



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2021 – 02:19 PM JST

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

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](mailto: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.

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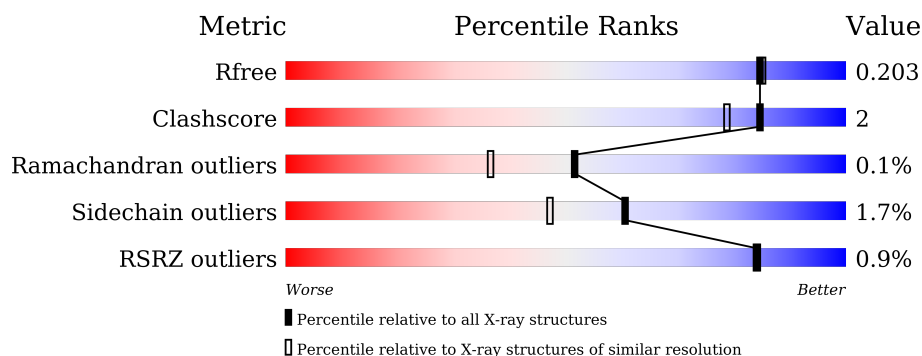
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.20  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.20

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## X-RAY DIFFRACTION

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













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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div><div></div><div></div><div></div></div> 91%9%
1	B	573	<div><div></div><div></div><div></div></div> 93%6%
1	C	573	<div><div></div><div></div><div></div></div> 94%6%
1	D	573	<div><div></div><div></div><div></div></div> 92%7%
1	G	573	<div><div></div><div></div><div></div></div> 92%8%
1	H	573	<div><div></div><div></div><div></div></div> 94%6%

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

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

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

## 2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	573	Total	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	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	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	K	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	L	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	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			

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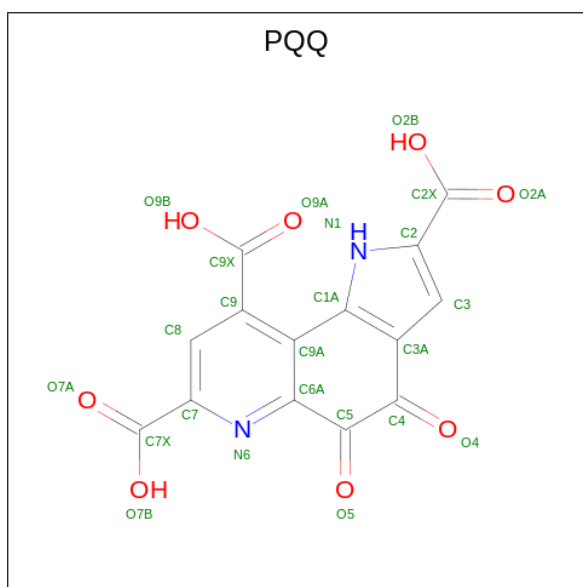
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			
2	P	71	Total	C	N	O	S	0	0	0
			568	356	100	109	3			

- Molecule 3 is CALCIUM ION (three-letter code: 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 (three-letter code: PQQ) (formula: C<sub>14</sub>H<sub>6</sub>N<sub>2</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



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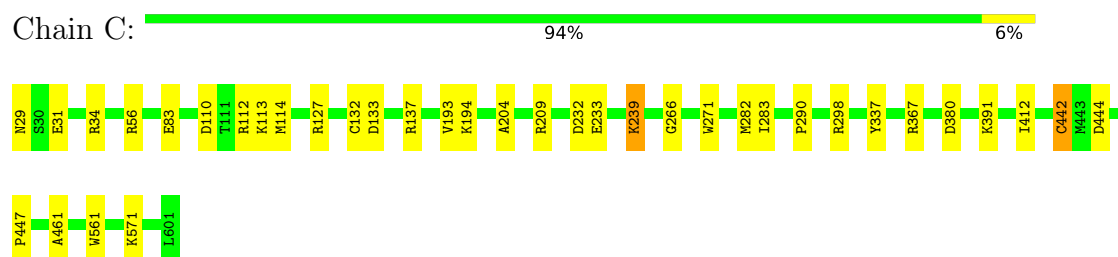
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	452	Total 452	O 452	0	0
5	E	84	Total 84	O 84	0	0
5	B	511	Total 511	O 511	0	0
5	F	81	Total 81	O 81	0	0
5	G	496	Total 496	O 496	0	0
5	I	78	Total 78	O 78	0	0
5	H	441	Total 441	O 441	0	0
5	J	60	Total 60	O 60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

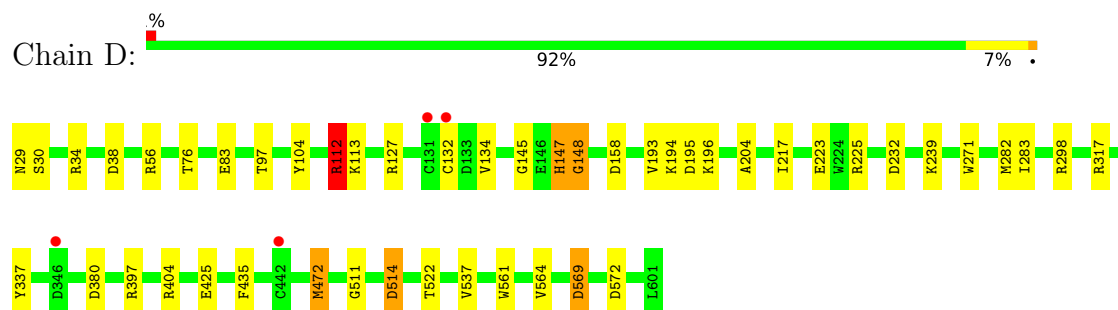
### 3 Residue-property plots [i](#)

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

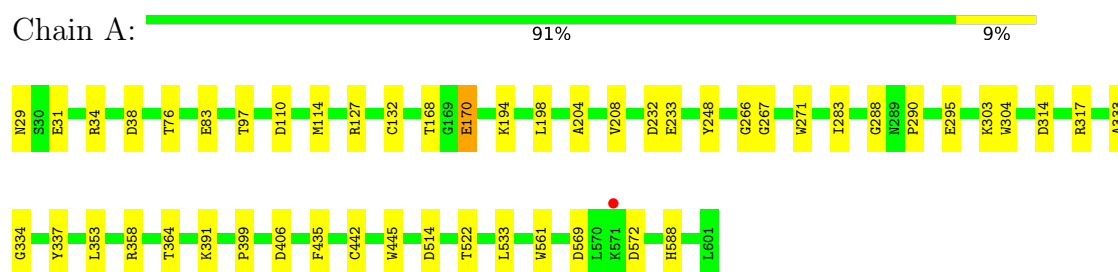
- Molecule 1: Methanol dehydrogenase protein, large subunit



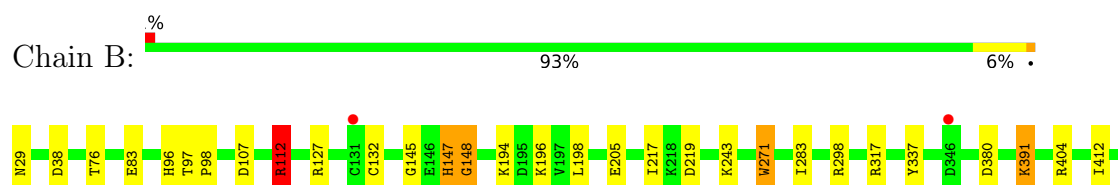
- Molecule 1: Methanol dehydrogenase protein, large subunit



- Molecule 1: Methanol dehydrogenase protein, large subunit



- Molecule 1: Methanol dehydrogenase protein, large subunit







- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain G: 92% 8% .



- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain H: 94% 6% .



- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain M: 92% 6% .



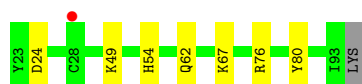
- Molecule 1: Methanol dehydrogenase protein, large subunit

Chain N: 92% 7% .

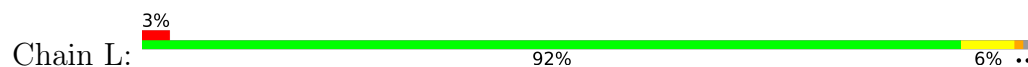


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2

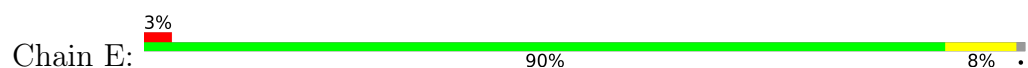
Chain K: 89% 10% .



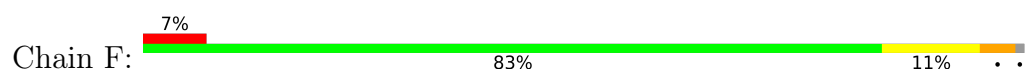
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



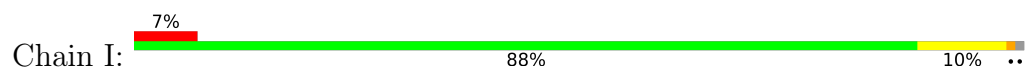
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



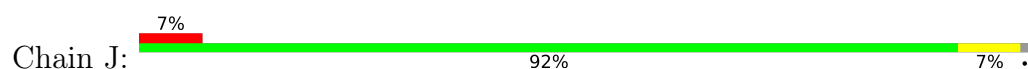
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



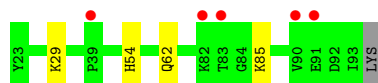
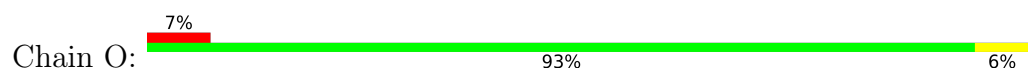
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2




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

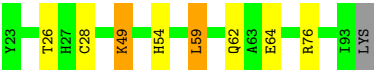


- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



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

Chain P:  88% 8% ..



## 4 Data and refinement statistics

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

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, PQQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	2
1	H	0	1
1	M	0	2
1	N	0	1
All	All	0	7

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	ARG	CD-NE	-10.34	1.28	1.46
1	N	112	ARG	CD-NE	-9.37	1.30	1.46
1	B	148	GLY	N-CA	-8.84	1.32	1.46
1	H	112	ARG	CD-NE	-8.82	1.31	1.46
1	A	170	GLU	CD-OE1	8.53	1.35	1.25
1	B	96	HIS	C-N	8.31	1.53	1.34
1	G	145	GLY	N-CA	-8.27	1.33	1.46
1	D	112	ARG	CD-NE	-7.86	1.33	1.46
1	G	148	GLY	N-CA	-7.56	1.34	1.46
1	H	148	GLY	N-CA	-7.53	1.34	1.46
2	P	62	GLN	CB-CG	-7.51	1.32	1.52
1	N	96	HIS	C-N	7.33	1.50	1.34
1	H	145	GLY	N-CA	-7.30	1.35	1.46
1	M	30	SER	CB-OG	-6.92	1.33	1.42
1	H	148	GLY	C-O	-6.79	1.12	1.23
1	H	205	GLU	CD-OE2	6.76	1.33	1.25
1	D	104	TYR	CB-CG	-6.48	1.42	1.51
1	G	148	GLY	C-O	-6.39	1.13	1.23
1	B	271	TRP	CE3-CZ3	6.36	1.49	1.38
1	D	148	GLY	N-CA	-6.36	1.36	1.46
1	M	148	GLY	N-CA	-6.22	1.36	1.46
1	G	205	GLU	CD-OE2	6.21	1.32	1.25
2	F	62	GLN	CB-CG	-6.17	1.35	1.52
1	M	96	HIS	C-N	6.06	1.48	1.34
1	D	30	SER	CB-OG	-5.99	1.34	1.42
1	B	489	GLU	CD-OE2	-5.94	1.19	1.25
1	B	148	GLY	C-O	-5.89	1.14	1.23
2	K	62	GLN	CB-CG	-5.89	1.36	1.52
1	N	205	GLU	CD-OE2	5.87	1.32	1.25
1	A	295	GLU	CG-CD	5.74	1.60	1.51
1	M	145	GLY	N-CA	-5.73	1.37	1.46
1	B	205	GLU	CD-OE2	5.69	1.31	1.25
1	A	233	GLU	CG-CD	5.61	1.60	1.51
1	G	233	GLU	CG-CD	5.55	1.60	1.51
2	P	49	LYS	CD-CE	5.55	1.65	1.51
1	N	170	GLU	CG-CD	5.51	1.60	1.51
1	G	295	GLU	CD-OE1	5.45	1.31	1.25
1	N	309	TRP	CB-CG	-5.45	1.40	1.50
1	N	233	GLU	CG-CD	5.45	1.60	1.51
1	H	96	HIS	C-N	5.42	1.46	1.34
1	G	145	GLY	C-O	-5.29	1.15	1.23
1	G	96	HIS	C-N	5.27	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	30	SER	CA-CB	5.20	1.60	1.52
1	H	427	TYR	CE1-CZ	5.16	1.45	1.38
1	M	363	TYR	CB-CG	-5.15	1.44	1.51
1	N	271	TRP	CG-CD1	5.13	1.44	1.36
1	N	595	SER	CB-OG	-5.11	1.35	1.42
1	D	569	ASP	CB-CG	-5.08	1.41	1.51
1	B	427	TYR	CG-CD2	5.08	1.45	1.39

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	ARG	NE-CZ-NH2	-27.97	106.31	120.30
1	H	112	ARG	NE-CZ-NH2	-25.44	107.58	120.30
1	H	112	ARG	NE-CZ-NH1	22.55	131.58	120.30
1	N	112	ARG	NE-CZ-NH1	20.35	130.48	120.30
1	N	112	ARG	NE-CZ-NH2	-19.91	110.35	120.30
1	B	112	ARG	NE-CZ-NH2	-19.50	110.55	120.30
1	D	112	ARG	NE-CZ-NH1	18.02	129.31	120.30
1	B	112	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	D	112	ARG	CD-NE-CZ	11.83	140.16	123.60
1	D	147	HIS	CA-C-N	11.82	139.84	116.20
1	N	572	ASP	CB-CG-OD1	11.32	128.49	118.30
1	B	147	HIS	CA-C-N	11.30	138.80	116.20
1	H	147	HIS	C-N-CA	10.90	145.20	122.30
1	H	147	HIS	CA-C-N	10.66	137.51	116.20
1	B	147	HIS	O-C-N	-10.46	105.42	123.20
1	D	147	HIS	C-N-CA	10.40	144.13	122.30
1	G	147	HIS	CA-C-N	10.33	136.87	116.20
1	G	572	ASP	CB-CG-OD1	9.82	127.14	118.30
1	D	147	HIS	O-C-N	-9.71	106.69	123.20
1	M	127	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	H	147	HIS	O-C-N	-9.47	107.10	123.20
1	M	147	HIS	CA-C-N	9.29	134.78	116.20
1	B	147	HIS	C-N-CA	9.22	141.66	122.30
1	M	147	HIS	C-N-CA	9.17	141.55	122.30
1	N	317	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	G	147	HIS	O-C-N	-8.92	108.04	123.20
1	C	444	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	B	444	ASP	CB-CG-OD1	8.77	126.19	118.30
1	M	572	ASP	CB-CG-OD2	-8.74	110.43	118.30
1	H	127	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	N	572	ASP	CB-CG-OD2	-8.61	110.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	N	367	ARG	NE-CZ-NH2	8.35	124.48	120.30
1	N	514	ASP	CB-CG-OD1	8.29	125.77	118.30
1	M	147	HIS	O-C-N	-8.23	109.20	123.20
1	D	127	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	404	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	E	76	ARG	NE-CZ-NH2	8.13	124.37	120.30
1	N	261	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	C	127	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	N	584	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	C	282	MET	CG-SD-CE	-7.94	87.50	100.20
1	D	298	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	G	147	HIS	C-N-CA	7.92	138.92	122.30
1	N	127	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	D	38	ASP	CB-CG-OD1	7.84	125.36	118.30
1	B	38	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	127	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	406	ASP	CB-CG-OD2	7.71	125.24	118.30
1	G	127	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	G	38	ASP	CB-CG-OD1	7.54	125.08	118.30
1	B	514	ASP	CB-CG-OD1	7.49	125.04	118.30
1	G	110	ASP	CB-CG-OD2	-7.48	111.56	118.30
1	B	444	ASP	CB-CG-OD2	-7.47	111.58	118.30
2	P	49	LYS	CD-CE-NZ	7.43	128.80	111.70
1	C	232	ASP	CB-CG-OD1	7.36	124.92	118.30
1	M	317	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	E	76	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	G	572	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	D	514	ASP	CB-CG-OD1	7.24	124.82	118.30
1	H	127	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	C	127	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	M	127	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	H	572	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	G	282	MET	CG-SD-CE	-7.03	88.95	100.20
1	D	397	ARG	NE-CZ-NH2	7.03	123.81	120.30
2	P	76	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	D	380	ASP	CB-CG-OD1	6.99	124.59	118.30
1	N	444	ASP	CB-CG-OD1	6.97	124.57	118.30
1	N	584	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	572	ASP	CB-CG-OD1	6.88	124.49	118.30
2	K	24	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	D	147	HIS	N-CA-C	6.85	129.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	298	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	A	38	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	472	MET	CB-CG-SD	6.79	132.78	112.40
1	D	127	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	D	158	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	127	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	G	520	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	N	110	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	232	ASP	CB-CG-OD1	6.42	124.08	118.30
1	C	367	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	C	110	ASP	CB-CG-OD1	6.37	124.03	118.30
1	G	144	ALA	CA-C-N	6.36	128.91	116.20
1	G	144	ALA	O-C-N	-6.34	112.42	123.20
1	G	38	ASP	CB-CG-OD2	-6.33	112.60	118.30
2	K	24	ASP	CB-CG-OD1	6.32	123.99	118.30
1	N	127	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	219	ASP	CB-CG-OD1	6.26	123.93	118.30
1	D	232	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	127	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	H	147	HIS	N-CA-C	6.22	127.78	111.00
1	H	572	ASP	CB-CG-OD1	6.21	123.89	118.30
2	F	28	CYS	CA-CB-SG	-6.21	102.83	114.00
1	M	282	MET	CG-SD-CE	-6.17	90.33	100.20
1	A	406	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	A	317	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	195	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	298	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	M	38	ASP	CB-CG-OD1	6.06	123.76	118.30
1	M	397	ARG	NE-CZ-NH1	-6.05	117.27	120.30
1	H	112	ARG	CD-NE-CZ	6.04	132.05	123.60
2	P	76	ARG	NE-CZ-NH2	6.01	123.31	120.30
2	K	76	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	G	110	ASP	CB-CG-OD1	5.96	123.66	118.30
1	G	453	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	N	453	ARG	CG-CD-NE	5.92	124.22	111.80
1	D	472	MET	CA-CB-CG	5.91	123.35	113.30
2	P	28	CYS	CA-CB-SG	-5.89	103.39	114.00
1	B	380	ASP	CB-CG-OD1	5.89	123.60	118.30
1	G	39	ASP	CB-CG-OD2	5.85	123.57	118.30
1	M	397	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	G	397	ARG	NE-CZ-NH1	-5.84	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	40	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	F	62	GLN	CB-CA-C	-5.82	98.77	110.40
1	G	147	HIS	N-CA-C	5.78	126.61	111.00
1	C	137	ARG	CG-CD-NE	-5.76	99.70	111.80
1	C	298	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	M	147	HIS	N-CA-C	5.74	126.50	111.00
1	A	127	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	D	158	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	N	38	ASP	CB-CG-OD1	5.70	123.43	118.30
1	G	569	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	38	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	K	62	GLN	CB-CA-C	-5.66	99.08	110.40
1	M	572	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	404	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	D	425	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	B	147	HIS	N-CA-C	5.64	126.24	111.00
2	J	28	CYS	CA-CB-SG	-5.64	103.84	114.00
1	N	232	ASP	CB-CG-OD1	5.64	123.38	118.30
1	G	144	ALA	C-N-CA	5.64	134.15	122.30
1	D	282	MET	CG-SD-CE	-5.63	91.19	100.20
2	F	59	LEU	CB-CG-CD1	5.60	120.52	111.00
1	D	104	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	D	225	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	H	314	ASP	CB-CG-OD1	5.53	123.28	118.30
2	L	28	CYS	CA-CB-SG	-5.53	104.05	114.00
1	B	317	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	N	317	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	572	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	34	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	F	51	ASP	CB-CG-OD1	5.46	123.21	118.30
1	G	298	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	248	TYR	CB-CG-CD1	5.45	124.27	121.00
1	N	406	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	107	ASP	CB-CG-OD1	5.44	123.20	118.30
2	L	59	LEU	CB-CG-CD1	5.43	120.23	111.00
1	H	196	LYS	CD-CE-NZ	5.42	124.18	111.70
1	D	56	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	N	112	ARG	CD-NE-CZ	5.42	131.19	123.60
1	N	158	ASP	CB-CG-OD1	5.42	123.18	118.30
1	G	520	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	514	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	444	ASP	CB-CG-OD1	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	572	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	148	GLY	C-N-CD	5.37	139.67	128.40
1	N	453	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	I	72	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	G	137	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	G	372	LEU	CA-CB-CG	5.35	127.61	115.30
1	M	90	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	H	40	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	P	59	LEU	CB-CG-CD1	5.30	120.01	111.00
1	N	33	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	380	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	317	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	389	ASP	CB-CG-OD1	5.21	122.99	118.30
1	N	110	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	298	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	A	110	ASP	CB-CG-OD1	5.21	122.98	118.30
1	N	219	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	572	ASP	CB-CG-OD1	5.17	122.95	118.30
2	K	76	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	H	317	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	G	311	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	N	520	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	H	34	ARG	CG-CD-NE	-5.06	101.17	111.80
1	N	367	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	572	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	219	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	N	298	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	C	209	ARG	NE-CZ-NH2	5.00	122.80	120.30

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4491	0	4322	22	0
1	B	4490	0	4322	22	0
1	C	4491	0	4322	15	0
1	D	4490	0	4322	18	0
1	G	4491	0	4322	16	0
1	H	4490	0	4322	16	0
1	M	4491	0	4322	21	0
1	N	4490	0	4322	11	0
2	E	568	0	545	4	0
2	F	568	0	545	4	0
2	I	568	0	545	6	0
2	J	568	0	545	2	0
2	K	568	0	545	4	0
2	L	568	0	545	2	0
2	O	568	0	545	4	0
2	P	568	0	545	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	24	0	4	5	0
4	B	24	0	3	7	0
4	C	24	0	3	4	0
4	D	24	0	3	5	0
4	G	24	0	3	7	0
4	H	24	0	4	4	0
4	M	24	0	4	3	0
4	N	24	0	3	2	0
5	A	452	0	0	4	0
5	B	511	0	0	8	0
5	C	483	0	0	4	0
5	D	516	0	0	4	0
5	E	84	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	81	0	0	1	0
5	G	496	0	0	5	0
5	H	441	0	0	6	0
5	I	78	0	0	3	0
5	J	60	0	0	0	0
5	K	87	0	0	2	0
5	L	98	0	0	0	0
5	M	440	0	0	8	0
5	N	488	0	0	4	0
5	O	60	0	0	1	0
5	P	90	0	0	6	0
All	All	45133	0	38963	181	0

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

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:601:LEU:C	5:H:820:HOH:O	1.80	1.15
1:D:112:ARG:O	1:D:112:ARG:HD3	1.51	1.10
1:H:112:ARG:HD3	1:H:112:ARG:O	1.63	0.97
2:P:26:THR:HB	5:P:102:HOH:O	0.79	0.96
1:N:112:ARG:O	1:N:112:ARG:HD3	1.68	0.93
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	0.82
1:B:112:ARG:O	1:B:112:ARG:HD3	1.82	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:N:204:ALA:HB3	4:N:702:PQQ:O7A	2.12	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
2:K:67:LYS:NZ	5:K:104:HOH:O	2.46	0.47
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: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:M:566:LEU:HD12	1:M:566:LEU:C	2.35	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: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:B:112:ARG:HD3	1:B:112:ARG:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:CZ2	4:A:702:PQQ:C6A	3.00	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
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
4:G:702:PQQ:C2	5:G:801:HOH:O	2.65	0.44
1:B:493:LYS:NZ	5:B:806:HOH:O	2.45	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
5:M:1115:HOH:O	2:O:54:HIS:HE1	2.00	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: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: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:C:31:GLU:OE2	1:C:34:ARG:NH2	2.41	0.43
1:A:114:MET:CE	1:B:591:GLN:HE21	2.32	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: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: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:H:332:TYR:O	1:H:333:ALA:C	2.57	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: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: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: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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/573 (100%)	543 (95%)	28 (5%)	0	100	100
1	B	571/573 (100%)	542 (95%)	29 (5%)	0	100	100
1	C	571/573 (100%)	541 (95%)	30 (5%)	0	100	100
1	D	571/573 (100%)	543 (95%)	27 (5%)	1 (0%)	47	33
1	G	571/573 (100%)	541 (95%)	28 (5%)	2 (0%)	34	19
1	H	571/573 (100%)	539 (94%)	32 (6%)	0	100	100
1	M	571/573 (100%)	544 (95%)	27 (5%)	0	100	100
1	N	571/573 (100%)	544 (95%)	25 (4%)	2 (0%)	34	19
2	E	69/72 (96%)	69 (100%)	0	0	100	100
2	F	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
2	I	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
2	J	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
2	K	69/72 (96%)	69 (100%)	0	0	100	100
2	L	69/72 (96%)	69 (100%)	0	0	100	100
2	O	69/72 (96%)	69 (100%)	0	0	100	100
2	P	69/72 (96%)	69 (100%)	0	0	100	100
All	All	5120/5160 (99%)	4884 (95%)	231 (4%)	5 (0%)	51	36

All (5) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	464/464 (100%)	459 (99%)	5 (1%)	73	65
1	B	464/464 (100%)	456 (98%)	8 (2%)	60	47
1	C	464/464 (100%)	459 (99%)	5 (1%)	73	65
1	D	464/464 (100%)	458 (99%)	6 (1%)	69	58
1	G	464/464 (100%)	460 (99%)	4 (1%)	78	72
1	H	464/464 (100%)	457 (98%)	7 (2%)	65	53
1	M	464/464 (100%)	456 (98%)	8 (2%)	60	47
1	N	464/464 (100%)	458 (99%)	6 (1%)	69	58
2	E	60/61 (98%)	58 (97%)	2 (3%)	38	21
2	F	60/61 (98%)	54 (90%)	6 (10%)	7	1
2	I	60/61 (98%)	56 (93%)	4 (7%)	16	4
2	J	60/61 (98%)	57 (95%)	3 (5%)	24	9
2	K	60/61 (98%)	58 (97%)	2 (3%)	38	21
2	L	60/61 (98%)	57 (95%)	3 (5%)	24	9
2	O	60/61 (98%)	59 (98%)	1 (2%)	60	47
2	P	60/61 (98%)	59 (98%)	1 (2%)	60	47
All	All	4192/4200 (100%)	4121 (98%)	71 (2%)	60	47

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	233	GLU
1	C	239	LYS
1	C	337	TYR
1	C	442	CYS
1	C	571	LYS
2	K	49	LYS
2	K	80	TYR
1	D	112	ARG

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Mol	Chain	Res	Type
1	D	239	LYS
1	D	337	TYR
1	D	472	MET
1	D	564	VAL
1	D	569	ASP
2	L	43	ASP
2	L	59	LEU
2	L	74	GLN
1	A	337	TYR
1	A	391	LYS
1	A	442	CYS
1	A	445	TRP
1	A	569	ASP
2	E	65	SER
2	E	80	TYR
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
2	F	82	LYS
2	F	91	GLU
1	G	146	GLU
1	G	337	TYR
1	G	523	ARG
1	G	584	ARG
2	I	67	LYS
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

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Mol	Chain	Res	Type
1	H	453	ARG
1	H	571	LYS
2	J	43	ASP
2	J	59	LEU
2	J	75	LYS
1	M	90	ASP
1	M	167	LYS
1	M	337	TYR
1	M	391	LYS
1	M	442	CYS
1	M	541	PRO
1	M	566	LEU
1	M	571	LYS
2	O	29	LYS
1	N	112	ARG
1	N	233	GLU
1	N	243	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 (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	270	ASN
2	K	54	HIS
1	D	117	GLN
1	D	216	ASN
1	D	464	ASN
2	L	54	HIS
2	L	74	GLN
1	A	117	GLN
1	A	588	HIS
1	A	591	GLN
2	E	54	HIS
1	B	117	GLN
1	B	216	ASN
1	B	464	ASN
1	B	591	GLN
2	F	54	HIS
2	F	74	GLN

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Mol	Chain	Res	Type
1	G	117	GLN
1	G	588	HIS
2	I	54	HIS
1	H	117	GLN
1	H	216	ASN
1	H	464	ASN
1	H	545	GLN
2	J	54	HIS
1	M	588	HIS
1	M	591	GLN
2	O	54	HIS
1	N	117	GLN
1	N	156	GLN
1	N	216	ASN
1	N	464	ASN
2	P	54	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PQQ	A	702	3	18,26,26	4.55	10 (55%)	14,40,40	2.54	7 (50%)
4	PQQ	B	702	3	18,26,26	4.52	10 (55%)	14,40,40	2.16	4 (28%)
4	PQQ	H	702	3	18,26,26	4.70	9 (50%)	14,40,40	2.39	5 (35%)
4	PQQ	C	702	3	18,26,26	4.75	10 (55%)	14,40,40	2.06	6 (42%)
4	PQQ	D	702	3	18,26,26	4.55	10 (55%)	14,40,40	3.06	7 (50%)
4	PQQ	M	702	3	18,26,26	4.57	10 (55%)	14,40,40	2.31	5 (35%)
4	PQQ	G	702	3	18,26,26	4.50	11 (61%)	14,40,40	2.68	6 (42%)
4	PQQ	N	702	3	18,26,26	4.56	10 (55%)	14,40,40	3.03	7 (50%)

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

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

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	702	PQQ	O4-C4	12.57	1.49	1.23
4	G	702	PQQ	O5-C5	11.33	1.47	1.23
4	N	702	PQQ	O4-C4	11.20	1.46	1.23
4	D	702	PQQ	O5-C5	11.19	1.46	1.23
4	A	702	PQQ	O4-C4	11.14	1.46	1.23
4	C	702	PQQ	O5-C5	11.10	1.46	1.23
4	D	702	PQQ	O4-C4	10.79	1.46	1.23
4	H	702	PQQ	O4-C4	10.75	1.46	1.23
4	G	702	PQQ	O4-C4	10.72	1.45	1.23
4	M	702	PQQ	O5-C5	10.64	1.45	1.23
4	H	702	PQQ	O5-C5	10.61	1.45	1.23
4	B	702	PQQ	O4-C4	10.57	1.45	1.23
4	M	702	PQQ	O4-C4	10.48	1.45	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	702	PQQ	O5-C5	10.24	1.44	1.23
4	B	702	PQQ	O5-C5	9.31	1.42	1.23
4	A	702	PQQ	O5-C5	9.13	1.42	1.23
4	H	702	PQQ	C9-C9X	8.89	1.56	1.47
4	B	702	PQQ	C9-C9X	8.48	1.55	1.47
4	A	702	PQQ	C9-C9X	8.09	1.55	1.47
4	M	702	PQQ	C9-C9X	7.89	1.55	1.47
4	N	702	PQQ	C9-C9X	7.81	1.55	1.47
4	C	702	PQQ	C9-C9X	6.85	1.54	1.47
4	D	702	PQQ	C9-C9X	6.70	1.53	1.47
4	G	702	PQQ	C9-C9X	5.46	1.52	1.47
4	H	702	PQQ	C5-C4	-4.73	1.37	1.53
4	G	702	PQQ	C9A-C6A	4.65	1.45	1.40
4	A	702	PQQ	C5-C4	-4.62	1.38	1.53
4	N	702	PQQ	C5-C4	-4.61	1.38	1.53
4	M	702	PQQ	C5-C4	-4.58	1.38	1.53
4	C	702	PQQ	C5-C4	-4.56	1.38	1.53
4	A	702	PQQ	C6A-C5	-4.52	1.44	1.50
4	B	702	PQQ	C5-C4	-4.51	1.38	1.53
4	G	702	PQQ	C5-C4	-4.36	1.39	1.53
4	B	702	PQQ	C6A-C5	-4.22	1.44	1.50
4	A	702	PQQ	C8-C9	4.18	1.46	1.39
4	D	702	PQQ	C8-C9	4.00	1.46	1.39
4	H	702	PQQ	C8-C9	3.93	1.46	1.39
4	H	702	PQQ	C6A-C5	-3.91	1.44	1.50
4	N	702	PQQ	C8-C9	3.86	1.46	1.39
4	B	702	PQQ	C8-C9	3.82	1.46	1.39
4	M	702	PQQ	C6A-C5	-3.81	1.45	1.50
4	M	702	PQQ	C9-C9A	3.80	1.48	1.41
4	C	702	PQQ	C8-C9	3.76	1.46	1.39
4	D	702	PQQ	C9-C9A	3.58	1.47	1.41
4	D	702	PQQ	C5-C4	-3.54	1.41	1.53
4	G	702	PQQ	C8-C9	3.40	1.45	1.39
4	B	702	PQQ	C9A-C6A	3.40	1.44	1.40
4	D	702	PQQ	C9A-C6A	3.37	1.44	1.40
4	C	702	PQQ	C9A-C6A	3.36	1.44	1.40
4	D	702	PQQ	C3A-C4	-3.36	1.41	1.48
4	M	702	PQQ	C8-C9	3.34	1.45	1.39
4	N	702	PQQ	C9-C9A	3.27	1.47	1.41
4	D	702	PQQ	C6A-C5	-3.25	1.45	1.50
4	A	702	PQQ	C3A-C4	-3.24	1.42	1.48
4	A	702	PQQ	C9-C9A	3.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	702	PQQ	C9A-C6A	3.14	1.44	1.40
4	H	702	PQQ	C3A-C4	-3.13	1.42	1.48
4	G	702	PQQ	C6A-C5	-3.11	1.46	1.50
4	N	702	PQQ	C3A-C4	-3.06	1.42	1.48
4	C	702	PQQ	C6A-C5	-3.06	1.46	1.50
4	B	702	PQQ	C3-C3A	2.97	1.46	1.40
4	N	702	PQQ	C3-C3A	2.92	1.46	1.40
4	A	702	PQQ	C3-C3A	2.86	1.46	1.40
4	B	702	PQQ	C9-C9A	2.79	1.46	1.41
4	G	702	PQQ	C3-C3A	2.72	1.45	1.40
4	D	702	PQQ	C3-C3A	2.69	1.45	1.40
4	M	702	PQQ	C3A-C4	-2.67	1.43	1.48
4	N	702	PQQ	C6A-C5	-2.62	1.46	1.50
4	C	702	PQQ	C3-C3A	2.58	1.45	1.40
4	M	702	PQQ	C3-C3A	2.57	1.45	1.40
4	M	702	PQQ	C9A-C6A	2.51	1.43	1.40
4	B	702	PQQ	C3A-C4	-2.51	1.43	1.48
4	A	702	PQQ	C9A-C6A	2.50	1.43	1.40
4	N	702	PQQ	C9A-C6A	2.41	1.43	1.40
4	C	702	PQQ	C9-C9A	2.40	1.45	1.41
4	G	702	PQQ	C8-C7	2.28	1.43	1.39
4	G	702	PQQ	C3A-C4	-2.25	1.43	1.48
4	H	702	PQQ	C9-C9A	2.19	1.45	1.41
4	G	702	PQQ	C9-C9A	2.14	1.45	1.41
4	C	702	PQQ	C3A-C1A	2.05	1.43	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	702	PQQ	C6A-N6-C7	5.84	126.90	118.19
4	H	702	PQQ	C9A-C1A-N1	5.27	135.26	124.25
4	M	702	PQQ	C6A-N6-C7	5.15	125.87	118.19
4	D	702	PQQ	C6A-N6-C7	5.11	125.82	118.19
4	A	702	PQQ	C9A-C1A-N1	5.00	134.69	124.25
4	A	702	PQQ	C6A-N6-C7	4.90	125.50	118.19
4	D	702	PQQ	C9A-C1A-N1	4.89	134.46	124.25
4	G	702	PQQ	C9A-C1A-N1	4.86	134.41	124.25
4	D	702	PQQ	O4-C4-C3A	-4.81	113.78	121.56
4	M	702	PQQ	C9A-C1A-N1	4.77	134.22	124.25
4	N	702	PQQ	C9A-C1A-N1	4.62	133.91	124.25
4	H	702	PQQ	C6A-N6-C7	4.58	125.02	118.19
4	B	702	PQQ	C9A-C1A-N1	4.47	133.60	124.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	PQQ	C3A-C4-C5	4.47	124.09	118.11
4	G	702	PQQ	C3A-C4-C5	4.31	123.88	118.11
4	C	702	PQQ	C9A-C1A-N1	4.28	133.19	124.25
4	N	702	PQQ	O5-C5-C6A	4.23	126.31	121.84
4	B	702	PQQ	C6A-N6-C7	4.21	124.46	118.19
4	G	702	PQQ	C6A-N6-C7	3.97	124.12	118.19
4	N	702	PQQ	C9-C8-C7	-3.92	115.85	120.41
4	G	702	PQQ	O5-C5-C6A	3.90	125.97	121.84
4	C	702	PQQ	C6A-N6-C7	3.70	123.71	118.19
4	G	702	PQQ	C9-C8-C7	-3.43	116.42	120.41
4	D	702	PQQ	C9-C8-C7	-3.39	116.47	120.41
4	H	702	PQQ	C3A-C4-C5	3.37	122.62	118.11
4	B	702	PQQ	C3A-C4-C5	3.29	122.50	118.11
4	N	702	PQQ	C3A-C4-C5	3.23	122.44	118.11
4	A	702	PQQ	C3A-C4-C5	3.20	122.39	118.11
4	G	702	PQQ	O4-C4-C5	-3.17	113.80	119.31
4	D	702	PQQ	O5-C5-C6A	3.16	125.18	121.84
4	C	702	PQQ	O4-C4-C5	-2.70	114.62	119.31
4	H	702	PQQ	O5-C5-C6A	2.67	124.67	121.84
4	N	702	PQQ	O4-C4-C5	-2.64	114.73	119.31
4	C	702	PQQ	C9-C8-C7	-2.63	117.35	120.41
4	M	702	PQQ	C3A-C4-C5	2.46	121.40	118.11
4	C	702	PQQ	C3A-C4-C5	2.44	121.37	118.11
4	N	702	PQQ	C9-C9A-C1A	2.39	128.17	122.86
4	A	702	PQQ	C9-C8-C7	-2.31	117.73	120.41
4	B	702	PQQ	O4-C4-C5	-2.30	115.32	119.31
4	A	702	PQQ	C9-C9A-C1A	2.26	127.88	122.86
4	D	702	PQQ	C3-C3A-C1A	2.18	109.53	106.65
4	H	702	PQQ	C8-C7-N6	-2.13	119.82	122.35
4	A	702	PQQ	C8-C7-N6	-2.10	119.85	122.35
4	M	702	PQQ	C9-C8-C7	-2.08	118.00	120.41
4	C	702	PQQ	C9-C9A-C1A	2.06	127.45	122.86
4	M	702	PQQ	C9-C9A-C1A	2.04	127.40	122.86
4	A	702	PQQ	O4-C4-C5	-2.01	115.82	119.31

There are no chirality outliers.

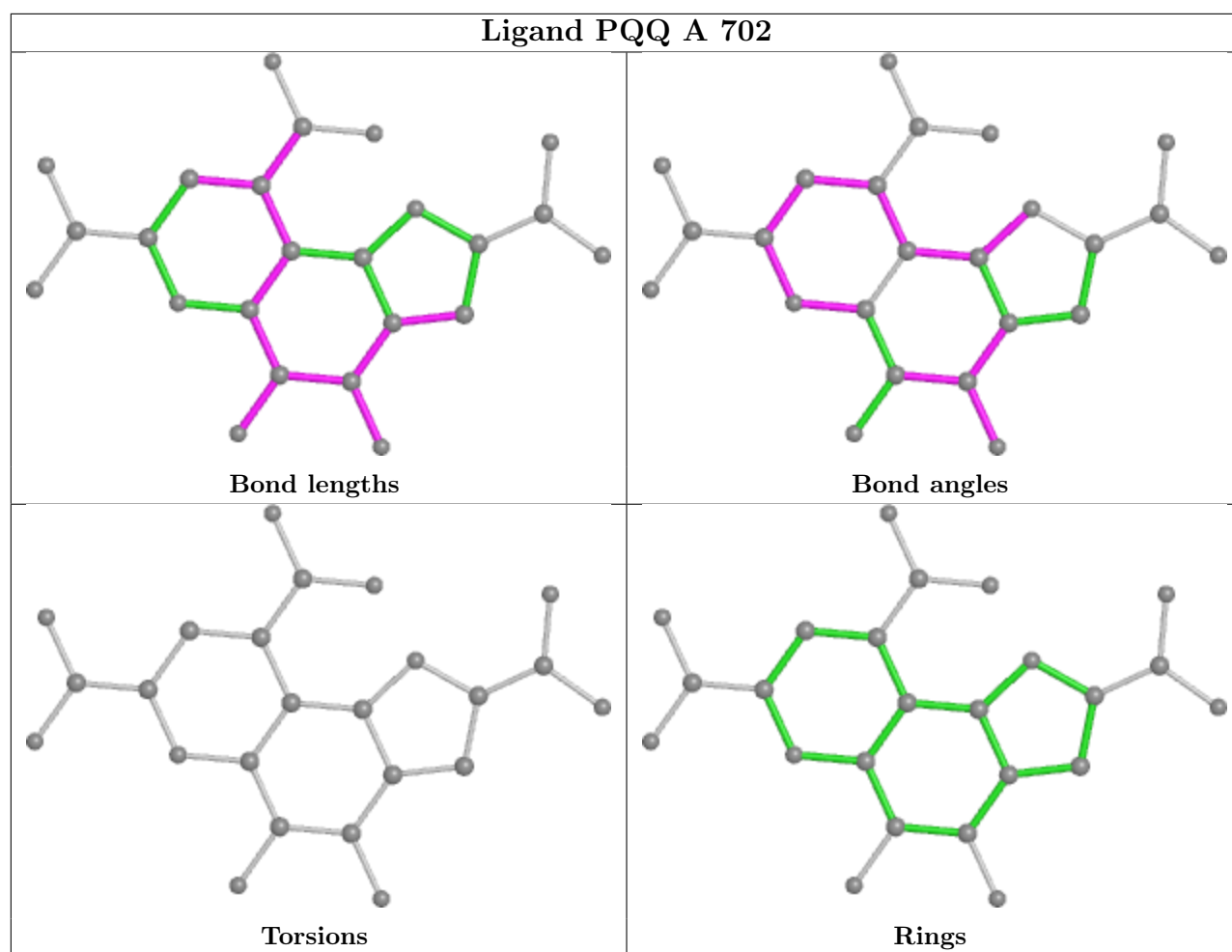
There are no torsion outliers.

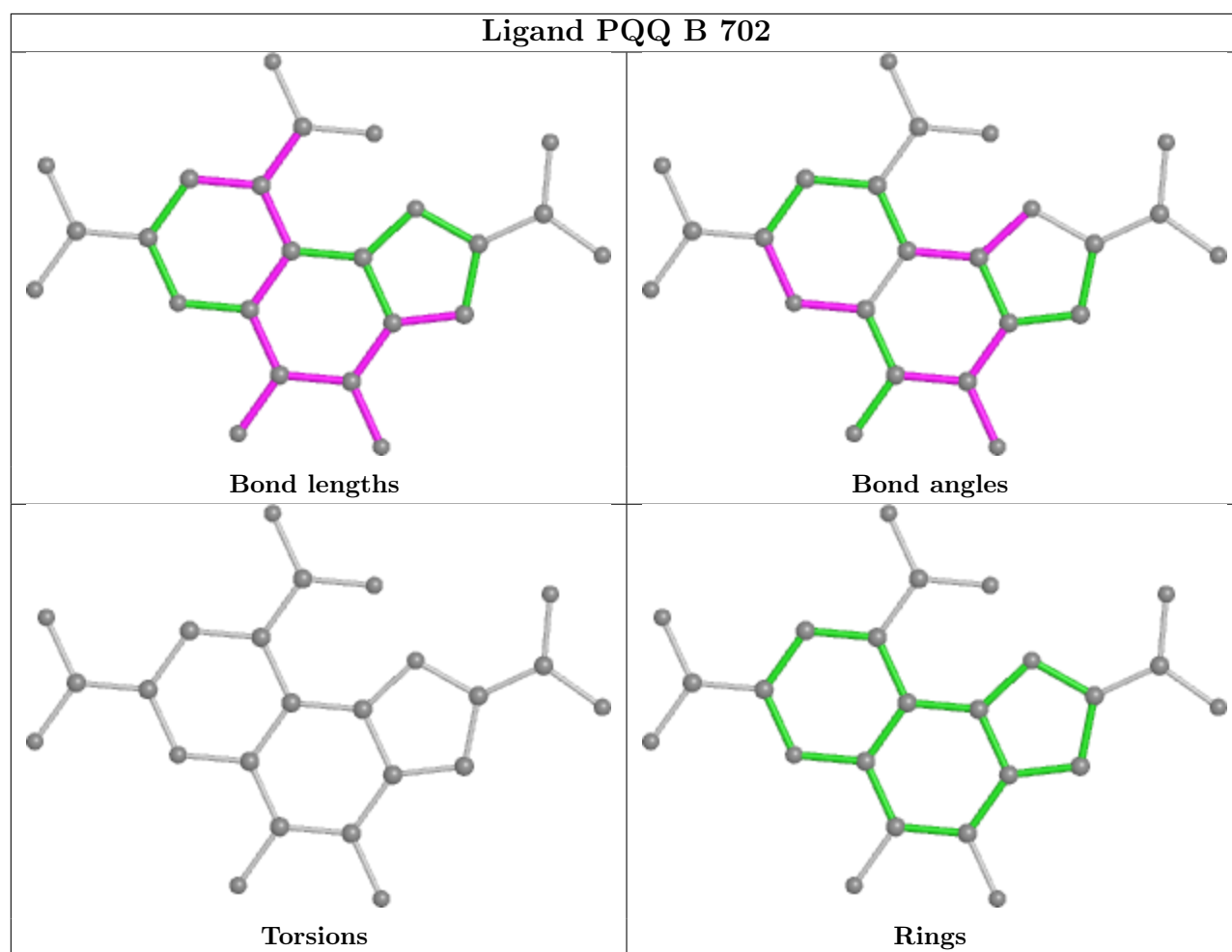
There are no ring outliers.

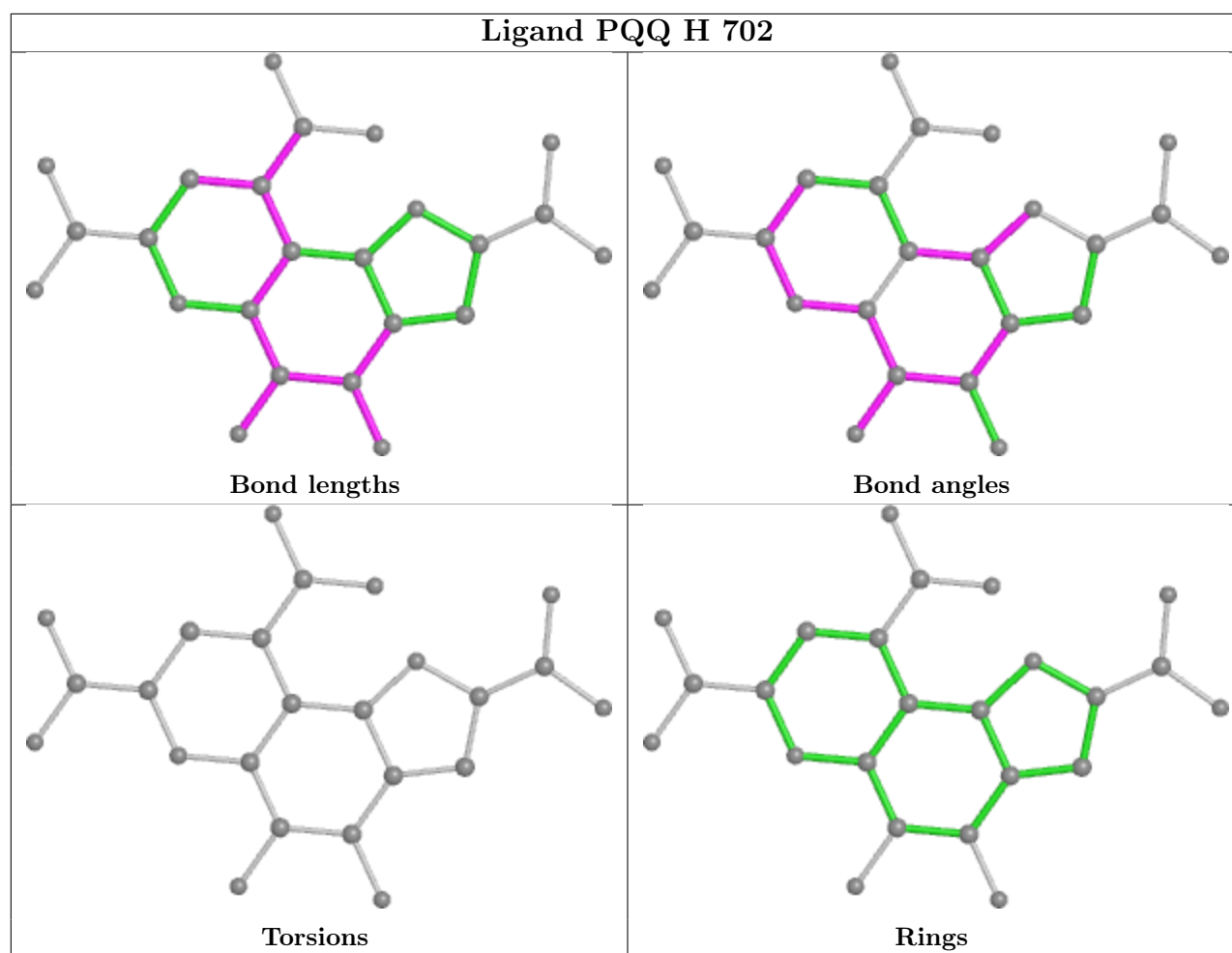
8 monomers are involved in 37 short contacts:

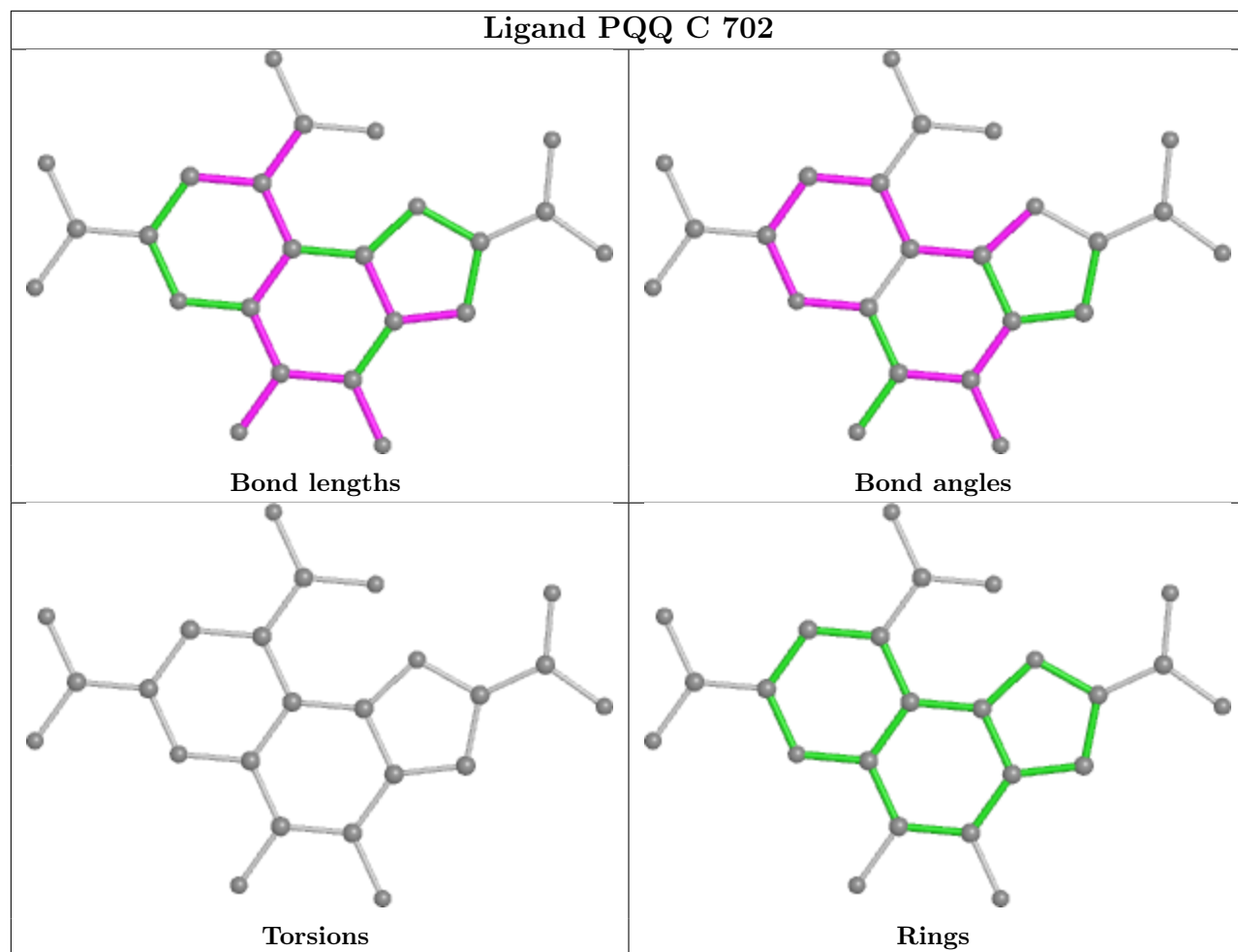
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	PQQ	5	0
4	B	702	PQQ	7	0
4	H	702	PQQ	4	0
4	C	702	PQQ	4	0
4	D	702	PQQ	5	0
4	M	702	PQQ	3	0
4	G	702	PQQ	7	0
4	N	702	PQQ	2	0

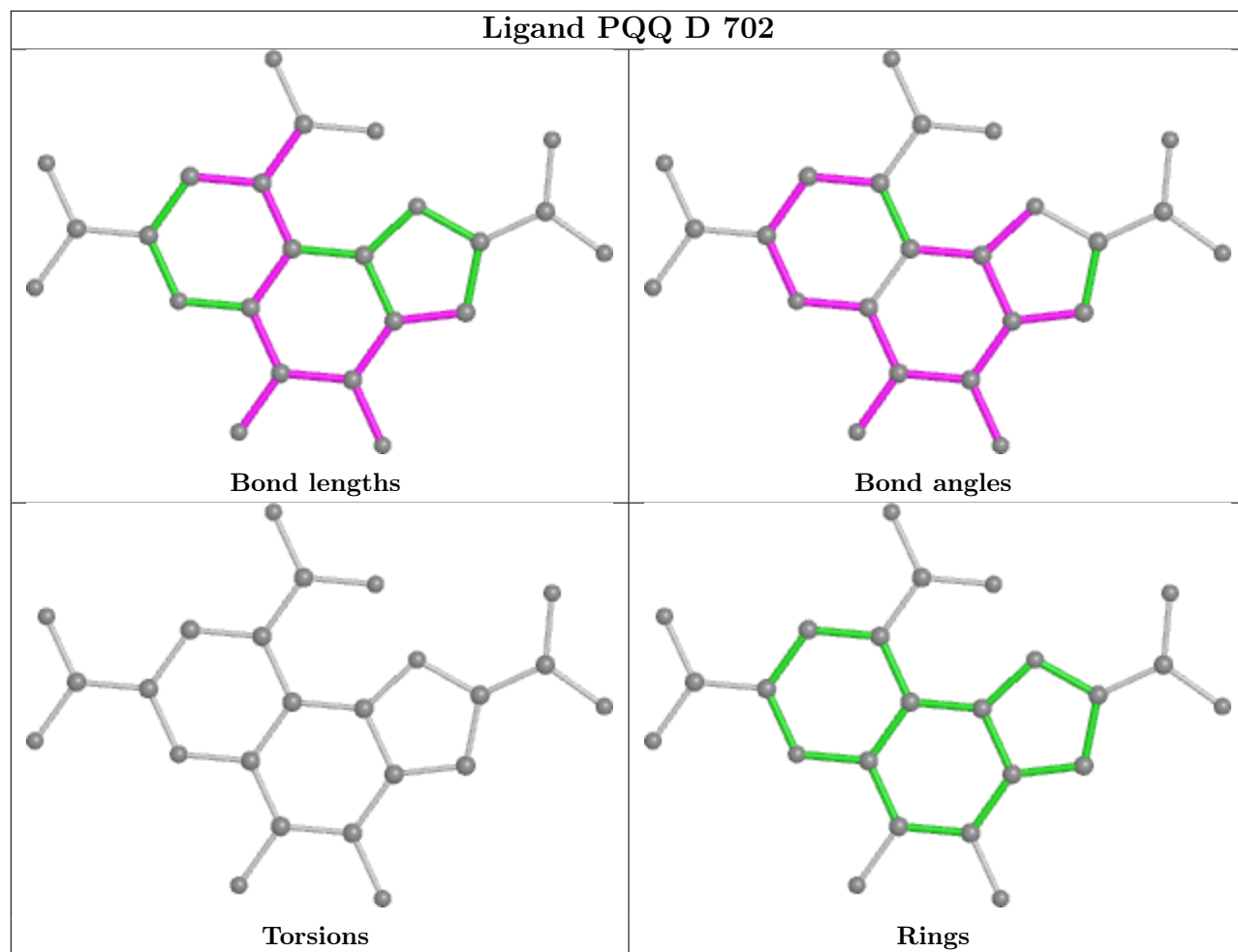
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



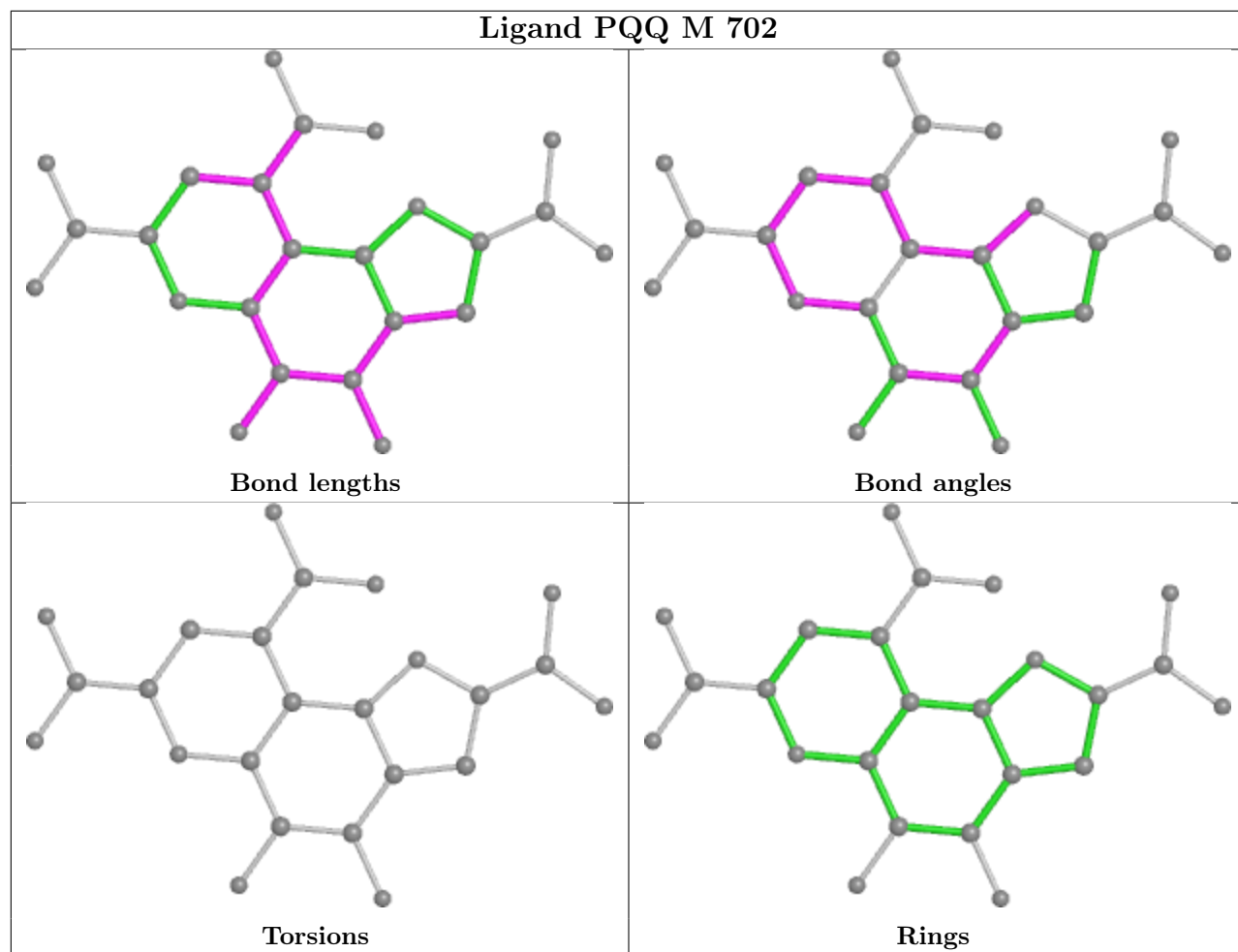


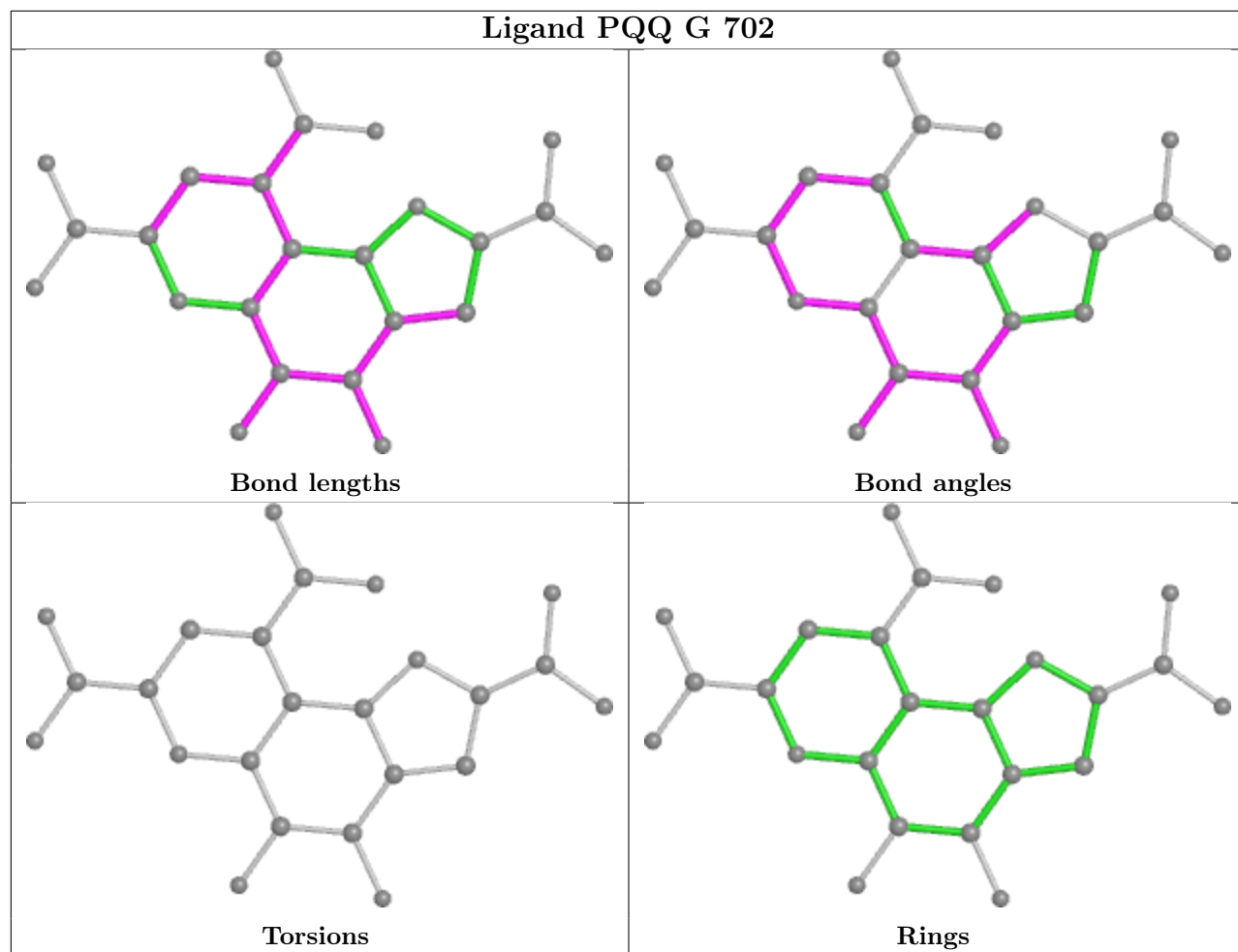


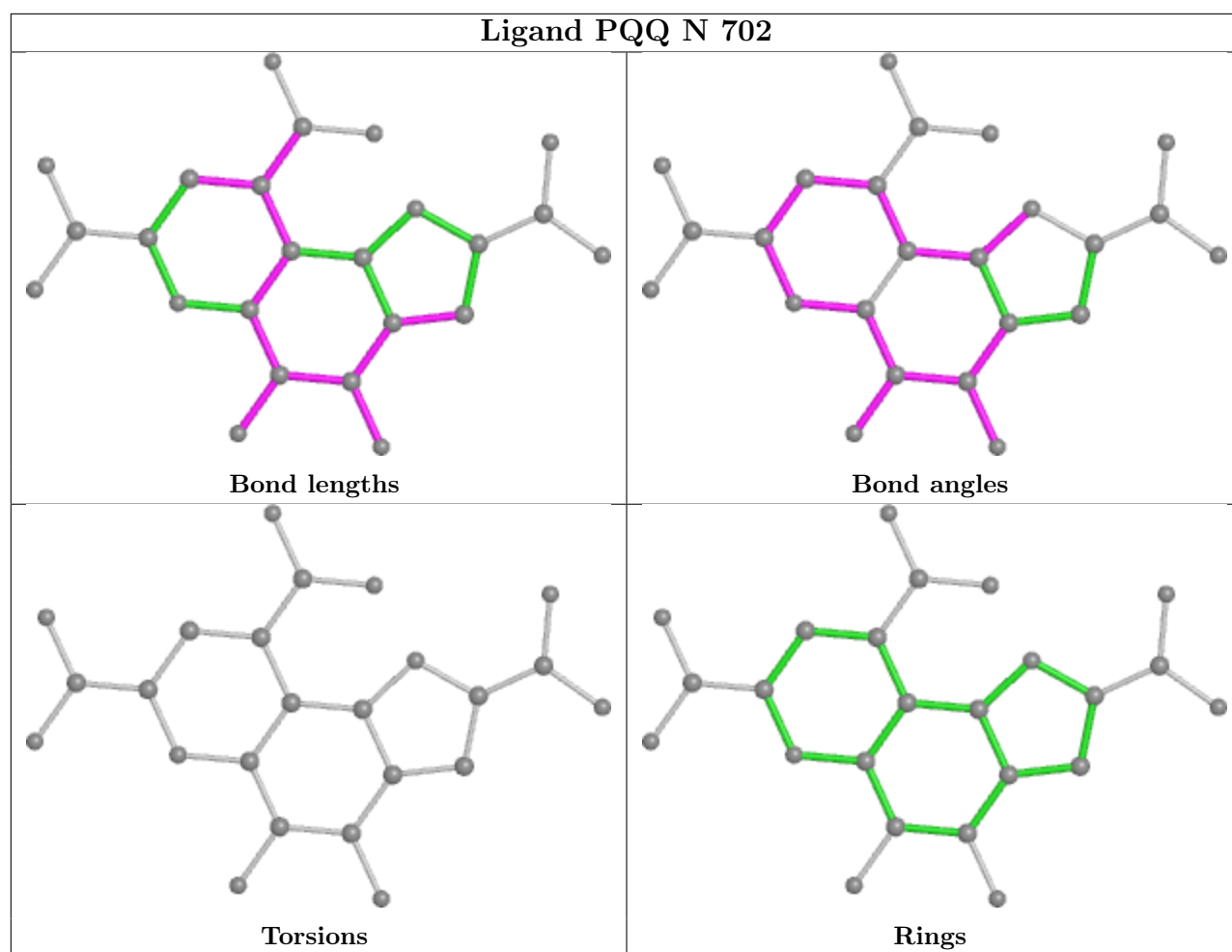












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	573/573 (100%)	-0.44	1 (0%) 95 94	13, 21, 33, 57	0
1	B	573/573 (100%)	-0.47	3 (0%) 91 91	12, 17, 30, 47	0
1	C	573/573 (100%)	-0.51	0 100 100	11, 17, 29, 45	0
1	D	573/573 (100%)	-0.46	4 (0%) 87 88	12, 18, 31, 50	0
1	G	573/573 (100%)	-0.49	1 (0%) 95 94	12, 18, 31, 48	0
1	H	573/573 (100%)	-0.39	4 (0%) 87 88	13, 23, 36, 53	0
1	M	573/573 (100%)	-0.34	2 (0%) 94 93	13, 22, 37, 55	0
1	N	573/573 (100%)	-0.55	4 (0%) 87 88	12, 17, 30, 47	0
2	E	71/72 (98%)	0.09	2 (2%) 53 52	20, 31, 46, 52	0
2	F	71/72 (98%)	0.04	5 (7%) 16 15	15, 24, 58, 87	0
2	I	71/72 (98%)	0.25	5 (7%) 16 15	17, 26, 65, 131	0
2	J	71/72 (98%)	0.51	5 (7%) 16 15	24, 36, 52, 67	0
2	K	71/72 (98%)	-0.25	1 (1%) 75 76	15, 24, 38, 52	0
2	L	71/72 (98%)	-0.07	2 (2%) 53 52	18, 26, 44, 61	0
2	O	71/72 (98%)	0.49	5 (7%) 16 15	26, 36, 53, 68	0
2	P	71/72 (98%)	-0.23	0 100 100	17, 22, 40, 53	0
All	All	5152/5160 (99%)	-0.39	44 (0%) 84 84	11, 20, 37, 131	0

All (44) RSRZ outliers are listed below:

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

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Mol	Chain	Res	Type	RSRZ
2	I	92	ASP	4.5
2	F	92	ASP	3.6
1	H	132	CYS	3.6
2	O	91	GLU	3.5
2	J	28	CYS	3.3
2	O	82	LYS	3.3
1	B	131	CYS	3.2
1	H	131	CYS	3.2
2	F	90	VAL	2.9
2	L	91	GLU	2.9
1	N	131	CYS	2.8
1	H	346	ASP	2.6
2	O	83	THR	2.6
1	H	347	GLY	2.5
2	J	91	GLU	2.5
1	G	346	ASP	2.5
1	A	571	LYS	2.5
2	K	28	CYS	2.5
1	B	571	LYS	2.4
2	E	93	ILE	2.4
1	N	346	ASP	2.4
2	E	28	CYS	2.4
1	D	132	CYS	2.4
1	D	131	CYS	2.4
2	L	93	ILE	2.4
2	J	31	PRO	2.3
2	I	89	LYS	2.3
1	M	346	ASP	2.3
1	M	131	CYS	2.3
1	N	132	CYS	2.3
2	J	93	ILE	2.2
2	J	47	GLY	2.2
2	O	39	PRO	2.1
2	F	82	LYS	2.1
1	D	346	ASP	2.1
1	N	146	GLU	2.1
2	O	90	VAL	2.1
1	B	346	ASP	2.0
1	D	442	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

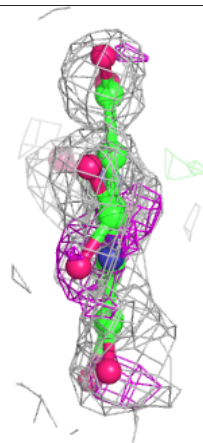
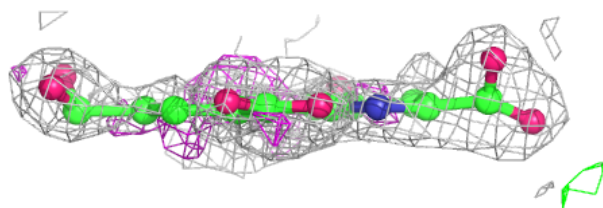
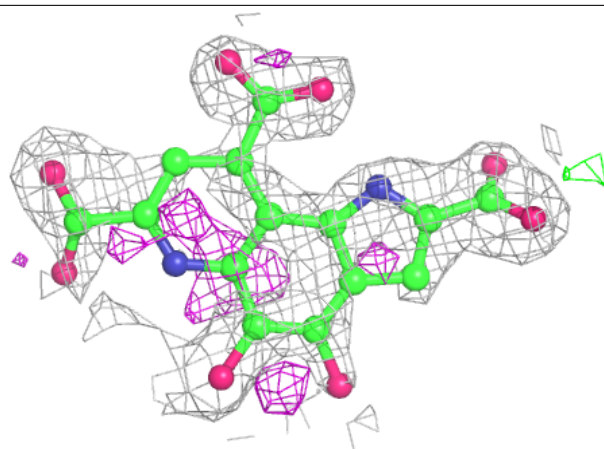
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

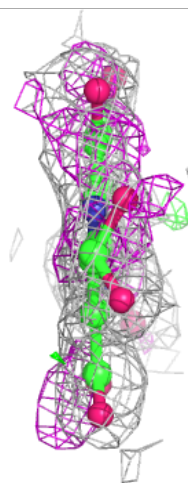
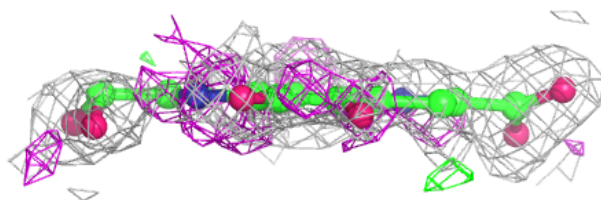
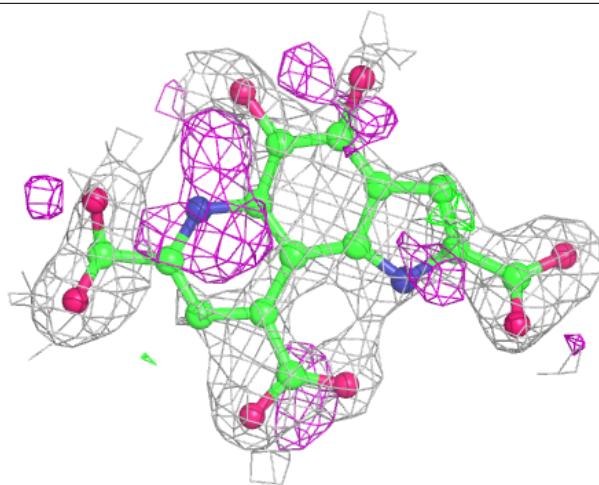
**Electron density around PQQ H 702:**

$2mF_o - DF_c$  (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:**

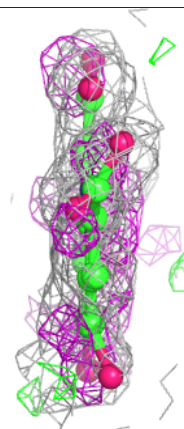
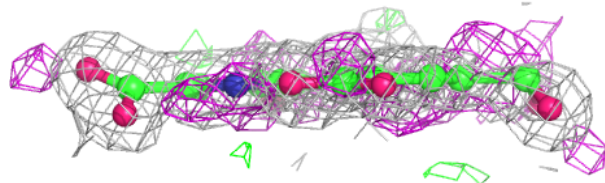
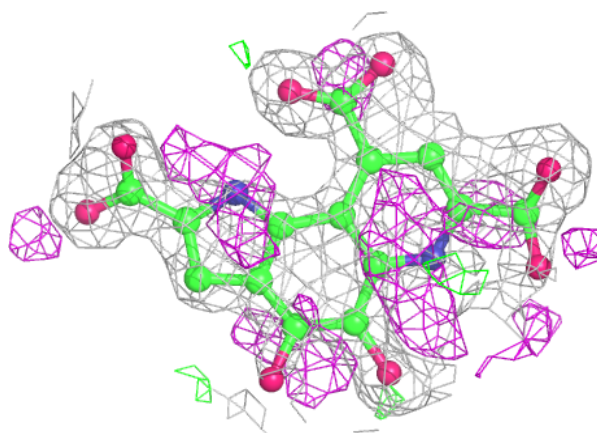
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





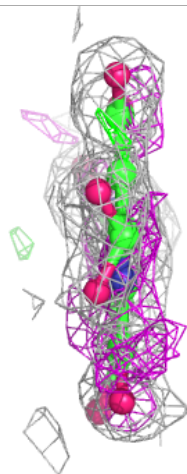
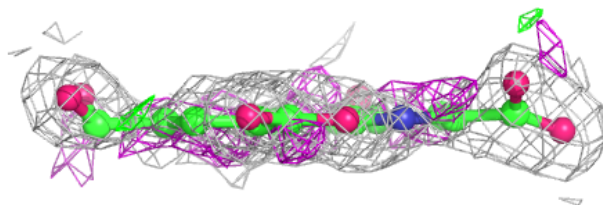
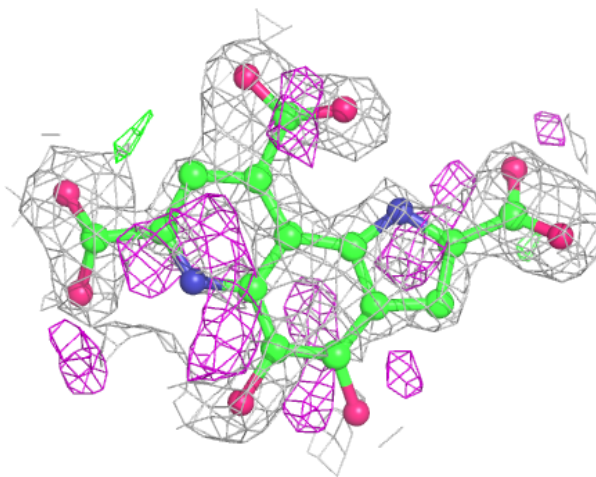
**Electron density around PQQ D 702:**

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



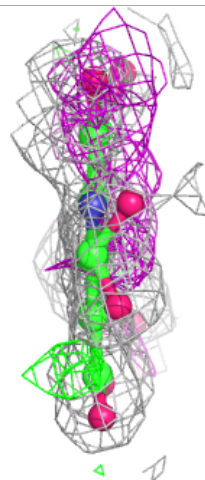
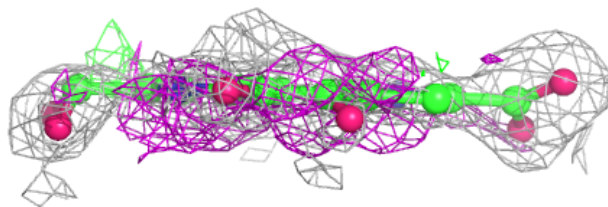
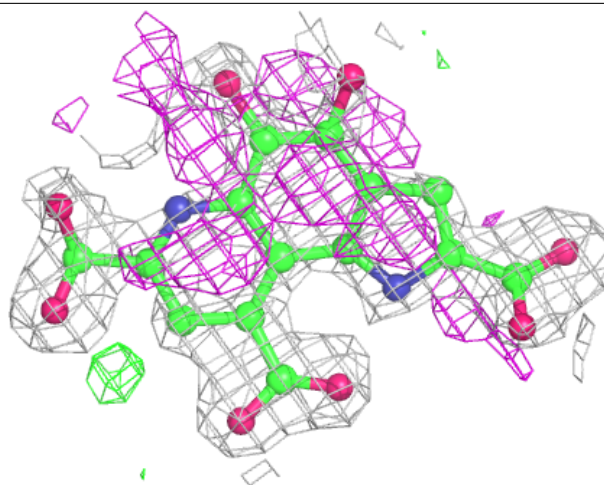
**Electron density around PQQ N 702:**

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



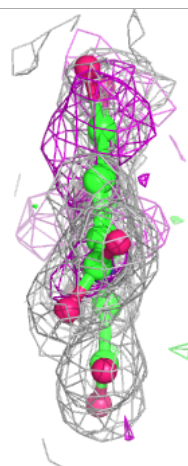
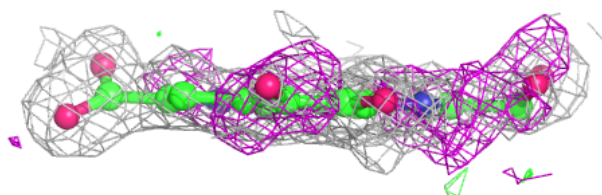
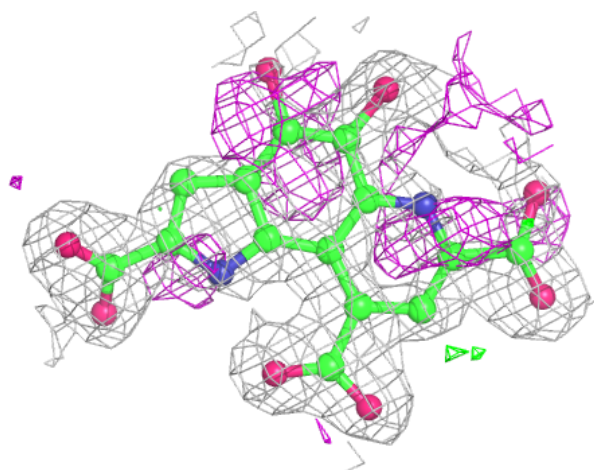
**Electron density around PQQ G 702:**

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



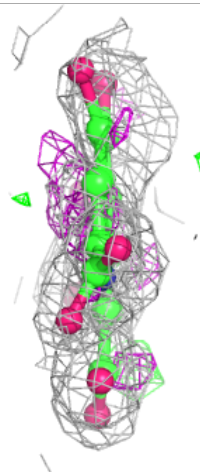
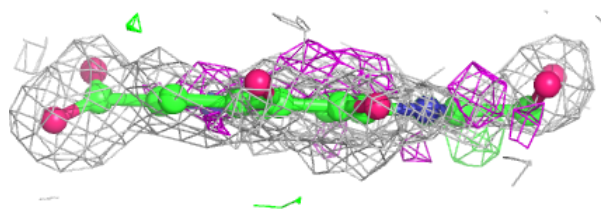
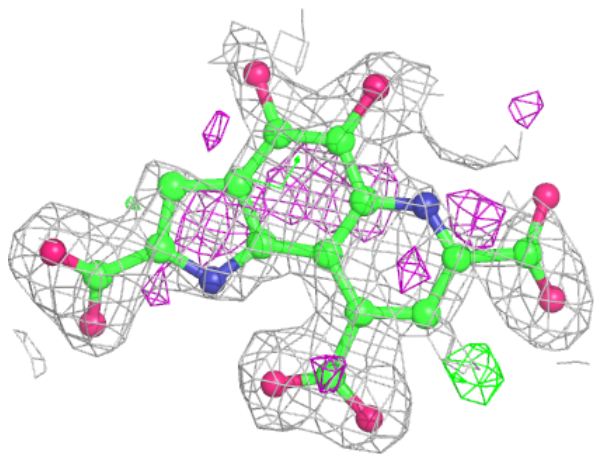
**Electron density around PQQ C 702:**

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



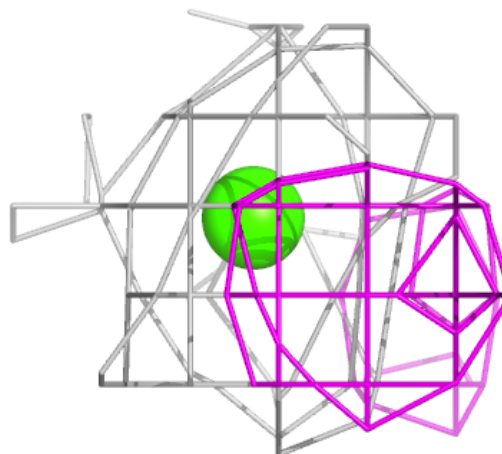
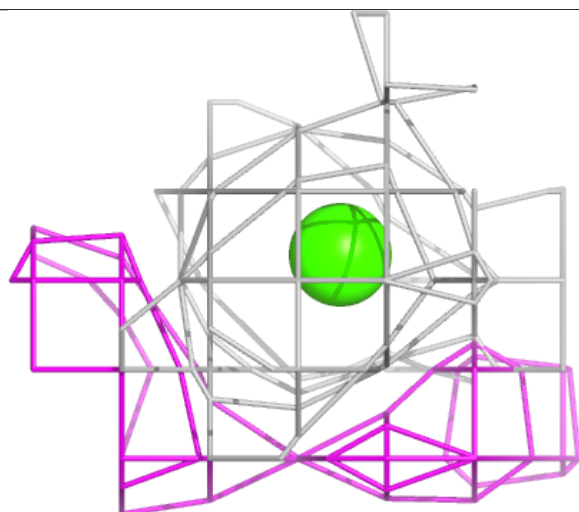
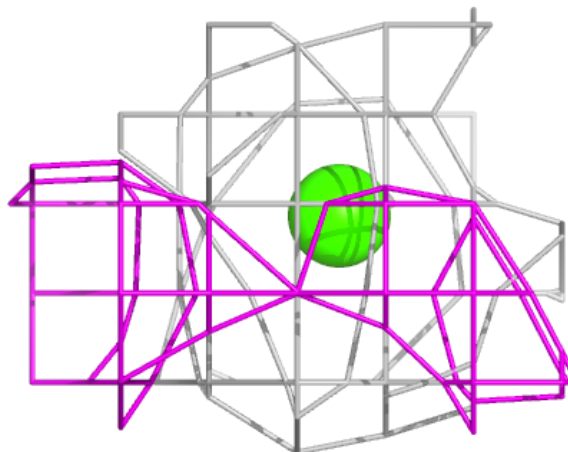
**Electron density around PQQ A 702:**

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



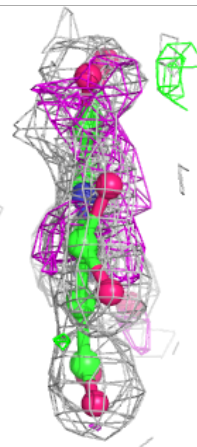
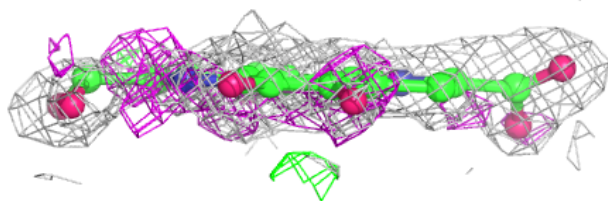
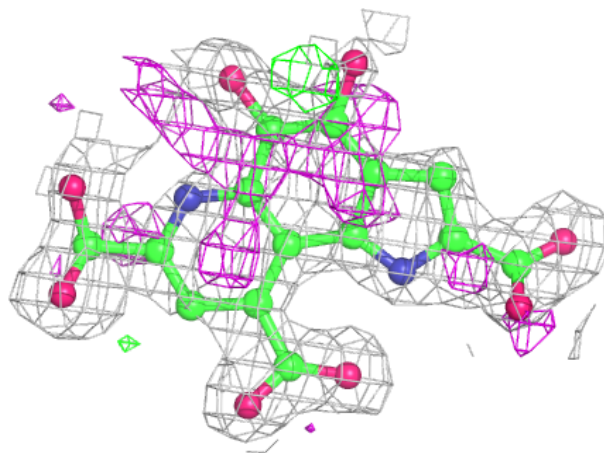
**Electron density around CA M 701:**

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



**Electron density around PQQ B 702:**

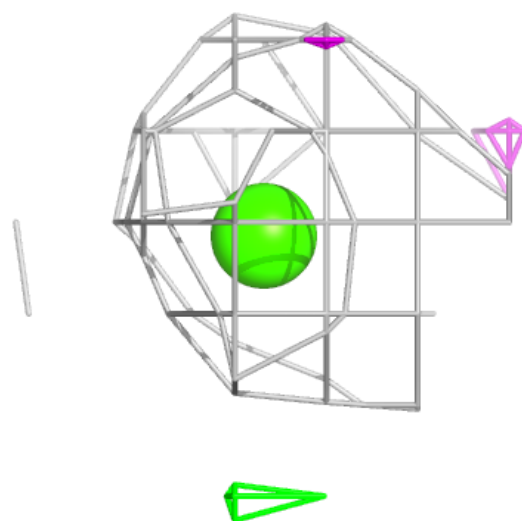
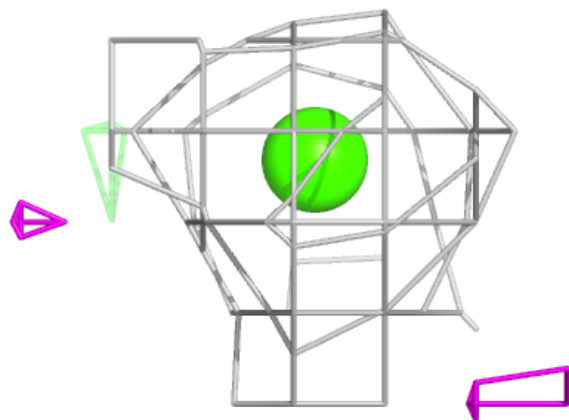
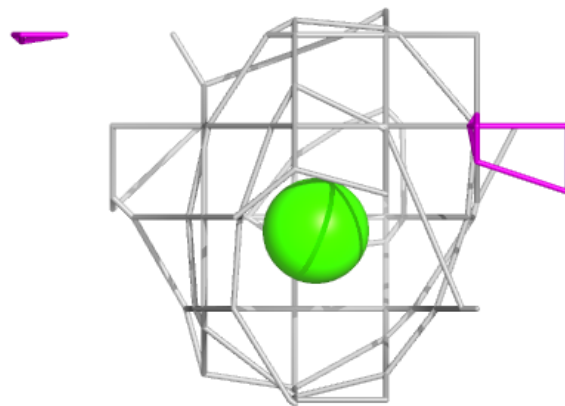
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CA H 701:**

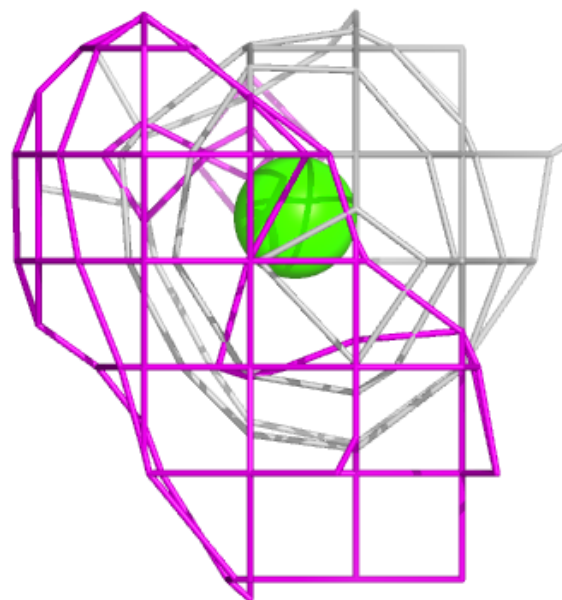
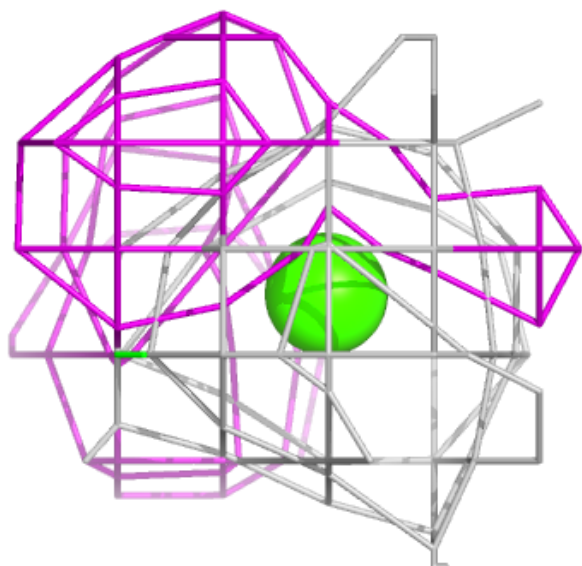
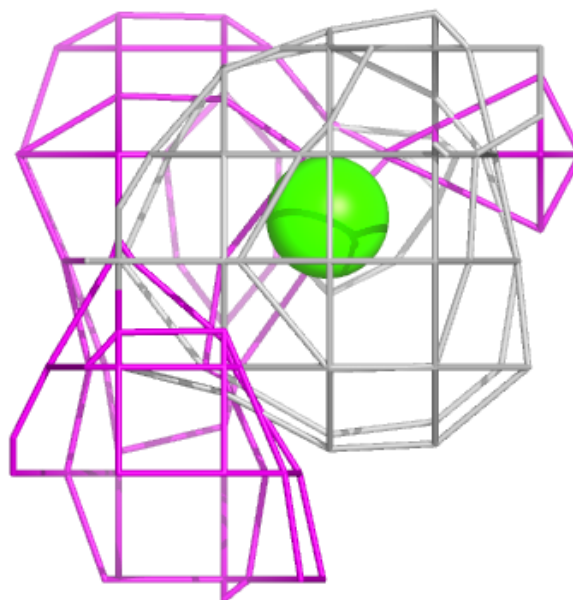
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





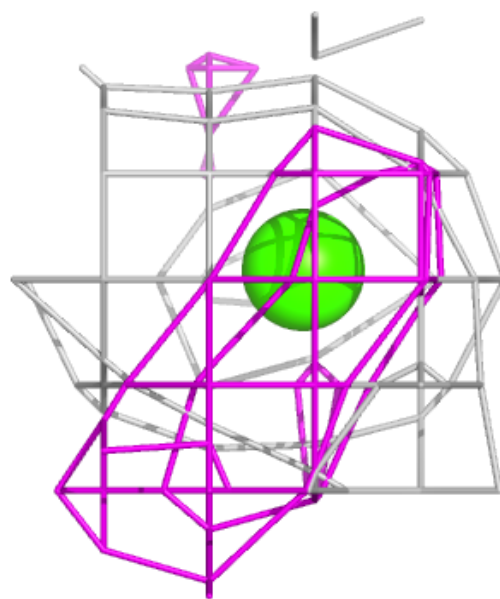
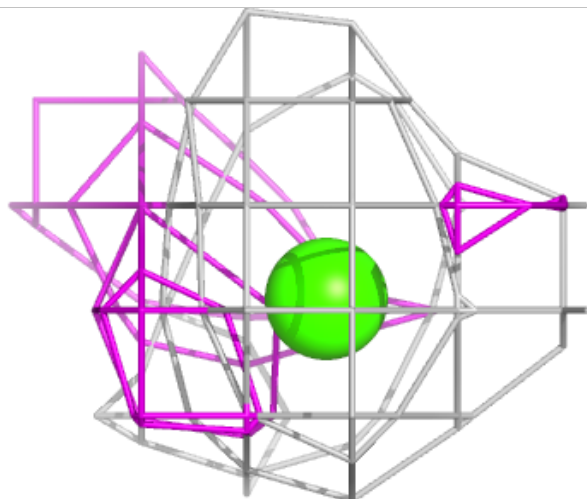
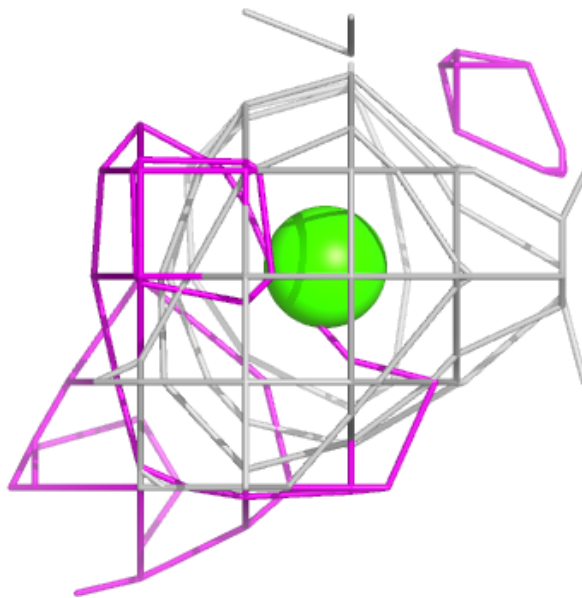
**Electron density around CA G 701:**

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



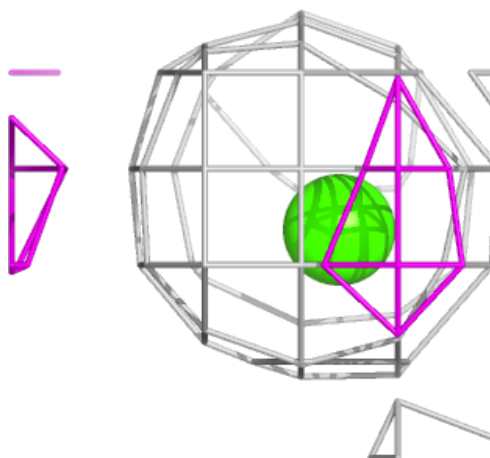
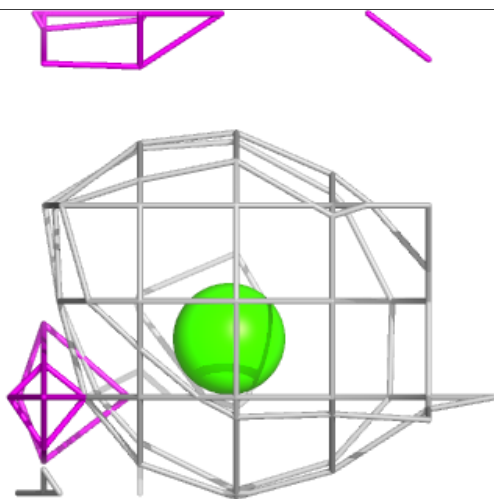
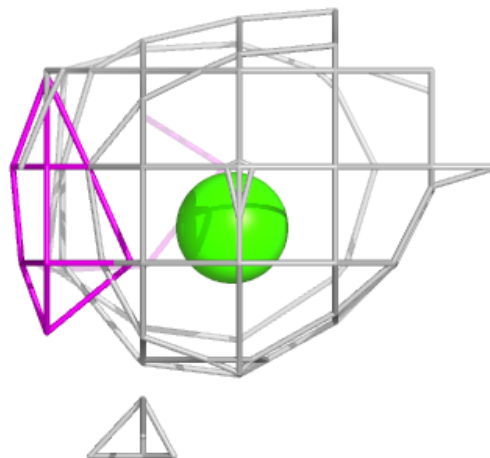
**Electron density around CA B 701:**

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



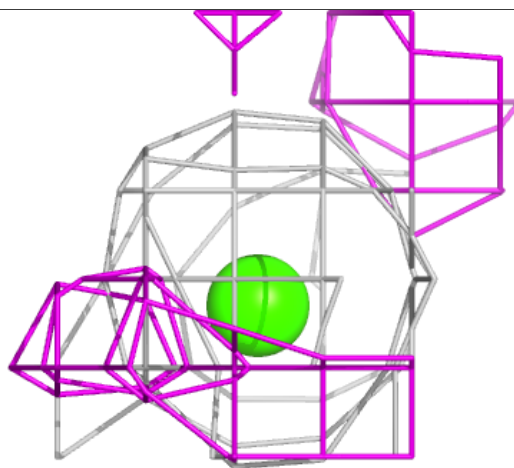
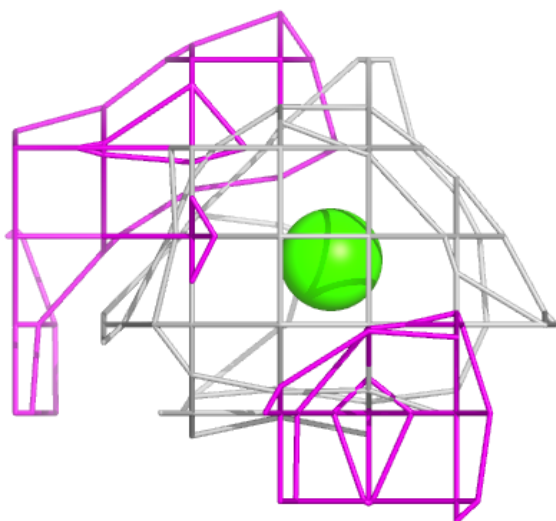
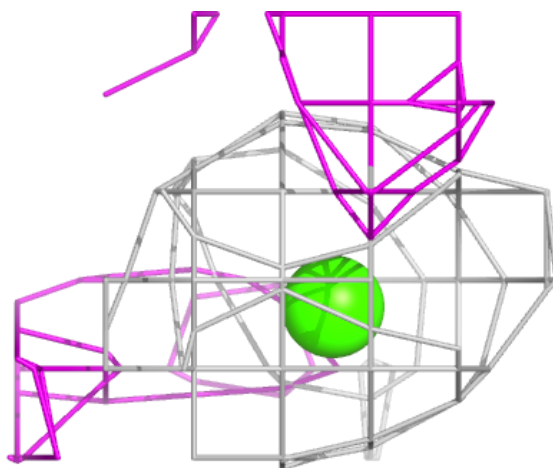
**Electron density around CA A 701:**

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



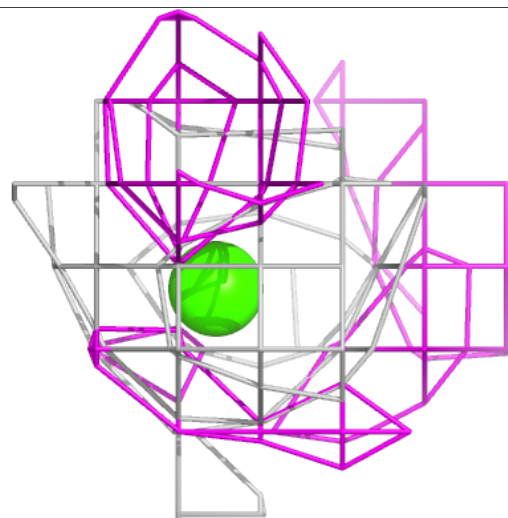
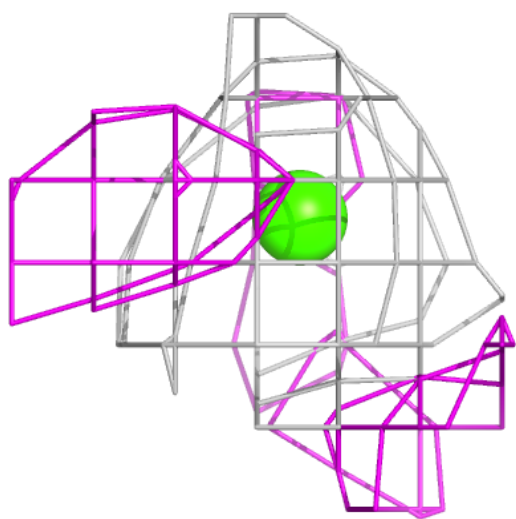
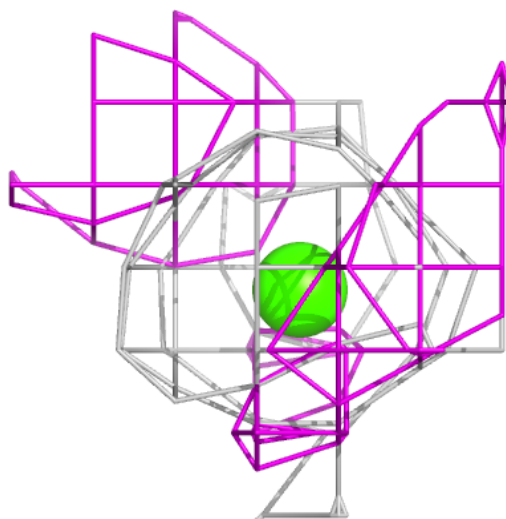
**Electron density around CA N 701:**

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



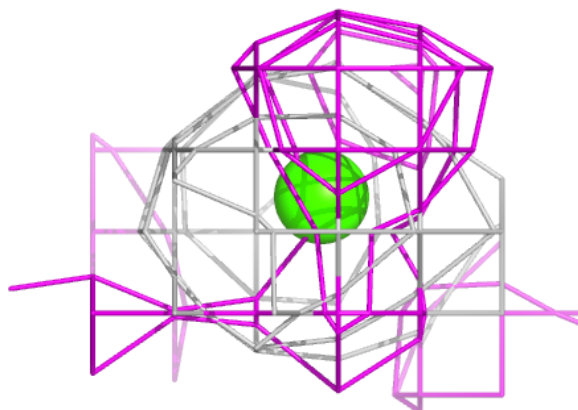
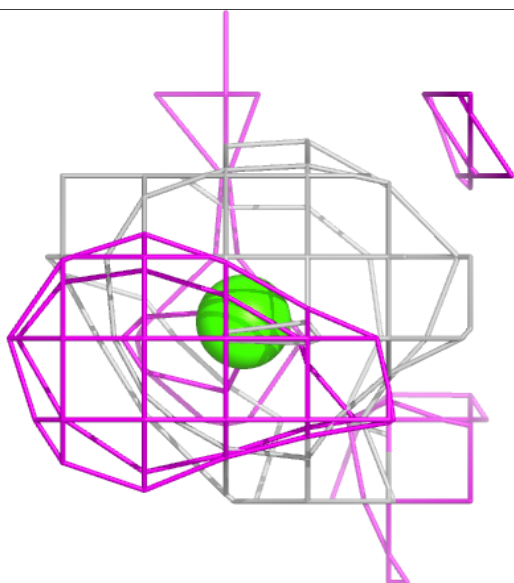
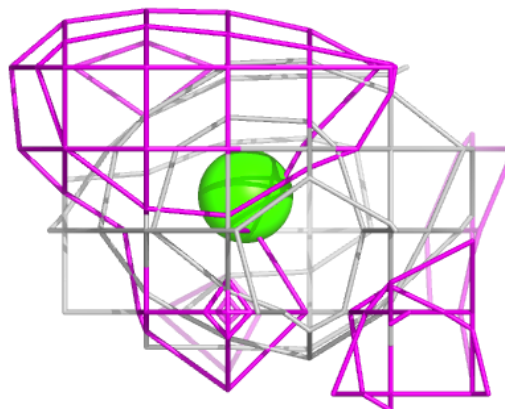
**Electron density around CA D 701:**

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



**Electron density around CA C 701:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.