



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 08:45 PM BST

PDB ID : 6SU0
Title : Crystal structure of dimethylated RSLex in complex with cucurbit[7]uril
Authors : Guagnini, F.; Engilberge, S.; Crowley, P.B.
Deposited on : 2019-09-12
Resolution : 1.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

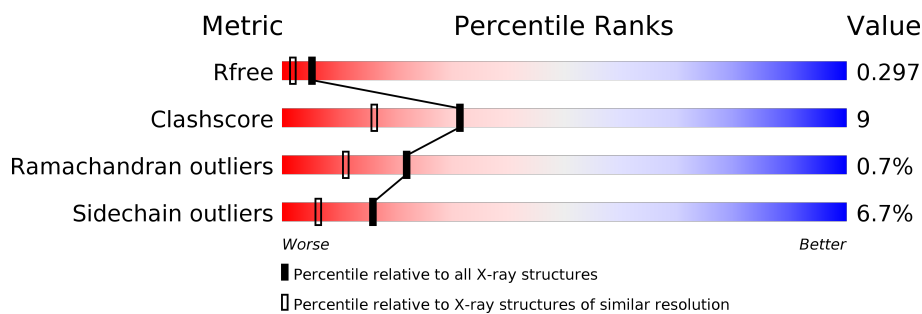
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	89	64% 34% .
1	B	89	67% 30% .
1	C	89	66% 30% .
1	D	89	84% 13% .
1	E	89	88% 11% .
1	F	89	73% 25% .
1	I	89	71% 27% .

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Mol	Chain	Length	Quality of chain
1	J	89	
1	K	89	
1	M	89	
1	N	89	
1	O	89	

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
1	MLY	C	34[A]	-	X	-	-
3	QQ7	A	202	X	-	-	-
3	QQ7	B	201	X	-	-	-
3	QQ7	C	204	X	-	-	-
3	QQ7	I	201	X	-	-	-
3	QQ7	J	201	X	-	-	-
3	QQ7	K	201	X	-	-	-
3	QQ7	M	201	X	-	-	-
3	QQ7	M	202	X	-	-	-
3	QQ7	N	201	X	-	-	-
3	QQ7	N	202	X	-	-	-
3	QQ7	O	201	X	-	-	-
3	QQ7	O	202	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9770 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 Fucose-binding lectin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	89	0
			696	443	117	134	2			
1	B	89	Total	C	N	O	S	0	89	0
			696	443	117	134	2			
1	C	89	Total	C	N	O	S	0	89	0
			696	443	117	134	2			
1	D	89	Total	C	N	O	S	0	89	0
			693	442	116	133	2			
1	E	89	Total	C	N	O	S	0	89	0
			696	443	117	134	2			
1	F	89	Total	C	N	O	S	0	89	0
			693	442	116	133	2			
1	I	89	Total	C	N	O	S	0	89	0
			695	443	117	133	2			
1	J	89	Total	C	N	O	S	0	89	0
			695	443	117	133	2			
1	K	89	Total	C	N	O	S	0	89	0
			695	443	117	133	2			
1	M	89	Total	C	N	O	S	0	89	0
			693	442	116	133	2			
1	N	89	Total	C	N	O	S	0	89	0
			695	443	117	133	2			
1	O	89	Total	C	N	O	S	0	89	0
			692	442	116	132	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MLY	ASN	conflict	UNP A0A0S4TLR1
A	82	TYR	THR	conflict	UNP A0A0S4TLR1
A	88	SER	ALA	conflict	UNP A0A0S4TLR1
B	79	MLY	ASN	conflict	UNP A0A0S4TLR1
B	82	TYR	THR	conflict	UNP A0A0S4TLR1

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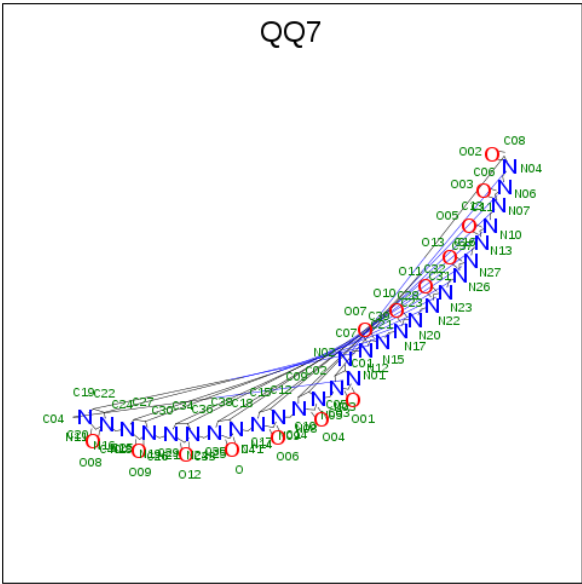
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Chain	Residue	Modelled	Actual	Comment	Reference
B	88	SER	ALA	conflict	UNP A0A0S4TLR1
C	79	MLY	ASN	conflict	UNP A0A0S4TLR1
C	82	TYR	THR	conflict	UNP A0A0S4TLR1
C	88	SER	ALA	conflict	UNP A0A0S4TLR1
D	79	MLY	ASN	conflict	UNP A0A0S4TLR1
D	82	TYR	THR	conflict	UNP A0A0S4TLR1
D	88	SER	ALA	conflict	UNP A0A0S4TLR1
E	79	MLY	ASN	conflict	UNP A0A0S4TLR1
E	82	TYR	THR	conflict	UNP A0A0S4TLR1
E	88	SER	ALA	conflict	UNP A0A0S4TLR1
F	79	MLY	ASN	conflict	UNP A0A0S4TLR1
F	82	TYR	THR	conflict	UNP A0A0S4TLR1
F	88	SER	ALA	conflict	UNP A0A0S4TLR1
I	79	MLY	ASN	conflict	UNP A0A0S4TLR1
I	82	TYR	THR	conflict	UNP A0A0S4TLR1
I	88	SER	ALA	conflict	UNP A0A0S4TLR1
J	79	MLY	ASN	conflict	UNP A0A0S4TLR1
J	82	TYR	THR	conflict	UNP A0A0S4TLR1
J	88	SER	ALA	conflict	UNP A0A0S4TLR1
K	79	MLY	ASN	conflict	UNP A0A0S4TLR1
K	82	TYR	THR	conflict	UNP A0A0S4TLR1
K	88	SER	ALA	conflict	UNP A0A0S4TLR1
M	79	MLY	ASN	conflict	UNP A0A0S4TLR1
M	82	TYR	THR	conflict	UNP A0A0S4TLR1
M	88	SER	ALA	conflict	UNP A0A0S4TLR1
N	79	MLY	ASN	conflict	UNP A0A0S4TLR1
N	82	TYR	THR	conflict	UNP A0A0S4TLR1
N	88	SER	ALA	conflict	UNP A0A0S4TLR1
O	79	MLY	ASN	conflict	UNP A0A0S4TLR1
O	82	TYR	THR	conflict	UNP A0A0S4TLR1
O	88	SER	ALA	conflict	UNP A0A0S4TLR1

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

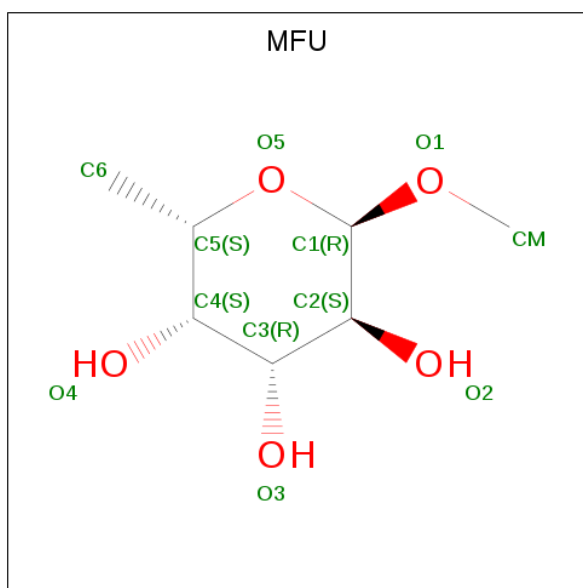
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	3	Total Na 3 3	0	0
2	F	1	Total Na 1 1	0	0

- Molecule 3 is cucurbit[7]uril (three-letter code: QQ7) (formula: C₄₂H₄₂N₂₈O₁₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			84	42	28	14		
3	B	1	Total	C	N	O	0	0
			84	42	28	14		
3	C	1	Total	C	N	O	0	0
			84	42	28	14		
3	I	1	Total	C	N	O	0	0
			84	42	28	14		
3	J	1	Total	C	N	O	0	0
			84	42	28	14		
3	K	1	Total	C	N	O	0	0
			84	42	28	14		
3	M	1	Total	C	N	O	0	0
			84	42	28	14		
3	M	1	Total	C	N	O	0	0
			84	42	28	14		
3	N	1	Total	C	N	O	0	0
			84	42	28	14		
3	N	1	Total	C	N	O	0	0
			84	42	28	14		
3	O	1	Total	C	N	O	0	0
			84	42	28	14		
3	O	1	Total	C	N	O	0	0
			84	42	28	14		

- Molecule 4 is methyl alpha-L-fucopyranoside (three-letter code: MFU) (formula: C₇H₁₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	7	5		
4	A	1	Total	C	O	0	0
			12	7	5		
4	B	1	Total	C	O	0	0
			12	7	5		
4	C	1	Total	C	O	0	0
			12	7	5		
4	C	1	Total	C	O	0	0
			12	7	5		
4	D	1	Total	C	O	0	0
			12	7	5		
4	E	1	Total	C	O	0	0
			12	7	5		
4	F	1	Total	C	O	0	0
			12	7	5		
4	I	1	Total	C	O	0	0
			12	7	5		
4	N	1	Total	C	O	0	0
			12	7	5		
4	O	1	Total	C	O	0	0
			12	7	5		
4	O	1	Total	C	O	0	0
			12	7	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	3
5	B	44	Total 44	O 44	0	1
5	C	39	Total 39	O 39	0	1
5	D	4	Total 4	O 4	0	0
5	E	2	Total 2	O 2	0	0
5	F	2	Total 2	O 2	0	0
5	I	33	Total 33	O 33	0	1
5	J	40	Total 40	O 40	0	0
5	K	35	Total 35	O 35	0	1
5	M	12	Total 12	O 12	0	0
5	N	12	Total 12	O 12	0	0
5	O	8	Total 8	O 8	0	0

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. 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. 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.

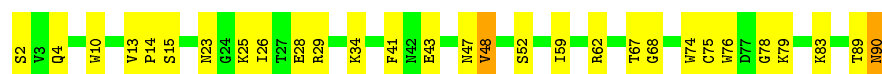
- Molecule 1: Fucose-binding lectin protein

Chain A: 



- Molecule 1: Fucose-binding lectin protein

Chain B: 




- Molecule 1: Fucose-binding lectin protein

Chain C: 




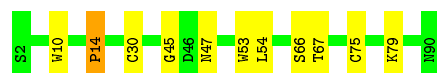
- Molecule 1: Fucose-binding lectin protein

Chain D: 



- Molecule 1: Fucose-binding lectin protein

Chain E: 



- Molecule 1: Fucose-binding lectin protein

Chain F: 



- Molecule 1: Fucose-binding lectin protein



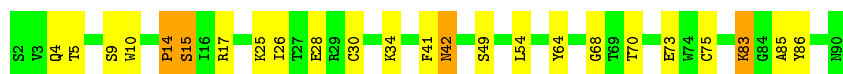
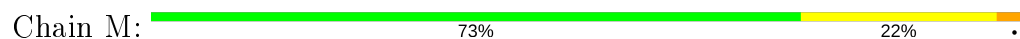
- Molecule 1: Fucose-binding lectin protein



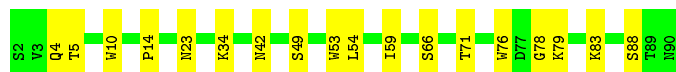
- Molecule 1: Fucose-binding lectin protein



- Molecule 1: Fucose-binding lectin protein



- Molecule 1: Fucose-binding lectin protein



- Molecule 1: Fucose-binding lectin protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	54.64Å 94.53Å 149.65Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	27.32 – 1.98 27.32 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.32-1.98) 99.1 (27.32-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.247 , 0.311 0.238 , 0.297	Depositor DCC
R_{free} test set	2583 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	1.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.326 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.310 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.326 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.316 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.438 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9770	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5835e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, QQ7, MLY, MFU

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	0.87	0/674	0.92	1/930 (0.1%)
1	B	0.83	0/674	0.94	0/930
1	C	0.81	0/674	0.90	2/930 (0.2%)
1	D	0.38	0/671	0.54	0/926
1	E	0.41	0/674	0.58	0/930
1	F	0.52	0/671	0.70	1/926 (0.1%)
1	I	0.72	0/673	0.91	1/929 (0.1%)
1	J	0.70	0/673	0.91	3/929 (0.3%)
1	K	0.70	0/673	0.87	0/929
1	M	0.53	0/671	0.77	0/926
1	N	0.58	0/673	0.78	0/929
1	O	0.54	0/670	0.80	1/925 (0.1%)
All	All	0.65	0/8071	0.81	9/11139 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	13[B]	VAL	N-CA-C	-6.12	94.47	111.00
1	I	55[B]	VAL	N-CA-C	-5.62	95.82	111.00
1	C	13[A]	VAL	N-CA-C	-5.58	95.94	111.00
1	J	55[B]	VAL	N-CA-C	-5.46	96.27	111.00
1	A	55[A]	VAL	N-CA-C	-5.31	96.66	111.00

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	696	0	552	20	0
1	B	696	0	557	16	0
1	C	696	0	562	22	0
1	D	693	0	567	8	0
1	E	696	0	569	6	0
1	F	693	0	548	10	0
1	I	695	0	564	22	0
1	J	695	0	550	21	0
1	K	695	0	561	21	0
1	M	693	0	558	12	0
1	N	695	0	565	9	0
1	O	692	0	556	11	0
2	A	1	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
3	A	84	0	42	0	0
3	B	84	0	42	0	0
3	C	84	0	42	0	0
3	I	84	0	42	0	0
3	J	84	0	42	1	0
3	K	84	0	42	0	0
3	M	168	0	84	0	0
3	N	168	0	84	0	0
3	O	168	0	84	0	0
4	A	24	0	28	0	0
4	B	12	0	14	0	0
4	C	24	0	28	0	0
4	D	12	0	14	1	0
4	E	12	0	14	0	0
4	F	12	0	14	2	0
4	I	12	0	14	0	0
4	N	12	0	14	0	0
4	O	24	0	28	1	0
5	A	46	0	0	1	0
5	B	44	0	0	2	0
5	C	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	4	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	I	33	0	0	0	0
5	J	40	0	0	1	0
5	K	35	0	0	2	0
5	M	12	0	0	0	0
5	N	12	0	0	0	0
5	O	8	0	0	0	0
All	All	9770	0	7381	152	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 9.

The worst 5 of 152 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:I:34[B]:MLY:CH2	1:I:34[B]:MLY:NZ	1.68	1.55
1:A:79[A]:MLY:NZ	1:A:79[A]:MLY:CH2	1.68	1.54
1:A:79[A]:MLY:CH1	1:A:79[A]:MLY:CH2	2.33	1.07
1:B:29[A]:ARG:HH12	1:C:90[A]:ASN:HB3	1.02	1.05
1:A:3[A]:VAL:HG12	1:B:68[A]:GLY:O	1.69	0.92

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	83/89 (93%)	82 (99%)	1 (1%)	0	100	100
1	B	83/89 (93%)	82 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	83/89 (93%)	79 (95%)	4 (5%)	0	100	100
1	D	83/89 (93%)	74 (89%)	7 (8%)	2 (2%)	6	1
1	E	83/89 (93%)	74 (89%)	8 (10%)	1 (1%)	13	4
1	F	83/89 (93%)	78 (94%)	4 (5%)	1 (1%)	13	4
1	I	83/89 (93%)	80 (96%)	3 (4%)	0	100	100
1	J	83/89 (93%)	81 (98%)	2 (2%)	0	100	100
1	K	83/89 (93%)	80 (96%)	3 (4%)	0	100	100
1	M	83/89 (93%)	79 (95%)	3 (4%)	1 (1%)	13	4
1	N	83/89 (93%)	75 (90%)	6 (7%)	2 (2%)	6	1
1	O	83/89 (93%)	75 (90%)	8 (10%)	0	100	100
All	All	996/1068 (93%)	939 (94%)	50 (5%)	7 (1%)	22	11

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	23[A]	ASN
1	M	68[B]	GLY
1	N	88[B]	SER
1	E	14[A]	PRO
1	N	23[B]	ASN

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	67/67 (100%)	60 (90%)	7 (10%)	7	1
1	B	67/67 (100%)	61 (91%)	6 (9%)	9	2
1	C	67/67 (100%)	63 (94%)	4 (6%)	19	8
1	D	66/67 (98%)	66 (100%)	0	100	100
1	E	67/67 (100%)	65 (97%)	2 (3%)	41	29
1	F	66/67 (98%)	61 (92%)	5 (8%)	13	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	66/67 (98%)	64 (97%)	2 (3%)	41	29
1	J	66/67 (98%)	56 (85%)	10 (15%)	3	0
1	K	66/67 (98%)	62 (94%)	4 (6%)	18	8
1	M	66/67 (98%)	60 (91%)	6 (9%)	9	2
1	N	66/67 (98%)	65 (98%)	1 (2%)	65	59
1	O	65/67 (97%)	59 (91%)	6 (9%)	9	2
All	All	795/804 (99%)	742 (93%)	53 (7%)	16	6

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	89[A]	THR
1	J	15[B]	SER
1	O	23[B]	ASN
1	I	8[B]	THR
1	J	2[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	22[B]	ASN
1	I	90[B]	ASN
1	O	22[B]	ASN
1	I	23[B]	ASN
1	I	60[B]	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	I	83[B]	1	9,10,11	1.10	0	6,11,13	0.88	0
1	MLY	J	79[B]	1	9,10,11	1.60	2 (22%)	6,11,13	3.20	2 (33%)
1	MLY	N	25[B]	1	9,10,11	0.93	0	6,11,13	0.96	0
1	MLY	B	83[A]	1	9,10,11	1.58	2 (22%)	6,11,13	2.06	3 (50%)
1	MLY	C	25[A]	1	9,10,11	1.77	1 (11%)	6,11,13	1.82	2 (33%)
1	MLY	F	34[A]	1	9,10,11	1.16	1 (11%)	6,11,13	1.81	1 (16%)
1	MLY	I	25[B]	1	9,10,11	1.07	1 (11%)	6,11,13	2.26	2 (33%)
1	MLY	A	25[A]	1	9,10,11	0.73	0	6,11,13	1.67	2 (33%)
1	MLY	M	25[B]	1	9,10,11	1.04	0	6,11,13	1.26	1 (16%)
1	MLY	E	25[A]	1	9,10,11	0.68	0	6,11,13	0.93	0
1	MLY	B	34[A]	1	9,10,11	1.73	2 (22%)	6,11,13	1.57	2 (33%)
1	MLY	B	25[A]	1	9,10,11	1.52	1 (11%)	6,11,13	2.61	1 (16%)
1	MLY	J	83[B]	1	9,10,11	2.10	1 (11%)	6,11,13	2.90	2 (33%)
1	MLY	F	83[A]	1	9,10,11	1.36	2 (22%)	6,11,13	1.36	1 (16%)
1	MLY	K	34[B]	1	9,10,11	2.00	3 (33%)	6,11,13	1.74	2 (33%)
1	MLY	O	34[B]	1	9,10,11	0.76	0	6,11,13	0.89	0
1	MLY	I	34[B]	1	9,10,11	2.52	1 (11%)	6,11,13	2.12	3 (50%)
1	MLY	A	34[A]	1	9,10,11	2.03	4 (44%)	6,11,13	3.08	4 (66%)
1	MLY	C	34[A]	1	9,10,11	2.62	2 (22%)	6,11,13	2.17	3 (50%)
1	MLY	F	25[A]	1	9,10,11	1.55	1 (11%)	6,11,13	1.35	1 (16%)
1	MLY	E	79[A]	1	9,10,11	1.08	1 (11%)	6,11,13	1.28	1 (16%)
1	MLY	M	79[B]	1	9,10,11	0.76	0	6,11,13	0.94	0
1	MLY	A	79[A]	1	9,10,11	2.63	1 (11%)	6,11,13	4.45	4 (66%)
1	MLY	I	79[B]	1	9,10,11	1.93	3 (33%)	6,11,13	0.90	0
1	MLY	N	34[B]	1	9,10,11	1.33	2 (22%)	6,11,13	2.15	1 (16%)
1	MLY	K	79[B]	1	9,10,11	1.89	2 (22%)	6,11,13	1.68	2 (33%)
1	MLY	D	25[A]	1	9,10,11	1.19	1 (11%)	6,11,13	1.38	1 (16%)
1	MLY	C	79[A]	1	9,10,11	1.08	1 (11%)	6,11,13	3.81	3 (50%)
1	MLY	O	79[B]	1	9,10,11	1.59	1 (11%)	6,11,13	1.06	0
1	MLY	F	79[A]	1	9,10,11	0.79	0	6,11,13	1.12	0
1	MLY	M	83[B]	1	9,10,11	1.44	1 (11%)	6,11,13	1.21	1 (16%)
1	MLY	D	34[A]	1	9,10,11	0.76	0	6,11,13	1.05	0
1	MLY	O	83[B]	1	9,10,11	1.19	0	6,11,13	1.54	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	N	83[B]	1	9,10,11	1.40	1 (11%)	6,11,13	2.07	3 (50%)
1	MLY	C	83[A]	1	9,10,11	0.79	0	6,11,13	2.93	3 (50%)
1	MLY	K	83[B]	1	9,10,11	1.35	2 (22%)	6,11,13	1.65	1 (16%)
1	MLY	E	34[A]	1	9,10,11	0.66	0	6,11,13	1.01	0
1	MLY	A	83[A]	1	9,10,11	1.44	1 (11%)	6,11,13	1.55	1 (16%)
1	MLY	M	34[B]	1	9,10,11	1.26	2 (22%)	6,11,13	1.30	1 (16%)
1	MLY	D	79[A]	1	9,10,11	0.75	0	6,11,13	0.79	0
1	MLY	E	83[A]	1	9,10,11	0.58	0	6,11,13	0.97	0
1	MLY	B	79[A]	1	9,10,11	3.24	4 (44%)	6,11,13	2.73	3 (50%)
1	MLY	J	34[B]	1	9,10,11	1.54	2 (22%)	6,11,13	1.23	1 (16%)
1	MLY	K	25[B]	1	9,10,11	1.38	2 (22%)	6,11,13	1.64	2 (33%)
1	MLY	D	83[A]	1	9,10,11	1.32	1 (11%)	6,11,13	1.25	1 (16%)
1	MLY	O	25[B]	1	9,10,11	0.95	0	6,11,13	0.95	0
1	MLY	N	79[B]	1	9,10,11	1.35	1 (11%)	6,11,13	1.38	1 (16%)
1	MLY	J	25[B]	1	9,10,11	1.24	1 (11%)	6,11,13	1.96	2 (33%)

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
1	MLY	I	83[B]	1	-	1/8/9/11	-
1	MLY	J	79[B]	1	-	6/8/9/11	-
1	MLY	N	25[B]	1	-	6/8/9/11	-
1	MLY	B	83[A]	1	-	6/8/9/11	-
1	MLY	C	25[A]	1	-	4/8/9/11	-
1	MLY	F	34[A]	1	-	6/8/9/11	-
1	MLY	I	25[B]	1	-	3/8/9/11	-
1	MLY	A	25[A]	1	-	5/8/9/11	-
1	MLY	M	25[B]	1	-	2/8/9/11	-
1	MLY	E	25[A]	1	-	5/8/9/11	-
1	MLY	B	34[A]	1	-	4/8/9/11	-
1	MLY	B	25[A]	1	-	2/8/9/11	-
1	MLY	J	83[B]	1	-	5/8/9/11	-
1	MLY	F	83[A]	1	-	2/8/9/11	-
1	MLY	K	34[B]	1	-	6/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	O	34[B]	1	-	4/8/9/11	-
1	MLY	I	34[B]	1	-	4/8/9/11	-
1	MLY	A	34[A]	1	-	3/8/9/11	-
1	MLY	C	34[A]	1	-	7/8/9/11	-
1	MLY	F	25[A]	1	-	7/8/9/11	-
1	MLY	E	79[A]	1	-	3/8/9/11	-
1	MLY	M	79[B]	1	-	5/8/9/11	-
1	MLY	A	79[A]	1	-	1/8/9/11	-
1	MLY	I	79[B]	1	-	3/8/9/11	-
1	MLY	N	34[B]	1	-	6/8/9/11	-
1	MLY	K	79[B]	1	-	2/8/9/11	-
1	MLY	D	25[A]	1	-	4/8/9/11	-
1	MLY	C	79[A]	1	-	2/8/9/11	-
1	MLY	O	79[B]	1	-	4/8/9/11	-
1	MLY	F	79[A]	1	-	5/8/9/11	-
1	MLY	M	83[B]	1	-	3/8/9/11	-
1	MLY	D	34[A]	1	-	5/8/9/11	-
1	MLY	O	83[B]	1	-	3/8/9/11	-
1	MLY	N	83[B]	1	-	2/8/9/11	-
1	MLY	C	83[A]	1	-	5/8/9/11	-
1	MLY	K	83[B]	1	-	3/8/9/11	-
1	MLY	E	34[A]	1	-	4/8/9/11	-
1	MLY	A	83[A]	1	-	3/8/9/11	-
1	MLY	M	34[B]	1	-	6/8/9/11	-
1	MLY	D	79[A]	1	-	3/8/9/11	-
1	MLY	E	83[A]	1	-	5/8/9/11	-
1	MLY	B	79[A]	1	-	0/8/9/11	-
1	MLY	J	34[B]	1	-	4/8/9/11	-
1	MLY	K	25[B]	1	-	3/8/9/11	-
1	MLY	D	83[A]	1	-	5/8/9/11	-
1	MLY	O	25[B]	1	-	3/8/9/11	-
1	MLY	N	79[B]	1	-	5/8/9/11	-
1	MLY	J	25[B]	1	-	6/8/9/11	-

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79[A]	MLY	CH2-NZ	7.27	1.68	1.46
1	I	34[B]	MLY	CH2-NZ	7.02	1.68	1.46
1	B	79[A]	MLY	CH2-NZ	6.53	1.66	1.46
1	C	34[A]	MLY	CB-CA	5.97	1.61	1.53
1	J	83[B]	MLY	CH1-NZ	5.74	1.64	1.46

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79[A]	MLY	CH2-NZ-CE	-7.41	81.37	110.74
1	A	79[A]	MLY	CH1-NZ-CE	-7.02	82.93	110.74
1	J	79[B]	MLY	CH1-NZ-CE	-6.91	83.37	110.74
1	J	83[B]	MLY	CH2-NZ-CE	-6.23	86.07	110.74
1	A	79[A]	MLY	CH2-NZ-CH1	-6.21	93.67	109.73

There are no chirality outliers.

5 of 191 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	79[B]	MLY	N-CA-CB-CG
1	J	79[B]	MLY	C-CA-CB-CG
1	N	25[B]	MLY	N-CA-CB-CG
1	N	25[B]	MLY	C-CA-CB-CG
1	C	25[A]	MLY	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	83[B]	MLY	1	0
1	I	34[B]	MLY	4	0
1	A	79[A]	MLY	4	0
1	M	83[B]	MLY	1	0
1	J	34[B]	MLY	1	0
1	D	83[A]	MLY	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 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	MFU	A	204	-	12,12,12	0.76	0	17,17,17	0.79	0
4	MFU	D	202	-	12,12,12	0.37	0	17,17,17	0.46	0
4	MFU	B	202	-	12,12,12	0.78	0	17,17,17	0.97	1 (5%)
3	QQ7	J	201	2	105,105,105	0.41	0	182,182,182	0.44	0
4	MFU	O	203	-	12,12,12	0.20	0	17,17,17	0.33	0
3	QQ7	B	201	2	105,105,105	0.34	0	182,182,182	0.44	0
3	QQ7	N	201	2	105,105,105	0.23	0	182,182,182	0.33	0
4	MFU	C	205	-	12,12,12	0.58	0	17,17,17	0.64	0
3	QQ7	C	204	2	105,105,105	0.42	0	182,182,182	0.47	1 (0%)
3	QQ7	M	201	2	105,105,105	0.21	0	182,182,182	0.32	0
3	QQ7	I	201	2	105,105,105	0.41	0	182,182,182	0.44	0
3	QQ7	A	202	2	105,105,105	0.37	0	182,182,182	0.44	0
3	QQ7	N	202	2	105,105,105	0.18	0	182,182,182	0.31	0
3	QQ7	O	201	2	105,105,105	0.19	0	182,182,182	0.31	0
4	MFU	F	202	-	12,12,12	0.29	0	17,17,17	0.91	0
4	MFU	N	203	-	12,12,12	0.19	0	17,17,17	0.53	0
4	MFU	O	204	-	12,12,12	0.26	0	17,17,17	0.49	0
4	MFU	E	101	-	12,12,12	0.36	0	17,17,17	0.91	0
3	QQ7	O	202	2	105,105,105	0.23	0	182,182,182	0.34	0
4	MFU	I	202	-	12,12,12	0.52	0	17,17,17	0.68	0
3	QQ7	M	202	2	105,105,105	0.22	0	182,182,182	0.33	0
4	MFU	C	206	-	12,12,12	0.65	0	17,17,17	0.83	1 (5%)
4	MFU	A	203	-	12,12,12	0.57	0	17,17,17	0.65	0
3	QQ7	K	201	2	105,105,105	0.37	0	182,182,182	0.45	0

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
4	MFU	A	204	-	-	0/2/22/22	0/1/1/1
3	QQ7	O	201	2	14/14/56/56	-	-
4	MFU	B	202	-	-	0/2/22/22	0/1/1/1
3	QQ7	J	201	2	12/12/56/56	-	-
4	MFU	D	202	-	-	0/2/22/22	0/1/1/1
3	QQ7	B	201	2	13/13/56/56	-	-
3	QQ7	N	201	2	14/14/56/56	-	-
4	MFU	C	205	-	-	0/2/22/22	0/1/1/1
3	QQ7	C	204	2	13/13/56/56	-	-
4	MFU	O	203	-	-	0/2/22/22	0/1/1/1
3	QQ7	M	201	2	14/14/56/56	-	-
3	QQ7	I	201	2	14/14/56/56	-	-
3	QQ7	A	202	2	12/12/56/56	-	-
3	QQ7	N	202	2	14/14/56/56	-	-
4	MFU	I	202	-	-	0/2/22/22	0/1/1/1
4	MFU	F	202	-	-	2/2/22/22	0/1/1/1
4	MFU	N	203	-	-	0/2/22/22	0/1/1/1
4	MFU	O	204	-	-	0/2/22/22	0/1/1/1
4	MFU	E	101	-	-	1/2/22/22	0/1/1/1
3	QQ7	O	202	2	14/14/56/56	-	-
3	QQ7	M	202	2	14/14/56/56	-	-
4	MFU	C	206	-	-	1/2/22/22	0/1/1/1
4	MFU	A	203	-	-	0/2/22/22	0/1/1/1
3	QQ7	K	201	2	12/12/56/56	-	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	202	MFU	O5-C1-O1	2.48	116.72	110.97
4	C	206	MFU	O4-C4-C3	2.36	115.81	110.35
3	C	204	QQ7	C33-N24-C29	2.20	125.61	122.35

5 of 160 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	201	QQ7	N14
3	J	201	QQ7	N01
3	J	201	QQ7	N08
3	J	201	QQ7	N03

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Mol	Chain	Res	Type	Atom
3	J	201	QQ7	N19

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	202	MFU	C2-C1-O1-CM
4	F	202	MFU	O5-C1-O1-CM
4	E	101	MFU	O5-C1-O1-CM
4	C	206	MFU	O5-C1-O1-CM

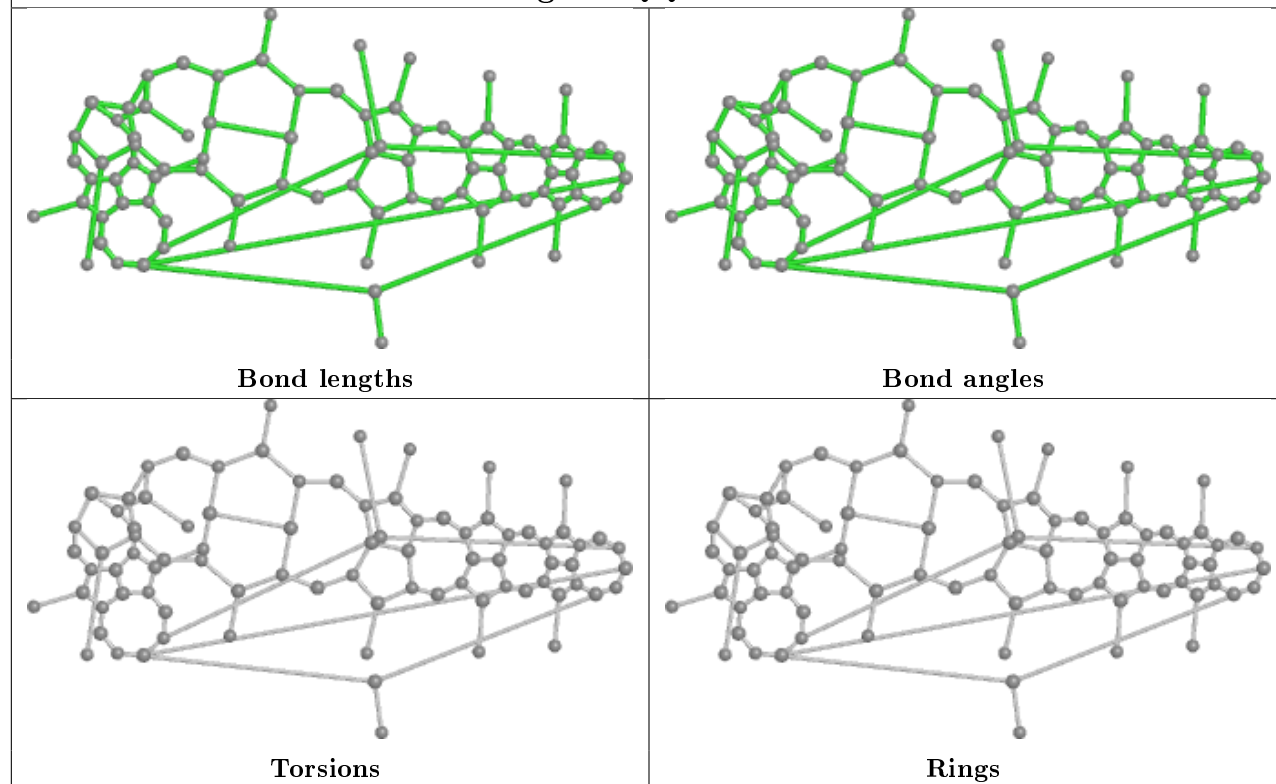
There are no ring outliers.

4 monomers are involved in 5 short contacts:

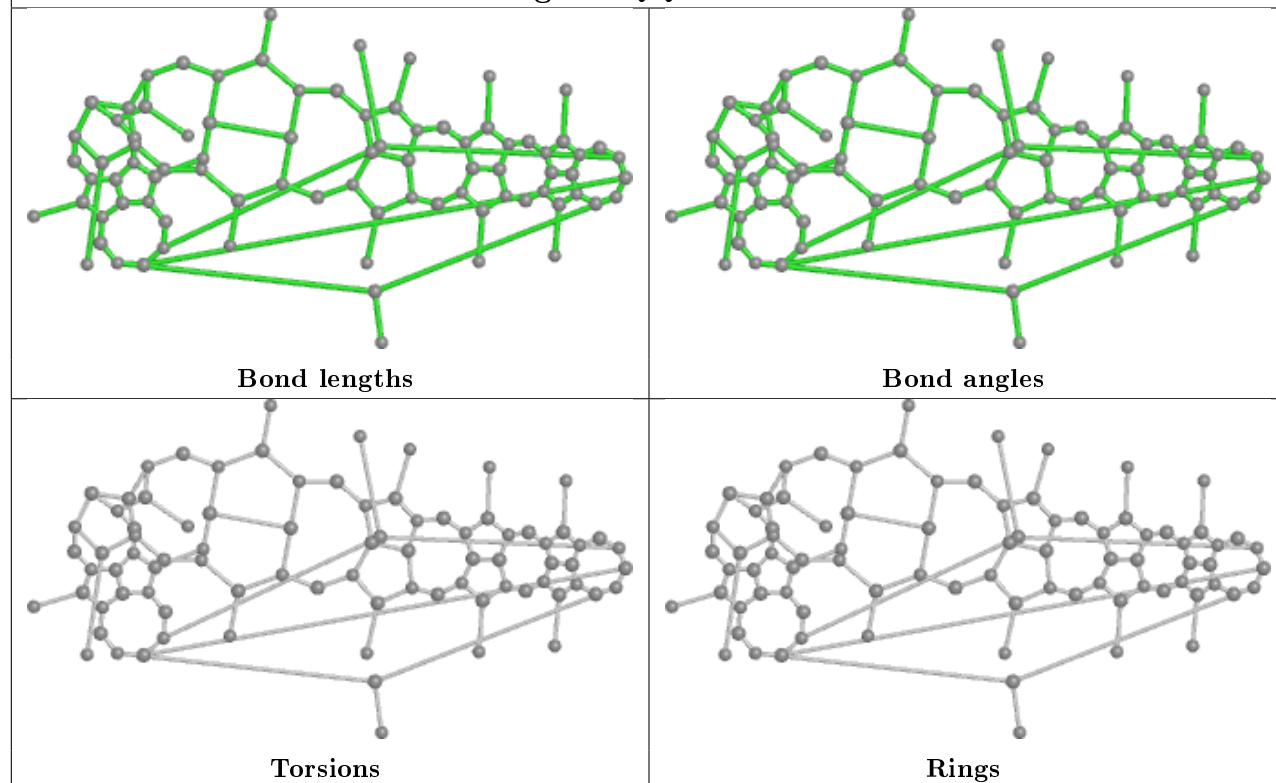
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	202	MFU	1	0
3	J	201	QQ7	1	0
4	F	202	MFU	2	0
4	O	204	MFU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

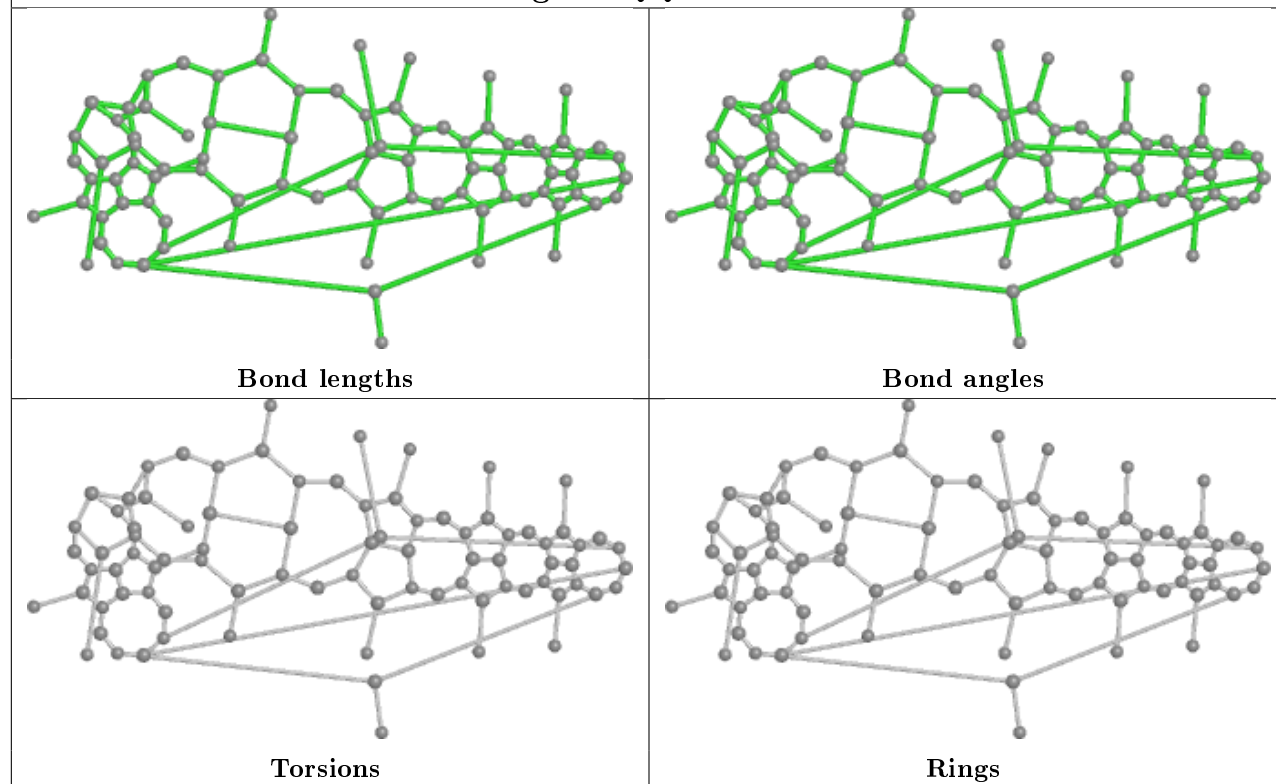
Ligand QQ7 J 201



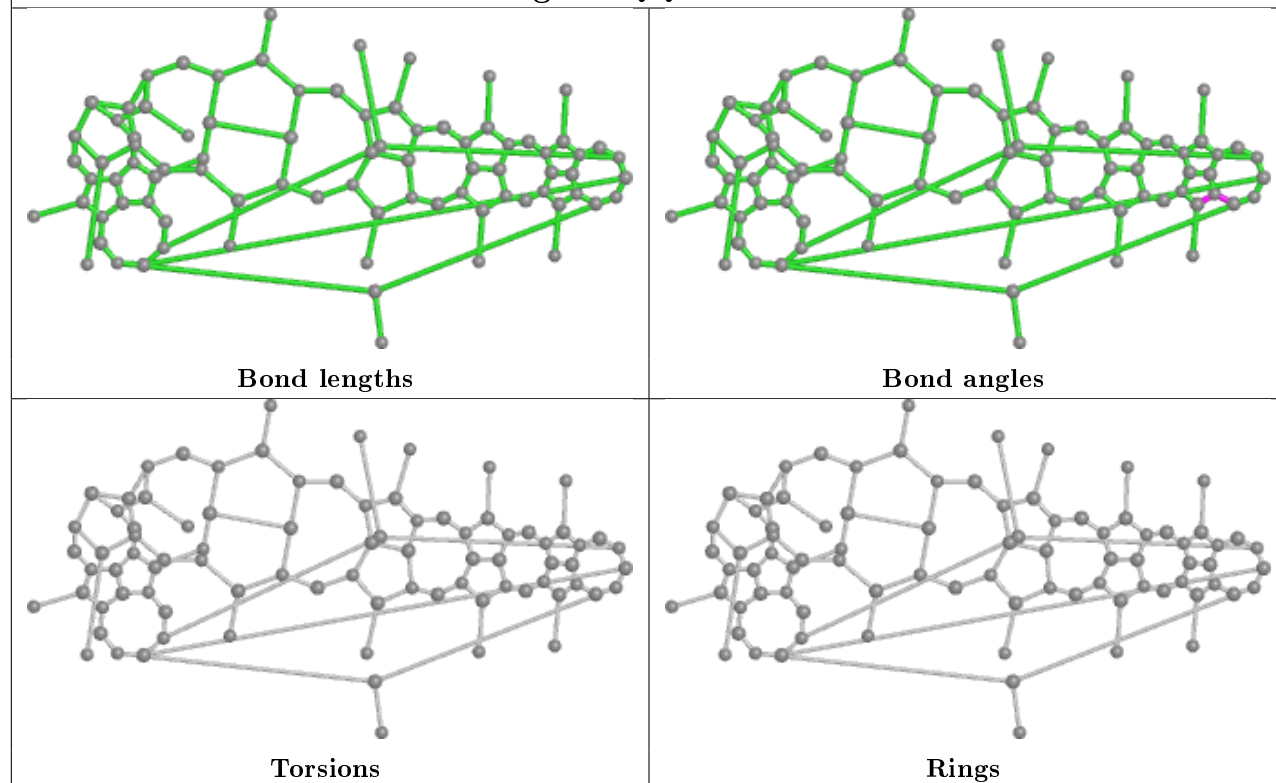
Ligand QQ7 B 201



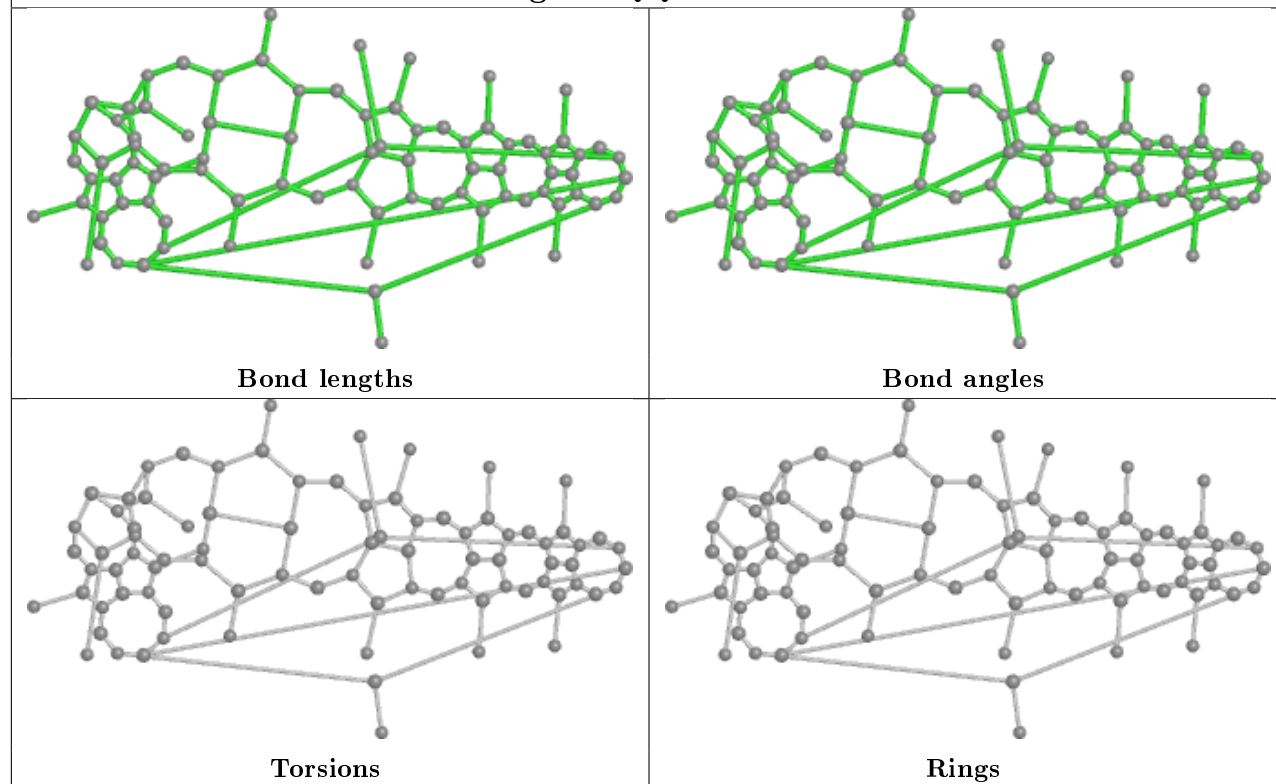
Ligand QQ7 N 201



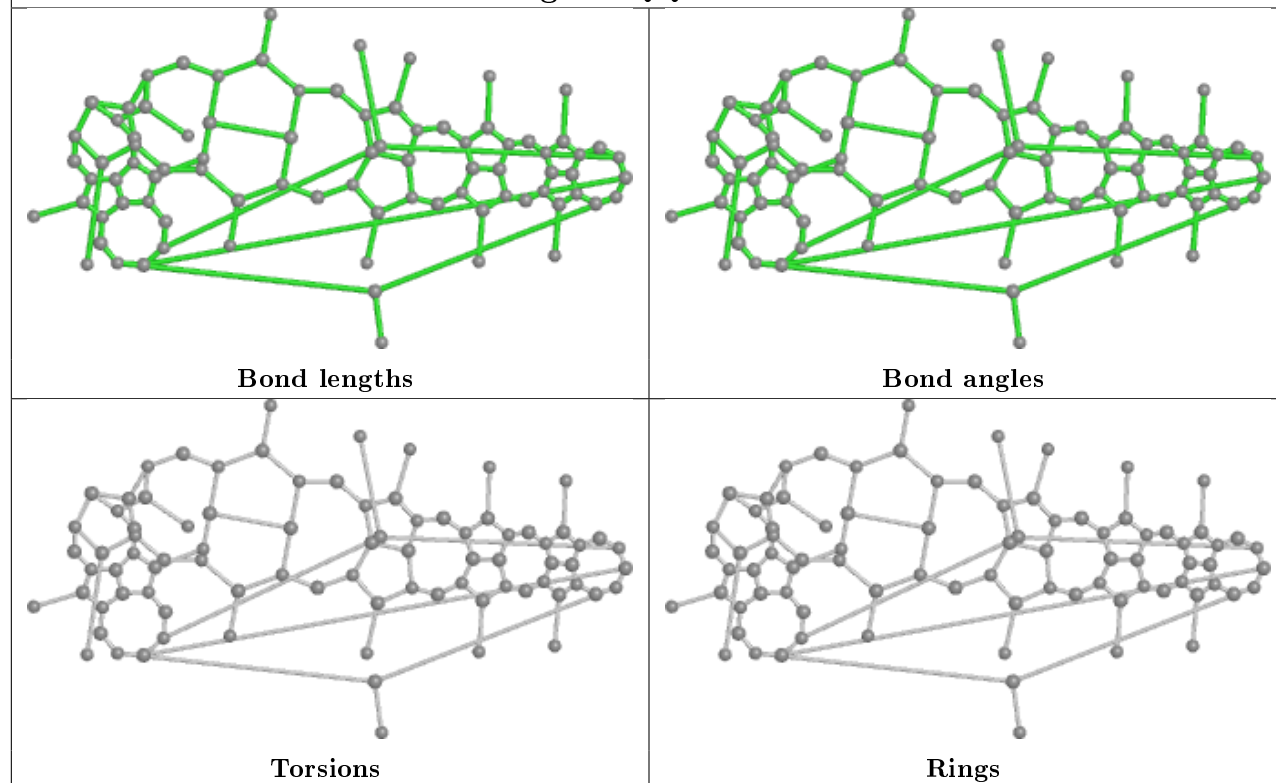
Ligand QQ7 C 204



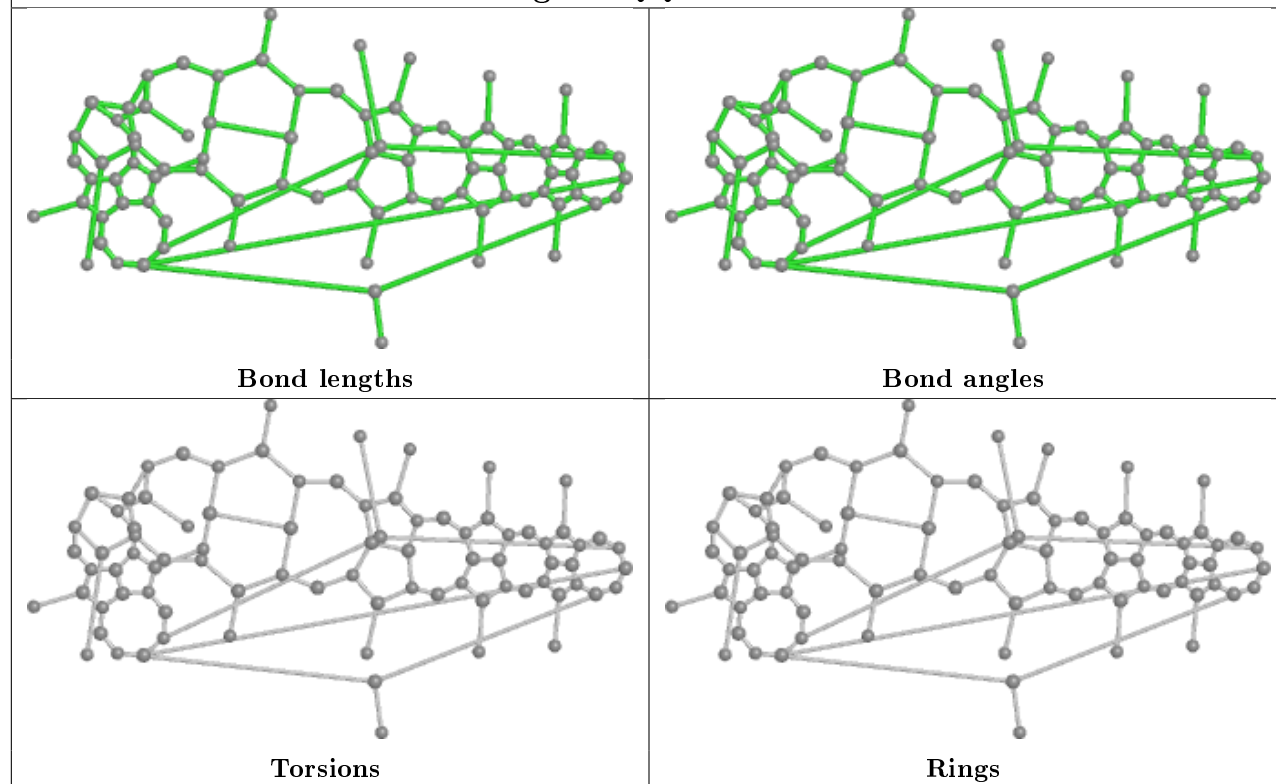
Ligand QQ7 M 201



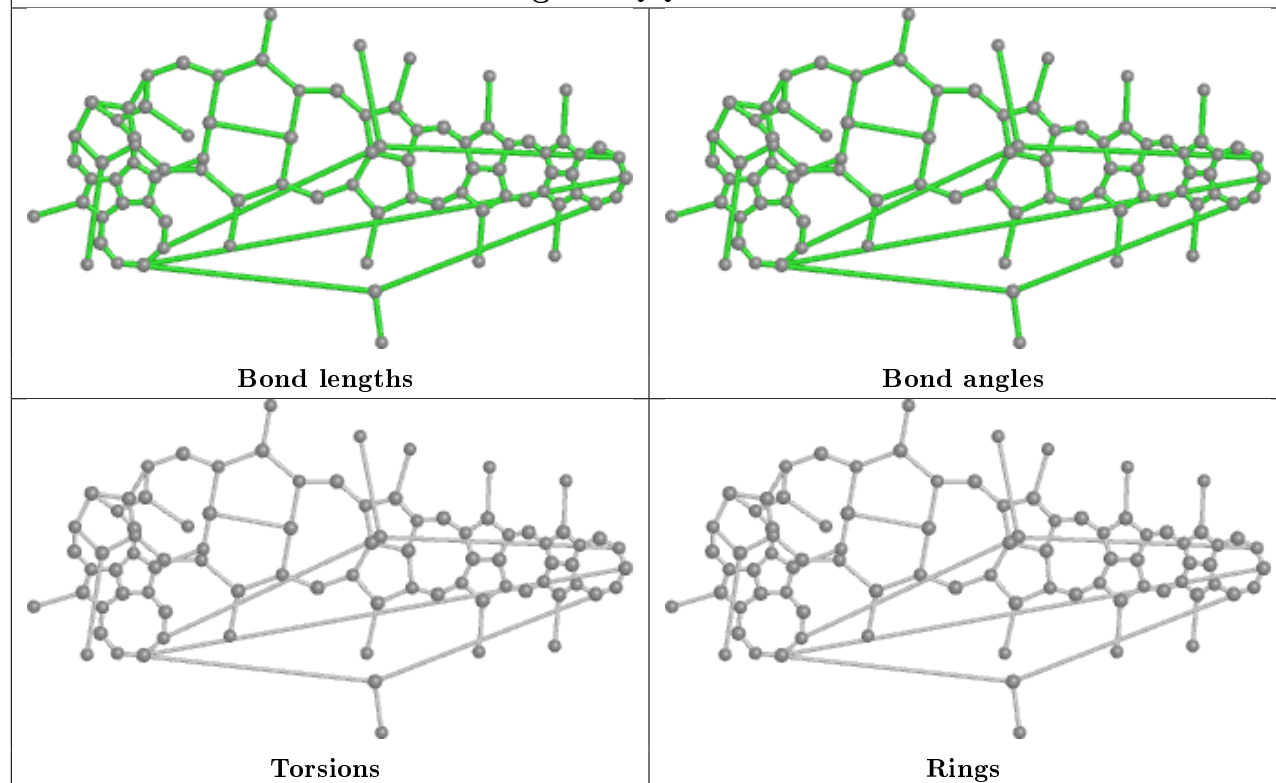
Ligand QQ7 I 201



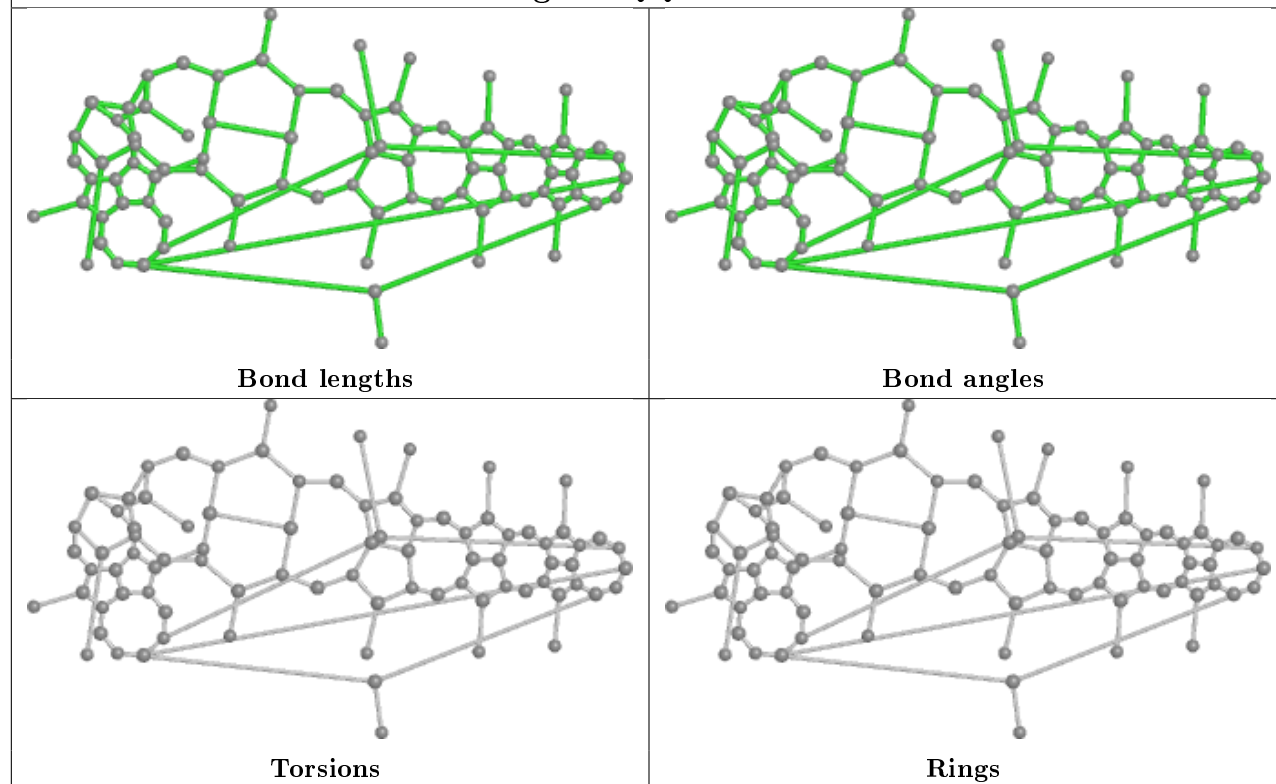
Ligand QQ7 A 202



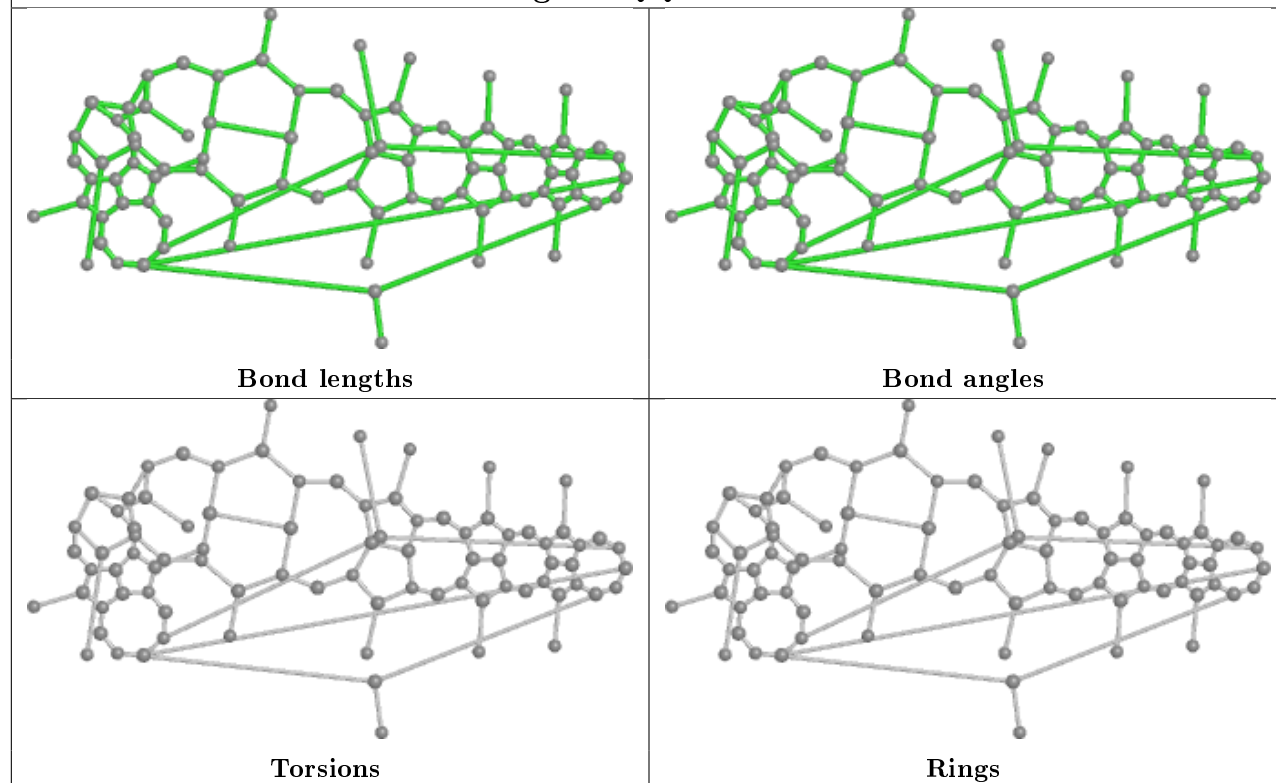
Ligand QQ7 N 202



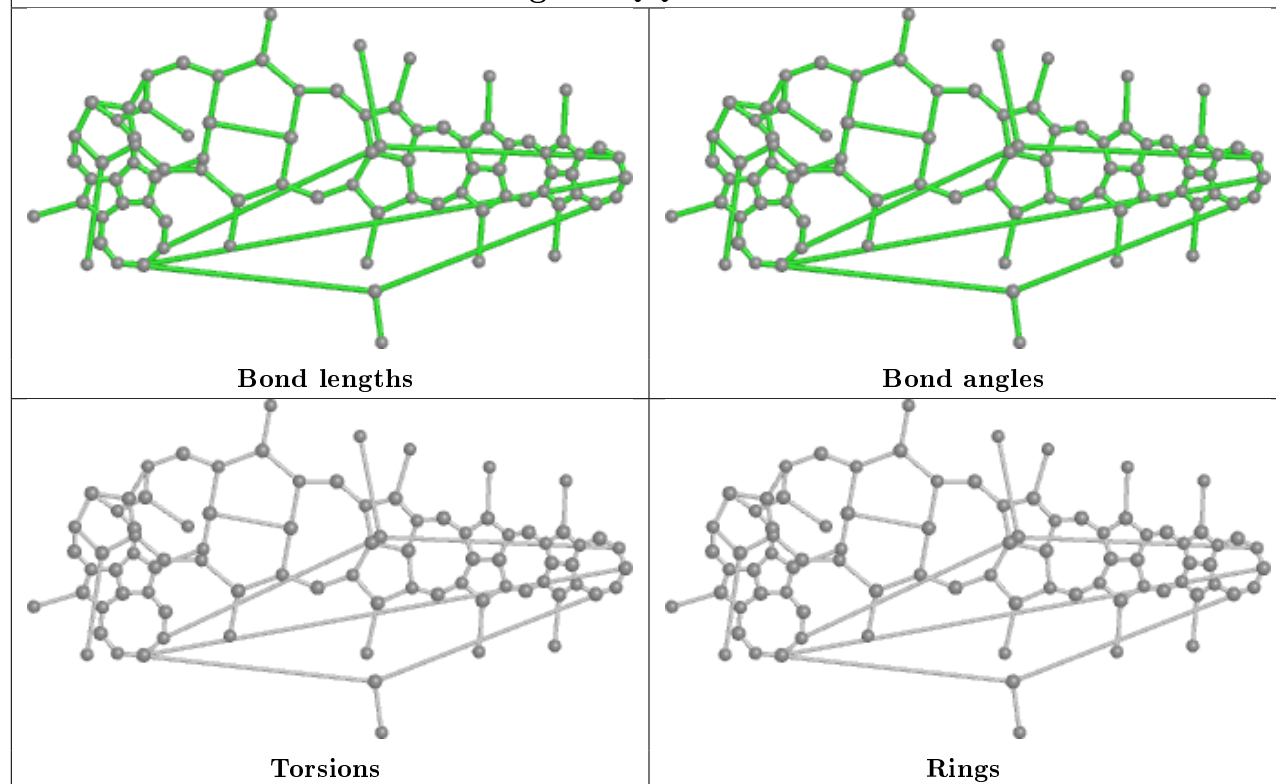
Ligand QQ7 O 201



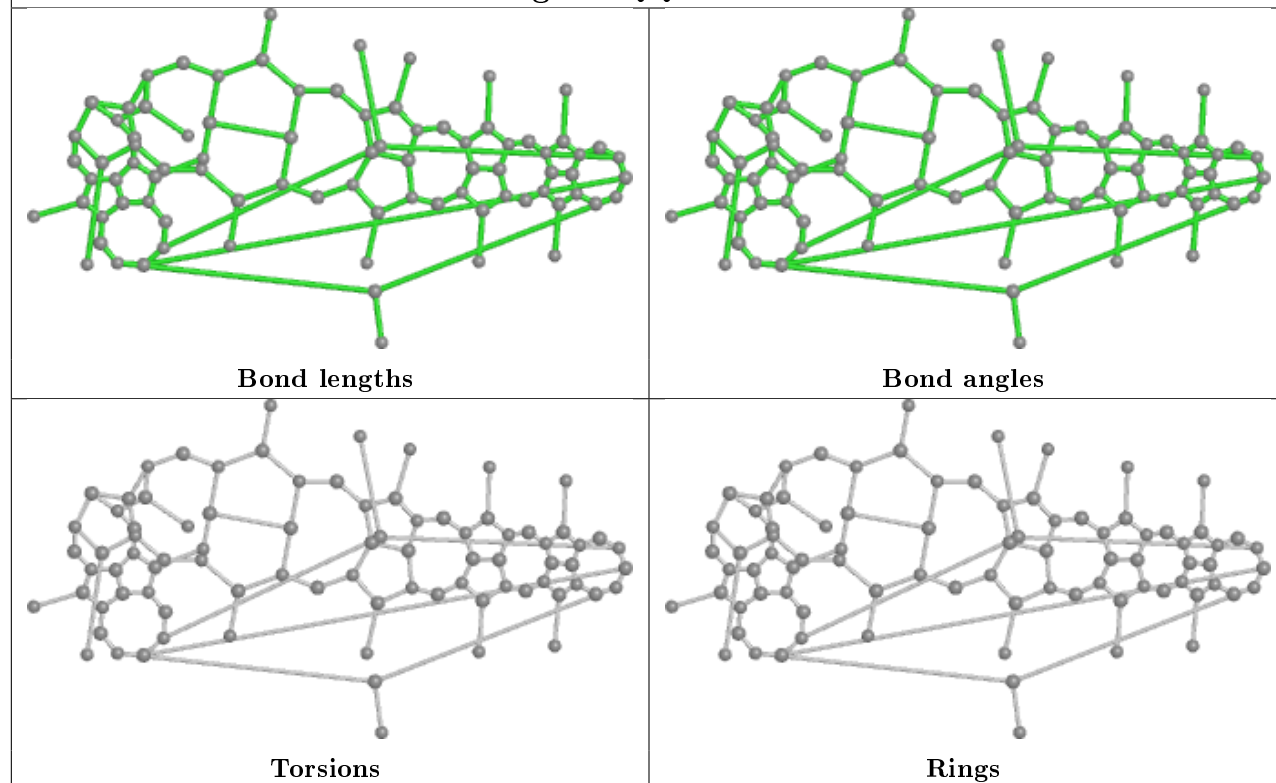
Ligand QQ7 O 202



Ligand QQ7 M 202



Ligand QQ7 K 201



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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

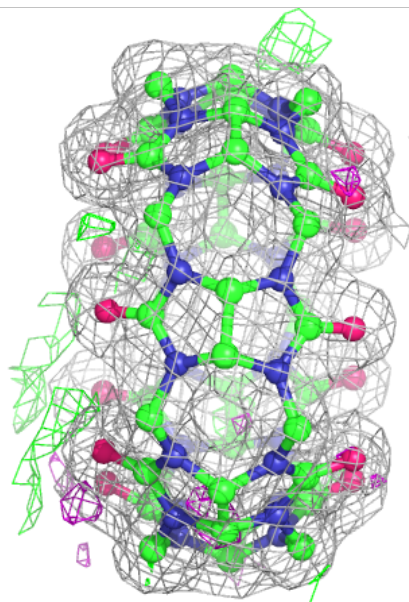
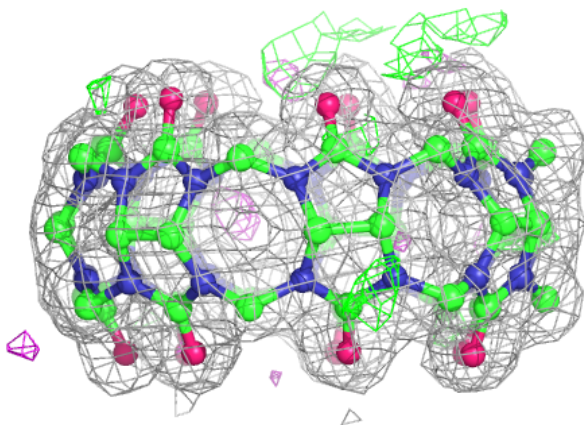
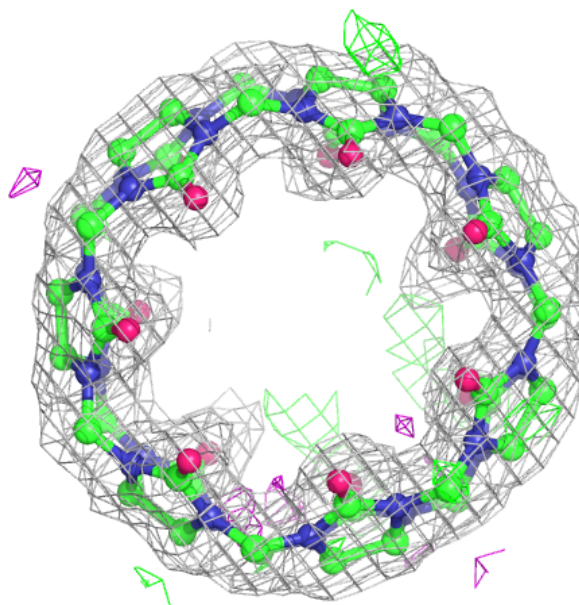
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

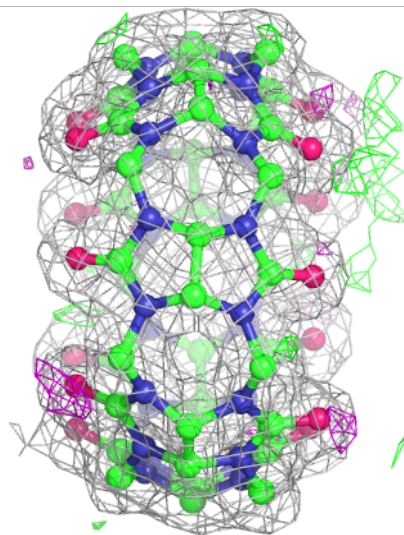
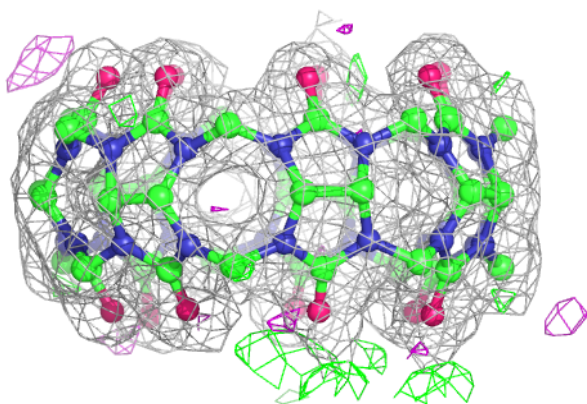
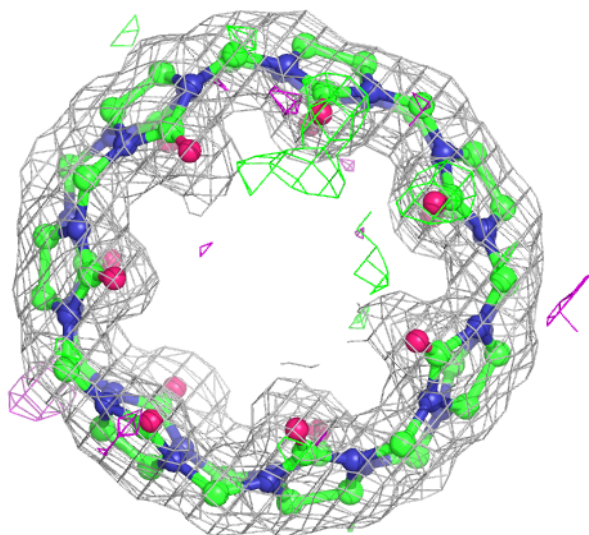
Electron density around QQ7 J 201:

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



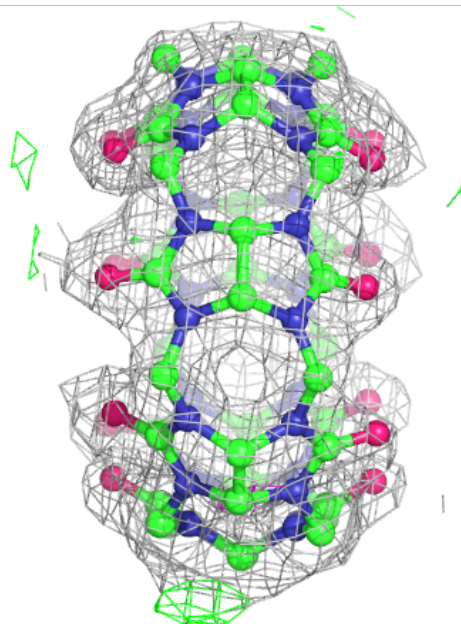
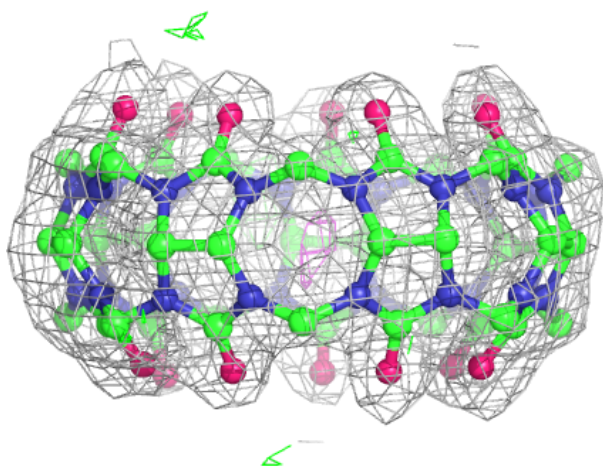
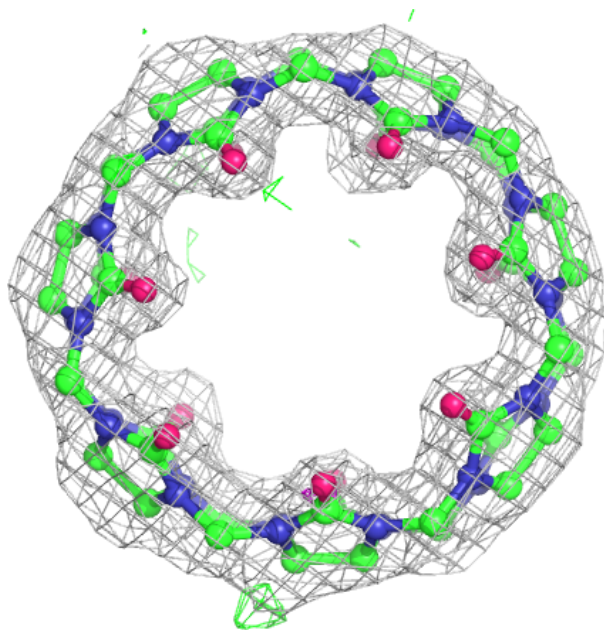
Electron density around QQ7 B 201:

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



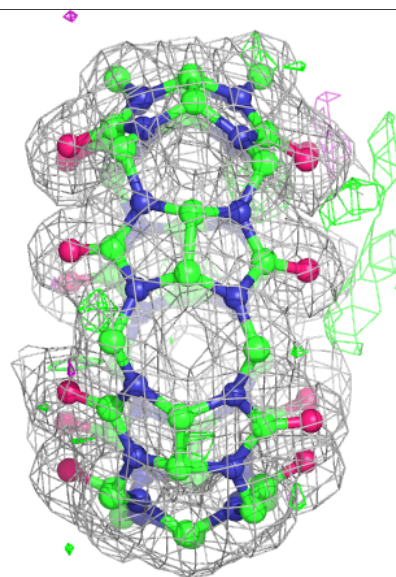
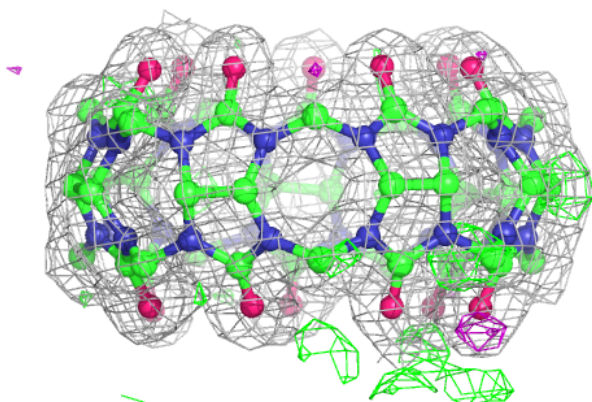
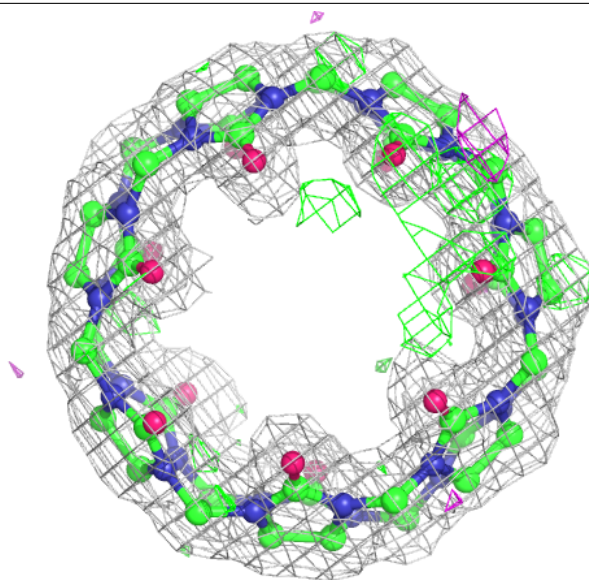
Electron density around QQ7 N 201:

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



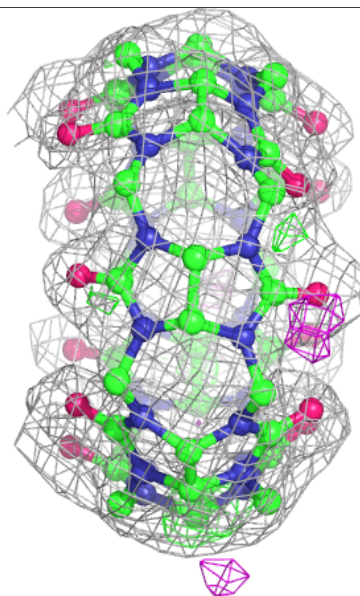
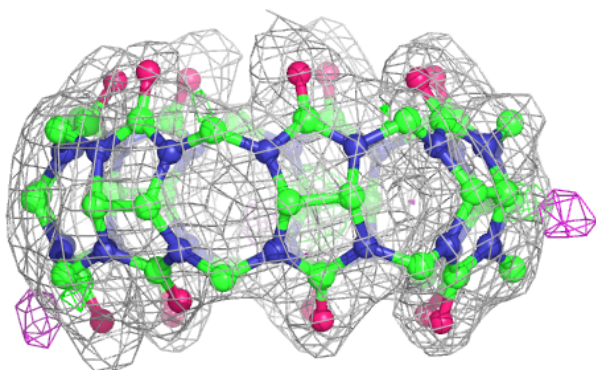
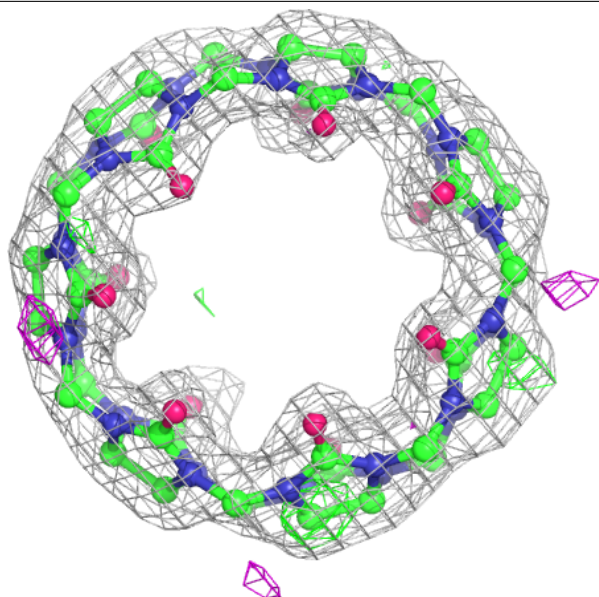
Electron density around QQ7 C 204:

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



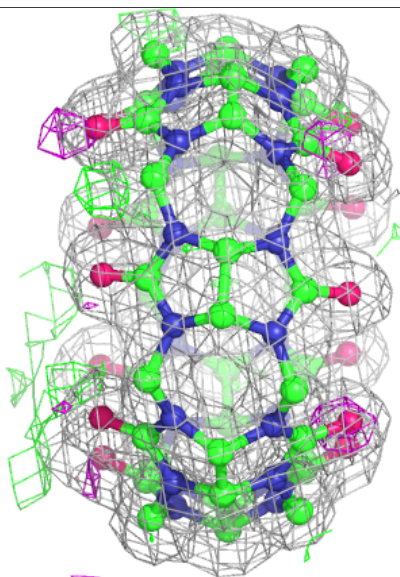
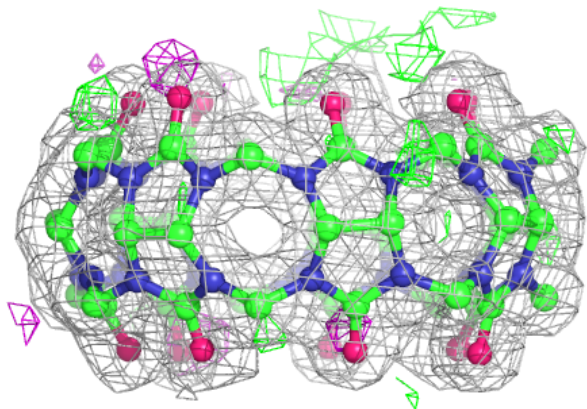
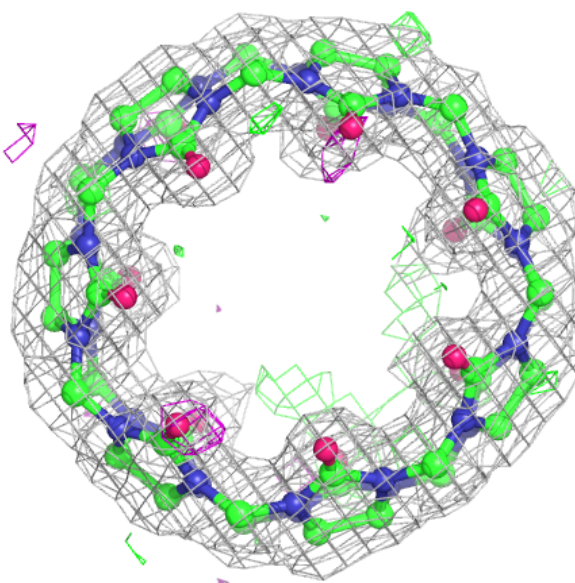
Electron density around QQ7 M 201:

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



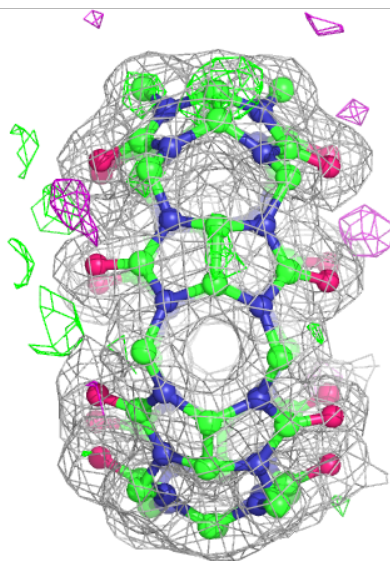
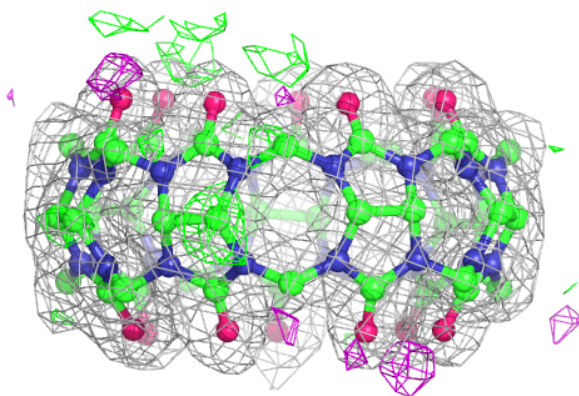
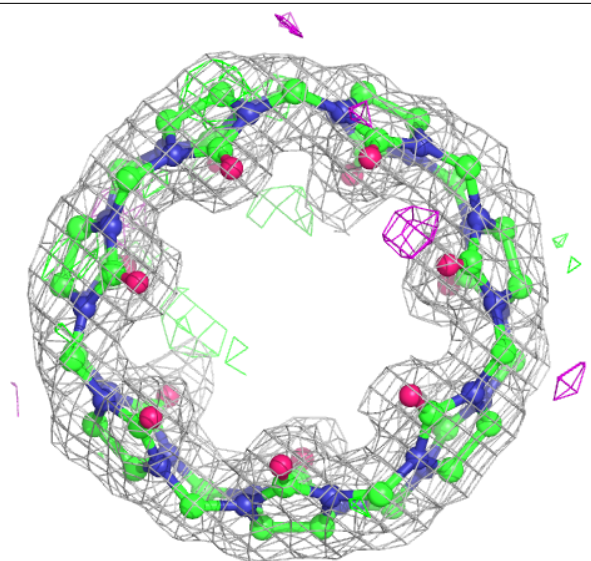
Electron density around QQ7 I 201:

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



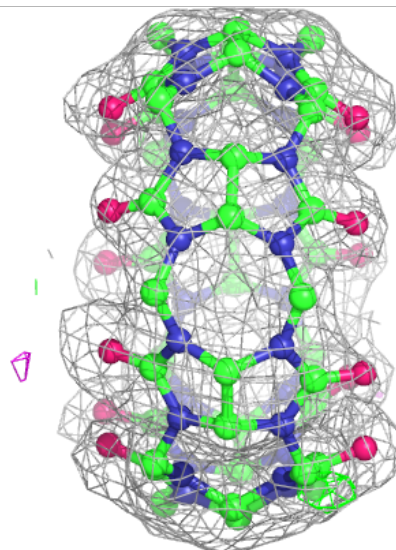
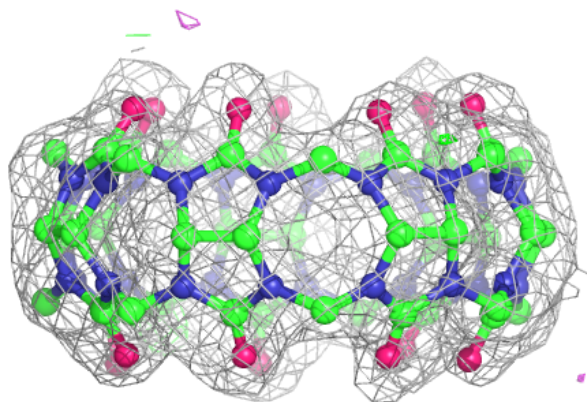
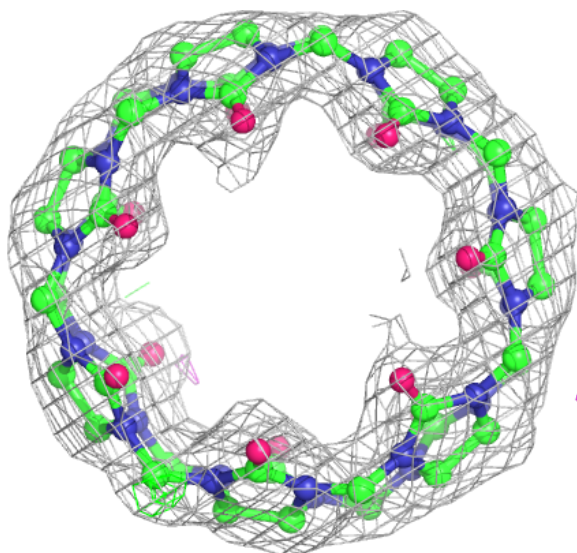
Electron density around QQ7 A 202:

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



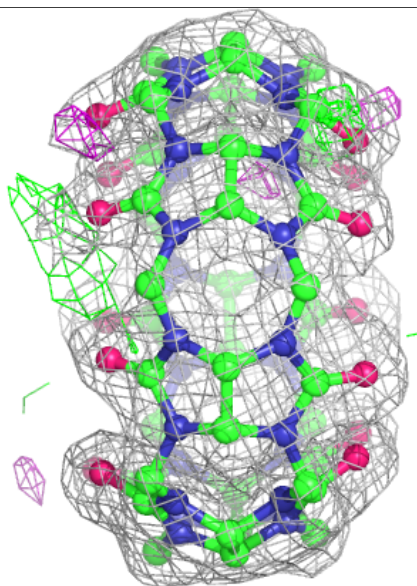
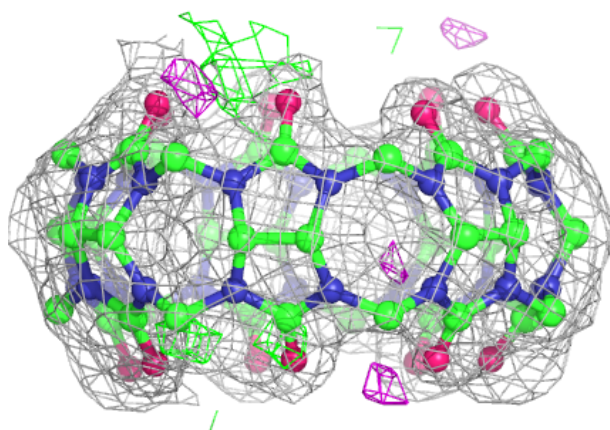
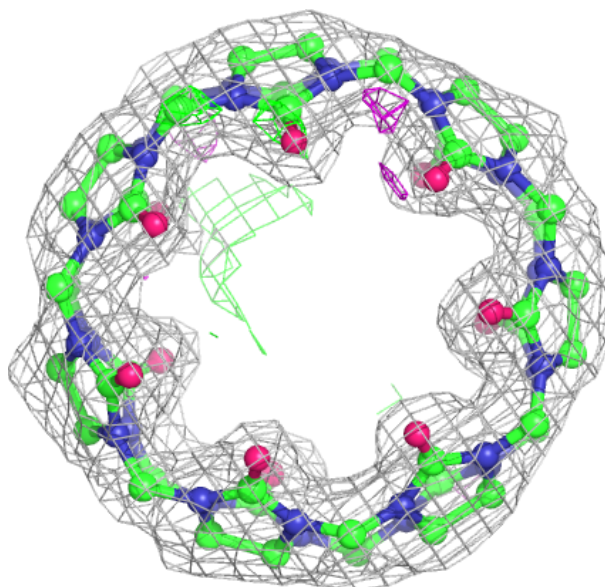
Electron density around QQ7 N 202:

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



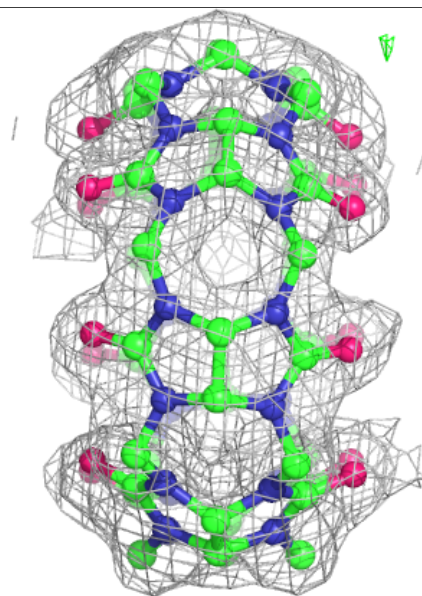
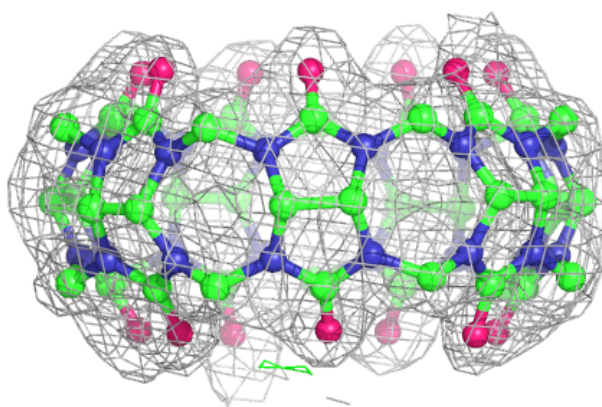
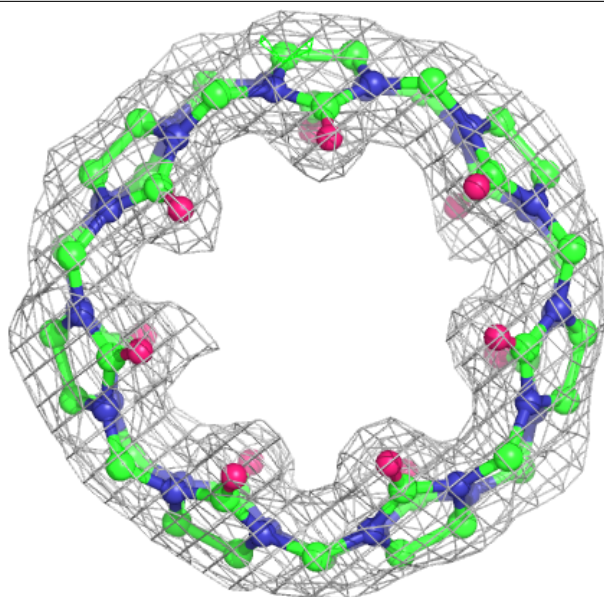
Electron density around QQ7 O 201:

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



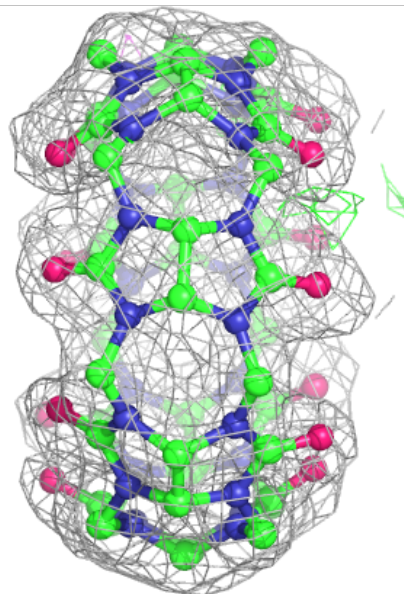
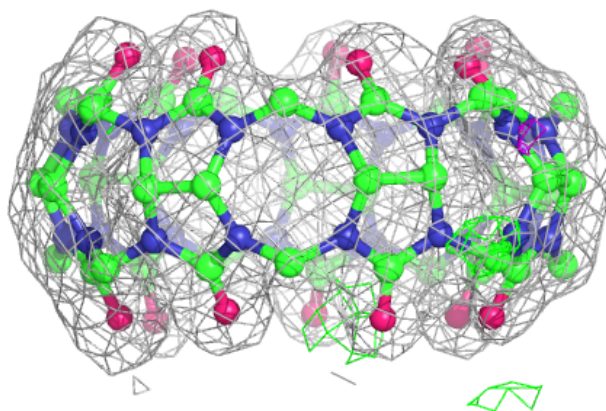
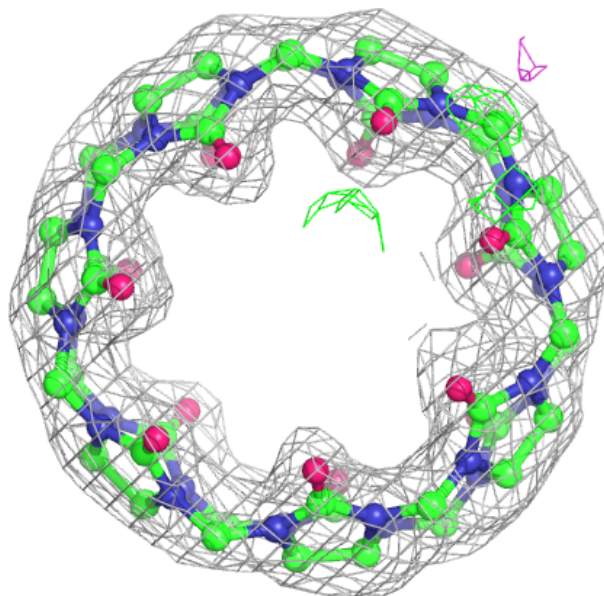
Electron density around QQ7 O 202:

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



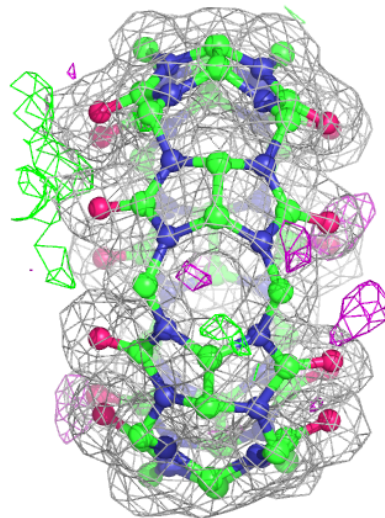
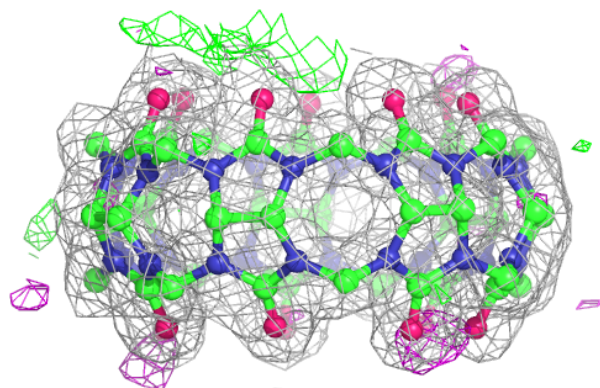
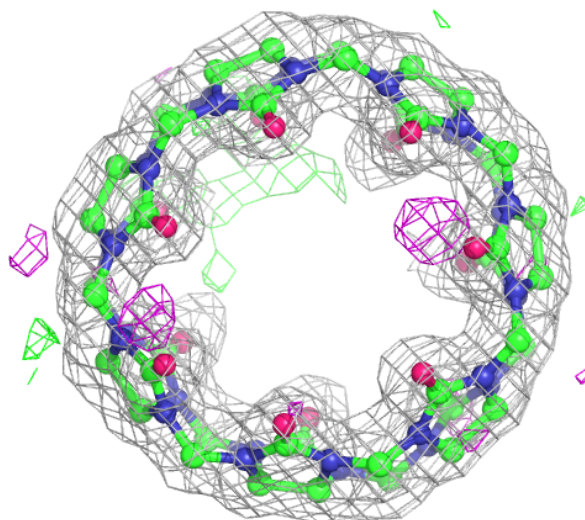
Electron density around QQ7 M 202:

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



Electron density around QQ7 K 201:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.