



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 04:19 PM EST

PDB ID : 5KBT  
EMDB ID: : EMD-8230  
Title : Cryo-EM structure of GluA2-1xSTZ complex at 6.4 Angstrom resolution  
Authors : Twomey, E.C.; Yelshanskaya, M.V.; Grassucci, R.A.; Frank, J.; Sobolevsky, A.I.  
Deposited on : 2016-06-03  
Resolution : 6.40 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

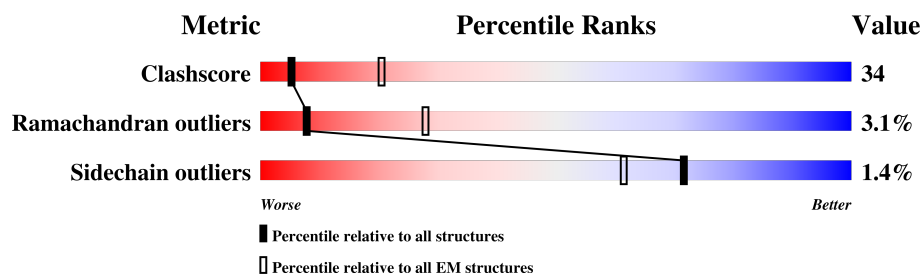
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.40 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1034	
1	B	1034	
1	C	1034	
1	D	1034	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24121 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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, Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	973	Total	C	N	O	S	0	0
			7110	4589	1138	1346	37		
1	B	779	Total	C	N	O	S	0	0
			5647	3635	902	1083	27		
1	C	779	Total	C	N	O	S	0	0
			5600	3605	891	1077	27		
1	D	779	Total	C	N	O	S	0	0
			5600	3605	891	1077	27		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	758	LEU	VAL	engineered mutation	UNP P19491
A	827	GLY	-	linker	UNP P19491
A	828	THR	-	linker	UNP P19491
A	1047	ASP	ASN	conflict	UNP O88602
A	1208	THR	-	expression tag	UNP O88602
A	1209	GLY	-	expression tag	UNP O88602
A	1210	GLY	-	expression tag	UNP O88602
A	1211	LEU	-	expression tag	UNP O88602
A	1212	VAL	-	expression tag	UNP O88602
A	1213	PRO	-	expression tag	UNP O88602

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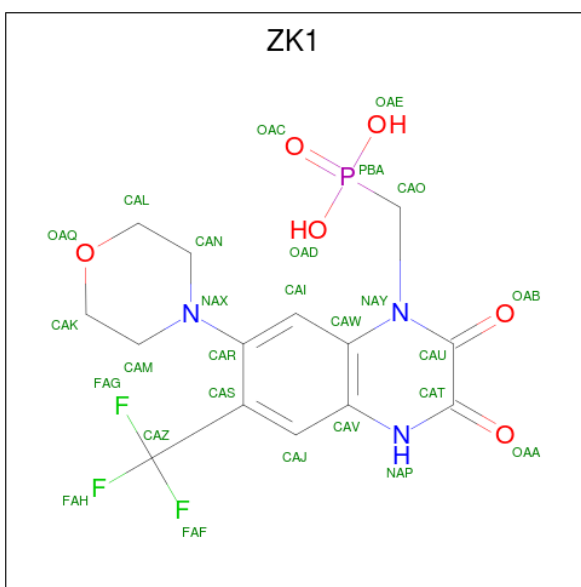
Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	ARG	-	expression tag	UNP O88602
A	1215	GLY	-	expression tag	UNP O88602
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
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B	392	GLN	ASN	conflict	UNP P19491
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B	827	GLY	-	linker	UNP P19491
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B	1047	ASP	ASN	conflict	UNP O88602
B	1208	THR	-	expression tag	UNP O88602
B	1209	GLY	-	expression tag	UNP O88602
B	1210	GLY	-	expression tag	UNP O88602
B	1211	LEU	-	expression tag	UNP O88602
B	1212	VAL	-	expression tag	UNP O88602
B	1213	PRO	-	expression tag	UNP O88602
B	1214	ARG	-	expression tag	UNP O88602
B	1215	GLY	-	expression tag	UNP O88602
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
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C	1208	THR	-	expression tag	UNP O88602
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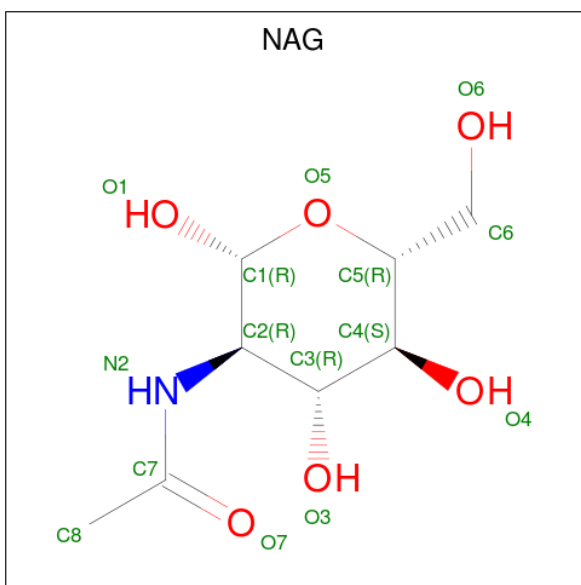
Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	GLY	-	expression tag	UNP O88602
C	1211	LEU	-	expression tag	UNP O88602
C	1212	VAL	-	expression tag	UNP O88602
C	1213	PRO	-	expression tag	UNP O88602
C	1214	ARG	-	expression tag	UNP O88602
C	1215	GLY	-	expression tag	UNP O88602
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	758	LEU	VAL	engineered mutation	UNP P19491
D	827	GLY	-	linker	UNP P19491
D	828	THR	-	linker	UNP P19491
D	1047	ASP	ASN	conflict	UNP O88602
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D	1210	GLY	-	expression tag	UNP O88602
D	1211	LEU	-	expression tag	UNP O88602
D	1212	VAL	-	expression tag	UNP O88602
D	1213	PRO	-	expression tag	UNP O88602
D	1214	ARG	-	expression tag	UNP O88602
D	1215	GLY	-	expression tag	UNP O88602

- 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						AltConf
2	A	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	B	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	C	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	
2	D	1	Total	C	F	N	O	P	0
			27	14	3	3	6	1	

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

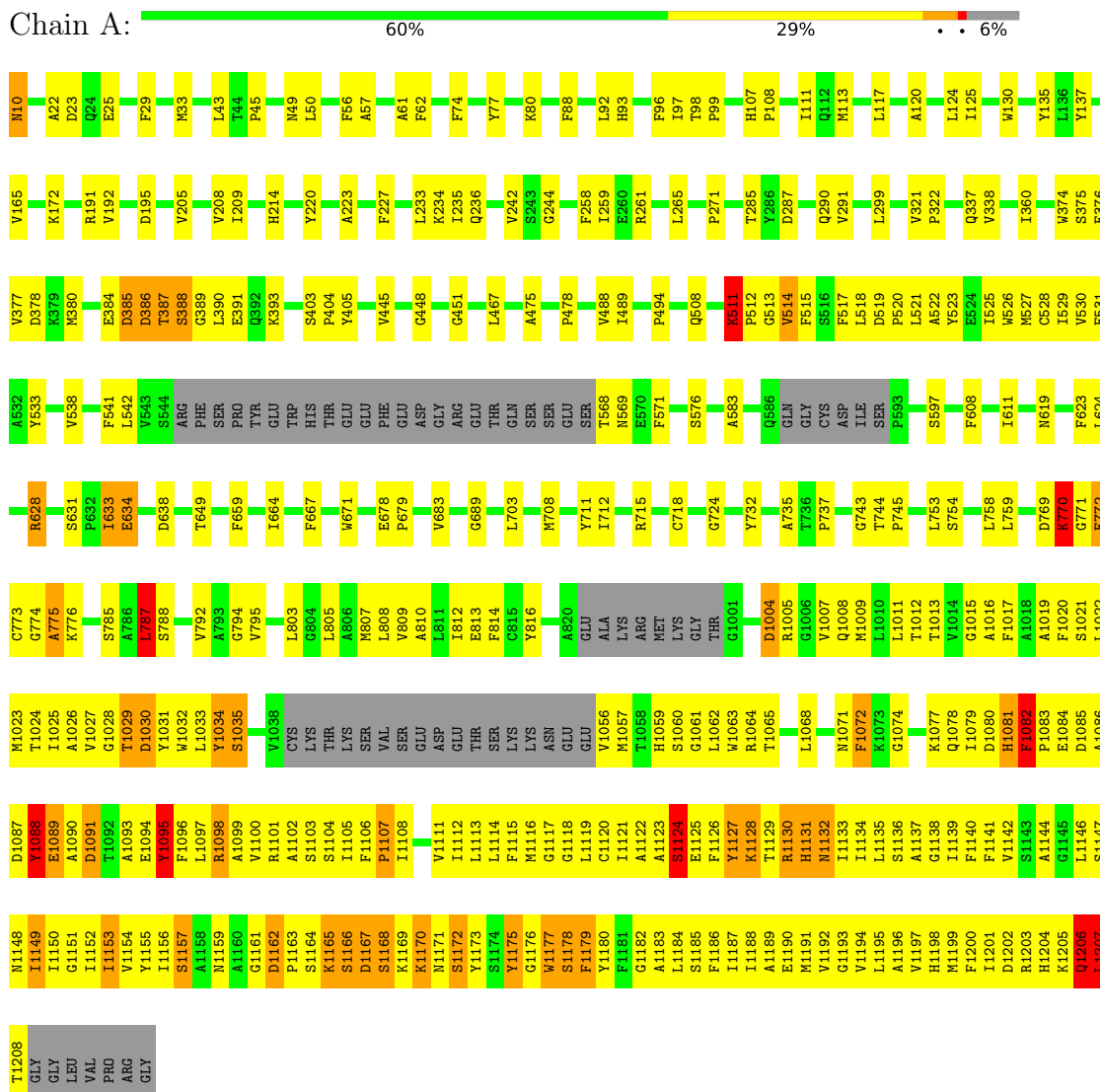


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

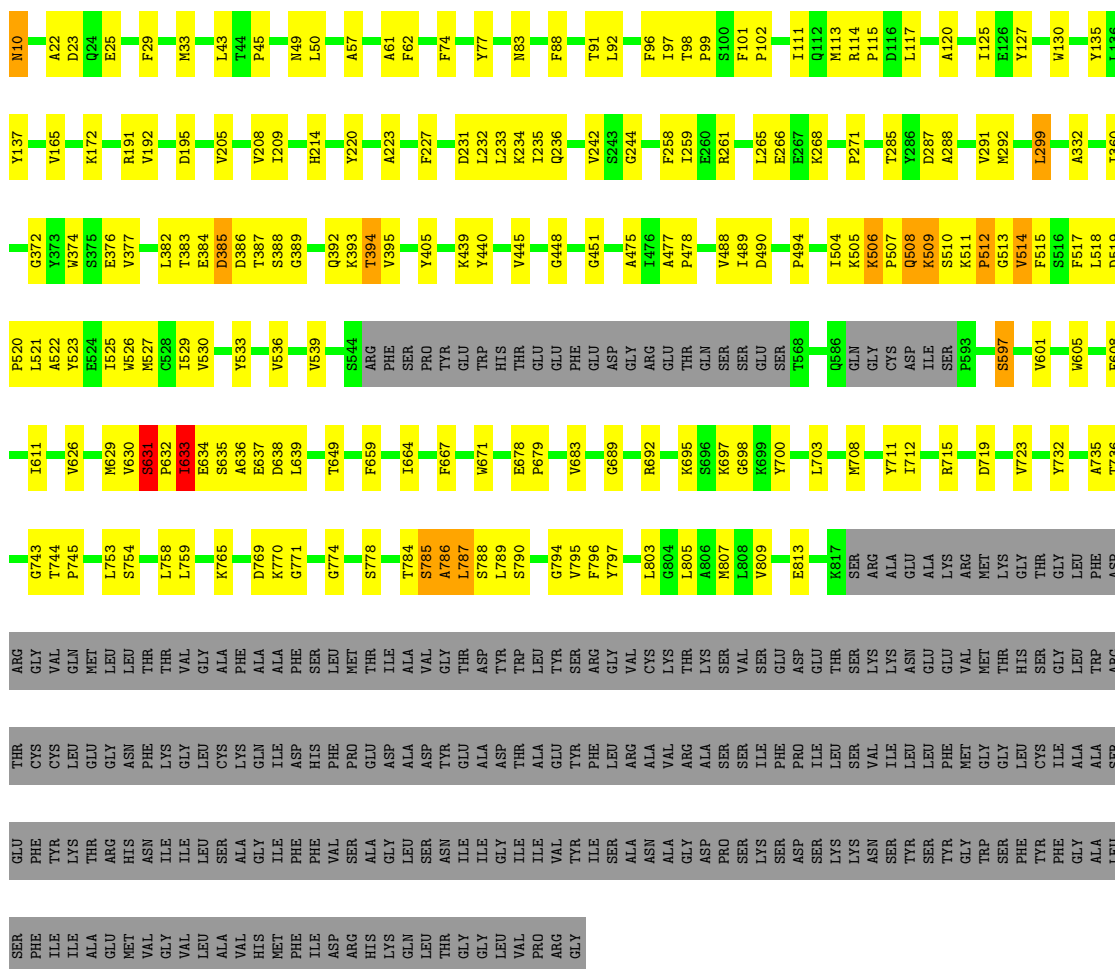
- Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit



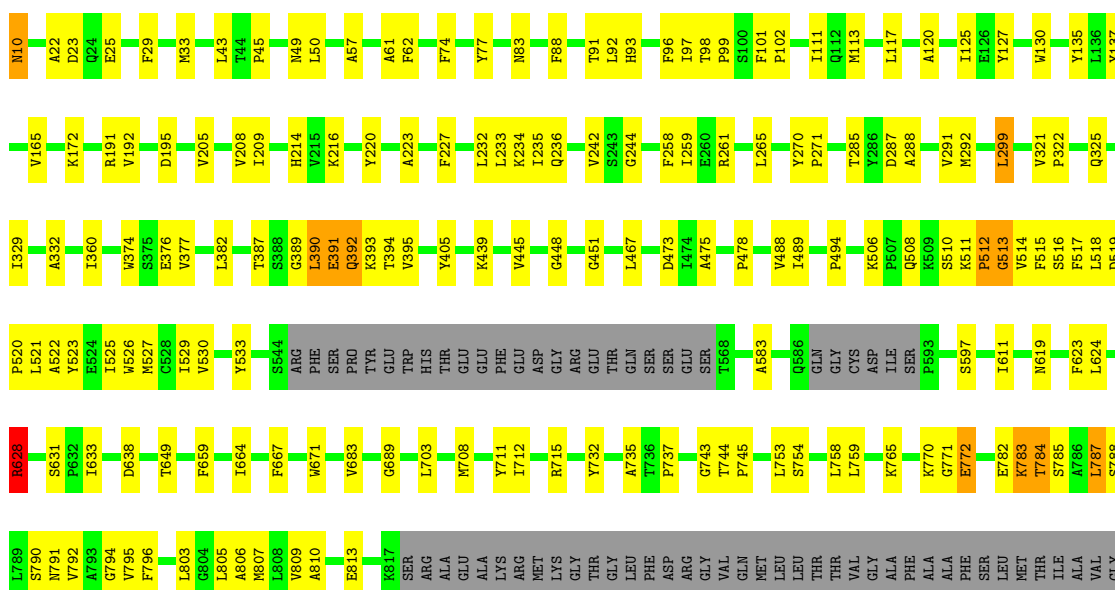
- Molecule 1: Glutamate receptor 2,Voltage-dependent calcium channel gamma-2 subunit







- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-2 subunit



[illegible]

- Molecule 1: Glutamate receptor 2, Voltage-dependent calcium channel gamma-2 subunit

Chain D:  57% 17% . 25%

VAL	HIS	GLY	ALA	LYS	PHE	L759	V626	V523	V377	M10
MET	MET	ILE	ILE	ILE	ALA	K765	E627	E524	R191	A22
PHE	PHE	PHE	ASP	ASP	ALA	K765	E628	I525	M380	D23
ILE	ILE	PHE	HIS	HIS	SER	K770	M629	V526	V381	D23
ASP	ASP	VAL	PHE	PHE	LEU	G771	S631	C528	L382	E25
ARG	ARG	SER	PRO	PRO	MET	E772	P632	I529	V205	E25
HIS	HIS	ALA	GLU	GLU	THR	C773	P633	V530	V208	F29
LYS	LYS	GLY	ASP	ASP	ILE	E634	E634		T209	F29
GLN	GLN	LEU	ALA	ALA	ALA	T784	S635	V533		M33
LEU	LEU	SER	ASP	ASP	VAL	S785	A636		H214	M33
THR	THR	ASN	TYR	TYR	GLY	A786	E637	S544		L43
GLY	GLY	ILE	GLU	GLU	THR	L787	D638	ARG	A223	T44
GLY	GLY	ILE	ALA	ALA	ASP	S788		PHE		P45
LEU	LEU	VAL	ASP	ASP	THR	L789	T649	SER	F227	
VAL	VAL	ILE	THR	THR	THR	S790		PRO		
PRO	PRO	ILE	ALA	ALA	LEU	N791	F659	TYR	L232	N49
ARG	ARG	VAL	VAL	GLU	TYR	V792	I664	GLU	L233	L50
GLY	GLY	TYR	TYR	TYR	SER	A793		TRP	K234	F56
		ILE	ILE	PHE	ARG	G794		HIS	P404	A57
		SER	SER	LEU	GLY	V795	F667	THR	Y405	
		ALA	ALA	ARG	VAL			GLU		A61
		ASN	ALA	ALA	CYS	L803	W671	GLU	Y440	F62
		ALA	ALA	VAL	LYS	G804		PHE	K441	
		GLY	ARG	ARG	THR	L805	E678	GLU	G244	F74
		ASP	ASP	PRO	SER	A906	P679	ASP		
		PRO	SER	SER	SER	M807		GLY	F258	Y77
		LYS	SER	ILE	VAL	L808	F683	ARG	T259	
		SER	SER	VAL	SER	V809		GLU	E260	K80
		SER	PHE	GLU	GLU		G689	THR	R261	
		ASP	PRO	ASP	ASP	E813		GLN		F88
		SER	SER	ILE	GLU	K817	L703	SER	L265	
		LYS	LYS	SER	THR		M708	SER	Y270	L92
		ASN	VAL	VAL	LYS			SER	P271	H93
		SER	SER	ILE	LYS		Y711	V568		F96
		TYR	LEU	LEU	ASN	GLU	I712		T285	I97
		SER	LEU	LEU	GLU	ALA		GLN	Y286	T98
		TYR	TYR	PHE	GLU	LYS	R715		D287	P99
		GLY	TRP	GLY	MET	ARG		CYS	A288	
		TRP	TRP	GLY	MET	MET	C718		V289	I111
		SER	SER	GLY	THR	LYS		ASP	Q290	Q112
		PHE	PHE	THR	HIS	GLY		ILE	V291	M113
		TYR	TYR	SER	SER	THR		SER	M292	
		PHE	ALA	ALA	TRP	PHE	G724	P693		L117
		GLY	GLY	ALA	LEU	LEU	Y732	L596		A120
		ALA	ALA	ALA	TRP	ASP		S507	L299	
		SER	SER	SER	ARG	ASP		Q508	K509	
		LEU	LEU	GLU	THR	THR	A735	S510	S510	L124
		SER	SER	GLU	ARG	ARG	T736	K511	P322	
		PHE	PHE	PHE	THR	GLY	P737	P608	A332	I125
		ILE	ILE	TYR	CYS	VAL		V514		V130
		ILE	ILE	LEU	LEU	GLN		1611		
		ALA	ALA	THR	GLU	MET	G743	F515	Q337	
		GLU	GLU	ARG	GLY	LEU	T744	S516	V338	Y135
		MET	MET	HIS	ASN	LEU	P745	F517	L136	
		VAL	VAL	ASN	PHE	THR		L620	T360	Y137
		GLY	GLY	ILE	LYS	THR	L753	P520		
		VAL	VAL	ILE	GLY	VAL	S754	P623	W374	V165
		LEU	LEU	LEU	LEU	GLY		L624	S375	
		ALA	ALA	SER	CYS		L758	F521	C276	Y172

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 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: NAG, 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.33	2/7267 (0.0%)	0.60	15/9925 (0.2%)
1	B	0.24	0/5768	0.37	2/7888 (0.0%)
1	C	0.24	0/5721	0.43	6/7837 (0.1%)
1	D	0.24	0/5721	0.37	1/7837 (0.0%)
All	All	0.27	2/24477 (0.0%)	0.46	24/33487 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1157	SER	C-N	-10.30	1.10	1.34
1	A	787	LEU	C-N	-5.18	1.22	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	LEU	O-C-N	-28.18	77.62	122.70
1	C	628	ARG	NE-CZ-NH1	-13.77	113.42	120.30
1	A	628	ARG	NE-CZ-NH2	-12.47	114.06	120.30
1	C	628	ARG	NE-CZ-NH2	11.86	126.23	120.30
1	A	628	ARG	NE-CZ-NH1	11.01	125.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1206	GLN	Mainchain
1	A	1207	LEU	Mainchain
1	A	787	LEU	Mainchain

## 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	7110	0	6571	1036	0
1	B	5647	0	5177	227	0
1	C	5600	0	5073	181	0
1	D	5600	0	5072	212	0
2	A	27	0	13	0	0
2	B	27	0	13	1	0
2	C	27	0	13	0	0
2	D	27	0	13	0	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	2	0
All	All	24121	0	21997	1576	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 1576 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:A:1114:LEU:CD1	1:A:1141:PHE:CZ	1.75	1.68
1:A:1083:PRO:HG2	1:A:1098:ARG:CG	1.16	1.62
1:A:1114:LEU:HD13	1:A:1141:PHE:CZ	1.31	1.60
1:C:512:PRO:CB	1:C:790:SER:HB2	1.23	1.59
1:A:1134:ILE:CG2	1:A:1200:PHE:HB3	1.21	1.58

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	963/1034 (93%)	844 (88%)	78 (8%)	41 (4%)	3	28
1	B	773/1034 (75%)	699 (90%)	56 (7%)	18 (2%)	7	41
1	C	773/1034 (75%)	700 (91%)	58 (8%)	15 (2%)	9	45
1	D	773/1034 (75%)	692 (90%)	54 (7%)	27 (4%)	4	32
All	All	3282/4136 (79%)	2935 (89%)	246 (8%)	101 (3%)	8	34

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	385	ASP
1	A	387	THR
1	A	389	GLY
1	A	511	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 PDB entries followed by that with respect to all EM entries.

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	693/876 (79%)	676 (98%)	17 (2%)	50	74
1	B	546/876 (62%)	540 (99%)	6 (1%)	76	88
1	C	534/876 (61%)	529 (99%)	5 (1%)	81	90
1	D	534/876 (61%)	529 (99%)	5 (1%)	81	90
All	All	2307/3504 (66%)	2274 (99%)	33 (1%)	71	85

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

Mol	Chain	Res	Type
1	A	1167	ASP
1	B	299	LEU
1	D	394	THR
1	A	1168	SER
1	A	1177	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1198	HIS
1	B	83	ASN
1	C	83	ASN
1	A	1148	ASN
1	B	619	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ZK1	A	1301	-	28,29,29	3.29	14 (50%)	36,45,45	1.60	5 (13%)
3	NAG	A	1302	1	14,14,15	0.48	0	17,19,21	0.75	0
2	ZK1	B	1101	-	28,29,29	3.28	14 (50%)	36,45,45	1.60	5 (13%)
3	NAG	B	1102	1	14,14,15	0.49	0	17,19,21	0.74	0
2	ZK1	C	1101	-	28,29,29	3.27	14 (50%)	36,45,45	1.60	5 (13%)
3	NAG	C	1102	1	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	ZK1	D	1101	-	28,29,29	3.28	14 (50%)	36,45,45	1.61	5 (13%)
3	NAG	D	1102	1	14,14,15	0.51	0	17,19,21	0.72	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	ZK1	A	1301	-	-	5/13/23/23	0/3/3/3
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	ZK1	B	1101	-	-	5/13/23/23	0/3/3/3
3	NAG	B	1102	1	-	0/6/23/26	0/1/1/1
2	ZK1	C	1101	-	-	5/13/23/23	0/3/3/3
3	NAG	C	1102	1	-	2/6/23/26	0/1/1/1
2	ZK1	D	1101	-	-	5/13/23/23	0/3/3/3
3	NAG	D	1102	1	-	2/6/23/26	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	ZK1	PBA-OAC	7.08	1.65	1.50
2	A	1301	ZK1	PBA-OAC	7.08	1.65	1.50
2	D	1101	ZK1	PBA-OAC	7.01	1.65	1.50
2	B	1101	ZK1	PBA-OAC	6.99	1.65	1.50
2	A	1301	ZK1	OAA-CAT	6.69	1.41	1.24

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	ZK1	CAN-NAX-CAM	4.68	121.61	111.53
2	A	1301	ZK1	CAN-NAX-CAM	4.64	121.51	111.53
2	D	1101	ZK1	CAN-NAX-CAM	4.61	121.45	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ZK1	CAN-NAX-CAM	4.60	121.44	111.53
2	D	1101	ZK1	CAV-CAW-NAY	3.37	120.29	117.71

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

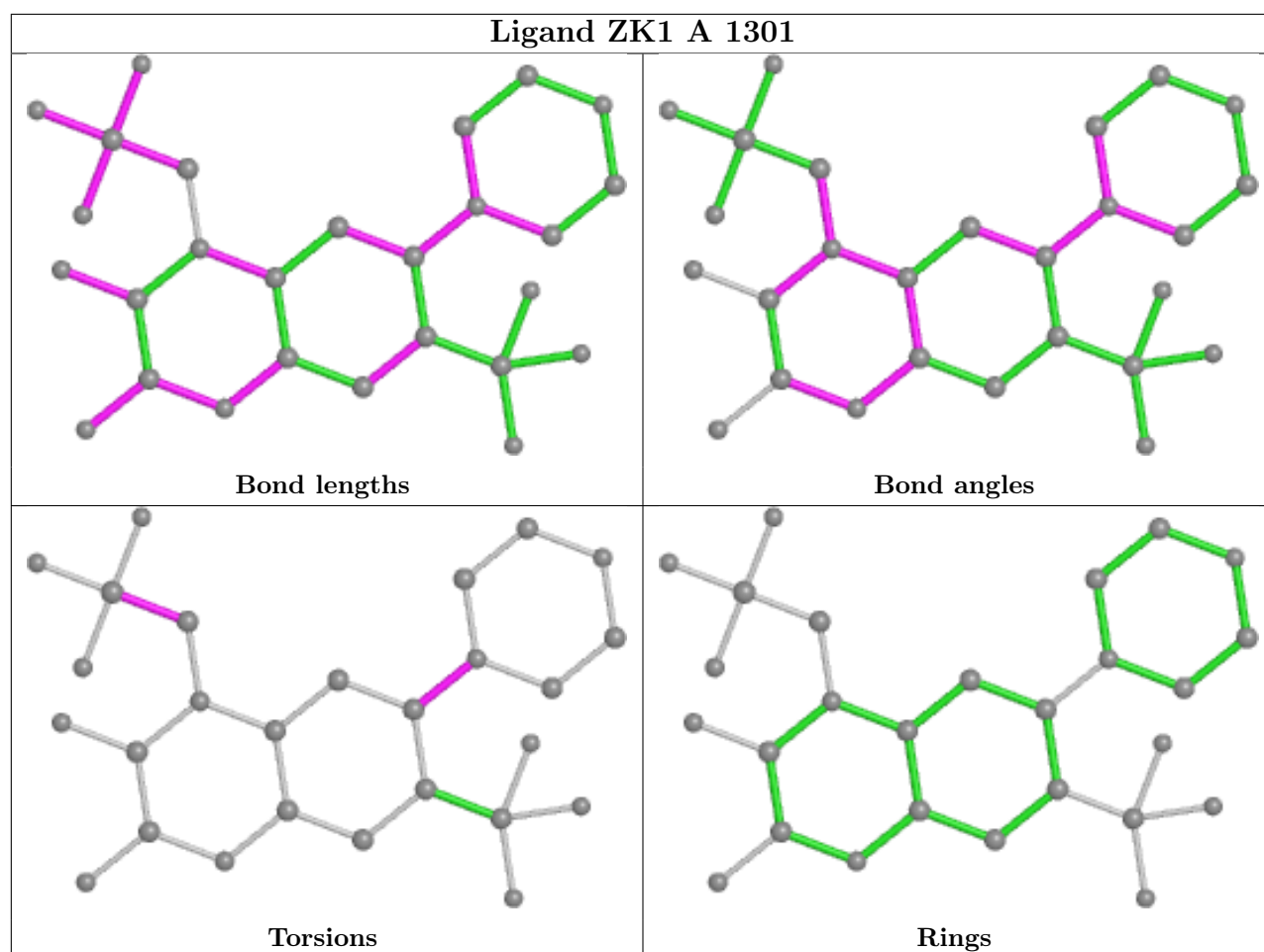
Mol	Chain	Res	Type	Atoms
2	A	1301	ZK1	NAY-CAO-PBA-OAC
2	A	1301	ZK1	NAY-CAO-PBA-OAE
2	C	1101	ZK1	NAY-CAO-PBA-OAC
2	C	1101	ZK1	NAY-CAO-PBA-OAE
2	D	1101	ZK1	NAY-CAO-PBA-OAC

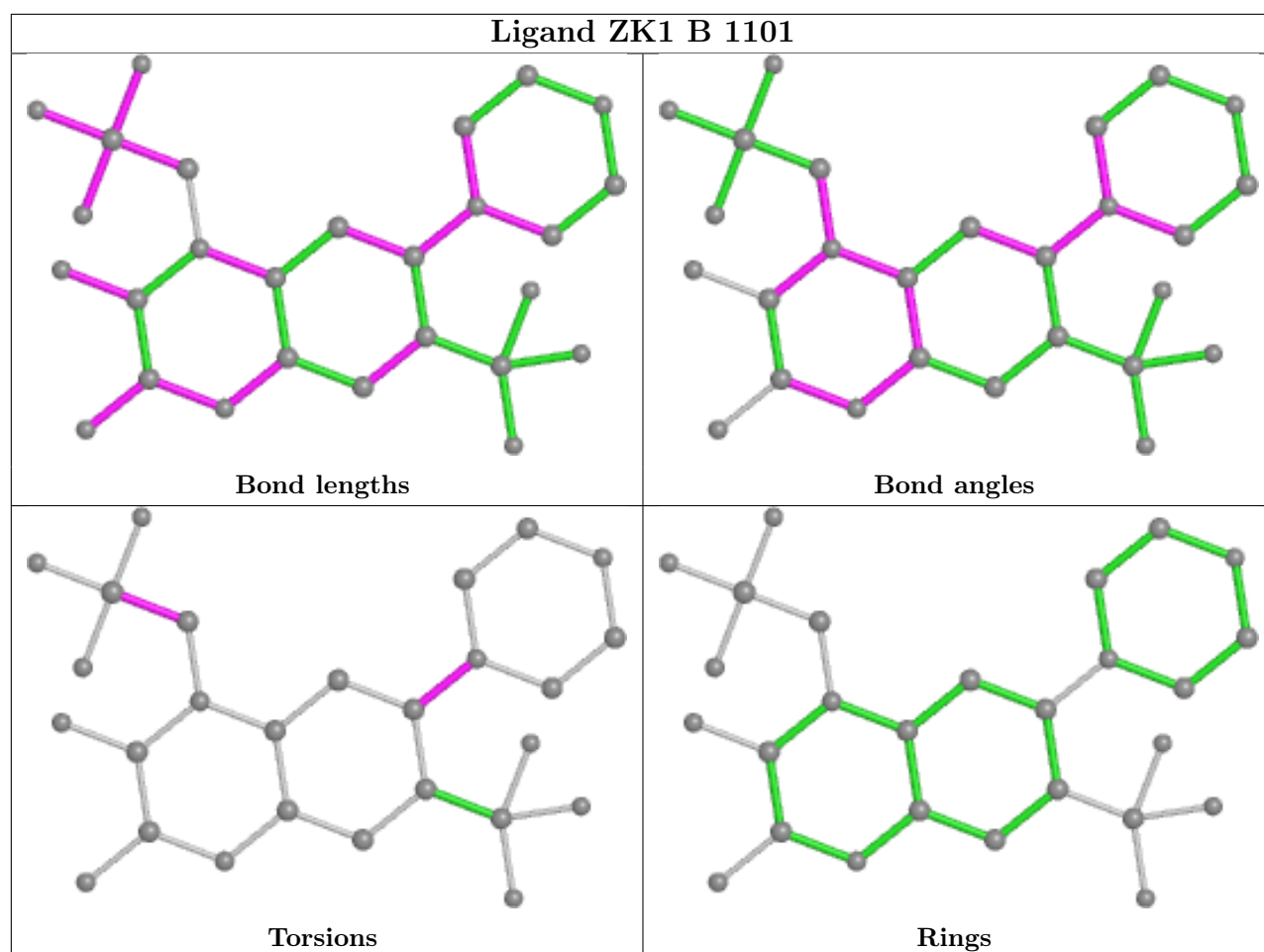
There are no ring outliers.

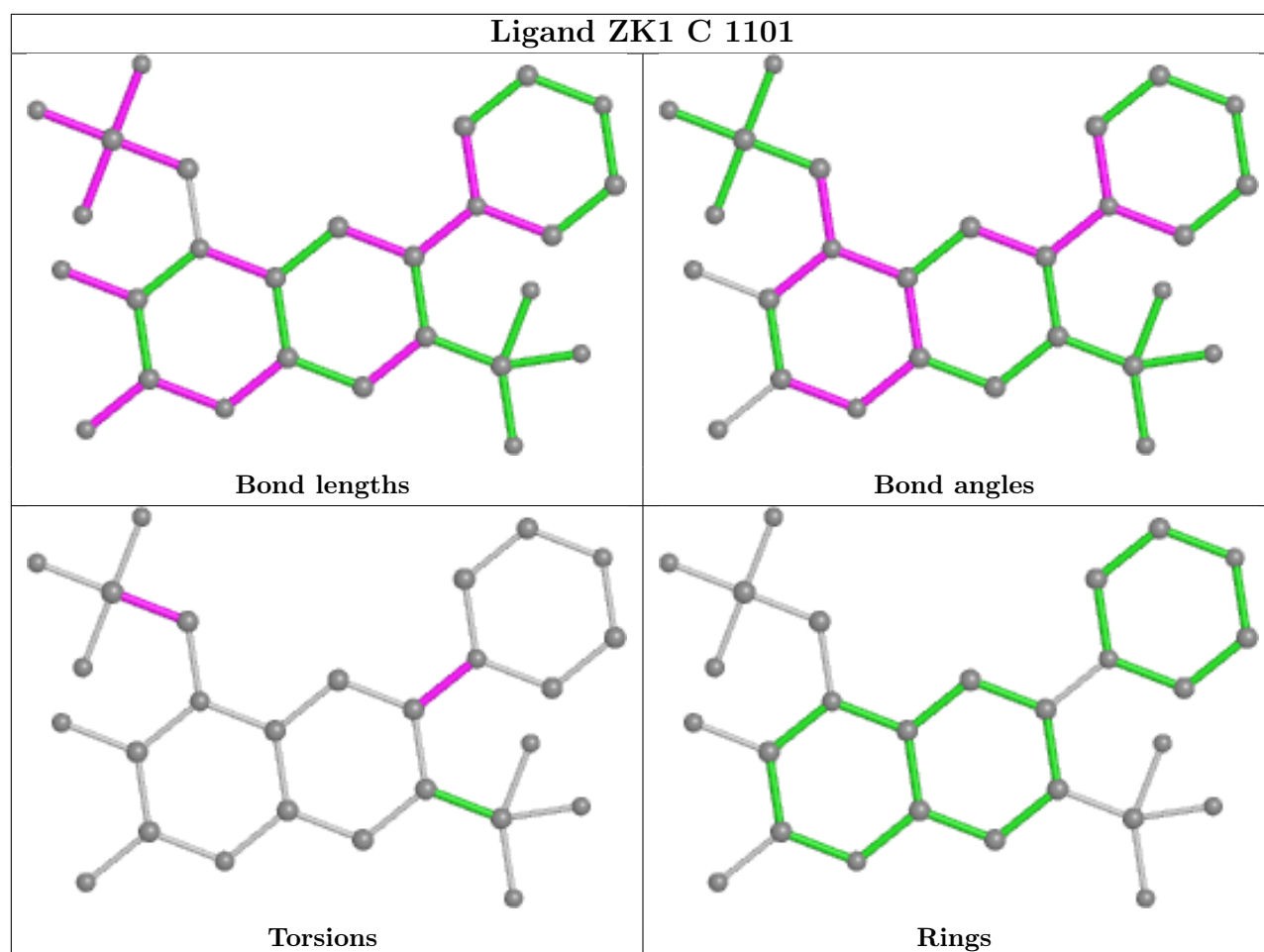
3 monomers are involved in 5 short contacts:

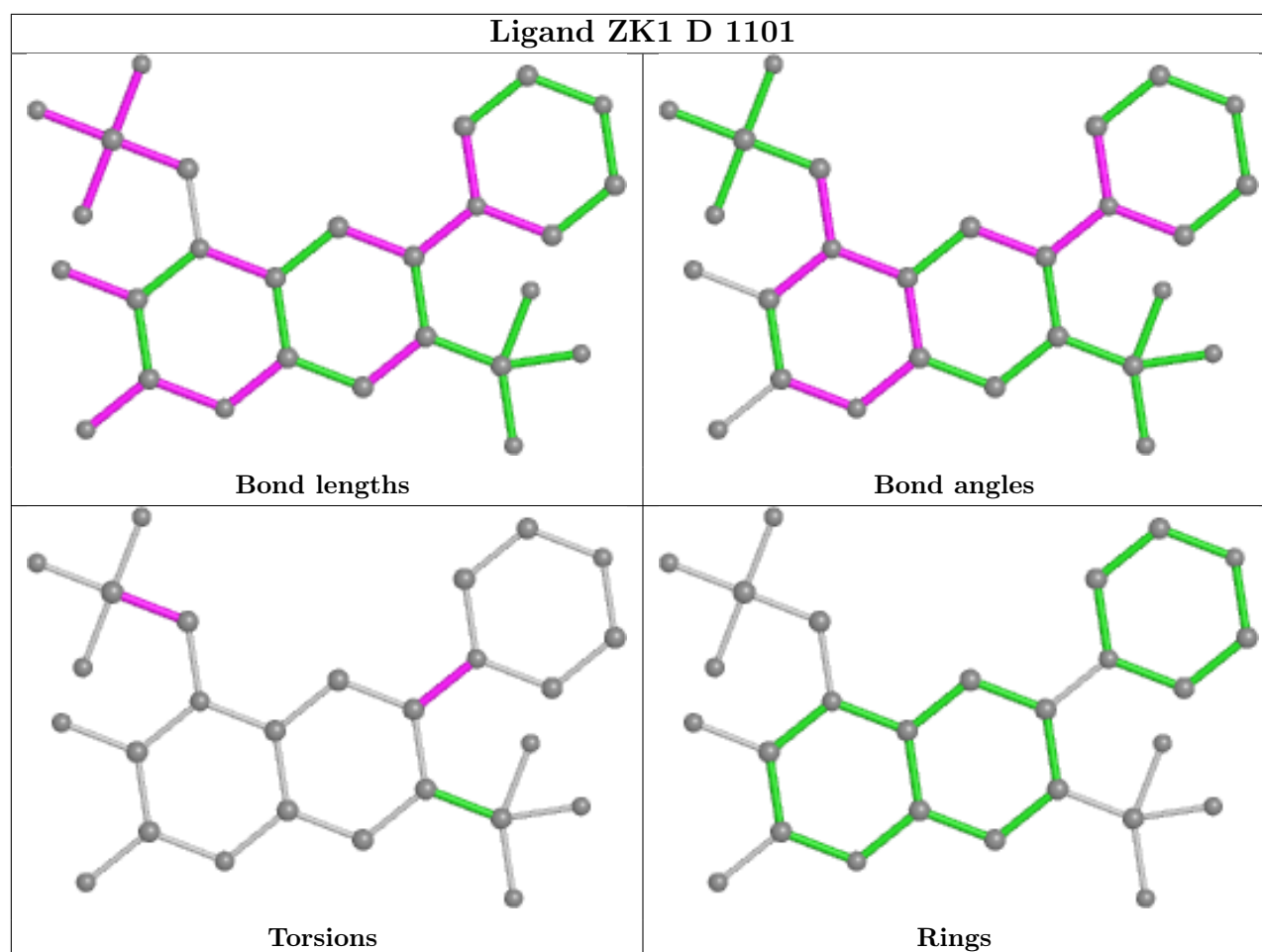
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	NAG	2	0
2	B	1101	ZK1	1	0
3	D	1102	NAG	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1157:SER	C	1158:ALA	N	1.10