



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2023 – 01:42 pm BST

PDB ID : 8OG6
Title : Crystal structure of human DCAF1 WD40 repeats (Q1250L) in complex with compound 1
Authors : Schroeder, M.; Vulpetti, A.; Renatus, M.
Deposited on : 2023-03-19
Resolution : 2.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

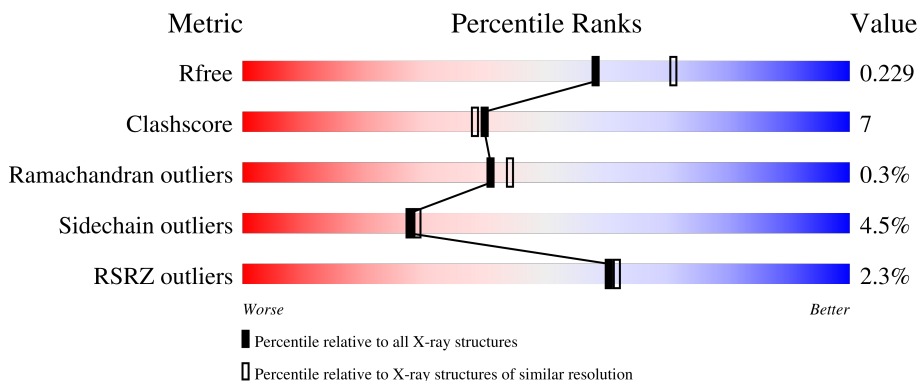
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	367	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5007 atoms, of which 2350 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.

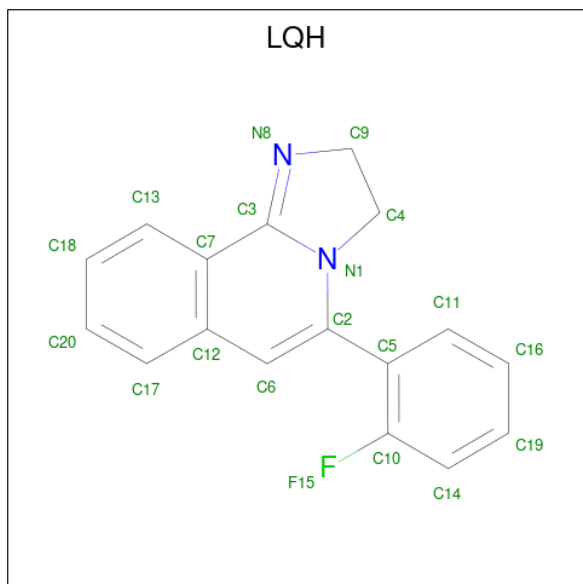
- Molecule 1 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	301	4763	1531	2347	413	454	18	87	4	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1035	GLY	-	expression tag	UNP Q9Y4B6
A	1036	GLY	-	expression tag	UNP Q9Y4B6
A	1037	GLY	-	expression tag	UNP Q9Y4B6
A	1038	ARG	-	expression tag	UNP Q9Y4B6
A	1250	LEU	GLN	engineered mutation	UNP Q9Y4B6

- Molecule 2 is 5-(2-fluorophenyl)-2,3-dihydroimidazo[2,1-a]isoquinoline (three-letter code: LQH) (formula: C₁₇H₁₃FN₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			20	17	1	2		
2	A	1	Total	C	F	N	0	0
			20	17	1	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	197	Total	O	0	0
			197	197		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.23Å 82.23Å 237.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.68 – 2.25 45.63 – 2.24	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.68-2.25) 100.0 (45.63-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.231 0.207 , 0.229	Depositor DCC
R_{free} test set	1139 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtrriage
Anisotropy	0.355	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5007	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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: LQH, ACT

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	1.20	17/2478 (0.7%)	1.15	4/3359 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1203	TYR	CG-CD1	10.27	1.52	1.39
1	A	1203	TYR	CE2-CZ	7.91	1.48	1.38
1	A	1247	ARG	C-O	7.73	1.38	1.23
1	A	1185	SER	CB-OG	7.44	1.51	1.42
1	A	1094	SER	C-O	7.15	1.36	1.23
1	A	1208	GLY	C-O	6.34	1.33	1.23
1	A	1289	HIS	C-O	6.34	1.35	1.23
1	A	1235	ASP	C-O	6.24	1.35	1.23
1	A	1386	LEU	C-O	5.97	1.34	1.23
1	A	1187	HIS	C-O	5.87	1.34	1.23
1	A	1203	TYR	CG-CD2	5.82	1.46	1.39
1	A	1095	GLY	C-O	5.78	1.32	1.23
1	A	1374	SER	C-O	5.75	1.34	1.23
1	A	1144	SER	C-O	5.71	1.34	1.23
1	A	1244	TRP	C-O	5.26	1.33	1.23
1	A	1203	TYR	CE1-CZ	5.21	1.45	1.38
1	A	1177	THR	C-O	5.20	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1245	ASP	CB-CG-OD1	-6.77	112.20	118.30
1	A	1247	ARG	CB-CA-C	-6.70	97.01	110.40
1	A	1203	TYR	CB-CG-CD1	-6.41	117.16	121.00
1	A	1385	ARG	O-C-N	5.11	130.88	122.70

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	2416	2347	2331	32	0
2	A	40	0	0	5	0
3	A	4	3	3	0	0
4	A	197	0	0	2	2
All	All	2657	2350	2334	35	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (35) 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:1117[B]:LEU:HD12	1:A:1133:CYS:SG	2.12	0.89
1:A:1117[B]:LEU:HD11	1:A:1152:THR:HG21	1.57	0.85
1:A:1156:TRP:O	1:A:1156:TRP:CE3	2.34	0.81
1:A:1314:GLN:HE21	1:A:1314:GLN:HA	1.47	0.78
2:A:1502:LQH:C4	2:A:1502:LQH:F15	2.22	0.78
1:A:1117[B]:LEU:HD11	1:A:1152:THR:CG2	2.16	0.76
1:A:1298:ARG:CZ	2:A:1501:LQH:C14	2.67	0.72
1:A:1117[B]:LEU:CD1	1:A:1133:CYS:SG	2.80	0.69
1:A:1117[B]:LEU:CD1	1:A:1152:THR:HG21	2.22	0.69
1:A:1233:THR:OG1	1:A:1235:ASP:OD1	2.11	0.68
1:A:1156:TRP:O	1:A:1156:TRP:CD2	2.47	0.68
1:A:1267:HIS:ND1	1:A:1268:PRO:HD2	2.13	0.64
1:A:1245:ASP:OD2	1:A:1248:SER:OG	2.17	0.61
2:A:1501:LQH:C18	4:A:1769:HOH:O	2.51	0.58
1:A:1298:ARG:NH1	2:A:1501:LQH:C14	2.71	0.53
1:A:1370:GLU:O	1:A:1382:THR:HA	2.08	0.52
1:A:1092:ASP:OD1	1:A:1092:ASP:N	2.42	0.52
2:A:1502:LQH:C4	2:A:1502:LQH:C10	2.90	0.50
1:A:1115:GLY:HA2	1:A:1138:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:HIS:CG	1:A:1210:LYS:HE2	2.51	0.45
1:A:1270:GLY:HA2	4:A:1601:HOH:O	2.17	0.44
1:A:1085:VAL:HA	1:A:1384:CYS:O	2.18	0.44
1:A:1105:GLU:O	1:A:1106:ARG:HB2	2.18	0.44
1:A:1201:HIS:CD2	1:A:1210:LYS:HZ3	2.36	0.43
1:A:1156:TRP:O	1:A:1156:TRP:CG	2.69	0.43
1:A:1083:ILE:HD11	1:A:1388:GLU:HB2	2.00	0.43
1:A:1201:HIS:CD2	1:A:1210:LYS:HE2	2.54	0.42
1:A:1117[B]:LEU:CD2	1:A:1141:LEU:HD12	2.49	0.42
1:A:1159:PRO:HG3	1:A:1175:SER:HB2	2.01	0.41
1:A:1117[B]:LEU:HD11	1:A:1152:THR:HG22	2.01	0.41
1:A:1326:MET:N	1:A:1326:MET:SD	2.93	0.41
1:A:1327:LYS:HA	1:A:1375:MET:HG2	2.03	0.40
1:A:1378:LEU:HD23	1:A:1378:LEU:HA	1.89	0.40
1:A:1187:HIS:HB3	1:A:1234:ASP:OD2	2.20	0.40
1:A:1204:ASP:HB2	1:A:1211:LEU:HD11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1789:HOH:O	4:A:1789:HOH:O[7_555]	1.98	0.22
4:A:1792:HOH:O	4:A:1792:HOH:O[12_555]	2.15	0.05

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	301/367 (82%)	288 (96%)	12 (4%)	1 (0%)	41 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1168	SER

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	268/321 (84%)	256 (96%)	12 (4%)	27 29

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

Mol	Chain	Res	Type
1	A	1084	SER
1	A	1092	ASP
1	A	1141	LEU
1	A	1168	SER
1	A	1235	ASP
1	A	1252	ILE
1	A	1259	ASN
1	A	1273	VAL
1	A	1314	GLN
1	A	1336	THR
1	A	1374	SER
1	A	1378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1158	GLN
1	A	1314	GLN
1	A	1379	ASN

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](#)

3 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
3	ACT	A	1503	-	3,3,3	0.96	0	3,3,3	0.90	0
2	LQH	A	1501	-	23,23,23	1.75	4 (17%)	29,33,33	1.84	5 (17%)
2	LQH	A	1502	-	23,23,23	1.87	5 (21%)	29,33,33	1.25	5 (17%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LQH	A	1501	-	-	1/4/10/10	0/4/4/4
2	LQH	A	1502	-	-	3/4/10/10	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1502	LQH	C12-C6	4.22	1.52	1.43
2	A	1501	LQH	C12-C6	4.16	1.52	1.43
2	A	1502	LQH	C3-N1	-3.92	1.31	1.38
2	A	1501	LQH	C3-N1	-3.82	1.31	1.38
2	A	1502	LQH	C7-C3	3.81	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	LQH	C7-C3	3.20	1.51	1.45
2	A	1502	LQH	C2-N1	-2.93	1.33	1.40
2	A	1501	LQH	C2-N1	-2.73	1.33	1.40
2	A	1502	LQH	C5-C2	2.62	1.53	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	LQH	C9-C4-N1	-5.66	97.50	101.24
2	A	1501	LQH	C14-C10-C5	-4.12	118.62	123.11
2	A	1501	LQH	C11-C5-C10	3.28	120.40	116.67
2	A	1501	LQH	C12-C6-C2	-3.26	118.56	122.25
2	A	1502	LQH	C9-C4-N1	-2.93	99.30	101.24
2	A	1502	LQH	C5-C2-N1	2.49	121.90	118.56
2	A	1502	LQH	C7-C3-N8	-2.36	122.17	127.00
2	A	1502	LQH	C14-C10-C5	-2.26	120.65	123.11
2	A	1502	LQH	C5-C2-C6	-2.22	117.53	123.02
2	A	1501	LQH	C6-C2-N1	2.09	122.62	119.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1502	LQH	N1-C2-C5-C11
2	A	1502	LQH	N1-C2-C5-C10
2	A	1502	LQH	C6-C2-C5-C10
2	A	1501	LQH	N1-C2-C5-C10

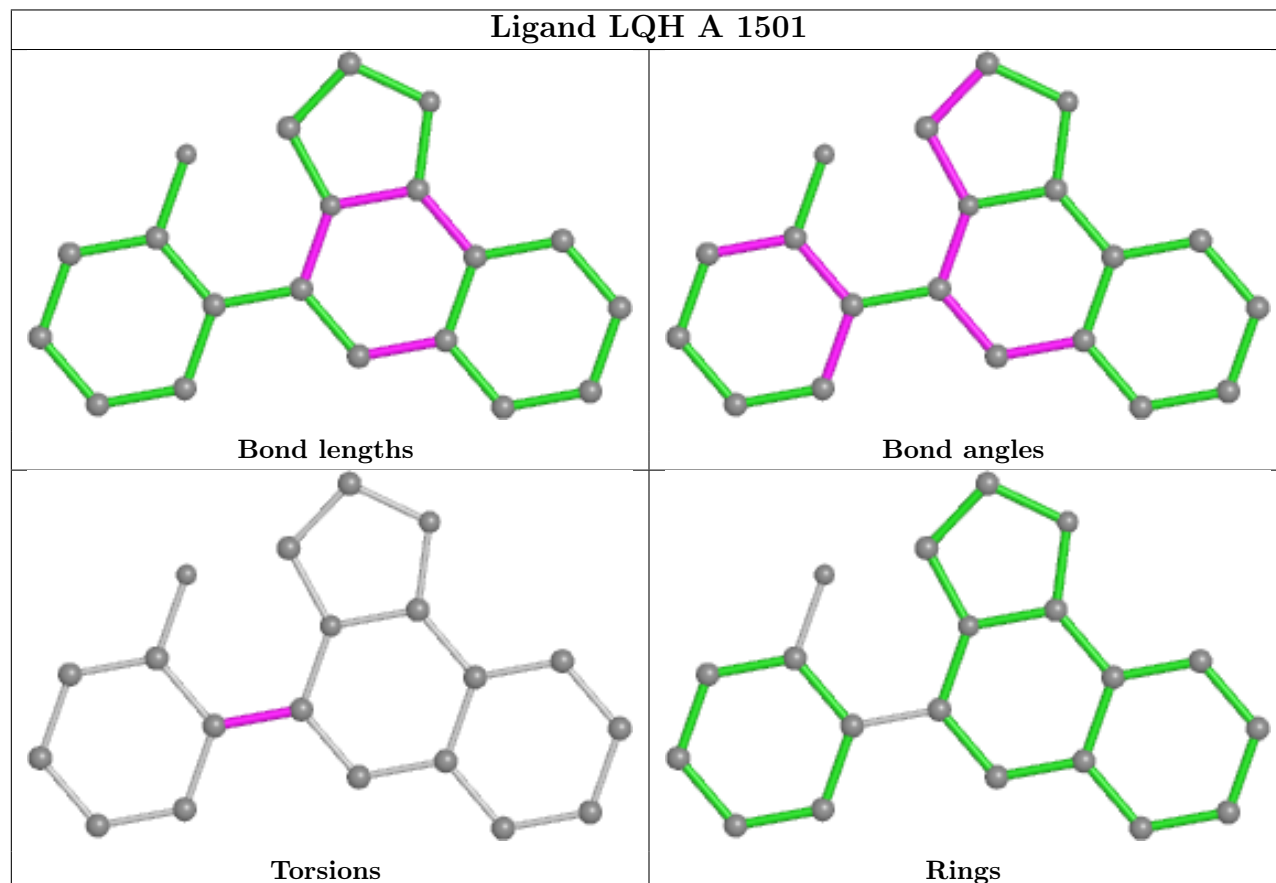
There are no ring outliers.

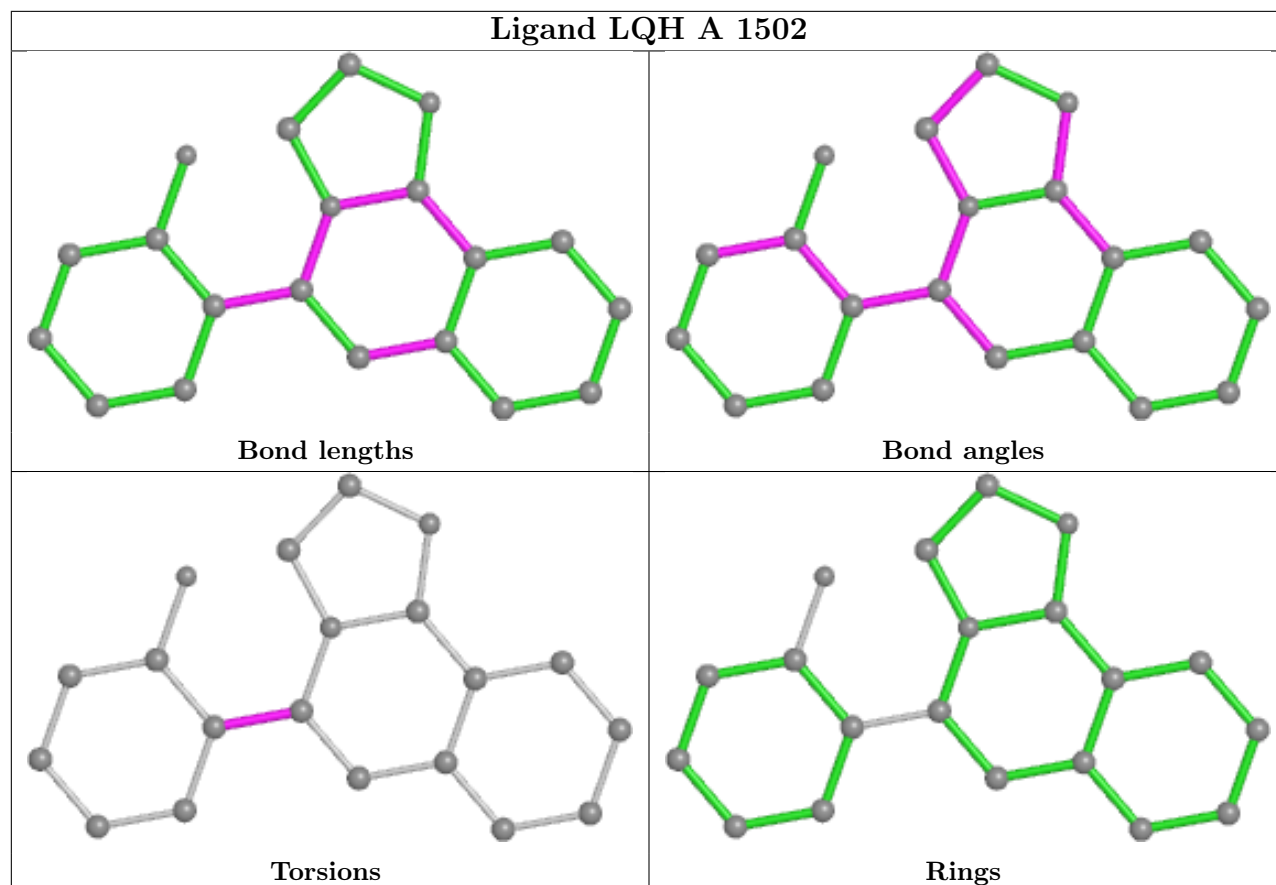
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	LQH	3	0
2	A	1502	LQH	2	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	301/367 (82%)	-0.07	7 (2%) 60 61	24, 48, 81, 104	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1169	VAL	3.0
1	A	1327	LYS	3.0
1	A	1375	MET	2.9
1	A	1326	MET	2.8
1	A	1390	GLY	2.7
1	A	1247	ARG	2.4
1	A	1315	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, 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.

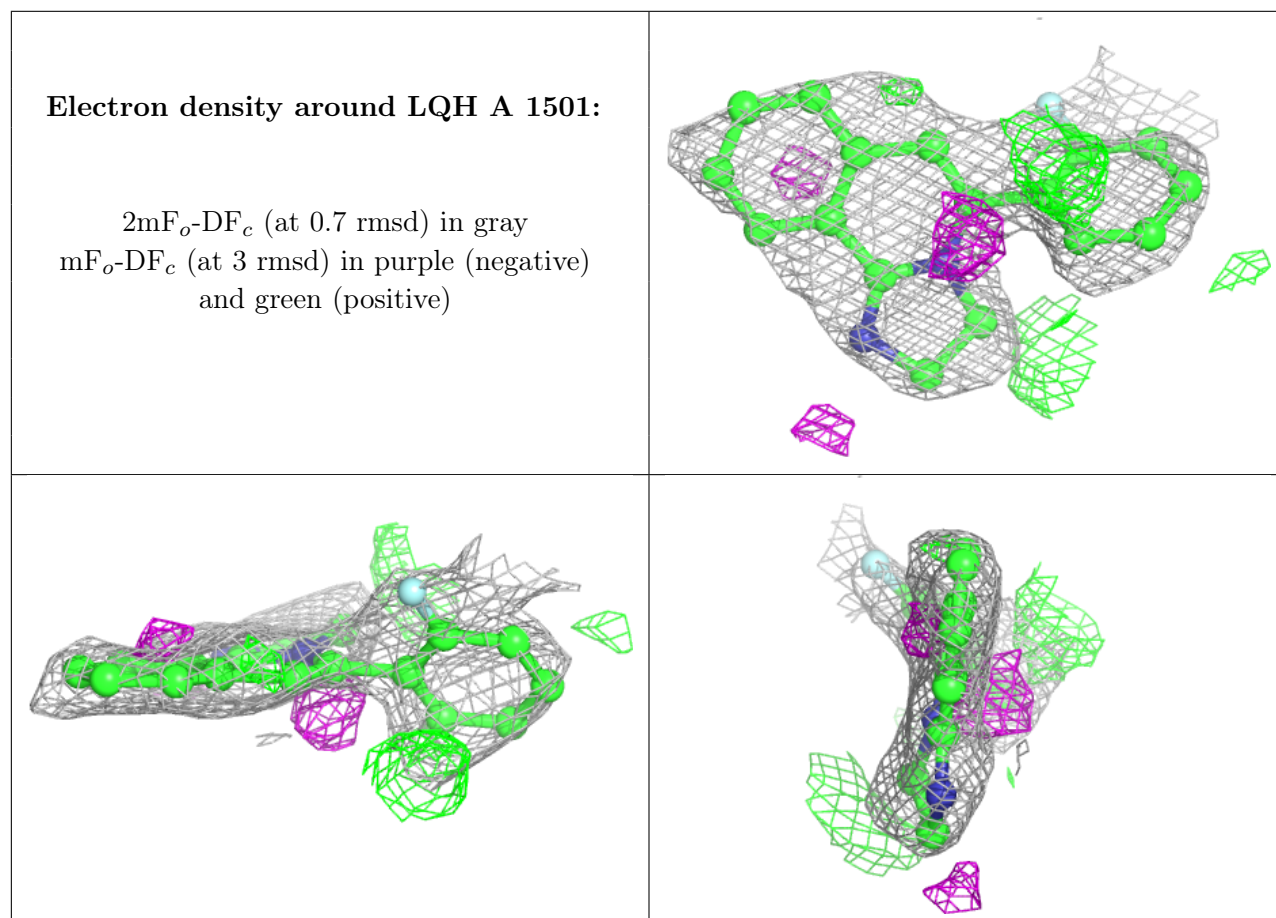
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LQH	A	1501	20/20	0.71	0.30	61,77,93,95	0

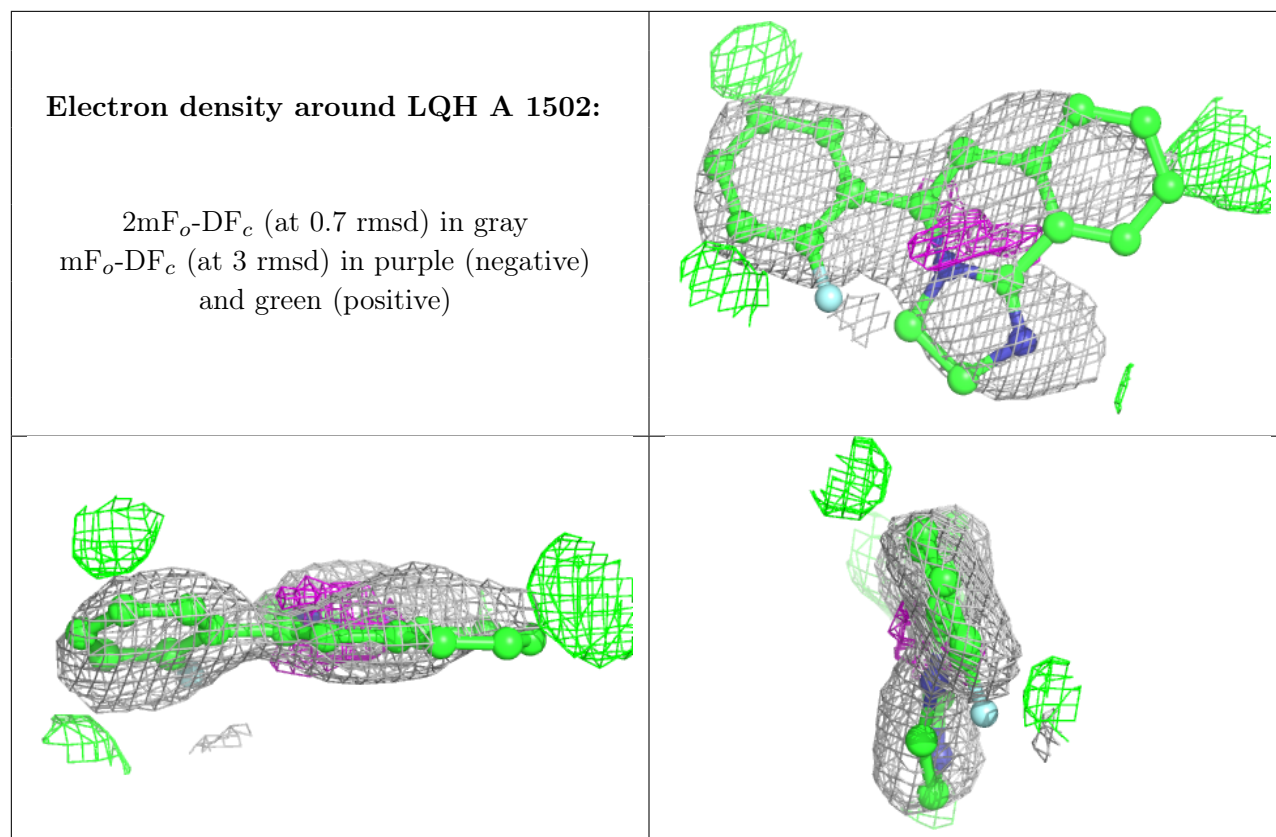
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LQH	A	1502	20/20	0.74	0.26	66,71,78,78	20
3	ACT	A	1503	4/4	0.99	0.07	27,28,29,29	7

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.