



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 11:03 AM BST

PDB ID : 2ZB2  
Title : Human liver glycogen phosphorylase a complexed with glucose and 5-chloro-N-[4-(1,2-dihydroxyethyl)phenyl]-1H-indole-2-carboxamide  
Authors : Katayama, N.; Onda, K.  
Deposited on : 2007-10-15  
Resolution : 2.45 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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

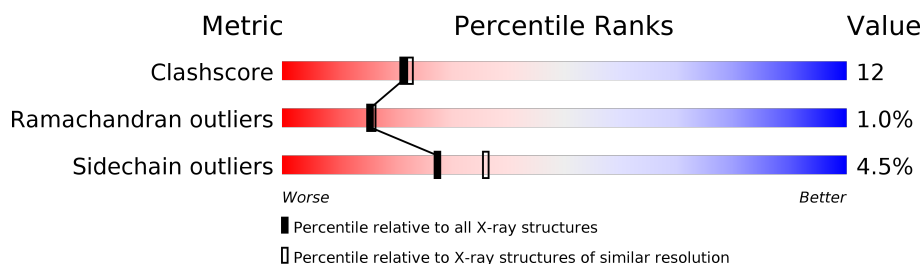
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)

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 on 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	849	
1	B	849	

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
6	MPD	B	852	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13413 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.

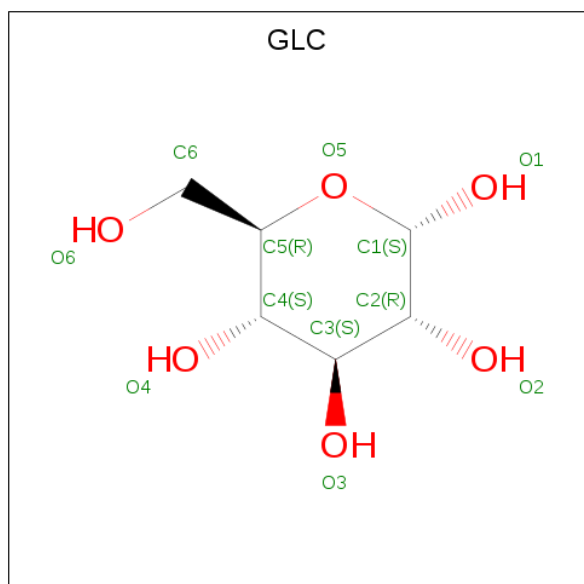
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	798	Total	C	N	O	S	0	0	0
			6466	4154	1097	1186	29			
1	B	791	Total	C	N	O	S	0	0	0
			6410	4116	1088	1177	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P06737
A	-1	SER	-	expression tag	UNP P06737
B	-2	GLY	-	expression tag	UNP P06737
B	-1	SER	-	expression tag	UNP P06737

- Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



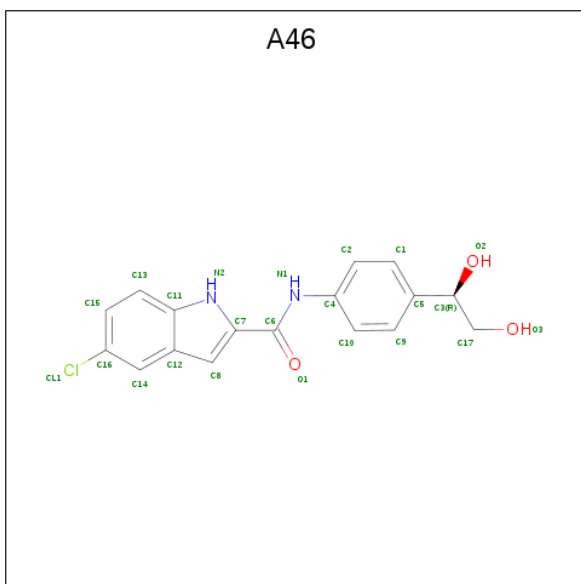
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 5 is 5-chloro-N-{4-[(1R)-1,2-dihydroxyethyl]phenyl}-1H-indole-2-carboxamide (three-letter code: A46) (formula:  $C_{17}H_{15}ClN_2O_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			23	17	1	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	
			23	17	1	2	3	
								0
								0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O		
			8	6	2		
						0	0
6	B	1	Total	C	O		
			8	6	2		
						0	0

- Molecule 7 is water.

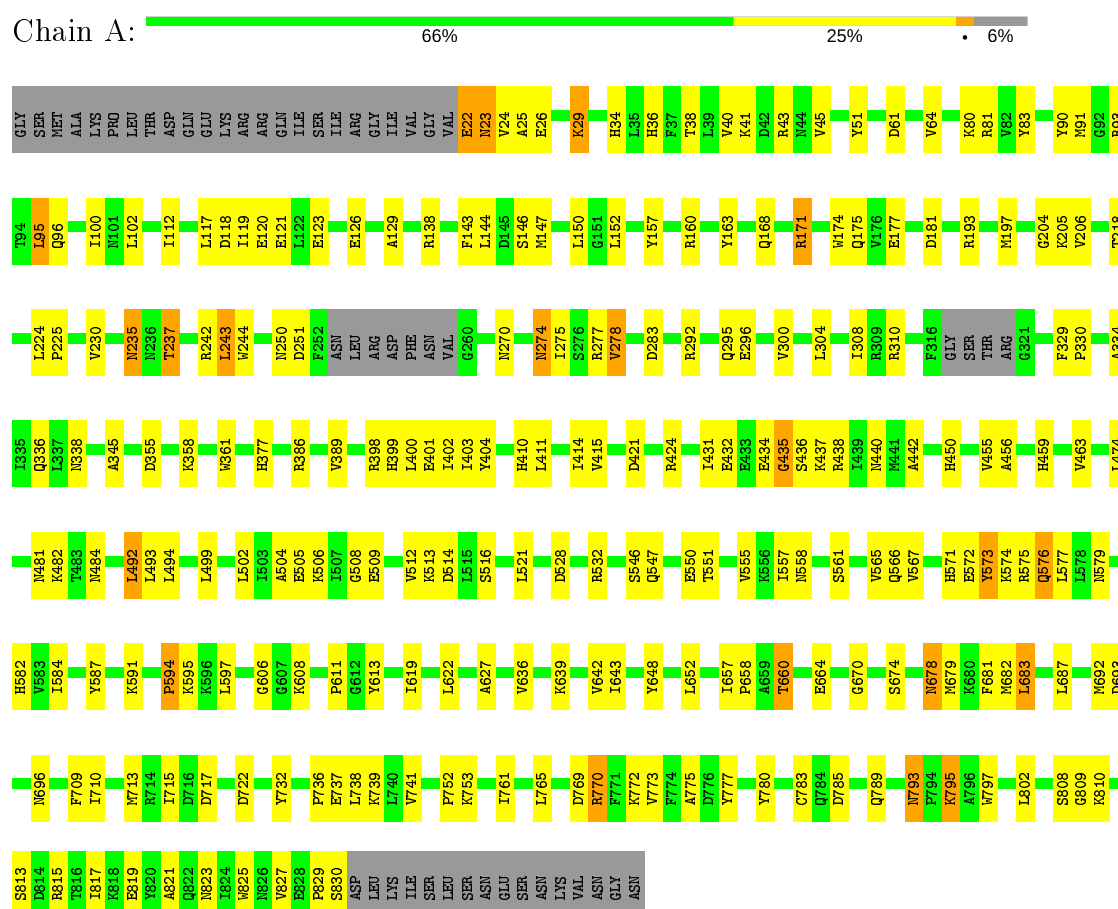
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O		
			199	199		
					0	0
7	B	198	Total	O		
			198	198		
					0	0

### 3 Residue-property plots

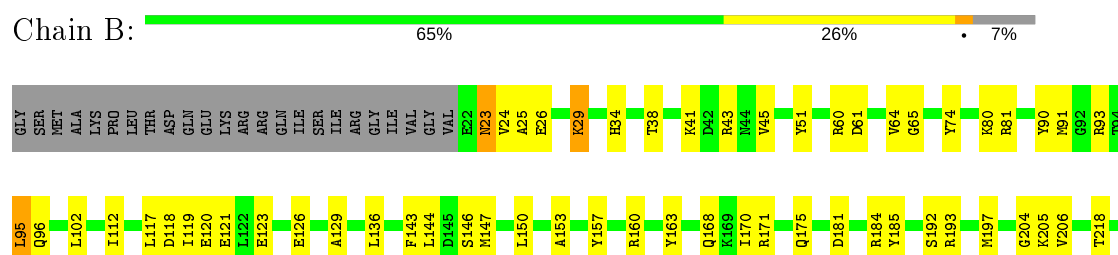
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: Glycogen phosphorylase, liver form



- Molecule 1: Glycogen phosphorylase, liver form



V221	ALA	N440	V567	A673	D785
I224	GLY	P441	K568	S674	Q789
P225	I324	A442	H571	N678	N793
Y226	F326	H450	E572	M679	P794
V230	P329	V455	Y573	K680	K795
N235	P330	A456	K574	F681	K796
N236	A334	K457	R575	M682	W797
T237	I458	N579	Q576	L683	L802
R242	H459	C580	N579	L687	S808
L243	T340	V463	V583	M692	G809
W244	H341	L474	Y587	D693	K810
N250	P342	N481	K591	N696	S813
ASP	A345	L492	P594	V697	R814
PHE	D355	L493	L597	E701	R815
ASN	K358	L494	L597	F709	T816
LEU	W361	L499	V603	I710	I817
ARG	K370	L502	I604	M713	K818
ASP	V379	I503	I605	R714	E819
PHE	R386	A504	G606	I715	V827
ASN	V389	E505	G607	D716	E828
VAL	R398	K506	Y613	D717	P829
G260	H399	G508	K617	D722	S830
V266	R399	E509	M618	Y732	ASP
N270	L400	V512	I619	P736	LEU
N274	E401	K513	L622	E737	LYS
I275	I402	D614	L627	L740	ILE
S276	I403	I515	V636	V741	SER
R277	Y404	S516	K639	P752	LEU
V278	E405	L521	L640	K753	SER
L291	I406	D528	V642	I761	ASN
R292	H410	R532	E646	L765	ASN
Q295	L411	S546	N647	D769	ASN
E296	I414	Q547	Y648	R770	GLY
V300	V415	E550	L652	F771	ASN
I304	D421	T551	I657	K772	
R310	R424	V555	P658	V773	
F311	I431	N558	A659	F774	
K312	E432	E434	T660	A775	
A313	E433	S561	S663	D776	
S314	E434	D564	E664	Y777	
LYS	G435	V565	Q665	C783	
PHE	S436	V565		Q784	
GLY	R437				
SER	R438				
THR	I439				
ARG					
GLY					



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.82Å 123.82Å 123.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.18 – 2.45	Depositor
% Data completeness (in resolution range)	99.4 (49.18-2.45)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.37	Depositor
Refinement program	CNX	Depositor
R, $R_{free}$	0.261 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A46, MPD, GLC, MES, PLP

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	0.54	0/6611	0.61	0/8940
1	B	0.52	0/6553	0.61	0/8865
All	All	0.53	0/13164	0.61	0/17805

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

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	6466	0	6451	160	0
1	B	6410	0	6394	153	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	12	0	12	3	0
3	B	12	0	13	3	0
4	A	15	0	7	0	0
4	B	15	0	7	0	0
5	A	23	0	15	0	0
5	B	23	0	15	1	0
6	B	16	0	28	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	199	0	0	8	0
7	B	198	0	0	13	0
All	All	13413	0	12966	312	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 12.

The worst 5 of 312 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:204:GLY:O	1:A:205:LYS:HD2	1.79	0.83
1:B:204:GLY:O	1:B:205:LYS:HD2	1.80	0.80
1:B:678:ASN:HD22	1:B:679:MET:H	1.29	0.77
1:A:678:ASN:HD22	1:A:679:MET:H	1.32	0.76
1:A:310:ARG:HE	3:A:848:MES:H72	1.50	0.76

There are no symmetry-related clashes.

## 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	792/849 (93%)	739 (93%)	45 (6%)	8 (1%)	15	16
1	B	785/849 (92%)	734 (94%)	43 (6%)	8 (1%)	15	16
All	All	1577/1698 (93%)	1473 (93%)	88 (6%)	16 (1%)	15	16

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ASP
1	A	435	GLY

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Mol	Chain	Res	Type
1	A	555	VAL
1	A	715	ILE
1	B	23	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	696/741 (94%)	663 (95%)	33 (5%)	26	34
1	B	691/741 (93%)	661 (96%)	30 (4%)	29	38
All	All	1387/1482 (94%)	1324 (96%)	63 (4%)	27	36

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	LEU
1	B	29	LYS
1	B	683	LEU
1	A	722	ASP
1	A	793	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	822	GLN
1	B	167	ASN
1	B	789	GLN
1	A	826	ASN
1	B	34	HIS

### 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 ⓘ

10 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	GLC	A	847	-	12,12,12	0.47	0	17,17,17	0.64	0
6	MPD	B	851	-	7,7,7	1.27	1 (14%)	9,10,10	1.23	0
4	PLP	A	849	1	15,15,16	1.81	4 (26%)	20,22,23	1.19	0
2	GLC	B	847	-	12,12,12	0.39	0	17,17,17	0.46	0
5	A46	B	850	-	22,25,25	2.04	7 (31%)	27,35,35	2.06	9 (33%)
5	A46	A	850	-	22,25,25	1.48	3 (13%)	27,35,35	1.84	7 (25%)
6	MPD	B	852	-	7,7,7	0.72	0	9,10,10	1.20	1 (11%)
3	MES	A	848	-	12,12,12	1.62	2 (16%)	14,16,16	2.67	5 (35%)
4	PLP	B	849	1	15,15,16	1.43	4 (26%)	20,22,23	1.12	0
3	MES	B	848	-	12,12,12	1.07	1 (8%)	14,16,16	2.15	5 (35%)

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	GLC	A	847	-	-	0/2/22/22	0/1/1/1
6	MPD	B	851	-	-	1/5/5/5	-
5	A46	B	850	-	-	0/11/14/14	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	847	-	-	0/2/22/22	0/1/1/1
4	PLP	A	849	1	-	0/6/6/8	0/1/1/1
5	A46	A	850	-	-	2/11/14/14	0/3/3/3
6	MPD	B	852	-	1/1/2/2	1/5/5/5	-
3	MES	A	848	-	-	4/6/14/14	0/1/1/1
4	PLP	B	849	1	-	0/6/6/8	0/1/1/1
3	MES	B	848	-	-	3/6/14/14	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	850	A46	C16-CL1	-5.43	1.62	1.74
3	A	848	MES	O3S-S	4.66	1.64	1.47
4	A	849	PLP	C5-C4	4.60	1.45	1.40
5	B	850	A46	C4-N1	-3.82	1.33	1.41
4	A	849	PLP	C3-C4	3.31	1.47	1.40

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	850	A46	C8-C12-C11	5.55	111.11	106.27
3	A	848	MES	C5-N4-C3	5.28	120.71	108.83
3	A	848	MES	O1S-S-C8	4.99	112.92	106.92
3	A	848	MES	O2S-S-C8	-4.50	101.50	106.92
5	B	850	A46	C7-C8-C12	-4.32	101.17	106.55

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	852	MPD	C4

5 of 11 torsion outliers are listed below:

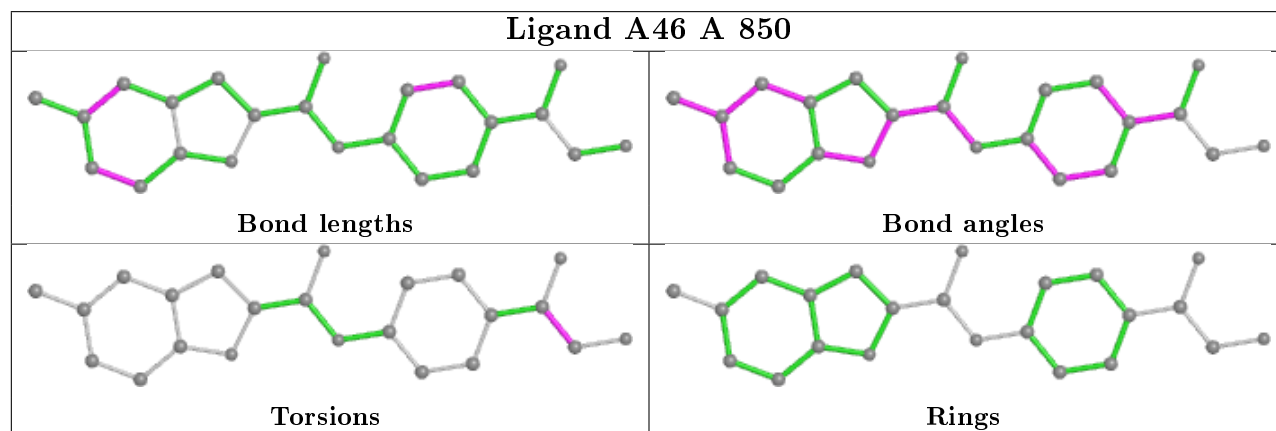
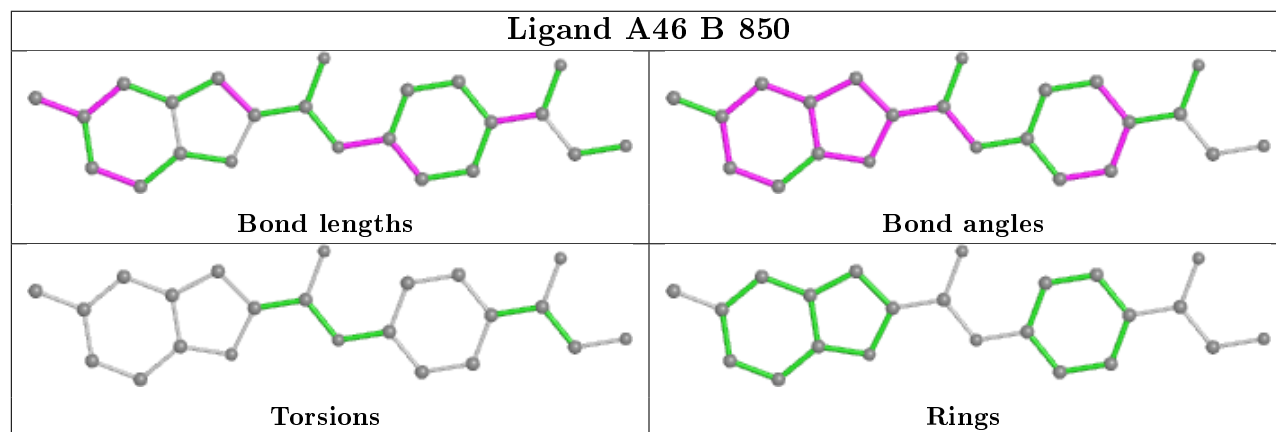
Mol	Chain	Res	Type	Atoms
6	B	851	MPD	C2-C3-C4-C5
5	A	850	A46	O3-C17-C3-O2
3	A	848	MES	C7-C8-S-O1S
3	A	848	MES	C7-C8-S-O3S
5	A	850	A46	O3-C17-C3-C5

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	851	MPD	2	0
5	B	850	A46	1	0
6	B	852	MPD	4	0
3	A	848	MES	3	0
3	B	848	MES	3	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.