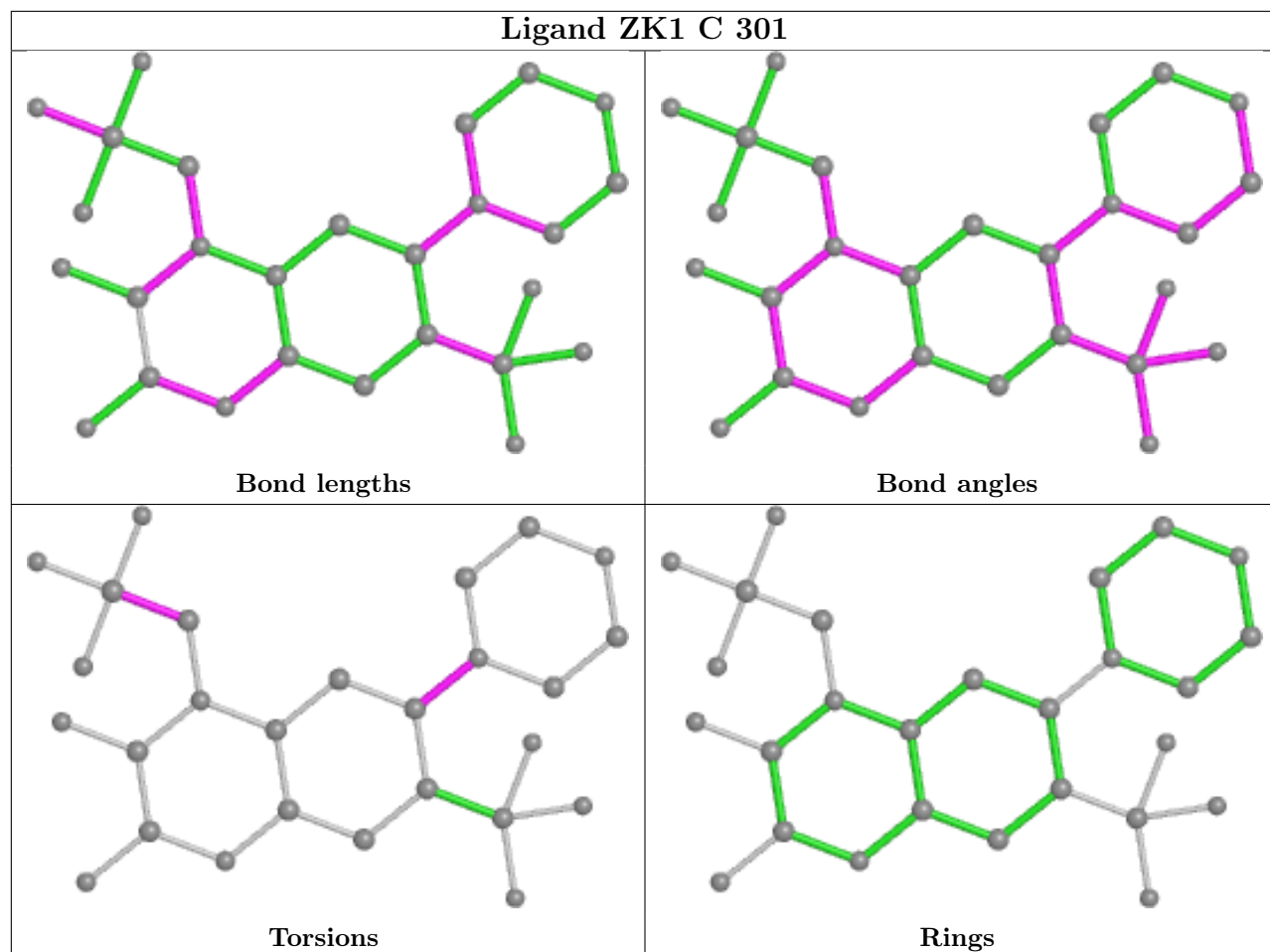


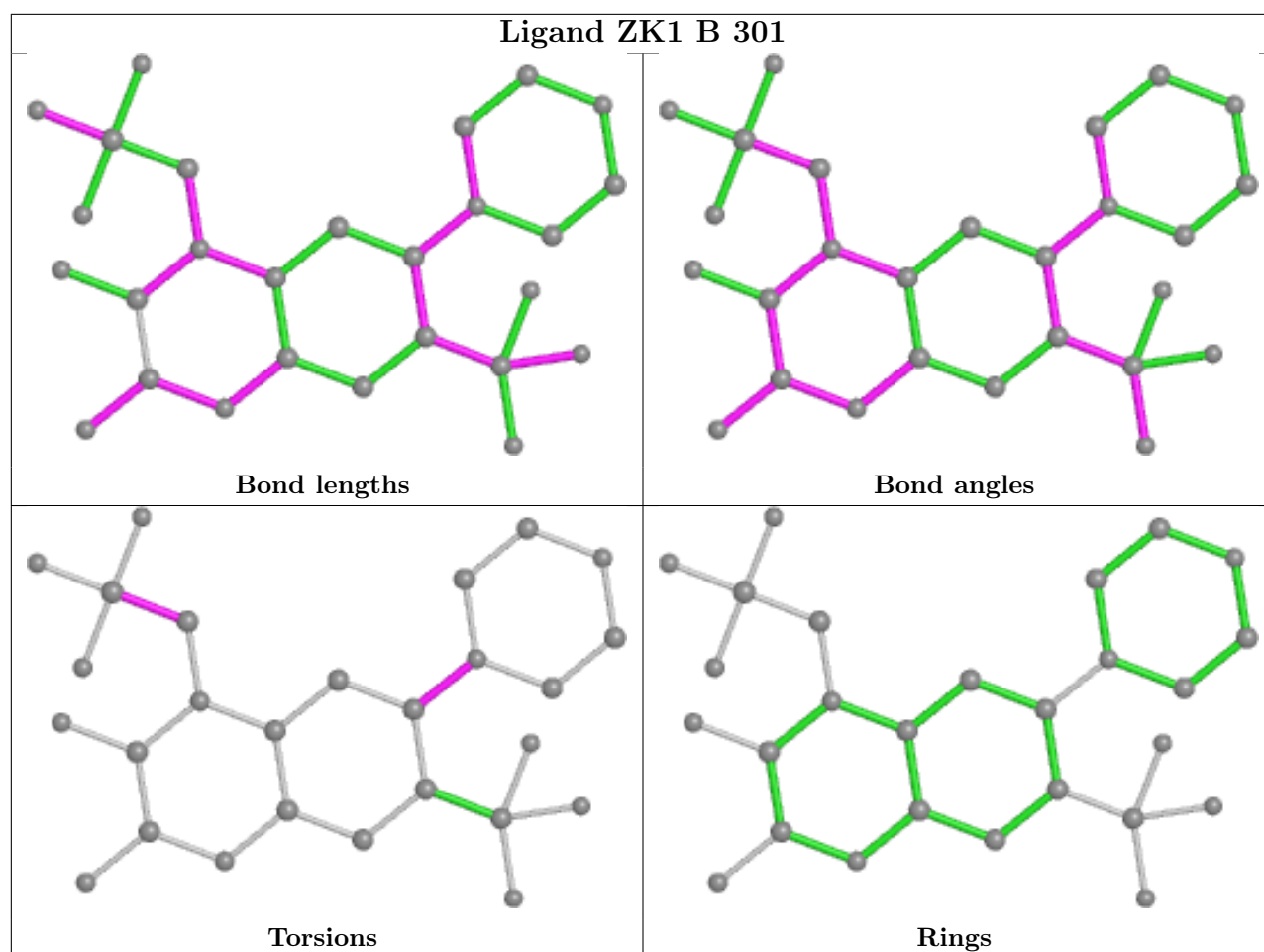
## Ligand ZK1 D 301











## 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	261/264 (98%)	0.24	4 (1%) 73 75	24, 42, 85, 144	0
1	B	258/264 (97%)	0.31	5 (1%) 66 69	24, 45, 96, 154	0
1	C	259/264 (98%)	0.35	7 (2%) 54 58	25, 48, 95, 127	0
1	D	259/264 (98%)	0.27	3 (1%) 79 80	23, 37, 83, 182	0
1	E	258/264 (97%)	0.20	4 (1%) 72 74	23, 36, 82, 129	0
1	F	258/264 (97%)	0.33	7 (2%) 54 58	21, 42, 90, 150	0
1	G	260/264 (98%)	0.25	5 (1%) 66 69	21, 44, 94, 178	0
1	H	260/264 (98%)	0.27	7 (2%) 54 58	25, 40, 91, 152	0
All	All	2073/2112 (98%)	0.28	42 (2%) 65 68	21, 42, 91, 182	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	PRO	7.1
1	H	263	SER	6.8
1	D	122	GLU	5.7
1	E	122	GLU	5.4
1	A	3	ASN	4.9

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

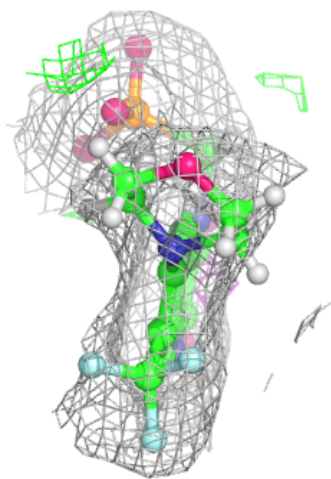
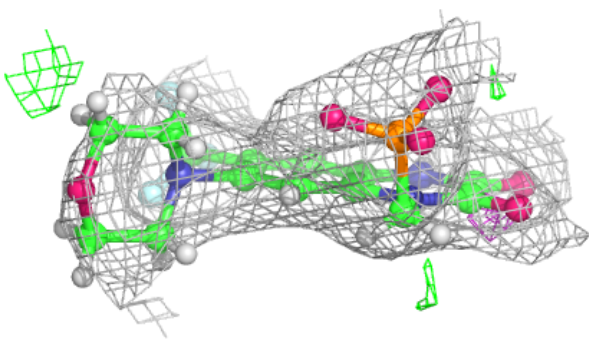
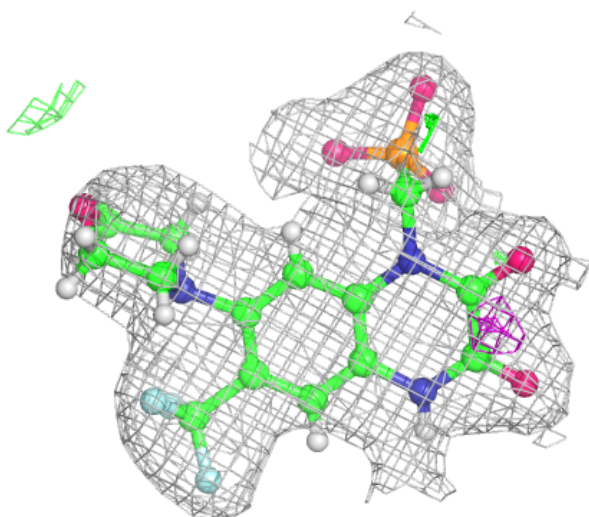
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	ZK1	B	301	27/27	0.92	0.17	25,55,91,99	0
2	ZK1	A	301	27/27	0.94	0.19	28,44,64,72	0
2	ZK1	F	301	27/27	0.94	0.18	22,49,91,106	0
2	ZK1	E	301	27/27	0.95	0.17	12,32,52,64	0
2	ZK1	C	301	27/27	0.96	0.16	19,51,73,83	0
2	ZK1	D	301	27/27	0.96	0.17	14,28,52,62	0
2	ZK1	G	301	27/27	0.96	0.17	18,38,59,67	0
2	ZK1	H	301	27/27	0.96	0.17	16,32,60,60	0

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

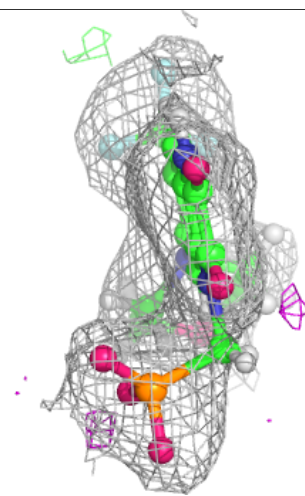
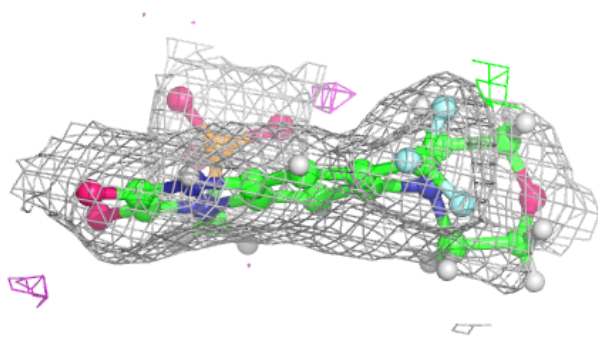
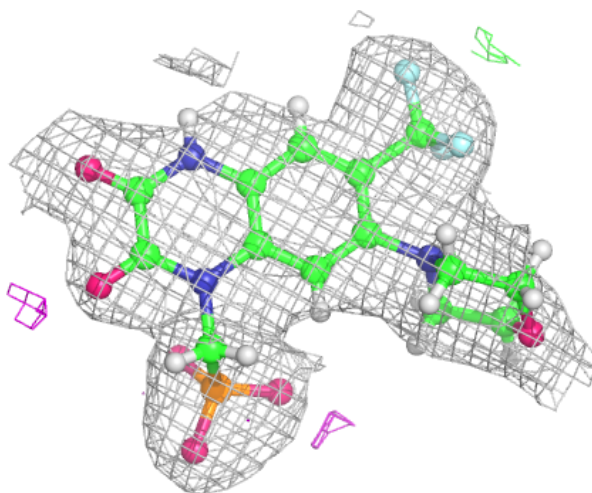
**Electron density around ZK1 B 301:**

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



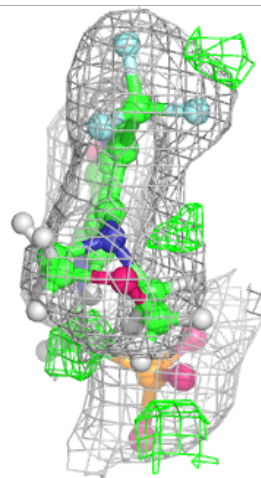
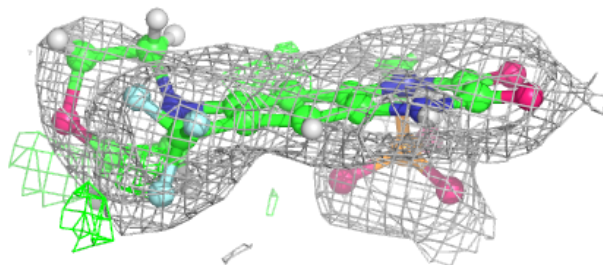
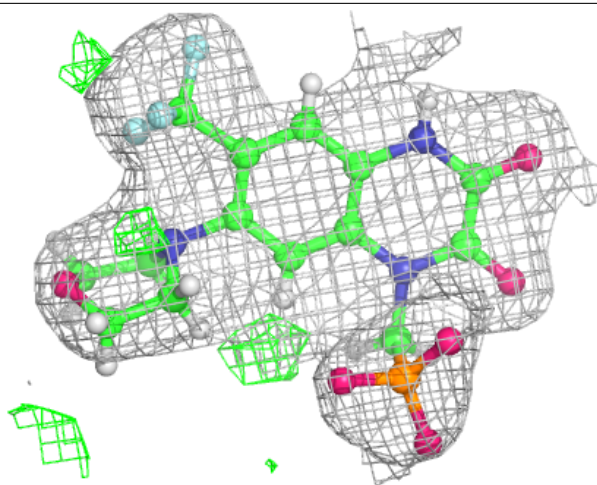
**Electron density around ZK1 A 301:**

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



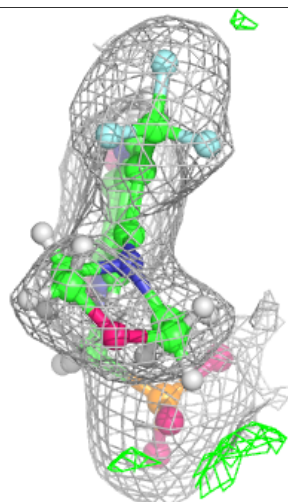
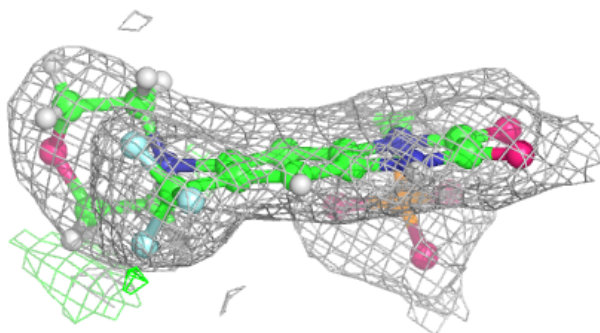
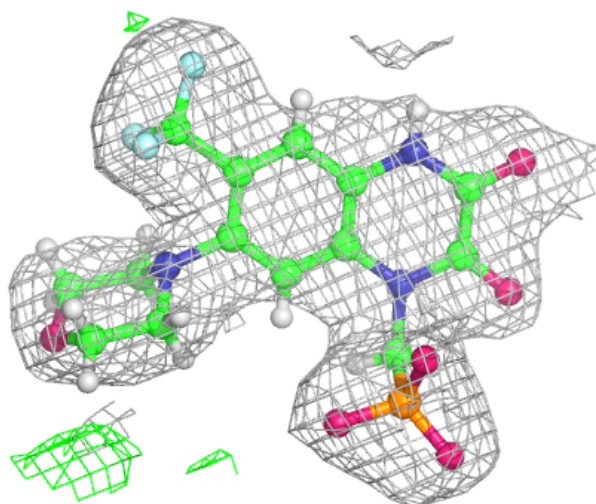
**Electron density around ZK1 F 301:**

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



**Electron density around ZK1 E 301:**

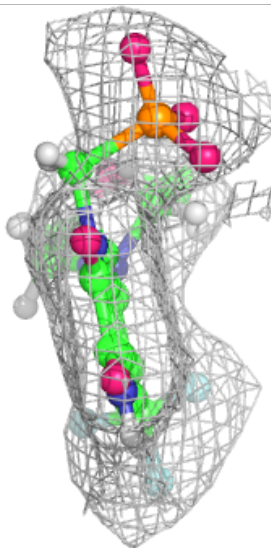
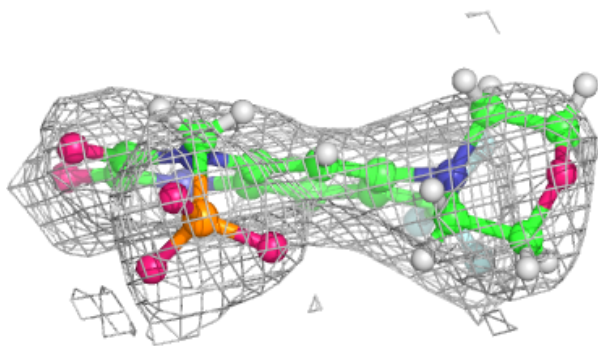
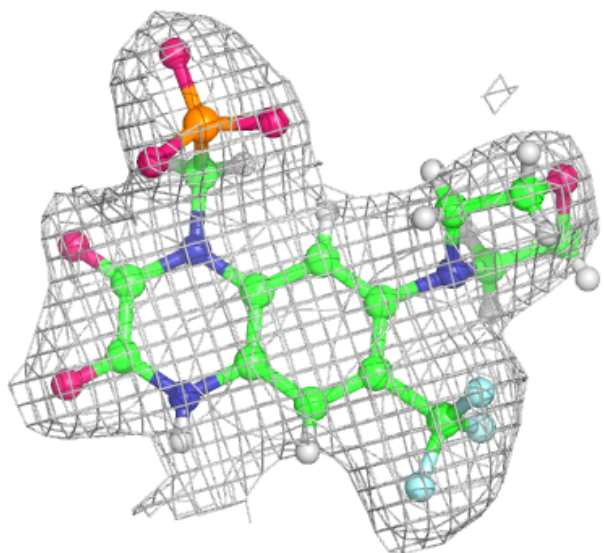
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





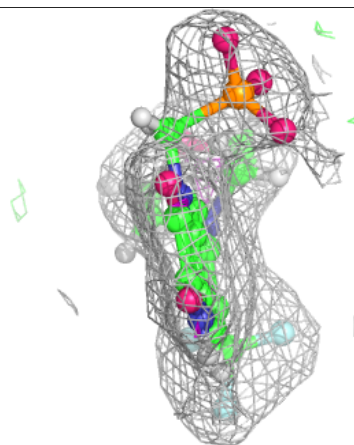
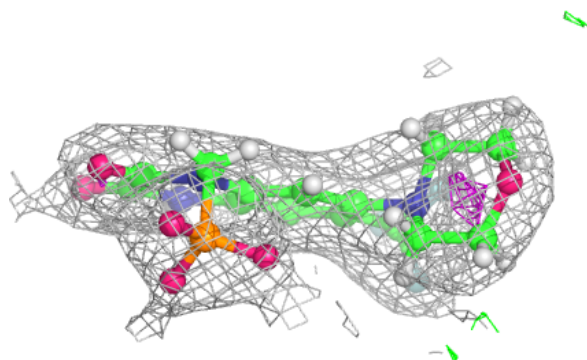
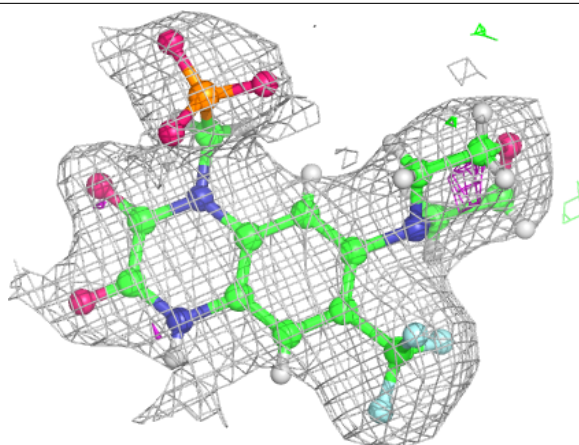
**Electron density around ZK1 C 301:**

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



**Electron density around ZK1 D 301:**

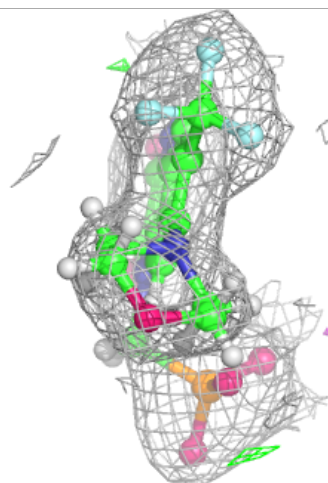
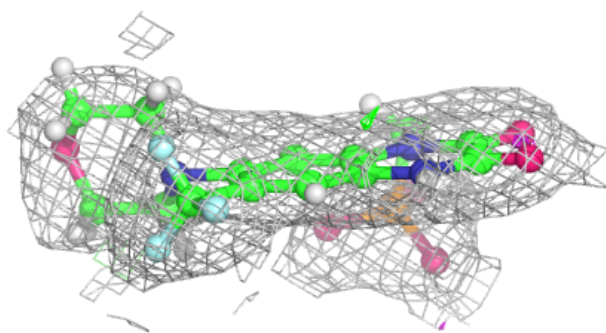
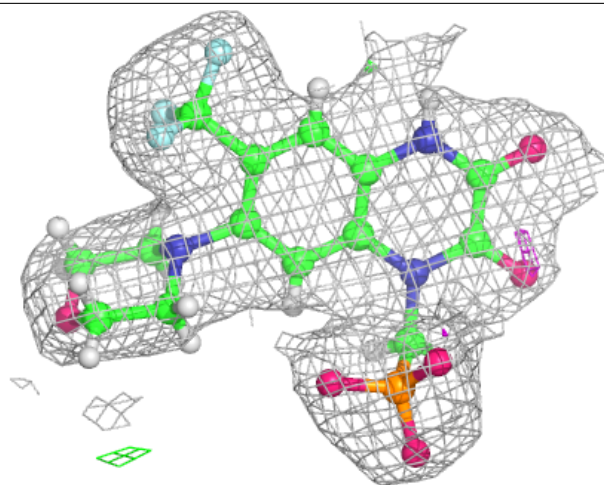
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





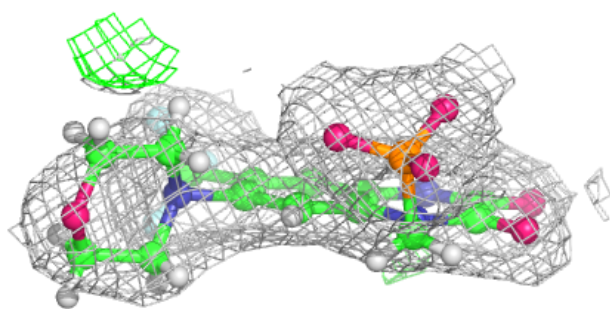
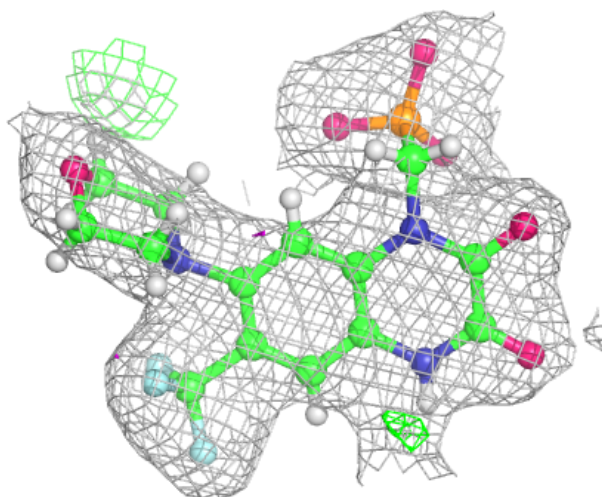
**Electron density around ZK1 G 301:**

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



**Electron density around ZK1 H 301:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.