



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:14 pm BST

PDB ID : 6IJD
Title : Crystal Structure of Arabidopsis thaliana UGT89C1 complexed with quercetin
Authors : Zong, G.; Wang, X.
Deposited on : 2018-10-09
Resolution : 3.21 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 : 2.11
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) : 2.11

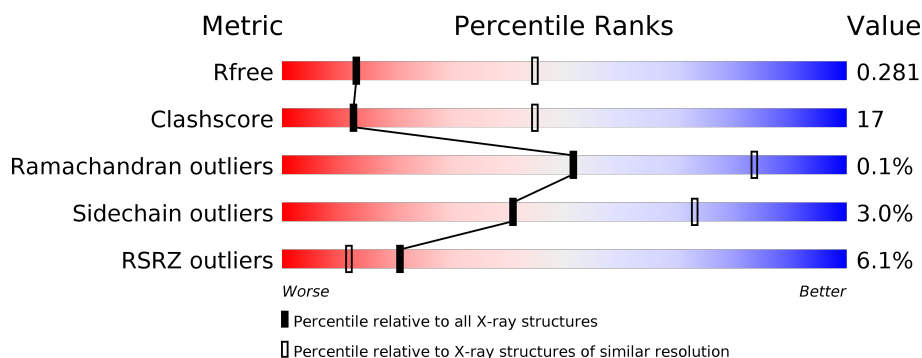
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	435	<div> <div>7%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>• 8%</div> </div> </div>
1	B	435	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>• 8%</div> </div> </div>

2 Entry composition [i](#)

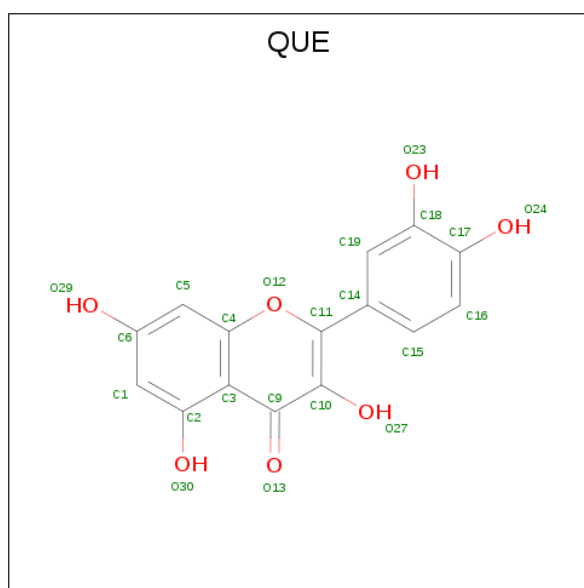
There are 3 unique types of molecules in this entry. The entry contains 6341 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-glycosyltransferase 89C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3133	2014	534	572	13			
1	B	402	Total	C	N	O	S	0	0	0
			3141	2022	530	576	13			

- Molecule 2 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: C₁₅H₁₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	15	7		
2	B	1	Total	C	O	0	0
			22	15	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	11	Total 11	O 11	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	81.10Å 81.10Å 341.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.55 – 3.21 47.60 – 3.21	Depositor EDS
% Data completeness (in resolution range)	89.7 (40.55-3.21) 90.0 (47.60-3.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.97 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.277 0.222 , 0.281	Depositor DCC
R_{free} test set	823 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.469 for -h,k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6341	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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

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	0.56	0/3213	0.71	2/4373 (0.0%)
1	B	0.58	0/3221	0.70	1/4384 (0.0%)
All	All	0.57	0/6434	0.71	3/8757 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	LEU	CB-CG-CD2	-6.52	99.92	111.00
1	A	391	LEU	CA-CB-CG	5.15	127.16	115.30
1	A	378	ARG	NE-CZ-NH2	5.12	122.86	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	CYS	Peptide
1	B	115	SER	Peptide
1	B	237	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	255	THR	Peptide

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	3133	0	3133	105	1
1	B	3141	0	3142	108	1
2	A	22	0	10	0	0
2	B	22	0	10	0	0
3	A	12	0	0	0	0
3	B	11	0	0	1	0
All	All	6341	0	6295	211	1

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 17.

All (211) 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:B:258:GLN:NE2	1:B:380:SER:O	2.06	0.88
1:A:141:LYS:NZ	1:A:432:GLU:O	2.12	0.83
1:A:72:SER:O	1:A:100:ARG:NH1	2.11	0.83
1:A:432:GLU:HG3	1:A:435:LEU:HD12	1.64	0.80
1:A:394:SER:HA	1:A:399:LEU:HD21	1.64	0.80
1:A:418:GLU:HA	1:A:423:TYR:CD2	2.19	0.77
1:B:254:LEU:HD21	1:B:275:TRP:CZ2	2.21	0.76
1:B:402:ARG:O	1:B:406:MET:HG2	1.86	0.76
1:A:258:GLN:NE2	1:A:380:SER:O	2.18	0.76
1:B:418:GLU:HA	1:B:423:TYR:CD2	2.23	0.73
1:A:402:ARG:O	1:A:406:MET:HG2	1.89	0.73
1:A:196:THR:HG21	1:A:197:ARG:NH1	2.05	0.72
1:B:432:GLU:HG3	1:B:435:LEU:HD12	1.73	0.71
1:A:239:GLU:O	1:A:242:SER:OG	2.10	0.69
1:A:377:ASN:H	1:A:380:SER:HB2	1.58	0.69
1:A:321:LEU:HA	1:A:326:VAL:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLN:HA	1:B:84:GLN:HE22	1.57	0.68
1:A:163:SER:OG	1:A:164:PHE:HA	1.93	0.68
1:B:321:LEU:HA	1:B:326:VAL:HG21	1.75	0.67
1:B:254:LEU:HD21	1:B:275:TRP:CH2	2.29	0.67
1:A:114:PRO:HA	1:A:117:LEU:HD13	1.77	0.66
1:A:18:GLN:HA	1:A:84:GLN:HE22	1.61	0.66
1:B:253:ARG:HD2	1:B:253:ARG:H	1.60	0.66
1:A:68:LEU:HD13	1:A:104:PRO:HB2	1.80	0.64
1:A:403:VAL:O	1:A:407:LYS:HG2	2.00	0.62
1:A:32:ILE:HG22	1:A:37:ALA:HB3	1.81	0.61
1:B:254:LEU:N	1:B:255:THR:OG1	2.34	0.61
1:A:377:ASN:OD1	1:A:378:ARG:N	2.35	0.60
1:A:125:SER:OG	1:A:172:THR:OG1	2.17	0.60
1:A:243:VAL:HG23	1:A:273:PHE:HA	1.83	0.59
1:A:372:VAL:HG23	1:A:401:GLU:HG3	1.85	0.59
1:A:46:LYS:NZ	1:B:46:LYS:HD3	2.17	0.59
1:A:365:VAL:HG22	1:A:371:ALA:HB3	1.84	0.59
1:B:388:ALA:HA	1:B:391:LEU:HD12	1.83	0.59
1:B:96:ASP:O	1:B:99:SER:HB3	2.03	0.59
1:A:224:SER:HB3	1:A:312:ARG:O	2.04	0.58
1:B:254:LEU:HD21	1:B:275:TRP:HZ2	1.69	0.58
1:B:317:GLN:HA	1:B:320:ILE:HD12	1.86	0.57
1:A:196:THR:HB	1:A:197:ARG:CZ	2.35	0.57
1:A:13:VAL:HG23	1:A:15:PRO:HD3	1.86	0.57
1:A:394:SER:O	1:A:397:GLU:HG3	2.05	0.56
1:B:245:TYR:HD2	1:B:321:LEU:HD21	1.70	0.56
1:B:121:ILE:HD12	1:B:135:ALA:HB2	1.88	0.56
1:B:222:GLN:HA	1:B:223:SER:HB2	1.87	0.56
1:A:196:THR:HB	1:A:197:ARG:NE	2.21	0.56
1:A:351:TRP:CD1	1:A:375:GLY:HA3	2.40	0.56
1:B:18:GLN:HA	1:B:84:GLN:NE2	2.21	0.55
1:B:386:LYS:HD3	1:B:389:ARG:HE	1.72	0.55
1:A:246:VAL:HG22	1:A:330:LEU:HB3	1.89	0.55
1:A:13:VAL:HG22	1:A:41:VAL:HG22	1.88	0.55
1:B:68:LEU:HD13	1:B:104:PRO:HB2	1.89	0.55
1:B:141:LYS:NZ	1:B:433:MET:O	2.39	0.54
1:B:246:VAL:O	1:B:275:TRP:HE3	1.91	0.54
1:A:46:LYS:HZ2	1:B:46:LYS:HD3	1.71	0.53
1:A:254:LEU:HD13	1:A:259:THR:HG21	1.90	0.53
1:A:96:ASP:O	1:A:99:SER:HB3	2.09	0.52
1:B:112:GLN:HB2	1:B:117:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ARG:HB2	1:A:378:ARG:CZ	2.39	0.52
1:A:385:ASP:O	1:A:389:ARG:HG3	2.09	0.52
1:B:309:LEU:HD12	1:B:310:VAL:H	1.74	0.51
1:A:25:HIS:O	1:A:29:THR:HG23	2.10	0.51
1:A:120:ALA:HA	1:A:140:ILE:HG22	1.92	0.51
1:B:234:LEU:HD11	1:B:323:HIS:HB3	1.91	0.51
1:B:241:ASN:HB3	1:B:397:GLU:OE1	2.11	0.51
1:B:125:SER:HA	1:B:128:SER:OG	2.11	0.51
1:B:105:LEU:HD23	1:B:134:VAL:HG11	1.93	0.51
1:A:186:LEU:HD21	1:A:335:TRP:HH2	1.76	0.51
1:A:386:LYS:O	1:A:386:LYS:HD3	2.11	0.51
1:B:120:ALA:HA	1:B:140:ILE:HG22	1.91	0.51
1:B:418:GLU:HG3	1:B:423:TYR:CE2	2.46	0.51
1:B:432:GLU:OE2	3:B:1001:HOH:O	2.19	0.51
1:A:42:LEU:HD22	1:A:105:LEU:HD13	1.93	0.50
1:B:334:GLY:O	1:B:338:VAL:HG23	2.12	0.50
1:A:245:TYR:CE2	1:A:317:GLN:HG2	2.47	0.50
1:B:195:LYS:HD2	1:B:204:ILE:HG22	1.92	0.50
1:B:19:SER:N	1:B:84:GLN:HE22	2.09	0.50
1:A:361:THR:HG21	1:A:373:ARG:HD2	1.92	0.50
1:B:13:VAL:HG22	1:B:41:VAL:HG22	1.94	0.50
1:B:73:HIS:CD2	1:B:75:CYS:H	2.30	0.50
1:A:350:ALA:HB3	1:A:373:ARG:HA	1.93	0.50
1:B:268:LYS:HB2	1:B:388:ALA:CB	2.41	0.49
1:B:28:LEU:O	1:B:32:ILE:HG12	2.12	0.49
1:A:334:GLY:O	1:A:338:VAL:HG23	2.12	0.49
1:B:234:LEU:CD1	1:B:323:HIS:HB3	2.42	0.49
1:A:297:PRO:HG2	1:A:301:GLU:HG3	1.94	0.49
1:A:173:THR:HG23	1:A:198:PHE:O	2.12	0.49
1:A:264:ALA:O	1:A:268:LYS:HG2	2.12	0.49
1:A:44:THR:HG22	1:A:81:GLU:OE1	2.12	0.49
1:A:59:SER:HB3	1:A:61:GLU:OE1	2.13	0.49
1:B:365:VAL:HG22	1:B:371:ALA:HB3	1.95	0.49
1:B:244:VAL:HG22	1:B:328:SER:HB2	1.95	0.48
1:B:13:VAL:HG23	1:B:15:PRO:HD3	1.94	0.48
1:B:377:ASN:OD1	1:B:378:ARG:N	2.47	0.48
1:A:418:GLU:HA	1:A:423:TYR:HD2	1.73	0.48
1:B:142:SER:O	1:B:175:SER:HB2	2.13	0.48
1:B:44:THR:CG2	1:B:70:PHE:HB2	2.43	0.48
1:A:353:MET:O	1:A:378:ARG:HG2	2.14	0.48
1:A:73:HIS:CG	1:A:74:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:HIS:HA	1:B:351:TRP:O	2.13	0.48
1:B:44:THR:HG22	1:B:81:GLU:OE1	2.14	0.48
1:B:264:ALA:O	1:B:268:LYS:HG2	2.13	0.48
1:B:153:ILE:HG23	1:B:157:TRP:CE3	2.48	0.48
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.74	0.47
1:A:243:VAL:HG23	1:A:273:PHE:CA	2.44	0.47
1:A:246:VAL:O	1:A:275:TRP:HE3	1.98	0.47
1:B:193:THR:O	1:B:197:ARG:HB2	2.15	0.47
1:B:19:SER:H	1:B:84:GLN:HE22	1.61	0.47
1:B:254:LEU:HD22	1:B:259:THR:HG23	1.96	0.47
1:A:32:ILE:HG22	1:A:37:ALA:CB	2.44	0.47
1:A:396:ARG:N	1:A:397:GLU:HA	2.29	0.47
1:B:187:GLU:O	1:B:191:VAL:HG23	2.14	0.47
1:B:397:GLU:C	1:B:399:LEU:H	2.16	0.47
1:B:40:THR:HA	1:B:64:LYS:O	2.15	0.47
1:A:187:GLU:O	1:A:191:VAL:HG23	2.15	0.47
1:A:190:PHE:O	1:A:194:VAL:HG23	2.15	0.47
1:A:42:LEU:HA	1:A:66:LEU:O	2.15	0.46
1:B:246:VAL:HG12	1:B:275:TRP:CE3	2.50	0.46
1:B:73:HIS:CD2	1:B:75:CYS:HB2	2.50	0.46
1:A:18:GLN:HG2	1:A:19:SER:N	2.28	0.46
1:B:246:VAL:HG22	1:B:330:LEU:HB3	1.97	0.46
1:B:32:ILE:HG22	1:B:37:ALA:HB3	1.98	0.46
1:A:245:TYR:HD2	1:A:321:LEU:HD21	1.80	0.46
1:A:332:HIS:O	1:A:352:PRO:HA	2.16	0.46
1:B:254:LEU:CB	1:B:255:THR:HA	2.45	0.46
1:B:361:THR:HG21	1:B:373:ARG:HD2	1.98	0.46
1:A:113:PRO:HG2	1:A:116:ASP:CG	2.36	0.46
1:A:153:ILE:HG23	1:A:157:TRP:CE3	2.50	0.46
1:A:44:THR:HG23	1:A:45:PRO:HD2	1.98	0.46
1:B:114:PRO:HG3	1:B:117:LEU:HD22	1.98	0.46
1:A:238:PRO:HG3	1:A:324:ARG:HH22	1.81	0.45
1:B:190:PHE:O	1:B:194:VAL:HG23	2.16	0.45
1:A:98:LEU:O	1:A:101:LEU:HB2	2.15	0.45
1:A:246:VAL:HG13	1:A:330:LEU:HD23	1.99	0.45
1:B:327:GLY:HA3	1:B:397:GLU:OE1	2.16	0.45
1:B:118:PRO:HG2	1:B:140:ILE:HD13	1.97	0.45
1:B:253:ARG:HD2	1:B:253:ARG:N	2.29	0.45
1:B:92:VAL:HB	1:B:164:PHE:CE2	2.51	0.45
1:A:402:ARG:HE	1:A:402:ARG:HB3	1.56	0.45
1:A:193:THR:O	1:A:197:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:O	1:A:32:ILE:HG12	2.17	0.45
1:A:103:ASP:HB2	1:A:104:PRO:HD3	1.98	0.45
1:B:252:ILE:HA	1:B:253:ARG:NH2	2.32	0.45
1:A:250:SER:HA	1:A:251:GLN:HA	1.40	0.45
1:A:8:LYS:HE2	1:A:35:ARG:O	2.16	0.45
1:A:18:GLN:HG2	1:A:19:SER:H	1.82	0.45
1:A:196:THR:CG2	1:A:197:ARG:NH1	2.79	0.44
1:A:95:PHE:CE1	1:A:126:PHE:HB3	2.52	0.44
1:B:243:VAL:HG12	1:B:325:ALA:O	2.16	0.44
1:A:333:LEU:HA	1:A:333:LEU:HD12	1.80	0.44
1:A:378:ARG:H	1:A:378:ARG:HG3	1.48	0.44
1:A:406:MET:O	1:A:410:GLU:HG3	2.17	0.44
1:A:83:LEU:HD12	1:A:86:LEU:HB2	1.99	0.44
1:B:83:LEU:HD21	1:B:91:ILE:HB	2.00	0.44
1:A:95:PHE:HE1	1:A:126:PHE:HB3	1.82	0.44
1:B:86:LEU:HB3	1:B:90:ALA:HB3	2.00	0.44
1:A:408:LEU:HA	1:A:408:LEU:HD23	1.84	0.43
1:B:73:HIS:HD2	1:B:75:CYS:H	1.65	0.43
1:B:73:HIS:HD2	1:B:75:CYS:HB2	1.83	0.43
1:A:83:LEU:HD21	1:A:91:ILE:HB	1.99	0.43
1:B:222:GLN:HA	1:B:223:SER:CB	2.48	0.43
1:A:163:SER:HA	1:A:165:PHE:N	2.34	0.43
1:A:40:THR:HA	1:A:64:LYS:O	2.19	0.43
1:B:227:PRO:O	1:B:230:VAL:HG22	2.18	0.43
1:B:347:MET:HB2	1:B:402:ARG:HD2	2.01	0.43
1:A:141:LYS:H	1:A:141:LYS:HG3	1.59	0.43
1:B:98:LEU:O	1:B:101:LEU:HB2	2.18	0.43
1:B:255:THR:HG22	1:B:256:ALA:H	1.84	0.43
1:B:80:VAL:HG11	1:B:86:LEU:HD13	2.01	0.43
1:A:238:PRO:HG3	1:A:324:ARG:NH2	2.34	0.43
1:B:32:ILE:HG22	1:B:37:ALA:CB	2.49	0.43
1:B:73:HIS:CG	1:B:74:PRO:HD2	2.54	0.43
1:A:411:LYS:HB2	1:A:411:LYS:HE3	1.81	0.43
1:A:24:PRO:HA	1:A:27:ASP:HB2	2.01	0.42
1:A:423:TYR:CD1	1:A:423:TYR:C	2.92	0.42
1:A:170:THR:O	1:A:174:GLU:HG3	2.19	0.42
1:A:254:LEU:HG	1:A:254:LEU:H	1.49	0.42
1:B:265:ALA:O	1:B:269:SER:OG	2.37	0.42
1:B:222:GLN:HG3	1:B:223:SER:HB3	2.00	0.42
1:B:418:GLU:HA	1:B:423:TYR:HD2	1.80	0.42
1:B:47:ASN:O	1:B:50:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:MET:O	1:B:410:GLU:HG3	2.19	0.42
1:A:368:LEU:HA	1:A:368:LEU:HD23	1.78	0.42
1:B:332:HIS:N	1:B:332:HIS:ND1	2.67	0.42
1:B:407:LYS:HD3	1:B:407:LYS:HA	1.97	0.42
1:A:113:PRO:HA	1:A:114:PRO:HD3	1.95	0.41
1:B:117:LEU:HA	1:B:117:LEU:HD12	1.85	0.41
1:B:125:SER:HB3	1:B:146:LEU:CD2	2.50	0.41
1:B:333:LEU:HD22	1:B:350:ALA:CB	2.50	0.41
1:A:272:ARG:HG2	1:A:307:LYS:HB3	2.02	0.41
1:B:333:LEU:HD22	1:B:350:ALA:HB2	2.02	0.41
1:A:423:TYR:HD1	1:A:423:TYR:C	2.23	0.41
1:A:7:LYS:C	1:A:8:LYS:HD2	2.40	0.41
1:B:420:GLY:O	1:B:424:LYS:HG3	2.21	0.41
1:A:162:ARG:HD3	1:A:166:ASN:OD1	2.20	0.41
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.89	0.41
1:B:195:LYS:HB2	1:B:204:ILE:HG21	2.01	0.41
1:B:335:TRP:CZ3	1:B:338:VAL:HG11	2.55	0.41
1:B:403:VAL:O	1:B:407:LYS:HG2	2.19	0.41
1:A:46:LYS:N	1:A:81:GLU:OE1	2.39	0.41
1:B:114:PRO:HA	1:B:115:SER:HA	1.70	0.41
1:B:183:PHE:CE2	1:B:186:LEU:HB2	2.56	0.41
1:B:351:TRP:C	1:B:351:TRP:CD1	2.94	0.41
1:B:24:PRO:HA	1:B:27:ASP:HB2	2.03	0.41
1:B:397:GLU:HB3	1:B:402:ARG:HD3	2.03	0.40
1:B:423:TYR:CD1	1:B:423:TYR:C	2.95	0.40
1:B:42:LEU:HA	1:B:66:LEU:O	2.21	0.40
1:A:335:TRP:CZ3	1:A:338:VAL:HG11	2.56	0.40
1:B:186:LEU:HD21	1:B:335:TRP:CH2	2.56	0.40
1:B:409:ARG:O	1:B:413:MET:HG2	2.21	0.40
1:A:77:PRO:HD2	1:A:86:LEU:HD21	2.04	0.40
1:B:43:VAL:O	1:B:67:ILE:HA	2.21	0.40

All (1) 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)
1:A:197:ARG:NH2	1:B:189:GLU:OE2[4_464]	1.93	0.27

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	396/435 (91%)	379 (96%)	17 (4%)	0	100	100
1	B	396/435 (91%)	373 (94%)	22 (6%)	1 (0%)	41	74
All	All	792/870 (91%)	752 (95%)	39 (5%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	ALA

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	346/377 (92%)	336 (97%)	10 (3%)	42	74
1	B	348/377 (92%)	337 (97%)	11 (3%)	39	71
All	All	694/754 (92%)	673 (97%)	21 (3%)	41	73

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	163	SER
1	A	197	ARG
1	A	240	ASP
1	A	275	TRP

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Mol	Chain	Res	Type
1	A	302	GLU
1	A	303	ARG
1	A	332	HIS
1	A	379	ASP
1	A	423	TYR
1	B	82	SER
1	B	99	SER
1	B	111	ARG
1	B	115	SER
1	B	250	SER
1	B	253	ARG
1	B	275	TRP
1	B	332	HIS
1	B	379	ASP
1	B	423	TYR
1	B	432	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	B	73	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	QUE	B	900	-	21,24,24	2.76	6 (28%)	28,36,36	1.89	9 (32%)
2	QUE	A	900	-	21,24,24	2.90	7 (33%)	28,36,36	2.09	9 (32%)

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	QUE	B	900	-	-	2/4/4/4	0/3/3/3
2	QUE	A	900	-	-	2/4/4/4	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	QUE	O13-C9	10.12	1.40	1.23
2	A	900	QUE	O13-C9	9.73	1.40	1.23
2	A	900	QUE	C3-C4	-4.30	1.35	1.41
2	A	900	QUE	O24-C17	3.90	1.44	1.36
2	B	900	QUE	C3-C4	-3.59	1.36	1.41
2	B	900	QUE	C5-C4	3.26	1.44	1.37
2	A	900	QUE	C5-C4	3.12	1.43	1.37
2	A	900	QUE	O29-C6	2.87	1.43	1.37
2	B	900	QUE	O24-C17	2.83	1.42	1.36
2	A	900	QUE	C14-C11	2.69	1.50	1.46
2	B	900	QUE	C14-C11	2.59	1.50	1.46
2	A	900	QUE	O23-C18	2.30	1.41	1.36
2	B	900	QUE	O23-C18	2.07	1.40	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	QUE	C5-C6-C1	-4.93	116.96	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	QUE	C15-C14-C11	-4.73	113.69	120.29
2	B	900	QUE	C15-C14-C11	-4.38	114.18	120.29
2	A	900	QUE	C14-C19-C18	-3.92	117.56	120.68
2	B	900	QUE	C14-C19-C18	-3.86	117.61	120.68
2	B	900	QUE	O12-C4-C5	3.25	119.91	116.11
2	B	900	QUE	C19-C14-C11	3.18	124.73	120.29
2	B	900	QUE	C15-C16-C17	-3.13	117.29	120.50
2	A	900	QUE	C19-C14-C11	3.06	124.56	120.29
2	A	900	QUE	O12-C4-C5	2.86	119.46	116.11
2	A	900	QUE	C19-C18-C17	2.82	122.35	119.86
2	B	900	QUE	C10-C9-C3	-2.67	117.64	121.38
2	A	900	QUE	O12-C4-C3	-2.62	118.45	121.03
2	B	900	QUE	C19-C18-C17	2.57	122.14	119.86
2	B	900	QUE	C5-C4-C3	-2.14	120.67	123.05
2	A	900	QUE	C15-C16-C17	-2.04	118.41	120.50
2	B	900	QUE	C5-C6-C1	-2.03	119.30	120.94
2	A	900	QUE	C2-C1-C6	2.02	121.53	119.70

There are no chirality outliers.

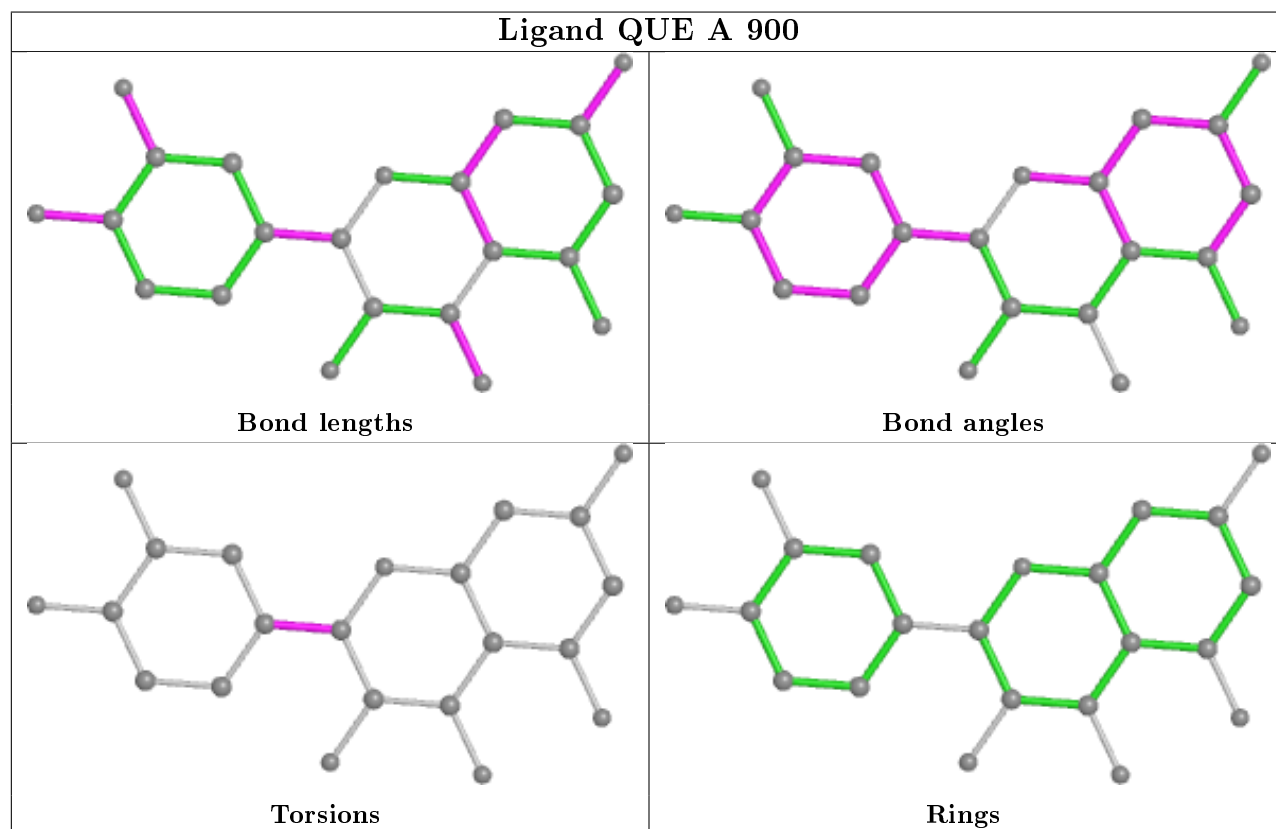
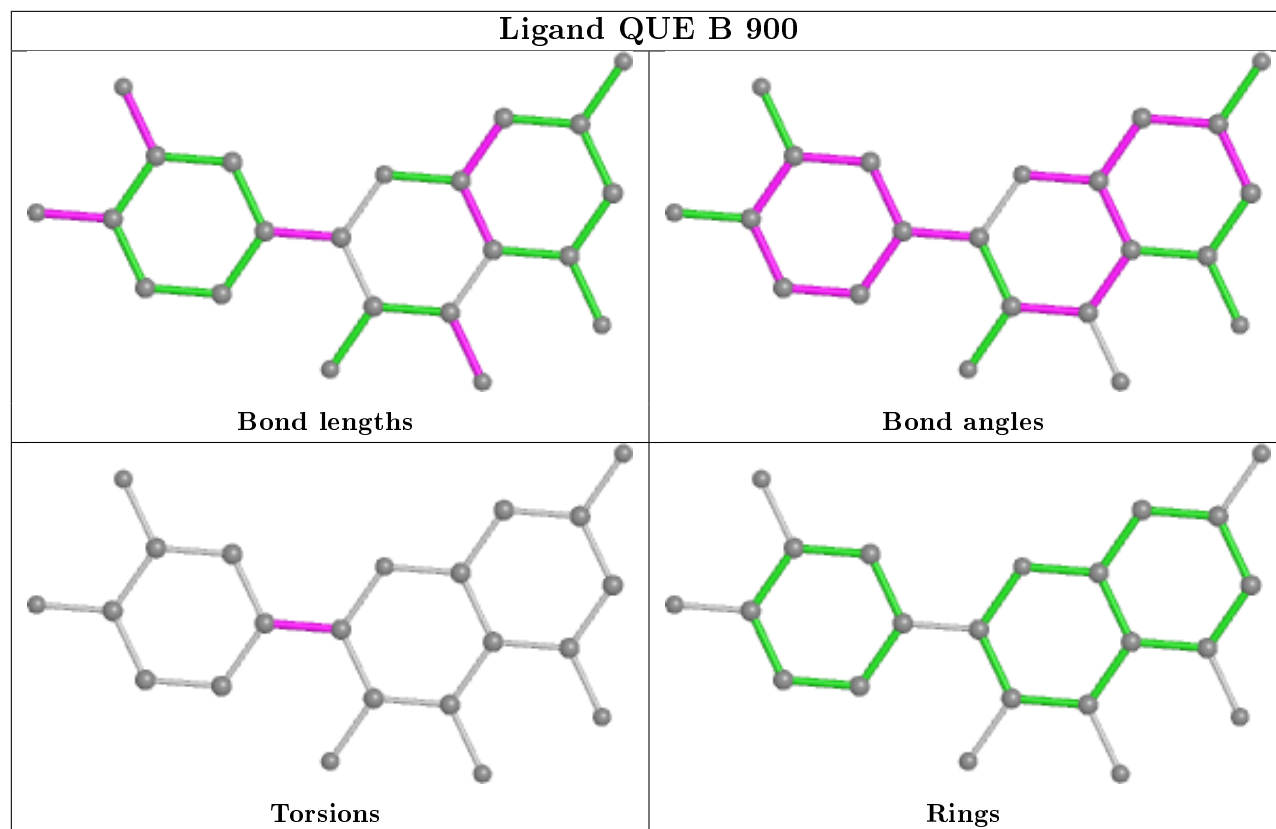
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	QUE	O12-C11-C14-C15
2	A	900	QUE	O12-C11-C14-C15
2	B	900	QUE	O12-C11-C14-C19
2	A	900	QUE	O12-C11-C14-C19

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	402/435 (92%)	0.22	29 (7%) 15 9	23, 46, 107, 153	0
1	B	402/435 (92%)	0.23	20 (4%) 28 16	21, 46, 103, 142	0
All	All	804/870 (92%)	0.22	49 (6%) 21 12	21, 46, 106, 153	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	ASP	5.2
1	A	270	SER	4.6
1	A	257	GLU	4.4
1	B	383	ASP	3.9
1	B	270	SER	3.7
1	B	257	GLU	3.6
1	B	396	ARG	3.5
1	A	387	LEU	3.4
1	B	256	ALA	3.4
1	B	385	ASP	3.3
1	A	394	SER	3.0
1	B	262	LEU	2.9
1	B	387	LEU	2.9
1	A	114	PRO	2.8
1	A	256	ALA	2.8
1	B	382	PRO	2.8
1	B	388	ALA	2.8
1	A	385	ASP	2.8
1	A	262	LEU	2.7
1	B	239	GLU	2.7
1	A	383	ASP	2.5
1	A	300	PHE	2.5
1	A	389	ARG	2.5
1	B	391	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	397	GLU	2.4
1	A	297	PRO	2.4
1	A	269	SER	2.4
1	B	7	LYS	2.4
1	A	398	ASP	2.4
1	A	255	THR	2.4
1	A	260	ALA	2.3
1	A	388	ALA	2.3
1	B	389	ARG	2.3
1	B	260	ALA	2.3
1	A	391	LEU	2.3
1	B	399	LEU	2.3
1	A	298	ALA	2.3
1	A	384	SER	2.3
1	A	301	GLU	2.2
1	B	275	TRP	2.2
1	A	273	PHE	2.2
1	B	273	PHE	2.2
1	A	275	TRP	2.2
1	A	253	ARG	2.2
1	A	392	ALA	2.1
1	B	266	LEU	2.1
1	A	396	ARG	2.0
1	A	238	PRO	2.0
1	A	309	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

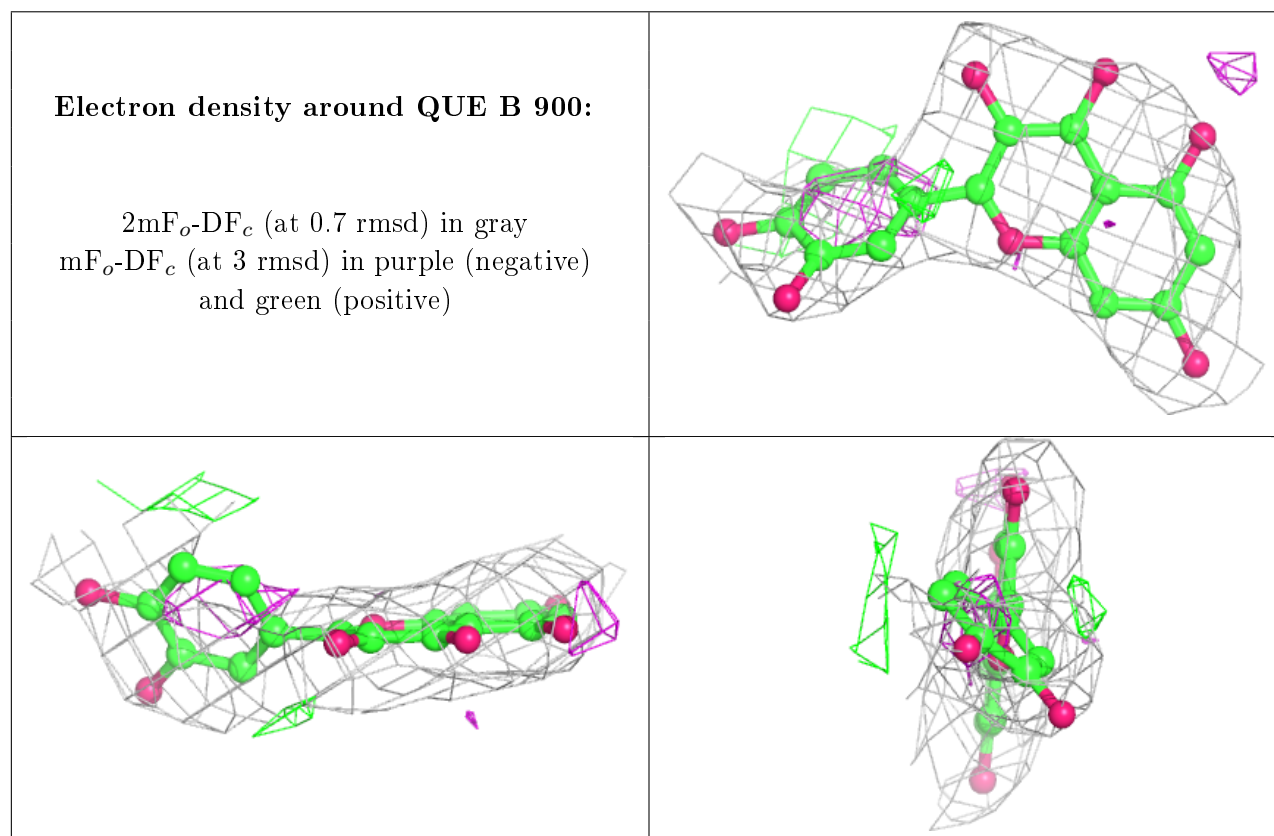
There are no carbohydrates in this entry.

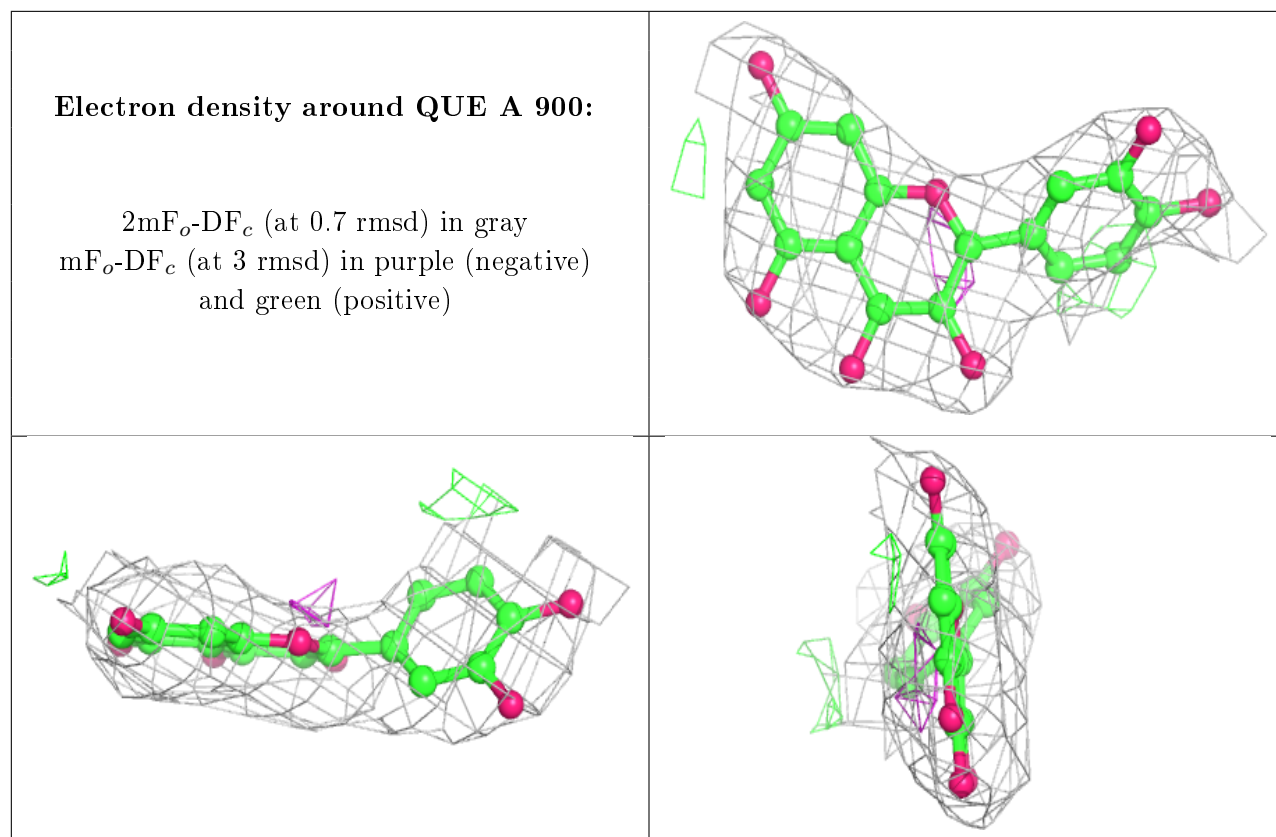
6.4 Ligands ⓘ

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	QUE	B	900	22/22	0.83	0.30	37,38,41,43	0
2	QUE	A	900	22/22	0.86	0.26	38,39,43,44	0

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.