



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 02:51 AM BST

PDB ID : 6UJS
Title : P-glycoprotein mutant-F728A and C952A-with BDE100
Authors : Aller, S.G.; Le, C.A.
Deposited on : 2019-10-03
Resolution : 4.17 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

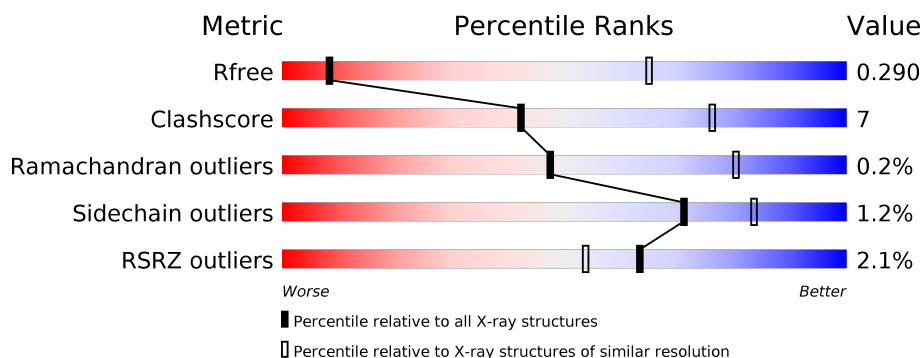
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.17 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	1034 (4.60-3.76)
Clashscore	141614	1030 (4.54-3.80)
Ramachandran outliers	138981	1006 (4.58-3.78)
Sidechain outliers	138945	1037 (4.60-3.76)
RSRZ outliers	127900	1056 (4.66-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1282	<div> <div>2%</div> <div>76%</div> <div>16%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9193 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.

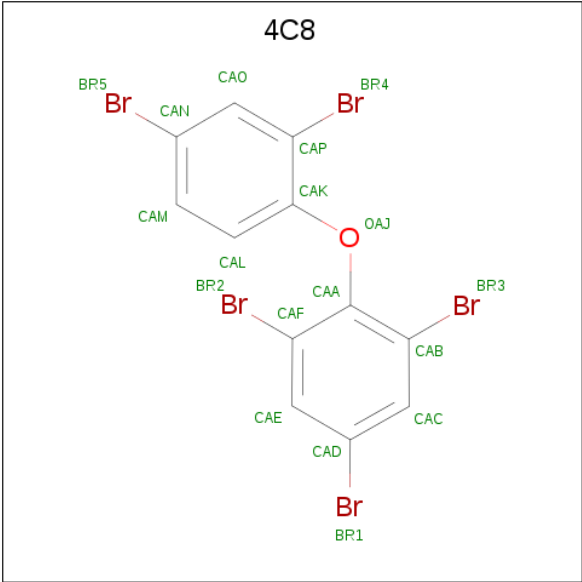
- Molecule 1 is a protein called ATP-dependent translocase ABCB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9157	5887	1553	1680	37			

There are 11 discrepancies between the modelled and reference sequences:


Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	engineered mutation	UNP P21447
A	87	GLN	ASN	engineered mutation	UNP P21447
A	90	GLN	ASN	engineered mutation	UNP P21447
A	728	ALA	PHE	engineered mutation	UNP P21447
A	952	ALA	CYS	engineered mutation	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447

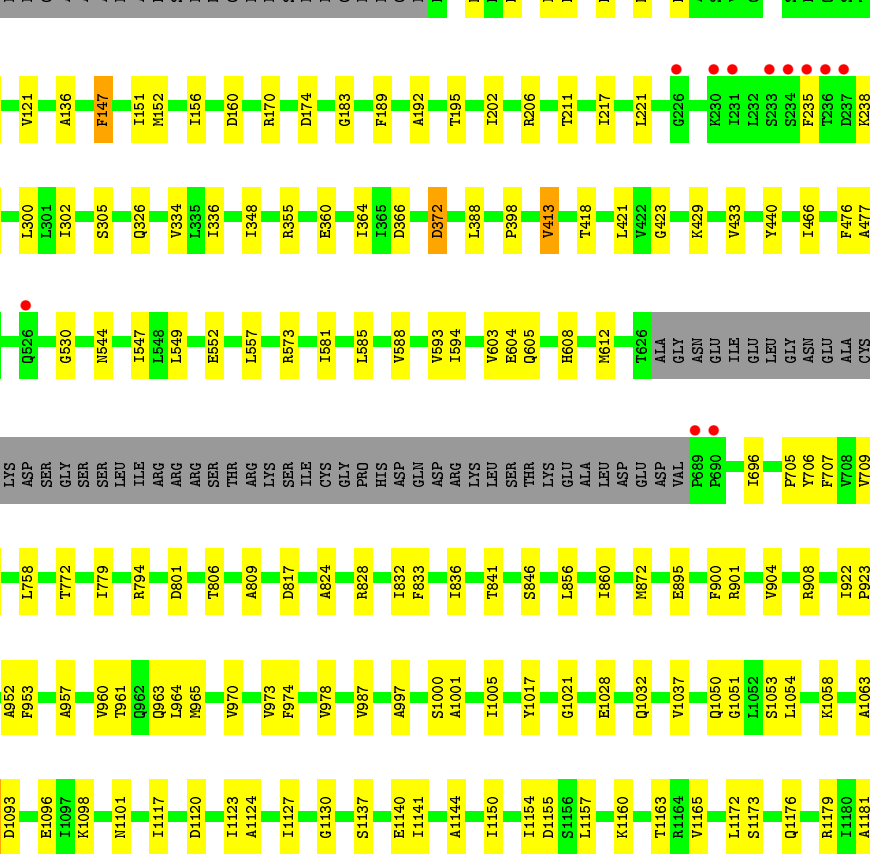
- Molecule 2 is 2,4-dibromophenyl 2,4,6-tribromophenyl ether (three-letter code: 4C8) (formula: C₁₂H₅Br₅O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	O	0	0
			18	5	12	1		
2	A	1	Total	Br	C	O	0	0
			18	5	12	1		

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: 



Row	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9	Col 10	Col 11	Col 12	Col 13	Col 14	Col 15	Col 16	Col 17	Col 18	Col 19	Col 20	Col 21	Col 22	Col 23	Col 24	Col 25	Col 26	Col 27	Col 28	Col 29	Col 30	Col 31	Col 32	Col 33	Col 34	Col 35	Col 36	Col 37	Col 38	Col 39	Col 40	Col 41	Col 42	Col 43	Col 44	Col 45	Col 46	Col 47	Col 48	Col 49	Col 50	Col 51	Col 52	Col 53	Col 54	Col 55	Col 56	Col 57	Col 58	Col 59	Col 60	Col 61	Col 62	Col 63	Col 64	Col 65	Col 66	Col 67	Col 68	Col 69	Col 70	Col 71	Col 72	Col 73	Col 74	Col 75	Col 76	Col 77	Col 78	Col 79	Col 80	Col 81	Col 82	Col 83	Col 84	Col 85	Col 86	Col 87	Col 88	Col 89	Col 90	Col 91	Col 92	Col 93	Col 94	Col 95	Col 96	Col 97	Col 98	Col 99	Col 100
Q1189	M944	F724	ASN	T518	Y110	MET																																																																																														
P1190	M945	I727	LEU	L519	GLU	GLU																																																																																														
L1194	Y946	A728	ASP	V520	LEU	LEU																																																																																														
L1195	F947	A728	ASP	G521	GLU	GLU																																																																																														
D1196	S948		SER	E522	GLU	ASP																																																																																														
T1199	A952	V731	LYS	R523	I117	LYS																																																																																														
L1202	E1093	L758	ASP	Q526	V121	LYS																																																																																														
D1203	E1096	T772	SER	G530	L301	GLY																																																																																														
T1204	K1098	I779	SER	N544	A136	ARG																																																																																														
E1205	M1101	T961	LEU	I547	F147	ASP																																																																																														
S1206	Q962	R794	ILE	L548	I151	LYS																																																																																														
E1207	Q963	D801	ARG	L549	M152	PHE																																																																																														
Q1211	L964	D806	ARG	E552	I156	LYS																																																																																														
E1219	V970	T806	SER	E557	D160	MET																																																																																														
I1226	V973	A809	THR	L557	R170	GLY																																																																																														
R1229	F974	D817	LYS	R573	R174	LYS																																																																																														
I1239	V978	A824	ILE	I581	D174	LYS																																																																																														
M1244	V987	R828	CYS	L585	G183	GLU																																																																																														
G1245	A997	I832	PRO	V588	F189	LYS																																																																																														
K1246	E1140	F833	HIS	V589	A192	LYS																																																																																														
V1247	I1141	I836	ASP	I594	T195	GLU																																																																																														
K1248	A1144	I836	GLN	V594	I202	LYS																																																																																														
H1253	I1150	T841	LYS	E603	R206	LYS																																																																																														
I1262	I1154	S846	THR	E604	T211	GLU																																																																																														
Y1263	D1155	L856	LYS	Q605	I217	LYS																																																																																														
A1273	S1156	L860	ALA	H608	I217	LYS																																																																																														
LYS	L1157	I860	LEU	M612	L221	LYS																																																																																														
ARG	K1160	M872	ASP	T626	G226	LYS																																																																																														
SER	Q1032		GLU	ALA	K429	LYS																																																																																														
HIS	T1163	E895	ASP	GLY	K429	LYS																																																																																														
HIS	R1164	V1037	VAL	ASN	I231	LYS																																																																																														
HIS	V1165	F900	P689	GLU	V433	LYS																																																																																														
HIS	L1172	Q1050	P690	ILE	V433	LYS																																																																																														
HIS	S1173	G1051	R901	GLU	Y440	LYS																																																																																														
HIS	Q1176	I1053	L696	LEU	I466	LYS																																																																																														
		L1054		GLY	I466	LYS																																																																																														
		K1058	P705	ASN	T236	LYS																																																																																														
	R1179		V706	GLU	Q87	LYS																																																																																														
		K1058	F707	GLU	S88	LYS																																																																																														
	L1180	A1063	V708	ALA	S88	LYS																																																																																														
	A1181	L1064	W109	CYS	Q90	LYS																																																																																														
	I1182		G740	LYS	D95	LYS																																																																																														
	A1183	C1070	F711	SER	A98	LYS																																																																																														
	R1184		F712	LYS	M99	LYS																																																																																														
	L1186	T1074	C713	ASP		LYS																																																																																														
	V1187	V1075	G719	GLU		LYS																																																																																														
	R1189	V1076		ILE		LYS																																																																																														
				ASP		LYS																																																																																														
				ILE		LYS																																																																																														
				ASP		LYS																																																																																														
				ILE		LYS																																																																																														

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.50Å 138.25Å 196.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 4.17 29.87 – 3.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.87-4.17) 90.3 (29.87-3.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.98Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.250 , 0.289 0.250 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (9.03%)	wwPDB-VP
Wilson B-factor (Å ²)	187.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 105.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9193	wwPDB-VP
Average B, all atoms (Å ²)	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4C8

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	0.25	0/9325	0.41	1/12605 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1092	LEU	CA-CB-CG	5.39	127.70	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9157	0	9346	128	0
2	A	36	0	0	2	0
All	All	9193	0	9346	128	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 7.

The worst 5 of 128 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:160:ASP:OD1	1:A:901:ARG:NH2	2.20	0.74
1:A:156:ILE:HD11	1:A:904:VAL:HG11	1.74	0.69
1:A:388:LEU:HD11	1:A:547:ILE:HD12	1.79	0.65
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.31	0.64
1:A:170:ARG:HG3	1:A:174:ASP:OD2	1.99	0.62

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	1178/1282 (92%)	1126 (96%)	50 (4%)	2 (0%)	47 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1204	THR
1	A	372	ASP

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	971/1061 (92%)	959 (99%)	12 (1%)	71 83

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	THR
1	A	593	VAL
1	A	1155	ASP
1	A	413	VAL
1	A	1032	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	4C8	A	1302	-	19,19,19	1.16	5 (26%)	27,27,27	0.78	0
2	4C8	A	1301	-	19,19,19	1.11	4 (21%)	27,27,27	0.94	1 (3%)

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	4C8	A	1302	-	-	0/4/4/4	0/2/2/2
2	4C8	A	1301	-	-	0/4/4/4	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1302	4C8	BR3-CAB	2.21	1.94	1.89
2	A	1302	4C8	BR1-CAD	2.12	1.94	1.90
2	A	1301	4C8	BR1-CAD	2.09	1.94	1.90
2	A	1302	4C8	BR5-CAN	2.06	1.94	1.90
2	A	1301	4C8	BR2-CAF	2.05	1.94	1.89

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	4C8	CAK-OAJ-CAA	-2.39	112.50	117.79

There are no chirality outliers.

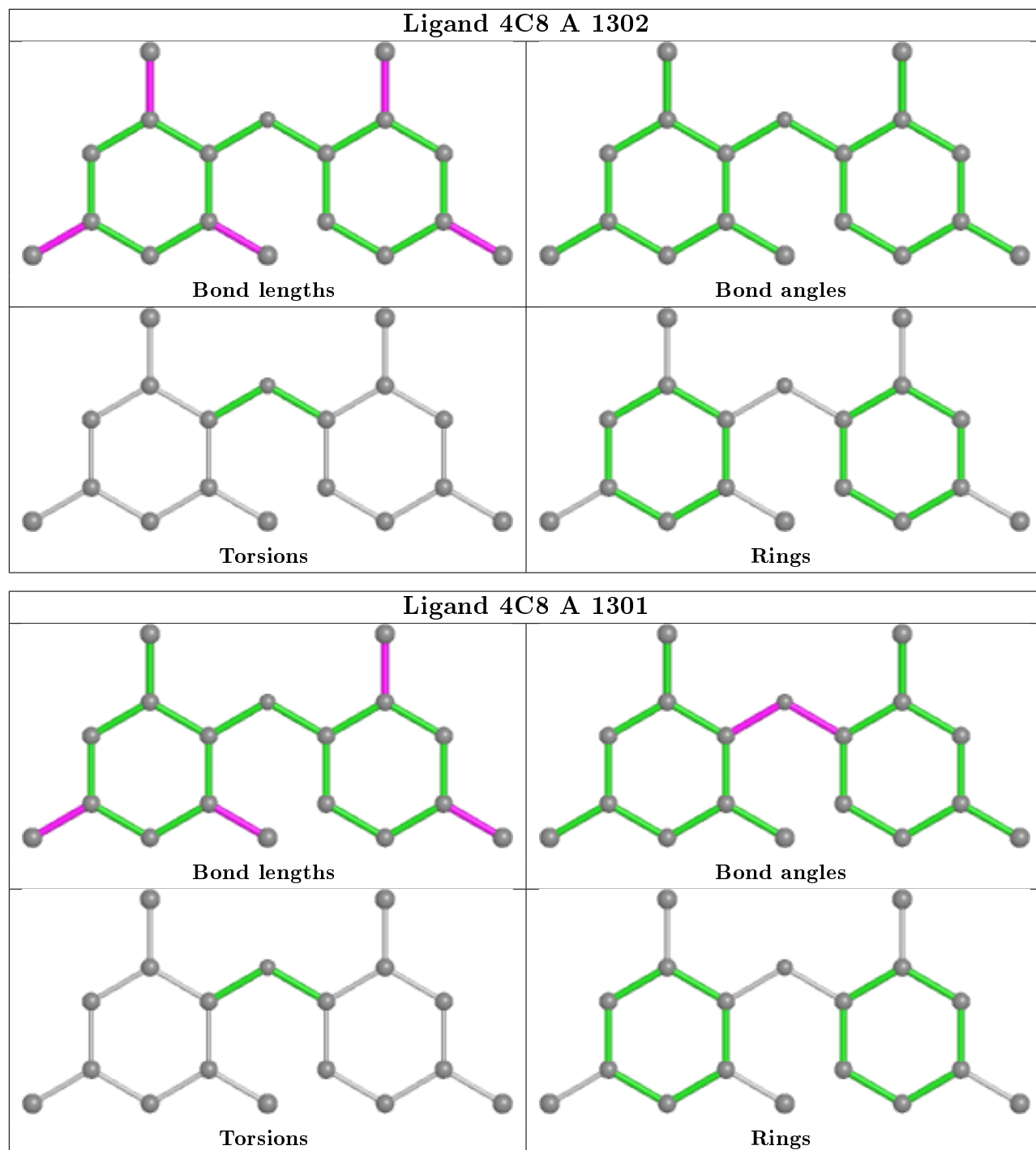
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	4C8	1	0
2	A	1301	4C8	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.



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, 95th 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 ²)	Q<0.9
1	A	1182/1282 (92%)	-0.44	25 (2%) 63 54	147, 205, 276, 327	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	690	PRO	7.3
1	A	1219	GLU	5.2
1	A	235	PHE	4.7
1	A	85	SER	4.4
1	A	689	PRO	4.1

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](#)

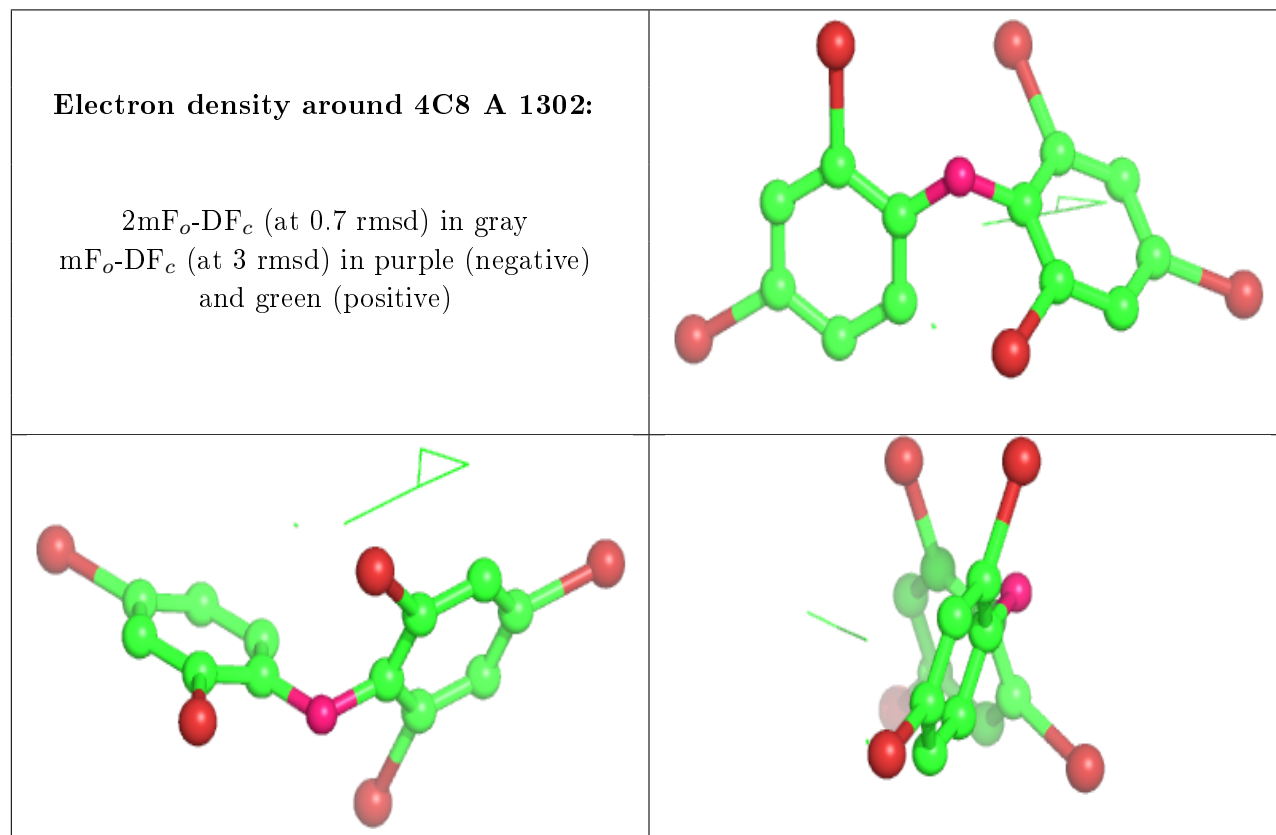
There are no monosaccharides in this entry.

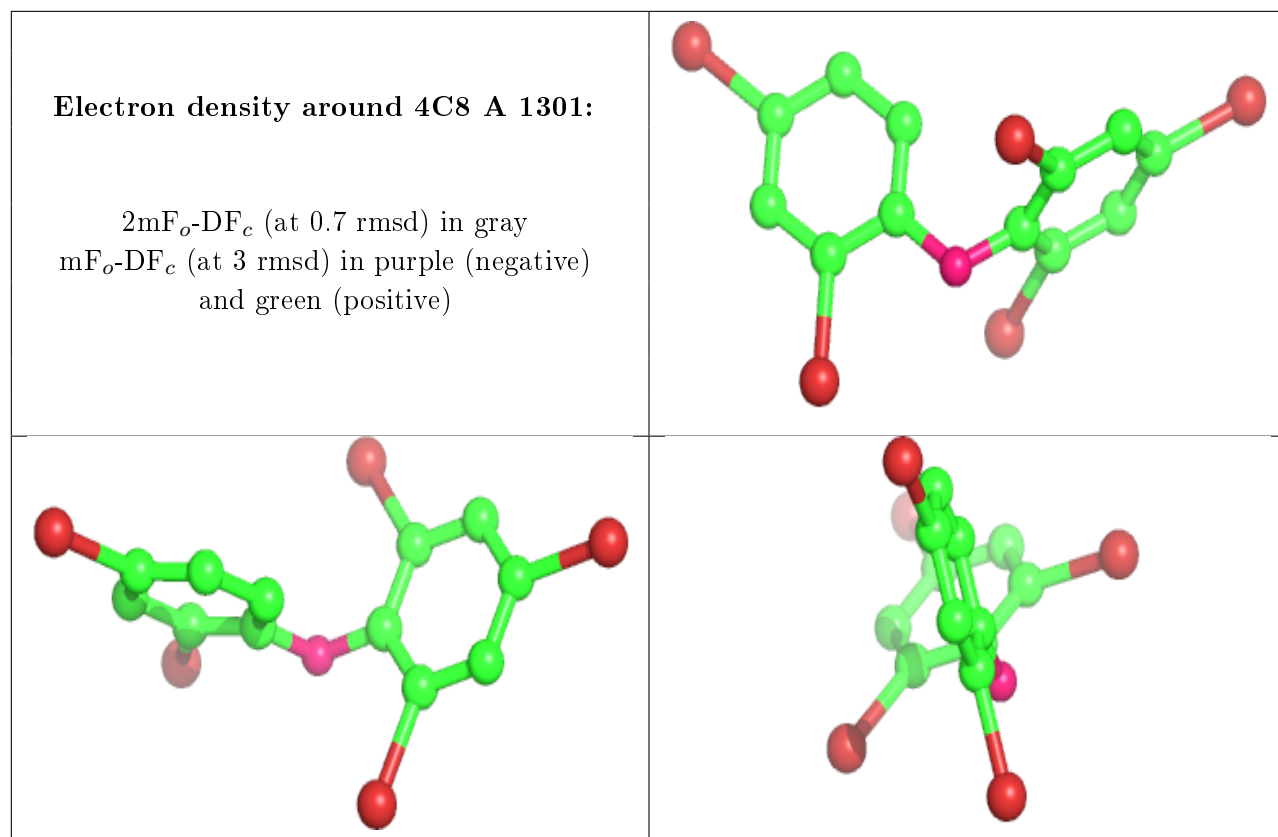
6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
2	4C8	A	1302	18/18	0.24	0.29	234,247,289,296	18
2	4C8	A	1301	18/18	0.59	0.30	229,239,256,284	18

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.