



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:02 AM UTC

PDB ID : 6V6O / pdb_00006v6o
Title : EGFR(T790M/V948R) in complex with LN2380
Authors : Heppner, D.E.; Eck, M.J.
Deposited on : 2019-12-05
Resolution : 2.10 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 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

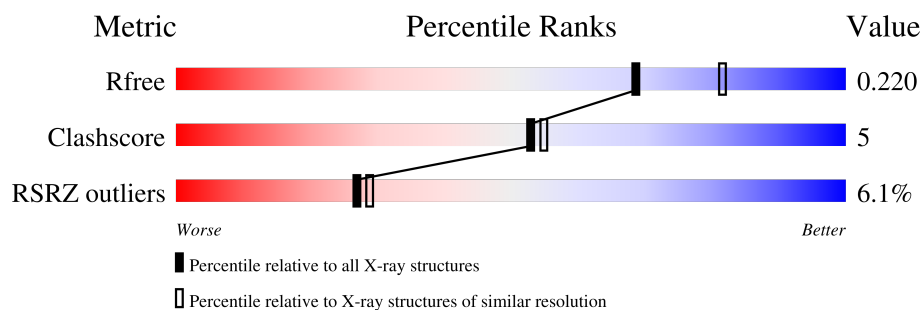
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



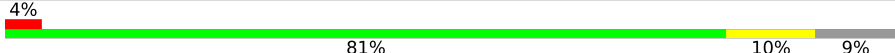
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 ≥ 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	327	5% 80% 14% 6%
1	B	327	% 87% 9% .
1	C	327	5% 83% 8% 9%
1	D	327	5% 82% 14% .
1	E	327	7% 82% 11% 7%
1	F	327	12% 79% 12% 9%
1	G	327	6% 81% 9% 10%

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Mol	Chain	Length	Quality of chain
1	H	327	

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
2	CL	C	1201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21480 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	314	Total	C	N	O	S	0	1	0
			2530	1619	428	464	19			
1	A	307	Total	C	N	O	S	0	0	0
			2470	1585	420	446	19			
1	B	314	Total	C	N	O	S	0	0	0
			2521	1614	427	461	19			
1	C	297	Total	C	N	O	S	0	0	0
			2390	1538	406	427	19			
1	E	303	Total	C	N	O	S	0	1	0
			2445	1568	414	444	19			
1	F	299	Total	C	N	O	S	0	1	0
			2419	1553	409	438	19			
1	G	294	Total	C	N	O	S	0	1	0
			2378	1526	404	429	19			
1	H	299	Total	C	N	O	S	0	1	0
			2413	1550	408	437	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
E	790	MET	THR	engineered mutation	UNP P00533
E	948	ARG	VAL	engineered mutation	UNP P00533
F	790	MET	THR	engineered mutation	UNP P00533
F	948	ARG	VAL	engineered mutation	UNP P00533
G	790	MET	THR	engineered mutation	UNP P00533

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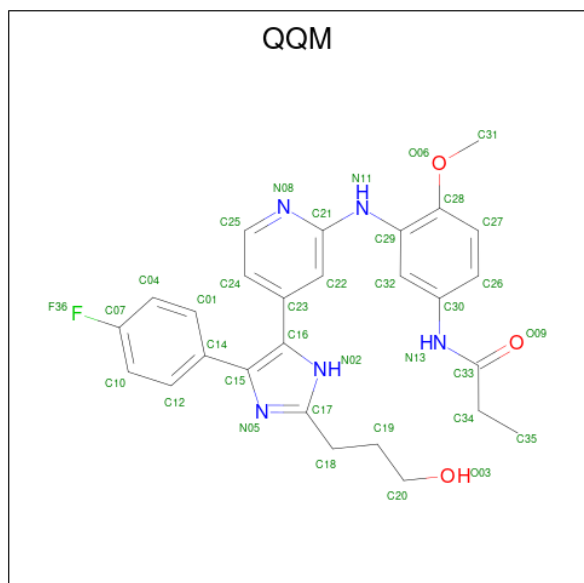
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Chain	Residue	Modelled	Actual	Comment	Reference
G	948	ARG	VAL	engineered mutation	UNP P00533
H	790	MET	THR	engineered mutation	UNP P00533
H	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0

- Molecule 3 is N-[3-(4-[4-(4-fluorophenyl)-2-(3-hydroxypropyl)-1H-imidazol-5-yl]pyridin-2-yl)amino)-4-methoxyphenyl]propanamide (CCD ID: QQM) (formula: C₂₇H₂₈FN₅O₃) (labeled as "Ligand of Interest" by depositor).

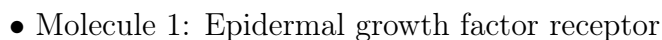


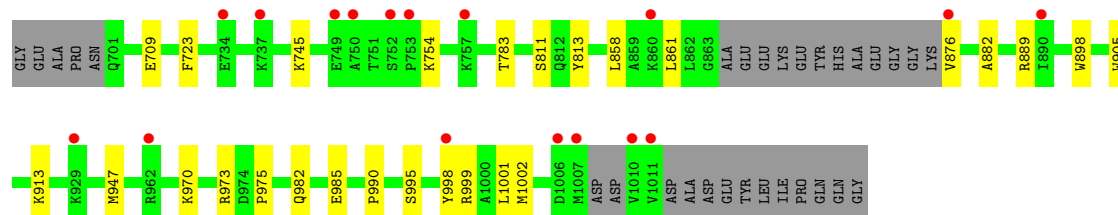
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	A	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	B	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	C	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	E	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	F	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	G	1	Total	C	F	N	O	0	0
			36	27	1	5	3		
3	H	1	Total	C	F	N	O	0	0
			36	27	1	5	3		

- Molecule 4 is water.

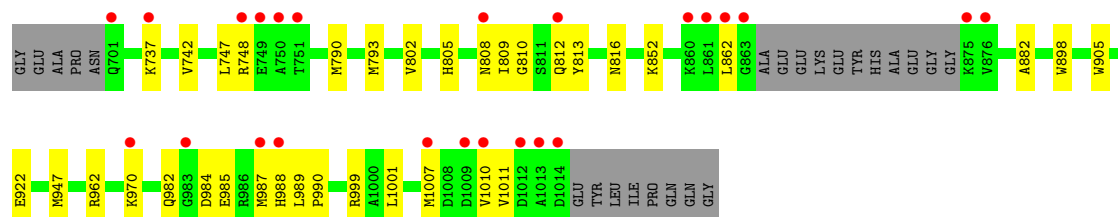
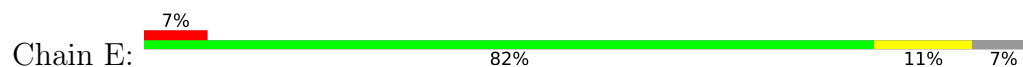
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	196	Total	O	0	0
			196	196		
4	A	172	Total	O	0	0
			172	172		
4	B	286	Total	O	0	0
			286	286		
4	C	219	Total	O	0	0
			219	219		
4	E	212	Total	O	0	0
			212	212		
4	F	156	Total	O	0	0
			156	156		
4	G	188	Total	O	0	0
			188	188		
4	H	189	Total	O	0	0
			189	189		

- Molecule 1: Epidermal growth factor receptor

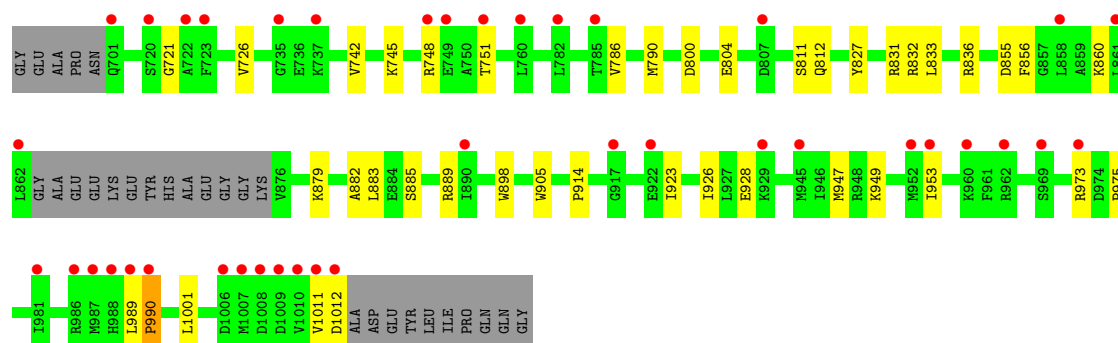
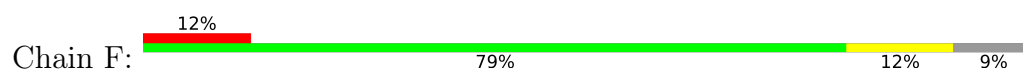




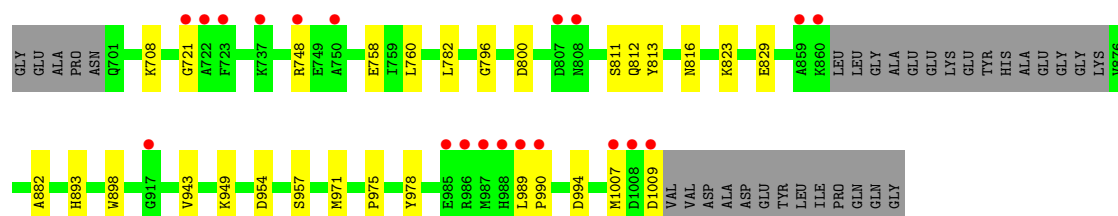
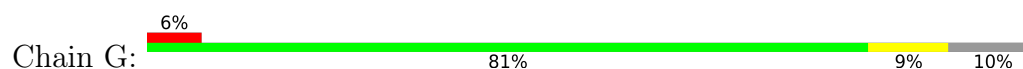
• Molecule 1: Epidermal growth factor receptor



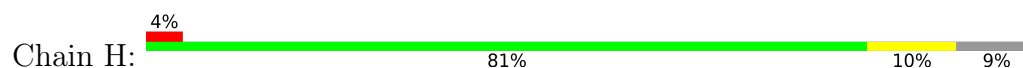
• Molecule 1: Epidermal growth factor receptor

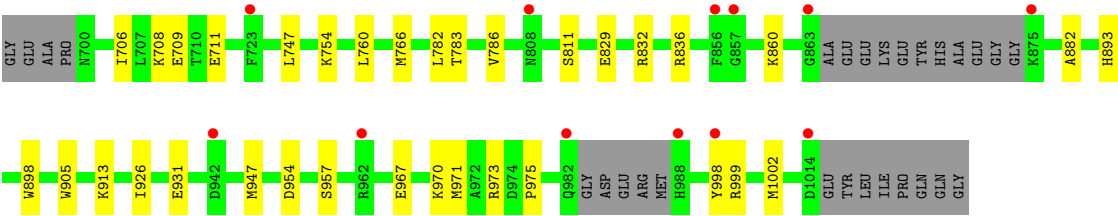


• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.55Å 102.36Å 173.57Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	69.83 – 2.10 69.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (69.83-2.10) 93.3 (69.83-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.195 , 0.221 (Not available) , 0.220	Depositor DCC
R_{free} test set	7020 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21480	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 54.79 % 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 3.4707e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/2525	0.41	0/3412
1	B	0.12	0/2576	0.38	0/3483
1	C	0.13	0/2441	0.38	0/3299
1	D	0.23	0/2585	0.45	1/3495 (0.0%)
1	E	0.15	0/2497	0.40	0/3376
1	F	0.28	1/2471 (0.0%)	0.50	0/3342
1	G	0.13	0/2430	0.33	0/3285
1	H	0.16	0/2464	0.41	0/3332
All	All	0.18	1/19989 (0.0%)	0.41	1/27024 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	990	PRO	C-O	-5.95	1.16	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	751	THR	CA-CB-OG1	-5.31	101.63	109.60

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	2470	0	2511	32	0
1	B	2521	0	2550	17	0
1	C	2390	0	2445	18	0
1	D	2530	0	2555	33	0
1	E	2445	0	2485	29	0
1	F	2419	0	2460	35	0
1	G	2378	0	2414	24	0
1	H	2413	0	2455	22	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
2	C	1	0	0	2	0
2	D	1	0	0	1	0
2	E	1	0	0	0	0
2	F	1	0	0	1	0
2	G	1	0	0	1	0
2	H	1	0	0	0	0
3	A	36	0	0	3	0
3	B	36	0	0	0	0
3	C	36	0	0	0	0
3	D	36	0	0	2	0
3	E	36	0	0	2	0
3	F	36	0	0	3	0
3	G	36	0	0	1	0
3	H	36	0	0	0	0
4	A	172	0	0	2	0
4	B	286	0	0	0	0
4	C	219	0	0	2	0
4	D	196	0	0	6	0
4	E	212	0	0	3	0
4	F	156	0	0	0	0
4	G	188	0	0	3	0
4	H	189	0	0	4	0
All	All	21480	0	19875	197	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 5.

The worst 5 of 197 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:F:973:ARG:CZ	1:F:1011:VAL:HG13	2.01	0.91
1:D:947:MET:SD	4:D:1478:HOH:O	2.36	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:ARG:NH1	1:D:1007:MET:SD	2.56	0.78
1:A:737:LYS:HE3	1:F:804:GLU:HB3	1.71	0.72
1:F:812:GLN:HG2	1:F:975:PRO:HG3	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QQM	G	1301	1	39,39,39	6.19	27 (69%)	52,53,53	1.62	11 (21%)
3	QQM	F	1202	1	39,39,39	6.19	28 (71%)	52,53,53	1.70	14 (26%)
3	QQM	B	1202	1	39,39,39	6.19	28 (71%)	52,53,53	1.68	10 (19%)
3	QQM	A	1202	1	39,39,39	6.19	28 (71%)	52,53,53	1.72	11 (21%)
3	QQM	D	1202	1	39,39,39	6.19	27 (69%)	52,53,53	1.73	12 (23%)
3	QQM	E	1202	1	39,39,39	6.20	28 (71%)	52,53,53	1.66	12 (23%)
3	QQM	C	1202	1	39,39,39	6.22	28 (71%)	52,53,53	2.21	12 (23%)
3	QQM	H	1202	1	39,39,39	6.18	27 (69%)	52,53,53	1.65	12 (23%)

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	QQM	G	1301	1	-	0/24/24/24	0/4/4/4
3	QQM	F	1202	1	-	2/24/24/24	0/4/4/4
3	QQM	B	1202	1	-	3/24/24/24	0/4/4/4
3	QQM	A	1202	1	-	3/24/24/24	0/4/4/4
3	QQM	D	1202	1	-	4/24/24/24	0/4/4/4
3	QQM	E	1202	1	-	3/24/24/24	0/4/4/4
3	QQM	C	1202	1	-	5/24/24/24	0/4/4/4
3	QQM	H	1202	1	-	3/24/24/24	0/4/4/4

The worst 5 of 221 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1202	QQM	C27-C26	10.76	1.56	1.38
3	A	1202	QQM	C27-C26	10.72	1.56	1.38
3	D	1202	QQM	C27-C26	10.71	1.56	1.38
3	F	1202	QQM	C27-C26	10.66	1.56	1.38
3	H	1202	QQM	C27-C26	10.66	1.56	1.38

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	QQM	O06-C28-C29	9.17	126.23	114.81
3	C	1202	QQM	O06-C28-C27	-5.64	114.78	124.30
3	D	1202	QQM	C14-C15-N05	4.57	126.28	119.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	QQM	C14-C15-N05	4.36	125.98	119.53
3	A	1202	QQM	C14-C15-N05	4.18	125.72	119.53

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1202	QQM	C29-C28-O06-C31
3	C	1202	QQM	C27-C28-O06-C31
3	D	1202	QQM	C18-C19-C20-O03
3	B	1202	QQM	C18-C19-C20-O03
3	C	1202	QQM	C18-C19-C20-O03

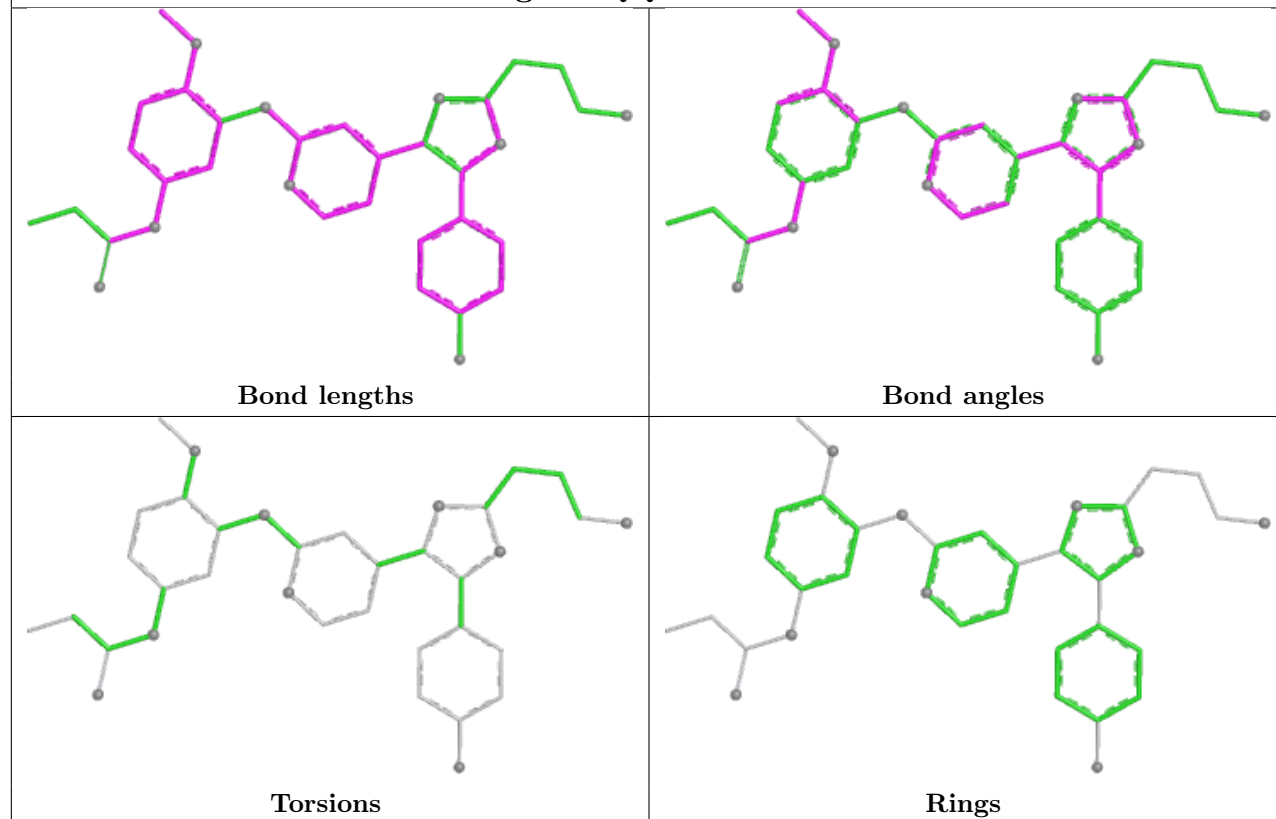
There are no ring outliers.

5 monomers are involved in 11 short contacts:

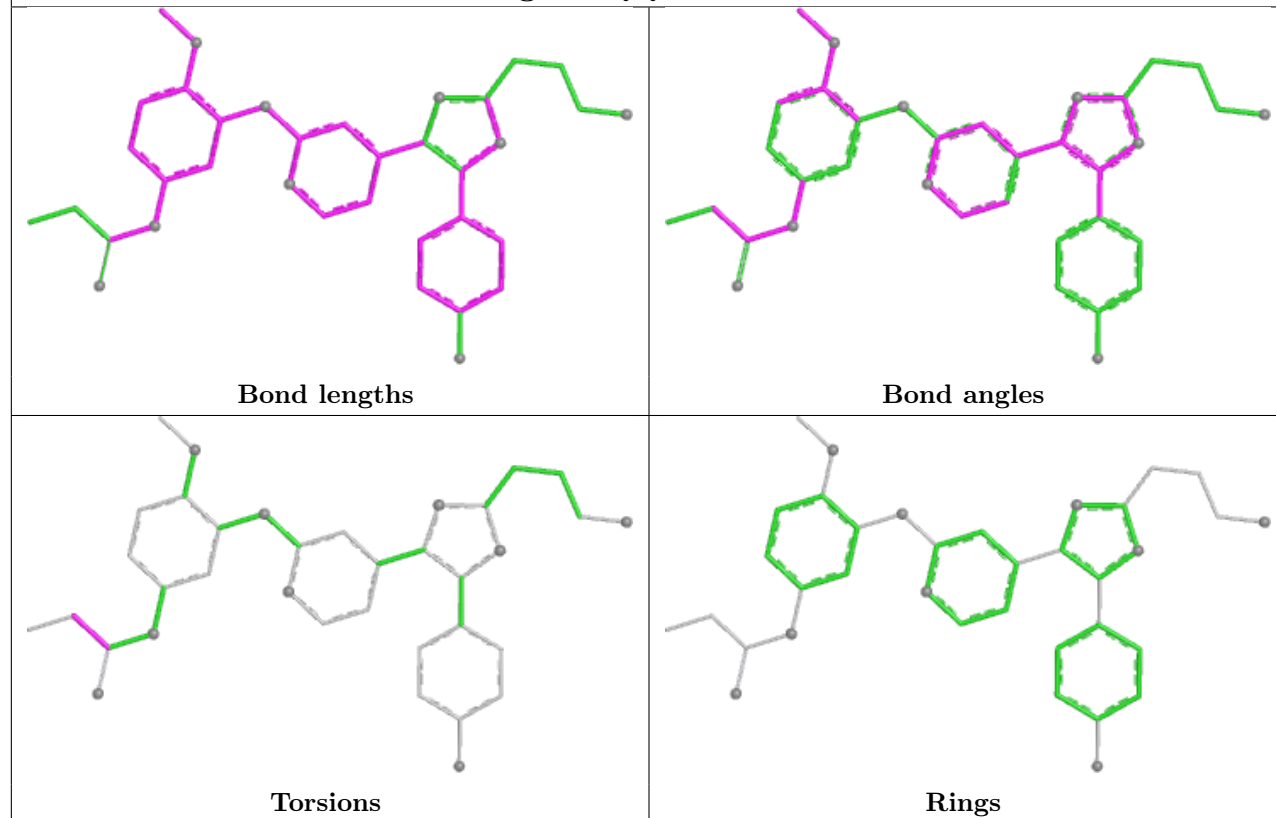
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1301	QQM	1	0
3	F	1202	QQM	3	0
3	A	1202	QQM	3	0
3	D	1202	QQM	2	0
3	E	1202	QQM	2	0

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.

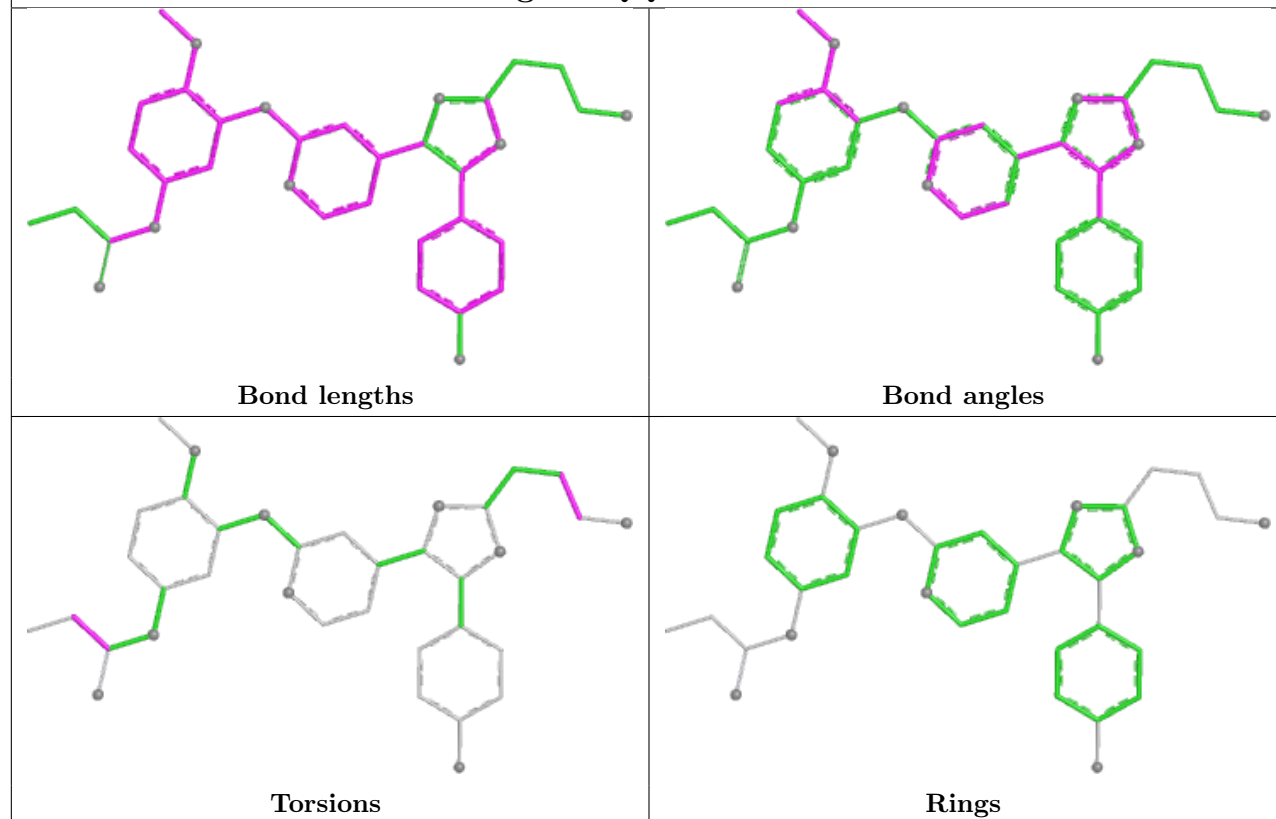
Ligand QQM G 1301



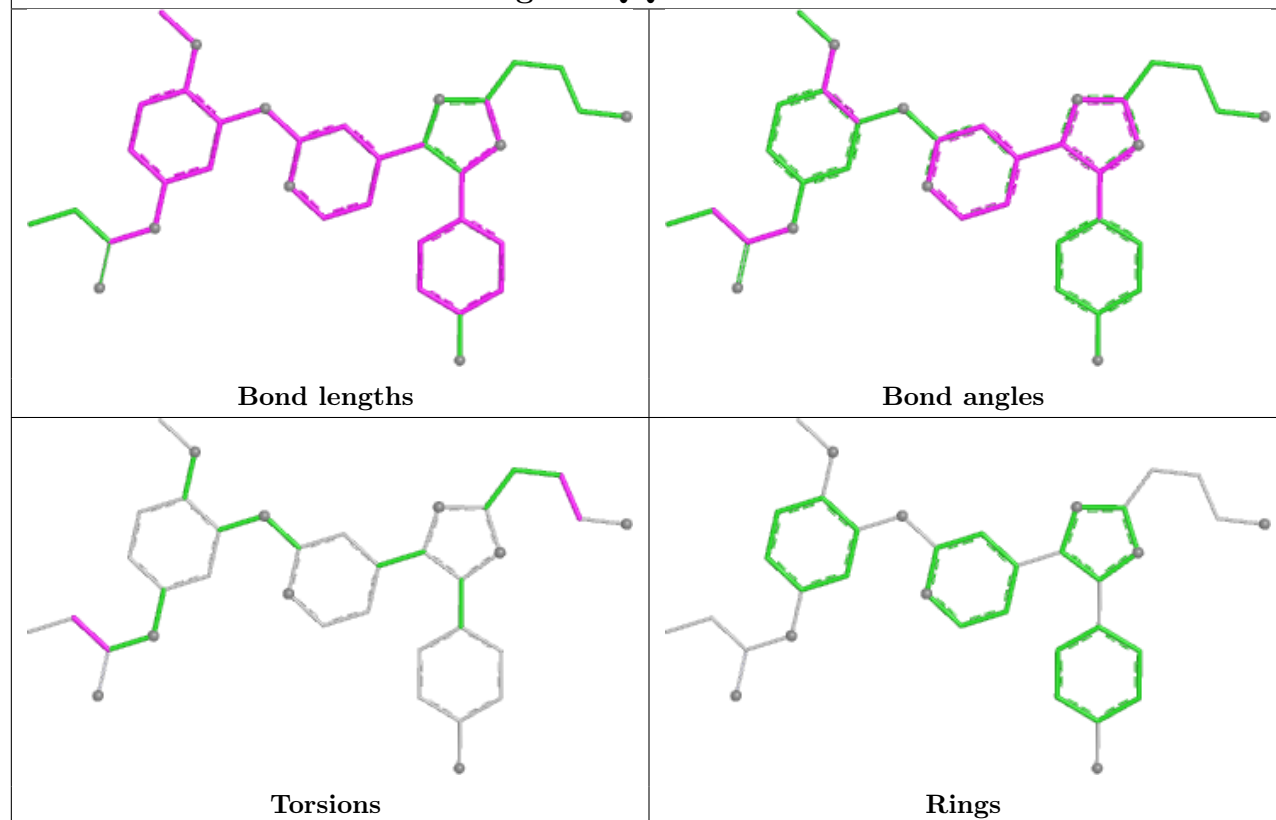
Ligand QQM F 1202



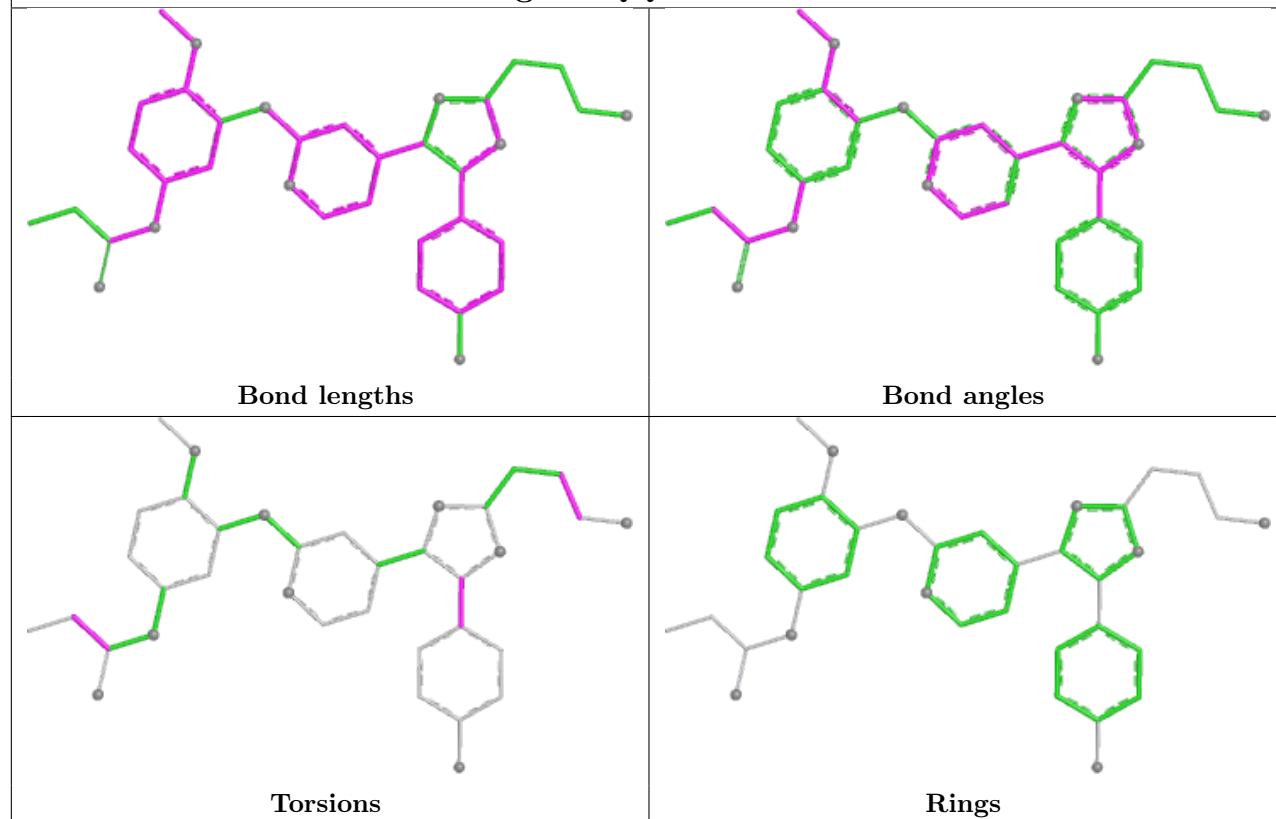
Ligand QQM B 1202



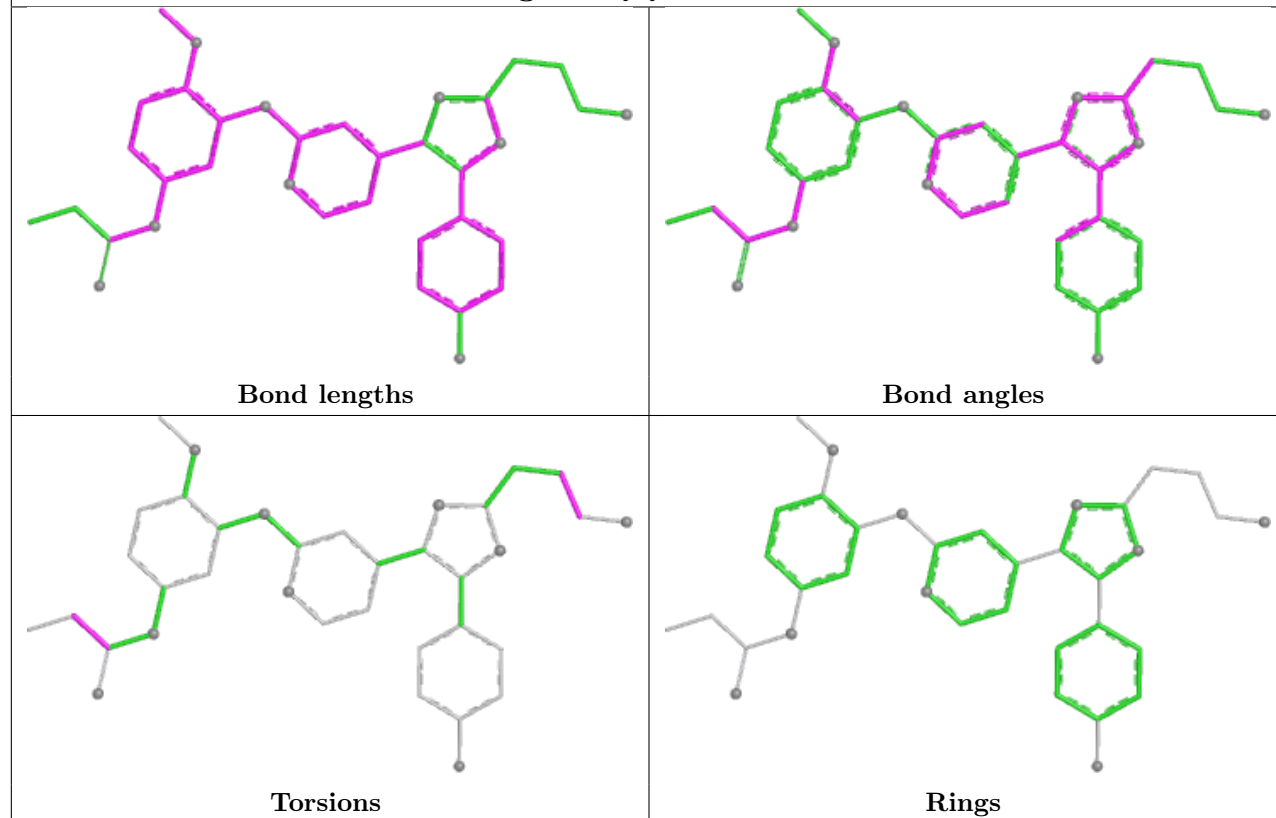
Ligand QQM A 1202



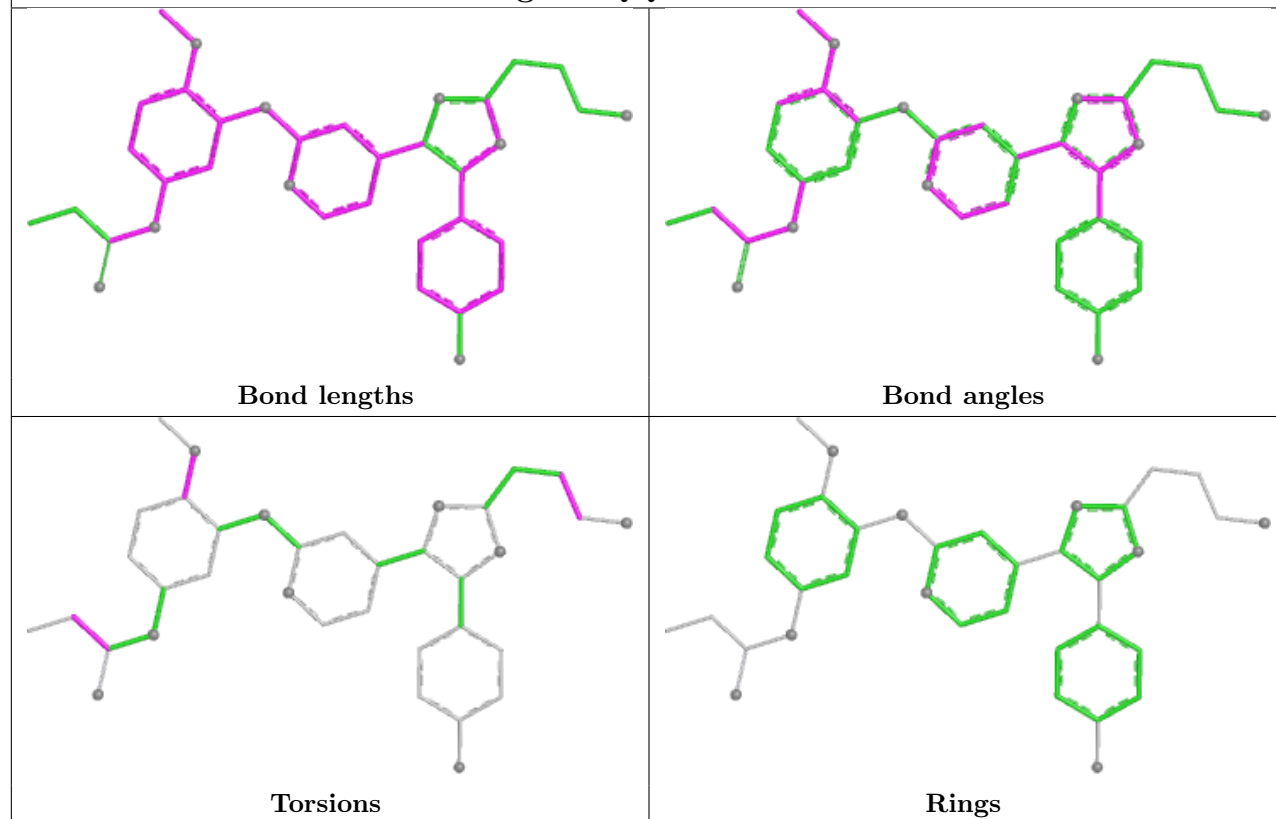
Ligand QQM D 1202



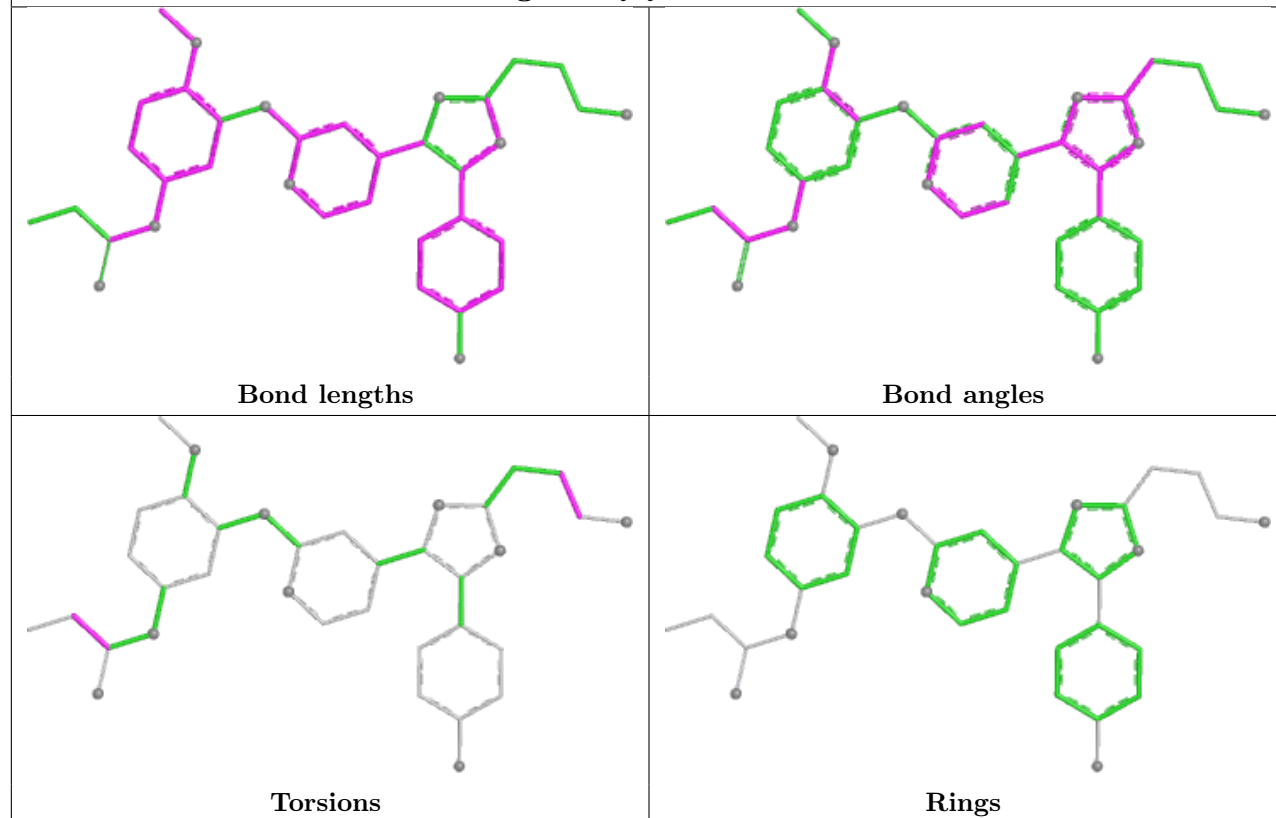
Ligand QQM E 1202



Ligand QQM C 1202



Ligand QQM H 1202



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, 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	307/327 (93%)	0.43	15 (4%) 35 37	14, 30, 58, 75	0
1	B	314/327 (96%)	-0.01	3 (0%) 79 81	12, 23, 40, 60	0
1	C	297/327 (90%)	0.23	17 (5%) 29 31	13, 26, 50, 71	0
1	D	314/327 (96%)	0.35	16 (5%) 33 35	16, 30, 55, 74	1 (0%)
1	E	303/327 (92%)	0.24	24 (7%) 18 20	13, 26, 57, 81	1 (0%)
1	F	299/327 (91%)	0.79	40 (13%) 7 7	17, 34, 64, 89	1 (0%)
1	G	294/327 (89%)	0.42	20 (6%) 23 25	13, 28, 60, 87	1 (0%)
1	H	299/327 (91%)	0.27	12 (4%) 42 44	14, 27, 51, 74	1 (0%)
All	All	2427/2616 (92%)	0.34	147 (6%) 27 29	12, 28, 56, 89	5 (0%)

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1010	VAL	6.9
1	G	1009	ASP	4.8
1	C	1011	VAL	4.5
1	F	1010	VAL	4.5
1	F	945	MET	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

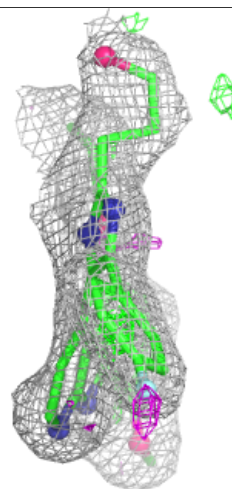
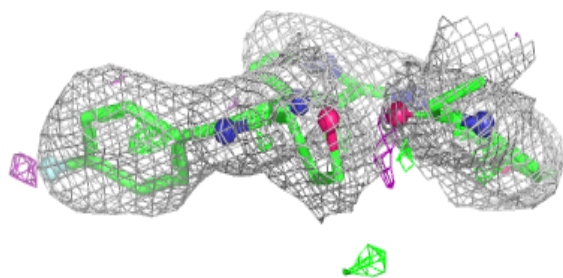
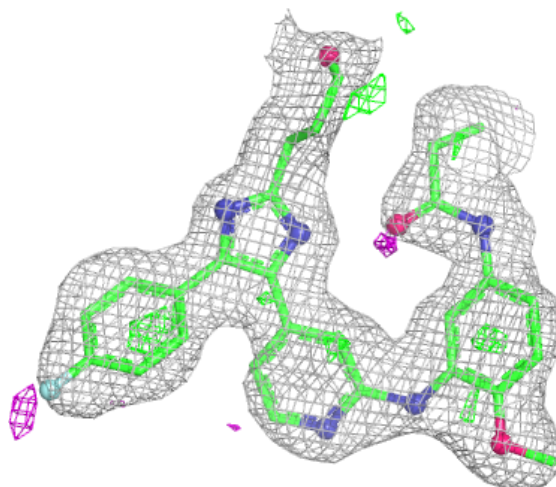
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	CL	G	1302	1/1	0.81	0.13	65,65,65,65	0
3	QQM	D	1202	36/36	0.88	0.12	18,27,34,40	0
2	CL	F	1201	1/1	0.89	0.17	65,65,65,65	0
2	CL	H	1201	1/1	0.90	0.11	56,56,56,56	0
3	QQM	A	1202	36/36	0.90	0.12	17,24,34,42	0
3	QQM	C	1202	36/36	0.90	0.12	13,19,31,34	0
3	QQM	E	1202	36/36	0.90	0.12	16,23,31,34	0
3	QQM	G	1301	36/36	0.90	0.11	17,23,34,38	0
3	QQM	F	1202	36/36	0.91	0.10	16,23,34,43	0
3	QQM	B	1202	36/36	0.91	0.10	15,18,33,33	0
3	QQM	H	1202	36/36	0.91	0.11	15,22,33,38	0
2	CL	D	1201	1/1	0.94	0.07	40,40,40,40	0
2	CL	E	1201	1/1	0.95	0.07	35,35,35,35	0
2	CL	A	1201	1/1	0.95	0.07	45,45,45,45	0
2	CL	C	1201	1/1	0.96	0.07	28,28,28,28	0
2	CL	B	1201	1/1	0.98	0.10	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.

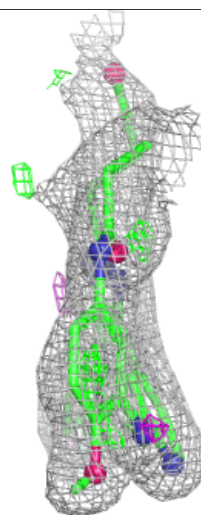
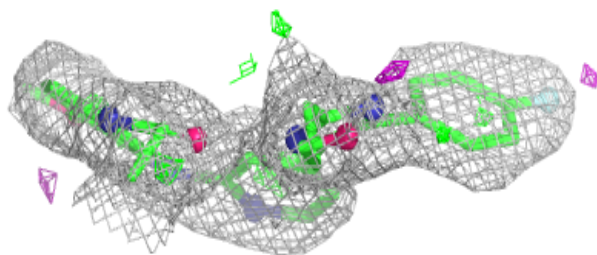
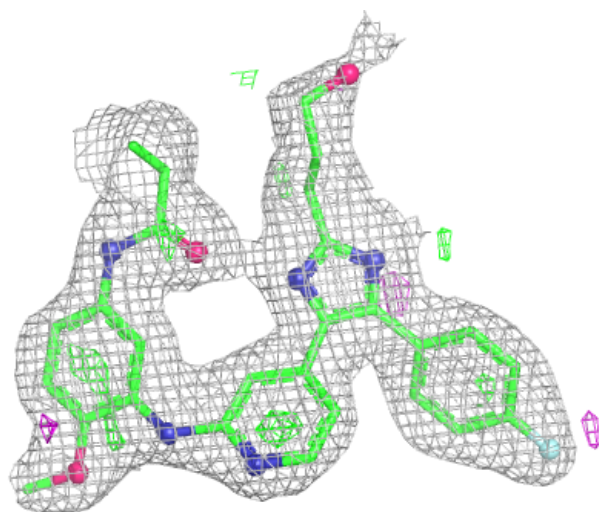
Electron density around QQM D 1202:

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



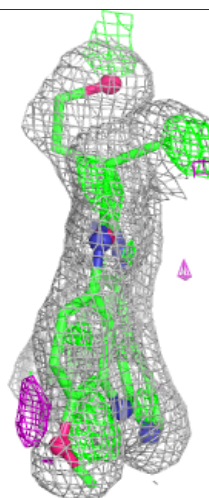
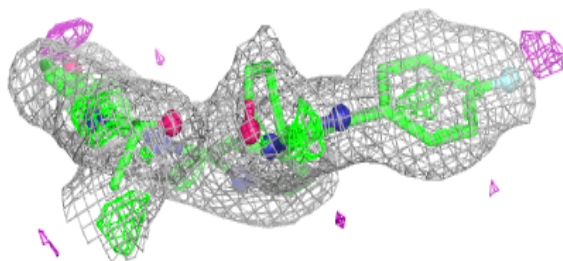
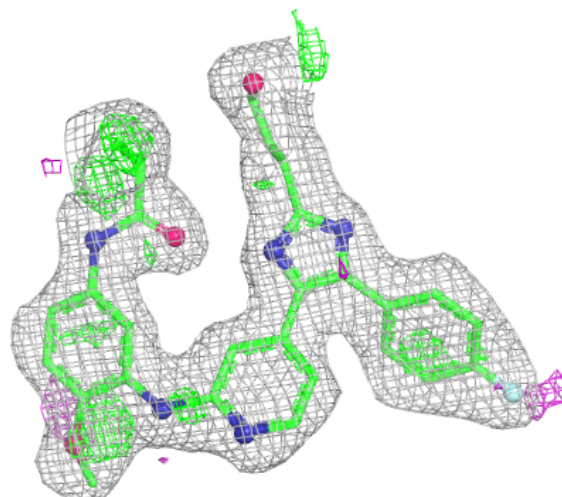
Electron density around QQM A 1202:

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



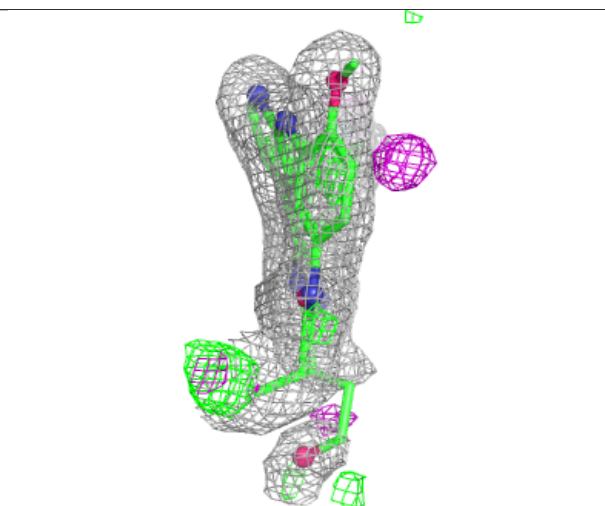
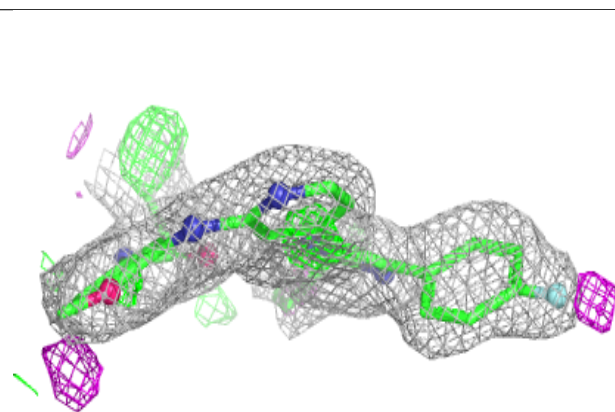
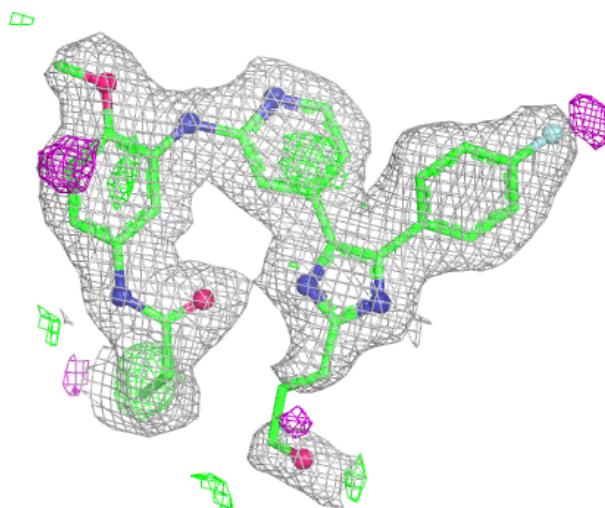
Electron density around QQM C 1202:

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



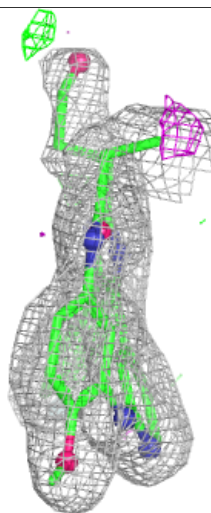
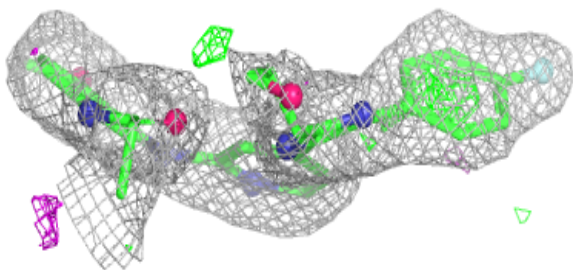
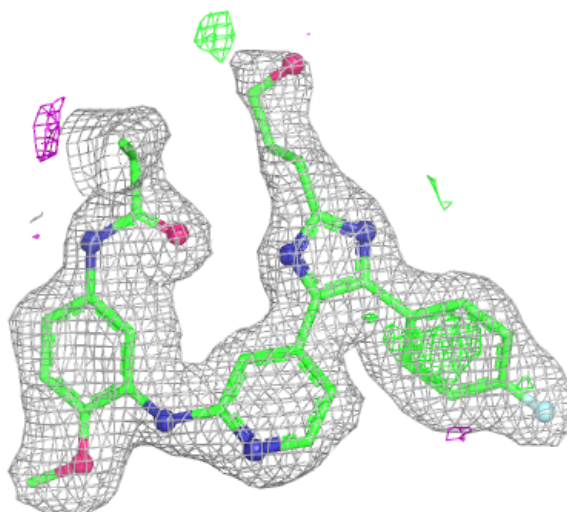
Electron density around QQM E 1202:

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



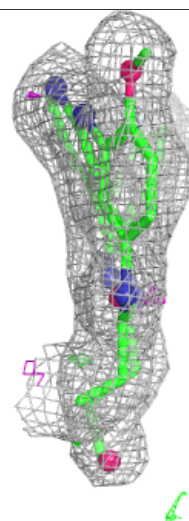
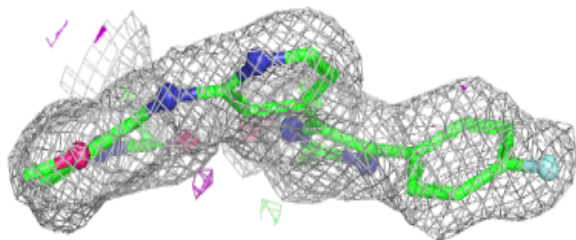
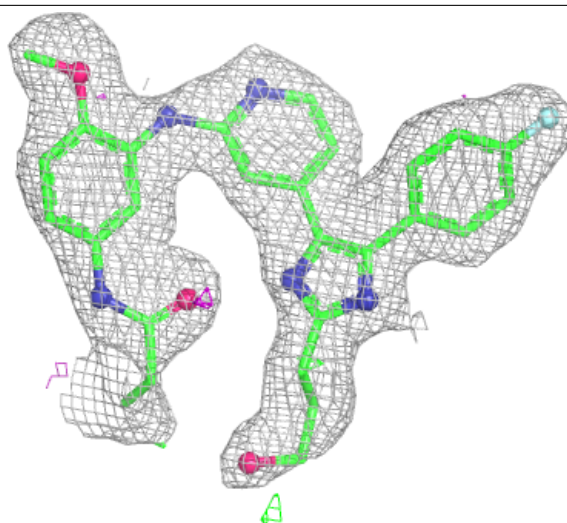
Electron density around QQM G 1301:

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



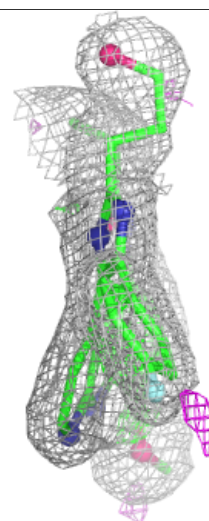
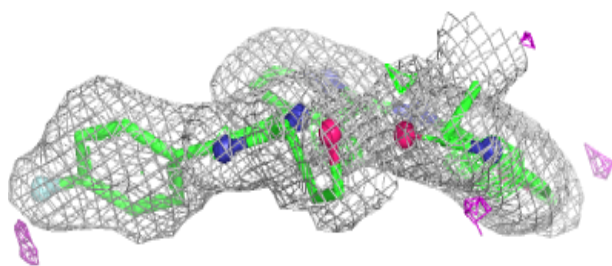
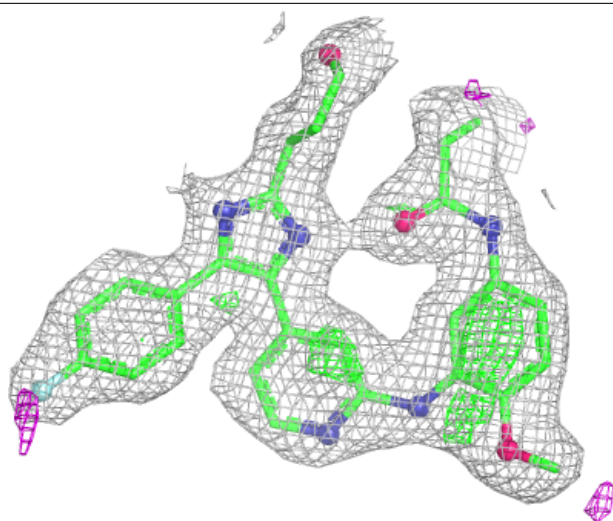
Electron density around QQM F 1202:

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



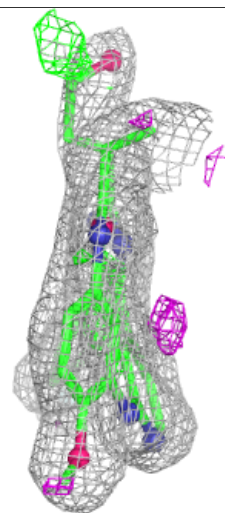
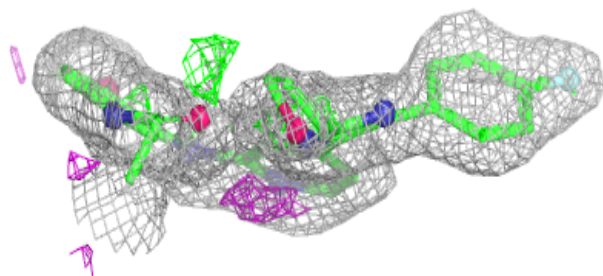
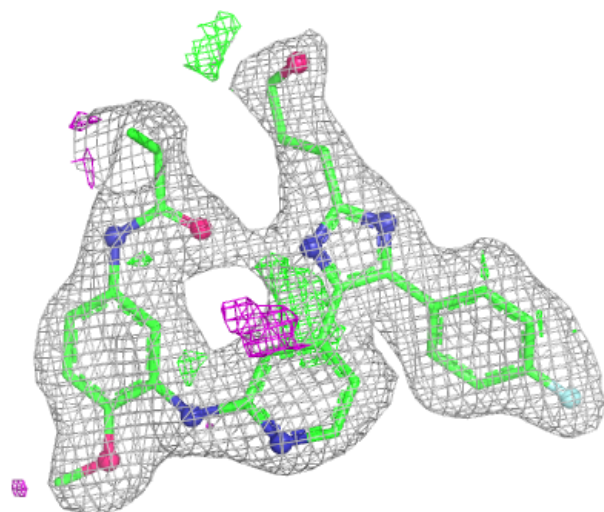
Electron density around QQM B 1202:

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



Electron density around QQM H 1202:

$2mF_o-DF_c$ (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.