



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:03 PM UTC

PDB ID : 7CE9 / pdb_00007ce9
Title : PQQ-soaked Apo-methanol dehydrogenase (MDH) from *Methylococcus capsulatus* (Bath)
Authors : Chuankhayan, P.; Chan, S.I.; Nareddy, P.K.R.; Tsai, I.K.; Tsai, Y.F.; Chen, K.H.-C.; Yu, S.S.-F.; Chen, C.J.
Deposited on : 2020-06-22
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

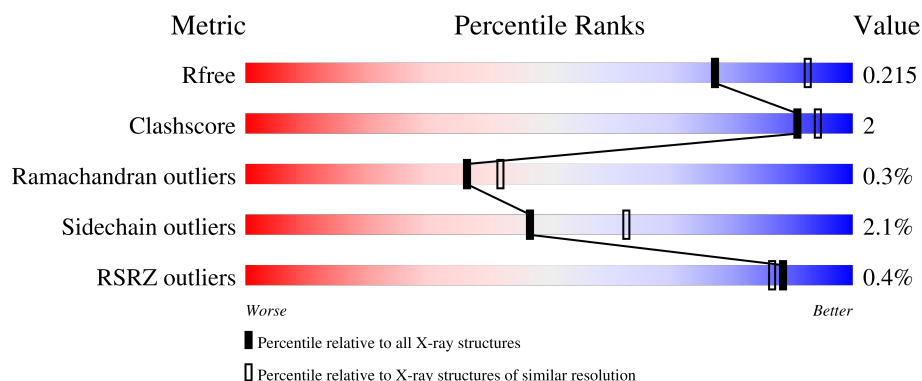
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



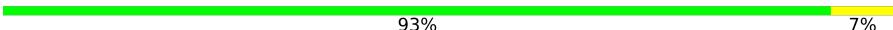
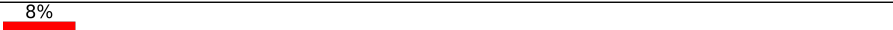
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	92% 7% .
1	B	573	95% . .
1	C	573	93% 6%
1	D	573	93% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	573	 93% 7%
1	H	573	 93% 6% .
1	M	573	 92% 8%
1	N	573	 94% 6% .
2	E	72	 93% 6% .
2	F	72	 11% 82% 15% ..
2	I	72	 3% 90% 7% ..
2	J	72	 90% 7% ..
2	K	72	 % 93% 6% .
2	L	72	 85% 11% ...
2	O	72	 8% 86% 11% ..
2	P	72	 4% 86% 11% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43200 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methanol dehydrogenase protein, large subunit.

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

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

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

Continued on next page...

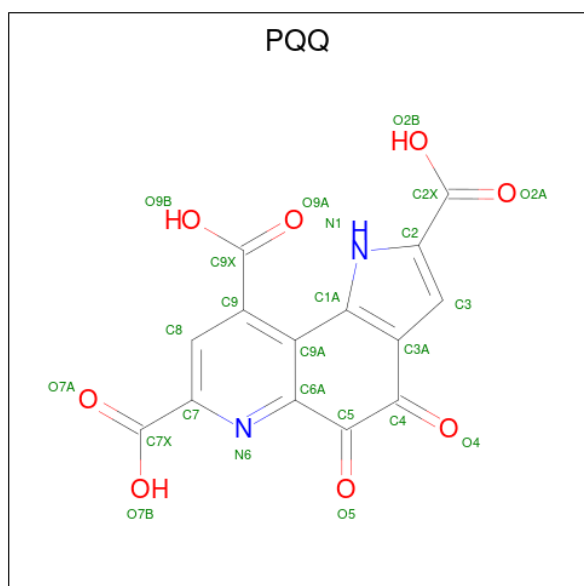
Continued from previous page...

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: C₁₄H₆N₂O₈) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	0
			254	254		
5	B	309	Total	O	0	0
			309	309		
5	C	286	Total	O	0	0
			286	286		
5	D	288	Total	O	0	0
			288	288		
5	E	34	Total	O	0	0
			34	34		
5	F	43	Total	O	0	0
			43	43		
5	G	250	Total	O	0	0
			250	250		
5	H	284	Total	O	0	0
			284	284		
5	I	25	Total	O	0	0
			25	25		
5	J	38	Total	O	0	0
			38	38		
5	K	48	Total	O	0	0
			48	48		
5	L	59	Total	O	0	0
			59	59		

Continued on next page...

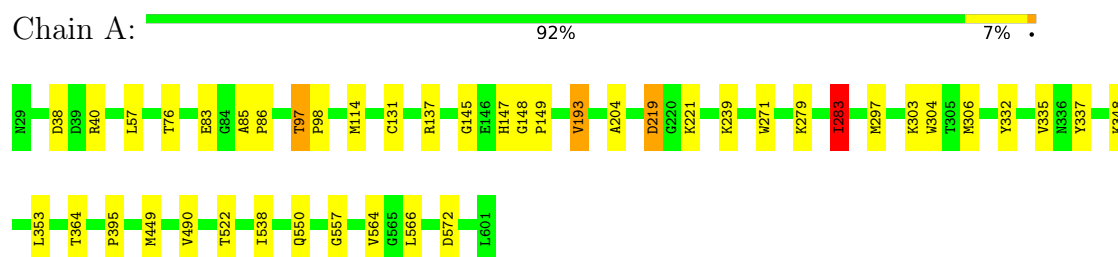
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	308	Total 308	O 308	0	0
5	N	238	Total 238	O 238	0	0
5	O	42	Total 42	O 42	0	0
5	P	26	Total 26	O 26	0	0

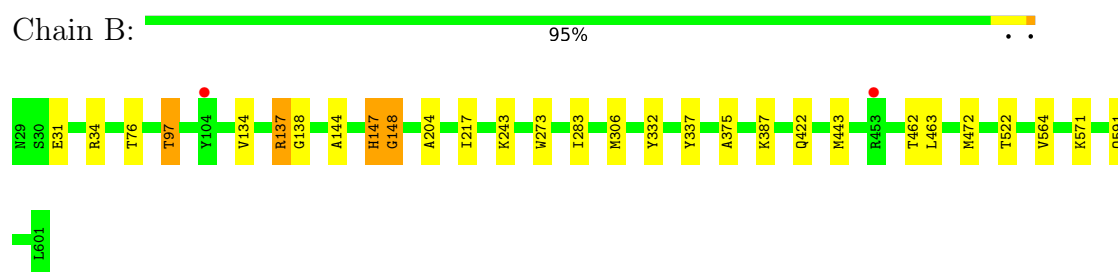
3 Residue-property plots

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.

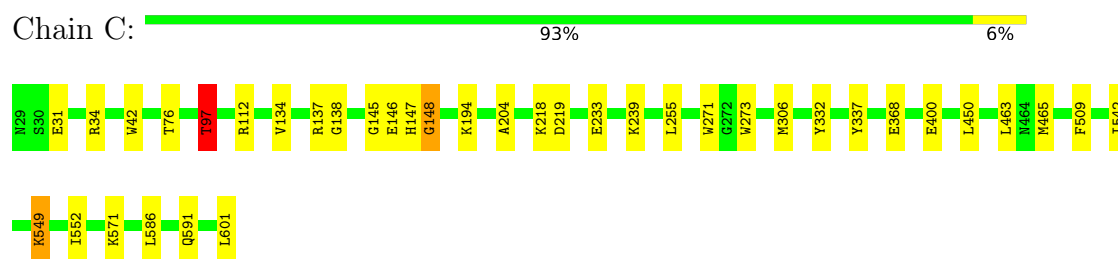
- Molecule 1: Methanol dehydrogenase protein, large subunit



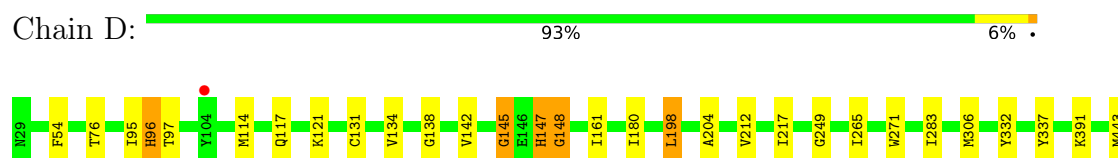
- Molecule 1: Methanol dehydrogenase protein, large subunit



- Molecule 1: Methanol dehydrogenase protein, large subunit



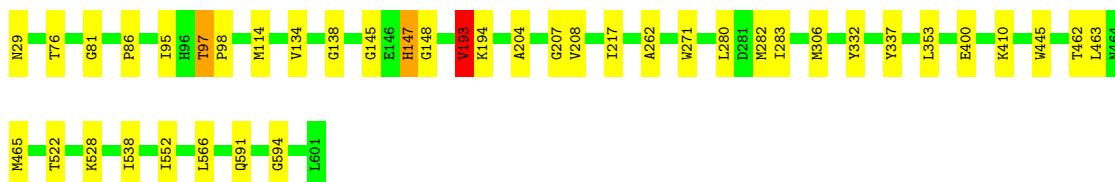
- Molecule 1: Methanol dehydrogenase protein, large subunit





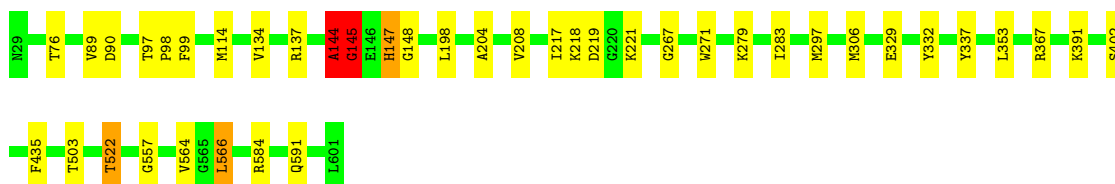
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain G: 93% 7%



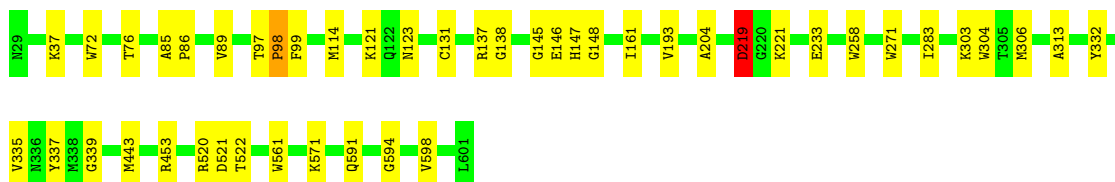
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain H: 93% 6%



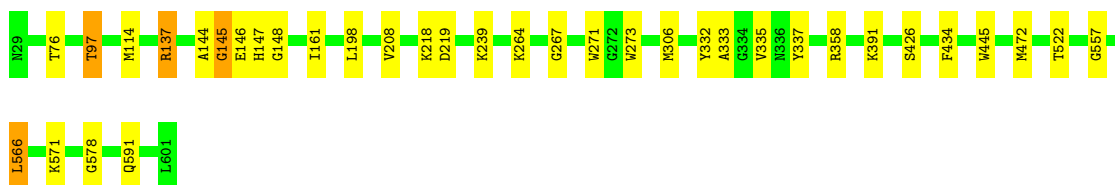
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain M: 92% 8%



- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain N: 94% 6%

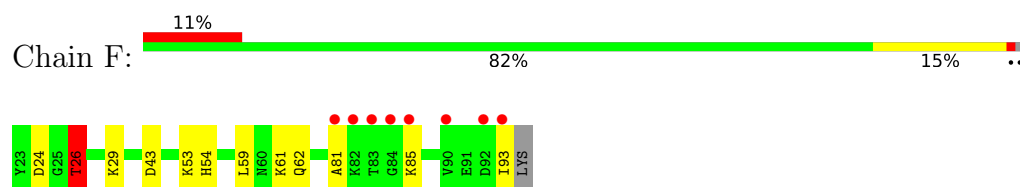


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

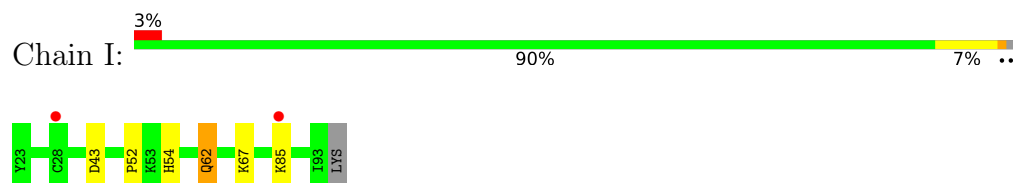
Chain E: 93% 6%



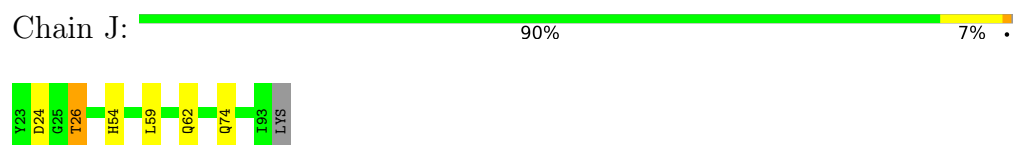
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



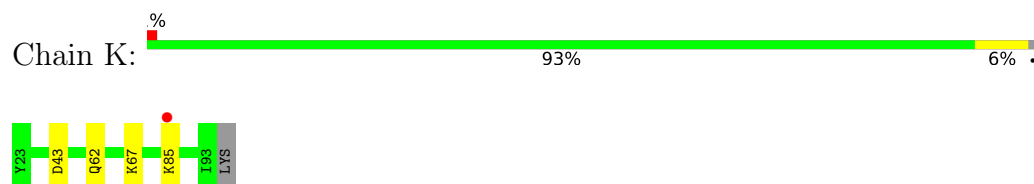
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



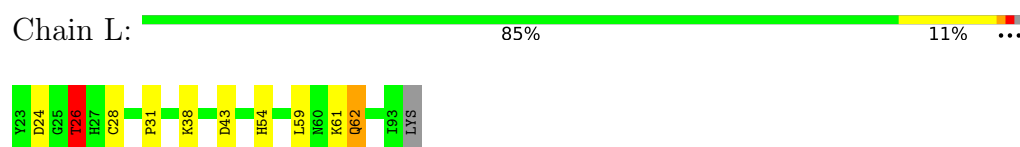
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



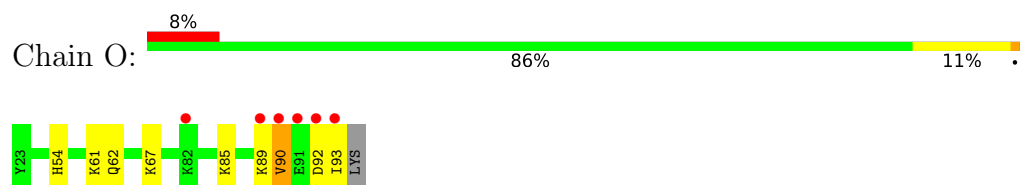
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



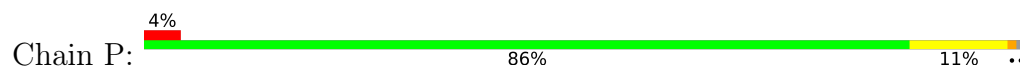
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.56Å 211.76Å 223.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.00 – 2.20 153.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.00-2.20) 99.9 (153.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.161 , 0.209 0.171 , 0.215	Depositor DCC
R_{free} test set	15016 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.2	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	0.95	EDS
Total number of atoms	43200	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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

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	1.15	8/4622 (0.2%)	1.07	9/6281 (0.1%)
1	B	1.17	4/4621 (0.1%)	1.10	9/6281 (0.1%)
1	C	1.18	8/4622 (0.2%)	1.10	14/6281 (0.2%)
1	D	1.19	5/4621 (0.1%)	1.08	9/6281 (0.1%)
1	G	1.14	4/4622 (0.1%)	1.06	6/6281 (0.1%)
1	H	1.17	2/4621 (0.0%)	1.10	8/6281 (0.1%)
1	M	1.14	8/4622 (0.2%)	1.08	11/6281 (0.2%)
1	N	1.12	3/4621 (0.1%)	1.06	9/6281 (0.1%)
2	E	1.19	1/583 (0.2%)	1.13	1/785 (0.1%)
2	F	1.25	1/583 (0.2%)	1.21	4/785 (0.5%)
2	I	1.10	1/583 (0.2%)	1.09	1/785 (0.1%)
2	J	1.22	0/583	1.23	1/785 (0.1%)
2	K	1.14	0/583	1.15	1/785 (0.1%)
2	L	1.17	1/583 (0.2%)	1.19	5/785 (0.6%)
2	O	1.26	0/583	1.11	2/785 (0.3%)
2	P	1.11	0/583	1.15	0/785
All	All	1.16	46/41636 (0.1%)	1.09	90/56528 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	G	0	1
1	H	0	3
1	M	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
All	All	0	10

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	96	HIS	C-N	10.77	1.46	1.32
1	C	97	THR	C-N	-7.60	1.22	1.33
1	B	522	THR	C-O	-7.44	1.14	1.24
1	A	98	PRO	CA-C	7.25	1.62	1.52
1	M	147	HIS	CA-C	7.04	1.62	1.52
1	N	522	THR	C-O	-6.85	1.15	1.24
1	N	97	THR	C-O	-6.67	1.17	1.24
1	D	212	VAL	C-O	-6.56	1.17	1.24
2	F	81	ALA	CA-C	6.52	1.61	1.52
1	A	149	PRO	N-CA	6.44	1.54	1.47
1	H	147	HIS	CA-C	6.43	1.61	1.52
1	M	561	TRP	C-O	-6.23	1.18	1.24
1	M	219	ASP	CB-CG	-6.14	1.36	1.52
2	I	62	GLN	CA-C	-6.09	1.45	1.52
1	B	147	HIS	CA-C	6.03	1.60	1.52
1	A	147	HIS	CA-C	6.02	1.60	1.52
1	H	522	THR	C-O	-5.80	1.16	1.24
1	B	148	GLY	N-CA	-5.64	1.36	1.45
1	C	400	GLU	CA-C	5.62	1.60	1.52
1	G	147	HIS	CA-C	5.58	1.60	1.52
1	C	148	GLY	N-CA	-5.57	1.36	1.45
1	M	339	GLY	N-CA	5.45	1.52	1.44
1	A	572	ASP	CA-C	5.43	1.59	1.52
1	C	586	LEU	C-O	-5.33	1.17	1.24
1	C	219	ASP	CA-CB	5.32	1.61	1.53
1	C	194	LYS	C-O	-5.31	1.19	1.24
1	C	368	GLU	C-O	-5.28	1.17	1.23
1	D	147	HIS	CA-C	5.28	1.60	1.52
1	D	522	THR	C-O	-5.27	1.17	1.24
1	G	208	VAL	C-O	-5.27	1.18	1.24
1	M	123	ASN	CA-C	5.26	1.59	1.52
1	M	98	PRO	CA-C	5.26	1.59	1.52
1	A	395	PRO	N-CA	-5.25	1.41	1.47
1	A	490	VAL	C-O	5.22	1.28	1.24
1	G	522	THR	C-O	-5.21	1.17	1.24
1	A	522	THR	C-O	-5.20	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	375	ALA	C-O	-5.18	1.17	1.23
2	E	80	TYR	C-O	-5.18	1.18	1.24
1	A	348	LYS	CA-C	5.15	1.58	1.52
1	N	566	LEU	C-O	-5.15	1.17	1.24
1	M	522	THR	C-N	-5.14	1.26	1.33
1	C	255	LEU	N-CA	5.11	1.52	1.46
2	L	31	PRO	CA-C	5.09	1.58	1.52
1	G	262	ALA	CA-C	5.08	1.59	1.52
1	D	54	PHE	CA-C	-5.04	1.46	1.52
1	M	98	PRO	C-O	-5.02	1.17	1.24

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	HIS	N-CA-C	14.88	130.73	112.87
1	M	147	HIS	N-CA-C	14.27	130.13	113.01
1	B	147	HIS	N-CA-C	11.80	127.17	113.01
1	H	147	HIS	N-CA-C	11.43	126.73	113.01
1	C	147	HIS	N-CA-C	11.41	126.70	113.01
1	N	147	HIS	N-CA-C	11.41	126.99	113.18
1	G	147	HIS	N-CA-C	10.93	126.41	113.18
1	A	147	HIS	N-CA-C	10.59	125.71	113.01
1	C	97	THR	O-C-N	-8.80	111.20	121.32
1	M	147	HIS	O-C-N	-8.04	111.37	122.46
1	D	147	HIS	O-C-N	-7.74	112.14	122.43
1	C	138	GLY	N-CA-C	7.67	122.73	111.76
1	A	147	HIS	CA-C-N	7.67	135.50	121.70
1	A	147	HIS	C-N-CA	7.67	135.50	121.70
1	B	148	GLY	CA-C-N	-7.60	112.86	120.31
1	B	148	GLY	C-N-CA	-7.60	112.86	120.31
1	C	219	ASP	N-CA-CB	-7.36	100.80	110.59
1	D	147	HIS	CA-C-N	7.34	134.90	121.70
1	D	147	HIS	C-N-CA	7.34	134.90	121.70
1	H	147	HIS	O-C-N	-7.16	112.59	122.46
1	M	147	HIS	CA-C-N	7.08	134.44	121.70
1	M	147	HIS	C-N-CA	7.08	134.44	121.70
2	J	62	GLN	CB-CA-C	-7.01	99.87	110.88
2	L	28	CYS	CA-C-N	7.01	129.98	120.38
2	L	28	CYS	C-N-CA	7.01	129.98	120.38
1	B	283	ILE	CB-CA-C	-6.89	101.26	110.98
1	D	148	GLY	CA-C-N	-6.89	113.21	120.03
1	D	148	GLY	C-N-CA	-6.89	113.21	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	26	THR	N-CA-CB	-6.86	100.25	110.61
2	O	61	LYS	N-CA-C	6.86	118.41	111.07
1	G	147	HIS	CA-C-N	6.79	133.93	121.70
1	G	147	HIS	C-N-CA	6.79	133.93	121.70
1	B	147	HIS	O-C-N	-6.72	113.19	122.46
2	F	61	LYS	N-CA-C	6.64	118.52	111.28
1	H	367	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	B	138	GLY	N-CA-C	6.50	120.04	111.52
1	H	297	MET	N-CA-C	6.46	120.88	113.19
1	A	147	HIS	O-C-N	-6.44	113.57	122.46
1	H	147	HIS	CA-C-N	6.40	133.22	121.70
1	H	147	HIS	C-N-CA	6.40	133.22	121.70
1	C	147	HIS	O-C-N	-6.23	113.86	122.46
2	L	62	GLN	CB-CA-C	-6.18	101.18	110.88
1	M	443	MET	N-CA-C	6.16	118.42	109.07
1	M	138	GLY	N-CA-C	6.14	120.55	111.76
2	F	29	LYS	CB-CA-C	-6.09	100.69	110.79
2	K	62	GLN	CB-CA-C	-6.07	101.34	110.88
1	N	147	HIS	CA-C-N	6.07	132.62	121.70
1	N	147	HIS	C-N-CA	6.07	132.62	121.70
1	G	193	VAL	CB-CA-C	6.03	118.32	110.12
1	N	578	GLY	N-CA-C	6.02	121.86	114.69
2	I	62	GLN	CB-CA-C	-5.92	101.58	110.88
1	G	138	GLY	N-CA-C	5.92	119.28	111.52
1	G	147	HIS	O-C-N	-5.80	113.96	122.43
1	C	450	LEU	N-CA-C	5.80	113.44	108.22
1	N	218	LYS	CA-C-N	5.76	132.26	122.36
1	N	218	LYS	C-N-CA	5.76	132.26	122.36
1	M	520	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	F	62	GLN	CB-CA-C	-5.68	101.72	110.81
2	O	62	GLN	CB-CA-C	-5.64	101.79	110.81
2	L	61	LYS	N-CA-C	5.62	117.09	111.07
1	H	144	ALA	O-C-N	-5.61	115.92	122.81
1	D	443	MET	N-CA-C	5.58	117.33	108.79
1	M	137	ARG	CG-CD-NE	-5.57	99.75	112.00
1	A	283	ILE	CB-CA-C	-5.54	102.57	110.83
1	N	147	HIS	O-C-N	-5.53	114.35	122.43
1	C	148	GLY	CA-C-N	-5.48	114.61	120.03
1	C	148	GLY	C-N-CA	-5.48	114.61	120.03
2	F	26	THR	N-CA-CB	-5.40	102.46	110.61
1	M	521	ASP	O-C-N	-5.36	115.88	123.01
1	B	137	ARG	CG-CD-NE	-5.36	100.21	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	THR	N-CA-C	5.30	118.73	109.82
1	A	219	ASP	N-CA-CB	-5.29	103.55	110.59
1	C	97	THR	CA-C-N	5.27	126.61	120.98
1	C	97	THR	C-N-CA	5.27	126.61	120.98
1	M	219	ASP	N-CA-CB	-5.26	103.03	110.81
1	B	422	GLN	N-CA-C	5.25	119.56	113.20
1	A	137	ARG	CG-CD-NE	-5.24	100.47	112.00
1	H	137	ARG	CG-CD-NE	-5.24	100.47	112.00
1	A	564	VAL	N-CA-C	5.18	116.53	110.62
1	C	147	HIS	CA-C-N	5.17	131.01	121.70
1	C	147	HIS	C-N-CA	5.17	131.01	121.70
1	B	443	MET	N-CA-C	5.16	116.68	108.79
1	N	219	ASP	CB-CA-C	-5.12	100.74	109.03
1	N	137	ARG	CG-CD-NE	-5.11	100.76	112.00
1	M	313	ALA	N-CA-C	5.04	116.77	111.28
2	E	62	GLN	CB-CA-C	-5.03	102.92	110.92
1	C	218	LYS	CA-C-N	5.03	131.01	122.36
1	C	218	LYS	C-N-CA	5.03	131.01	122.36
1	D	249	GLY	N-CA-C	-5.02	105.14	111.72
1	D	180	ILE	N-CA-C	5.02	115.74	110.62

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	CYS	Peptide
1	B	97	THR	Mainchain
1	C	97	THR	Mainchain
1	D	131	CYS	Peptide
1	G	97	THR	Mainchain
1	H	144	ALA	Peptide
1	H	145	GLY	Peptide
1	H	218	LYS	Peptide
1	M	131	CYS	Peptide
2	O	90	VAL	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	4320	15	0
1	B	4490	0	4320	9	0
1	C	4491	0	4320	13	0
1	D	4490	0	4320	14	0
1	G	4491	0	4320	20	0
1	H	4490	0	4320	20	0
1	M	4491	0	4320	15	0
1	N	4490	0	4320	17	0
2	E	568	0	545	1	0
2	F	568	0	545	3	0
2	I	568	0	545	2	0
2	J	568	0	545	2	0
2	K	568	0	545	0	0
2	L	568	0	545	5	0
2	O	568	0	545	3	0
2	P	568	0	545	3	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	3	1	0
4	B	24	0	3	2	0
4	C	24	0	3	2	0
4	D	24	0	3	2	0
4	G	24	0	3	2	0
4	H	24	0	3	2	0
4	M	24	0	3	2	0
4	N	24	0	3	1	0
5	A	254	0	0	1	0
5	B	309	0	0	1	0
5	C	286	0	0	0	0
5	D	288	0	0	3	0
5	E	34	0	0	0	0
5	F	43	0	0	0	0
5	G	250	0	0	0	0
5	H	284	0	0	2	0
5	I	25	0	0	0	0
5	J	38	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	48	0	0	0	0
5	L	59	0	0	2	0
5	M	308	0	0	2	0
5	N	238	0	0	1	0
5	O	42	0	0	1	0
5	P	26	0	0	0	0
All	All	43200	0	38944	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (134) 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:90:ASP:HB2	5:H:1055:HOH:O	1.76	0.84
2:O:90:VAL:HG12	2:O:93:ILE:HD12	1.61	0.82
1:N:145:GLY:HA3	1:N:148:GLY:O	1.83	0.76
1:A:114:MET:HE1	1:B:591:GLN:HE21	1.53	0.72
1:C:591:GLN:HE21	1:D:114:MET:HE1	1.55	0.71
2:O:67:LYS:HE3	5:O:117:HOH:O	1.90	0.71
2:L:38:LYS:N	5:L:101:HOH:O	2.23	0.68
1:G:97:THR:HB	1:G:98:PRO:HD2	1.74	0.67
5:B:1009:HOH:O	2:F:54:HIS:HD2	1.79	0.66
1:H:145:GLY:O	1:H:148:GLY:HA2	1.96	0.66
2:P:24:ASP:OD1	2:P:26:THR:HG22	1.96	0.65
1:H:198:LEU:HD11	1:H:283:ILE:HD13	1.78	0.64
1:N:264:LYS:NZ	2:P:60:ASN:OD1	2.31	0.64
1:D:147:HIS:CD2	1:D:217:ILE:HD11	2.34	0.62
1:C:145:GLY:O	1:C:148:GLY:HA2	2.00	0.62
2:J:24:ASP:OD1	2:J:26:THR:HB	2.00	0.62
1:M:114:MET:HE1	1:N:591:GLN:HE21	1.64	0.62
1:M:145:GLY:O	1:M:148:GLY:HA2	1.99	0.61
1:B:76:THR:HB	1:B:97:THR:HG22	1.83	0.61
1:A:145:GLY:O	1:A:148:GLY:HA2	2.00	0.60
1:H:145:GLY:HA3	1:H:148:GLY:O	2.00	0.60
1:A:204:ALA:HB3	4:A:702:PQQ:O7B	2.02	0.59
1:C:31:GLU:OE2	1:C:34:ARG:NH2	2.30	0.58
5:N:926:HOH:O	2:P:54:HIS:HD2	1.85	0.58
1:H:566:LEU:C	1:H:566:LEU:HD12	2.28	0.58
1:D:198:LEU:HD11	1:D:283:ILE:HD13	1.86	0.58
1:D:306:MET:HE1	1:D:332:TYR:C	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:THR:HB	1:H:97:THR:HG22	1.86	0.57
1:D:204:ALA:HB3	4:D:702:PQQ:O7B	2.05	0.57
5:H:1015:HOH:O	2:J:54:HIS:HD2	1.88	0.55
1:G:145:GLY:O	1:G:148:GLY:HA2	2.07	0.54
1:C:463:LEU:HD23	1:C:465:MET:HE2	1.89	0.53
5:M:903:HOH:O	2:O:54:HIS:HD2	1.90	0.53
1:M:76:THR:HB	1:M:97:THR:HG22	1.91	0.53
2:L:62:GLN:HG3	5:L:139:HOH:O	2.09	0.52
1:A:353:LEU:O	1:A:364:THR:HA	2.10	0.52
1:D:76:THR:HB	1:D:97:THR:HG22	1.91	0.52
1:M:591:GLN:HG2	1:N:114:MET:HE1	1.91	0.52
1:N:145:GLY:CA	1:N:148:GLY:O	2.56	0.52
1:C:76:THR:HB	1:C:97:THR:HG22	1.93	0.51
1:G:306:MET:HE1	1:G:332:TYR:C	2.36	0.51
1:H:208:VAL:O	1:H:267:GLY:HA2	2.10	0.51
1:M:204:ALA:HB3	4:M:702:PQQ:O7A	2.11	0.51
1:D:95:ILE:HD12	1:D:596:VAL:HG21	1.93	0.50
1:B:204:ALA:HB3	4:B:702:PQQ:O7A	2.12	0.49
1:G:76:THR:HB	1:G:97:THR:HG22	1.93	0.49
1:G:147:HIS:CD2	1:G:217:ILE:HD11	2.47	0.49
1:C:204:ALA:HB3	4:C:702:PQQ:O7A	2.13	0.49
1:G:81:GLY:HA3	1:G:538:ILE:HD11	1.95	0.49
1:M:258:TRP:C	5:M:858:HOH:O	2.54	0.49
1:N:208:VAL:O	1:N:267:GLY:HA2	2.12	0.49
1:G:591:GLN:HE21	1:H:114:MET:HE1	1.78	0.49
1:A:57:LEU:HD13	1:A:550:GLN:HG3	1.95	0.48
1:N:271:TRP:CZ2	4:N:702:PQQ:C6A	2.96	0.48
1:A:38:ASP:OD2	1:A:40:ARG:NH2	2.45	0.48
1:N:144:ALA:HA	1:N:148:GLY:O	2.14	0.48
1:G:271:TRP:CZ2	4:G:702:PQQ:C6A	2.97	0.47
4:B:702:PQQ:O9A	4:B:702:PQQ:N1	2.45	0.47
1:H:145:GLY:HA2	1:H:147:HIS:CD2	2.50	0.47
1:C:271:TRP:CZ2	4:C:702:PQQ:C6A	2.97	0.47
5:D:888:HOH:O	2:L:54:HIS:HD2	1.97	0.47
1:D:145:GLY:O	1:D:148:GLY:HA2	2.15	0.47
1:G:353:LEU:HD12	1:G:353:LEU:C	2.39	0.47
1:M:193:VAL:HG21	1:M:283:ILE:HD11	1.97	0.47
1:H:435:PHE:CZ	1:H:522:THR:HB	2.50	0.47
1:M:306:MET:HE1	1:M:332:TYR:C	2.40	0.47
1:M:271:TRP:CE2	1:M:335:VAL:HG21	2.50	0.46
1:N:145:GLY:O	1:N:148:GLY:HA2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:OE2	1:B:34:ARG:NH2	2.44	0.46
1:B:137:ARG:HB3	1:B:273:TRP:CH2	2.51	0.46
1:N:137:ARG:HB3	1:N:273:TRP:CH2	2.50	0.46
1:N:76:THR:HB	1:N:97:THR:HG22	1.98	0.46
2:L:24:ASP:OD1	2:L:26:THR:HB	2.15	0.46
1:M:219:ASP:HB3	1:M:221:LYS:H	1.80	0.46
1:D:271:TRP:CZ2	4:D:702:PQQ:C6A	2.98	0.46
1:H:98:PRO:O	1:H:99:PHE:C	2.59	0.46
1:H:219:ASP:HB3	1:H:221:LYS:H	1.81	0.46
1:A:297:MET:HG2	1:A:449:MET:HE1	1.97	0.46
1:C:137:ARG:HB3	1:C:273:TRP:CH2	2.51	0.46
1:A:306:MET:HE1	1:A:332:TYR:C	2.40	0.46
1:C:42:TRP:CE2	1:C:542:ILE:HG22	2.50	0.46
1:B:306:MET:HE1	1:B:332:TYR:C	2.41	0.45
1:D:96:HIS:CE1	1:D:138:GLY:HA2	2.51	0.45
1:H:271:TRP:CZ2	4:H:702:PQQ:C6A	3.00	0.45
1:G:81:GLY:CA	1:G:538:ILE:HD11	2.46	0.45
1:G:114:MET:HE1	1:H:591:GLN:HE21	1.81	0.45
1:A:193:VAL:HG11	1:A:283:ILE:CD1	2.47	0.45
1:N:271:TRP:CE2	1:N:335:VAL:HG21	2.51	0.45
5:A:1007:HOH:O	2:E:54:HIS:HE1	2.00	0.45
1:G:204:ALA:HB3	4:G:702:PQQ:O7B	2.16	0.45
1:H:353:LEU:C	1:H:353:LEU:HD12	2.42	0.45
1:G:462:THR:C	1:G:463:LEU:HD12	2.43	0.44
1:A:303:LYS:HA	1:A:304:TRP:HA	1.84	0.44
1:C:112:ARG:HD3	1:D:514:ASP:O	2.17	0.44
1:H:144:ALA:HA	1:H:148:GLY:O	2.17	0.44
1:H:306:MET:HE1	1:H:332:TYR:C	2.42	0.44
1:H:204:ALA:HB3	4:H:702:PQQ:O7A	2.18	0.43
1:G:193:VAL:HG11	1:G:283:ILE:HD11	1.99	0.43
5:D:981:HOH:O	2:L:54:HIS:HE1	2.00	0.43
1:G:463:LEU:HD23	1:G:465:MET:HE2	2.00	0.43
1:A:85:ALA:HB1	1:A:86:PRO:CD	2.49	0.43
1:G:29:ASN:N	1:G:194:LYS:H	2.16	0.43
2:F:24:ASP:OD1	2:F:26:THR:HG22	2.19	0.42
1:M:85:ALA:HB1	1:M:86:PRO:CD	2.49	0.42
1:H:329:GLU:OE2	1:H:402:SER:HB2	2.19	0.42
1:N:332:TYR:O	1:N:333:ALA:C	2.62	0.42
1:B:147:HIS:CD2	1:B:217:ILE:HD11	2.55	0.42
1:M:271:TRP:CZ2	4:M:702:PQQ:C6A	3.02	0.42
1:N:306:MET:HE1	1:N:332:TYR:C	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:333:ALA:O	1:N:358:ARG:HG3	2.18	0.42
1:A:83:GLU:HG3	1:A:538:ILE:HD12	2.00	0.42
1:C:549:LYS:NZ	1:C:601:LEU:OXT	2.53	0.42
1:G:207:GLY:O	2:I:62:GLN:NE2	2.52	0.42
1:B:144:ALA:HA	1:B:148:GLY:O	2.20	0.42
1:A:76:THR:HB	1:A:97:THR:HG22	2.02	0.42
1:A:271:TRP:CE2	1:A:335:VAL:HG21	2.54	0.42
1:H:217:ILE:HG21	1:H:217:ILE:HD13	1.78	0.42
1:D:142:VAL:HG11	1:D:217:ILE:HD12	2.02	0.41
1:M:98:PRO:O	1:M:99:PHE:C	2.63	0.41
1:N:445:TRP:CD1	1:N:445:TRP:C	2.98	0.41
1:D:265:ILE:HD12	1:D:458:PHE:CE2	2.55	0.41
1:G:445:TRP:CD1	1:G:445:TRP:C	2.99	0.41
1:M:72:TRP:CZ2	1:M:598:VAL:HG21	2.54	0.41
1:N:426:SER:O	1:N:434:PHE:HA	2.21	0.41
1:G:280:LEU:HB3	1:G:282:MET:HE3	2.03	0.41
1:A:219:ASP:HB3	1:A:221:LYS:H	1.86	0.41
1:C:306:MET:HE1	1:C:332:TYR:C	2.46	0.41
1:D:591:GLN:NE2	5:D:809:HOH:O	2.54	0.41
1:B:462:THR:C	1:B:463:LEU:HD12	2.46	0.40
1:C:509:PHE:CZ	1:C:552:ILE:CD1	3.05	0.40
1:G:86:PRO:HG3	1:G:95:ILE:CD1	2.51	0.40
1:M:303:LYS:HA	1:M:304:TRP:HA	1.91	0.40
2:F:24:ASP:OD1	2:F:26:THR:HB	2.21	0.40
2:I:52:PRO:HB2	2:I:54:HIS:CE1	2.57	0.40

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%)	539 (94%)	31 (5%)	1 (0%)	43	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	571/573 (100%)	538 (94%)	32 (6%)	1 (0%)	43	51
1	C	571/573 (100%)	540 (95%)	30 (5%)	1 (0%)	43	51
1	D	571/573 (100%)	535 (94%)	34 (6%)	2 (0%)	30	34
1	G	571/573 (100%)	542 (95%)	27 (5%)	2 (0%)	30	34
1	H	571/573 (100%)	541 (95%)	27 (5%)	3 (0%)	24	27
1	M	571/573 (100%)	539 (94%)	31 (5%)	1 (0%)	43	51
1	N	571/573 (100%)	539 (94%)	30 (5%)	2 (0%)	30	34
2	E	69/72 (96%)	69 (100%)	0	0	100	100
2	F	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	I	69/72 (96%)	68 (99%)	1 (1%)	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%)	69 (100%)	0	0	100	100
2	O	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	P	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
All	All	5120/5160 (99%)	4861 (95%)	246 (5%)	13 (0%)	36	42

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	145	GLY
1	N	145	GLY
1	H	557	GLY
1	H	145	GLY
1	A	557	GLY
1	H	134	VAL
1	N	557	GLY
1	B	134	VAL
1	C	134	VAL
1	D	134	VAL
1	G	594	GLY
1	M	594	GLY
1	G	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%)	458 (99%)	6 (1%)	61	76
1	B	464/464 (100%)	458 (99%)	6 (1%)	61	76
1	C	464/464 (100%)	458 (99%)	6 (1%)	61	76
1	D	464/464 (100%)	455 (98%)	9 (2%)	50	66
1	G	464/464 (100%)	457 (98%)	7 (2%)	57	73
1	H	464/464 (100%)	456 (98%)	8 (2%)	53	69
1	M	464/464 (100%)	454 (98%)	10 (2%)	45	61
1	N	464/464 (100%)	455 (98%)	9 (2%)	50	66
2	E	60/61 (98%)	59 (98%)	1 (2%)	53	69
2	F	60/61 (98%)	54 (90%)	6 (10%)	7	7
2	I	60/61 (98%)	57 (95%)	3 (5%)	22	28
2	J	60/61 (98%)	57 (95%)	3 (5%)	22	28
2	K	60/61 (98%)	57 (95%)	3 (5%)	22	28
2	L	60/61 (98%)	57 (95%)	3 (5%)	22	28
2	O	60/61 (98%)	57 (95%)	3 (5%)	22	28
2	P	60/61 (98%)	54 (90%)	6 (10%)	7	7
All	All	4192/4200 (100%)	4103 (98%)	89 (2%)	47	63

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	VAL
1	A	239	LYS
1	A	279	LYS
1	A	283	ILE
1	A	337	TYR
1	A	566	LEU
1	B	243	LYS
1	B	337	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	387	LYS
1	B	472	MET
1	B	564	VAL
1	B	571	LYS
1	C	146	GLU
1	C	233	GLU
1	C	239	LYS
1	C	337	TYR
1	C	549	LYS
1	C	571	LYS
1	D	117	GLN
1	D	121	LYS
1	D	161	ILE
1	D	198	LEU
1	D	337	TYR
1	D	391	LYS
1	D	472	MET
1	D	564	VAL
1	D	571	LYS
2	E	65	SER
2	F	26	THR
2	F	43	ASP
2	F	53	LYS
2	F	59	LEU
2	F	85	LYS
2	F	93	ILE
1	G	193	VAL
1	G	337	TYR
1	G	400	GLU
1	G	410	LYS
1	G	528	LYS
1	G	552	ILE
1	G	566	LEU
1	H	89	VAL
1	H	279	LYS
1	H	337	TYR
1	H	391	LYS
1	H	503	THR
1	H	564	VAL
1	H	566	LEU
1	H	584	ARG
2	I	43	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	67	LYS
2	I	85	LYS
2	J	26	THR
2	J	59	LEU
2	J	74	GLN
2	K	43	ASP
2	K	67	LYS
2	K	85	LYS
2	L	26	THR
2	L	43	ASP
2	L	59	LEU
1	M	37	LYS
1	M	89	VAL
1	M	121	LYS
1	M	146	GLU
1	M	161	ILE
1	M	219	ASP
1	M	233	GLU
1	M	337	TYR
1	M	453	ARG
1	M	571	LYS
1	N	146	GLU
1	N	161	ILE
1	N	198	LEU
1	N	239	LYS
1	N	337	TYR
1	N	391	LYS
1	N	472	MET
1	N	566	LEU
1	N	571	LYS
2	O	85	LYS
2	O	89	LYS
2	O	92	ASP
2	P	26	THR
2	P	43	ASP
2	P	53	LYS
2	P	59	LEU
2	P	74	GLN
2	P	91	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	407	HIS
1	B	67	ASN
1	B	117	GLN
1	B	155	ASN
1	B	177	ASN
1	B	270	ASN
1	B	408	ASN
1	B	464	ASN
1	B	591	GLN
1	C	177	ASN
1	C	546	HIS
1	C	591	GLN
1	D	67	ASN
1	D	117	GLN
1	D	177	ASN
1	D	270	ASN
1	D	407	HIS
1	D	408	ASN
1	D	464	ASN
1	D	546	HIS
1	D	547	ASN
2	E	27	HIS
2	E	54	HIS
2	F	54	HIS
1	G	136	ASN
1	G	407	HIS
1	G	591	GLN
1	H	117	GLN
1	H	156	GLN
1	H	216	ASN
1	H	323	GLN
1	H	545	GLN
2	I	27	HIS
2	J	54	HIS
2	J	74	GLN
2	K	27	HIS
2	K	54	HIS
2	L	54	HIS
1	M	177	ASN
1	N	117	GLN
1	N	136	ASN
1	N	155	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	177	ASN
1	N	408	ASN
1	N	464	ASN
1	N	475	GLN
1	N	545	GLN
1	N	588	HIS
1	N	591	GLN
2	O	54	HIS
2	O	79	ASN
2	P	27	HIS
2	P	54	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	G	702	3	26,26,26	3.61	10 (38%)	34,40,40	2.15	12 (35%)
4	PQQ	B	702	3	26,26,26	3.42	10 (38%)	34,40,40	1.96	10 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PQQ	H	702	3	26,26,26	3.59	7 (26%)	34,40,40	1.97	12 (35%)
4	PQQ	M	702	3	26,26,26	3.66	7 (26%)	34,40,40	2.37	16 (47%)
4	PQQ	N	702	3	26,26,26	3.64	9 (34%)	34,40,40	2.32	13 (38%)
4	PQQ	D	702	3	26,26,26	3.35	8 (30%)	34,40,40	2.32	16 (47%)
4	PQQ	C	702	3	26,26,26	3.40	8 (30%)	34,40,40	2.00	13 (38%)
4	PQQ	A	702	3	26,26,26	3.64	10 (38%)	34,40,40	2.25	16 (47%)

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	G	702	3	-	2/12/28/28	0/3/3/3
4	PQQ	B	702	3	-	4/12/28/28	0/3/3/3
4	PQQ	H	702	3	-	3/12/28/28	0/3/3/3
4	PQQ	M	702	3	-	2/12/28/28	0/3/3/3
4	PQQ	N	702	3	-	3/12/28/28	0/3/3/3
4	PQQ	D	702	3	-	2/12/28/28	0/3/3/3
4	PQQ	C	702	3	-	3/12/28/28	0/3/3/3
4	PQQ	A	702	3	-	5/12/28/28	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	702	PQQ	C5-C4	-12.75	1.36	1.54
4	A	702	PQQ	C5-C4	-12.32	1.37	1.54
4	M	702	PQQ	C5-C4	-12.24	1.37	1.54
4	B	702	PQQ	C5-C4	-11.97	1.37	1.54
4	H	702	PQQ	C5-C4	-11.67	1.38	1.54
4	G	702	PQQ	C5-C4	-11.17	1.38	1.54
4	D	702	PQQ	C5-C4	-11.07	1.39	1.54
4	C	702	PQQ	C5-C4	-10.38	1.40	1.54
4	H	702	PQQ	O5-C5	9.46	1.43	1.23
4	M	702	PQQ	O5-C5	9.09	1.42	1.23
4	D	702	PQQ	O5-C5	7.96	1.39	1.23
4	G	702	PQQ	O4-C4	7.87	1.41	1.23
4	C	702	PQQ	O5-C5	7.87	1.39	1.23
4	A	702	PQQ	O5-C5	7.63	1.39	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	PQQ	O4-C4	7.45	1.40	1.23
4	N	702	PQQ	O5-C5	7.29	1.38	1.23
4	G	702	PQQ	O5-C5	7.26	1.38	1.23
4	H	702	PQQ	O4-C4	6.87	1.38	1.23
4	A	702	PQQ	O4-C4	6.79	1.38	1.23
4	G	702	PQQ	C6A-C5	-6.73	1.42	1.50
4	B	702	PQQ	O5-C5	6.68	1.37	1.23
4	B	702	PQQ	O4-C4	6.30	1.37	1.23
4	D	702	PQQ	O4-C4	6.10	1.37	1.23
4	N	702	PQQ	C6A-C5	-6.07	1.42	1.50
4	C	702	PQQ	C6A-C5	-5.98	1.43	1.50
4	M	702	PQQ	O4-C4	5.82	1.36	1.23
4	N	702	PQQ	O4-C4	5.67	1.36	1.23
4	A	702	PQQ	C6A-C5	-5.19	1.44	1.50
4	M	702	PQQ	C6A-C5	-5.18	1.44	1.50
4	B	702	PQQ	C6A-C5	-5.04	1.44	1.50
4	H	702	PQQ	C6A-C5	-4.70	1.44	1.50
4	D	702	PQQ	C6A-C5	-4.36	1.45	1.50
4	A	702	PQQ	C2-N1	-3.86	1.31	1.37
4	N	702	PQQ	C2-N1	-3.52	1.31	1.37
4	M	702	PQQ	C9-C9A	3.47	1.46	1.41
4	N	702	PQQ	C9-C9A	3.40	1.46	1.41
4	D	702	PQQ	C9-C9A	3.32	1.46	1.41
4	C	702	PQQ	C9-C9A	3.29	1.46	1.41
4	G	702	PQQ	C3A-C4	-3.13	1.37	1.46
4	M	702	PQQ	C7-N6	-3.01	1.30	1.34
4	H	702	PQQ	O2B-C2X	-2.92	1.22	1.30
4	H	702	PQQ	C9-C9A	2.91	1.45	1.41
4	B	702	PQQ	C2-N1	-2.84	1.33	1.37
4	N	702	PQQ	C3A-C4	-2.82	1.38	1.46
4	B	702	PQQ	C9-C9A	2.77	1.45	1.41
4	N	702	PQQ	C9-C9X	2.61	1.55	1.49
4	B	702	PQQ	O9A-C9X	2.50	1.30	1.22
4	A	702	PQQ	C9-C9A	2.45	1.44	1.41
4	A	702	PQQ	C3A-C4	-2.43	1.39	1.46
4	C	702	PQQ	C1A-N1	-2.43	1.33	1.37
4	G	702	PQQ	O7B-C7X	-2.42	1.23	1.30
4	B	702	PQQ	O2B-C2X	-2.41	1.24	1.30
4	B	702	PQQ	C7-N6	-2.37	1.31	1.34
4	D	702	PQQ	C3A-C4	-2.31	1.39	1.46
4	D	702	PQQ	O2B-C2X	-2.30	1.24	1.30
4	A	702	PQQ	C8-C9	2.27	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	702	PQQ	C3A-C4	-2.27	1.39	1.46
4	A	702	PQQ	O2B-C2X	-2.26	1.24	1.30
4	A	702	PQQ	O7B-C7X	-2.24	1.23	1.30
4	D	702	PQQ	O9B-C9X	-2.23	1.23	1.30
4	G	702	PQQ	C2-N1	-2.22	1.34	1.37
4	C	702	PQQ	C2-N1	-2.21	1.34	1.37
4	C	702	PQQ	O7B-C7X	-2.19	1.24	1.30
4	G	702	PQQ	C7-N6	-2.19	1.31	1.34
4	H	702	PQQ	O9A-C9X	2.17	1.29	1.22
4	N	702	PQQ	C9A-C1A	-2.12	1.43	1.46
4	B	702	PQQ	C8-C9	2.06	1.43	1.39
4	G	702	PQQ	O2A-C2X	2.04	1.27	1.22
4	G	702	PQQ	O2B-C2X	-2.04	1.25	1.30

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	702	PQQ	O9B-C9X-O9A	-5.31	111.94	123.35
4	M	702	PQQ	C3-C2-C2X	-4.93	121.17	132.53
4	D	702	PQQ	O9B-C9X-O9A	-4.78	113.08	123.35
4	A	702	PQQ	C3-C2-C2X	-4.71	121.69	132.53
4	B	702	PQQ	C3-C2-C2X	-4.62	121.88	132.53
4	M	702	PQQ	C3A-C3-C2	-4.55	103.26	107.94
4	G	702	PQQ	O2B-C2X-C2	4.43	123.81	114.27
4	N	702	PQQ	C8-C9-C9A	-4.31	114.80	120.33
4	A	702	PQQ	C3A-C3-C2	-4.30	103.52	107.94
4	H	702	PQQ	O7B-C7X-C7	4.25	124.81	114.71
4	H	702	PQQ	C3-C2-C2X	-4.12	123.03	132.53
4	C	702	PQQ	C3-C2-C2X	-4.08	123.13	132.53
4	A	702	PQQ	O2B-C2X-C2	3.98	122.85	114.27
4	G	702	PQQ	C6A-N6-C7	3.95	123.20	118.01
4	M	702	PQQ	O2B-C2X-C2	3.94	122.76	114.27
4	A	702	PQQ	C8-C9-C9A	-3.90	115.32	120.33
4	G	702	PQQ	O2A-C2X-C2	-3.90	113.09	121.01
4	C	702	PQQ	C8-C9-C9A	-3.90	115.33	120.33
4	D	702	PQQ	C6A-N6-C7	3.88	123.11	118.01
4	B	702	PQQ	C6A-N6-C7	3.87	123.10	118.01
4	D	702	PQQ	C1A-C3A-C4	-3.85	119.09	122.33
4	D	702	PQQ	O2B-C2X-C2	3.76	122.39	114.27
4	N	702	PQQ	C9A-C9-C9X	3.71	129.63	121.49
4	M	702	PQQ	C6A-N6-C7	3.66	122.82	118.01
4	D	702	PQQ	C3-C2-C2X	-3.64	124.14	132.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	PQQ	C3A-C3-C2	-3.63	104.20	107.94
4	C	702	PQQ	C3A-C3-C2	-3.61	104.22	107.94
4	N	702	PQQ	O7B-C7X-O7A	-3.59	115.63	123.35
4	D	702	PQQ	O9B-C9X-C9	3.56	125.40	115.28
4	G	702	PQQ	C3-C2-C2X	-3.55	124.35	132.53
4	H	702	PQQ	O2A-C2X-C2	3.55	128.22	121.01
4	M	702	PQQ	O9B-C9X-C9	3.53	125.32	115.28
4	N	702	PQQ	C3A-C3-C2	-3.50	104.34	107.94
4	M	702	PQQ	O2A-C2X-C2	-3.50	113.92	121.01
4	N	702	PQQ	C3A-C4-C5	3.49	120.98	117.03
4	N	702	PQQ	C3-C2-C2X	-3.48	124.50	132.53
4	M	702	PQQ	C3A-C4-C5	3.47	120.96	117.03
4	N	702	PQQ	C9-C8-C7	3.44	122.76	119.93
4	A	702	PQQ	O9B-C9X-C9	3.36	124.84	115.28
4	A	702	PQQ	O2A-C2X-C2	-3.34	114.23	121.01
4	G	702	PQQ	O7B-C7X-O7A	-3.33	116.19	123.35
4	B	702	PQQ	C8-C9-C9A	-3.20	116.23	120.33
4	H	702	PQQ	C6A-N6-C7	3.14	122.14	118.01
4	C	702	PQQ	C9A-C9-C9X	3.14	128.38	121.49
4	H	702	PQQ	C3A-C4-C5	3.14	120.58	117.03
4	B	702	PQQ	C3A-C3-C2	-3.13	104.71	107.94
4	G	702	PQQ	C3A-C3-C2	-3.12	104.73	107.94
4	D	702	PQQ	O7B-C7X-O7A	-3.07	116.76	123.35
4	G	702	PQQ	O9B-C9X-C9	3.06	123.98	115.28
4	C	702	PQQ	O9B-C9X-C9	3.05	123.96	115.28
4	M	702	PQQ	C8-C9-C9A	-3.00	116.49	120.33
4	B	702	PQQ	O7B-C7X-C7	2.99	121.80	114.71
4	M	702	PQQ	O7B-C7X-O7A	-2.98	116.95	123.35
4	C	702	PQQ	O9A-C9X-C9	-2.97	114.89	121.97
4	D	702	PQQ	C3A-C4-C5	2.93	120.35	117.03
4	C	702	PQQ	O7B-C7X-O7A	-2.92	117.07	123.35
4	A	702	PQQ	O7B-C7X-O7A	-2.92	117.08	123.35
4	B	702	PQQ	C3A-C4-C5	2.91	120.33	117.03
4	M	702	PQQ	O7B-C7X-C7	2.90	121.60	114.71
4	N	702	PQQ	O5-C5-C6A	2.88	125.04	121.76
4	G	702	PQQ	O9B-C9X-O9A	-2.86	117.21	123.35
4	N	702	PQQ	C6A-N6-C7	2.81	121.70	118.01
4	H	702	PQQ	O7A-C7X-C7	-2.80	115.66	121.30
4	H	702	PQQ	O7B-C7X-O7A	-2.80	117.33	123.35
4	A	702	PQQ	C3A-C4-C5	2.79	120.20	117.03
4	A	702	PQQ	C9A-C9-C9X	2.79	127.62	121.49
4	A	702	PQQ	O9B-C9X-O9A	-2.77	117.40	123.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	PQQ	O7B-C7X-C7	2.63	120.96	114.71
4	D	702	PQQ	O7B-C7X-C7	2.62	120.94	114.71
4	N	702	PQQ	O9B-C9X-C9	2.62	122.73	115.28
4	H	702	PQQ	O2B-C2X-O2A	-2.60	117.71	123.90
4	C	702	PQQ	C9-C8-C7	2.59	122.06	119.93
4	A	702	PQQ	O5-C5-C6A	2.59	124.72	121.76
4	M	702	PQQ	O9B-C9X-O9A	-2.57	117.82	123.35
4	N	702	PQQ	O5-C5-C4	-2.56	114.80	118.14
4	B	702	PQQ	C3-C2-N1	2.55	111.99	107.74
4	M	702	PQQ	O9A-C9X-C9	-2.51	115.98	121.97
4	M	702	PQQ	C9A-C9-C9X	2.50	126.98	121.49
4	M	702	PQQ	C2X-C2-N1	2.48	126.89	120.52
4	D	702	PQQ	O5-C5-C4	-2.44	114.96	118.14
4	H	702	PQQ	O5-C5-C6A	2.37	124.47	121.76
4	M	702	PQQ	C3-C2-N1	2.37	111.69	107.74
4	C	702	PQQ	O5-C5-C6A	-2.34	119.08	121.76
4	H	702	PQQ	C2X-C2-N1	2.33	126.50	120.52
4	G	702	PQQ	C9A-C9-C9X	2.33	126.59	121.49
4	D	702	PQQ	C8-C9-C9A	-2.31	117.36	120.33
4	C	702	PQQ	C3A-C4-C5	2.30	119.64	117.03
4	A	702	PQQ	C2X-C2-N1	2.27	126.36	120.52
4	C	702	PQQ	C1A-C3A-C4	-2.25	120.44	122.33
4	G	702	PQQ	C8-C9-C9A	-2.23	117.47	120.33
4	G	702	PQQ	C3A-C4-C5	2.22	119.55	117.03
4	H	702	PQQ	C9A-C9-C9X	2.22	126.37	121.49
4	C	702	PQQ	C2X-C2-N1	2.19	126.14	120.52
4	A	702	PQQ	C3-C2-N1	2.18	111.38	107.74
4	H	702	PQQ	C3A-C3-C2	-2.18	105.70	107.94
4	A	702	PQQ	C6A-N6-C7	2.18	120.87	118.01
4	D	702	PQQ	C9A-C9-C9X	2.16	126.24	121.49
4	B	702	PQQ	O9B-C9X-O9A	-2.16	118.71	123.35
4	M	702	PQQ	O5-C5-C6A	2.16	124.22	121.76
4	B	702	PQQ	O5-C5-C6A	2.15	124.21	121.76
4	D	702	PQQ	C3-C2-N1	2.10	111.25	107.74
4	N	702	PQQ	C1A-C3A-C4	-2.09	120.58	122.33
4	D	702	PQQ	O5-C5-C6A	2.05	124.10	121.76
4	G	702	PQQ	C2X-C2-N1	2.04	125.76	120.52
4	C	702	PQQ	O2B-C2X-O2A	-2.03	119.07	123.90
4	A	702	PQQ	O5-C5-C4	-2.03	115.49	118.14
4	D	702	PQQ	O2B-C2X-O2A	-2.02	119.08	123.90
4	B	702	PQQ	O7B-C7X-O7A	-2.00	119.05	123.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	PQQ	C3-C2-C2X-O2A
4	B	702	PQQ	N1-C2-C2X-O2A
4	B	702	PQQ	N1-C2-C2X-O2B
4	B	702	PQQ	C3-C2-C2X-O2A
4	B	702	PQQ	C3-C2-C2X-O2B
4	C	702	PQQ	N1-C2-C2X-O2B
4	C	702	PQQ	C3-C2-C2X-O2A
4	C	702	PQQ	C3-C2-C2X-O2B
4	H	702	PQQ	N1-C2-C2X-O2B
4	H	702	PQQ	C3-C2-C2X-O2B
4	N	702	PQQ	N1-C2-C2X-O2B
4	N	702	PQQ	C3-C2-C2X-O2A
4	N	702	PQQ	C3-C2-C2X-O2B
4	A	702	PQQ	N1-C2-C2X-O2A
4	A	702	PQQ	N6-C7-C7X-O7A
4	D	702	PQQ	C3-C2-C2X-O2A
4	H	702	PQQ	C3-C2-C2X-O2A
4	A	702	PQQ	C8-C7-C7X-O7A
4	D	702	PQQ	N1-C2-C2X-O2A
4	G	702	PQQ	N1-C2-C2X-O2A
4	G	702	PQQ	N1-C2-C2X-O2B
4	M	702	PQQ	N1-C2-C2X-O2A
4	A	702	PQQ	C3-C2-C2X-O2B
4	M	702	PQQ	C3-C2-C2X-O2A

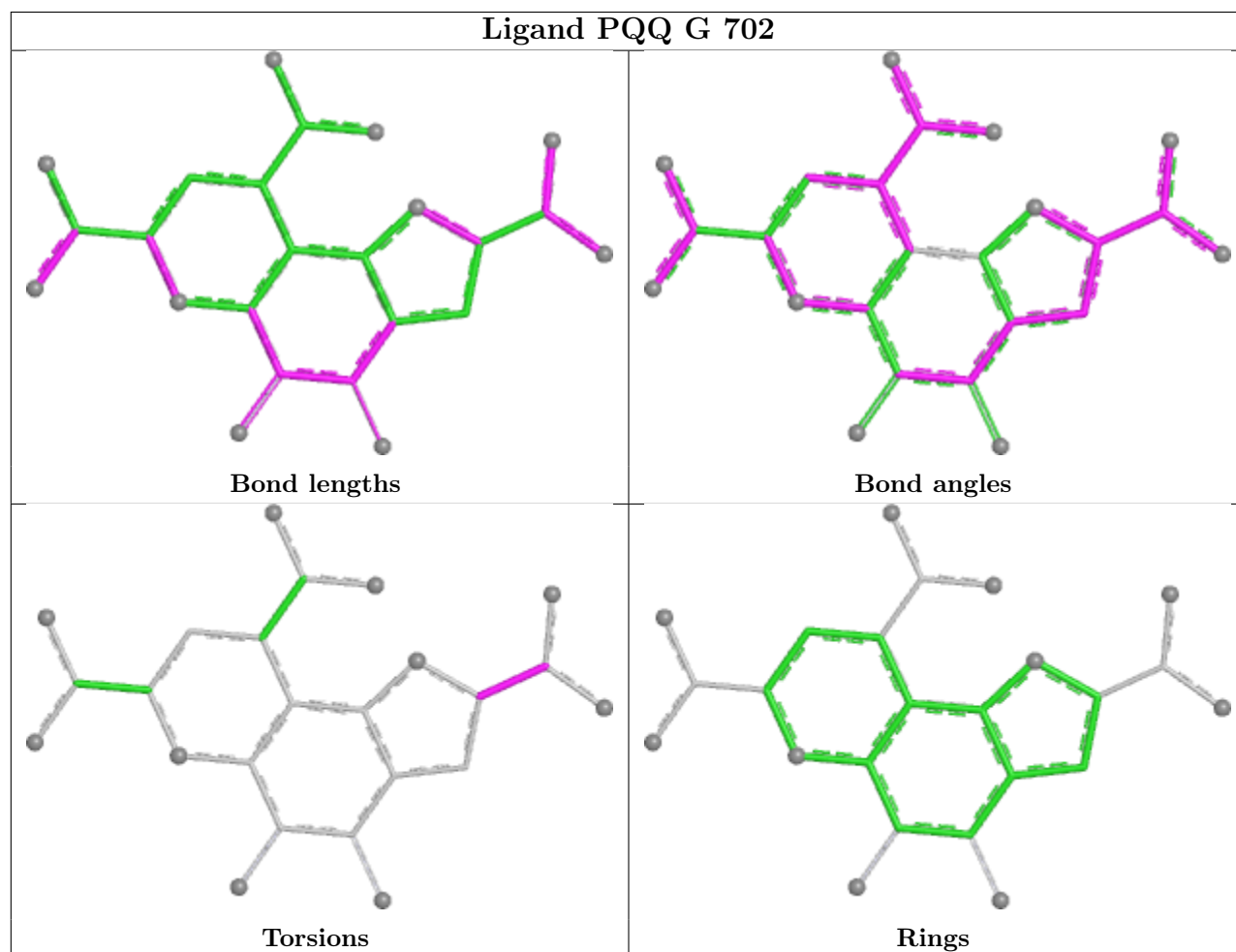
There are no ring outliers.

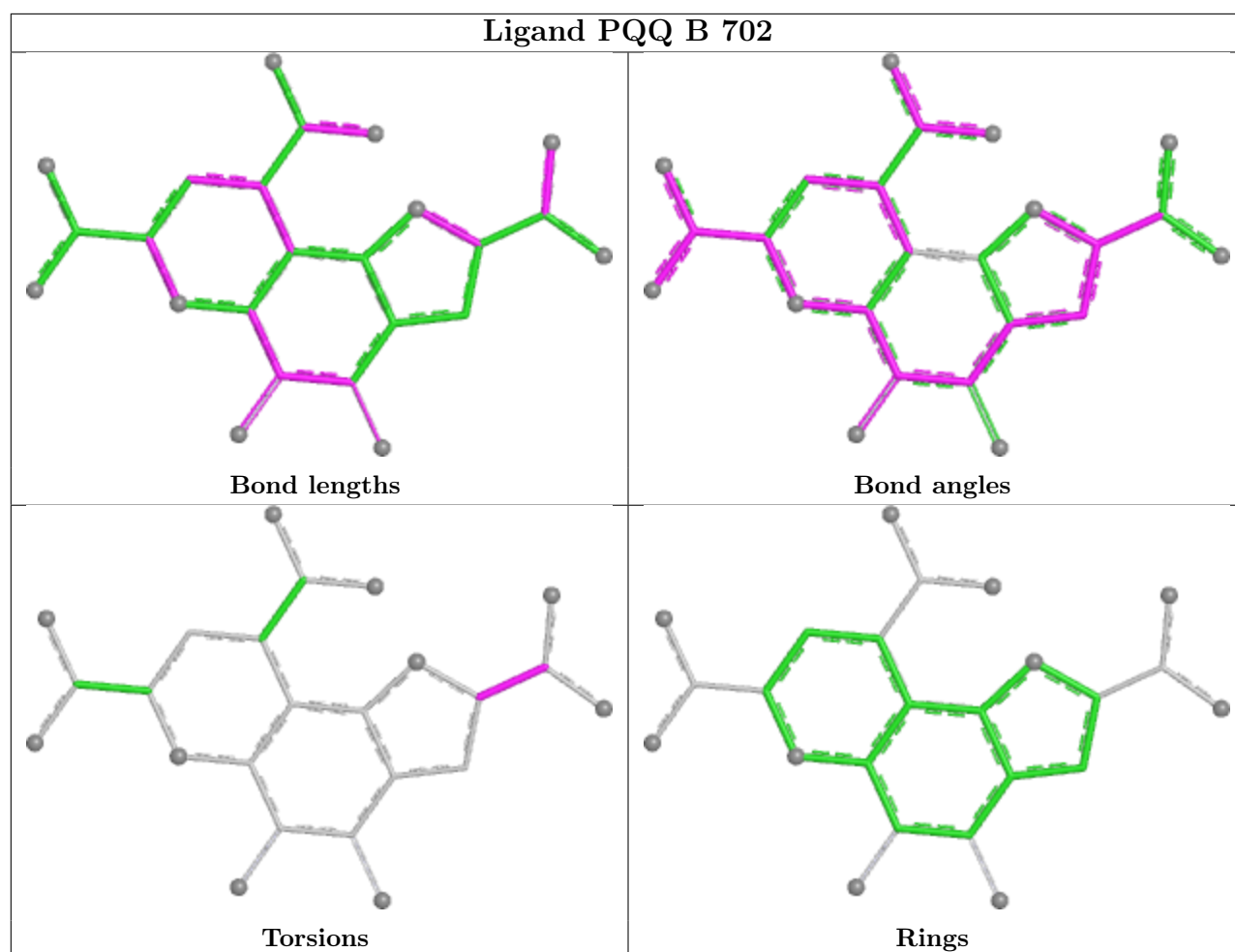
8 monomers are involved in 14 short contacts:

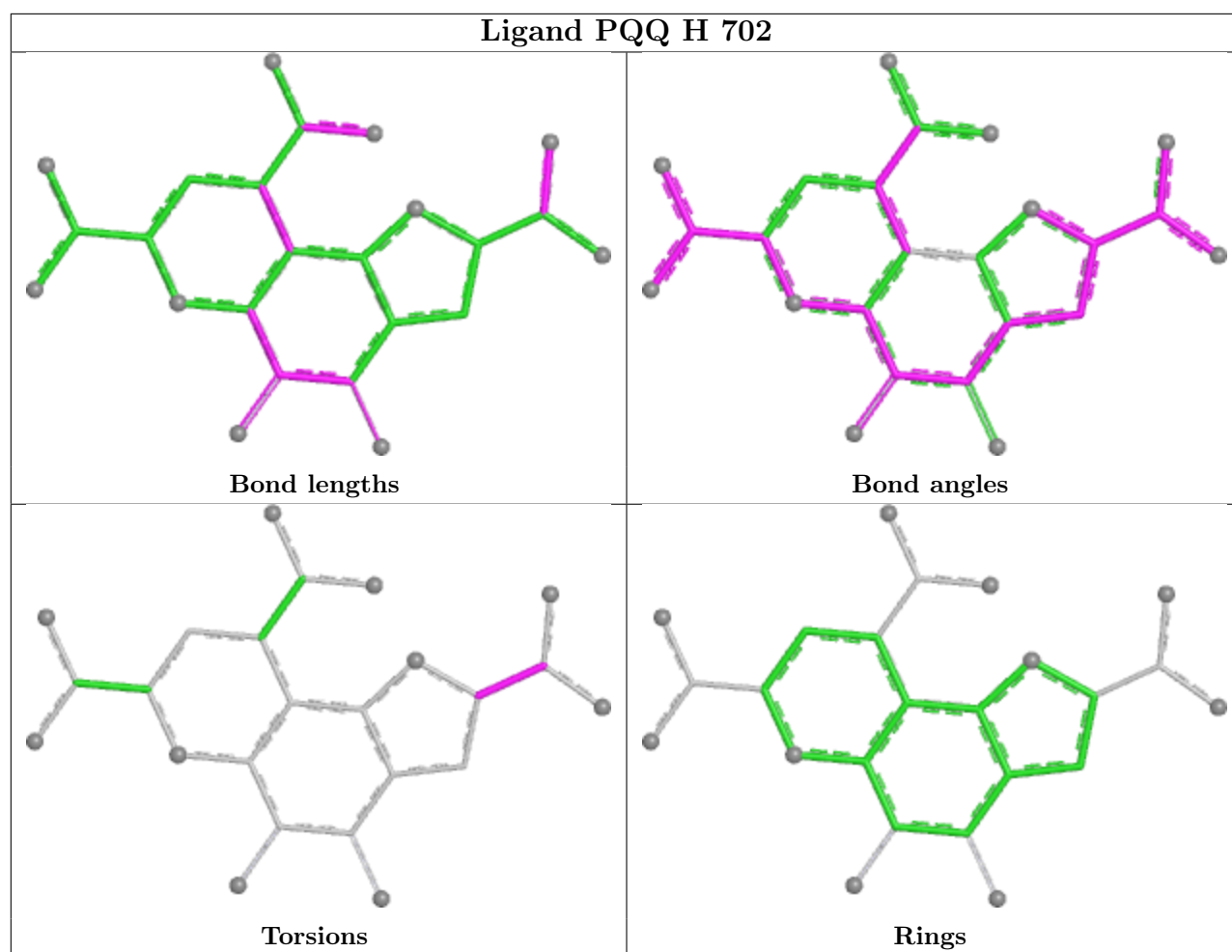
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	702	PQQ	2	0
4	B	702	PQQ	2	0
4	H	702	PQQ	2	0
4	M	702	PQQ	2	0
4	N	702	PQQ	1	0
4	D	702	PQQ	2	0
4	C	702	PQQ	2	0
4	A	702	PQQ	1	0

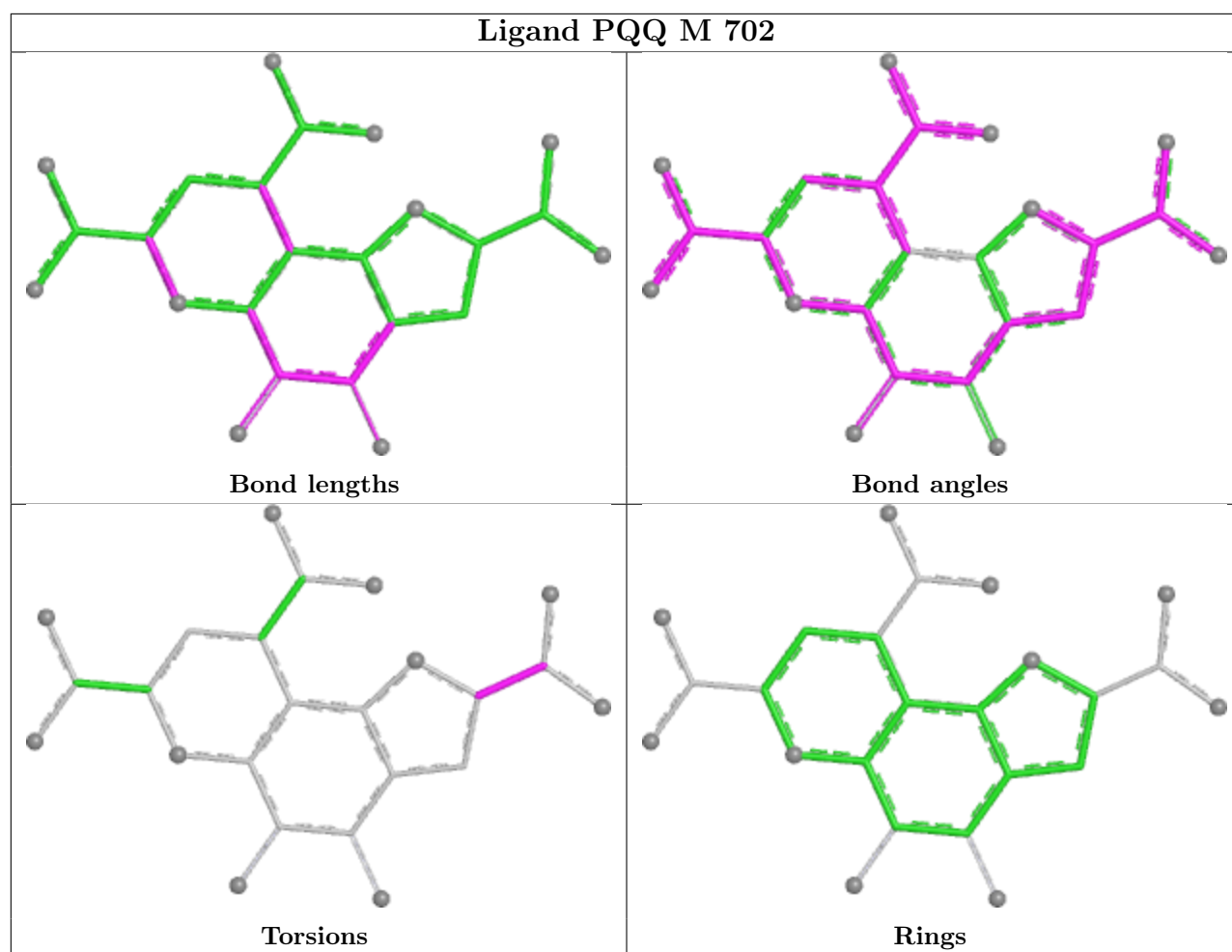
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

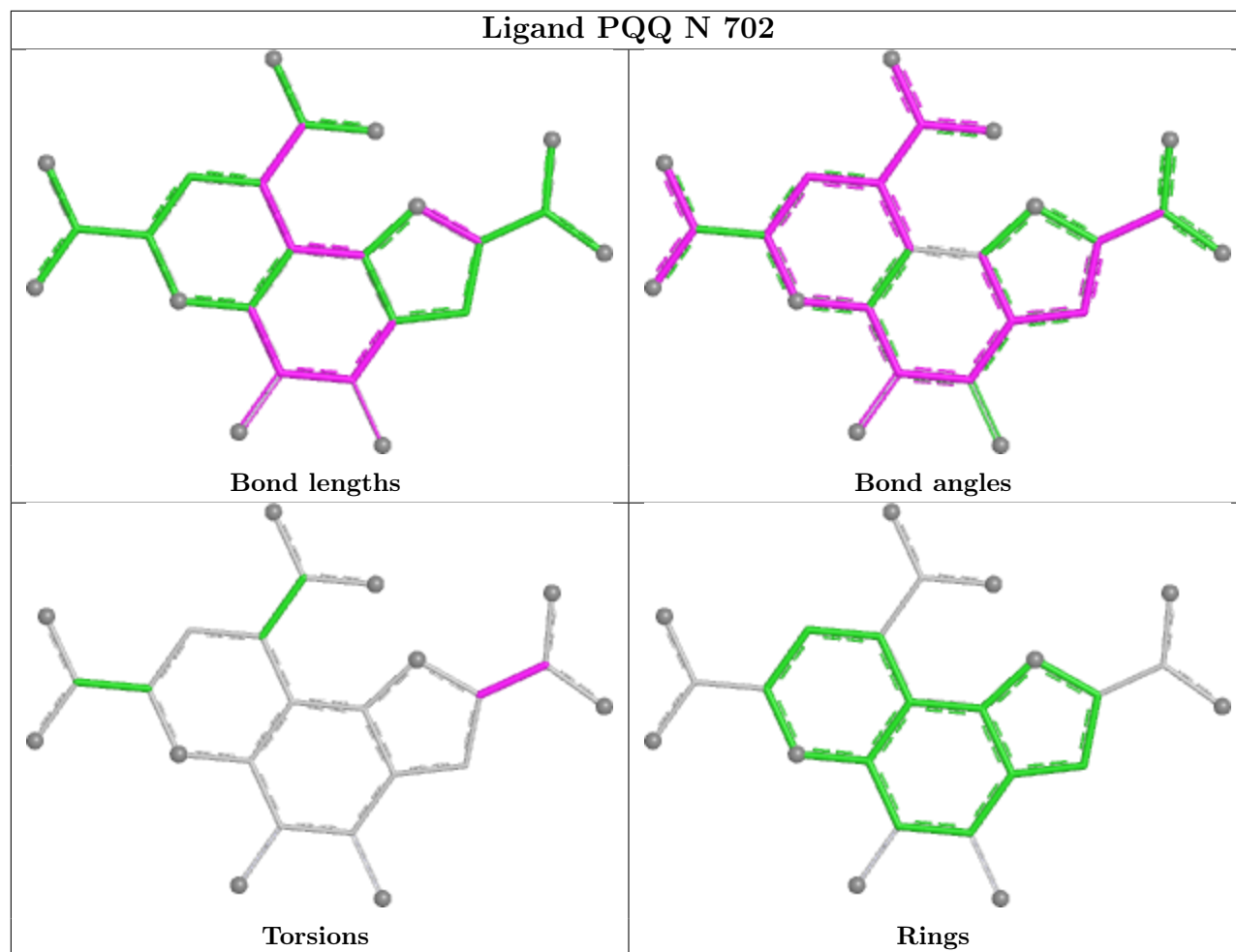
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

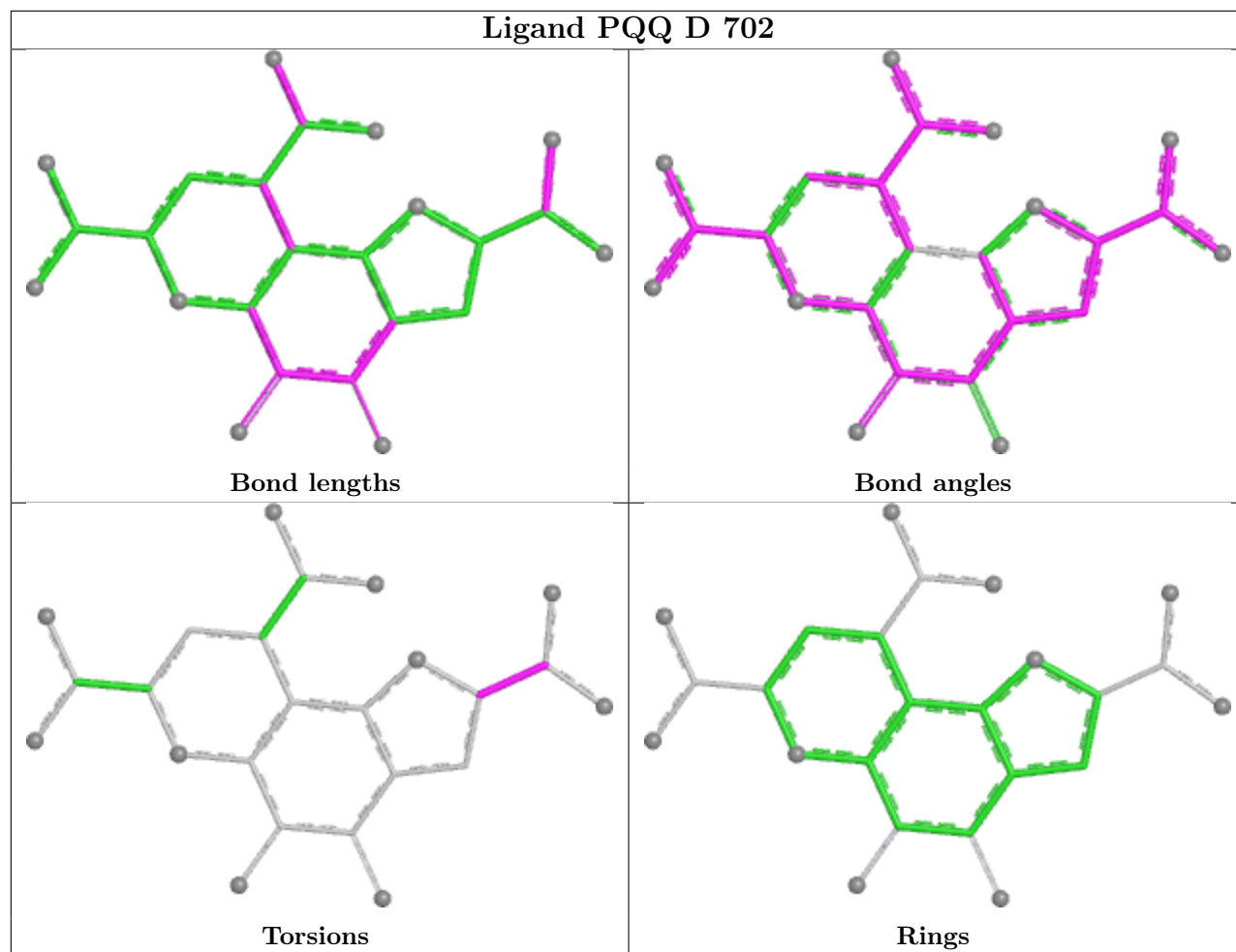


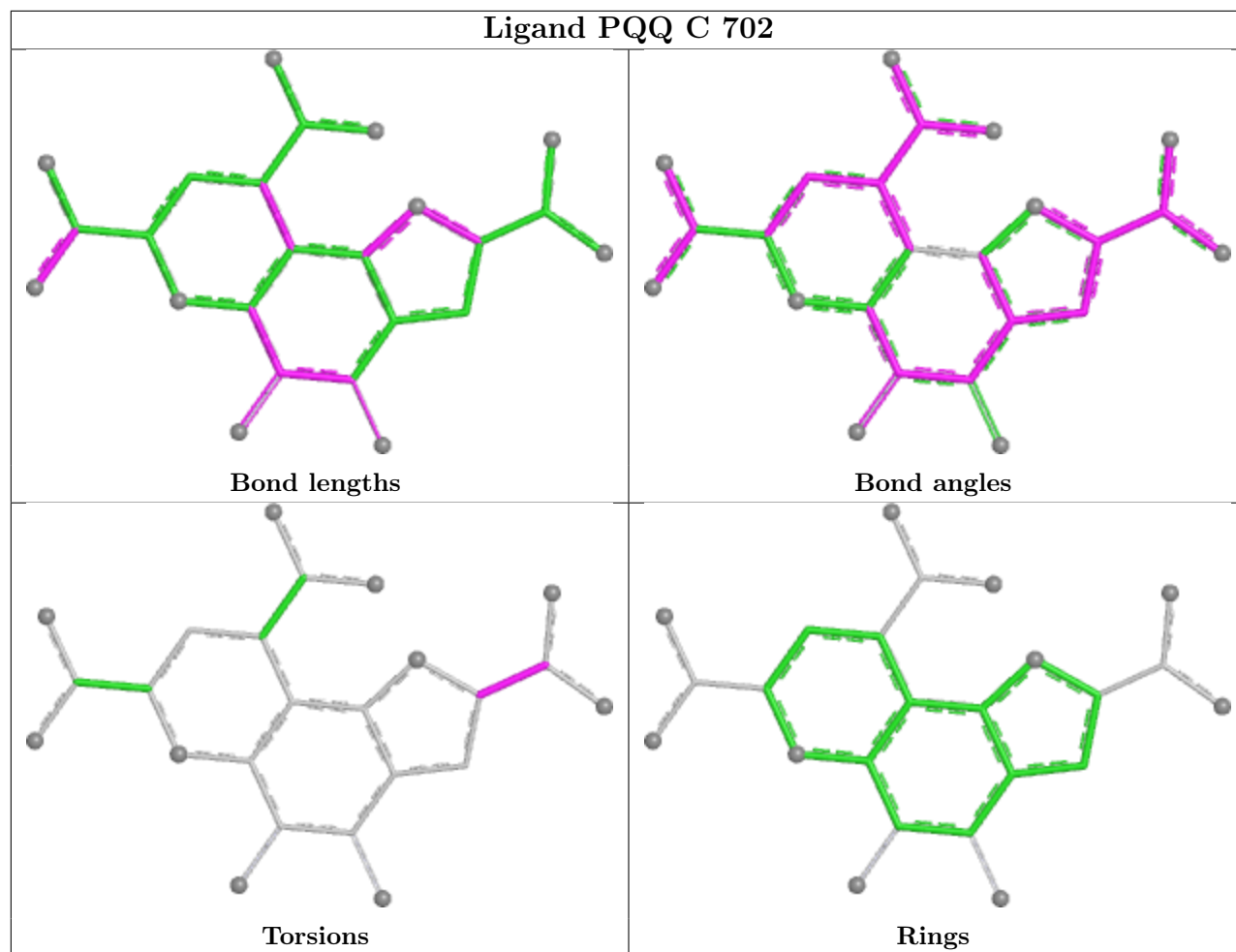


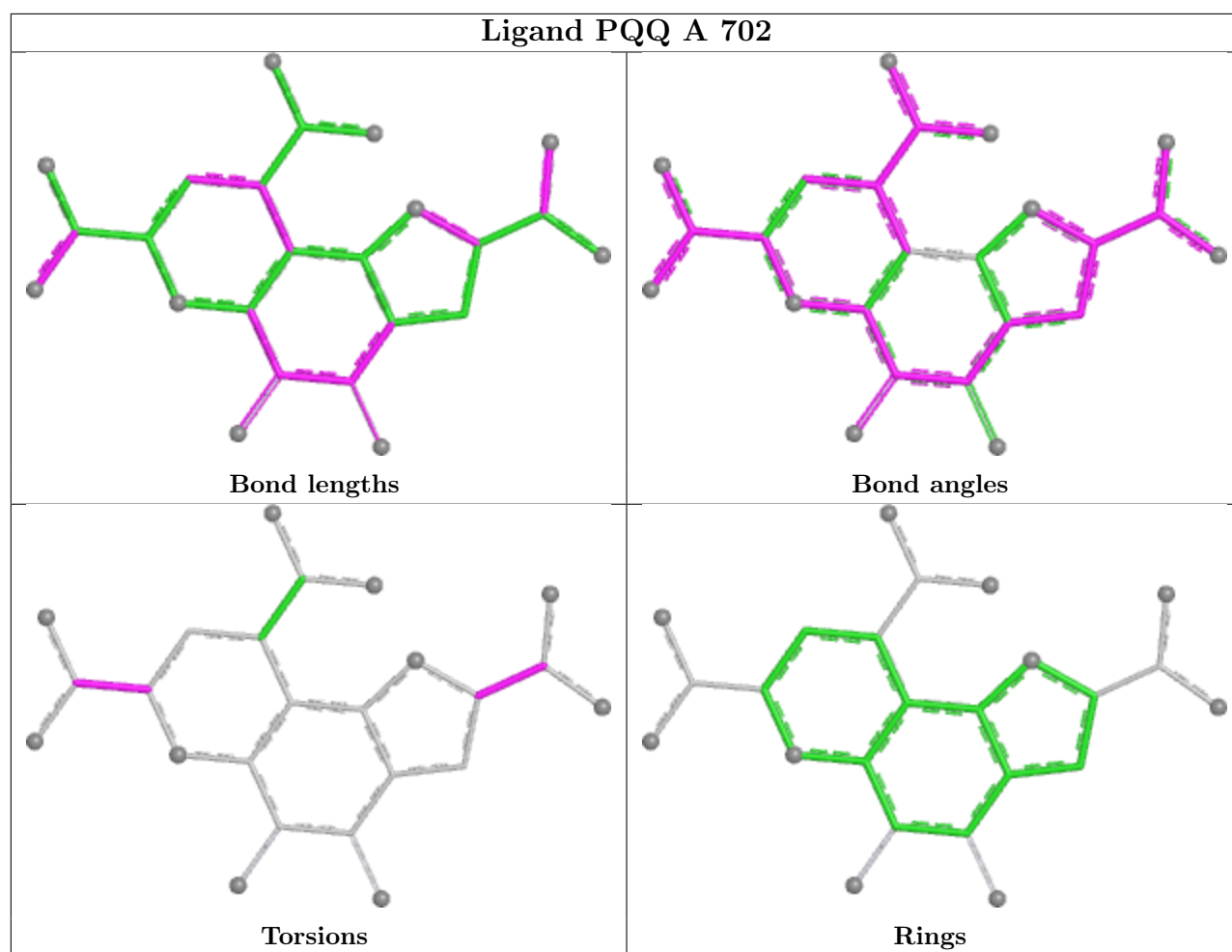












5.7 Other polymers [i](#)

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%)	-0.58	0 100 100	14, 22, 35, 67	0
1	B	573/573 (100%)	-0.66	2 (0%) 90 88	13, 20, 34, 54	0
1	C	573/573 (100%)	-0.69	0 100 100	13, 19, 31, 52	0
1	D	573/573 (100%)	-0.69	1 (0%) 91 90	13, 19, 33, 52	0
1	G	573/573 (100%)	-0.55	0 100 100	13, 23, 38, 62	0
1	H	573/573 (100%)	-0.66	0 100 100	14, 19, 34, 55	0
1	M	573/573 (100%)	-0.66	0 100 100	14, 20, 33, 53	0
1	N	573/573 (100%)	-0.49	0 100 100	14, 25, 40, 62	0
2	E	71/72 (98%)	-0.14	0 100 100	21, 32, 49, 66	0
2	F	71/72 (98%)	0.18	8 (11%) 10 8	16, 26, 78, 113	0
2	I	71/72 (98%)	0.20	2 (2%) 55 52	25, 37, 55, 74	0
2	J	71/72 (98%)	-0.24	0 100 100	18, 25, 48, 63	0
2	K	71/72 (98%)	-0.29	1 (1%) 73 71	17, 26, 45, 58	0
2	L	71/72 (98%)	-0.30	0 100 100	18, 28, 49, 68	0
2	O	71/72 (98%)	0.15	6 (8%) 16 14	20, 28, 80, 130	0
2	P	71/72 (98%)	0.29	3 (4%) 40 37	30, 39, 58, 72	0
All	All	5152/5160 (99%)	-0.56	23 (0%) 88 87	13, 21, 41, 130	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	90	VAL	6.2
2	O	93	ILE	5.9
2	F	93	ILE	5.4
2	O	91	GLU	4.4
2	F	82	LYS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	81	ALA	3.8
2	O	92	ASP	3.8
2	F	84	GLY	3.2
1	B	104	TYR	3.1
2	F	85	LYS	2.9
2	O	89	LYS	2.9
2	F	92	ASP	2.9
2	I	85	LYS	2.8
2	F	90	VAL	2.6
2	O	82	LYS	2.5
1	D	104	TYR	2.5
2	K	85	LYS	2.3
2	F	83	THR	2.1
2	P	85	LYS	2.1
2	P	89	LYS	2.1
2	P	93	ILE	2.1
1	B	453	ARG	2.1
2	I	28	CYS	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 oligosaccharides 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(Å ²)	Q<0.9
3	CA	M	701	1/1	0.94	0.15	58,58,58,58	0
3	CA	N	701	1/1	0.94	0.13	77,77,77,77	0
3	CA	B	701	1/1	0.95	0.21	61,61,61,61	0
3	CA	G	701	1/1	0.95	0.15	67,67,67,67	0
4	PQQ	A	702	24/24	0.95	0.06	18,23,26,31	0

Continued on next page...

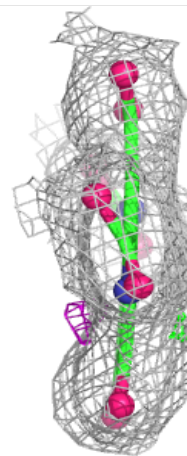
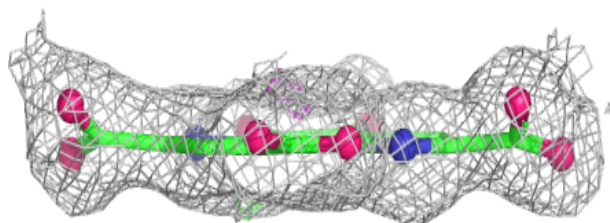
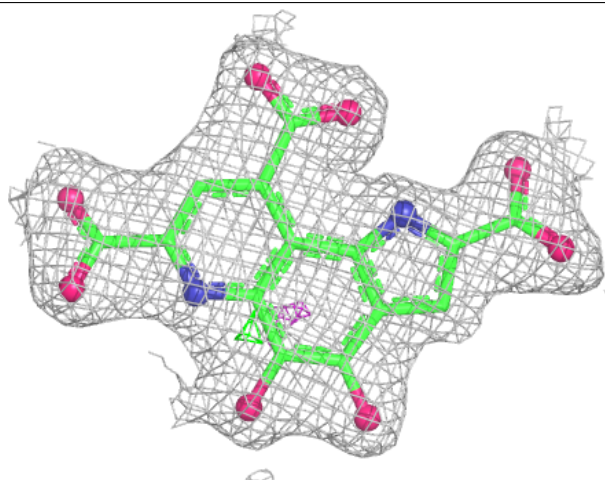
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PQQ	H	702	24/24	0.95	0.06	20,24,25,27	0
4	PQQ	N	702	24/24	0.95	0.06	20,24,27,28	0
3	CA	H	701	1/1	0.96	0.23	60,60,60,60	0
4	PQQ	C	702	24/24	0.96	0.05	16,22,27,27	0
4	PQQ	D	702	24/24	0.96	0.05	16,19,21,24	0
4	PQQ	G	702	24/24	0.96	0.05	17,23,25,27	0
3	CA	D	701	1/1	0.96	0.21	59,59,59,59	0
4	PQQ	M	702	24/24	0.96	0.06	16,21,23,28	0
3	CA	A	701	1/1	0.96	0.16	57,57,57,57	0
4	PQQ	B	702	24/24	0.97	0.05	16,19,20,23	0
3	CA	C	701	1/1	0.98	0.19	54,54,54,54	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.

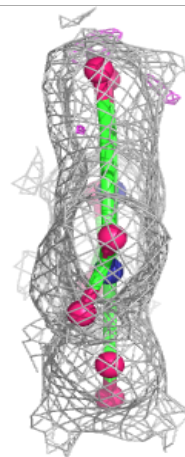
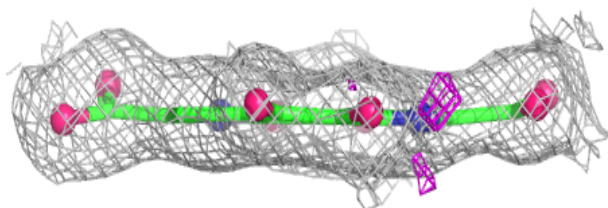
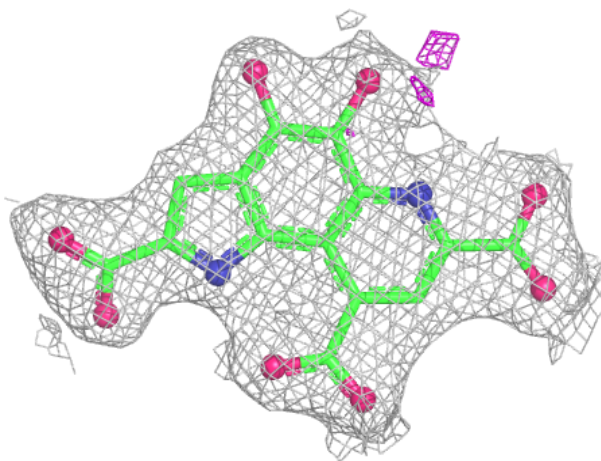
Electron density around PQQ A 702:

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



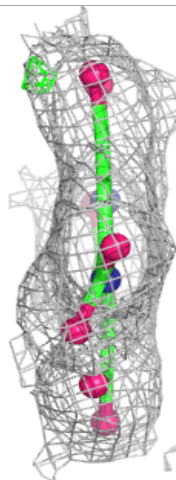
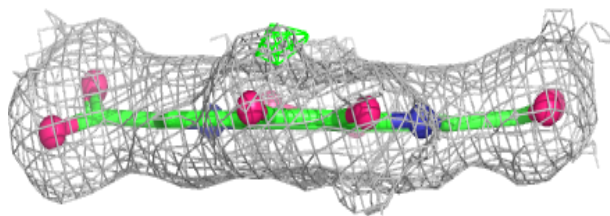
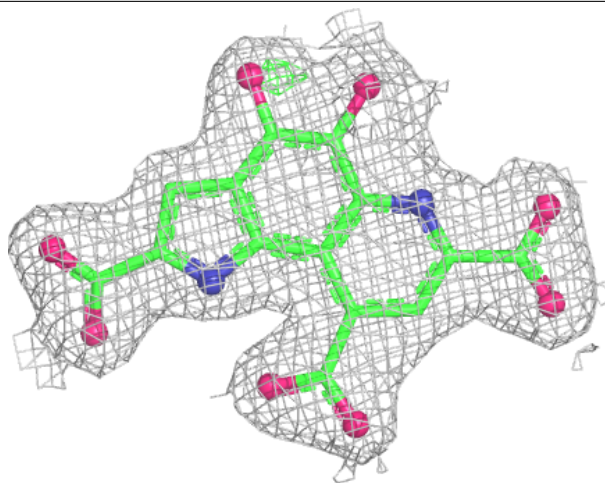
Electron density around PQQ H 702:

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



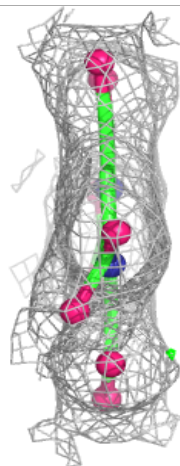
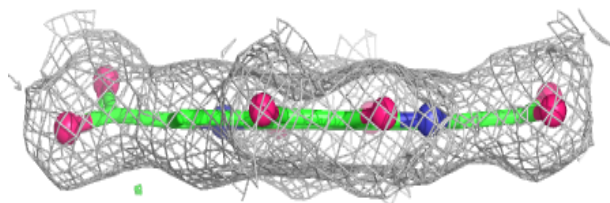
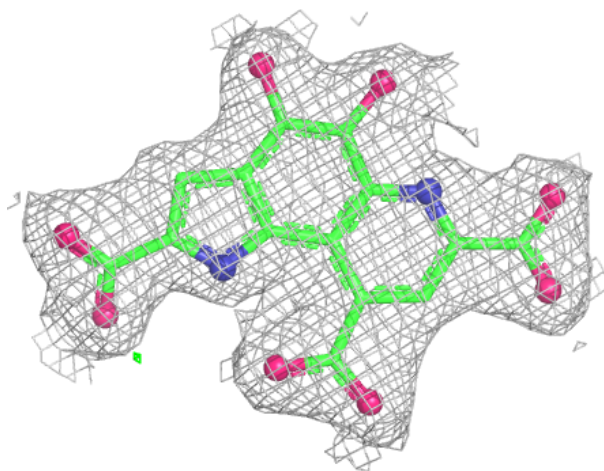
Electron density around PQQ N 702:

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



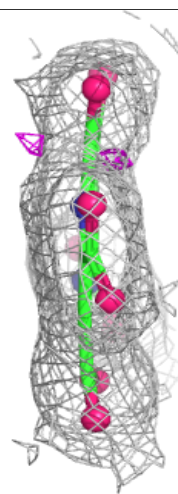
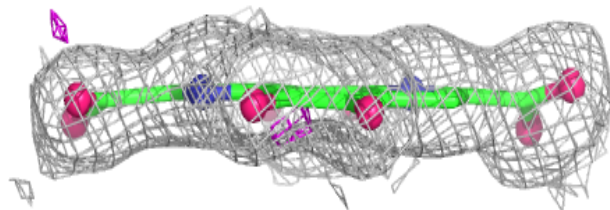
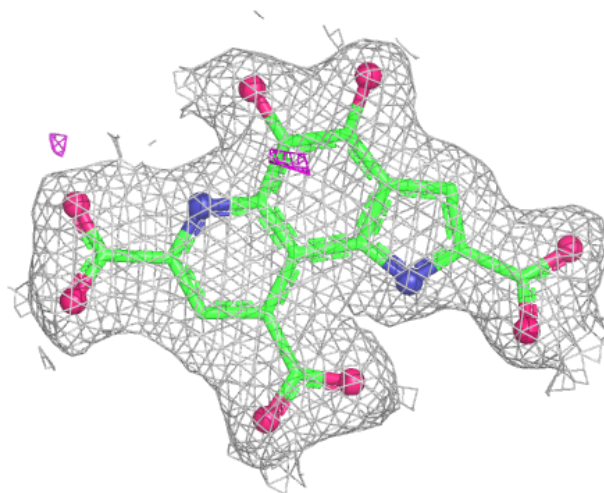
Electron density around PQQ C 702:

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



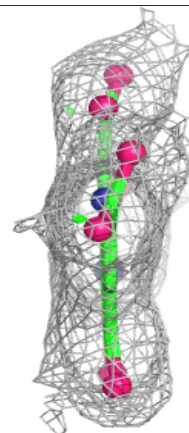
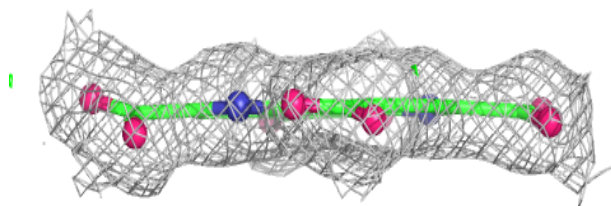
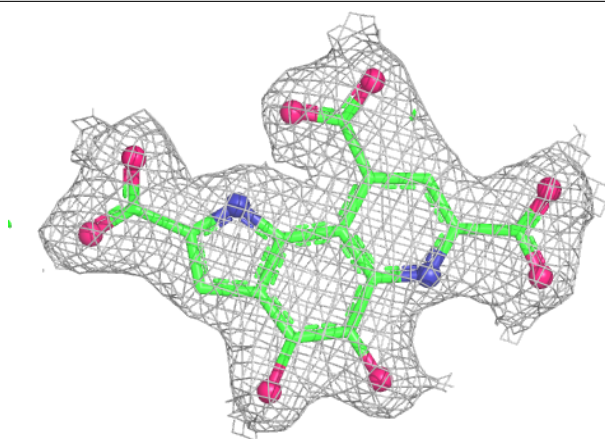
Electron density around PQQ D 702:

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



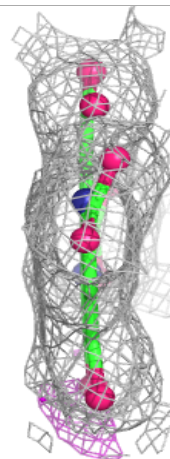
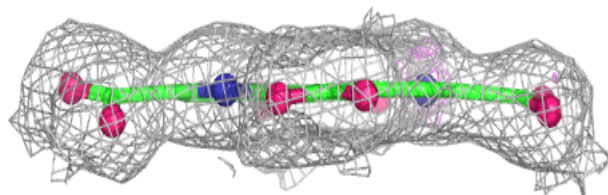
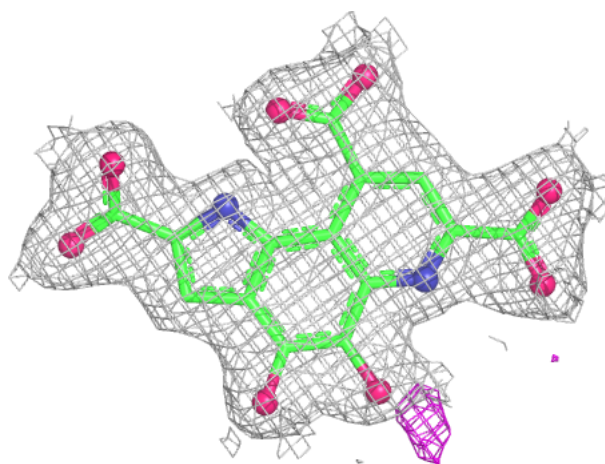
Electron density around PQQ G 702:

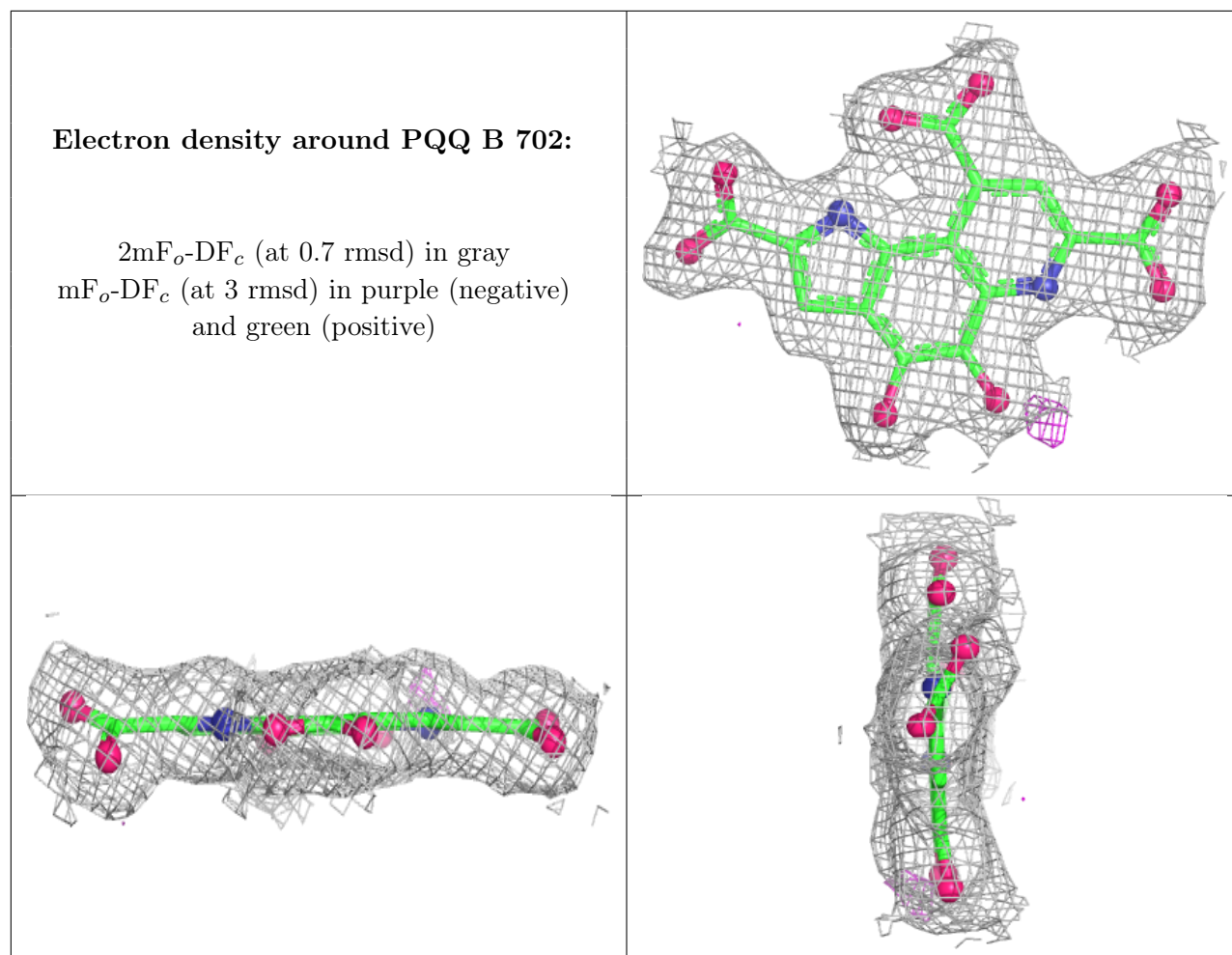
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PQQ 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.