WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 01:34 AM JST

|		
PDB ID	:	7CDL
Title	:	holo-methanol dehydrogenase (MDH) with Cys131-Cys132 reduced 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	:	2020-06-20
Resolution	:	1.85 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.85 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.
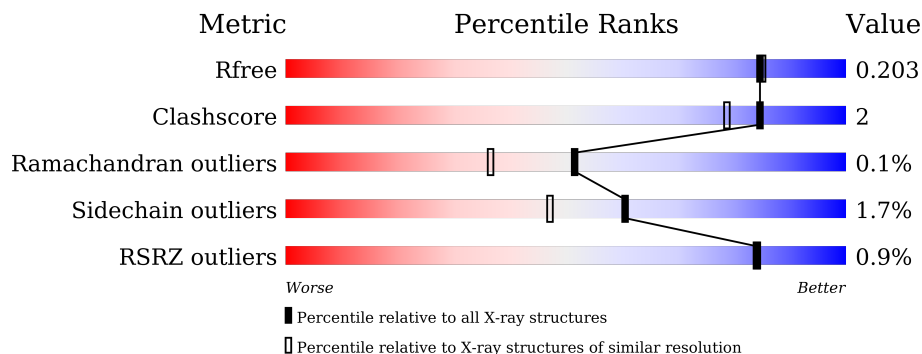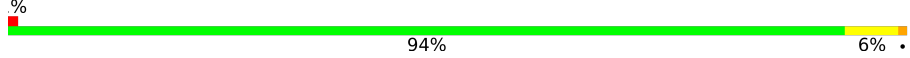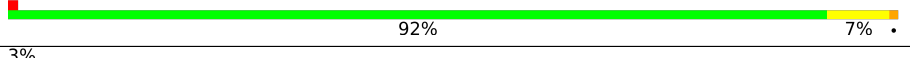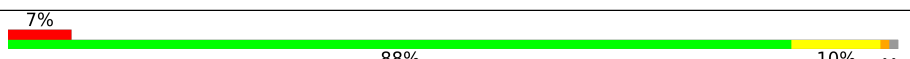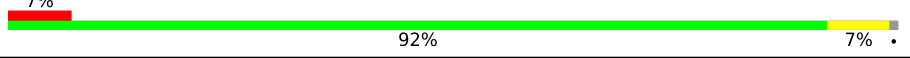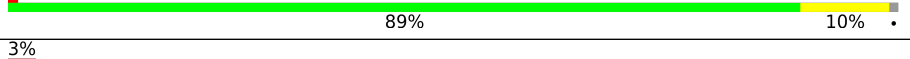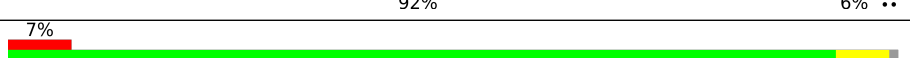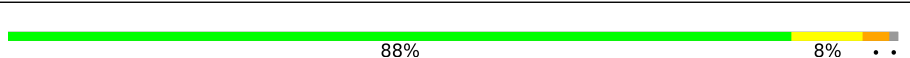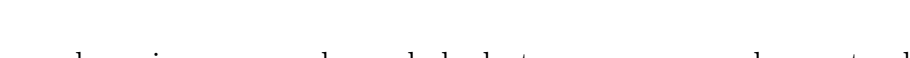

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	91% / 9%
1	B	573	93% / 6% ·
1	C	573	94% / 6%
1	D	573	92% / 7% ·
1	G	573	92% / 8% ·

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Mol	Chain	Length	Quality of chain
1	H	573	94% ... 6%
1	M	573	92% ... 6%
1	N	573	92% ... 7%
2	E	72	3% ... 90% ... 8%
2	F	72	7% ... 83% ... 11%
2	I	72	7% ... 88% ... 10%
2	J	72	7% ... 92% ... 7%
2	K	72	89% ... 10%
2	L	72	3% ... 92% ... 6%
2	O	72	7% ... 93% ... 6%
2	P	72	88% ... 8%

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	PQQ	B	702	-	-	X	-
4	PQQ	G	702	-	-	X	-
4	PQQ	H	702	-	X	-	-
4	PQQ	N	702	-	X	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 45133 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	C	573	Total 4491	C 2871	N 765	O 832	S 23	0	0	0
1	D	573	Total 4490	C 2871	N 765	O 831	S 23	0	0	0
1	A	573	Total 4491	C 2871	N 765	O 832	S 23	0	0	0
1	B	573	Total 4490	C 2871	N 765	O 831	S 23	0	0	0
1	G	573	Total 4491	C 2871	N 765	O 832	S 23	0	0	0
1	H	573	Total 4490	C 2871	N 765	O 831	S 23	0	0	0
1	M	573	Total 4491	C 2871	N 765	O 832	S 23	0	0	0
1	N	573	Total 4490	C 2871	N 765	O 831	S 23	0	0	0

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

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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: $C_{14}H_6N_2O_8$) (labeled as "Ligand of Interest" by depositor).

PQQ

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	483	Total 483	O 483	0	0
5	K	87	Total 87	O 87	0	0
5	D	516	Total 516	O 516	0	0
5	L	98	Total 98	O 98	0	0

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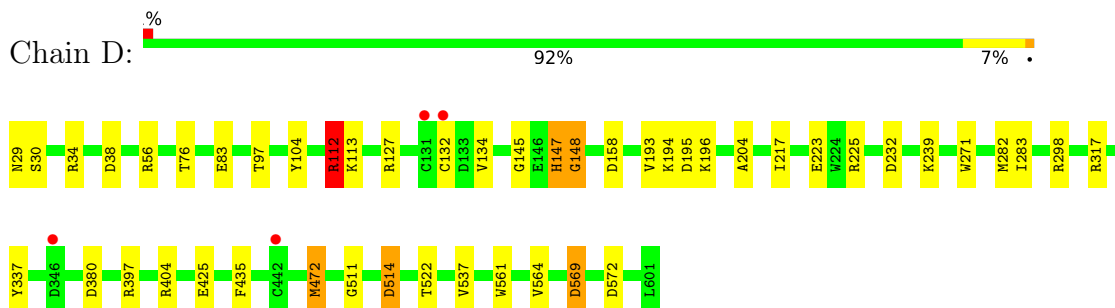| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	452	Total 452	O 452	0	0
5	E	84	Total 84	O 84	0	0
5	B	511	Total 511	O 511	0	0
5	F	81	Total 81	O 81	0	0
5	G	496	Total 496	O 496	0	0
5	I	78	Total 78	O 78	0	0
5	H	441	Total 441	O 441	0	0
5	J	60	Total 60	O 60	0	0
5	M	440	Total 440	O 440	0	0
5	O	60	Total 60	O 60	0	0
5	N	488	Total 488	O 488	0	0
5	P	90	Total 90	O 90	0	0

3 Residue-property plots ⓘ

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.
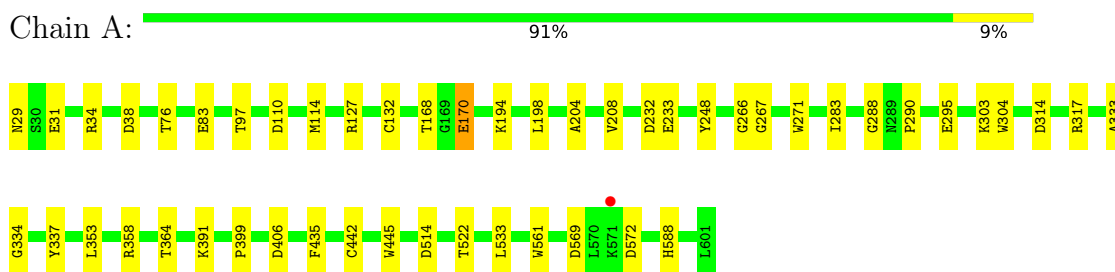
• Molecule 1: Methanol dehydrogenase protein, large subunit
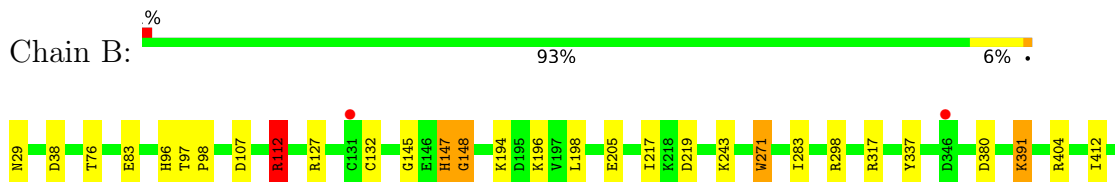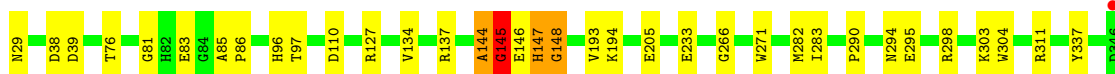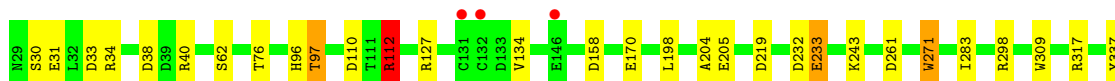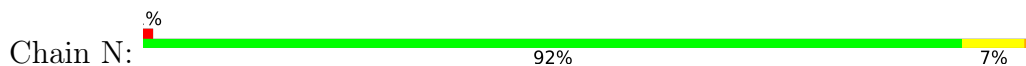
Chain C:

• Molecule 1: Methanol dehydrogenase protein, large subunit
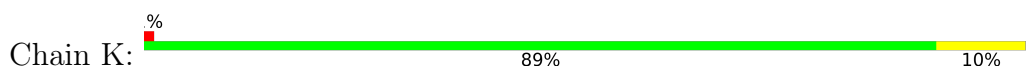
Chain D:

• Molecule 1: Methanol dehydrogenase protein, large subunit

Chain A:

• Molecule 1: Methanol dehydrogenase protein, large subunit

Chain B:

Y427 C442 M443 D444 E489 K493 D514 W561 L566 K571 D572 R584 Q591 L601

- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain G:
92%
8%

N29 D38 D39 T76 G81 H82 E83 G84 A85 P86 H96 T97 D110 R127 V134 R137 A144 G145 E146 H147 G148 V193 K194 E205 E233 G266 W271 M282 I283 P290 N294 E295 R298 K303 W304 R311 Y337 D346

L372 D389 R397 F435 R453 R520 D521 T522 R523 I538 W561 D569 D572 R584 L601

- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain H:
%
94%
6%

N29 R34 R40 K66 T76 E83 H96 T97 R112 R127 C131 C132 A144 G145 E146 H147 G148 V193 K196 E205 V208 G267 W271 Y276 K279 I283 D314 R317 Y332 A333 Y337 D346 G347 I412

Y427 C442 R453 W561 K571 D572 L601

- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain M:
92%
6%

N29 S30 D38 K66 E83 D90 H96 T97 P98 Y104 Q117 R127 C131 A144 G145 E146 H147 G148 K167 V193 K194 I217 W271 Y276 M282 I283 R317 Y337 D346 Y363 K391 R397 I412 C442 P447

A461 F509 L533 I538 P541 I552 W561 L566 K571 D572 H588 L601

- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain N:
%
92%
7%

N29 S30 E31 L32 D33 R34 D38 D39 R40 S62 T76 H96 T97 D110 T111 R112 R127 C131 C132 D133 V134 E146 D158 E170 L198 A204 E205 D219 D232 E233 K243 D261 W271 I283 R298 W309 R317 Y337

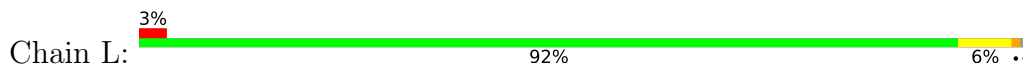D346 R367 D406 I412 C442 M443 D444 Y452 R453 L507 D514 R520 G557 K571 D572 R584 S595 L601

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

Chain K:
%
89%
10%

● Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2
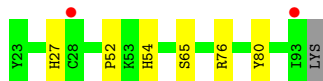
Chain L:

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

Chain E:

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

Chain F:

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

Chain I:
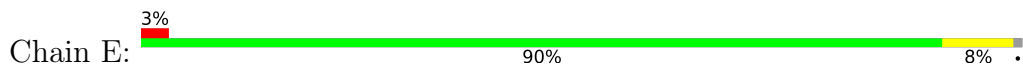

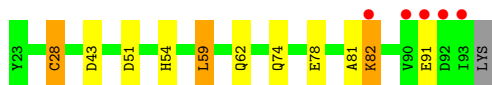● Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2
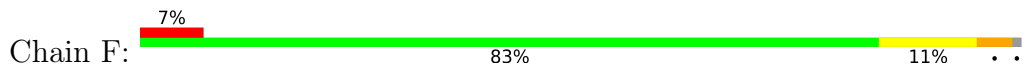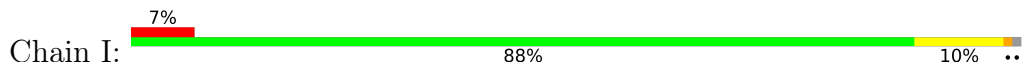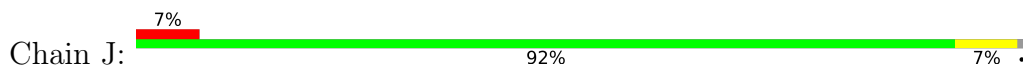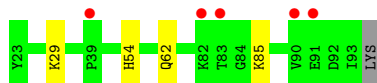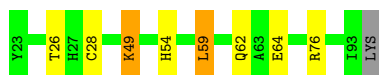
Chain J:

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

Chain O:

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

Chain P:

88%   8%

Y23 T26 H27 C28 K49 H54 L59 Q62 A63 E64 R76 I93 LYS

4 Data and refinement statistics $\textcircled{i}$

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.11Å 211.11Å 222.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 29.75 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-1.85) 99.8 (29.75-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.152 , 0.195 0.165 , 0.203	Depositor DCC
R_{free} test set	25548 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	45133	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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:
PQQ, CA

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	1.04	3/4622 (0.1%)	1.00	13/6281 (0.2%)
1	B	1.10	8/4621 (0.2%)	1.12	23/6281 (0.4%)
1	C	1.06	0/4622	1.04	14/6281 (0.2%)
1	D	1.08	5/4621 (0.1%)	1.19	30/6281 (0.5%)
1	G	1.09	8/4622 (0.2%)	1.08	26/6281 (0.4%)
1	H	1.04	7/4621 (0.2%)	1.12	16/6281 (0.3%)
1	M	1.07	5/4622 (0.1%)	1.02	14/6281 (0.2%)
1	N	1.09	9/4621 (0.2%)	1.15	29/6281 (0.5%)
2	E	0.95	0/583	0.94	2/785 (0.3%)
2	F	1.10	1/583 (0.2%)	1.08	4/785 (0.5%)
2	I	1.09	0/583	1.04	1/785 (0.1%)
2	J	0.92	0/583	0.94	1/785 (0.1%)
2	K	1.10	1/583 (0.2%)	1.08	5/785 (0.6%)
2	L	1.01	0/583	0.99	2/785 (0.3%)
2	O	0.90	0/583	0.90	0/785
2	P	1.11	2/583 (0.3%)	1.07	5/785 (0.6%)
All	All	1.07	49/41636 (0.1%)	1.08	185/56528 (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	D	0	1
1	G	0	2
1	H	0	1
1	M	0	2
1	N	0	1
All	All	0	7

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	ARG	CD-NE	-10.34	1.28	1.46
1	N	112	ARG	CD-NE	-9.37	1.30	1.46
1	B	148	GLY	N-CA	-8.84	1.32	1.46
1	H	112	ARG	CD-NE	-8.82	1.31	1.46
1	A	170	GLU	CD-OE1	8.53	1.35	1.25

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	ARG	NE-CZ-NH2	-27.97	106.31	120.30
1	H	112	ARG	NE-CZ-NH2	-25.44	107.58	120.30
1	H	112	ARG	NE-CZ-NH1	22.55	131.58	120.30
1	N	112	ARG	NE-CZ-NH1	20.35	130.48	120.30
1	N	112	ARG	NE-CZ-NH2	-19.91	110.35	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	112	ARG	Sidechain
1	G	144	ALA	Peptide
1	G	145	GLY	Peptide
1	H	144	ALA	Peptide
1	M	144	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	4491	0	4322	22	0
1	B	4490	0	4322	22	0
1	C	4491	0	4322	15	0
1	D	4490	0	4322	18	0
1	G	4491	0	4322	16	0
1	H	4490	0	4322	16	0
1	M	4491	0	4322	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4490	0	4322	11	0
2	E	568	0	545	4	0
2	F	568	0	545	4	0
2	I	568	0	545	6	0
2	J	568	0	545	2	0
2	K	568	0	545	4	0
2	L	568	0	545	2	0
2	O	568	0	545	4	0
2	P	568	0	545	10	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	24	0	4	5	0
4	B	24	0	3	7	0
4	C	24	0	3	4	0
4	D	24	0	3	5	0
4	G	24	0	3	7	0
4	H	24	0	4	4	0
4	M	24	0	4	3	0
4	N	24	0	3	2	0
5	A	452	0	0	4	0
5	B	511	0	0	8	0
5	C	483	0	0	4	0
5	D	516	0	0	4	0
5	E	84	0	0	2	0
5	F	81	0	0	1	0
5	G	496	0	0	5	0
5	H	441	0	0	6	0
5	I	78	0	0	3	0
5	J	60	0	0	0	0
5	K	87	0	0	2	0
5	L	98	0	0	0	0
5	M	440	0	0	8	0
5	N	488	0	0	4	0
5	O	60	0	0	1	0
5	P	90	0	0	6	0
All	All	45133	0	38963	181	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.

The worst 5 of 181 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:H:601:LEU:C	5:H:820:HOH:O	1.80	1.15
1:D:112:ARG:O	1:D:112:ARG:HD3	1.51	1.10
1:H:112:ARG:HD3	1:H:112:ARG:O	1.63	0.97
2:P:26:THR:HB	5:P:102:HOH:O	0.79	0.96
1:N:112:ARG:O	1:N:112:ARG:HD3	1.68	0.93

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/573 (100%)	543 (95%)	28 (5%)	0	100	100
1	B	571/573 (100%)	542 (95%)	29 (5%)	0	100	100
1	C	571/573 (100%)	541 (95%)	30 (5%)	0	100	100
1	D	571/573 (100%)	543 (95%)	27 (5%)	1 (0%)	47	33
1	G	571/573 (100%)	541 (95%)	28 (5%)	2 (0%)	34	19
1	H	571/573 (100%)	539 (94%)	32 (6%)	0	100	100
1	M	571/573 (100%)	544 (95%)	27 (5%)	0	100	100
1	N	571/573 (100%)	544 (95%)	25 (4%)	2 (0%)	34	19
2	E	69/72 (96%)	69 (100%)	0	0	100	100
2	F	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
2	I	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	J	69/72 (96%)	67 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	69 (100%)	0	0	100	100
2	P	69/72 (96%)	69 (100%)	0	0	100	100
All	All	5120/5160 (99%)	4884 (95%)	231 (4%)	5 (0%)	51	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	294	ASN
1	D	134	VAL
1	G	134	VAL
1	N	557	GLY
1	N	134	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	464/464 (100%)	459 (99%)	5 (1%)	73	65
1	B	464/464 (100%)	456 (98%)	8 (2%)	60	47
1	C	464/464 (100%)	459 (99%)	5 (1%)	73	65
1	D	464/464 (100%)	458 (99%)	6 (1%)	69	58
1	G	464/464 (100%)	460 (99%)	4 (1%)	78	72
1	H	464/464 (100%)	457 (98%)	7 (2%)	65	53
1	M	464/464 (100%)	456 (98%)	8 (2%)	60	47
1	N	464/464 (100%)	458 (99%)	6 (1%)	69	58
2	E	60/61 (98%)	58 (97%)	2 (3%)	38	21
2	F	60/61 (98%)	54 (90%)	6 (10%)	7	1
2	I	60/61 (98%)	56 (93%)	4 (7%)	16	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	60/61 (98%)	57 (95%)	3 (5%)	24	9
2	K	60/61 (98%)	58 (97%)	2 (3%)	38	21
2	L	60/61 (98%)	57 (95%)	3 (5%)	24	9
2	O	60/61 (98%)	59 (98%)	1 (2%)	60	47
2	P	60/61 (98%)	59 (98%)	1 (2%)	60	47
All	All	4192/4200 (100%)	4121 (98%)	71 (2%)	60	47

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	337	TYR
1	M	442	CYS
1	N	233	GLU
1	B	196	LYS
1	B	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	117	GLN
1	N	156	GLN
2	P	54	HIS
1	B	216	ASN
1	B	117	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	PQQ	N	702	3	23,26,26	4.22	14 (60%)	29,40,40	3.76	18 (62%)
4	PQQ	C	702	3	23,26,26	4.51	12 (52%)	29,40,40	2.87	14 (48%)
4	PQQ	G	702	3	23,26,26	4.28	12 (52%)	29,40,40	3.28	16 (55%)
4	PQQ	M	702	3	23,26,26	4.28	13 (56%)	29,40,40	3.33	12 (41%)
4	PQQ	D	702	3	23,26,26	4.44	14 (60%)	29,40,40	3.76	17 (58%)
4	PQQ	A	702	3	23,26,26	4.31	15 (65%)	29,40,40	3.13	10 (34%)
4	PQQ	H	702	3	23,26,26	4.36	12 (52%)	29,40,40	3.49	19 (65%)
4	PQQ	B	702	3	23,26,26	4.13	13 (56%)	29,40,40	3.24	14 (48%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PQQ	N	702	3	-	9/10/28/28	0/3/3/3
4	PQQ	C	702	3	-	5/10/28/28	0/3/3/3
4	PQQ	G	702	3	-	5/10/28/28	0/3/3/3
4	PQQ	M	702	3	-	4/10/28/28	0/3/3/3
4	PQQ	D	702	3	-	5/10/28/28	0/3/3/3
4	PQQ	A	702	3	-	5/10/28/28	0/3/3/3
4	PQQ	H	702	3	-	10/10/28/28	0/3/3/3
4	PQQ	B	702	3	-	9/10/28/28	0/3/3/3

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	PQQ	O4-C4	12.57	1.49	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	702	PQQ	O5-C5	11.33	1.47	1.23
4	N	702	PQQ	O4-C4	11.20	1.46	1.23
4	D	702	PQQ	O5-C5	11.19	1.46	1.23
4	A	702	PQQ	O4-C4	11.14	1.46	1.23

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	702	PQQ	O7A-C7X-C7	-10.28	100.39	121.24
4	D	702	PQQ	C3A-C4-C5	10.23	124.09	118.14
4	G	702	PQQ	C3A-C4-C5	9.86	123.88	118.14
4	H	702	PQQ	C3A-C4-C5	7.71	122.62	118.14
4	B	702	PQQ	C3A-C4-C5	7.51	122.50	118.14

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	702	PQQ	N1-C2-C2X-O2A
4	C	702	PQQ	C8-C7-C7X-O7B
4	D	702	PQQ	N1-C2-C2X-O2A
4	D	702	PQQ	C8-C7-C7X-O7B
4	A	702	PQQ	N1-C2-C2X-O2A

There are no ring outliers.

8 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	702	PQQ	2	0
4	C	702	PQQ	4	0
4	G	702	PQQ	7	0
4	M	702	PQQ	3	0
4	D	702	PQQ	5	0
4	A	702	PQQ	5	0
4	H	702	PQQ	4	0
4	B	702	PQQ	7	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 PQQ N 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PQQ C 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PQQ G 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PQQ M 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PQQ D 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PQQ A 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PQQ H 702

Bond lengths

Bond angles

Torsions

Rings

Ligand PQQ B 702

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	573/573 (100%)	-0.44	1 (0%)	95	94	13, 21, 33, 57	0
1	B	573/573 (100%)	-0.47	3 (0%)	91	91	12, 17, 30, 47	0
1	C	573/573 (100%)	-0.51	0	100	100	11, 17, 29, 45	0
1	D	573/573 (100%)	-0.46	4 (0%)	87	88	12, 18, 31, 50	0
1	G	573/573 (100%)	-0.49	1 (0%)	95	94	12, 18, 31, 48	0
1	H	573/573 (100%)	-0.39	4 (0%)	87	88	13, 23, 36, 53	0
1	M	573/573 (100%)	-0.34	2 (0%)	94	93	13, 22, 37, 55	0
1	N	573/573 (100%)	-0.55	4 (0%)	87	88	12, 17, 30, 47	0
2	E	71/72 (98%)	0.09	2 (2%)	53	52	20, 31, 46, 52	0
2	F	71/72 (98%)	0.04	5 (7%)	16	15	15, 24, 58, 87	0
2	I	71/72 (98%)	0.25	5 (7%)	16	15	17, 26, 65, 131	0
2	J	71/72 (98%)	0.51	5 (7%)	16	15	24, 36, 52, 67	0
2	K	71/72 (98%)	-0.25	1 (1%)	75	76	15, 24, 38, 52	0
2	L	71/72 (98%)	-0.07	2 (2%)	53	52	18, 26, 44, 61	0
2	O	71/72 (98%)	0.49	5 (7%)	16	15	26, 36, 53, 68	0
2	P	71/72 (98%)	-0.23	0	100	100	17, 22, 40, 53	0
All	All	5152/5160 (99%)	-0.39	44 (0%)	84	84	11, 20, 37, 131	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	90	VAL	11.2
2	I	91	GLU	9.1
2	F	93	ILE	5.7
2	F	91	GLU	5.2
2	I	93	ILE	4.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PQQ	H	702	24/24	0.81	0.25	33,56,64,67	0
4	PQQ	M	702	24/24	0.82	0.22	30,51,56,62	0
4	PQQ	D	702	24/24	0.85	0.23	24,39,44,55	0
4	PQQ	N	702	24/24	0.85	0.22	23,46,52,70	0
4	PQQ	G	702	24/24	0.87	0.23	23,45,49,62	0
4	PQQ	C	702	24/24	0.88	0.21	20,35,40,45	0
4	PQQ	A	702	24/24	0.88	0.24	26,46,52,54	0
3	CA	M	701	1/1	0.90	0.10	68,68,68,68	0
4	PQQ	B	702	24/24	0.91	0.22	25,41,47,49	0
3	CA	H	701	1/1	0.93	0.14	63,63,63,63	0
3	CA	G	701	1/1	0.96	0.15	50,50,50,50	0
3	CA	B	701	1/1	0.97	0.15	52,52,52,52	0
3	CA	A	701	1/1	0.97	0.18	56,56,56,56	0
3	CA	N	701	1/1	0.98	0.12	48,48,48,48	0
3	CA	D	701	1/1	0.98	0.13	47,47,47,47	0
3	CA	C	701	1/1	0.98	0.15	44,44,44,44	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 PQQ H 702:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
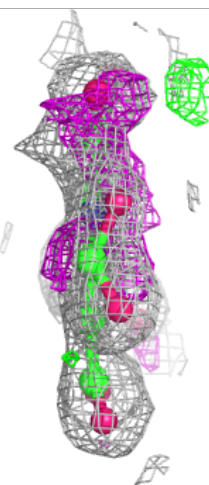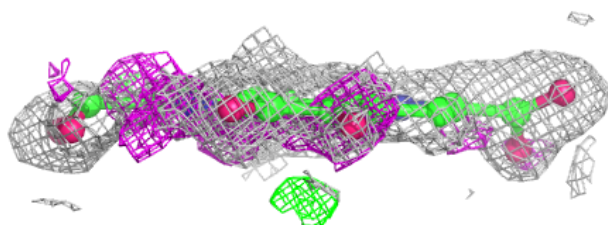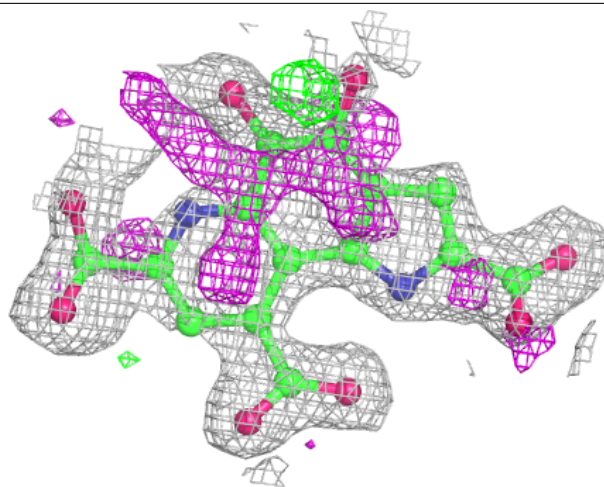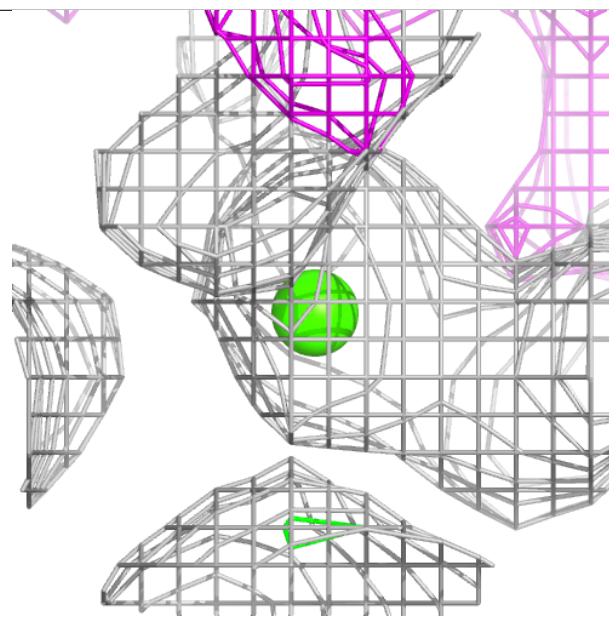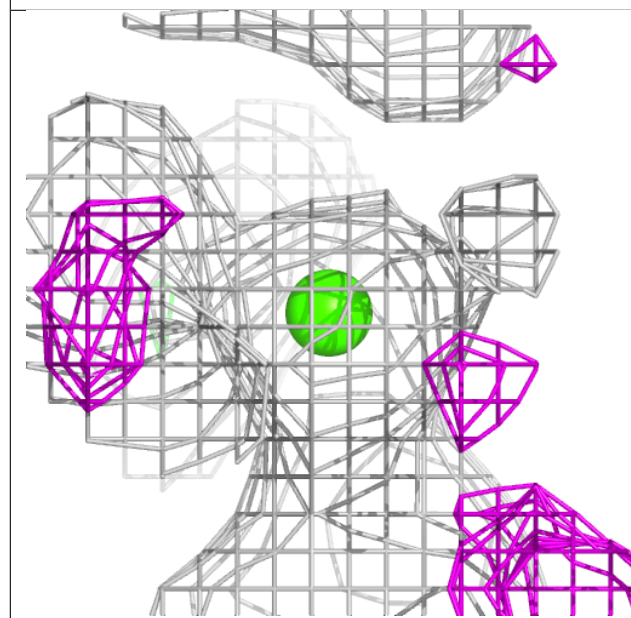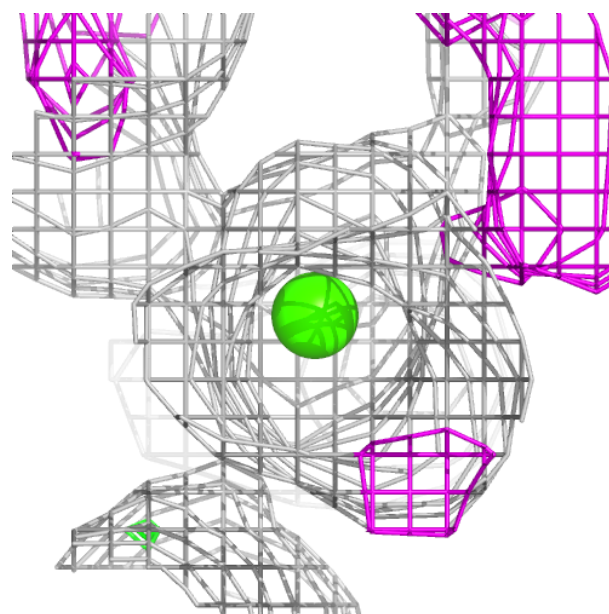and green (positive)
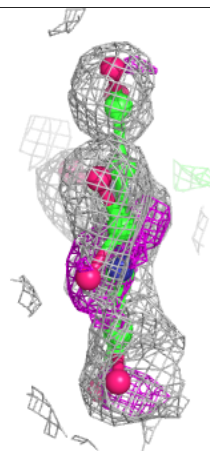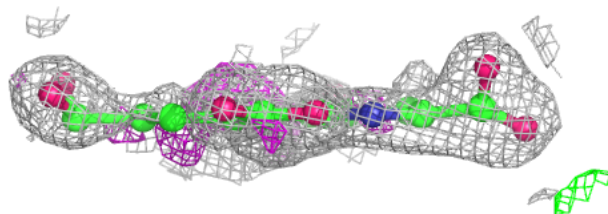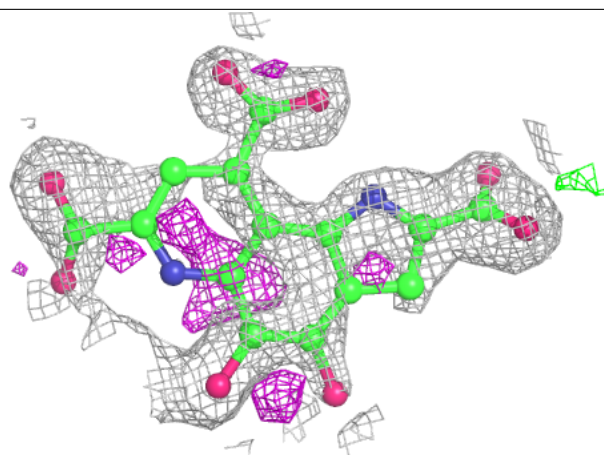
Electron density around PQQ M 702:

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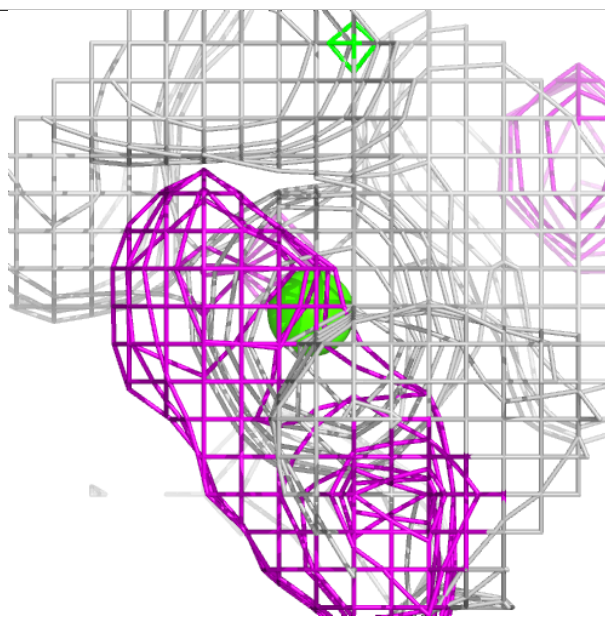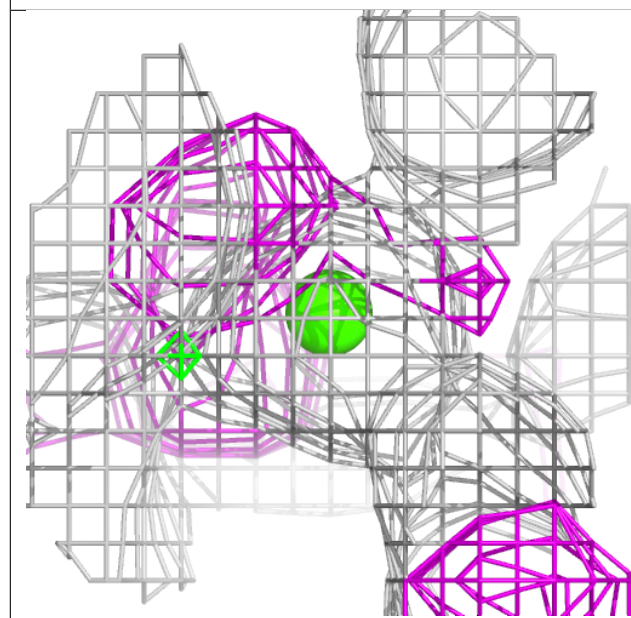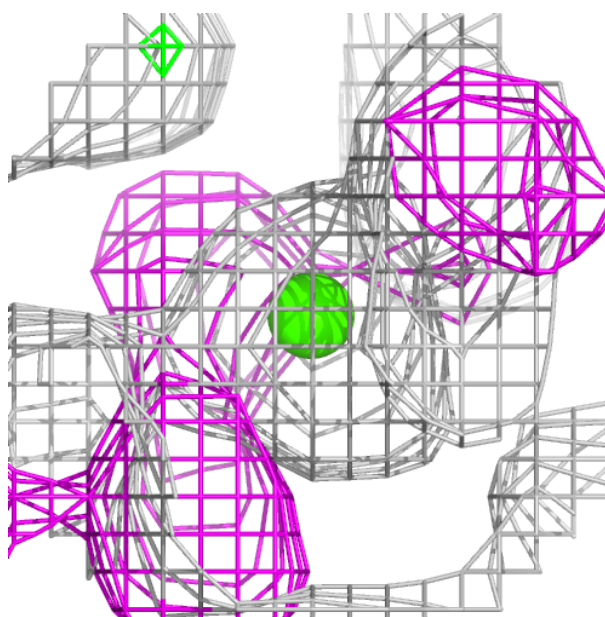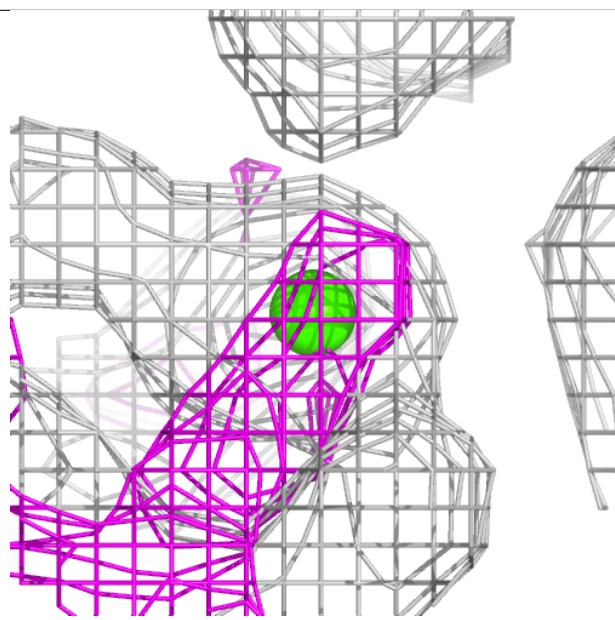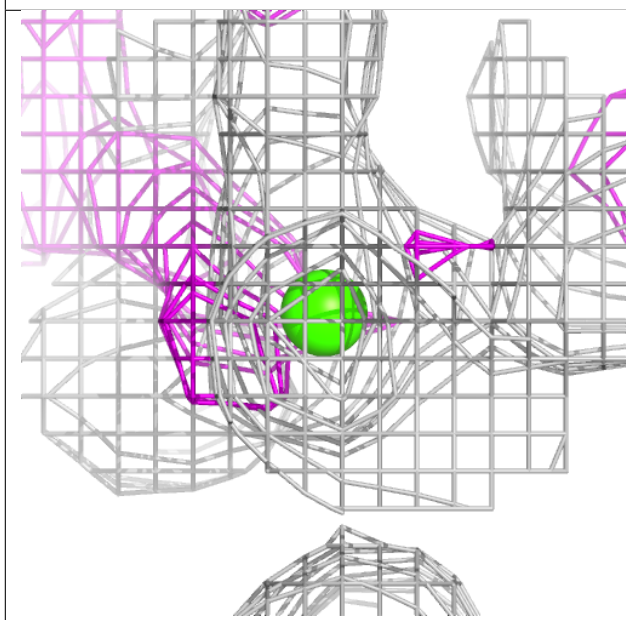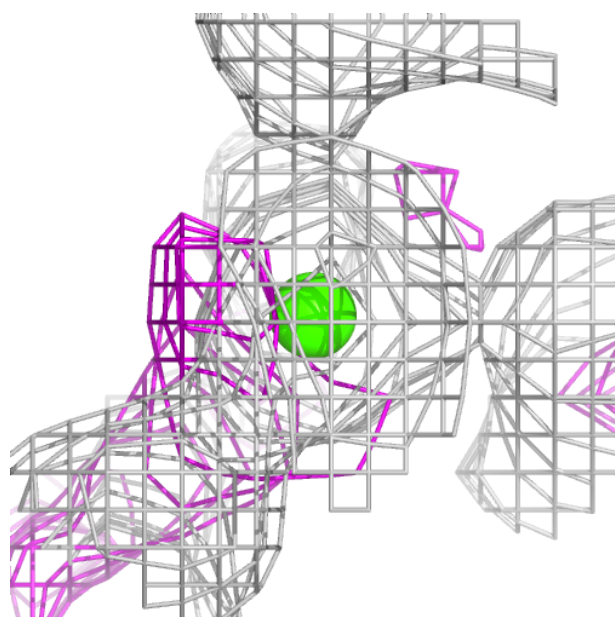mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PQQ 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)
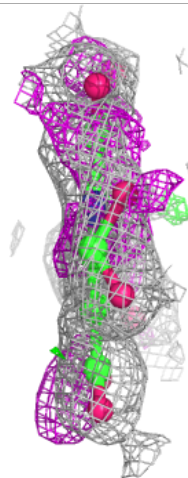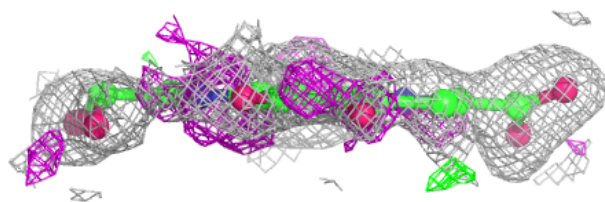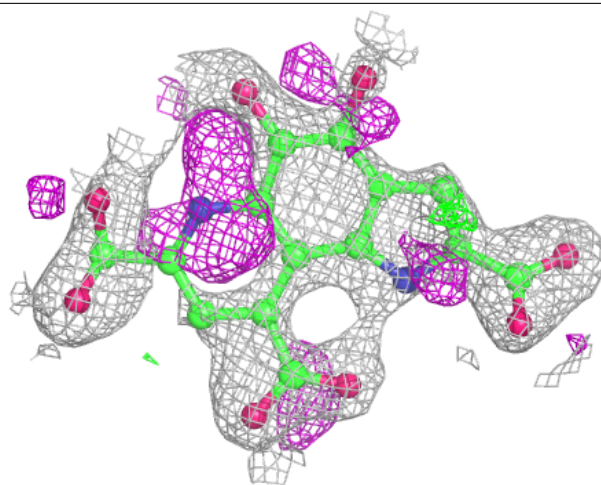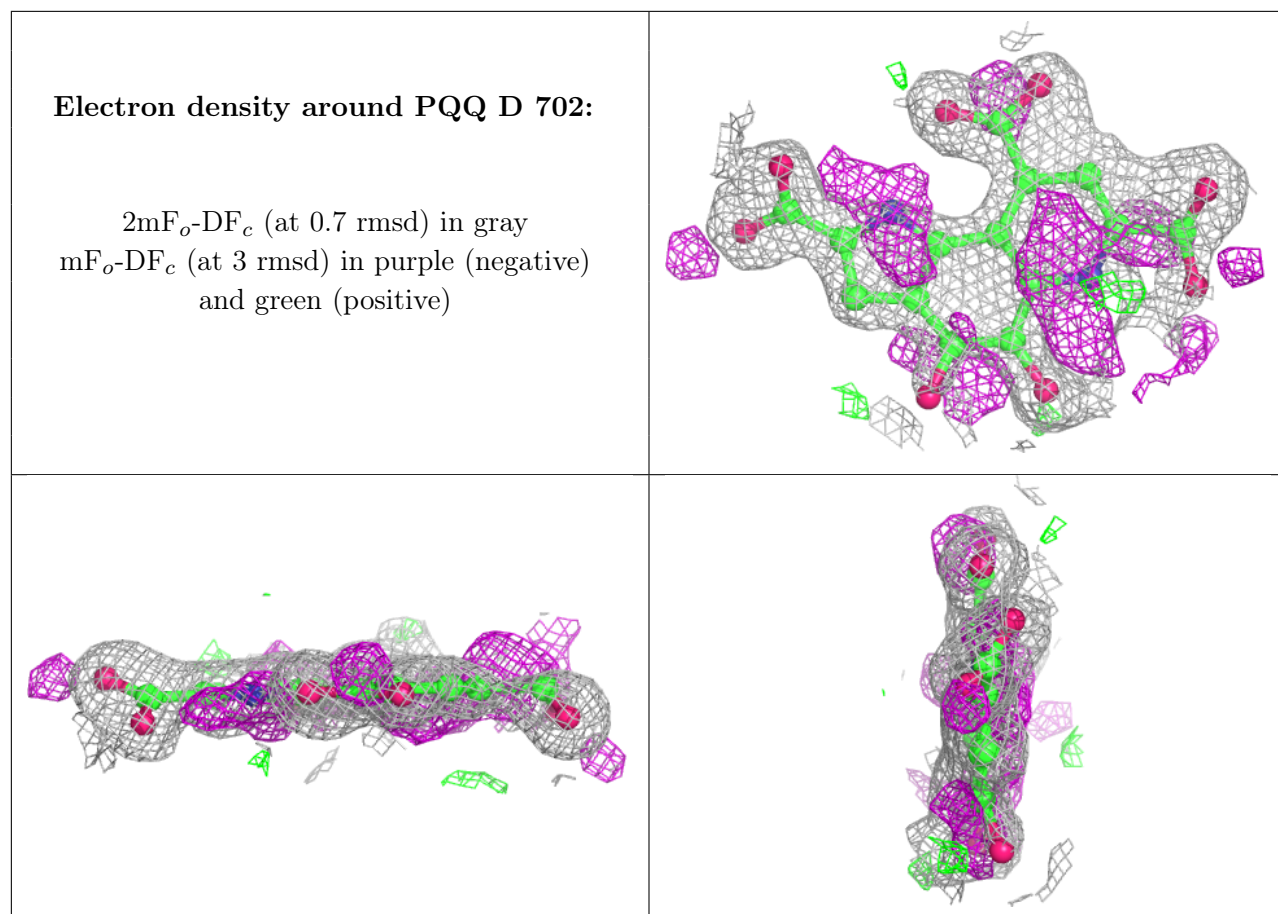
Electron density around PQQ N 702:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
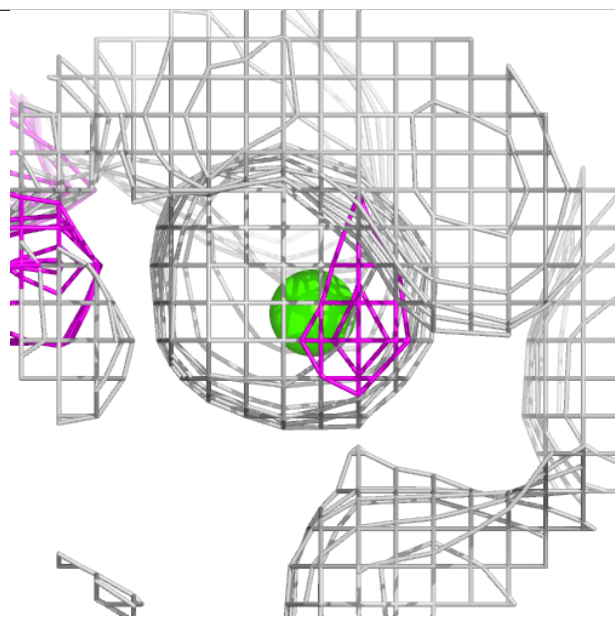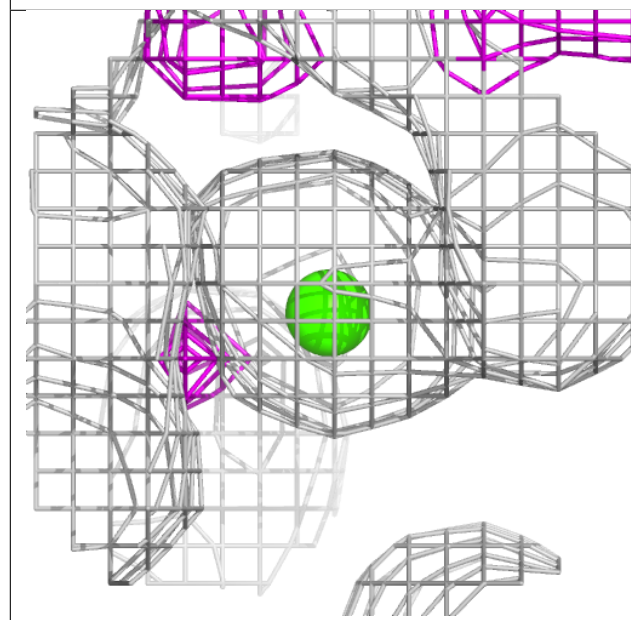and green (positive)
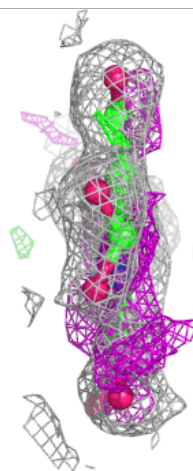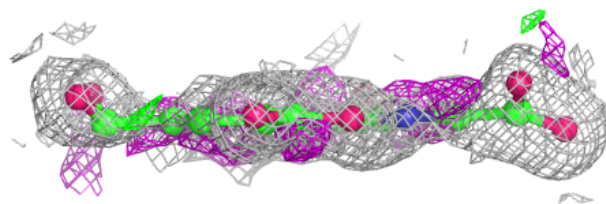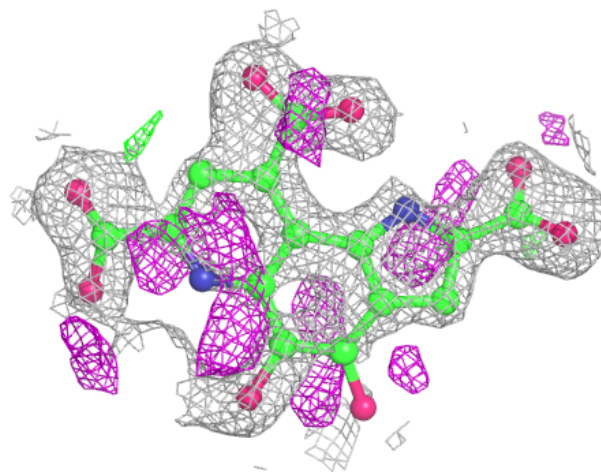
Electron density around PQQ G 702:

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

Electron density around PQQ C 702:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
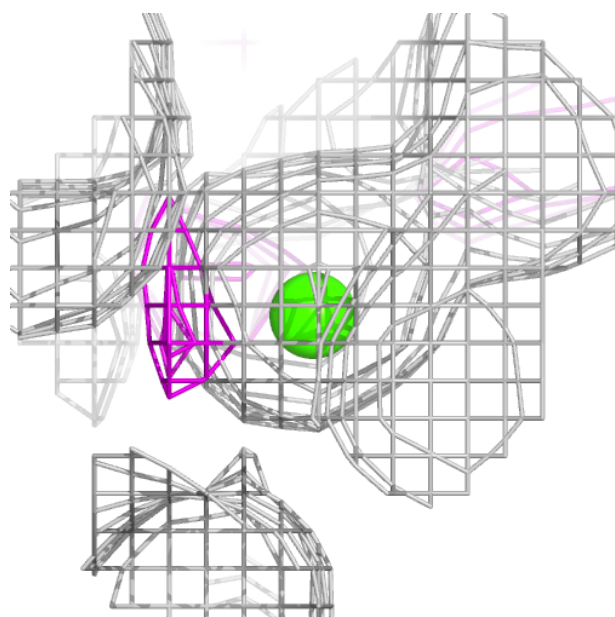and green (positive)
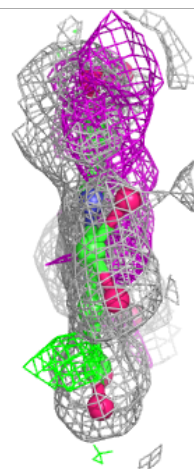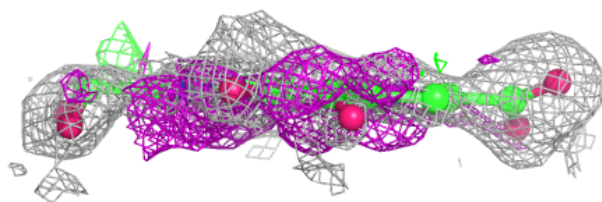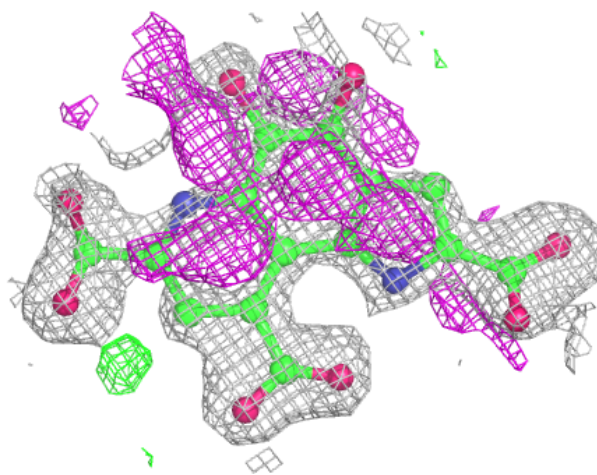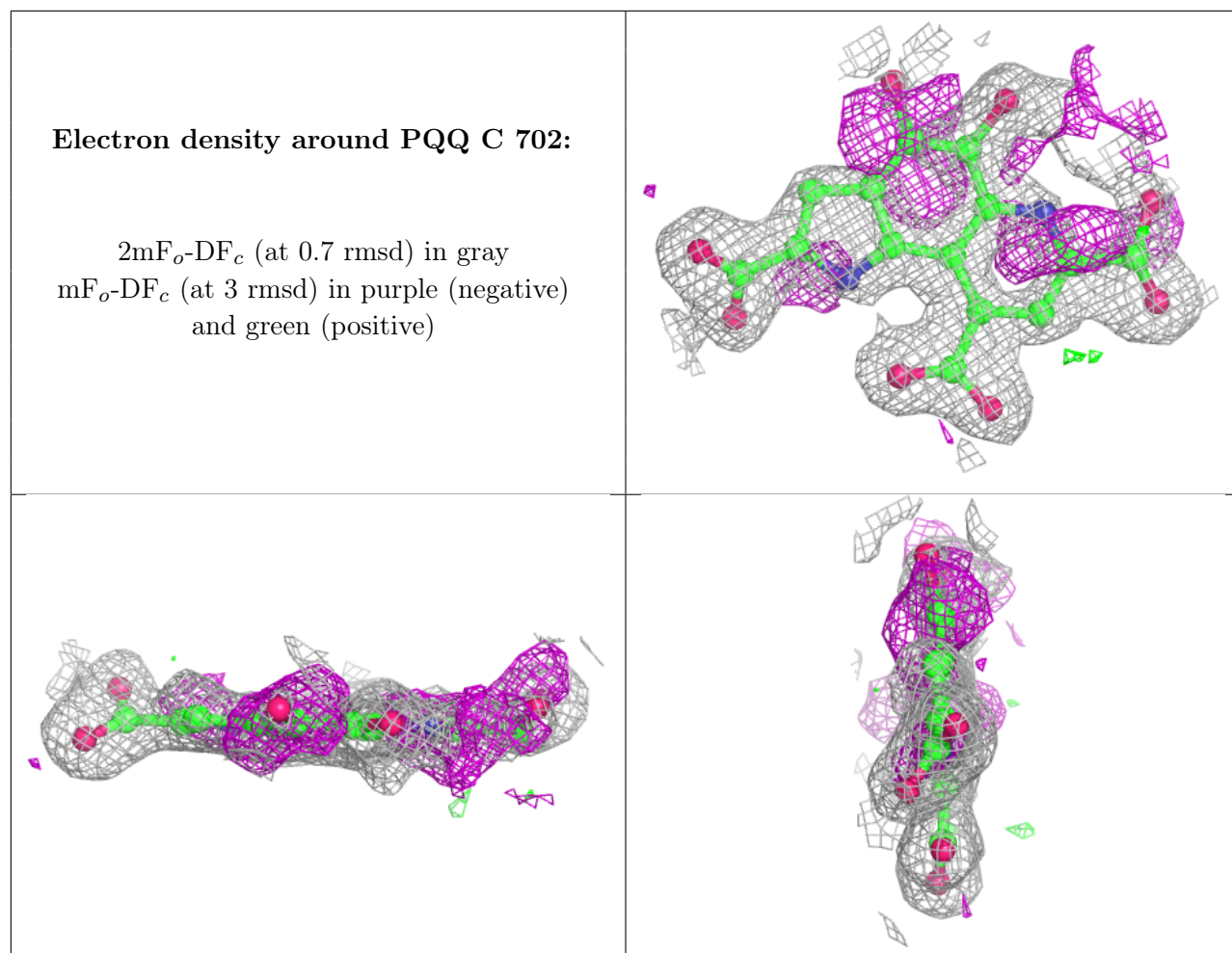
Electron density around PQQ A 702:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
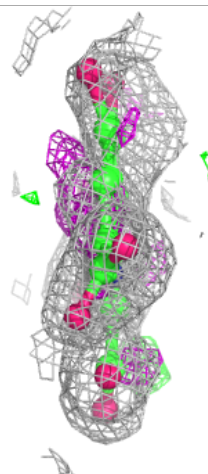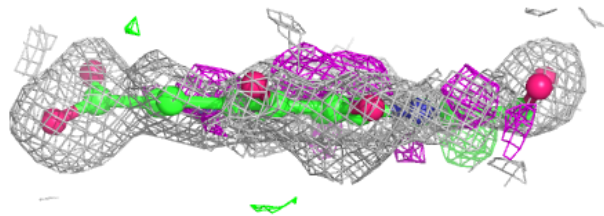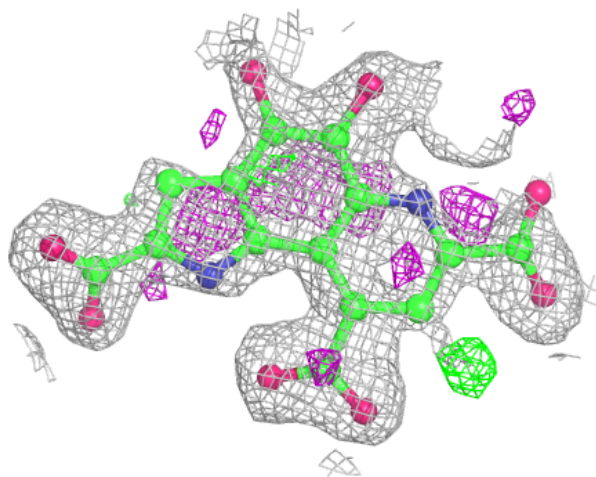
Electron density around CA M 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
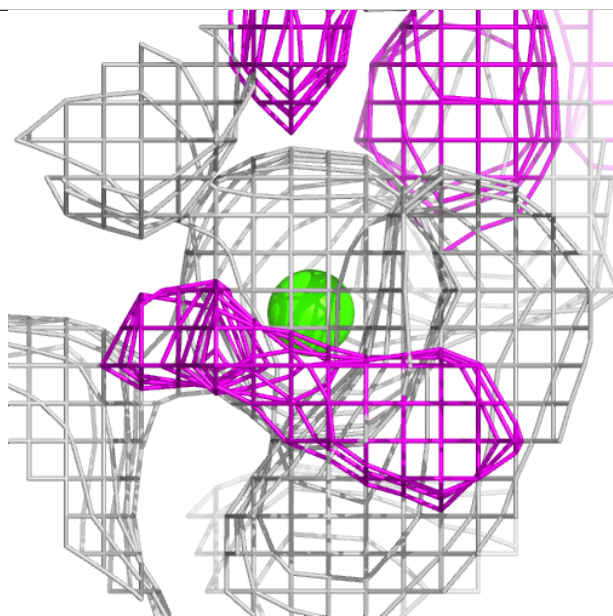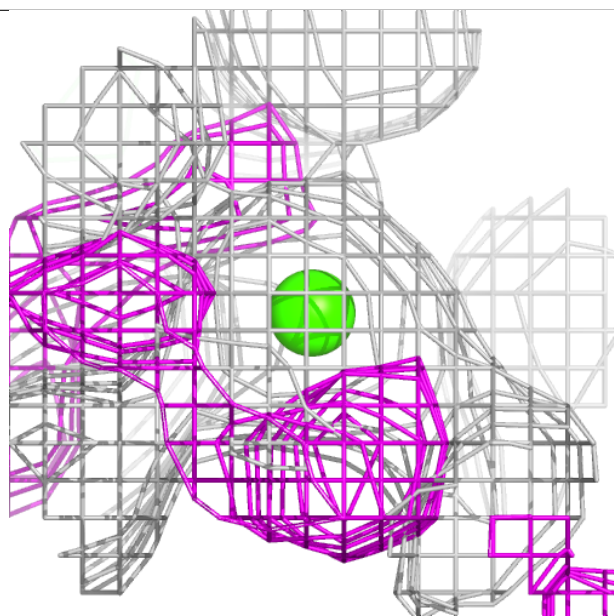and green (positive)
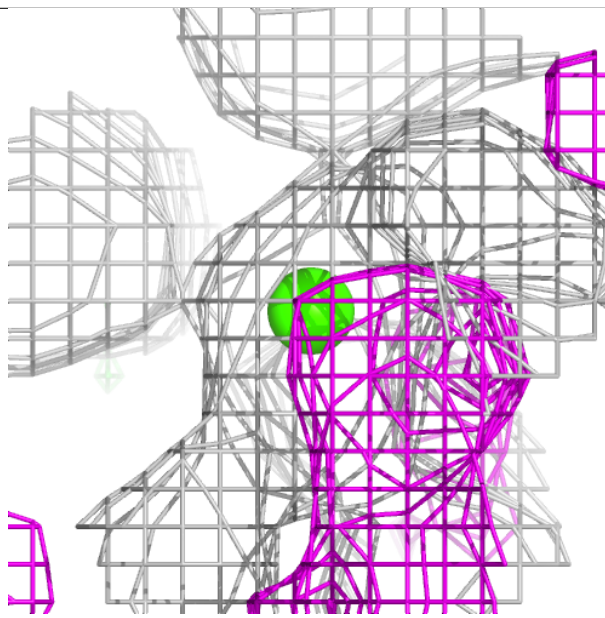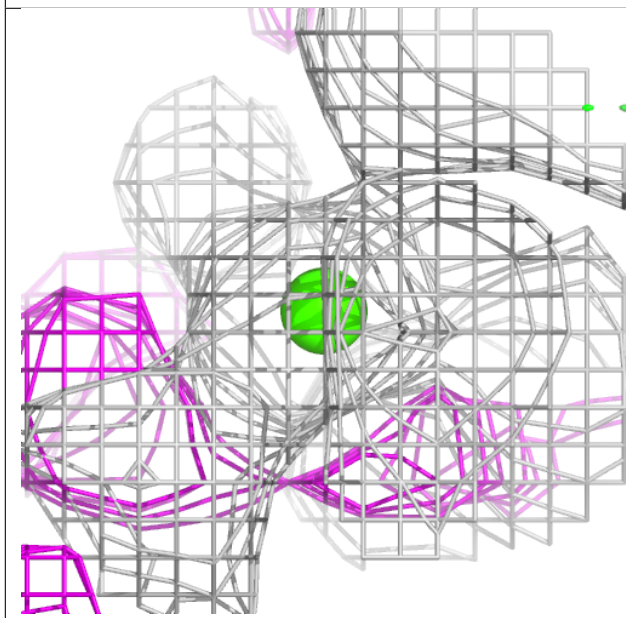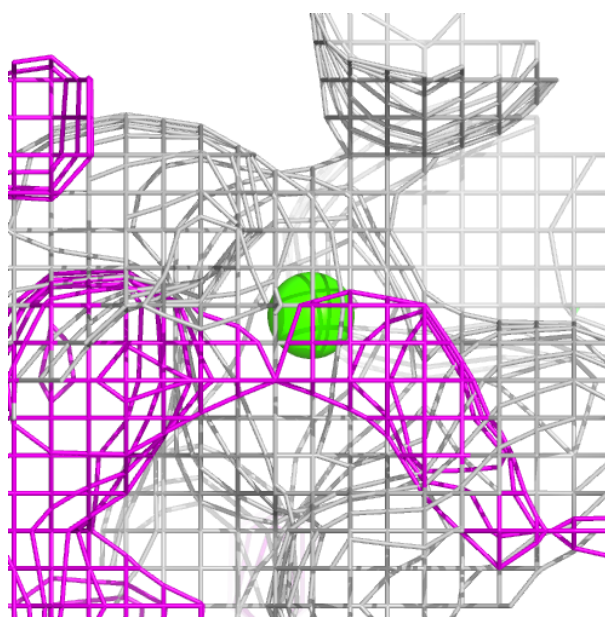
Electron density around PQQ B 702:

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 CA H 701:

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

Electron density around CA G 701:

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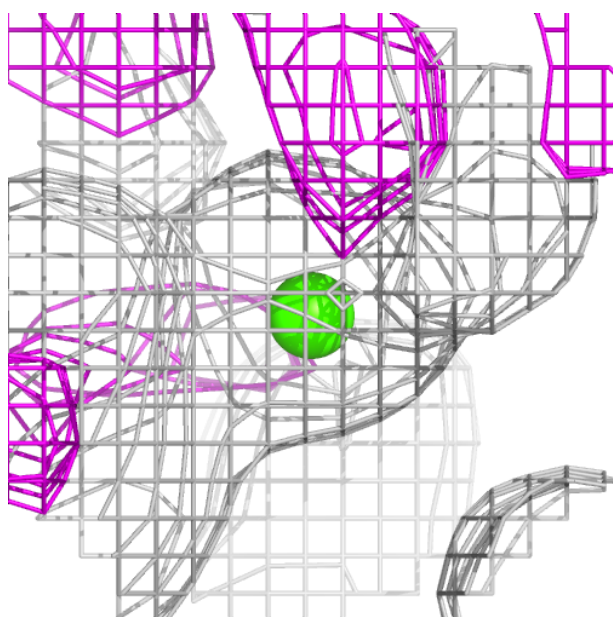$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CA B 701:

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

Electron density around CA A 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
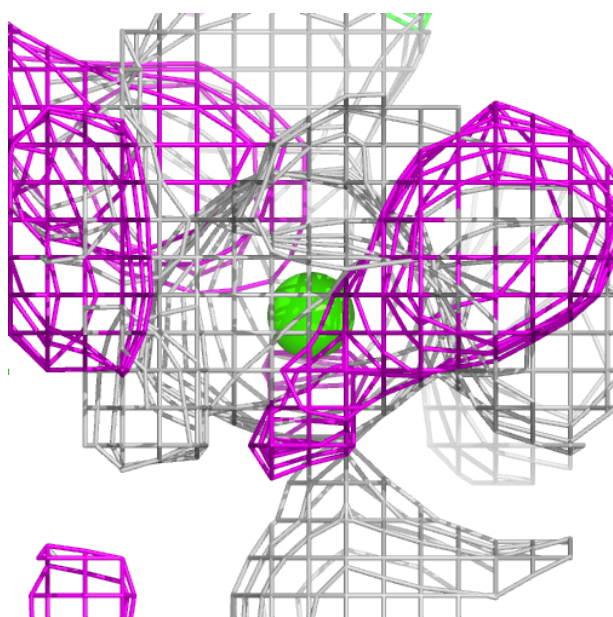and green (positive)
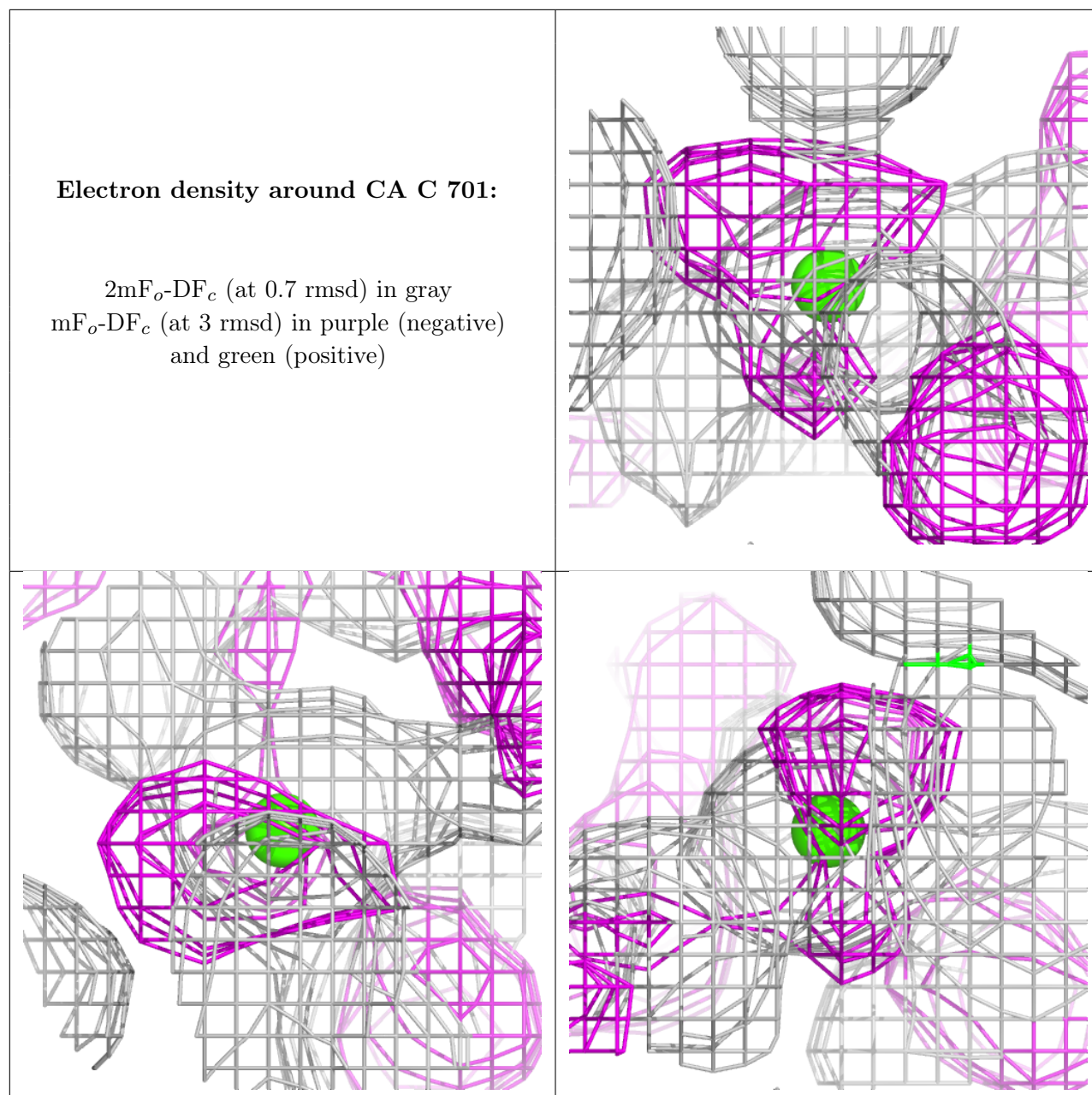
Electron density around CA N 701:

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

Electron density around CA D 701:

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 CA C 701:

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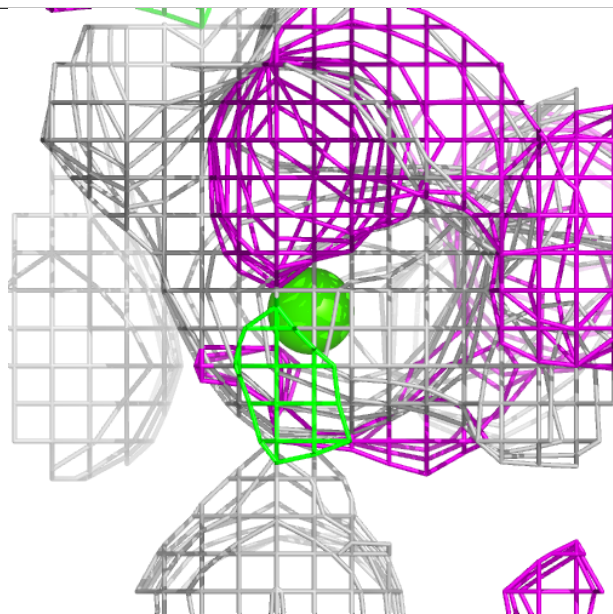
6.5 Other polymers ⓘ

There are no such residues in this entry.