



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2019 – 06:55 PM EST

PDB ID : 4TQO
Title : The crystal structure of methanol dehydrogenase from *Methylococcus capsulatus* (Bath)
Authors : Culpepper, M.A.; Rosenzweig, A.C.
Deposited on : 2014-06-11
Resolution : 2.57 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

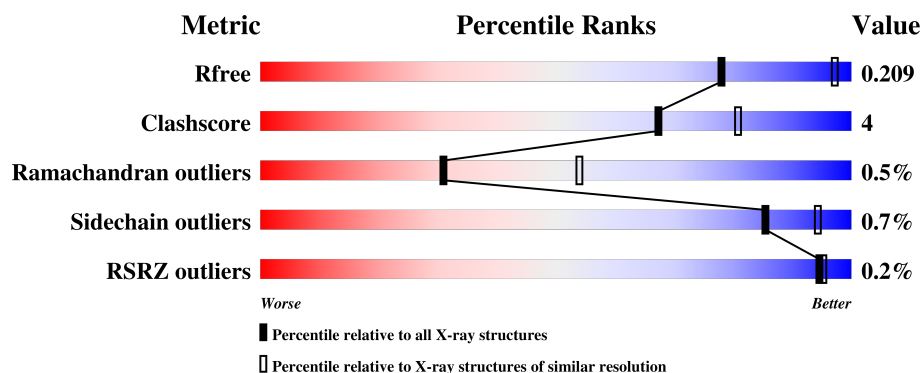
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	111664	3182 (2.60-2.56)
Clashscore	122126	3541 (2.60-2.56)
Ramachandran outliers	120053	3489 (2.60-2.56)
Sidechain outliers	120020	3489 (2.60-2.56)
RSRZ outliers	108989	3120 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>90%</div> <div>9% .</div> </div>
1	B	573	<div> <div>89%</div> <div>9% ..</div> </div>
1	C	573	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>
1	D	573	<div> <div>92%</div> <div>7% .</div> </div>
1	E	573	<div> <div>92%</div> <div>8% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	573	 90% 10%
1	G	573	 89% 11%
1	H	573	 91% 9%
2	I	72	 90% 8% .
2	J	72	 93% 6% .
2	K	72	 3% 96% . .
2	L	72	 94% . .
2	M	72	 82% 18%
2	N	72	 89% 10% .
2	O	72	 90% 10%
2	P	72	 90% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43059 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	B	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	A	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	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	E	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	23			
1	F	573	Total	C	N	O	S	0	0	0
			4491	2871	765	832	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
			4491	2871	765	832	23			

- Molecule 2 is a protein called Methanol dehydrogenase, small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
2	M	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			
2	N	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			

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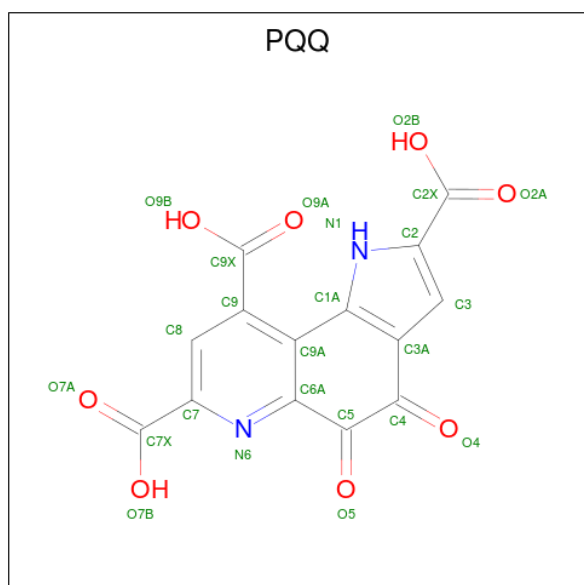
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			
2	P	72	Total	C	N	O	S	0	0	0
			577	362	102	110	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	H	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	A	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: C₁₄H₆N₂O₈).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	276	Total	O	0	0
			276	276		
5	I	57	Total	O	0	0
			57	57		
5	A	288	Total	O	0	0
			288	288		
5	J	45	Total	O	0	0
			45	45		
5	C	237	Total	O	0	0
			237	237		
5	K	29	Total	O	0	0
			29	29		
5	D	247	Total	O	0	0
			247	247		
5	L	46	Total	O	0	0
			46	46		
5	E	241	Total	O	0	0
			241	241		
5	M	33	Total	O	0	0
			33	33		
5	F	251	Total	O	0	0
			251	251		
5	N	39	Total	O	0	0
			39	39		

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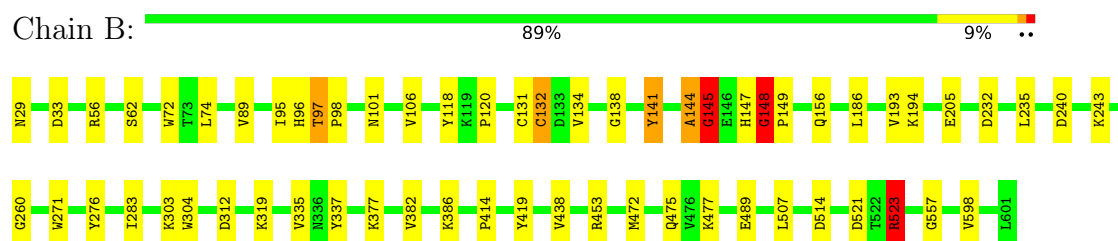
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	244	Total 244	O 244	0	0
5	O	35	Total 35	O 35	0	0
5	H	254	Total 254	O 254	0	0
5	P	30	Total 30	O 30	0	0

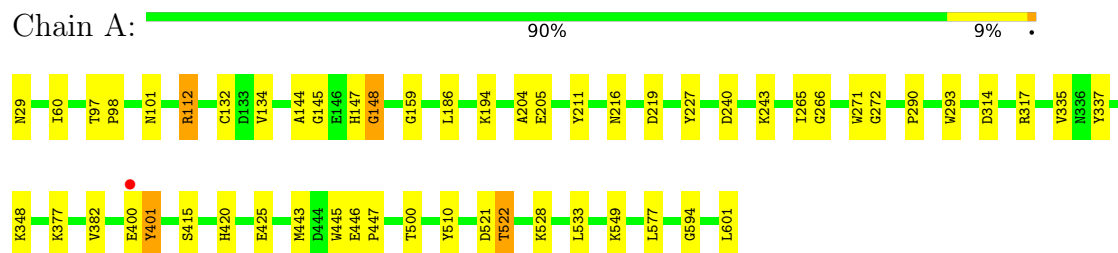
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

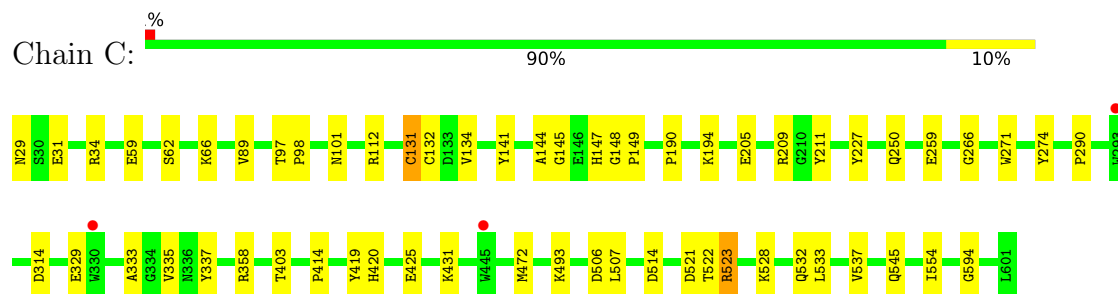
- Molecule 1: Methanol dehydrogenase protein, large subunit



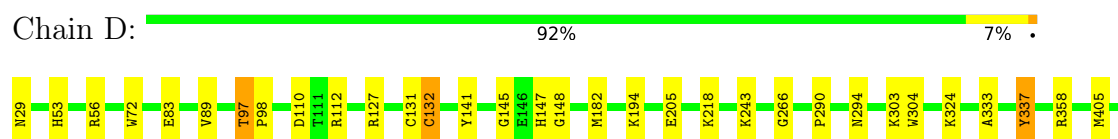
- Molecule 1: Methanol dehydrogenase protein, large subunit



- Molecule 1: Methanol dehydrogenase protein, large subunit



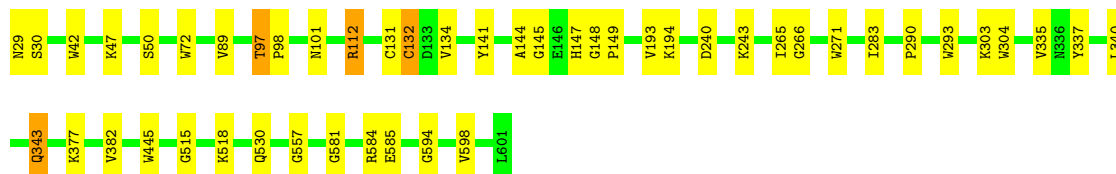
- Molecule 1: Methanol dehydrogenase protein, large subunit





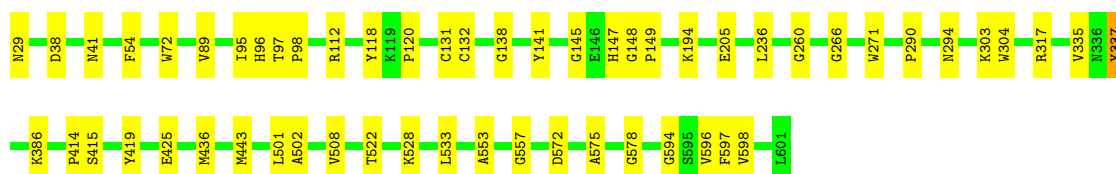
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain E: 92% 8%



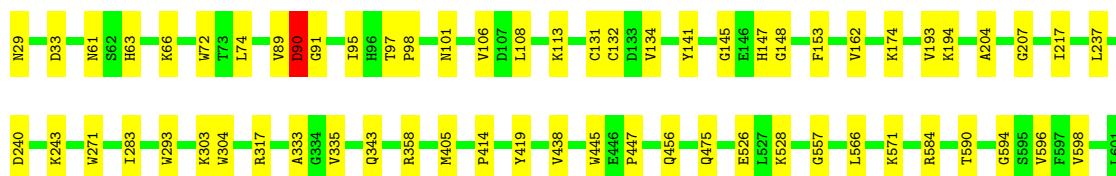
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain F: 90% 10%



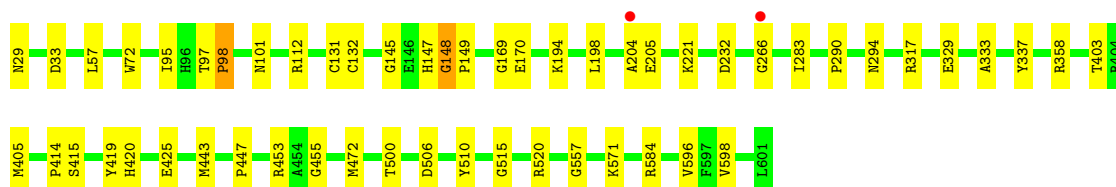
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain G: 89% 11%



- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain H: 91% 9%



- Molecule 2: Methanol dehydrogenase, small subunit

Chain I: 90% 8%



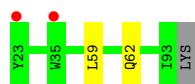
- Molecule 2: Methanol dehydrogenase, small subunit

Chain J:  93% 6%



- Molecule 2: Methanol dehydrogenase, small subunit

Chain K:  3% 96%




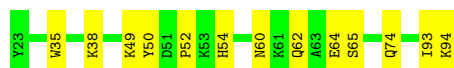
- Molecule 2: Methanol dehydrogenase, small subunit

Chain L:  94%



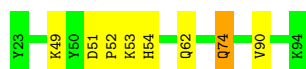
- Molecule 2: Methanol dehydrogenase, small subunit

Chain M:  82% 18%



- Molecule 2: Methanol dehydrogenase, small subunit

Chain N:  89% 10%



- Molecule 2: Methanol dehydrogenase, small subunit

Chain O:  90% 10%



- Molecule 2: Methanol dehydrogenase, small subunit

Chain P:  90% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.49Å 210.29Å 231.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.15 – 2.57 105.14 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.9 (105.15-2.57) 100.0 (105.14-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.158 , 0.208 0.163 , 0.209	Depositor DCC
R_{free} test set	9931 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	43059	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	2/4622 (0.0%)	0.49	0/6281
1	B	0.42	3/4622 (0.1%)	0.52	4/6281 (0.1%)
1	C	0.30	0/4622	0.47	0/6281
1	D	0.34	0/4621	0.49	0/6281
1	E	0.29	0/4622	0.48	0/6281
1	F	0.37	2/4622 (0.0%)	0.48	0/6281
1	G	0.27	0/4622	0.48	0/6281
1	H	0.28	0/4622	0.48	0/6281
2	I	0.34	0/583	0.42	0/785
2	J	0.28	0/583	0.43	0/785
2	K	0.25	0/583	0.41	0/785
2	L	0.27	0/583	0.42	0/785
2	M	0.31	0/592	0.54	0/796
2	N	0.33	0/592	0.53	1/796 (0.1%)
2	O	0.25	0/592	0.41	0/796
2	P	0.26	0/592	0.41	0/796
All	All	0.33	7/41675 (0.0%)	0.48	5/56572 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	TYR	CD1-CE1	-6.59	1.29	1.39
1	B	141	TYR	CD2-CE2	-5.91	1.30	1.39
1	A	401	TYR	CD2-CE2	-5.77	1.30	1.39
1	A	401	TYR	CD1-CE1	-5.66	1.30	1.39
1	B	148	GLY	C-O	-5.50	1.14	1.23
1	F	337	TYR	CD2-CE2	-5.37	1.31	1.39
1	F	337	TYR	CE2-CZ	-5.14	1.31	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	523	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	523	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	N	74	GLN	CA-CB-CG	6.28	127.21	113.40
1	B	144	ALA	C-N-CA	-5.72	110.28	122.30
1	B	145	GLY	N-CA-C	5.25	126.21	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4491	0	4320	47	0
1	B	4491	0	4320	40	0
1	C	4491	0	4320	38	0
1	D	4490	0	4320	31	0
1	E	4491	0	4320	31	0
1	F	4491	0	4320	37	0
1	G	4491	0	4320	42	0
1	H	4491	0	4320	36	0
2	I	568	0	545	6	0
2	J	568	0	545	3	0
2	K	568	0	545	2	0
2	L	568	0	545	3	0
2	M	577	0	558	12	0
2	N	577	0	558	9	0
2	O	577	0	558	5	0
2	P	577	0	558	5	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	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	24	0	3	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	3	3	0
4	C	24	0	3	1	0
4	D	24	0	3	1	0
4	E	24	0	3	0	0
4	F	24	0	3	2	0
4	G	24	0	3	2	0
4	H	24	0	3	2	0
5	A	288	0	0	3	0
5	B	276	0	0	5	1
5	C	237	0	0	9	0
5	D	247	0	0	7	1
5	E	241	0	0	3	0
5	F	251	0	0	8	0
5	G	244	0	0	9	0
5	H	254	0	0	9	1
5	I	57	0	0	3	1
5	J	45	0	0	1	1
5	K	29	0	0	1	0
5	L	46	0	0	2	0
5	M	33	0	0	3	0
5	N	39	0	0	2	1
5	O	35	0	0	0	0
5	P	30	0	0	0	0
All	All	43059	0	38996	337	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:OE1	1:A:401:TYR:CE2	1.71	1.41
1:A:400:GLU:OE1	1:A:401:TYR:CZ	1.79	1.33
1:A:400:GLU:OE1	1:A:401:TYR:CD2	2.09	1.03
2:M:35:TRP:O	5:M:706:HOH:O	1.80	0.98
1:A:400:GLU:OE1	1:A:401:TYR:CE1	2.26	0.89
1:G:89:VAL:O	5:G:926:HOH:O	1.92	0.87
1:A:533:LEU:O	1:E:112:ARG:NH2	2.08	0.86
2:I:79:ASN:HD22	2:I:93:ILE:HG23	1.43	0.83
1:D:324:LYS:O	5:D:863:HOH:O	1.96	0.82
1:B:240:ASP:HB3	1:B:243:LYS:HD3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:SER:O	5:E:887:HOH:O	2.00	0.79
1:D:110:ASP:OD2	5:D:820:HOH:O	2.00	0.79
1:B:523:ARG:NH2	1:C:506:ASP:OD2	2.15	0.78
1:C:250:GLN:O	5:C:995:HOH:O	2.02	0.78
1:C:190:PRO:O	5:C:841:HOH:O	2.03	0.76
2:M:52:PRO:HB2	2:M:54:HIS:CD2	2.20	0.76
2:J:70:GLU:OE2	5:J:708:HOH:O	2.05	0.74
1:C:533:LEU:O	1:D:112:ARG:NH2	2.19	0.74
1:B:260:GLY:O	5:B:914:HOH:O	2.05	0.73
1:G:113:LYS:O	5:G:868:HOH:O	2.06	0.73
1:F:533:LEU:O	1:H:112:ARG:NH2	2.21	0.73
2:I:74:GLN:OE1	5:I:741:HOH:O	2.08	0.72
2:K:59:LEU:O	5:K:715:HOH:O	2.09	0.71
1:H:198:LEU:HD11	1:H:283:ILE:HD13	1.73	0.71
1:G:89:VAL:O	1:G:90:ASP:HB2	1.90	0.70
1:A:147:HIS:N	1:A:148:GLY:HA2	2.06	0.70
1:G:456:GLN:HG3	5:G:801:HOH:O	1.92	0.70
1:F:145:GLY:HA3	1:F:148:GLY:O	1.92	0.70
1:G:147:HIS:H	1:G:148:GLY:HA2	1.55	0.70
1:D:147:HIS:N	1:D:148:GLY:HA2	2.06	0.69
2:M:52:PRO:HB2	2:M:54:HIS:NE2	2.07	0.69
1:A:97:THR:HG22	1:A:98:PRO:O	1.92	0.69
1:A:60:ILE:O	5:A:831:HOH:O	2.11	0.69
1:H:57:LEU:O	5:H:842:HOH:O	2.09	0.69
1:G:240:ASP:HB3	1:G:243:LYS:HD3	1.74	0.68
1:D:147:HIS:H	1:D:148:GLY:HA2	1.58	0.68
1:A:400:GLU:CD	1:A:401:TYR:CZ	2.67	0.68
1:H:33:ASP:OD1	5:H:824:HOH:O	2.11	0.68
1:H:97:THR:HG22	1:H:98:PRO:O	1.93	0.68
1:C:147:HIS:N	1:C:148:GLY:HA2	2.09	0.68
1:G:97:THR:HG22	1:G:98:PRO:O	1.93	0.68
1:C:66:LYS:NZ	5:C:986:HOH:O	2.27	0.68
1:G:147:HIS:N	1:G:148:GLY:HA2	2.09	0.67
1:H:506:ASP:OD2	5:H:1052:HOH:O	2.12	0.67
2:I:36:GLU:OE1	5:I:711:HOH:O	2.12	0.67
1:F:147:HIS:N	1:F:148:GLY:HA2	2.08	0.67
1:E:147:HIS:N	1:E:148:GLY:HA2	2.10	0.67
1:H:145:GLY:HA3	1:H:148:GLY:O	1.96	0.66
1:H:147:HIS:N	1:H:148:GLY:HA2	2.10	0.66
1:A:147:HIS:H	1:A:148:GLY:HA2	1.61	0.66
1:A:29:ASN:HB3	1:A:194:LYS:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LYS:NZ	1:A:314:ASP:OD2	2.26	0.66
1:A:112:ARG:HH21	1:E:515:GLY:HA3	1.61	0.65
1:C:97:THR:HG22	1:C:98:PRO:O	1.96	0.65
1:F:97:THR:HG22	1:F:98:PRO:O	1.95	0.65
1:C:274:TYR:O	5:C:892:HOH:O	2.14	0.65
1:B:147:HIS:N	1:B:148:GLY:HA2	2.11	0.65
1:B:144:ALA:O	1:B:145:GLY:C	2.29	0.64
1:F:112:ARG:HH21	1:H:515:GLY:HA3	1.63	0.64
2:L:76:ARG:O	5:L:727:HOH:O	2.14	0.64
1:E:147:HIS:H	1:E:148:GLY:HA2	1.63	0.64
1:A:400:GLU:OE1	1:A:401:TYR:CG	2.52	0.63
1:H:221:LYS:HD3	2:P:77:VAL:HG11	1.79	0.63
2:P:52:PRO:HB2	2:P:54:HIS:CE1	2.33	0.63
1:A:549:LYS:NZ	1:A:601:LEU:OXT	2.31	0.62
1:E:585:GLU:OE1	5:E:813:HOH:O	2.16	0.62
2:I:26:THR:HG21	1:A:317:ARG:HH12	1.64	0.62
1:C:29:ASN:N	1:C:194:LYS:H	1.98	0.61
1:B:521:ASP:OD1	1:B:523:ARG:HD3	2.00	0.61
1:G:145:GLY:HA3	1:G:148:GLY:O	2.01	0.60
1:H:147:HIS:H	1:H:148:GLY:HA2	1.65	0.60
1:H:169:GLY:O	5:H:909:HOH:O	2.16	0.60
1:F:147:HIS:H	1:F:148:GLY:HA2	1.67	0.59
1:E:145:GLY:HA3	1:E:148:GLY:O	2.03	0.59
1:D:97:THR:HG22	1:D:98:PRO:O	2.03	0.58
2:I:26:THR:HG22	1:A:317:ARG:HH22	1.68	0.58
1:A:400:GLU:OE1	1:A:401:TYR:CD1	2.57	0.58
1:E:518:LYS:HG2	1:E:530:GLN:HG2	1.86	0.58
4:A:702:PQQ:O9B	4:A:702:PQQ:N1	2.36	0.57
1:E:29:ASN:N	1:E:194:LYS:H	2.03	0.57
1:G:528:LYS:O	5:G:1000:HOH:O	2.17	0.57
1:G:90:ASP:HB2	5:G:926:HOH:O	2.03	0.57
1:F:522:THR:HG21	5:F:814:HOH:O	2.04	0.57
1:C:145:GLY:HA3	1:C:148:GLY:O	2.04	0.57
1:B:147:HIS:H	1:B:148:GLY:HA2	1.70	0.57
1:F:578:GLY:O	5:F:847:HOH:O	2.18	0.57
1:G:33:ASP:OD1	5:G:833:HOH:O	2.17	0.57
1:F:271:TRP:CZ2	1:F:335:VAL:HG21	2.40	0.56
1:C:314:ASP:OD2	1:F:386:LYS:NZ	2.38	0.56
1:G:61:ASN:OD1	1:G:63:HIS:HB2	2.06	0.56
4:D:702:PQQ:O9A	4:D:702:PQQ:N1	2.34	0.56
1:B:62:SER:HA	1:B:507:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:702:PQQ:N1	4:G:702:PQQ:O9A	2.33	0.56
1:B:377:LYS:HD3	1:B:382:VAL:HB	1.88	0.56
1:F:528:LYS:NZ	5:F:872:HOH:O	2.39	0.55
4:F:702:PQQ:O9B	4:F:702:PQQ:N1	2.37	0.55
1:C:131:CYS:SG	1:C:132:CYS:N	2.80	0.55
2:O:52:PRO:HB2	2:O:54:HIS:CE1	2.42	0.55
1:B:97:THR:O	1:B:101:ASN:HA	2.08	0.54
1:C:420:HIS:NE2	1:C:425:GLU:OE2	2.34	0.54
1:A:400:GLU:CD	1:A:400:GLU:O	2.47	0.53
1:C:59:GLU:OE1	5:C:914:HOH:O	2.19	0.53
1:G:571:LYS:O	1:G:584:ARG:NH2	2.40	0.53
1:E:97:THR:HG22	1:E:98:PRO:O	2.08	0.53
2:N:74:GLN:HA	2:N:74:GLN:HE21	1.73	0.53
1:A:145:GLY:HA3	1:A:148:GLY:O	2.09	0.53
1:H:500:THR:HG22	1:H:510:TYR:HB3	1.91	0.53
1:B:144:ALA:O	1:B:148:GLY:O	2.27	0.52
1:C:545:GLN:NE2	5:C:937:HOH:O	2.16	0.52
1:G:162:VAL:HG22	1:G:174:LYS:HG3	1.91	0.52
1:H:29:ASN:N	1:H:194:LYS:H	2.07	0.52
1:B:97:THR:HG22	1:B:98:PRO:O	2.09	0.52
1:B:74:LEU:HD11	1:B:106:VAL:HG21	1.93	0.51
1:H:405:MET:HA	1:H:447:PRO:HG2	1.92	0.51
1:A:272:GLY:HA3	1:A:335:VAL:O	2.11	0.51
1:H:571:LYS:O	1:H:584:ARG:NH1	2.42	0.51
4:B:702:PQQ:N1	4:B:702:PQQ:O9B	2.42	0.51
1:C:31:GLU:OE2	1:C:34:ARG:NH2	2.35	0.51
2:O:52:PRO:HB2	2:O:54:HIS:ND1	2.26	0.51
1:B:514:ASP:OD2	5:B:925:HOH:O	2.19	0.51
1:A:420:HIS:NE2	1:A:425:GLU:OE2	2.37	0.50
1:D:145:GLY:HA3	1:D:148:GLY:O	2.11	0.50
1:D:83:GLU:HG2	1:D:538:ILE:HG13	1.92	0.50
1:E:193:VAL:HG21	1:E:283:ILE:HD12	1.93	0.50
1:G:566:LEU:HD11	1:G:590:THR:O	2.11	0.50
1:B:29:ASN:N	1:B:194:LYS:H	2.08	0.50
1:H:415:SER:HB2	1:H:443:MET:HB3	1.94	0.50
1:F:148:GLY:H	1:F:149:PRO:HD2	1.76	0.50
2:N:90:VAL:O	5:N:701:HOH:O	2.19	0.50
2:I:29:LYS:HD3	5:I:712:HOH:O	2.13	0.49
2:P:52:PRO:HB2	2:P:54:HIS:ND1	2.27	0.49
1:C:514:ASP:N	1:C:514:ASP:OD1	2.38	0.49
4:C:702:PQQ:O9A	4:C:702:PQQ:N1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ASN:N	1:D:194:LYS:H	2.09	0.49
2:M:60:ASN:O	2:M:64:GLU:HG2	2.12	0.49
1:B:144:ALA:O	1:B:145:GLY:O	2.29	0.49
1:H:455:GLY:N	5:H:885:HOH:O	2.40	0.49
1:A:415:SER:HB2	1:A:443:MET:HB3	1.94	0.49
1:C:259:GLU:OE1	5:C:864:HOH:O	2.19	0.49
2:L:73:ASN:OD1	2:L:76:ARG:NH2	2.46	0.49
1:E:131:CYS:SG	1:E:132:CYS:N	2.85	0.48
1:E:343:GLN:HG2	5:E:983:HOH:O	2.12	0.48
1:G:89:VAL:HG11	1:G:141:TYR:CE1	2.47	0.48
2:O:28:CYS:HA	2:O:34:CYS:HA	1.93	0.48
1:C:148:GLY:H	1:C:149:PRO:HD2	1.79	0.48
2:M:49:LYS:HE3	2:M:50:TYR:CZ	2.49	0.48
1:C:205:GLU:HB2	5:C:879:HOH:O	2.13	0.48
1:D:266:GLY:O	1:D:290:PRO:HA	2.13	0.48
4:B:702:PQQ:C5	5:B:1034:HOH:O	2.61	0.48
1:H:205:GLU:OE1	5:H:878:HOH:O	2.20	0.48
1:G:271:TRP:CZ2	1:G:335:VAL:HG21	2.49	0.48
1:B:193:VAL:HG21	1:B:283:ILE:HD12	1.96	0.48
1:D:72:TRP:CZ2	1:D:598:VAL:HG21	2.49	0.48
1:F:38:ASP:HB3	1:F:41:ASN:HD22	1.78	0.48
1:G:29:ASN:N	1:G:194:LYS:H	2.12	0.48
1:B:453:ARG:HG3	1:B:453:ARG:HH11	1.77	0.48
1:F:29:ASN:N	1:F:194:LYS:H	2.11	0.48
1:A:348:LYS:HE2	1:A:348:LYS:HB2	1.59	0.48
1:C:532:GLN:HG3	1:D:112:ARG:HH21	1.79	0.48
1:H:520:ARG:NH2	5:H:1004:HOH:O	2.46	0.48
1:B:477:LYS:HG2	1:B:489:GLU:HG2	1.96	0.47
1:D:56:ARG:NH1	5:D:949:HOH:O	2.44	0.47
1:H:232:ASP:OD1	5:H:819:HOH:O	2.20	0.47
1:F:260:GLY:O	5:F:991:HOH:O	2.20	0.47
1:B:96:HIS:CE1	1:B:138:GLY:HA2	2.49	0.47
1:B:148:GLY:O	1:B:149:PRO:C	2.50	0.47
1:A:271:TRP:CE2	1:A:335:VAL:HG21	2.50	0.47
1:G:571:LYS:HB3	1:G:571:LYS:HE2	1.67	0.47
1:D:127:ARG:NH1	5:D:999:HOH:O	2.28	0.47
1:D:182:MET:HG3	5:L:720:HOH:O	2.15	0.47
1:F:271:TRP:CE2	1:F:335:VAL:HG21	2.50	0.47
1:B:453:ARG:NH1	1:B:453:ARG:HG3	2.30	0.47
1:H:333:ALA:O	1:H:358:ARG:HG3	2.15	0.47
2:O:89:LYS:HG2	2:O:91:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:65:SER:HB3	5:M:729:HOH:O	2.14	0.47
1:A:97:THR:O	1:A:101:ASN:HA	2.15	0.47
1:G:72:TRP:CZ2	1:G:598:VAL:HG21	2.50	0.47
1:C:209:ARG:N	2:K:62:GLN:OE1	2.39	0.47
2:M:93:ILE:HG22	2:M:94:LYS:HG3	1.97	0.47
1:E:148:GLY:H	1:E:149:PRO:HD2	1.79	0.47
1:H:329:GLU:HB3	1:H:403:THR:OG1	2.15	0.47
1:A:293:TRP:CH2	1:A:577:LEU:HD13	2.49	0.46
1:F:425:GLU:HG3	1:F:436:MET:HG2	1.97	0.46
1:G:97:THR:O	1:G:101:ASN:HA	2.15	0.46
1:G:414:PRO:HB3	1:G:419:TYR:CD1	2.50	0.46
1:G:204:ALA:HB3	4:G:702:PQQ:O7A	2.15	0.46
1:C:414:PRO:HB3	1:C:419:TYR:CD1	2.49	0.46
1:G:193:VAL:HG21	1:G:283:ILE:HD12	1.97	0.46
1:B:438:VAL:HB	1:B:475:GLN:HB2	1.98	0.46
2:N:51:ASP:HB3	2:N:53:LYS:HE3	1.96	0.46
1:B:118:TYR:O	1:B:120:PRO:HD3	2.15	0.46
1:D:131:CYS:SG	1:D:132:CYS:N	2.88	0.46
1:G:131:CYS:SG	1:G:132:CYS:N	2.89	0.46
1:E:145:GLY:HA2	1:E:147:HIS:CD2	2.50	0.46
1:F:72:TRP:CZ2	1:F:598:VAL:HG21	2.50	0.46
1:G:237:LEU:O	1:G:317:ARG:NH1	2.46	0.46
1:C:89:VAL:HG11	1:C:141:TYR:CZ	2.51	0.46
2:M:74:GLN:HE21	2:M:74:GLN:HA	1.80	0.46
1:C:97:THR:O	1:C:101:ASN:HA	2.15	0.46
1:G:91:GLY:HA2	1:G:108:LEU:HD12	1.98	0.46
1:H:472:MET:H	1:H:472:MET:HG2	1.49	0.46
1:D:358:ARG:HD3	5:D:835:HOH:O	2.15	0.45
1:H:112:ARG:HD3	1:H:112:ARG:O	2.16	0.45
2:M:38:LYS:HG3	5:M:713:HOH:O	2.16	0.45
1:A:205:GLU:HB2	5:A:832:HOH:O	2.17	0.45
1:B:33:ASP:OD1	5:B:854:HOH:O	2.21	0.45
1:D:415:SER:HB2	1:D:443:MET:HB3	1.98	0.45
1:F:118:TYR:O	1:F:120:PRO:HD3	2.17	0.45
1:G:95:ILE:HD12	1:G:596:VAL:HG21	1.98	0.45
1:A:446:GLU:HA	1:A:447:PRO:HD3	1.80	0.45
1:F:266:GLY:O	1:F:290:PRO:HA	2.16	0.45
1:H:131:CYS:SG	1:H:132:CYS:N	2.90	0.45
1:E:265:ILE:HG22	2:M:62:GLN:NE2	2.32	0.45
1:B:271:TRP:CZ2	4:B:702:PQQ:C6A	3.00	0.45
1:F:89:VAL:HG11	1:F:141:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:ARG:NE	5:H:1016:HOH:O	2.30	0.45
1:A:337:TYR:OH	1:A:425:GLU:HB2	2.17	0.45
1:G:207:GLY:O	2:O:62:GLN:NE2	2.44	0.45
1:H:95:ILE:HD12	1:H:596:VAL:HG21	1.99	0.45
1:H:72:TRP:CZ2	1:H:598:VAL:HG21	2.52	0.45
1:C:211:TYR:HB3	1:C:227:TYR:CD2	2.52	0.45
1:D:333:ALA:O	1:D:358:ARG:HG3	2.16	0.45
1:F:112:ARG:HD2	1:F:112:ARG:HA	1.57	0.45
1:H:414:PRO:HB3	1:H:419:TYR:CD1	2.51	0.45
1:B:276:TYR:HD1	1:B:283:ILE:HD13	1.81	0.44
1:A:159:GLY:HA2	1:A:186:LEU:HG	1.99	0.44
1:E:265:ILE:HD11	2:M:54:HIS:CE1	2.52	0.44
1:C:271:TRP:CE2	1:C:335:VAL:HG21	2.53	0.44
1:E:240:ASP:HB3	1:E:243:LYS:HD3	1.98	0.44
1:A:265:ILE:HG22	2:J:62:GLN:NE2	2.32	0.44
1:F:271:TRP:CZ2	4:F:702:PQQ:C6A	3.01	0.44
1:B:131:CYS:SG	1:B:132:CYS:N	2.91	0.44
1:F:131:CYS:SG	1:F:132:CYS:N	2.90	0.44
1:A:500:THR:HG22	1:A:510:TYR:HB3	1.99	0.44
1:D:405:MET:HA	1:D:447:PRO:HG2	1.98	0.44
1:F:96:HIS:CE1	1:F:138:GLY:HA2	2.53	0.44
1:C:266:GLY:O	1:C:290:PRO:HA	2.17	0.44
1:D:205:GLU:HB2	5:D:849:HOH:O	2.17	0.44
1:F:414:PRO:HB3	1:F:419:TYR:CD1	2.53	0.44
1:A:144:ALA:HA	1:A:145:GLY:HA3	1.65	0.43
1:F:54:PHE:HA	1:F:502:ALA:O	2.18	0.43
1:G:303:LYS:HA	1:G:304:TRP:HA	1.78	0.43
1:C:329:GLU:HB3	1:C:403:THR:OG1	2.18	0.43
1:C:62:SER:HA	1:C:507:LEU:HD21	2.01	0.43
1:B:303:LYS:HA	1:B:304:TRP:HA	1.76	0.43
1:C:333:ALA:O	1:C:358:ARG:HG3	2.17	0.43
1:E:377:LYS:HD3	1:E:382:VAL:HB	2.00	0.43
1:A:522:THR:HG21	5:A:836:HOH:O	2.17	0.43
1:E:293:TRP:HB3	1:E:445:TRP:CZ2	2.54	0.43
1:F:415:SER:HB2	1:F:443:MET:HB3	1.99	0.43
1:G:438:VAL:HB	1:G:475:GLN:HB2	1.99	0.43
1:G:405:MET:HA	1:G:447:PRO:HG2	2.01	0.43
1:F:303:LYS:HA	1:F:304:TRP:HA	1.70	0.43
1:F:205:GLU:HB2	5:F:868:HOH:O	2.18	0.43
1:G:89:VAL:O	1:G:90:ASP:CB	2.61	0.43
1:F:145:GLY:HA2	1:F:147:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:CZ2	4:A:702:PQQ:C6A	3.02	0.43
1:E:581:GLY:O	1:E:584:ARG:HG2	2.19	0.43
4:H:702:PQQ:O9A	4:H:702:PQQ:N1	2.52	0.43
1:C:144:ALA:HA	1:C:145:GLY:HA3	1.65	0.42
1:E:303:LYS:HA	1:E:304:TRP:HA	1.73	0.42
1:F:236:LEU:HA	1:F:236:LEU:HD12	1.88	0.42
1:B:72:TRP:CZ2	1:B:598:VAL:HG21	2.54	0.42
1:D:89:VAL:HG11	1:D:141:TYR:CE1	2.54	0.42
1:E:271:TRP:CE2	1:E:335:VAL:HG21	2.54	0.42
1:G:74:LEU:HD11	1:G:106:VAL:HG21	2.01	0.42
1:E:266:GLY:O	1:E:290:PRO:HA	2.20	0.42
2:N:52:PRO:HB2	2:N:54:HIS:CE1	2.54	0.42
1:D:515:GLY:HA2	1:D:536:GLY:HA2	2.01	0.42
1:E:42:TRP:CZ2	1:E:47:LYS:HB2	2.55	0.42
1:H:204:ALA:HB3	4:H:702:PQQ:O7B	2.19	0.42
2:N:49:LYS:HB3	2:N:49:LYS:HE2	1.77	0.42
2:P:28:CYS:HA	2:P:34:CYS:HA	2.01	0.42
1:B:232:ASP:HA	1:B:235:LEU:HD12	2.01	0.42
1:C:431:LYS:HE2	1:C:523:ARG:HG2	2.01	0.42
1:C:521:ASP:HB2	1:C:528:LYS:HD2	2.02	0.42
1:E:97:THR:O	1:E:101:ASN:HA	2.19	0.42
1:H:266:GLY:O	1:H:290:PRO:HA	2.20	0.42
1:H:420:HIS:NE2	1:H:425:GLU:OE2	2.38	0.42
5:F:1028:HOH:O	2:N:49:LYS:HD2	2.19	0.42
1:B:514:ASP:N	1:B:514:ASP:OD1	2.53	0.42
1:D:243:LYS:HB2	1:D:243:LYS:HE3	1.89	0.42
2:J:52:PRO:HB2	2:J:54:HIS:CE1	2.54	0.42
1:A:112:ARG:HD3	1:A:112:ARG:HA	1.76	0.42
1:G:145:GLY:HA2	1:G:147:HIS:CD2	2.55	0.42
1:F:553:ALA:HA	1:F:597:PHE:O	2.20	0.41
1:B:89:VAL:HG11	1:B:141:TYR:CE2	2.55	0.41
1:C:493:LYS:HE3	5:C:1014:HOH:O	2.20	0.41
1:D:584:ARG:NH1	5:D:1040:HOH:O	2.52	0.41
1:G:526:GLU:OE1	5:G:874:HOH:O	2.22	0.41
1:D:417:MET:HG2	1:D:561:TRP:CE3	2.56	0.41
1:F:572:ASP:HB3	1:F:575:ALA:HB2	2.02	0.41
1:A:377:LYS:HD3	1:A:382:VAL:HB	2.02	0.41
1:G:153:PHE:HZ	1:G:217:ILE:HG23	1.84	0.41
1:H:148:GLY:H	1:H:149:PRO:HD2	1.84	0.41
1:A:293:TRP:HB3	1:A:445:TRP:CZ2	2.54	0.41
1:B:56:ARG:HD3	1:B:56:ARG:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:ARG:NE	5:F:927:HOH:O	2.40	0.41
1:G:343:GLN:NE2	5:G:866:HOH:O	2.27	0.41
1:B:271:TRP:CZ2	1:B:335:VAL:HG21	2.55	0.41
1:D:303:LYS:HA	1:D:304:TRP:HA	1.76	0.41
1:F:501:LEU:O	1:F:508:VAL:HA	2.21	0.41
1:B:414:PRO:HB3	1:B:419:TYR:CD1	2.55	0.41
1:C:537:VAL:HG11	1:C:554:ILE:HD11	2.02	0.41
1:D:337:TYR:CZ	1:D:425:GLU:HB2	2.56	0.41
1:F:95:ILE:HD12	1:F:596:VAL:HG21	2.03	0.41
1:A:521:ASP:HB2	1:A:528:LYS:HD2	2.02	0.41
1:B:156:GLN:O	1:B:186:LEU:HB2	2.20	0.41
1:E:50:SER:HB3	1:E:340:LEU:HB2	2.02	0.41
1:H:145:GLY:HA2	1:H:147:HIS:CD2	2.55	0.41
1:A:216:ASN:HB3	1:A:219:ASP:OD1	2.20	0.41
1:A:266:GLY:O	1:A:290:PRO:HA	2.21	0.41
1:E:145:GLY:HA2	1:E:147:HIS:NE2	2.36	0.41
1:G:293:TRP:HB3	1:G:445:TRP:CZ2	2.56	0.41
2:N:74:GLN:HA	2:N:74:GLN:NE2	2.35	0.41
1:A:204:ALA:HB3	4:A:702:PQQ:O7A	2.21	0.41
1:A:271:TRP:CD2	1:A:335:VAL:HG21	2.56	0.41
1:G:66:LYS:HE3	5:G:965:HOH:O	2.20	0.41
1:A:211:TYR:HB3	1:A:227:TYR:CD2	2.56	0.40
1:A:337:TYR:CZ	1:A:425:GLU:HB2	2.56	0.40
1:B:205:GLU:HB2	5:B:981:HOH:O	2.21	0.40
1:D:112:ARG:HD3	1:D:112:ARG:O	2.20	0.40
1:E:144:ALA:HA	1:E:145:GLY:HA3	1.64	0.40
1:H:98:PRO:O	1:H:101:ASN:N	2.42	0.40
2:N:49:LYS:NZ	5:N:716:HOH:O	2.53	0.40
5:F:1013:HOH:O	2:N:62:GLN:HG3	2.21	0.40
1:C:112:ARG:HH11	1:D:532:GLN:HG3	1.85	0.40
1:G:333:ALA:O	1:G:358:ARG:HG3	2.21	0.40
1:B:312:ASP:HB2	1:B:319:LYS:HE3	2.03	0.40
1:A:240:ASP:HB3	1:A:243:LYS:HD3	2.03	0.40
1:C:419:TYR:HA	1:C:419:TYR:HD1	1.74	0.40
1:D:147:HIS:HB2	1:D:218:LYS:HB2	2.03	0.40
1:E:89:VAL:HG11	1:E:141:TYR:CZ	2.56	0.40
1:E:72:TRP:CZ2	1:E:598:VAL:HG21	2.57	0.40
2:L:53:LYS:HD3	2:L:53:LYS:HA	1.89	0.40
2:M:54:HIS:N	2:M:54:HIS:CD2	2.89	0.40
2:P:79:ASN:HA	2:P:82:LYS:HE2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:705:HOH:O	5:J:702:HOH:O[4_444]	2.00	0.20
5:B:811:HOH:O	5:H:810:HOH:O[3_554]	2.04	0.16
5:D:810:HOH:O	5:N:707:HOH:O[3_654]	2.10	0.10

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%)	25 (4%)	3 (0%)	31	54
1	B	571/573 (100%)	539 (94%)	28 (5%)	4 (1%)	24	45
1	C	571/573 (100%)	537 (94%)	32 (6%)	2 (0%)	36	59
1	D	571/573 (100%)	536 (94%)	33 (6%)	2 (0%)	36	59
1	E	571/573 (100%)	541 (95%)	27 (5%)	3 (0%)	31	54
1	F	571/573 (100%)	533 (93%)	35 (6%)	3 (0%)	31	54
1	G	571/573 (100%)	538 (94%)	29 (5%)	4 (1%)	24	45
1	H	571/573 (100%)	536 (94%)	31 (5%)	4 (1%)	24	45
2	I	69/72 (96%)	69 (100%)	0	0	100	100
2	J	69/72 (96%)	69 (100%)	0	0	100	100
2	K	69/72 (96%)	69 (100%)	0	0	100	100
2	L	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	M	70/72 (97%)	70 (100%)	0	0	100	100
2	N	70/72 (97%)	68 (97%)	2 (3%)	0	100	100
2	O	70/72 (97%)	70 (100%)	0	0	100	100
2	P	70/72 (97%)	70 (100%)	0	0	100	100
All	All	5124/5160 (99%)	4856 (95%)	243 (5%)	25 (0%)	31	54

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	GLY
1	D	294	ASN
1	G	90	ASP
1	H	294	ASN
1	F	294	ASN
1	B	134	VAL
1	B	148	GLY
1	A	134	VAL
1	A	148	GLY
1	C	134	VAL
1	E	557	GLY
1	F	557	GLY
1	G	557	GLY
1	H	557	GLY
1	D	594	GLY
1	E	594	GLY
1	H	98	PRO
1	B	557	GLY
1	A	594	GLY
1	F	594	GLY
1	G	134	VAL
1	G	594	GLY
1	C	594	GLY
1	E	134	VAL
1	H	148	GLY

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%)	461 (99%)	3 (1%)	87	95
1	B	464/464 (100%)	458 (99%)	6 (1%)	71	87
1	C	464/464 (100%)	459 (99%)	5 (1%)	76	89
1	D	464/464 (100%)	460 (99%)	4 (1%)	81	92
1	E	464/464 (100%)	459 (99%)	5 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	464/464 (100%)	463 (100%)	1 (0%)	94	98
1	G	464/464 (100%)	463 (100%)	1 (0%)	94	98
1	H	464/464 (100%)	461 (99%)	3 (1%)	87	95
2	I	60/61 (98%)	60 (100%)	0	100	100
2	J	60/61 (98%)	60 (100%)	0	100	100
2	K	60/61 (98%)	60 (100%)	0	100	100
2	L	60/61 (98%)	60 (100%)	0	100	100
2	M	61/61 (100%)	61 (100%)	0	100	100
2	N	61/61 (100%)	61 (100%)	0	100	100
2	O	61/61 (100%)	61 (100%)	0	100	100
2	P	61/61 (100%)	61 (100%)	0	100	100
All	All	4196/4200 (100%)	4168 (99%)	28 (1%)	85	94

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	ILE
1	B	97	THR
1	B	132	CYS
1	B	337	TYR
1	B	472	MET
1	B	523	ARG
1	A	112	ARG
1	A	132	CYS
1	A	522	THR
1	C	131	CYS
1	C	337	TYR
1	C	472	MET
1	C	522	THR
1	C	523	ARG
1	D	53	HIS
1	D	97	THR
1	D	132	CYS
1	D	337	TYR
1	E	97	THR
1	E	112	ARG
1	E	132	CYS
1	E	337	TYR

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Mol	Chain	Res	Type
1	E	343	GLN
1	F	337	TYR
1	G	90	ASP
1	H	170	GLU
1	H	337	TYR
1	H	453	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	ASN
2	I	79	ASN
1	A	588	HIS
2	M	74	GLN
2	N	74	GLN
2	N	79	ASN
1	G	63	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	702	-	18,26,26	1.46	2 (11%)	15,40,40	1.64	3 (20%)
4	PQQ	B	702	-	18,26,26	1.44	2 (11%)	15,40,40	1.75	4 (26%)
4	PQQ	C	702	-	18,26,26	1.64	2 (11%)	15,40,40	1.53	3 (20%)
4	PQQ	D	702	-	18,26,26	1.59	2 (11%)	15,40,40	1.55	3 (20%)
4	PQQ	E	702	-	18,26,26	1.43	2 (11%)	15,40,40	1.65	4 (26%)
4	PQQ	F	702	-	18,26,26	1.33	2 (11%)	15,40,40	1.72	5 (33%)
4	PQQ	G	702	-	18,26,26	1.45	2 (11%)	15,40,40	1.59	4 (26%)
4	PQQ	H	702	-	18,26,26	1.38	2 (11%)	15,40,40	1.67	4 (26%)

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	A	702	-	-	0/0/28/28	0/3/3/3
4	PQQ	B	702	-	-	0/0/28/28	0/3/3/3
4	PQQ	C	702	-	-	0/0/28/28	0/3/3/3
4	PQQ	D	702	-	-	0/0/28/28	0/3/3/3
4	PQQ	E	702	-	-	0/0/28/28	0/3/3/3
4	PQQ	F	702	-	-	0/0/28/28	0/3/3/3
4	PQQ	G	702	-	-	0/0/28/28	0/3/3/3
4	PQQ	H	702	-	-	0/0/28/28	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	PQQ	C9-C9X	5.82	1.53	1.47
4	D	702	PQQ	C9-C9X	5.41	1.52	1.47
4	G	702	PQQ	C9-C9X	4.96	1.52	1.47
4	A	702	PQQ	C9-C9X	4.90	1.52	1.47
4	B	702	PQQ	C9-C9X	4.80	1.52	1.47
4	E	702	PQQ	C9-C9X	4.73	1.52	1.47
4	H	702	PQQ	C9-C9X	4.43	1.51	1.47
4	F	702	PQQ	C9-C9X	4.25	1.51	1.47
4	H	702	PQQ	C5-C4	-2.79	1.44	1.53
4	F	702	PQQ	C5-C4	-2.74	1.44	1.53
4	C	702	PQQ	C5-C4	-2.73	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	PQQ	C5-C4	-2.66	1.44	1.53
4	E	702	PQQ	C5-C4	-2.66	1.44	1.53
4	G	702	PQQ	C5-C4	-2.64	1.44	1.53
4	D	702	PQQ	C5-C4	-2.57	1.44	1.53
4	B	702	PQQ	C5-C4	-2.57	1.44	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	702	PQQ	C9A-C1A-N1	3.74	132.07	124.25
4	F	702	PQQ	C9A-C1A-N1	3.63	131.83	124.25
4	E	702	PQQ	C9A-C1A-N1	3.62	131.82	124.25
4	A	702	PQQ	C9A-C1A-N1	3.56	131.69	124.25
4	B	702	PQQ	C9A-C1A-N1	3.46	131.49	124.25
4	D	702	PQQ	C9A-C1A-N1	3.43	131.41	124.25
4	C	702	PQQ	C9A-C1A-N1	3.34	131.23	124.25
4	G	702	PQQ	C9A-C1A-N1	3.32	131.19	124.25
4	B	702	PQQ	C6A-N6-C7	3.10	122.98	118.14
4	H	702	PQQ	C6A-N6-C7	3.01	122.83	118.14
4	F	702	PQQ	C6A-N6-C7	2.99	122.81	118.14
4	E	702	PQQ	C6A-N6-C7	2.89	122.64	118.14
4	G	702	PQQ	C6A-N6-C7	2.82	122.54	118.14
4	A	702	PQQ	C6A-N6-C7	2.71	122.36	118.14
4	D	702	PQQ	C6A-N6-C7	2.64	122.26	118.14
4	B	702	PQQ	C8-C7-N6	-2.58	119.26	122.35
4	C	702	PQQ	C6A-N6-C7	2.52	122.07	118.14
4	F	702	PQQ	C8-C7-N6	-2.46	119.40	122.35
4	H	702	PQQ	C8-C7-N6	-2.42	119.45	122.35
4	D	702	PQQ	C9A-C6A-N6	-2.23	120.57	123.66
4	G	702	PQQ	C8-C7-N6	-2.22	119.69	122.35
4	F	702	PQQ	C9A-C6A-N6	-2.22	120.59	123.66
4	B	702	PQQ	C9A-C6A-N6	-2.19	120.63	123.66
4	G	702	PQQ	C9A-C6A-N6	-2.18	120.64	123.66
4	H	702	PQQ	C9A-C6A-N6	-2.18	120.64	123.66
4	E	702	PQQ	C9A-C6A-N6	-2.13	120.71	123.66
4	E	702	PQQ	C8-C7-N6	-2.13	119.80	122.35
4	A	702	PQQ	C8-C7-N6	-2.11	119.83	122.35
4	C	702	PQQ	C9A-C6A-N6	-2.10	120.76	123.66
4	F	702	PQQ	C5-C6A-N6	2.04	118.42	114.96

There are no chirality outliers.

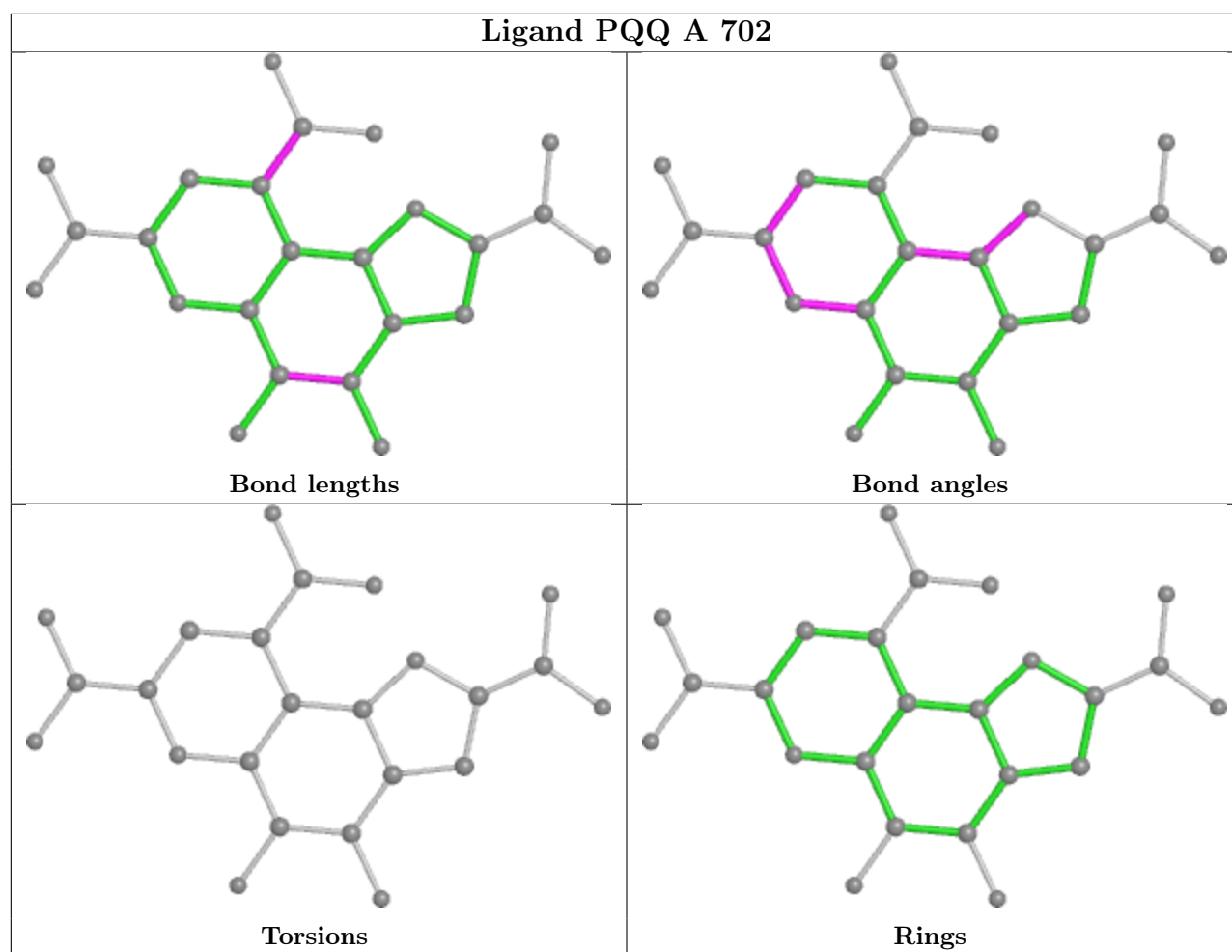
There are no torsion outliers.

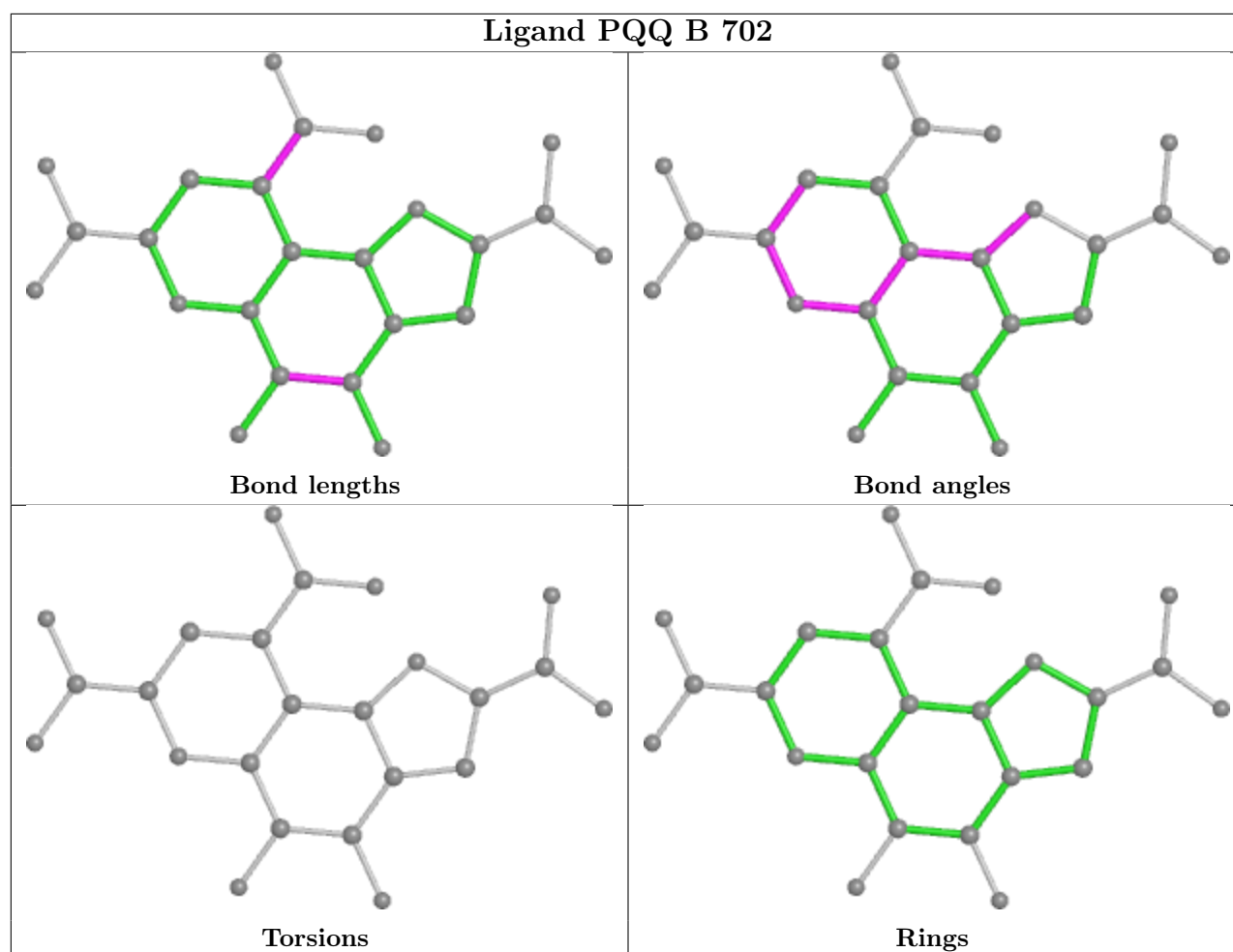
There are no ring outliers.

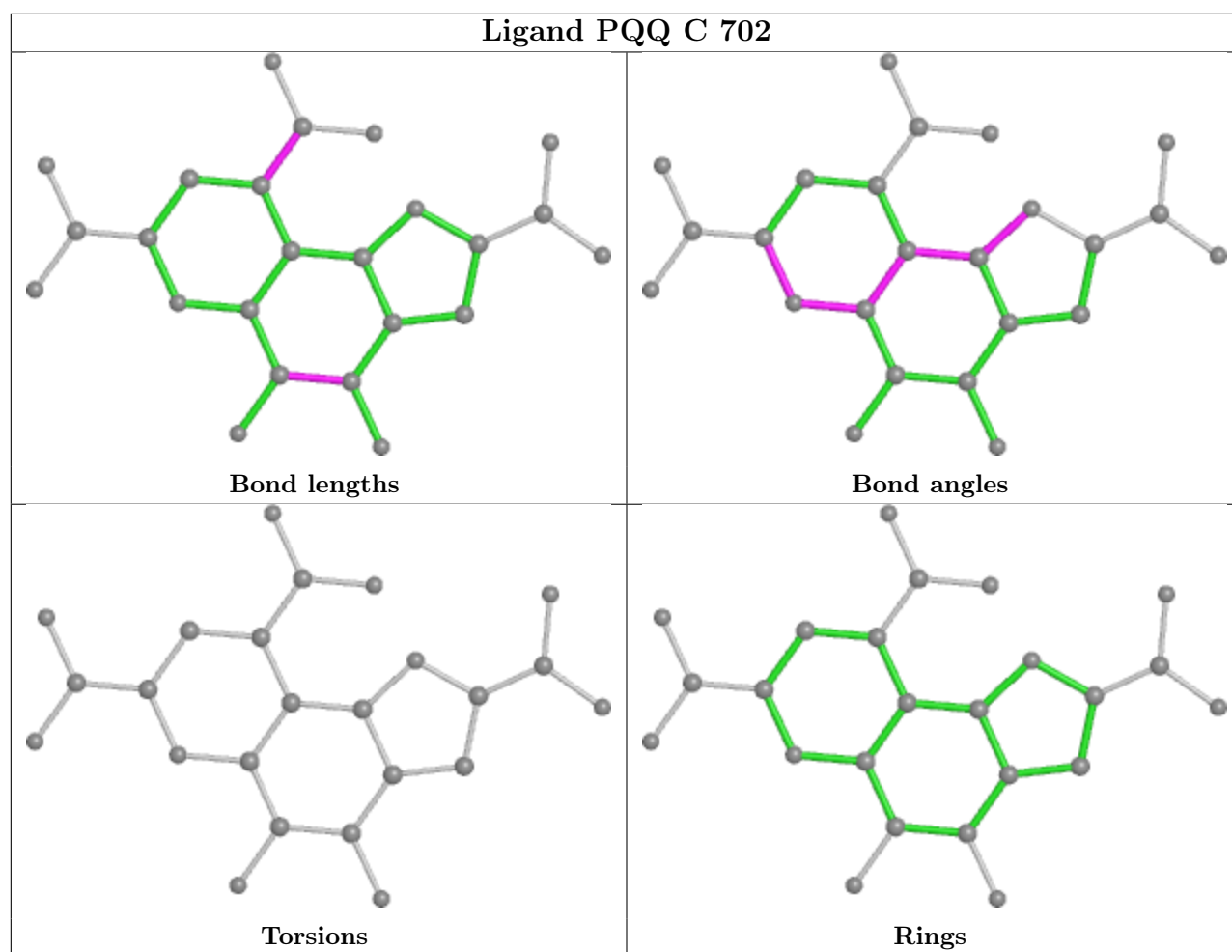
7 monomers are involved in 14 short contacts:

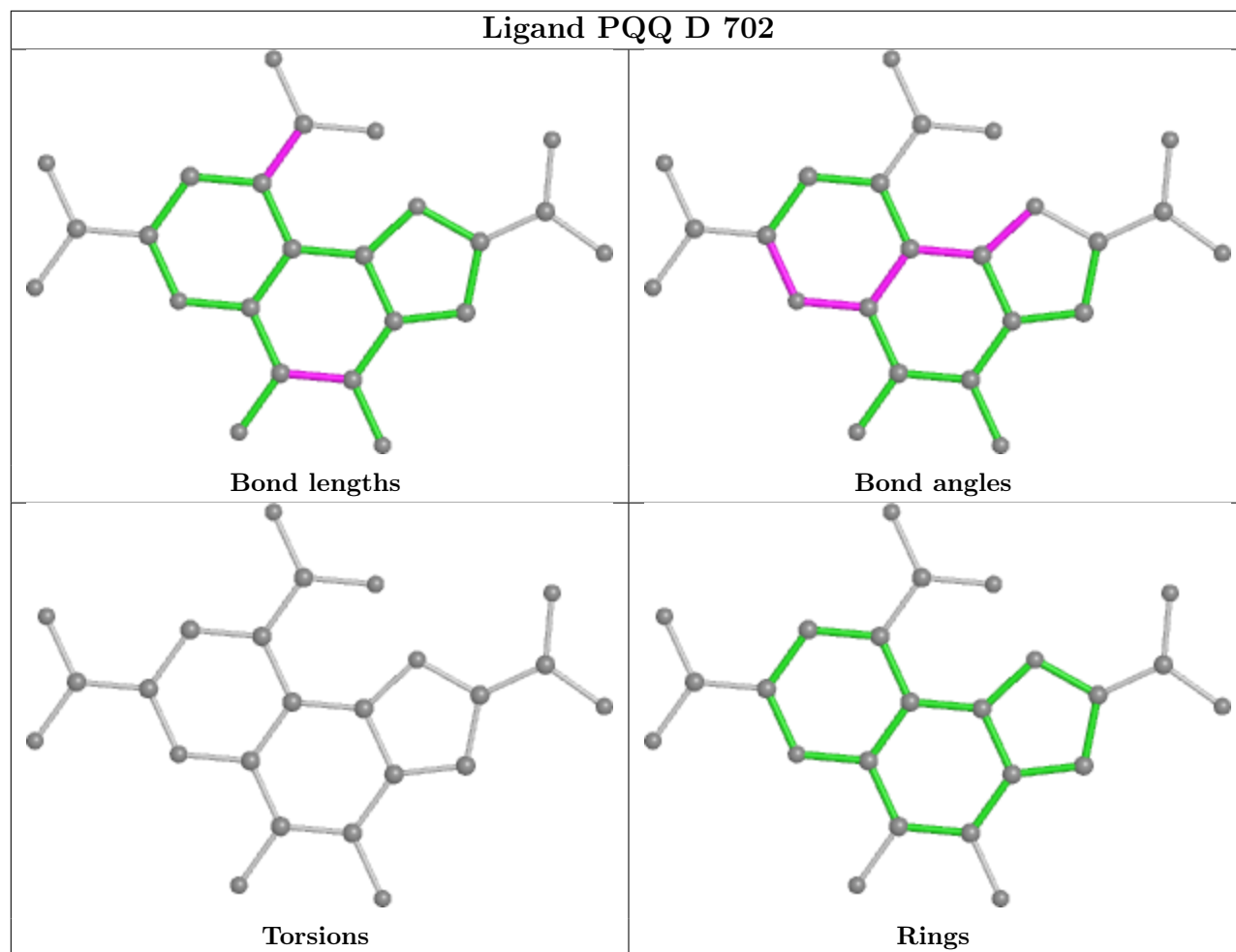
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	PQQ	3	0
4	B	702	PQQ	3	0
4	C	702	PQQ	1	0
4	D	702	PQQ	1	0
4	F	702	PQQ	2	0
4	G	702	PQQ	2	0
4	H	702	PQQ	2	0

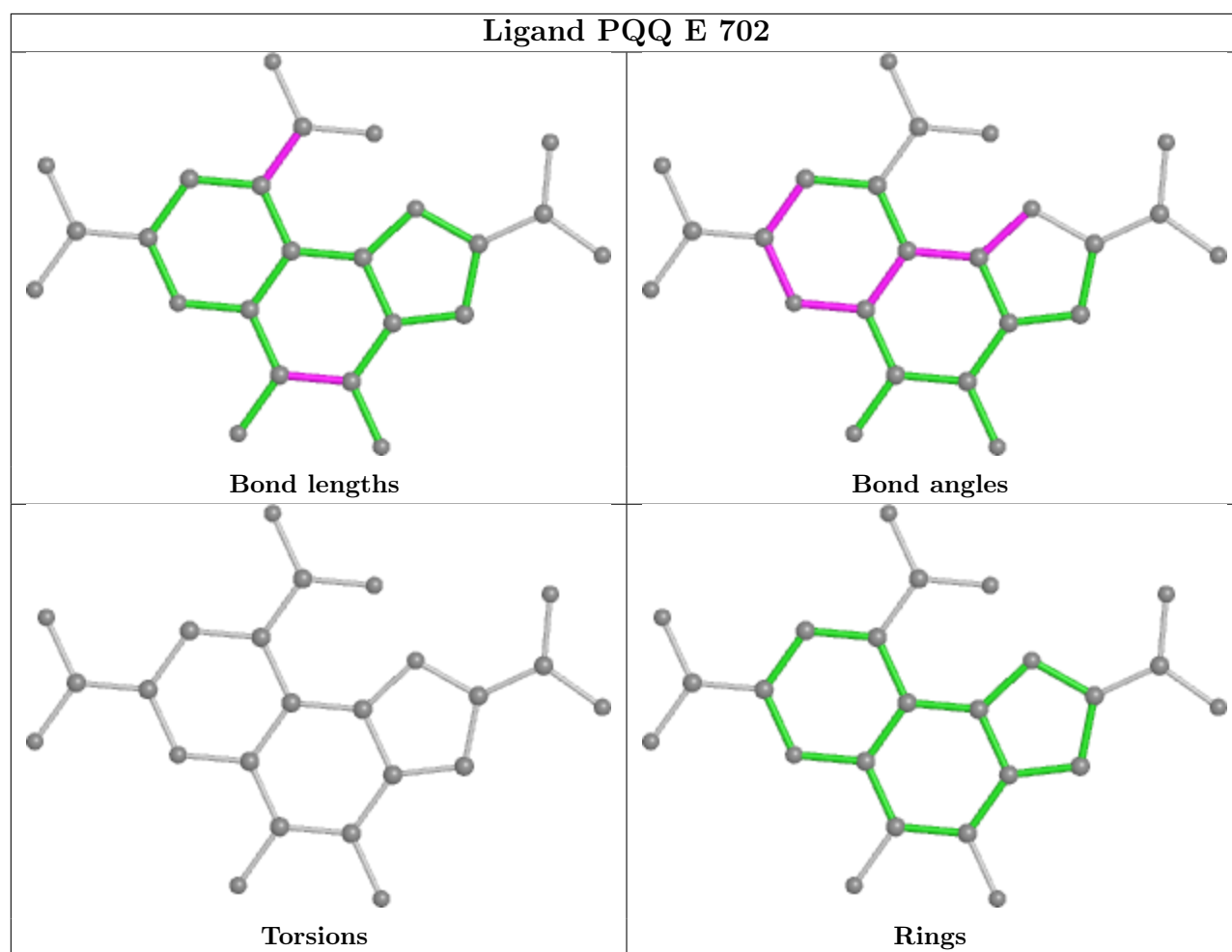
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

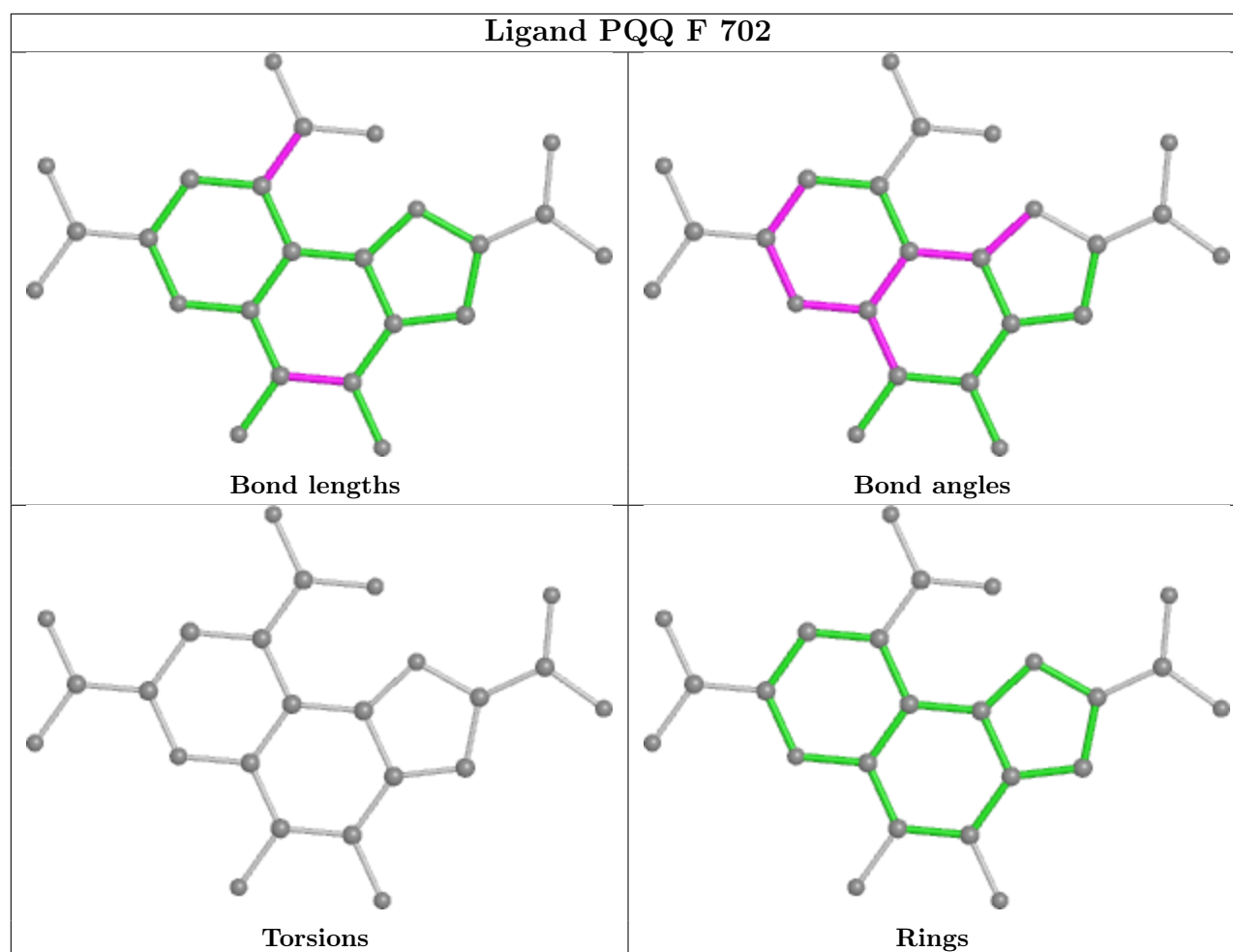


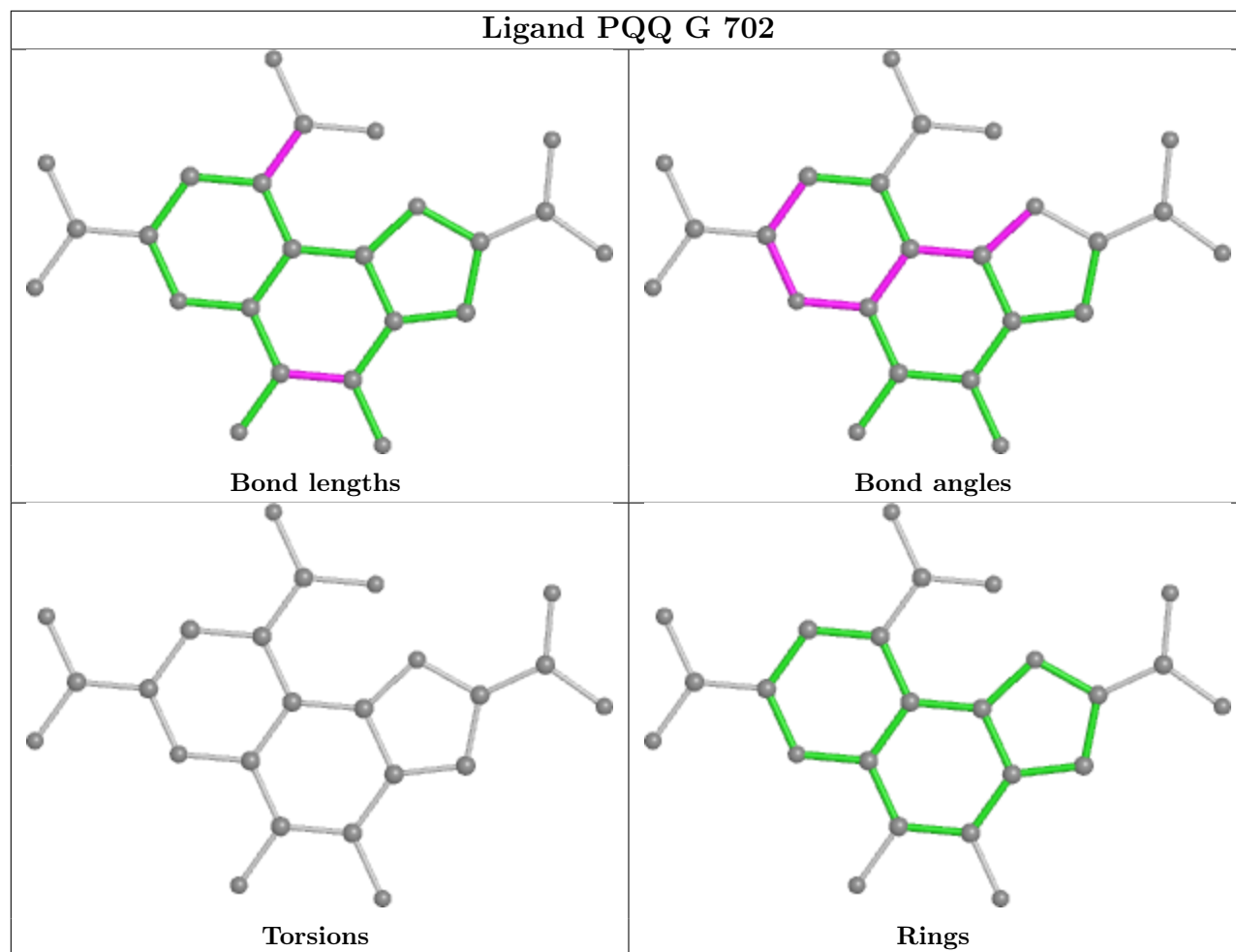


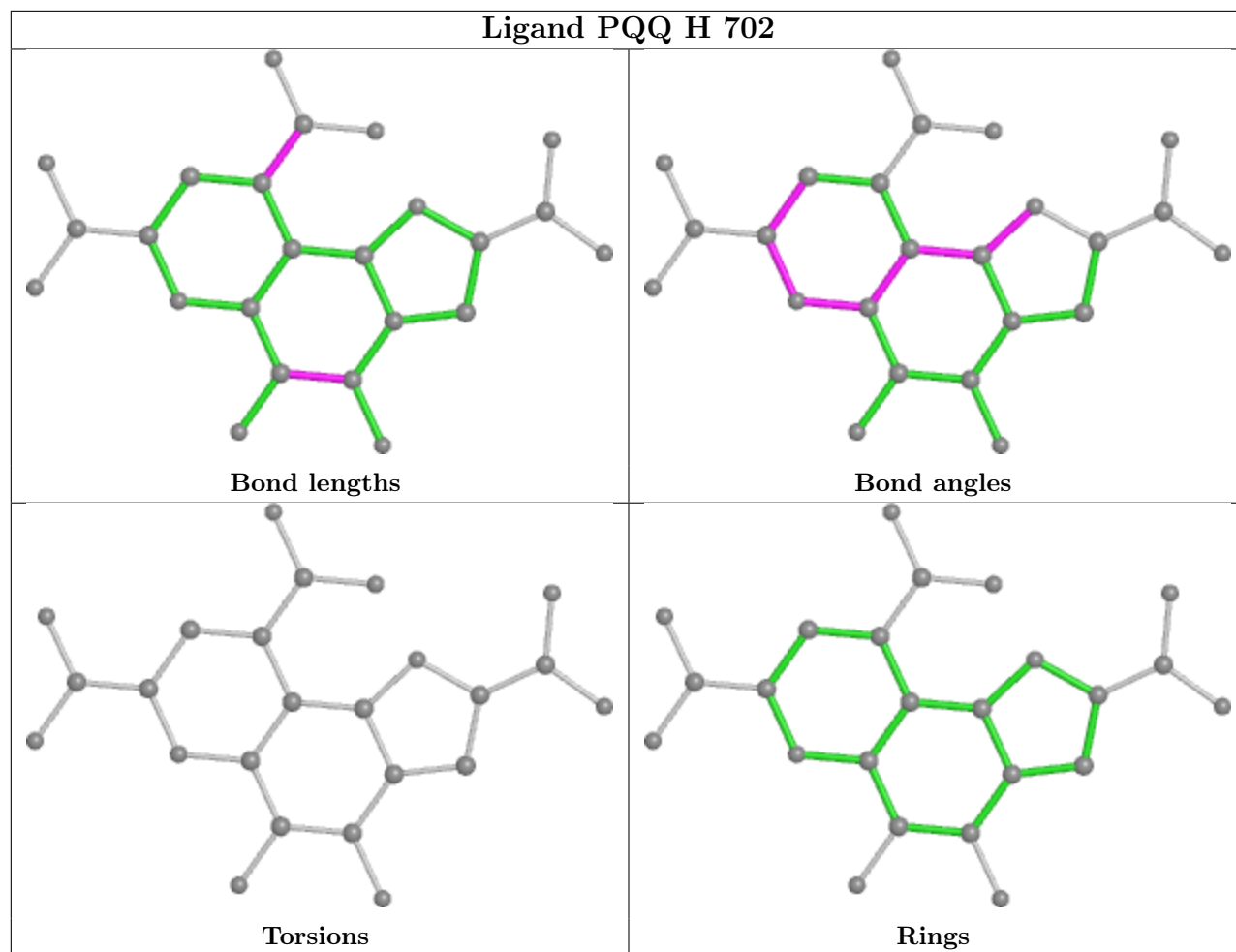












5.7 Other polymers [i](#)

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%)	-0.34	1 (0%) 94 95	15, 21, 32, 46	0
1	B	573/573 (100%)	-0.40	0 100 100	15, 22, 33, 49	0
1	C	573/573 (100%)	-0.19	3 (0%) 90 90	15, 25, 36, 53	0
1	D	573/573 (100%)	-0.38	0 100 100	16, 23, 34, 50	0
1	E	573/573 (100%)	-0.37	0 100 100	16, 23, 35, 48	0
1	F	573/573 (100%)	-0.40	0 100 100	15, 24, 34, 45	0
1	G	573/573 (100%)	-0.36	0 100 100	15, 24, 35, 50	0
1	H	573/573 (100%)	-0.22	2 (0%) 93 94	16, 24, 36, 52	0
2	I	71/72 (98%)	-0.17	0 100 100	21, 27, 45, 53	0
2	J	71/72 (98%)	-0.26	0 100 100	22, 27, 41, 48	0
2	K	71/72 (98%)	0.05	2 (2%) 53 49	28, 36, 46, 51	0
2	L	71/72 (98%)	-0.34	0 100 100	19, 31, 44, 55	0
2	M	72/72 (100%)	-0.15	0 100 100	24, 31, 48, 64	0
2	N	72/72 (100%)	-0.31	0 100 100	25, 32, 44, 48	0
2	O	72/72 (100%)	-0.18	0 100 100	25, 36, 48, 59	0
2	P	72/72 (100%)	0.16	0 100 100	23, 32, 47, 59	0
All	All	5156/5160 (99%)	-0.31	8 (0%) 94 95	15, 24, 38, 64	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	293	TRP	2.6
1	A	400	GLU	2.3
1	C	330	TRP	2.2
1	C	445	TRP	2.1
2	K	23	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	204	ALA	2.0
2	K	35	TRP	2.0
1	H	266	GLY	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 carbohydrates in this entry.

6.4 Ligands [i](#)

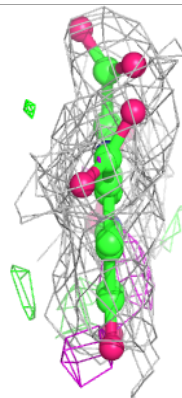
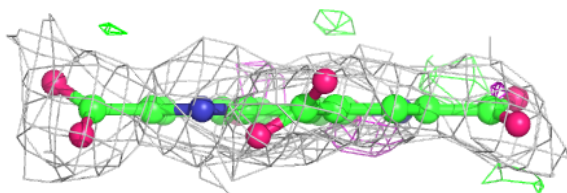
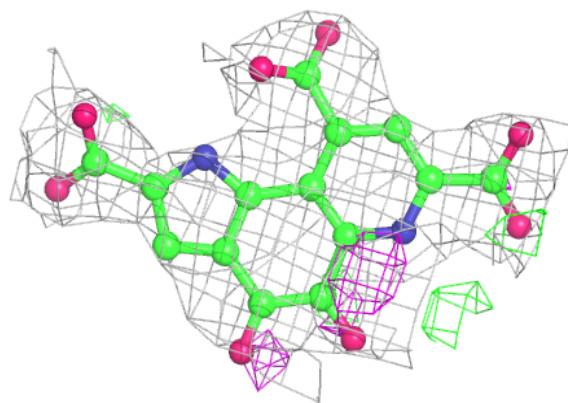
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	H	701	1/1	0.67	0.16	97,97,97,97	0
4	PQQ	H	702	24/24	0.90	0.33	30,42,48,50	0
4	PQQ	E	702	24/24	0.91	0.28	27,40,43,45	0
4	PQQ	F	702	24/24	0.91	0.25	28,38,42,45	0
4	PQQ	B	702	24/24	0.91	0.29	27,36,40,43	0
4	PQQ	C	702	24/24	0.92	0.27	26,36,42,44	0
4	PQQ	D	702	24/24	0.92	0.27	29,39,45,47	0
4	PQQ	G	702	24/24	0.93	0.27	25,38,43,44	0
4	PQQ	A	702	24/24	0.94	0.25	25,33,36,38	0
3	CA	F	701	1/1	0.95	0.06	49,49,49,49	0
3	CA	D	701	1/1	0.95	0.07	44,44,44,44	0
3	CA	C	701	1/1	0.97	0.14	46,46,46,46	0
3	CA	G	701	1/1	0.97	0.14	43,43,43,43	0
3	CA	A	701	1/1	0.98	0.15	40,40,40,40	0
3	CA	E	701	1/1	0.98	0.10	39,39,39,39	0
3	CA	B	701	1/1	0.99	0.08	37,37,37,37	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.

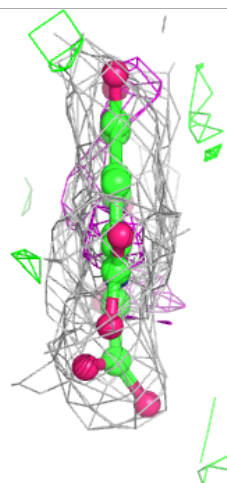
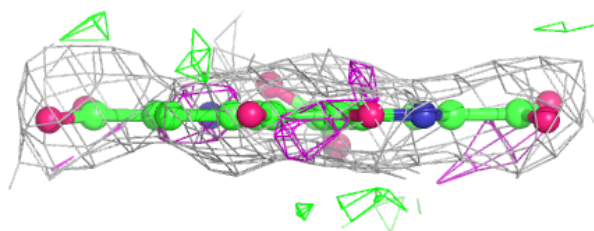
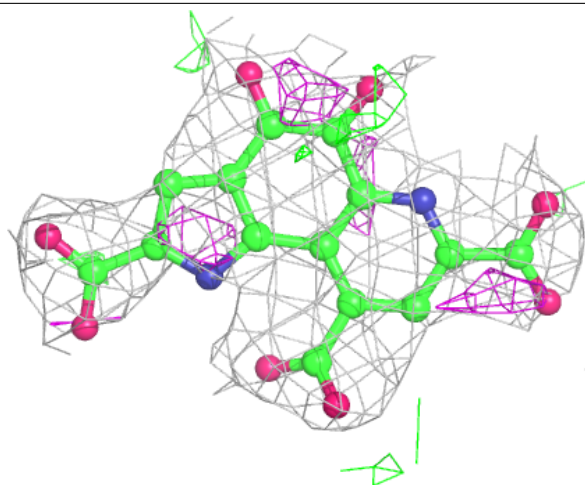
Electron density around PQQ H 702:

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



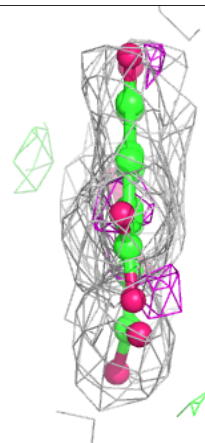
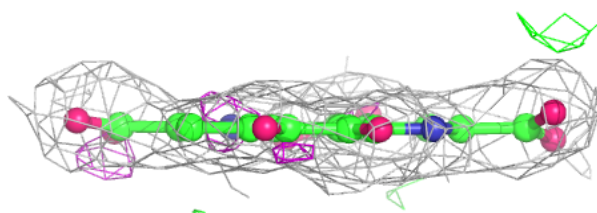
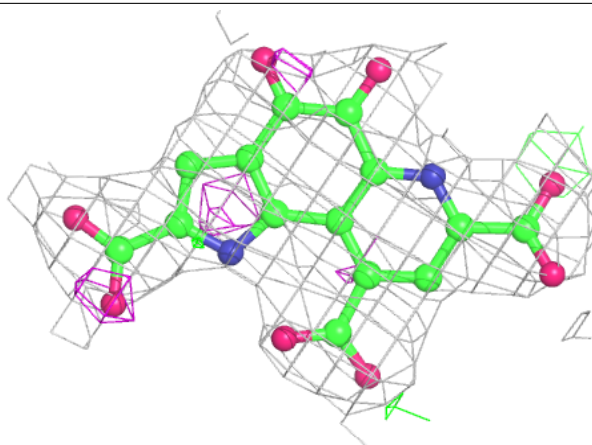
Electron density around PQQ E 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



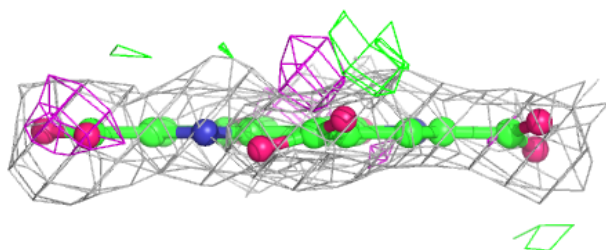
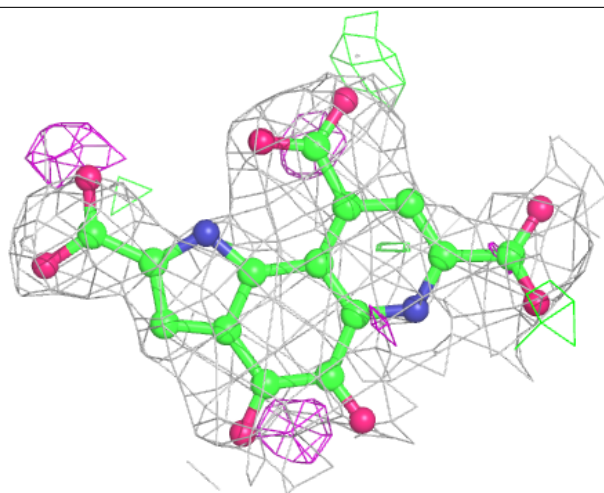
Electron density around PQQ F 702:

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



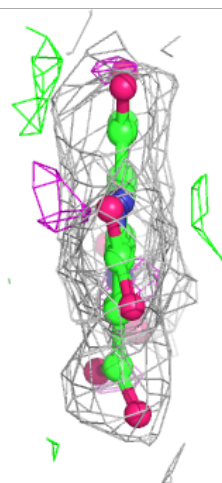
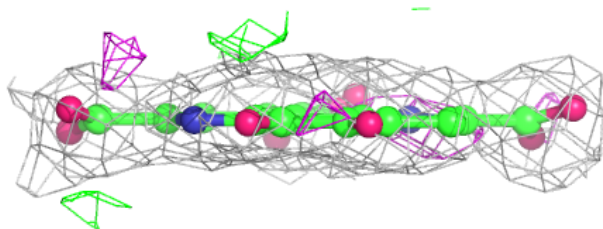
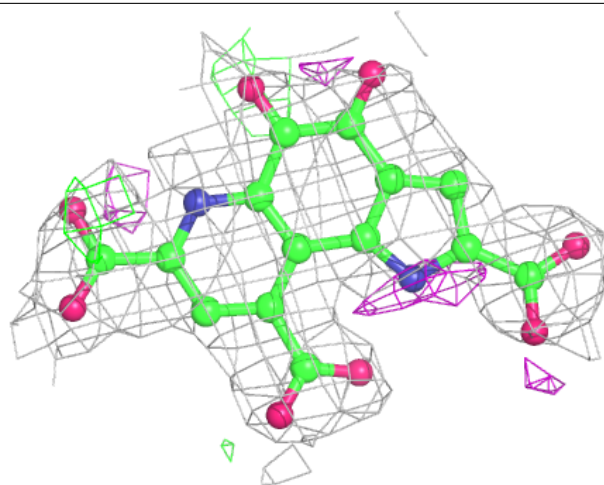
Electron density around PQQ B 702:

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



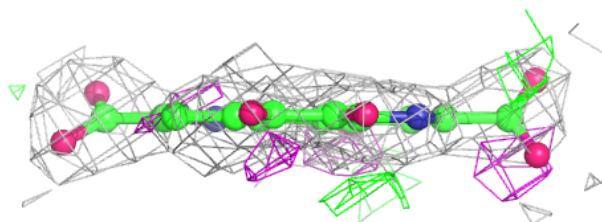
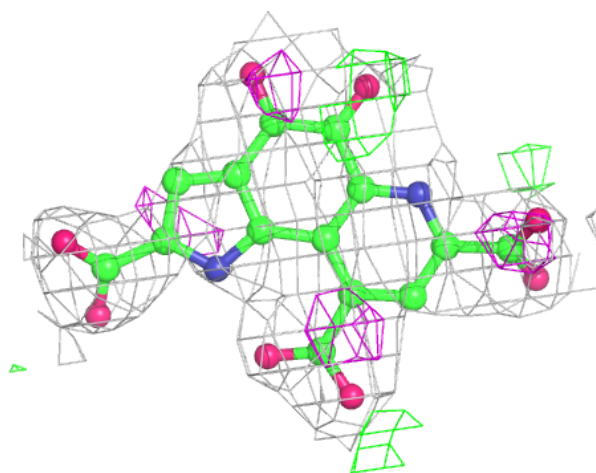
Electron density around PQQ C 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



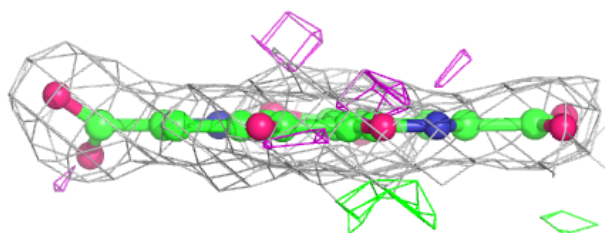
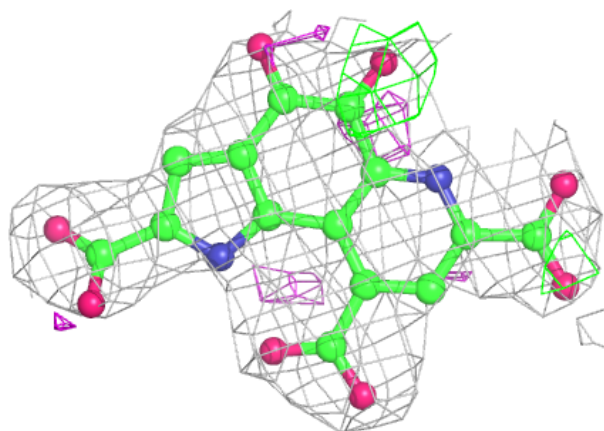
Electron density around PQQ D 702:

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



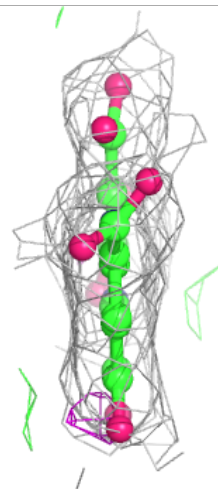
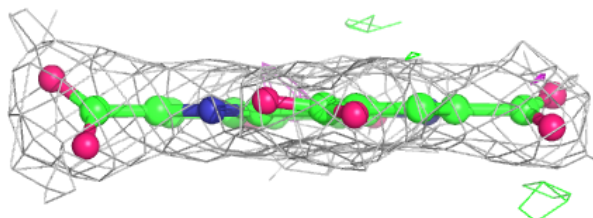
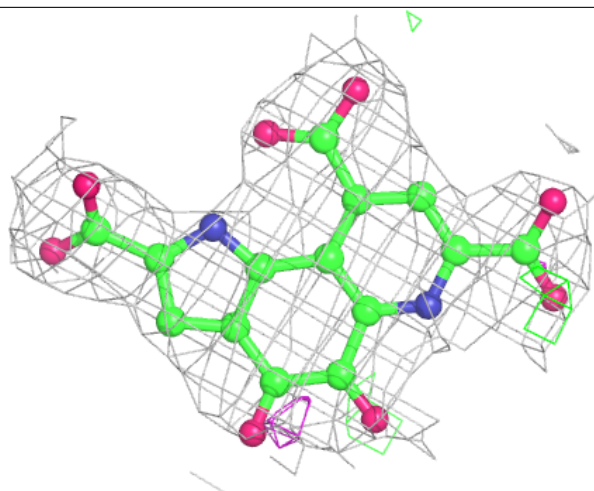
Electron density around PQQ G 702:

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



Electron density around PQQ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.