



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:32 AM UTC

PDB ID : 9R0W / pdb_00009r0w
Title : Crystal structure of glutathione transferase iota 1 from *Synechocystis* sp. PCC 6803 in complex with FMN
Authors : Didierjean, C.; Hecker, A.; Morette, L.
Deposited on : 2025-04-24
Resolution : 2.71 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

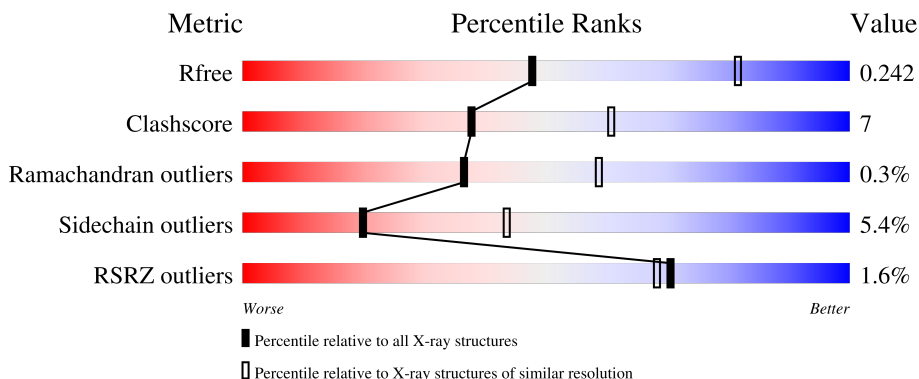
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	399	79% 19% .
1	B	399	78% 21% .
1	C	399	78% 20% .
1	D	399	3% 81% 16% .
1	E	399	2% 77% 20% .

2 Entry composition [i](#)

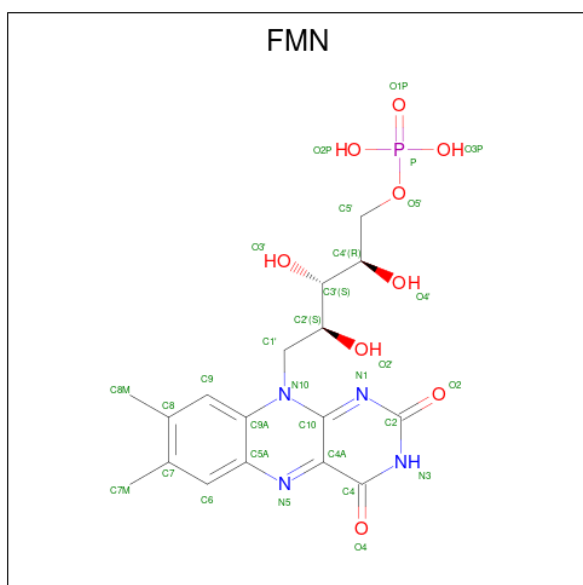
There are 4 unique types of molecules in this entry. The entry contains 16352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sll1902 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3238	2061	567	592	18			
1	B	399	Total	C	N	O	S	0	0	0
			3238	2061	567	592	18			
1	C	399	Total	C	N	O	S	0	0	0
			3238	2061	567	592	18			
1	D	399	Total	C	N	O	S	0	0	0
			3238	2061	567	592	18			
1	E	399	Total	C	N	O	S	0	0	0
			3238	2061	567	592	18			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

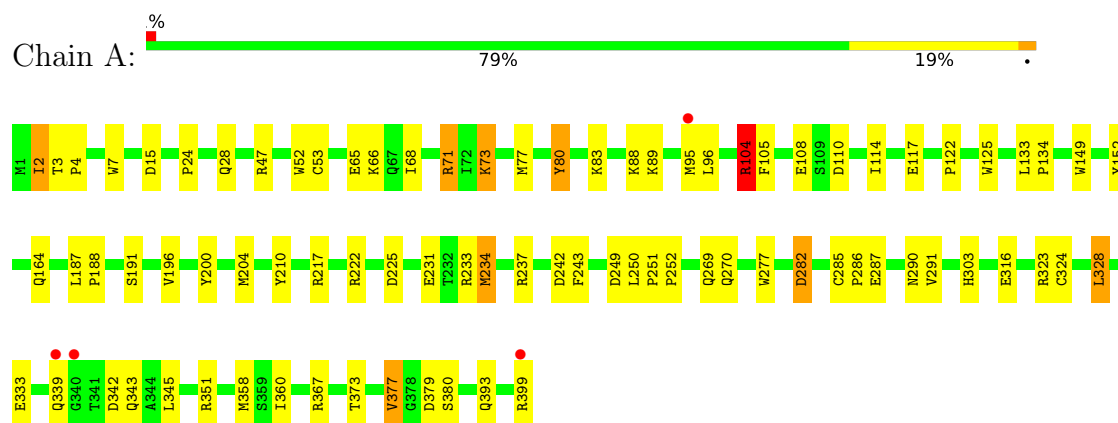
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

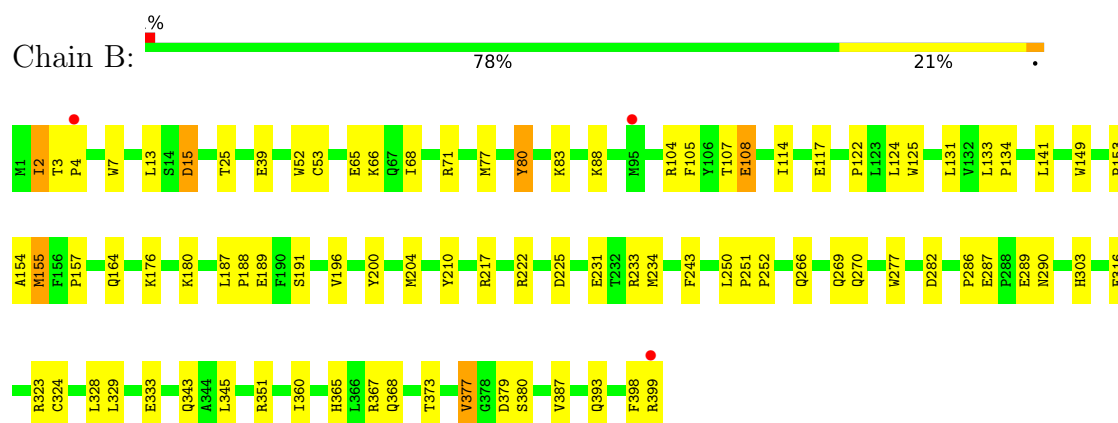
3 Residue-property plots [i](#)

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.

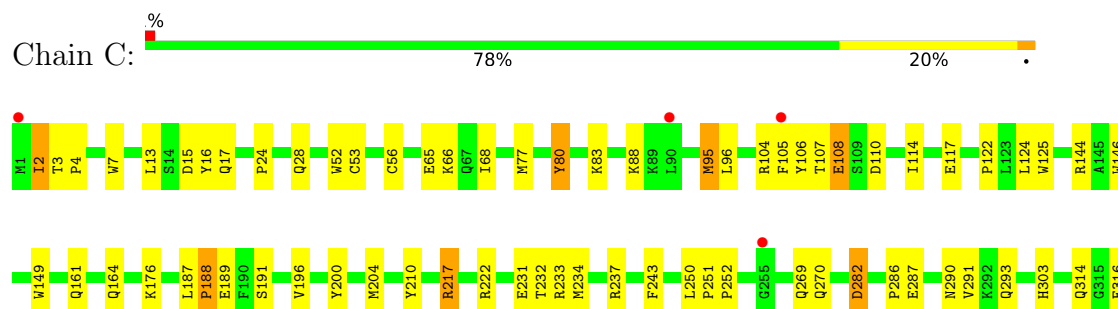
• Molecule 1: Sll1902 protein

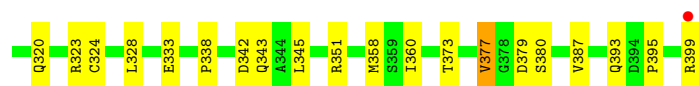


• Molecule 1: Sll1902 protein

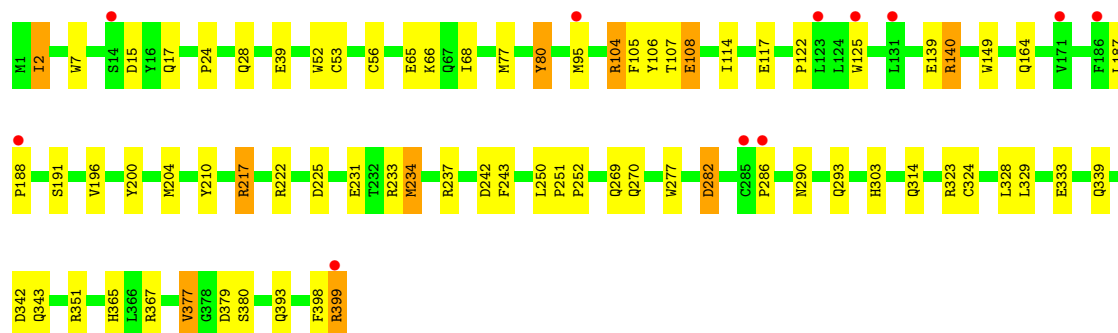
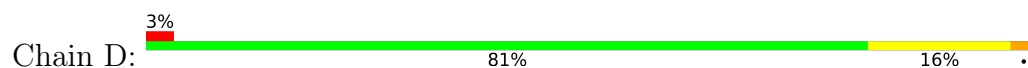


• Molecule 1: Sll1902 protein

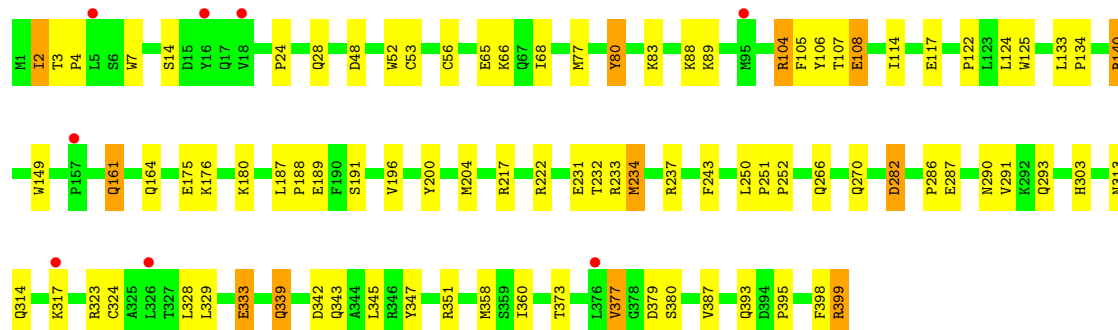
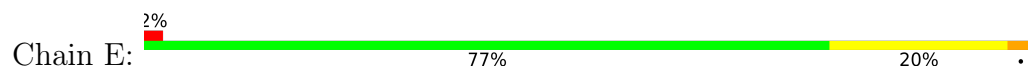




• Molecule 1: Sll1902 protein



• Molecule 1: Sll1902 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.31Å 173.93Å 318.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 2.71 48.79 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.79-2.71) 99.8 (48.79-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.208 , 0.242 0.208 , 0.242	Depositor DCC
R_{free} test set	4660 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16352	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/3326	1.29	18/4520 (0.4%)
1	B	0.60	0/3326	1.30	16/4520 (0.4%)
1	C	0.60	0/3326	1.28	14/4520 (0.3%)
1	D	0.60	0/3326	1.28	16/4520 (0.4%)
1	E	0.56	0/3326	1.27	15/4520 (0.3%)
All	All	0.60	0/16630	1.28	79/22600 (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	A	0	2
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	MET	CG-SD-CE	12.53	128.47	100.90
1	E	140	ARG	CG-CD-NE	10.27	134.60	112.00
1	D	140	ARG	CG-CD-NE	9.86	133.69	112.00
1	E	398	PHE	CA-CB-CG	7.19	120.99	113.80
1	D	286	PRO	CB-CA-C	6.83	121.53	111.22
1	A	270	GLN	CB-CA-C	6.58	121.20	110.88
1	D	17	GLN	CB-CA-C	-6.50	98.40	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	GLU	N-CA-CB	-6.47	97.83	109.68
1	A	287	GLU	N-CA-CB	-6.42	98.24	109.73
1	B	176	LYS	CA-CB-CG	6.36	126.81	114.10
1	E	339	GLN	CB-CA-C	6.33	121.12	109.46
1	C	379	ASP	CB-CA-C	-6.28	99.33	109.13
1	B	287	GLU	N-CA-CB	-6.28	98.50	109.73
1	A	104	ARG	CB-CG-CD	6.27	125.72	111.30
1	E	287	GLU	N-CA-CB	-6.26	98.23	109.68
1	D	270	GLN	CB-CA-C	6.22	120.64	110.88
1	E	270	GLN	CB-CA-C	6.19	120.59	110.88
1	C	270	GLN	CB-CA-C	6.17	120.56	110.88
1	B	270	GLN	CB-CA-C	6.05	120.39	110.88
1	C	15	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	398	PHE	CA-CB-CG	6.00	119.80	113.80
1	C	286	PRO	CB-CA-C	5.98	118.83	111.12
1	A	71	ARG	CB-CG-CD	5.94	124.97	111.30
1	B	105	PHE	CA-CB-CG	-5.84	107.96	113.80
1	B	80	TYR	N-CA-CB	5.79	119.29	110.95
1	A	80	TYR	N-CA-CB	5.76	119.25	110.95
1	B	104	ARG	CB-CG-CD	5.72	124.47	111.30
1	C	80	TYR	N-CA-CB	5.70	119.15	110.95
1	A	73	LYS	CB-CG-CD	5.69	124.38	111.30
1	E	282	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	398	PHE	CA-CB-CG	5.67	119.47	113.80
1	D	15	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	286	PRO	CB-CA-C	5.64	118.39	111.12
1	A	225	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	342	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	342	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	242	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	282	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	242	ASP	CA-CB-CG	5.51	118.11	112.60
1	E	161	GLN	CB-CA-C	5.51	119.93	110.79
1	D	105	PHE	CA-CB-CG	-5.48	108.32	113.80
1	E	379	ASP	CB-CA-C	-5.47	100.60	109.13
1	E	286	PRO	CB-CA-C	5.42	118.11	111.12
1	D	282	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	105	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	316	GLU	CB-CG-CD	-5.38	103.46	112.60
1	C	316	GLU	CB-CG-CD	-5.34	103.53	112.60
1	D	139	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	379	ASP	CB-CA-C	-5.31	100.84	109.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	GLN	CB-CA-C	5.31	119.23	109.46
1	E	175	GLU	CB-CG-CD	5.29	121.59	112.60
1	D	80	TYR	N-CA-CB	5.27	118.54	110.95
1	C	282	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	342	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	339	GLN	CB-CA-C	5.25	119.21	109.54
1	B	286	PRO	CB-CA-C	5.24	117.88	111.12
1	E	80	TYR	N-CA-CB	5.23	118.48	110.95
1	E	232	THR	CA-CB-OG1	-5.22	101.77	109.60
1	E	180	LYS	CB-CG-CD	5.21	123.29	111.30
1	B	15	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	379	ASP	CB-CA-C	-5.21	101.01	109.13
1	B	316	GLU	CB-CG-CD	-5.19	103.78	112.60
1	E	342	ASP	CA-CB-CG	5.18	117.78	112.60
1	E	105	PHE	CA-CB-CG	-5.18	108.62	113.80
1	D	95	MET	CG-SD-CE	5.17	112.28	100.90
1	B	379	ASP	CB-CA-C	-5.16	101.08	109.13
1	C	232	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	71	ARG	CG-CD-NE	-5.12	100.74	112.00
1	D	225	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	249	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	17	GLN	CB-CA-C	-5.10	100.79	109.51
1	B	157	PRO	CB-CA-C	5.08	118.02	111.46
1	B	180	LYS	N-CA-CB	5.05	117.34	110.01
1	B	71	ARG	CG-CD-NE	-5.03	100.93	112.00
1	C	188	PRO	CB-CA-C	5.03	119.04	111.44
1	A	110	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	110	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	225	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	287	GLU	CB-CA-C	5.01	117.49	109.62

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	A	71	ARG	Sidechain
1	C	144	ARG	Sidechain
1	D	140	ARG	Sidechain
1	E	140	ARG	Sidechain

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	3238	0	3153	43	1
1	B	3238	0	3153	44	0
1	C	3238	0	3155	47	0
1	D	3238	0	3155	41	0
1	E	3238	0	3155	49	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	1	0
2	D	31	0	19	0	0
2	E	31	0	19	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	16352	0	15866	223	1

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 7.

All (223) 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:E:53:CYS:HG	1:E:56:CYS:HG	0.94	0.90
1:D:53:CYS:HG	1:D:56:CYS:HG	1.05	0.86
1:A:234:MET:HE3	1:A:237:ARG:HH12	1.46	0.79
1:B:25:THR:H	1:B:234:MET:HE3	1.47	0.78
1:E:234:MET:HE3	1:E:237:ARG:HH12	1.49	0.78
1:B:153:PRO:HB2	1:B:155:MET:HE3	1.67	0.75
1:C:234:MET:HE3	1:C:237:ARG:HH12	1.51	0.74
1:D:234:MET:HE3	1:D:237:ARG:HH12	1.53	0.73
1:E:14:SER:HA	1:E:293:GLN:HE21	1.54	0.71
1:B:66:LYS:HB3	1:B:68:ILE:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LYS:HB3	1:C:68:ILE:CD1	2.22	0.70
1:C:125:TRP:CH2	1:C:188:PRO:HD2	2.27	0.69
1:D:66:LYS:HB3	1:D:68:ILE:CD1	2.22	0.69
1:E:66:LYS:HB3	1:E:68:ILE:CD1	2.22	0.69
1:A:66:LYS:HB3	1:A:68:ILE:CD1	2.22	0.69
1:D:125:TRP:CH2	1:D:188:PRO:HD2	2.28	0.69
1:E:125:TRP:CH2	1:E:188:PRO:HD2	2.29	0.68
1:B:125:TRP:CH2	1:B:188:PRO:HD2	2.29	0.67
1:A:125:TRP:CH2	1:A:188:PRO:HD2	2.29	0.67
1:E:133:LEU:HB3	1:E:134:PRO:HD3	1.78	0.64
1:E:104:ARG:HH11	1:E:104:ARG:HB2	1.65	0.61
1:A:2:ILE:HD11	1:A:333:GLU:O	2.00	0.61
1:B:117:GLU:HG2	1:B:122:PRO:HA	1.82	0.61
1:B:124:LEU:HD22	1:B:189:GLU:HB3	1.83	0.61
1:B:52:TRP:HB2	1:B:77:MET:HE1	1.83	0.61
1:E:399:ARG:HD2	1:E:399:ARG:N	2.15	0.61
1:A:117:GLU:HG2	1:A:122:PRO:HA	1.81	0.60
1:B:2:ILE:HD11	1:B:333:GLU:O	2.02	0.59
1:D:290:ASN:N	1:D:290:ASN:OD1	2.35	0.59
1:C:117:GLU:HG2	1:C:122:PRO:HA	1.84	0.59
1:D:2:ILE:HD11	1:D:333:GLU:O	2.02	0.58
1:B:290:ASN:N	1:B:290:ASN:OD1	2.36	0.58
1:A:290:ASN:OD1	1:A:290:ASN:N	2.37	0.58
1:C:290:ASN:OD1	1:C:290:ASN:N	2.36	0.58
1:D:117:GLU:HG2	1:D:122:PRO:HA	1.86	0.58
1:C:95:MET:HE3	1:C:96:LEU:H	1.68	0.57
1:A:77:MET:HE3	1:A:80:TYR:HE2	1.70	0.57
1:B:133:LEU:HB3	1:B:134:PRO:HD3	1.86	0.57
1:D:66:LYS:HB3	1:D:68:ILE:HD11	1.86	0.57
1:C:68:ILE:N	1:C:68:ILE:HD12	2.20	0.57
1:C:66:LYS:HB3	1:C:68:ILE:HD11	1.87	0.56
1:A:77:MET:HE3	1:A:80:TYR:CE2	2.41	0.56
1:A:133:LEU:HB3	1:A:134:PRO:HD3	1.87	0.56
1:A:68:ILE:N	1:A:68:ILE:HD12	2.21	0.56
1:E:290:ASN:OD1	1:E:290:ASN:N	2.37	0.56
1:A:2:ILE:CG1	1:A:333:GLU:HB3	2.36	0.56
1:A:2:ILE:HG13	1:A:333:GLU:HB3	1.88	0.56
1:C:395:PRO:HA	2:C:401:FMN:O2	2.06	0.55
1:D:104:ARG:HD3	1:D:106:TYR:OH	2.07	0.55
1:E:117:GLU:HG2	1:E:122:PRO:HA	1.87	0.55
1:E:2:ILE:HD11	1:E:333:GLU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:MET:HE3	1:C:80:TYR:CE2	2.42	0.55
1:C:83:LYS:HB3	1:C:88:LYS:HE2	1.89	0.55
1:E:68:ILE:N	1:E:68:ILE:HD12	2.22	0.55
1:E:313:ASN:ND2	1:E:317:LYS:HB2	2.22	0.55
1:B:65:GLU:CD	1:B:233:ARG:HH21	2.14	0.54
1:E:66:LYS:HB3	1:E:68:ILE:HD11	1.89	0.54
1:A:217:ARG:NH2	1:A:231:GLU:OE1	2.40	0.54
1:B:83:LYS:HB3	1:B:88:LYS:HE2	1.89	0.54
1:B:66:LYS:HB3	1:B:68:ILE:HD11	1.89	0.54
1:E:347:TYR:CE1	1:E:351:ARG:CZ	2.91	0.54
1:D:68:ILE:HD12	1:D:68:ILE:N	2.22	0.54
1:D:251:PRO:HB2	1:D:252:PRO:HD3	1.90	0.54
1:A:65:GLU:CD	1:A:233:ARG:HH21	2.16	0.54
1:C:251:PRO:HB2	1:C:252:PRO:HD3	1.89	0.54
1:C:2:ILE:HD11	1:C:333:GLU:O	2.07	0.54
1:B:68:ILE:HD12	1:B:68:ILE:N	2.23	0.54
1:A:52:TRP:HB2	1:A:77:MET:HE1	1.89	0.53
1:D:77:MET:HE3	1:D:80:TYR:CE2	2.42	0.53
1:C:52:TRP:HB2	1:C:77:MET:HE1	1.91	0.53
1:B:217:ARG:NH2	1:B:231:GLU:OE1	2.41	0.53
1:D:77:MET:HE3	1:D:80:TYR:HE2	1.73	0.53
1:C:65:GLU:CD	1:C:233:ARG:HH21	2.17	0.53
1:B:251:PRO:HB2	1:B:252:PRO:HD3	1.90	0.53
1:C:217:ARG:NH2	1:C:231:GLU:OE1	2.42	0.53
1:C:77:MET:HE3	1:C:80:TYR:HE2	1.74	0.52
1:D:351:ARG:HB3	1:D:393:GLN:HE22	1.74	0.52
1:E:217:ARG:NH2	1:E:231:GLU:OE1	2.42	0.52
1:C:53:CYS:CB	1:C:56:CYS:HG	2.23	0.52
1:E:52:TRP:HB2	1:E:77:MET:HE1	1.92	0.52
1:D:2:ILE:CG1	1:D:333:GLU:HB3	2.40	0.52
1:A:328:LEU:HD12	1:A:328:LEU:O	2.10	0.52
1:D:328:LEU:HD12	1:D:328:LEU:O	2.10	0.51
1:B:52:TRP:HB2	1:B:77:MET:CE	2.40	0.51
1:E:77:MET:HE3	1:E:80:TYR:CE2	2.45	0.51
1:D:217:ARG:NH2	1:D:231:GLU:OE1	2.43	0.51
1:E:65:GLU:CD	1:E:233:ARG:HH21	2.18	0.51
1:D:65:GLU:CD	1:D:233:ARG:HH21	2.17	0.51
1:A:351:ARG:HB3	1:A:393:GLN:HE22	1.75	0.51
1:E:2:ILE:HD11	1:E:333:GLU:HB3	1.93	0.51
1:C:351:ARG:HB3	1:C:393:GLN:HE22	1.74	0.51
1:A:83:LYS:HB3	1:A:88:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ILE:HD11	1:C:333:GLU:HB3	1.94	0.50
1:A:52:TRP:HB2	1:A:77:MET:CE	2.41	0.50
1:A:66:LYS:HB3	1:A:68:ILE:HD11	1.91	0.50
1:B:328:LEU:HD12	1:B:328:LEU:O	2.11	0.50
1:E:200:TYR:HB3	1:E:204:MET:HE3	1.94	0.50
1:D:24:PRO:HB3	1:D:234:MET:SD	2.52	0.50
1:B:77:MET:HE3	1:B:80:TYR:CE2	2.47	0.50
1:C:52:TRP:HB2	1:C:77:MET:CE	2.42	0.50
1:E:24:PRO:HB3	1:E:234:MET:SD	2.52	0.49
1:E:77:MET:HE3	1:E:80:TYR:HE2	1.77	0.49
1:A:7:TRP:CE2	1:A:303:HIS:CD2	3.01	0.49
1:B:351:ARG:HB3	1:B:393:GLN:HE22	1.76	0.49
1:B:7:TRP:CE2	1:B:303:HIS:CD2	3.01	0.49
1:D:7:TRP:CE2	1:D:303:HIS:CD2	3.00	0.49
1:D:52:TRP:HB2	1:D:77:MET:HE1	1.94	0.49
1:D:343:GLN:HE21	1:D:380:SER:HB3	1.78	0.49
1:E:7:TRP:CE2	1:E:303:HIS:CD2	3.01	0.49
1:D:377:VAL:O	1:D:377:VAL:HG23	2.13	0.49
1:E:2:ILE:CG1	1:E:333:GLU:HB3	2.43	0.48
1:C:7:TRP:CE2	1:C:303:HIS:CD2	3.01	0.48
1:E:377:VAL:HG23	1:E:377:VAL:O	2.13	0.48
1:A:377:VAL:HG23	1:A:377:VAL:O	2.12	0.48
1:B:2:ILE:CG1	1:B:333:GLU:HB3	2.43	0.48
1:D:200:TYR:HB3	1:D:204:MET:HE3	1.95	0.48
1:E:3:THR:HB	1:E:4:PRO:HD2	1.96	0.48
1:C:200:TYR:HB3	1:C:204:MET:HE3	1.96	0.48
1:D:53:CYS:CB	1:D:56:CYS:HG	2.26	0.48
1:E:83:LYS:HB3	1:E:88:LYS:HE2	1.96	0.48
1:E:328:LEU:HD12	1:E:328:LEU:O	2.13	0.47
1:E:351:ARG:HB3	1:E:393:GLN:HE22	1.79	0.47
1:C:2:ILE:CG1	1:C:333:GLU:HB3	2.44	0.47
1:D:243:PHE:CD1	1:D:282:ASP:HB3	2.50	0.47
1:A:251:PRO:HB2	1:A:252:PRO:HD3	1.97	0.47
1:D:52:TRP:HB2	1:D:77:MET:CE	2.44	0.47
1:E:251:PRO:HB2	1:E:252:PRO:HD3	1.97	0.47
1:E:395:PRO:HA	2:E:401:FMN:O2	2.15	0.47
1:C:243:PHE:CD1	1:C:282:ASP:HB3	2.50	0.46
1:B:329:LEU:HD11	1:B:365:HIS:HB3	1.97	0.46
1:E:52:TRP:HB2	1:E:77:MET:CE	2.44	0.46
1:E:104:ARG:HD3	1:E:106:TYR:CZ	2.49	0.46
1:B:2:ILE:HD11	1:B:333:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:PHE:CD1	1:E:282:ASP:HB3	2.50	0.46
1:B:343:GLN:HE21	1:B:380:SER:HB3	1.81	0.46
1:B:377:VAL:HG23	1:B:377:VAL:O	2.14	0.46
1:D:66:LYS:CB	1:D:68:ILE:CD1	2.94	0.46
1:D:210:TYR:CZ	1:D:269:GLN:HG3	2.51	0.46
1:E:343:GLN:HE21	1:E:380:SER:HB3	1.81	0.46
1:B:107:THR:O	1:B:108:GLU:HB2	2.15	0.46
1:D:2:ILE:HG13	1:D:333:GLU:HB3	1.97	0.46
1:A:2:ILE:HD11	1:A:333:GLU:HB3	1.98	0.45
1:B:77:MET:HE3	1:B:80:TYR:HE2	1.80	0.45
1:B:187:LEU:HB3	1:B:188:PRO:CD	2.46	0.45
1:C:358:MET:HE2	1:C:358:MET:HB3	1.71	0.45
1:D:187:LEU:HB3	1:D:188:PRO:CD	2.46	0.45
1:B:243:PHE:CD1	1:B:282:ASP:HB3	2.51	0.45
1:B:200:TYR:HB3	1:B:204:MET:HE3	1.98	0.45
1:E:377:VAL:O	1:E:377:VAL:CG2	2.65	0.45
1:A:66:LYS:CB	1:A:68:ILE:CD1	2.94	0.45
1:A:200:TYR:HB3	1:A:204:MET:HE3	1.99	0.45
1:C:377:VAL:HG23	1:C:377:VAL:O	2.17	0.45
1:E:107:THR:O	1:E:108:GLU:HB2	2.16	0.45
1:B:250:LEU:N	1:B:251:PRO:CD	2.80	0.45
1:C:345:LEU:HD11	1:C:373:THR:HG22	1.99	0.45
1:D:107:THR:O	1:D:108:GLU:HB2	2.17	0.45
1:A:377:VAL:O	1:A:377:VAL:CG2	2.65	0.45
1:C:104:ARG:HD2	1:C:106:TYR:OH	2.17	0.45
1:C:149:TRP:CZ2	1:C:164:GLN:HB2	2.52	0.45
1:C:250:LEU:N	1:C:251:PRO:CD	2.80	0.45
1:A:250:LEU:N	1:A:251:PRO:CD	2.80	0.44
1:C:343:GLN:HE21	1:C:380:SER:HB3	1.81	0.44
1:E:250:LEU:N	1:E:251:PRO:CD	2.80	0.44
1:A:95:MET:HE3	1:A:96:LEU:H	1.82	0.44
1:C:234:MET:CE	1:C:237:ARG:HH12	2.27	0.44
1:C:328:LEU:O	1:C:328:LEU:HD12	2.17	0.44
1:D:7:TRP:CE2	1:D:323:ARG:HD3	2.53	0.44
1:D:250:LEU:N	1:D:251:PRO:CD	2.80	0.44
1:A:7:TRP:CE2	1:A:323:ARG:HD3	2.53	0.44
1:B:7:TRP:CE2	1:B:323:ARG:HD3	2.53	0.44
1:C:24:PRO:HB3	1:C:234:MET:SD	2.58	0.44
1:A:187:LEU:HB3	1:A:188:PRO:CD	2.48	0.44
1:E:124:LEU:HD22	1:E:189:GLU:HB2	2.00	0.44
1:D:2:ILE:HD11	1:D:333:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:VAL:O	1:D:377:VAL:CG2	2.66	0.44
1:A:24:PRO:HB3	1:A:234:MET:SD	2.57	0.43
1:A:210:TYR:CZ	1:A:269:GLN:HG2	2.53	0.43
1:A:343:GLN:HE21	1:A:380:SER:HB3	1.83	0.43
1:B:377:VAL:O	1:B:377:VAL:CG2	2.66	0.43
1:C:107:THR:O	1:C:108:GLU:HB2	2.19	0.43
1:E:66:LYS:CB	1:E:68:ILE:CD1	2.95	0.43
1:C:377:VAL:O	1:C:377:VAL:CG2	2.66	0.43
1:E:187:LEU:HB3	1:E:188:PRO:CD	2.48	0.43
1:B:343:GLN:HG2	1:B:380:SER:HB2	2.00	0.43
1:B:345:LEU:HD11	1:B:373:THR:HG22	2.00	0.43
1:A:243:PHE:CD1	1:A:282:ASP:HB3	2.53	0.43
1:D:277:TRP:NE1	1:D:367:ARG:HD2	2.34	0.43
1:A:277:TRP:NE1	1:A:367:ARG:HD2	2.34	0.43
1:A:104:ARG:HB2	1:A:104:ARG:HH11	1.83	0.43
1:C:16:TYR:HD1	1:C:16:TYR:H	1.67	0.43
1:C:210:TYR:CZ	1:C:269:GLN:HG2	2.54	0.43
1:D:149:TRP:CZ2	1:D:164:GLN:HB2	2.53	0.43
1:E:7:TRP:CE2	1:E:323:ARG:HD3	2.54	0.43
1:E:149:TRP:CZ2	1:E:164:GLN:HB2	2.53	0.43
1:D:329:LEU:HD11	1:D:365:HIS:HB3	2.01	0.43
1:A:2:ILE:H	1:A:2:ILE:HD12	1.83	0.42
1:C:187:LEU:HB3	1:C:188:PRO:CD	2.49	0.42
1:B:66:LYS:CB	1:B:68:ILE:CD1	2.95	0.42
1:C:7:TRP:CE2	1:C:323:ARG:HD3	2.54	0.42
1:C:124:LEU:HD22	1:C:189:GLU:HB2	2.02	0.42
1:B:149:TRP:CZ2	1:B:164:GLN:HB2	2.55	0.42
1:B:3:THR:HB	1:B:4:PRO:HD2	2.01	0.42
1:B:125:TRP:CZ2	1:C:2:ILE:HG21	2.56	0.41
1:E:347:TYR:CE1	1:E:351:ARG:NE	2.89	0.41
1:E:329:LEU:HD12	1:E:329:LEU:HA	1.86	0.41
1:A:2:ILE:CD1	1:A:333:GLU:HB3	2.51	0.41
1:A:358:MET:HB3	1:A:358:MET:HE2	1.68	0.41
1:C:3:THR:HB	1:C:4:PRO:HD2	2.02	0.41
1:D:399:ARG:CG	1:D:399:ARG:HH11	2.34	0.41
1:E:358:MET:HE2	1:E:358:MET:HB3	1.74	0.41
1:B:154:ALA:O	1:B:155:MET:HE2	2.21	0.41
1:B:277:TRP:NE1	1:B:367:ARG:HD2	2.36	0.41
1:B:210:TYR:CZ	1:B:269:GLN:HG2	2.56	0.41
1:C:320:GLN:HG2	1:C:338:PRO:HD3	2.03	0.41
1:C:343:GLN:HG2	1:C:380:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:GLN:HE21	1:D:269:GLN:HB2	1.44	0.41
1:E:48:ASP:HB2	1:E:77:MET:HG3	2.02	0.41
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.98	0.40
1:A:3:THR:HB	1:A:4:PRO:HD2	2.03	0.40
1:A:345:LEU:HD11	1:A:373:THR:HG22	2.02	0.40
1:A:149:TRP:CZ2	1:A:164:GLN:HB2	2.56	0.40
1:C:146:TRP:CD1	1:C:204:MET:HG2	2.57	0.40
1:E:345:LEU:HD11	1:E:373:THR:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:OH	1:A:152:TYR:OH[3_454]	2.12	0.08

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	397/399 (100%)	381 (96%)	15 (4%)	1 (0%)	36	59
1	B	397/399 (100%)	379 (96%)	17 (4%)	1 (0%)	36	59
1	C	397/399 (100%)	381 (96%)	15 (4%)	1 (0%)	36	59
1	D	397/399 (100%)	379 (96%)	17 (4%)	1 (0%)	36	59
1	E	397/399 (100%)	381 (96%)	15 (4%)	1 (0%)	36	59
All	All	1985/1995 (100%)	1901 (96%)	79 (4%)	5 (0%)	36	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLU

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Mol	Chain	Res	Type
1	B	108	GLU
1	C	108	GLU
1	D	108	GLU
1	E	108	GLU

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	345/345 (100%)	325 (94%)	20 (6%)	18	41
1	B	345/345 (100%)	327 (95%)	18 (5%)	21	45
1	C	345/345 (100%)	326 (94%)	19 (6%)	19	43
1	D	345/345 (100%)	330 (96%)	15 (4%)	26	52
1	E	345/345 (100%)	324 (94%)	21 (6%)	17	38
All	All	1725/1725 (100%)	1632 (95%)	93 (5%)	20	43

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	15	ASP
1	A	28	GLN
1	A	53	CYS
1	A	73	LYS
1	A	89	LYS
1	A	104	ARG
1	A	105	PHE
1	A	114	ILE
1	A	191	SER
1	A	196	VAL
1	A	222	ARG
1	A	234	MET
1	A	285	CYS
1	A	291	VAL

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Mol	Chain	Res	Type
1	A	324	CYS
1	A	328	LEU
1	A	360	ILE
1	A	377	VAL
1	A	399	ARG
1	B	2	ILE
1	B	13	LEU
1	B	15	ASP
1	B	39	GLU
1	B	53	CYS
1	B	114	ILE
1	B	141	LEU
1	B	191	SER
1	B	196	VAL
1	B	222	ARG
1	B	266	GLN
1	B	289	GLU
1	B	324	CYS
1	B	360	ILE
1	B	368	GLN
1	B	377	VAL
1	B	387	VAL
1	B	399	ARG
1	C	2	ILE
1	C	13	LEU
1	C	28	GLN
1	C	95	MET
1	C	114	ILE
1	C	161	GLN
1	C	176	LYS
1	C	191	SER
1	C	196	VAL
1	C	217	ARG
1	C	222	ARG
1	C	291	VAL
1	C	293	GLN
1	C	314	GLN
1	C	324	CYS
1	C	360	ILE
1	C	377	VAL
1	C	387	VAL
1	C	399	ARG

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Mol	Chain	Res	Type
1	D	2	ILE
1	D	28	GLN
1	D	39	GLU
1	D	104	ARG
1	D	114	ILE
1	D	191	SER
1	D	196	VAL
1	D	217	ARG
1	D	222	ARG
1	D	234	MET
1	D	293	GLN
1	D	314	GLN
1	D	324	CYS
1	D	377	VAL
1	D	399	ARG
1	E	2	ILE
1	E	28	GLN
1	E	89	LYS
1	E	104	ARG
1	E	114	ILE
1	E	161	GLN
1	E	176	LYS
1	E	191	SER
1	E	196	VAL
1	E	222	ARG
1	E	234	MET
1	E	266	GLN
1	E	291	VAL
1	E	314	GLN
1	E	324	CYS
1	E	333	GLU
1	E	339	GLN
1	E	360	ILE
1	E	377	VAL
1	E	387	VAL
1	E	399	ARG

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

Mol	Chain	Res	Type
1	A	148	ASN
1	A	161	GLN

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Mol	Chain	Res	Type
1	D	269	GLN
1	E	42	GLN
1	E	293	GLN
1	E	303	HIS
1	E	313	ASN

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 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\# Z > 2$
2	FMN	B	401	-	33,33,33	0.76	0	48,50,50	0.95	2 (4%)
2	FMN	A	401	-	33,33,33	0.85	1 (3%)	48,50,50	1.01	2 (4%)
2	FMN	C	401	-	33,33,33	0.73	0	48,50,50	1.32	6 (12%)
2	FMN	D	401	-	33,33,33	0.69	0	48,50,50	0.85	1 (2%)
2	FMN	E	401	-	33,33,33	0.64	0	48,50,50	1.04	4 (8%)

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
2	FMN	B	401	-	-	0/18/18/18	0/3/3/3
2	FMN	A	401	-	-	4/18/18/18	0/3/3/3
2	FMN	C	401	-	-	5/18/18/18	0/3/3/3
2	FMN	D	401	-	-	3/18/18/18	0/3/3/3
2	FMN	E	401	-	-	0/18/18/18	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C1'-C2'	-3.40	1.47	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FMN	O5'-C5'-C4'	-3.94	98.85	109.36
2	C	401	FMN	C4'-C3'-C2'	3.49	119.38	113.57
2	E	401	FMN	C4'-C3'-C2'	3.48	119.36	113.57
2	B	401	FMN	O3P-P-O5'	-2.97	98.92	106.67
2	C	401	FMN	O3P-P-O2P	2.69	117.89	107.80
2	C	401	FMN	O2P-P-O5'	-2.62	99.83	106.67
2	D	401	FMN	C4'-C3'-C2'	2.57	117.85	113.57
2	E	401	FMN	O5'-C5'-C4'	-2.47	102.78	109.36
2	C	401	FMN	O2'-C2'-C3'	2.43	114.94	109.25
2	C	401	FMN	C1'-C2'-C3'	-2.33	103.34	109.66
2	A	401	FMN	C4-N3-C2	-2.29	121.57	125.64
2	E	401	FMN	C4-N3-C2	-2.25	121.64	125.64
2	B	401	FMN	C9-C9A-N10	2.22	124.84	121.85
2	A	401	FMN	O4-C4-C4A	-2.15	120.85	126.53
2	E	401	FMN	C4A-C4-N3	2.01	118.36	113.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FMN	C5'-O5'-P-O2P
2	A	401	FMN	C5'-O5'-P-O3P
2	C	401	FMN	C3'-C4'-C5'-O5'
2	C	401	FMN	O4'-C4'-C5'-O5'

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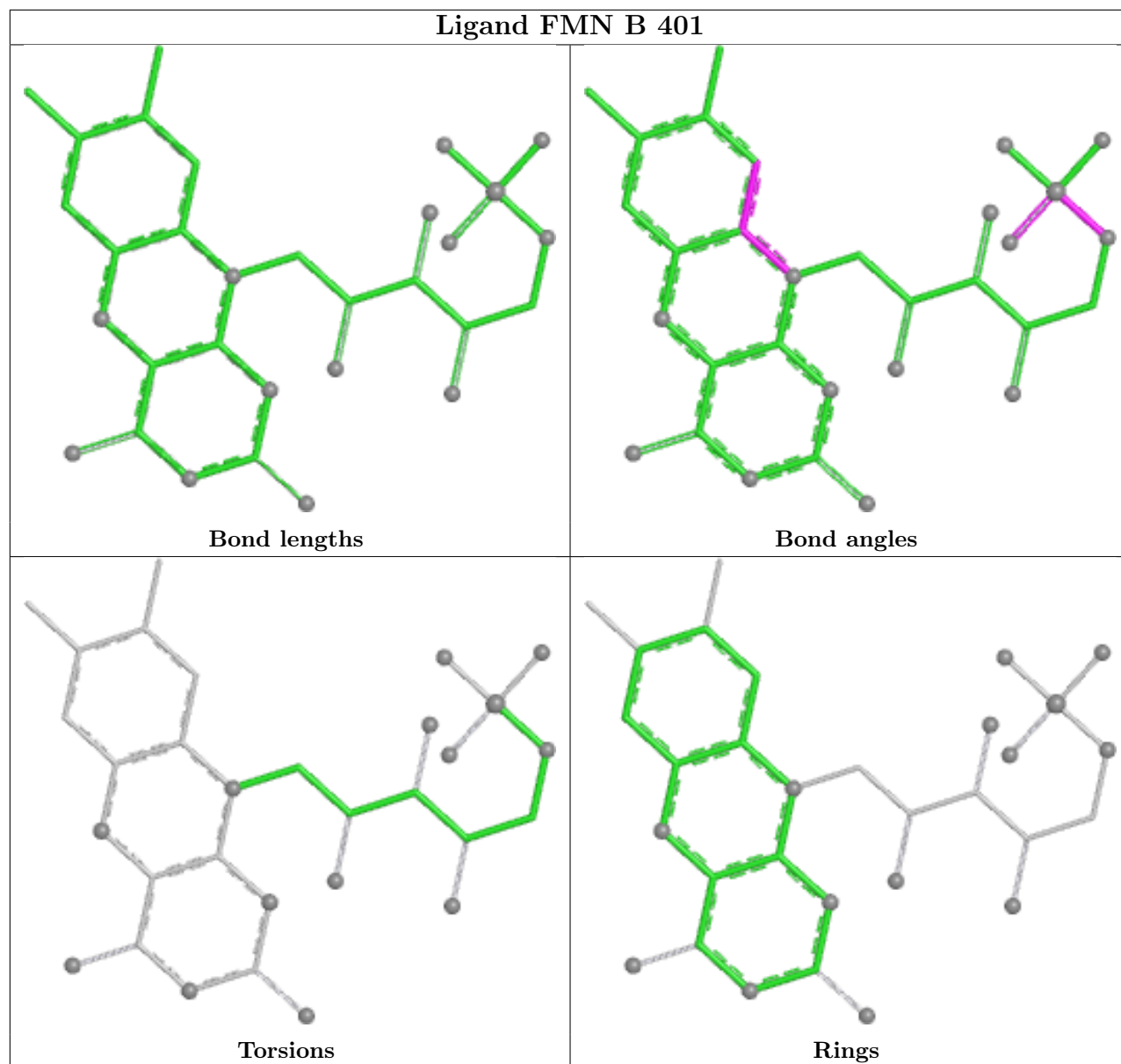
Mol	Chain	Res	Type	Atoms
2	C	401	FMN	C5'-O5'-P-O2P
2	C	401	FMN	C5'-O5'-P-O3P
2	D	401	FMN	C5'-O5'-P-O2P
2	D	401	FMN	C5'-O5'-P-O3P
2	A	401	FMN	C5'-O5'-P-O1P
2	C	401	FMN	C5'-O5'-P-O1P
2	D	401	FMN	C5'-O5'-P-O1P
2	A	401	FMN	C4'-C5'-O5'-P

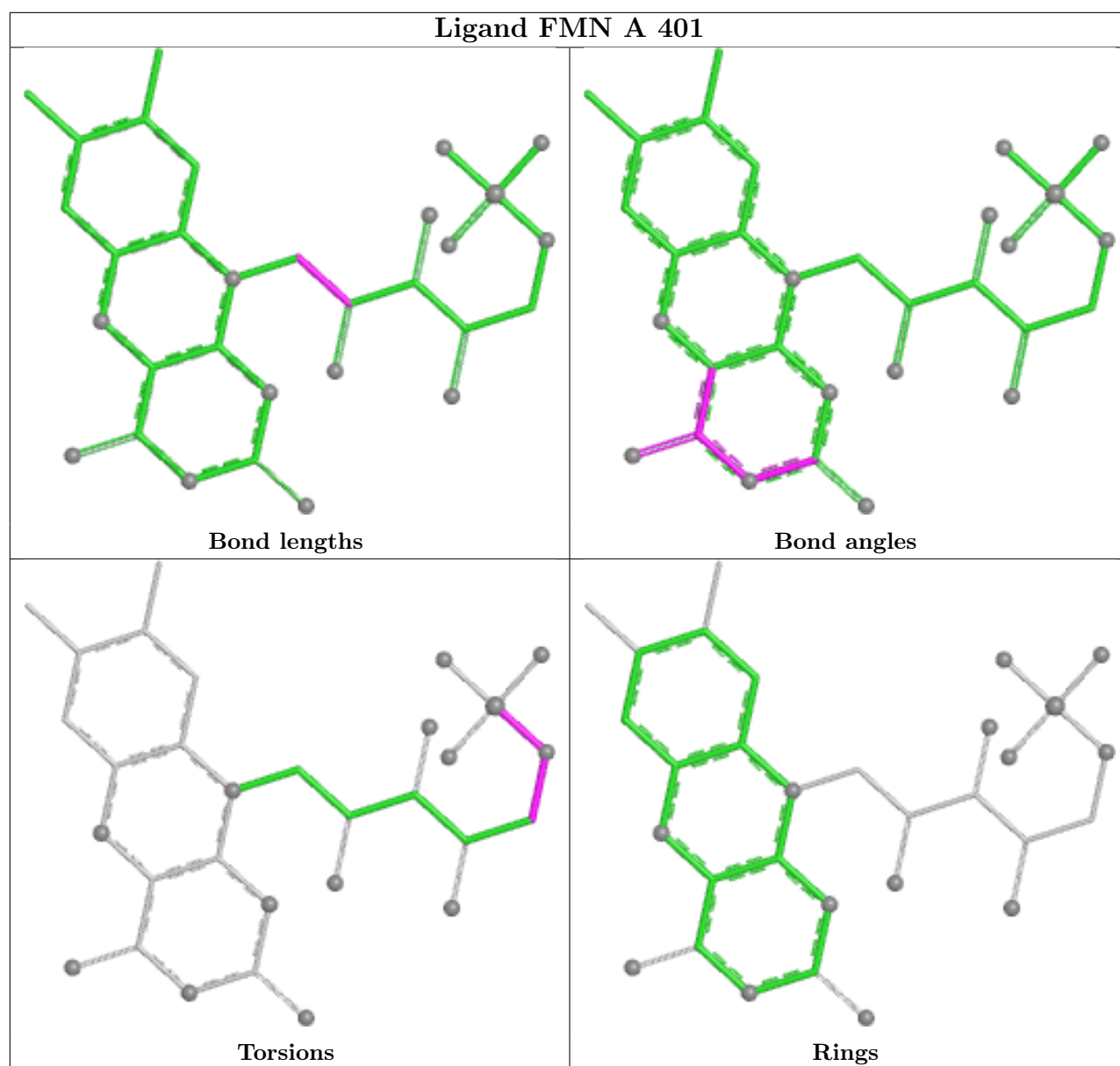
There are no ring outliers.

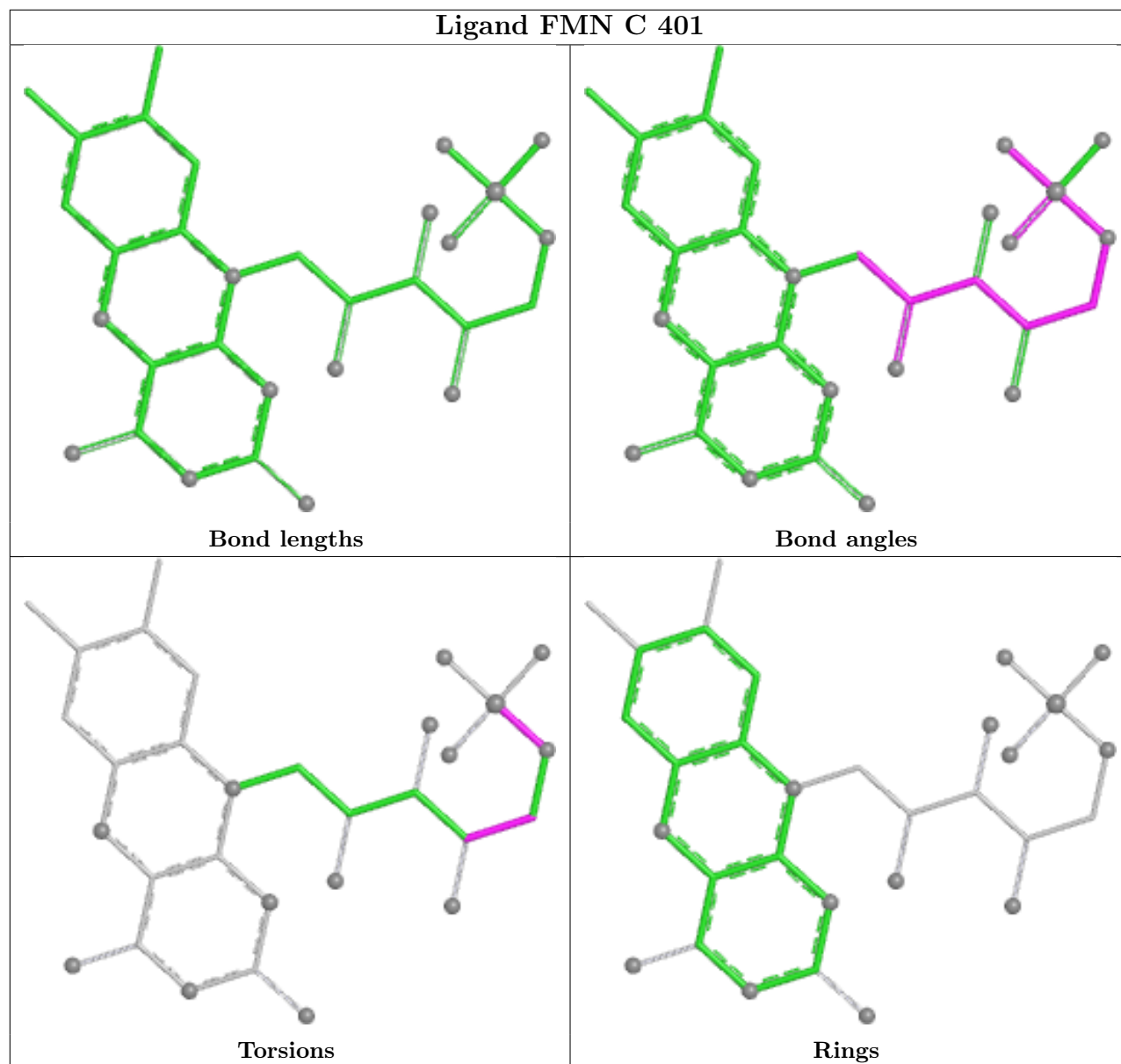
2 monomers are involved in 2 short contacts:

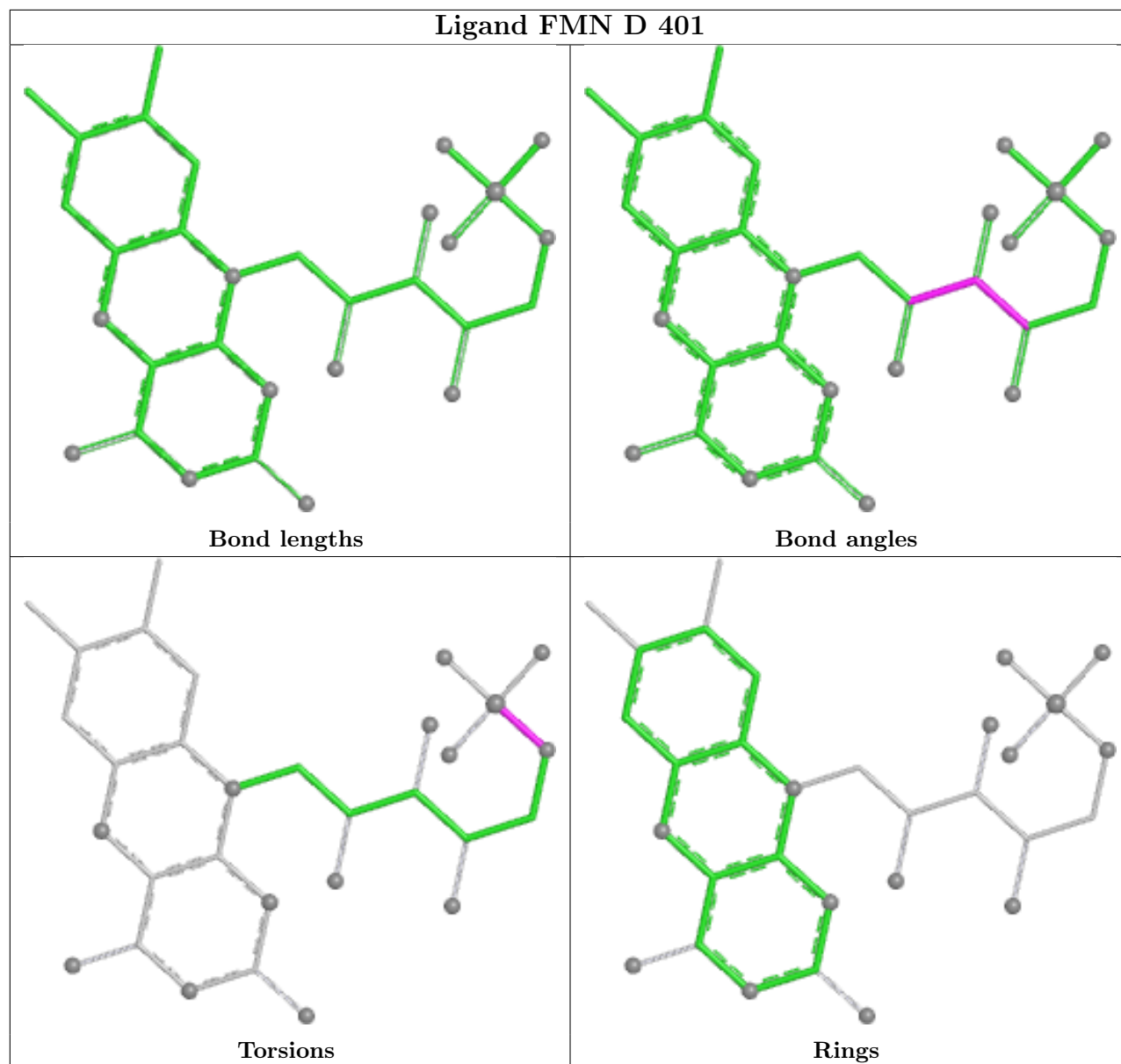
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	FMN	1	0
2	E	401	FMN	1	0

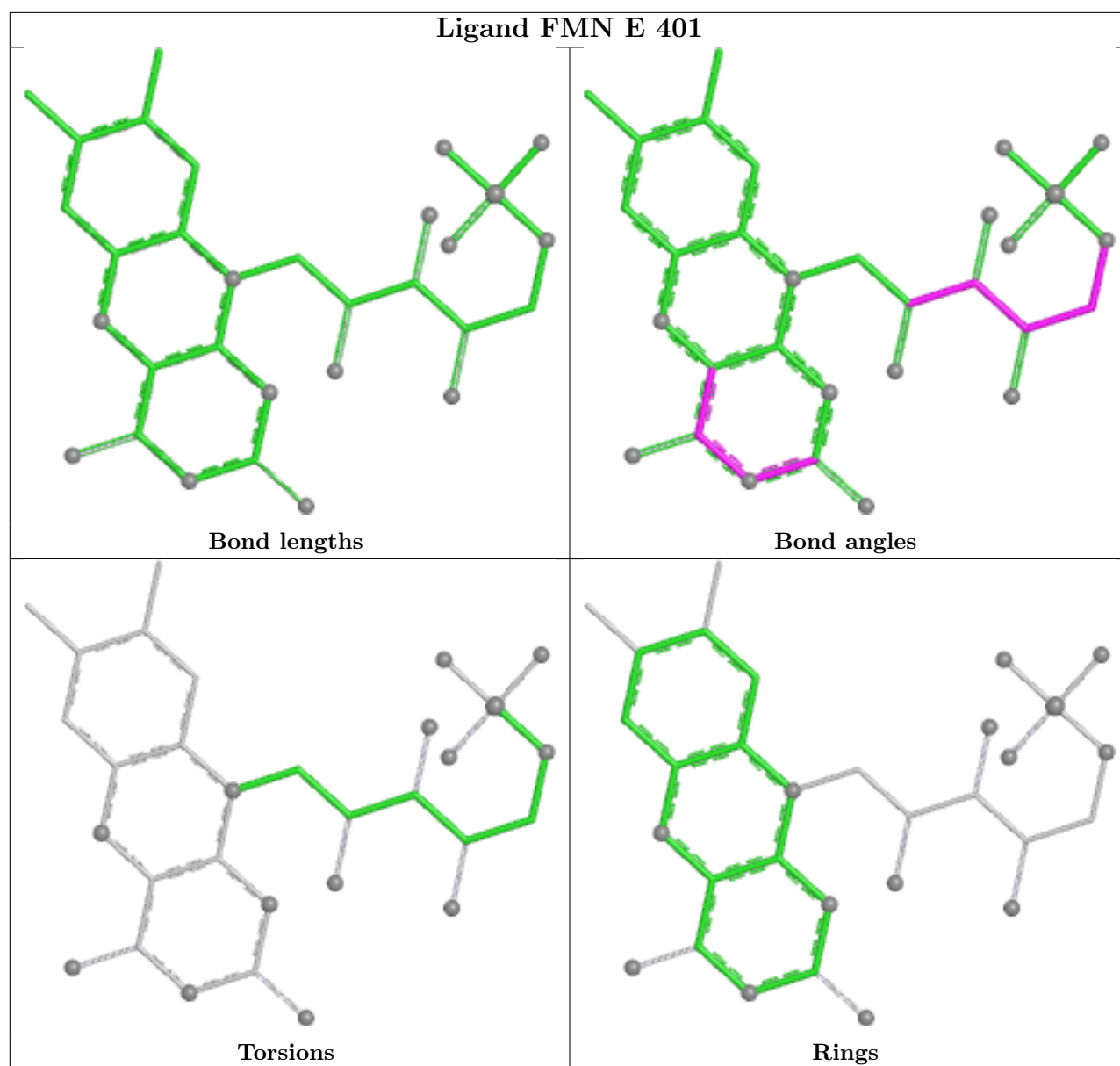
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/399 (100%)	-0.43	4 (1%) 79 78	37, 57, 89, 126	0
1	B	399/399 (100%)	-0.22	3 (0%) 82 81	43, 67, 97, 120	0
1	C	399/399 (100%)	0.21	5 (1%) 75 73	51, 73, 106, 137	0
1	D	399/399 (100%)	0.19	11 (2%) 55 52	49, 78, 115, 145	0
1	E	399/399 (100%)	0.31	8 (2%) 65 62	57, 89, 147, 170	0
All	All	1995/1995 (100%)	0.01	31 (1%) 70 68	37, 73, 121, 170	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	286	PRO	4.0
1	B	95	MET	3.8
1	A	95	MET	3.4
1	E	18	VAL	3.4
1	A	340	GLY	3.3
1	E	95	MET	3.2
1	D	285	CYS	3.2
1	D	131	LEU	3.1
1	E	376	LEU	3.0
1	E	157	PRO	3.0
1	D	399	ARG	2.7
1	E	317	LYS	2.7
1	A	399	ARG	2.6
1	D	186	PHE	2.6
1	B	399	ARG	2.6
1	D	188	PRO	2.5
1	D	14	SER	2.5
1	D	95	MET	2.4
1	C	105	PHE	2.4
1	E	326	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	255	GLY	2.3
1	C	1	MET	2.2
1	E	16	TYR	2.2
1	A	339	GLN	2.2
1	D	125	TRP	2.1
1	D	123	LEU	2.1
1	C	399	ARG	2.1
1	D	171	VAL	2.1
1	E	5	LEU	2.0
1	B	4	PRO	2.0
1	C	90	LEU	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](#)

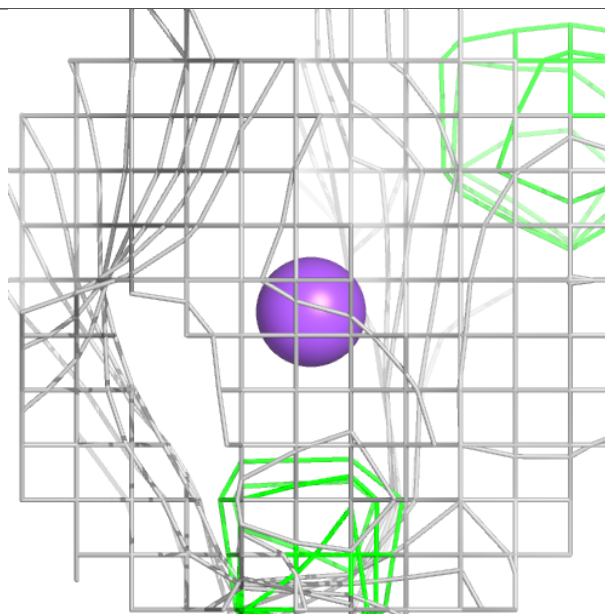
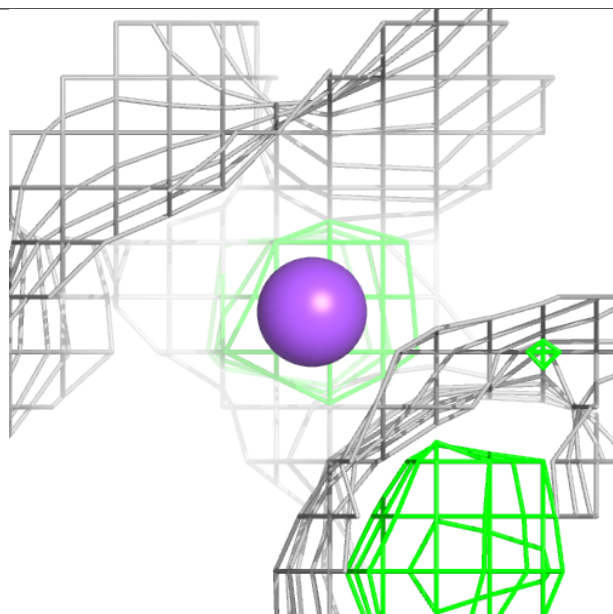
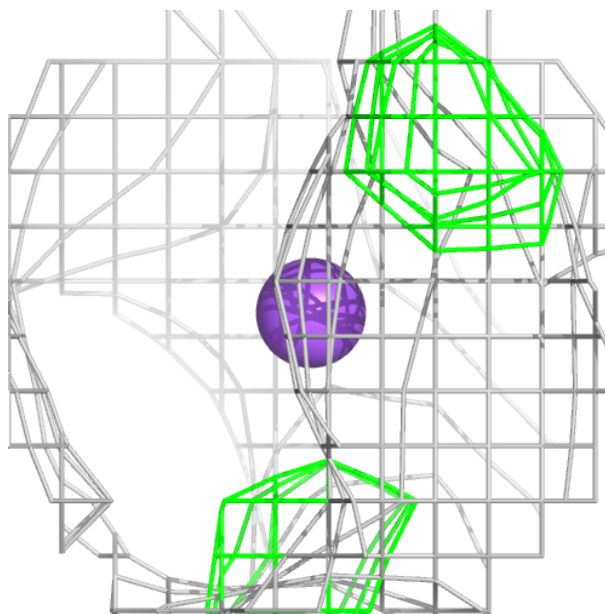
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	NA	C	403	1/1	0.82	0.15	96,96,96,96	0
3	CL	D	402	1/1	0.91	0.10	71,71,71,71	0
4	NA	A	403	1/1	0.92	0.11	65,65,65,65	0
2	FMN	E	401	31/31	0.94	0.09	73,95,111,121	0
2	FMN	C	401	31/31	0.94	0.08	48,67,88,97	0
3	CL	C	402	1/1	0.96	0.07	64,64,64,64	0
2	FMN	B	401	31/31	0.97	0.06	39,54,62,68	0
3	CL	E	402	1/1	0.97	0.07	64,64,64,64	0
3	CL	B	402	1/1	0.97	0.08	60,60,60,60	0
2	FMN	D	401	31/31	0.97	0.06	46,63,71,77	0
2	FMN	A	401	31/31	0.98	0.05	36,44,53,57	0
3	CL	A	402	1/1	0.99	0.04	56,56,56,56	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.

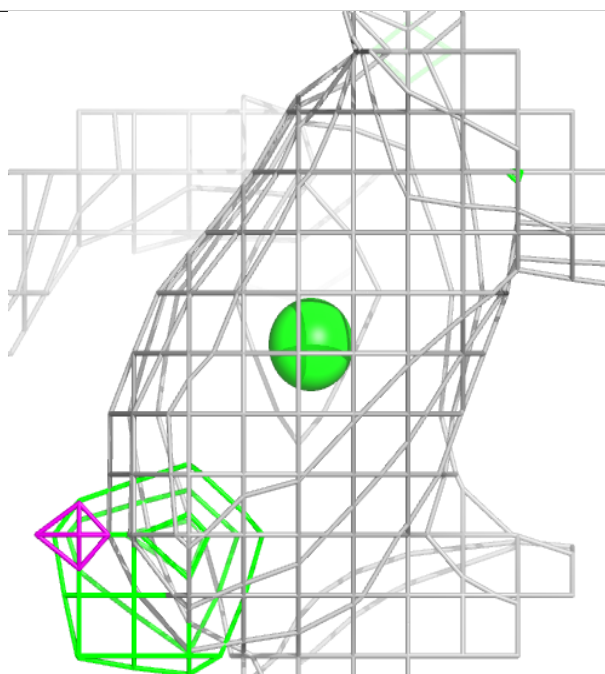
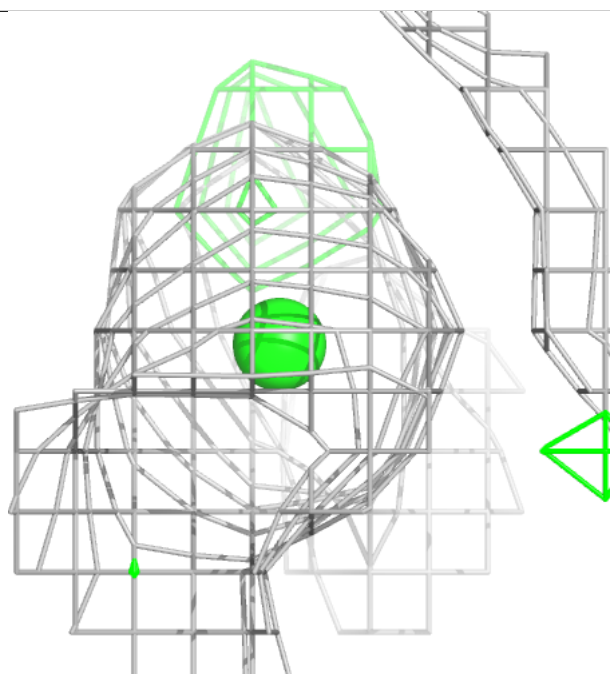
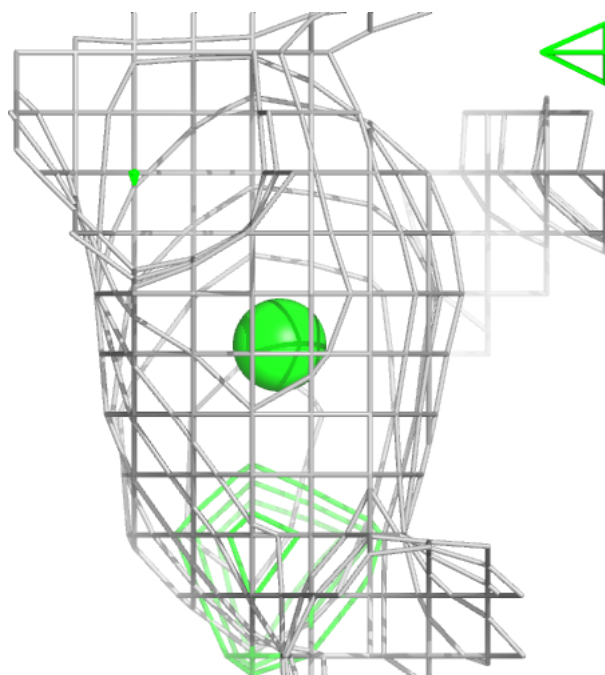
Electron density around NA C 403:

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



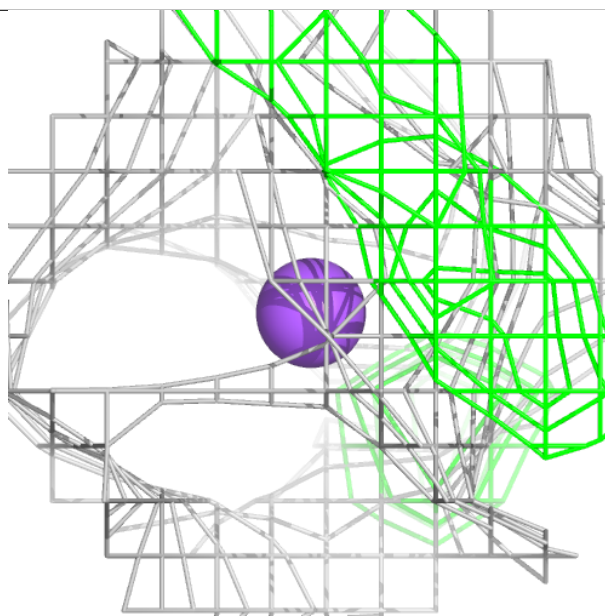
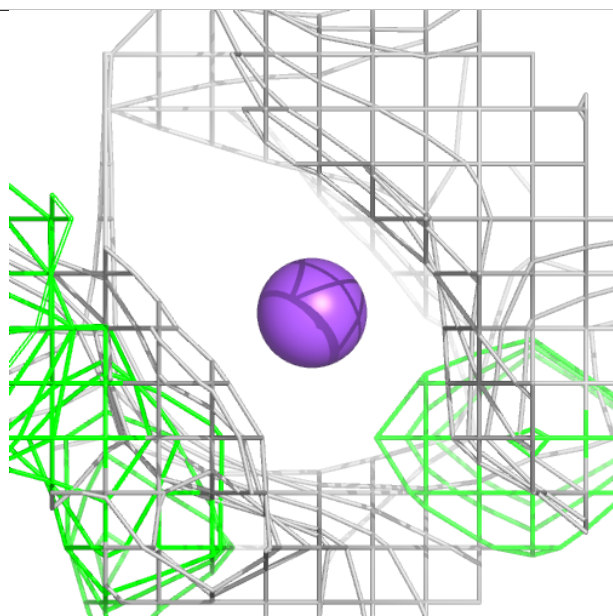
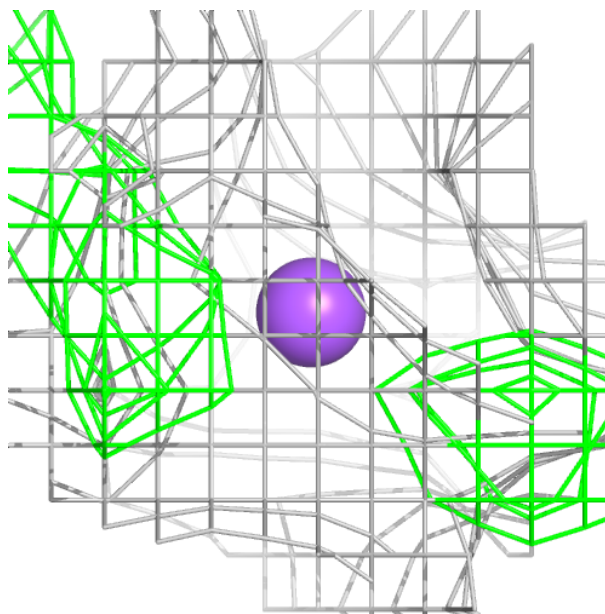
Electron density around CL D 402:

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



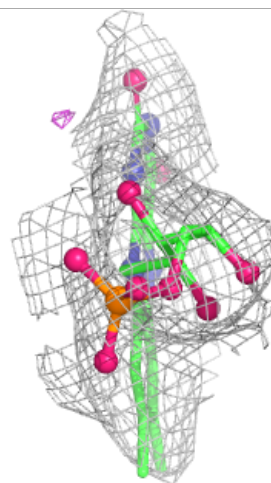
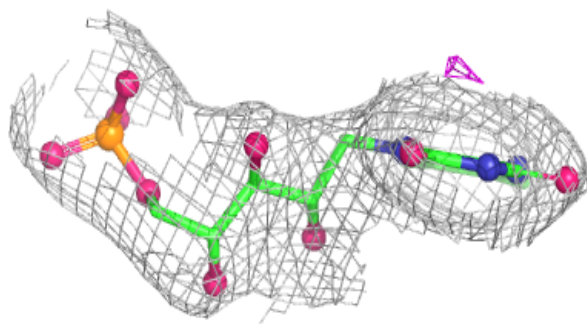
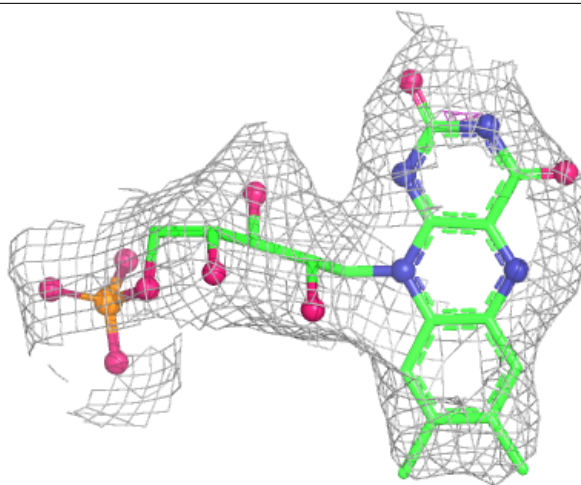
Electron density around NA A 403:

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and green (positive)



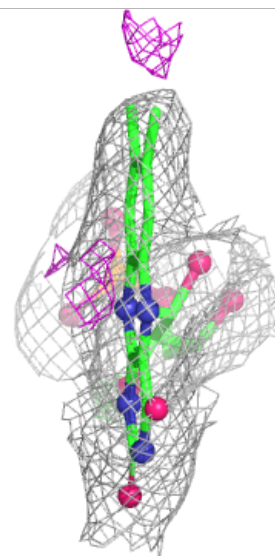
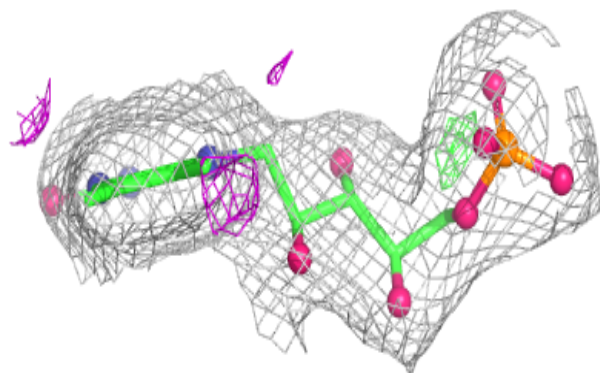
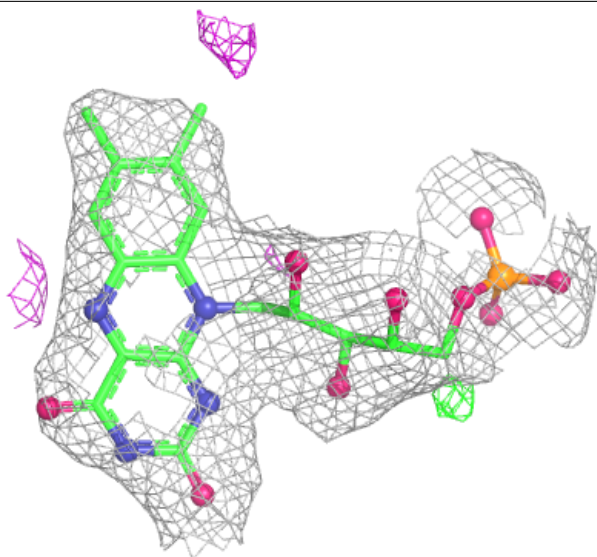
Electron density around FMN E 401:

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and green (positive)



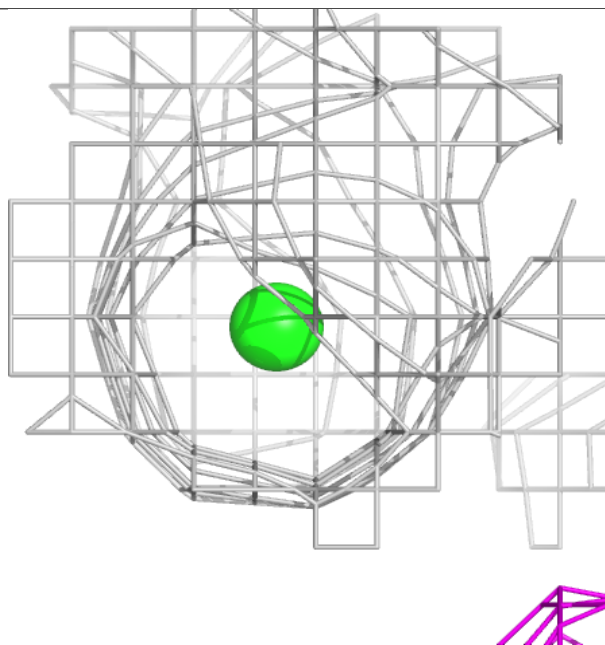
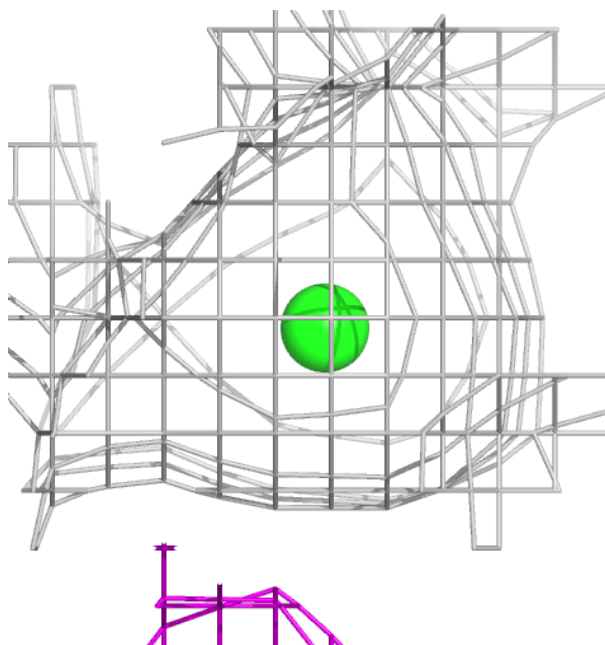
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and green (positive)



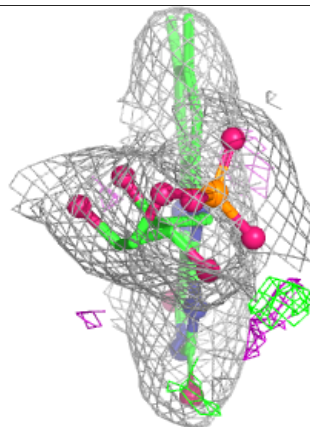
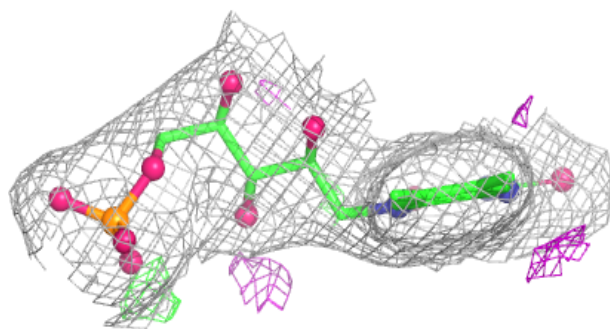
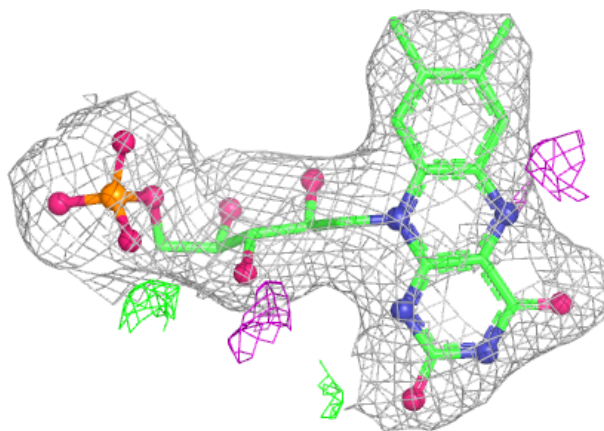
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and green (positive)



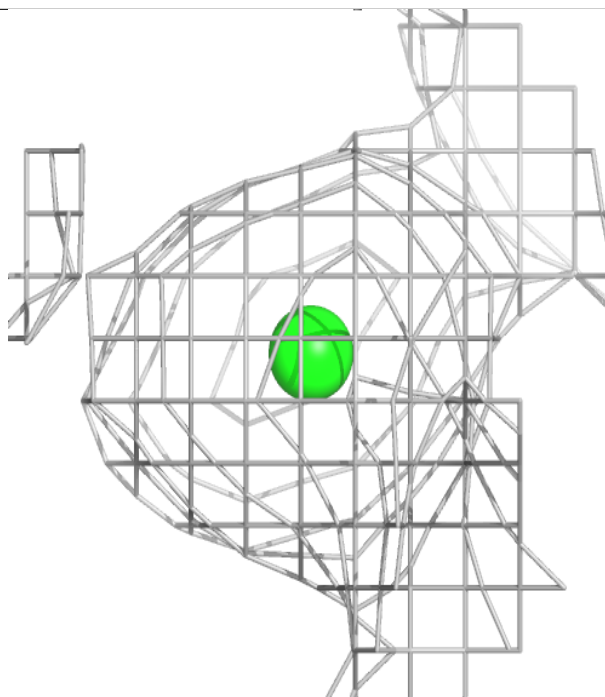
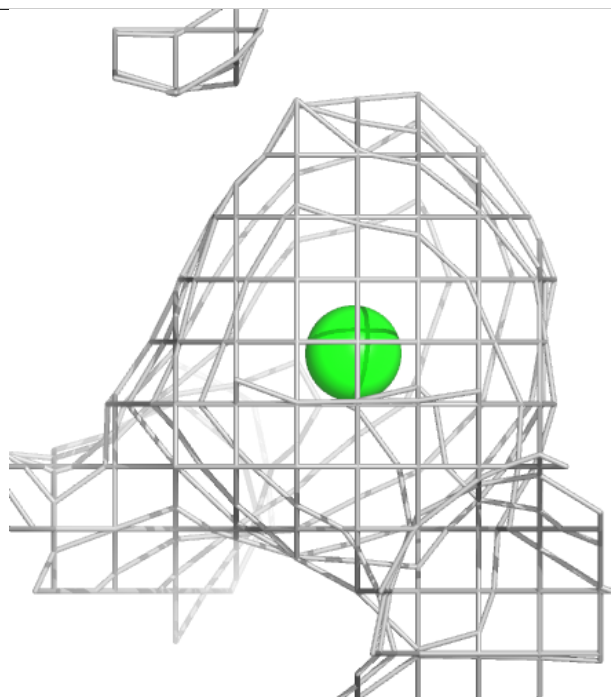
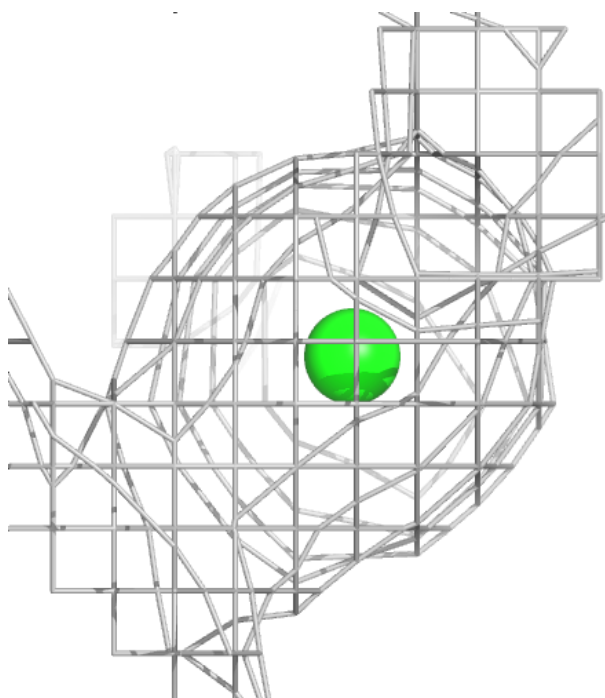
Electron density around FMN B 401:

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and green (positive)



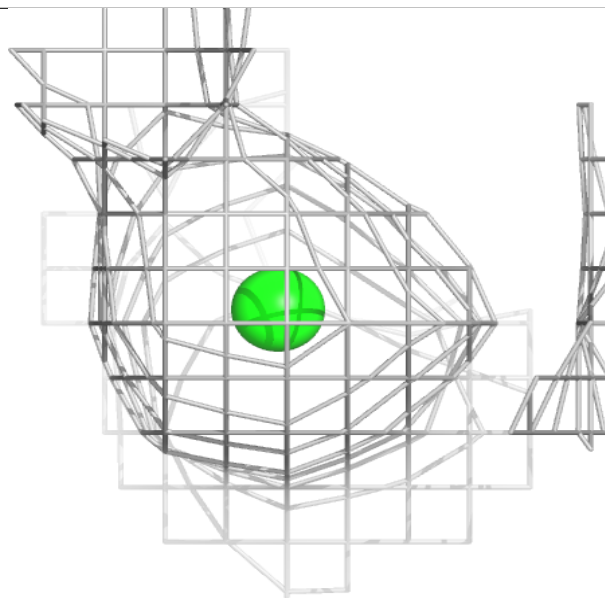
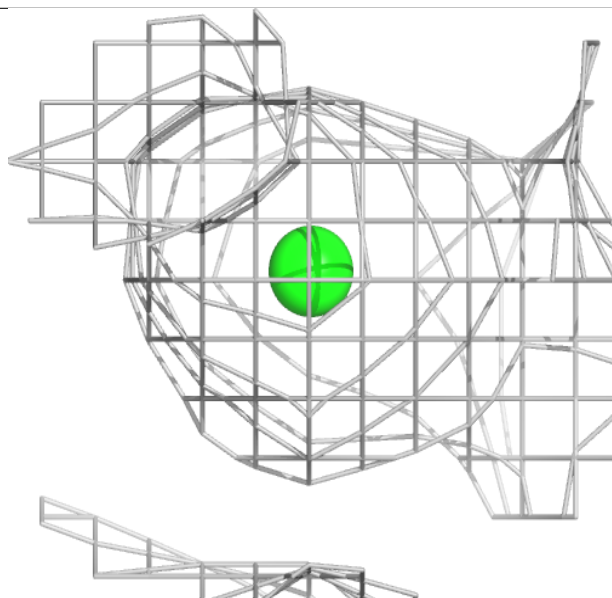
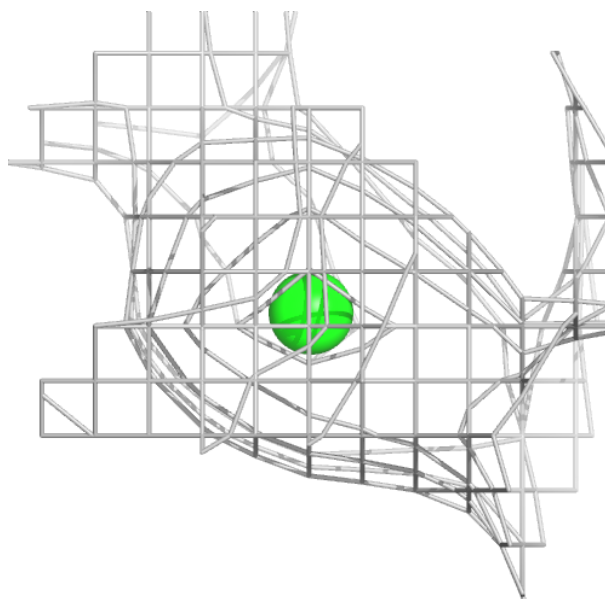
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



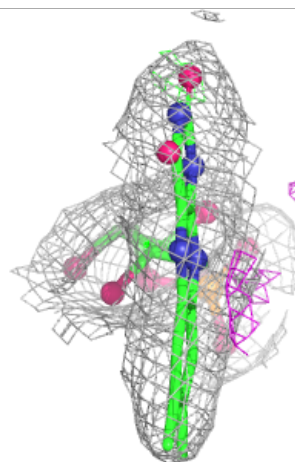
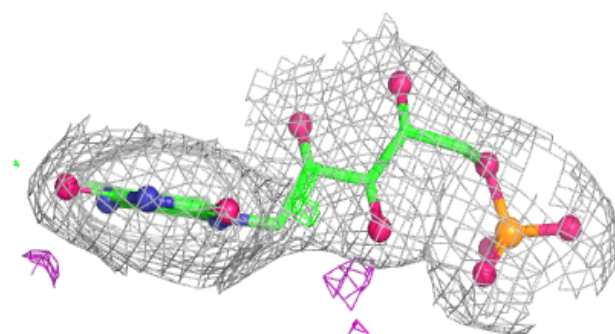
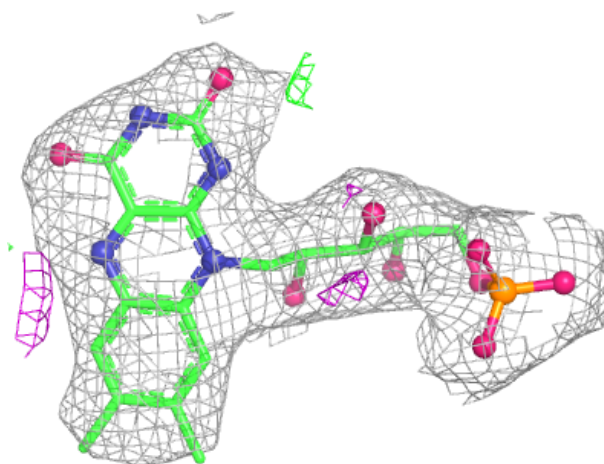
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and green (positive)



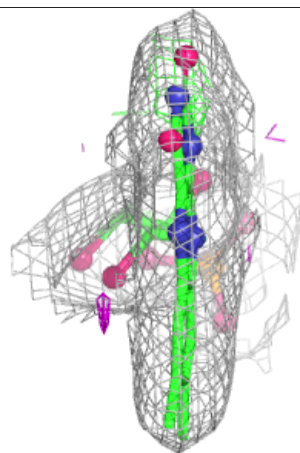
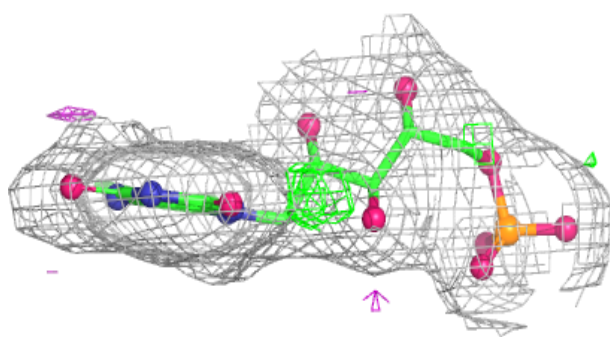
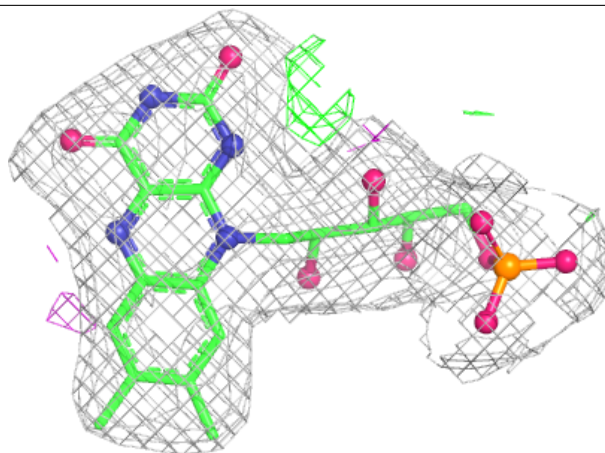
Electron density around FMN D 401:

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



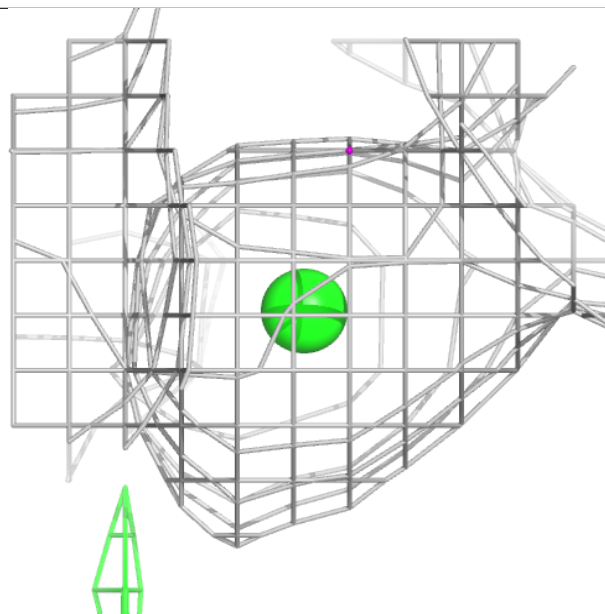
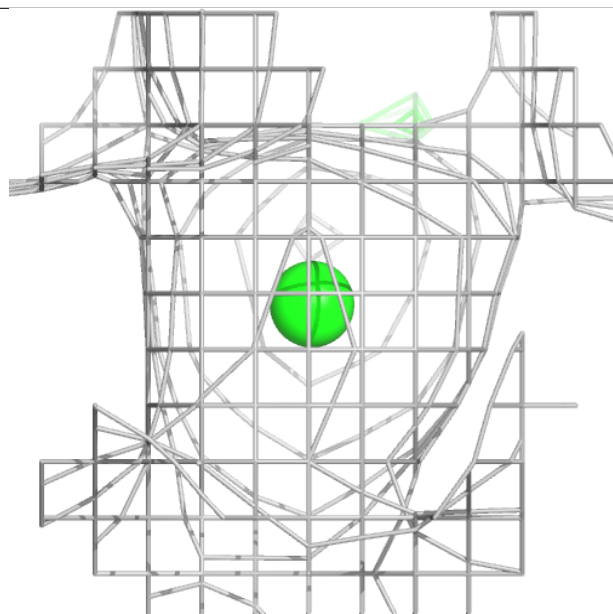
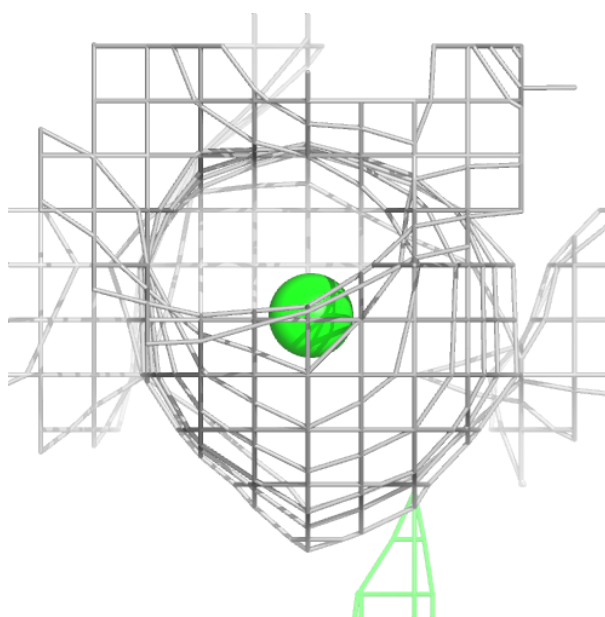
Electron density around FMN A 401:

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and green (positive)



Electron density around CL A 402:

$2mF_o-DF_c$ (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.