



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:07 AM BST

PDB ID : 6UJN
Title : P-glycoprotein mutant-C952A-with BDE100
Authors : Aller, S.G.; Le, C.A.
Deposited on : 2019-10-03
Resolution : 3.98 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

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

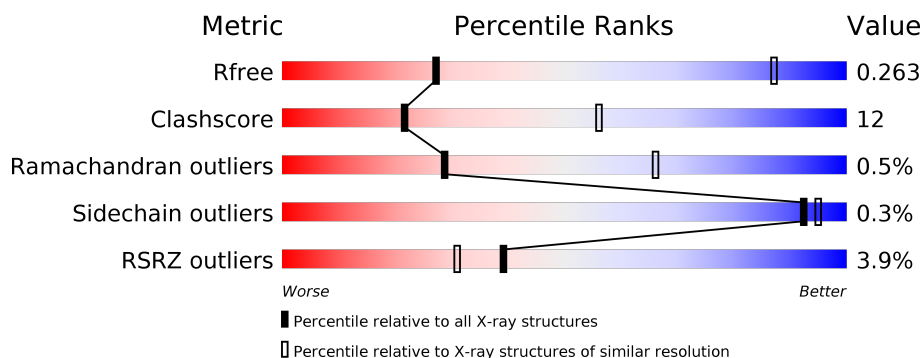
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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>4%</div> <div>68%</div> <div>24%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9181 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.

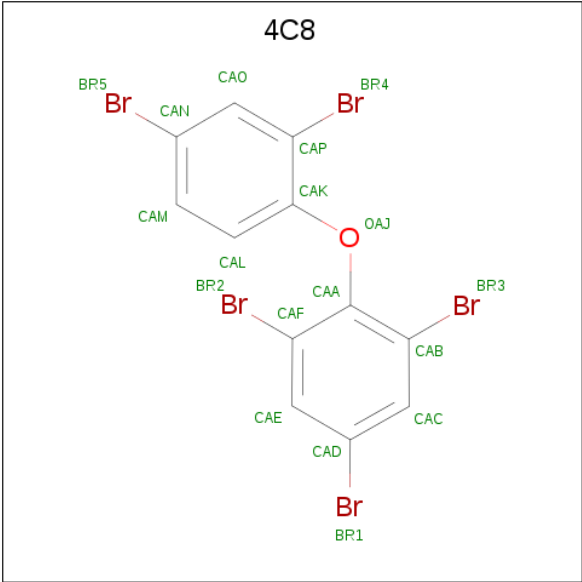
- Molecule 1 is a protein called ATP-dependent translocase ABCB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9163	5893	1553	1680	37			

There are 10 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	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).



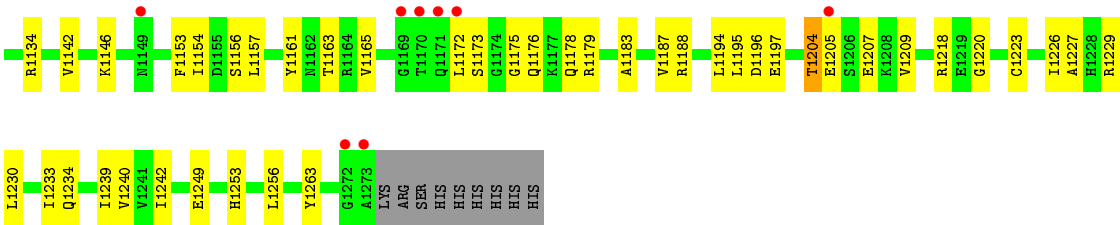
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
2	A	1	18	5	12	1	0	0

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: 68% 24% 8% 4%

The sequence logo displays the conservation of amino acid residues across 100 positions. The residues are listed on the y-axis, and the positions are numbered 1 to 100 on the x-axis. The conservation is indicated by the height of the colored bars, with a color scale from green (68%) to red (4%).

Position	Residue	Conservation (%)
1	GLU	68
2	GLU	68
3	GLU	68
4	GLU	68
5	GLU	68
6	GLU	68
7	GLU	68
8	GLU	68
9	GLU	68
10	GLU	68
11	GLU	68
12	GLU	68
13	GLU	68
14	GLU	68
15	GLU	68
16	GLU	68
17	GLU	68
18	GLU	68
19	GLU	68
20	GLU	68
21	GLU	68
22	GLU	68
23	GLU	68
24	GLU	68
25	GLU	68
26	GLU	68
27	GLU	68
28	GLU	68
29	GLU	68
30	GLU	68
31	GLU	24
32	GLU	24
33	GLU	24
34	GLU	24
35	GLU	24
36	GLU	24
37	GLU	24
38	GLU	24
39	GLU	24
40	GLU	24
41	GLU	24
42	GLU	24
43	GLU	24
44	GLU	24
45	GLU	24
46	GLU	24
47	GLU	24
48	GLU	24
49	GLU	24
50	GLU	24
51	GLU	24
52	GLU	24
53	GLU	24
54	GLU	24
55	GLU	24
56	GLU	24
57	GLU	24
58	GLU	24
59	GLU	24
60	GLU	24
61	GLU	68
62	GLU	68
63	GLU	68
64	GLU	68
65	GLU	68
66	GLU	68
67	GLU	68
68	GLU	68
69	GLU	68
70	GLU	68
71	GLU	68
72	GLU	68
73	GLU	68
74	GLU	68
75	GLU	68
76	GLU	68
77	GLU	68
78	GLU	68
79	GLU	68
80	GLU	68
81	GLU	68
82	GLU	68
83	GLU	68
84	GLU	68
85	GLU	68
86	GLU	68
87	GLU	68
88	GLU	68
89	GLU	68
90	GLU	68
91	GLU	68
92	GLU	68
93	GLU	68
94	GLU	68
95	GLU	68
96	GLU	68
97	GLU	68
98	GLU	68
99	GLU	68
100	GLU	68



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.57Å 137.54Å 184.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.98 29.95 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-3.98) 88.3 (29.95-3.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 3.75Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.243 , 0.264 0.243 , 0.263	Depositor DCC
R_{free} test set	1997 reflections (8.52%)	wwPDB-VP
Wilson B-factor (Å ²)	165.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 95.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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	0.27	0/9332	0.46	0/12614

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 [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	9163	0	9350	220	0
2	A	18	0	0	1	0
All	All	9181	0	9350	220	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.

All (220) 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:281:LYS:HD2	1:A:779:ILE:HG22	1.61	0.82
1:A:160:ASP:OD2	1:A:440:TYR:OH	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HD11	1:A:904:VAL:HG11	1.60	0.80
1:A:160:ASP:OD1	1:A:901:ARG:NH2	2.15	0.79
1:A:239:GLU:HB2	1:A:287:LYS:HZ2	1.46	0.78
1:A:170:ARG:HG3	1:A:174:ASP:OD2	1.83	0.78
1:A:307:ALA:HB2	1:A:755:PHE:HE2	1.49	0.78
1:A:235:PHE:HB3	1:A:287:LYS:HE2	1.65	0.78
1:A:1092:LEU:HG	1:A:1093:ASP:H	1.49	0.76
1:A:1064:LEU:HB3	1:A:1226:ILE:HG22	1.69	0.75
1:A:278:GLU:OE2	1:A:782:LYS:NZ	2.14	0.72
1:A:42:ALA:HB2	1:A:139:GLN:NE2	2.06	0.70
1:A:1054:LEU:HD11	1:A:1240:VAL:HG11	1.73	0.70
1:A:720:LEU:HD21	1:A:761:ILE:HG23	1.73	0.69
1:A:817:ASP:HA	1:A:1000:SER:HB3	1.74	0.69
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.77	0.67
1:A:486:TYR:HE1	1:A:911:LYS:HE2	1.60	0.66
1:A:1207:GLU:OE1	1:A:1229:ARG:NH2	2.29	0.65
1:A:239:GLU:HB2	1:A:287:LYS:NZ	2.11	0.65
1:A:257:ILE:HG12	1:A:800:PHE:CE2	2.32	0.64
1:A:38:MET:HA	1:A:362:PHE:HE2	1.62	0.64
1:A:395:PHE:HZ	1:A:440:TYR:CD2	2.15	0.64
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.79	0.64
1:A:307:ALA:HB2	1:A:755:PHE:CE2	2.31	0.63
1:A:388:LEU:HD11	1:A:547:ILE:HD12	1.80	0.63
1:A:213:VAL:HG21	1:A:312:TYR:HE2	1.64	0.61
1:A:421:LEU:HB2	1:A:581:ILE:HG13	1.81	0.61
1:A:94:ALA:HA	1:A:97:ARG:HE	1.65	0.61
1:A:1249:GLU:HG2	1:A:1256:LEU:HD22	1.81	0.61
1:A:65:PRO:HB2	1:A:202:ILE:HD12	1.82	0.61
1:A:257:ILE:HG21	1:A:800:PHE:HD2	1.65	0.60
1:A:954:ARG:HH21	1:A:958:TYR:HB2	1.66	0.60
1:A:42:ALA:HB2	1:A:139:GLN:HE21	1.66	0.60
1:A:237:ASP:O	1:A:241:HIS:ND1	2.30	0.60
1:A:256:ALA:HB2	1:A:1117:ILE:HG12	1.82	0.60
1:A:963:GLN:HG2	1:A:964:LEU:H	1.67	0.60
1:A:1157:LEU:HD22	1:A:1163:THR:HG21	1.84	0.59
1:A:1172:LEU:HD13	1:A:1176:GLN:HB2	1.84	0.59
1:A:1070:CYS:O	1:A:1074:THR:N	2.27	0.59
1:A:900:PHE:HA	1:A:903:VAL:HG12	1.83	0.59
1:A:1196:ASP:OD1	1:A:1226:ILE:HD11	2.03	0.58
1:A:390:PHE:HE2	1:A:432:THR:HB	1.67	0.58
1:A:437:GLN:HB2	1:A:439:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ALA:HB2	1:A:534:ARG:HB3	1.86	0.57
1:A:1082:PHE:C	1:A:1083:TYR:HD1	2.07	0.57
1:A:258:ARG:NH2	1:A:801:ASP:OD1	2.36	0.57
1:A:1123:ILE:HD11	1:A:1161:TYR:HA	1.87	0.57
1:A:762:SER:HA	1:A:765:THR:HG22	1.87	0.57
1:A:409:LEU:HD21	1:A:597:PHE:HE1	1.70	0.57
1:A:206:ARG:HH11	1:A:326:GLN:HG2	1.70	0.56
1:A:324:ILE:HD13	1:A:735:PHE:HD2	1.69	0.56
1:A:512:LEU:HD12	1:A:513:PRO:HD2	1.86	0.56
1:A:147:PHE:CD1	1:A:361:VAL:HG13	2.41	0.56
1:A:1001:ALA:HA	1:A:1004:ILE:HG22	1.86	0.55
1:A:508:PHE:HE2	1:A:531:GLN:HB3	1.71	0.55
1:A:471:GLN:HB2	1:A:552:GLU:HB2	1.89	0.55
1:A:997:ALA:O	1:A:1001:ALA:N	2.38	0.55
1:A:419:VAL:HG23	1:A:593:VAL:HG23	1.88	0.55
1:A:1107:ALA:HA	1:A:1188:ARG:NH1	2.22	0.55
1:A:35:VAL:HG13	1:A:36:LEU:HD12	1.89	0.54
1:A:121:VAL:HA	1:A:124:VAL:HG22	1.89	0.54
1:A:794:ARG:NH1	1:A:1017:TYR:HB2	2.22	0.54
1:A:324:ILE:HD13	1:A:735:PHE:CD2	2.44	0.53
1:A:1092:LEU:HD22	1:A:1097:ILE:HG22	1.91	0.53
1:A:488:ARG:HA	1:A:908:ARG:HH11	1.74	0.53
1:A:151:ILE:HD12	1:A:167:LEU:HD21	1.91	0.53
1:A:711:ILE:HD12	1:A:833:PHE:HD2	1.74	0.53
1:A:1153:PHE:CE2	1:A:1176:GLN:HG2	2.44	0.52
1:A:696:ILE:HG23	1:A:697:LEU:HD12	1.92	0.52
1:A:147:PHE:O	1:A:151:ILE:HG12	2.09	0.52
1:A:439:LEU:C	1:A:440:TYR:HD1	2.13	0.52
1:A:1173:SER:OG	1:A:1176:GLN:OE1	2.16	0.52
1:A:189:PHE:CE1	1:A:348:ILE:HD11	2.45	0.52
1:A:217:ILE:HD12	1:A:305:SER:HB3	1.91	0.52
1:A:479:THR:HA	1:A:518:THR:O	2.09	0.51
1:A:573:ARG:C	1:A:575:GLY:H	2.14	0.51
1:A:856:LEU:HD22	1:A:955:PHE:CD2	2.46	0.51
1:A:1061:THR:HG21	1:A:1218:ARG:NH1	2.25	0.51
1:A:466:ILE:HG12	1:A:547:ILE:HB	1.93	0.51
1:A:573:ARG:O	1:A:575:GLY:N	2.39	0.51
1:A:1090:VAL:C	1:A:1091:PHE:HD1	2.14	0.51
1:A:257:ILE:HG12	1:A:800:PHE:CD2	2.45	0.51
1:A:1024:PRO:HD2	1:A:1104:TRP:CZ3	2.45	0.51
1:A:1037:VAL:HG22	1:A:1050:GLN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HG22	1:A:144:ARG:NH1	2.26	0.50
1:A:1091:PHE:N	1:A:1091:PHE:HD1	2.09	0.50
1:A:530:GLY:N	1:A:557:LEU:HD11	2.27	0.50
1:A:829:LEU:HA	1:A:832:ILE:HG22	1.94	0.50
1:A:728:PHE:HB2	2:A:1301:4C8:CAL	2.42	0.50
1:A:488:ARG:HE	1:A:542:VAL:HG12	1.77	0.50
1:A:719:GLY:HA2	1:A:841:THR:OG1	2.11	0.49
1:A:1091:PHE:N	1:A:1091:PHE:CD1	2.79	0.49
1:A:1153:PHE:O	1:A:1156:SER:N	2.46	0.49
1:A:200:PHE:HE1	1:A:215:LEU:HD11	1.77	0.49
1:A:853:LEU:HD23	1:A:955:PHE:HB3	1.95	0.49
1:A:894:THR:O	1:A:898:GLU:HG2	2.13	0.49
1:A:388:LEU:HB2	1:A:413:VAL:CG1	2.43	0.48
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.94	0.48
1:A:856:LEU:HD22	1:A:955:PHE:HD2	1.78	0.48
1:A:1112:VAL:HB	1:A:1195:LEU:HD13	1.94	0.48
1:A:481:ALA:O	1:A:485:ARG:HB2	2.13	0.48
1:A:417:GLN:HA	1:A:592:ASP:OD2	2.13	0.48
1:A:832:ILE:HG13	1:A:987:VAL:HG22	1.96	0.48
1:A:1197:GLU:HA	1:A:1227:ALA:HA	1.96	0.48
1:A:140:ILE:HG22	1:A:144:ARG:HH11	1.79	0.48
1:A:550:LEU:HB2	1:A:580:VAL:HG23	1.96	0.48
1:A:1153:PHE:CD2	1:A:1176:GLN:HG2	2.49	0.47
1:A:390:PHE:HB3	1:A:393:ILE:HD12	1.96	0.47
1:A:806:THR:HG23	1:A:809:ALA:H	1.79	0.47
1:A:1032:GLN:HB2	1:A:1091:PHE:HB2	1.95	0.47
1:A:384:ILE:HG23	1:A:450:ASP:OD2	2.15	0.47
1:A:40:ARG:HD2	1:A:41:TYR:CZ	2.49	0.47
1:A:589:ARG:NH1	1:A:608:HIS:CD2	2.82	0.47
1:A:1183:ALA:O	1:A:1187:VAL:HG23	2.15	0.47
1:A:257:ILE:HA	1:A:260:VAL:HG12	1.97	0.47
1:A:534:ARG:HG3	1:A:565:VAL:HG22	1.96	0.47
1:A:477:ALA:HA	1:A:520:VAL:O	2.15	0.47
1:A:846:SER:HB3	1:A:973:VAL:HG13	1.96	0.47
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.47	0.47
1:A:528:SER:HB3	1:A:531:GLN:HG3	1.97	0.47
1:A:785:ARG:HE	1:A:818:ALA:HB3	1.80	0.47
1:A:1092:LEU:HD21	1:A:1100:LEU:HD22	1.97	0.46
1:A:558:ASP:OD1	1:A:561:SER:HB3	2.15	0.46
1:A:1028:GLU:HB2	1:A:1058:LYS:HD2	1.96	0.46
1:A:221:LEU:HD22	1:A:302:ILE:HG12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:GLN:HB3	1:A:997:ALA:HA	1.98	0.46
1:A:938:PHE:O	1:A:942:GLN:HG2	2.16	0.46
1:A:1131:ASP:OD2	1:A:1134:ARG:NH1	2.44	0.46
1:A:1142:VAL:HG22	1:A:1161:TYR:CZ	2.50	0.46
1:A:296:GLY:HA3	1:A:763:PHE:HD1	1.80	0.46
1:A:438:ARG:NH1	1:A:455:ARG:HA	2.30	0.46
1:A:76:ASP:HA	1:A:79:ALA:HB3	1.97	0.46
1:A:955:PHE:O	1:A:960:VAL:HB	2.16	0.46
1:A:114:TYR:HE2	1:A:953:PHE:HD2	1.62	0.46
1:A:833:PHE:HA	1:A:836:ILE:HG12	1.97	0.46
1:A:200:PHE:CE1	1:A:215:LEU:HD11	2.51	0.46
1:A:843:ILE:HD11	1:A:858:LEU:HD21	1.97	0.45
1:A:1021:GLY:HA3	1:A:1101:ASN:HB2	1.99	0.45
1:A:1061:THR:HA	1:A:1223:CYS:HB3	1.97	0.45
1:A:228:TRP:CZ2	1:A:295:MET:HG2	2.52	0.45
1:A:395:PHE:HZ	1:A:440:TYR:HD2	1.58	0.45
1:A:1083:TYR:N	1:A:1083:TYR:CD1	2.85	0.45
1:A:1083:TYR:HD1	1:A:1083:TYR:N	2.15	0.45
1:A:126:TYR:OH	1:A:932:HIS:ND1	2.39	0.45
1:A:237:ASP:C	1:A:241:HIS:HD1	2.18	0.45
1:A:505:ALA:HB1	1:A:508:PHE:HE1	1.82	0.45
1:A:824:ALA:HA	1:A:828:ARG:HD3	1.99	0.45
1:A:64:LEU:HD12	1:A:336:ILE:HG21	1.99	0.45
1:A:414:LYS:HB3	1:A:417:GLN:CD	2.38	0.45
1:A:360:GLU:O	1:A:364:ILE:HG12	2.17	0.44
1:A:725:SER:HB3	1:A:975:SER:OG	2.17	0.44
1:A:113:TYR:O	1:A:117:ILE:HG12	2.17	0.44
1:A:607:ASN:OD1	1:A:608:HIS:N	2.46	0.44
1:A:1234:GLN:HG2	1:A:1253:HIS:CE1	2.52	0.44
1:A:1120:ASP:HA	1:A:1165:VAL:O	2.17	0.44
1:A:799:TRP:CE3	1:A:800:PHE:HE1	2.35	0.44
1:A:799:TRP:HE3	1:A:800:PHE:HE1	1.66	0.44
1:A:1092:LEU:HG	1:A:1093:ASP:N	2.26	0.44
1:A:840:GLY:O	1:A:843:ILE:HG22	2.18	0.44
1:A:864:ILE:HG22	1:A:944:MET:HB3	2.00	0.44
1:A:102:LYS:HE2	1:A:105:GLU:OE2	2.17	0.44
1:A:1096:GLU:HG2	1:A:1098:LYS:H	1.83	0.44
1:A:151:ILE:HD12	1:A:167:LEU:HD11	1.99	0.43
1:A:801:ASP:OD2	1:A:1083:TYR:OH	2.30	0.43
1:A:805:ASN:HB3	1:A:810:LEU:HD21	2.00	0.43
1:A:1116:PRO:HG3	1:A:1178:GLN:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:LEU:O	1:A:860:ILE:HG12	2.18	0.43
1:A:168:ASN:ND2	1:A:894:THR:OG1	2.44	0.43
1:A:1123:ILE:HD13	1:A:1154:ILE:HD12	2.00	0.43
1:A:121:VAL:HG11	1:A:946:TYR:HE2	1.83	0.43
1:A:270:LEU:HD21	1:A:786:TYR:CE1	2.53	0.43
1:A:243:TYR:CD1	1:A:785:ARG:NH1	2.87	0.43
1:A:1016:SER:OG	1:A:1103:GLN:OE1	2.37	0.43
1:A:372:ASP:OD2	1:A:375:SER:HB3	2.18	0.43
1:A:703:GLU:HG2	1:A:779:ILE:HD11	2.01	0.43
1:A:144:ARG:HD3	1:A:920:LEU:HD22	2.01	0.43
1:A:1037:VAL:HG22	1:A:1051:GLY:H	1.84	0.42
1:A:1107:ALA:HA	1:A:1188:ARG:HH11	1.83	0.42
1:A:1131:ASP:OD2	1:A:1134:ARG:HD3	2.19	0.42
1:A:1124:ALA:HB2	1:A:1161:TYR:HB3	2.00	0.42
1:A:799:TRP:HE3	1:A:800:PHE:CE1	2.37	0.42
1:A:839:LEU:O	1:A:843:ILE:N	2.50	0.42
1:A:121:VAL:HG11	1:A:946:TYR:CE2	2.53	0.42
1:A:1239:ILE:HG21	1:A:1263:TYR:CE1	2.55	0.42
1:A:963:GLN:HG2	1:A:964:LEU:N	2.34	0.42
1:A:1218:ARG:C	1:A:1220:GLY:H	2.21	0.42
1:A:400:ARG:HG2	1:A:401:LYS:H	1.85	0.42
1:A:916:TYR:CE2	1:A:920:LEU:HD11	2.55	0.42
1:A:1230:LEU:O	1:A:1233:ILE:HG22	2.20	0.42
1:A:171:LEU:HD21	1:A:916:TYR:OH	2.19	0.42
1:A:730:LYS:O	1:A:734:VAL:HG12	2.19	0.42
1:A:764:ILE:O	1:A:768:LEU:HD13	2.19	0.42
1:A:395:PHE:HD1	1:A:442:PRO:HA	1.85	0.42
1:A:1175:GLY:O	1:A:1179:ARG:HG3	2.19	0.42
1:A:211:THR:HG22	1:A:334:VAL:HG21	2.01	0.42
1:A:400:ARG:HG2	1:A:401:LYS:N	2.35	0.42
1:A:904:VAL:HG23	1:A:909:GLU:OE2	2.20	0.42
1:A:1092:LEU:CG	1:A:1093:ASP:H	2.26	0.41
1:A:296:GLY:HA3	1:A:763:PHE:CD1	2.55	0.41
1:A:892:ILE:HD11	1:A:916:TYR:HA	2.02	0.41
1:A:74:MET:HG2	1:A:110:TYR:CD2	2.55	0.41
1:A:156:ILE:HG13	1:A:439:LEU:HD22	2.02	0.41
1:A:433:VAL:HG13	1:A:549:LEU:HD13	2.03	0.41
1:A:453:ASP:OD1	1:A:454:ILE:N	2.54	0.41
1:A:1002:SER:O	1:A:1006:ARG:HG2	2.20	0.41
1:A:1153:PHE:HA	1:A:1156:SER:HB3	2.03	0.41
1:A:1179:ARG:HH21	1:A:1209:VAL:HG11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:LEU:HD11	1:A:1242:ILE:HD11	2.02	0.41
1:A:235:PHE:CD1	1:A:238:LYS:HD2	2.56	0.41
1:A:1063:ALA:HB3	1:A:1239:ILE:HG13	2.02	0.41
1:A:440:TYR:CD1	1:A:440:TYR:N	2.87	0.41
1:A:711:ILE:HD12	1:A:833:PHE:CD2	2.55	0.41
1:A:721:GLN:HG2	1:A:979:PHE:HE2	1.85	0.41
1:A:758:LEU:HA	1:A:761:ILE:HG22	2.03	0.41
1:A:1154:ILE:HG21	1:A:1161:TYR:CE1	2.56	0.40
1:A:1142:VAL:O	1:A:1146:LYS:HG2	2.20	0.40
1:A:604:GLU:HG2	1:A:611:LEU:HG	2.03	0.40
1:A:160:ASP:OD2	1:A:440:TYR:CZ	2.75	0.40
1:A:178:ILE:HD11	1:A:358:ALA:HA	2.04	0.40
1:A:512:LEU:HD21	1:A:518:THR:HG21	2.03	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%)	1114 (95%)	58 (5%)	6 (0%)	29 66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	ASN
1	A	574	GLU
1	A	1204	THR
1	A	398	PRO
1	A	705	PRO
1	A	44	TRP

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	972/1062 (92%)	969 (100%)	3 (0%)	92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	440	TYR
1	A	1083	TYR
1	A	1091	PHE

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

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](#)

1 ligand is 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	1301	-	19,19,19	1.06	1 (5%)	27,27,27	0.97	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	1301	-	-	0/4/4/4	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	4C8	BR3-CAB	2.14	1.94	1.89

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	4C8	BR2-CAF-CAA	2.32	121.89	118.51

There are no chirality outliers.

There are no torsion outliers.

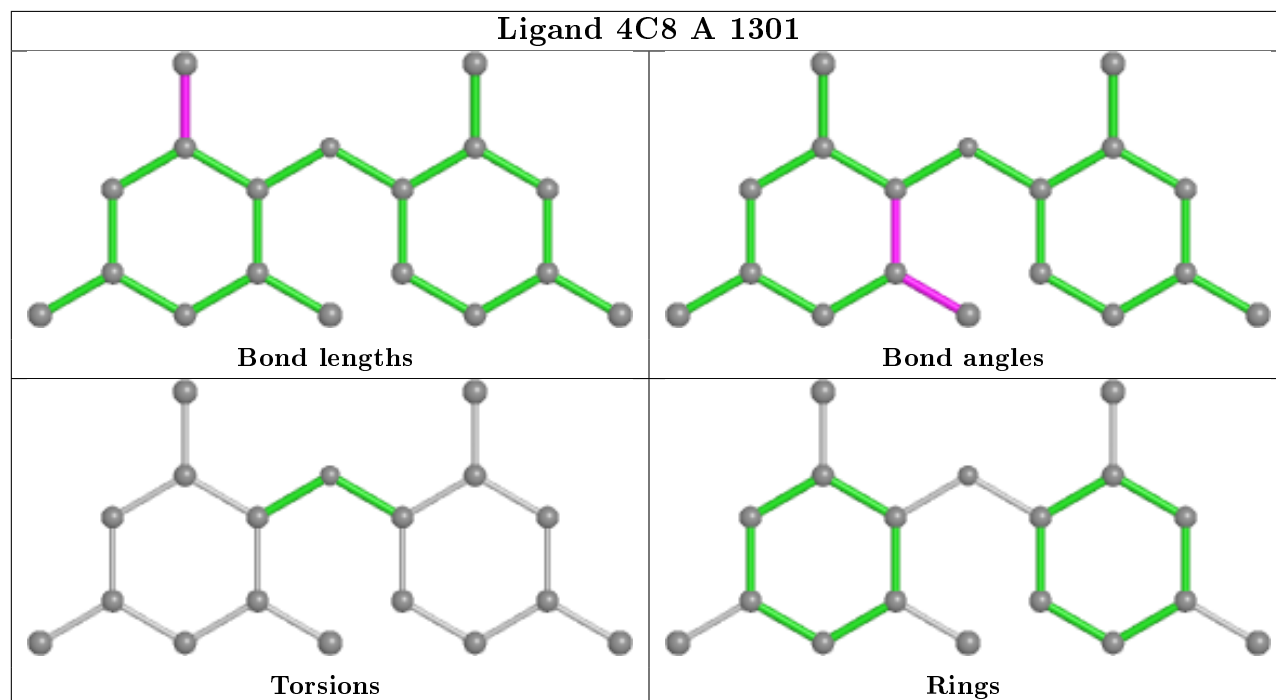
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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, 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%)	-0.16	46 (3%)	39 31	130, 186, 248, 298	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	GLN	7.7
1	A	692	SER	6.4
1	A	88	SER	5.3
1	A	226	GLY	5.1
1	A	704	TRP	4.8
1	A	229	ALA	4.8
1	A	89	THR	4.7
1	A	85	SER	4.5
1	A	98	ALA	4.0
1	A	507	ASP	3.8
1	A	1172	LEU	3.6
1	A	506	TYR	3.4
1	A	1149	ASN	3.3
1	A	1273	ALA	3.3
1	A	691	ALA	3.3
1	A	99	MET	3.2
1	A	322	TYR	3.1
1	A	623	MET	3.0
1	A	1171	GLN	3.0
1	A	95	ASP	3.0
1	A	93	GLU	2.9
1	A	91	MET	2.9
1	A	244	ALA	2.8
1	A	227	ILE	2.6
1	A	1272	GLY	2.6
1	A	97	ARG	2.6
1	A	321	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	690	PRO	2.5
1	A	523	ARG	2.4
1	A	209	LYS	2.4
1	A	1170	THR	2.3
1	A	405	ILE	2.3
1	A	84	VAL	2.3
1	A	1205	GLU	2.3
1	A	233	SER	2.3
1	A	225	ALA	2.3
1	A	964	LEU	2.3
1	A	230	LYS	2.2
1	A	1023	LYS	2.2
1	A	1169	GLY	2.1
1	A	955	PHE	2.1
1	A	959	LEU	2.1
1	A	87	GLN	2.1
1	A	228	TRP	2.1
1	A	133	CYS	2.1
1	A	705	PRO	2.0

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.

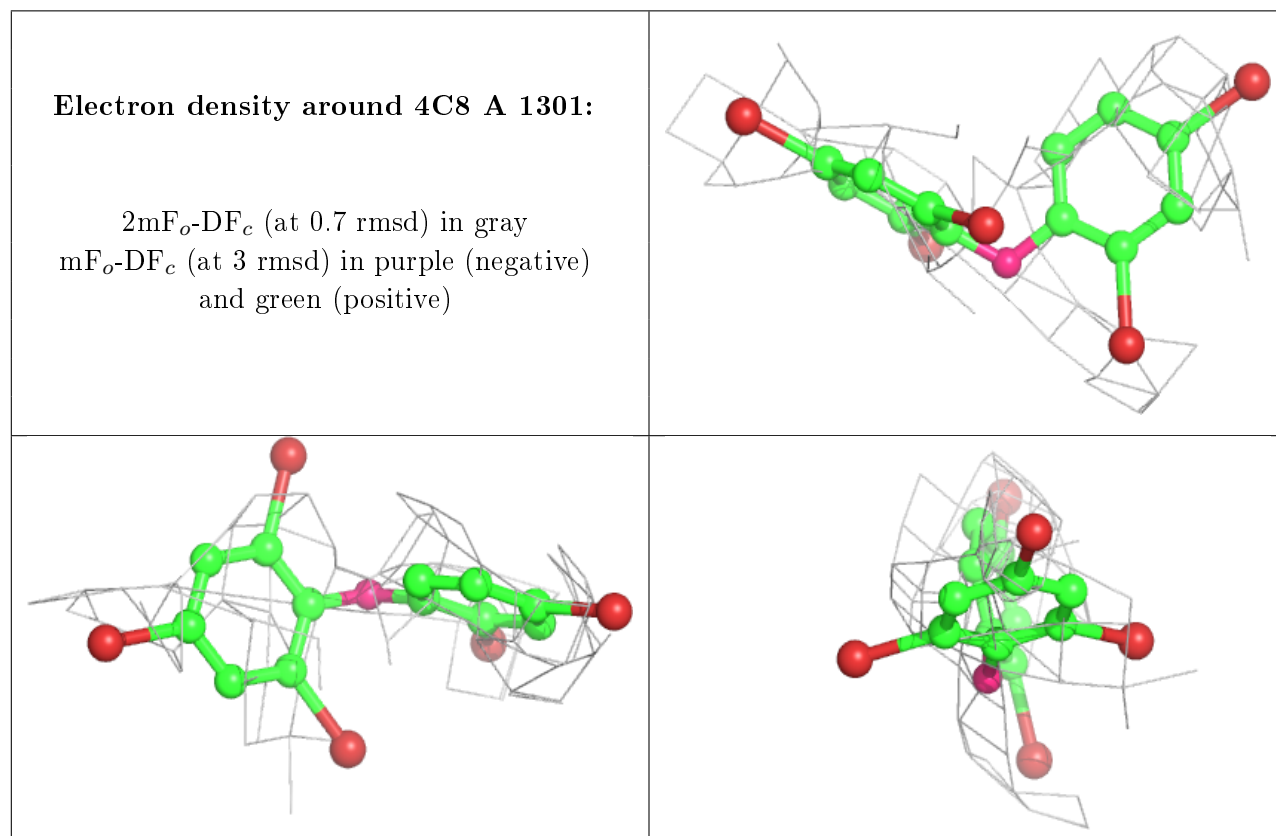
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	4C8	A	1301	18/18	0.78	0.28	192,205,226,237	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.