Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 01:36 AM JST

PDB ID	:	7CE5
Title	:	Methanol-PQQ bound methanol dehydrogenase (MDH) from Methylococcus capsulatus (Bath)
Authors	:	Chuankhayan, P.; Chan, S.I.; Nareddy, P.K.R.; Tsai, I.K.; Tsai, Y.F.; Chen, K.H.-C.; Yu, S.S.-F.; Chen, C.J.
Deposited on	:	2020-06-22
Resolution	:	1.80 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 ⓘ 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:

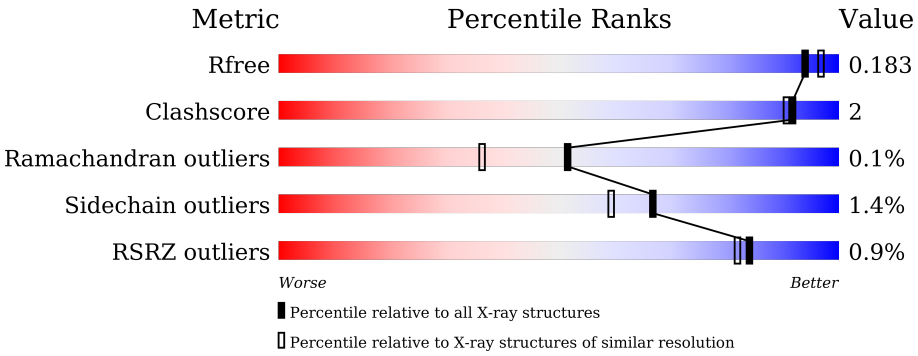
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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)
RSRZ outliers	127900	5850 (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 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	573	94% 6%
1	B	573	93% 6%
1	C	573	92% 7%
1	D	573	94% 5% •
1	G	573	94% 6%

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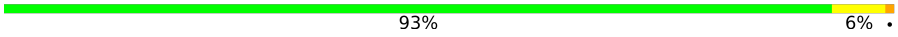
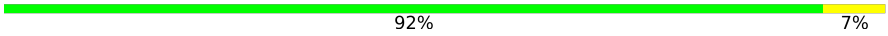
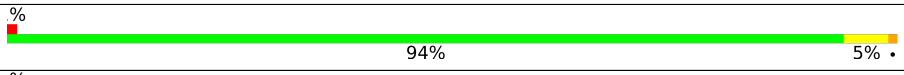
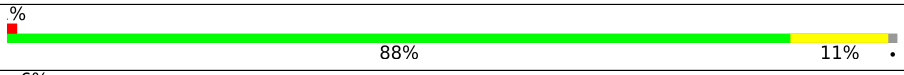
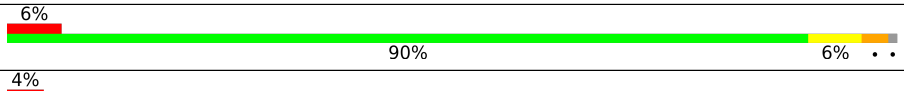
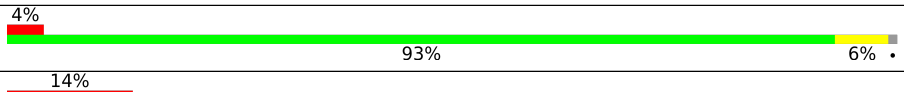
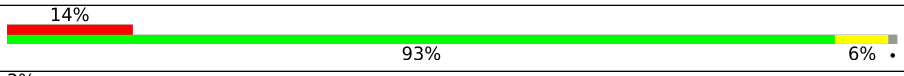
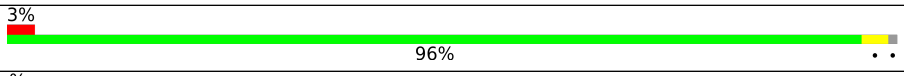
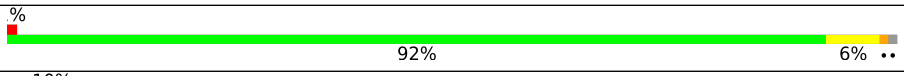
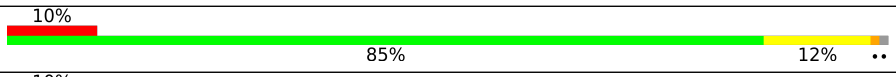
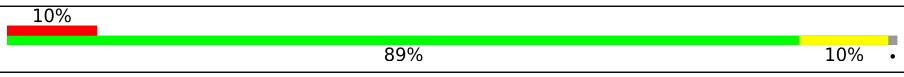
Mol	Chain	Length	Quality of chain
1	H	573	
1	M	573	
1	N	573	
2	E	72	
2	F	72	
2	I	72	
2	J	72	
2	K	72	
2	L	72	
2	O	72	
2	P	72	

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	MOH	A	702	-	-	X	X
4	MOH	B	702	-	-	X	X
4	MOH	C	703	-	-	-	X
4	MOH	D	702	-	-	X	-
4	MOH	G	702	-	-	X	X
4	MOH	H	702	-	-	X	X
4	MOH	N	702	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 46034 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 Methanol dehydrogenase protein, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	B	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			
1	C	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	D	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			
1	G	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	H	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			
1	M	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	N	573	Total	C	N	O	S	0	0	0
			4490	2871	765	831	23			

- Molecule 2 is a protein called Methanol dehydrogenase [cytochrome c] subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	F	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	I	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	J	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	K	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	L	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			

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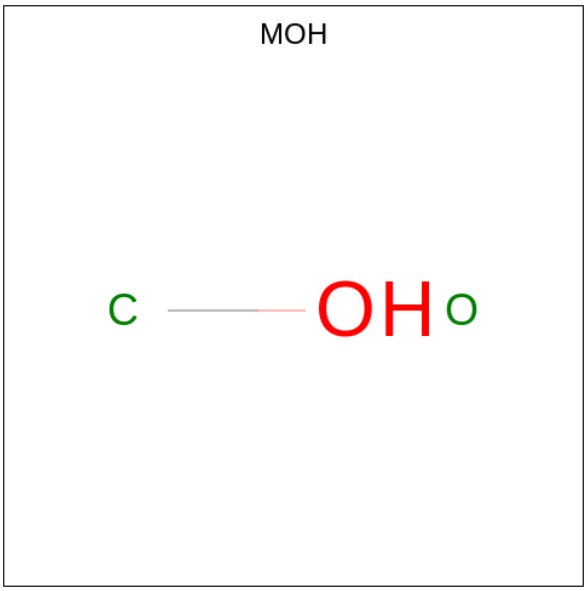
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	P	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

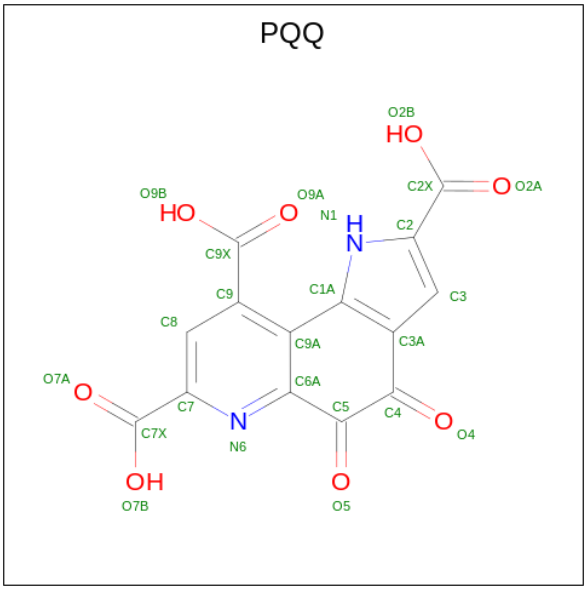
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	N	1	Total	Ca	0	0
			1	1		

- Molecule 4 is METHANOL (three-letter code: MOH) (formula: CH_4O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 2 1 1	0	0
4	B	1	Total C O 2 1 1	0	0
4	C	1	Total C O 2 1 1	0	0
4	D	1	Total C O 2 1 1	0	0
4	G	1	Total C O 2 1 1	0	0
4	H	1	Total C O 2 1 1	0	0
4	M	1	Total C O 2 1 1	0	0
4	N	1	Total C O 2 1 1	0	0

- Molecule 5 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: $C_{14}H_6N_2O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 24 14 2 8	0	0
5	B	1	Total C N O 24 14 2 8	0	0
5	C	1	Total C N O 24 14 2 8	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			24	14	2	8		
5	G	1	Total	C	N	O	0	0
			24	14	2	8		
5	H	1	Total	C	N	O	0	0
			24	14	2	8		
5	M	1	Total	C	N	O	0	0
			24	14	2	8		
5	N	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	580	Total	O	0	0
			580	580		
6	B	585	Total	O	0	0
			585	585		
6	C	590	Total	O	0	0
			590	590		
6	D	567	Total	O	0	0
			567	567		
6	E	113	Total	O	0	0
			113	113		
6	F	104	Total	O	0	0
			104	104		
6	G	598	Total	O	0	0
			598	598		
6	H	491	Total	O	0	0
			491	491		
6	I	106	Total	O	0	0
			106	106		
6	J	74	Total	O	0	0
			74	74		
6	K	109	Total	O	0	0
			109	109		
6	L	114	Total	O	0	0
			114	114		
6	M	590	Total	O	0	0
			590	590		
6	N	545	Total	O	0	0
			545	545		

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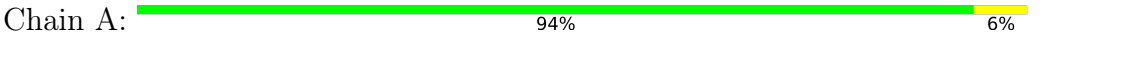
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	94	Total O 94 94	0	0
6	P	90	Total O 90 90	0	0

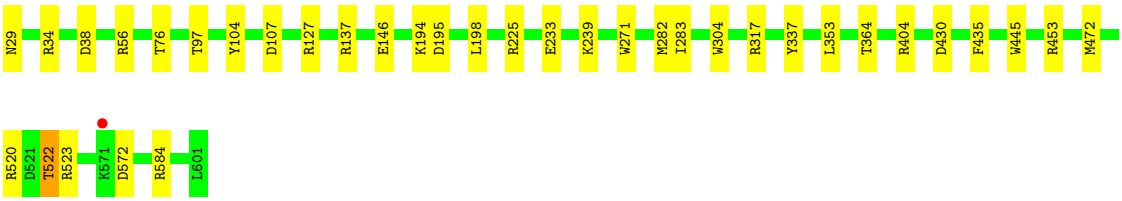
3 Residue-property plots (i)

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: Methanol dehydrogenase protein, large subunit

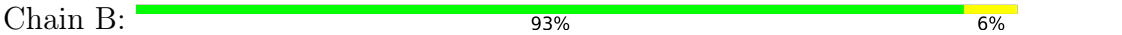
Chain A:

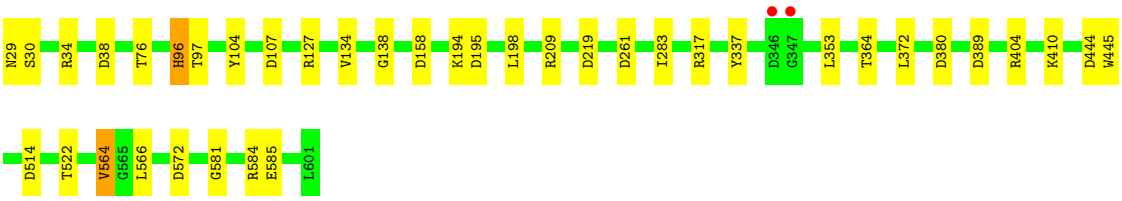




• Molecule 1: Methanol dehydrogenase protein, large subunit

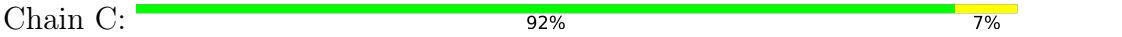
Chain B:





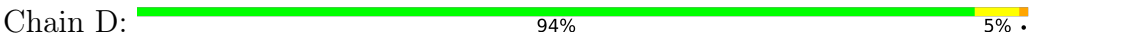
• Molecule 1: Methanol dehydrogenase protein, large subunit

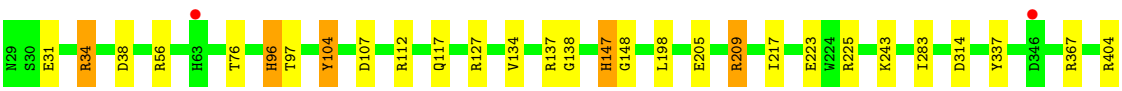
Chain C:

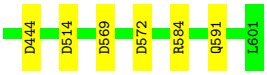


• Molecule 1: Methanol dehydrogenase protein, large subunit

Chain D:

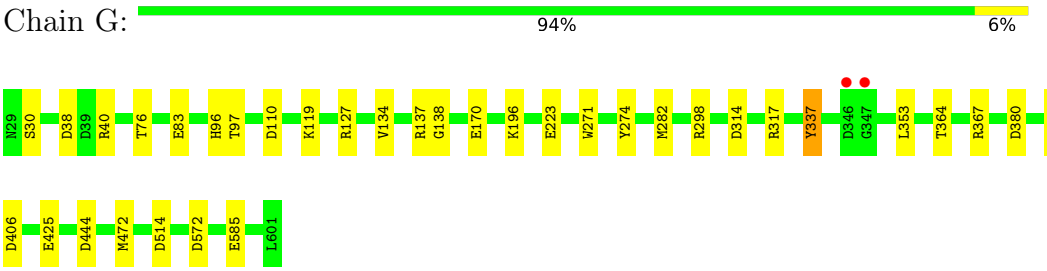






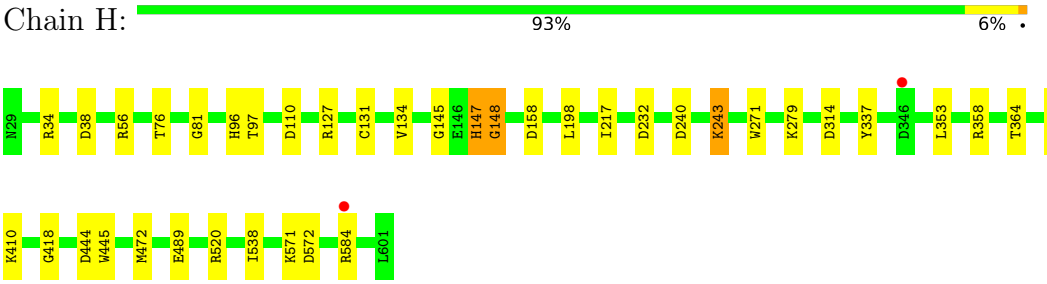
• Molecule 1: Methanol dehydrogenase protein, large subunit

Chain G:



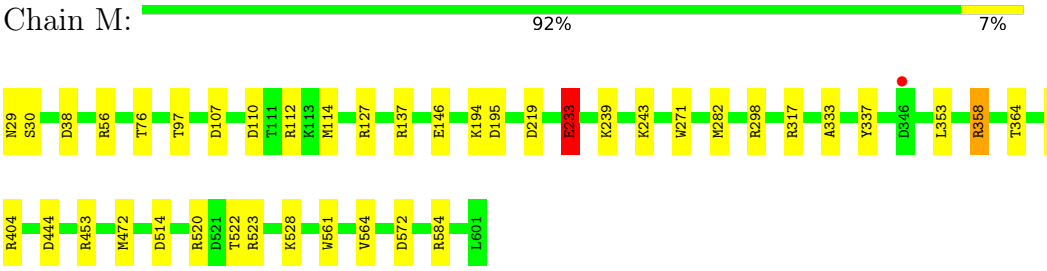
• Molecule 1: Methanol dehydrogenase protein, large subunit

Chain H:



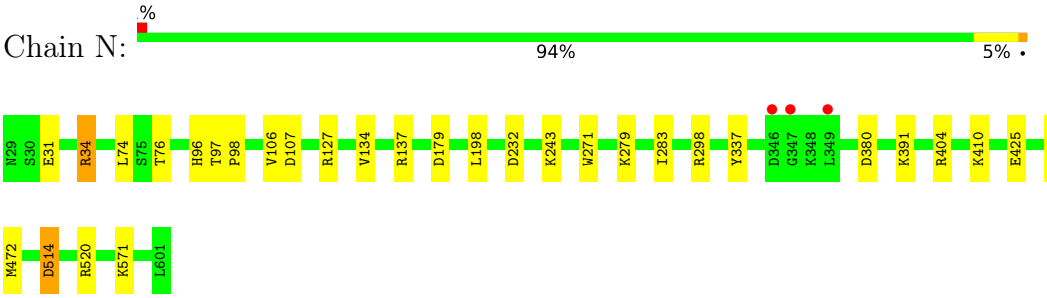
• Molecule 1: Methanol dehydrogenase protein, large subunit

Chain M:



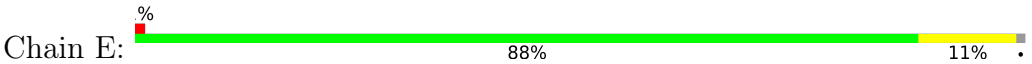
• Molecule 1: Methanol dehydrogenase protein, large subunit

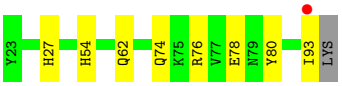
Chain N:



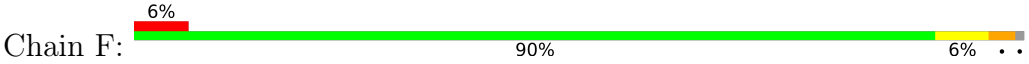
• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

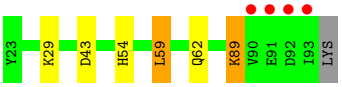
Chain E:



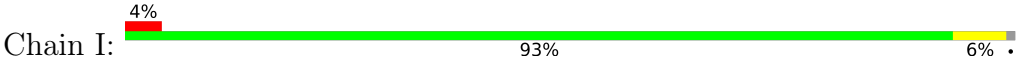


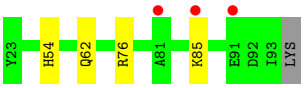
• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



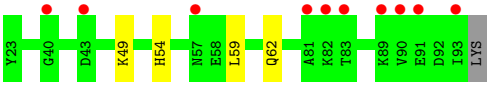


• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

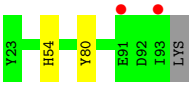




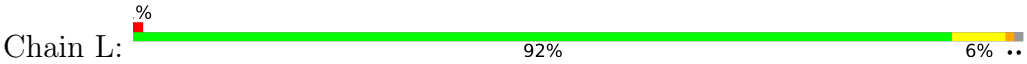
• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

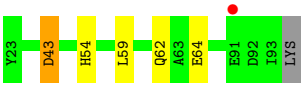


• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

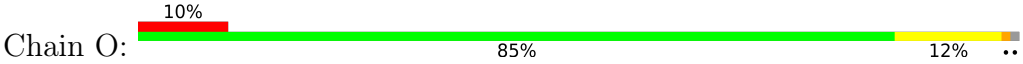


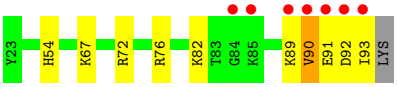
• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2





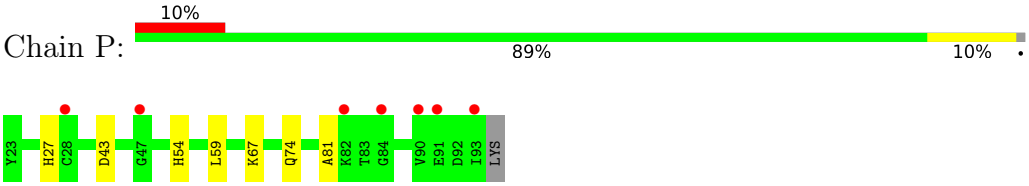
• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2





• Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

Chain P:


10%
89%
10%
Y23
H27
C28
D43
G47
H54
L59
K67
Q74
A81
K82
T83
G84
V90
E91
D92
I93
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.61Å 211.83Å 223.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.00 – 1.80 29.72 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.00-1.80) 99.9 (29.72-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.140 , 0.170 0.154 , 0.183	Depositor DCC
R_{free} test set	27905 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	46034	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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: CA, PQQ, MOH

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	1.01	4/4622 (0.1%)	1.06	18/6281 (0.3%)
1	B	1.03	4/4621 (0.1%)	1.06	26/6281 (0.4%)
1	C	1.04	8/4622 (0.2%)	1.05	18/6281 (0.3%)
1	D	1.01	4/4621 (0.1%)	1.04	20/6281 (0.3%)
1	G	1.03	5/4622 (0.1%)	1.06	23/6281 (0.4%)
1	H	1.02	3/4621 (0.1%)	1.05	19/6281 (0.3%)
1	M	0.99	3/4622 (0.1%)	1.05	25/6281 (0.4%)
1	N	0.98	1/4621 (0.0%)	1.00	16/6281 (0.3%)
2	E	1.04	1/583 (0.2%)	0.97	1/785 (0.1%)
2	F	1.01	1/583 (0.2%)	0.99	2/785 (0.3%)
2	I	1.12	1/583 (0.2%)	0.97	2/785 (0.3%)
2	J	0.89	0/583	0.92	1/785 (0.1%)
2	K	1.09	2/583 (0.3%)	0.95	0/785
2	L	1.10	2/583 (0.3%)	0.96	0/785
2	O	1.02	0/583	1.04	2/785 (0.3%)
2	P	1.01	0/583	0.95	0/785
All	All	1.02	39/41636 (0.1%)	1.04	173/56528 (0.3%)

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	C	0	2
1	D	0	1
1	G	0	1
1	H	0	1
1	M	0	1
1	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
All	All	0	9

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	TYR	CB-CG	-9.63	1.37	1.51
1	A	104	TYR	CE1-CZ	9.12	1.50	1.38
1	G	170	GLU	CD-OE1	8.97	1.35	1.25
1	C	148	GLY	N-CA	-8.96	1.32	1.46
1	B	104	TYR	CE1-CZ	8.77	1.50	1.38
2	I	62	GLN	CB-CG	-8.71	1.29	1.52
1	H	96	HIS	C-N	7.26	1.50	1.34
1	D	148	GLY	N-CA	-7.05	1.35	1.46
1	A	104	TYR	CB-CG	-6.97	1.41	1.51
1	B	96	HIS	C-N	6.94	1.50	1.34
2	E	62	GLN	CB-CG	-6.74	1.34	1.52
2	K	80	TYR	CG-CD2	6.72	1.47	1.39
1	M	233	GLU	CG-CD	6.44	1.61	1.51
1	H	489	GLU	CD-OE2	-6.38	1.18	1.25
2	K	80	TYR	CE1-CZ	6.32	1.46	1.38
2	F	62	GLN	CB-CG	-6.16	1.35	1.52
1	C	446	GLU	CD-OE2	6.15	1.32	1.25
1	C	104	TYR	CE1-CZ	6.06	1.46	1.38
1	C	104	TYR	CB-CG	-5.98	1.42	1.51
1	G	30	SER	CB-OG	-5.93	1.34	1.42
1	H	148	GLY	N-CA	-5.75	1.37	1.46
1	M	233	GLU	CD-OE2	5.69	1.31	1.25
1	M	30	SER	CB-OG	-5.67	1.34	1.42
1	D	96	HIS	C-N	5.66	1.47	1.34
1	A	233	GLU	CG-CD	5.63	1.60	1.51
1	D	205	GLU	CD-OE2	5.55	1.31	1.25
1	C	148	GLY	C-O	-5.48	1.14	1.23
1	G	83	GLU	CD-OE1	5.46	1.31	1.25
1	G	337	TYR	CG-CD2	-5.32	1.32	1.39
1	C	223	GLU	CD-OE1	5.31	1.31	1.25
1	D	104	TYR	CB-CG	-5.20	1.43	1.51
2	L	64	GLU	CD-OE2	5.17	1.31	1.25
1	B	30	SER	CB-OG	-5.15	1.35	1.42
2	L	43	ASP	CB-CG	-5.13	1.41	1.51
1	C	59	GLU	CD-OE1	-5.13	1.20	1.25
1	G	274	TYR	CE1-CZ	5.09	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	96	HIS	C-N	5.09	1.45	1.34
1	A	304	TRP	CE3-CZ3	5.09	1.47	1.38
1	C	83	GLU	CD-OE1	5.03	1.31	1.25

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	147	HIS	C-N-CA	13.79	151.26	122.30
1	D	147	HIS	CA-C-N	12.30	140.80	116.20
1	D	147	HIS	C-N-CA	11.69	146.86	122.30
1	C	147	HIS	CA-C-N	11.65	139.51	116.20
1	H	147	HIS	CA-C-N	11.47	139.14	116.20
1	H	147	HIS	C-N-CA	10.97	145.35	122.30
1	M	282	MET	CG-SD-CE	-10.89	82.78	100.20
1	C	147	HIS	O-C-N	-10.68	105.04	123.20
1	G	298	ARG	NE-CZ-NH2	10.54	125.57	120.30
1	D	127	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	G	572	ASP	CB-CG-OD1	10.22	127.50	118.30
1	G	404	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	D	147	HIS	O-C-N	-10.02	106.17	123.20
1	M	38	ASP	CB-CG-OD1	9.75	127.07	118.30
1	H	147	HIS	O-C-N	-9.70	106.72	123.20
1	H	380	ASP	CB-CG-OD1	9.51	126.86	118.30
1	C	127	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	C	127	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	195	ASP	CB-CG-OD1	8.68	126.11	118.30
1	A	127	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	G	127	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	B	209	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	G	367	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	A	127	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	G	298	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	G	404	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	C	444	ASP	CB-CG-OD1	7.97	125.47	118.30
1	N	127	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	M	317	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	M	572	ASP	CB-CG-OD1	7.85	125.37	118.30
1	N	127	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	D	127	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	G	38	ASP	CB-CG-OD1	7.67	125.21	118.30
1	B	404	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	564	VAL	CG1-CB-CG2	7.55	122.99	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	38	ASP	CB-CG-OD1	7.50	125.05	118.30
1	M	404	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	M	219	ASP	CB-CG-OD1	7.43	124.99	118.30
1	D	107	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	572	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	317	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	G	282	MET	CG-SD-CE	-7.28	88.55	100.20
1	M	298	ARG	NE-CZ-NH1	-7.23	116.69	120.30
1	G	514	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	572	ASP	CB-CG-OD1	7.14	124.73	118.30
1	D	56	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	B	127	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	444	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	56	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	317	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	H	572	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	M	404	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	M	127	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	104	TYR	CB-CG-CD2	-6.78	116.94	121.00
1	C	522	THR	O-C-N	-6.73	111.93	122.70
2	O	76	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	H	127	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	G	406	ASP	CB-CG-OD2	6.66	124.29	118.30
1	M	127	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	B	514	ASP	CB-CG-OD1	6.64	124.27	118.30
1	G	127	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	M	107	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	572	ASP	CB-CG-OD1	6.54	124.18	118.30
1	B	380	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	572	ASP	CB-CG-OD1	6.51	124.16	118.30
1	G	367	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	M	520	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	M	367	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	C	232	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	D	314	ASP	CB-CG-OD1	6.43	124.09	118.30
1	G	317	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	C	232	ASP	CB-CG-OD1	6.38	124.04	118.30
1	G	444	ASP	CB-CG-OD1	6.34	124.00	118.30
1	H	520	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	C	104	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	G	425	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	G	314	ASP	CB-CG-OD1	6.28	123.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	444	ASP	CB-CG-OD1	6.27	123.94	118.30
1	M	298	ARG	NE-CZ-NH2	6.22	123.41	120.30
2	E	76	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	H	127	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	C	486	MET	CG-SD-CE	-6.14	90.37	100.20
1	N	34	ARG	CG-CD-NE	-6.11	98.98	111.80
1	A	404	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	N	520	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	N	380	ASP	CB-CG-OD1	6.06	123.75	118.30
1	N	453	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	O	72	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	38	ASP	CB-CG-OD1	6.02	123.72	118.30
1	M	56	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	G	572	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	N	444	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	C	430	ASP	CB-CG-OD1	5.92	123.62	118.30
1	M	195	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	261	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	G	380	ASP	CB-CG-OD1	5.85	123.57	118.30
1	G	119	LYS	CD-CE-NZ	-5.84	98.26	111.70
1	B	107	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	34	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	B	404	ARG	NE-CZ-NH1	5.81	123.20	120.30
2	I	62	GLN	CB-CA-C	-5.80	98.81	110.40
1	M	386	LYS	CD-CE-NZ	5.80	125.03	111.70
1	H	314	ASP	CB-CG-OD1	5.79	123.51	118.30
1	G	386	LYS	CD-CE-NZ	5.77	124.96	111.70
1	B	195	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	M	572	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	H	38	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	520	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	N	298	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	H	110	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	104	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	225	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	F	62	GLN	CB-CA-C	-5.59	99.21	110.40
1	C	56	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	38	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	404	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	H	147	HIS	N-CA-C	5.55	125.97	111.00
2	F	59	LEU	CB-CG-CD1	5.54	120.41	111.00
1	M	522	THR	O-C-N	-5.54	113.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	147	HIS	N-CA-C	5.52	125.90	111.00
1	G	40	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	34	ARG	CG-CD-NE	-5.47	100.31	111.80
1	M	520	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	N	425	GLU	OE1-CD-OE2	-5.47	116.74	123.30
1	H	34	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	522	THR	O-C-N	-5.45	113.99	122.70
1	N	107	ASP	CB-CG-OD1	5.44	123.19	118.30
1	G	317	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	34	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	N	444	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	522	THR	O-C-N	-5.40	114.06	122.70
1	H	56	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	34	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	H	158	ASP	CB-CG-OD1	5.35	123.12	118.30
1	H	232	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	430	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	389	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	419	TYR	CB-CG-CD1	5.29	124.17	121.00
1	N	232	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	404	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	H	444	ASP	CB-CG-OD1	5.26	123.04	118.30
1	M	358	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	261	ASP	CB-CG-OD1	5.26	123.03	118.30
1	H	572	ASP	CB-CG-OD1	5.25	123.03	118.30
1	M	358	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	B	572	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	225	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	M	444	ASP	CB-CG-OD1	5.21	122.98	118.30
1	M	528	LYS	CD-CE-NZ	-5.19	99.77	111.70
1	B	127	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	444	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	430	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	372	LEU	CA-CB-CG	5.16	127.18	115.30
1	D	107	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	D	367	ARG	NE-CZ-NH1	-5.15	117.73	120.30
2	J	62	GLN	CB-CA-C	-5.14	100.11	110.40
1	N	514	ASP	CB-CG-OD1	5.14	122.93	118.30
1	N	404	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	158	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	209	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	D	572	ASP	CB-CG-OD2	-5.13	113.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	104	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	B	38	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	I	76	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	C	209	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	B	219	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	N	34	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	N	179	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	282	MET	CG-SD-CE	-5.04	92.14	100.20
1	A	107	ASP	CB-CG-OD1	5.03	122.83	118.30
1	M	514	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	572	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	H	198	LEU	CB-CG-CD2	5.01	119.51	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	C	131	CYS	Peptide
1	C	137	ARG	Sidechain
1	D	137	ARG	Sidechain
1	G	137	ARG	Sidechain
1	H	131	CYS	Peptide
1	M	137	ARG	Sidechain
1	N	137	ARG	Sidechain
2	O	90	VAL	Peptide

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	4491	0	4320	6	0
1	B	4490	0	4320	6	0
1	C	4491	0	4319	15	0
1	D	4490	0	4320	14	0
1	G	4491	0	4320	10	0
1	H	4490	0	4320	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	4491	0	4320	18	0
1	N	4490	0	4320	8	0
2	E	568	0	545	5	0
2	F	568	0	545	3	0
2	I	568	0	545	2	0
2	J	568	0	545	3	0
2	K	568	0	545	2	0
2	L	568	0	545	4	0
2	O	568	0	545	6	0
2	P	568	0	545	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	2	0	0	2	0
4	B	2	0	0	3	0
4	C	2	0	0	1	0
4	D	2	0	0	2	0
4	G	2	0	0	2	0
4	H	2	0	0	2	0
4	M	2	0	0	1	0
4	N	2	0	0	2	0
5	A	24	0	3	3	0
5	B	24	0	3	3	0
5	C	24	0	3	2	0
5	D	24	0	3	2	0
5	G	24	0	3	3	0
5	H	24	0	3	3	0
5	M	24	0	3	3	0
5	N	24	0	3	3	0
6	A	580	0	0	2	0
6	B	585	0	0	2	0
6	C	590	0	0	2	0
6	D	567	0	0	3	0
6	E	113	0	0	2	0
6	F	104	0	0	0	0
6	G	598	0	0	4	0
6	H	491	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	106	0	0	0	0
6	J	74	0	0	1	0
6	K	109	0	0	0	0
6	L	114	0	0	0	0
6	M	590	0	0	8	0
6	N	545	0	0	7	0
6	O	94	0	0	2	0
6	P	90	0	0	3	0
All	All	46034	0	38943	125	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 2.

All (125) 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)
2:P:74:GLN:HG2	6:P:174:HOH:O	1.49	1.10
4:M:702:MOH:O	5:M:703:PQQ:C5	2.06	1.03
1:M:114:MET:HE2	6:M:856:HOH:O	1.62	1.00
4:B:702:MOH:O	5:B:703:PQQ:C5	2.11	0.99
4:H:702:MOH:O	5:H:703:PQQ:C5	2.11	0.99
4:N:702:MOH:O	5:N:703:PQQ:C5	2.11	0.99
4:D:702:MOH:O	5:D:703:PQQ:C5	2.14	0.95
5:C:702:PQQ:C5	4:C:703:MOH:O	2.14	0.95
1:M:114:MET:CE	6:M:856:HOH:O	2.13	0.95
4:G:702:MOH:O	5:G:703:PQQ:C5	2.14	0.94
1:M:110:ASP:OD1	6:M:801:HOH:O	1.84	0.94
4:A:702:MOH:O	5:A:703:PQQ:C5	2.21	0.88
2:O:82:LYS:NZ	6:O:101:HOH:O	1.81	0.86
2:O:90:VAL:HG12	2:O:93:ILE:HD12	1.66	0.76
1:G:585:GLU:HG3	6:G:1229:HOH:O	1.83	0.75
1:N:391:LYS:NZ	6:N:801:HOH:O	2.25	0.69
1:D:209:ARG:H	2:L:62:GLN:HE22	1.42	0.66
6:N:1122:HOH:O	2:P:54:HIS:HD2	1.80	0.64
1:H:147:HIS:CD2	1:H:217:ILE:HD11	2.33	0.63
1:G:110:ASP:OD1	6:G:801:HOH:O	2.15	0.63
6:D:1128:HOH:O	2:L:54:HIS:HD2	1.81	0.63
6:H:1011:HOH:O	2:J:54:HIS:HD2	1.83	0.61
1:M:114:MET:CE	6:N:836:HOH:O	2.47	0.61
1:C:145:GLY:O	1:C:148:GLY:HA2	2.01	0.60
6:C:1069:HOH:O	2:K:54:HIS:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:GLY:O	1:H:148:GLY:HA2	2.01	0.59
6:M:1116:HOH:O	2:O:54:HIS:HD2	1.88	0.57
6:G:1105:HOH:O	2:I:54:HIS:HD2	1.89	0.56
6:D:1180:HOH:O	2:L:54:HIS:HE1	1.89	0.56
1:M:239:LYS:NZ	6:M:802:HOH:O	2.38	0.56
1:G:196:LYS:HE3	1:G:223:GLU:HG3	1.86	0.56
1:D:209:ARG:H	2:L:62:GLN:NE2	2.04	0.55
6:B:1086:HOH:O	2:F:54:HIS:HD2	1.90	0.55
1:C:104:TYR:HD2	1:C:117:GLN:HG2	1.72	0.54
6:A:1077:HOH:O	2:E:54:HIS:HD2	1.90	0.54
2:O:90:VAL:HG12	2:O:93:ILE:CD1	2.36	0.53
2:E:27:HIS:HE1	6:E:116:HOH:O	1.91	0.53
1:B:198:LEU:HD11	1:B:283:ILE:HD13	1.89	0.53
6:B:1124:HOH:O	2:F:54:HIS:HE1	1.90	0.53
6:M:1148:HOH:O	2:O:54:HIS:HE1	1.92	0.53
2:P:27:HIS:HE1	6:P:114:HOH:O	1.92	0.53
1:A:29:ASN:N	1:A:194:LYS:H	2.07	0.52
4:D:702:MOH:O	5:D:703:PQQ:C4	2.57	0.52
1:C:591:GLN:NE2	1:D:104:TYR:CZ	2.78	0.52
1:M:114:MET:HE1	6:N:836:HOH:O	2.08	0.52
1:M:114:MET:HE3	6:N:836:HOH:O	2.09	0.52
6:N:1100:HOH:O	2:P:54:HIS:HE1	1.93	0.52
1:D:198:LEU:HD11	1:D:283:ILE:HD13	1.92	0.51
2:E:74:GLN:NE2	2:E:78:GLU:OE2	2.44	0.51
1:A:76:THR:HB	1:A:97:THR:HG22	1.93	0.51
2:F:89:LYS:HE3	2:F:89:LYS:HA	1.93	0.51
1:N:31:GLU:OE1	1:N:34:ARG:NH1	2.44	0.51
1:M:114:MET:HE1	6:M:856:HOH:O	1.95	0.50
1:G:76:THR:HB	1:G:97:THR:HG22	1.94	0.50
4:N:702:MOH:O	5:N:703:PQQ:C6A	2.60	0.49
2:E:93:ILE:O	6:E:101:HOH:O	2.19	0.49
1:H:240:ASP:HB3	1:H:243:LYS:HG2	1.94	0.49
1:C:104:TYR:CZ	1:D:591:GLN:NE2	2.80	0.49
1:D:147:HIS:CD2	1:D:217:ILE:HD11	2.48	0.49
6:G:1176:HOH:O	2:I:54:HIS:HE1	1.95	0.49
1:M:76:THR:HB	1:M:97:THR:HG22	1.94	0.48
1:M:584:ARG:HB3	1:M:584:ARG:CZ	2.44	0.48
6:H:998:HOH:O	2:J:54:HIS:HE1	1.96	0.48
1:C:29:ASN:N	1:C:194:LYS:H	2.12	0.47
1:D:223:GLU:CD	6:D:820:HOH:O	2.51	0.47
6:C:1143:HOH:O	2:K:54:HIS:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:LYS:HD2	1:G:223:GLU:HG3	1.97	0.46
6:A:1141:HOH:O	2:E:54:HIS:HE1	1.97	0.46
1:G:271:TRP:CZ2	5:G:703:PQQ:C6A	2.98	0.46
4:G:702:MOH:O	5:G:703:PQQ:C6A	2.64	0.46
1:H:571:LYS:O	1:H:584:ARG:NH1	2.49	0.46
1:C:591:GLN:NE2	1:D:104:TYR:CE1	2.84	0.46
1:H:76:THR:HB	1:H:97:THR:HG22	1.98	0.46
2:O:67:LYS:HD3	6:O:168:HOH:O	2.15	0.46
1:H:271:TRP:CZ2	5:H:703:PQQ:C6A	3.00	0.45
4:H:702:MOH:O	5:H:703:PQQ:C4	2.62	0.45
1:C:104:TYR:CD2	1:C:117:GLN:HG2	2.49	0.45
1:G:196:LYS:CE	1:G:223:GLU:HG3	2.46	0.45
1:C:76:THR:HB	1:C:97:THR:HG22	1.99	0.45
1:D:96:HIS:CE1	1:D:138:GLY:HA2	2.52	0.45
1:M:271:TRP:CZ2	5:M:703:PQQ:C6A	3.00	0.45
1:D:76:THR:HB	1:D:97:THR:HG22	1.99	0.44
1:B:76:THR:HB	1:B:97:THR:HG22	1.98	0.44
1:C:266:GLY:O	1:C:290:PRO:HA	2.17	0.44
1:M:29:ASN:N	1:M:194:LYS:H	2.15	0.44
1:M:561:TRP:O	1:M:564:VAL:HG22	2.18	0.44
1:A:353:LEU:O	1:A:364:THR:HA	2.18	0.44
1:N:271:TRP:CZ2	5:N:703:PQQ:C6A	3.01	0.43
1:D:31:GLU:OE2	1:D:34:ARG:NH2	2.49	0.43
1:A:271:TRP:CZ2	5:A:703:PQQ:C6A	3.00	0.43
5:M:703:PQQ:O9A	5:M:703:PQQ:N1	2.50	0.43
4:A:702:MOH:O	5:A:703:PQQ:C6A	2.67	0.42
1:C:112:ARG:HD3	1:D:514:ASP:O	2.19	0.42
1:H:358:ARG:HD2	1:H:418:GLY:HA3	2.01	0.42
1:B:581:GLY:O	1:B:584:ARG:NH1	2.52	0.42
1:C:514:ASP:O	1:D:112:ARG:HD3	2.19	0.42
1:N:76:THR:HB	1:N:97:THR:HG22	2.01	0.42
1:B:29:ASN:N	1:B:194:LYS:H	2.18	0.42
4:B:702:MOH:O	5:B:703:PQQ:C6A	2.64	0.42
2:P:67:LYS:HE2	6:P:172:HOH:O	2.19	0.42
4:B:702:MOH:C	5:B:703:PQQ:C5	2.96	0.42
1:M:233:GLU:HB2	6:M:891:HOH:O	2.20	0.42
6:N:1055:HOH:O	2:P:81:ALA:HB2	2.19	0.42
1:G:196:LYS:CD	1:G:223:GLU:HG3	2.50	0.42
1:H:81:GLY:HA3	1:H:538:ILE:HD11	2.02	0.42
1:H:353:LEU:O	1:H:364:THR:HA	2.20	0.42
1:B:353:LEU:O	1:B:364:THR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:TRP:CZ2	5:C:702:PQQ:C6A	3.03	0.42
1:C:447:PRO:HA	1:C:461:ALA:HA	2.03	0.41
1:A:198:LEU:HD21	1:A:283:ILE:HD13	2.03	0.41
1:C:85:ALA:HB1	1:C:86:PRO:CD	2.50	0.41
1:D:104:TYR:HD1	1:D:117:GLN:HG2	1.86	0.41
1:A:435:PHE:CZ	1:A:522:THR:HB	2.56	0.41
1:B:96:HIS:CE1	1:B:138:GLY:HA2	2.55	0.41
1:M:243:LYS:HA	1:M:243:LYS:HD3	1.79	0.41
1:N:74:LEU:HD11	1:N:106:VAL:HG21	2.02	0.41
1:N:198:LEU:HD11	1:N:283:ILE:HD13	2.02	0.41
1:C:31:GLU:OE2	1:C:34:ARG:NH2	2.46	0.41
1:G:96:HIS:CE1	1:G:138:GLY:HA2	2.55	0.41
1:M:353:LEU:O	1:M:364:THR:HA	2.20	0.41
1:G:353:LEU:O	1:G:364:THR:HA	2.21	0.40
1:M:112:ARG:HD3	1:N:514:ASP:O	2.21	0.40
2:J:49:LYS:HB2	6:J:130:HOH:O	2.20	0.40
1:M:333:ALA:O	1:M:358:ARG:HG3	2.21	0.40
1:N:97:THR:HB	1:N:98:PRO:HD2	2.02	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	571/573 (100%)	543 (95%)	28 (5%)	0	100	100
1	B	571/573 (100%)	546 (96%)	24 (4%)	1 (0%)	47	33
1	C	571/573 (100%)	543 (95%)	27 (5%)	1 (0%)	47	33
1	D	571/573 (100%)	541 (95%)	29 (5%)	1 (0%)	47	33
1	G	571/573 (100%)	546 (96%)	24 (4%)	1 (0%)	47	33
1	H	571/573 (100%)	541 (95%)	29 (5%)	1 (0%)	47	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	571/573 (100%)	542 (95%)	29 (5%)	0	100 100
1	N	571/573 (100%)	540 (95%)	30 (5%)	1 (0%)	47 33
2	E	69/72 (96%)	69 (100%)	0	0	100 100
2	F	69/72 (96%)	69 (100%)	0	0	100 100
2	I	69/72 (96%)	69 (100%)	0	0	100 100
2	J	69/72 (96%)	68 (99%)	1 (1%)	0	100 100
2	K	69/72 (96%)	69 (100%)	0	0	100 100
2	L	69/72 (96%)	69 (100%)	0	0	100 100
2	O	69/72 (96%)	67 (97%)	2 (3%)	0	100 100
2	P	69/72 (96%)	69 (100%)	0	0	100 100
All	All	5120/5160 (99%)	4891 (96%)	223 (4%)	6 (0%)	51 36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	134	VAL
1	D	134	VAL
1	N	134	VAL
1	B	134	VAL
1	C	134	VAL
1	G	134	VAL

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	464/464 (100%)	456 (98%)	8 (2%)	60 51
1	B	464/464 (100%)	458 (99%)	6 (1%)	69 62
1	C	464/464 (100%)	459 (99%)	5 (1%)	73 68
1	D	464/464 (100%)	460 (99%)	4 (1%)	78 75
1	G	464/464 (100%)	462 (100%)	2 (0%)	91 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	464/464 (100%)	457 (98%)	7 (2%)	65 56
1	M	464/464 (100%)	458 (99%)	6 (1%)	69 62
1	N	464/464 (100%)	457 (98%)	7 (2%)	65 56
2	E	60/61 (98%)	59 (98%)	1 (2%)	60 51
2	F	60/61 (98%)	56 (93%)	4 (7%)	16 5
2	I	60/61 (98%)	59 (98%)	1 (2%)	60 51
2	J	60/61 (98%)	59 (98%)	1 (2%)	60 51
2	K	60/61 (98%)	60 (100%)	0	100 100
2	L	60/61 (98%)	58 (97%)	2 (3%)	38 23
2	O	60/61 (98%)	57 (95%)	3 (5%)	24 10
2	P	60/61 (98%)	58 (97%)	2 (3%)	38 23
All	All	4192/4200 (100%)	4133 (99%)	59 (1%)	67 59

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	239	LYS
1	A	337	TYR
1	A	445	TRP
1	A	453	ARG
1	A	472	MET
1	A	523	ARG
1	A	584	ARG
1	B	337	TYR
1	B	410	LYS
1	B	445	TRP
1	B	564	VAL
1	B	566	LEU
1	B	585	GLU
1	C	121	LYS
1	C	337	TYR
1	C	453	ARG
1	C	472	MET
1	C	523	ARG
1	D	243	LYS
1	D	337	TYR
1	D	569	ASP

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Mol	Chain	Res	Type
1	D	584	ARG
2	E	80	TYR
2	F	29	LYS
2	F	43	ASP
2	F	59	LEU
2	F	89	LYS
1	G	337	TYR
1	G	472	MET
1	H	243	LYS
1	H	279	LYS
1	H	337	TYR
1	H	387	LYS
1	H	410	LYS
1	H	445	TRP
1	H	472	MET
2	I	85	LYS
2	J	59	LEU
2	L	43	ASP
2	L	59	LEU
1	M	146	GLU
1	M	233	GLU
1	M	337	TYR
1	M	453	ARG
1	M	472	MET
1	M	523	ARG
1	N	243	LYS
1	N	279	LYS
1	N	337	TYR
1	N	410	LYS
1	N	453	ARG
1	N	472	MET
1	N	571	LYS
2	O	89	LYS
2	O	91	GLU
2	O	92	ASP
2	P	43	ASP
2	P	59	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	588	HIS

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Mol	Chain	Res	Type
1	A	591	GLN
1	B	156	GLN
1	B	216	ASN
1	B	464	ASN
1	B	588	HIS
1	C	117	GLN
1	D	117	GLN
1	D	156	GLN
1	D	216	ASN
2	E	27	HIS
2	E	54	HIS
2	E	74	GLN
2	F	54	HIS
1	G	216	ASN
1	G	588	HIS
1	H	117	GLN
1	H	216	ASN
1	H	545	GLN
1	H	588	HIS
2	I	54	HIS
2	J	54	HIS
2	K	54	HIS
2	L	54	HIS
2	L	62	GLN
1	M	270	ASN
1	M	588	HIS
1	N	156	GLN
1	N	216	ASN
1	N	464	ASN
1	N	545	GLN
2	O	54	HIS
2	P	54	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	MOH	N	702	-	1,1,1	0.05	0	-		
5	PQQ	C	702	3	23,26,26	1.85	6 (26%)	29,40,40	2.21	7 (24%)
5	PQQ	H	703	3	23,26,26	1.71	7 (30%)	29,40,40	2.17	9 (31%)
5	PQQ	A	703	3	23,26,26	1.66	5 (21%)	29,40,40	2.32	7 (24%)
4	MOH	A	702	-	1,1,1	0.04	0	-		
4	MOH	G	702	-	1,1,1	0.07	0	-		
4	MOH	D	702	-	1,1,1	0.01	0	-		
5	PQQ	G	703	3	23,26,26	1.41	5 (21%)	29,40,40	2.51	12 (41%)
5	PQQ	B	703	3	23,26,26	1.45	3 (13%)	29,40,40	2.19	11 (37%)
4	MOH	H	702	-	1,1,1	0.09	0	-		
4	MOH	B	702	-	1,1,1	0.15	0	-		
4	MOH	M	702	-	1,1,1	0.30	0	-		
5	PQQ	M	703	3	23,26,26	1.78	4 (17%)	29,40,40	2.04	4 (13%)
5	PQQ	N	703	3	23,26,26	2.23	8 (34%)	29,40,40	2.26	9 (31%)
5	PQQ	D	703	3	23,26,26	1.84	5 (21%)	29,40,40	2.36	8 (27%)
4	MOH	C	703	-	1,1,1	0.02	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
5	PQQ	C	702	3	-	0/10/28/28	0/3/3/3
5	PQQ	H	703	3	-	0/10/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PQQ	A	703	3	-	0/10/28/28	0/3/3/3
5	PQQ	G	703	3	-	4/10/28/28	0/3/3/3
5	PQQ	B	703	3	-	4/10/28/28	0/3/3/3
5	PQQ	M	703	3	-	0/10/28/28	0/3/3/3
5	PQQ	N	703	3	-	4/10/28/28	0/3/3/3
5	PQQ	D	703	3	-	0/10/28/28	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	703	PQQ	C6A-N6	6.40	1.37	1.32
5	M	703	PQQ	C6A-C9A	4.96	1.48	1.42
5	N	703	PQQ	C6A-C9A	4.48	1.47	1.42
5	H	703	PQQ	C6A-N6	4.35	1.36	1.32
5	D	703	PQQ	C2-C2X	-4.20	1.44	1.50
5	C	702	PQQ	C6A-C9A	4.01	1.47	1.42
5	D	703	PQQ	C6A-C9A	3.37	1.46	1.42
5	A	703	PQQ	C2-C2X	-3.34	1.46	1.50
5	A	703	PQQ	O5-C5	3.32	1.30	1.23
5	H	703	PQQ	C9-C9A	3.21	1.48	1.41
5	C	702	PQQ	O5-C5	3.18	1.30	1.23
5	A	703	PQQ	C6A-C9A	3.10	1.46	1.42
5	C	702	PQQ	C7-N6	3.08	1.39	1.34
5	N	703	PQQ	C9-C9A	3.03	1.47	1.41
5	G	703	PQQ	C6A-C9A	2.95	1.46	1.42
5	M	703	PQQ	C7-N6	-2.89	1.30	1.34
5	B	703	PQQ	C8-C9	2.83	1.43	1.37
5	D	703	PQQ	C9-C9A	2.73	1.47	1.41
5	D	703	PQQ	C6A-N6	2.73	1.34	1.32
5	C	702	PQQ	C9-C9A	2.72	1.47	1.41
5	H	703	PQQ	C2-C2X	-2.60	1.47	1.50
5	H	703	PQQ	O5-C5	2.56	1.28	1.23
5	C	702	PQQ	O7B-C7X	-2.54	1.22	1.30
5	B	703	PQQ	C6A-C5	2.48	1.53	1.50
5	G	703	PQQ	O7B-C7X	-2.47	1.23	1.30
5	A	703	PQQ	C6A-N6	-2.45	1.30	1.32
5	N	703	PQQ	C3-C2	-2.40	1.35	1.39
5	M	703	PQQ	O5-C5	2.36	1.28	1.23
5	N	703	PQQ	C5-C4	-2.33	1.45	1.53
5	G	703	PQQ	O2B-C2X	-2.31	1.23	1.30
5	C	702	PQQ	C5-C4	-2.29	1.45	1.53
5	N	703	PQQ	O2B-C2X	-2.27	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	703	PQQ	O9B-C9X	-2.27	1.23	1.30
5	N	703	PQQ	C6A-C5	-2.24	1.47	1.50
5	N	703	PQQ	C8-C9	2.21	1.42	1.37
5	A	703	PQQ	C5-C4	-2.20	1.46	1.53
5	H	703	PQQ	C6A-C5	-2.15	1.47	1.50
5	H	703	PQQ	C6A-C9A	2.14	1.45	1.42
5	G	703	PQQ	C8-C7	-2.12	1.34	1.40
5	G	703	PQQ	O5-C5	2.10	1.27	1.23
5	B	703	PQQ	C9-C9A	2.05	1.45	1.41
5	H	703	PQQ	C5-C4	-2.01	1.46	1.53
5	D	703	PQQ	O5-C5	2.00	1.27	1.23

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	703	PQQ	C9-C9A-C1A	8.28	129.68	122.88
5	A	703	PQQ	C9-C9A-C1A	7.85	129.32	122.88
5	C	702	PQQ	C9-C9A-C1A	7.09	128.69	122.88
5	M	703	PQQ	C9-C9A-C1A	7.05	128.66	122.88
5	G	703	PQQ	C9-C9A-C1A	6.44	128.16	122.88
5	N	703	PQQ	C9-C9A-C1A	6.14	127.92	122.88
5	D	703	PQQ	C9-C9A-C6A	-5.45	114.40	121.68
5	M	703	PQQ	C9-C9A-C6A	-5.37	114.51	121.68
5	A	703	PQQ	C9-C9A-C6A	-5.37	114.51	121.68
5	H	703	PQQ	C9-C9A-C6A	-5.12	114.84	121.68
5	B	703	PQQ	C9-C9A-C6A	-4.96	115.06	121.68
5	N	703	PQQ	C9-C9A-C6A	-4.84	115.21	121.68
5	C	702	PQQ	C9-C9A-C6A	-4.82	115.25	121.68
5	B	703	PQQ	C9-C9A-C1A	4.60	126.66	122.88
5	G	703	PQQ	O2A-C2X-C2	-4.59	111.92	121.24
5	H	703	PQQ	C9-C9A-C1A	4.57	126.62	122.88
5	G	703	PQQ	O2B-C2X-C2	4.41	124.74	114.69
5	G	703	PQQ	C9-C9A-C6A	-4.25	116.00	121.68
5	N	703	PQQ	O2A-C2X-C2	-4.15	112.82	121.24
5	H	703	PQQ	C3A-C4-C5	3.97	120.45	118.14
5	G	703	PQQ	O9A-C9X-C9	-3.61	112.59	122.23
5	H	703	PQQ	O7A-C7X-C7	-3.59	113.96	121.24
5	B	703	PQQ	O9B-C9X-C9	3.54	124.42	114.39
5	H	703	PQQ	C8-C9-C9X	-3.50	114.32	118.27
5	D	703	PQQ	C2-N1-C1A	3.42	110.93	103.90
5	H	703	PQQ	C2-N1-C1A	3.41	110.90	103.90
5	B	703	PQQ	C2-N1-C1A	3.36	110.80	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	703	PQQ	O9B-C9X-C9	3.31	123.76	114.39
5	G	703	PQQ	O7B-C7X-O7A	-3.26	116.10	123.35
5	B	703	PQQ	C8-C9-C9X	-3.23	114.63	118.27
5	H	703	PQQ	O7B-C7X-C7	3.22	122.02	114.69
5	G	703	PQQ	C2-N1-C1A	3.19	110.45	103.90
5	C	702	PQQ	C8-C9-C9A	-3.17	115.75	120.06
5	A	703	PQQ	O7B-C7X-C7	3.06	121.66	114.69
5	A	703	PQQ	C2-N1-C1A	3.03	110.12	103.90
5	G	703	PQQ	O9B-C9X-C9	3.01	122.93	114.39
5	N	703	PQQ	O9B-C9X-O9A	-2.93	116.86	123.35
5	G	703	PQQ	C8-C9-C9X	-2.87	115.03	118.27
5	B	703	PQQ	O2B-C2X-C2	2.85	121.17	114.69
5	B	703	PQQ	O2A-C2X-C2	-2.84	115.47	121.24
5	N	703	PQQ	C2-N1-C1A	2.84	109.74	103.90
5	A	703	PQQ	C6A-N6-C7	2.76	122.55	117.91
5	C	702	PQQ	O2B-C2X-C2	2.73	120.91	114.69
5	N	703	PQQ	O7B-C7X-C7	2.65	120.73	114.69
5	C	702	PQQ	O2A-C2X-C2	-2.64	115.88	121.24
5	M	703	PQQ	C2-N1-C1A	2.63	109.31	103.90
5	N	703	PQQ	O2B-C2X-C2	2.59	120.58	114.69
5	N	703	PQQ	O7A-C7X-C7	-2.59	115.99	121.24
5	B	703	PQQ	C9A-C9-C9X	2.57	127.59	123.95
5	D	703	PQQ	O9B-C9X-O9A	-2.46	117.90	123.35
5	B	703	PQQ	O9A-C9X-C9	-2.42	115.78	122.23
5	D	703	PQQ	C8-C9-C9X	-2.34	115.63	118.27
5	A	703	PQQ	C8-C9-C9X	-2.33	115.64	118.27
5	C	702	PQQ	C9-C8-C7	2.28	123.95	120.33
5	D	703	PQQ	C3A-C1A-C9A	2.28	124.57	121.54
5	G	703	PQQ	C3A-C1A-N1	-2.28	104.37	108.77
5	A	703	PQQ	C3A-C1A-N1	-2.18	104.56	108.77
5	B	703	PQQ	C3A-C4-C5	-2.17	116.88	118.14
5	G	703	PQQ	O7A-C7X-C7	2.15	125.59	121.24
5	D	703	PQQ	O7B-C7X-C7	2.12	119.51	114.69
5	C	702	PQQ	O7B-C7X-O7A	-2.11	118.66	123.35
5	D	703	PQQ	C7X-C7-N6	-2.10	113.37	116.48
5	M	703	PQQ	C8-C9-C9A	-2.07	117.24	120.06
5	G	703	PQQ	O5-C5-C6A	2.06	124.01	121.84
5	H	703	PQQ	O9B-C9X-O9A	-2.04	118.81	123.35
5	H	703	PQQ	C3A-C1A-N1	-2.01	104.88	108.77
5	B	703	PQQ	C3-C2-C2X	-2.01	122.37	128.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	703	PQQ	C9A-C9-C9X-O9B
5	G	703	PQQ	C9A-C9-C9X-O9B
5	N	703	PQQ	C9A-C9-C9X-O9B
5	B	703	PQQ	C9A-C9-C9X-O9A
5	G	703	PQQ	C9A-C9-C9X-O9A
5	N	703	PQQ	C9A-C9-C9X-O9A
5	B	703	PQQ	C8-C9-C9X-O9A
5	B	703	PQQ	C8-C9-C9X-O9B
5	G	703	PQQ	C8-C9-C9X-O9A
5	G	703	PQQ	C8-C9-C9X-O9B
5	N	703	PQQ	C8-C9-C9X-O9A
5	N	703	PQQ	C8-C9-C9X-O9B

There are no ring outliers.

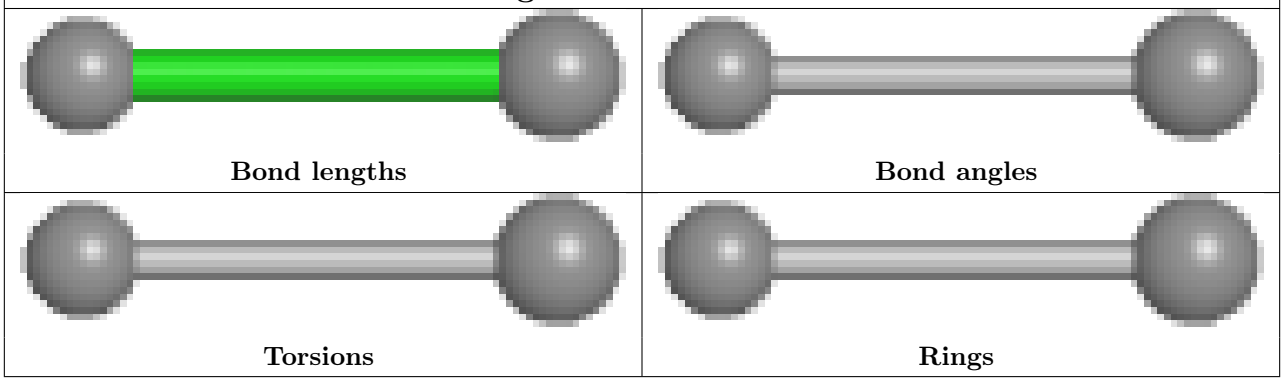
16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	702	MOH	2	0
5	C	702	PQQ	2	0
5	H	703	PQQ	3	0
5	A	703	PQQ	3	0
4	A	702	MOH	2	0
4	G	702	MOH	2	0
4	D	702	MOH	2	0
5	G	703	PQQ	3	0
5	B	703	PQQ	3	0
4	H	702	MOH	2	0
4	B	702	MOH	3	0
4	M	702	MOH	1	0
5	M	703	PQQ	3	0
5	N	703	PQQ	3	0
5	D	703	PQQ	2	0
4	C	703	MOH	1	0

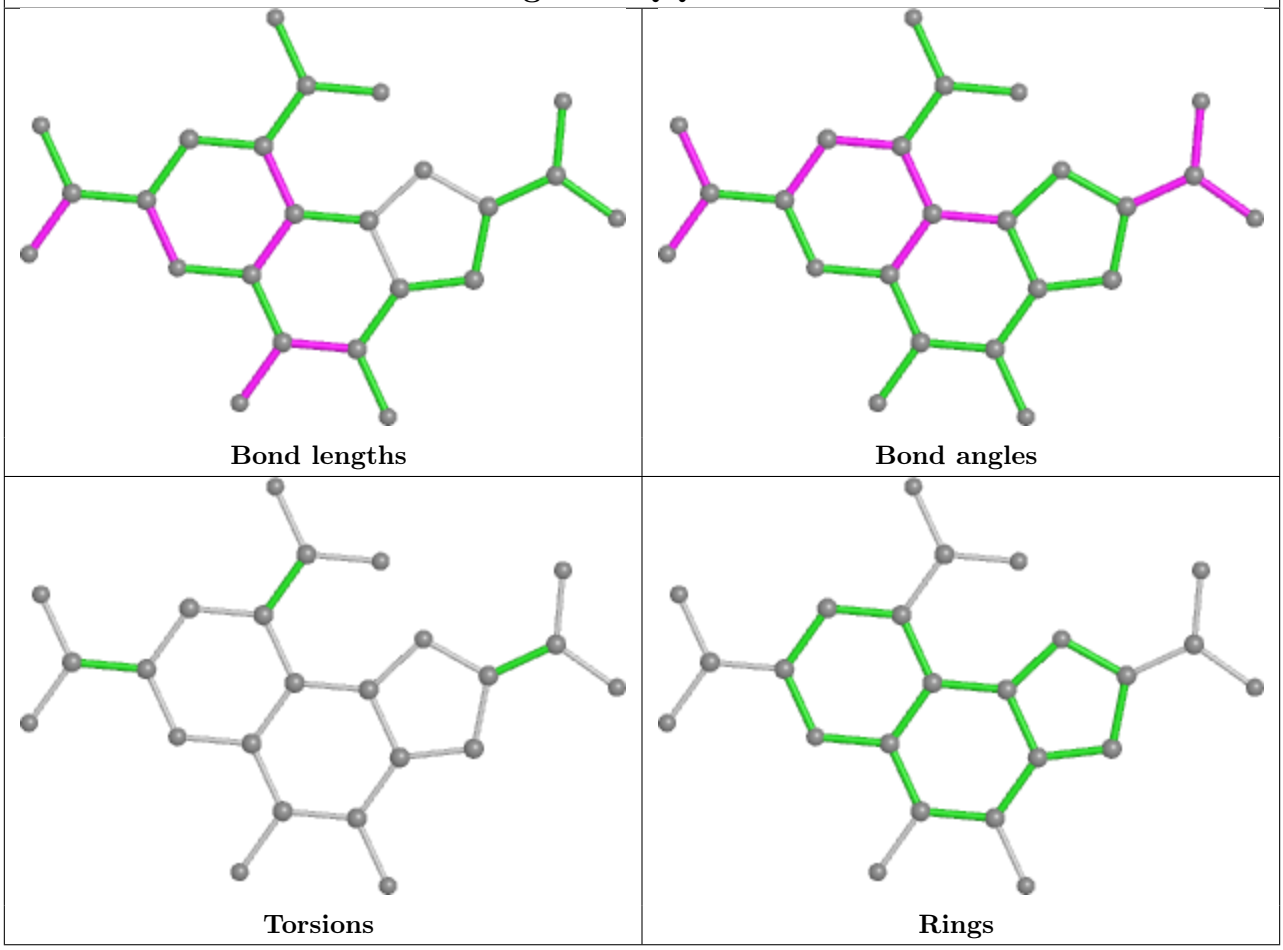
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

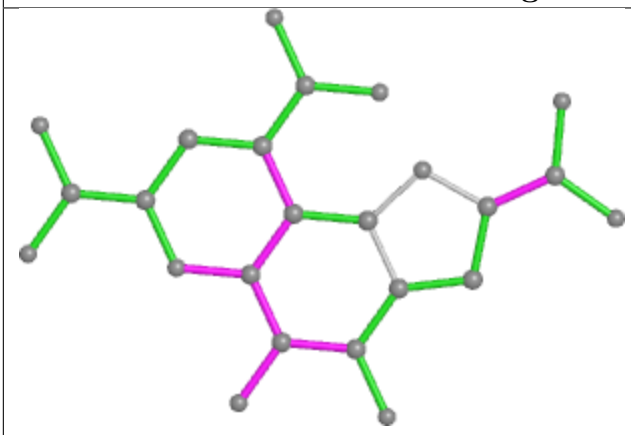
Ligand MOH N 702



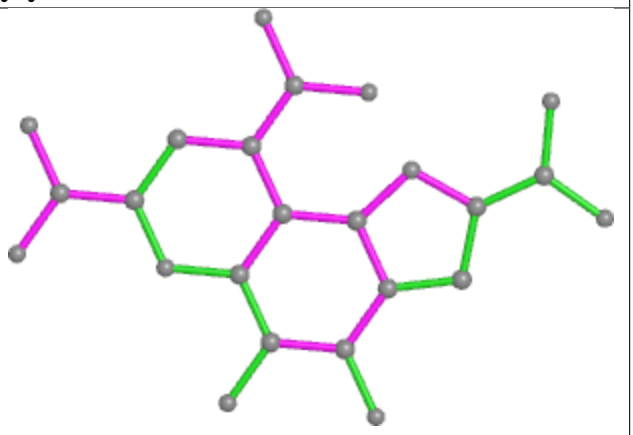
Ligand PQQ C 702



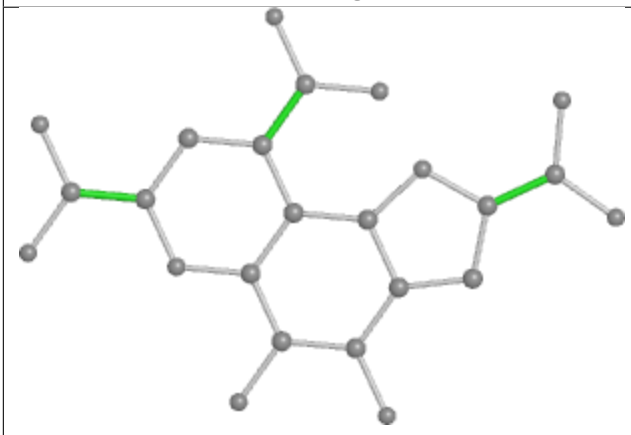
Ligand PQQ H 703



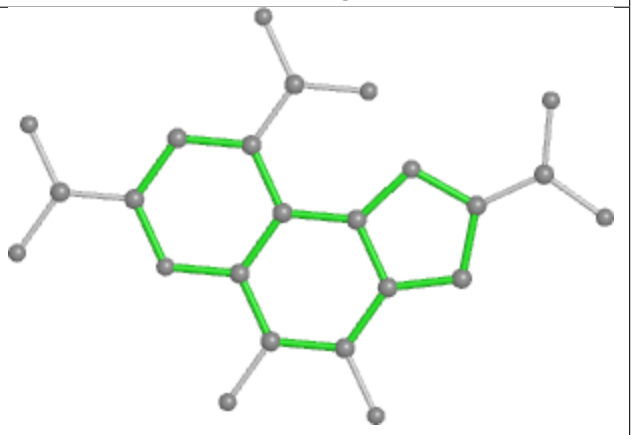
Bond lengths



Bond angles

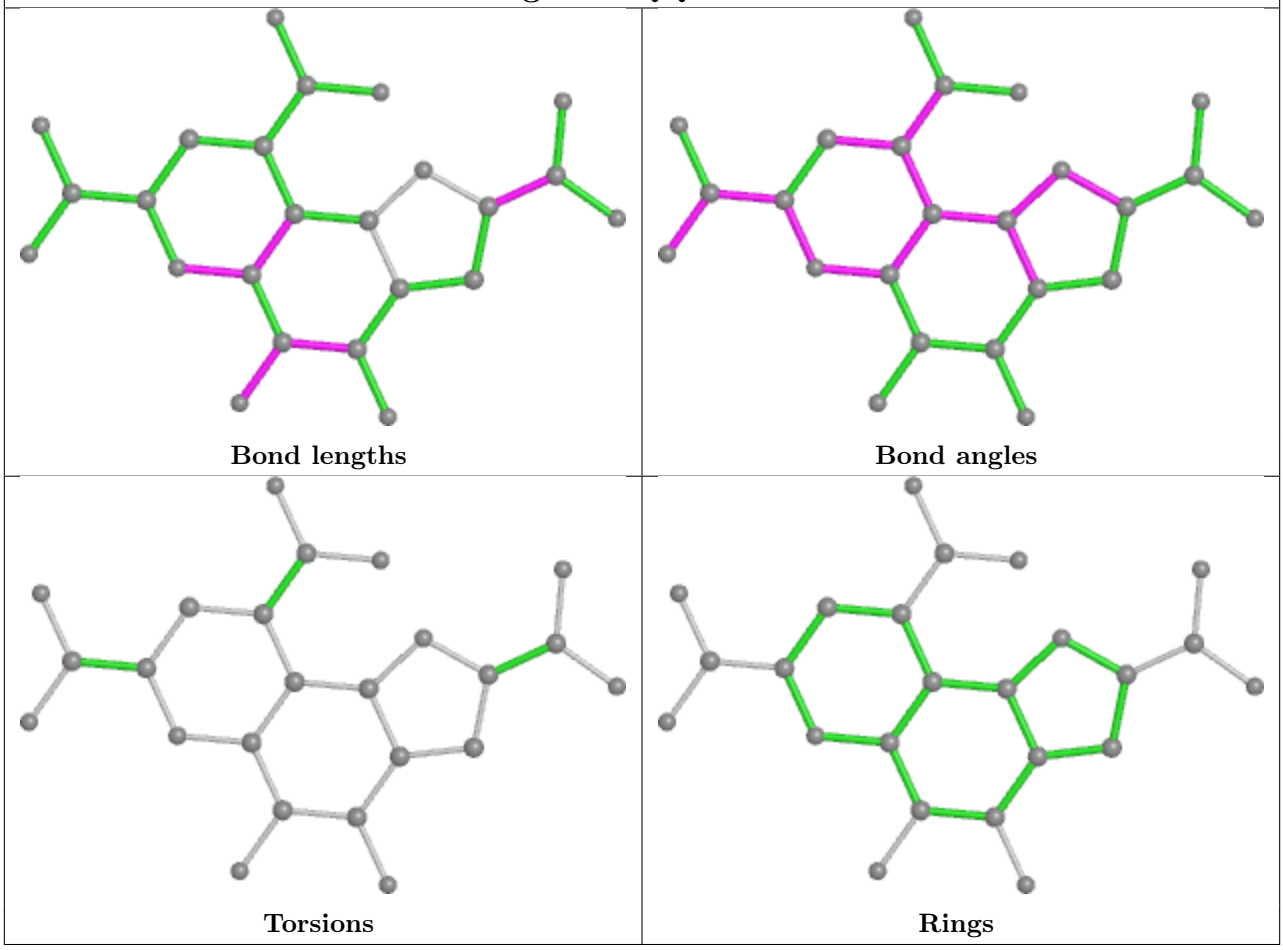


Torsions

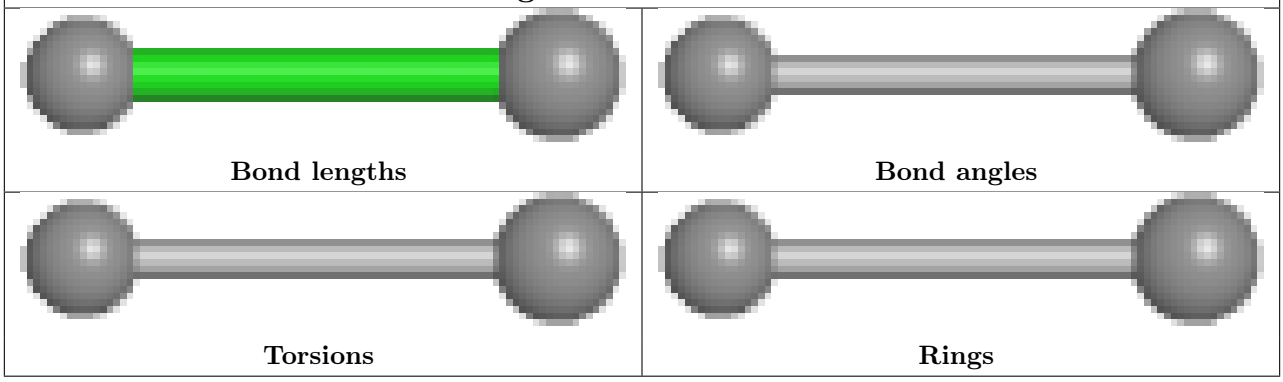


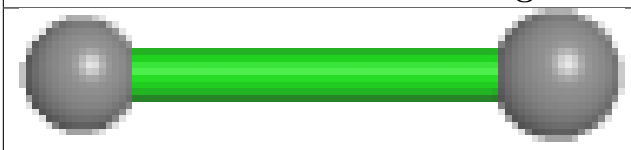
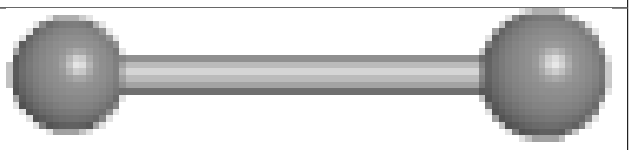
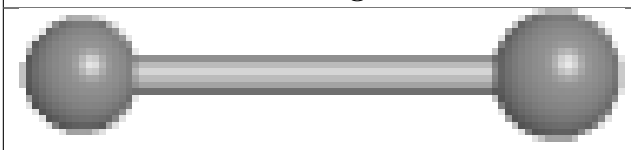
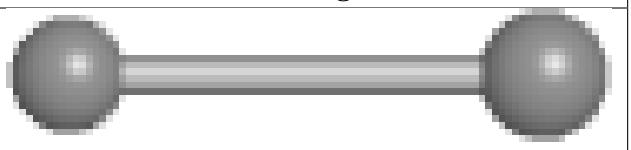
Rings

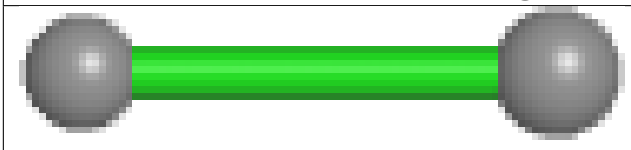
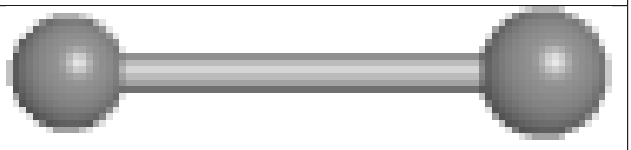
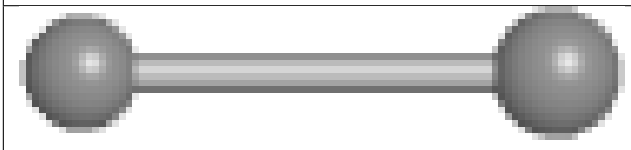
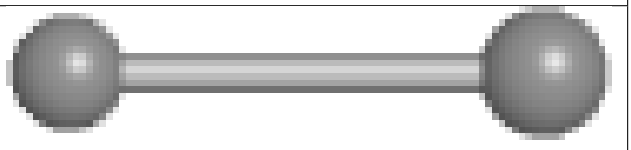
Ligand PQQ A 703



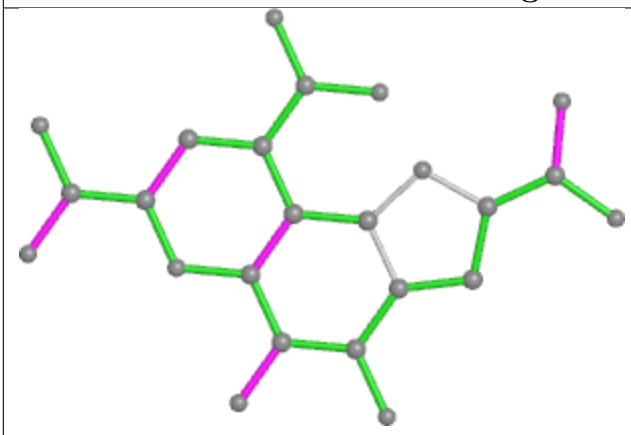
Ligand MOH A 702



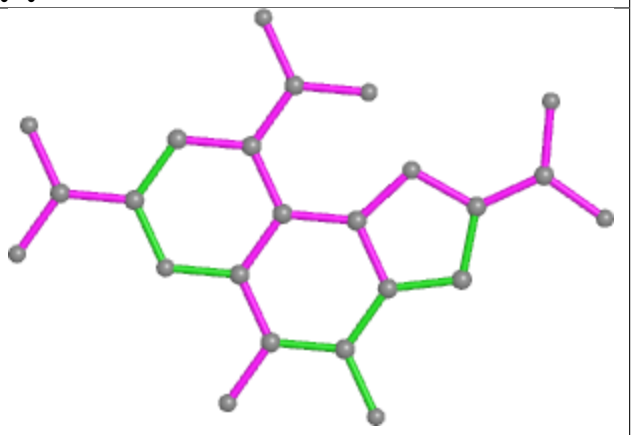
Ligand MOH G 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MOH D 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

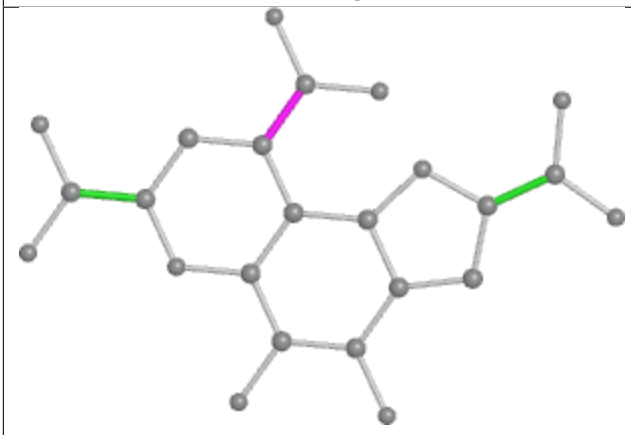
Ligand PQQ G 703



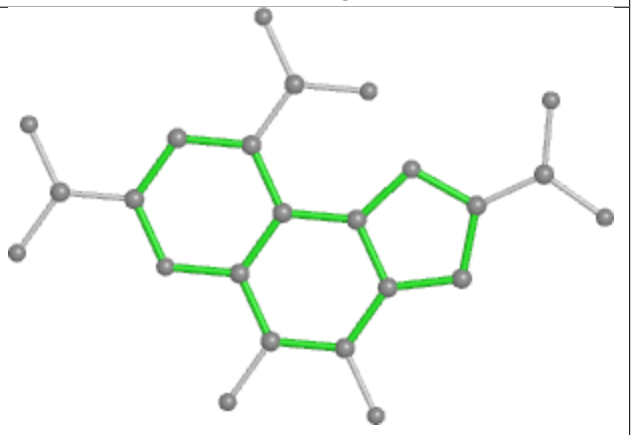
Bond lengths



Bond angles

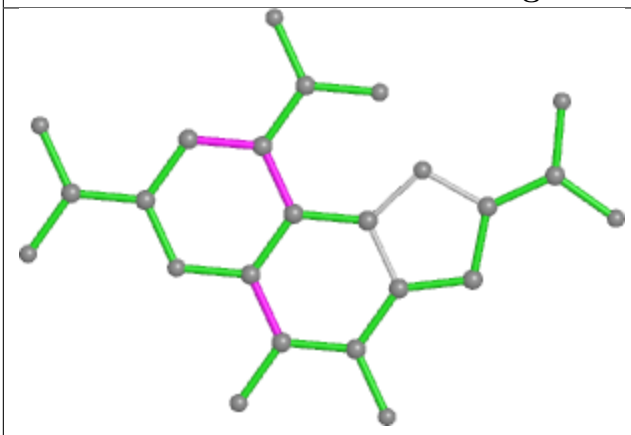


Torsions

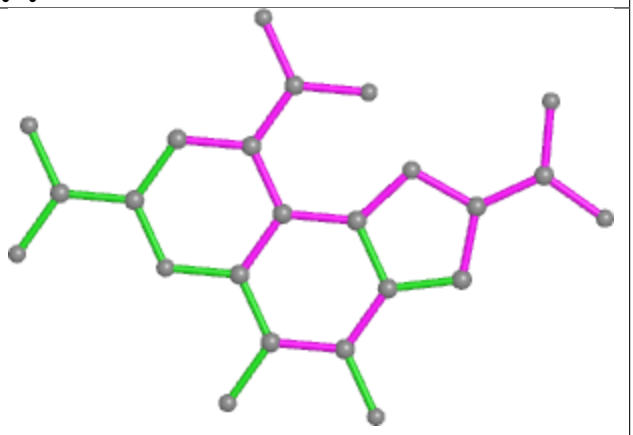


Rings

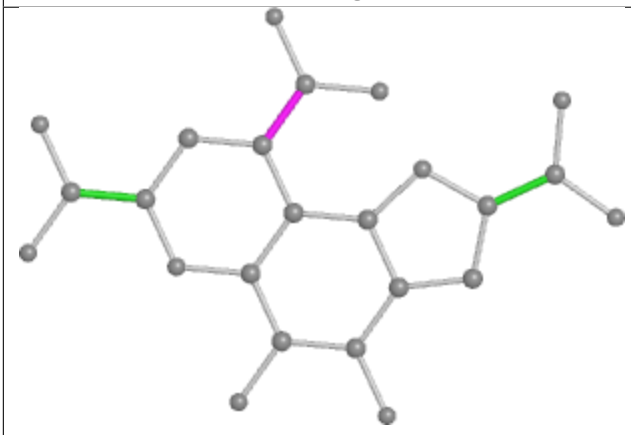
Ligand PQQ B 703



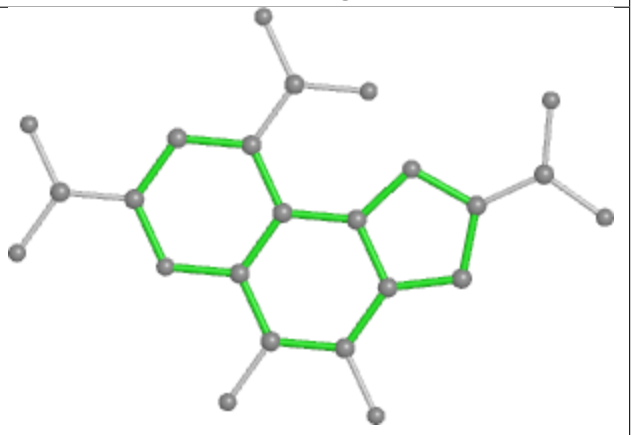
Bond lengths



Bond angles

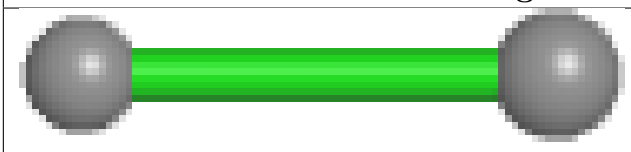


Torsions

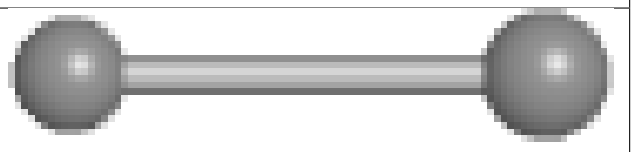


Rings

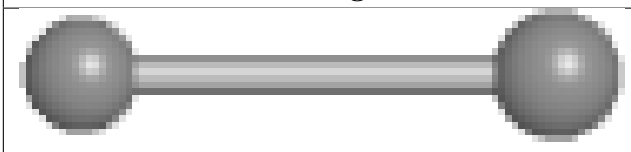
Ligand MOH H 702



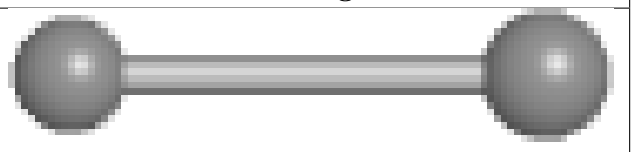
Bond lengths



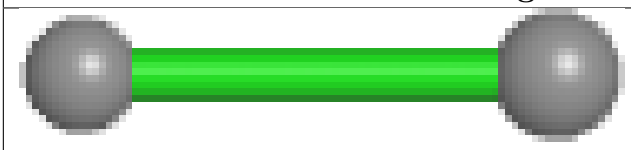
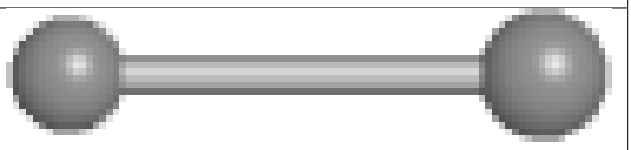
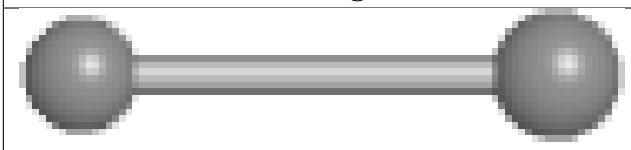
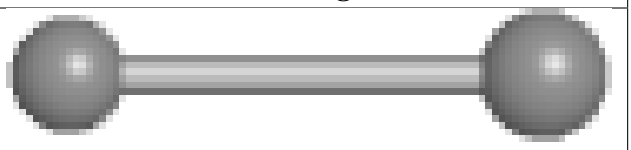
Bond angles

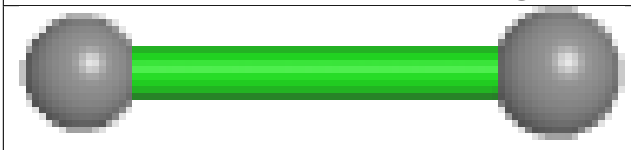
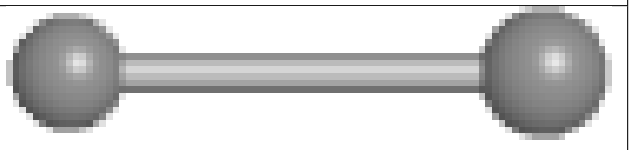
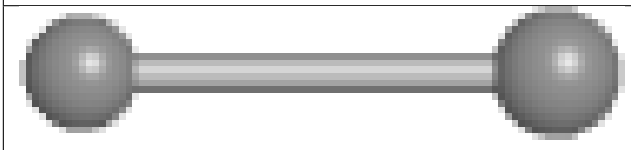
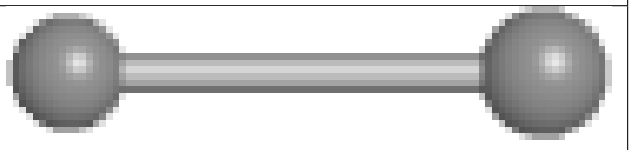


Torsions

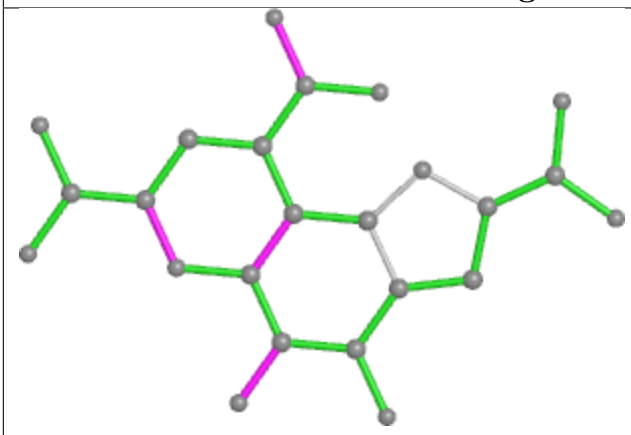


Rings

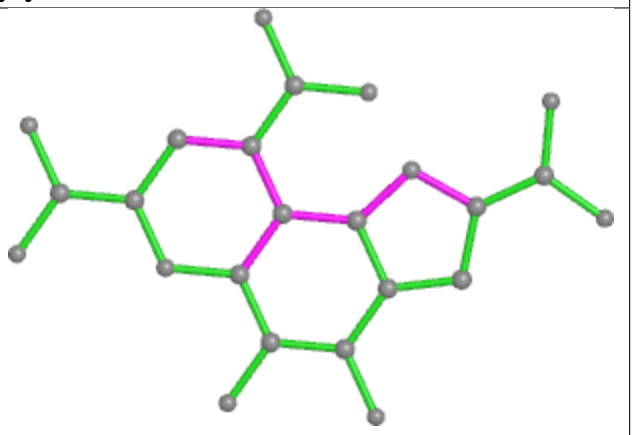
Ligand MOH B 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MOH M 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

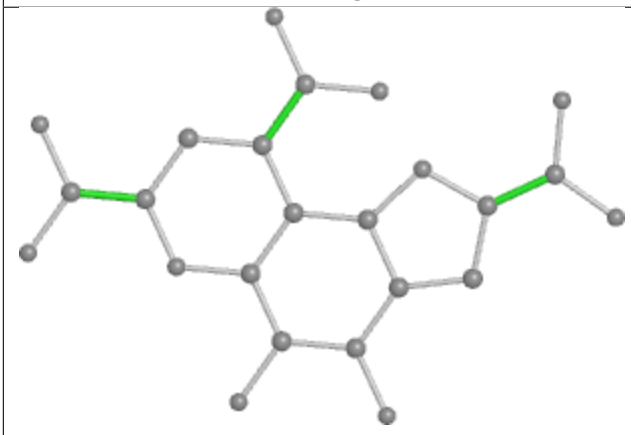
Ligand PQQ M 703



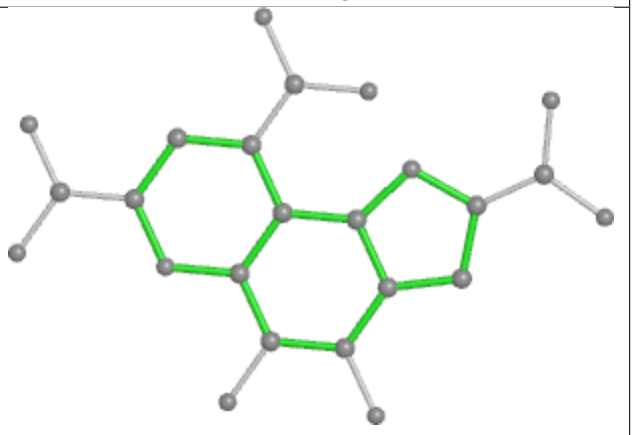
Bond lengths



Bond angles

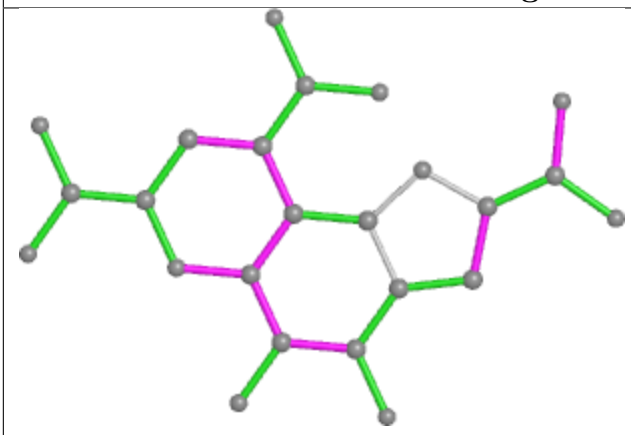


Torsions

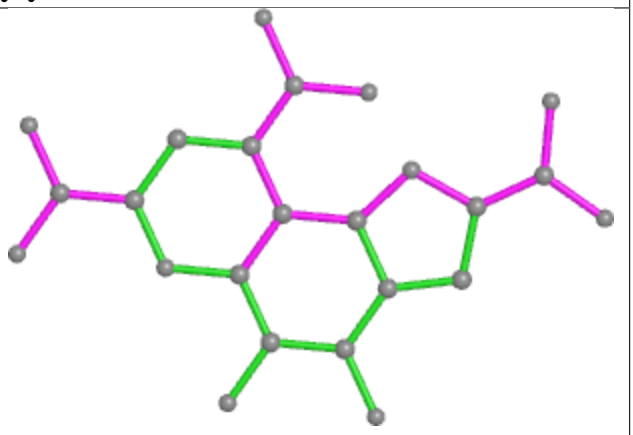


Rings

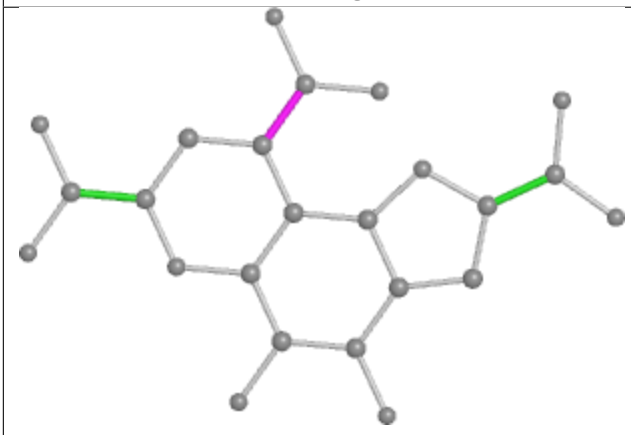
Ligand PQQ N 703



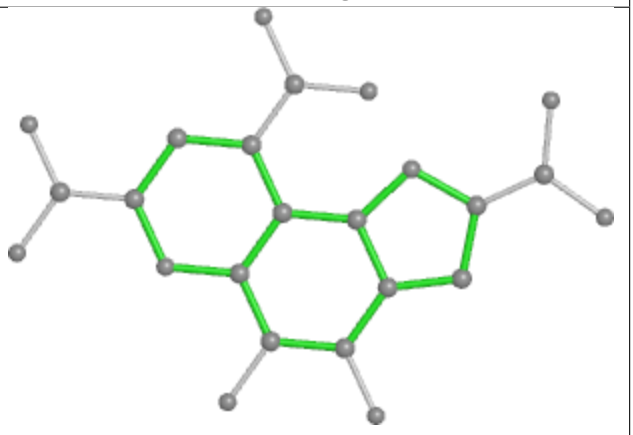
Bond lengths



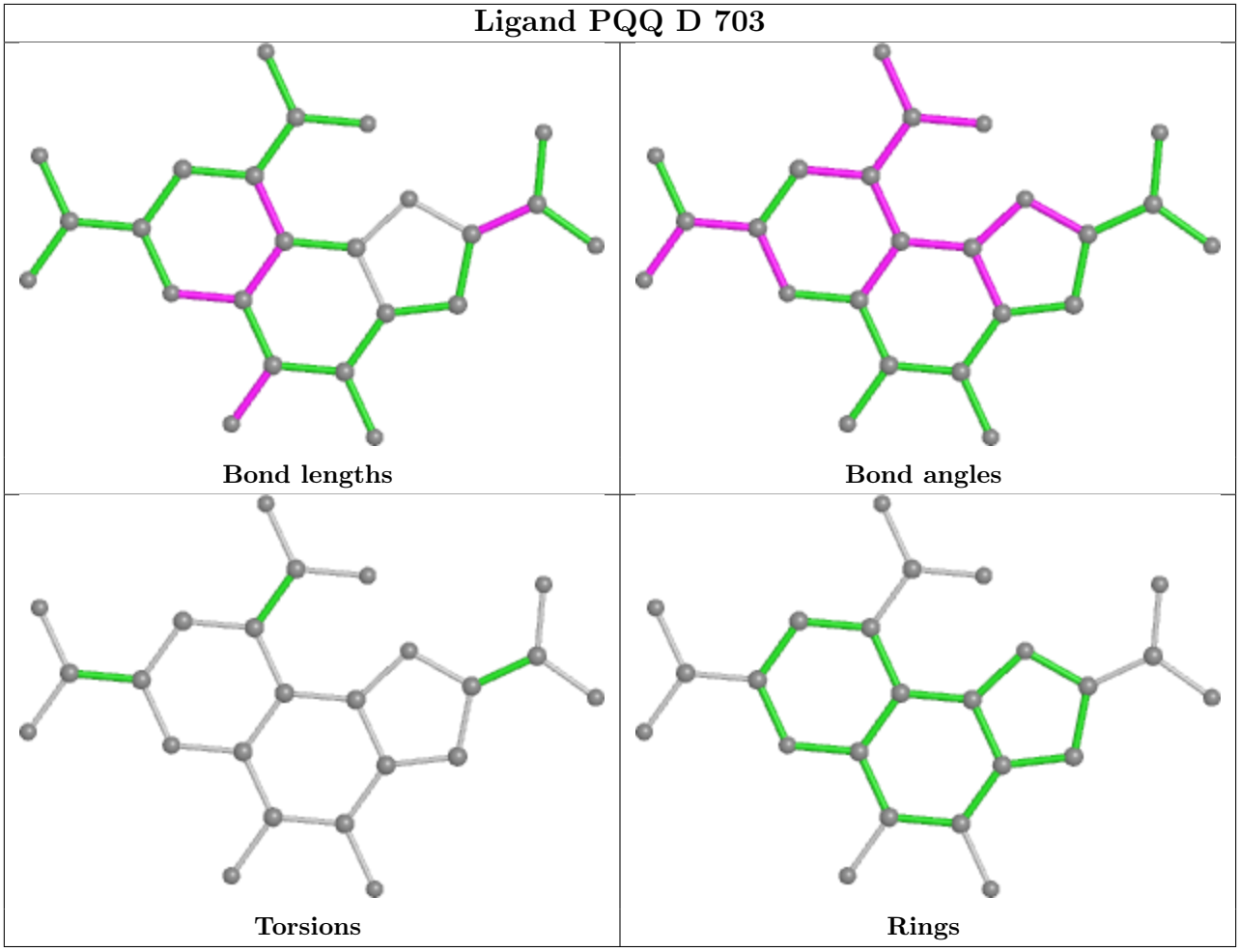
Bond angles

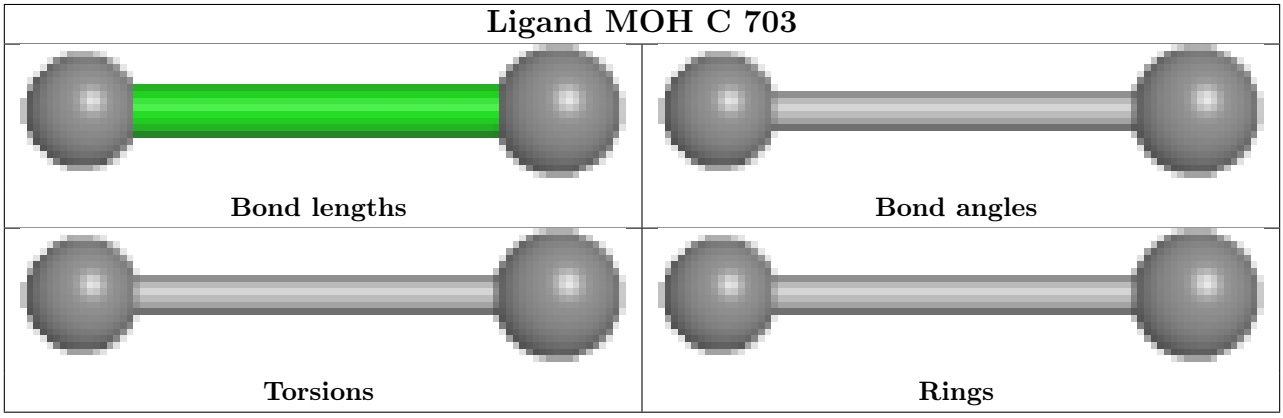


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	573/573 (100%)	-0.48	1 (0%) 95 93	11, 16, 28, 45	0
1	B	573/573 (100%)	-0.44	2 (0%) 94 92	11, 15, 28, 43	0
1	C	573/573 (100%)	-0.51	0 100 100	11, 15, 25, 43	0
1	D	573/573 (100%)	-0.46	2 (0%) 94 92	11, 16, 27, 48	0
1	G	573/573 (100%)	-0.51	2 (0%) 94 92	11, 15, 25, 40	0
1	H	573/573 (100%)	-0.36	2 (0%) 94 92	12, 20, 32, 52	0
1	M	573/573 (100%)	-0.50	1 (0%) 95 93	11, 15, 26, 42	0
1	N	573/573 (100%)	-0.40	3 (0%) 91 89	12, 19, 30, 46	0
2	E	71/72 (98%)	-0.05	1 (1%) 75 72	16, 22, 38, 49	0
2	F	71/72 (98%)	-0.14	4 (5%) 24 19	14, 21, 47, 90	0
2	I	71/72 (98%)	-0.14	3 (4%) 36 30	14, 20, 40, 51	0
2	J	71/72 (98%)	0.58	10 (14%) 2 1	23, 32, 51, 65	0
2	K	71/72 (98%)	-0.16	2 (2%) 53 47	14, 20, 34, 46	0
2	L	71/72 (98%)	-0.18	1 (1%) 75 72	16, 22, 36, 51	0
2	O	71/72 (98%)	0.16	7 (9%) 7 5	15, 22, 65, 95	0
2	P	71/72 (98%)	0.37	7 (9%) 7 5	21, 28, 47, 57	0
All	All	5152/5160 (99%)	-0.40	48 (0%) 84 82	11, 17, 32, 95	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	93	ILE	7.7
2	O	92	ASP	7.3
2	O	93	ILE	6.8
2	O	90	VAL	6.2
2	F	92	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
2	O	91	GLU	4.3
2	F	91	GLU	4.1
2	J	82	LYS	3.9
2	E	93	ILE	3.2
2	J	90	VAL	3.2
1	H	346	ASP	3.0
2	P	91	GLU	2.9
1	H	584	ARG	2.9
2	P	28	CYS	2.9
2	F	90	VAL	2.8
2	P	90	VAL	2.8
1	N	347	GLY	2.7
2	J	91	GLU	2.7
1	G	346	ASP	2.7
1	B	347	GLY	2.6
1	N	346	ASP	2.6
2	L	91	GLU	2.6
2	J	57	ASN	2.6
2	P	82	LYS	2.6
2	P	47	GLY	2.5
1	D	346	ASP	2.4
2	K	91	GLU	2.4
2	I	81	ALA	2.3
1	D	63	HIS	2.3
2	J	40	GLY	2.3
2	J	43	ASP	2.3
2	O	89	LYS	2.3
2	I	91	GLU	2.3
2	J	81	ALA	2.3
2	J	83	THR	2.3
2	O	85	LYS	2.2
2	J	93	ILE	2.2
1	G	347	GLY	2.2
2	O	84	GLY	2.2
1	N	349	LEU	2.2
1	M	346	ASP	2.1
2	I	85	LYS	2.1
2	K	93	ILE	2.1
2	P	84	GLY	2.1
2	J	89	LYS	2.1
1	B	346	ASP	2.0
2	P	93	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	571	LYS	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	MOH	H	702	2/2	0.34	0.66	64,64,64,72	0
4	MOH	G	702	2/2	0.42	0.57	43,43,43,54	0
4	MOH	B	702	2/2	0.57	0.74	50,50,50,56	0
4	MOH	A	702	2/2	0.61	0.54	67,67,67,74	0
4	MOH	D	702	2/2	0.70	0.36	56,56,56,59	0
4	MOH	M	702	2/2	0.72	0.39	42,42,42,45	0
4	MOH	C	703	2/2	0.73	0.41	44,44,44,53	0
4	MOH	N	702	2/2	0.74	0.27	48,48,48,49	0
5	PQQ	H	703	24/24	0.96	0.07	16,18,21,22	0
5	PQQ	A	703	24/24	0.97	0.07	12,15,19,21	0
5	PQQ	C	702	24/24	0.97	0.07	13,15,19,22	0
5	PQQ	D	703	24/24	0.97	0.06	13,14,17,19	0
5	PQQ	G	703	24/24	0.97	0.07	13,15,18,20	0
3	CA	H	701	1/1	0.97	0.10	45,45,45,45	0
5	PQQ	M	703	24/24	0.97	0.07	12,15,17,19	0
5	PQQ	N	703	24/24	0.97	0.07	14,16,19,20	0
3	CA	M	701	1/1	0.98	0.15	40,40,40,40	0
5	PQQ	B	703	24/24	0.98	0.07	12,14,16,17	0
3	CA	G	701	1/1	0.98	0.15	44,44,44,44	0
3	CA	A	701	1/1	0.98	0.16	41,41,41,41	0
3	CA	C	701	1/1	0.99	0.21	42,42,42,42	0
3	CA	D	701	1/1	0.99	0.13	43,43,43,43	0

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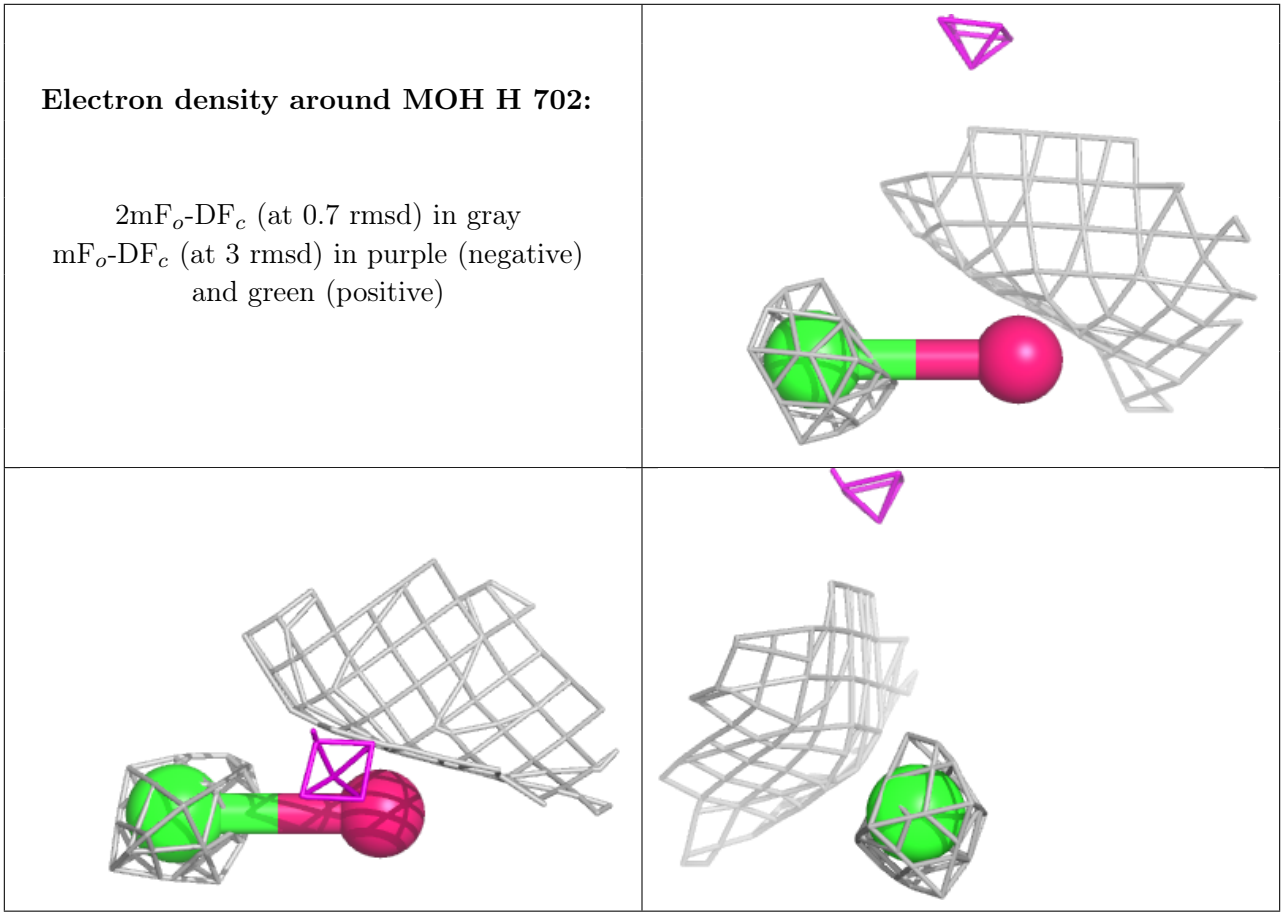
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	B	701	1/1	0.99	0.12	42,42,42,42	0
3	CA	N	701	1/1	1.00	0.16	51,51,51,51	0

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.

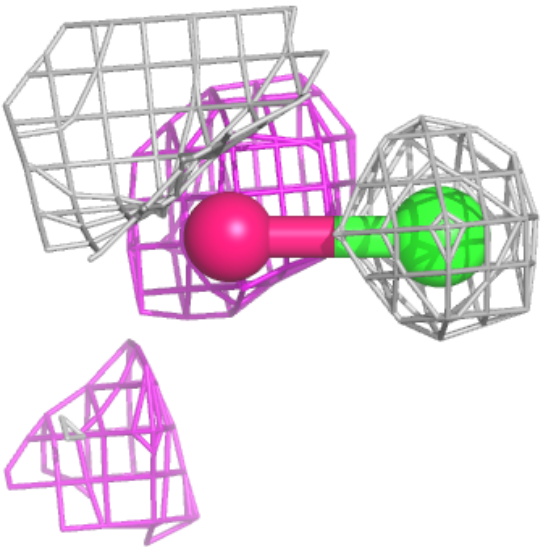
Electron density around MOH H 702:

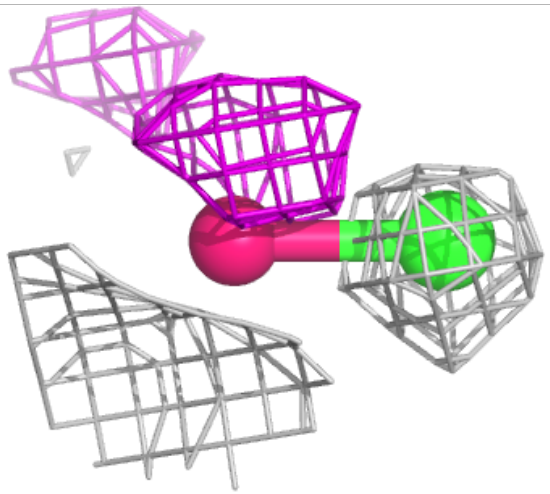
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

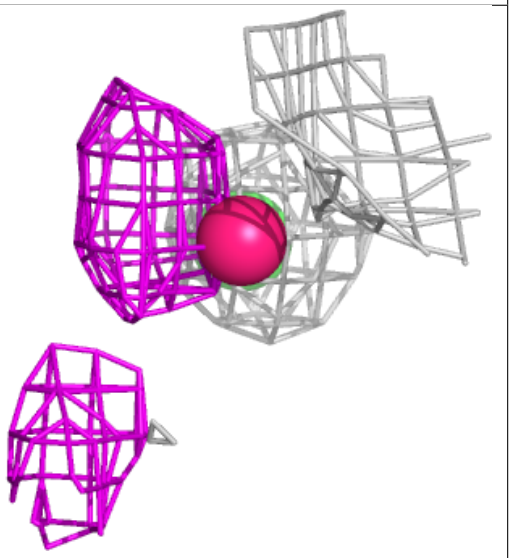


Electron density around MOH G 702:

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

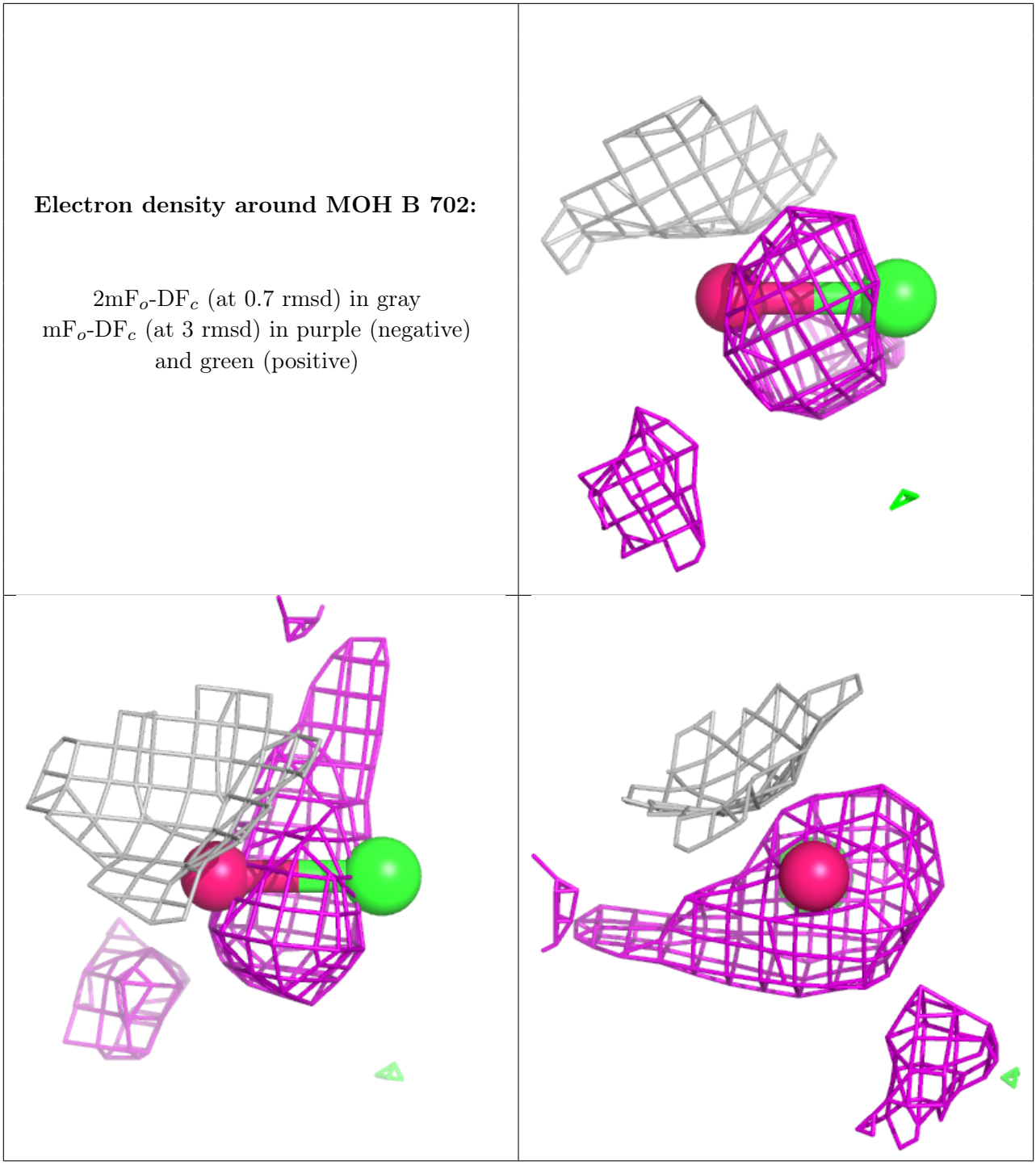






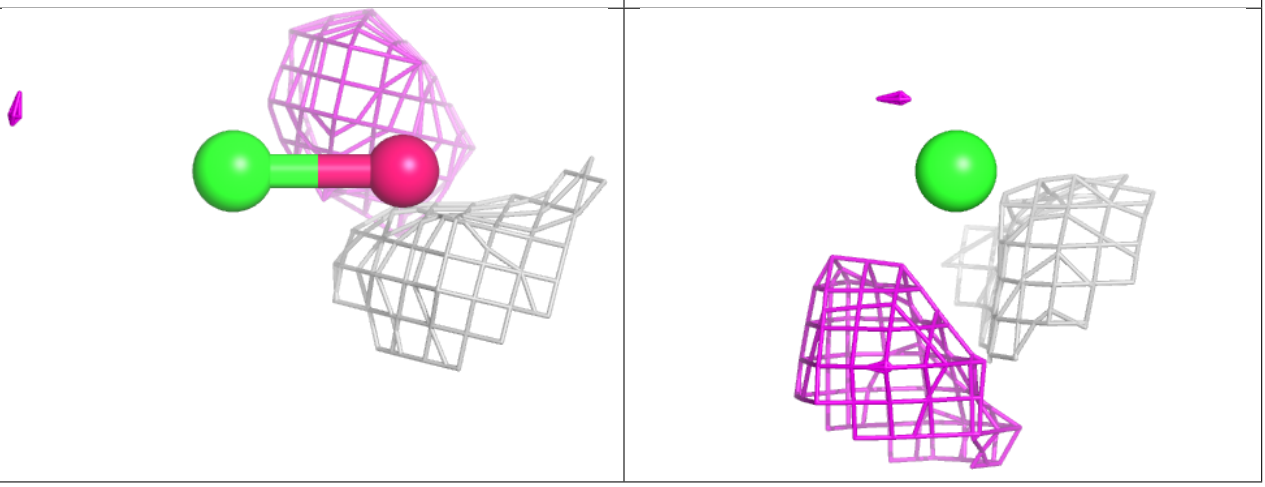
Electron density around MOH B 702:

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



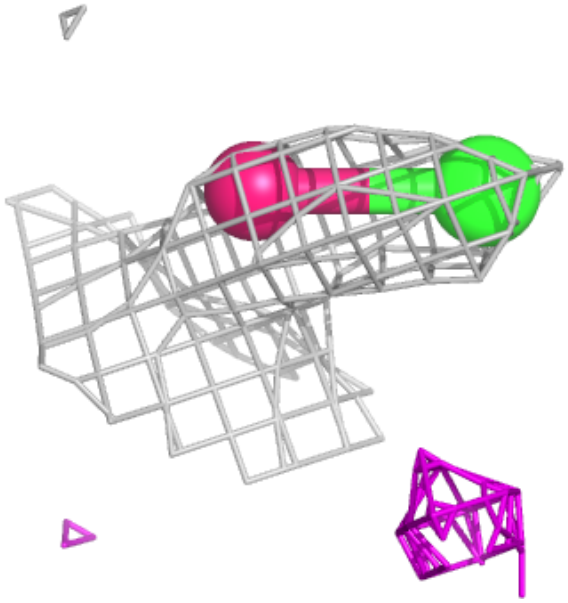
Electron density around MOH A 702:

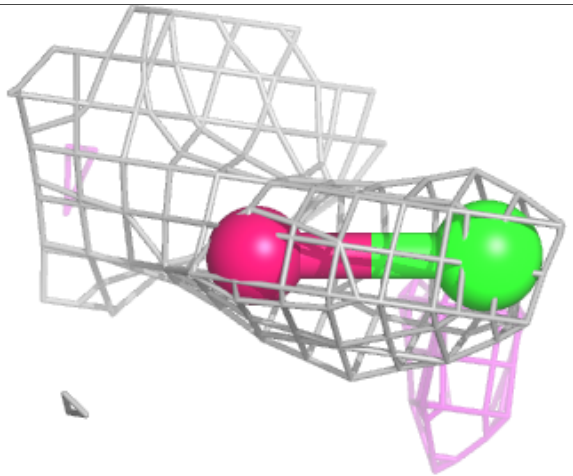
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

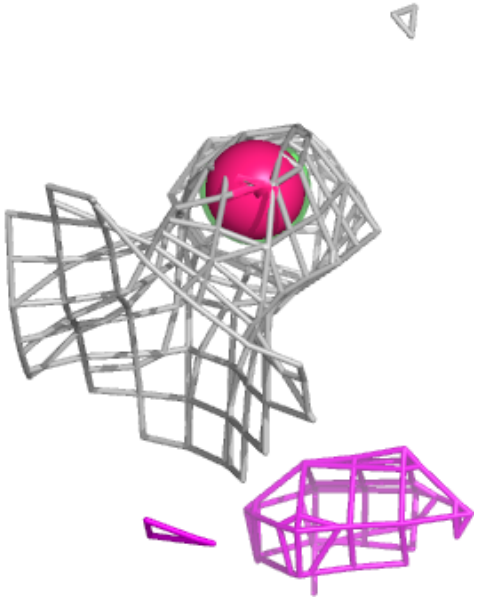


Electron density around MOH D 702:

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

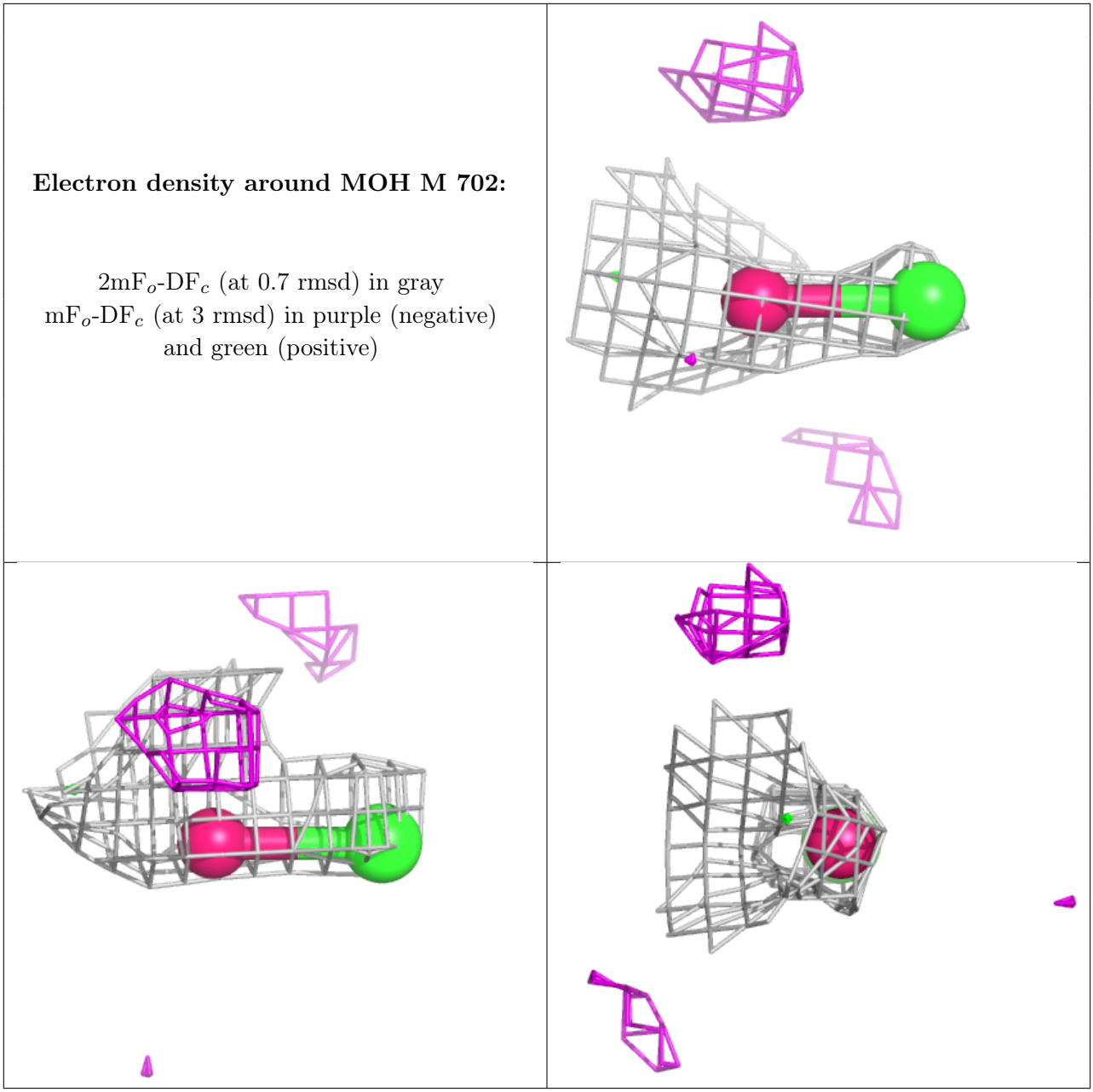






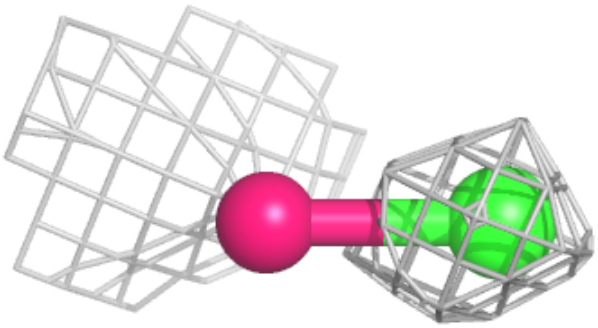
Electron density around MOH M 702:

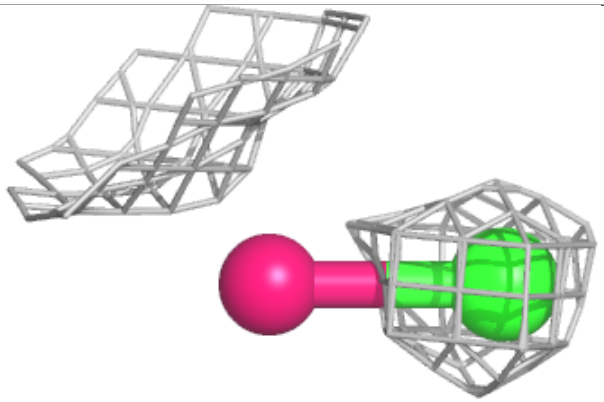
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

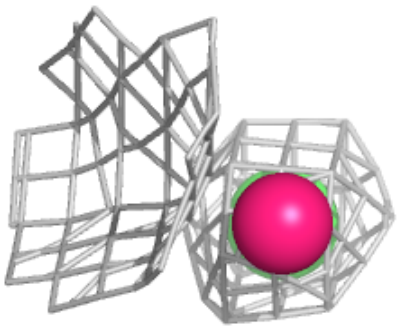


Electron density around MOH C 703:

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

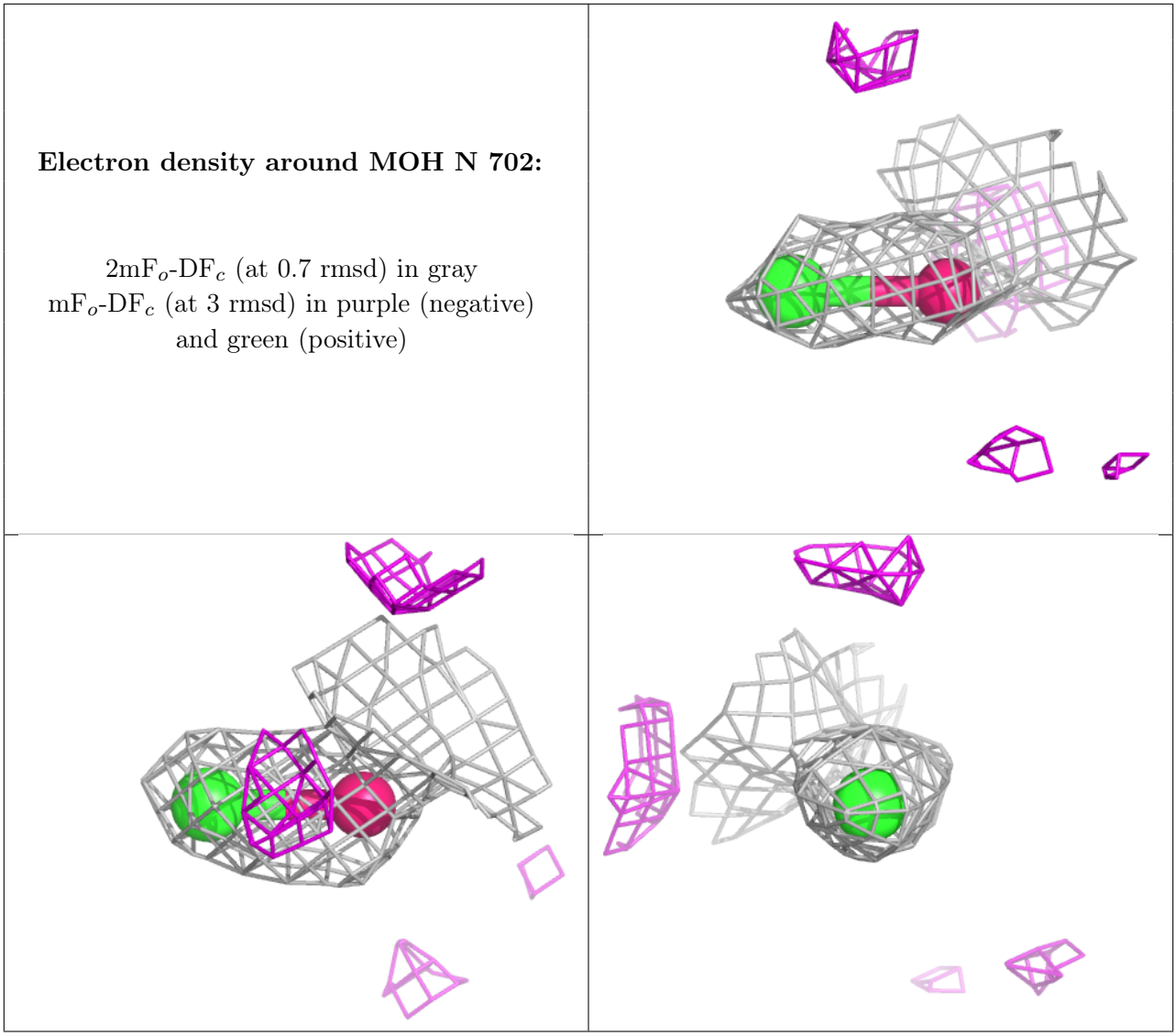






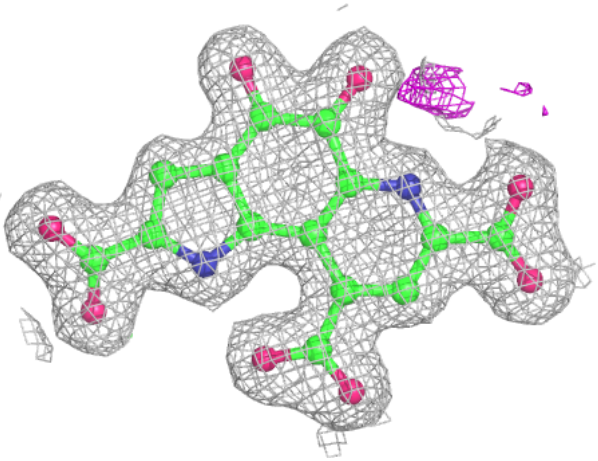
Electron density around MOH N 702:

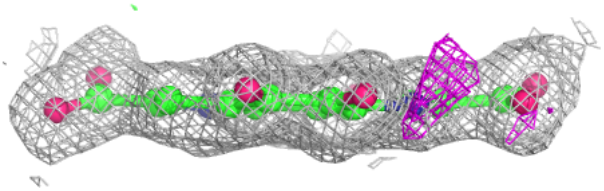
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

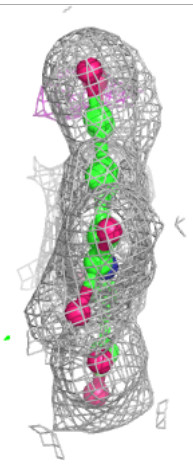


Electron density around PQQ H 703:

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

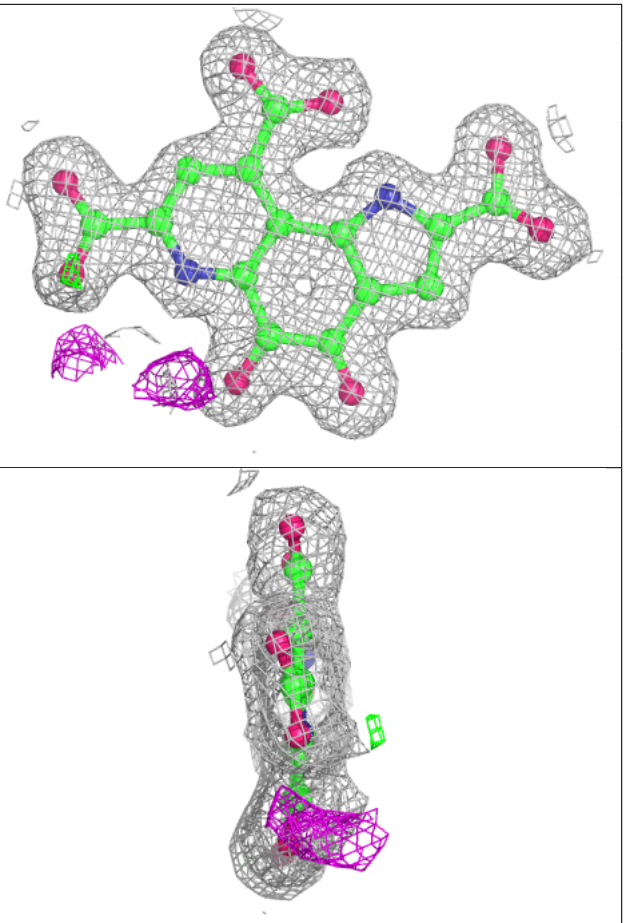


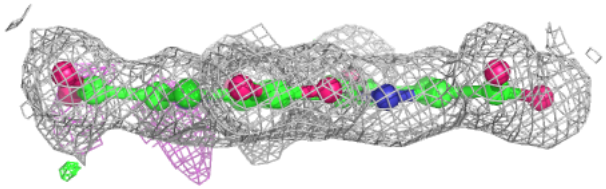




Electron density around PQQ A 703:

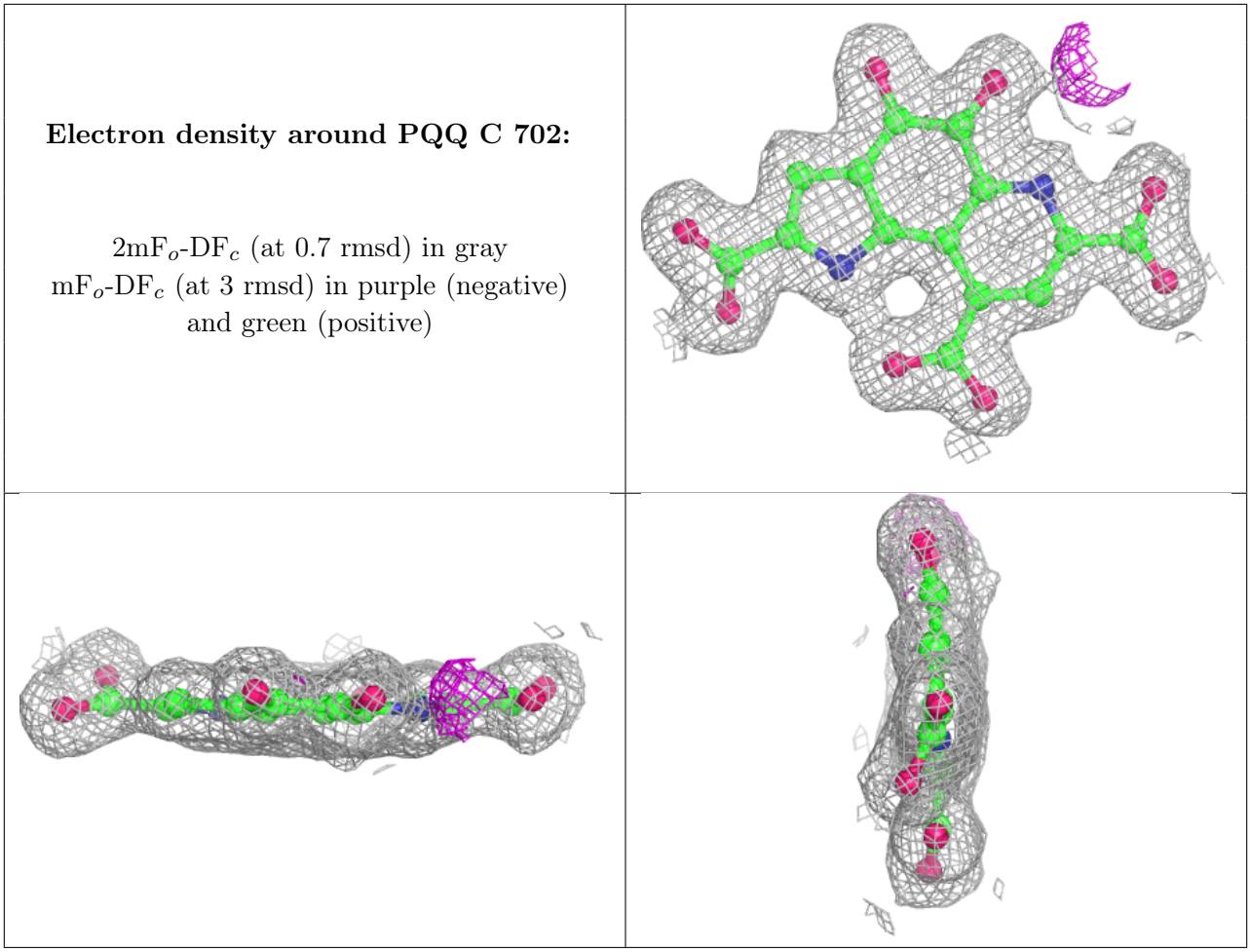
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





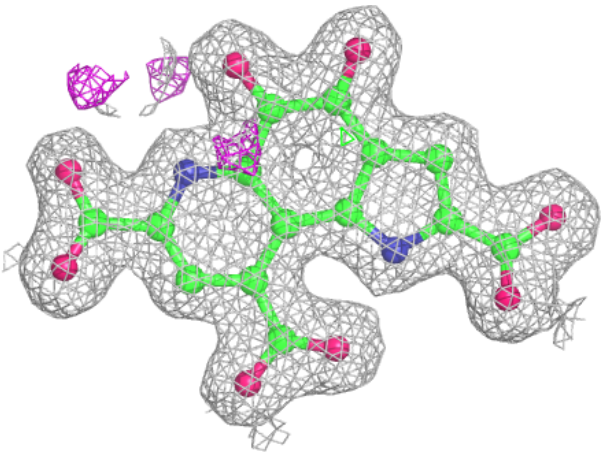
Electron density around PQQ C 702:

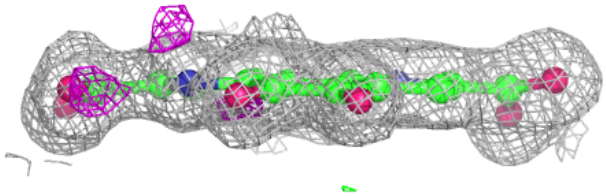
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

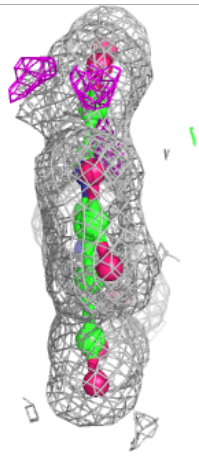


Electron density around PQQ D 703:

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

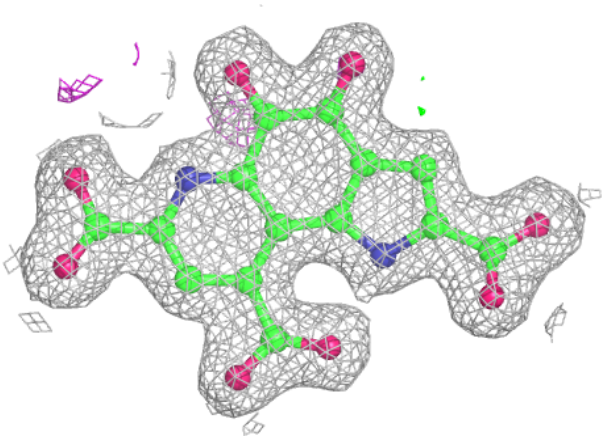


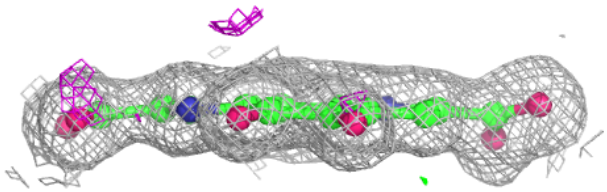


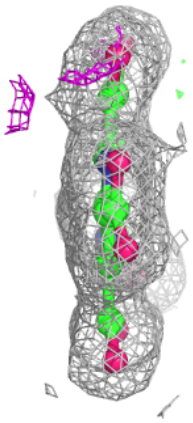


Electron density around PQQ G 703:

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

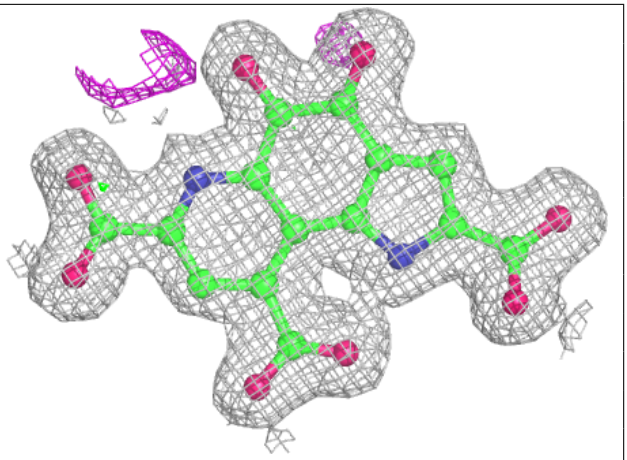


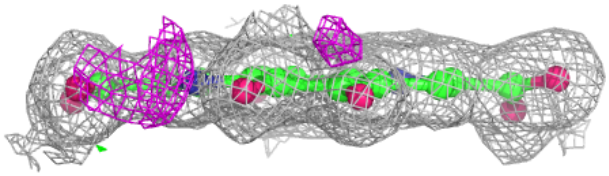


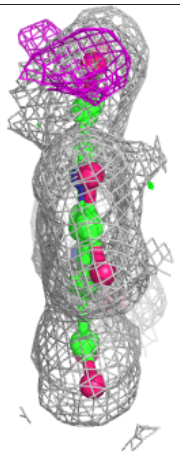


Electron density around PQQ M 703:

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

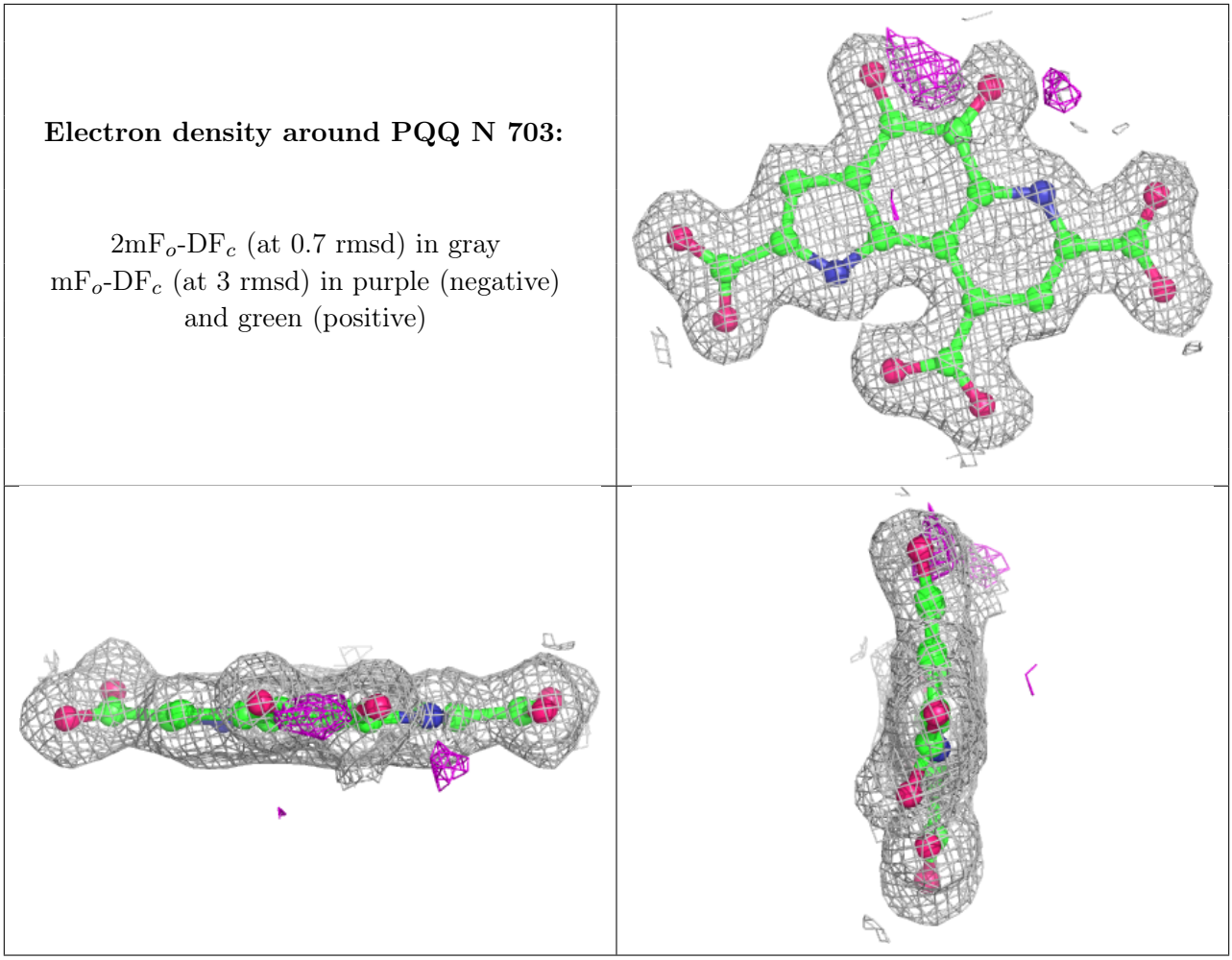






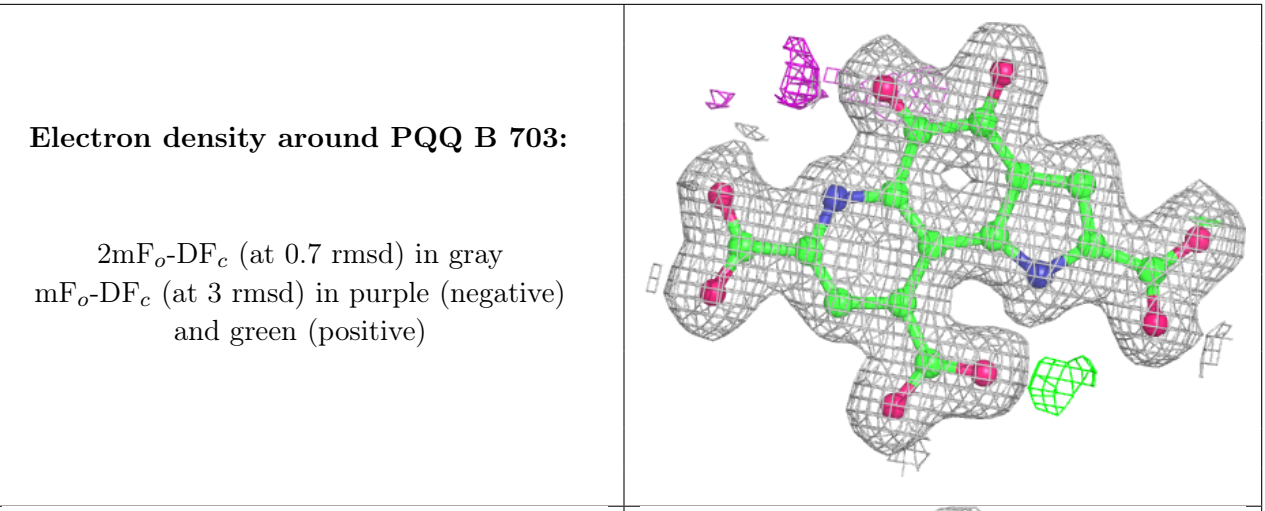
Electron density around PQQ N 703:

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



Electron density around PQQ B 703:

$2mF_o$-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.