



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:10 am BST

PDB ID : 5FLI  
Title : enzyme-substrate complex of Ni-queracetinase  
Authors : Jeoung, J.-H.; Nianios, D.; Fetzner, S.; Dobbek, H.  
Deposited on : 2015-10-26  
Resolution : 2.15 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 : 2.11  
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

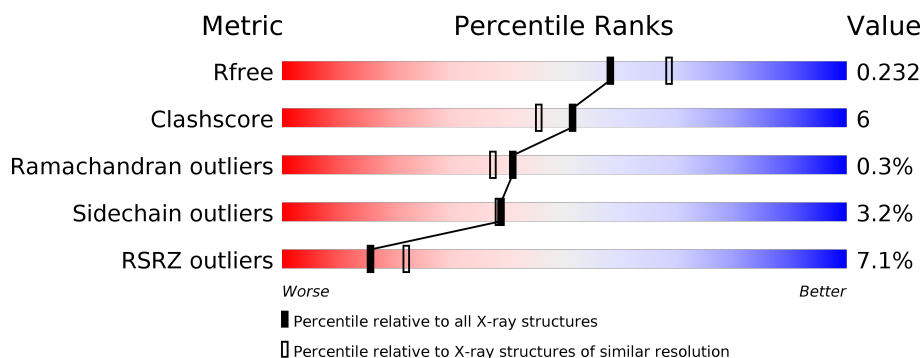
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	186	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	186	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	C	186	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	D	186	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
1	E	186	<div> <div>12%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	F	186	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	186	<div><div></div><div>9%</div><div>77%</div><div>20%</div><div></div><div>• •</div></div>
1	H	186	<div><div></div><div>5%</div><div>85%</div><div>11%</div><div></div><div>• •</div></div>
1	I	186	<div><div></div><div>11%</div><div>85%</div><div>12%</div><div></div><div>• •</div></div>
1	J	186	<div><div></div><div>9%</div><div>84%</div><div>14%</div><div></div><div>• •</div></div>
1	K	186	<div><div></div><div>5%</div><div>75%</div><div>23%</div><div></div><div>• •</div></div>
1	L	186	<div><div></div><div>11%</div><div>85%</div><div>13%</div><div></div><div>•</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18870 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 QUERCETINASE QUED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			
1	B	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			
1	C	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			
1	D	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			
1	E	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			
1	F	183	Total	C	N	O	S	0	1	0
			1482	951	258	270	3			
1	G	183	Total	C	N	O	S	0	2	0
			1484	952	256	272	4			
1	H	183	Total	C	N	O	S	0	0	0
			1472	945	255	269	3			
1	I	183	Total	C	N	O	S	0	1	0
			1482	951	258	270	3			
1	J	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			
1	K	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			
1	L	183	Total	C	N	O	S	0	1	0
			1475	947	255	269	4			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

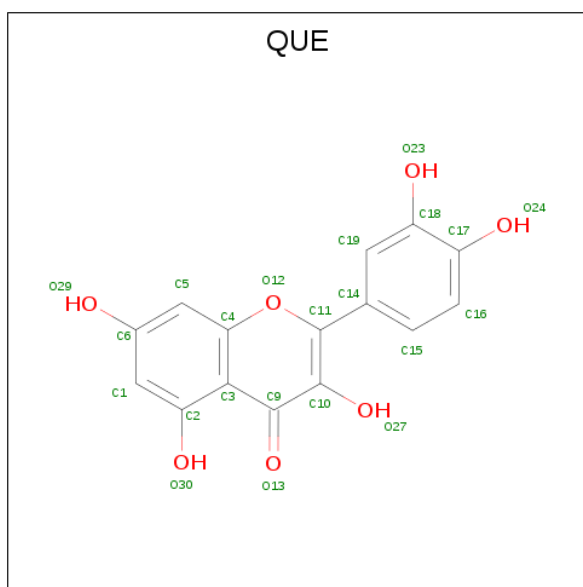
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ni	0	0
			1	1		
2	J	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ni	0	0
			1	1		
2	K	1	Total	Ni	0	0
			1	1		
2	E	1	Total	Ni	0	0
			1	1		
2	H	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		
2	I	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		
2	L	1	Total	Ni	0	0
			1	1		
2	F	1	Total	Ni	0	0
			1	1		

- Molecule 3 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula:  $C_{15}H_{10}O_7$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			22	15	7		
3	C	1	Total	C	O	0	0
			22	15	7		
3	D	1	Total	C	O	0	0
			22	15	7		
3	E	1	Total	C	O	0	0
			22	15	7		
3	F	1	Total	C	O	0	0
			22	15	7		
3	G	1	Total	C	O	0	0
			22	15	7		
3	H	1	Total	C	O	0	0
			22	15	7		
3	J	1	Total	C	O	0	0
			22	15	7		
3	K	1	Total	C	O	0	0
			22	15	7		
3	L	1	Total	C	O	0	0
			22	15	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	91	Total	O	0	0
			91	91		
4	C	70	Total	O	0	0
			70	70		
4	D	71	Total	O	0	0
			71	71		
4	E	92	Total	O	0	0
			92	92		
4	F	65	Total	O	0	0
			65	65		
4	G	60	Total	O	0	0
			60	60		
4	H	86	Total	O	0	0
			86	86		
4	I	72	Total	O	0	0
			72	72		

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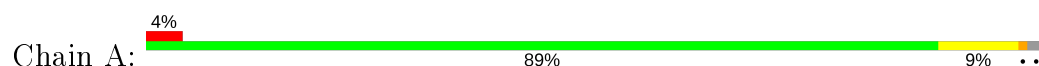
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	65	Total 65	O 65	0	0
4	K	65	Total 65	O 65	0	0
4	L	63	Total 63	O 63	0	0

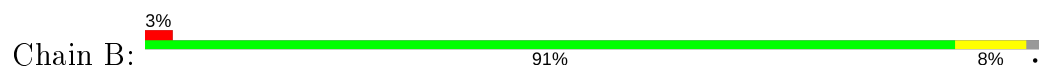
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

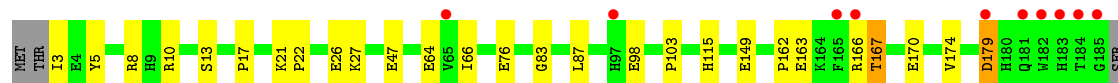
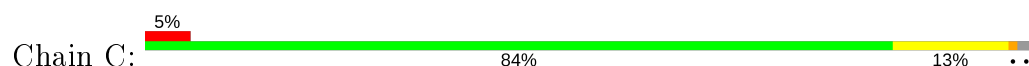
- Molecule 1: QUERCETINASE QUED



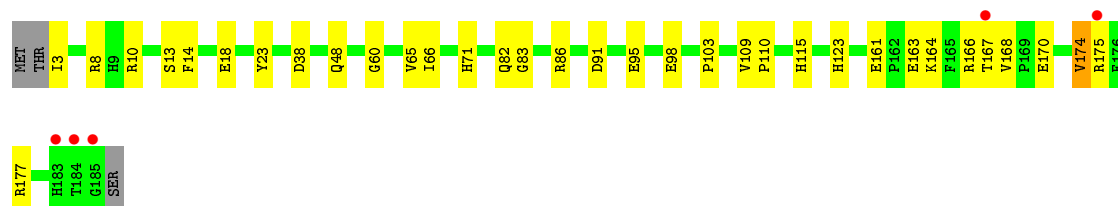
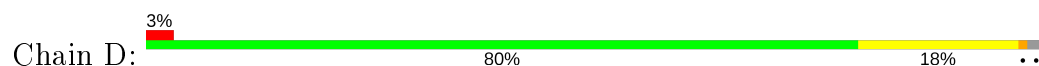
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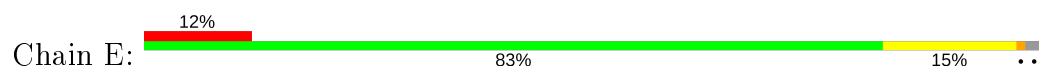
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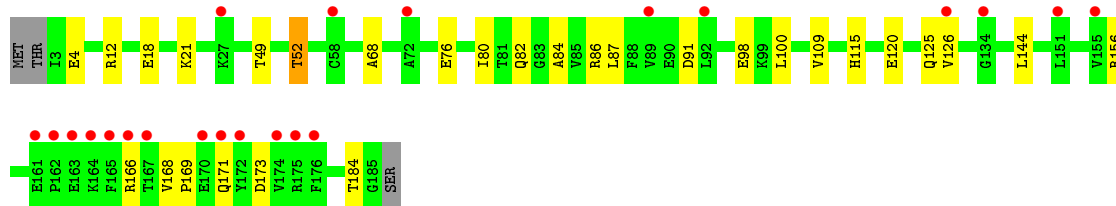
- Molecule 1: QUERCETINASE QUED



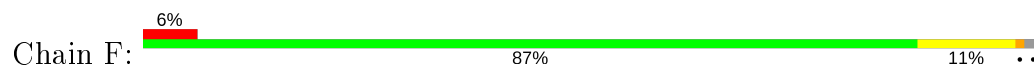
- Molecule 1: QUERCETINASE QUED



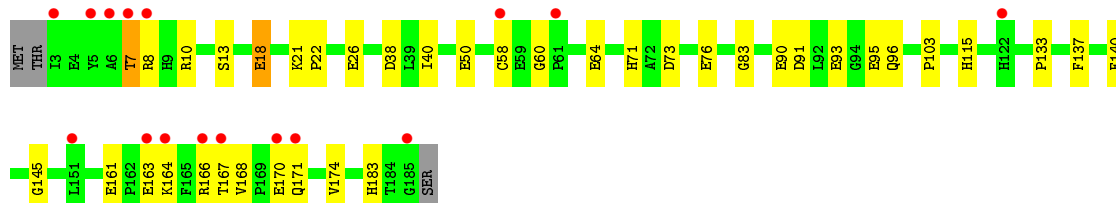
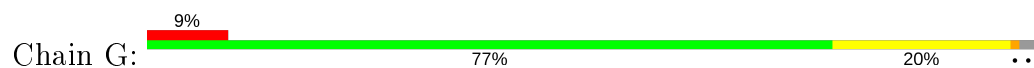




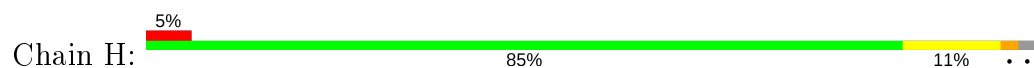
- Molecule 1: QUERCETINASE QUED



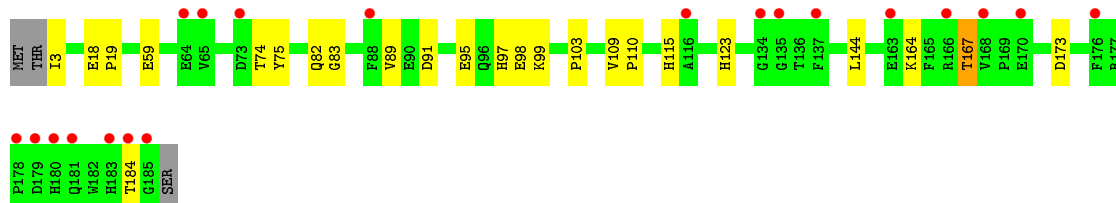
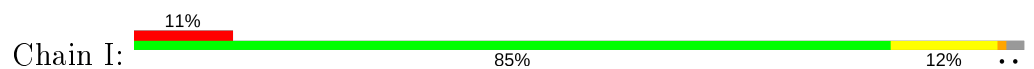
- Molecule 1: QUERCETINASE QUED



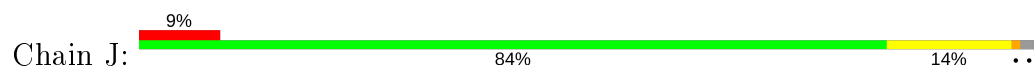
- Molecule 1: QUERCETINASE QUED

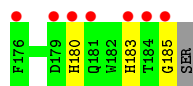


- Molecule 1: QUERCETINASE QUED

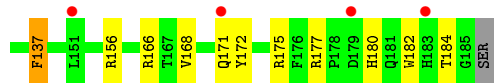
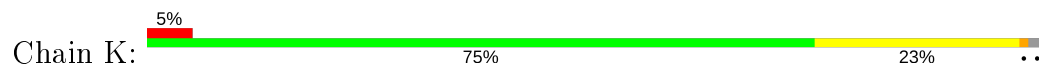


- Molecule 1: QUERCETINASE QUED

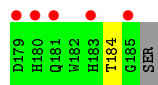
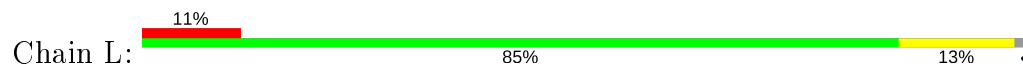




• Molecule 1: QUERCETINASE QUED



• Molecule 1: QUERCETINASE QUED



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.40Å 113.75Å 105.00Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	47.51 – 2.15 47.50 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.51-2.15) 99.4 (47.50-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.195 , 0.232 0.196 , 0.232	Depositor DCC
$R_{free}$ test set	6407 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: NI, 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	0.41	0/1528	0.56	0/2075
1	B	0.40	0/1528	0.58	0/2075
1	C	0.40	0/1528	0.55	0/2075
1	D	0.44	0/1528	0.58	0/2075
1	E	0.39	0/1528	0.55	0/2075
1	F	0.38	0/1533	0.55	0/2082
1	G	0.37	0/1537	0.53	0/2087
1	H	0.42	0/1522	0.55	0/2067
1	I	0.38	0/1533	0.53	0/2082
1	J	0.37	0/1528	0.54	0/2075
1	K	0.36	0/1528	0.53	0/2075
1	L	0.38	0/1528	0.56	0/2075
All	All	0.39	0/18349	0.55	0/24918

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	1475	0	1390	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1475	0	1390	9	0
1	C	1475	0	1390	14	0
1	D	1475	0	1390	19	0
1	E	1475	0	1390	19	0
1	F	1482	0	1391	15	0
1	G	1484	0	1395	23	0
1	H	1472	0	1385	19	0
1	I	1482	0	1391	17	0
1	J	1475	0	1390	11	0
1	K	1475	0	1390	29	0
1	L	1475	0	1390	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	22	0	5	2	0
3	B	22	0	6	1	0
3	C	22	0	6	2	0
3	D	22	0	6	0	0
3	E	22	0	5	3	0
3	F	22	0	6	1	0
3	G	22	0	5	2	0
3	H	22	0	6	1	0
3	J	22	0	6	1	0
3	K	22	0	5	3	0
3	L	22	0	5	2	0
4	A	96	0	0	0	0
4	B	91	0	0	6	0
4	C	70	0	0	1	2
4	D	71	0	0	1	0
4	E	92	0	0	7	1
4	F	65	0	0	0	0
4	G	60	0	0	0	0
4	H	86	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	72	0	0	4	0
4	J	65	0	0	2	0
4	K	65	0	0	4	0
4	L	63	0	0	0	1
All	All	18870	0	16743	195	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 6.

All (195) 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:K:76:GLU:OE2	3:K:301:QUE:O27	2.02	0.78
1:B:173:ASP:N	4:B:2082:HOH:O	2.23	0.70
1:I:59:GLU:OE2	4:I:2034:HOH:O	2.11	0.69
1:D:163:GLU:OE2	1:D:166:ARG:NH2	2.26	0.68
1:K:12:ARG:O	4:K:2008:HOH:O	2.12	0.67
1:A:82:GLN:NE2	1:I:82:GLN:OE1	2.29	0.65
1:A:21:LYS:HD2	1:A:22:PRO:HD2	1.76	0.65
1:E:76:GLU:OE2	3:E:301:QUE:O27	2.13	0.65
1:E:173:ASP:N	4:E:2090:HOH:O	2.31	0.63
1:H:76:GLU:OE2	3:H:301:QUE:O27	2.17	0.62
1:J:96:GLN:OE1	1:J:183:HIS:N	2.28	0.62
1:C:163:GLU:HG3	1:C:166:ARG:HH21	1.64	0.61
1:A:59:GLU:HG2	1:A:125:GLN:HG3	1.81	0.61
1:K:76:GLU:OE2	3:K:301:QUE:H19	2.00	0.61
4:E:2070:HOH:O	1:G:26:GLU:OE2	2.16	0.60
1:H:4:GLU:OE2	1:H:12:ARG:NE	2.33	0.59
1:H:64:GLU:OE2	4:H:2045:HOH:O	2.16	0.59
1:D:3:ILE:HG23	1:D:14:PHE:HE1	1.68	0.59
1:E:84:ALA:HB1	1:E:100:LEU:HD11	1.84	0.59
1:E:156:ARG:NH1	4:E:2086:HOH:O	2.35	0.58
1:E:49:THR:O	1:E:52:THR:OG1	2.20	0.58
1:H:161:GLU:H	1:H:161:GLU:CD	2.07	0.57
1:L:76:GLU:OE2	3:L:301:QUE:O27	2.22	0.57
3:F:301:QUE:O27	3:F:301:QUE:H19	2.04	0.57
1:I:74:THR:OG1	1:I:173:ASP:OD2	2.19	0.57
1:D:167:THR:O	1:D:170:GLU:HG2	2.04	0.57
1:H:90:GLU:HB3	1:H:114:VAL:HG13	1.86	0.56
1:I:144:LEU:HD12	1:I:164:LYS:HB3	1.87	0.56
1:J:173:ASP:N	4:J:2062:HOH:O	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:ILE:N	4:I:2001:HOH:O	2.38	0.55
1:D:175:ARG:HH12	1:D:177:ARG:HH11	1.55	0.55
1:K:65:VAL:HG22	1:K:118:ARG:HB2	1.89	0.55
1:I:83:GLY:O	1:I:103:PRO:HD3	2.07	0.55
1:J:75:TYR:HD1	1:J:110:PRO:HA	1.72	0.55
1:L:71:HIS:NE2	1:L:76:GLU:OE2	2.39	0.55
1:F:10:ARG:HB2	1:F:13:SER:HB2	1.89	0.54
1:H:150:GLU:CD	1:H:150:GLU:H	2.09	0.54
1:C:76:GLU:OE2	1:C:115:HIS:NE2	2.40	0.54
1:J:185:GLY:N	4:J:2065:HOH:O	2.40	0.53
4:E:2070:HOH:O	1:H:99:LYS:NZ	2.41	0.53
1:L:162:PRO:HA	1:L:165:PHE:HD2	1.73	0.53
1:F:169:PRO:HB3	1:F:174:VAL:O	2.08	0.53
1:K:52:THR:HG23	1:K:53:PHE:HD1	1.73	0.53
1:D:175:ARG:HH12	1:D:177:ARG:NH1	2.05	0.53
1:K:82:GLN:OE1	4:K:2042:HOH:O	2.18	0.53
3:L:301:QUE:H19	3:L:301:QUE:O27	2.10	0.52
1:J:83:GLY:O	1:J:103:PRO:HD3	2.08	0.52
1:D:38:ASP:OD1	1:D:60:GLY:HA3	2.09	0.52
1:J:114:VAL:HG11	1:J:180:HIS:CD2	2.45	0.52
1:C:76:GLU:HB2	3:C:301:QUE:O23	2.10	0.51
1:D:164:LYS:O	1:D:168:VAL:HG12	2.10	0.51
1:F:34:HIS:CG	1:F:154:PRO:HG3	2.45	0.51
1:K:168:VAL:HG13	1:K:172:TYR:HD2	1.75	0.51
1:D:103:PRO:HG2	1:I:103:PRO:HG2	1.92	0.51
1:K:76:GLU:OE1	1:K:115:HIS:NE2	2.44	0.51
1:G:90:GLU:HG3	1:G:96:GLN:HG2	1.92	0.51
1:D:91:ASP:OD1	1:D:95:GLU:N	2.43	0.51
4:C:2038:HOH:O	1:D:8:ARG:NH1	2.36	0.50
1:D:71:HIS:CD2	1:D:115:HIS:HE1	2.29	0.50
1:G:76[A]:GLU:OE2	3:G:301:QUE:O27	2.29	0.50
1:F:34:HIS:CD2	1:F:154:PRO:HG3	2.45	0.50
1:K:52:THR:HG21	1:L:132:GLY:HA2	1.92	0.50
1:D:86:ARG:HD3	1:D:98:GLU:OE1	2.11	0.50
1:K:82:GLN:HB2	1:K:125:GLN:HB3	1.94	0.49
1:L:75:TYR:HD1	1:L:110:PRO:HA	1.77	0.49
1:J:140:PHE:CE1	1:J:174:VAL:HG21	2.47	0.49
1:D:161:GLU:HG3	1:F:3:ILE:HA	1.93	0.49
1:G:83:GLY:O	1:G:103:PRO:HD3	2.12	0.49
1:L:16:PRO:HB3	1:L:21:LYS:HD3	1.93	0.49
1:J:18:GLU:N	1:J:18:GLU:OE1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:PRO:O	4:B:2015:HOH:O	2.19	0.48
1:E:82:GLN:HB2	1:E:125:GLN:HB3	1.95	0.48
1:H:156:ARG:HD2	4:H:2075:HOH:O	2.12	0.48
1:K:49:THR:O	1:K:52:THR:HG22	2.13	0.48
1:H:64:GLU:OE1	4:H:2046:HOH:O	2.19	0.48
1:L:109:VAL:HG11	1:L:115:HIS:CG	2.48	0.48
1:C:167:THR:O	1:C:170:GLU:HG2	2.13	0.48
1:C:8:ARG:NH1	1:C:47:GLU:HG2	2.27	0.48
1:E:144:LEU:HB2	1:E:168:VAL:HG21	1.95	0.48
1:E:68:ALA:N	4:E:2045:HOH:O	2.44	0.48
1:B:99:LYS:HE3	4:B:2063:HOH:O	2.13	0.48
1:C:8:ARG:HH11	1:C:47:GLU:HG2	1.79	0.48
1:K:66:ILE:HG12	1:K:117:TYR:H	1.79	0.47
3:A:301:QUE:H19	3:A:301:QUE:O27	2.14	0.47
1:B:38:ASP:OD1	1:B:60:GLY:HA3	2.14	0.47
1:G:161:GLU:HG2	1:G:163:GLU:H	1.79	0.47
1:G:7:THR:OG1	1:G:8:ARG:N	2.47	0.47
1:I:109:VAL:HG11	1:I:115:HIS:CG	2.49	0.47
1:E:18:GLU:HG2	1:E:21:LYS:HG3	1.97	0.47
1:G:38:ASP:OD1	1:G:60:GLY:HA3	2.15	0.47
1:I:75:TYR:HD1	1:I:110:PRO:HA	1.80	0.47
1:H:161:GLU:OE1	1:H:161:GLU:N	2.48	0.47
1:E:109:VAL:HG11	1:E:115:HIS:CG	2.50	0.47
1:G:137:PHE:CZ	1:G:174:VAL:HG22	2.51	0.46
1:D:10:ARG:HB2	1:D:13:SER:HB2	1.96	0.46
1:E:76:GLU:OE2	3:E:301:QUE:H19	2.15	0.46
1:A:76:GLU:HB2	3:A:301:QUE:O23	2.16	0.46
1:G:145:GLY:O	1:G:164:LYS:NZ	2.48	0.46
1:A:83:GLY:O	1:A:103:PRO:HD3	2.16	0.46
1:H:140:PHE:CE1	1:H:174:VAL:HG21	2.50	0.46
1:C:10:ARG:HB2	1:C:13:SER:HB2	1.98	0.46
1:C:21:LYS:HD2	1:C:22:PRO:HD2	1.98	0.46
1:G:50:GLU:OE2	1:H:75:TYR:OH	2.28	0.46
1:A:167:THR:O	1:A:170:GLU:HG2	2.16	0.45
1:G:137:PHE:HZ	1:G:174:VAL:HG22	1.81	0.45
1:F:170:GLU:OE2	1:K:177:ARG:HD2	2.16	0.45
1:L:75:TYR:CD1	1:L:110:PRO:HA	2.51	0.45
1:L:138:GLU:OE1	1:L:138:GLU:N	2.35	0.45
1:E:86:ARG:NE	1:E:120:GLU:OE2	2.37	0.45
1:A:161:GLU:OE1	1:A:163:GLU:HB3	2.16	0.45
1:I:98:GLU:HG2	1:I:184:THR:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:ARG:NH1	1:K:47:GLU:HG2	2.32	0.45
1:K:73:ASP:O	1:K:132:GLY:HA3	2.16	0.45
1:K:52:THR:HG23	1:K:53:PHE:CD1	2.52	0.45
1:C:179:ASP:OD1	1:C:179:ASP:N	2.38	0.45
1:G:21:LYS:HA	1:G:22:PRO:HD3	1.84	0.45
1:J:109:VAL:HG11	1:J:115:HIS:ND1	2.31	0.45
1:B:105:ASP:OD2	4:B:2063:HOH:O	2.21	0.45
1:B:76:GLU:OE2	3:B:301:QUE:O27	2.34	0.45
1:D:71:HIS:CE1	1:D:174:VAL:HG13	2.51	0.45
3:E:301:QUE:O27	3:E:301:QUE:H19	2.17	0.45
1:H:161:GLU:HG2	1:H:164:LYS:HG3	1.98	0.45
1:G:91:ASP:OD1	1:G:95:GLU:N	2.49	0.45
1:L:140:PHE:CE1	1:L:174:VAL:HG21	2.52	0.44
1:F:73:ASP:O	1:F:132:GLY:HA3	2.17	0.44
1:I:75:TYR:CD1	1:I:110:PRO:HA	2.53	0.44
1:I:99:LYS:NZ	4:I:2054:HOH:O	2.51	0.44
1:E:18:GLU:N	1:E:18:GLU:OE1	2.47	0.44
1:K:9:HIS:HE1	1:K:47:GLU:OE2	1.99	0.44
1:D:23:TYR:OH	1:D:48:GLN:HG2	2.17	0.44
1:K:83:GLY:O	1:K:103:PRO:HD3	2.18	0.44
1:C:76:GLU:OE1	3:C:301:QUE:H19	2.17	0.44
1:E:166:ARG:O	1:E:169:PRO:HD2	2.17	0.44
1:F:168:VAL:HG13	1:F:169:PRO:HD3	1.99	0.44
1:K:122:HIS:HB2	4:K:2015:HOH:O	2.17	0.44
1:C:5:TYR:HB3	1:C:17:PRO:HD3	2.00	0.43
1:G:168:VAL:O	1:G:171:GLN:HG2	2.18	0.43
1:E:87:LEU:HD23	1:F:24:PHE:HE1	1.82	0.43
1:G:73:ASP:HB3	1:G:133:PRO:O	2.18	0.43
1:K:166:ARG:HD3	1:K:166:ARG:HA	1.83	0.43
1:I:97:HIS:HE1	4:I:2051:HOH:O	2.01	0.43
1:E:169:PRO:HA	4:E:2090:HOH:O	2.18	0.43
1:G:76[A]:GLU:OE2	3:G:301:QUE:H19	2.19	0.43
3:J:301:QUE:H19	3:J:301:QUE:O27	2.18	0.43
1:B:144:LEU:HD12	1:B:164:LYS:HB3	1.99	0.43
1:F:140:PHE:CE1	1:F:174:VAL:HG21	2.53	0.43
3:K:301:QUE:H19	3:K:301:QUE:O27	2.18	0.43
1:I:18:GLU:HG2	1:I:18:GLU:H	1.68	0.43
1:D:65:VAL:HG22	1:D:66:ILE:O	2.19	0.43
1:E:4:GLU:OE1	1:E:12:ARG:HB3	2.19	0.43
1:B:169:PRO:HA	4:B:2082:HOH:O	2.18	0.43
1:K:49:THR:HB	1:K:52:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLY:O	1:C:103:PRO:HD3	2.19	0.42
1:K:156:ARG:NH1	4:K:2063:HOH:O	2.28	0.42
1:H:109:VAL:HG11	1:H:115:HIS:CG	2.55	0.42
1:I:109:VAL:HG11	1:I:115:HIS:CD2	2.55	0.42
1:K:73:ASP:O	1:K:133:PRO:HD2	2.20	0.42
1:L:10:ARG:HB2	1:L:13:SER:HB2	2.01	0.42
1:G:40:ILE:HG13	1:G:58[A]:CYS:SG	2.59	0.42
1:J:59:GLU:HG2	1:J:125:GLN:HG3	2.02	0.42
1:D:83:GLY:O	1:D:103:PRO:HD3	2.20	0.42
1:F:168:VAL:CG1	1:F:169:PRO:HD3	2.50	0.42
1:G:10:ARG:HB2	1:G:13:SER:HB2	2.01	0.42
1:K:114:VAL:HG11	1:K:180:HIS:NE2	2.35	0.42
1:H:183:HIS:ND1	1:H:183:HIS:O	2.52	0.41
1:G:18:GLU:HG2	1:G:21:LYS:HD3	2.03	0.41
1:G:71:HIS:CD2	1:G:115:HIS:HE1	2.38	0.41
1:F:66:ILE:HB	1:F:67:PRO:HD2	2.03	0.41
1:K:109:VAL:HA	1:K:110:PRO:HD3	1.84	0.41
1:A:109:VAL:HG11	1:A:115:HIS:CG	2.56	0.41
1:H:83:GLY:O	1:H:103:PRO:HD3	2.21	0.41
1:C:87:LEU:O	1:C:98:GLU:HA	2.20	0.41
1:E:91:ASP:HB2	4:E:2061:HOH:O	2.21	0.41
1:G:140:PHE:CE1	1:G:174:VAL:HG21	2.55	0.41
1:G:167:THR:O	1:G:170:GLU:HG2	2.20	0.41
1:K:22:PRO:HB2	1:L:89:VAL:HG21	2.02	0.41
1:H:110:PRO:HG2	1:H:113:CYS:SG	2.61	0.41
1:H:109:VAL:HG11	1:H:115:HIS:ND1	2.36	0.41
1:B:72:ALA:HA	1:B:112:ASN:OD1	2.21	0.41
1:H:21:LYS:HA	1:H:22:PRO:HD2	1.96	0.41
1:I:91:ASP:OD2	1:I:95:GLU:HB3	2.20	0.41
1:K:137:PHE:O	1:K:137:PHE:CG	2.73	0.41
1:L:85:VAL:HG22	1:L:119:MET:HG2	2.03	0.41
1:E:80:ILE:HD12	1:E:126:VAL:HG22	2.03	0.40
4:B:2061:HOH:O	1:C:26:GLU:OE2	2.21	0.40
1:F:76:GLU:HB2	1:F:109:VAL:HB	2.03	0.40
1:I:18:GLU:HA	1:I:19:PRO:HD2	1.83	0.40
1:J:21:LYS:HD2	1:J:22:PRO:HD2	2.03	0.40
1:K:14:PHE:HD2	1:K:29:LEU:O	2.05	0.40
1:K:3:ILE:HG23	1:K:14:PHE:CE1	2.57	0.40
1:F:109:VAL:HG11	1:F:115:HIS:ND1	2.36	0.40
1:D:109:VAL:HA	1:D:110:PRO:HD3	1.84	0.40
4:D:2064:HOH:O	1:F:3:ILE:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:GLU:HG3	1:G:166:ARG:HH21	1.87	0.40
1:L:18:GLU:HA	1:L:19:PRO:HD3	1.88	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:C:2042:HOH:O	4:L:2021:HOH:O[2_454]	2.13	0.07
4:C:2065:HOH:O	4:E:2001:HOH:O[2_554]	2.17	0.03

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	182/186 (98%)	179 (98%)	3 (2%)	0	100	100
1	B	182/186 (98%)	179 (98%)	3 (2%)	0	100	100
1	C	182/186 (98%)	174 (96%)	7 (4%)	1 (0%)	29	22
1	D	182/186 (98%)	176 (97%)	6 (3%)	0	100	100
1	E	182/186 (98%)	177 (97%)	4 (2%)	1 (0%)	29	22
1	F	182/186 (98%)	178 (98%)	4 (2%)	0	100	100
1	G	183/186 (98%)	175 (96%)	8 (4%)	0	100	100
1	H	181/186 (97%)	177 (98%)	4 (2%)	0	100	100
1	I	182/186 (98%)	175 (96%)	6 (3%)	1 (0%)	29	22
1	J	182/186 (98%)	177 (97%)	4 (2%)	1 (0%)	29	22
1	K	182/186 (98%)	173 (95%)	8 (4%)	1 (0%)	29	22
1	L	182/186 (98%)	176 (97%)	4 (2%)	2 (1%)	14	8
All	All	2184/2232 (98%)	2116 (97%)	61 (3%)	7 (0%)	41	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	184	THR
1	J	173	ASP
1	K	182	TRP
1	L	173	ASP
1	E	184	THR
1	I	167	THR
1	C	162	PRO

### 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	154/156 (99%)	149 (97%)	5 (3%)	39	38
1	B	154/156 (99%)	152 (99%)	2 (1%)	69	74
1	C	154/156 (99%)	146 (95%)	8 (5%)	23	19
1	D	154/156 (99%)	150 (97%)	4 (3%)	46	47
1	E	154/156 (99%)	151 (98%)	3 (2%)	57	61
1	F	154/156 (99%)	150 (97%)	4 (3%)	46	47
1	G	155/156 (99%)	150 (97%)	5 (3%)	39	38
1	H	153/156 (98%)	147 (96%)	6 (4%)	32	30
1	I	154/156 (99%)	151 (98%)	3 (2%)	57	61
1	J	154/156 (99%)	146 (95%)	8 (5%)	23	19
1	K	154/156 (99%)	146 (95%)	8 (5%)	23	19
1	L	154/156 (99%)	152 (99%)	2 (1%)	69	74
All	All	1848/1872 (99%)	1790 (97%)	58 (3%)	39	39

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	62	LYS

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Mol	Chain	Res	Type
1	A	64	GLU
1	A	161	GLU
1	A	168	VAL
1	B	65	VAL
1	B	175	ARG
1	C	3	ILE
1	C	27	LYS
1	C	64	GLU
1	C	66	ILE
1	C	149	GLU
1	C	167	THR
1	C	174	VAL
1	C	179	ASP
1	D	18	GLU
1	D	82	GLN
1	D	123	HIS
1	D	174	VAL
1	E	52	THR
1	E	98	GLU
1	E	171	GLN
1	F	123	HIS
1	F	159	VAL
1	F	163	GLU
1	F	174	VAL
1	G	7	THR
1	G	18	GLU
1	G	64	GLU
1	G	93	GLU
1	G	183	HIS
1	H	93	GLU
1	H	114	VAL
1	H	123	HIS
1	H	150	GLU
1	H	161	GLU
1	H	174	VAL
1	I	89	VAL
1	I	123	HIS
1	I	167	THR
1	J	4	GLU
1	J	8	ARG
1	J	51	ASN
1	J	52	THR

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Mol	Chain	Res	Type
1	J	65	VAL
1	J	93	GLU
1	J	156	ARG
1	J	171	GLN
1	K	4	GLU
1	K	18	GLU
1	K	51	ASN
1	K	92	LEU
1	K	137	PHE
1	K	171	GLN
1	K	175	ARG
1	K	184	THR
1	L	123	HIS
1	L	167	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	115	HIS
1	J	180	HIS
1	K	9	HIS
1	K	71	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](#)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 for Mogul analysis.

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	QUE	G	301	2	21,24,24	1.93	4 (19%)	28,36,36	1.60	3 (10%)
3	QUE	A	301	2	21,24,24	1.96	4 (19%)	28,36,36	1.52	3 (10%)
3	QUE	C	301	2	21,24,24	1.98	4 (19%)	28,36,36	1.73	5 (17%)
3	QUE	J	301	2	21,24,24	1.97	5 (23%)	28,36,36	1.49	4 (14%)
3	QUE	L	301	2	21,24,24	1.99	5 (23%)	28,36,36	1.45	3 (10%)
3	QUE	H	301	2	21,24,24	1.99	5 (23%)	28,36,36	1.52	4 (14%)
3	QUE	B	301	2	21,24,24	1.97	4 (19%)	28,36,36	1.60	4 (14%)
3	QUE	D	301	2	21,24,24	1.97	5 (23%)	28,36,36	1.61	4 (14%)
3	QUE	F	301	2	21,24,24	1.94	4 (19%)	28,36,36	1.52	3 (10%)
3	QUE	K	301	2	21,24,24	1.85	4 (19%)	28,36,36	1.50	3 (10%)
3	QUE	E	301	2	21,24,24	1.91	4 (19%)	28,36,36	1.59	4 (14%)

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
3	QUE	G	301	2	-	2/4/4/4	0/3/3/3
3	QUE	A	301	2	-	2/4/4/4	0/3/3/3
3	QUE	C	301	2	-	2/4/4/4	0/3/3/3
3	QUE	J	301	2	-	2/4/4/4	0/3/3/3
3	QUE	L	301	2	-	2/4/4/4	0/3/3/3
3	QUE	H	301	2	-	2/4/4/4	0/3/3/3
3	QUE	B	301	2	-	2/4/4/4	0/3/3/3
3	QUE	D	301	2	-	2/4/4/4	0/3/3/3
3	QUE	F	301	2	-	2/4/4/4	0/3/3/3
3	QUE	K	301	2	-	2/4/4/4	0/3/3/3
3	QUE	E	301	2	-	2/4/4/4	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	QUE	C18-C17	5.40	1.48	1.40
3	H	301	QUE	C3-C4	5.37	1.48	1.41
3	J	301	QUE	C18-C17	5.36	1.48	1.40
3	F	301	QUE	C3-C4	5.34	1.48	1.41
3	B	301	QUE	C3-C4	5.32	1.48	1.41
3	K	301	QUE	C18-C17	5.32	1.48	1.40
3	L	301	QUE	C3-C4	5.31	1.48	1.41
3	J	301	QUE	C3-C4	5.26	1.48	1.41
3	L	301	QUE	C18-C17	5.25	1.48	1.40
3	D	301	QUE	C18-C17	5.24	1.48	1.40
3	A	301	QUE	C3-C4	5.22	1.48	1.41
3	E	301	QUE	C3-C4	5.19	1.48	1.41
3	G	301	QUE	C3-C4	5.19	1.48	1.41
3	C	301	QUE	C18-C17	5.18	1.48	1.40
3	C	301	QUE	C3-C4	5.15	1.48	1.41
3	E	301	QUE	C18-C17	5.12	1.48	1.40
3	D	301	QUE	C3-C4	5.12	1.48	1.41
3	A	301	QUE	C18-C17	5.11	1.48	1.40
3	G	301	QUE	C18-C17	5.09	1.48	1.40
3	B	301	QUE	C18-C17	4.98	1.48	1.40
3	F	301	QUE	C18-C17	4.85	1.47	1.40
3	K	301	QUE	C3-C4	4.82	1.47	1.41
3	C	301	QUE	C2-C3	3.64	1.49	1.43
3	L	301	QUE	C2-C3	3.44	1.49	1.43
3	B	301	QUE	C2-C3	3.28	1.49	1.43
3	D	301	QUE	C2-C3	3.22	1.49	1.43
3	J	301	QUE	C2-C3	3.19	1.48	1.43
3	A	301	QUE	C2-C3	3.13	1.48	1.43
3	H	301	QUE	C2-C3	3.11	1.48	1.43
3	E	301	QUE	C2-C3	3.05	1.48	1.43
3	G	301	QUE	C2-C3	3.04	1.48	1.43
3	F	301	QUE	C2-C3	3.02	1.48	1.43
3	K	301	QUE	C2-C3	2.53	1.47	1.43
3	C	301	QUE	C9-C10	2.47	1.49	1.41
3	J	301	QUE	C9-C10	2.33	1.49	1.41
3	D	301	QUE	C9-C10	2.25	1.49	1.41
3	L	301	QUE	C9-C10	2.21	1.48	1.41
3	A	301	QUE	C9-C10	2.19	1.48	1.41
3	E	301	QUE	C9-C10	2.19	1.48	1.41
3	D	301	QUE	C14-C11	2.19	1.50	1.46
3	K	301	QUE	C9-C10	2.18	1.48	1.41
3	H	301	QUE	C14-C11	2.14	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	QUE	C9-C10	2.10	1.48	1.41
3	L	301	QUE	C14-C11	2.10	1.50	1.46
3	F	301	QUE	C14-C11	2.07	1.49	1.46
3	J	301	QUE	C14-C11	2.04	1.49	1.46
3	H	301	QUE	C9-C10	2.03	1.48	1.41
3	G	301	QUE	C9-C10	2.02	1.48	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	QUE	O12-C4-C5	4.75	121.67	116.11
3	F	301	QUE	O12-C4-C5	4.68	121.59	116.11
3	A	301	QUE	O12-C4-C5	4.62	121.52	116.11
3	E	301	QUE	C5-C4-C3	-4.61	117.94	123.05
3	G	301	QUE	C5-C4-C3	-4.57	117.99	123.05
3	D	301	QUE	O12-C4-C5	4.48	121.35	116.11
3	B	301	QUE	C5-C4-C3	-4.47	118.10	123.05
3	B	301	QUE	O12-C4-C5	4.45	121.32	116.11
3	F	301	QUE	C5-C4-C3	-4.45	118.12	123.05
3	E	301	QUE	O12-C4-C5	4.44	121.31	116.11
3	L	301	QUE	C5-C4-C3	-4.41	118.16	123.05
3	A	301	QUE	C5-C4-C3	-4.31	118.28	123.05
3	K	301	QUE	O12-C4-C5	4.26	121.10	116.11
3	C	301	QUE	C15-C14-C11	-4.21	114.41	120.29
3	J	301	QUE	O12-C4-C5	4.18	121.01	116.11
3	J	301	QUE	C5-C4-C3	-4.13	118.47	123.05
3	D	301	QUE	C5-C4-C3	-4.12	118.48	123.05
3	L	301	QUE	O12-C4-C5	4.07	120.88	116.11
3	K	301	QUE	C5-C4-C3	-3.98	118.64	123.05
3	H	301	QUE	C5-C4-C3	-3.96	118.67	123.05
3	H	301	QUE	O12-C4-C5	3.76	120.51	116.11
3	C	301	QUE	O12-C4-C5	3.56	120.28	116.11
3	C	301	QUE	C5-C4-C3	-3.48	119.19	123.05
3	C	301	QUE	C19-C14-C11	3.32	124.92	120.29
3	K	301	QUE	C10-C9-C3	-2.99	117.19	121.38
3	H	301	QUE	C10-C9-C3	-2.70	117.61	121.38
3	D	301	QUE	C15-C14-C11	-2.69	116.54	120.29
3	B	301	QUE	C15-C14-C11	-2.67	116.56	120.29
3	C	301	QUE	C14-C19-C18	-2.55	118.65	120.68
3	E	301	QUE	C10-C9-C3	-2.54	117.82	121.38
3	L	301	QUE	C10-C9-C3	-2.45	117.95	121.38
3	D	301	QUE	C19-C14-C11	2.45	123.70	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	QUE	C10-C9-C3	-2.44	117.96	121.38
3	F	301	QUE	C10-C9-C3	-2.40	118.02	121.38
3	J	301	QUE	C10-C9-C3	-2.37	118.07	121.38
3	E	301	QUE	C15-C14-C11	-2.30	117.09	120.29
3	B	301	QUE	C10-C9-C3	-2.24	118.24	121.38
3	J	301	QUE	C15-C14-C11	-2.22	117.20	120.29
3	A	301	QUE	C10-C9-C3	-2.11	118.42	121.38
3	H	301	QUE	C15-C14-C11	-2.08	117.38	120.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	QUE	C10-C11-C14-C15
3	C	301	QUE	C10-C11-C14-C19
3	J	301	QUE	C10-C11-C14-C15
3	J	301	QUE	C10-C11-C14-C19
3	B	301	QUE	C10-C11-C14-C15
3	B	301	QUE	C10-C11-C14-C19
3	E	301	QUE	C10-C11-C14-C15
3	E	301	QUE	C10-C11-C14-C19
3	G	301	QUE	C10-C11-C14-C15
3	G	301	QUE	C10-C11-C14-C19
3	L	301	QUE	C10-C11-C14-C15
3	L	301	QUE	C10-C11-C14-C19
3	D	301	QUE	C10-C11-C14-C15
3	D	301	QUE	C10-C11-C14-C19
3	K	301	QUE	C10-C11-C14-C15
3	K	301	QUE	C10-C11-C14-C19
3	A	301	QUE	C10-C11-C14-C15
3	A	301	QUE	C10-C11-C14-C19
3	H	301	QUE	C10-C11-C14-C15
3	H	301	QUE	C10-C11-C14-C19
3	F	301	QUE	C10-C11-C14-C15
3	F	301	QUE	C10-C11-C14-C19

There are no ring outliers.

10 monomers are involved in 18 short contacts:

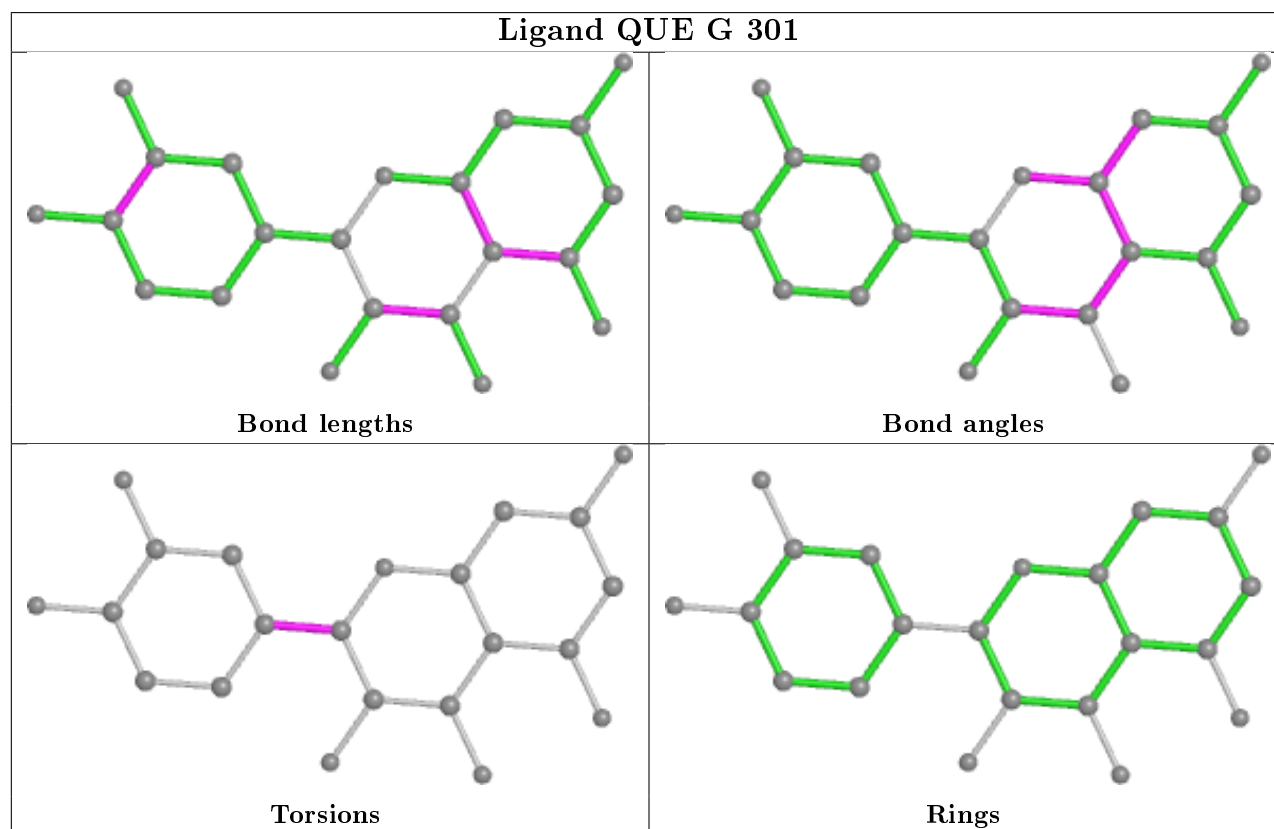
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	QUE	2	0

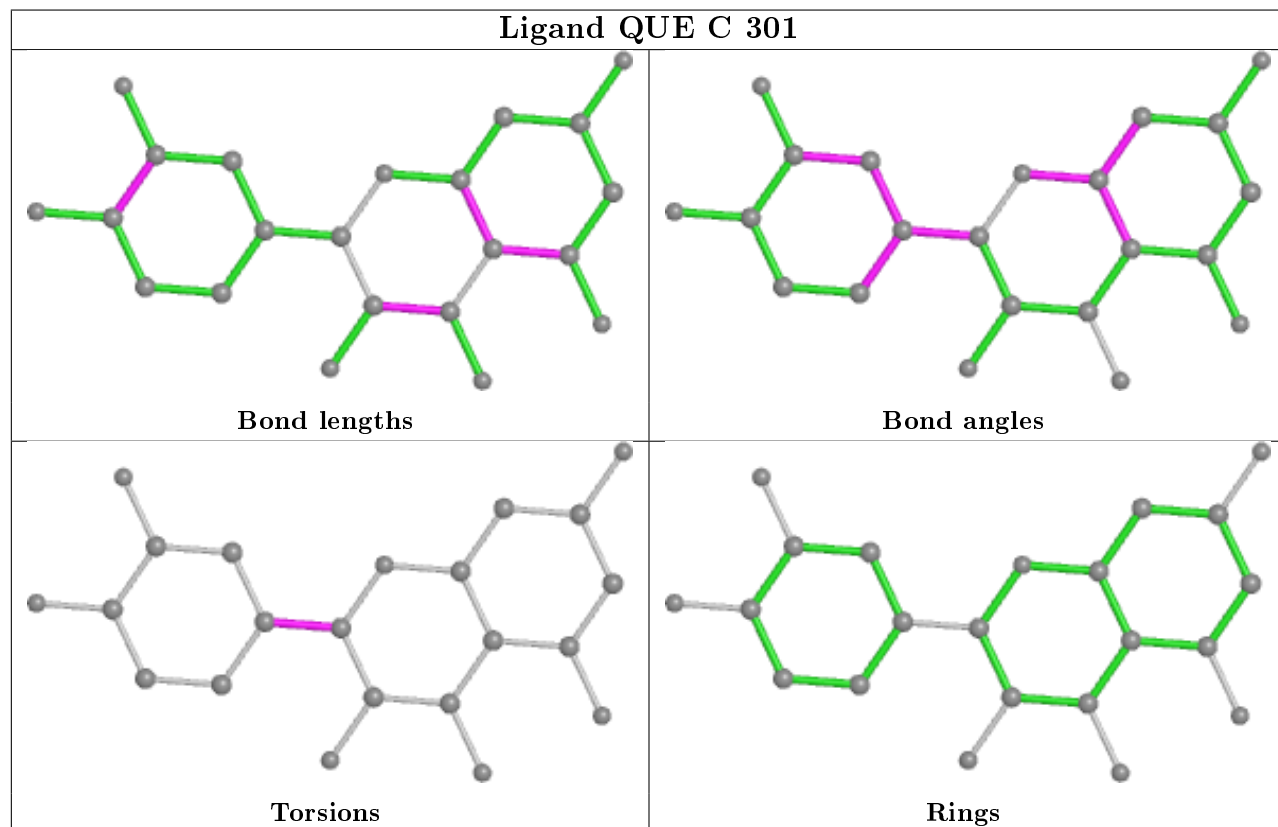
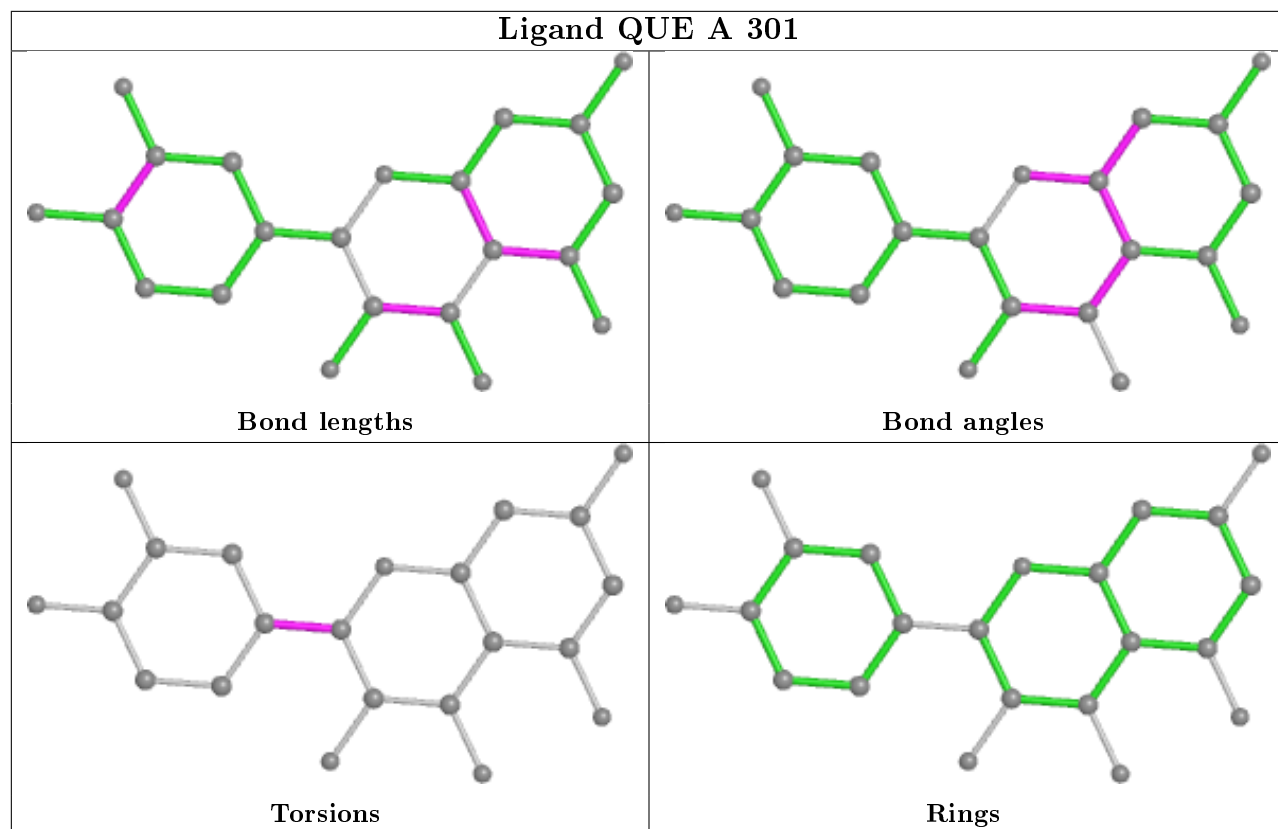
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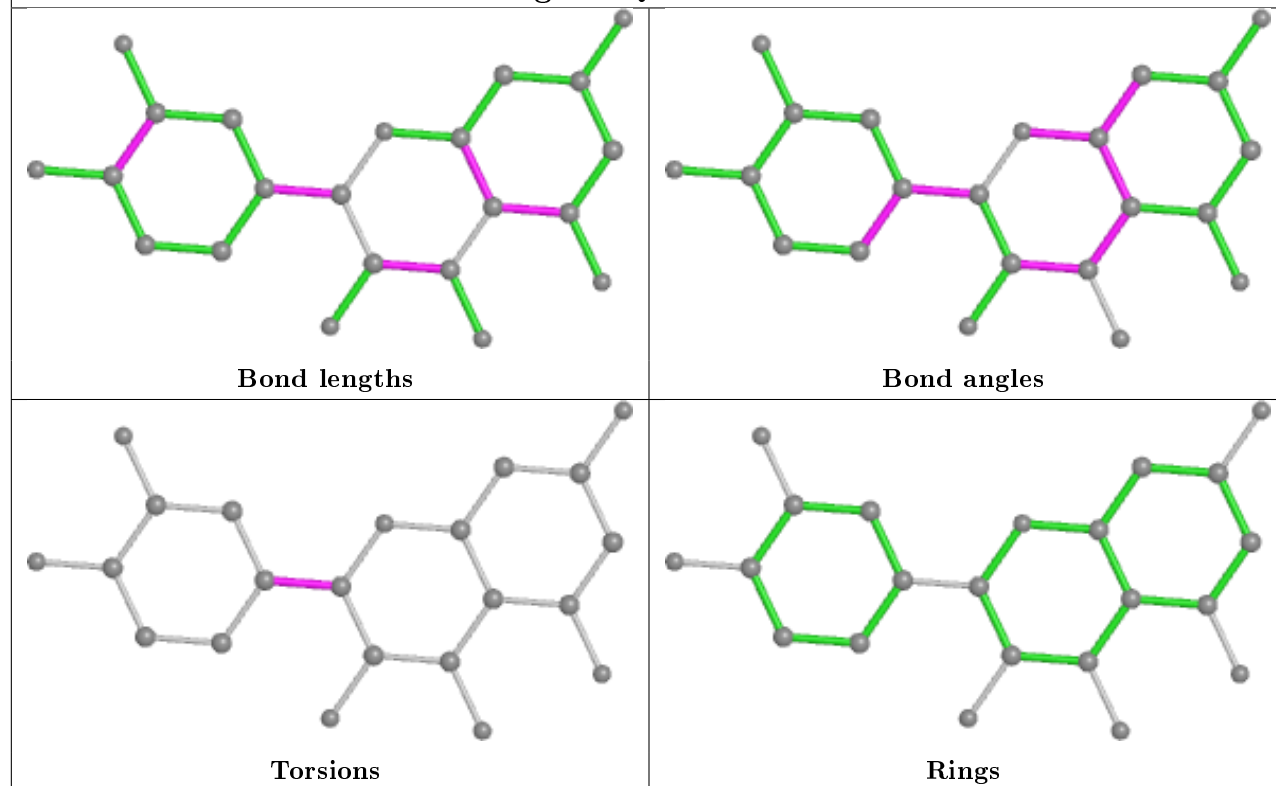
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	QUE	2	0
3	C	301	QUE	2	0
3	J	301	QUE	1	0
3	L	301	QUE	2	0
3	H	301	QUE	1	0
3	B	301	QUE	1	0
3	F	301	QUE	1	0
3	K	301	QUE	3	0
3	E	301	QUE	3	0

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.

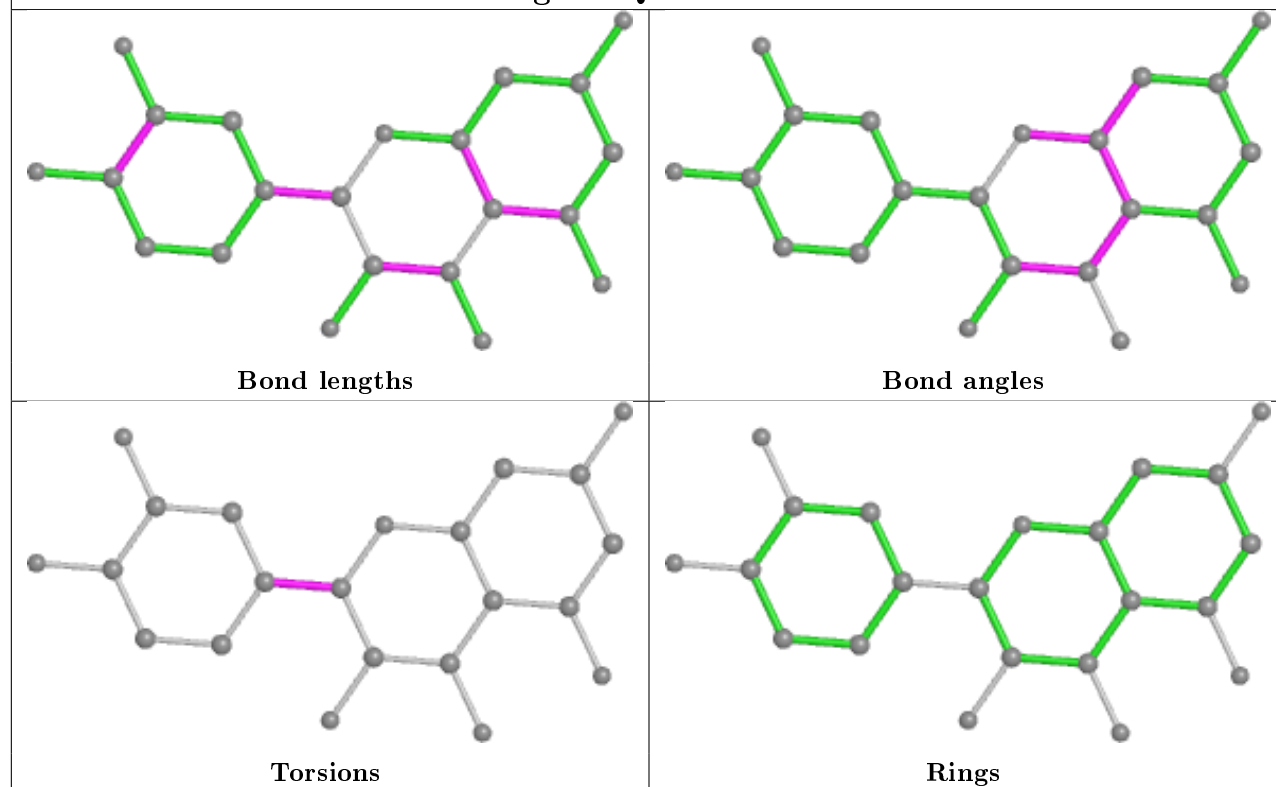


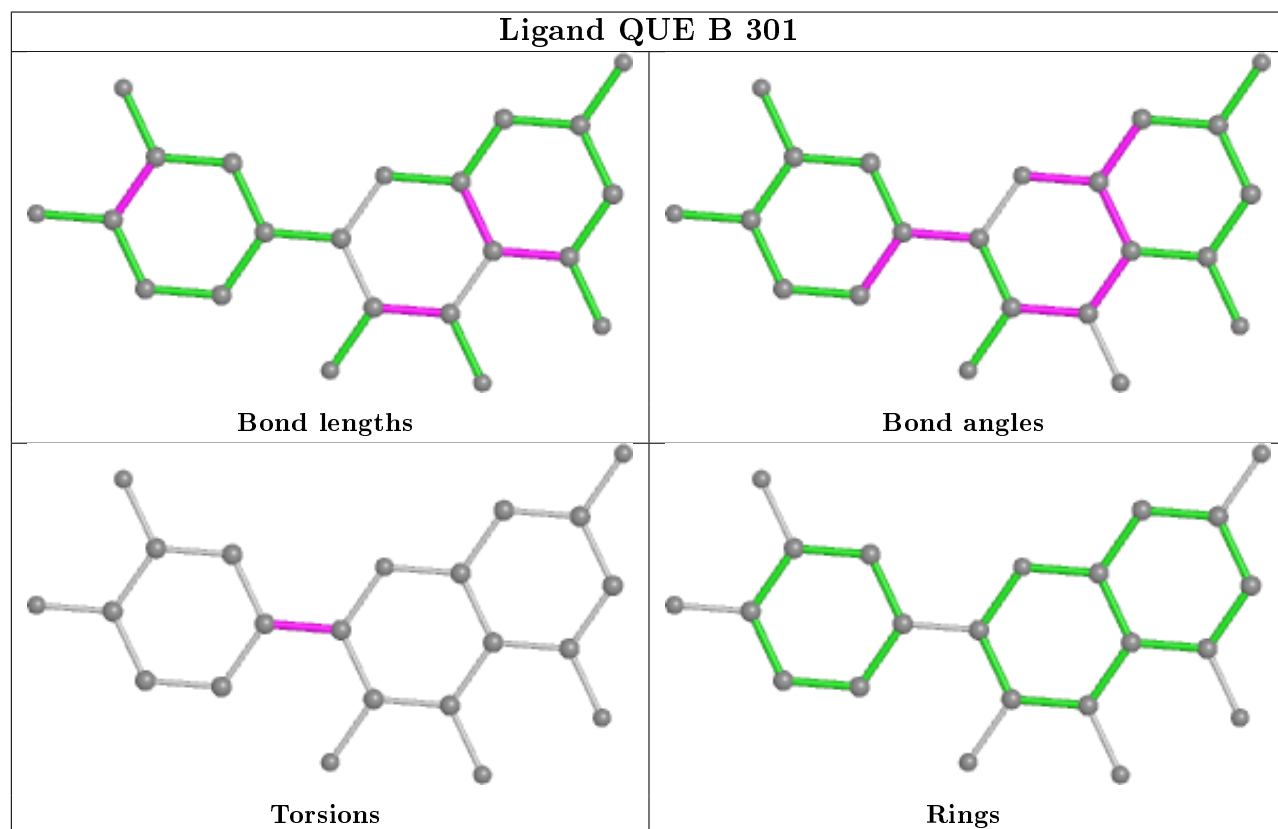
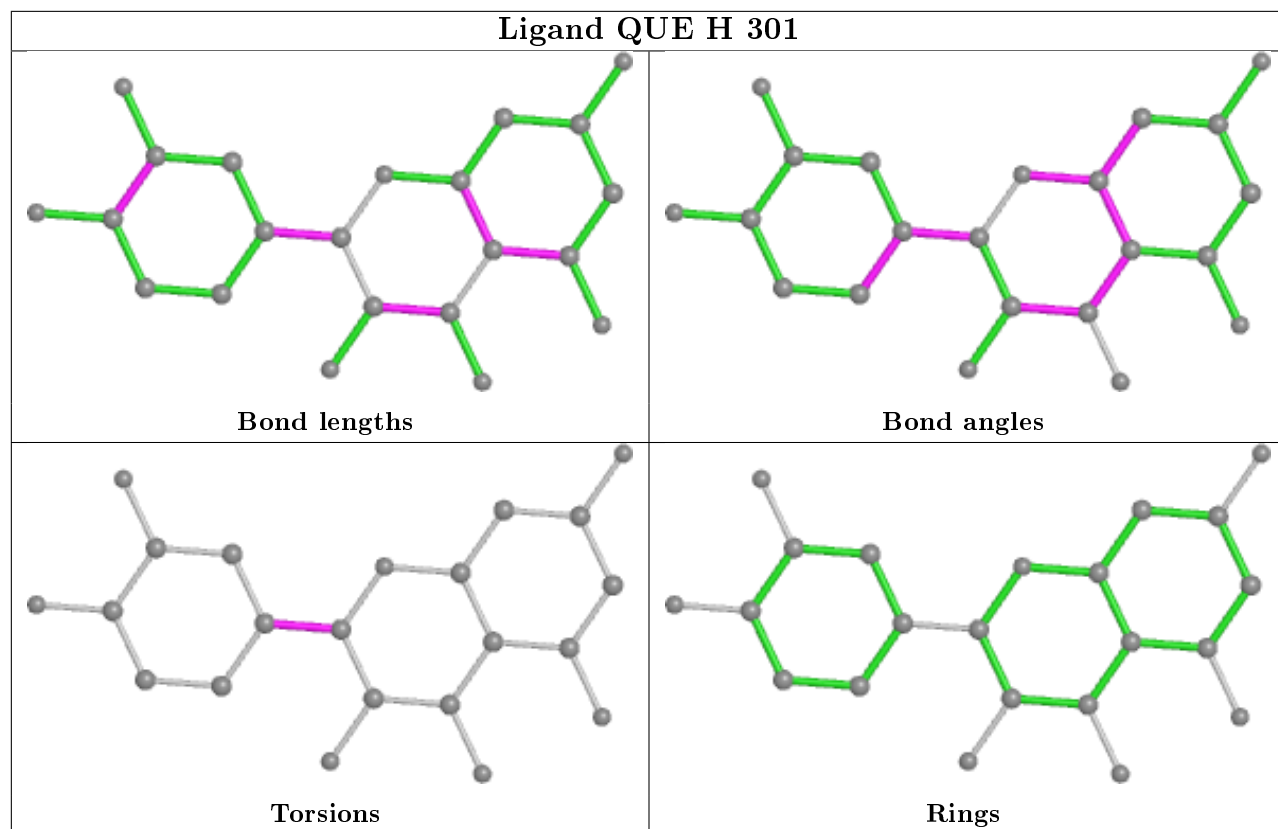


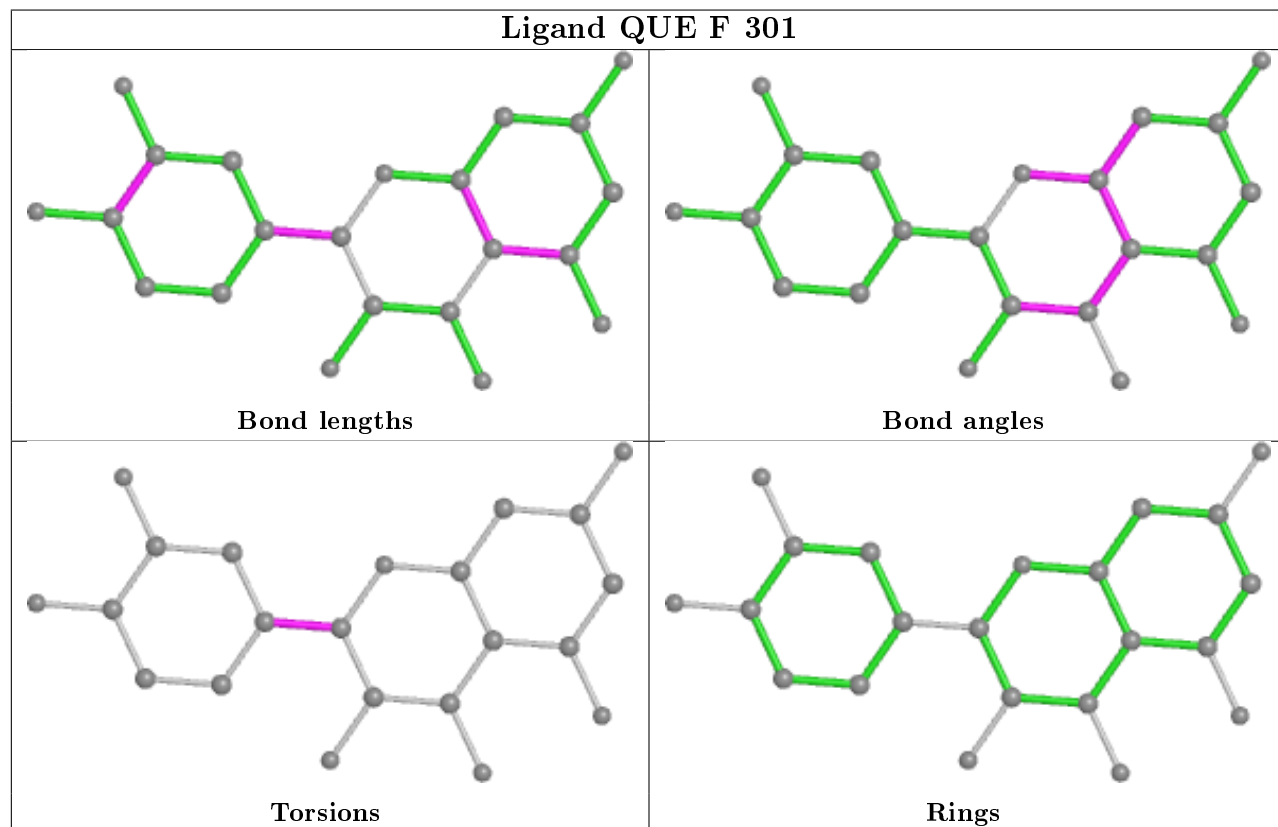
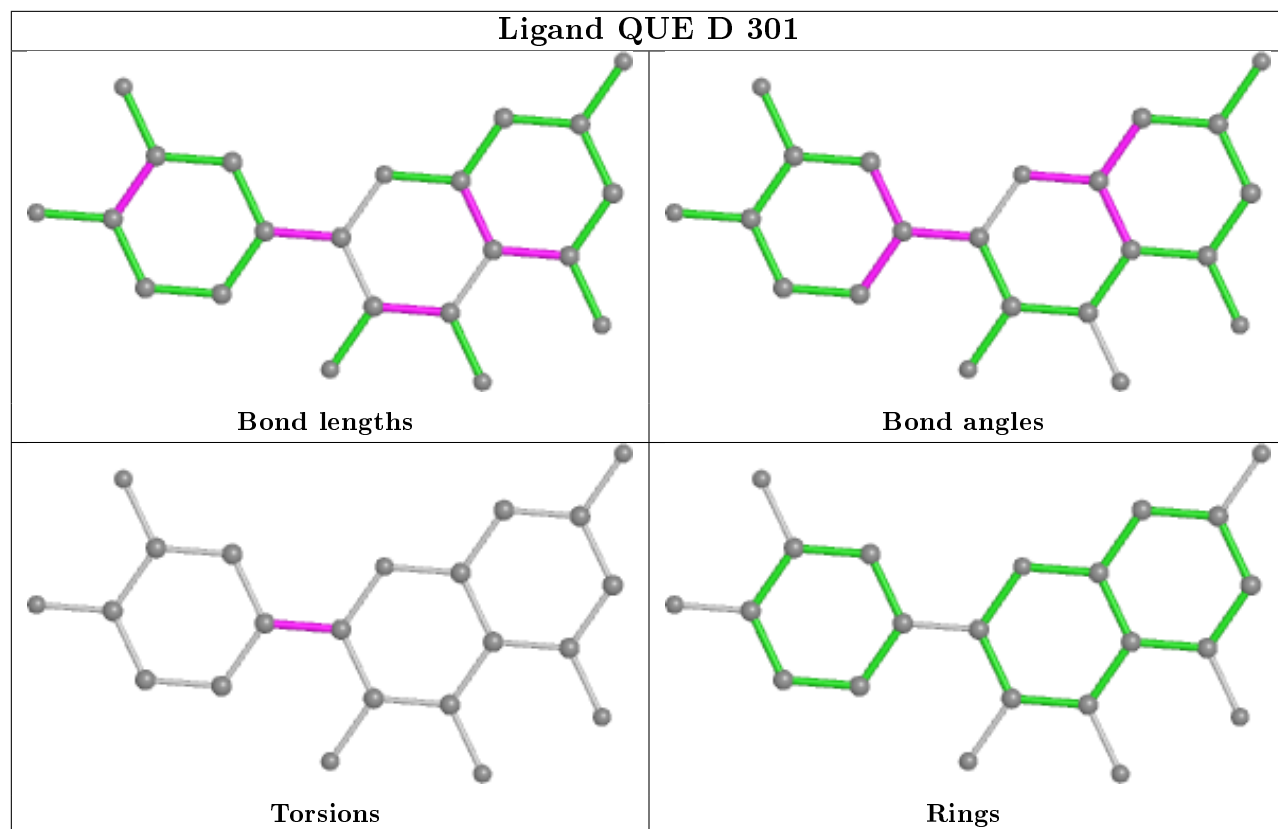
## Ligand QUE J 301

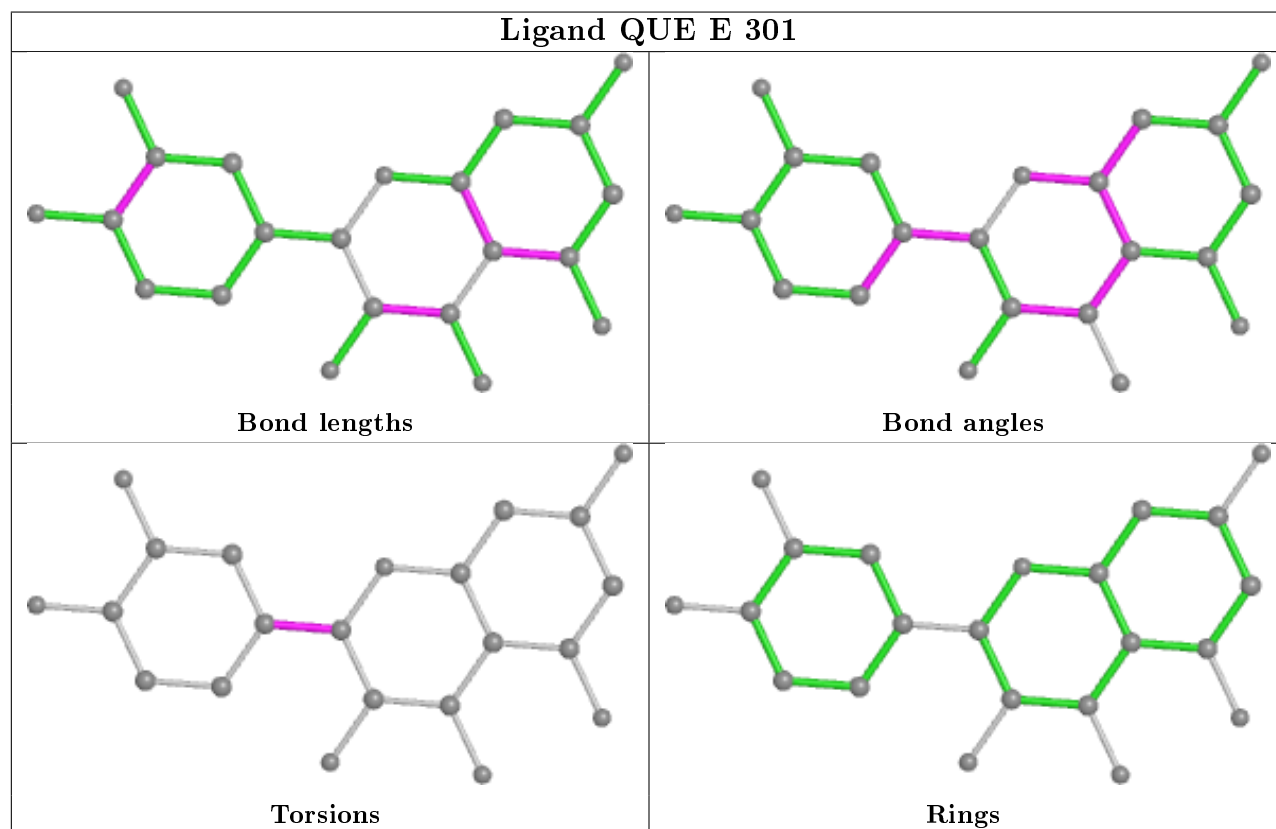
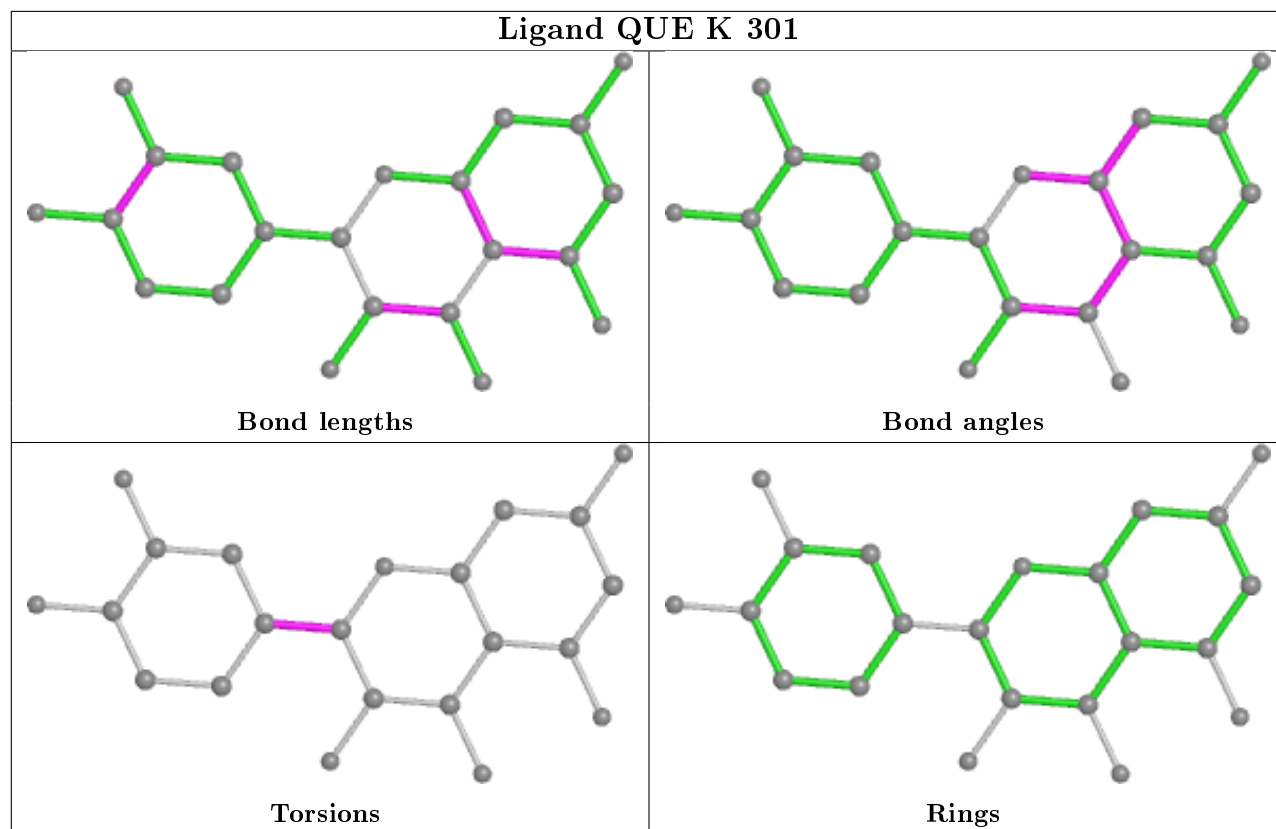


## Ligand QUE L 301











## 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, 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	183/186 (98%)	0.21	7 (3%) 40 49	7, 24, 54, 104	0
1	B	183/186 (98%)	0.25	6 (3%) 46 55	12, 27, 57, 85	0
1	C	183/186 (98%)	0.32	10 (5%) 25 34	11, 27, 60, 88	0
1	D	183/186 (98%)	0.16	5 (2%) 54 63	9, 25, 54, 108	0
1	E	183/186 (98%)	0.77	22 (12%) 4 6	8, 30, 66, 82	0
1	F	183/186 (98%)	0.52	12 (6%) 18 24	7, 33, 77, 109	0
1	G	183/186 (98%)	0.65	16 (8%) 10 14	6, 32, 70, 100	0
1	H	183/186 (98%)	0.31	9 (4%) 29 38	6, 25, 56, 105	0
1	I	183/186 (98%)	0.46	20 (10%) 5 8	10, 35, 71, 94	0
1	J	183/186 (98%)	0.68	17 (9%) 8 13	13, 32, 68, 110	0
1	K	183/186 (98%)	0.55	10 (5%) 25 34	15, 38, 77, 120	0
1	L	183/186 (98%)	0.64	21 (11%) 4 6	8, 32, 72, 95	0
All	All	2196/2232 (98%)	0.46	155 (7%) 16 22	6, 30, 69, 120	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	185	GLY	10.0
1	D	185	GLY	6.6
1	F	185	GLY	6.0
1	I	185	GLY	6.0
1	C	185	GLY	5.5
1	E	164	LYS	5.2
1	L	134	GLY	5.2
1	K	92	LEU	4.9
1	K	183	HIS	4.8
1	G	170	GLU	4.7
1	H	181	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	166	ARG	4.4
1	J	163	GLU	4.3
1	G	6	ALA	4.3
1	G	3	ILE	4.3
1	A	184	THR	4.2
1	H	184	THR	4.2
1	L	181	GLN	3.9
1	D	184	THR	3.8
1	H	92	LEU	3.8
1	H	3	ILE	3.8
1	L	166	ARG	3.7
1	B	3	ILE	3.6
1	J	184	THR	3.6
1	H	185	GLY	3.6
1	B	183	HIS	3.6
1	I	183	HIS	3.6
1	G	167	THR	3.5
1	I	134	GLY	3.5
1	C	166	ARG	3.5
1	K	93	GLU	3.5
1	I	170	GLU	3.4
1	J	183	HIS	3.4
1	E	171	GLN	3.4
1	I	176	PHE	3.4
1	E	172	TYR	3.4
1	I	181	GLN	3.2
1	I	65	VAL	3.2
1	C	179	ASP	3.2
1	J	166	ARG	3.2
1	E	170	GLU	3.1
1	I	184	THR	3.1
1	L	21	LYS	3.1
1	L	133	PRO	3.1
1	J	159	VAL	3.0
1	G	5	TYR	3.0
1	L	172	TYR	3.0
1	L	178	PRO	3.0
1	A	183	HIS	3.0
1	C	184	THR	3.0
1	A	3	ILE	2.9
1	L	175	ARG	2.9
1	J	162	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	184	THR	2.9
1	F	163	GLU	2.8
1	J	179	ASP	2.8
1	J	168	VAL	2.8
1	L	180	HIS	2.8
1	E	92	LEU	2.8
1	A	185	GLY	2.8
1	C	183	HIS	2.8
1	J	92	LEU	2.8
1	F	104	GLY	2.7
1	A	179	ASP	2.7
1	B	58[A]	CYS	2.7
1	E	174	VAL	2.7
1	K	151	LEU	2.7
1	G	7	THR	2.7
1	J	175	ARG	2.7
1	J	176	PHE	2.7
1	F	166	ARG	2.6
1	F	92	LEU	2.6
1	D	175	ARG	2.6
1	K	67	PRO	2.6
1	A	181	GLN	2.6
1	I	166	ARG	2.6
1	L	170	GLU	2.6
1	L	137	PHE	2.6
1	F	21	LYS	2.6
1	I	178	PRO	2.6
1	F	93	GLU	2.5
1	F	162	PRO	2.5
1	L	171	GLN	2.5
1	E	175	ARG	2.5
1	D	183	HIS	2.5
1	H	183	HIS	2.5
1	G	171	GLN	2.5
1	E	167	THR	2.5
1	K	171	GLN	2.5
1	H	179	ASP	2.5
1	G	151	LEU	2.5
1	K	3	ILE	2.4
1	F	181	GLN	2.4
1	I	168	VAL	2.4
1	C	181	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	166	ARG	2.4
1	B	184	THR	2.4
1	L	183	HIS	2.4
1	K	134	GLY	2.4
1	D	167	THR	2.4
1	G	58[A]	CYS	2.4
1	L	174	VAL	2.4
1	C	97	HIS	2.3
1	L	135	GLY	2.3
1	G	163	GLU	2.3
1	K	95	GLU	2.3
1	E	162	PRO	2.3
1	C	65	VAL	2.3
1	E	163	GLU	2.3
1	L	179	ASP	2.3
1	I	64	GLU	2.3
1	E	134	GLY	2.3
1	H	5	TYR	2.3
1	J	134	GLY	2.3
1	E	165	PHE	2.3
1	I	88	PHE	2.3
1	J	180	HIS	2.3
1	G	185	GLY	2.3
1	I	180	HIS	2.3
1	B	126	VAL	2.2
1	E	126	VAL	2.2
1	K	179	ASP	2.2
1	C	165	PHE	2.2
1	E	58[A]	CYS	2.2
1	L	167	THR	2.2
1	L	160	PRO	2.2
1	J	181	GLN	2.2
1	I	73	ASP	2.2
1	E	27	LYS	2.2
1	G	164	LYS	2.2
1	L	162	PRO	2.2
1	G	122	HIS	2.1
1	L	185	GLY	2.1
1	I	163	GLU	2.1
1	H	180	HIS	2.1
1	E	89	VAL	2.1
1	B	5	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	8	ARG	2.1
1	I	137	PHE	2.1
1	J	161	GLU	2.1
1	E	161	GLU	2.1
1	J	170	GLU	2.1
1	L	176	PHE	2.1
1	E	72	ALA	2.1
1	C	182	TRP	2.1
1	I	135	GLY	2.1
1	I	179	ASP	2.0
1	F	171	GLN	2.0
1	I	116	ALA	2.0
1	G	61	PRO	2.0
1	A	180	HIS	2.0
1	E	155	VAL	2.0
1	E	176	PHE	2.0
1	F	88	PHE	2.0
1	E	151	LEU	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 carbohydrates 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(Å <sup>2</sup> )	Q<0.9
3	QUE	J	301	22/22	0.69	0.31	46,46,46,46	22
3	QUE	G	301	22/22	0.72	0.27	47,47,47,47	22
3	QUE	A	301	22/22	0.78	0.29	33,33,33,33	22
3	QUE	B	301	22/22	0.82	0.29	37,37,37,37	22
3	QUE	L	301	22/22	0.83	0.20	44,44,44,44	0

*Continued on next page...*

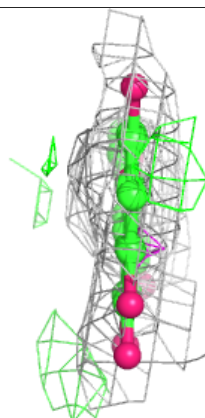
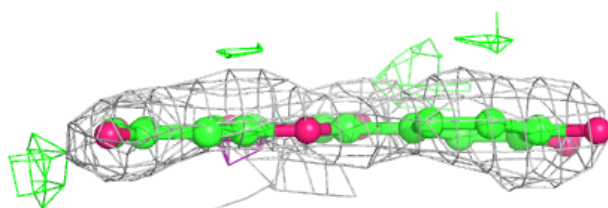
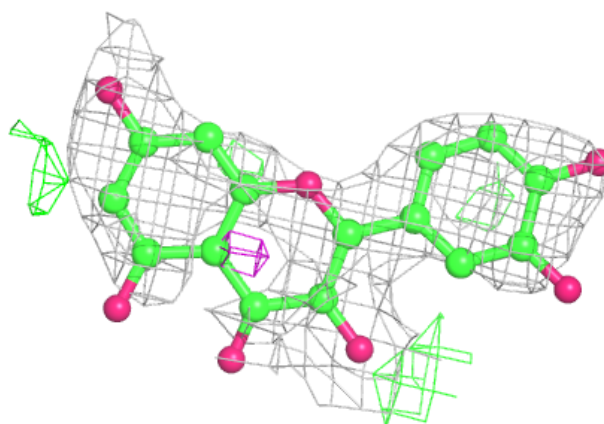
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	QUE	F	301	22/22	0.83	0.19	37,37,37,37	22
3	QUE	E	301	22/22	0.84	0.21	37,37,37,37	22
3	QUE	K	301	22/22	0.85	0.22	40,40,40,40	22
3	QUE	C	301	22/22	0.87	0.24	50,50,50,50	22
3	QUE	D	301	22/22	0.88	0.22	27,27,27,27	22
3	QUE	H	301	22/22	0.94	0.11	22,22,22,22	22
2	NI	I	300	1/1	0.96	0.12	32,32,32,32	0
2	NI	J	300	1/1	0.98	0.10	37,37,37,37	0
2	NI	K	300	1/1	0.98	0.12	43,43,43,43	0
2	NI	G	300	1/1	0.99	0.09	23,23,23,23	0
2	NI	B	300	1/1	0.99	0.12	21,21,21,21	0
2	NI	D	300	1/1	0.99	0.10	17,17,17,17	0
2	NI	F	300	1/1	0.99	0.12	34,34,34,34	0
2	NI	E	300	1/1	0.99	0.12	28,28,28,28	0
2	NI	L	300	1/1	0.99	0.10	28,28,28,28	0
2	NI	H	300	1/1	0.99	0.10	22,22,22,22	0
2	NI	C	300	1/1	1.00	0.09	25,25,25,25	0
2	NI	A	300	1/1	1.00	0.12	22,22,22,22	0

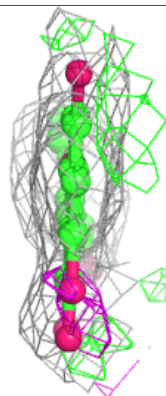
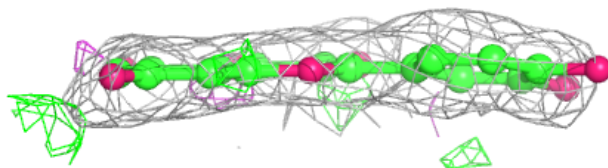
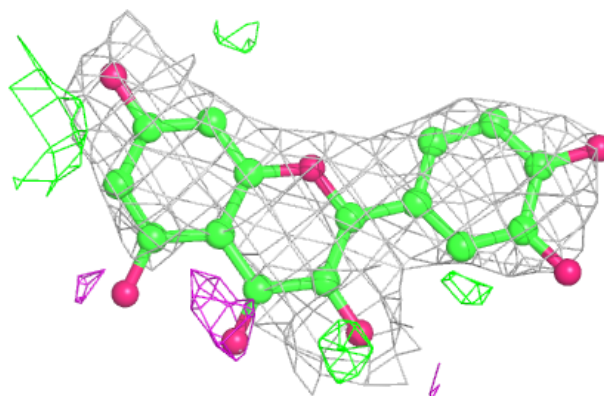
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around QUE J 301:**

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

**Electron density around QUE G 301:**

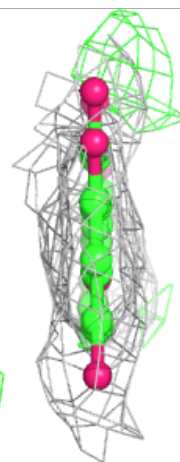
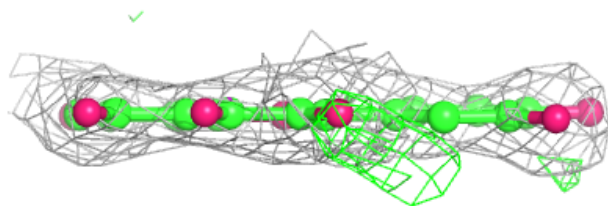
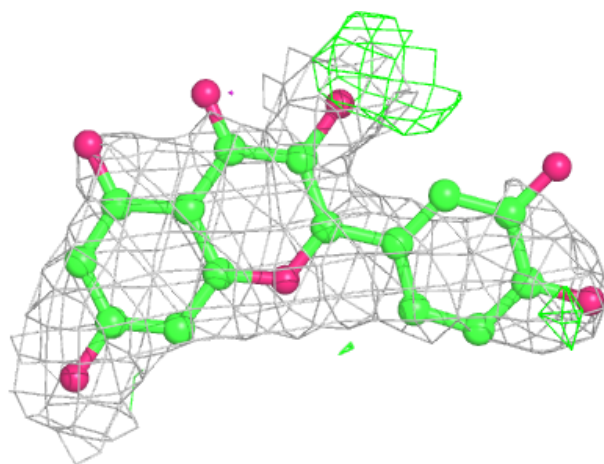
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





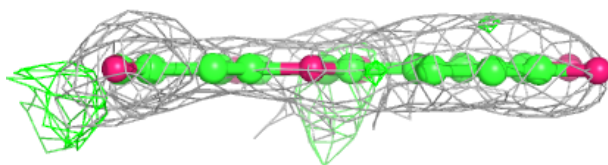
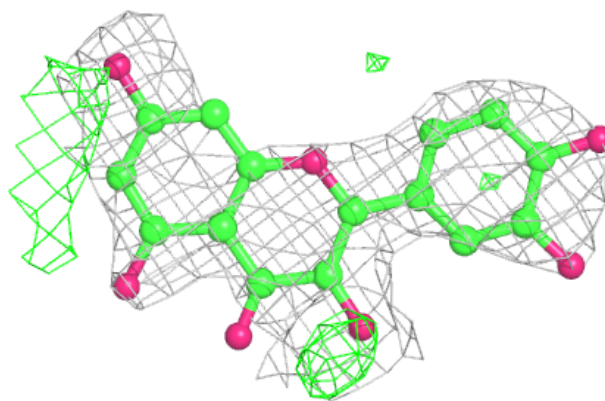
**Electron density around QUE A 301:**

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

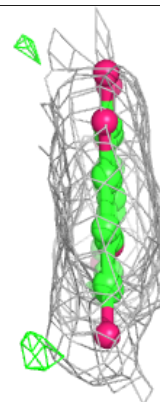
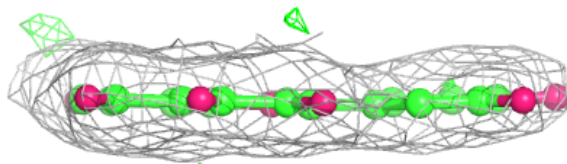
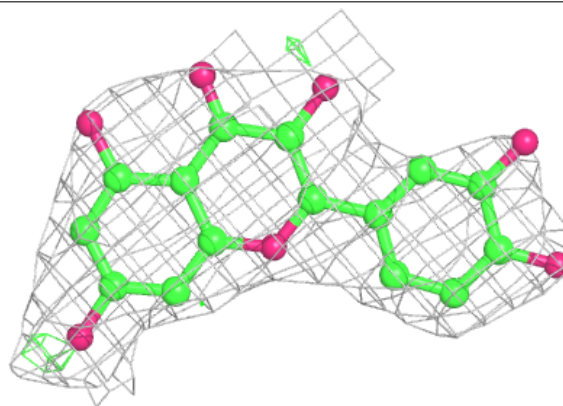


**Electron density around QUE B 301:**

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

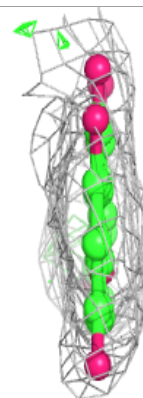
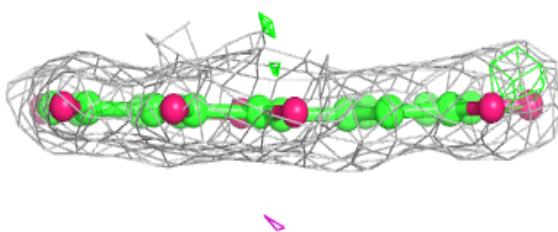
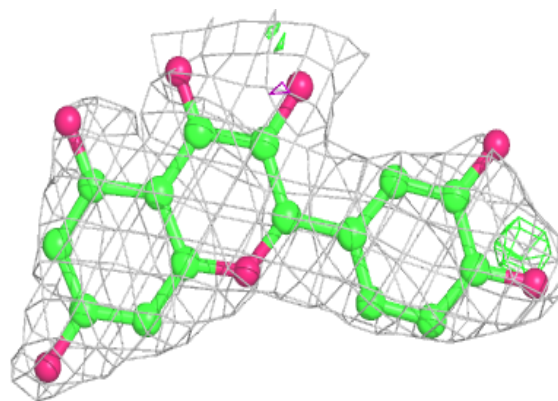
**Electron density around QUE L 301:**

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

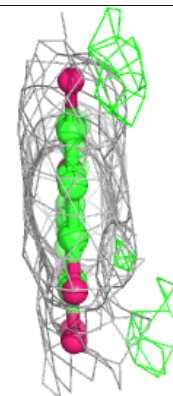
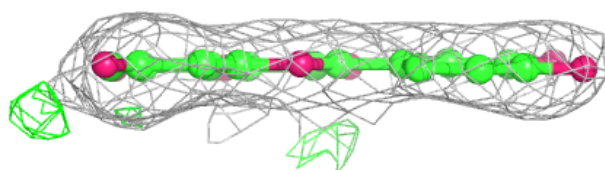
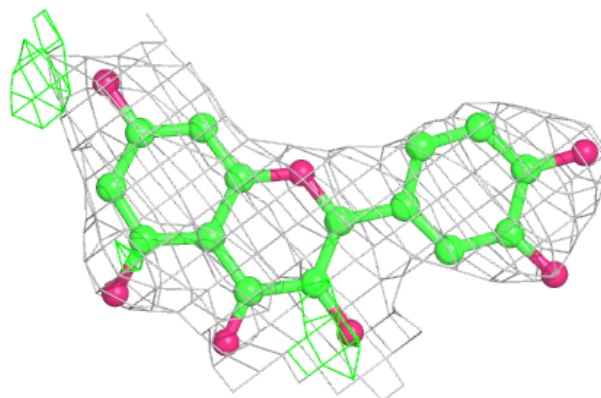


**Electron density around QUE F 301:**

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

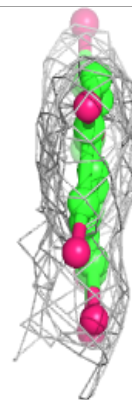
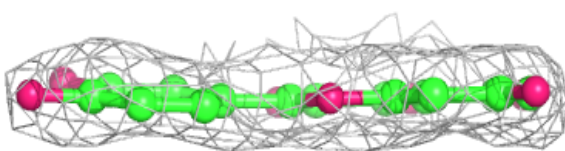
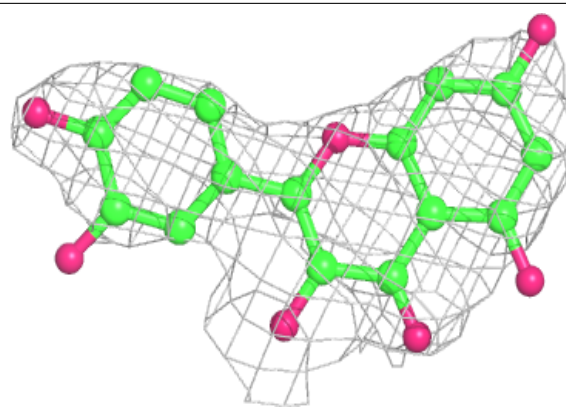
**Electron density around QUE E 301:**

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

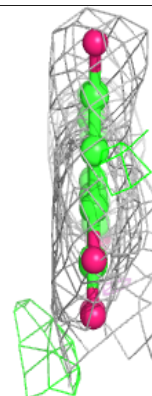
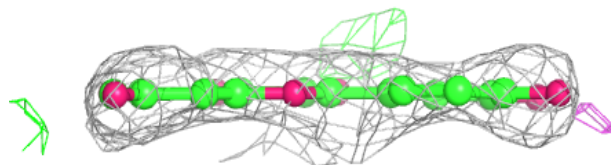
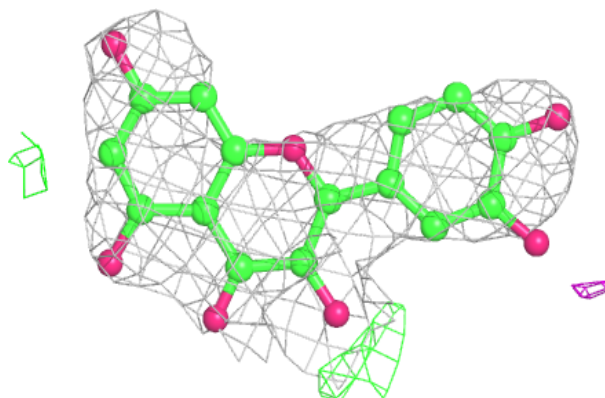


**Electron density around QUE K 301:**

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

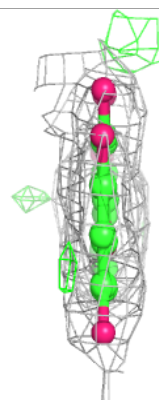
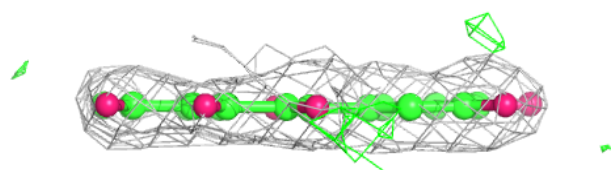
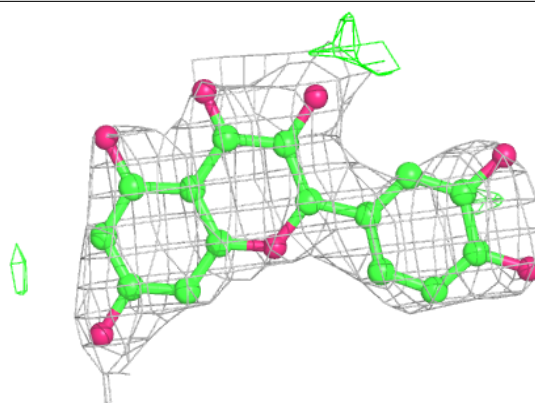
**Electron density around QUE C 301:**

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

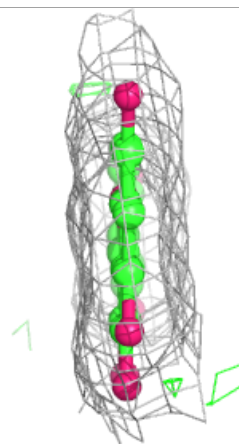
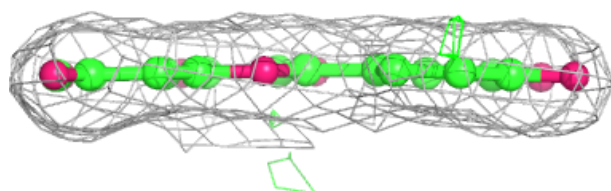
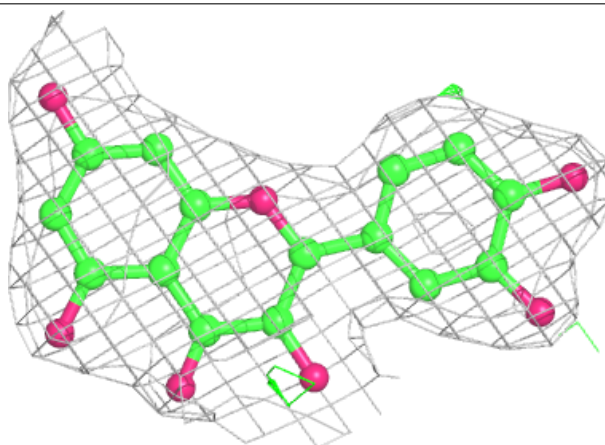


**Electron density around QUE D 301:**

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

**Electron density around QUE H 301:**

$2mF_o-DF_c$  (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.