



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 03:21 PM BST

PDB ID : 6V7C
Title : Human Arginase1 Complexed with Bicyclic Inhibitor Compound 3
Authors : Palte, R.L.
Deposited on : 2019-12-08
Resolution : 1.80 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

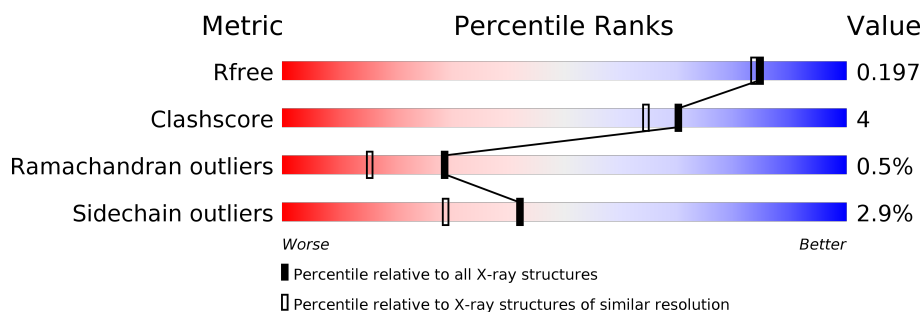
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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	322	92% (green), 7% (yellow), 1% (orange), 0% (red), 0% (grey)
1	B	322	88% (green), 10% (yellow), 1% (orange), 0% (red), 0% (grey)
1	C	322	91% (green), 7% (yellow), 1% (orange), 0% (red), 0% (grey)
1	D	322	85% (green), 13% (yellow), 1% (orange), 0% (red), 0% (grey)
1	E	322	91% (green), 8% (yellow), 1% (orange), 0% (red), 0% (grey)
1	F	322	84% (green), 14% (yellow), 1% (orange), 0% (red), 0% (grey)

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15342 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.

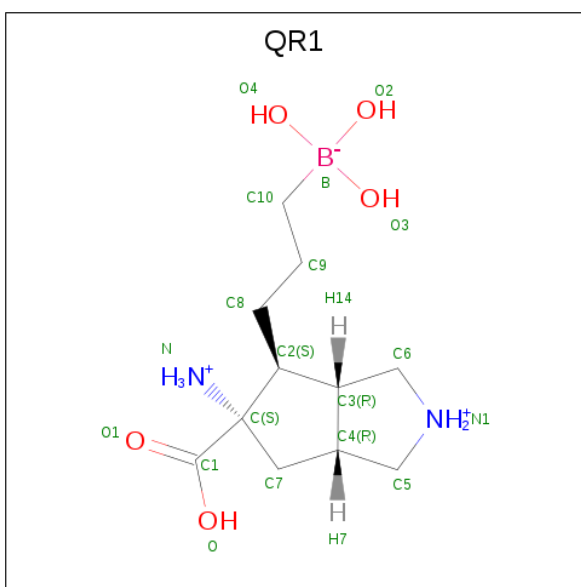
- Molecule 1 is a protein called Arginase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	B	318	Total	C	N	O	S	0	0	0
			2416	1540	412	458	6			
1	C	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	D	318	Total	C	N	O	S	0	0	0
			2415	1538	412	459	6			
1	E	319	Total	C	N	O	S	0	0	0
			2422	1543	413	460	6			
1	F	316	Total	C	N	O	S	0	0	0
			2402	1531	409	456	6			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is {3-[(3aR,4S,5S,6aR)-5-azaniumyl-5-carboxyoctahydrocyclopenta[c]pyrrol-2-ium-4-yl]propyl}(trihydroxy)borate(1-) (three-letter code: QR1) (formula: C₁₁H₂₄BN₂O₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			19	1	11	2	5		
3	B	1	Total	B	C	N	O	0	0
			19	1	11	2	5		
3	C	1	Total	B	C	N	O	0	0
			19	1	11	2	5		
3	D	1	Total	B	C	N	O	0	0
			19	1	11	2	5		
3	E	1	Total	B	C	N	O	0	0
			19	1	11	2	5		
3	F	1	Total	B	C	N	O	0	0
			19	1	11	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		
4	B	134	Total	O	0	0
			134	134		
4	C	132	Total	O	0	0
			132	132		
4	D	131	Total	O	0	0
			131	131		
4	E	91	Total	O	0	0
			91	91		
4	F	102	Total	O	0	0
			102	102		

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.

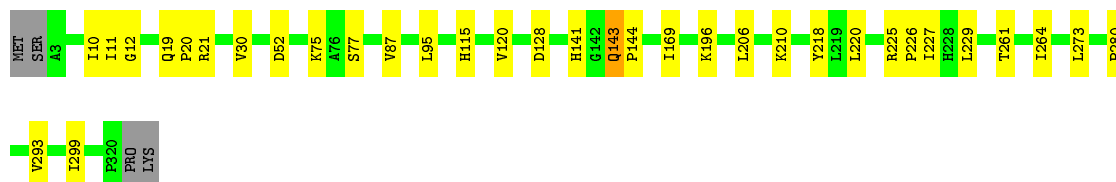
- Molecule 1: Arginase-1

Chain A: 



- Molecule 1: Arginase-1

Chain B: 




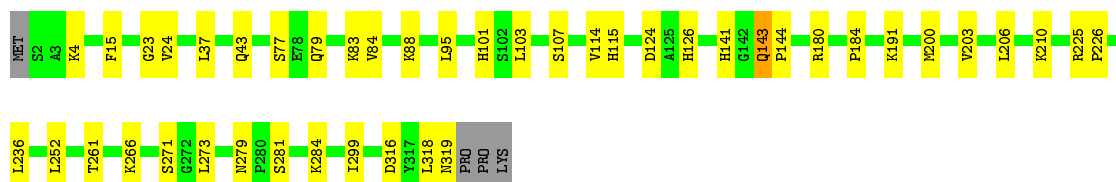
- Molecule 1: Arginase-1

Chain C: 



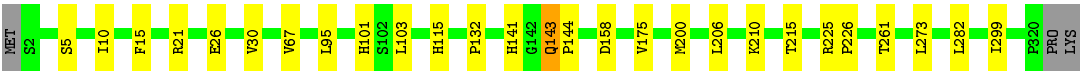
- Molecule 1: Arginase-1

Chain D: 

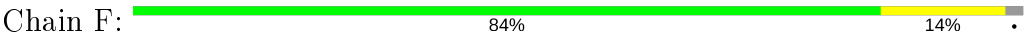


- Molecule 1: Arginase-1

Chain E: 



● Molecule 1: Arginase-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.98Å 281.38Å 67.26Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	35.84 – 1.80 35.84 – 1.81	Depositor EDS
% Data completeness (in resolution range)	94.4 (35.84-1.80) 94.1 (35.84-1.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.81Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.216 , 0.264 0.164 , 0.197	Depositor DCC
R_{free} test set	8416 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 18.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15342	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QR1, MN

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	0.53	0/2459	0.62	0/3336
1	B	0.51	0/2467	0.63	0/3348
1	C	0.52	0/2459	0.64	0/3336
1	D	0.50	0/2465	0.63	0/3344
1	E	0.46	0/2473	0.61	0/3356
1	F	0.47	0/2453	0.61	0/3330
All	All	0.50	0/14776	0.62	0/20050

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	2409	0	2456	19	0
1	B	2416	0	2463	18	0
1	C	2409	0	2456	10	0
1	D	2415	0	2461	19	0
1	E	2422	0	2468	16	0
1	F	2402	0	2445	26	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	19	0	0	1	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0
3	D	19	0	0	0	0
3	E	19	0	0	0	0
3	F	19	0	0	0	0
4	A	153	0	0	10	0
4	B	134	0	0	0	0
4	C	132	0	0	0	0
4	D	131	0	0	2	0
4	E	91	0	0	0	0
4	F	102	0	0	6	0
All	All	15342	0	14749	106	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 4.

The worst 5 of 106 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:C:155:LYS:HD2	1:D:318:LEU:HD13	1.61	0.82
1:F:244:THR:HG21	4:F:595:HOH:O	1.94	0.67
1:A:68:LYS:HE3	4:A:518:HOH:O	1.94	0.67
1:D:261:THR:HG21	1:D:299:ILE:HG23	1.77	0.66
1:C:210:LYS:HG3	1:C:214:GLU:OE2	1.96	0.66

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	315/322 (98%)	301 (96%)	13 (4%)	1 (0%)	41	27
1	B	316/322 (98%)	305 (96%)	10 (3%)	1 (0%)	41	27
1	C	315/322 (98%)	303 (96%)	9 (3%)	3 (1%)	15	5
1	D	316/322 (98%)	307 (97%)	8 (2%)	1 (0%)	41	27
1	E	317/322 (98%)	303 (96%)	13 (4%)	1 (0%)	41	27
1	F	314/322 (98%)	302 (96%)	10 (3%)	2 (1%)	25	12
All	All	1893/1932 (98%)	1821 (96%)	63 (3%)	9 (0%)	29	15

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	221	GLY
1	C	180	ARG
1	A	143	GLN
1	E	143	GLN
1	B	143	GLN

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	265/270 (98%)	260 (98%)	5 (2%)	57	46
1	B	266/270 (98%)	261 (98%)	5 (2%)	57	46
1	C	265/270 (98%)	258 (97%)	7 (3%)	46	32
1	D	266/270 (98%)	253 (95%)	13 (5%)	25	11
1	E	267/270 (99%)	262 (98%)	5 (2%)	57	46
1	F	265/270 (98%)	254 (96%)	11 (4%)	30	15
All	All	1594/1620 (98%)	1548 (97%)	46 (3%)	42	29

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	43	GLN
1	D	191	LYS
1	F	166	THR
1	D	77	SER
1	D	101	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	319	ASN
1	F	69	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	QR1	B	403	2	11,20,20	0.21	0	11,31,31	1.21	1 (9%)
3	QR1	C	403	2	11,20,20	0.27	0	11,31,31	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QR1	F	403	2	11,20,20	0.31	0	11,31,31	1.29	1 (9%)
3	QR1	A	403	2	11,20,20	0.24	0	11,31,31	1.35	1 (9%)
3	QR1	D	403	2	11,20,20	0.24	0	11,31,31	1.35	1 (9%)
3	QR1	E	403	2	11,20,20	0.27	0	11,31,31	1.08	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
3	QR1	B	403	2	-	0/4/38/38	0/2/2/2
3	QR1	C	403	2	-	0/4/38/38	0/2/2/2
3	QR1	F	403	2	-	0/4/38/38	0/2/2/2
3	QR1	A	403	2	-	1/4/38/38	0/2/2/2
3	QR1	D	403	2	-	0/4/38/38	0/2/2/2
3	QR1	E	403	2	-	0/4/38/38	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	QR1	C6-N1-C5	2.91	111.44	108.07
3	A	403	QR1	O3-B-O4	-2.53	100.09	109.18
3	F	403	QR1	C9-C8-C2	2.22	119.02	114.07
3	B	403	QR1	C5-C4-C7	-2.08	107.64	115.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	QR1	C3-C2-C8-C9

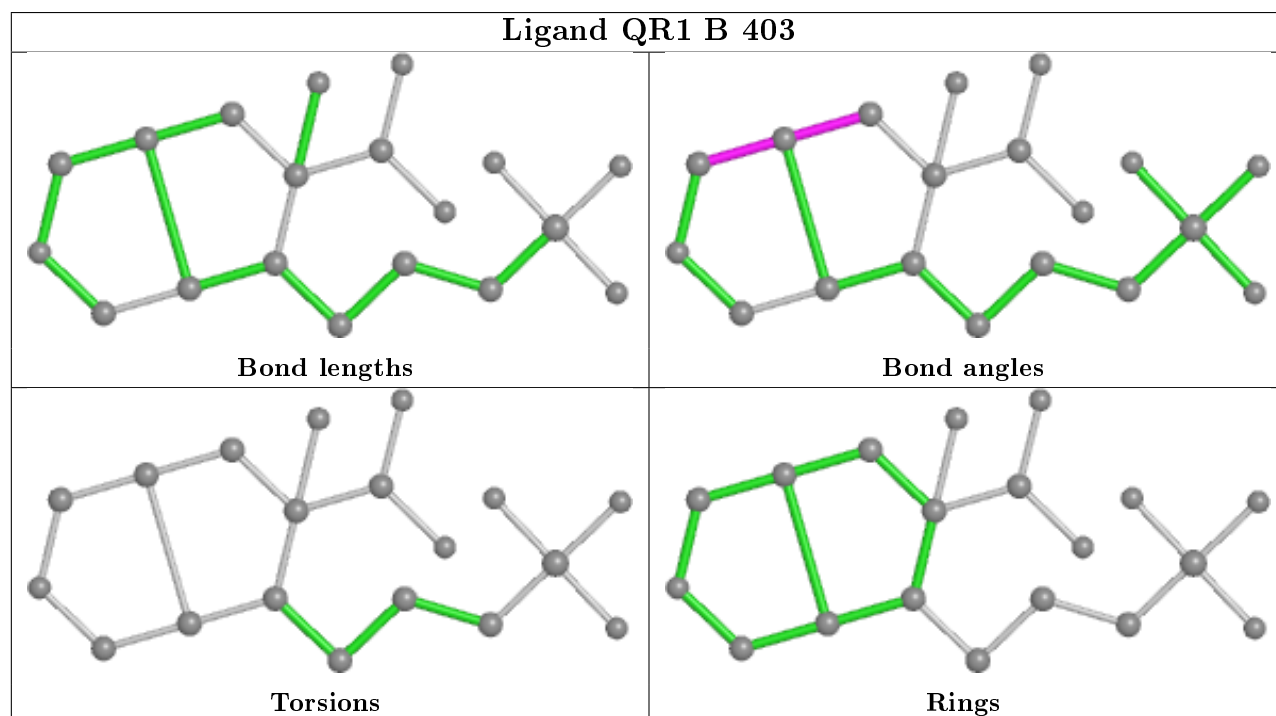
There are no ring outliers.

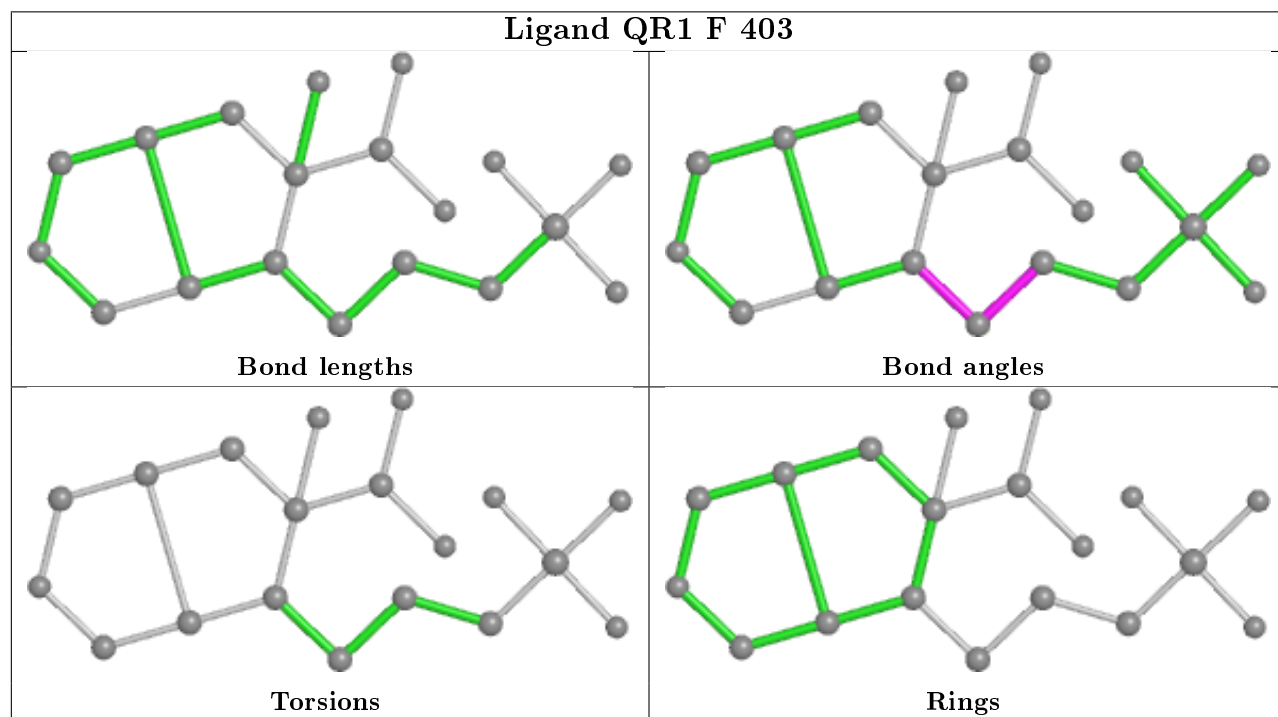
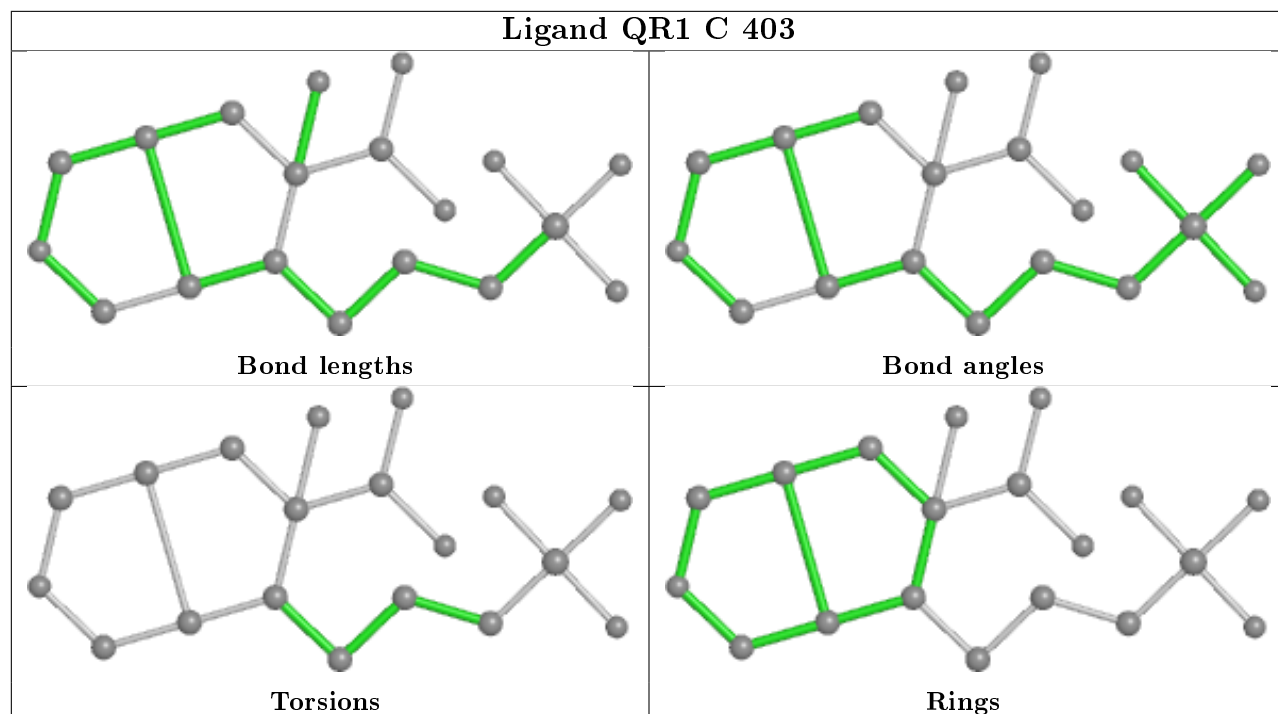
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	QR1	1	0

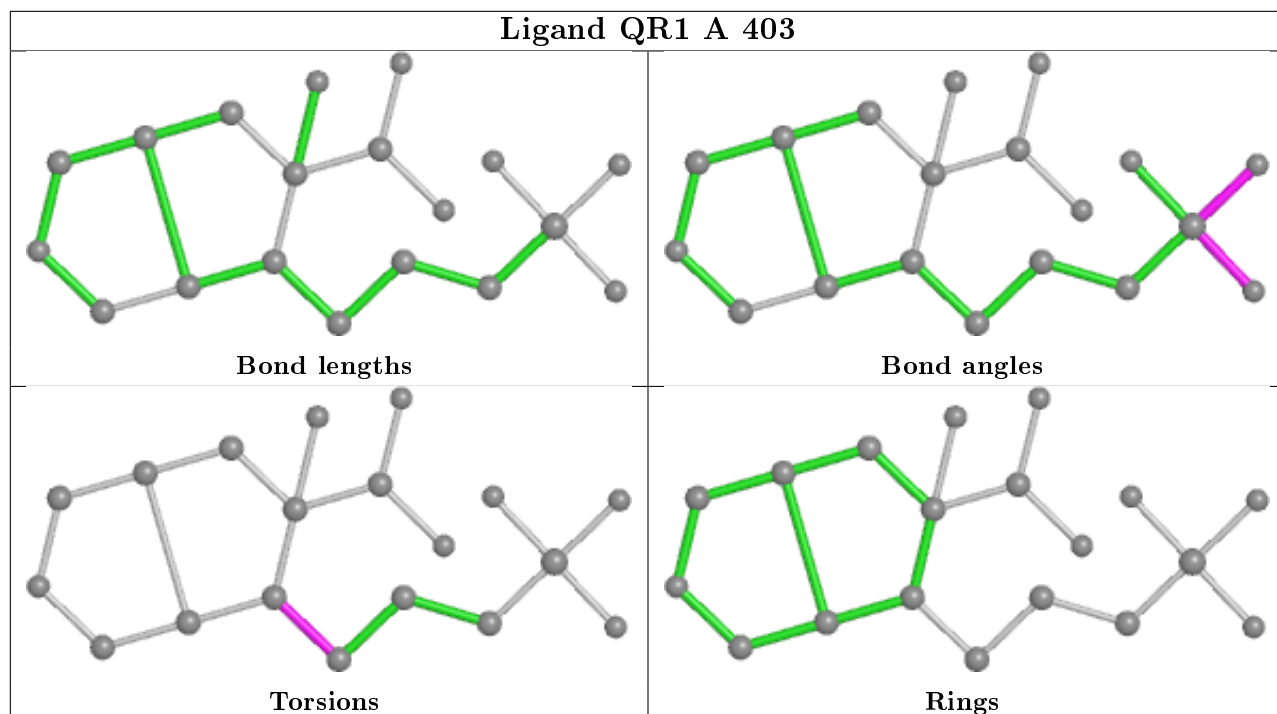
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

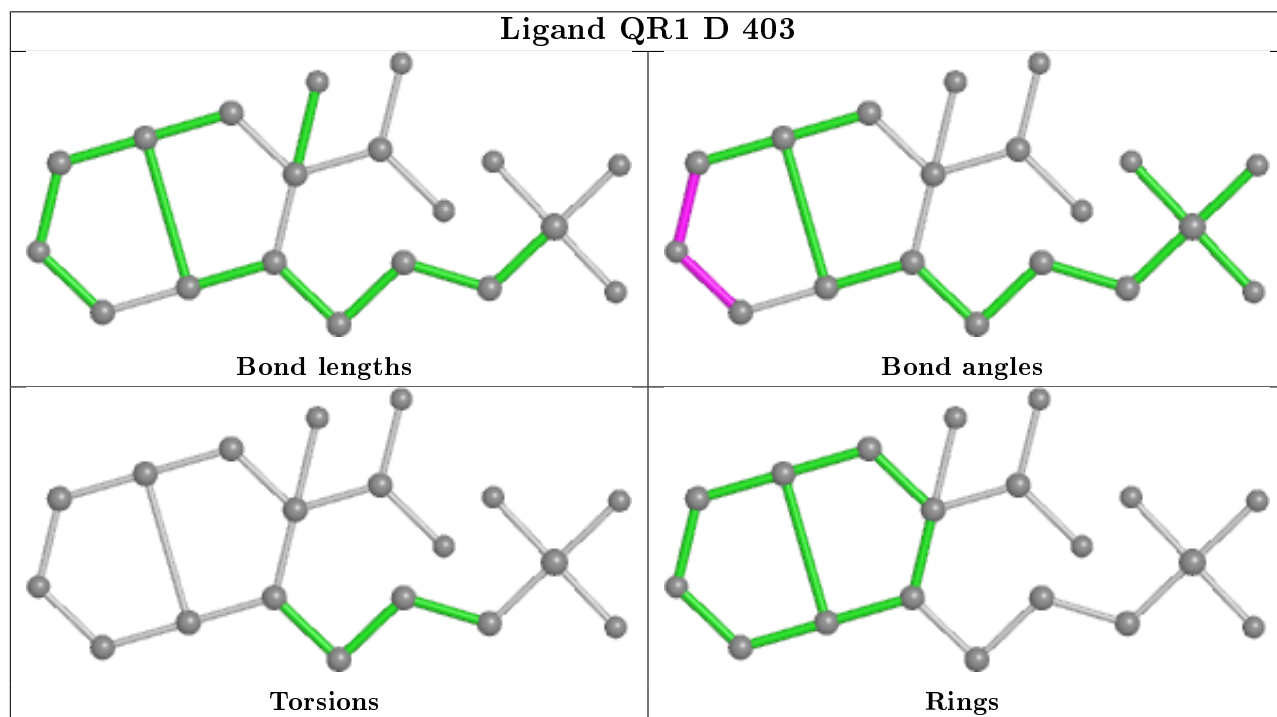


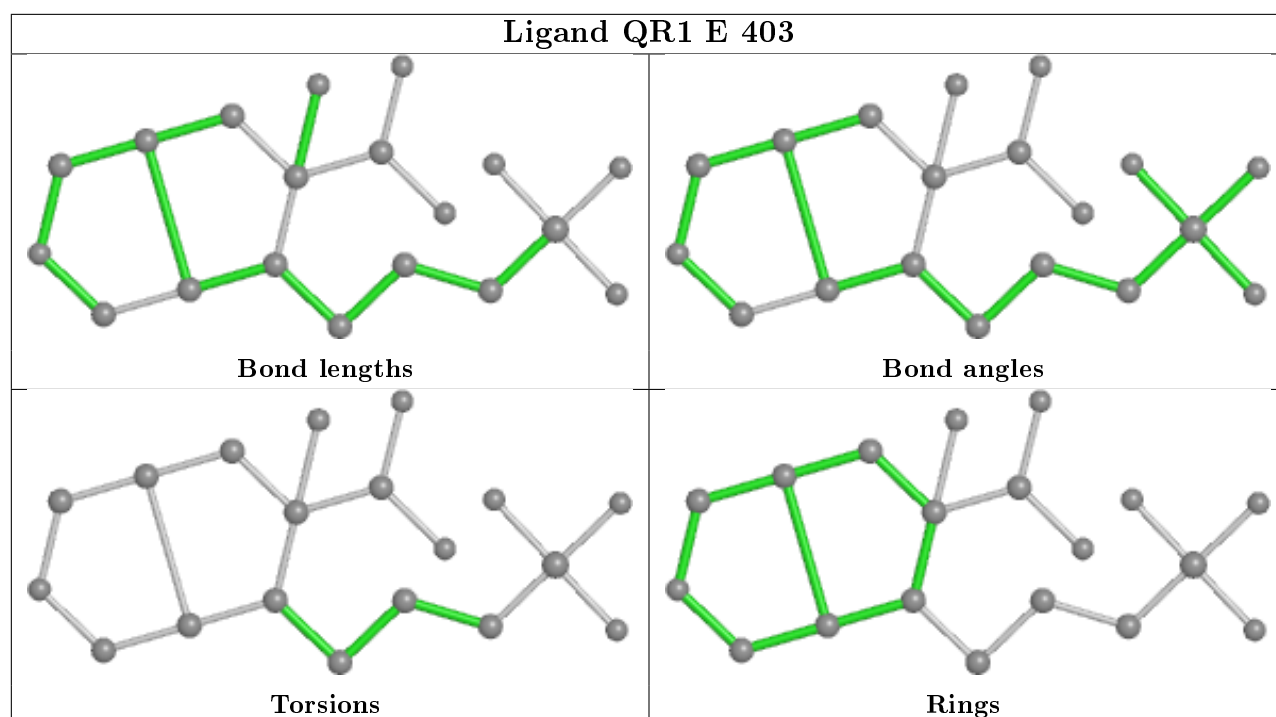


Ligand QR1 A 403



Ligand QR1 D 403





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.

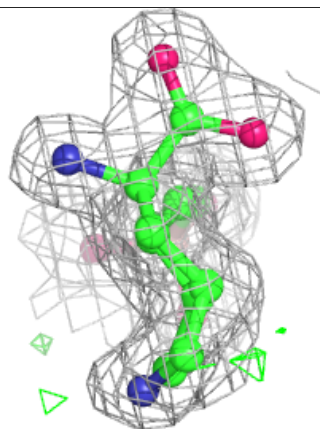
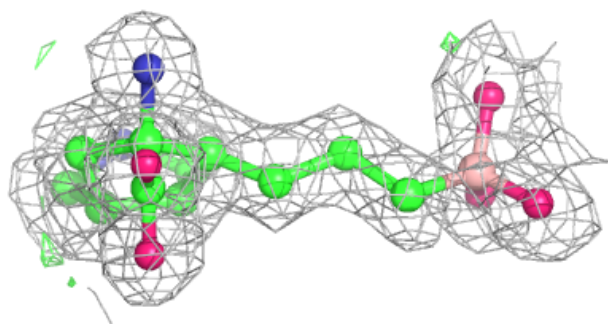
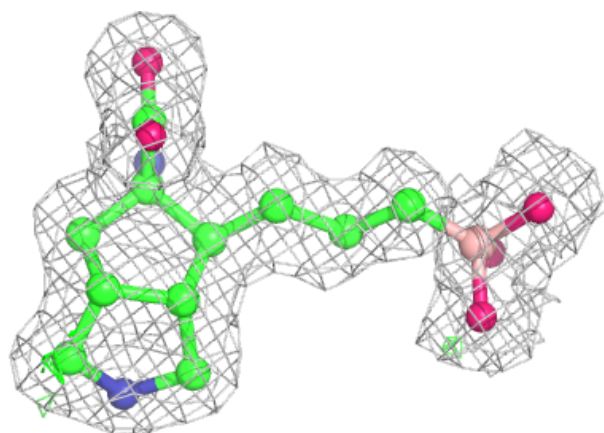
6.4 Ligands ⓘ

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.

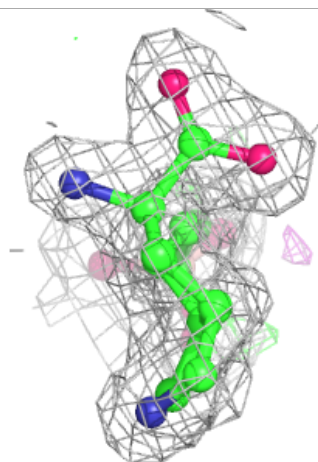
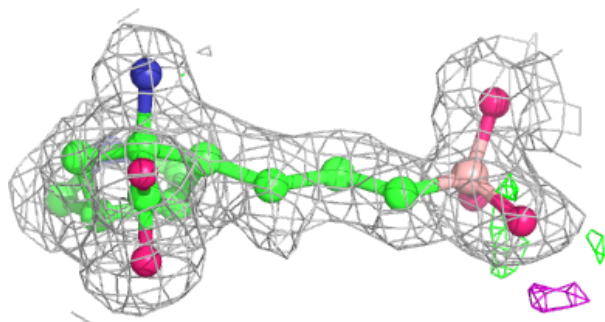
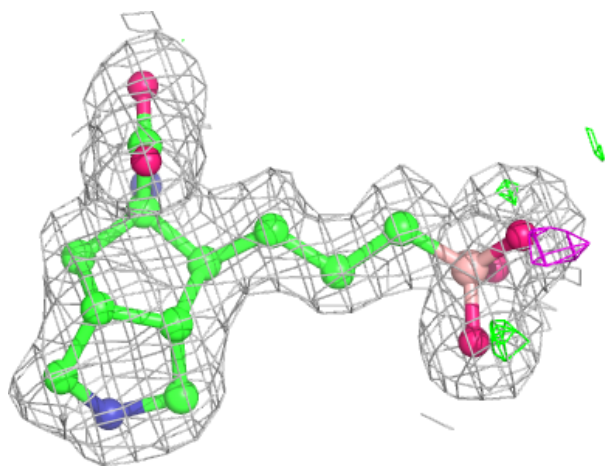
Electron density around QR1 A 403:

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



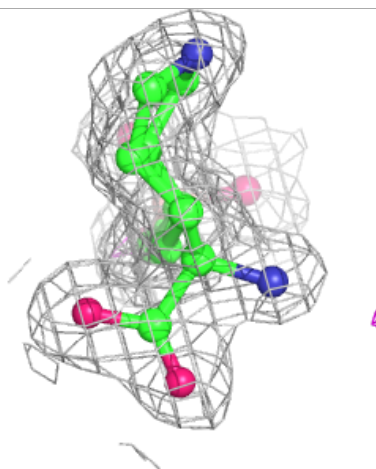
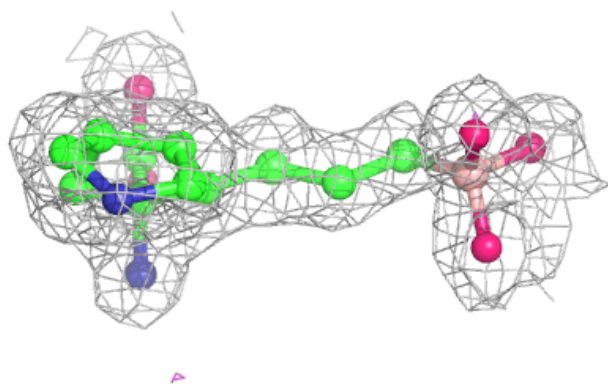
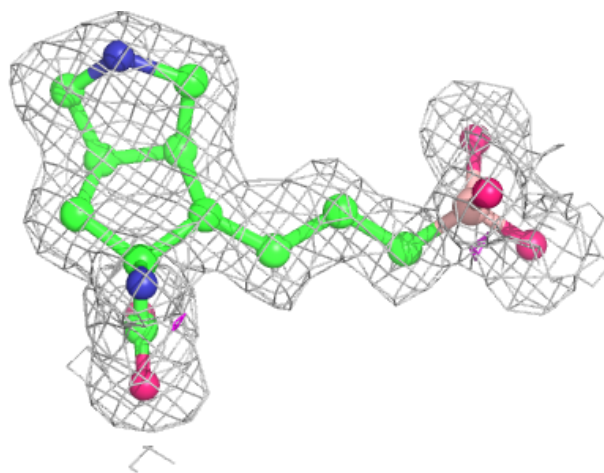
Electron density around QR1 B 403:

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



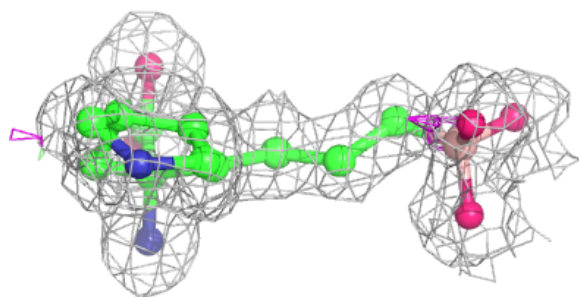
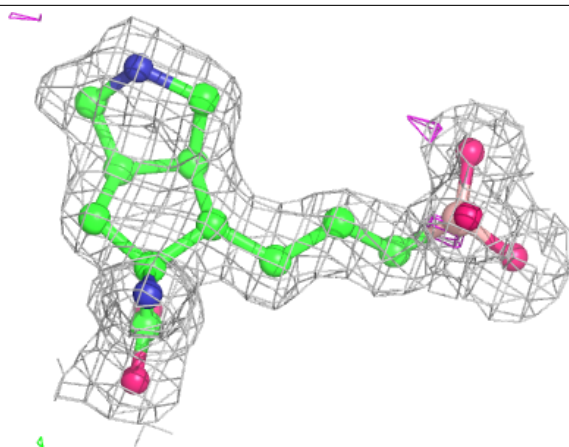
Electron density around QR1 C 403:

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



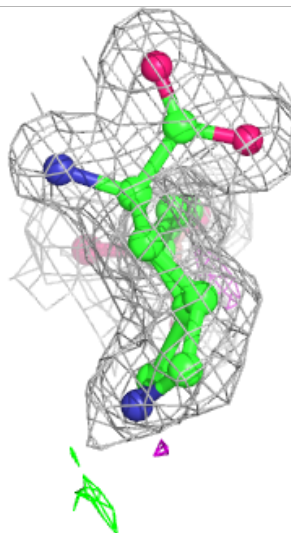
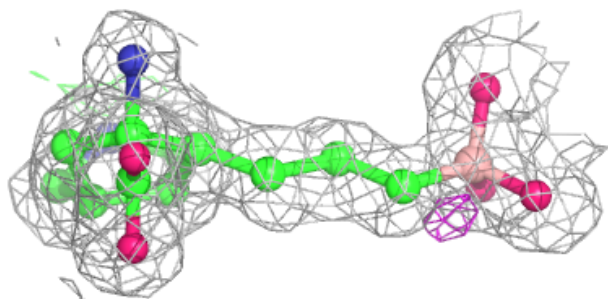
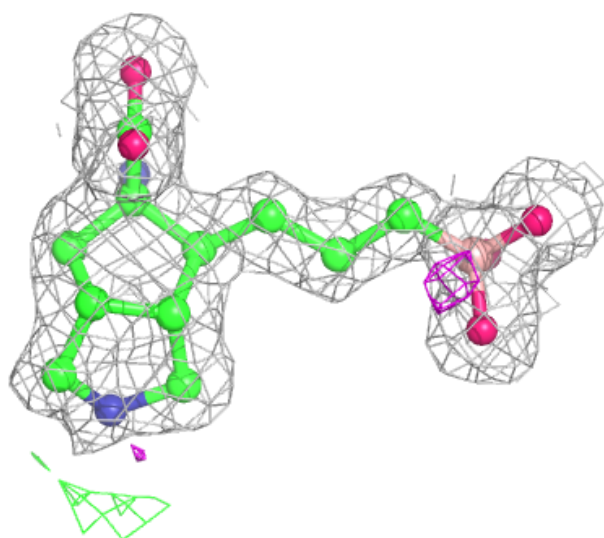
Electron density around QR1 D 403:

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



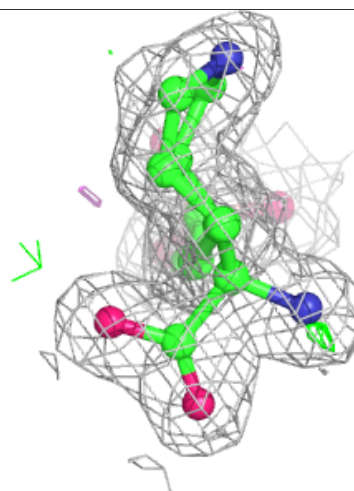
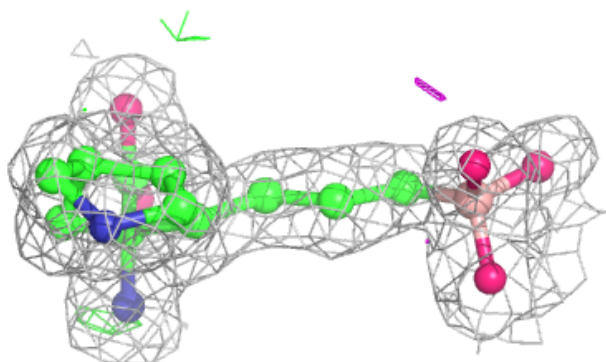
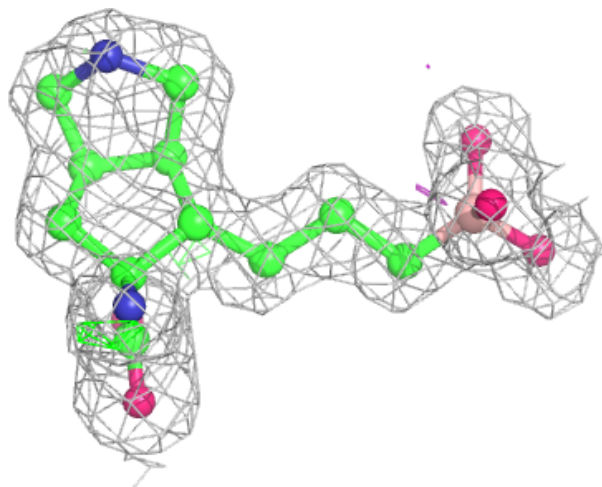
Electron density around QR1 F 403:

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



Electron density around QR1 E 403:

$2mF_o-DF_c$ (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 depositor's R factor - this section is therefore empty.