Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 01:33 AM EDT

PDB ID	:	7T5K
Title	:	E. coli dihydroorotate dehydrogenase bound to the inhibitor HQNO
Authors	:	Horwitz, S.M.; Ambarian, J.A.; Davis, K.M.
Deposited on	:	2021-12-12
Resolution	:	2.25 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

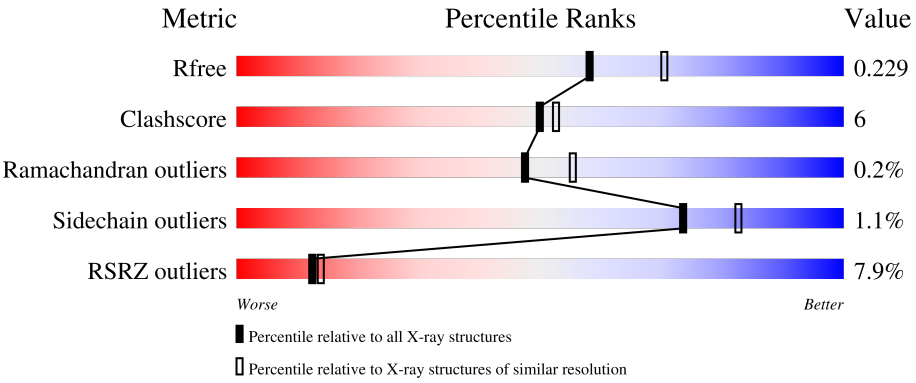
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	368	5% 80% 11% 9%
1	B	368	9% 78% 12% • 9%

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
4	ORO	A	403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5324 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 Dihydroorotate dehydrogenase (quinone).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2536	1608	444	474	10			
1	B	335	Total	C	N	O	S	0	1	0
			2534	1601	452	471	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	HIS	-	expression tag	UNP P0A7E1
A	-30	HIS	-	expression tag	UNP P0A7E1
A	-29	HIS	-	expression tag	UNP P0A7E1
A	-28	HIS	-	expression tag	UNP P0A7E1
A	-27	HIS	-	expression tag	UNP P0A7E1
A	-26	HIS	-	expression tag	UNP P0A7E1
A	-25	SER	-	expression tag	UNP P0A7E1
A	-24	SER	-	expression tag	UNP P0A7E1
A	-23	GLY	-	expression tag	UNP P0A7E1
A	-22	LEU	-	expression tag	UNP P0A7E1
A	-21	VAL	-	expression tag	UNP P0A7E1
A	-20	PRO	-	expression tag	UNP P0A7E1
A	-19	ARG	-	expression tag	UNP P0A7E1
A	-18	GLY	-	expression tag	UNP P0A7E1
A	-17	SER	-	expression tag	UNP P0A7E1
A	-16	HIS	-	expression tag	UNP P0A7E1
A	-15	MET	-	expression tag	UNP P0A7E1
A	-14	ALA	-	expression tag	UNP P0A7E1
A	-13	SER	-	expression tag	UNP P0A7E1
A	-12	MET	-	expression tag	UNP P0A7E1
A	-11	THR	-	expression tag	UNP P0A7E1
A	-10	GLY	-	expression tag	UNP P0A7E1
A	-9	GLY	-	expression tag	UNP P0A7E1
A	-8	GLN	-	expression tag	UNP P0A7E1
A	-7	GLN	-	expression tag	UNP P0A7E1

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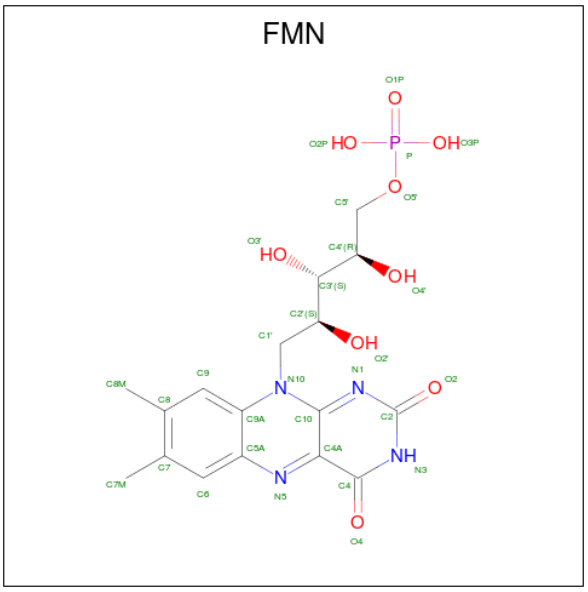
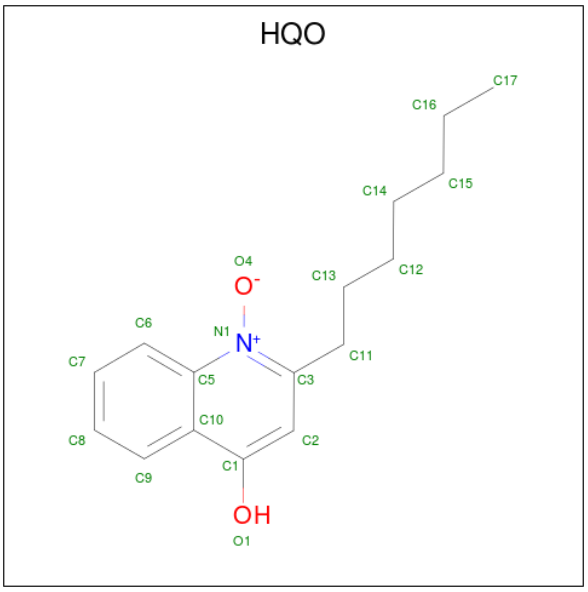
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P0A7E1
A	-5	GLY	-	expression tag	UNP P0A7E1
A	-4	ARG	-	expression tag	UNP P0A7E1
A	-3	GLY	-	expression tag	UNP P0A7E1
A	-2	SER	-	expression tag	UNP P0A7E1
A	-1	GLU	-	expression tag	UNP P0A7E1
A	0	PHE	-	expression tag	UNP P0A7E1
B	-31	HIS	-	expression tag	UNP P0A7E1
B	-30	HIS	-	expression tag	UNP P0A7E1
B	-29	HIS	-	expression tag	UNP P0A7E1
B	-28	HIS	-	expression tag	UNP P0A7E1
B	-27	HIS	-	expression tag	UNP P0A7E1
B	-26	HIS	-	expression tag	UNP P0A7E1
B	-25	SER	-	expression tag	UNP P0A7E1
B	-24	SER	-	expression tag	UNP P0A7E1
B	-23	GLY	-	expression tag	UNP P0A7E1
B	-22	LEU	-	expression tag	UNP P0A7E1
B	-21	VAL	-	expression tag	UNP P0A7E1
B	-20	PRO	-	expression tag	UNP P0A7E1
B	-19	ARG	-	expression tag	UNP P0A7E1
B	-18	GLY	-	expression tag	UNP P0A7E1
B	-17	SER	-	expression tag	UNP P0A7E1
B	-16	HIS	-	expression tag	UNP P0A7E1
B	-15	MET	-	expression tag	UNP P0A7E1
B	-14	ALA	-	expression tag	UNP P0A7E1
B	-13	SER	-	expression tag	UNP P0A7E1
B	-12	MET	-	expression tag	UNP P0A7E1
B	-11	THR	-	expression tag	UNP P0A7E1
B	-10	GLY	-	expression tag	UNP P0A7E1
B	-9	GLY	-	expression tag	UNP P0A7E1
B	-8	GLN	-	expression tag	UNP P0A7E1
B	-7	GLN	-	expression tag	UNP P0A7E1
B	-6	MET	-	expression tag	UNP P0A7E1
B	-5	GLY	-	expression tag	UNP P0A7E1
B	-4	ARG	-	expression tag	UNP P0A7E1
B	-3	GLY	-	expression tag	UNP P0A7E1
B	-2	SER	-	expression tag	UNP P0A7E1
B	-1	GLU	-	expression tag	UNP P0A7E1
B	0	PHE	-	expression tag	UNP P0A7E1

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			30	17	4	8	1		

- Molecule 3 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: $C_{16}H_{21}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	16	1	2		

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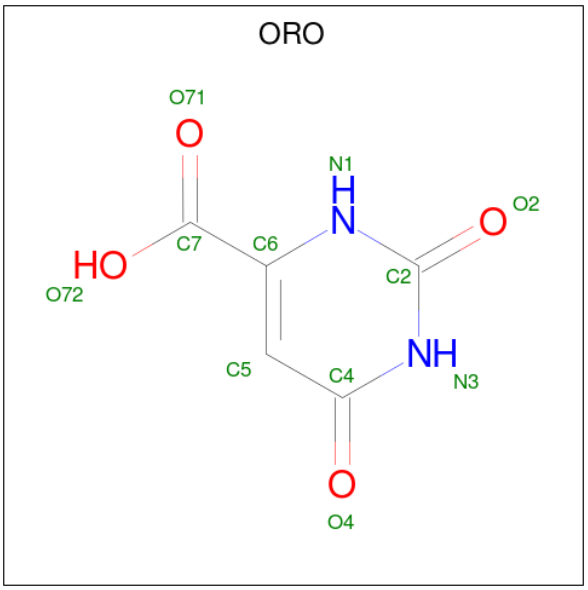
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 19 16 1 2	0	0

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 11 5 2 4	0	0
4	B	1	Total C N O 11 5 2 4	0	0

- Molecule 5 is water.

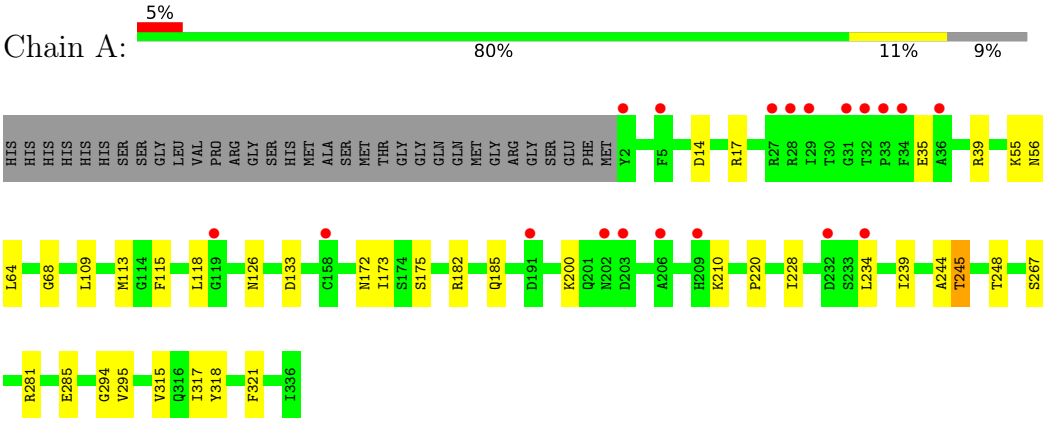
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	71	Total O 71 71	0	0
5	B	62	Total O 62 62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

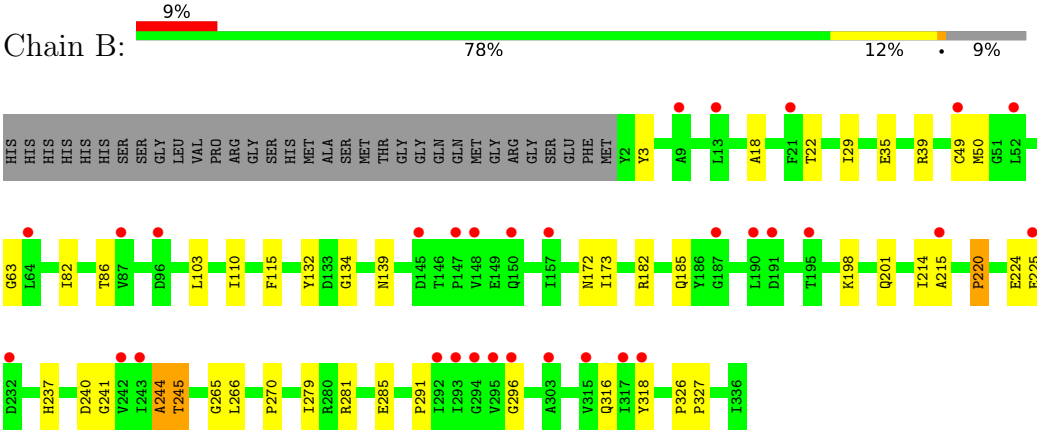
• Molecule 1: Dihydroorotate dehydrogenase (quinone)

Chain A:



• Molecule 1: Dihydroorotate dehydrogenase (quinone)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.05Å 169.33Å 129.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.25 49.61 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.30-2.25) 99.6 (49.61-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.217 , 0.232 0.214 , 0.229	Depositor DCC
R_{free} test set	2001 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5324	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: FMN, HQO, ORO

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	0/2579	0.68	0/3493
1	B	0.51	0/2575	0.69	0/3486
All	All	0.52	0/5154	0.68	0/6979

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ALA	Peptide
1	B	244	ALA	Peptide

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	2536	0	2566	29	0
1	B	2534	0	2551	31	0
2	A	31	0	19	1	0
2	B	30	0	17	1	0
3	A	19	0	21	0	0
3	B	19	0	21	0	0
4	A	11	0	3	6	0
4	B	11	0	3	3	0
5	A	71	0	0	0	0
5	B	62	0	0	0	0
All	All	5324	0	5201	60	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 6.

All (60) 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:B:3:TYR:CG	1:B:3:TYR:CE1	2.41	1.03
1:B:115:PHE:CE1	4:B:503:ORO:H5	2.06	0.89
1:B:115:PHE:HE1	4:B:503:ORO:H5	1.35	0.88
1:A:115:PHE:CE1	4:A:403:ORO:H5	2.12	0.84
1:A:172:ASN:ND2	4:A:403:ORO:O4	2.19	0.73
1:A:115:PHE:HE1	4:A:403:ORO:H5	1.53	0.72
1:B:220:PRO:HB3	1:B:245:THR:HG21	1.71	0.72
1:A:220:PRO:HB3	1:A:245:THR:HG21	1.74	0.69
1:A:175:SER:HB2	4:A:403:ORO:C4	2.26	0.65
1:B:173:ILE:HD12	1:B:185:GLN:HB3	1.80	0.64
1:B:220:PRO:HB3	1:B:245:THR:CG2	2.27	0.64
1:A:55:LYS:NZ	1:A:133:ASP:OD2	2.29	0.61
1:A:182:ARG:O	1:A:185:GLN:HG2	2.00	0.60
1:A:245:THR:H	1:A:295:VAL:HG13	1.70	0.56
1:A:317:ILE:HD12	1:A:321:PHE:HB2	1.87	0.56
1:B:281[A]:ARG:NH1	1:B:285:GLU:OE1	2.37	0.54
1:B:266:LEU:HD21	1:B:270:PRO:HB2	1.91	0.52
1:B:139:ASN:OD1	1:B:172:ASN:HB2	2.10	0.52
1:A:35:GLU:HB3	1:A:39:ARG:HH21	1.74	0.52
1:B:201:GLN:HB2	1:B:214:ILE:CD1	2.41	0.51
1:B:29:ILE:HD12	1:B:35:GLU:HA	1.93	0.50
1:A:63:GLY:HA3	2:A:401:FMN:N5	2.26	0.50
1:B:201:GLN:HB2	1:B:214:ILE:HD11	1.94	0.50
1:B:244:ALA:O	1:B:279:ILE:HD11	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ALA:HA	1:B:241:GLY:O	2.12	0.49
1:B:18:ALA:O	1:B:22:THR:HG23	2.13	0.49
1:B:63:GLY:HA3	2:B:502:FMN:N5	2.27	0.49
1:B:225:GLU:H	1:B:225:GLU:CD	2.16	0.49
1:B:132:TYR:CZ	1:B:134:GLY:HA3	2.48	0.49
1:B:172:ASN:ND2	4:B:503:ORO:O4	2.37	0.48
1:B:59:GLY:O	1:B:316:GLN:HA	2.14	0.47
1:B:224:GLU:O	1:B:228:ILE:HG13	2.14	0.47
1:B:35:GLU:HG3	1:B:39:ARG:HH21	1.79	0.46
1:B:182:ARG:O	1:B:185:GLN:HG2	2.15	0.46
1:B:240:ASP:O	1:B:291:PRO:HD2	2.15	0.46
1:B:110:ILE:HA	1:B:265:GLY:O	2.16	0.45
1:A:68:GLY:O	1:A:126:ASN:HB3	2.17	0.45
1:B:60:LEU:HD23	1:B:82:ILE:HG23	1.98	0.45
1:A:228:ILE:HA	1:A:285:GLU:HG2	1.99	0.43
1:A:173:ILE:HD12	1:A:185:GLN:HB3	2.00	0.43
1:B:103:LEU:HD11	1:B:110:ILE:HD12	2.01	0.43
1:A:234:LEU:HD23	1:A:239:ILE:HG13	2.00	0.42
1:A:56:ASN:HB2	1:A:57:PRO:CD	2.50	0.42
1:A:248:THR:HB	1:A:271:LEU:HD13	2.01	0.42
1:B:198:LYS:HG3	1:B:237:HIS:O	2.20	0.42
1:A:220:PRO:HA	1:A:278:ILE:HG13	2.02	0.42
1:B:49:CYS:O	1:B:50:MET:HB2	2.20	0.42
1:B:326:PRO:N	1:B:327:PRO:CD	2.82	0.42
1:A:14:ASP:OD1	1:A:17:ARG:HB2	2.20	0.42
1:A:113:MET:HB2	4:A:403:ORO:C7	2.50	0.42
1:B:281[A]:ARG:HA	1:B:281[A]:ARG:HD2	1.89	0.42
1:A:109:LEU:HB2	1:A:267:SER:OG	2.19	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.88	0.41
1:A:294:GLY:O	1:A:315:VAL:HA	2.20	0.41
1:A:210:LYS:HB2	1:A:210:LYS:HE3	1.74	0.41
1:A:115:PHE:CD1	4:A:403:ORO:H5	2.55	0.41
1:A:64:LEU:HA	1:A:64:LEU:HD12	1.87	0.40
1:A:281:ARG:HA	1:A:281:ARG:HD2	1.82	0.40
1:A:200:LYS:HA	1:A:200:LYS:HD3	1.60	0.40
1:A:58:LEU:HD11	1:A:317:ILE:HG12	2.03	0.40

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	333/368 (90%)	327 (98%)	6 (2%)	0	100 100
1	B	334/368 (91%)	324 (97%)	9 (3%)	1 (0%)	41 46
All	All	667/736 (91%)	651 (98%)	15 (2%)	1 (0%)	47 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	GLY

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	267/304 (88%)	265 (99%)	2 (1%)	84 90
1	B	262/304 (86%)	258 (98%)	4 (2%)	65 75
All	All	529/608 (87%)	523 (99%)	6 (1%)	73 82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	THR
1	A	318	TYR
1	B	86	THR
1	B	220	PRO
1	B	245	THR

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Mol	Chain	Res	Type
1	B	318	TYR

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

Mol	Chain	Res	Type
1	B	12	GLN
1	B	24	GLN

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)

6 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	$\#\|Z\| > 2$
2	FMN	A	401	-	33,33,33	1.11	2 (6%)	48,50,50	1.40	9 (18%)
4	ORO	A	403	-	9,11,11	1.46	2 (22%)	8,15,15	3.42	3 (37%)
4	ORO	B	503	-	9,11,11	1.45	2 (22%)	8,15,15	3.39	3 (37%)
3	HQO	B	501	-	20,20,20	1.29	3 (15%)	18,26,26	1.90	5 (27%)
2	FMN	B	502	-	32,32,33	1.17	2 (6%)	47,48,50	1.42	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HQO	A	402	-	20,20,20	1.37	3 (15%)	18,26,26	1.95	2 (11%)

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	FMN	A	401	-	-	6/18/18/18	0/3/3/3
4	ORO	A	403	-	-	4/4/4/4	0/1/1/1
4	ORO	B	503	-	-	4/4/4/4	0/1/1/1
3	HQO	B	501	-	-	2/7/7/7	0/2/2/2
2	FMN	B	502	-	-	4/15/15/18	0/3/3/3
3	HQO	A	402	-	-	3/7/7/7	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HQO	O4-N1	3.88	1.43	1.38
2	B	502	FMN	C4A-N5	3.70	1.37	1.30
2	A	401	FMN	C4A-N5	3.64	1.37	1.30
3	B	501	HQO	C10-C5	-3.33	1.37	1.42
2	B	502	FMN	C10-N1	3.01	1.39	1.33
4	A	403	ORO	O72-C7	-2.88	1.21	1.30
3	A	402	HQO	C10-C5	-2.87	1.38	1.42
4	B	503	ORO	O72-C7	-2.85	1.21	1.30
3	B	501	HQO	O4-N1	2.72	1.41	1.38
4	B	503	ORO	C4-N3	2.70	1.37	1.33
4	A	403	ORO	C4-N3	2.69	1.37	1.33
2	A	401	FMN	C10-N1	2.51	1.38	1.33
3	A	402	HQO	C1-C10	-2.09	1.38	1.42
3	B	501	HQO	C1-C10	-2.09	1.38	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	403	ORO	C5-C4-N3	-7.83	114.94	124.08
4	B	503	ORO	C5-C4-N3	-7.79	114.98	124.08
3	A	402	HQO	O1-C1-C10	6.63	124.59	116.31
4	A	403	ORO	C6-C5-C4	4.51	119.64	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	HQO	O1-C1-C10	4.49	121.92	116.31
3	B	501	HQO	C13-C11-C3	-4.37	102.31	113.82
4	B	503	ORO	C6-C5-C4	4.32	119.52	116.73
2	A	401	FMN	C5A-C9A-N10	3.60	121.67	117.95
2	B	502	FMN	C1'-N10-C10	3.20	122.04	118.14
2	A	401	FMN	C4-N3-C2	-3.08	119.95	125.64
2	B	502	FMN	C4-N3-C2	-2.97	120.15	125.64
2	A	401	FMN	C4A-C10-N10	2.82	120.61	116.48
2	B	502	FMN	C4A-C10-N1	-2.81	118.21	124.73
2	B	502	FMN	C4A-C4-N3	2.72	120.09	113.19
3	A	402	HQO	C11-C3-C2	-2.72	116.08	120.74
2	B	502	FMN	C4A-C10-N10	2.72	120.45	116.48
2	A	401	FMN	C4A-C4-N3	2.63	119.87	113.19
2	B	502	FMN	C10-N1-C2	2.39	121.67	116.90
2	A	401	FMN	C9A-C5A-N5	-2.35	119.88	122.43
2	B	502	FMN	O3'-C3'-C4'	2.32	114.48	109.72
2	B	502	FMN	C10-C4A-N5	-2.29	120.00	124.86
2	A	401	FMN	O4-C4-C4A	-2.28	120.54	126.60
2	A	401	FMN	C4A-C10-N1	-2.28	119.44	124.73
3	B	501	HQO	C11-C3-C2	-2.18	117.01	120.74
3	B	501	HQO	C14-C12-C13	-2.18	103.37	114.42
4	B	503	ORO	O71-C7-C6	-2.16	116.86	121.24
2	A	401	FMN	O2'-C2'-C3'	2.15	114.34	109.10
4	A	403	ORO	O71-C7-C6	-2.15	116.88	121.24
3	B	501	HQO	C2-C3-N1	2.05	121.19	118.94
2	A	401	FMN	C9-C9A-N10	-2.01	119.12	121.84

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FMN	C5'-O5'-P-O1P
2	B	502	FMN	C2'-C3'-C4'-O4'
2	B	502	FMN	O3'-C3'-C4'-O4'
3	B	501	HQO	C3-C11-C13-C12
4	A	403	ORO	N1-C6-C7-O71
4	A	403	ORO	N1-C6-C7-O72
4	A	403	ORO	C5-C6-C7-O71
4	A	403	ORO	C5-C6-C7-O72
4	B	503	ORO	N1-C6-C7-O71
4	B	503	ORO	N1-C6-C7-O72
4	B	503	ORO	C5-C6-C7-O71

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Mol	Chain	Res	Type	Atoms
4	B	503	ORO	C5-C6-C7-O72
3	A	402	HQO	C3-C11-C13-C12
2	A	401	FMN	O3'-C3'-C4'-C5'
2	A	401	FMN	C2'-C3'-C4'-C5'
2	A	401	FMN	C2'-C3'-C4'-O4'
3	A	402	HQO	C13-C12-C14-C15
3	B	501	HQO	C12-C14-C15-C16
2	A	401	FMN	O3'-C3'-C4'-O4'
3	A	402	HQO	C14-C15-C16-C17
2	A	401	FMN	C4'-C5'-O5'-P
2	B	502	FMN	C4'-C5'-O5'-P
2	B	502	FMN	O3'-C3'-C4'-C5'

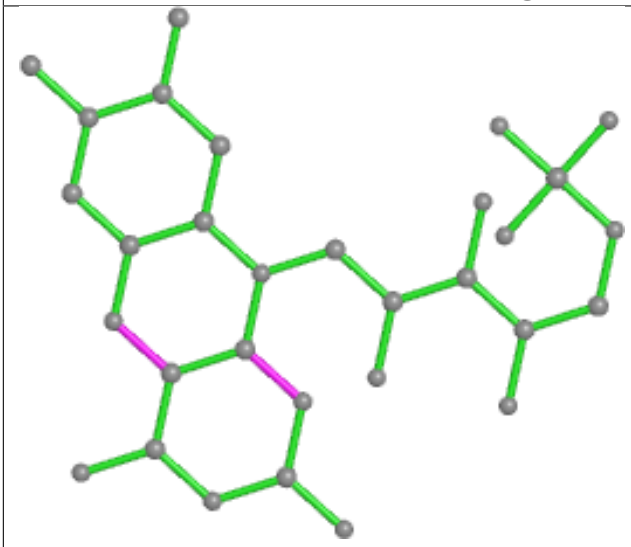
There are no ring outliers.

4 monomers are involved in 11 short contacts:

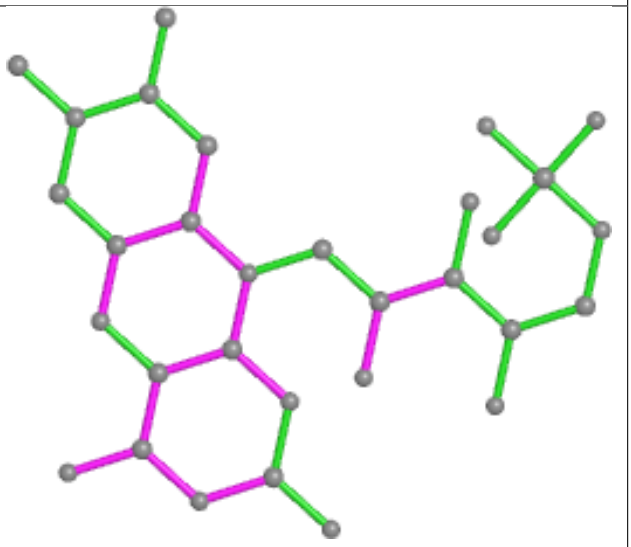
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FMN	1	0
4	A	403	ORO	6	0
4	B	503	ORO	3	0
2	B	502	FMN	1	0

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 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.

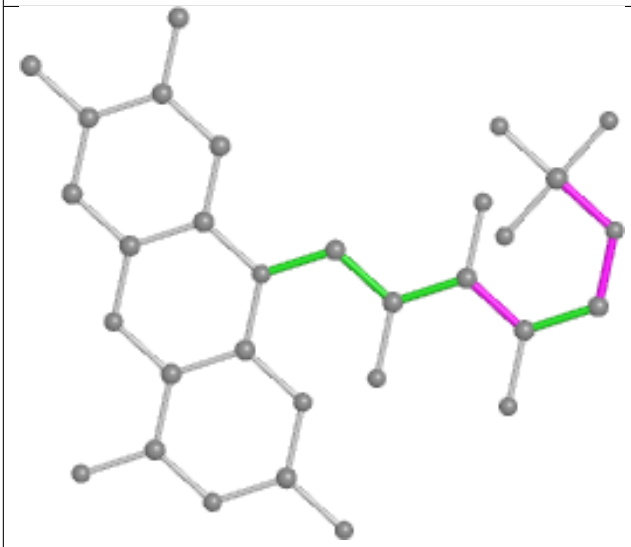
Ligand FMN A 401



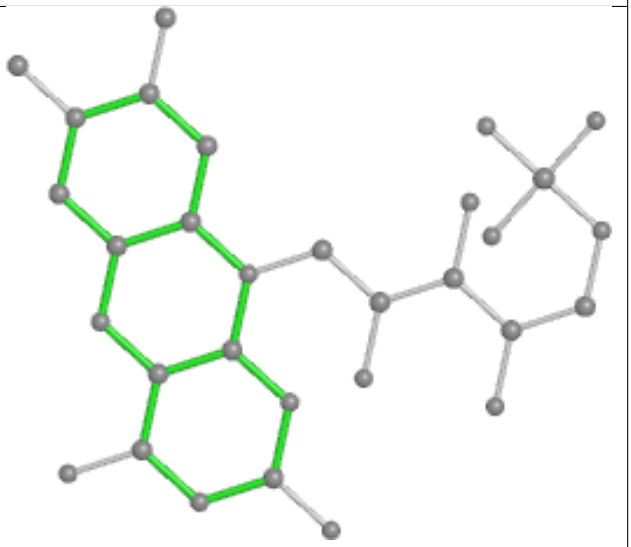
Bond lengths



Bond angles

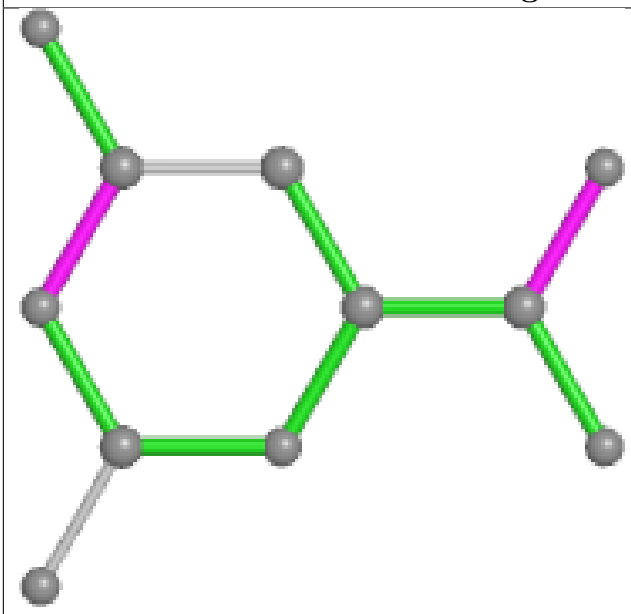


Torsions

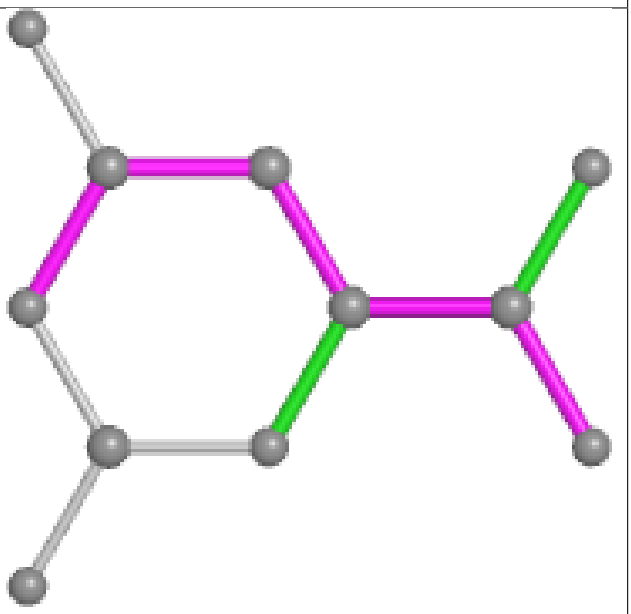


Rings

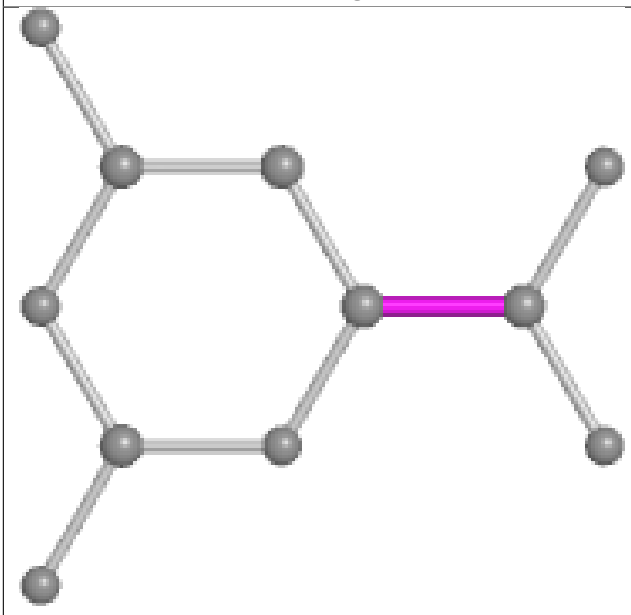
Ligand ORO A 403



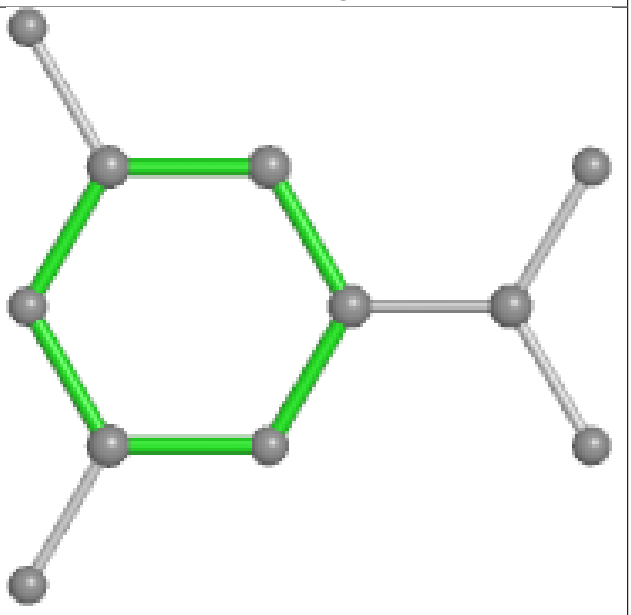
Bond lengths



Bond angles

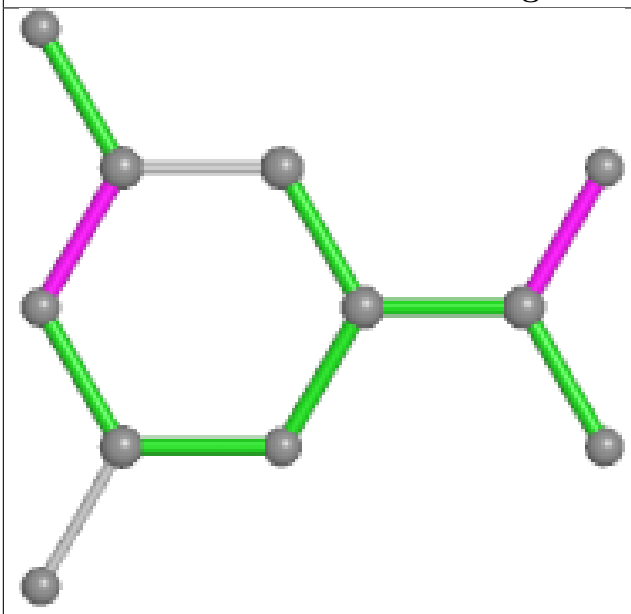


Torsions

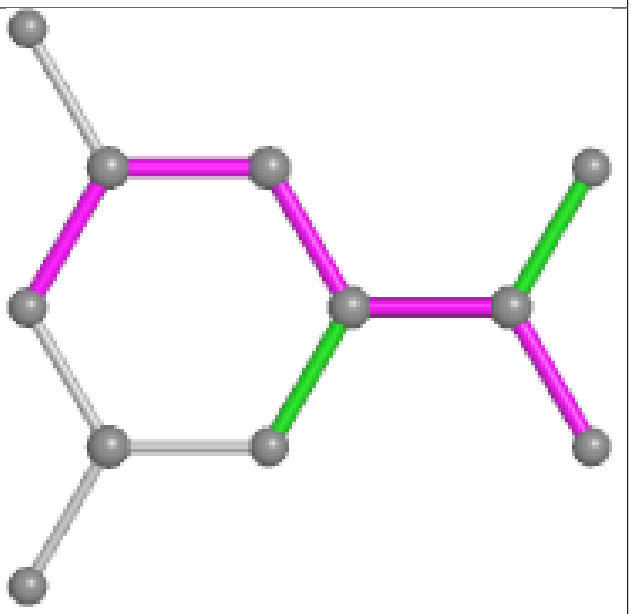


Rings

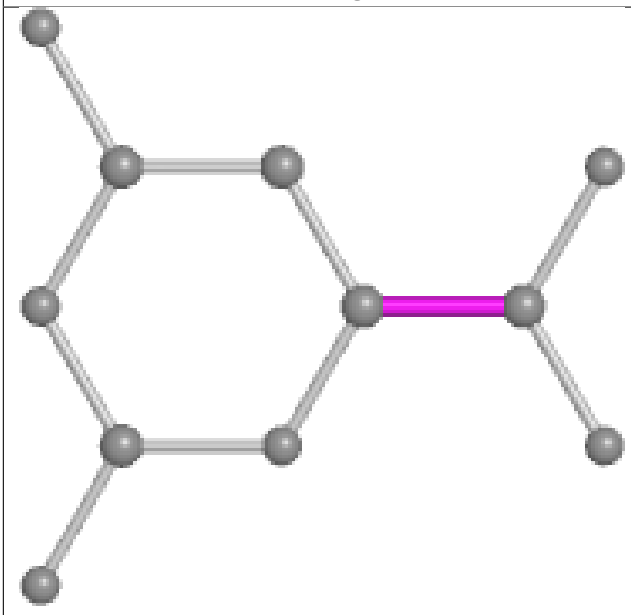
Ligand ORO B 503



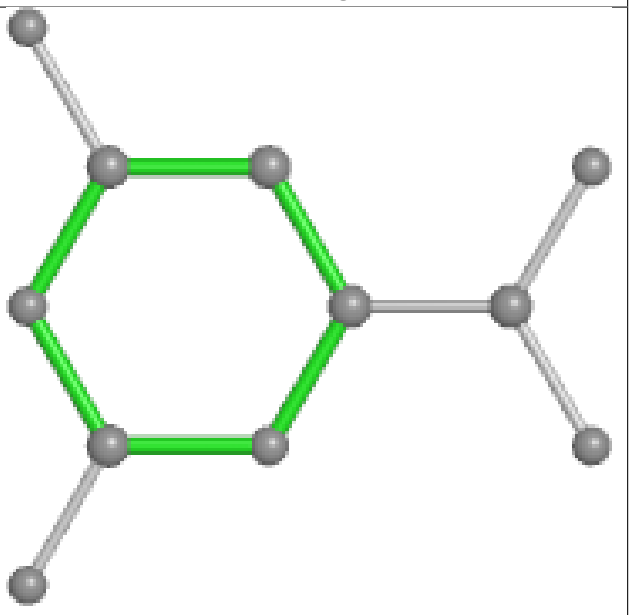
Bond lengths



Bond angles

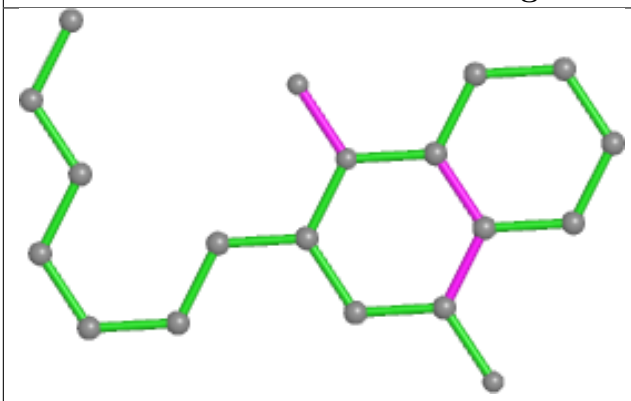


Torsions

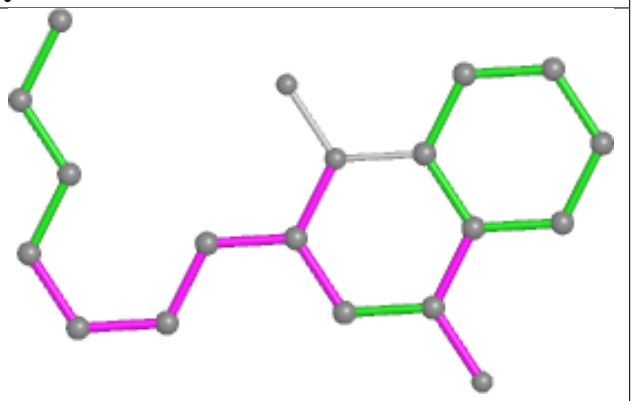


Rings

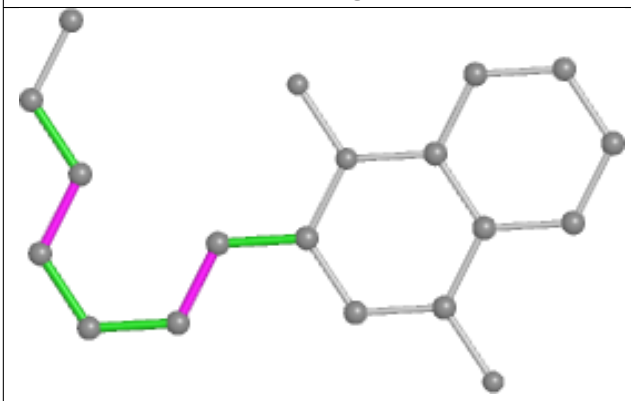
Ligand HQO B 501



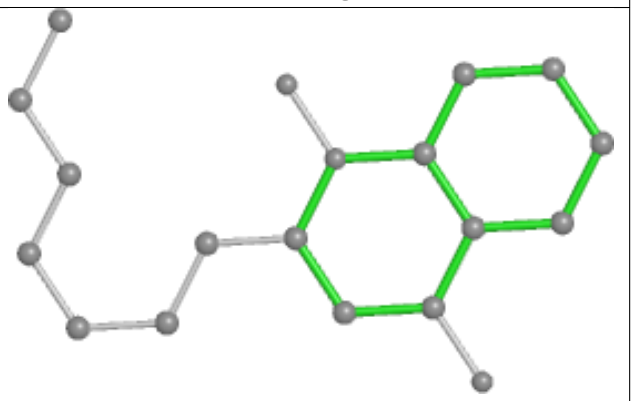
Bond lengths



Bond angles

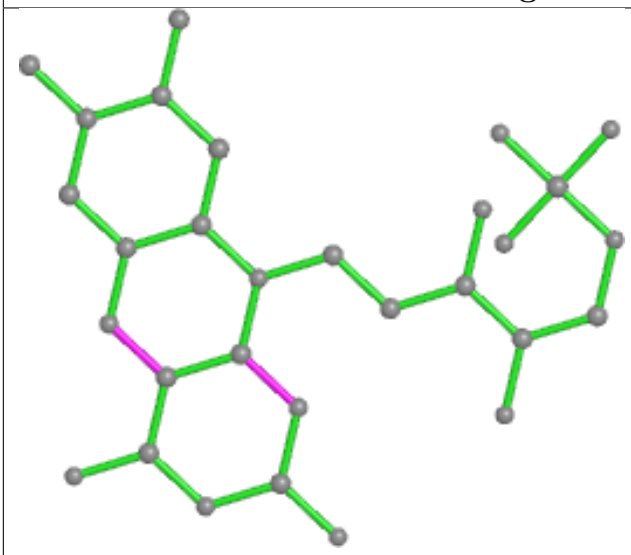


Torsions

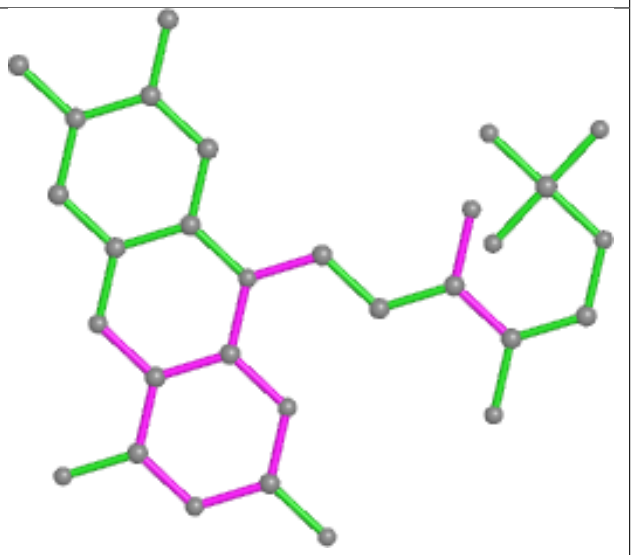


Rings

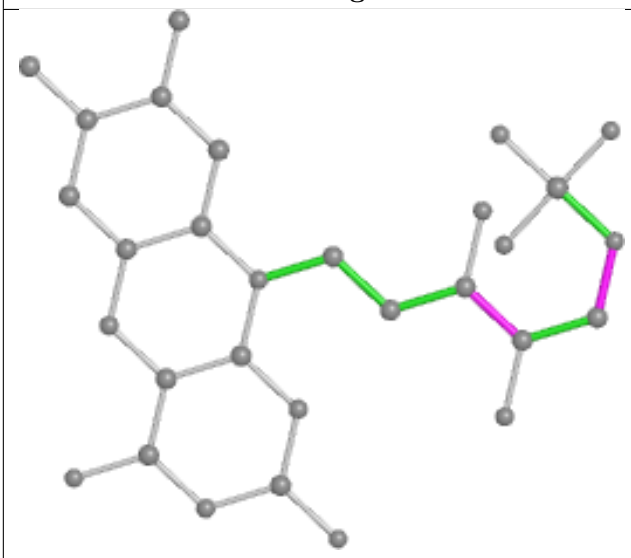
Ligand FMN B 502



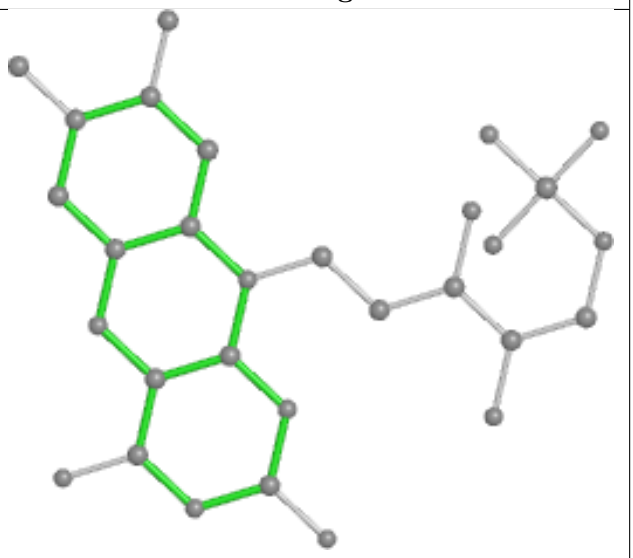
Bond lengths



Bond angles

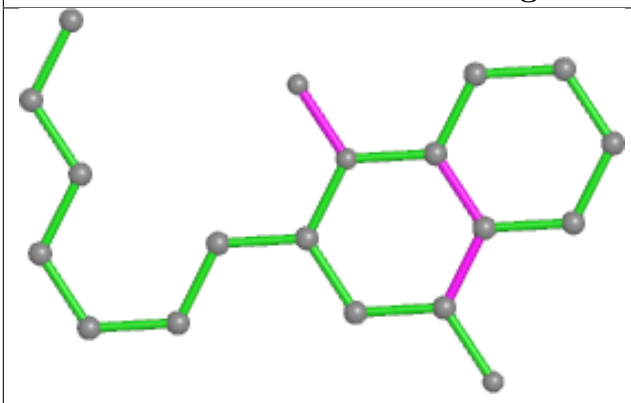


Torsions

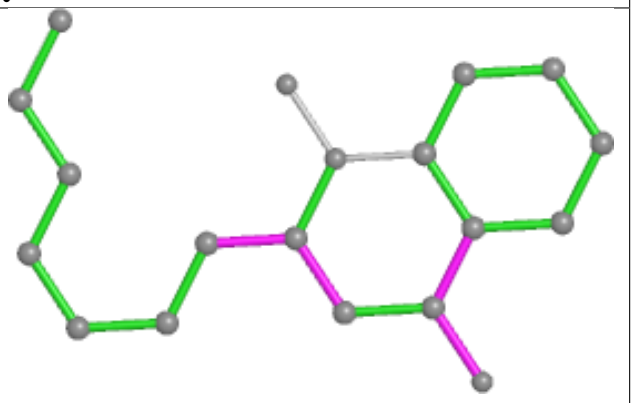


Rings

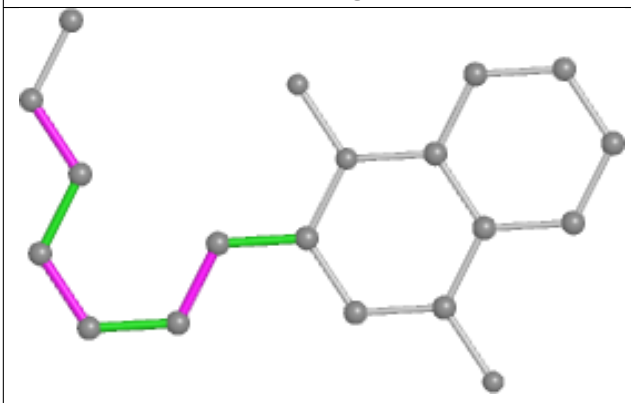
Ligand HQO A 402



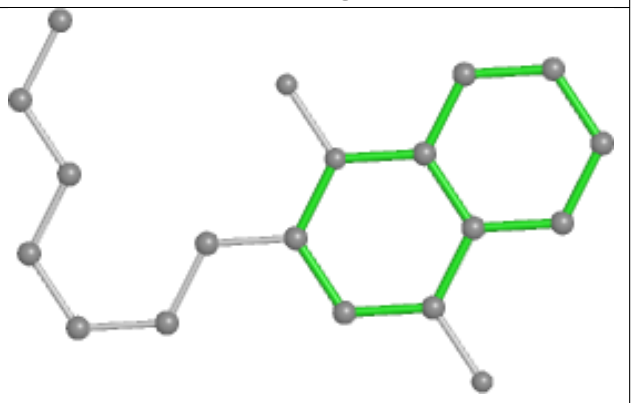
Bond lengths



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	335/368 (91%)	0.70	20 (5%) 21 23	40, 55, 77, 104	0
1	B	335/368 (91%)	0.95	33 (9%) 7 7	44, 61, 81, 92	0
All	All	670/736 (91%)	0.82	53 (7%) 12 14	40, 58, 80, 104	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	PRO	4.3
1	B	62	ALA	3.9
1	B	145	ASP	3.8
1	B	243	ILE	3.7
1	A	34	PHE	3.5
1	B	195	THR	3.5
1	A	232	ASP	3.4
1	B	13	LEU	3.2
1	B	187	GLY	3.2
1	B	293	ILE	3.2
1	B	295	VAL	3.1
1	A	5	PHE	3.1
1	A	191	ASP	3.1
1	B	148	VAL	3.0
1	B	191	ASP	3.0
1	A	29	ILE	3.0
1	B	9	ALA	2.9
1	A	36	ALA	2.8
1	A	203	ASP	2.7
1	A	209	HIS	2.7
1	B	315	VAL	2.7
1	B	147	PRO	2.6
1	B	232	ASP	2.6
1	B	52	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	215	ALA	2.5
1	A	31	GLY	2.5
1	A	27	ARG	2.5
1	B	96	ASP	2.5
1	B	157	ILE	2.5
1	A	234	LEU	2.5
1	B	21	PHE	2.4
1	A	2	TYR	2.4
1	B	294	GLY	2.4
1	B	190	LEU	2.3
1	A	119	GLY	2.3
1	B	292	ILE	2.3
1	B	229	GLN	2.3
1	B	150	GLN	2.3
1	B	296	GLY	2.3
1	A	28	ARG	2.3
1	B	225	GLU	2.2
1	A	202	ASN	2.2
1	B	242	VAL	2.2
1	A	32	THR	2.2
1	B	49	CYS	2.2
1	B	317	ILE	2.2
1	A	158	CYS	2.2
1	B	303	ALA	2.1
1	A	271	LEU	2.1
1	B	87	VAL	2.1
1	B	64	LEU	2.0
1	B	318	TYR	2.0
1	A	206	ALA	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

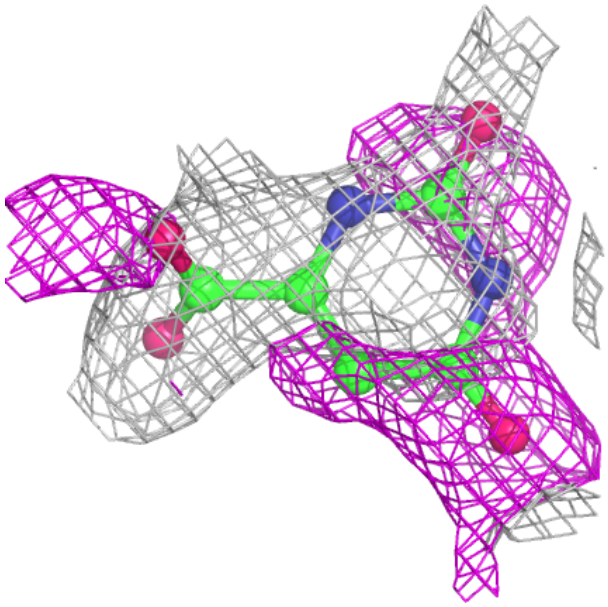
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

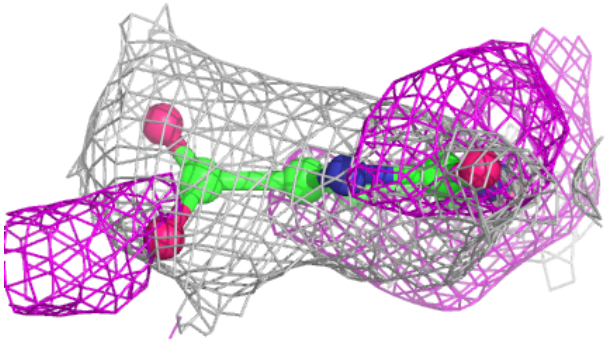
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ORO	A	403	11/11	0.80	0.36	59,70,75,80	0
3	HQO	A	402	19/19	0.81	0.22	49,60,72,76	0
4	ORO	B	503	11/11	0.81	0.26	74,79,86,86	0
3	HQO	B	501	19/19	0.88	0.17	55,65,81,82	0
2	FMN	B	502	30/31	0.91	0.20	44,57,63,64	0
2	FMN	A	401	31/31	0.93	0.15	40,48,54,57	0

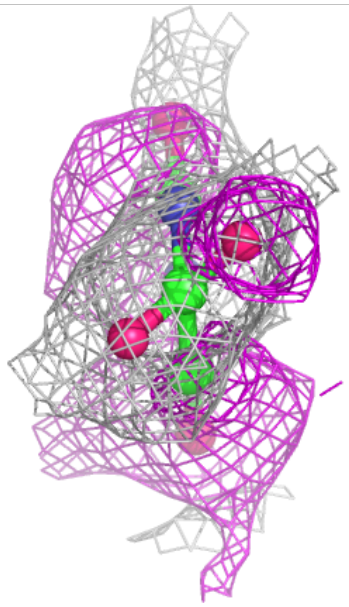
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ORO 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)

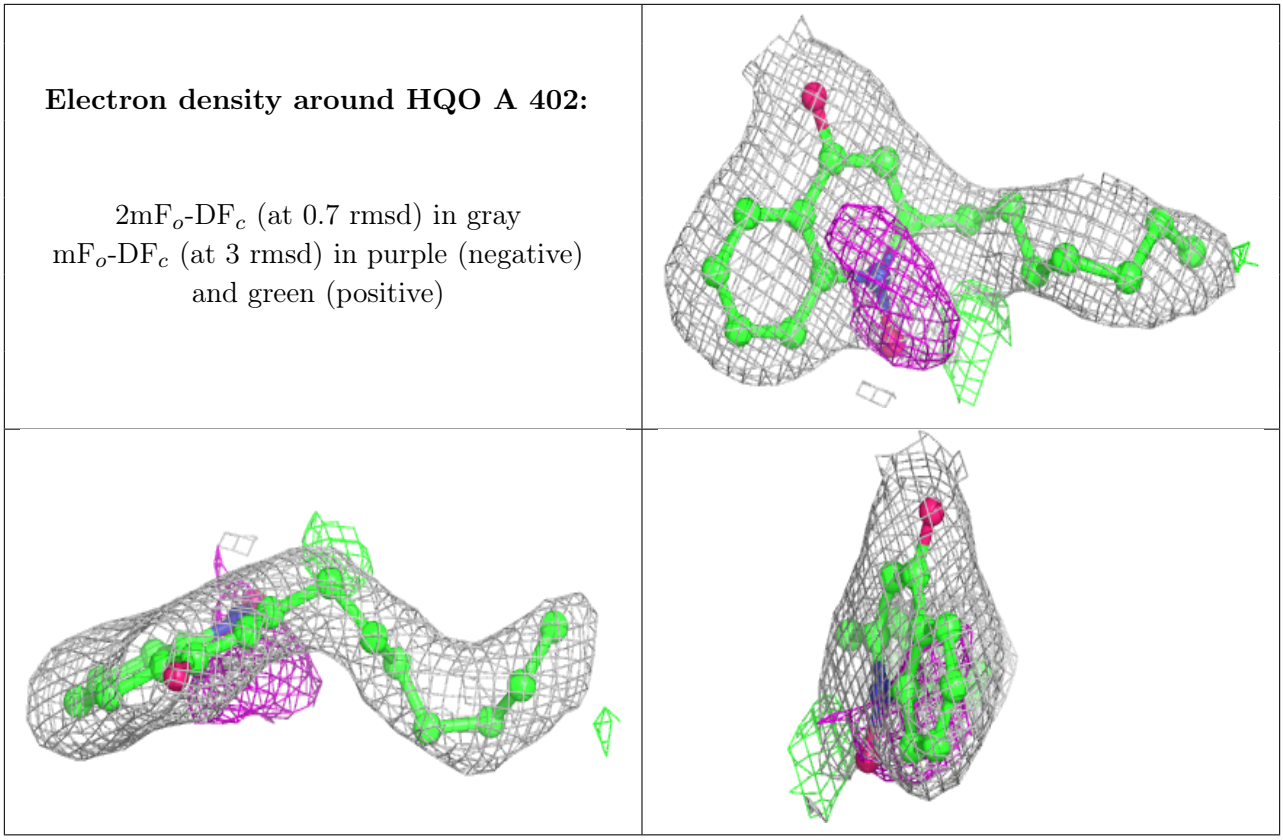






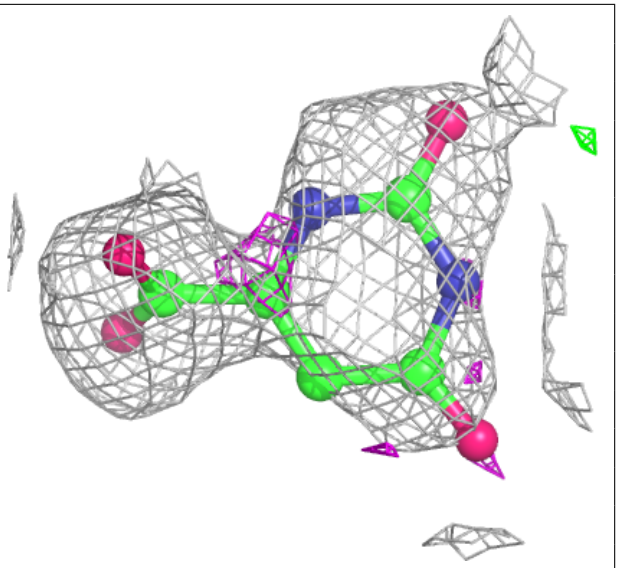
Electron density around HQO A 402:

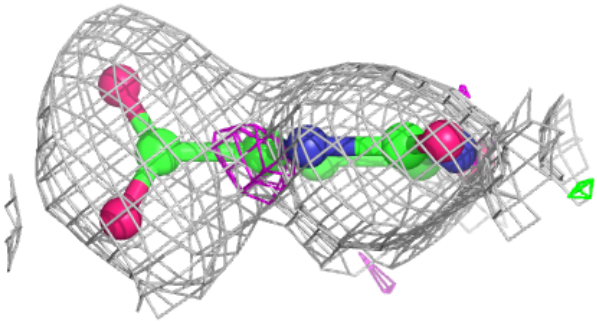
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

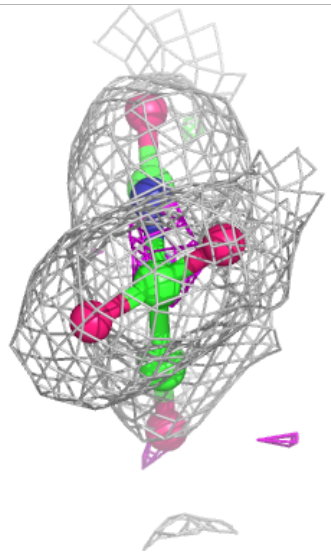


Electron density around ORO B 503:

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

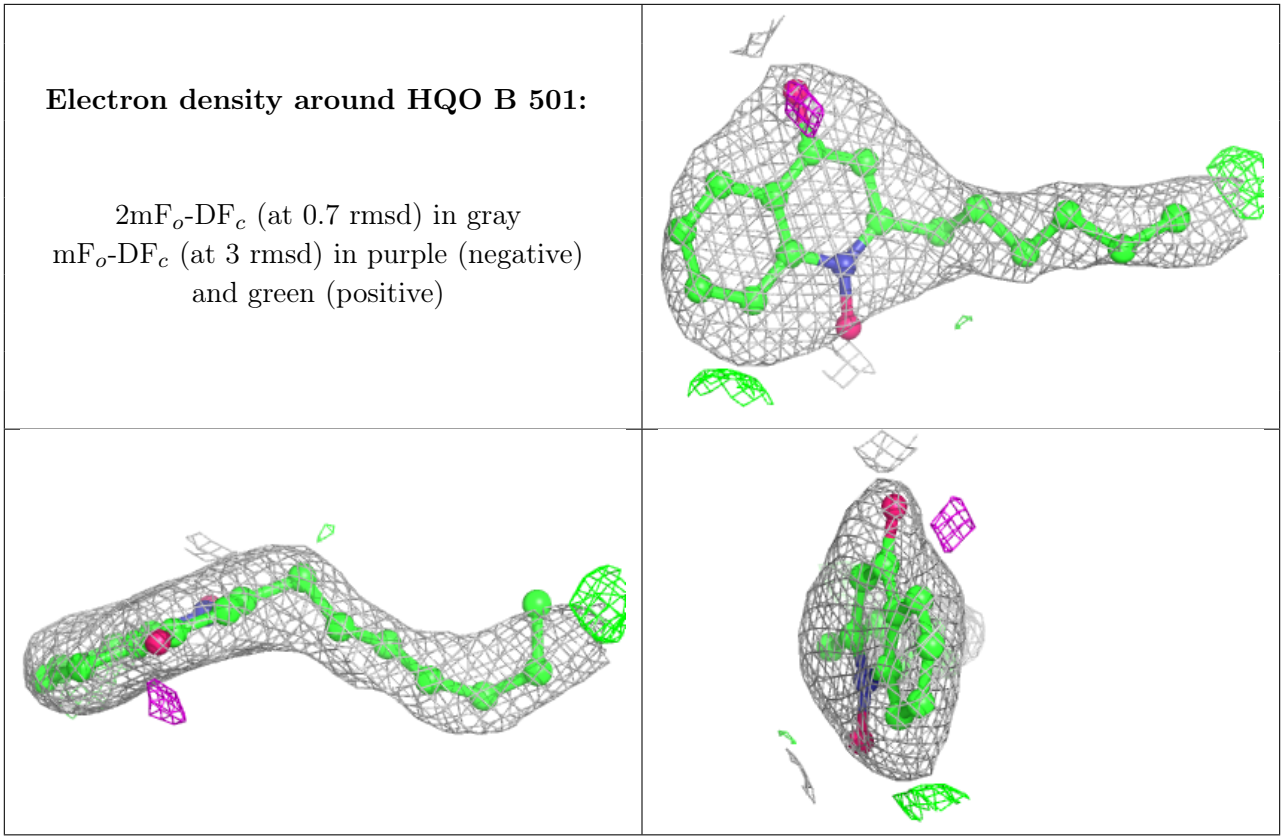






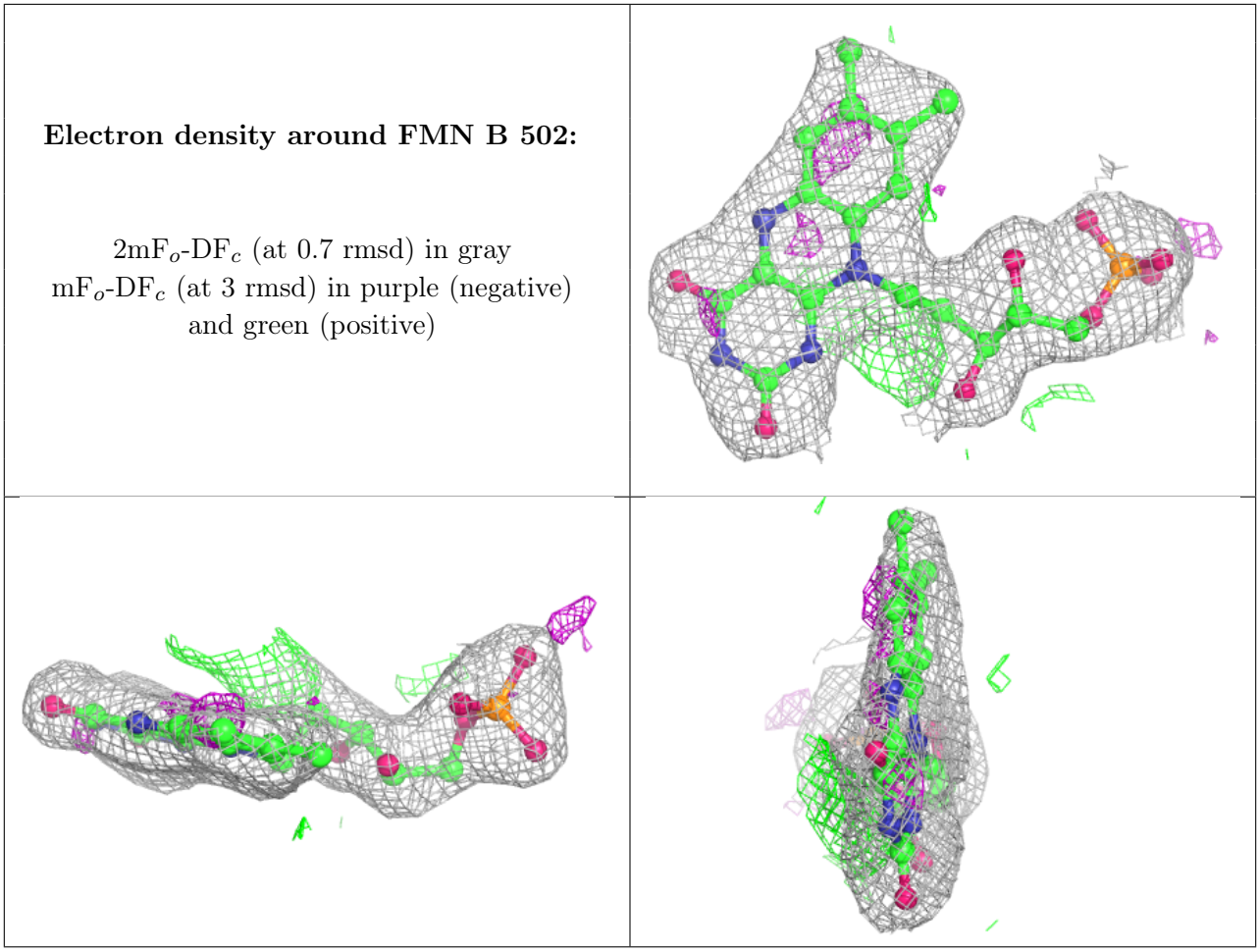
Electron density around HQO B 501:

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



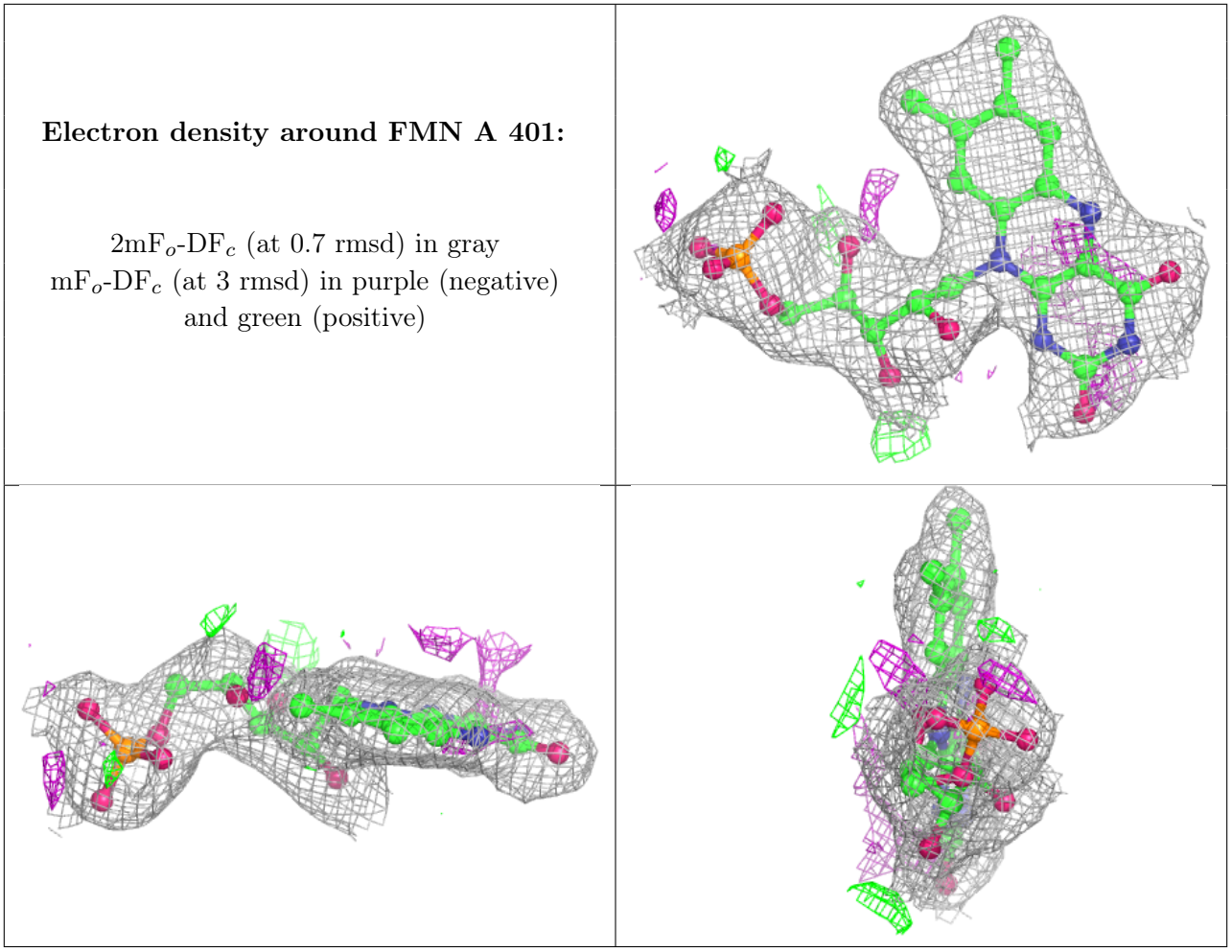
Electron density around FMN B 502:

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



Electron density around FMN A 401:

$2mF_o$-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.