



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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) : 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

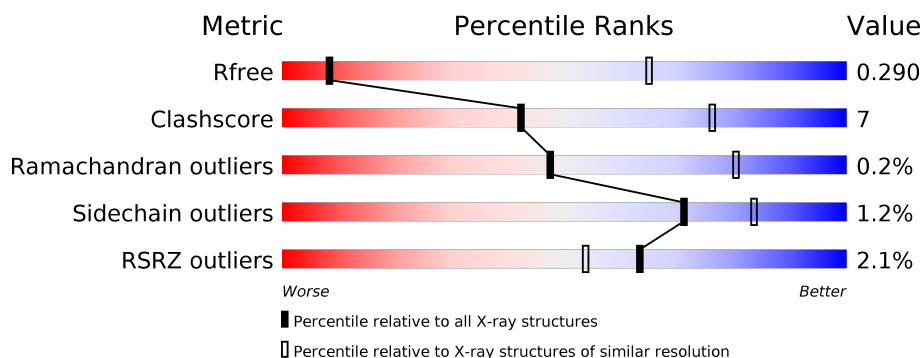
# 1 Overall quality at a glance

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  $\geq 3$ , 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	1282	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>8%</div> </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.

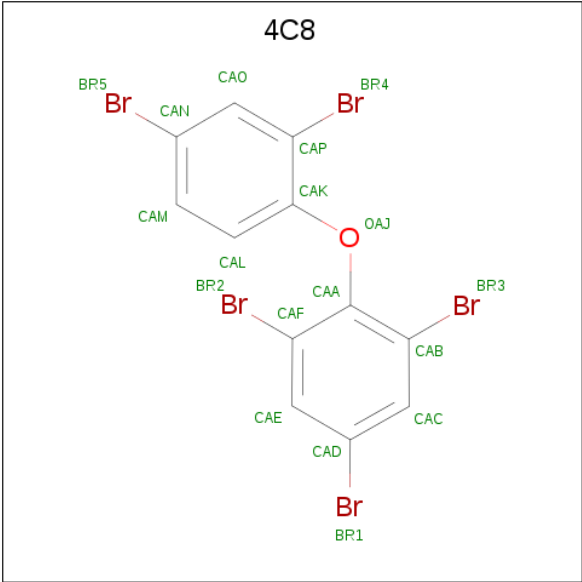
- Molecule 1 is a protein called ATP-dependent translocase ABCB1.

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

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: C<sub>12</sub>H<sub>5</sub>Br<sub>5</sub>O) (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 ( $\text{RSRZ} > 2$ ). 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: 29% 76% 16% 8%

Q1189	M944	F724	ASN	T518	Y110	MET
P1190	N945	I727	LEU	L519	F263	GLU
L1194	Y946	A728	ASP	G521	L270	ASP
L1195	F947		MET	E522	K287	GLU
D1196	S948		SER	R523		ASP
	A952		LYS			LEU
T1199	F953	L758	ASP	Q526	L300	LYS
L1202	A957	T772	SER	G530	L301	GLY
D1203	V960	I779	SER	N544	A136	ARG
T1204	T961	R794	ILE	I547	F147	ALA
E1205	Q962	R794	ARG	L548	Q326	LYS
S1206	Q963	D801	ARG	L549	M152	ASN
E1207	L964	D801	ARG	L549	V334	PHE
Q1211	N965	T806	ARG	E552	I156	SER
	V970		SER		I336	LYS
E1219	V973	A809	THR	L557	D160	MET
I1226	V974	D817	LYS	R573	R170	GLY
	V978	A824	ILE	I581	D174	LYS
R1229	V987	R828	CYS	L585	E360	LYS
I1239	A997	I832	GLY	V588	G183	GLU
N1244	S1000	F833	PRO	I594	I364	LYS
G1245	A1001	I836	HIS	V603	I365	LYS
K1246	I1141	I836	ASP	E604	D366	GLU
V1247	A1144	I836	GLN	Q605	A192	LYS
K1248	I1150	T841	ASP	V593	D372	K30
H1253	I1154	S846	ARG	I594	T195	K38
I1262	D1155	L856	LYS	V603	I202	F39
Y1263	S1156	L860	SER	E604	R206	R40
L1273	L1157	I860	THR	Q605	T211	L64
	K1160	M872	LYS	H608	I217	P65
	T1163	E895	ALA	M612		F71
H15	R1164	F900	ASP	T626	L221	M74
H15	V1165	R901	VAL	ALA	G226	F78
H15	L1172	Q1050	ASP	GLY	K429	A79
H15	S1173	G1051	P690	ASN	I231	S80
	Q1176	I1052		ILE	L232	V81
	R1179	V904	I696	GLU	S233	G82
	I1180	R908	P705	LEU	S234	S85
A1181	L1182	I922	V706	GLY	F235	K36
L1182	L1084	P923	F707	ASN	T236	Q87
A1183	C1070	K930	V708	ALA	F476	S88
R1184	F1111	F938	W09	CYS	A477	T89
L1186	T1074	V942	G740	LYS	T478	Q90
V1187	V1075	V942	F712	SER	I479	
R1189			C743	LYS	A481	D95
			G719	ASP	A242	
				GLU	A256	A98
				ILE	R485	N99
				ASP		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	187.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 105.9	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	0.89	EDS
Total number of atoms	9193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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 [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.

All (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
1:A:846:SER:HB3	1:A:973:VAL:HG13	1.81	0.61
1:A:239:GLU:HB2	1:A:287:LYS:HZ2	1.67	0.60
1:A:421:LEU:HB2	1:A:581:ILE:HG13	1.83	0.60
1:A:711:ILE:HD12	1:A:833:PHE:HD2	1.68	0.58
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.86	0.58
1:A:952:ALA:HB1	1:A:974:PHE:CZ	2.40	0.57
1:A:1207:GLU:OE1	1:A:1229:ARG:NH2	2.38	0.57
1:A:817:ASP:HA	1:A:1000:SER:HB3	1.87	0.56
1:A:256:ALA:HB2	1:A:1117:ILE:HG12	1.87	0.56
1:A:1050:GLN:NE2	1:A:1244:ASN:O	2.35	0.56
1:A:263:PHE:HA	1:A:1188:ARG:HH22	1.71	0.55
1:A:1196:ASP:HA	1:A:1226:ILE:HG12	1.88	0.55
1:A:1157:LEU:HD13	1:A:1163:THR:HG21	1.89	0.54
1:A:1124:ALA:HB1	1:A:1141:ILE:HD12	1.89	0.53
1:A:64:LEU:HD12	1:A:336:ILE:HG21	1.89	0.53
1:A:1092:LEU:HG	1:A:1093:ASP:H	1.71	0.53
1:A:930:LYS:NZ	1:A:930:LYS:HB3	2.23	0.53
1:A:160:ASP:OD2	1:A:440:TYR:OH	2.25	0.53
1:A:1096:GLU:HG2	1:A:1098:LYS:H	1.73	0.53
1:A:603:VAL:HG12	1:A:604:GLU:HG3	1.89	0.53
1:A:1202:LEU:HB3	1:A:1207:GLU:HG2	1.91	0.52
1:A:1079:LEU:HD23	1:A:1194:LEU:HD21	1.90	0.52
1:A:388:LEU:HB2	1:A:413:VAL:HG13	1.92	0.52
1:A:71:PHE:HE1	1:A:953:PHE:HZ	1.59	0.51
1:A:152:MET:HA	1:A:900:PHE:HE2	1.75	0.51
1:A:1173:SER:OG	1:A:1176:GLN:OE1	2.27	0.51
1:A:238:LYS:O	1:A:242:ALA:N	2.43	0.51
1:A:1123:ILE:HD13	1:A:1154:ILE:HD12	1.92	0.51
1:A:1050:GLN:O	1:A:1246:LYS:HG3	2.11	0.51
1:A:1239:ILE:HG21	1:A:1263:TYR:CE1	2.46	0.51
1:A:235:PHE:HB3	1:A:287:LYS:HE2	1.92	0.51
1:A:160:ASP:HB2	1:A:398:PRO:HG2	1.94	0.50
1:A:114:TYR:HE2	1:A:953:PHE:HD2	1.60	0.50
1:A:1064:LEU:HB3	1:A:1226:ILE:HG22	1.93	0.50
1:A:360:GLU:O	1:A:364:ILE:HG12	2.11	0.50
1:A:1202:LEU:HD23	1:A:1207:GLU:HA	1.95	0.49
1:A:544:ASN:ND2	1:A:544:ASN:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ILE:HG12	1:A:547:ILE:HB	1.94	0.49
1:A:1063:ALA:HB3	1:A:1239:ILE:HG13	1.94	0.49
1:A:113:TYR:O	1:A:117:ILE:HG12	2.12	0.49
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.94	0.49
1:A:221:LEU:HD22	1:A:302:ILE:HG12	1.95	0.48
1:A:206:ARG:HH11	1:A:326:GLN:HG2	1.78	0.48
1:A:719:GLY:HA2	1:A:841:THR:OG1	2.13	0.48
1:A:824:ALA:HA	1:A:828:ARG:HD3	1.96	0.48
1:A:938:PHE:O	1:A:942:GLN:HG2	2.14	0.48
1:A:263:PHE:CD2	1:A:1130:GLY:HA2	2.48	0.48
1:A:423:GLY:N	1:A:429:LYS:HD3	2.28	0.48
1:A:856:LEU:O	1:A:860:ILE:HG12	2.14	0.48
1:A:963:GLN:HG2	1:A:964:LEU:H	1.78	0.48
1:A:418:THR:HG21	1:A:573:ARG:HE	1.79	0.47
1:A:711:ILE:HD12	1:A:833:PHE:CD2	2.47	0.47
1:A:74:MET:HG2	1:A:110:TYR:CD2	2.50	0.47
1:A:801:ASP:OD2	1:A:1083:TYR:OH	2.32	0.47
1:A:944:MET:O	1:A:948:SER:OG	2.16	0.47
1:A:479:THR:HA	1:A:518:THR:O	2.15	0.47
1:A:832:ILE:HG13	1:A:987:VAL:HG22	1.96	0.47
1:A:1070:CYS:O	1:A:1074:THR:N	2.39	0.47
1:A:1199:THR:HG21	1:A:1211:GLN:HG2	1.97	0.47
1:A:477:ALA:HA	1:A:520:VAL:O	2.15	0.47
1:A:707:PHE:O	1:A:711:ILE:HG12	2.15	0.47
1:A:189:PHE:CE1	1:A:348:ILE:HD11	2.51	0.47
1:A:997:ALA:O	1:A:1001:ALA:N	2.45	0.46
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.97	0.46
1:A:217:ILE:HD12	1:A:305:SER:HB3	1.97	0.46
1:A:1021:GLY:HA3	1:A:1101:ASN:HB2	1.98	0.46
1:A:1120:ASP:HA	1:A:1165:VAL:O	2.17	0.45
1:A:960:VAL:HG13	1:A:965:MET:HB2	1.98	0.45
1:A:696:ILE:HB	1:A:1005:ILE:HD11	1.99	0.45
1:A:65:PRO:HB2	1:A:202:ILE:HD12	1.98	0.45
1:A:709:VAL:O	1:A:713:CYS:HB2	2.16	0.45
1:A:833:PHE:HA	1:A:836:ILE:HG12	1.98	0.45
1:A:1127:ILE:HA	1:A:1184:ARG:HB3	1.98	0.45
1:A:433:VAL:HG13	1:A:549:LEU:HD13	1.98	0.45
1:A:978:VAL:HG21	2:A:1302:4C8:BR2	2.73	0.44
1:A:585:LEU:HD12	1:A:588:VAL:HG11	1.98	0.44
1:A:530:GLY:N	1:A:557:LEU:HD11	2.32	0.44
1:A:136:ALA:HB2	1:A:183:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:PHE:CE1	1:A:758:LEU:HB3	2.52	0.44
1:A:211:THR:HG22	1:A:334:VAL:HG21	1.99	0.44
1:A:78:PHE:HE1	1:A:961:THR:HG21	1.82	0.44
1:A:192:ALA:O	1:A:195:THR:OG1	2.31	0.44
1:A:552:GLU:N	1:A:581:ILE:O	2.41	0.44
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.44	0.44
1:A:147:PHE:O	1:A:151:ILE:HG12	2.18	0.43
1:A:1144:ALA:HB2	1:A:1187:VAL:HG23	2.01	0.43
1:A:608:HIS:O	1:A:612:MET:HG2	2.18	0.43
1:A:121:VAL:HG21	1:A:946:TYR:CD1	2.52	0.43
1:A:728:ALA:HB2	2:A:1301:4C8:BR3	2.74	0.43
1:A:481:ALA:O	1:A:485:ARG:HB2	2.19	0.43
1:A:1248:LYS:HG2	1:A:1262:ILE:HD12	2.00	0.43
1:A:170:ARG:O	1:A:174:ASP:HB2	2.19	0.43
1:A:1050:GLN:H	1:A:1245:GLY:HA3	1.84	0.42
1:A:1037:VAL:HG22	1:A:1051:GLY:H	1.83	0.42
1:A:1253:HIS:ND1	1:A:1263:TYR:OH	2.38	0.42
1:A:1186:LEU:HA	1:A:1190:PRO:HD3	2.01	0.42
1:A:957:ALA:HA	1:A:961:THR:OG1	2.19	0.42
1:A:1154:ILE:O	1:A:1160:LYS:HA	2.19	0.42
1:A:806:THR:HG23	1:A:809:ALA:H	1.84	0.42
1:A:908:ARG:HA	1:A:908:ARG:HD3	1.80	0.42
1:A:1181:ALA:HA	1:A:1184:ARG:HG2	2.02	0.42
1:A:1137:SER:HB2	1:A:1140:GLU:HB2	2.02	0.41
1:A:38:MET:SD	1:A:355:ARG:HG2	2.60	0.41
1:A:40:ARG:NH1	1:A:366:ASP:OD1	2.47	0.41
1:A:476:PHE:HB3	1:A:895:GLU:OE2	2.20	0.41
1:A:1028:GLU:HB2	1:A:1058:LYS:HD2	2.02	0.41
1:A:930:LYS:HZ3	1:A:930:LYS:HB3	1.85	0.41
1:A:1150:ILE:HB	1:A:1179:ARG:HB3	2.03	0.41
1:A:1154:ILE:HA	1:A:1157:LEU:HD12	2.03	0.41
1:A:705:PRO:C	1:A:707:PHE:H	2.23	0.41
1:A:794:ARG:HB2	1:A:1017:TYR:CE2	2.55	0.41
1:A:1130:GLY:HA3	1:A:1184:ARG:O	2.21	0.41
1:A:594:ILE:O	1:A:605:GLN:HA	2.20	0.41
1:A:235:PHE:O	1:A:287:LYS:NZ	2.51	0.41
1:A:1053:SER:O	1:A:1054:LEU:HD13	2.21	0.41
1:A:727:ILE:O	1:A:731:VAL:HG23	2.21	0.41
1:A:779:ILE:H	1:A:779:ILE:HG12	1.76	0.41
1:A:1144:ALA:CB	1:A:1187:VAL:HG23	2.51	0.41
1:A:239:GLU:HB2	1:A:287:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD12	1:A:300:LEU:HA	1.94	0.41
1:A:706:TYR:O	1:A:772:THR:HB	2.21	0.40
1:A:1150:ILE:HD13	1:A:1179:ARG:HH11	1.86	0.40
1:A:970:VAL:HG12	1:A:974:PHE:CE2	2.56	0.40

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

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	PHE
1	A	260	VAL
1	A	270	LEU
1	A	372	ASP
1	A	413	VAL
1	A	518	THR
1	A	593	VAL
1	A	872	MET
1	A	1032	GLN
1	A	1155	ASP
1	A	1172	LEU
1	A	1182	ILE

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

All (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
2	A	1302	4C8	BR2-CAF	2.04	1.94	1.89
2	A	1301	4C8	BR5-CAN	2.04	1.94	1.90
2	A	1302	4C8	BR4-CAP	2.02	1.94	1.89
2	A	1301	4C8	BR4-CAP	2.01	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.

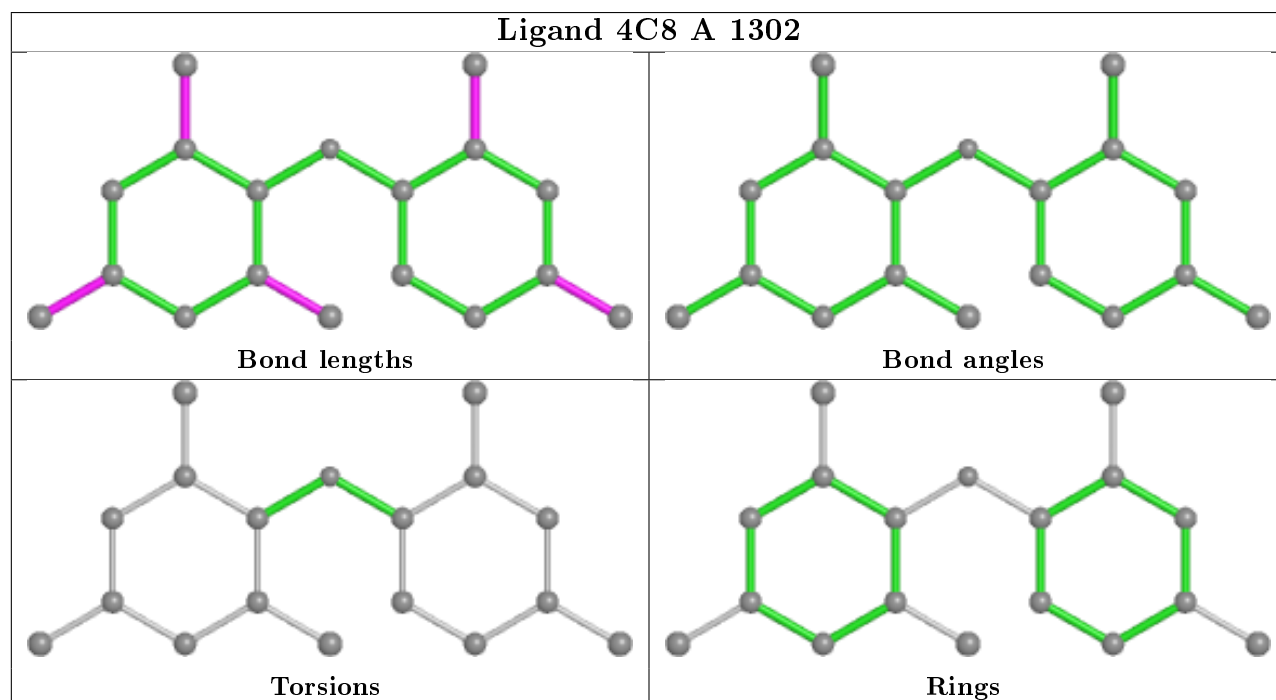
There are no ring outliers.

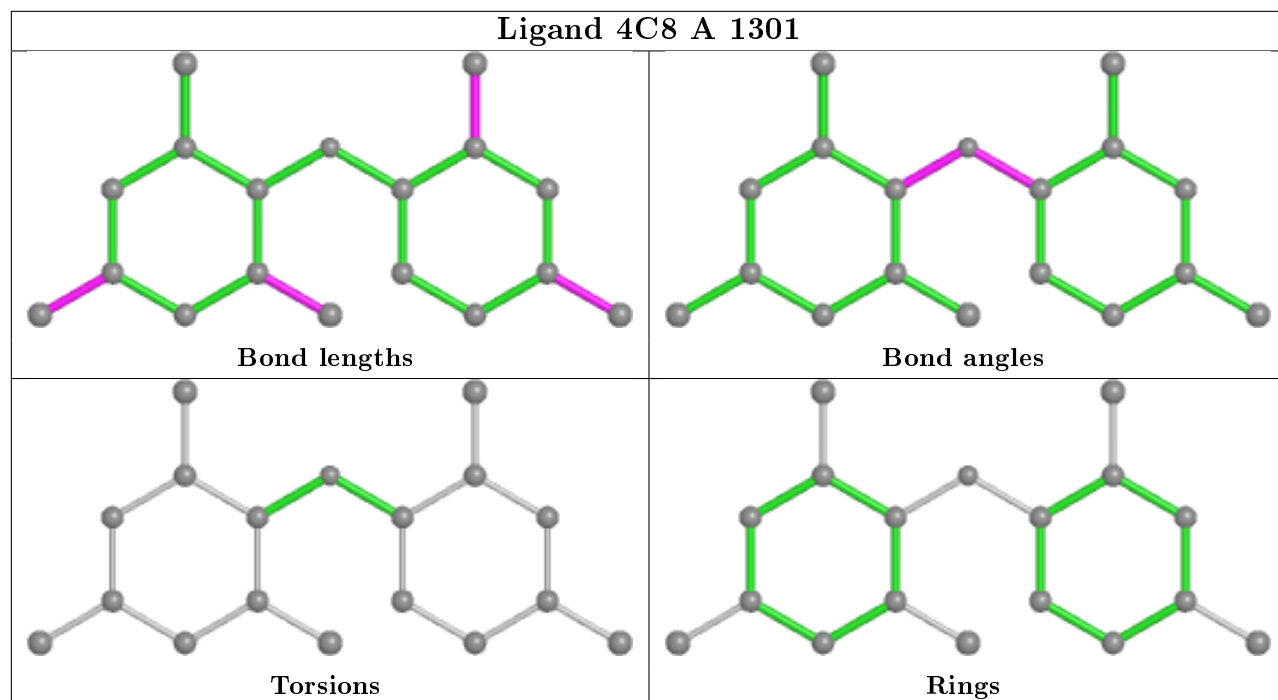
2 monomers are involved in 2 short contacts:

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

### 6.1 Protein, DNA and RNA chains

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	1182/1282 (92%)	-0.44	25 (2%) 63 54	147, 205, 276, 327	0

All (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
1	A	88	SER	4.0
1	A	95	ASP	3.9
1	A	230	LYS	3.9
1	A	234	SER	3.7
1	A	236	THR	3.3
1	A	522	GLU	3.3
1	A	82	GLY	3.2
1	A	231	ILE	3.1
1	A	523	ARG	3.0
1	A	81	VAL	2.9
1	A	89	THR	2.9
1	A	90	GLN	2.9
1	A	99	MET	2.7
1	A	80	SER	2.6
1	A	237	ASP	2.6
1	A	526	GLN	2.5
1	A	226	GLY	2.5
1	A	86	LYS	2.3
1	A	233	SER	2.2
1	A	98	ALA	2.1



## 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](#)

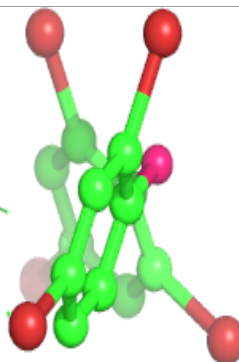
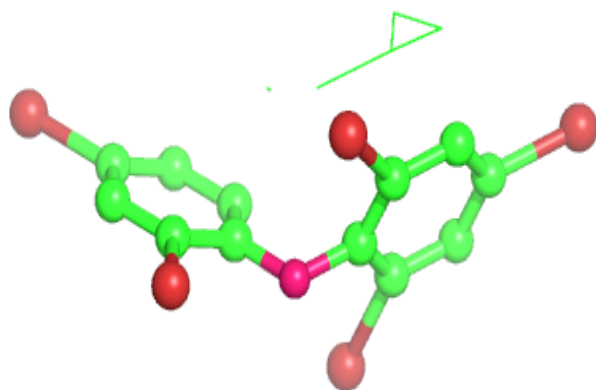
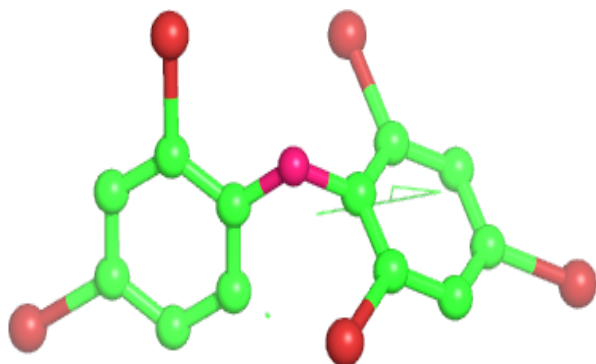
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	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

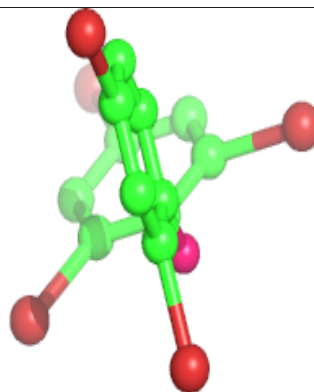
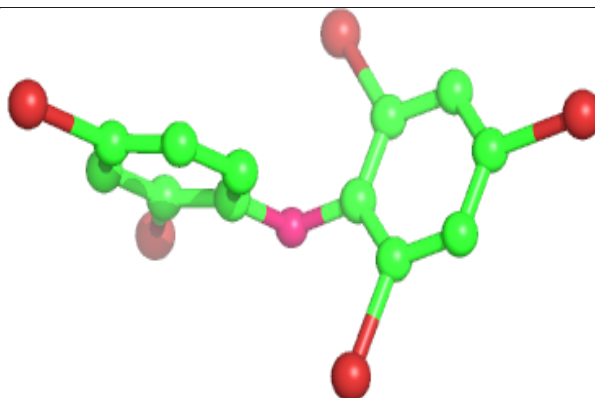
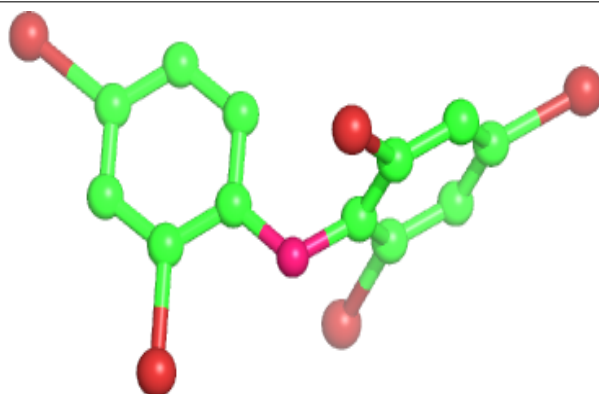
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 4C8 A 1302:**

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

**Electron density around 4C8 A 1301:**

$2mF_o-DF_c$  (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.