



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 10:19 AM EDT

PDB ID : 2X6J  
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH PIK-93  
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.  
Deposited on : 2010-02-17  
Resolution : 3.50 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)

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<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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2



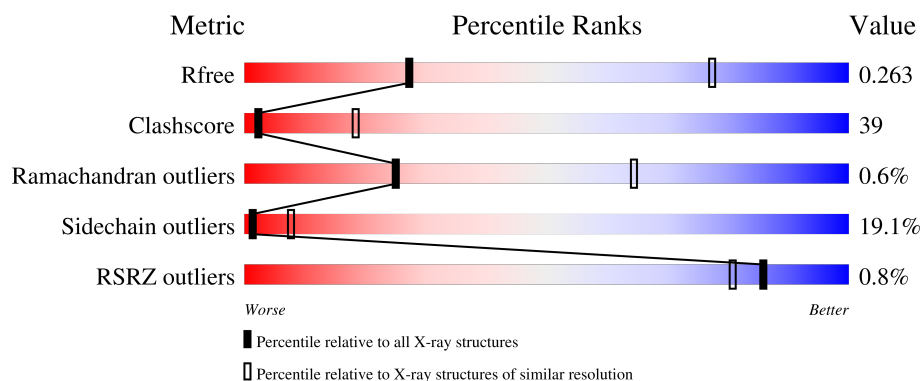
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	696	
1	B	696	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	093	B	1950	-	X	-	-



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8967 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 PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

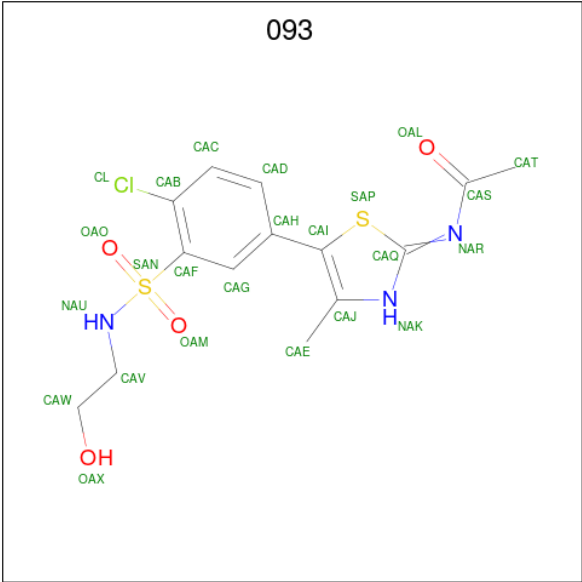
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4457	2882	757	791	27			
1	B	546	Total	C	N	O	S	0	0	0
			4462	2886	759	790	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q9W1M7
A	255	SER	-	expression tag	UNP Q9W1M7
A	256	HIS	-	expression tag	UNP Q9W1M7
A	257	MET	-	expression tag	UNP Q9W1M7
A	455	ALA	GLY	engineered mutation	UNP Q9W1M7
B	254	GLY	-	expression tag	UNP Q9W1M7
B	255	SER	-	expression tag	UNP Q9W1M7
B	256	HIS	-	expression tag	UNP Q9W1M7
B	257	MET	-	expression tag	UNP Q9W1M7
B	455	ALA	GLY	engineered mutation	UNP Q9W1M7

- Molecule 2 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C<sub>14</sub>H<sub>16</sub>ClN<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		
2	B	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		



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.

Chain A:										34%										34%										10%										22%									
M885	V886	D887	A888	R889	V890	H807	L808	D809	N810	L811	L895	E896	P897	D898	K903	L908	Q909	L912	T913	D914	E915	E916	A917	V918	Q919	H920	R829	R830	M835	L924	L925	D926	V927	S928	T929	A930	V932	L936	I940	T944	R946	L948	L95						
L801	G802	V803	R806	H807	L808	D809	N810	L811	L812	L813	T814	T815	N816	G817	K818	L819	F820	H821	T822	D823	E824	G825	Y826	L827	Q828	R829	R830	M835	L924	L925	D926	V927	S928	T929	A930	V932	L936	I940	T944	R946	L948	L95							
P655	L656	L657	P658	F659	T660	Y661	L662	K664	T667	M668	S669	T670	S671	L672	F673	K674	S675	A676	L677	M678	P679	A680	K681	L682	T683	F684	V685	T686	F687	L688	K689	T690	K691	H692	G693	K694	H695	G696	L697	T698	L699	L700							
R722	N723	N724	L727	K728	L729	V734	T737	S738	S739	K740	H741	L744	V747	D748	T749	C750	T751	E754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778							
P655	L656	L657	P658	F659	T660	Y661	L662	K664	T667	M668	S669	T670	S671	L672	F673	K674	S675	A676	L677	M678	P679	A680	K681	L682	T683	F684	V685	T686	F687	L688	K689	T690	K691	H692	G693	K694	H695	G696	L697	T698	L699	L700							
R722	N723	N724	L727	K728	L729	V734	T737	S738	S739	K740	H741	L744	V747	D748	T749	C750	T751	E754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778							
P655	L656	L657	P658	F659	T660	Y661	L662	K664	T667	M668	S669	T670	S671	L672	F673	K674	S675	A676	L677	M678	P679	A680	K681	L682	T683	F684	V685	T686	F687	L688	K689	T690	K691	H692	G693	K694	H695	G696	L697	T698	L699	L700							
R722	N723	N724	L727	K728	L729	V734	T737	S738	S739	K740	H741	L744	V747	D748	T749	C750	T751	E754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778							
P655	L656	L657	P658	F659	T660	Y661	L662	K664	T667	M668	S669	T670	S671	L672	F673	K674	S675	A676	L677	M678	P679	A680	K681	L682	T683	F684	V685	T686	F687	L688	K689	T690	K691	H692	G693	K694	H695	G696	L697	T698	L699	L700							
R722	N723	N724	L727	K728	L729	V734	T737	S738	S739	K740	H741	L744	V747	D748	T749	C750	T751	E754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778							
P655	L656	L657	P658	F659	T660	Y661	L662	K664	T667	M668	S669	T670	S671	L672	F673	K674	S675	A676	L677	M678	P679	A680	K681	L682	T683	F684	V685	T686	F687	L688	K689	T690	K691	H692	G693	K694	H695	G696	L697	T698	L699	L700							
R722	N723	N724	L727	K728	L729	V734	T737	S738	S739	K740	H741	L744	V747	D748	T749	C750	T751	E754	L755	L756	L757	L758	L759</																										

Chain B:  34% 34% 10% 22%



F882	D805	Y732	P653	K581	LEU	THR	E314	GLY
A888	R806	K733	F654	M582	PRO	SER	Q315	SER
T889	H807	V734	P655		CYS	SER	D316	HIS
V890	L808	L735	L656	V586	ASP	GLY	L317	MET
P891	D809	A736	P658	L587	SER	LEU	V318	ASP
D892	N810	T737	P658		ASN	HIS	W319	SER
L811	L811	D737		G590	SER	ALA	K320	GLU
T893	L812	S738	V661	N591	ASN	SER	F321	ILE
A894	L813	S739	T663		ALA	VAL	R322	GLN
L895	T814	K740	T663	L594	LEU	ILE		MET
E896	T815	H741	K664	R595	LEU		L325	GLU
P897	N816	G742			MET	PRO		GLU
D898	G817	F743	P667	F598	LEU	ALA	L398	ASN
K899	K818	L744		V599	ALA	ASN	S327	LEU
	L819		T670	N600	GLU	GLN	H328	VAL
K903	F820	V747	S671	L601	GLY	ARG	K330	GLU
	H821	D748	L672	R602	ILE	ALA	K331	ARG
E906	T822	S749	F673	K603	SER	ALA	A332	LYS
N907	D823	G750	F673	Q604	PHE	SER	L405	HIS
L908	F824	T751	L677	R605	GLY	VAL	K406	ARG
Q909	G825	V752	N678		SER	LEU	Y407	ARG
L912	Y826	A753	P679	I608	VAL	ALA	E408	LEU
T913	L827	E754		D609	PRO	ALA	D409	ALA
	L828	V755	V685	E610	ASP	ILE	P410	ARG
E916	G829	A757	T686	L611	N532	LYS	R411	SER
A917	R830	R758	H691	L614	T543	ASP	H412	GLU
V918	H835	E759			M544	LYS	I413	ARG
Q919	P837		L696	V618	M545	SER	U341	SER
	H838	N764	F697		A548	ILE	K342	GLY
Q922	R839	F765	K698	E621	L547	VAL	L343	ILE
S923	K840	G766	H699	P622	A548	SER	E419	SER
	L841	R767	G700	G623	M549	PRO	D345	ASP
V927			D701	N624		GLY	E346	ASP
	S842	P771	L703	R625	Y552	SER	F421	ASP
A931	K843	C772	D702	K626	W553	ALA	P422	ALA
V932	A848	D773	L704	L703	Y554	GLY	E423	LYS
N933	N849	G778	Q705	K628	L555	GLY	ARG	PRO
P934	G850	P776	D706	T629	L557	SER	VAL	THR
	G851	Y777	Q707	E630		GLY	VAL	A291
E938	L852	G778	L708	K631	E560	GLY	ARG	S292
Q939	S853	L779	T709	F632	GLU	GLY	SER	T293
F943	S854	T779	L710	Q633	VAL	GLN	ILE	R294
T944	E855	E782	Q711	K634	GLU	GLY	L368	Q296
Q945		V783	N712	L635	SER	SER	L297	H298
Y946	E859	T786	L714	L636	VAL	ALA	ASN	T299
N947	F860	Y787	L715	Q639	ARG	LEU	GLY	I300
R948	R861	L788	N716	D640	K567	PRO	SER	V301
K949	K862		D717	N641	Q568	ASN	LEU	Y302
		C791	K718	F642	E570	PRO	LEU	R303
				K643		SER	ASP	Y304
	T865					ALA	GLN	P305
	T866	Y794	R721	V644	H573	PRO	SER	P306
			R722	N645	D574	ALA	SER	T307
	N876		E723	F646	M575	THR	LEU	Y308
	H877	T798	N724	T647	Y576	PRO	SER	V309
	H878	Y799	L725	N648	A577	GLY	ASP	L310
	L879			F649	M578	SER	LEU	S311
	N880	V803	K728		V579	SER	ALA	S312
	L881	G804	L729	T652	L580	SER	ALA	E313



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.95Å 156.33Å 242.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.62 – 3.50 61.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.62-3.50) 99.5 (61.62-3.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.04 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.230 , 0.272 0.225 , 0.263	Depositor DCC
$R_{free}$ test set	1313 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: 093

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	0.61	1/4566 (0.0%)	0.84	1/6183 (0.0%)
1	B	0.48	0/4571	0.69	2/6189 (0.0%)
All	All	0.55	1/9137 (0.0%)	0.77	3/12372 (0.0%)

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	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	864	CYS	CB-SG	-6.21	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	A	818	LYS	N-CA-C	-5.24	96.86	111.00
1	B	710	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	591	ASN	Mainchain
1	A	663	THR	Mainchain
1	A	680	ALA	Peptide
1	A	737	THR	Mainchain

## 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	4457	0	4490	348	1
1	B	4462	0	4499	348	1
2	A	24	0	16	8	0
2	B	24	0	16	6	0
All	All	8967	0	9021	697	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 39.

The worst 5 of 697 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:375:HIS:CD2	1:A:377:GLN:H	1.54	1.24
1:B:311:SER:HB3	1:B:314:GLU:CB	1.76	1.15
1:B:299:THR:HB	1:B:303:ARG:HH11	1.10	1.14
1:A:705:GLN:HG2	1:A:890:VAL:HG13	1.22	1.13
1:A:629:THR:HB	1:A:672:LEU:HD12	1.18	1.10

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)
1:A:661:TYR:OH	1:A:782:GLU:OE1[6_555]	2.07	0.13
1:B:391:ASP:OD2	1:B:724:ASN:ND2[8_565]	2.18	0.02



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	539/696 (77%)	505 (94%)	30 (6%)	4 (1%)	22	61
1	B	540/696 (78%)	517 (96%)	20 (4%)	3 (1%)	25	64
All	All	1079/1392 (78%)	1022 (95%)	50 (5%)	7 (1%)	25	64

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	SER
1	A	305	PRO
1	B	408	GLU
1	A	304	TYR
1	A	591	ASN

### 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	490/612 (80%)	398 (81%)	92 (19%)	1	8
1	B	490/612 (80%)	395 (81%)	95 (19%)	1	7
All	All	980/1224 (80%)	793 (81%)	187 (19%)	1	8

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	398	LEU

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Mol	Chain	Res	Type
1	B	654	PHE
1	B	544	ASN
1	B	599	TYR
1	B	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	810	ASN
1	B	907	ASN
1	B	403	GLN
1	B	807	HIS
1	A	922	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	093	B	1950	-	19,25,25	4.25	14 (73%)	23,36,36	3.12	11 (47%)
2	093	A	1949	-	19,25,25	4.02	12 (63%)	23,36,36	2.89	11 (47%)

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	093	B	1950	-	-	9/13/19/19	0/2/2/2
2	093	A	1949	-	-	2/13/19/19	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1950	093	CAG-CAF	11.88	1.49	1.37
2	A	1949	093	CAG-CAF	10.80	1.48	1.37
2	A	1949	093	SAN-NAU	7.86	1.73	1.61
2	B	1950	093	SAN-NAU	7.48	1.72	1.61
2	B	1950	093	CAD-CAC	5.17	1.47	1.36

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1949	093	OAO-SAN-OAM	-8.88	108.74	119.52
2	B	1950	093	OAO-SAN-OAM	-7.10	110.90	119.52
2	B	1950	093	CAT-CAS-NAR	6.79	124.91	114.84
2	B	1950	093	CAB-CAF-SAN	-5.44	119.44	123.19
2	B	1950	093	CAF-CAB-CL	-5.27	117.70	121.52

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1950	093	OAL-CAS-NAR-CAQ
2	B	1950	093	CAT-CAS-NAR-CAQ
2	B	1950	093	NAU-CAV-CAW-OAX
2	B	1950	093	CAV-NAU-SAN-OAM
2	B	1950	093	CAV-NAU-SAN-OAO

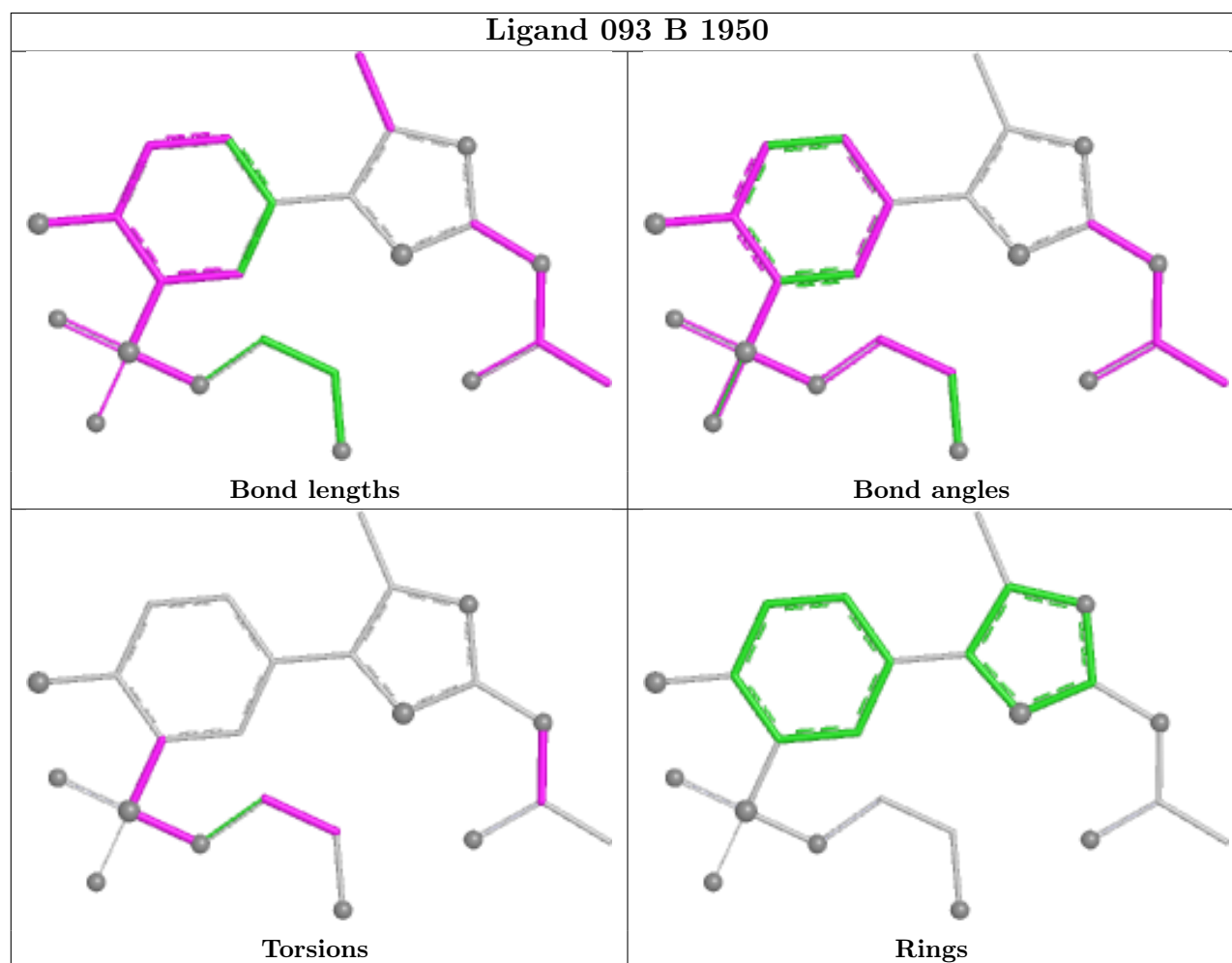
There are no ring outliers.



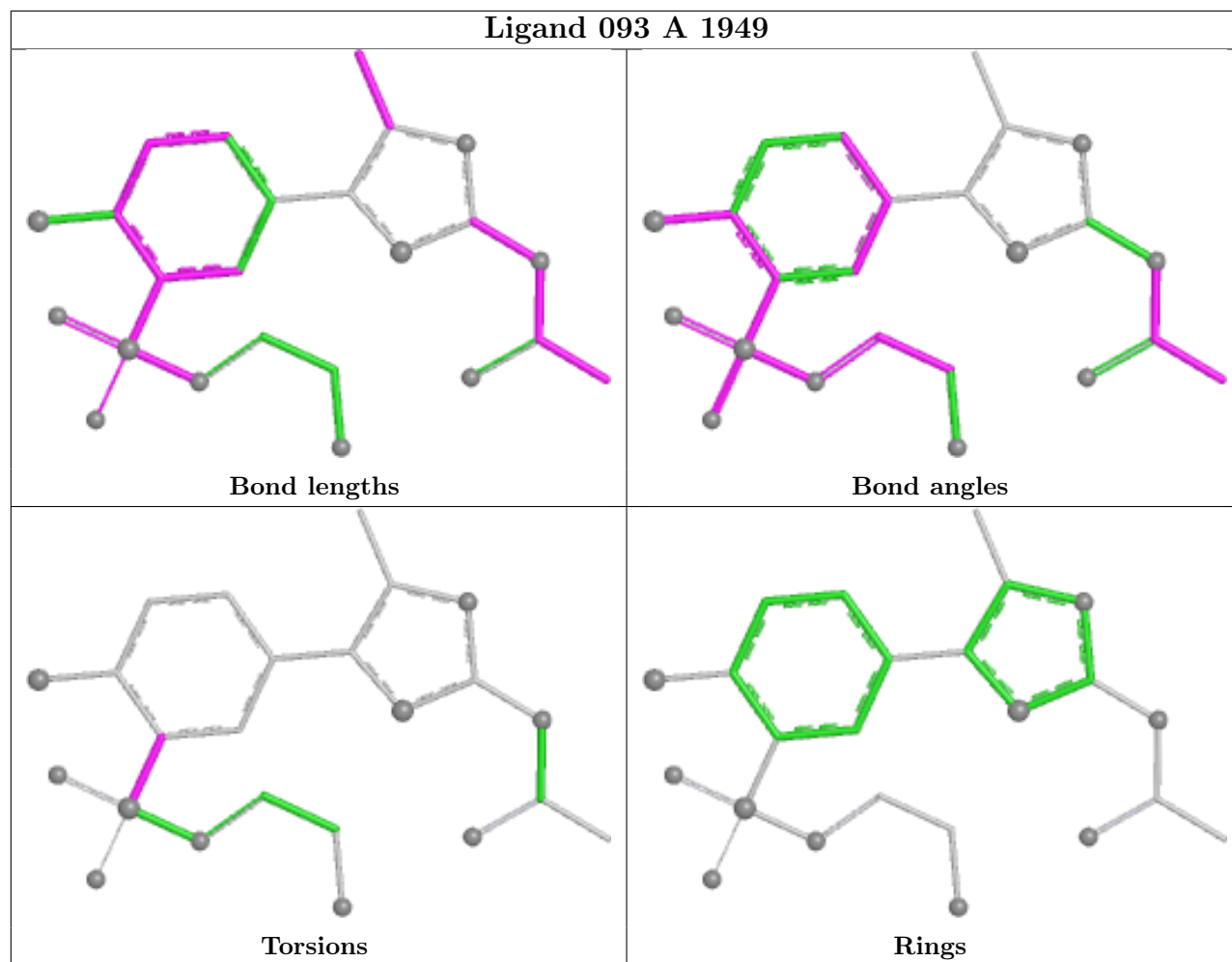
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1950	093	6	0
2	A	1949	093	8	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	545/696 (78%)	-0.29	3 (0%) 89 86	32, 55, 105, 116	0
1	B	546/696 (78%)	-0.18	6 (1%) 80 75	43, 65, 116, 123	0
All	All	1091/1392 (78%)	-0.23	9 (0%) 86 81	32, 61, 107, 123	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	TRP	3.1
1	A	302	TYR	2.7
1	B	636	LEU	2.5
1	A	322	ARG	2.2
1	A	298	HIS	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no 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.

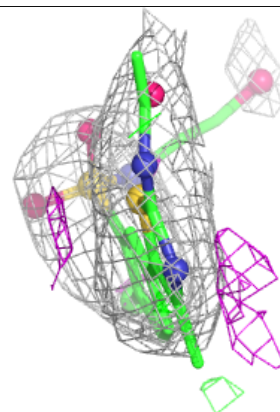
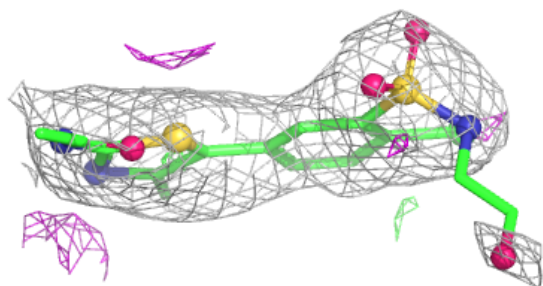
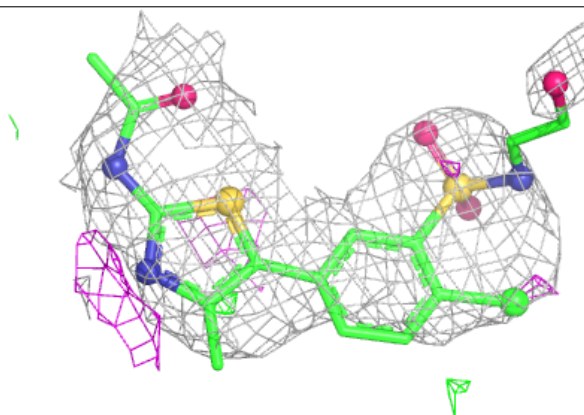


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	093	A	1949	24/24	0.89	0.31	87,97,104,107	0
2	093	B	1950	24/24	0.91	0.35	101,108,117,119	0

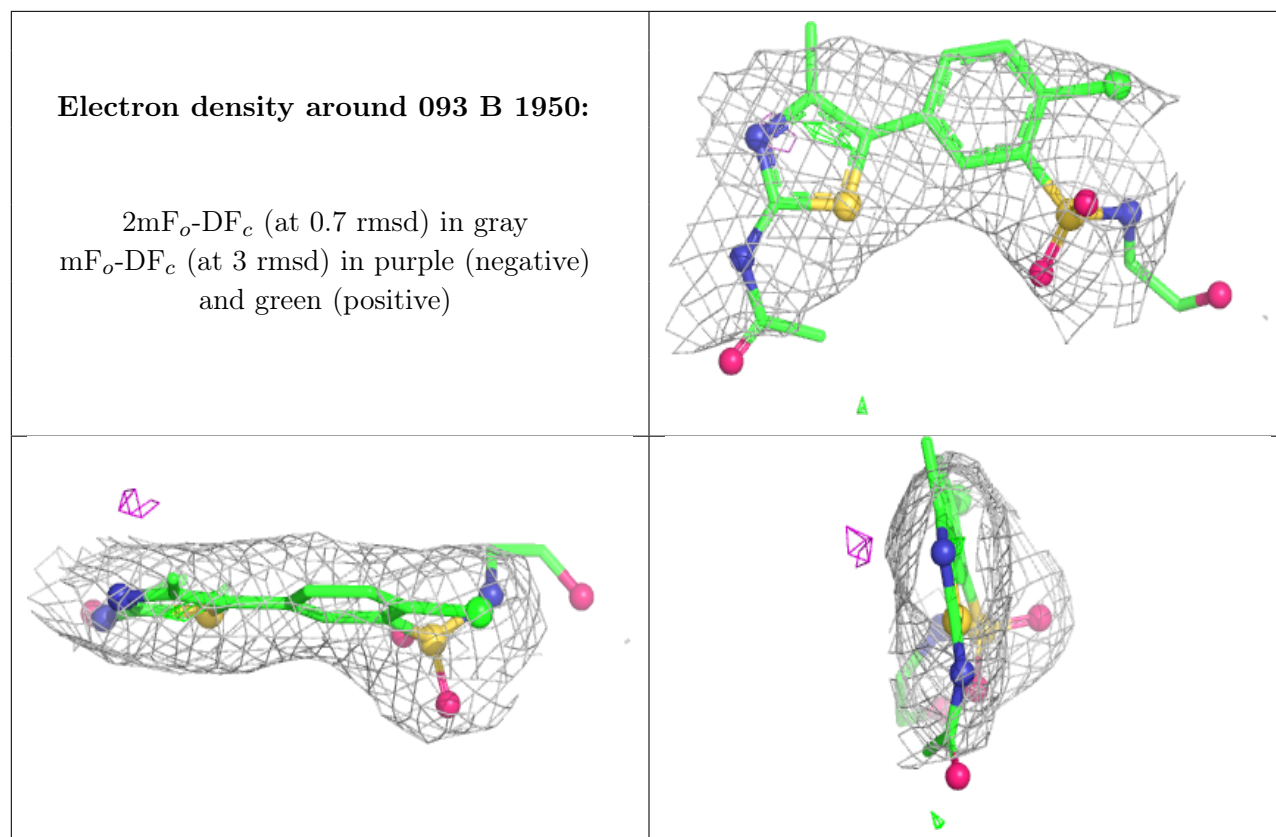
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 093 A 1949:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.