wwPDB X-ray Structure Validation Summary Report (i)

Oct 29, 2020 – 12:16 PM GMT

PDB ID	:	6ZQZ
Title	:	[1,2,4]Triazolo[1,5-a]pyrimidine Phosphodiesterase 2 Inhibitors
Authors	:	Tresadern, G.; Leonard, P.M.
Deposited on	:	2020-07-10
Resolution	:	1.88 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 (i) symbol.

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

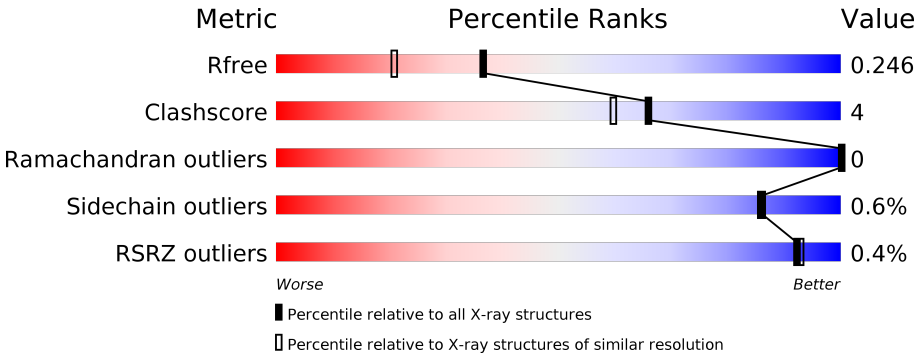
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	353	88% 8%
1	B	353	% 89% 7% 5%
1	C	353	% 84% 9% 7%
1	D	353	86% 8% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11809 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	1	0
			2738	1747	462	504	25			
1	B	337	Total	C	N	O	S	0	1	0
			2707	1728	460	494	25			
1	C	327	Total	C	N	O	S	0	1	0
			2610	1668	441	476	25			
1	D	336	Total	C	N	O	S	0	0	0
			2727	1737	466	499	25			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	MET	-	initiating methionine	UNP O00408
A	577	GLY	-	expression tag	UNP O00408
A	922	ARG	-	expression tag	UNP O00408
A	923	HIS	-	expression tag	UNP O00408
A	924	HIS	-	expression tag	UNP O00408
A	925	HIS	-	expression tag	UNP O00408
A	926	HIS	-	expression tag	UNP O00408
A	927	HIS	-	expression tag	UNP O00408
A	928	HIS	-	expression tag	UNP O00408
B	576	MET	-	initiating methionine	UNP O00408
B	577	GLY	-	expression tag	UNP O00408
B	922	ARG	-	expression tag	UNP O00408
B	923	HIS	-	expression tag	UNP O00408
B	924	HIS	-	expression tag	UNP O00408
B	925	HIS	-	expression tag	UNP O00408
B	926	HIS	-	expression tag	UNP O00408
B	927	HIS	-	expression tag	UNP O00408
B	928	HIS	-	expression tag	UNP O00408
C	576	MET	-	initiating methionine	UNP O00408
C	577	GLY	-	expression tag	UNP O00408
C	922	ARG	-	expression tag	UNP O00408

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Chain	Residue	Modelled	Actual	Comment	Reference
C	923	HIS	-	expression tag	UNP O00408
C	924	HIS	-	expression tag	UNP O00408
C	925	HIS	-	expression tag	UNP O00408
C	926	HIS	-	expression tag	UNP O00408
C	927	HIS	-	expression tag	UNP O00408
C	928	HIS	-	expression tag	UNP O00408
D	576	MET	-	initiating methionine	UNP O00408
D	577	GLY	-	expression tag	UNP O00408
D	922	ARG	-	expression tag	UNP O00408
D	923	HIS	-	expression tag	UNP O00408
D	924	HIS	-	expression tag	UNP O00408
D	925	HIS	-	expression tag	UNP O00408
D	926	HIS	-	expression tag	UNP O00408
D	927	HIS	-	expression tag	UNP O00408
D	928	HIS	-	expression tag	UNP O00408

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

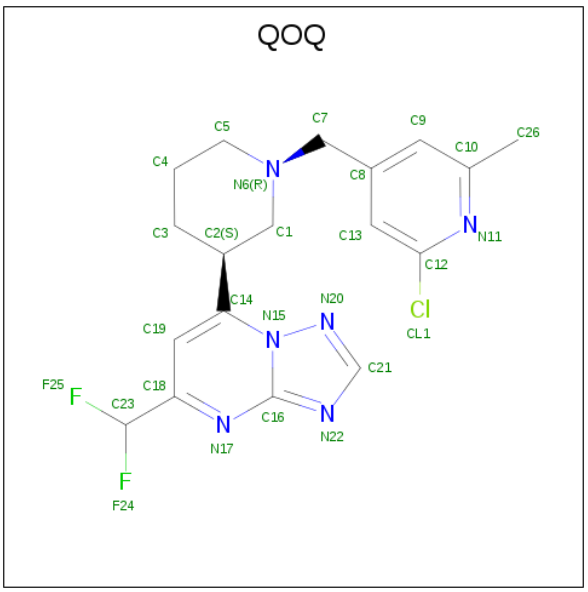
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 5-[bis(fluoranyl)methyl]-7-[(3 {S})-1-[(2-chloranyl-6-methyl-pyridin-4-yl) methyl]piperidin-3-yl]-[1,2,4]triazolo[1,5-a]pyrimidine (three-letter code: QOQ) (formula:

$C_{18}H_{19}ClF_2N_6$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	0	0
			27	18	1	2	6		
4	B	1	Total	C	Cl	F	N	0	0
			27	18	1	2	6		
4	C	1	Total	C	Cl	F	N	0	0
			27	18	1	2	6		
4	D	1	Total	C	Cl	F	N	0	0
			27	18	1	2	6		

- Molecule 5 is water.

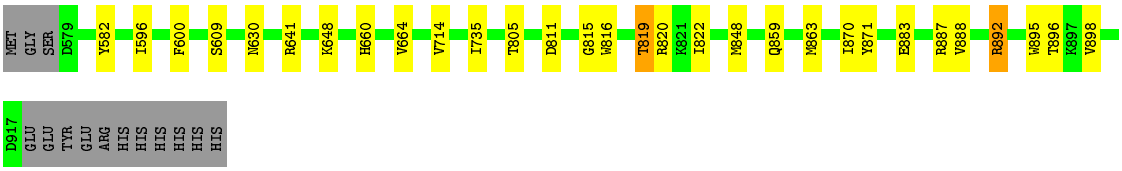
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	249	Total	O	0	0
			249	249		
5	B	240	Total	O	0	0
			240	240		
5	C	173	Total	O	0	0
			173	173		
5	D	248	Total	O	0	0
			248	248		

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.

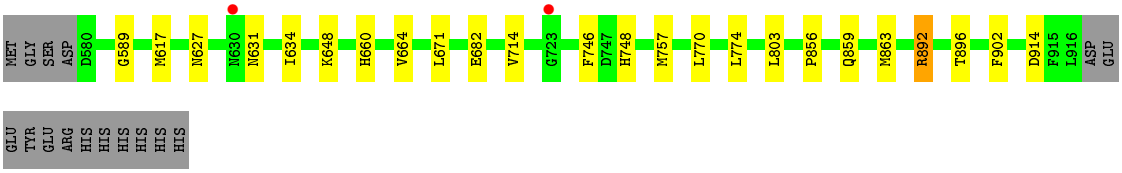
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain A:



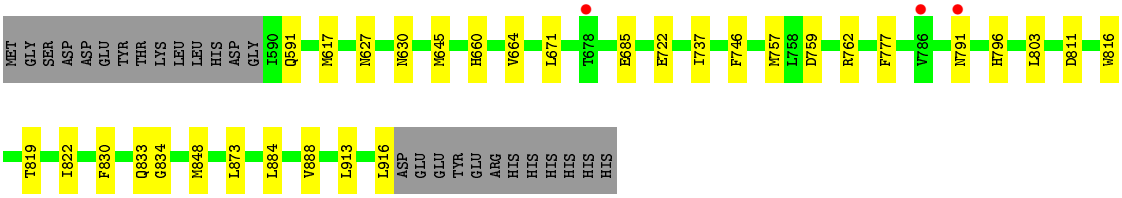
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain B:



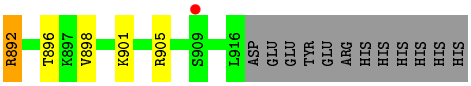
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain C:



- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

Chain D:


R892
T896
K897
V898
K901
R905
S909
L916
ASP
GLU
GLU
TYR
GLU
ARG
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.96Å 73.46Å 92.23Å 109.16° 91.37° 91.26°	Depositor
Resolution (Å)	87.07 – 1.88 47.21 – 1.88	Depositor EDS
% Data completeness (in resolution range)	93.4 (87.07-1.88) 93.4 (47.21-1.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.244 0.201 , 0.246	Depositor DCC
R_{free} test set	5262 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11809	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, QOQ

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	1/2808 (0.0%)	0.59	0/3798
1	B	0.52	0/2778	0.58	0/3762
1	C	0.49	0/2678	0.56	0/3630
1	D	0.52	1/2794 (0.0%)	0.62	2/3778 (0.1%)
All	All	0.52	2/11058 (0.0%)	0.59	2/14968 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	895	TRP	CD2-CE2	5.23	1.47	1.41
1	D	816	TRP	CD2-CE2	5.12	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	762	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	762	ARG	NE-CZ-NH2	-5.75	117.42	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2738	0	2642	21	0
1	B	2707	0	2591	20	0
1	C	2610	0	2491	21	0
1	D	2727	0	2635	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	27	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	0	0
5	A	249	0	0	5	0
5	B	240	0	0	5	0
5	C	173	0	0	1	0
5	D	248	0	0	13	0
All	All	11809	0	10359	84	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 84 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:714:VAL:HG12	5:A:1305:HOH:O	1.52	1.10
1:D:763:ASP:HB3	5:D:1103:HOH:O	1.70	0.91
1:D:868:MET:HG2	5:D:1101:HOH:O	1.77	0.84
1:C:833:GLN:HB3	1:C:848:MET:HE1	1.72	0.71
1:B:892:ARG:NH2	1:B:896:THR:OG1	2.24	0.70

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	338/353 (96%)	334 (99%)	4 (1%)	0	100	100
1	B	336/353 (95%)	331 (98%)	5 (2%)	0	100	100
1	C	326/353 (92%)	322 (99%)	4 (1%)	0	100	100
1	D	334/353 (95%)	331 (99%)	3 (1%)	0	100	100
All	All	1334/1412 (94%)	1318 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	298/319 (93%)	294 (99%)	4 (1%)	69	64
1	B	291/319 (91%)	290 (100%)	1 (0%)	92	92
1	C	279/319 (88%)	279 (100%)	0	100	100
1	D	297/319 (93%)	295 (99%)	2 (1%)	84	83
All	All	1165/1276 (91%)	1158 (99%)	7 (1%)	86	86

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	898	VAL
1	D	892	ARG
1	B	892	ARG

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Mol	Chain	Res	Type
1	A	819	THR
1	D	683	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	708	GLN
1	D	842	ASN
1	B	842	ASN
1	B	627	ASN
1	B	894	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	QOQ	A	1003	-	25,30,30	1.14	2 (8%)	22,43,43	1.51	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	QOQ	D	1003	-	25,30,30	1.22	2 (8%)	22,43,43	1.67	4 (18%)
4	QOQ	B	1003	-	25,30,30	1.05	2 (8%)	22,43,43	1.53	4 (18%)
4	QOQ	C	1003	-	25,30,30	1.18	2 (8%)	22,43,43	1.40	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	QOQ	A	1003	-	-	1/12/22/22	0/4/4/4
4	QOQ	D	1003	-	-	2/12/22/22	0/4/4/4
4	QOQ	B	1003	-	-	2/12/22/22	0/4/4/4
4	QOQ	C	1003	-	-	2/12/22/22	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1003	QOQ	C18-N17	3.66	1.35	1.32
4	D	1003	QOQ	C18-N17	3.30	1.35	1.32
4	B	1003	QOQ	C18-N17	3.16	1.35	1.32
4	A	1003	QOQ	C18-N17	2.90	1.35	1.32
4	D	1003	QOQ	C12-CL1	2.83	1.80	1.74

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1003	QOQ	C13-C12-N11	-4.54	120.52	125.50
4	B	1003	QOQ	C13-C12-N11	-4.00	121.11	125.50
4	A	1003	QOQ	C13-C12-N11	-3.55	121.60	125.50
4	B	1003	QOQ	C3-C2-C14	3.46	116.39	112.06
4	C	1003	QOQ	C13-C12-N11	-3.05	122.16	125.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1003	QOQ	N17-C18-C23-F24
4	B	1003	QOQ	N17-C18-C23-F25
4	C	1003	QOQ	N17-C18-C23-F24

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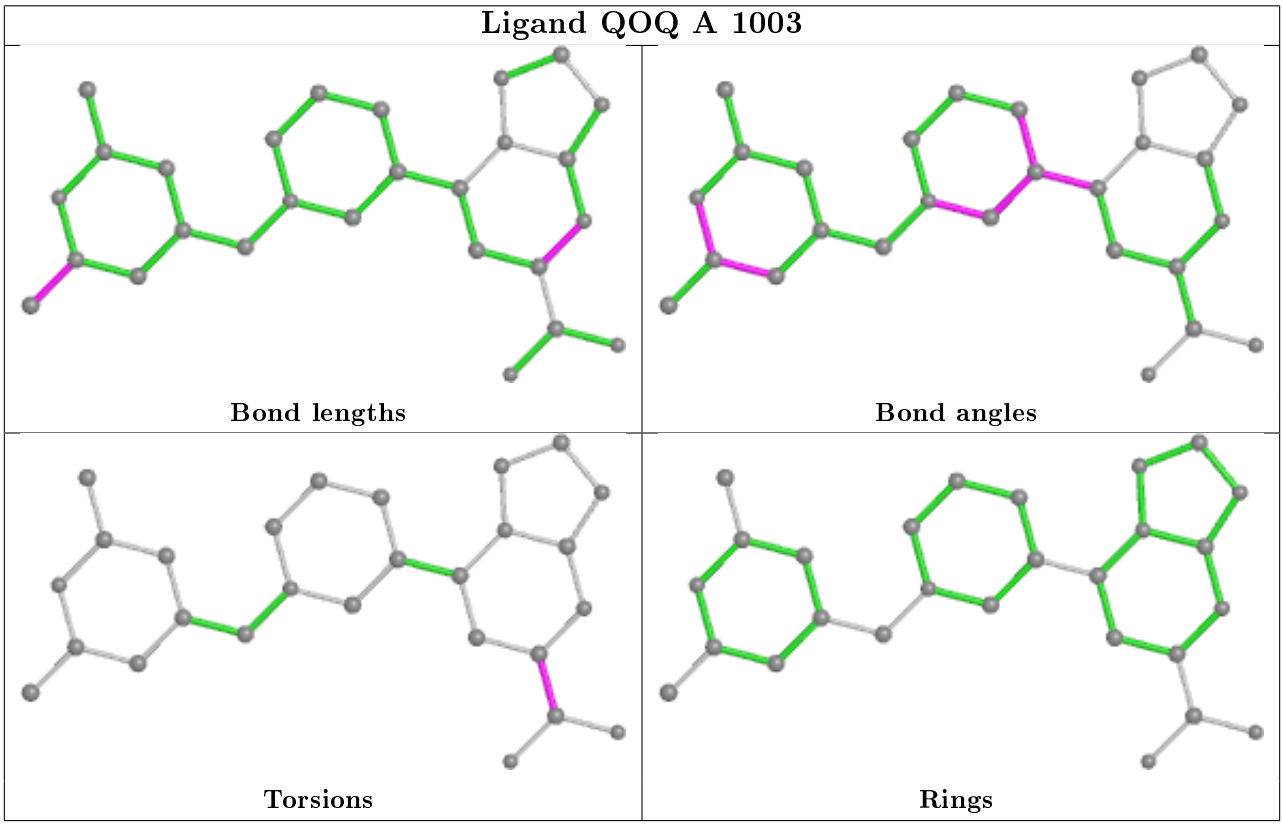
Mol	Chain	Res	Type	Atoms
4	C	1003	QOQ	N17-C18-C23-F25
4	D	1003	QOQ	N17-C18-C23-F24

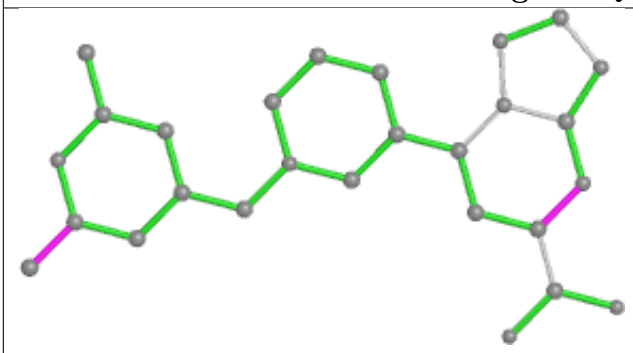
There are no ring outliers.

No monomer is involved in short contacts.

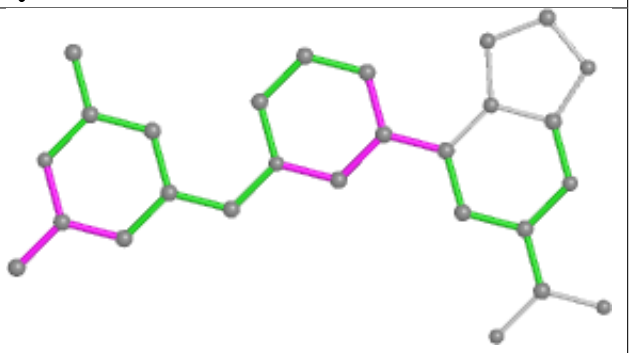
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



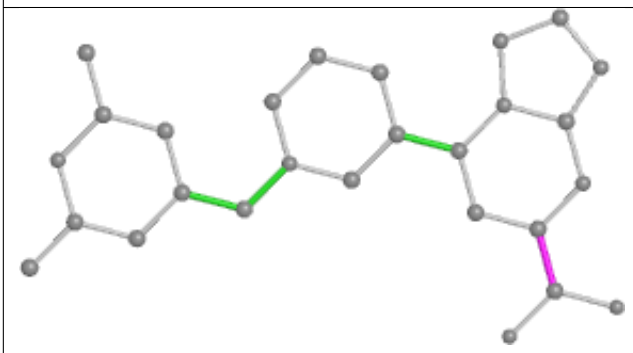
Ligand QOQ D 1003



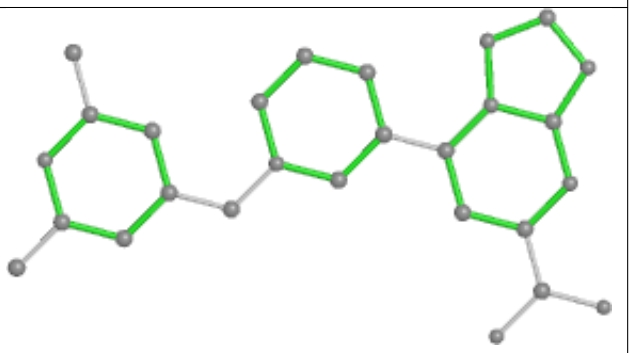
Bond lengths



Bond angles

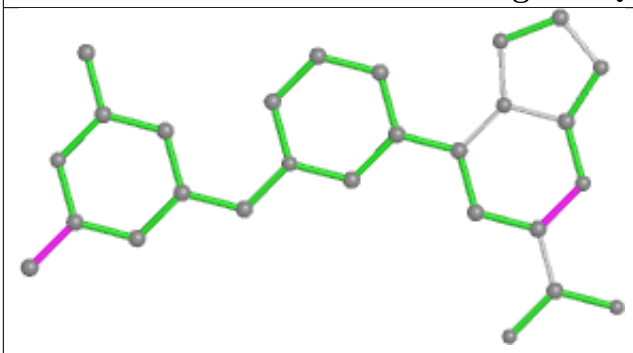


Torsions

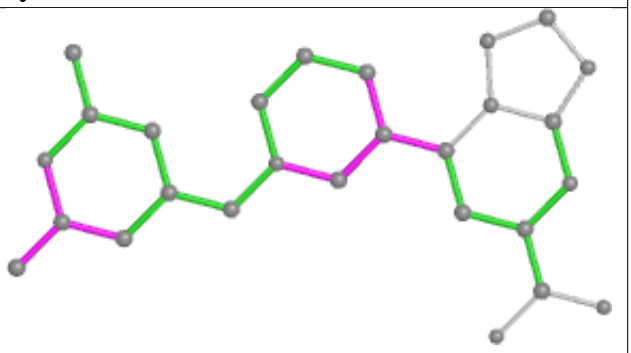


Rings

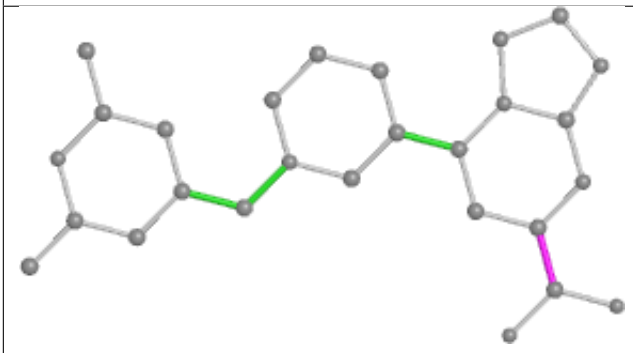
Ligand QOQ B 1003



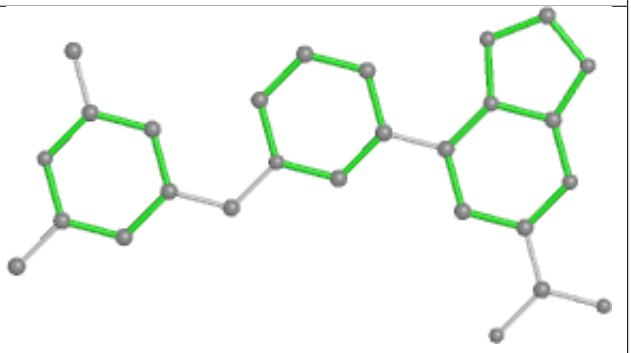
Bond lengths



Bond angles

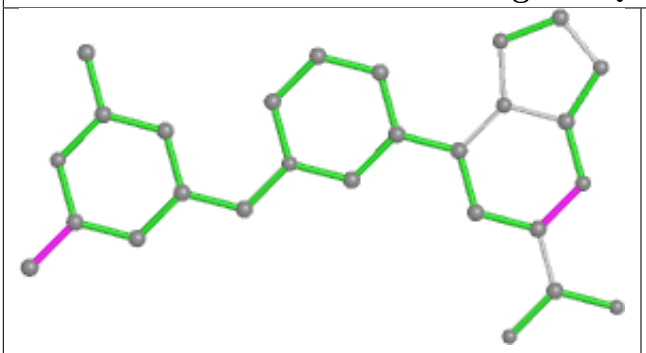


Torsions

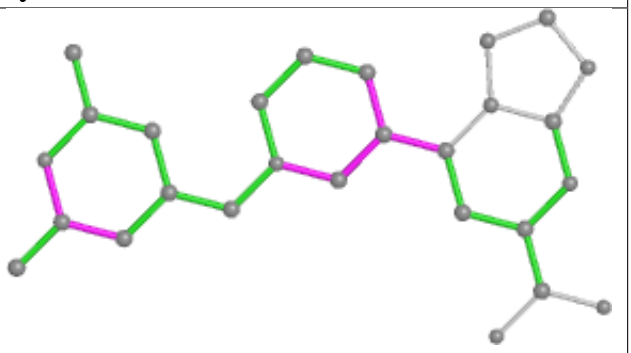


Rings

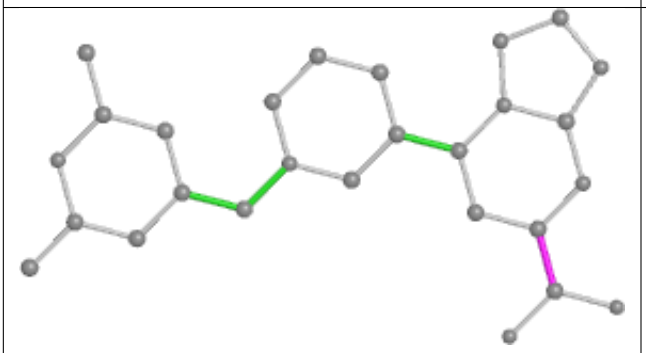
Ligand QOQ C 1003



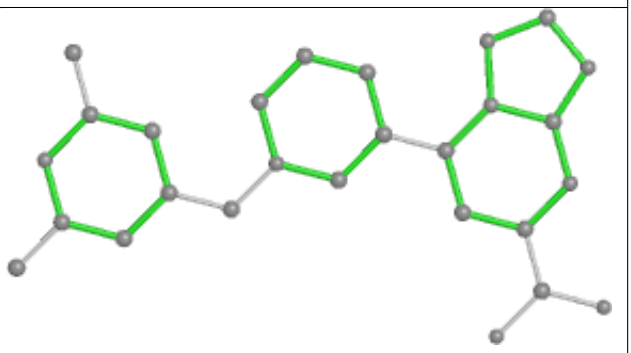
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	339/353 (96%)	-0.26	0	100	100	8, 18, 32, 53	0
1	B	337/353 (95%)	-0.23	2 (0%)	89	90	10, 21, 34, 47	0
1	C	327/353 (92%)	-0.12	3 (0%)	84	85	11, 25, 39, 54	0
1	D	336/353 (95%)	-0.23	1 (0%)	94	94	10, 20, 33, 44	0
All	All	1339/1412 (94%)	-0.21	6 (0%)	92	93	8, 21, 36, 54	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	786	VAL	3.0
1	B	723	GLY	2.8
1	B	630	ASN	2.7
1	D	909	SER	2.4
1	C	791	ASN	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

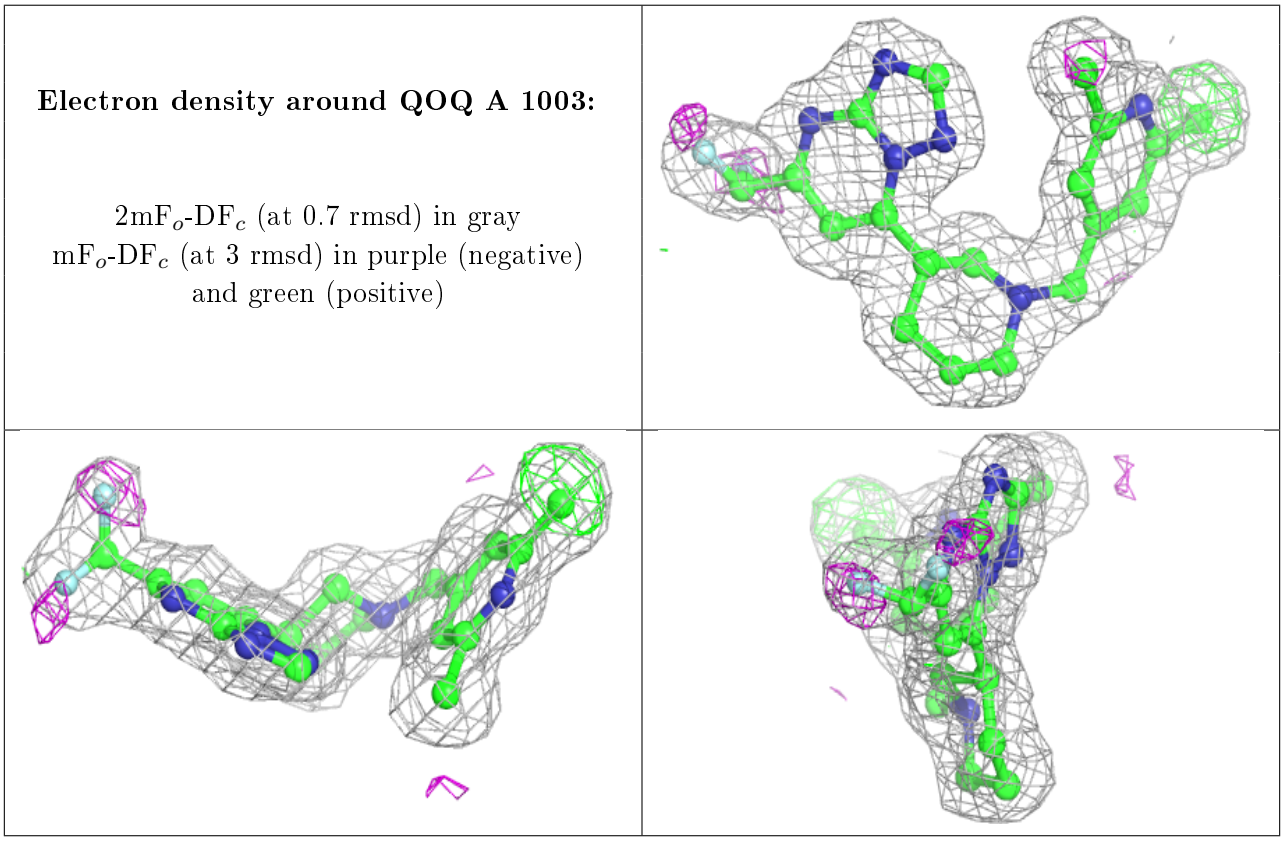
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	QOQ	A	1003	27/27	0.89	0.10	14,16,19,22	0
4	QOQ	D	1003	27/27	0.89	0.12	20,21,25,28	0
4	QOQ	B	1003	27/27	0.91	0.10	18,20,25,27	0
4	QOQ	C	1003	27/27	0.91	0.10	20,21,25,28	0
3	MG	B	1004	1/1	0.93	0.05	27,27,27,27	0
3	MG	D	1002	1/1	0.98	0.04	11,11,11,11	0
3	MG	B	1002	1/1	0.98	0.07	12,12,12,12	0
3	MG	A	1002	1/1	0.98	0.07	11,11,11,11	0
3	MG	C	1002	1/1	0.99	0.08	10,10,10,10	0
2	ZN	D	1001	1/1	1.00	0.05	14,14,14,14	0
2	ZN	C	1001	1/1	1.00	0.06	15,15,15,15	0
2	ZN	B	1001	1/1	1.00	0.05	15,15,15,15	0
2	ZN	A	1001	1/1	1.00	0.03	13,13,13,13	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.

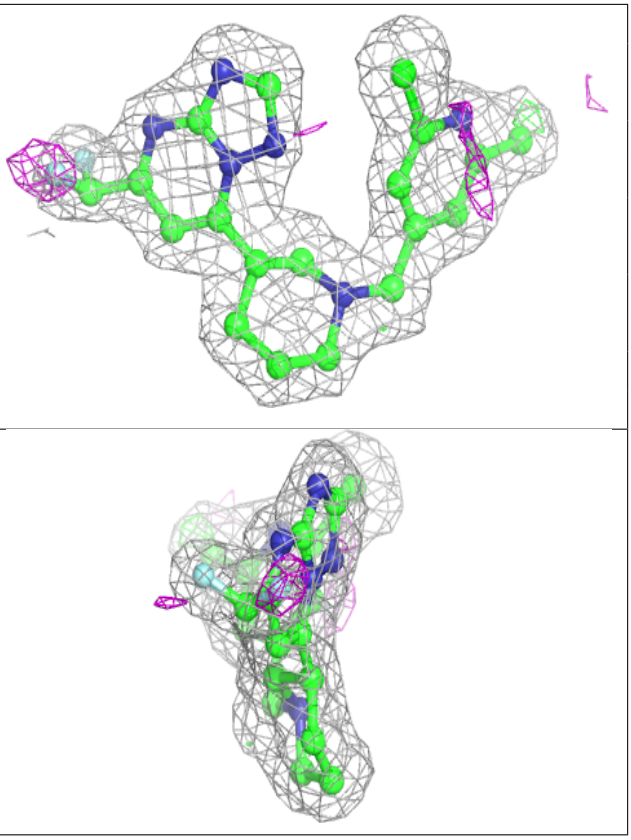
Electron density around QOQ A 1003:

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



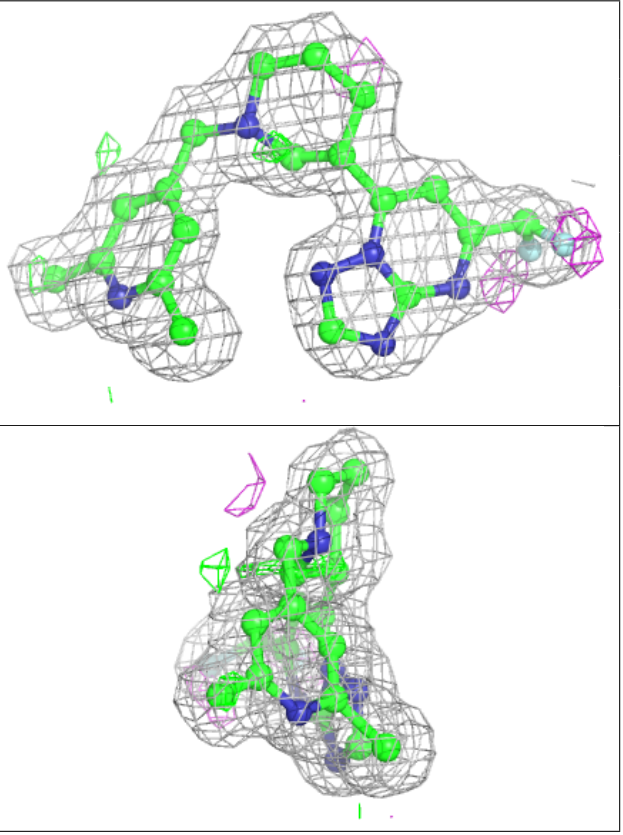
Electron density around QOQ D 1003:

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



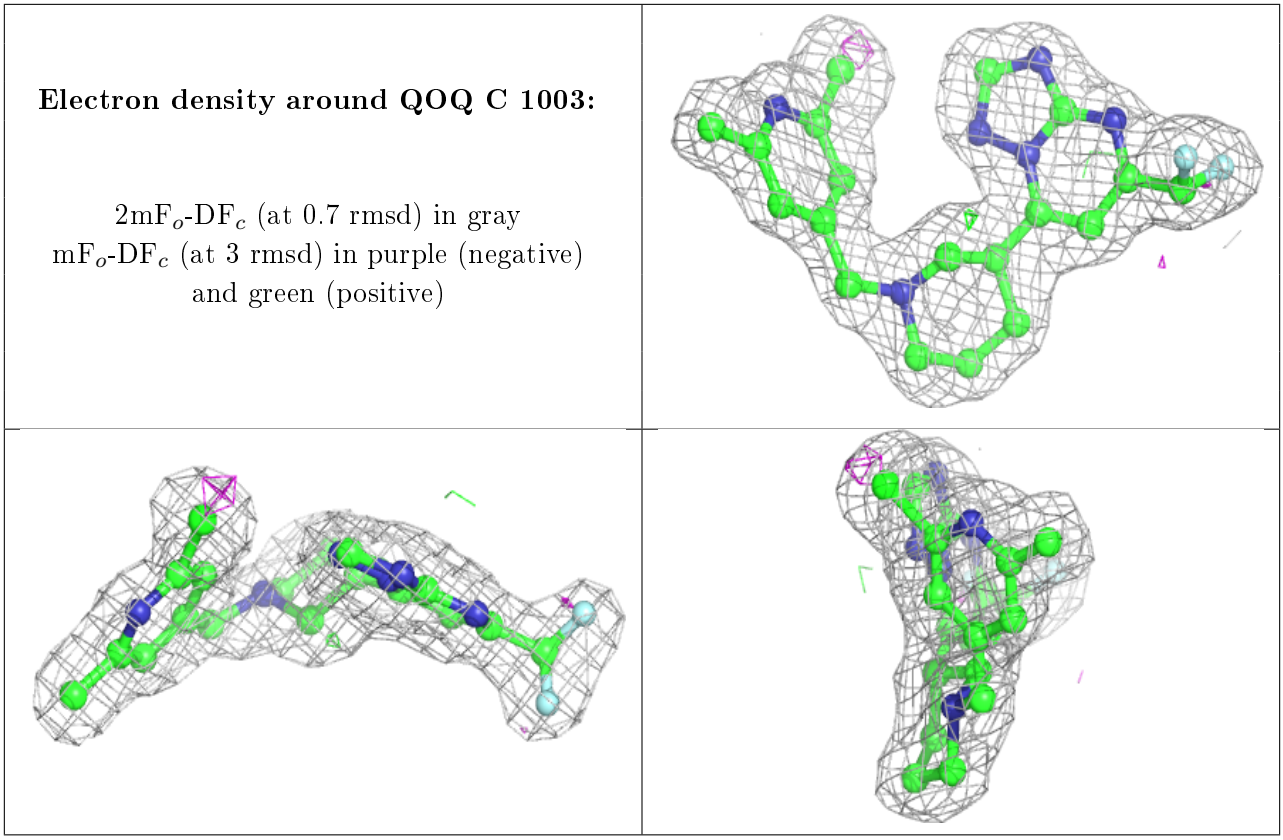
Electron density around QOQ B 1003:

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



Electron density around QOQ C 1003:

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



6.5 Other polymers

There are no such residues in this entry.