



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:59 AM UTC

PDB ID : 7CDL / pdb_00007cdl
Title : holo-methanol dehydrogenase (MDH) with Cys131-Cys132 reduced from Methylococcus capsulatus (Bath)
Authors : Chuankhayan, P.; Chan, S.I.; Nareddy, P.K.R.; Tsai, I.K.; Tsai, Y.F.; Chen, K.H.-C.; Yu, S.S.-F.; Chen, C.J.
Deposited on : 2020-06-20
Resolution : 1.85 Å(reported)

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

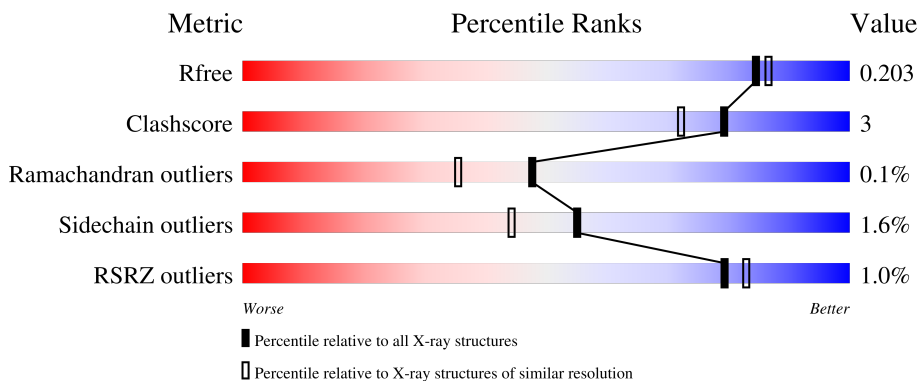
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

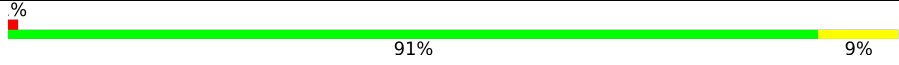
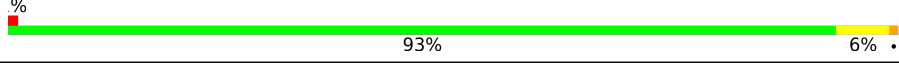
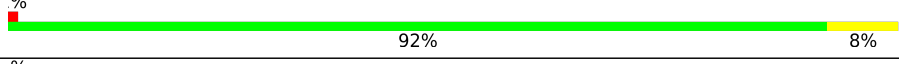
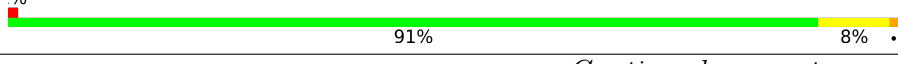
The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 91% 9%
1	B	573	 93% 6%
1	C	573	 92% 8%
1	D	573	 91% 8%

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Mol	Chain	Length	Quality of chain	
1	G	573		92% 6% .
1	H	573		93% 6% .
1	M	573		90% 9% .
1	N	573		92% 8%
2	E	72		92% 7% .
2	F	72		82% 14% ..
2	I	72		88% 6% 6% .
2	J	72		86% 12% .
2	K	72		92% 7% .
2	L	72		89% 10% .
2	O	72		88% 10% ..
2	P	72		86% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PQQ	B	702	-	-	X	-
4	PQQ	G	702	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 45133 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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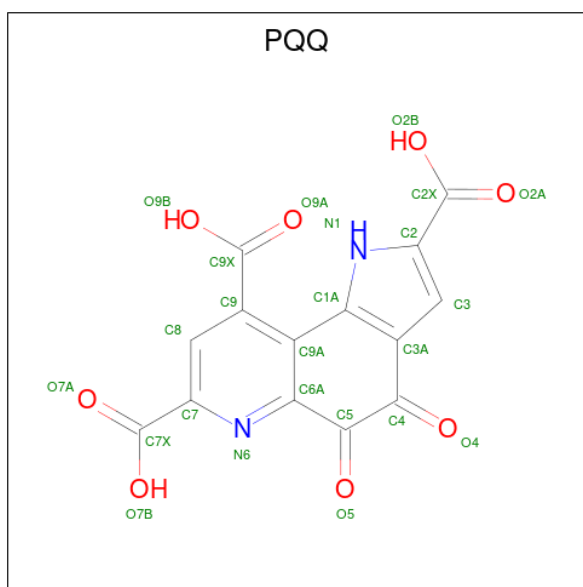
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	P	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	B	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
			Total	C	N	O		
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	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	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	C	483	Total	O	0	0
			483	483		
5	K	87	Total	O	0	0
			87	87		
5	D	516	Total	O	0	0
			516	516		
5	L	98	Total	O	0	0
			98	98		

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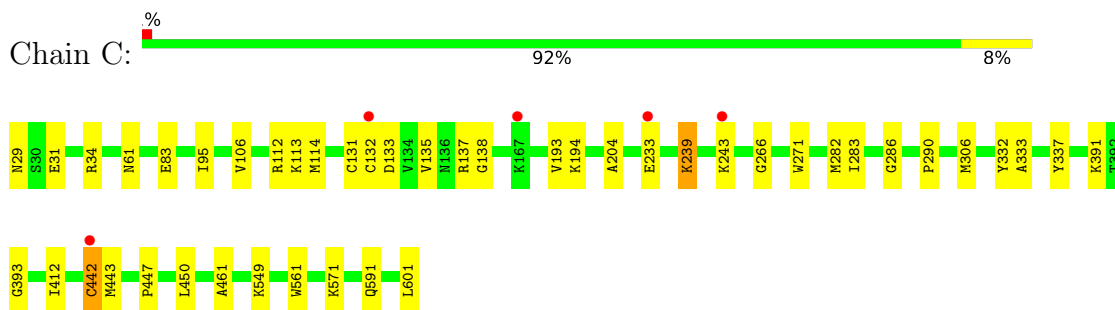
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	452	Total 452	O 452	0	0
5	E	84	Total 84	O 84	0	0
5	B	511	Total 511	O 511	0	0
5	F	81	Total 81	O 81	0	0
5	G	496	Total 496	O 496	0	0
5	I	78	Total 78	O 78	0	0
5	H	441	Total 441	O 441	0	0
5	J	60	Total 60	O 60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

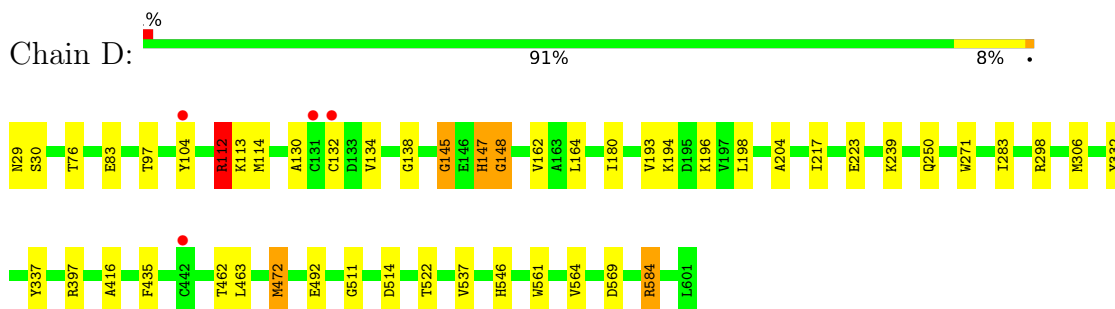
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

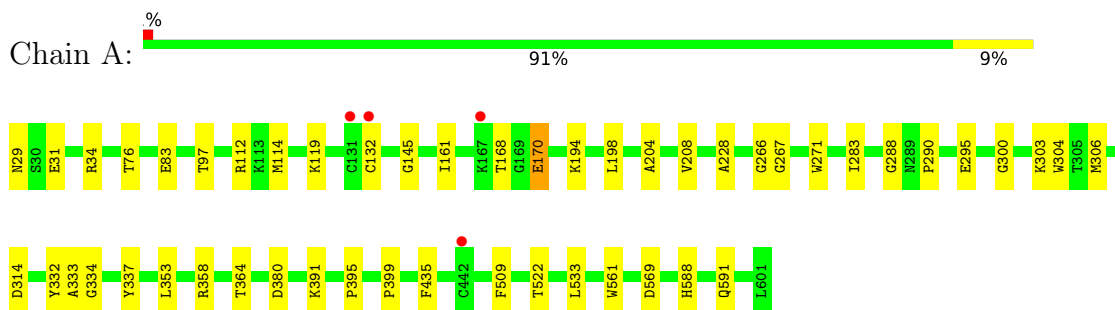
- Molecule 1: Methanol dehydrogenase protein, large subunit



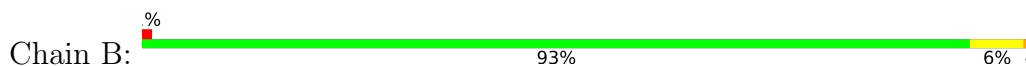
- Molecule 1: Methanol dehydrogenase protein, large subunit

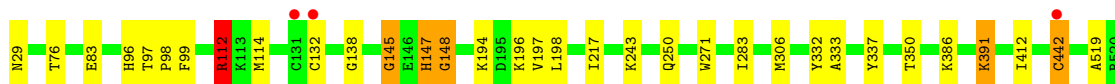


- Molecule 1: Methanol dehydrogenase protein, large subunit

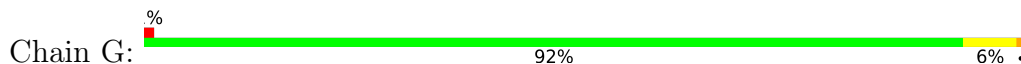


- Molecule 1: Methanol dehydrogenase protein, large subunit

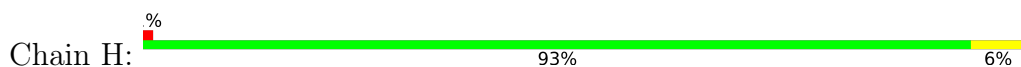




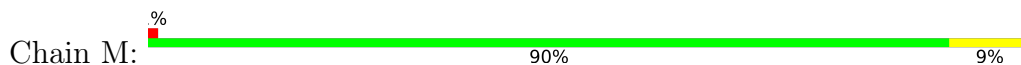
- Molecule 1: Methanol dehydrogenase protein, large subunit



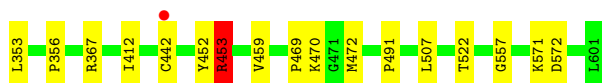
- Molecule 1: Methanol dehydrogenase protein, large subunit



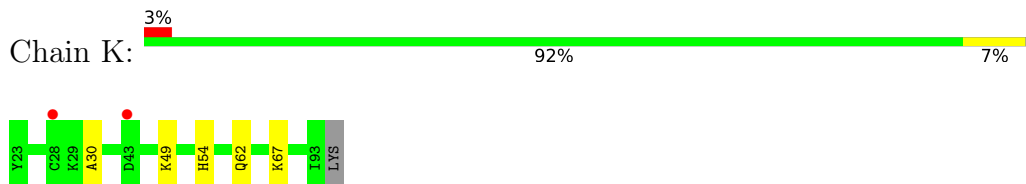
- Molecule 1: Methanol dehydrogenase protein, large subunit



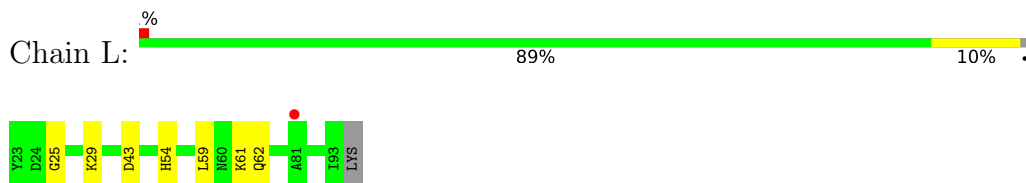
- Molecule 1: Methanol dehydrogenase protein, large subunit



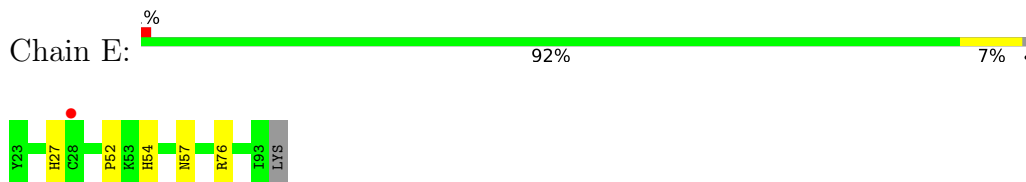
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



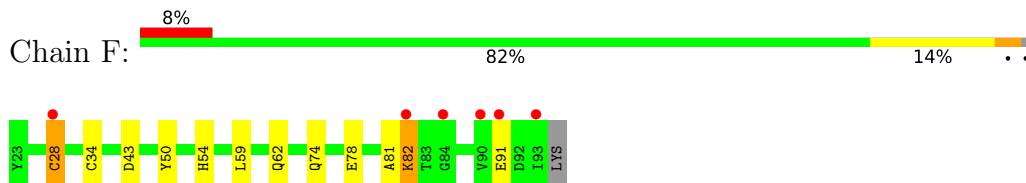
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



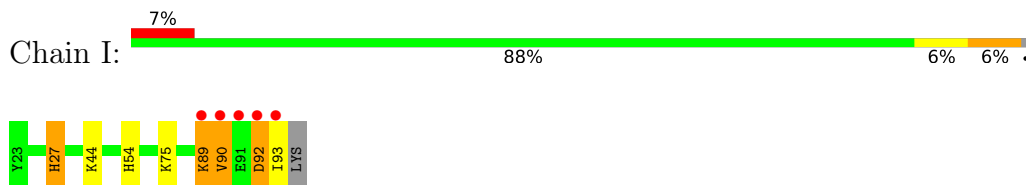
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



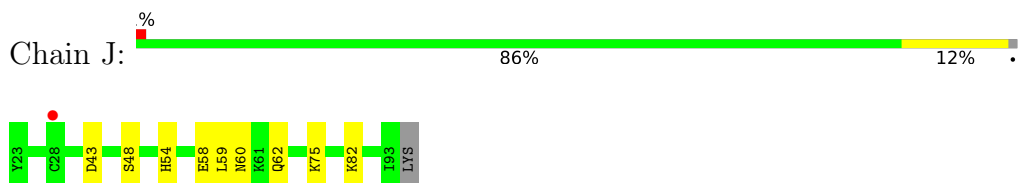
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



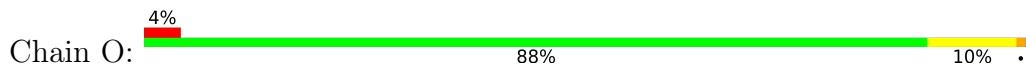
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

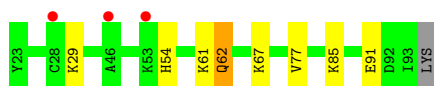


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

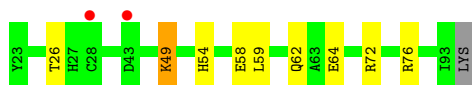
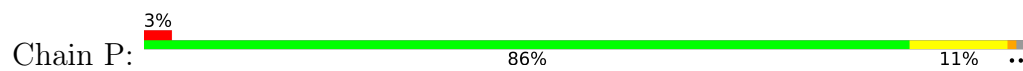


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2





- 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	128.11Å 211.11Å 222.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-1.85) 99.8 (30.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.152 , 0.195 0.165 , 0.203	Depositor DCC
R_{free} test set	25548 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	45133	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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

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	1.31	11/4622 (0.2%)	1.08	0/6281
1	B	1.36	12/4621 (0.3%)	1.16	10/6281 (0.2%)
1	C	1.31	6/4622 (0.1%)	1.12	8/6281 (0.1%)
1	D	1.33	11/4621 (0.2%)	1.21	18/6281 (0.3%)
1	G	1.33	13/4622 (0.3%)	1.16	11/6281 (0.2%)
1	H	1.29	15/4621 (0.3%)	1.17	10/6281 (0.2%)
1	M	1.38	23/4622 (0.5%)	1.15	12/6281 (0.2%)
1	N	1.34	15/4621 (0.3%)	1.14	7/6281 (0.1%)
2	E	1.24	0/583	1.11	1/785 (0.1%)
2	F	1.39	3/583 (0.5%)	1.29	2/785 (0.3%)
2	I	1.42	3/583 (0.5%)	1.24	3/785 (0.4%)
2	J	1.21	1/583 (0.2%)	1.18	4/785 (0.5%)
2	K	1.35	2/583 (0.3%)	1.21	1/785 (0.1%)
2	L	1.32	2/583 (0.3%)	1.20	3/785 (0.4%)
2	O	1.20	0/583	1.14	3/785 (0.4%)
2	P	1.31	3/583 (0.5%)	1.24	3/785 (0.4%)
All	All	1.33	120/41636 (0.3%)	1.15	96/56528 (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	D	0	1
1	G	0	2
1	H	0	1
1	M	0	2
1	N	0	1
All	All	0	7

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	ARG	CD-NE	-12.42	1.28	1.46
1	N	112	ARG	CD-NE	-11.23	1.30	1.46
1	H	112	ARG	CD-NE	-10.57	1.31	1.46
1	B	96	HIS	C-N	9.47	1.53	1.33
1	D	112	ARG	CD-NE	-9.40	1.33	1.46
1	N	96	HIS	C-N	8.39	1.50	1.33
1	G	145	GLY	N-CA	-8.09	1.33	1.45
1	B	148	GLY	N-CA	-7.97	1.32	1.45
1	B	350	THR	CA-C	7.77	1.59	1.52
1	B	521	ASP	C-N	-7.67	1.23	1.33
1	G	382	VAL	C-O	7.44	1.31	1.24
1	M	438	VAL	C-O	7.32	1.31	1.24
1	H	145	GLY	N-CA	-7.08	1.35	1.45
1	M	326	PRO	CA-C	-7.03	1.43	1.52
1	M	96	HIS	C-N	6.97	1.48	1.33
1	H	521	ASP	C-N	-6.95	1.24	1.33
1	H	279	LYS	C-O	-6.89	1.16	1.24
1	N	300	GLY	C-O	6.83	1.29	1.23
1	G	148	GLY	N-CA	-6.78	1.34	1.45
1	H	148	GLY	N-CA	-6.75	1.34	1.45
2	P	62	GLN	CB-CG	-6.73	1.32	1.52
1	D	145	GLY	C-O	-6.68	1.19	1.23
1	C	286	GLY	CA-C	-6.62	1.47	1.52
1	B	99	PHE	N-CA	6.60	1.53	1.45
1	C	95	ILE	C-O	6.56	1.30	1.24
1	B	386	LYS	C-O	-6.53	1.16	1.24
1	A	295	GLU	N-CA	6.51	1.54	1.46
1	G	145	GLY	C-O	-6.47	1.15	1.23
1	G	163	ALA	C-O	6.46	1.31	1.24
1	M	147	HIS	CA-C	6.29	1.61	1.52
1	H	96	HIS	C-N	6.27	1.46	1.33
1	A	509	PHE	CA-C	6.19	1.60	1.52
1	G	96	HIS	C-N	6.10	1.46	1.33
1	H	236	LEU	CA-C	-6.09	1.47	1.53
1	M	375	ALA	CA-C	-6.05	1.46	1.53
2	J	60	ASN	CA-C	5.99	1.60	1.52
1	G	286	GLY	CA-C	-5.98	1.48	1.52
2	L	25	GLY	C-N	5.95	1.42	1.33
1	M	522	THR	C-N	-5.93	1.25	1.33
1	D	147	HIS	CA-C	5.87	1.60	1.52
1	G	522	THR	C-N	-5.85	1.25	1.33
1	A	395	PRO	N-CA	-5.82	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	66	LYS	CA-C	5.81	1.60	1.52
1	C	393	GLY	CA-C	5.80	1.59	1.51
1	G	110	ASP	CG-OD1	5.78	1.36	1.25
2	P	58	GLU	CA-C	-5.77	1.45	1.52
2	I	44	LYS	CA-C	-5.75	1.45	1.52
1	M	417	MET	N-CA	5.71	1.53	1.46
1	B	519	ALA	N-CA	-5.70	1.39	1.46
1	M	424	ILE	CA-CB	-5.67	1.47	1.54
1	D	148	GLY	N-CA	-5.65	1.36	1.45
1	M	521	ASP	C-N	-5.64	1.26	1.33
1	G	285	TYR	C-O	5.57	1.30	1.23
1	M	226	ALA	CA-C	-5.56	1.46	1.52
1	M	145	GLY	C-O	-5.56	1.16	1.23
1	M	283	ILE	CA-C	-5.53	1.46	1.52
2	F	62	GLN	CB-CG	-5.52	1.35	1.52
1	M	148	GLY	N-CA	-5.52	1.36	1.45
1	A	161	ILE	CA-CB	5.52	1.60	1.54
1	B	541	PRO	CA-CB	5.49	1.60	1.53
1	N	251	PHE	N-CA	-5.47	1.39	1.45
1	C	61	ASN	C-O	-5.46	1.17	1.23
1	A	119	LYS	N-CA	-5.46	1.40	1.46
1	M	145	GLY	N-CA	-5.46	1.37	1.45
1	C	106	VAL	C-O	-5.45	1.18	1.24
1	D	546	HIS	N-CA	-5.44	1.39	1.46
1	A	112	ARG	C-O	-5.42	1.17	1.24
1	N	153	PHE	N-CA	5.42	1.52	1.46
1	D	250	GLN	CA-C	-5.41	1.49	1.52
1	A	145	GLY	C-O	-5.40	1.18	1.23
2	I	27	HIS	C-O	-5.39	1.17	1.23
1	M	125	ALA	C-O	-5.39	1.17	1.24
1	N	469	PRO	C-O	-5.39	1.17	1.24
1	G	546	HIS	C-O	5.39	1.30	1.24
1	H	148	GLY	C-O	-5.38	1.12	1.23
1	N	342	GLU	N-CA	5.36	1.52	1.46
2	L	25	GLY	C-O	-5.36	1.16	1.24
1	D	162	VAL	CA-C	-5.34	1.46	1.52
1	N	103	VAL	C-O	-5.32	1.18	1.24
1	B	197	VAL	C-O	5.31	1.29	1.24
1	D	164	LEU	CA-C	-5.30	1.46	1.52
1	D	416	ALA	CA-CB	-5.28	1.44	1.53
1	A	228	ALA	CA-C	5.28	1.59	1.52
2	F	34	CYS	N-CA	-5.28	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	62	GLN	CB-CG	-5.27	1.36	1.52
1	H	262	ALA	CA-C	5.27	1.59	1.52
1	N	131	CYS	C-O	-5.26	1.18	1.24
1	M	361	LEU	CA-C	-5.25	1.46	1.52
2	F	50	TYR	CA-CB	-5.22	1.46	1.53
1	N	459	VAL	C-O	-5.22	1.17	1.24
1	H	62	SER	C-O	-5.22	1.17	1.24
1	H	423	GLY	N-CA	5.21	1.52	1.45
1	C	131	CYS	C-O	-5.21	1.18	1.24
2	K	30	ALA	N-CA	5.21	1.51	1.46
2	I	90	VAL	N-CA	5.21	1.52	1.46
1	A	300	GLY	C-O	5.21	1.28	1.23
1	H	327	HIS	C-O	5.20	1.30	1.23
1	N	470	LYS	CA-C	-5.17	1.45	1.52
1	D	492	GLU	CA-C	5.16	1.58	1.52
2	P	72	ARG	C-O	5.16	1.30	1.24
1	D	104	TYR	CA-C	-5.15	1.46	1.52
1	G	130	ALA	C-N	-5.13	1.27	1.33
1	H	356	PRO	C-O	-5.13	1.19	1.24
1	M	550	GLN	C-O	-5.12	1.17	1.23
1	H	202	ALA	C-O	-5.12	1.17	1.23
1	M	324	LYS	CA-C	-5.12	1.46	1.52
1	A	380	ASP	N-CA	5.11	1.53	1.46
1	N	522	THR	C-N	-5.11	1.26	1.33
1	A	170	GLU	CD-OE1	5.10	1.35	1.25
1	N	102	ASN	CA-C	-5.08	1.46	1.52
1	G	148	GLY	C-O	-5.07	1.13	1.23
1	N	254	GLY	CA-C	-5.07	1.44	1.51
1	M	209	ARG	N-CA	-5.06	1.39	1.46
1	N	145	GLY	N-CA	5.05	1.50	1.45
1	B	145	GLY	C-O	-5.02	1.18	1.23
1	H	469	PRO	C-O	-5.02	1.18	1.24
1	M	315	THR	CA-C	-5.01	1.46	1.52
1	M	148	GLY	C-N	5.01	1.39	1.33
1	M	350	THR	CA-C	5.00	1.56	1.52
1	B	250	GLN	N-CA	-5.00	1.39	1.45

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	ARG	NE-CZ-NH2	-14.32	106.31	119.20
1	D	147	HIS	N-CA-C	13.74	129.50	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	147	HIS	CA-C-N	13.05	145.20	121.70
1	H	147	HIS	C-N-CA	13.05	145.20	121.70
1	H	112	ARG	NE-CZ-NH2	-12.91	107.58	119.20
1	D	147	HIS	CA-C-N	12.46	144.13	121.70
1	D	147	HIS	C-N-CA	12.46	144.13	121.70
1	H	147	HIS	N-CA-C	12.43	127.78	112.87
1	B	147	HIS	O-C-N	-12.35	105.42	122.46
1	H	147	HIS	O-C-N	-11.53	107.10	122.43
1	D	147	HIS	O-C-N	-11.43	106.69	122.46
1	G	147	HIS	N-CA-C	11.34	126.61	113.01
1	D	112	ARG	CD-NE-CZ	11.26	140.16	124.40
1	M	147	HIS	N-CA-C	11.25	126.50	113.01
1	B	147	HIS	CA-C-N	11.09	141.66	121.70
1	B	147	HIS	C-N-CA	11.09	141.66	121.70
1	M	147	HIS	CA-C-N	11.03	141.55	121.70
1	M	147	HIS	C-N-CA	11.03	141.55	121.70
1	B	147	HIS	N-CA-C	11.03	126.24	113.01
1	B	148	GLY	CA-C-N	-10.55	110.08	120.52
1	B	148	GLY	C-N-CA	-10.55	110.08	120.52
1	G	147	HIS	O-C-N	-10.45	108.04	122.46
1	H	112	ARG	NE-CZ-NH1	10.08	131.58	121.50
1	N	112	ARG	NE-CZ-NH2	-9.84	110.35	119.20
1	B	112	ARG	NE-CZ-NH2	-9.61	110.55	119.20
1	M	147	HIS	O-C-N	-9.61	109.20	122.46
1	G	147	HIS	CA-C-N	9.57	138.92	121.70
1	G	147	HIS	C-N-CA	9.57	138.92	121.70
1	G	144	ALA	O-C-N	-9.10	112.42	122.79
1	N	112	ARG	NE-CZ-NH1	8.98	130.48	121.50
2	L	29	LYS	N-CA-C	-8.04	102.49	111.82
1	D	112	ARG	NE-CZ-NH1	7.81	129.31	121.50
2	F	62	GLN	CB-CA-C	-7.71	98.77	110.88
1	B	138	GLY	N-CA-C	7.58	120.95	111.85
2	K	62	GLN	CB-CA-C	-7.51	99.08	110.88
1	M	148	GLY	CA-C-N	-7.35	112.75	120.03
1	M	148	GLY	C-N-CA	-7.35	112.75	120.03
1	H	210	GLY	N-CA-C	7.14	119.72	111.36
1	B	112	ARG	NE-CZ-NH1	7.12	128.62	121.50
1	C	131	CYS	N-CA-C	7.09	119.09	111.36
1	D	472	MET	CB-CG-SD	6.69	132.78	112.70
1	G	148	GLY	CA-C-N	-6.68	113.42	120.03
1	G	148	GLY	C-N-CA	-6.68	113.42	120.03
1	C	138	GLY	N-CA-C	6.67	120.23	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	144	ALA	CA-C-N	6.50	134.15	121.41
1	G	144	ALA	C-N-CA	6.50	134.15	121.41
1	N	356	PRO	CB-CA-C	-6.42	106.48	111.87
2	P	62	GLN	CB-CA-C	-6.40	100.83	110.88
1	H	548	GLY	N-CA-C	6.17	123.54	115.40
1	C	282	MET	CG-SD-CE	-6.09	87.50	100.90
1	C	443	MET	N-CA-C	6.08	118.31	109.07
1	N	131	CYS	N-CA-C	6.00	117.82	111.28
1	D	148	GLY	CA-C-N	-5.99	114.46	120.21
1	D	148	GLY	C-N-CA	-5.99	114.46	120.21
1	M	144	ALA	O-C-N	-5.94	116.01	122.79
1	N	367	ARG	NE-CZ-NH2	5.86	124.48	119.20
2	E	76	ARG	NE-CZ-NH2	5.74	124.37	119.20
2	J	58	GLU	N-CA-C	-5.72	105.13	111.36
1	M	468	GLY	CA-C-N	5.70	125.55	119.28
1	M	468	GLY	C-N-CA	5.70	125.55	119.28
2	L	61	LYS	N-CA-C	5.69	117.56	111.36
2	O	61	LYS	N-CA-C	5.65	117.43	111.28
1	D	298	ARG	NE-CZ-NH2	5.62	124.26	119.20
2	O	77	VAL	CB-CA-C	-5.62	104.78	111.97
1	D	180	ILE	N-CA-C	5.61	118.06	111.05
1	C	137	ARG	CG-CD-NE	-5.59	99.70	112.00
1	N	453	ARG	CG-CD-NE	5.55	124.22	112.00
1	M	138	GLY	N-CA-C	5.50	118.72	111.52
1	H	112	ARG	CD-NE-CZ	5.47	132.05	124.40
1	G	282	MET	CG-SD-CE	-5.43	88.95	100.90
1	M	473	LEU	N-CA-C	5.43	119.90	113.28
1	D	584	ARG	CB-CA-C	-5.40	101.50	110.68
2	I	89	LYS	CA-C-N	5.38	129.74	121.19
2	I	89	LYS	C-N-CA	5.38	129.74	121.19
1	C	135	VAL	CA-C-N	5.37	130.34	122.39
1	C	135	VAL	C-N-CA	5.37	130.34	122.39
1	N	572	ASP	N-CA-C	-5.34	102.92	109.65
1	G	474	GLY	N-CA-C	5.34	118.92	110.96
1	M	522	THR	O-C-N	-5.33	115.11	122.46
1	D	30	SER	CB-CA-C	-5.32	101.96	110.79
2	J	62	GLN	CB-CA-C	-5.29	102.34	110.81
2	P	49	LYS	CD-CE-NZ	5.28	128.80	111.90
2	O	62	GLN	CB-CA-C	-5.22	101.97	110.85
1	D	130	ALA	CA-C-N	-5.21	112.90	120.29
1	D	130	ALA	C-N-CA	-5.21	112.90	120.29
1	H	144	ALA	O-C-N	-5.16	116.71	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	GLY	N-CA-C	5.14	118.28	111.70
2	L	62	GLN	CB-CA-C	-5.14	102.26	110.79
2	J	48	SER	CA-C-N	5.14	127.88	120.38
2	J	48	SER	C-N-CA	5.14	127.88	120.38
2	I	75	LYS	CG-CD-CE	5.13	123.10	111.30
1	D	397	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	P	76	ARG	N-CA-C	5.09	116.83	111.28
1	B	522	THR	O-C-N	-5.06	115.48	122.46
2	F	28	CYS	CA-CB-SG	-5.03	102.83	114.40
1	C	450	LEU	N-CA-C	5.00	112.72	108.22

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	112	ARG	Sidechain
1	G	144	ALA	Peptide
1	G	145	GLY	Peptide
1	H	144	ALA	Peptide
1	M	144	ALA	Peptide
1	M	145	GLY	Peptide
1	N	97	THR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4491	0	4322	24	0
1	B	4490	0	4322	25	0
1	C	4491	0	4322	19	0
1	D	4490	0	4322	22	0
1	G	4491	0	4322	20	0
1	H	4490	0	4322	20	0
1	M	4491	0	4322	27	0
1	N	4490	0	4322	20	0
2	E	568	0	545	4	0
2	F	568	0	545	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	568	0	545	6	0
2	J	568	0	545	2	0
2	K	568	0	545	3	0
2	L	568	0	545	2	0
2	O	568	0	545	4	0
2	P	568	0	545	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	24	0	4	5	0
4	B	24	0	3	7	0
4	C	24	0	3	4	0
4	D	24	0	3	5	0
4	G	24	0	3	7	0
4	H	24	0	4	4	0
4	M	24	0	4	3	0
4	N	24	0	3	2	0
5	A	452	0	0	4	0
5	B	511	0	0	7	0
5	C	483	0	0	4	0
5	D	516	0	0	4	0
5	E	84	0	0	2	0
5	F	81	0	0	1	0
5	G	496	0	0	5	0
5	H	441	0	0	6	0
5	I	78	0	0	3	0
5	J	60	0	0	0	0
5	K	87	0	0	1	0
5	L	98	0	0	0	0
5	M	440	0	0	8	0
5	N	488	0	0	4	0
5	O	60	0	0	1	0
5	P	90	0	0	6	0
All	All	45133	0	38963	211	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 3.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:601:LEU:C	5:H:820:HOH:O	1.80	1.19
1:D:112:ARG:O	1:D:112:ARG:HD3	1.51	1.10
1:H:112:ARG:HD3	1:H:112:ARG:O	1.63	0.97
2:P:26:THR:HB	5:P:102:HOH:O	0.79	0.96
1:N:112:ARG:O	1:N:112:ARG:HD3	1.68	0.93
2:I:90:VAL:HG12	5:I:157:HOH:O	1.73	0.87
1:M:90:ASP:CG	5:M:801:HOH:O	2.18	0.86
1:B:112:ARG:O	1:B:112:ARG:HD3	1.82	0.80
1:G:591:GLN:HE21	1:H:114:MET:HE1	1.50	0.76
1:H:112:ARG:O	1:H:112:ARG:CD	2.35	0.75
1:C:239:LYS:HD3	5:C:1115:HOH:O	1.90	0.72
5:N:839:HOH:O	2:P:26:THR:HG23	1.89	0.71
1:B:112:ARG:O	1:B:112:ARG:CD	2.40	0.70
2:I:92:ASP:OD2	5:I:101:HOH:O	2.10	0.69
1:B:132:CYS:O	5:B:801:HOH:O	2.11	0.69
1:B:561:TRP:CZ3	4:B:702:PQQ:O4	2.46	0.68
1:M:90:ASP:OD1	5:M:801:HOH:O	2.12	0.68
2:I:27:HIS:CD2	5:I:149:HOH:O	2.48	0.67
1:M:147:HIS:CD2	1:M:217:ILE:HD11	2.30	0.66
1:A:31:GLU:OE2	1:A:34:ARG:NH2	2.28	0.64
1:B:145:GLY:O	1:B:148:GLY:HA2	1.98	0.63
5:H:1066:HOH:O	2:J:54:HIS:HD2	1.82	0.63
2:P:49:LYS:CD	5:P:174:HOH:O	2.46	0.63
1:G:472:MET:HE2	1:G:491:PRO:HB3	1.82	0.62
2:P:49:LYS:HD3	5:P:174:HOH:O	1.98	0.62
5:D:1143:HOH:O	2:L:54:HIS:HE1	1.83	0.61
2:F:81:ALA:HB2	5:F:109:HOH:O	1.98	0.61
1:B:112:ARG:HD3	1:B:112:ARG:C	2.22	0.60
5:N:1103:HOH:O	2:P:54:HIS:HD2	1.83	0.60
1:A:561:TRP:CZ3	4:A:702:PQQ:O4	2.54	0.60
1:A:591:GLN:HE21	1:B:114:MET:HE1	1.67	0.60
1:N:112:ARG:O	1:N:112:ARG:CD	2.44	0.60
2:P:64:GLU:HG2	5:P:103:HOH:O	2.02	0.59
5:B:971:HOH:O	2:F:54:HIS:HD2	1.85	0.59
5:D:1102:HOH:O	2:L:54:HIS:HD2	1.86	0.59
1:N:31:GLU:OE1	1:N:34:ARG:NH1	2.37	0.58
1:A:204:ALA:HB3	4:A:702:PQQ:O7A	2.04	0.58
1:H:145:GLY:O	1:H:148:GLY:HA2	2.03	0.58
1:C:561:TRP:CZ3	4:C:702:PQQ:O4	2.56	0.58
1:M:561:TRP:CZ3	4:M:702:PQQ:O4	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:HIS:CD2	1:D:217:ILE:HD11	2.39	0.57
5:G:1038:HOH:O	2:I:54:HIS:HD2	1.87	0.57
1:A:114:MET:HE1	1:B:591:GLN:HE21	1.69	0.57
5:M:947:HOH:O	2:O:54:HIS:HD2	1.88	0.57
1:D:145:GLY:O	1:D:148:GLY:HA2	2.04	0.57
1:G:145:GLY:O	1:G:148:GLY:HA2	2.05	0.56
1:G:145:GLY:HA2	1:G:147:HIS:CD2	2.40	0.56
1:N:271:TRP:CZ2	4:N:702:PQQ:C6A	2.89	0.56
5:A:1023:HOH:O	2:E:54:HIS:HD2	1.88	0.56
2:E:27:HIS:CE1	5:E:117:HOH:O	2.59	0.55
1:H:453:ARG:HG2	5:H:1209:HOH:O	2.05	0.55
1:D:561:TRP:CZ3	4:D:702:PQQ:O4	2.60	0.54
5:N:1131:HOH:O	2:P:54:HIS:HE1	1.89	0.54
2:F:78:GLU:O	2:F:82:LYS:HD2	2.07	0.54
1:D:193:VAL:HG21	1:D:283:ILE:CD1	2.38	0.53
1:G:193:VAL:HG21	1:G:283:ILE:HD11	1.90	0.53
4:H:702:PQQ:C5	5:H:801:HOH:O	2.57	0.53
1:N:198:LEU:HD11	1:N:283:ILE:HD13	1.91	0.53
1:C:271:TRP:CZ2	4:C:702:PQQ:C6A	2.91	0.53
5:C:1026:HOH:O	2:K:54:HIS:HD2	1.91	0.53
1:M:306:MET:HE1	1:M:332:TYR:C	2.34	0.53
1:B:561:TRP:CE3	4:B:702:PQQ:O4	2.62	0.52
5:C:1143:HOH:O	2:K:54:HIS:HE1	1.92	0.52
1:C:591:GLN:HE21	1:D:114:MET:HE1	1.73	0.52
1:M:412:ILE:O	1:M:442:CYS:SG	2.68	0.52
1:C:391:LYS:HE2	5:C:1216:HOH:O	2.10	0.52
1:A:533:LEU:O	1:B:112:ARG:NH2	2.42	0.52
1:C:112:ARG:HD3	1:D:514:ASP:O	2.10	0.52
4:G:702:PQQ:C2X	5:G:801:HOH:O	2.58	0.52
2:I:92:ASP:OD1	2:I:92:ASP:N	2.43	0.52
5:B:1148:HOH:O	2:F:54:HIS:HE1	1.93	0.52
1:C:29:ASN:N	1:C:194:LYS:H	2.09	0.51
1:M:566:LEU:HD12	1:M:566:LEU:C	2.35	0.51
1:A:132:CYS:O	5:A:801:HOH:O	2.19	0.51
1:H:276:TYR:HD1	1:H:283:ILE:HD13	1.75	0.50
1:N:412:ILE:O	1:N:442:CYS:SG	2.69	0.50
1:C:204:ALA:HB3	4:C:702:PQQ:O7A	2.11	0.50
4:G:702:PQQ:C5	5:G:803:HOH:O	2.60	0.50
4:B:702:PQQ:C5	5:B:979:HOH:O	2.59	0.50
1:N:452:TYR:O	1:N:453:ARG:HD3	2.10	0.50
1:G:271:TRP:CZ2	4:G:702:PQQ:C6A	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:204:ALA:HB3	4:N:702:PQQ:O7A	2.12	0.49
1:G:306:MET:HE1	1:G:332:TYR:C	2.37	0.49
1:D:271:TRP:CZ2	4:D:702:PQQ:C6A	2.96	0.49
1:B:271:TRP:CZ2	4:B:702:PQQ:C6A	2.96	0.49
1:M:271:TRP:CZ2	4:M:702:PQQ:C6A	2.96	0.49
2:P:26:THR:O	2:P:26:THR:HG22	2.12	0.49
1:D:83:GLU:OE1	4:D:702:PQQ:O2B	2.31	0.48
1:G:83:GLU:OE1	4:G:702:PQQ:O2B	2.32	0.48
5:H:1060:HOH:O	2:J:54:HIS:HE1	1.97	0.48
1:D:196:LYS:HD2	1:D:223:GLU:HG3	1.96	0.47
1:G:81:GLY:CA	1:G:538:ILE:HD11	2.45	0.47
1:D:196:LYS:HE3	1:D:223:GLU:HG3	1.95	0.47
1:B:391:LYS:HD2	1:B:391:LYS:N	2.29	0.47
1:N:306:MET:HE1	1:N:332:TYR:C	2.39	0.47
1:H:561:TRP:CZ3	4:H:702:PQQ:O4	2.68	0.47
1:M:29:ASN:N	1:M:194:LYS:H	2.12	0.47
2:P:26:THR:CB	5:P:102:HOH:O	1.70	0.47
1:A:168:THR:OG1	1:A:170:GLU:HG2	2.15	0.46
1:D:112:ARG:HD3	1:D:112:ARG:C	2.20	0.46
1:A:76:THR:HB	1:A:97:THR:HG22	1.97	0.46
1:B:29:ASN:N	1:B:194:LYS:H	2.13	0.46
1:G:81:GLY:HA3	1:G:538:ILE:HD11	1.96	0.46
1:C:83:GLU:OE1	4:C:702:PQQ:O2A	2.33	0.46
1:H:332:TYR:O	1:H:333:ALA:C	2.57	0.46
1:H:453:ARG:CG	5:H:1209:HOH:O	2.64	0.46
1:C:193:VAL:HG21	1:C:283:ILE:HD11	1.98	0.46
1:H:271:TRP:CZ2	4:H:702:PQQ:C6A	2.99	0.46
1:M:591:GLN:HE21	1:N:114:MET:HE1	1.80	0.46
1:D:435:PHE:CZ	1:D:522:THR:HB	2.51	0.46
1:H:76:THR:HB	1:H:97:THR:HG22	1.98	0.46
1:G:561:TRP:CZ3	4:G:702:PQQ:O4	2.68	0.45
1:H:276:TYR:CD1	1:H:283:ILE:HD13	2.51	0.45
1:D:561:TRP:CE3	4:D:702:PQQ:O4	2.70	0.45
1:A:271:TRP:CZ2	4:A:702:PQQ:C6A	3.00	0.45
1:C:306:MET:HE1	1:C:332:TYR:C	2.42	0.45
1:D:132:CYS:O	5:D:801:HOH:O	2.21	0.45
1:A:588:HIS:HD2	5:B:1104:HOH:O	2.00	0.45
1:G:76:THR:HB	1:G:97:THR:HG22	1.98	0.45
1:C:132:CYS:O	1:C:133:ASP:CB	2.64	0.45
1:B:198:LEU:HD11	1:B:283:ILE:HD13	1.98	0.45
1:M:97:THR:HB	1:M:98:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LEU:C	1:B:566:LEU:HD12	2.41	0.45
1:M:167:LYS:HD3	5:M:950:HOH:O	2.16	0.44
1:M:509:PHE:CE2	1:M:552:ILE:HD13	2.52	0.44
1:M:591:GLN:HG2	1:N:114:MET:HE1	1.99	0.44
1:A:306:MET:HE1	1:A:332:TYR:C	2.42	0.44
4:G:702:PQQ:C2	5:G:801:HOH:O	2.65	0.44
4:G:702:PQQ:O9A	4:G:702:PQQ:N1	2.49	0.44
5:G:1157:HOH:O	2:I:54:HIS:HE1	2.00	0.44
1:H:353:LEU:C	1:H:353:LEU:HD12	2.42	0.44
5:M:1115:HOH:O	2:O:54:HIS:HE1	2.00	0.44
1:B:332:TYR:O	1:B:333:ALA:C	2.60	0.44
4:B:702:PQQ:C2X	5:B:801:HOH:O	2.66	0.44
1:H:412:ILE:O	1:H:442:CYS:SG	2.76	0.44
1:M:588:HIS:HD2	5:N:1091:HOH:O	2.00	0.44
1:C:412:ILE:O	1:C:442:CYS:SG	2.76	0.44
1:M:193:VAL:HG21	1:M:283:ILE:HD11	2.00	0.44
1:M:549:LYS:NZ	1:M:601:LEU:OXT	2.41	0.44
1:H:83:GLU:OE1	4:H:702:PQQ:O2A	2.36	0.43
1:A:29:ASN:N	1:A:194:LYS:H	2.16	0.43
1:M:533:LEU:O	1:N:112:ARG:NH2	2.50	0.43
1:A:353:LEU:O	1:A:364:THR:HA	2.17	0.43
1:D:29:ASN:N	1:D:194:LYS:H	2.16	0.43
1:M:353:LEU:C	1:M:353:LEU:HD12	2.43	0.43
1:A:266:GLY:O	1:A:290:PRO:HA	2.19	0.43
1:G:85:ALA:HB1	1:G:86:PRO:CD	2.48	0.43
2:K:67:LYS:HE3	5:K:159:HOH:O	2.19	0.43
1:H:306:MET:HE1	1:H:332:TYR:C	2.44	0.43
1:C:31:GLU:OE2	1:C:34:ARG:NH2	2.41	0.43
1:N:331:ASP:CG	1:N:331:ASP:O	2.60	0.43
2:E:52:PRO:HB2	2:E:54:HIS:CE1	2.54	0.43
1:D:204:ALA:HB3	4:D:702:PQQ:O7A	2.18	0.43
1:B:97:THR:HB	1:B:98:PRO:HD2	2.01	0.43
5:A:1089:HOH:O	2:E:54:HIS:HE1	2.02	0.42
1:H:208:VAL:O	1:H:267:GLY:HA2	2.18	0.42
1:M:83:GLU:HG3	1:M:538:ILE:HD12	2.01	0.42
2:O:85:LYS:HG2	5:O:154:HOH:O	2.19	0.42
1:A:83:GLU:OE1	4:A:702:PQQ:O2B	2.36	0.42
4:A:702:PQQ:C5	5:A:837:HOH:O	2.67	0.42
1:N:62:SER:HA	1:N:507:LEU:HD21	2.00	0.42
1:A:303:LYS:HA	1:A:304:TRP:HA	1.86	0.42
1:B:112:ARG:HD3	1:B:112:ARG:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLU:OE1	4:B:702:PQQ:O2A	2.37	0.42
1:N:472:MET:HE2	1:N:491:PRO:HB3	2.01	0.42
1:D:113:LYS:NZ	5:D:813:HOH:O	2.52	0.42
1:G:266:GLY:O	1:G:290:PRO:HA	2.20	0.42
1:M:276:TYR:HD1	1:M:283:ILE:HD13	1.84	0.42
1:A:399:PRO:HB3	5:E:164:HOH:O	2.18	0.42
1:A:194:LYS:NZ	1:A:314:ASP:OD1	2.51	0.42
1:G:331:ASP:CG	1:G:331:ASP:O	2.60	0.42
1:N:353:LEU:HD12	1:N:353:LEU:C	2.44	0.42
1:B:306:MET:HE1	1:B:332:TYR:C	2.45	0.42
1:G:85:ALA:HB1	1:G:86:PRO:HD2	2.01	0.42
1:G:29:ASN:N	1:G:194:LYS:H	2.17	0.42
1:C:266:GLY:O	1:C:290:PRO:HA	2.20	0.41
1:A:208:VAL:O	1:A:267:GLY:HA2	2.20	0.41
1:N:112:ARG:HD3	1:N:112:ARG:C	2.23	0.41
1:C:549:LYS:NZ	1:C:601:LEU:OXT	2.48	0.41
1:D:306:MET:HE1	1:D:332:TYR:C	2.46	0.41
1:M:66:LYS:HE2	5:M:1183:HOH:O	2.19	0.41
1:A:198:LEU:HD21	1:A:283:ILE:HD13	2.03	0.41
1:M:104:TYR:HD1	1:M:117:GLN:HG2	1.84	0.41
1:B:584:ARG:HB2	5:B:1230:HOH:O	2.20	0.41
1:C:113:LYS:HG3	1:C:114:MET:N	2.36	0.41
1:B:147:HIS:CD2	1:B:217:ILE:HD11	2.55	0.41
1:M:412:ILE:C	1:M:442:CYS:SG	3.04	0.41
1:B:412:ILE:O	1:B:442:CYS:SG	2.79	0.41
1:D:76:THR:HB	1:D:97:THR:HG22	2.02	0.41
1:B:76:THR:HB	1:B:97:THR:HG22	2.02	0.41
1:H:112:ARG:HD3	1:H:112:ARG:C	2.21	0.41
1:C:332:TYR:O	1:C:333:ALA:C	2.64	0.41
1:D:462:THR:C	1:D:463:LEU:HD12	2.46	0.41
1:A:333:ALA:O	1:A:358:ARG:HG3	2.21	0.41
1:G:303:LYS:HA	1:G:304:TRP:HA	1.89	0.41
1:H:193:VAL:HG11	1:H:283:ILE:HD11	2.03	0.41
1:M:561:TRP:CE3	4:M:702:PQQ:O4	2.74	0.40
1:N:76:THR:HB	1:N:97:THR:HG22	2.03	0.40
1:A:288:GLY:HA2	1:A:334:GLY:H	1.86	0.40
1:M:167:LYS:HE2	5:M:1175:HOH:O	2.21	0.40
1:M:447:PRO:HA	1:M:461:ALA:HA	2.04	0.40
5:M:1020:HOH:O	2:O:62:GLN:HG3	2.20	0.40
1:N:98:PRO:O	1:N:99:PHE:C	2.64	0.40
1:N:412:ILE:C	1:N:442:CYS:SG	3.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:PRO:HA	1:C:461:ALA:HA	2.02	0.40
1:D:511:GLY:HA3	1:D:537:VAL:HG11	2.02	0.40
1:A:435:PHE:CZ	1:A:522:THR:HB	2.57	0.40
1:G:435:PHE:CZ	1:G:522:THR:HB	2.57	0.40
2:P:49:LYS:HD2	5:P:174:HOH:O	2.15	0.40
1:B:561:TRP:HZ3	4:B:702:PQQ:O4	2.00	0.40
1:G:145:GLY:HA3	1:G:148:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/573 (100%)	543 (95%)	28 (5%)	0	100	100
1	B	571/573 (100%)	542 (95%)	29 (5%)	0	100	100
1	C	571/573 (100%)	541 (95%)	30 (5%)	0	100	100
1	D	571/573 (100%)	543 (95%)	27 (5%)	1 (0%)	43	31
1	G	571/573 (100%)	541 (95%)	28 (5%)	2 (0%)	30	17
1	H	571/573 (100%)	539 (94%)	32 (6%)	0	100	100
1	M	571/573 (100%)	544 (95%)	27 (5%)	0	100	100
1	N	571/573 (100%)	544 (95%)	25 (4%)	2 (0%)	30	17
2	E	69/72 (96%)	69 (100%)	0	0	100	100
2	F	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
2	I	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	J	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
2	K	69/72 (96%)	69 (100%)	0	0	100	100
2	L	69/72 (96%)	69 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	69/72 (96%)	69 (100%)	0	0	100	100
2	P	69/72 (96%)	69 (100%)	0	0	100	100
All	All	5120/5160 (99%)	4884 (95%)	231 (4%)	5 (0%)	48	35

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	464/464 (100%)	461 (99%)	3 (1%)	78	73
1	B	464/464 (100%)	456 (98%)	8 (2%)	53	42
1	C	464/464 (100%)	458 (99%)	6 (1%)	61	51
1	D	464/464 (100%)	456 (98%)	8 (2%)	53	42
1	G	464/464 (100%)	461 (99%)	3 (1%)	78	73
1	H	464/464 (100%)	457 (98%)	7 (2%)	57	47
1	M	464/464 (100%)	458 (99%)	6 (1%)	61	51
1	N	464/464 (100%)	457 (98%)	7 (2%)	57	47
2	E	60/61 (98%)	59 (98%)	1 (2%)	53	42
2	F	60/61 (98%)	54 (90%)	6 (10%)	7	1
2	I	60/61 (98%)	57 (95%)	3 (5%)	22	8
2	J	60/61 (98%)	56 (93%)	4 (7%)	15	4
2	K	60/61 (98%)	59 (98%)	1 (2%)	53	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	60/61 (98%)	58 (97%)	2 (3%)	33	18
2	O	60/61 (98%)	57 (95%)	3 (5%)	22	8
2	P	60/61 (98%)	59 (98%)	1 (2%)	53	42
All	All	4192/4200 (100%)	4123 (98%)	69 (2%)	55	44

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	233	GLU
1	C	239	LYS
1	C	243	LYS
1	C	337	TYR
1	C	442	CYS
1	C	571	LYS
2	K	49	LYS
1	D	112	ARG
1	D	198	LEU
1	D	239	LYS
1	D	337	TYR
1	D	472	MET
1	D	564	VAL
1	D	569	ASP
1	D	584	ARG
2	L	43	ASP
2	L	59	LEU
1	A	337	TYR
1	A	391	LYS
1	A	569	ASP
2	E	57	ASN
1	B	112	ARG
1	B	196	LYS
1	B	243	LYS
1	B	337	TYR
1	B	391	LYS
1	B	442	CYS
1	B	566	LEU
1	B	584	ARG
2	F	28	CYS
2	F	43	ASP
2	F	59	LEU
2	F	74	GLN

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Mol	Chain	Res	Type
2	F	82	LYS
2	F	91	GLU
1	G	146	GLU
1	G	193	VAL
1	G	337	TYR
2	I	89	LYS
2	I	92	ASP
2	I	93	ILE
1	H	66	LYS
1	H	112	ARG
1	H	132	CYS
1	H	279	LYS
1	H	337	TYR
1	H	453	ARG
1	H	571	LYS
2	J	43	ASP
2	J	59	LEU
2	J	75	LYS
2	J	82	LYS
1	M	167	LYS
1	M	337	TYR
1	M	391	LYS
1	M	442	CYS
1	M	566	LEU
1	M	571	LYS
2	O	29	LYS
2	O	67	LYS
2	O	91	GLU
1	N	112	ARG
1	N	233	GLU
1	N	243	LYS
1	N	279	LYS
1	N	337	TYR
1	N	453	ARG
1	N	571	LYS
2	P	59	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	117	GLN
1	C	156	GLN

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Mol	Chain	Res	Type
1	C	177	ASN
1	C	270	ASN
1	C	408	ASN
1	C	546	HIS
1	C	591	GLN
2	K	54	HIS
1	D	63	HIS
1	D	117	GLN
1	D	177	ASN
1	D	216	ASN
1	D	464	ASN
2	L	54	HIS
1	A	117	GLN
1	A	407	HIS
1	A	588	HIS
1	A	591	GLN
2	E	54	HIS
1	B	117	GLN
1	B	250	GLN
1	B	270	ASN
1	B	408	ASN
1	B	464	ASN
1	B	591	GLN
2	F	54	HIS
1	G	117	GLN
1	G	155	ASN
1	G	250	GLN
1	G	270	ASN
1	G	408	ASN
1	G	588	HIS
1	G	591	GLN
2	I	54	HIS
1	H	117	GLN
1	H	177	ASN
1	H	216	ASN
1	H	464	ASN
1	H	545	GLN
2	J	54	HIS
1	M	156	GLN
1	M	216	ASN
1	M	270	ASN
1	M	407	HIS

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Mol	Chain	Res	Type
1	M	588	HIS
1	M	591	GLN
2	O	54	HIS
1	N	117	GLN
1	N	155	ASN
1	N	177	ASN
1	N	216	ASN
1	N	464	ASN
1	N	546	HIS
2	P	54	HIS
2	P	74	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	M	702	3	26,26,26	4.39	12 (46%)	34,40,40	2.89	13 (38%)
4	PQQ	N	702	3	26,26,26	4.34	10 (38%)	34,40,40	3.36	19 (55%)

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	4.48	11 (42%)	34,40,40	3.16	19 (55%)
4	PQQ	B	702	3	26,26,26	4.29	12 (46%)	34,40,40	2.96	16 (47%)
4	PQQ	G	702	3	26,26,26	4.34	10 (38%)	34,40,40	2.91	16 (47%)
4	PQQ	A	702	3	26,26,26	4.37	11 (42%)	34,40,40	2.61	14 (41%)
4	PQQ	C	702	3	26,26,26	4.64	12 (46%)	34,40,40	2.51	16 (47%)
4	PQQ	D	702	3	26,26,26	4.31	12 (46%)	34,40,40	3.13	18 (52%)

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	M	702	3	-	8/12/28/28	0/3/3/3
4	PQQ	N	702	3	-	8/12/28/28	0/3/3/3
4	PQQ	H	702	3	-	8/12/28/28	0/3/3/3
4	PQQ	B	702	3	-	7/12/28/28	0/3/3/3
4	PQQ	G	702	3	-	8/12/28/28	0/3/3/3
4	PQQ	A	702	3	-	8/12/28/28	0/3/3/3
4	PQQ	C	702	3	-	7/12/28/28	0/3/3/3
4	PQQ	D	702	3	-	8/12/28/28	0/3/3/3

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	702	PQQ	C5-C4	-11.97	1.37	1.54
4	C	702	PQQ	O4-C4	11.80	1.49	1.23
4	A	702	PQQ	C5-C4	-11.71	1.38	1.54
4	N	702	PQQ	C5-C4	-11.69	1.38	1.54
4	M	702	PQQ	C5-C4	-11.64	1.38	1.54
4	C	702	PQQ	C5-C4	-11.58	1.38	1.54
4	G	702	PQQ	O5-C5	11.49	1.47	1.23
4	B	702	PQQ	C5-C4	-11.47	1.38	1.54
4	D	702	PQQ	O5-C5	11.35	1.46	1.23
4	C	702	PQQ	O5-C5	11.25	1.46	1.23
4	G	702	PQQ	C5-C4	-11.13	1.39	1.54
4	M	702	PQQ	O5-C5	10.79	1.45	1.23
4	H	702	PQQ	O5-C5	10.76	1.45	1.23
4	N	702	PQQ	O4-C4	10.50	1.46	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	PQQ	O4-C4	10.44	1.46	1.23
4	N	702	PQQ	O5-C5	10.38	1.44	1.23
4	D	702	PQQ	O4-C4	10.11	1.46	1.23
4	H	702	PQQ	O4-C4	10.08	1.46	1.23
4	G	702	PQQ	O4-C4	10.05	1.45	1.23
4	B	702	PQQ	O4-C4	9.90	1.45	1.23
4	M	702	PQQ	O4-C4	9.82	1.45	1.23
4	B	702	PQQ	O5-C5	9.44	1.42	1.23
4	A	702	PQQ	O5-C5	9.26	1.42	1.23
4	D	702	PQQ	C5-C4	-9.24	1.41	1.54
4	C	702	PQQ	O7A-C7X	8.61	1.47	1.22
4	D	702	PQQ	O7A-C7X	8.15	1.46	1.22
4	H	702	PQQ	O7A-C7X	7.99	1.45	1.22
4	B	702	PQQ	O7A-C7X	7.78	1.45	1.22
4	G	702	PQQ	O7A-C7X	7.58	1.44	1.22
4	A	702	PQQ	O7A-C7X	7.42	1.44	1.22
4	M	702	PQQ	O7A-C7X	7.39	1.43	1.22
4	N	702	PQQ	O7A-C7X	7.18	1.43	1.22
4	A	702	PQQ	C6A-C5	-5.05	1.44	1.50
4	M	702	PQQ	C9-C9A	4.75	1.48	1.41
4	B	702	PQQ	C6A-C5	-4.72	1.44	1.50
4	A	702	PQQ	C8-C9	4.48	1.46	1.39
4	D	702	PQQ	C9-C9A	4.47	1.47	1.41
4	H	702	PQQ	C6A-C5	-4.37	1.44	1.50
4	D	702	PQQ	C8-C9	4.29	1.46	1.39
4	M	702	PQQ	C6A-C5	-4.26	1.45	1.50
4	H	702	PQQ	C8-C9	4.21	1.46	1.39
4	N	702	PQQ	C8-C9	4.13	1.46	1.39
4	B	702	PQQ	C8-C9	4.09	1.46	1.39
4	N	702	PQQ	C9-C9A	4.09	1.47	1.41
4	C	702	PQQ	C8-C9	4.03	1.46	1.39
4	A	702	PQQ	C9-C9A	3.97	1.47	1.41
4	D	702	PQQ	C6A-C5	-3.65	1.45	1.50
4	G	702	PQQ	C8-C9	3.65	1.45	1.39
4	M	702	PQQ	C8-C9	3.58	1.45	1.39
4	G	702	PQQ	C6A-C5	-3.50	1.46	1.50
4	A	702	PQQ	C7-C7X	3.50	1.56	1.50
4	B	702	PQQ	C9-C9A	3.49	1.46	1.41
4	C	702	PQQ	C6A-C5	-3.43	1.46	1.50
4	D	702	PQQ	C7-C7X	3.39	1.56	1.50
4	C	702	PQQ	O2B-C2X	-3.37	1.21	1.30
4	H	702	PQQ	C7-C7X	3.35	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	702	PQQ	O2B-C2X	-3.06	1.22	1.30
4	B	702	PQQ	C7-C7X	3.04	1.56	1.50
4	C	702	PQQ	C7-C7X	3.02	1.56	1.50
4	C	702	PQQ	C9-C9A	3.01	1.45	1.41
4	B	702	PQQ	O2B-C2X	-2.99	1.22	1.30
4	H	702	PQQ	C9-C9X	2.99	1.56	1.49
4	N	702	PQQ	C6A-C5	-2.95	1.46	1.50
4	G	702	PQQ	C9A-C6A	2.94	1.45	1.41
4	N	702	PQQ	C7-C7X	2.89	1.55	1.50
4	G	702	PQQ	O2B-C2X	-2.84	1.22	1.30
4	N	702	PQQ	O2B-C2X	-2.82	1.22	1.30
4	B	702	PQQ	C9-C9X	2.81	1.55	1.49
4	M	702	PQQ	C7-C7X	2.78	1.55	1.50
4	H	702	PQQ	C9-C9A	2.76	1.45	1.41
4	G	702	PQQ	C9-C9A	2.69	1.45	1.41
4	A	702	PQQ	O2B-C2X	-2.66	1.23	1.30
4	H	702	PQQ	O7B-C7X	2.66	1.38	1.30
4	A	702	PQQ	C9-C9X	2.63	1.55	1.49
4	M	702	PQQ	C9-C9X	2.54	1.55	1.49
4	N	702	PQQ	C9-C9X	2.50	1.55	1.49
4	M	702	PQQ	O7B-C7X	2.50	1.37	1.30
4	G	702	PQQ	C7-C7X	2.38	1.54	1.50
4	A	702	PQQ	O7B-C7X	2.32	1.37	1.30
4	D	702	PQQ	O9A-C9X	2.24	1.29	1.22
4	M	702	PQQ	O2B-C2X	-2.22	1.24	1.30
4	C	702	PQQ	C9-C9X	2.07	1.54	1.49
4	C	702	PQQ	C1A-N1	-2.06	1.34	1.37
4	B	702	PQQ	C9A-C6A	2.04	1.44	1.41
4	D	702	PQQ	O7B-C7X	2.02	1.36	1.30
4	D	702	PQQ	C9A-C6A	2.02	1.44	1.41
4	B	702	PQQ	O7B-C7X	2.01	1.36	1.30
4	M	702	PQQ	C2-C2X	2.01	1.53	1.48
4	C	702	PQQ	C9A-C6A	2.00	1.44	1.41
4	D	702	PQQ	C9-C9X	2.00	1.53	1.49

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	702	PQQ	O7A-C7X-C7	-10.39	100.39	121.30
4	D	702	PQQ	O7A-C7X-C7	-7.43	106.36	121.30
4	G	702	PQQ	O7B-C7X-O7A	-7.35	107.55	123.35
4	A	702	PQQ	O7B-C7X-O7A	-7.10	108.09	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	PQQ	O7A-C7X-C7	-7.00	107.22	121.30
4	H	702	PQQ	O7A-C7X-C7	-6.86	107.51	121.30
4	N	702	PQQ	C6A-N6-C7	6.77	126.90	118.01
4	N	702	PQQ	O2B-C2X-C2	6.76	128.84	114.27
4	H	702	PQQ	O2B-C2X-C2	6.57	128.43	114.27
4	D	702	PQQ	C3A-C4-C5	6.24	124.09	117.03
4	N	702	PQQ	O7B-C7X-O7A	-6.19	110.05	123.35
4	G	702	PQQ	C3A-C4-C5	6.05	123.88	117.03
4	M	702	PQQ	C6A-N6-C7	5.98	125.87	118.01
4	D	702	PQQ	C6A-N6-C7	5.94	125.82	118.01
4	B	702	PQQ	O9A-C9X-C9	-5.94	107.78	121.97
4	D	702	PQQ	O7B-C7X-O7A	-5.89	110.69	123.35
4	N	702	PQQ	O7A-C7X-C7	-5.85	109.54	121.30
4	C	702	PQQ	O7A-C7X-C7	-5.83	109.56	121.30
4	H	702	PQQ	O7B-C7X-O7A	-5.71	111.08	123.35
4	G	702	PQQ	O7A-C7X-C7	-5.70	109.82	121.30
4	A	702	PQQ	C6A-N6-C7	5.70	125.50	118.01
4	A	702	PQQ	O7A-C7X-C7	-5.47	110.29	121.30
4	N	702	PQQ	O9A-C9X-C9	-5.43	109.00	121.97
4	H	702	PQQ	C3-C2-C2X	-5.39	120.11	132.53
4	M	702	PQQ	O7B-C7X-O7A	-5.36	111.82	123.35
4	H	702	PQQ	C6A-N6-C7	5.34	125.02	118.01
4	B	702	PQQ	O2B-C2X-C2	5.23	125.55	114.27
4	N	702	PQQ	C9-C8-C7	-4.97	115.85	119.93
4	H	702	PQQ	C3A-C4-C5	4.94	122.62	117.03
4	B	702	PQQ	C6A-N6-C7	4.91	124.46	118.01
4	H	702	PQQ	O2A-C2X-C2	-4.88	111.10	121.01
4	B	702	PQQ	C3A-C4-C5	4.83	122.50	117.03
4	C	702	PQQ	C9A-C6A-C5	4.78	126.03	121.59
4	N	702	PQQ	C3A-C4-C5	4.77	122.44	117.03
4	A	702	PQQ	C3A-C4-C5	4.73	122.39	117.03
4	G	702	PQQ	C6A-N6-C7	4.65	124.12	118.01
4	H	702	PQQ	O9A-C9X-C9	-4.59	111.02	121.97
4	G	702	PQQ	C3-C2-C2X	-4.44	122.29	132.53
4	B	702	PQQ	O2A-C2X-C2	-4.38	112.12	121.01
4	C	702	PQQ	C6A-N6-C7	4.34	123.71	118.01
4	G	702	PQQ	C9-C8-C7	-4.28	116.42	119.93
4	D	702	PQQ	C9-C8-C7	-4.22	116.47	119.93
4	C	702	PQQ	O2B-C2X-C2	4.10	123.12	114.27
4	B	702	PQQ	O7B-C7X-O7A	-4.09	114.56	123.35
4	D	702	PQQ	C1A-C3A-C4	-4.03	118.94	122.33
4	N	702	PQQ	O5-C5-C6A	3.99	126.31	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	702	PQQ	O2A-C2X-C2	-3.96	112.97	121.01
4	A	702	PQQ	C3A-C3-C2	-3.91	103.91	107.94
4	D	702	PQQ	C3A-C3-C2	-3.91	103.92	107.94
4	C	702	PQQ	O7B-C7X-O7A	-3.90	114.96	123.35
4	B	702	PQQ	C3-C2-C2X	-3.87	123.60	132.53
4	M	702	PQQ	C3A-C4-C5	3.86	121.40	117.03
4	C	702	PQQ	C3A-C4-C5	3.83	121.37	117.03
4	N	702	PQQ	C3A-C3-C2	-3.74	104.09	107.94
4	H	702	PQQ	O9B-C9X-C9	3.73	125.89	115.28
4	G	702	PQQ	O4-C4-C5	-3.71	113.80	118.37
4	G	702	PQQ	O5-C5-C6A	3.68	125.97	121.76
4	B	702	PQQ	C3A-C3-C2	-3.67	104.16	107.94
4	D	702	PQQ	O2B-C2X-O2A	-3.64	115.22	123.90
4	B	702	PQQ	O9B-C9X-C9	3.58	125.45	115.28
4	N	702	PQQ	C9A-C6A-N6	-3.57	118.41	123.58
4	D	702	PQQ	C9A-C6A-N6	-3.49	118.53	123.58
4	M	702	PQQ	C9A-C6A-C5	3.46	124.80	121.59
4	H	702	PQQ	C2X-C2-N1	3.37	129.17	120.52
4	D	702	PQQ	O4-C4-C3A	-3.33	113.78	121.92
4	A	702	PQQ	C3-C2-C2X	-3.32	124.87	132.53
4	M	702	PQQ	O2A-C2X-C2	3.27	127.66	121.01
4	C	702	PQQ	C9-C8-C7	-3.14	117.35	119.93
4	D	702	PQQ	O2B-C2X-C2	3.11	120.97	114.27
4	M	702	PQQ	C9A-C6A-N6	-3.11	119.08	123.58
4	H	702	PQQ	C9A-C6A-C5	3.10	124.47	121.59
4	C	702	PQQ	O4-C4-C5	-3.05	114.62	118.37
4	D	702	PQQ	O5-C5-C6A	3.00	125.18	121.76
4	N	702	PQQ	C9A-C6A-C5	2.97	124.35	121.59
4	D	702	PQQ	C9A-C9-C9X	2.97	128.00	121.49
4	N	702	PQQ	O4-C4-C5	-2.95	114.73	118.37
4	A	702	PQQ	C1A-C3A-C4	-2.95	119.85	122.33
4	M	702	PQQ	C9A-C9-C9X	2.91	127.88	121.49
4	G	702	PQQ	C9A-C6A-N6	-2.89	119.39	123.58
4	C	702	PQQ	C9A-C9-C9X	2.88	127.82	121.49
4	B	702	PQQ	C9A-C6A-C5	2.87	124.26	121.59
4	G	702	PQQ	O2A-C2X-C2	2.86	126.81	121.01
4	N	702	PQQ	C3-C2-C2X	-2.81	126.05	132.53
4	G	702	PQQ	C2X-C2-N1	2.80	127.71	120.52
4	G	702	PQQ	O7B-C7X-C7	-2.78	108.11	114.71
4	G	702	PQQ	C9A-C6A-C5	2.77	124.17	121.59
4	N	702	PQQ	C8-C7-C7X	2.75	125.69	119.61
4	C	702	PQQ	O7B-C7X-C7	-2.71	108.28	114.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	702	PQQ	O9B-C9X-C9	2.68	122.91	115.28
4	A	702	PQQ	C9-C8-C7	-2.68	117.73	119.93
4	D	702	PQQ	C1A-N1-C2	2.61	114.43	110.20
4	H	702	PQQ	O5-C5-C6A	2.55	124.67	121.76
4	M	702	PQQ	C3A-C3-C2	-2.55	105.32	107.94
4	C	702	PQQ	C3-C2-C2X	-2.54	126.67	132.53
4	N	702	PQQ	O2B-C2X-O2A	-2.53	117.88	123.90
4	D	702	PQQ	C3A-C1A-N1	-2.51	103.93	107.23
4	H	702	PQQ	C9A-C9-C9X	2.50	126.99	121.49
4	C	702	PQQ	C9A-C6A-N6	-2.48	119.98	123.58
4	B	702	PQQ	O4-C4-C5	-2.47	115.32	118.37
4	G	702	PQQ	C3A-C3-C2	-2.43	105.43	107.94
4	M	702	PQQ	C3-C2-C2X	-2.43	126.92	132.53
4	D	702	PQQ	O9B-C9X-C9	-2.43	108.38	115.28
4	H	702	PQQ	C8-C7-C7X	2.37	124.85	119.61
4	M	702	PQQ	O2B-C2X-O2A	-2.36	118.27	123.90
4	D	702	PQQ	C8-C9-C9X	-2.36	111.26	117.89
4	M	702	PQQ	C9-C8-C7	-2.36	118.00	119.93
4	C	702	PQQ	C8-C7-C7X	2.34	124.79	119.61
4	B	702	PQQ	C9A-C6A-N6	-2.32	120.22	123.58
4	M	702	PQQ	C8-C7-C7X	2.28	124.66	119.61
4	B	702	PQQ	C9A-C9-C9X	2.24	126.41	121.49
4	C	702	PQQ	C7X-C7-N6	-2.22	113.14	116.46
4	G	702	PQQ	O9B-C9X-C9	-2.21	108.99	115.28
4	A	702	PQQ	C9A-C9-C9X	2.21	126.34	121.49
4	H	702	PQQ	O2B-C2X-O2A	-2.21	118.65	123.90
4	N	702	PQQ	O9B-C9X-O9A	2.20	128.08	123.35
4	H	702	PQQ	C9A-C6A-N6	-2.15	120.46	123.58
4	A	702	PQQ	C9A-C6A-N6	-2.15	120.47	123.58
4	C	702	PQQ	C3A-C3-C2	-2.14	105.74	107.94
4	N	702	PQQ	C1A-C3A-C4	-2.14	120.53	122.33
4	G	702	PQQ	O2B-C2X-O2A	-2.13	118.84	123.90
4	C	702	PQQ	O2B-C2X-O2A	-2.09	118.92	123.90
4	B	702	PQQ	C8-C7-C7X	2.08	124.22	119.61
4	A	702	PQQ	O4-C4-C5	-2.07	115.82	118.37
4	H	702	PQQ	C8-C7-N6	-2.07	119.82	123.41
4	A	702	PQQ	C8-C7-N6	-2.05	119.85	123.41
4	A	702	PQQ	O2B-C2X-O2A	-2.05	119.03	123.90
4	D	702	PQQ	C8-C7-C7X	2.03	124.10	119.61
4	A	702	PQQ	O7B-C7X-C7	-2.02	109.92	114.71
4	B	702	PQQ	C3-C2-N1	2.01	111.09	107.74
4	H	702	PQQ	O7B-C7X-C7	-2.00	109.96	114.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	702	PQQ	O4-C4-C5	-2.00	115.90	118.37

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	702	PQQ	N1-C2-C2X-O2A
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	C	702	PQQ	C8-C7-C7X-O7B
4	D	702	PQQ	N1-C2-C2X-O2A
4	D	702	PQQ	N1-C2-C2X-O2B
4	D	702	PQQ	C3-C2-C2X-O2A
4	D	702	PQQ	C3-C2-C2X-O2B
4	D	702	PQQ	C8-C7-C7X-O7B
4	A	702	PQQ	N1-C2-C2X-O2A
4	A	702	PQQ	N1-C2-C2X-O2B
4	A	702	PQQ	C3-C2-C2X-O2A
4	A	702	PQQ	C3-C2-C2X-O2B
4	A	702	PQQ	N6-C7-C7X-O7B
4	A	702	PQQ	C8-C7-C7X-O7B
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	B	702	PQQ	C8-C7-C7X-O7B
4	G	702	PQQ	N1-C2-C2X-O2A
4	G	702	PQQ	N1-C2-C2X-O2B
4	G	702	PQQ	C3-C2-C2X-O2A
4	G	702	PQQ	C3-C2-C2X-O2B
4	G	702	PQQ	N6-C7-C7X-O7A
4	G	702	PQQ	C8-C7-C7X-O7A
4	H	702	PQQ	N1-C2-C2X-O2A
4	H	702	PQQ	N1-C2-C2X-O2B
4	H	702	PQQ	C3-C2-C2X-O2A
4	H	702	PQQ	C3-C2-C2X-O2B
4	H	702	PQQ	N6-C7-C7X-O7A
4	H	702	PQQ	C8-C7-C7X-O7A
4	M	702	PQQ	N1-C2-C2X-O2A
4	M	702	PQQ	N1-C2-C2X-O2B
4	M	702	PQQ	C3-C2-C2X-O2A

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Mol	Chain	Res	Type	Atoms
4	M	702	PQQ	C3-C2-C2X-O2B
4	N	702	PQQ	N1-C2-C2X-O2A
4	N	702	PQQ	N1-C2-C2X-O2B
4	N	702	PQQ	C3-C2-C2X-O2A
4	D	702	PQQ	N6-C7-C7X-O7B
4	C	702	PQQ	N6-C7-C7X-O7B
4	B	702	PQQ	N6-C7-C7X-O7B
4	M	702	PQQ	N6-C7-C7X-O7B
4	M	702	PQQ	C8-C7-C7X-O7A
4	N	702	PQQ	N6-C7-C7X-O7B
4	N	702	PQQ	C8-C7-C7X-O7A
4	M	702	PQQ	C8-C7-C7X-O7B
4	M	702	PQQ	N6-C7-C7X-O7A
4	N	702	PQQ	N6-C7-C7X-O7A
4	N	702	PQQ	C8-C7-C7X-O7B
4	N	702	PQQ	C3-C2-C2X-O2B
4	G	702	PQQ	N6-C7-C7X-O7B
4	D	702	PQQ	N6-C7-C7X-O7A
4	H	702	PQQ	N6-C7-C7X-O7B
4	H	702	PQQ	C8-C7-C7X-O7B
4	D	702	PQQ	C8-C7-C7X-O7A
4	A	702	PQQ	C8-C7-C7X-O7A
4	G	702	PQQ	C8-C7-C7X-O7B
4	A	702	PQQ	N6-C7-C7X-O7A
4	B	702	PQQ	N6-C7-C7X-O7A
4	C	702	PQQ	N6-C7-C7X-O7A

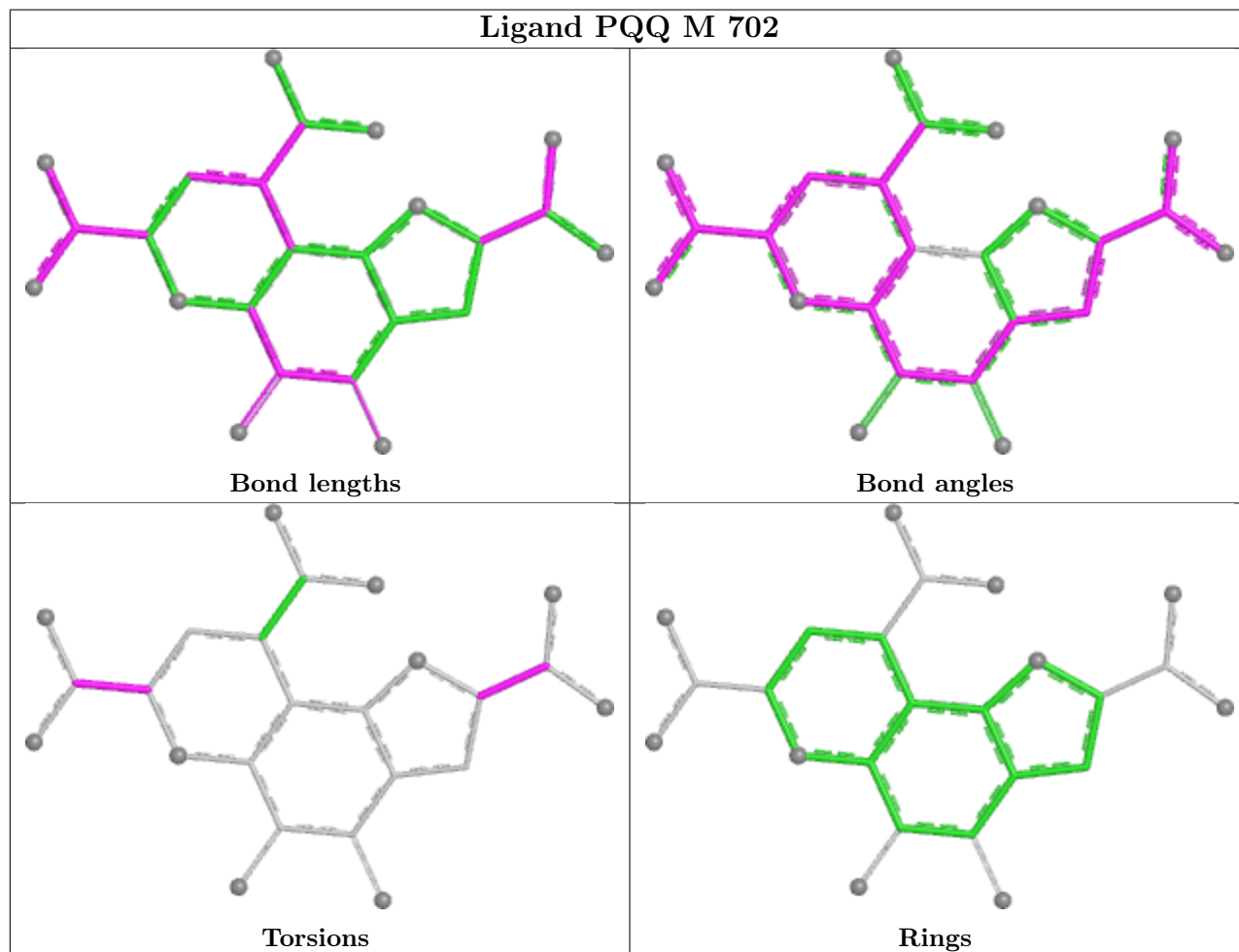
There are no ring outliers.

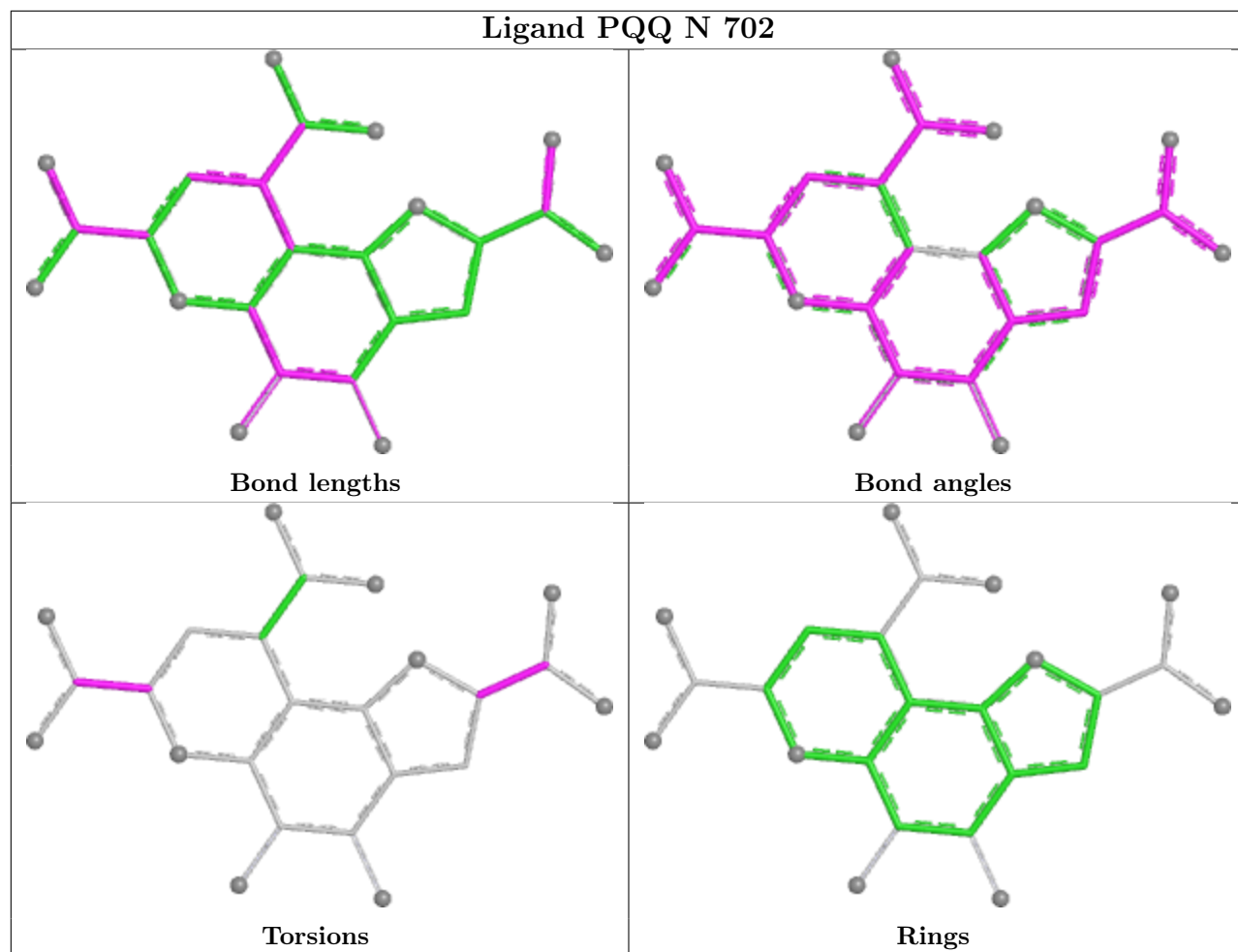
8 monomers are involved in 37 short contacts:

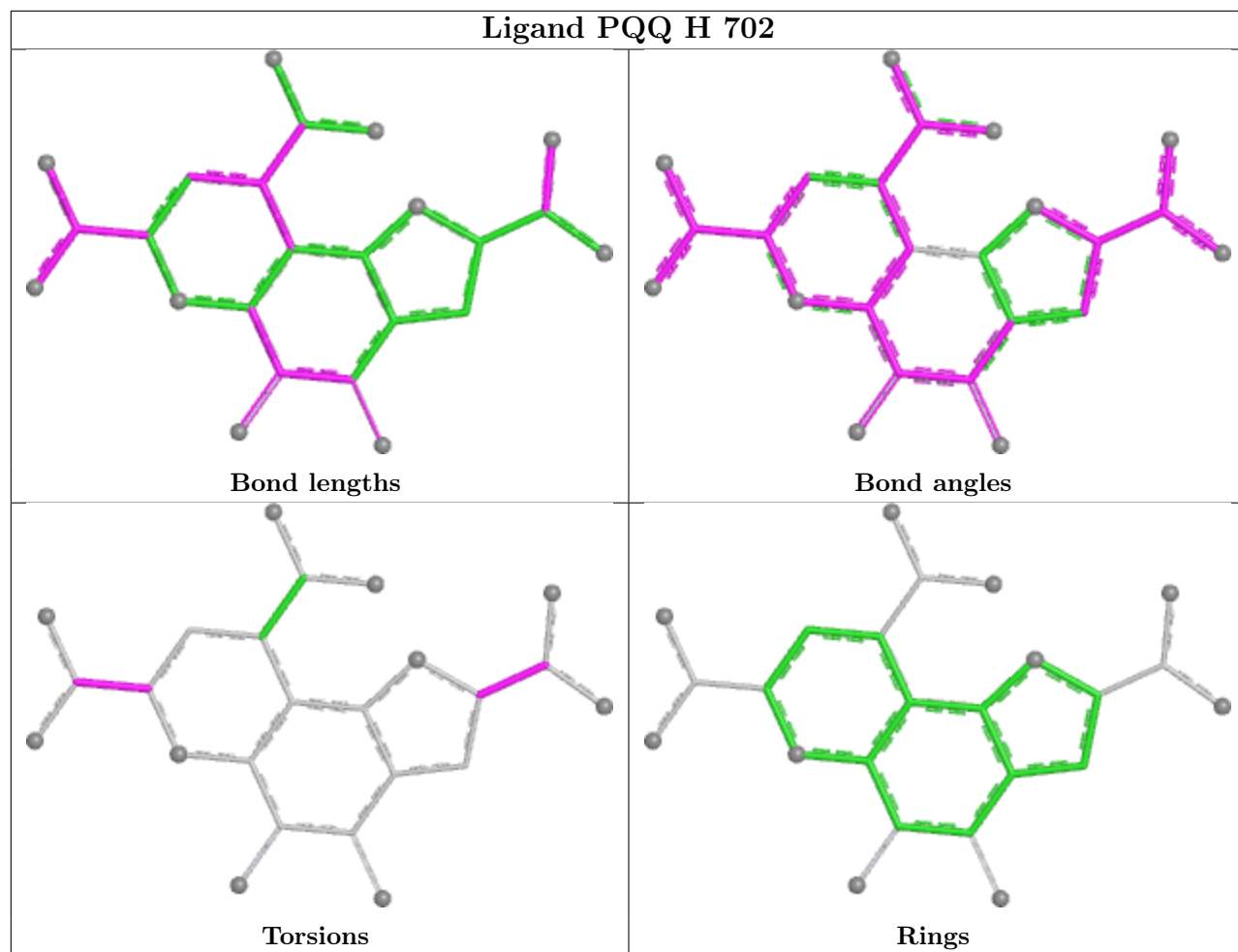
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	702	PQQ	3	0
4	N	702	PQQ	2	0
4	H	702	PQQ	4	0
4	B	702	PQQ	7	0
4	G	702	PQQ	7	0
4	A	702	PQQ	5	0
4	C	702	PQQ	4	0
4	D	702	PQQ	5	0

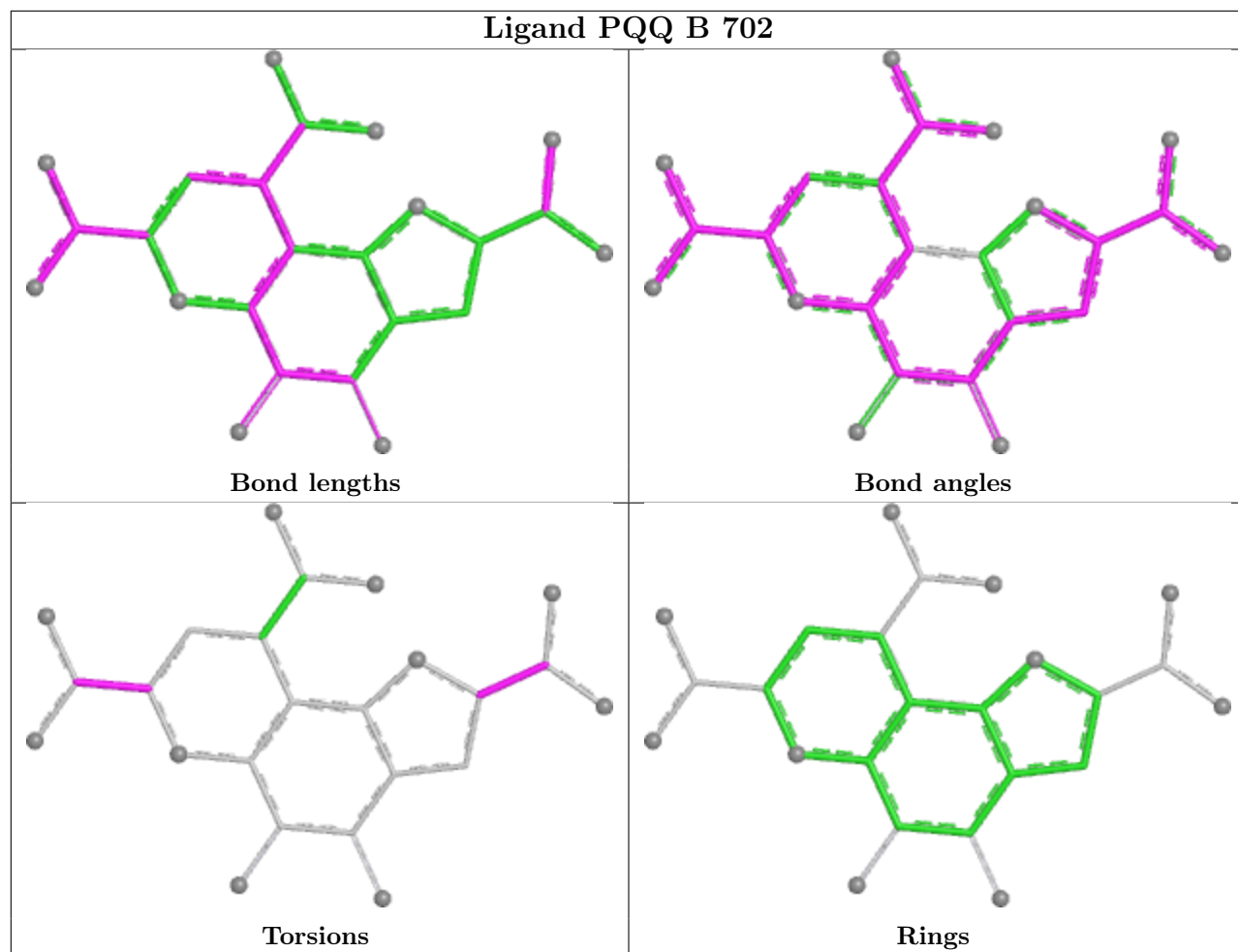
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

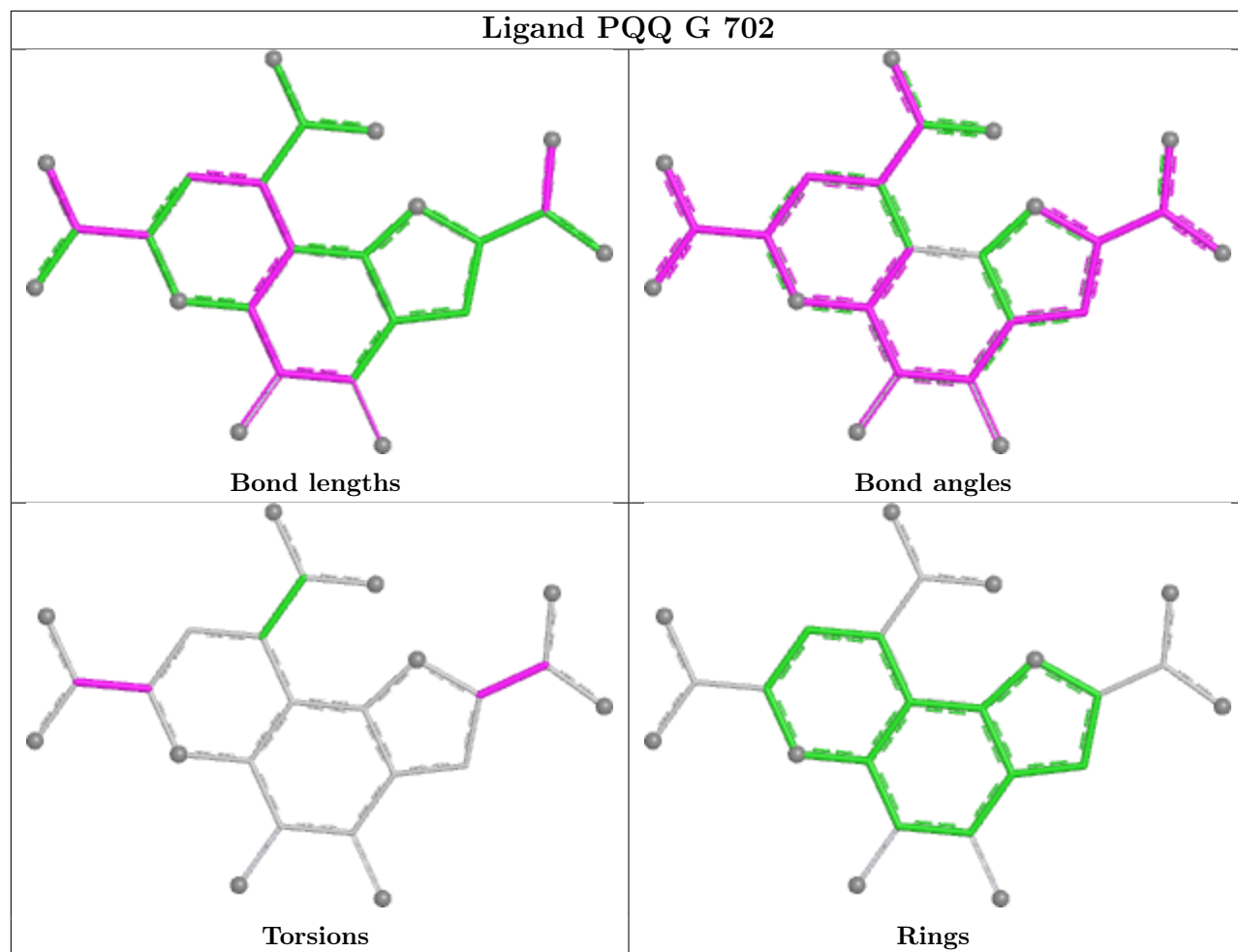
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

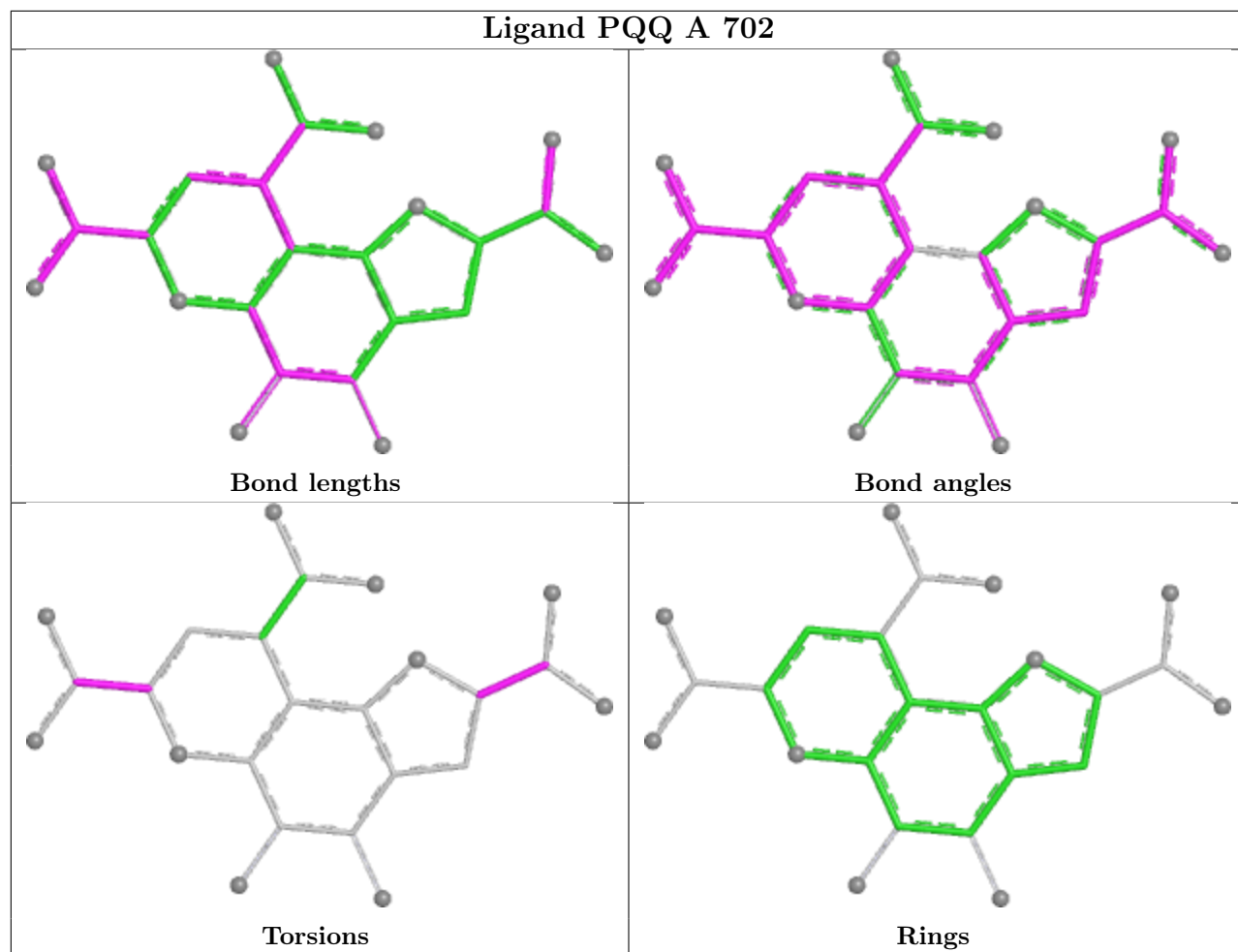


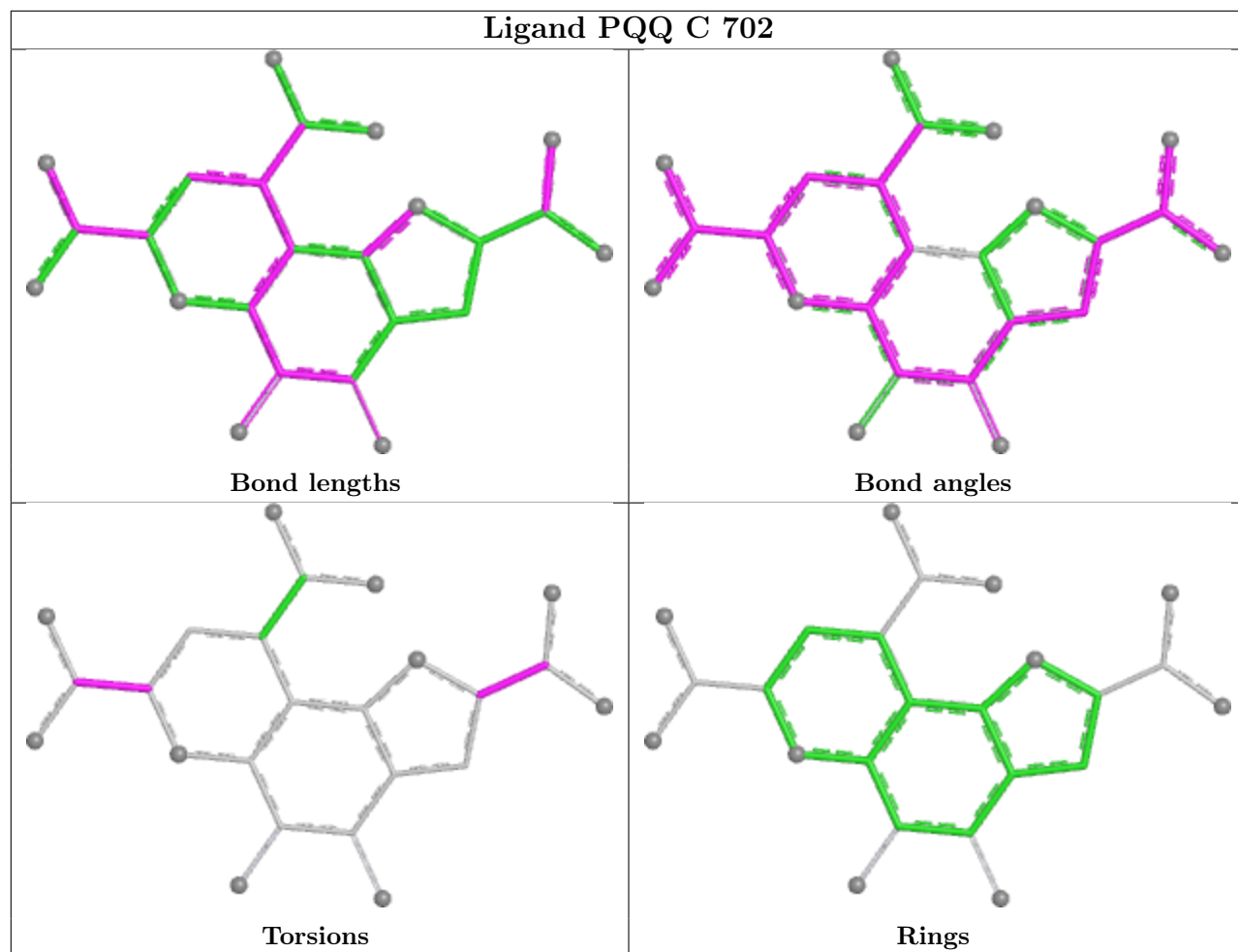


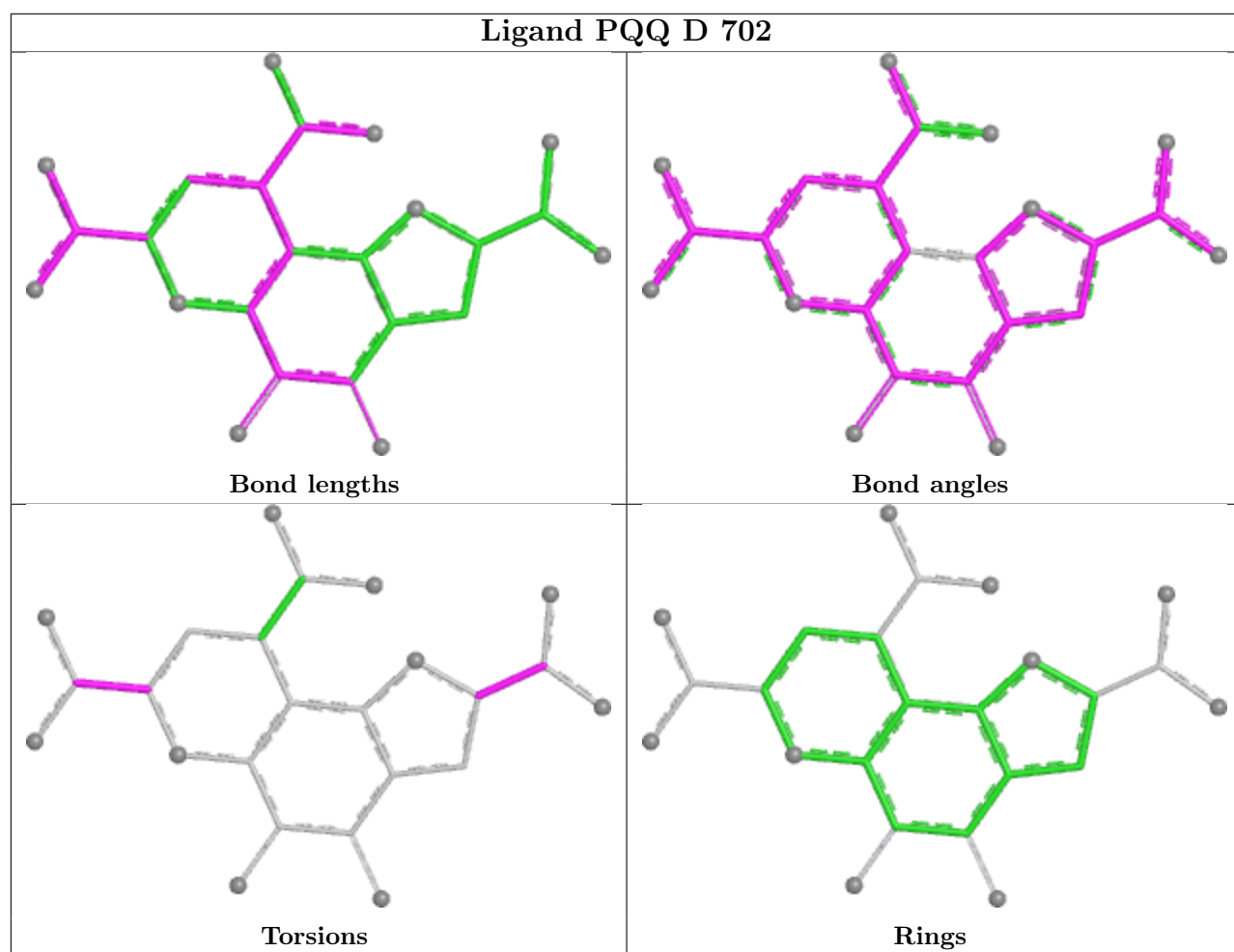












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.39	4 (0%) 84 87	13, 21, 33, 57	0
1	B	573/573 (100%)	-0.58	3 (0%) 87 90	12, 17, 30, 47	0
1	C	573/573 (100%)	-0.59	5 (0%) 81 84	11, 17, 29, 45	0
1	D	573/573 (100%)	-0.53	4 (0%) 84 87	12, 18, 31, 50	0
1	G	573/573 (100%)	-0.49	4 (0%) 84 87	12, 18, 31, 48	0
1	H	573/573 (100%)	-0.31	3 (0%) 87 90	13, 23, 36, 53	0
1	M	573/573 (100%)	-0.29	3 (0%) 87 90	13, 22, 37, 55	0
1	N	573/573 (100%)	-0.55	3 (0%) 87 90	12, 17, 30, 47	0
2	E	71/72 (98%)	0.19	1 (1%) 73 77	20, 31, 46, 52	0
2	F	71/72 (98%)	0.27	6 (8%) 16 17	15, 24, 58, 87	0
2	I	71/72 (98%)	0.36	5 (7%) 22 24	17, 26, 65, 131	0
2	J	71/72 (98%)	0.61	1 (1%) 73 77	24, 36, 52, 67	0
2	K	71/72 (98%)	-0.01	2 (2%) 55 58	15, 24, 38, 52	0
2	L	71/72 (98%)	0.04	1 (1%) 73 77	18, 26, 44, 61	0
2	O	71/72 (98%)	0.61	3 (4%) 40 44	26, 36, 53, 68	0
2	P	71/72 (98%)	-0.04	2 (2%) 55 58	17, 22, 40, 53	0
All	All	5152/5160 (99%)	-0.38	50 (0%) 79 83	11, 20, 37, 131	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	90	VAL	8.8
2	I	93	ILE	6.8
1	H	132	CYS	4.4
2	F	93	ILE	4.4
1	D	442	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	131	CYS	4.2
2	F	28	CYS	4.1
1	A	442	CYS	4.1
1	C	442	CYS	4.0
2	F	82	LYS	3.9
1	B	442	CYS	3.9
1	N	132	CYS	3.9
1	N	442	CYS	3.9
1	B	132	CYS	3.8
2	O	28	CYS	3.8
2	I	91	GLU	3.7
1	N	131	CYS	3.6
1	M	131	CYS	3.6
1	H	131	CYS	3.5
1	M	442	CYS	3.5
1	H	442	CYS	3.5
2	J	28	CYS	3.4
2	I	89	LYS	3.4
2	E	28	CYS	3.4
1	D	132	CYS	3.3
1	D	131	CYS	3.2
2	I	92	ASP	3.2
1	G	442	CYS	3.1
1	M	132	CYS	3.0
1	A	132	CYS	3.0
2	F	90	VAL	3.0
2	K	28	CYS	2.9
1	G	131	CYS	2.9
1	G	132	CYS	2.8
1	C	132	CYS	2.5
1	D	104	TYR	2.4
2	P	28	CYS	2.4
1	A	131	CYS	2.3
1	C	233	GLU	2.3
1	C	243	LYS	2.3
2	F	91	GLU	2.2
1	G	145	GLY	2.2
2	O	46	ALA	2.2
1	C	167	LYS	2.2
2	F	84	GLY	2.1
1	A	167	LYS	2.1
2	L	81	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	K	43	ASP	2.0
2	P	43	ASP	2.0
2	O	53	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

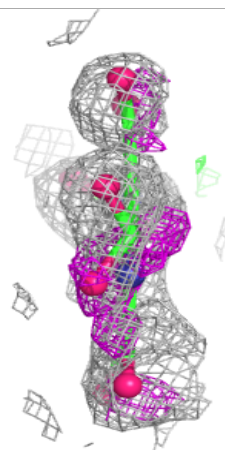
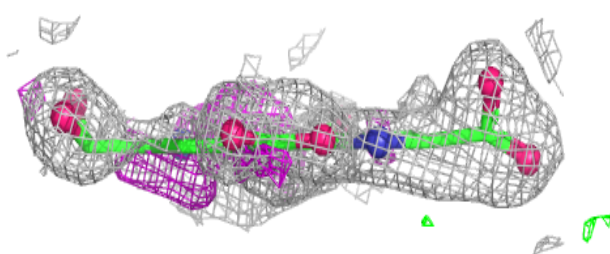
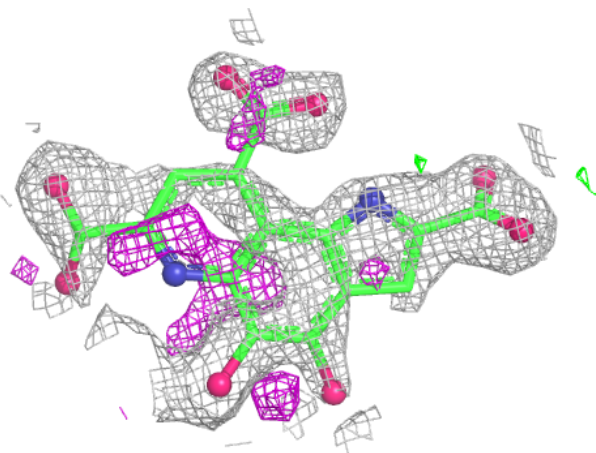
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PQQ	H	702	24/24	0.82	0.14	33,56,64,67	0
4	PQQ	M	702	24/24	0.82	0.14	30,51,56,62	0
4	PQQ	A	702	24/24	0.85	0.12	26,46,52,54	0
4	PQQ	D	702	24/24	0.86	0.12	24,39,44,55	0
4	PQQ	G	702	24/24	0.86	0.13	23,45,49,62	0
4	PQQ	N	702	24/24	0.86	0.14	23,46,52,70	0
4	PQQ	C	702	24/24	0.89	0.11	20,35,40,45	0
4	PQQ	B	702	24/24	0.89	0.10	25,41,47,49	0
3	CA	M	701	1/1	0.89	0.20	68,68,68,68	0
3	CA	H	701	1/1	0.91	0.19	63,63,63,63	0
3	CA	A	701	1/1	0.95	0.24	56,56,56,56	0
3	CA	B	701	1/1	0.95	0.24	52,52,52,52	0
3	CA	D	701	1/1	0.95	0.21	47,47,47,47	0
3	CA	C	701	1/1	0.96	0.22	44,44,44,44	0
3	CA	G	701	1/1	0.96	0.25	50,50,50,50	0
3	CA	N	701	1/1	0.97	0.21	48,48,48,48	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.

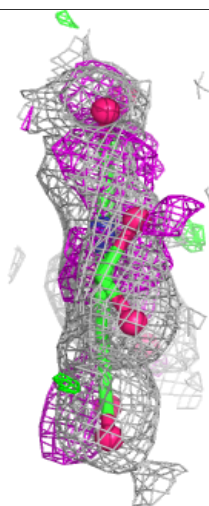
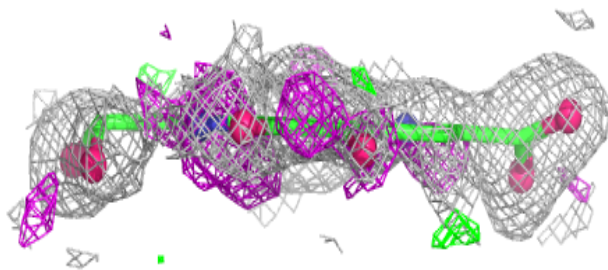
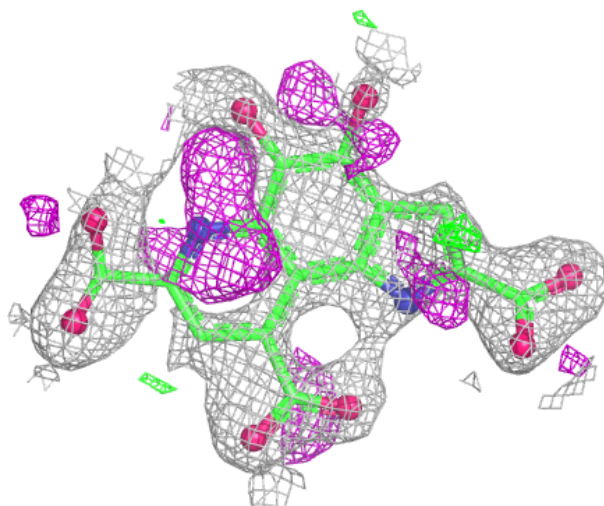
Electron density around PQQ H 702:

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



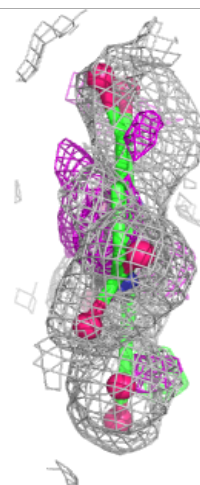
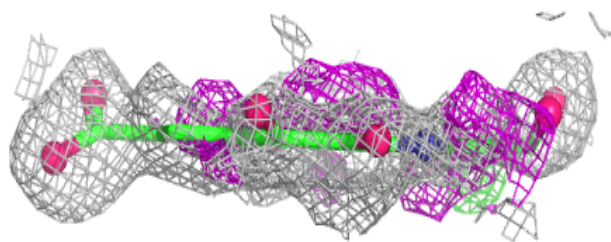
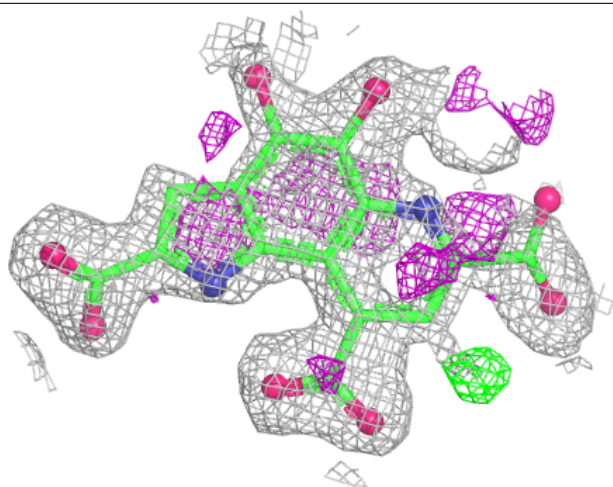
Electron density around PQQ M 702:

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



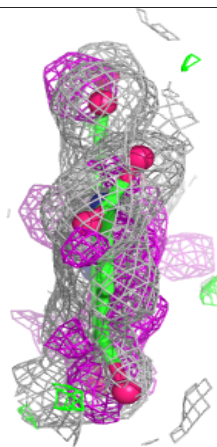
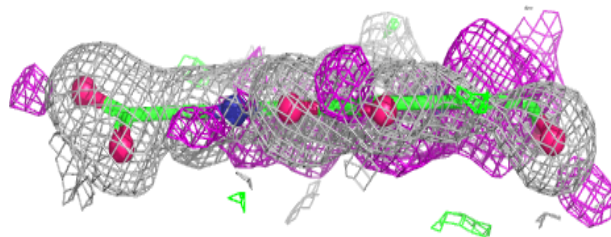
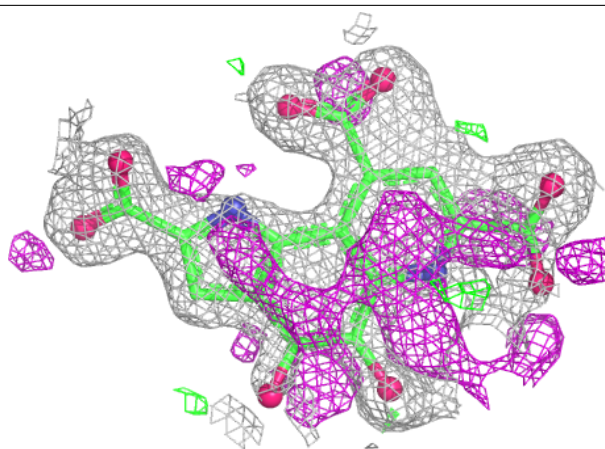
Electron density around PQQ A 702:

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



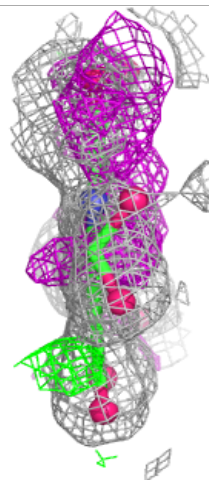
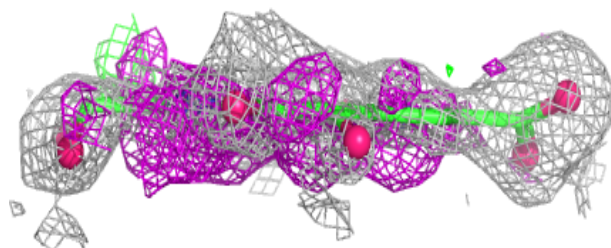
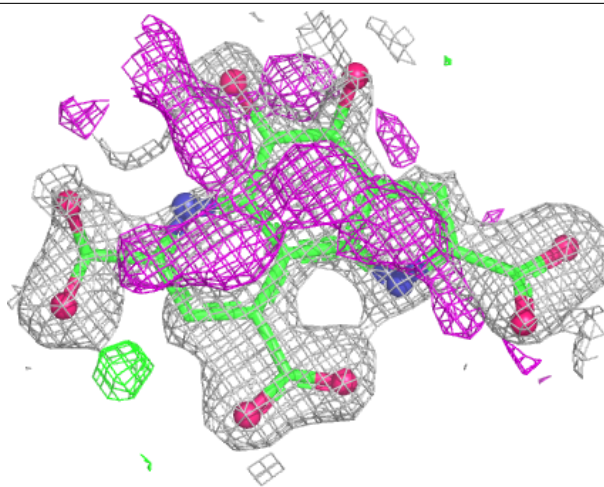
Electron density around PQQ D 702:

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



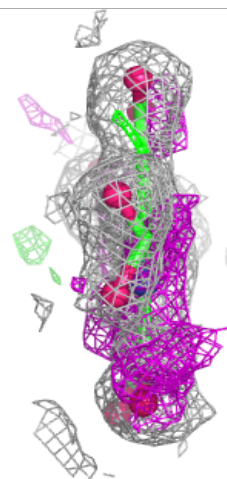
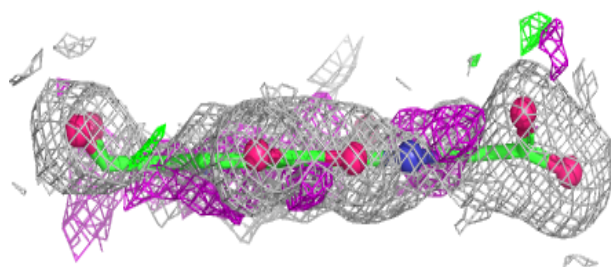
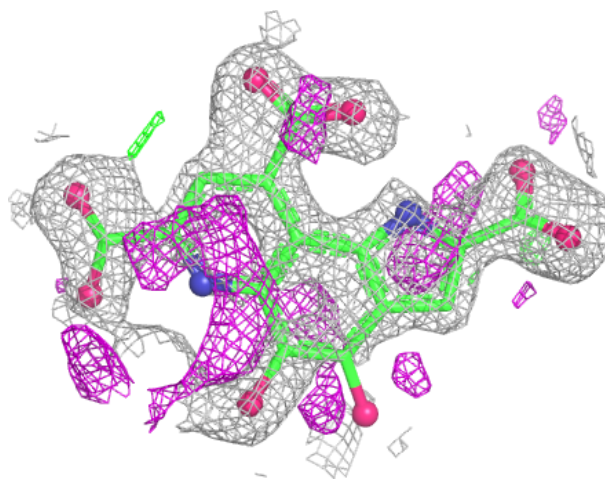
Electron density around PQQ G 702:

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



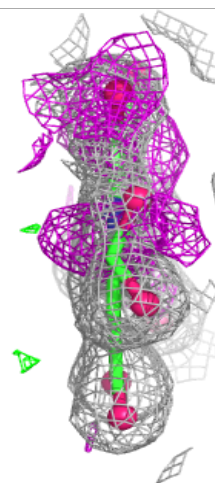
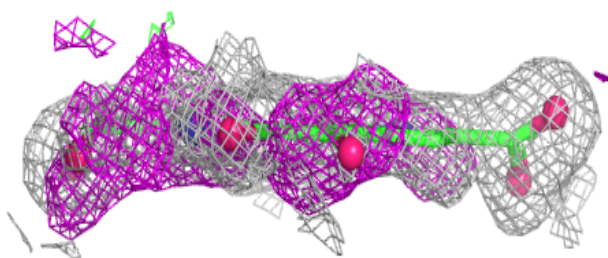
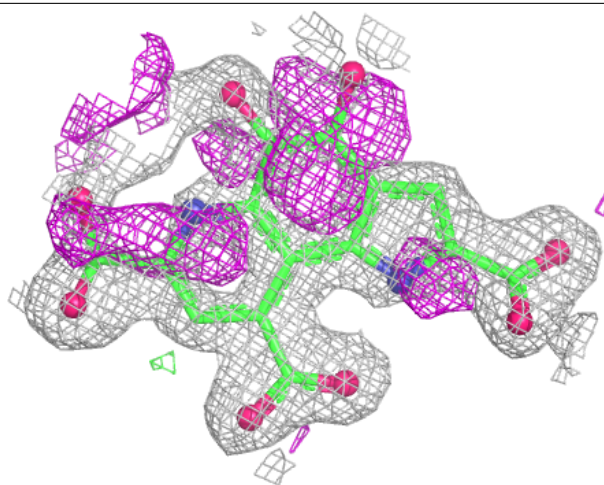
Electron density around PQQ N 702:

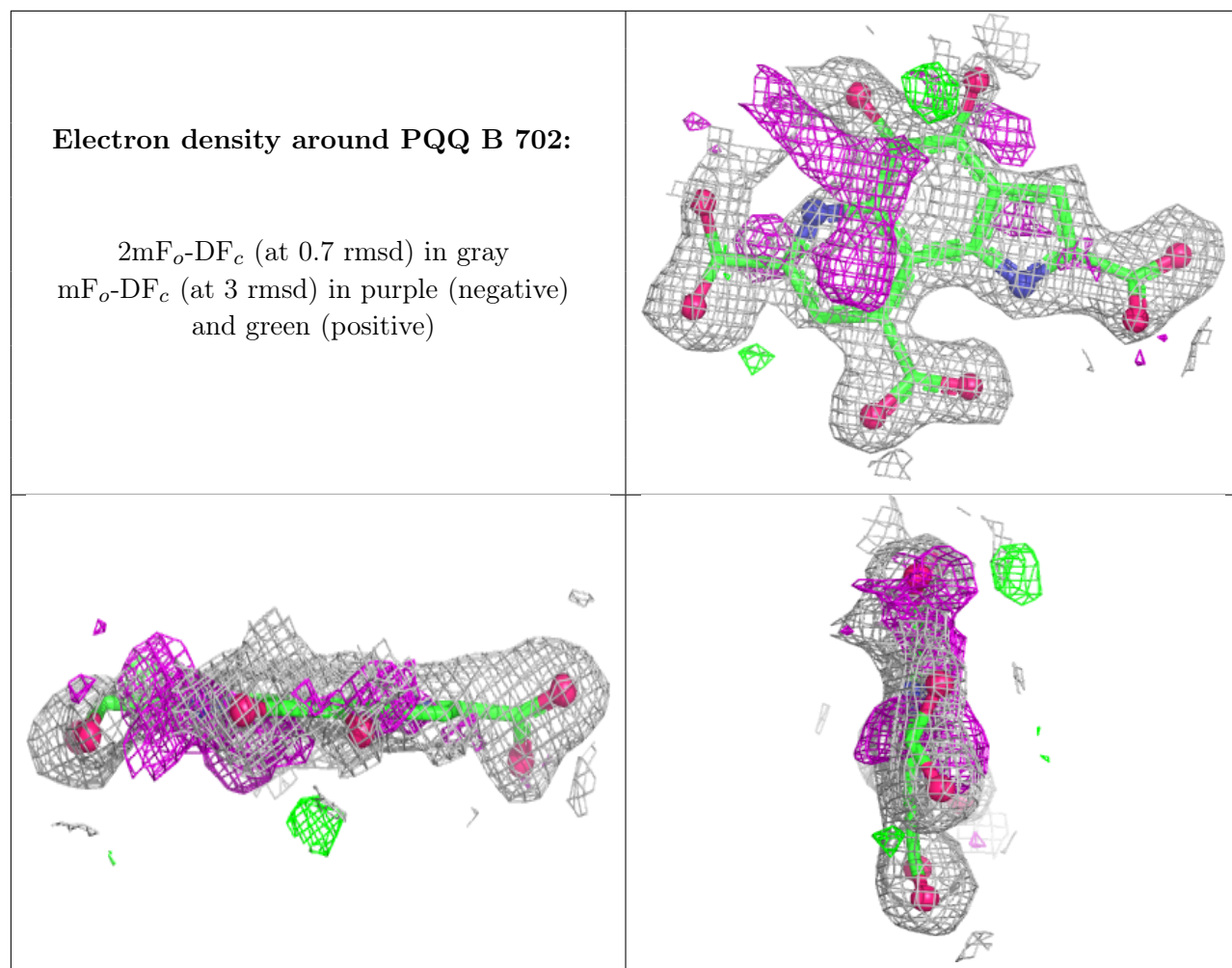
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PQQ C 702:

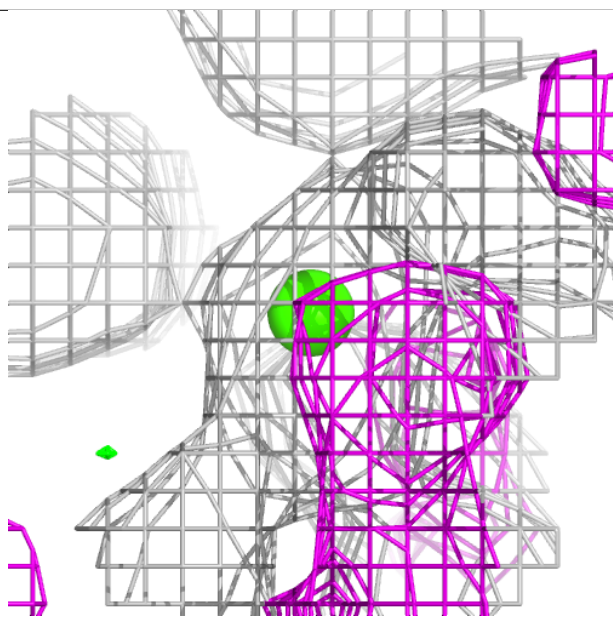
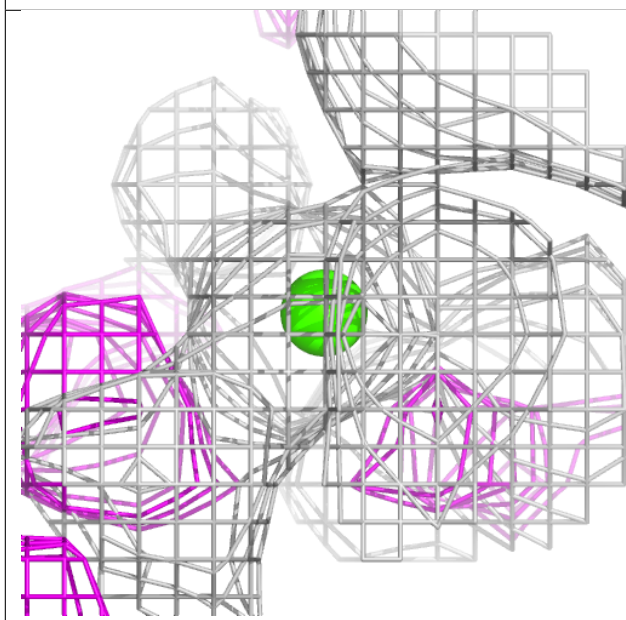
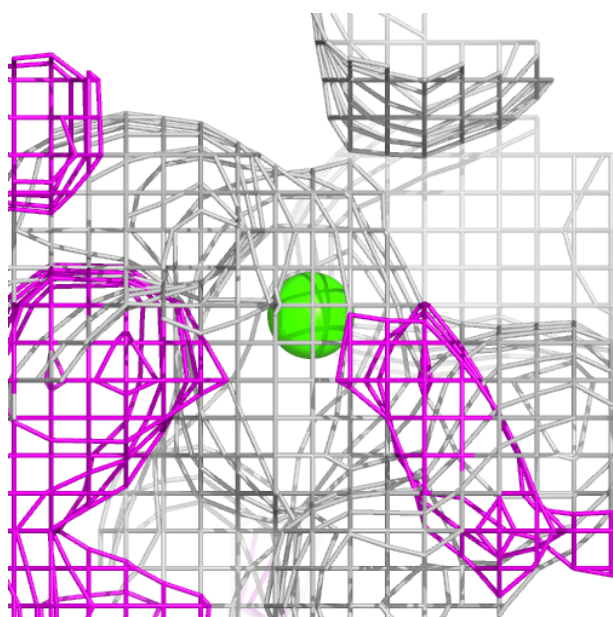
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





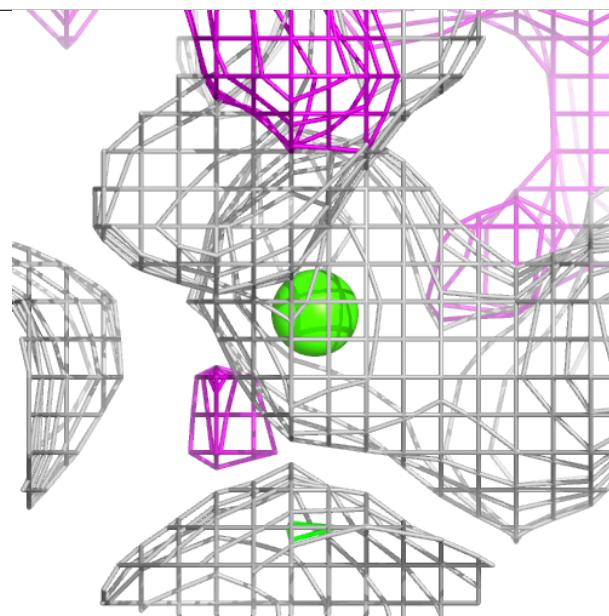
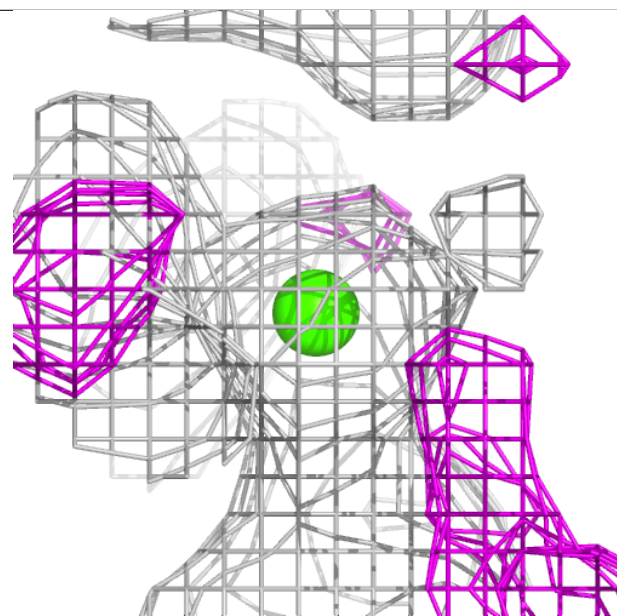
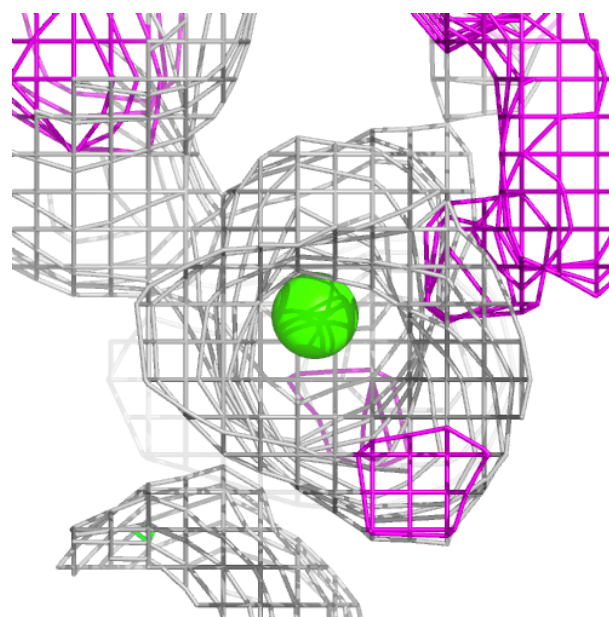
Electron density around CA M 701:

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



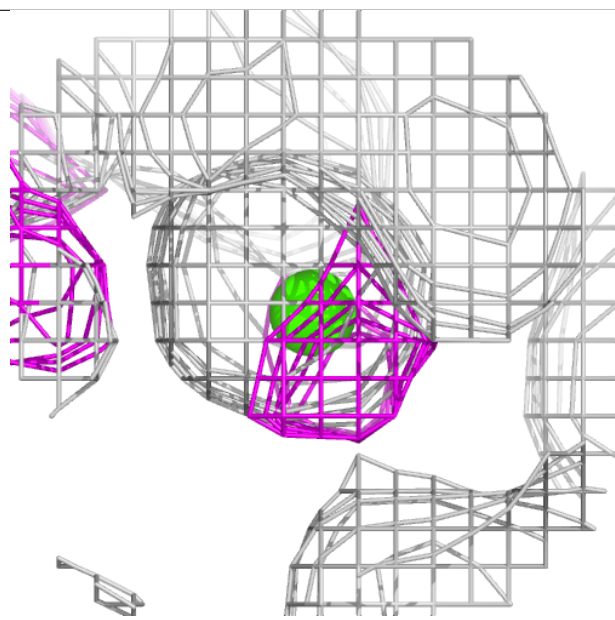
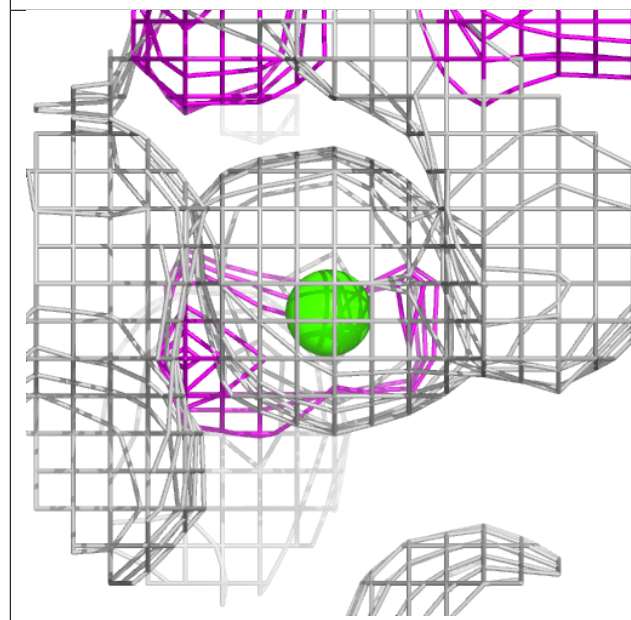
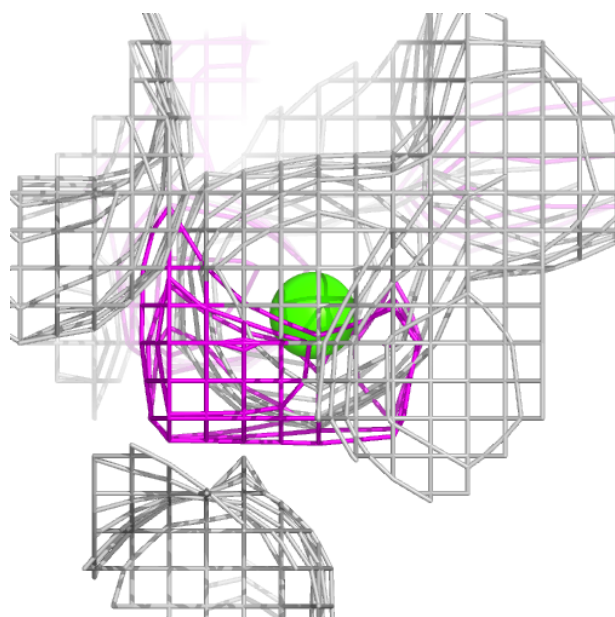
Electron density around CA H 701:

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



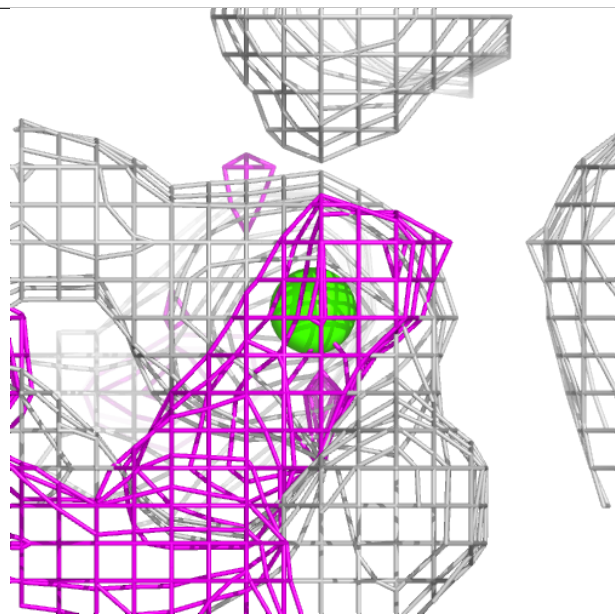
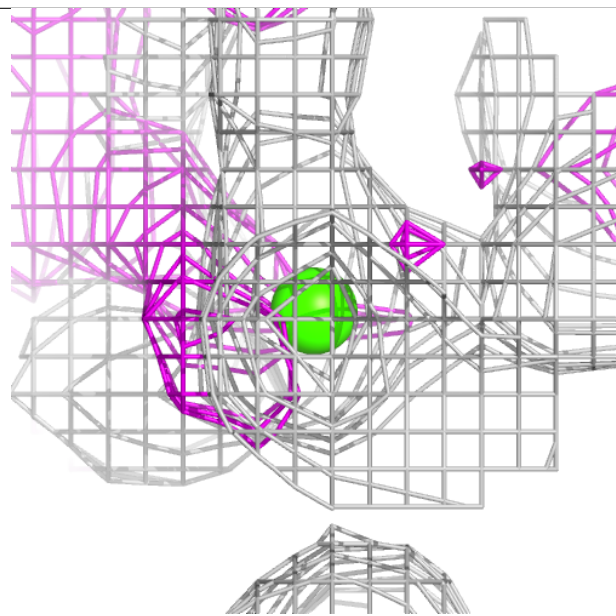
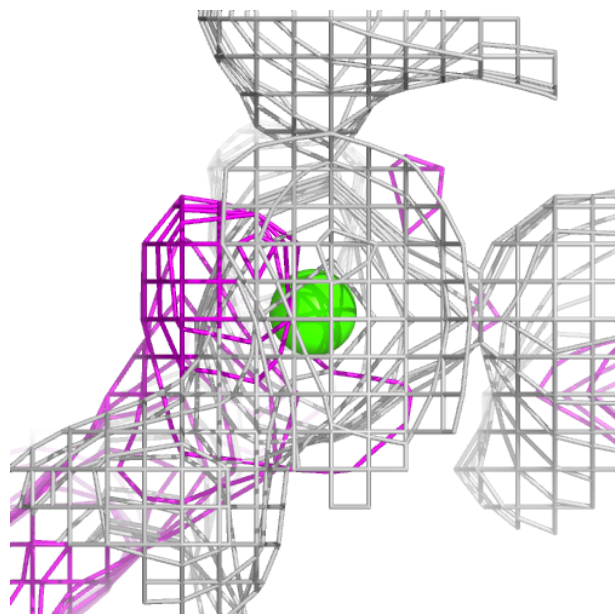
Electron density around CA A 701:

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



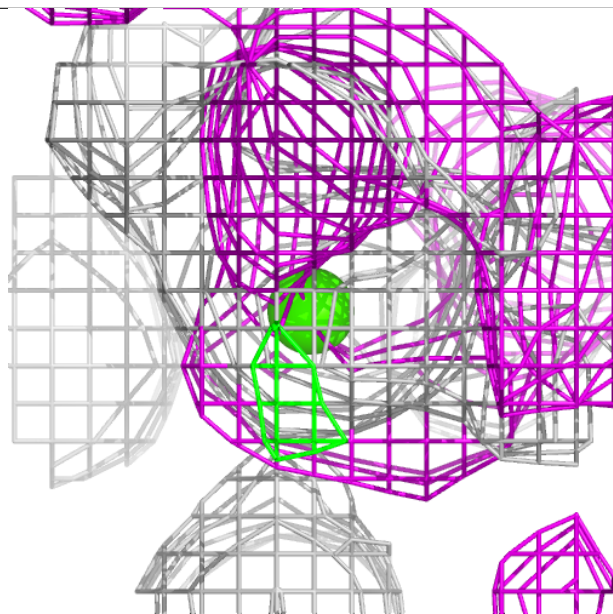
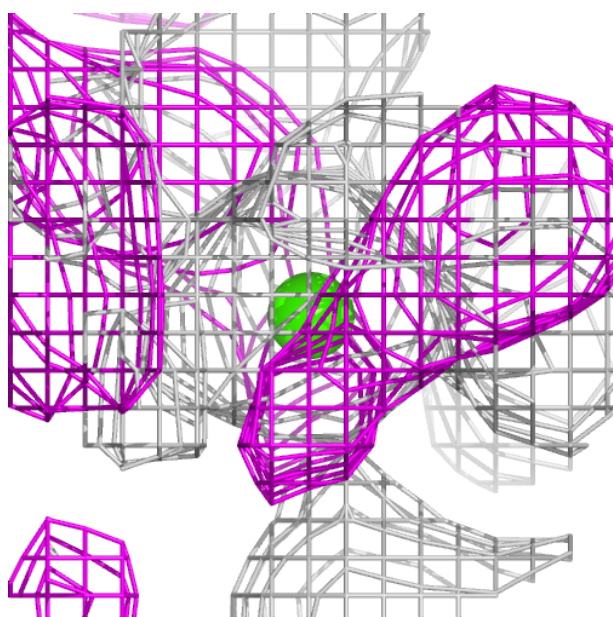
Electron density around CA B 701:

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



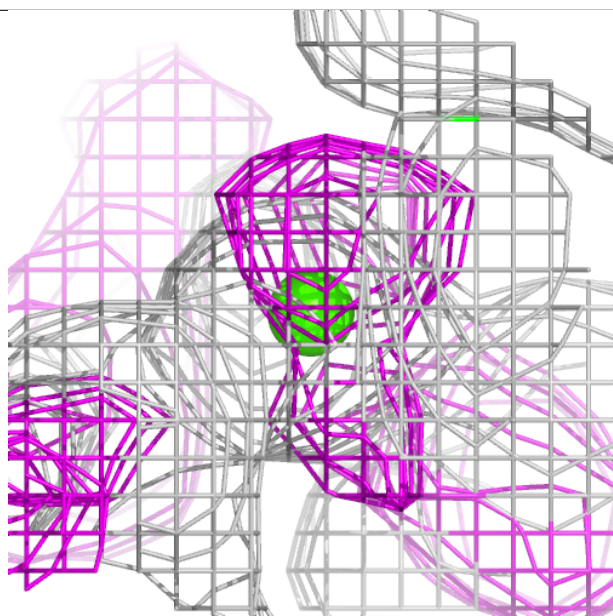
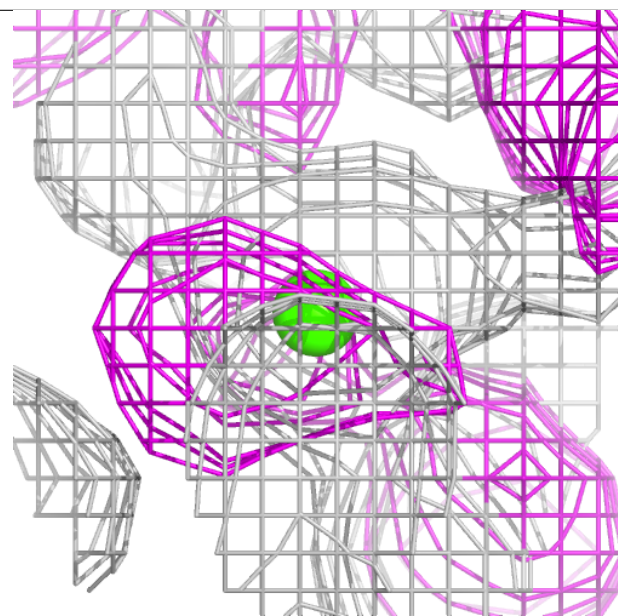
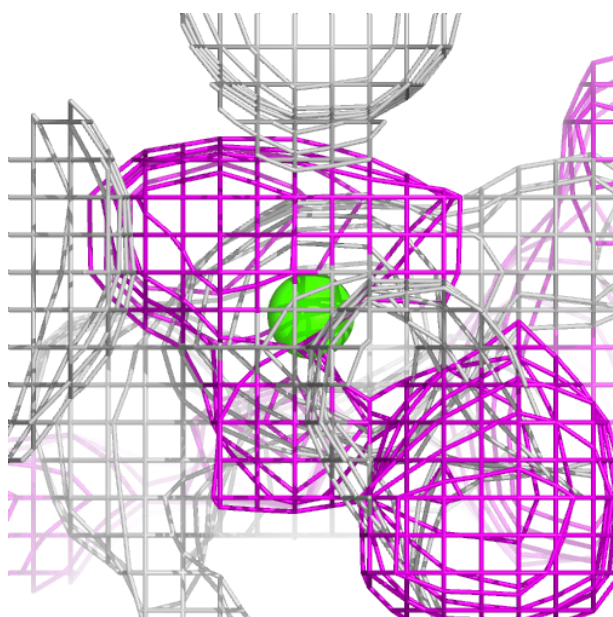
Electron density around CA D 701:

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



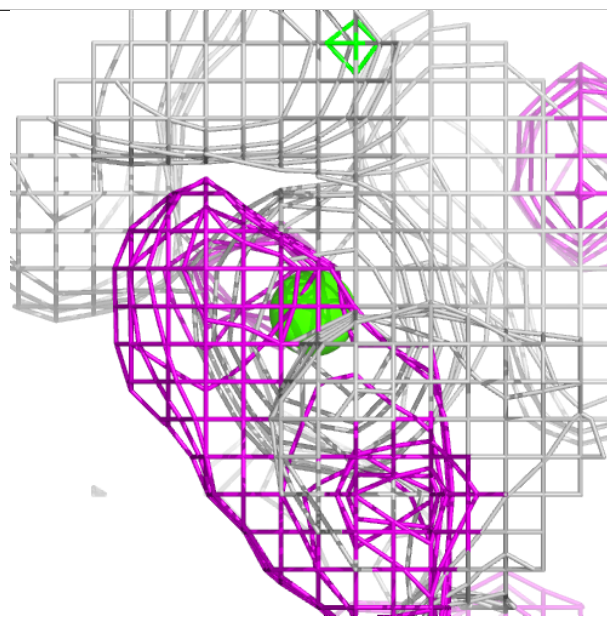
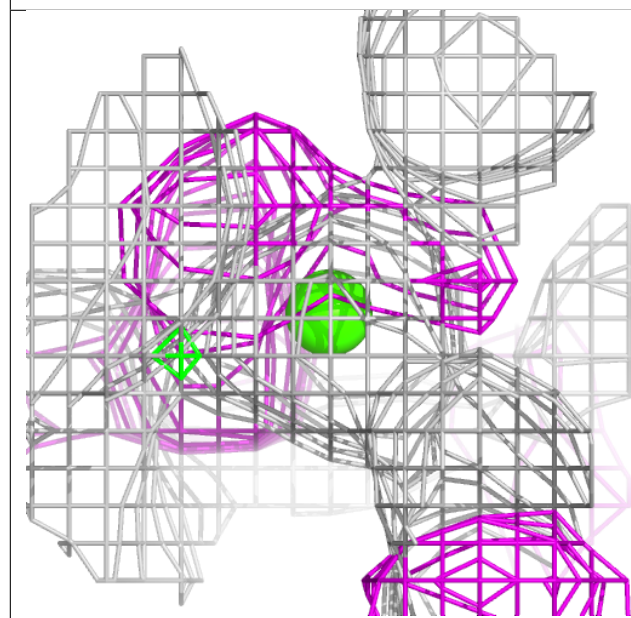
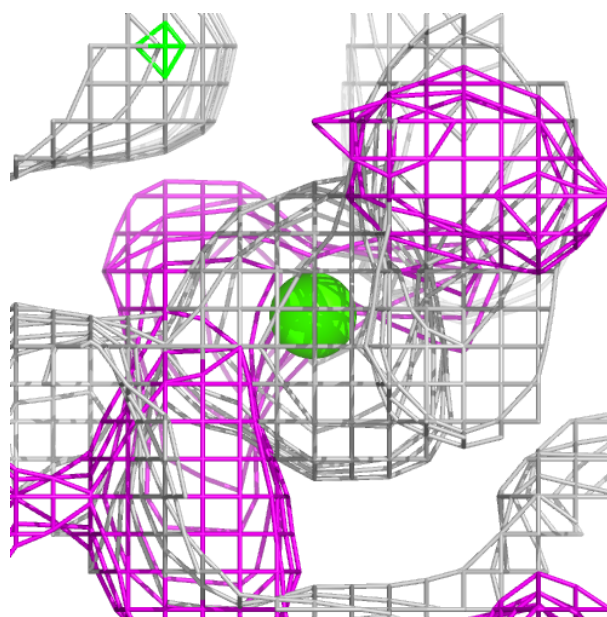
Electron density around CA C 701:

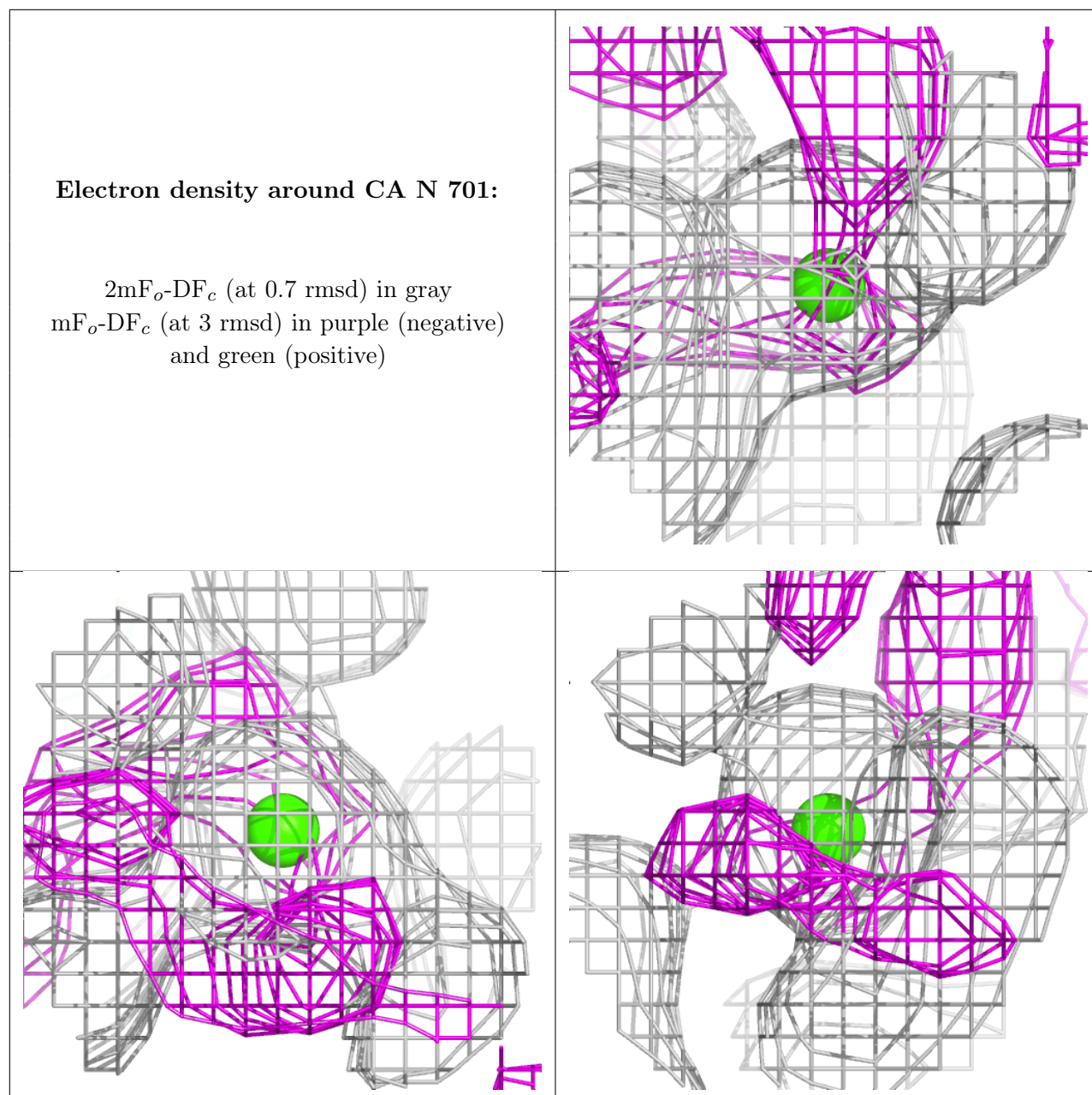
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA G 701:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.