



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2022 – 10:08 pm BST

PDB ID : 7PCJ  
Title : X-ray structure of CypA-C52AK125C/CsA/aromatic foldamer complex  
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Deposited on : 2021-08-03  
Resolution : 1.91 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.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

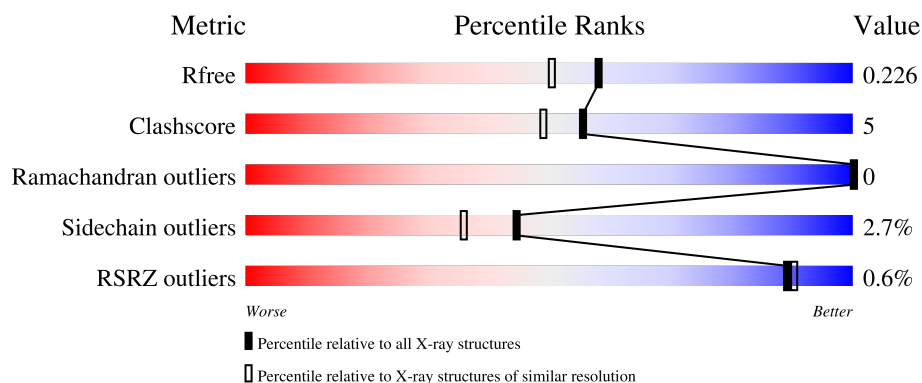
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	165	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>..</div> </div> </div>
1	D	165	<div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	11	<div> <div>27%</div> <div>55%</div> <div>18%</div> </div>
2	E	11	<div> <div>45%</div> <div>36%</div> <div>18%</div> </div>

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
3	7I7	A	201	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3009 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 Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1249	793	213	235	8			
1	D	164	Total	C	N	O	S	0	0	0
			1248	792	215	233	8			

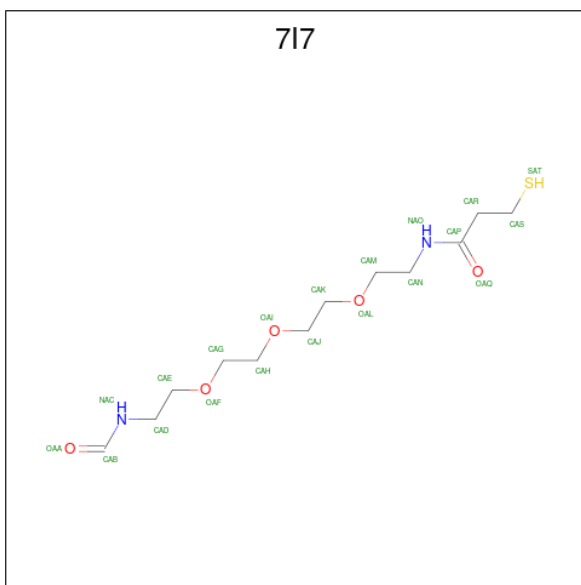
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	CYS	LYS	engineered mutation	UNP P62937
D	127	CYS	LYS	engineered mutation	UNP P62937

- Molecule 2 is a protein (with D amino acids) called Cyclosporin A.

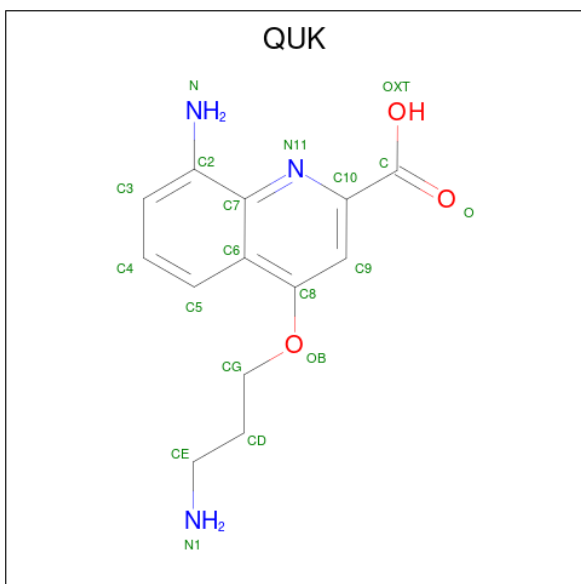
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			85	62	11	12			
2	E	11	Total	C	N	O	0	0	0
			85	62	11	12			

- Molecule 3 is N-[2-[2-[2-(2-formamidoethoxy)ethoxy]ethoxy]ethyl]-3-sulfanyl-propanamide (three-letter code: 7I7) (formula: C<sub>12</sub>H<sub>24</sub>N<sub>2</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	12	2	5	1		
3	D	1	Total	C	N	O	S	0	0
			20	12	2	5	1		

- Molecule 4 is 8-azanyl-4-(3-azanylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUK) (formula: C<sub>13</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>).



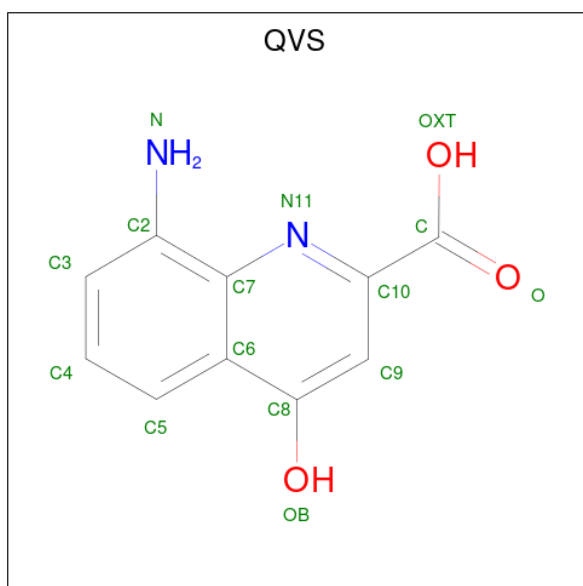
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	13	3	2		

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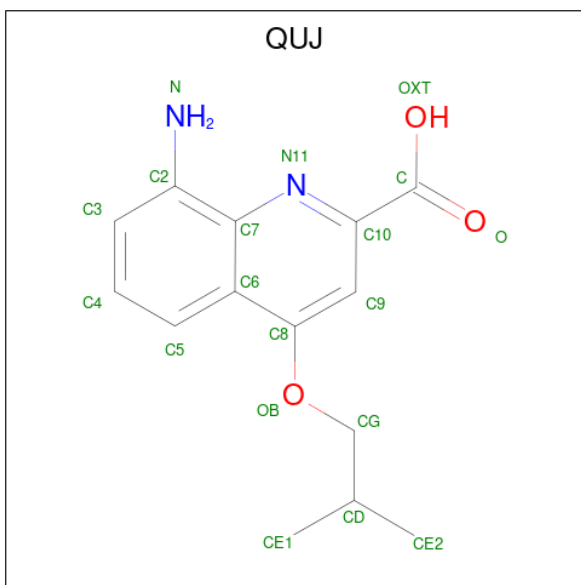
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	13	3	2		
4	D	1	Total	C	N	O	0	0
			18	13	3	2		
4	D	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 5 is 8-azanyl-4-oxidanyl-quinoline-2-carboxylic acid (three-letter code: QVS) (formula:  $C_{10}H_8N_2O_3$ ).



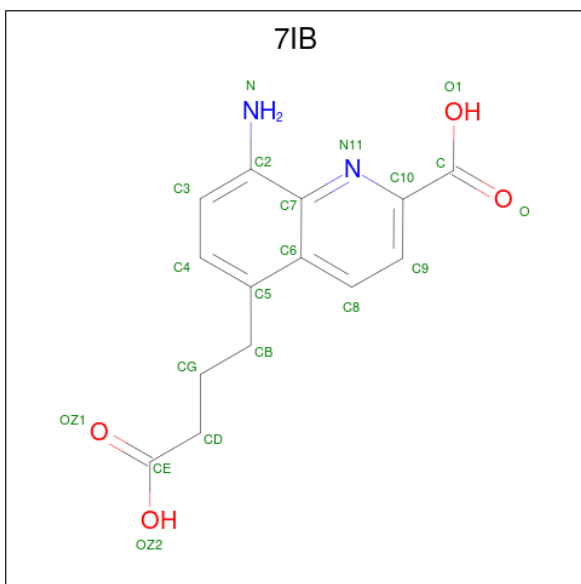
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	10	2	2		
5	D	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 6 is 8-azanyl-4-(2-methylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUJ) (formula:  $C_{14}H_{16}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	14	2	2		
6	D	1	Total	C	N	O	0	0
			18	14	2	2		

- Molecule 7 is 8-azanyl-5-(4-oxidanyl-4-oxidanylidene-butyl)quinoline-2-carboxylic acid (three-letter code: 7IB) (formula: C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			20	14	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			20	14	2	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	67	Total	O	0	0
			67	67		
8	B	3	Total	O	0	0
			3	3		
8	D	51	Total	O	0	0
			51	51		
8	E	5	Total	O	0	0
			5	5		

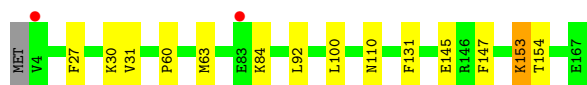


### 3 Residue-property plots [i](#)

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: Peptidyl-prolyl cis-trans isomerase A

Chain A:  91% 8% ..



- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

Chain D:  90% 9% .



- Molecule 2: Cyclosporin A

Chain B:  27% 55% 18%



- Molecule 2: Cyclosporin A

Chain E:  45% 36% 18%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.47Å 70.89Å 64.09Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	62.52 – 1.91 62.52 – 1.91	Depositor EDS
% Data completeness (in resolution range)	89.1 (62.52-1.91) 89.1 (62.52-1.91)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.177 , 0.219 0.185 , 0.226	Depositor DCC
$R_{free}$ test set	1272 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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: MVA, SAR, 7IB, MLE, DAL, ABA, 7I7, QUK, BMT, QVS, QUJ

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	0.75	0/1277	0.77	0/1714
1	D	0.74	0/1276	0.76	0/1713
2	B	0.40	0/10	0.64	0/11
2	E	0.61	0/10	0.69	0/11
All	All	0.74	0/2573	0.77	0/3449

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	1249	0	1206	6	0
1	D	1248	0	1204	9	0
2	B	85	0	109	7	0
2	E	85	0	110	5	0
3	A	20	0	0	0	0
3	D	20	0	0	0	0
4	A	36	0	0	1	0
4	D	36	0	0	0	0
5	A	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	14	0	0	0	0
6	A	18	0	0	0	0
6	D	18	0	0	0	0
7	A	20	0	0	2	0
7	D	20	0	0	0	0
8	A	67	0	0	1	1
8	B	3	0	0	0	0
8	D	51	0	0	2	1
8	E	5	0	0	0	0
All	All	3009	0	2629	28	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:O	1:A:154:THR:HA	2.06	0.56
1:A:60:PRO:HA	1:A:145:GLU:HG3	1.92	0.51
1:D:147:PHE:CE1	1:D:156:LYS:HD2	2.46	0.51
7:A:206:7IB:C8	7:A:206:7IB:CG	2.89	0.50
1:A:84:LYS:HA	1:A:110:ASN:O	2.12	0.49
1:D:86:GLU:CD	1:D:86:GLU:H	2.15	0.49
1:D:7:THR:HA	1:D:24:PHE:O	2.15	0.46
2:E:3:MLE:HB2	2:E:4:MVA:HN1	1.97	0.46
1:D:151:ASN:ND2	8:D:303:HOH:O	2.49	0.45
1:D:147:PHE:CD1	1:D:156:LYS:HD2	2.52	0.44
4:A:205:QUK:O	7:A:206:7IB:C3	2.65	0.43
2:B:4:MVA:HA	2:B:5:BMT:HN1	1.83	0.43
1:D:120:LYS:O	8:D:301:HOH:O	2.22	0.43
2:E:4:MVA:HA	2:E:5:BMT:HN1	1.76	0.43
1:A:100:LEU:HG	1:A:131:PHE:CZ	2.54	0.43
1:D:14:VAL:HG22	1:D:158:ILE:HD12	2.01	0.43
2:E:3:MLE:O	2:E:3:MLE:HN3	2.18	0.42
2:B:1:DAL:C	2:B:3:MLE:HN1	2.48	0.42
2:E:9:VAL:HA	2:E:10:MLE:HN1	1.75	0.42
2:B:5:BMT:HN2	2:B:5:BMT:OG1	2.20	0.41
2:B:3:MLE:HA	2:B:4:MVA:HN1	1.89	0.41
1:D:104:ASN:O	2:E:5:BMT:HA	2.20	0.41
1:A:153:LYS:HD2	8:A:340:HOH:O	2.19	0.41
2:B:10:MLE:HN2	2:B:10:MLE:HB3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:PRO:O	1:D:109:THR:HG23	2.21	0.41
1:A:27:PHE:CD2	1:A:92:LEU:HD13	2.56	0.41
2:B:9:VAL:HA	2:B:10:MLE:HN1	1.68	0.40
2:B:1:DAL:HA	2:B:2:MLE:HN1	1.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:343:HOH:O	8:D:301:HOH:O[2_657]	1.52	0.68

## 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	162/165 (98%)	157 (97%)	5 (3%)	0	100	100
1	D	162/165 (98%)	156 (96%)	6 (4%)	0	100	100
2	B	1/11 (9%)	1 (100%)	0	0	100	100
2	E	1/11 (9%)	1 (100%)	0	0	100	100
All	All	326/352 (93%)	315 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	130/133 (98%)	126 (97%)	4 (3%)	40	30
1	D	129/133 (97%)	126 (98%)	3 (2%)	50	43
2	B	1/1 (100%)	1 (100%)	0	100	100
2	E	1/1 (100%)	1 (100%)	0	100	100
All	All	261/268 (97%)	254 (97%)	7 (3%)	44	36

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	31	VAL
1	A	63	MET
1	A	153	LYS
1	D	31	VAL
1	D	63	MET
1	D	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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	$\# Z  > 2$
2	MLE	B	10	2	7,8,9	0.59	0	6,9,11	0.69	0
2	SAR	B	7	2	4,4,5	1.36	1 (25%)	1,3,5	1.73	0
2	ABA	B	6	2	4,5,6	0.64	0	1,5,7	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLE	E	3	2	7,8,9	0.40	0	6,9,11	1.00	1 (16%)
2	MLE	E	10	2	7,8,9	0.74	0	6,9,11	0.74	0
2	MLE	B	2	2	7,8,9	0.67	0	6,9,11	0.56	0
2	MVA	E	4	2	6,7,8	0.66	0	7,8,10	0.80	0
2	MLE	E	2	2	7,8,9	0.59	0	6,9,11	0.69	0
2	MVA	B	4	2	6,7,8	0.70	0	7,8,10	1.29	1 (14%)
2	ABA	E	6	2	4,5,6	0.48	0	1,5,7	0.07	0
2	MLE	E	8	2	7,8,9	0.45	0	6,9,11	1.01	0
2	MLE	B	8	2	7,8,9	0.55	0	6,9,11	0.98	0
2	BMT	E	5	2	11,12,13	0.61	0	12,14,16	1.12	1 (8%)
2	SAR	E	7	2	4,4,5	1.50	1 (25%)	1,3,5	1.70	0
2	BMT	B	5	2	11,12,13	0.65	0	12,14,16	0.69	0
2	MLE	B	3	2	7,8,9	0.37	0	6,9,11	1.03	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	B	10	2	-	2/5/8/10	-
2	SAR	B	7	2	-	1/1/2/3	-
2	ABA	B	6	2	-	0/3/4/6	-
2	MLE	E	3	2	-	0/5/8/10	-
2	MLE	E	10	2	-	0/5/8/10	-
2	MLE	B	2	2	-	0/5/8/10	-
2	MVA	E	4	2	-	1/6/8/10	-
2	MLE	E	2	2	-	0/5/8/10	-
2	MVA	B	4	2	-	3/6/8/10	-
2	ABA	E	6	2	-	0/3/4/6	-
2	MLE	E	8	2	-	1/5/8/10	-
2	MLE	B	8	2	-	1/5/8/10	-
2	BMT	E	5	2	-	3/13/16/18	-
2	SAR	E	7	2	-	1/1/2/3	-
2	BMT	B	5	2	-	1/13/16/18	-
2	MLE	B	3	2	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	7	SAR	CA-N	2.66	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	SAR	CA-N	2.37	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	BMT	CB-CA-N	2.76	116.90	111.41
2	B	4	MVA	CB-CA-C	-2.68	109.68	113.04
2	B	3	MLE	O-C-CA	-2.17	119.08	124.78
2	E	3	MLE	O-C-CA	-2.07	119.34	124.78

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MVA	N-CA-CB-CG2
2	B	5	BMT	CB-CA-N-CN
2	B	8	MLE	O-C-CA-CB
2	E	8	MLE	O-C-CA-CB
2	B	10	MLE	CA-CB-CG-CD1
2	B	10	MLE	CA-CB-CG-CD2
2	B	4	MVA	N-CA-CB-CG1
2	E	5	BMT	CE-CD2-CG2-CB
2	E	5	BMT	CB-CA-N-CN
2	B	4	MVA	CB-CA-N-CN
2	E	4	MVA	CB-CA-N-CN
2	E	5	BMT	CE-CD2-CG2-CD1
2	B	7	SAR	C-CA-N-CN
2	E	7	SAR	C-CA-N-CN

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	10	MLE	2	0
2	E	3	MLE	2	0
2	E	10	MLE	1	0
2	B	2	MLE	1	0
2	E	4	MVA	2	0
2	B	4	MVA	2	0
2	E	5	BMT	2	0
2	B	5	BMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	MLE	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	QUJ	A	204	4,5	19,19,20	2.05	1 (5%)	23,26,28	2.19	7 (30%)
4	QUK	D	201	3,5	19,19,20	1.82	2 (10%)	22,25,27	3.14	9 (40%)
4	QUK	A	202	3,5	19,19,20	2.18	1 (5%)	22,25,27	1.72	3 (13%)
4	QUK	D	204	6,7	19,19,20	1.94	2 (10%)	22,25,27	2.02	4 (18%)
4	QUK	A	205	6,7	19,19,20	2.06	2 (10%)	22,25,27	1.97	5 (22%)
6	QUJ	D	203	4,5	19,19,20	1.87	2 (10%)	23,26,28	1.98	6 (26%)
7	7IB	A	206	4	21,21,21	1.96	2 (9%)	28,29,29	1.86	9 (32%)
3	7I7	A	201	4,1	18,19,19	0.94	0	16,19,19	0.45	0
5	QVS	A	203	4,6	15,15,16	2.37	2 (13%)	19,21,23	2.02	5 (26%)
5	QVS	D	202	4,6	15,15,16	2.12	3 (20%)	19,21,23	2.23	6 (31%)
7	7IB	D	205	4	21,21,21	1.96	3 (14%)	28,29,29	1.55	7 (25%)
3	7I7	D	206	4,1	18,19,19	0.83	0	16,19,19	0.89	1 (6%)

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
6	QUJ	A	204	4,5	-	2/7/7/9	0/2/2/2
4	QUK	D	201	3,5	-	3/7/7/9	0/2/2/2
4	QUK	A	202	3,5	-	3/7/7/9	0/2/2/2
4	QUK	D	204	6,7	-	3/7/7/9	0/2/2/2
4	QUK	A	205	6,7	-	1/7/7/9	0/2/2/2
6	QUJ	D	203	4,5	-	0/7/7/9	0/2/2/2
7	7IB	A	206	4	-	5/10/10/10	0/2/2/2
3	7I7	A	201	4,1	-	7/18/18/18	-
5	QVS	A	203	4,6	-	0/2/2/4	0/2/2/2
5	QVS	D	202	4,6	-	2/2/2/4	0/2/2/2
7	7IB	D	205	4	-	3/10/10/10	0/2/2/2
3	7I7	D	206	4,1	-	8/18/18/18	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	202	QUK	C10-C	-8.81	1.39	1.48
5	A	203	QVS	C10-C	-8.00	1.40	1.48
4	A	205	QUK	C10-C	-7.97	1.40	1.48
6	A	204	QUJ	C10-C	-7.72	1.40	1.48
4	D	204	QUK	C10-C	-7.65	1.40	1.48
7	A	206	7IB	C10-C	-7.37	1.40	1.50
6	D	203	QUJ	C10-C	-6.99	1.41	1.48
7	D	205	7IB	C10-C	-6.92	1.41	1.50
5	D	202	QVS	C10-C	-6.29	1.42	1.48
4	D	201	QUK	C10-C	-6.08	1.42	1.48
4	D	201	QUK	C10-N11	4.44	1.37	1.33
5	D	202	QVS	C2-C7	-3.16	1.37	1.42
7	D	205	7IB	CB-C5	-2.96	1.43	1.51
7	A	206	7IB	CB-C5	-2.61	1.44	1.51
4	A	205	QUK	C10-N11	2.50	1.35	1.33
4	D	204	QUK	C10-N11	2.28	1.35	1.33
5	D	202	QVS	C10-N11	2.14	1.35	1.33
6	D	203	QUJ	C10-N11	2.12	1.35	1.33
5	A	203	QVS	C10-N11	2.09	1.35	1.33
7	D	205	7IB	C2-C7	-2.01	1.39	1.42

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	QUK	C-C10-N11	7.22	121.74	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	203	QUJ	C10-N11-C7	6.83	123.29	118.11
6	A	204	QUJ	C10-N11-C7	6.80	123.27	118.11
4	D	204	QUK	C10-N11-C7	6.60	123.12	118.11
4	D	201	QUK	C7-C2-N	6.44	130.35	118.07
4	A	205	QUK	C10-N11-C7	6.34	122.91	118.11
5	A	203	QVS	C10-N11-C7	6.16	122.78	118.11
5	D	202	QVS	C10-N11-C7	6.12	122.75	118.11
4	A	202	QUK	C10-N11-C7	5.96	122.63	118.11
4	D	201	QUK	C2-C7-N11	5.53	124.11	118.64
4	D	201	QUK	C10-N11-C7	5.29	122.12	118.11
4	D	201	QUK	C3-C2-N	-4.60	111.17	120.36
5	D	202	QVS	C3-C2-N	3.86	128.08	120.36
7	A	206	7IB	CB-C5-C6	3.75	129.11	120.93
7	A	206	7IB	C9-C10-N11	-3.72	118.81	123.42
5	D	202	QVS	C7-C2-N	-3.62	111.17	118.07
6	A	204	QUJ	C3-C2-N	3.48	127.31	120.36
7	D	205	7IB	C9-C10-N11	-3.42	119.18	123.42
7	A	206	7IB	C-C10-N11	3.37	121.66	116.28
6	A	204	QUJ	CG-OB-C8	3.33	129.14	118.25
5	D	202	QVS	C9-C10-C	3.24	124.02	121.23
4	D	201	QUK	O-C-C10	-3.20	121.19	124.22
6	A	204	QUJ	C9-C10-C	3.18	123.98	121.23
6	A	204	QUJ	C7-C2-N	-3.15	112.06	118.07
4	D	204	QUK	O-C-C10	-3.15	121.24	124.22
6	A	204	QUJ	O-C-C10	-3.11	121.28	124.22
4	D	201	QUK	C9-C10-C	-3.09	118.55	121.23
4	A	205	QUK	O-C-C10	-3.05	121.33	124.22
4	D	204	QUK	C-C10-N11	2.98	117.58	114.66
7	A	206	7IB	CB-CG-CD	-2.97	104.55	114.34
4	A	202	QUK	C-C10-N11	2.97	117.57	114.66
7	D	205	7IB	C3-C2-N	2.95	126.26	120.36
5	A	203	QVS	C9-C10-C	2.94	123.77	121.23
6	D	203	QUJ	C3-C2-N	2.88	126.12	120.36
6	D	203	QUJ	O-C-C10	-2.84	121.53	124.22
3	D	206	7I7	OAA-CAB-NAC	-2.83	122.03	124.89
6	D	203	QUJ	C9-C10-C	2.79	123.63	121.23
4	A	205	QUK	C3-C2-N	2.77	125.91	120.36
4	D	204	QUK	C3-C2-N	2.77	125.90	120.36
4	A	205	QUK	C-C10-N11	2.75	117.35	114.66
5	A	203	QVS	C3-C2-N	2.69	125.73	120.36
5	D	202	QVS	O-C-C10	-2.68	121.68	124.22
6	D	203	QUJ	C-C10-N11	2.67	117.28	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	206	7IB	CB-C5-C4	-2.66	112.21	120.09
6	D	203	QUJ	C7-C2-N	-2.63	113.05	118.07
7	D	205	7IB	C-C10-N11	2.63	120.47	116.28
5	A	203	QVS	C7-C2-N	-2.44	113.42	118.07
7	A	206	7IB	C10-N11-C7	2.42	122.35	117.24
7	D	205	7IB	C7-C2-N	-2.42	113.45	118.07
4	D	201	QUK	C6-C7-N11	-2.42	117.79	122.78
7	D	205	7IB	C10-N11-C7	2.40	122.30	117.24
4	D	201	QUK	C5-C6-C8	-2.40	117.05	122.58
7	D	205	7IB	O1-C-C10	2.39	120.13	114.69
4	A	205	QUK	OB-C8-C6	2.36	121.62	115.01
5	D	202	QVS	C-C10-N11	2.30	116.91	114.66
7	A	206	7IB	O1-C-C10	2.16	119.60	114.69
6	A	204	QUJ	C-C10-N11	2.15	116.77	114.66
7	D	205	7IB	CB-CG-CD	-2.09	107.45	114.34
4	A	202	QUK	O-C-C10	-2.08	122.25	124.22
7	A	206	7IB	O1-C-O	-2.06	118.78	123.35
7	A	206	7IB	OZ1-CE-CD	-2.05	116.49	123.08
5	A	203	QVS	C-C10-N11	2.01	116.63	114.66

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	7I7	CAP-CAR-CAS-SAT
4	A	202	QUK	O-C-C10-C9
4	D	201	QUK	O-C-C10-N11
4	D	201	QUK	O-C-C10-C9
5	D	202	QVS	O-C-C10-C9
7	A	206	7IB	C6-C5-CB-CG
7	A	206	7IB	C4-C5-CB-CG
3	A	201	7I7	OAI-CAJ-CAK-OAL
3	A	201	7I7	NAC-CAD-CAE-OAF
3	A	201	7I7	OAL-CAM-CAN-NAO
4	D	204	QUK	CE-CD-CG-OB
6	A	204	QUJ	C6-C8-OB-CG
3	D	206	7I7	OAL-CAM-CAN-NAO
6	A	204	QUJ	C9-C8-OB-CG
7	D	205	7IB	CE-CD-CG-CB
3	A	201	7I7	OAF-CAG-CAH-OAI
7	A	206	7IB	C5-CB-CG-CD
4	A	205	QUK	CG-CD-CE-N1

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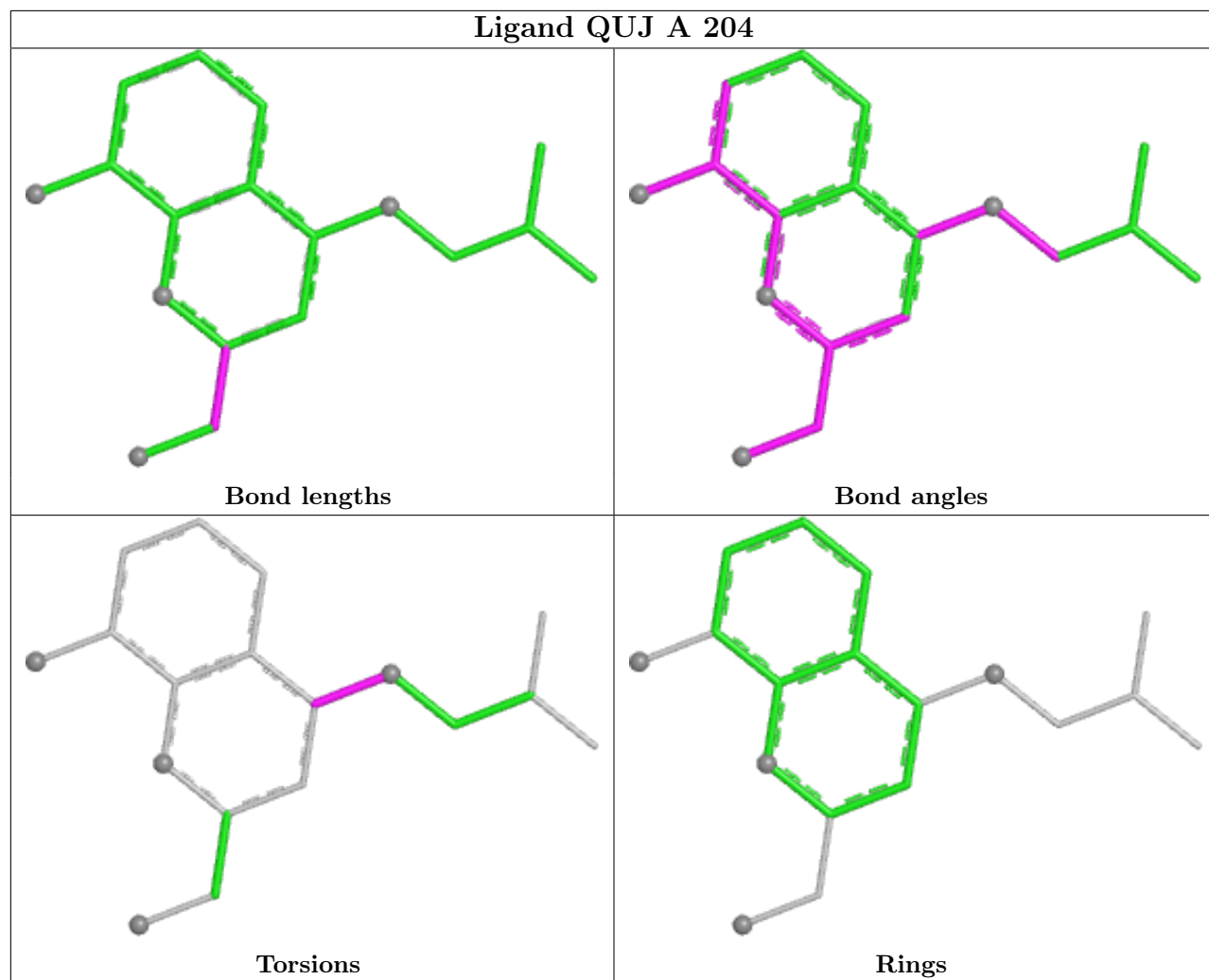
Mol	Chain	Res	Type	Atoms
4	D	201	QUK	CG-CD-CE-N1
4	D	204	QUK	C6-C8-OB-CG
4	D	204	QUK	C9-C8-OB-CG
3	D	206	7I7	CAK-CAJ-OAI-CAH
3	D	206	7I7	CAJ-CAK-OAL-CAM
5	D	202	QVS	O-C-C10-N11
3	D	206	7I7	OAA-CAB-NAC-CAD
3	D	206	7I7	CAD-CAE-OAF-CAG
3	A	201	7I7	CAH-CAG-OAF-CAE
3	A	201	7I7	CAG-CAH-OAI-CAJ
7	D	205	7IB	CG-CD-CE-OZ2
7	D	205	7IB	CG-CD-CE-OZ1
3	D	206	7I7	CAN-CAM-OAL-CAK
7	A	206	7IB	CG-CD-CE-OZ2
4	A	202	QUK	CE-CD-CG-OB
7	A	206	7IB	CG-CD-CE-OZ1
4	A	202	QUK	O-C-C10-N11
3	D	206	7I7	NAC-CAD-CAE-OAF
3	D	206	7I7	NAO-CAP-CAR-CAS

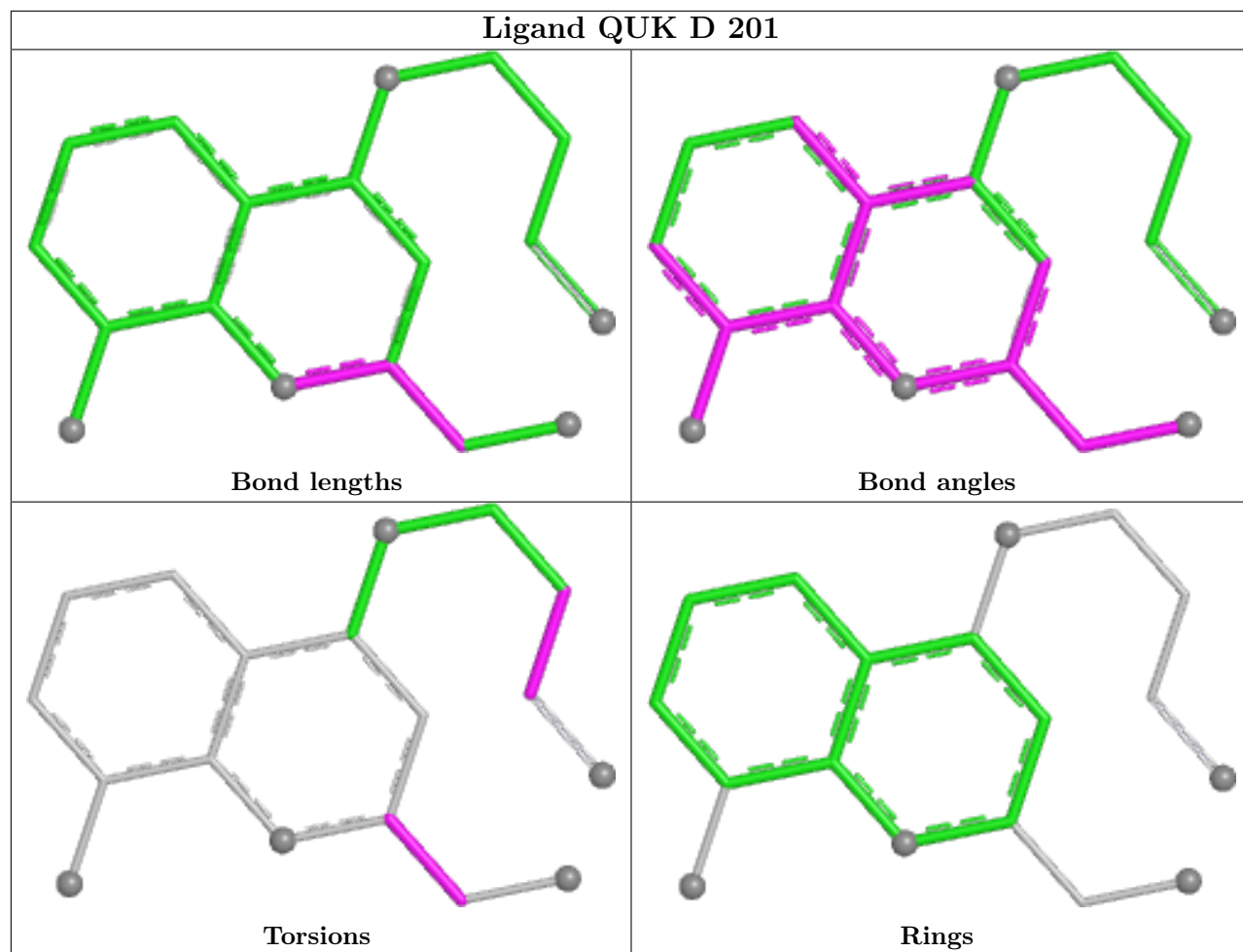
There are no ring outliers.

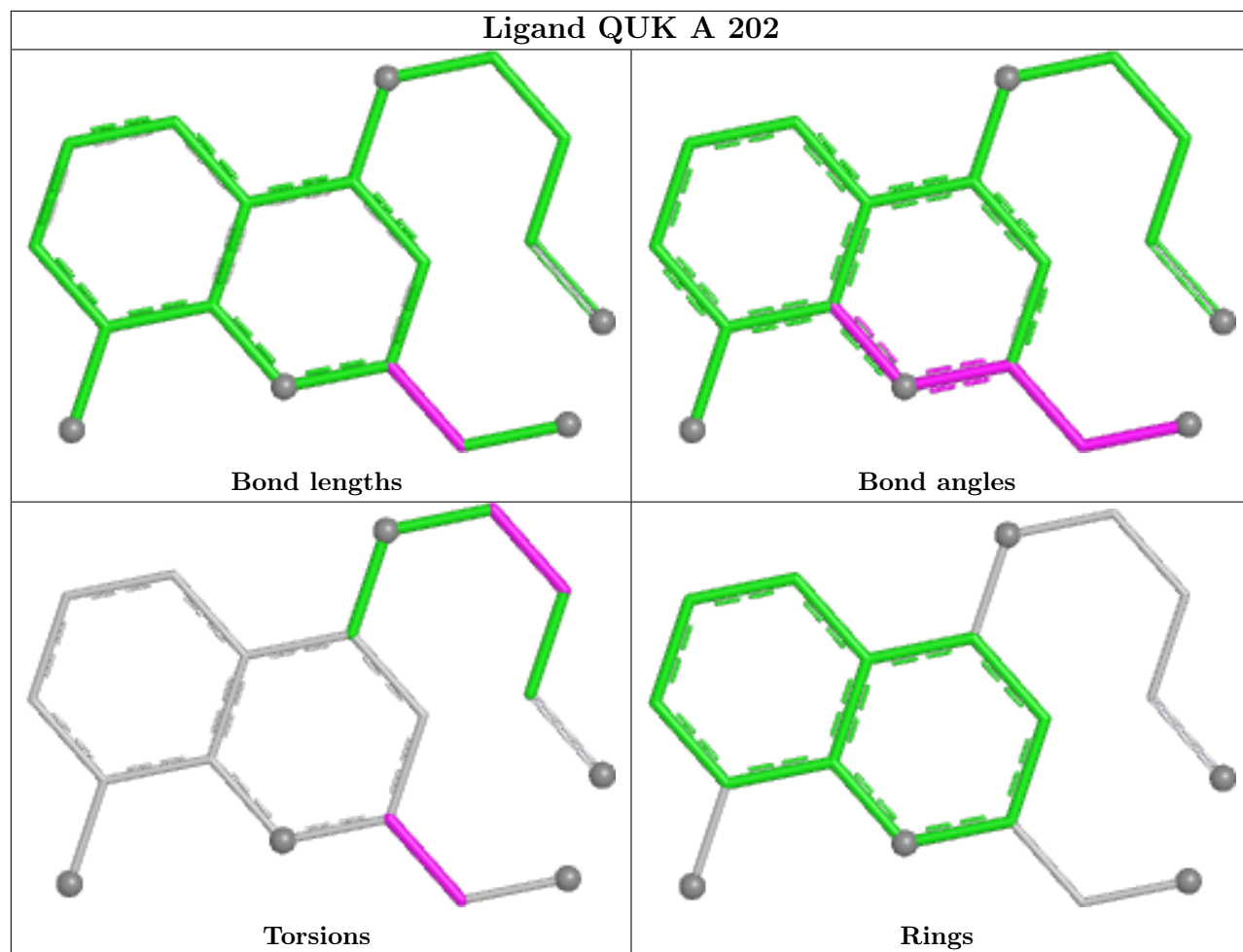
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	205	QUK	1	0
7	A	206	7IB	2	0

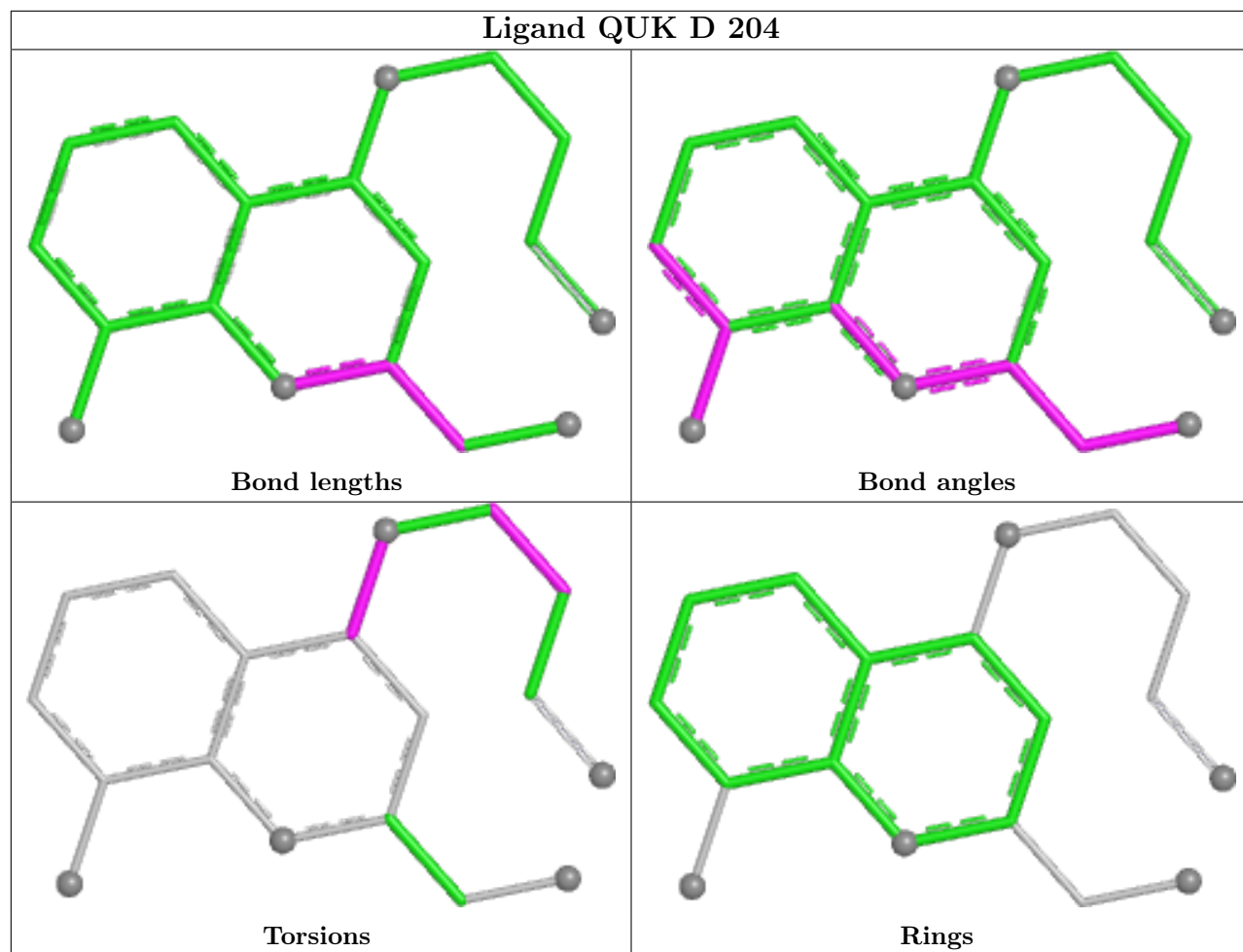
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

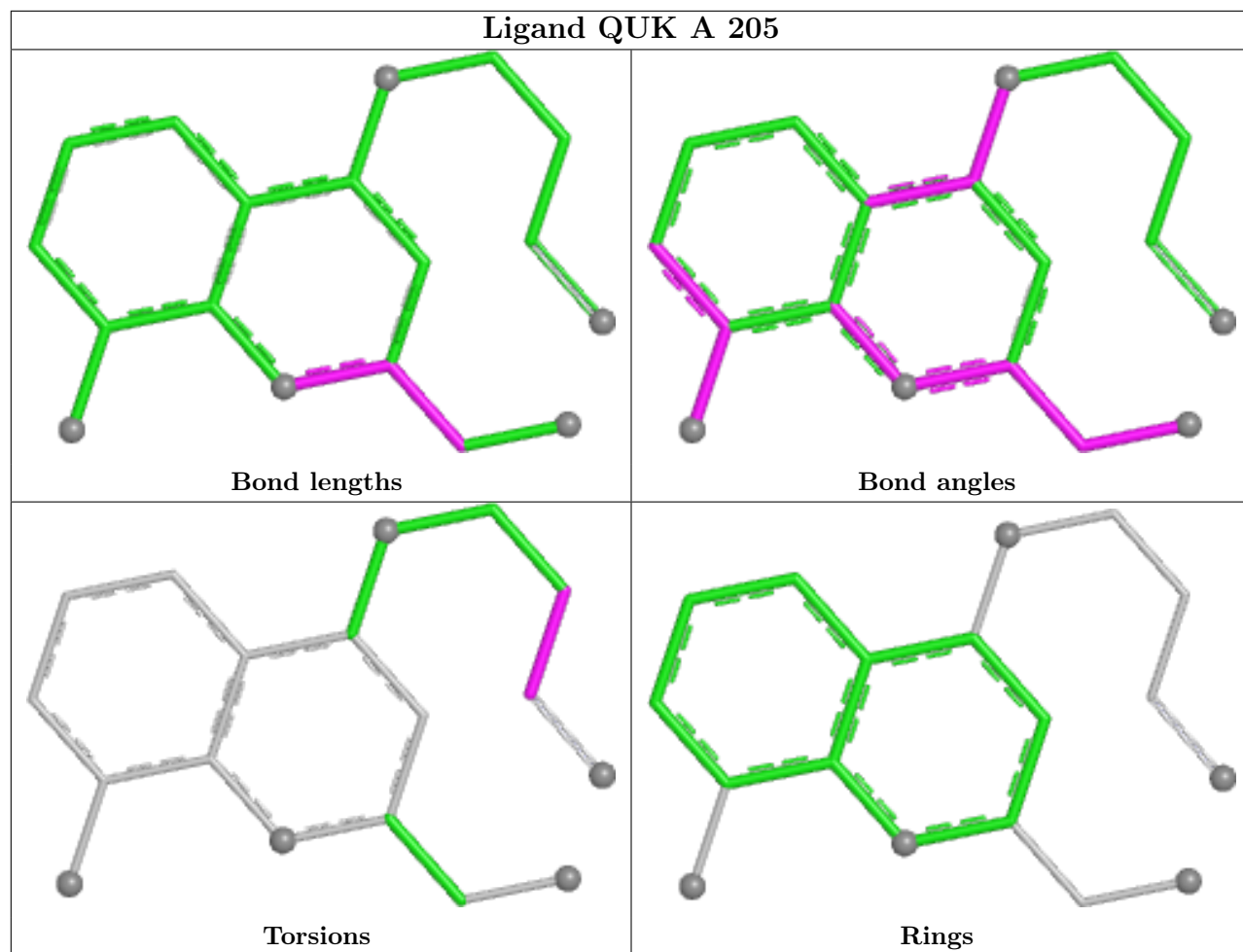




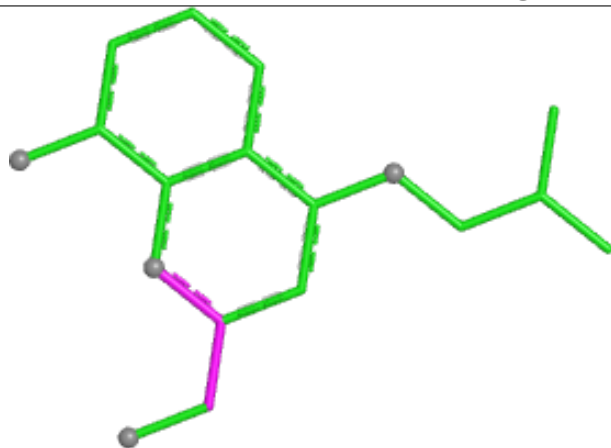




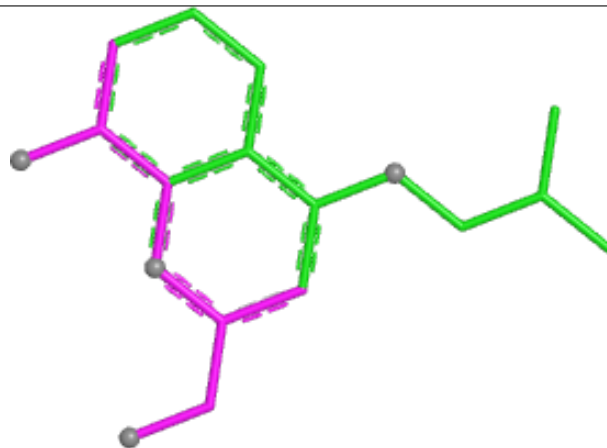




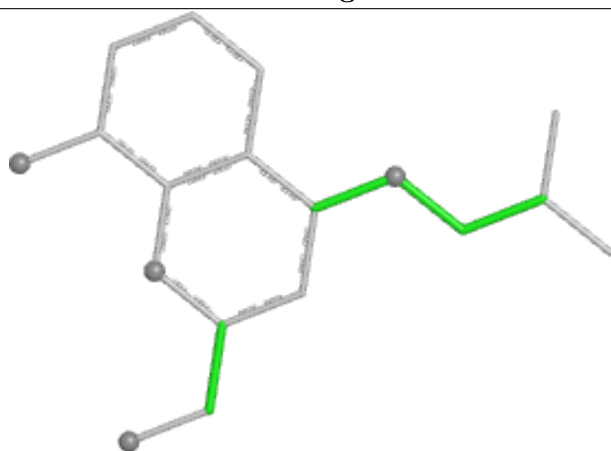
## Ligand QUJ D 203



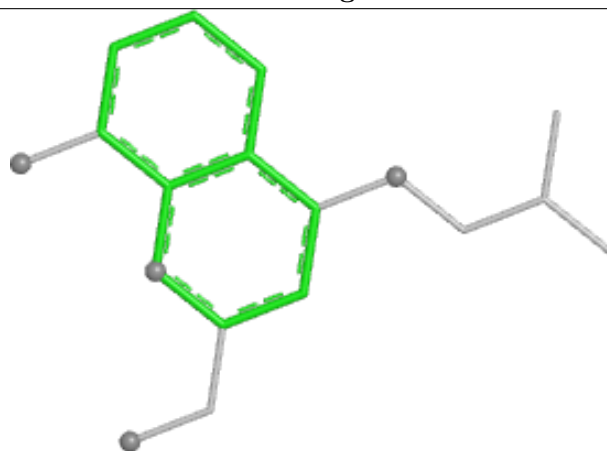
Bond lengths



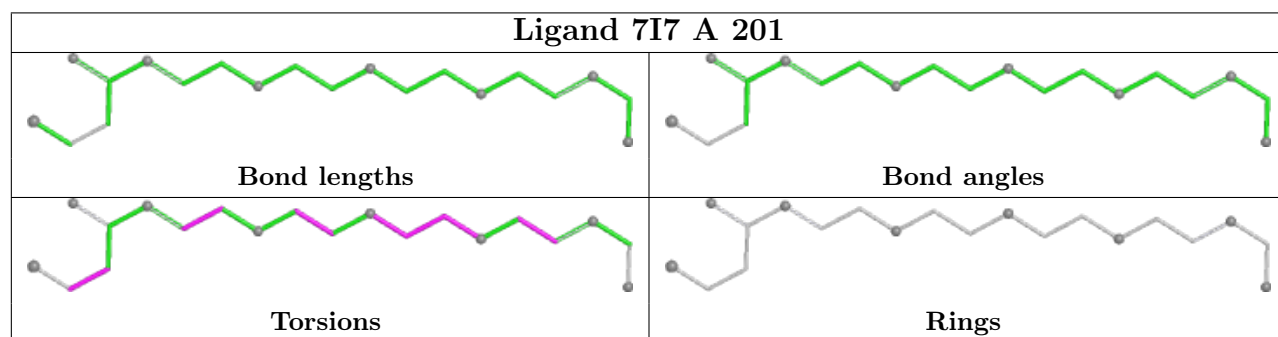
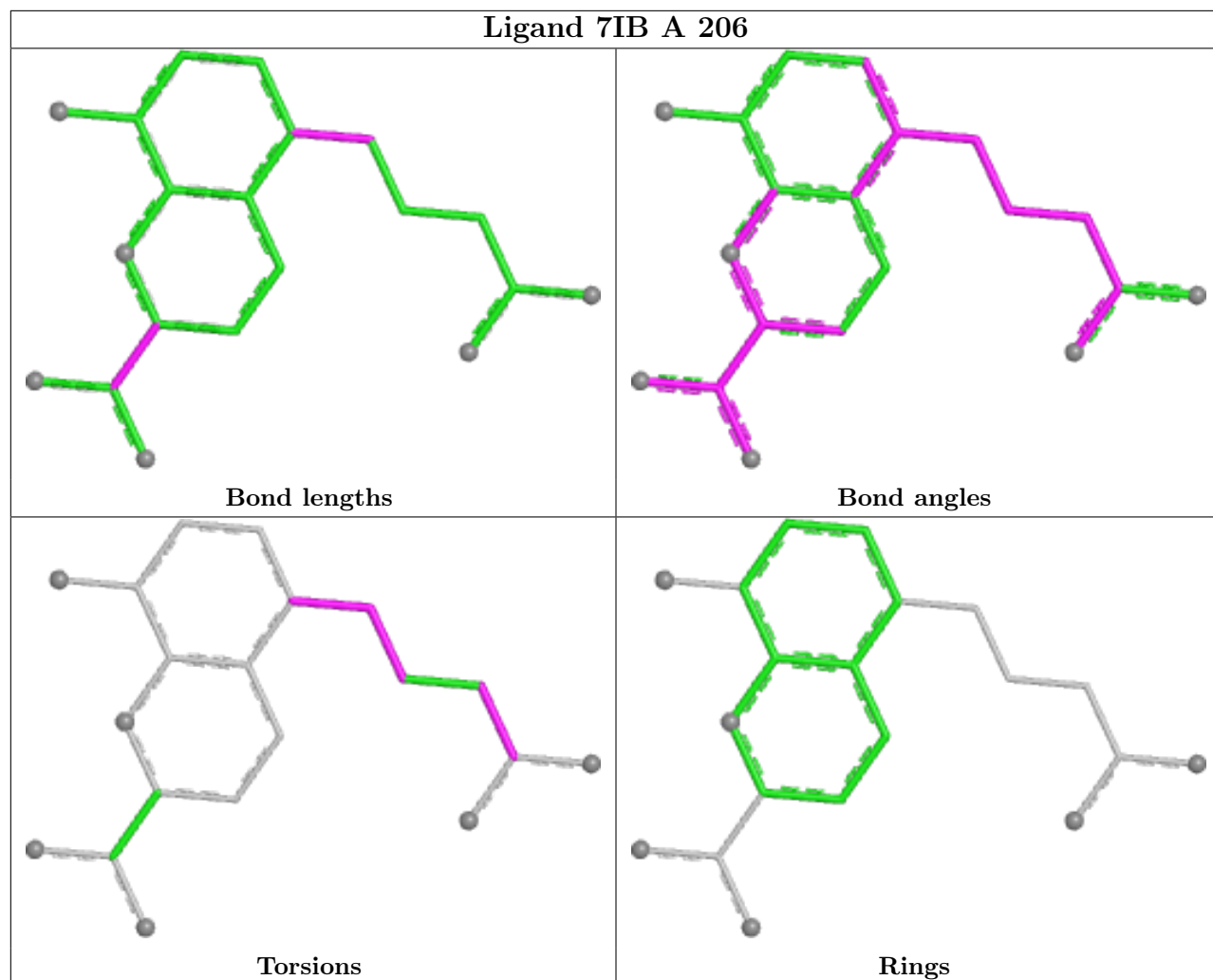
Bond angles

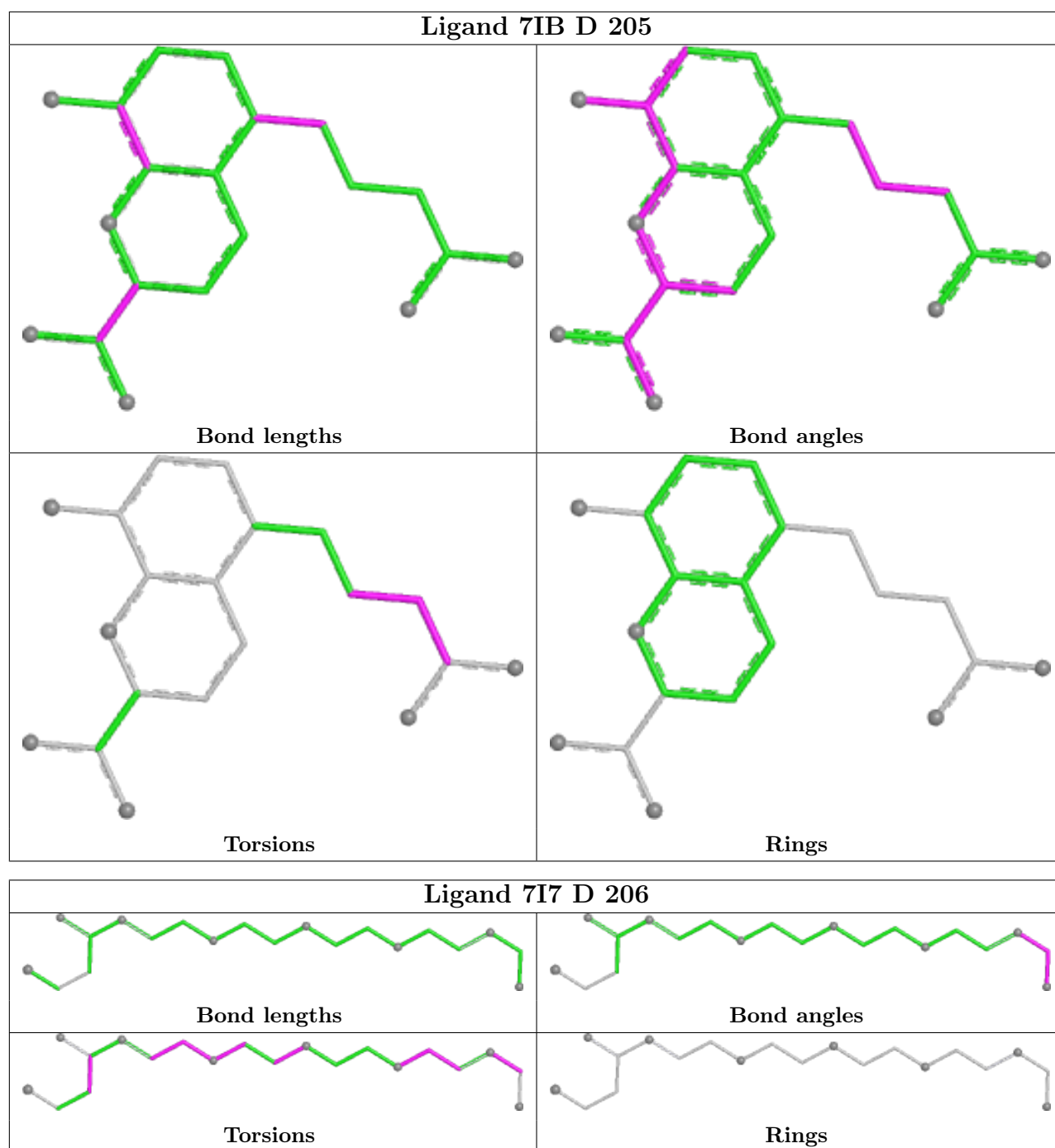


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	164/165 (99%)	-0.22	2 (1%) 79 81	24, 35, 55, 72	0
1	D	164/165 (99%)	-0.18	0 100 100	26, 38, 54, 66	0
2	B	2/11 (18%)	-0.08	0 100 100	31, 31, 31, 34	0
2	E	2/11 (18%)	-0.27	0 100 100	31, 31, 31, 32	0
All	All	332/352 (94%)	-0.20	2 (0%) 89 90	24, 37, 55, 72	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	GLU	2.6
1	A	4	VAL	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DAL	B	1	5/6	0.94	0.11	29,31,32,34	0
2	ABA	E	6	6/7	0.94	0.09	29,34,35,37	0
2	BMT	B	5	13/14	0.95	0.12	23,26,35,38	0
2	BMT	E	5	13/14	0.95	0.12	23,27,37,40	0
2	MLE	B	2	9/10	0.95	0.10	26,28,29,30	0
2	SAR	E	7	5/6	0.95	0.09	35,35,37,37	0
2	MLE	B	8	9/10	0.96	0.10	32,37,45,46	0
2	MLE	B	10	9/10	0.96	0.11	31,34,44,45	0
2	MLE	E	10	9/10	0.96	0.10	28,31,44,46	0
2	MVA	B	4	8/9	0.97	0.08	23,25,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MVA	E	4	8/9	0.97	0.08	23,25,26,26	0
2	DAL	E	1	5/6	0.97	0.08	29,29,30,32	0
2	MLE	E	8	9/10	0.97	0.11	31,36,58,60	0
2	MLE	B	3	9/10	0.97	0.08	24,27,32,33	0
2	ABA	B	6	6/7	0.97	0.09	28,30,32,33	0
2	SAR	B	7	5/6	0.98	0.07	34,34,37,37	0
2	MLE	E	2	9/10	0.98	0.08	24,29,31,33	0
2	MLE	E	3	9/10	0.98	0.10	22,24,29,31	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

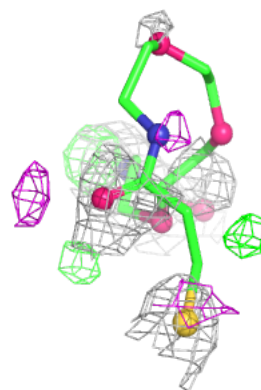
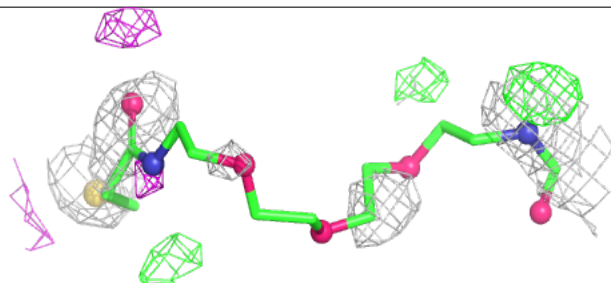
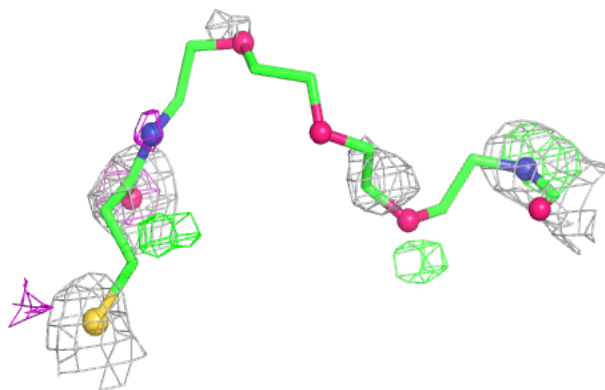
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	7I7	A	201	20/20	0.70	0.41	75,99,112,113	0
3	7I7	D	206	20/20	0.72	0.33	58,84,101,102	0
5	QVS	D	202	14/15	0.85	0.12	42,45,54,56	0
4	QUK	D	201	18/19	0.89	0.11	51,56,70,72	0
4	QUK	A	205	18/19	0.92	0.11	38,45,71,74	0
6	QUJ	A	204	18/19	0.92	0.11	45,51,68,72	0
6	QUJ	D	203	18/19	0.92	0.14	40,50,68,69	0
7	7IB	D	205	20/20	0.92	0.12	45,48,67,68	0
4	QUK	A	202	18/19	0.93	0.15	49,54,74,80	0
5	QVS	A	203	14/15	0.93	0.08	46,48,52,60	0
7	7IB	A	206	20/20	0.94	0.11	39,49,82,98	0
4	QUK	D	204	18/19	0.95	0.11	41,45,57,61	0

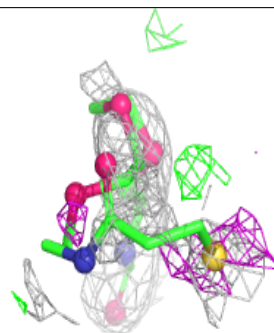
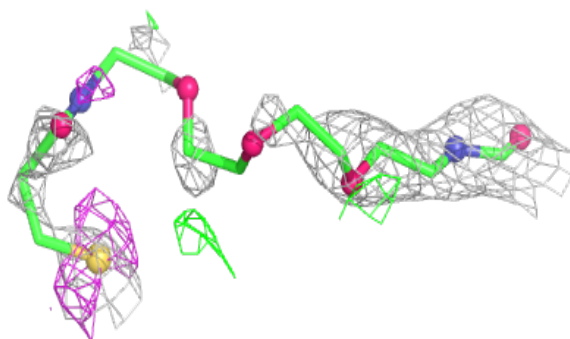
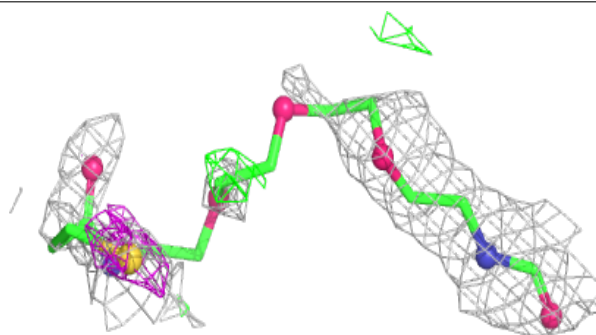
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 7I7 A 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 7I7 D 206:**

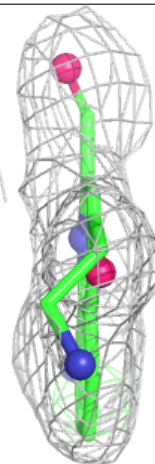
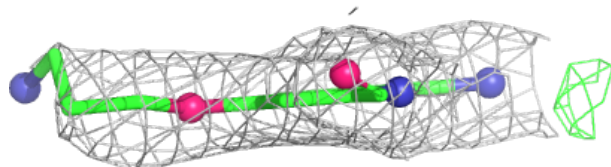
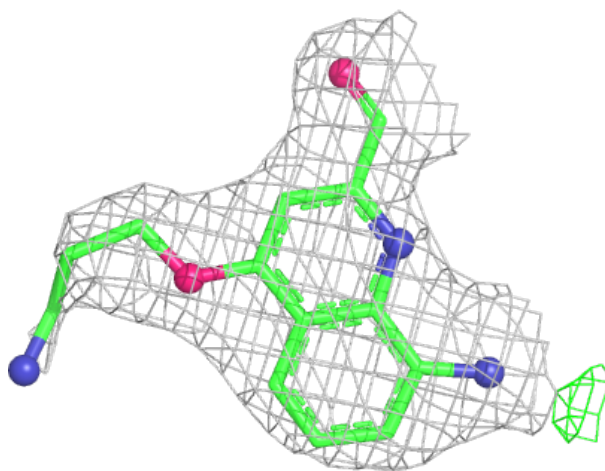
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





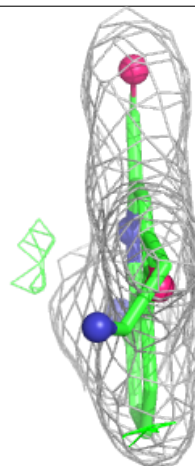
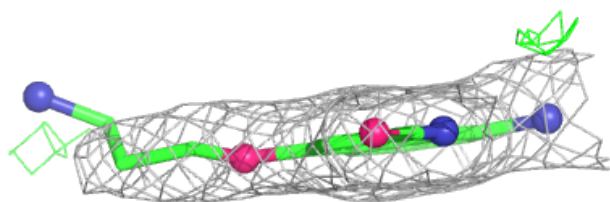
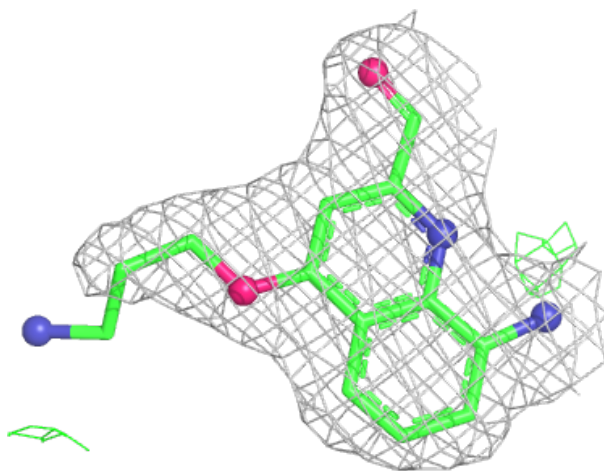
**Electron density around QUK D 201:**

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



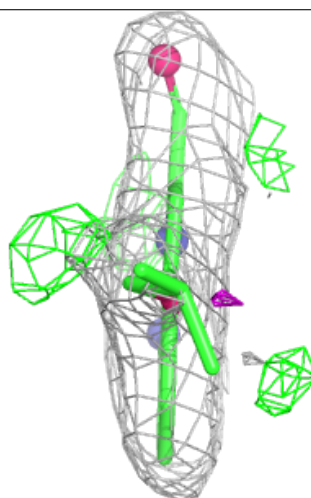
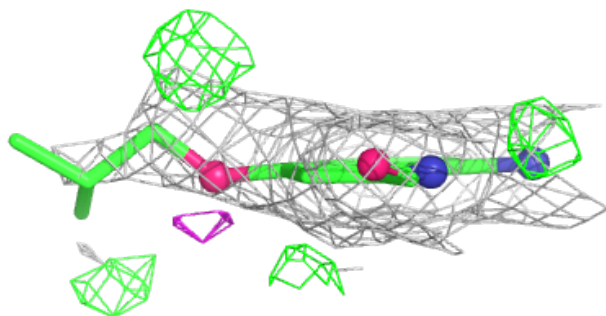
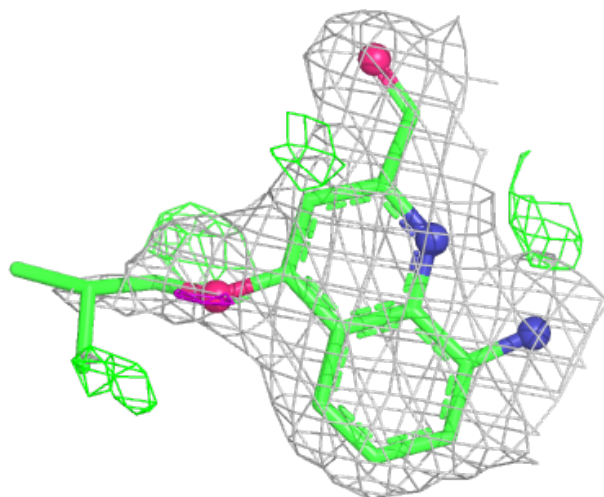
**Electron density around QUK A 205:**

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



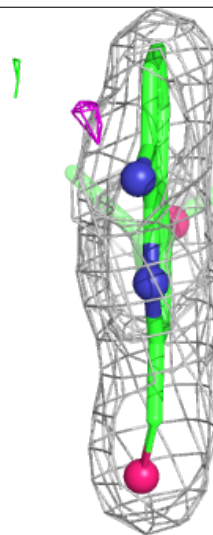
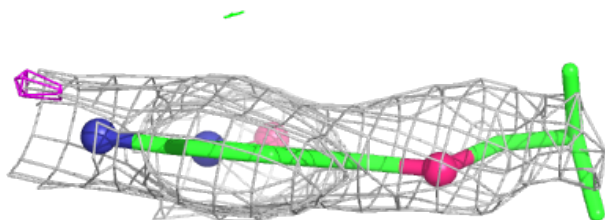
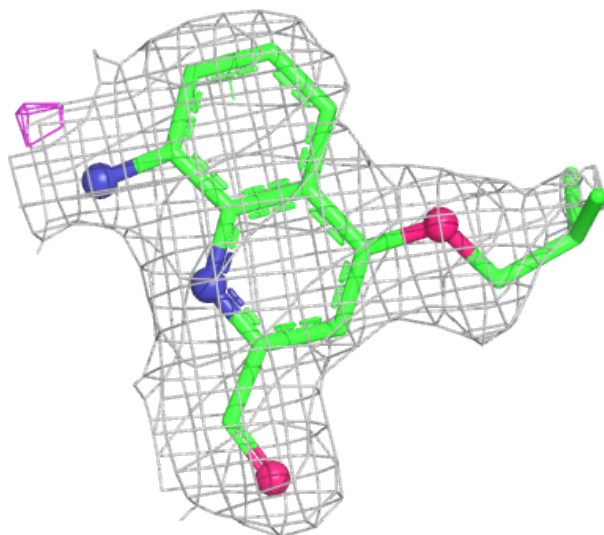
**Electron density around Q UJ A 204:**

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



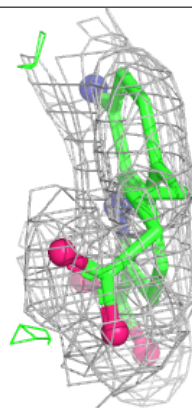
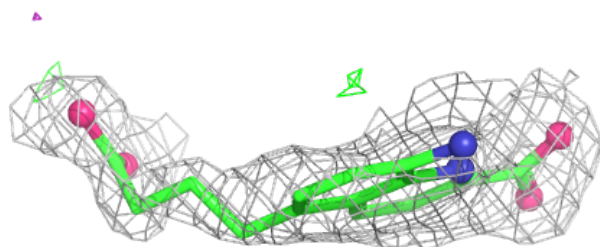
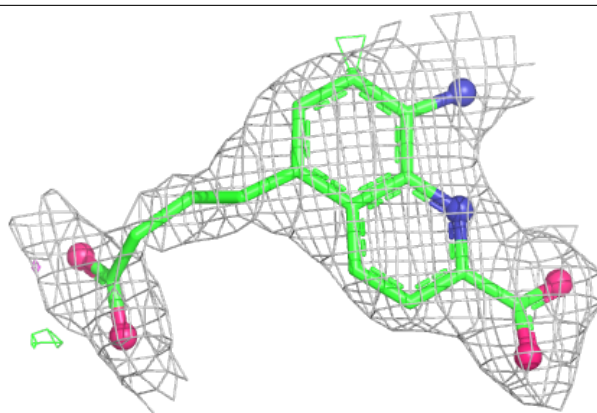
**Electron density around QUJ D 203:**

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



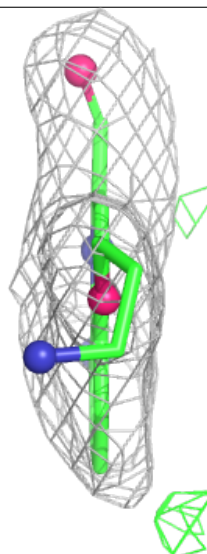
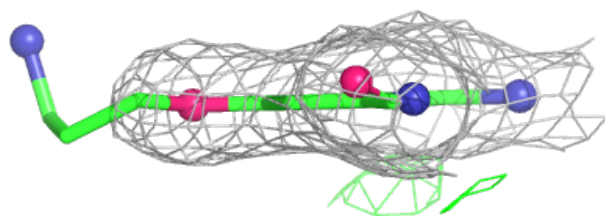
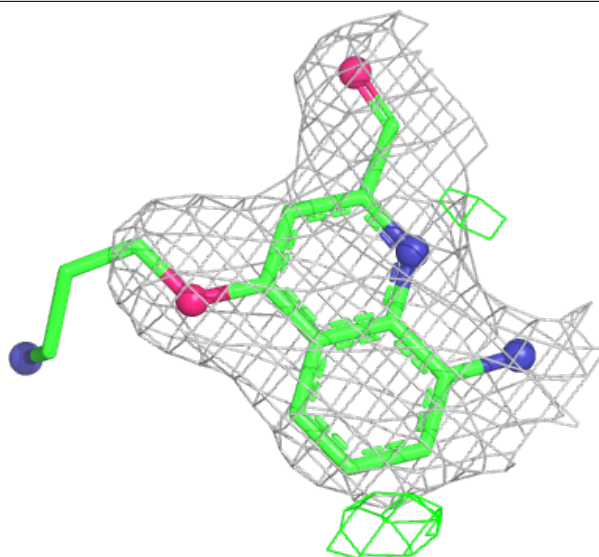
**Electron density around 7IB D 205:**

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



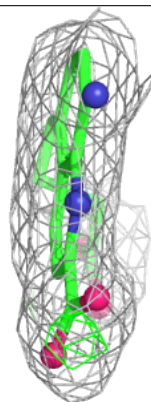
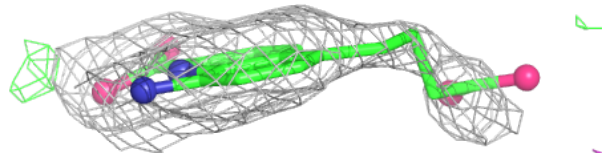
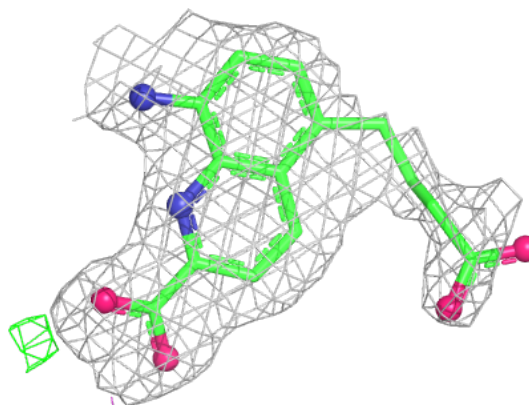
**Electron density around QUK A 202:**

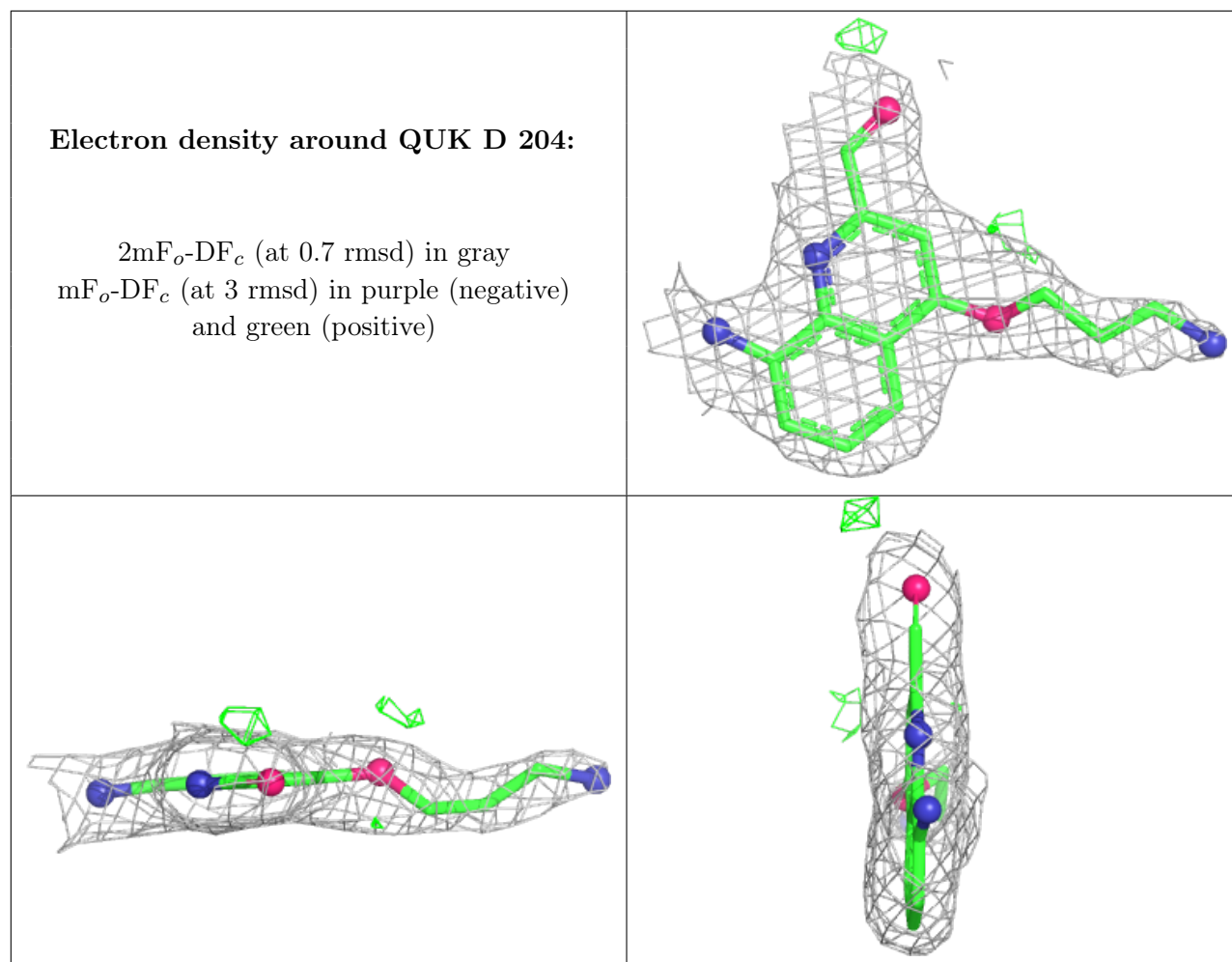
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 7IB A 206:**

$2mF_o - DF_c$  (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.