



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:57 PM UTC

PDB ID : 5FLJ / pdb_00005flj
Title : enzyme-substrate-dioxygen complex of Ni-quercetinase
Authors : Jeoung, J.-H.; Nianios, D.; Fetzner, S.; Dobbek, H.
Deposited on : 2015-10-26
Resolution : 1.82 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	F	186	 2% 92% 5% ..
1	G	186	 2% 91% 7% ..
1	H	186	 3% 90% 8% ..
1	I	186	 2% 91% 7% .
1	J	186	 3% 87% 12% .
1	K	186	 3% 91% 6% ..
1	L	186	 1% 91% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OXY	C	302	-	-	X	-
5	OXY	F	302	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19465 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	182	Total	C	N	O	S	0	3	0
			1484	956	256	269	3			
1	B	183	Total	C	N	O	S	0	3	0
			1493	959	261	270	3			
1	C	183	Total	C	N	O	S	0	6	0
			1511	971	266	270	4			
1	D	183	Total	C	N	O	S	0	4	0
			1493	959	259	271	4			
1	E	183	Total	C	N	O	S	0	3	0
			1486	954	256	272	4			
1	F	183	Total	C	N	O	S	0	1	0
			1479	950	257	269	3			
1	G	183	Total	C	N	O	S	0	3	0
			1488	956	258	270	4			
1	H	183	Total	C	N	O	S	0	3	0
			1488	956	257	271	4			
1	I	183	Total	C	N	O	S	0	2	0
			1485	954	258	270	3			
1	J	183	Total	C	N	O	S	0	1	0
			1478	949	256	270	3			
1	K	183	Total	C	N	O	S	0	1	0
			1479	950	257	269	3			
1	L	184	Total	C	N	O	S	0	1	0
			1485	953	257	272	3			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

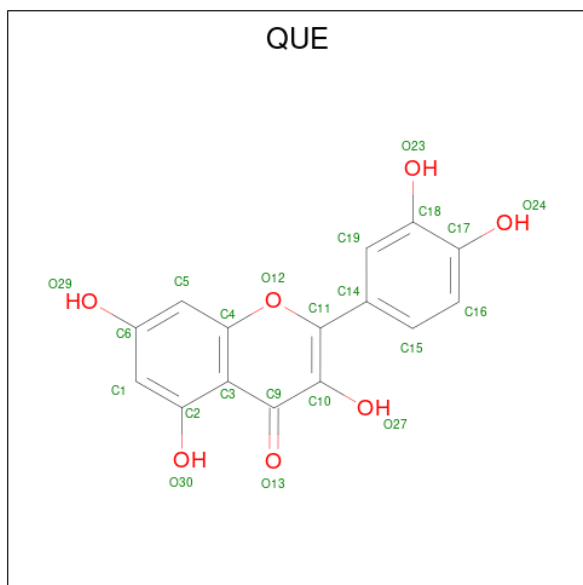
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		

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

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



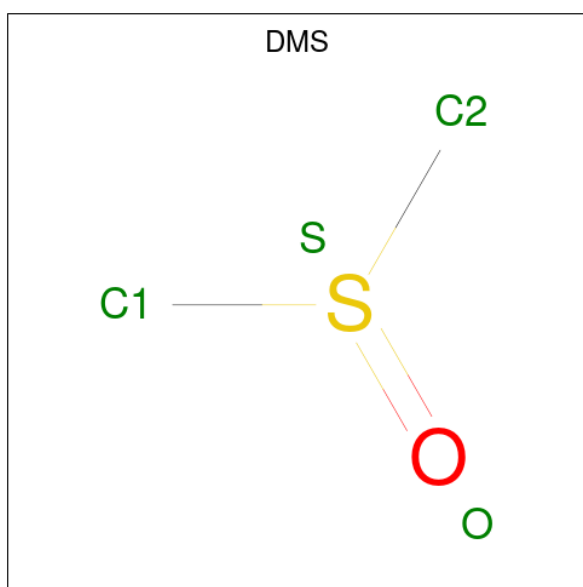
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	15	7		

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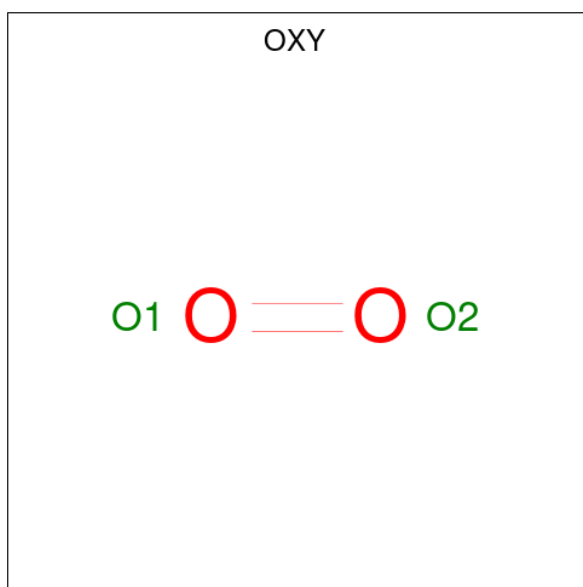
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			22	15	7		
3	C	1	Total	C	O	0	0
			22	15	7		
3	D	1	Total	C	O	0	0
			22	15	7		
3	E	1	Total	C	O	0	0
			22	15	7		
3	F	1	Total	C	O	0	0
			22	15	7		
3	G	1	Total	C	O	0	0
			22	15	7		
3	H	1	Total	C	O	0	0
			22	15	7		
3	I	1	Total	C	O	0	0
			22	15	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 DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 1	S 1	0	0
4	B	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	D	1	Total 4	C 2	O 1	S 1	0	0
4	E	1	Total 4	C 2	O 1	S 1	0	0
4	E	1	Total 4	C 2	O 1	S 1	0	0
4	F	1	Total 4	C 2	O 1	S 1	0	0
4	G	1	Total 4	C 2	O 1	S 1	0	0
4	H	1	Total 4	C 2	O 1	S 1	0	0
4	H	1	Total 4	C 2	O 1	S 1	0	0
4	I	1	Total 4	C 2	O 1	S 1	0	0
4	J	1	Total 4	C 2	O 1	S 1	0	0
4	K	1	Total 4	C 2	O 1	S 1	0	0
4	L	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 2 2	0	0
5	F	1	Total O 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	112	Total O 112 112	0	0
6	B	119	Total O 119 119	0	0
6	C	124	Total O 124 124	0	0
6	D	119	Total O 119 119	0	0
6	E	121	Total O 121 121	0	0
6	F	105	Total O 105 105	0	0
6	G	123	Total O 123 123	0	0
6	H	105	Total O 105 105	0	0
6	I	100	Total O 100 100	0	0
6	J	81	Total O 81 81	0	0

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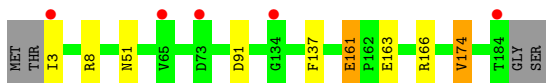
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	82	Total	O	0	0
			82	82		
6	L	85	Total	O	0	0
			85	85		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

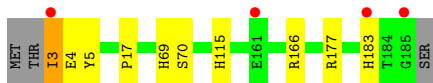
- Molecule 1: QUERCETINASE QUED



- Molecule 1: QUERCETINASE QUED



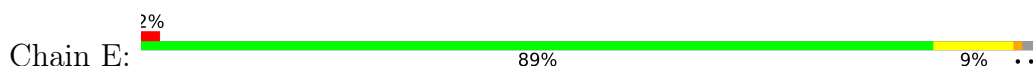
- Molecule 1: QUERCETINASE QUED



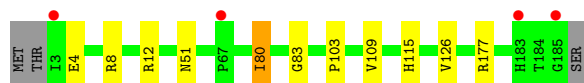
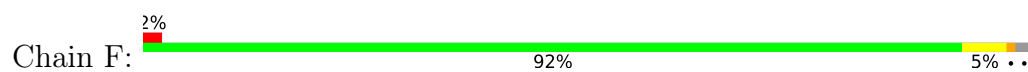
- Molecule 1: QUERCETINASE QUED



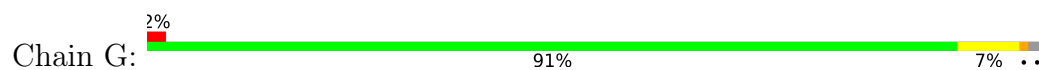
- Molecule 1: QUERCETINASE QUED



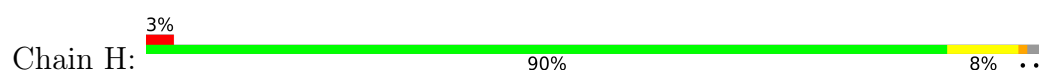
- Molecule 1: QUERCETINASE QUED



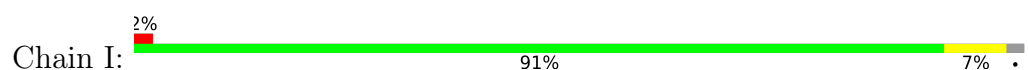
• Molecule 1: QUERCETINASE QUED



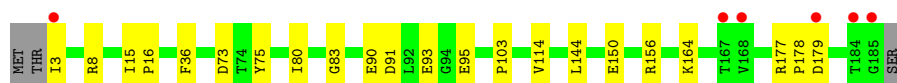
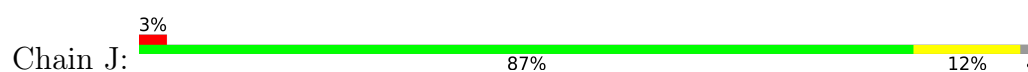
• Molecule 1: QUERCETINASE QUED



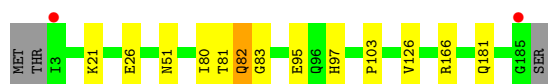
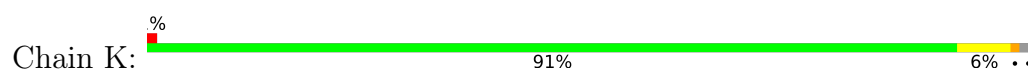
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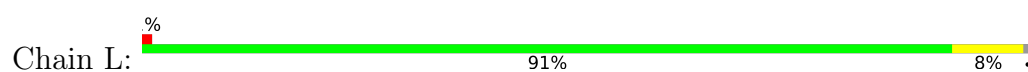
• Molecule 1: QUERCETINASE QUED



• 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, α , β , γ	102.81Å 114.59Å 105.99Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	38.80 – 1.82 38.80 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.1 (38.80-1.82) 96.1 (38.80-1.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.82Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.164 , 0.208 0.167 , 0.209	Depositor DCC
R_{free} test set	10534 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for l,k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19465	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: OXY, QUE, DMS, NI

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	0.47	0/1543	0.78	0/2095
1	B	0.49	0/1553	0.77	0/2108
1	C	0.51	0/1581	0.80	0/2147
1	D	0.52	0/1556	0.77	0/2113
1	E	0.51	0/1545	0.79	0/2098
1	F	0.53	0/1533	0.79	2/2082 (0.1%)
1	G	0.52	0/1548	0.83	1/2102 (0.0%)
1	H	0.53	0/1548	0.81	2/2102 (0.1%)
1	I	0.49	0/1542	0.77	0/2094
1	J	0.47	0/1531	0.80	3/2079 (0.1%)
1	K	0.51	0/1533	0.81	0/2082
1	L	0.46	0/1538	0.77	0/2089
All	All	0.50	0/18551	0.79	8/25191 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	135	GLY	N-CA-C	7.45	121.55	110.97
1	H	66	ILE	CA-C-N	-5.95	113.81	119.76
1	H	66	ILE	C-N-CA	-5.95	113.81	119.76
1	J	177	ARG	CA-C-N	5.49	126.70	119.84
1	J	177	ARG	C-N-CA	5.49	126.70	119.84
1	J	36	PHE	CB-CA-C	-5.41	110.32	116.54
1	F	177	ARG	CA-C-N	5.25	124.92	119.56
1	F	177	ARG	C-N-CA	5.25	124.92	119.56

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	1484	0	1412	4	0
1	B	1493	0	1413	3	0
1	C	1511	0	1438	6	0
1	D	1493	0	1411	9	0
1	E	1486	0	1402	15	0
1	F	1479	0	1392	5	0
1	G	1488	0	1405	6	0
1	H	1488	0	1403	9	0
1	I	1485	0	1400	8	0
1	J	1478	0	1393	12	0
1	K	1479	0	1392	8	0
1	L	1485	0	1400	12	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	6	0	0
3	B	22	0	6	0	0
3	C	22	0	7	3	0
3	D	22	0	8	0	0
3	E	22	0	6	0	0
3	F	22	0	6	2	0
3	G	22	0	7	0	0
3	H	22	0	6	0	0
3	I	22	0	6	0	0
3	J	22	0	7	0	0
3	K	22	0	7	0	0
3	L	22	0	6	0	0
4	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	1	0
4	D	12	0	18	2	0
4	E	8	0	12	5	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	8	0	12	0	0
4	I	4	0	6	2	0
4	J	4	0	6	2	0
4	K	4	0	6	0	0
4	L	4	0	6	1	0
5	C	2	0	0	3	0
5	F	2	0	0	3	0
6	A	112	0	0	1	0
6	B	119	0	0	1	0
6	C	124	0	0	1	0
6	D	119	0	0	2	0
6	E	121	0	0	5	0
6	F	105	0	0	0	0
6	G	123	0	0	2	0
6	H	105	0	0	1	0
6	I	100	0	0	1	0
6	J	81	0	0	5	0
6	K	82	0	0	0	0
6	L	85	0	0	0	0
All	All	19465	0	17029	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (96) 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)
3:F:301:QUE:C10	5:F:302:OXY:O1	2.34	0.76
3:C:301:QUE:C10	5:C:302:OXY:O2	2.34	0.75
4:I:1186:DMS:O	6:I:2057:HOH:O	2.03	0.74
1:H:82:GLN:HE22	1:L:82[B]:GLN:HE22	1.36	0.72
1:H:163:GLU:OE2	1:H:166:ARG:NH2	2.23	0.71
6:G:2054:HOH:O	1:K:26:GLU:OE1	2.10	0.69
1:G:82[A]:GLN:NE2	1:K:82:GLN:OE1	2.26	0.67
1:F:115:HIS:CD2	5:F:302:OXY:O2	2.50	0.65
1:F:80:ILE:HD12	1:F:126:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:SER:OG	1:C:177[B]:ARG:NH2	2.33	0.62
1:C:115:HIS:CD2	5:C:302:OXY:O1	2.52	0.62
1:E:80:ILE:HD12	1:E:126:VAL:HG22	1.83	0.60
6:J:2027:HOH:O	1:L:156:ARG:NH1	2.34	0.60
1:E:95:GLU:HG3	1:E:97:HIS:CE1	2.37	0.60
1:K:95:GLU:HG3	1:K:97:HIS:CE1	2.37	0.58
6:H:2055:HOH:O	1:L:26:GLU:OE1	2.17	0.58
1:J:179:ASP:N	6:J:2081:HOH:O	2.36	0.57
1:H:161:GLU:HG2	1:H:164:LYS:HG3	1.88	0.56
1:K:95:GLU:HG3	1:K:97:HIS:HE1	1.71	0.56
1:G:59:GLU:OE2	1:G:123:HIS:HE1	1.89	0.55
1:B:3:ILE:N	6:B:2001:HOH:O	2.39	0.54
1:I:82[A]:GLN:HE21	4:J:1186:DMS:H22	1.73	0.54
1:D:150:GLU:H	1:D:150:GLU:CD	2.16	0.53
1:E:181:GLN:NE2	6:E:2119:HOH:O	2.42	0.52
1:D:161:GLU:HG3	1:D:164:LYS:HG3	1.90	0.52
1:F:83:GLY:O	1:F:103:PRO:HD3	2.09	0.52
1:J:73:ASP:OD1	6:J:2046:HOH:O	2.19	0.52
1:J:90:GLU:HB3	1:J:114:VAL:HG12	1.91	0.52
1:D:58[B]:CYS:SG	1:D:126:VAL:HB	2.50	0.52
1:E:150:GLU:H	1:E:150:GLU:CD	2.21	0.49
1:H:82:GLN:NE2	1:L:82[B]:GLN:HE22	2.08	0.49
1:F:109:VAL:HG11	1:F:115:HIS:CG	2.48	0.48
1:K:81:THR:C	1:K:82:GLN:HG2	2.38	0.48
1:H:4:GLU:OE1	1:H:12:ARG:NE	2.46	0.48
1:H:155:VAL:HG11	1:J:150:GLU:HG3	1.97	0.46
1:L:80:ILE:HD12	1:L:126:VAL:HG22	1.96	0.46
1:K:83:GLY:O	1:K:103:PRO:HD3	2.15	0.46
1:E:34:HIS:CD2	1:E:154:PRO:HB3	2.51	0.46
1:E:71:HIS:CD2	1:E:76:GLU:OE2	2.56	0.46
1:L:103:PRO:HB3	4:L:1186:DMS:H13	1.98	0.46
1:C:5:TYR:HB3	1:C:17:PRO:HD3	1.98	0.46
1:L:167:THR:O	1:L:170:GLU:HG2	2.16	0.46
1:H:164:LYS:O	1:H:168:VAL:HG22	2.16	0.45
4:I:1186:DMS:H21	6:J:2025:HOH:O	2.16	0.45
1:H:83:GLY:O	1:H:103:PRO:HD3	2.16	0.45
1:I:183:HIS:O	1:I:183:HIS:ND1	2.50	0.45
1:I:66:ILE:HB	1:I:67:PRO:HD2	1.99	0.45
3:F:301:QUE:C11	5:F:302:OXY:O1	2.64	0.45
1:I:50:GLU:OE2	1:J:75:TYR:OH	2.34	0.44
1:L:83:GLY:O	1:L:103:PRO:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:QUE:C11	5:C:302:OXY:O2	2.64	0.44
1:A:137:PHE:CE1	1:A:174:VAL:HG22	2.53	0.44
1:F:4:GLU:OE1	1:F:12:ARG:HD2	2.18	0.44
1:G:161:GLU:HG3	1:G:164:LYS:HG3	2.01	0.43
1:E:32:ARG:HH12	4:E:1187:DMS:C1	2.31	0.43
1:E:91:ASP:HB2	6:E:2083:HOH:O	2.17	0.43
1:C:183[B]:HIS:ND1	6:C:2126:HOH:O	2.36	0.43
1:D:21:LYS:NZ	6:D:2027:HOH:O	2.41	0.43
1:D:173:ASP:H	4:D:1188:DMS:C2	2.31	0.43
1:J:83:GLY:O	1:J:103:PRO:HD3	2.18	0.43
1:E:67:PRO:HB2	6:E:2069:HOH:O	2.19	0.43
1:A:163:GLU:OE2	1:A:166:ARG:NH1	2.51	0.43
1:D:83:GLY:O	1:D:103:PRO:HD3	2.19	0.43
1:A:161:GLU:H	1:A:161:GLU:HG3	1.62	0.42
1:C:69:HIS:NE2	3:C:301:QUE:O13	2.52	0.42
1:E:47:GLU:HG2	6:E:2007:HOH:O	2.18	0.42
1:E:99:LYS:NZ	6:E:2087:HOH:O	2.53	0.42
1:I:21:LYS:HB2	1:I:21:LYS:HE3	1.70	0.42
1:I:95:GLU:HG2	1:I:97:HIS:CE1	2.55	0.42
1:E:32:ARG:HH12	4:E:1187:DMS:H13	1.85	0.41
1:J:3:ILE:N	6:J:2001:HOH:O	2.54	0.41
1:D:71:HIS:CD2	1:D:115:HIS:HE1	2.39	0.41
1:E:32:ARG:HH22	4:E:1187:DMS:H22	1.85	0.41
1:L:66:ILE:HG12	1:L:117:TYR:H	1.85	0.41
1:I:159:VAL:HA	1:I:160:PRO:HD3	1.92	0.41
1:J:91:ASP:OD2	1:J:95:GLU:HB3	2.21	0.41
1:J:156:ARG:HH22	1:L:150:GLU:CD	2.27	0.41
1:J:15:ILE:HA	1:J:16:PRO:HD3	1.95	0.41
1:J:156:ARG:NH2	1:L:150:GLU:OE2	2.50	0.41
1:B:27:LYS:NZ	4:B:1186:DMS:H12	2.36	0.41
1:D:173:ASP:H	4:D:1188:DMS:H23	1.86	0.41
1:E:104:GLY:CA	4:E:1186:DMS:H22	2.51	0.41
6:G:2034:HOH:O	1:K:82:GLN:NE2	2.54	0.41
1:C:3:ILE:HD12	1:C:4:GLU:O	2.21	0.40
1:H:66:ILE:HB	1:H:67:PRO:HD2	2.03	0.40
1:L:21:LYS:HE2	1:L:21:LYS:HB2	1.75	0.40
1:I:82[A]:GLN:HE21	4:J:1186:DMS:C2	2.35	0.40
1:J:144:LEU:O	1:J:164:LYS:HE3	2.21	0.40
1:D:156:ARG:HD2	6:D:2105:HOH:O	2.21	0.40
1:G:83:GLY:O	1:G:103:PRO:HD3	2.22	0.40
1:A:91:ASP:HB2	6:A:2080:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:ILE:HG13	1:G:4:GLU:HG3	2.02	0.40
1:B:163:GLU:HA	1:B:166:ARG:NH2	2.37	0.40
1:E:104:GLY:HA3	4:E:1186:DMS:H22	2.03	0.40
1:G:5:TYR:HB3	1:G:17:PRO:HD3	2.03	0.40
1:K:80:ILE:HD12	1:K:126:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
1	B	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
1	C	187/186 (100%)	185 (99%)	2 (1%)	0	100	100
1	D	185/186 (100%)	184 (100%)	1 (0%)	0	100	100
1	E	184/186 (99%)	182 (99%)	2 (1%)	0	100	100
1	F	182/186 (98%)	179 (98%)	3 (2%)	0	100	100
1	G	184/186 (99%)	182 (99%)	2 (1%)	0	100	100
1	H	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
1	I	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
1	J	182/186 (98%)	177 (97%)	4 (2%)	1 (0%)	24	14
1	K	182/186 (98%)	181 (100%)	1 (0%)	0	100	100
1	L	183/186 (98%)	182 (100%)	1 (0%)	0	100	100
All	All	2203/2232 (99%)	2172 (99%)	30 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	178	PRO

5.3.2 Protein sidechains ⓘ

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	156/156 (100%)	151 (97%)	5 (3%)	34	16
1	B	156/156 (100%)	150 (96%)	6 (4%)	29	11
1	C	159/156 (102%)	157 (99%)	2 (1%)	61	50
1	D	157/156 (101%)	155 (99%)	2 (1%)	61	50
1	E	156/156 (100%)	154 (99%)	2 (1%)	61	50
1	F	154/156 (99%)	151 (98%)	3 (2%)	50	37
1	G	156/156 (100%)	153 (98%)	3 (2%)	50	37
1	H	156/156 (100%)	154 (99%)	2 (1%)	61	50
1	I	155/156 (99%)	152 (98%)	3 (2%)	50	37
1	J	154/156 (99%)	151 (98%)	3 (2%)	50	37
1	K	154/156 (99%)	149 (97%)	5 (3%)	34	16
1	L	155/156 (99%)	153 (99%)	2 (1%)	61	50
All	All	1868/1872 (100%)	1830 (98%)	38 (2%)	47	35

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	8	ARG
1	A	51	ASN
1	A	161	GLU
1	A	174	VAL
1	B	3	ILE
1	B	161	GLU
1	B	163	GLU
1	B	171	GLN
1	B	179	ASP

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Mol	Chain	Res	Type
1	B	183	HIS
1	C	3	ILE
1	C	166	ARG
1	D	3	ILE
1	D	66	ILE
1	E	80	ILE
1	E	161	GLU
1	F	8	ARG
1	F	51	ASN
1	F	80	ILE
1	G	18	GLU
1	G	65	VAL
1	G	161	GLU
1	H	51	ASN
1	H	184	THR
1	I	4	GLU
1	I	80	ILE
1	I	99	LYS
1	J	8	ARG
1	J	80	ILE
1	J	93	GLU
1	K	21	LYS
1	K	51	ASN
1	K	82	GLN
1	K	166	ARG
1	K	181	GLN
1	L	3	ILE
1	L	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	97	HIS
1	A	125	GLN
1	B	97	HIS
1	B	171	GLN
1	B	180	HIS
1	C	125	GLN
1	E	34	HIS
1	E	97	HIS
1	F	82	GLN

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Mol	Chain	Res	Type
1	G	97	HIS
1	G	123	HIS
1	H	51	ASN
1	H	82	GLN
1	H	97	HIS
1	H	171	GLN
1	J	125	GLN
1	J	180	HIS
1	K	82	GLN
1	K	97	HIS
1	L	51	ASN
1	L	125	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 12 are monoatomic - leaving 29 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	$\# Z > 2$
4	DMS	H	1186	-	3,3,3	0.64	0	3,3,3	0.64	0
3	QUE	C	301	2	24,24,24	2.44	3 (12%)	36,36,36	2.15	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QUE	F	301	2	24,24,24	2.53	3 (12%)	36,36,36	2.12	9 (25%)
4	DMS	D	1188	-	3,3,3	0.67	0	3,3,3	0.76	0
4	DMS	H	1187	-	3,3,3	0.66	0	3,3,3	0.60	0
4	DMS	J	1186	-	3,3,3	0.61	0	3,3,3	0.47	0
3	QUE	A	301	2	24,24,24	1.26	2 (8%)	36,36,36	1.23	4 (11%)
4	DMS	D	1186	-	3,3,3	0.61	0	3,3,3	0.48	0
3	QUE	H	301	2	24,24,24	1.53	5 (20%)	36,36,36	1.49	6 (16%)
4	DMS	K	1186	-	3,3,3	0.60	0	3,3,3	0.33	0
4	DMS	E	1187	-	3,3,3	0.66	0	3,3,3	0.64	0
3	QUE	J	301	2	24,24,24	1.25	3 (12%)	36,36,36	1.15	3 (8%)
4	DMS	A	1185	-	3,3,3	0.61	0	3,3,3	0.54	0
4	DMS	B	1186	-	3,3,3	0.54	0	3,3,3	0.46	0
3	QUE	K	301	2	24,24,24	1.38	4 (16%)	36,36,36	1.27	7 (19%)
4	DMS	D	1187	-	3,3,3	0.65	0	3,3,3	0.57	0
3	QUE	E	301	2	24,24,24	1.65	5 (20%)	36,36,36	1.27	4 (11%)
3	QUE	B	301	2	24,24,24	1.09	1 (4%)	36,36,36	1.40	6 (16%)
3	QUE	I	301	2	24,24,24	1.49	4 (16%)	36,36,36	1.20	2 (5%)
4	DMS	E	1186	-	3,3,3	0.58	0	3,3,3	0.44	0
4	DMS	I	1186	-	3,3,3	0.55	0	3,3,3	0.38	0
5	OXY	C	302	2	1,1,1	0.34	0	-		
4	DMS	L	1186	-	3,3,3	0.66	0	3,3,3	0.60	0
4	DMS	G	1186	-	3,3,3	0.72	0	3,3,3	0.30	0
4	DMS	F	1186	-	3,3,3	0.61	0	3,3,3	0.70	0
3	QUE	L	301	2	24,24,24	1.34	5 (20%)	36,36,36	1.34	5 (13%)
5	OXY	F	302	2	1,1,1	0.33	0	-		
3	QUE	D	301	2	24,24,24	1.57	4 (16%)	36,36,36	1.47	6 (16%)
3	QUE	G	301	2	24,24,24	1.67	4 (16%)	36,36,36	1.42	5 (13%)

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	J	301	2	-	0/4/4/4	0/3/3/3
3	QUE	C	301	2	-	0/4/4/4	0/3/3/3
3	QUE	K	301	2	-	0/4/4/4	0/3/3/3
3	QUE	F	301	2	-	0/4/4/4	0/3/3/3
3	QUE	E	301	2	-	0/4/4/4	0/3/3/3
3	QUE	A	301	2	-	0/4/4/4	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QUE	L	301	2	-	0/4/4/4	0/3/3/3
3	QUE	B	301	2	-	0/4/4/4	0/3/3/3
3	QUE	H	301	2	-	0/4/4/4	0/3/3/3
3	QUE	I	301	2	-	0/4/4/4	0/3/3/3
3	QUE	D	301	2	-	0/4/4/4	0/3/3/3
3	QUE	G	301	2	-	0/4/4/4	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	QUE	C10-C11	11.38	1.47	1.36
3	C	301	QUE	C10-C11	11.02	1.47	1.36
3	E	301	QUE	C14-C11	4.87	1.54	1.47
3	H	301	QUE	C10-C11	4.53	1.40	1.36
3	G	301	QUE	C14-C11	4.18	1.53	1.47
3	I	301	QUE	C10-C11	4.17	1.40	1.36
3	G	301	QUE	C10-C11	4.14	1.40	1.36
3	D	301	QUE	C10-C11	4.08	1.40	1.36
3	K	301	QUE	C10-C11	3.92	1.40	1.36
3	L	301	QUE	C10-C11	3.62	1.40	1.36
3	E	301	QUE	C10-C11	3.57	1.40	1.36
3	B	301	QUE	C10-C11	3.44	1.39	1.36
3	D	301	QUE	C14-C11	3.41	1.52	1.47
3	J	301	QUE	C14-C11	3.37	1.52	1.47
3	A	301	QUE	C10-C11	3.32	1.39	1.36
3	A	301	QUE	C14-C11	3.20	1.52	1.47
3	D	301	QUE	C16-C15	3.13	1.43	1.38
3	E	301	QUE	C19-C18	3.11	1.43	1.38
3	F	301	QUE	C3-C9	-3.02	1.38	1.46
3	G	301	QUE	C19-C18	2.99	1.43	1.38
3	C	301	QUE	C3-C9	-2.94	1.39	1.46
3	K	301	QUE	C14-C11	2.85	1.51	1.47
3	D	301	QUE	C15-C14	2.78	1.43	1.39
3	I	301	QUE	C14-C11	2.74	1.51	1.47
3	J	301	QUE	C10-C11	2.66	1.39	1.36
3	H	301	QUE	C14-C11	2.58	1.51	1.47
3	H	301	QUE	C5-C4	2.53	1.43	1.38
3	L	301	QUE	C15-C14	2.44	1.43	1.39
3	F	301	QUE	O27-C10	-2.44	1.25	1.33
3	C	301	QUE	O27-C10	-2.36	1.25	1.33
3	E	301	QUE	C18-C17	-2.34	1.36	1.40
3	G	301	QUE	C5-C6	2.33	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	QUE	O24-C17	-2.28	1.31	1.36
3	I	301	QUE	C15-C14	2.28	1.42	1.39
3	I	301	QUE	C19-C18	2.20	1.42	1.38
3	H	301	QUE	C18-C17	-2.20	1.36	1.40
3	L	301	QUE	O27-C10	2.19	1.41	1.33
3	J	301	QUE	C19-C18	2.15	1.42	1.38
3	K	301	QUE	C16-C15	2.13	1.42	1.38
3	L	301	QUE	C14-C11	2.07	1.50	1.47
3	E	301	QUE	C5-C4	2.05	1.42	1.38
3	L	301	QUE	C19-C18	2.04	1.41	1.38
3	K	301	QUE	C19-C18	2.01	1.41	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	QUE	O27-C10-C11	7.27	128.26	120.74
3	C	301	QUE	O27-C10-C11	6.62	127.59	120.74
3	F	301	QUE	C11-C10-C9	-5.61	117.51	121.52
3	C	301	QUE	O12-C11-C14	4.93	117.77	110.87
3	C	301	QUE	C11-C10-C9	-4.79	118.10	121.52
3	G	301	QUE	O27-C10-C11	4.34	125.23	120.74
3	F	301	QUE	O12-C11-C14	4.08	116.58	110.87
3	D	301	QUE	O27-C10-C11	4.06	124.95	120.74
3	H	301	QUE	O27-C10-C11	3.86	124.73	120.74
3	H	301	QUE	C15-C14-C11	-3.18	116.03	120.71
3	C	301	QUE	C2-C3-C4	3.09	120.36	117.41
3	C	301	QUE	O12-C11-C10	-3.08	117.27	120.19
3	H	301	QUE	C14-C19-C18	-3.07	117.41	120.09
3	F	301	QUE	C2-C3-C4	3.05	120.32	117.41
3	C	301	QUE	C19-C14-C11	3.05	124.96	120.65
3	B	301	QUE	C15-C14-C11	-3.04	116.24	120.71
3	C	301	QUE	C14-C11-C10	-3.02	123.69	128.44
3	E	301	QUE	C15-C14-C11	-3.00	116.30	120.71
3	C	301	QUE	C15-C14-C11	-2.96	116.36	120.71
3	L	301	QUE	O12-C11-C10	2.85	122.89	120.19
3	A	301	QUE	C15-C14-C11	-2.83	116.55	120.71
3	B	301	QUE	O27-C10-C11	2.76	123.60	120.74
3	E	301	QUE	C14-C19-C18	-2.72	117.72	120.09
3	B	301	QUE	C14-C19-C18	-2.70	117.73	120.09
3	G	301	QUE	C14-C19-C18	-2.63	117.79	120.09
3	F	301	QUE	O12-C11-C10	-2.61	117.71	120.19
3	L	301	QUE	C15-C14-C11	-2.61	116.86	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	QUE	C15-C14-C11	-2.60	116.88	120.71
3	J	301	QUE	C15-C14-C11	-2.58	116.92	120.71
3	G	301	QUE	C15-C14-C11	-2.56	116.94	120.71
3	L	301	QUE	C14-C19-C18	-2.53	117.88	120.09
3	I	301	QUE	C15-C14-C11	-2.52	117.01	120.71
3	K	301	QUE	C15-C14-C11	-2.48	117.07	120.71
3	D	301	QUE	C15-C16-C17	-2.46	118.04	120.50
3	G	301	QUE	C15-C16-C17	-2.45	118.05	120.50
3	K	301	QUE	C14-C19-C18	-2.43	117.97	120.09
3	E	301	QUE	O27-C10-C11	2.41	123.24	120.74
3	A	301	QUE	C14-C19-C18	-2.40	117.99	120.09
3	F	301	QUE	O12-C4-C5	2.36	119.18	115.83
3	L	301	QUE	C3-C9-C10	-2.33	113.58	116.88
3	D	301	QUE	C5-C6-C1	2.29	123.61	120.47
3	J	301	QUE	C14-C19-C18	-2.29	118.09	120.09
3	C	301	QUE	C3-C9-C10	2.27	120.10	116.88
3	F	301	QUE	C14-C11-C10	-2.27	124.87	128.44
3	K	301	QUE	C3-C9-C10	-2.27	113.66	116.88
3	B	301	QUE	O13-C9-C3	2.27	126.16	122.06
3	B	301	QUE	O12-C11-C10	2.24	122.30	120.19
3	A	301	QUE	O13-C9-C3	2.21	126.06	122.06
3	F	301	QUE	C15-C16-C17	-2.20	118.30	120.50
3	C	301	QUE	O12-C4-C5	2.18	118.92	115.83
3	H	301	QUE	C15-C16-C17	-2.16	118.34	120.50
3	K	301	QUE	C15-C16-C17	-2.15	118.34	120.50
3	D	301	QUE	C14-C19-C18	-2.13	118.23	120.09
3	L	301	QUE	O13-C9-C3	2.13	125.91	122.06
3	K	301	QUE	O13-C9-C3	2.12	125.91	122.06
3	A	301	QUE	O27-C10-C11	2.12	122.93	120.74
3	G	301	QUE	C2-C1-C6	-2.12	117.72	119.67
3	H	301	QUE	O13-C9-C3	2.12	125.89	122.06
3	K	301	QUE	C5-C6-C1	2.09	123.33	120.47
3	J	301	QUE	O13-C9-C3	2.07	125.81	122.06
3	K	301	QUE	C19-C18-C17	2.04	121.78	119.89
3	B	301	QUE	C2-C1-C6	-2.04	117.79	119.67
3	H	301	QUE	O12-C11-C10	2.03	122.11	120.19
3	D	301	QUE	O13-C9-C3	2.03	125.73	122.06
3	E	301	QUE	C19-C14-C11	2.02	123.50	120.65
3	I	301	QUE	O27-C10-C11	2.02	122.83	120.74
3	F	301	QUE	C3-C9-C10	2.01	119.73	116.88

There are no chirality outliers.

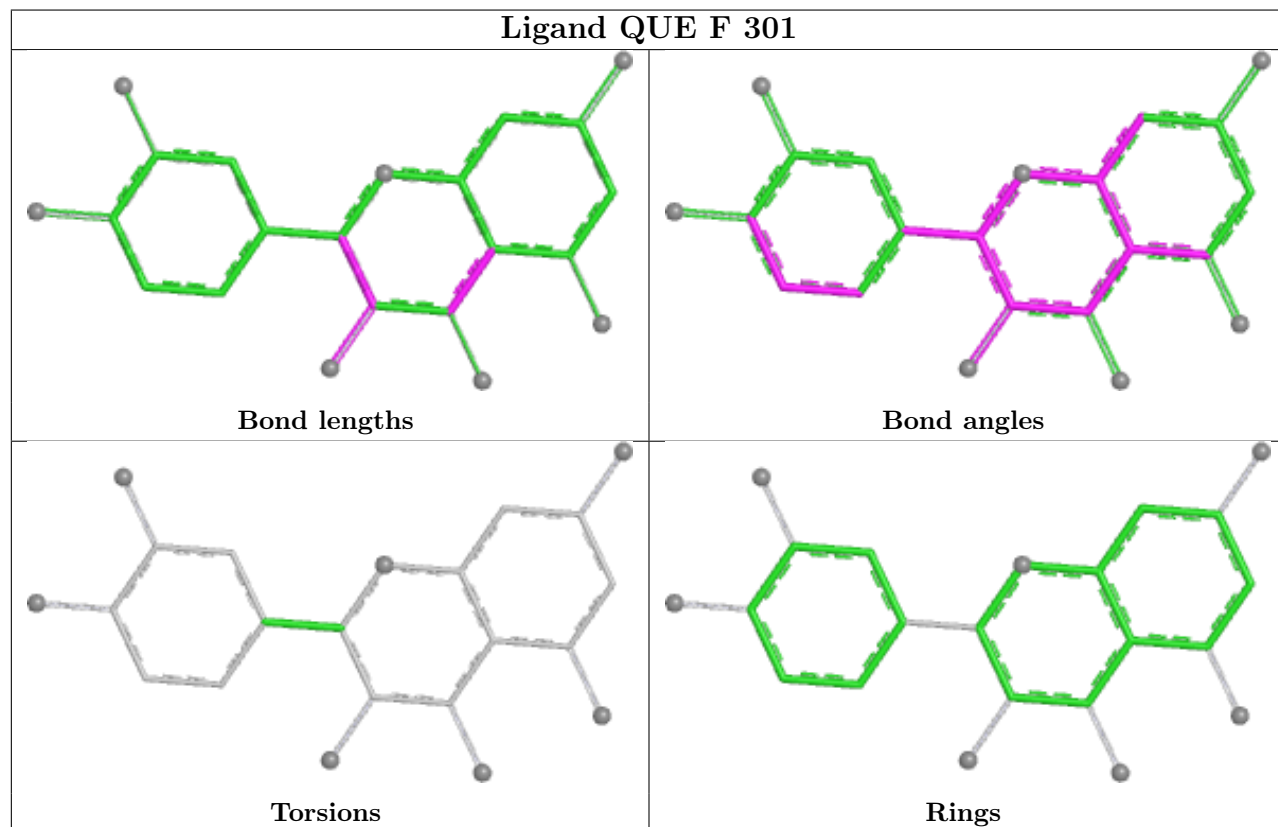
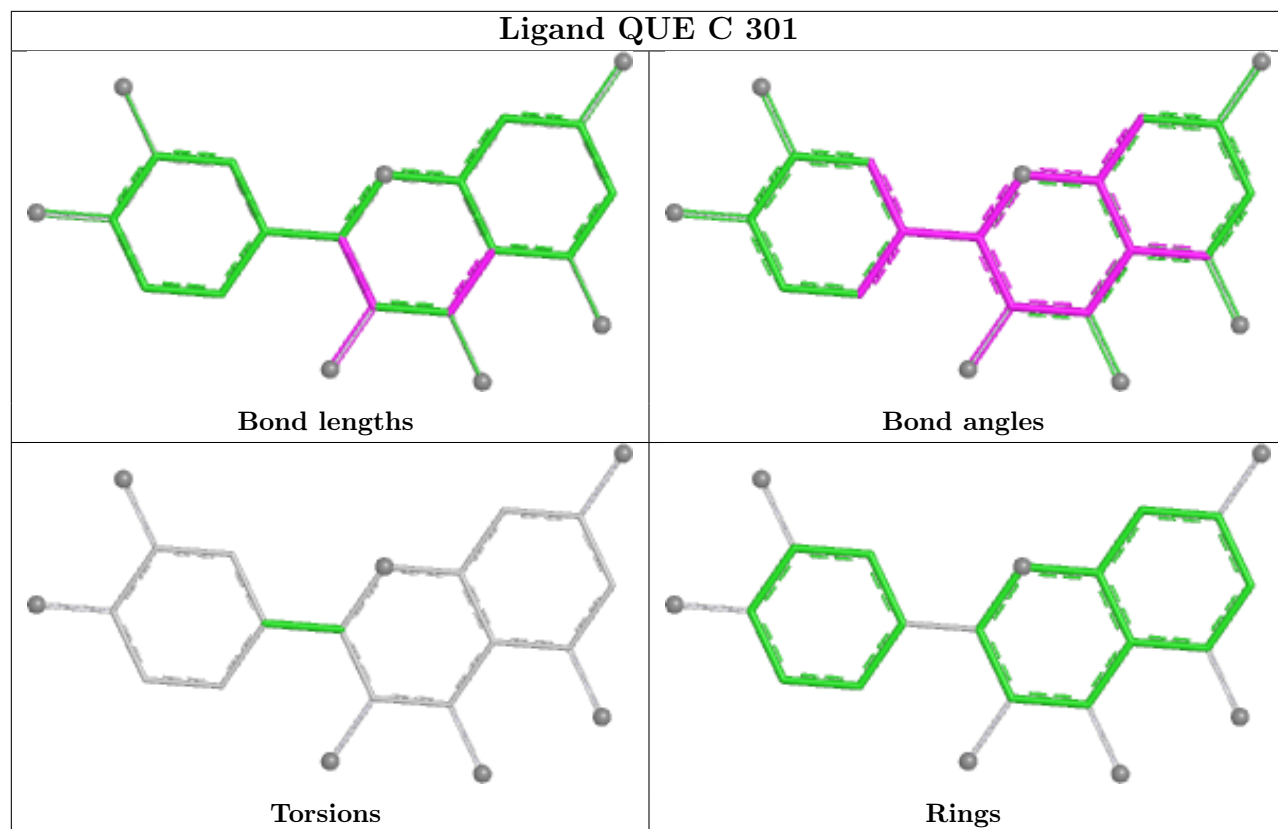
There are no torsion outliers.

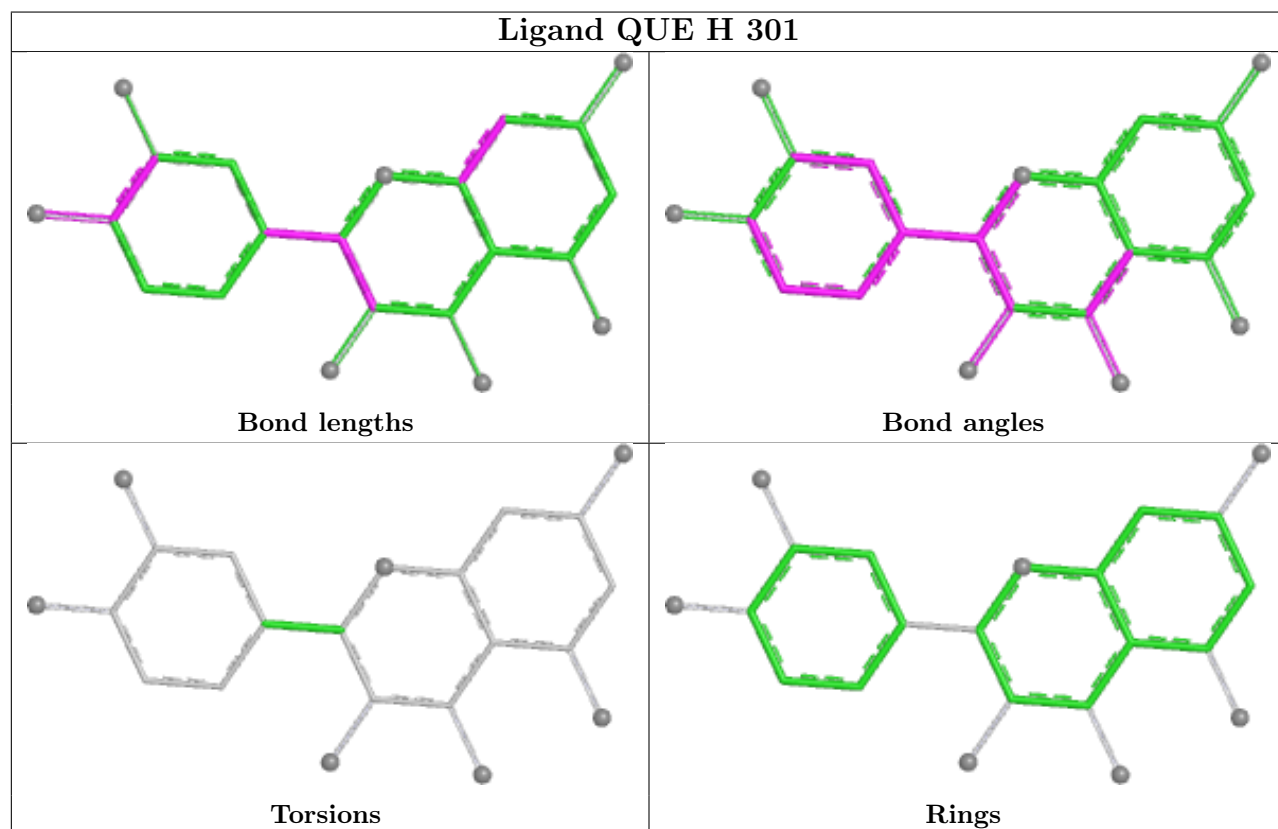
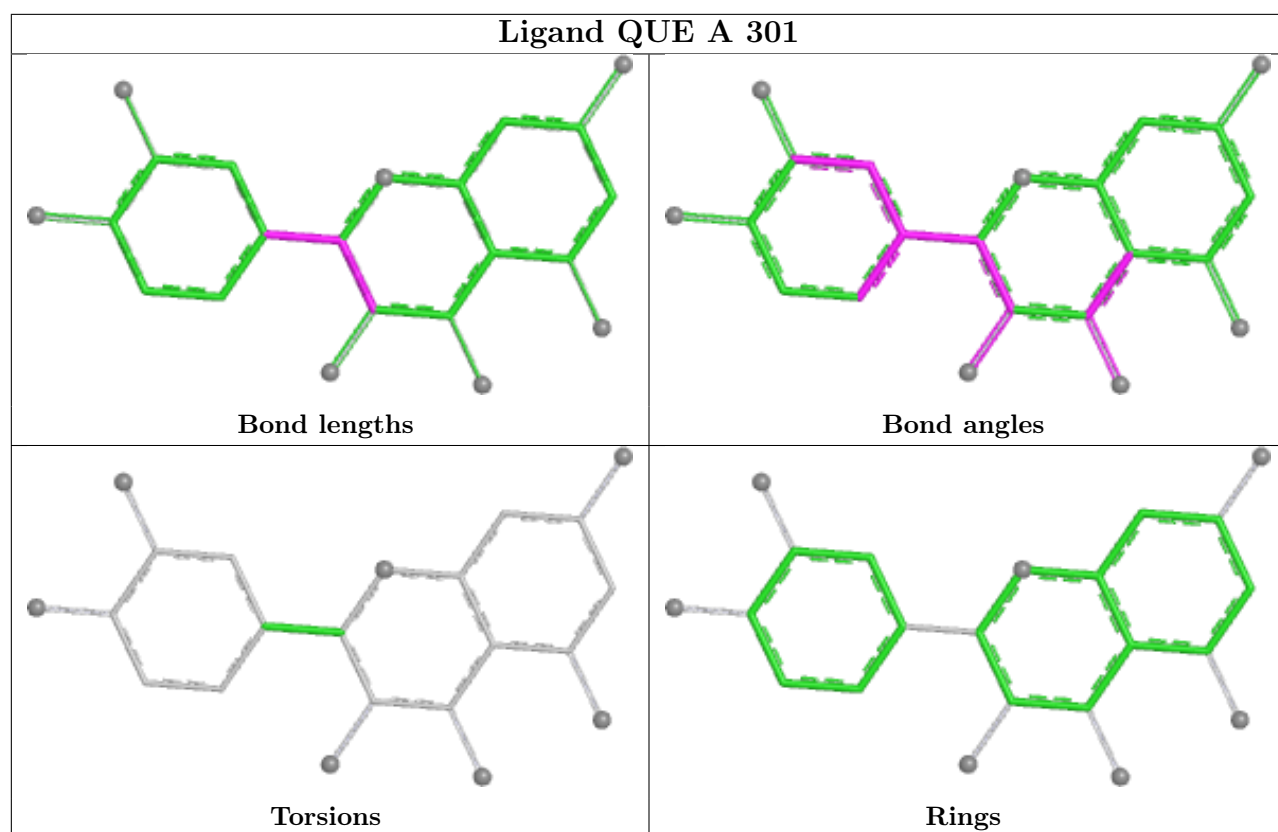
There are no ring outliers.

11 monomers are involved in 20 short contacts:

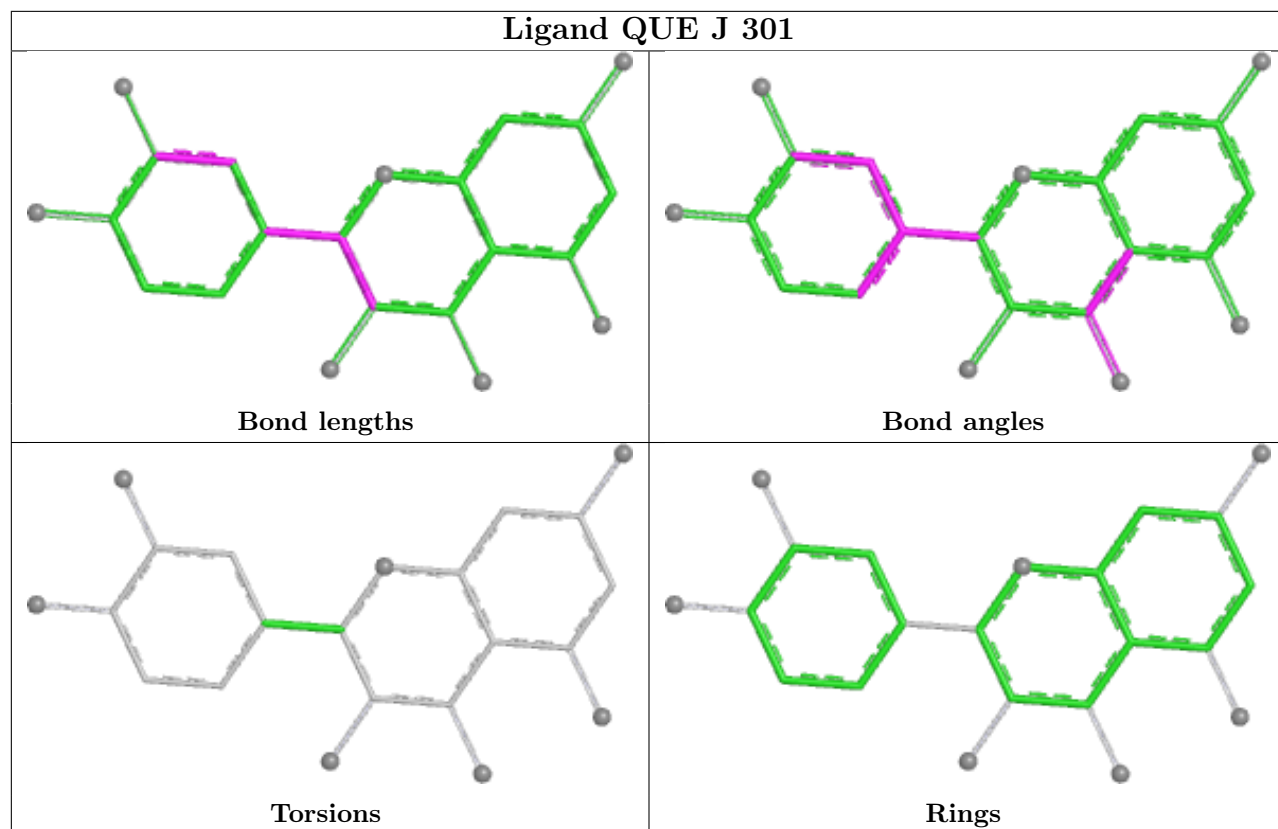
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	QUE	3	0
3	F	301	QUE	2	0
4	D	1188	DMS	2	0
4	J	1186	DMS	2	0
4	E	1187	DMS	3	0
4	B	1186	DMS	1	0
4	E	1186	DMS	2	0
4	I	1186	DMS	2	0
5	C	302	OXY	3	0
4	L	1186	DMS	1	0
5	F	302	OXY	3	0

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.

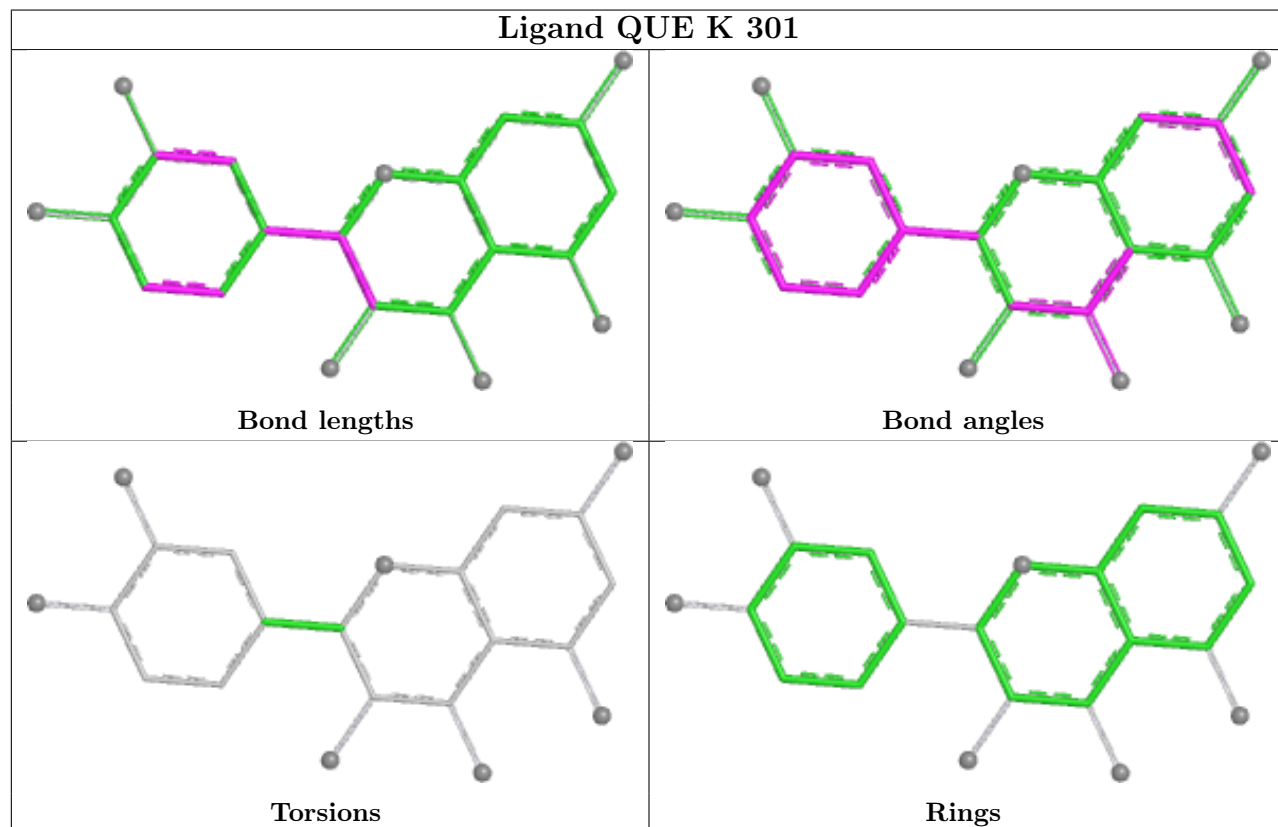




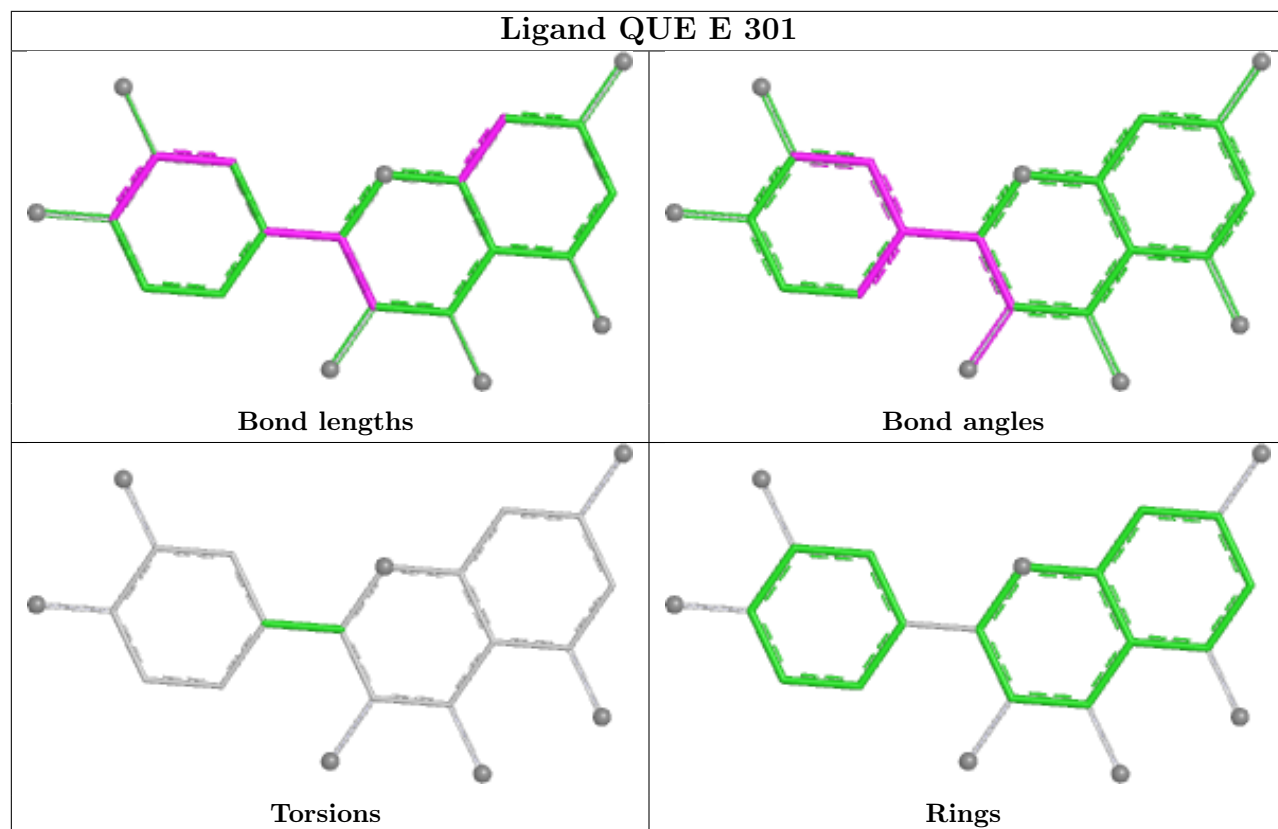
Ligand QUE J 301



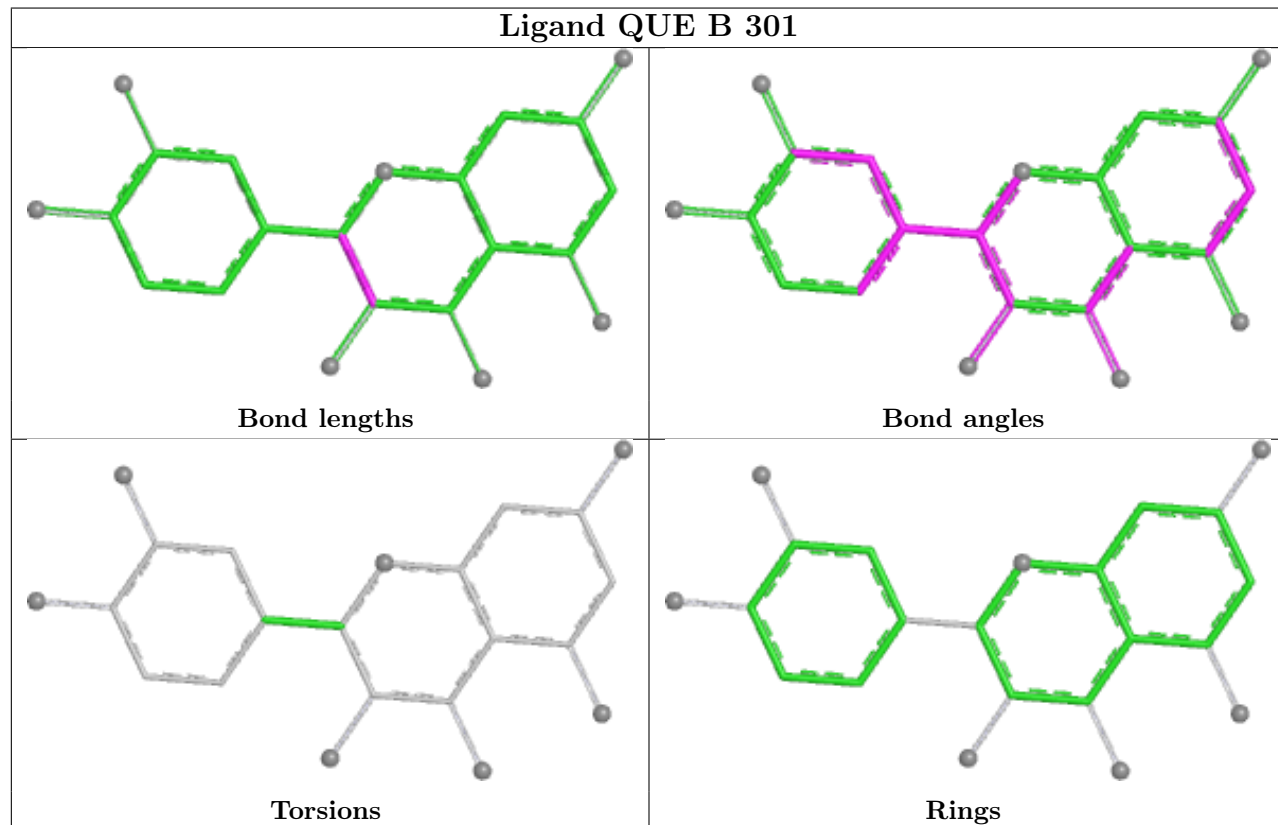
Ligand QUE K 301



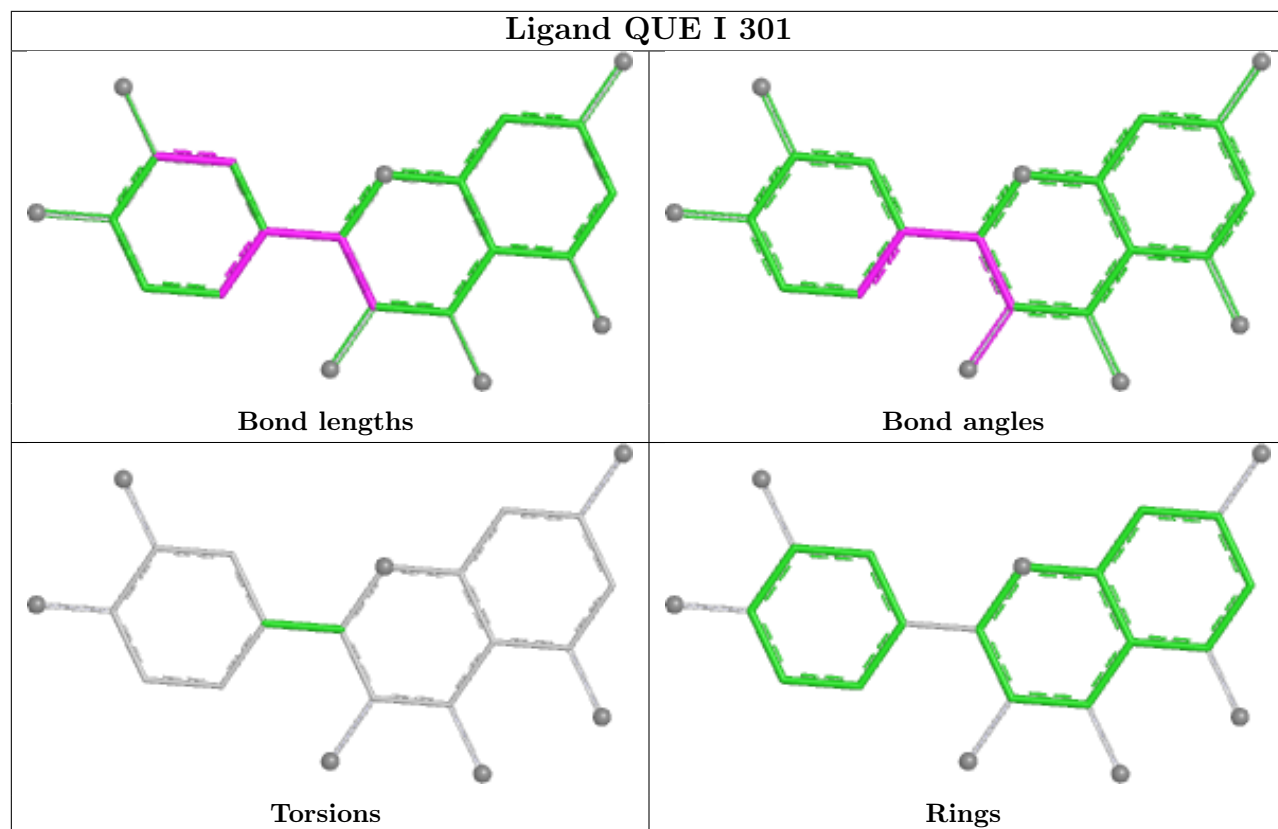
Ligand QUE E 301



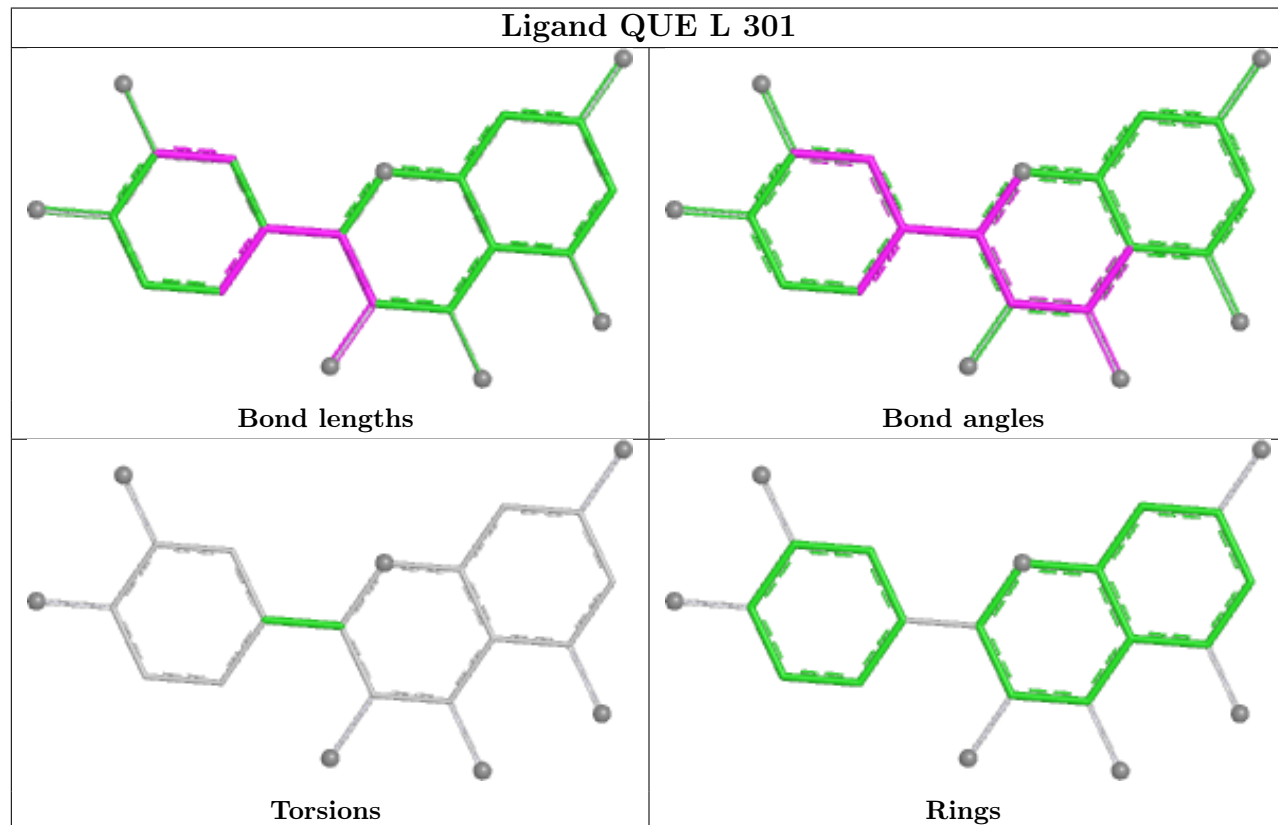
Ligand QUE B 301

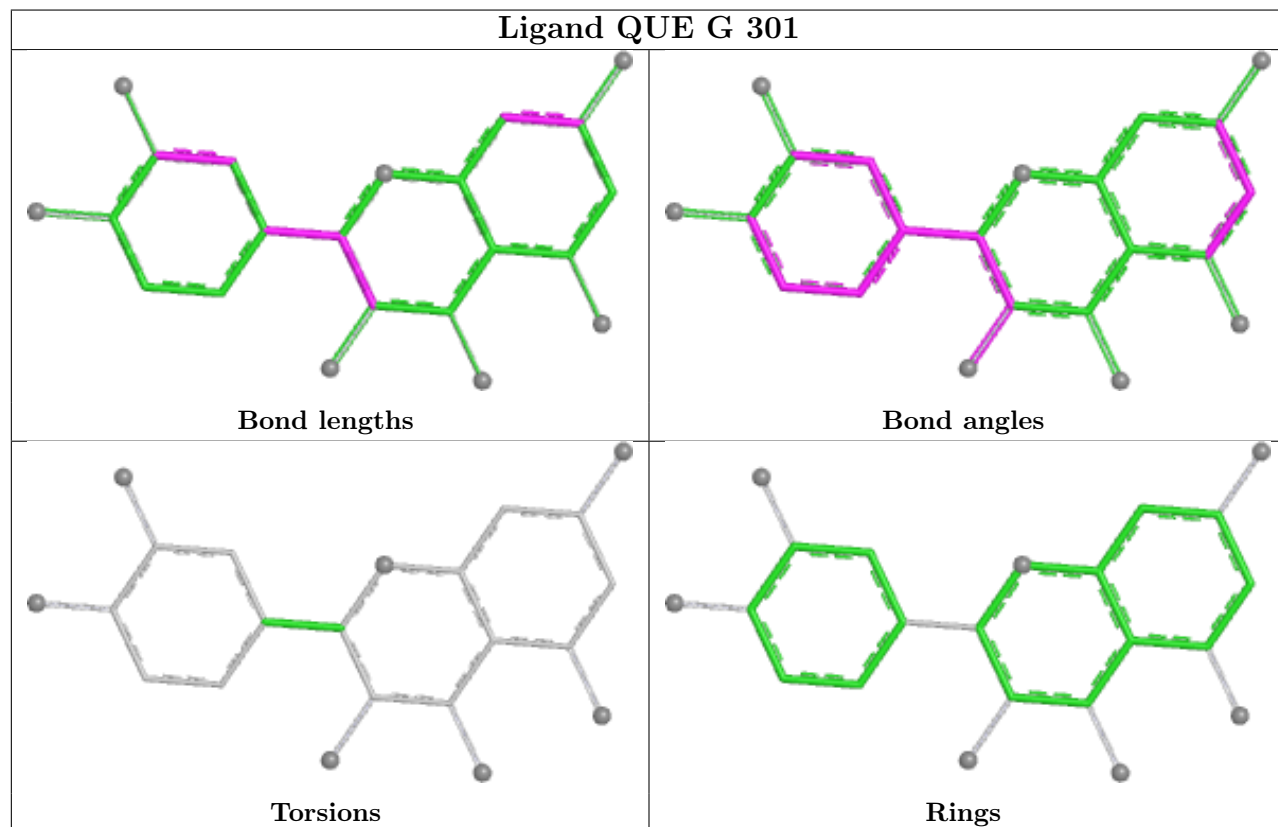
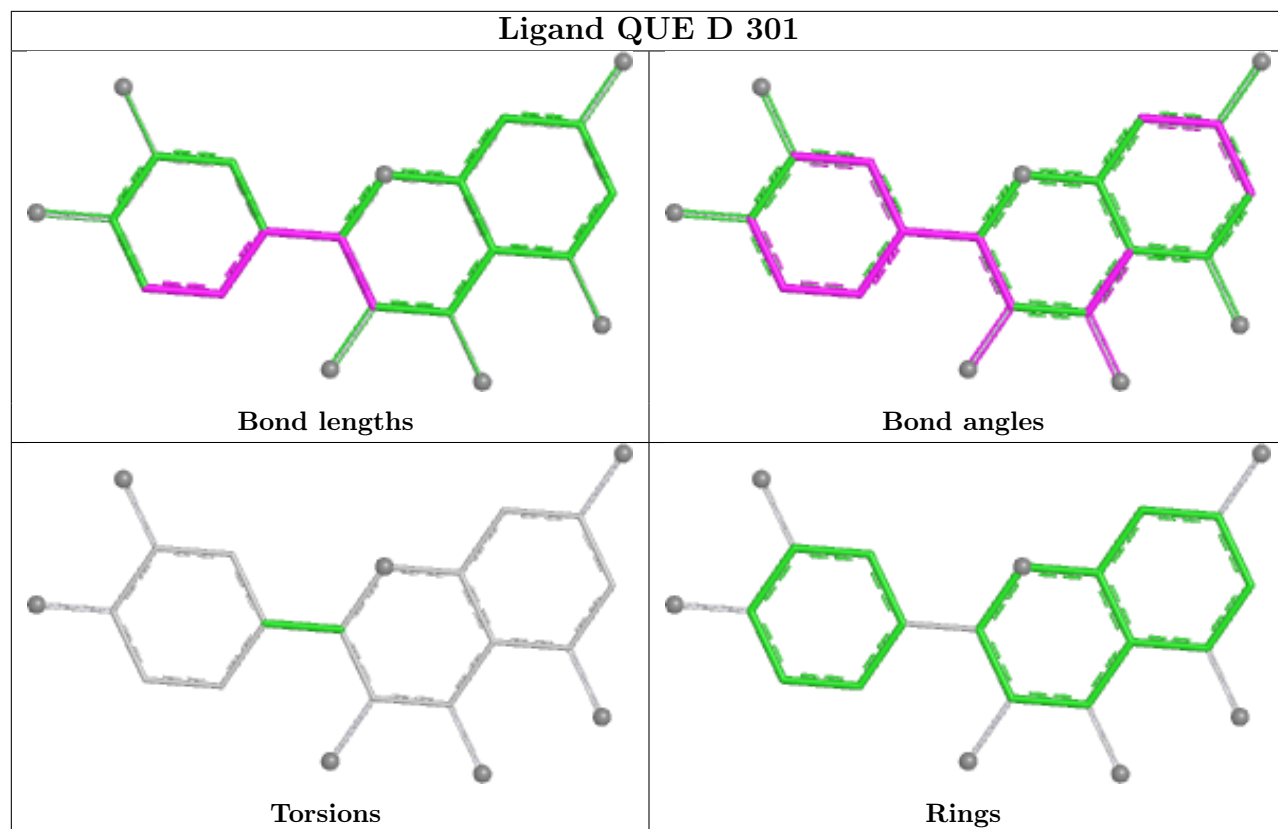


Ligand QUE I 301



Ligand QUE L 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	182/186 (97%)	0.01	5 (2%)	56	61	15, 40, 72, 89	3 (1%)
1	B	183/186 (98%)	-0.05	5 (2%)	56	61	15, 39, 70, 86	3 (1%)
1	C	183/186 (98%)	-0.02	4 (2%)	62	69	16, 37, 70, 112	6 (3%)
1	D	183/186 (98%)	-0.14	2 (1%)	78	82	16, 34, 66, 86	4 (2%)
1	E	183/186 (98%)	-0.05	4 (2%)	62	69	18, 36, 67, 95	3 (1%)
1	F	183/186 (98%)	-0.04	4 (2%)	62	69	20, 37, 71, 102	1 (0%)
1	G	183/186 (98%)	-0.14	4 (2%)	62	69	18, 34, 66, 102	3 (1%)
1	H	183/186 (98%)	-0.13	5 (2%)	56	61	17, 34, 64, 94	3 (1%)
1	I	183/186 (98%)	0.05	3 (1%)	70	77	16, 42, 74, 105	2 (1%)
1	J	183/186 (98%)	0.21	6 (3%)	49	56	18, 46, 87, 98	1 (0%)
1	K	183/186 (98%)	0.12	2 (1%)	78	82	17, 43, 74, 114	1 (0%)
1	L	184/186 (98%)	0.11	2 (1%)	78	82	20, 46, 79, 94	1 (0%)
All	All	2196/2232 (98%)	-0.01	46 (2%)	63	70	15, 39, 74, 114	31 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ILE	4.8
1	G	3	ILE	4.7
1	D	185	GLY	4.2
1	E	3	ILE	4.2
1	F	185	GLY	3.9
1	C	185	GLY	3.8
1	J	185	GLY	3.7
1	D	3	ILE	3.7
1	I	185	GLY	3.5
1	H	168	VAL	3.5
1	K	3	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	184	THR	2.8
1	J	3	ILE	2.8
1	K	185	GLY	2.8
1	L	185	GLY	2.8
1	G	185	GLY	2.7
1	H	3	ILE	2.7
1	J	168	VAL	2.7
1	G	134	GLY	2.6
1	I	183	HIS	2.5
1	G	183	HIS	2.5
1	J	184	THR	2.5
1	B	185	GLY	2.5
1	F	3	ILE	2.4
1	F	183	HIS	2.4
1	H	183	HIS	2.4
1	A	3	ILE	2.4
1	I	184	THR	2.3
1	A	65[A]	VAL	2.3
1	E	65	VAL	2.3
1	B	3	ILE	2.3
1	H	185	GLY	2.3
1	C	183[A]	HIS	2.3
1	E	185	GLY	2.2
1	A	134	GLY	2.2
1	B	184	THR	2.2
1	B	183	HIS	2.1
1	E	66	ILE	2.1
1	L	134	GLY	2.1
1	H	171	GLN	2.1
1	A	73	ASP	2.1
1	B	166	ARG	2.1
1	J	167	THR	2.1
1	J	179	ASP	2.1
1	F	67	PRO	2.0
1	C	161	GLU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	DMS	D	1187	4/4	0.77	0.25	32,51,57,59	4
3	QUE	E	301	22/22	0.83	0.22	21,38,44,52	22
4	DMS	D	1188	4/4	0.84	0.21	19,45,70,72	4
4	DMS	E	1187	4/4	0.84	0.20	43,53,57,60	4
4	DMS	F	1186	4/4	0.84	0.21	46,49,53,59	4
4	DMS	H	1186	4/4	0.84	0.22	45,49,61,82	4
4	DMS	G	1186	4/4	0.85	0.19	38,39,40,43	4
3	QUE	L	301	22/22	0.85	0.13	35,43,53,54	22
3	QUE	F	301	22/22	0.87	0.13	33,40,47,51	22
4	DMS	B	1186	4/4	0.88	0.17	25,31,55,65	4
4	DMS	L	1186	4/4	0.88	0.20	34,57,61,82	4
3	QUE	H	301	22/22	0.89	0.13	27,39,47,59	22
3	QUE	J	301	22/22	0.89	0.12	38,49,56,56	22
3	QUE	B	301	22/22	0.89	0.11	33,41,49,62	22
4	DMS	J	1186	4/4	0.89	0.18	46,51,59,75	4
4	DMS	A	1185	4/4	0.89	0.23	51,53,60,64	4
3	QUE	I	301	22/22	0.90	0.11	35,43,49,56	22
3	QUE	C	301	22/22	0.90	0.09	28,34,42,47	22
4	DMS	D	1186	4/4	0.90	0.20	21,41,44,57	4
3	QUE	K	301	22/22	0.90	0.10	31,38,46,53	22
4	DMS	H	1187	4/4	0.90	0.20	32,49,53,58	4
4	DMS	I	1186	4/4	0.90	0.15	24,33,64,66	4
3	QUE	A	301	22/22	0.90	0.11	32,43,51,60	22
4	DMS	K	1186	4/4	0.90	0.20	40,42,97,103	4
4	DMS	E	1186	4/4	0.90	0.27	59,63,65,66	4
3	QUE	D	301	22/22	0.93	0.08	26,31,34,43	22
3	QUE	G	301	22/22	0.93	0.08	25,33,41,43	22
5	OXY	C	302	2/2	0.94	0.12	34,34,34,36	2
5	OXY	F	302	2/2	0.94	0.13	35,35,35,36	2
2	NI	L	300	1/1	0.96	0.05	37,37,37,37	0
2	NI	K	300	1/1	0.97	0.05	36,36,36,36	0
2	NI	J	300	1/1	0.98	0.05	42,42,42,42	0

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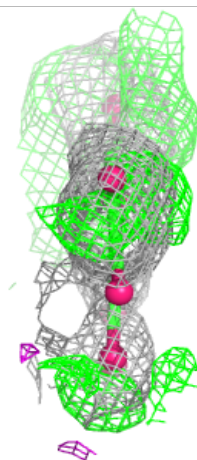
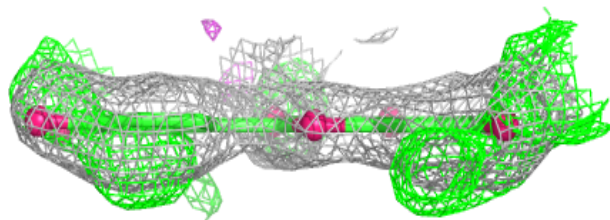
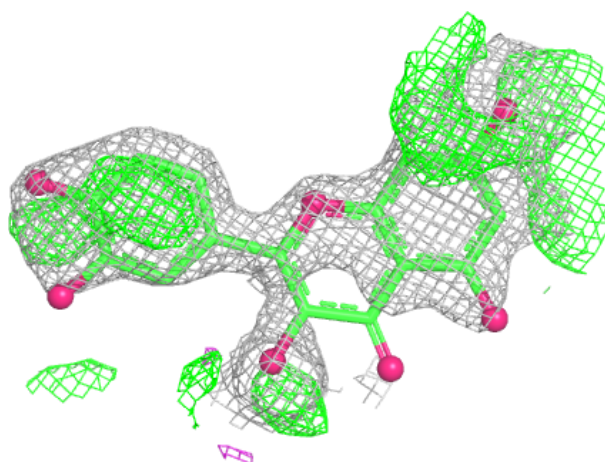
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	A	300	1/1	0.98	0.03	35,35,35,35	0
2	NI	C	300	1/1	0.98	0.03	30,30,30,30	0
2	NI	I	300	1/1	0.98	0.05	35,35,35,35	0
2	NI	F	300	1/1	0.99	0.03	31,31,31,31	0
2	NI	G	300	1/1	0.99	0.03	28,28,28,28	0
2	NI	H	300	1/1	0.99	0.02	30,30,30,30	0
2	NI	B	300	1/1	0.99	0.02	34,34,34,34	0
2	NI	D	300	1/1	0.99	0.02	30,30,30,30	0
2	NI	E	300	1/1	0.99	0.02	31,31,31,31	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.

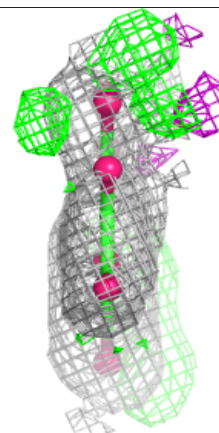
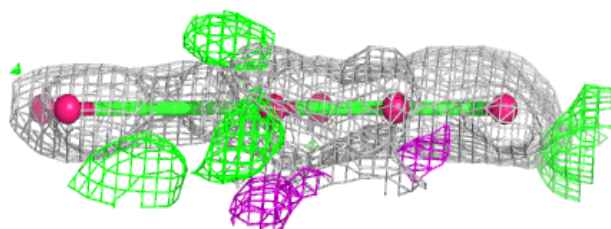
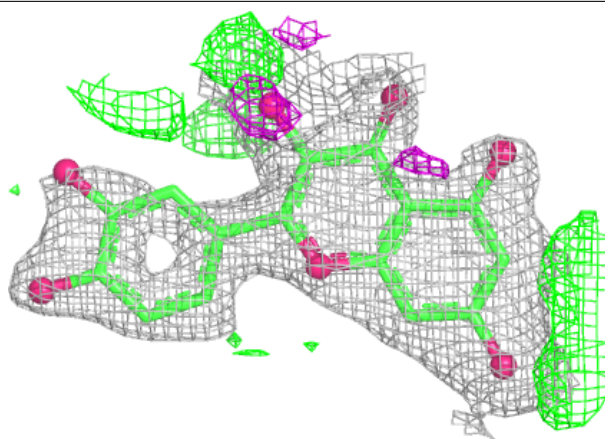
Electron density around QUE E 301:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

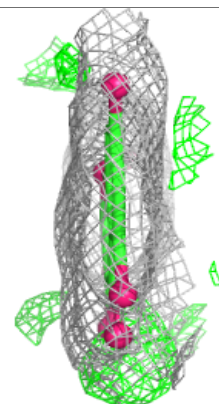
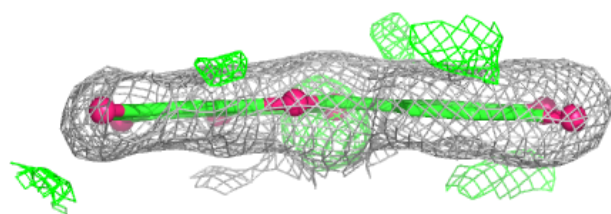
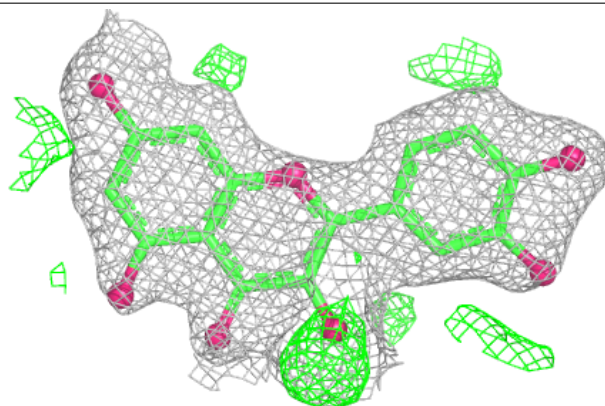


Electron density around QUE L 301:

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and green (positive)

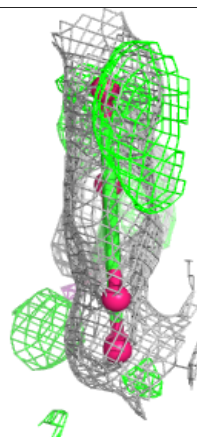
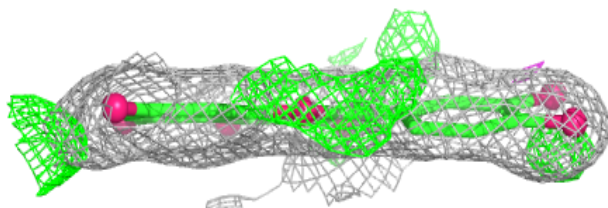
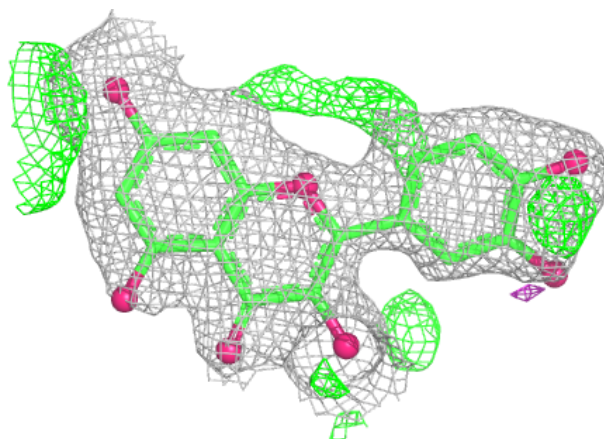
**Electron density around QUE F 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



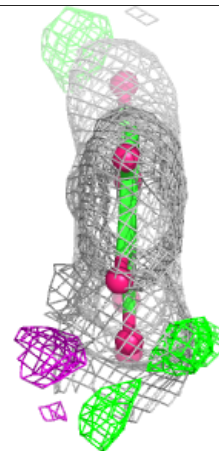
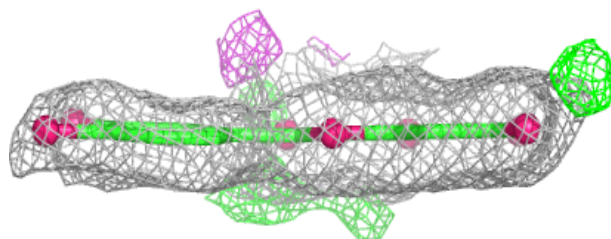
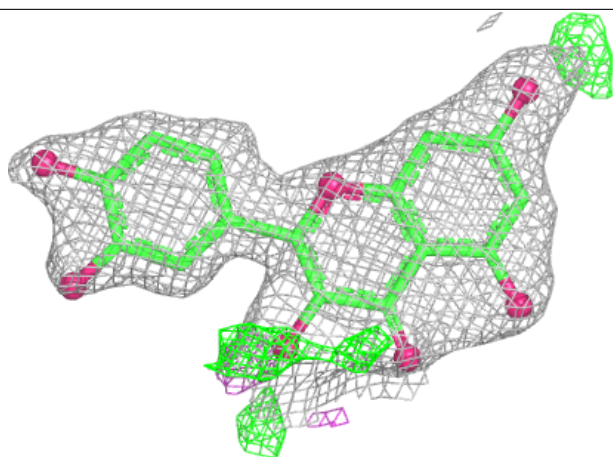
Electron density around QUE H 301:

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and green (positive)

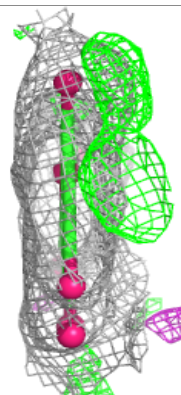
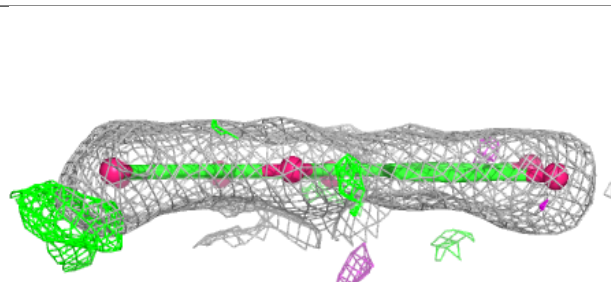
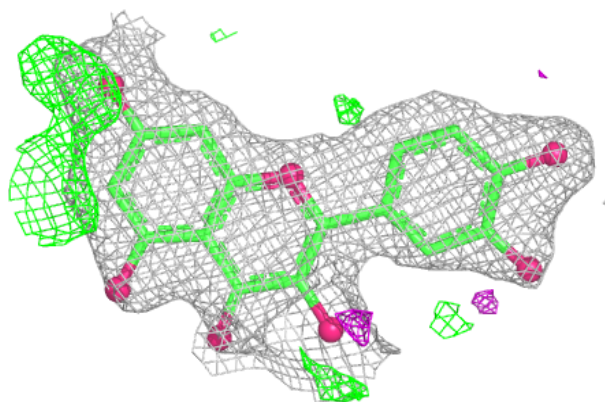


Electron density around QUE J 301:

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and green (positive)

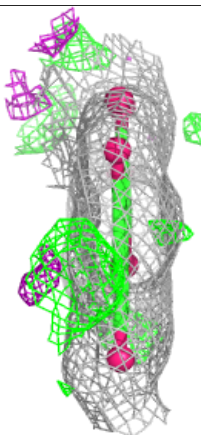
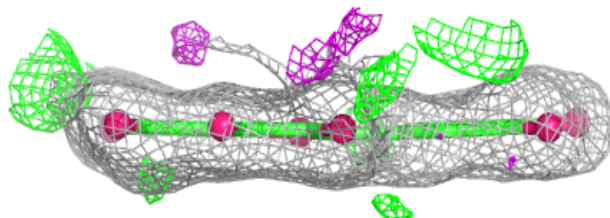
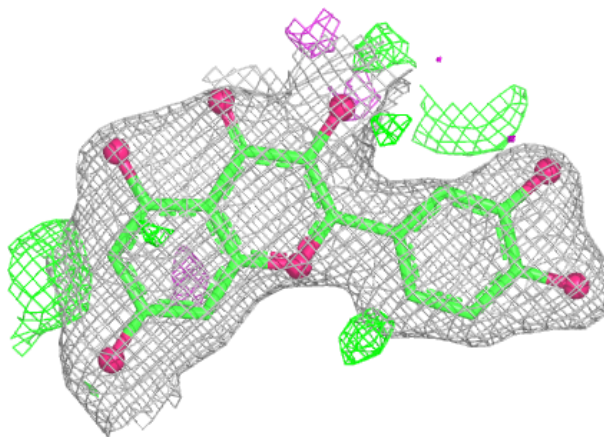
**Electron density around QUE B 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

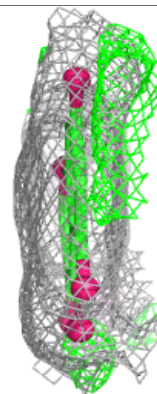
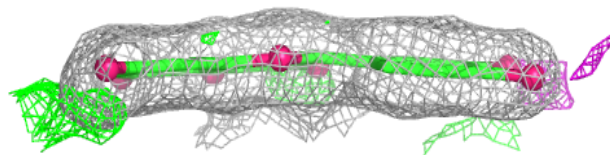
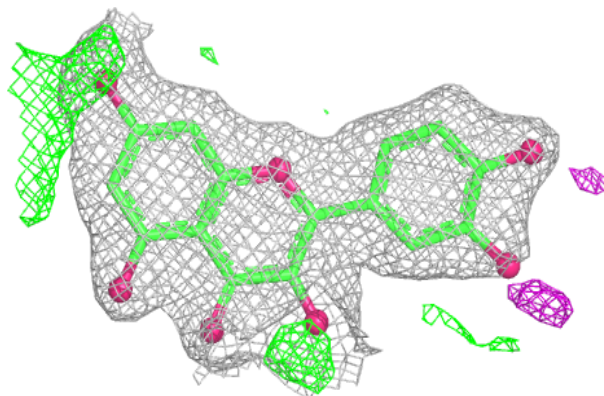


Electron density around QUE I 301:

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and green (positive)

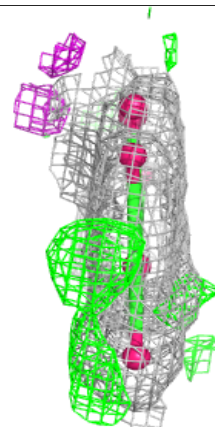
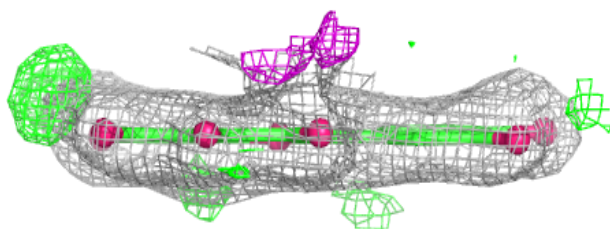
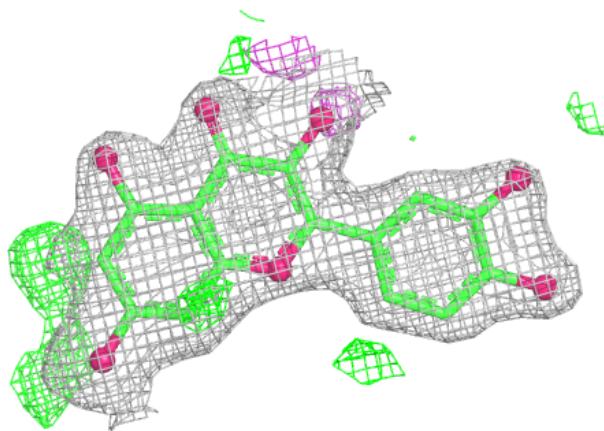
**Electron density around QUE C 301:**

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



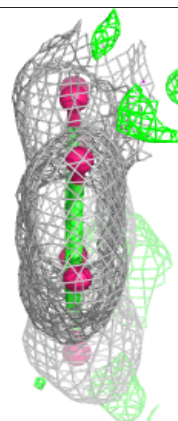
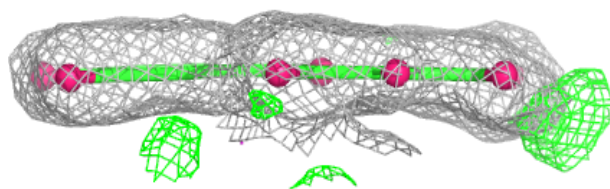
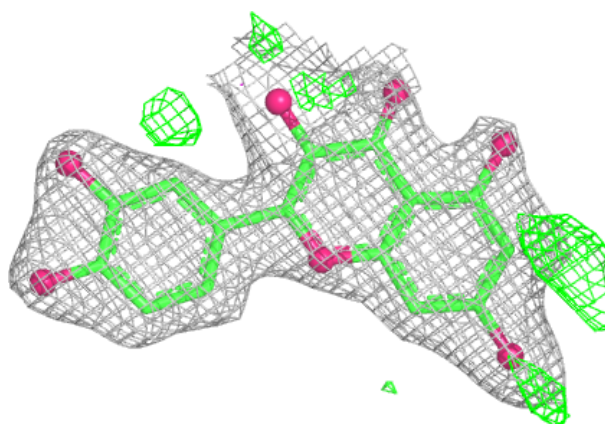
Electron density around QUE K 301:

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



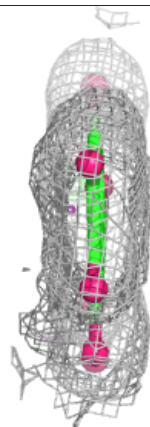
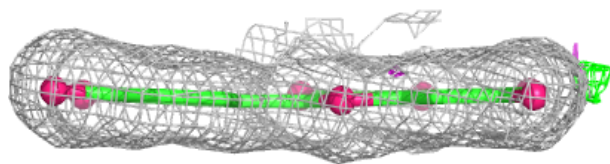
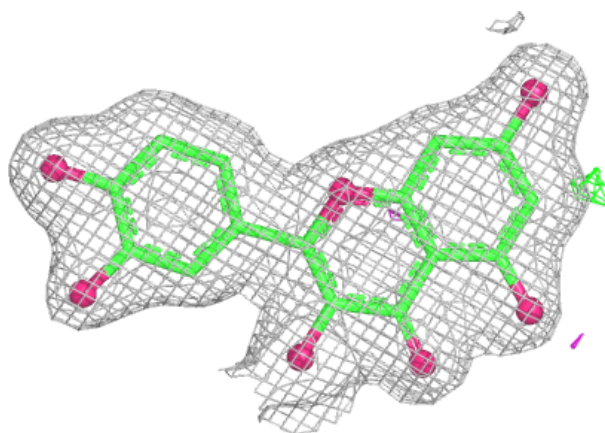
Electron density around QUE A 301:

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



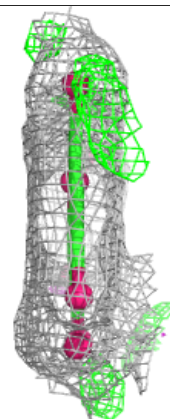
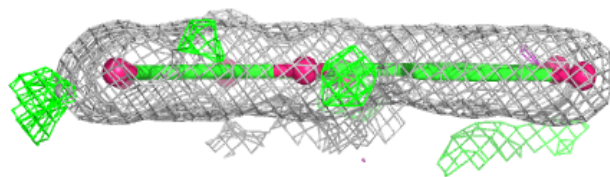
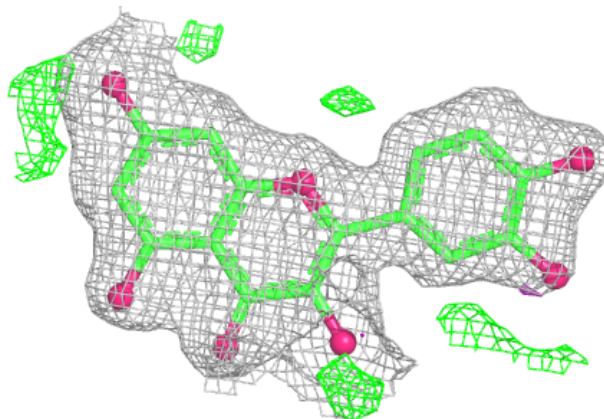
Electron density around QUE D 301:

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



Electron density around QUE 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.