



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 8QZI / pdb_00008qzi
Title : Crystal structure of PptT-ACP from Mycobacterium tuberculosis
Authors : Gavalda, S.; Mourey, L.; Pedelacq, J.D.
Deposited on : 2023-10-27
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

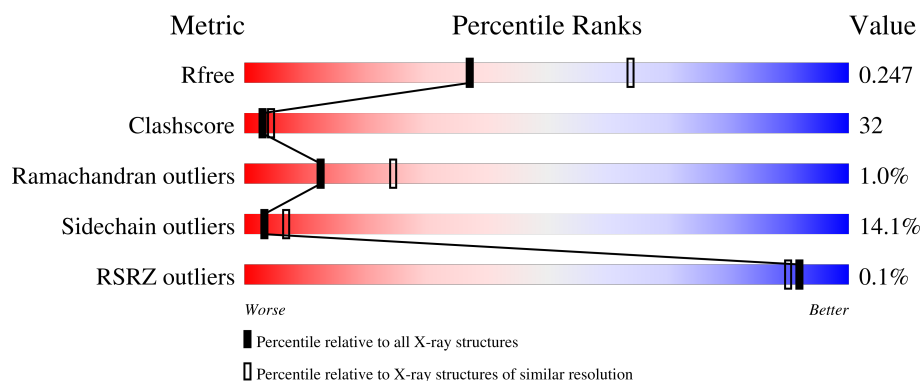
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	247	
1	B	247	
1	C	247	
1	D	247	
2	E	172	

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Mol	Chain	Length	Quality of chain
2	F	172	19% 20% 11% 49%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8405 atoms, of which 16 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 4'-phosphopantetheinyl transferase PptT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1720	1100	301	312	7			
1	B	225	Total	C	N	O	S	0	0	0
			1720	1100	301	312	7			
1	C	225	Total	C	N	O	S	0	0	0
			1720	1100	301	312	7			
1	D	225	Total	C	N	O	S	0	1	0
			1732	1107	304	314	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O33336
A	-18	GLY	-	expression tag	UNP O33336
A	-17	SER	-	expression tag	UNP O33336
A	-16	SER	-	expression tag	UNP O33336
A	-15	HIS	-	expression tag	UNP O33336
A	-14	HIS	-	expression tag	UNP O33336
A	-13	HIS	-	expression tag	UNP O33336
A	-12	HIS	-	expression tag	UNP O33336
A	-11	HIS	-	expression tag	UNP O33336
A	-10	HIS	-	expression tag	UNP O33336
A	-9	SER	-	expression tag	UNP O33336
A	-8	SER	-	expression tag	UNP O33336
A	-7	GLY	-	expression tag	UNP O33336
A	-6	LEU	-	expression tag	UNP O33336
A	-5	VAL	-	expression tag	UNP O33336
A	-4	PRO	-	expression tag	UNP O33336
A	-3	ARG	-	expression tag	UNP O33336
A	-2	GLY	-	expression tag	UNP O33336
A	-1	SER	-	expression tag	UNP O33336
A	0	HIS	-	expression tag	UNP O33336
B	-19	MET	-	initiating methionine	UNP O33336

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O33336
B	-17	SER	-	expression tag	UNP O33336
B	-16	SER	-	expression tag	UNP O33336
B	-15	HIS	-	expression tag	UNP O33336
B	-14	HIS	-	expression tag	UNP O33336
B	-13	HIS	-	expression tag	UNP O33336
B	-12	HIS	-	expression tag	UNP O33336
B	-11	HIS	-	expression tag	UNP O33336
B	-10	HIS	-	expression tag	UNP O33336
B	-9	SER	-	expression tag	UNP O33336
B	-8	SER	-	expression tag	UNP O33336
B	-7	GLY	-	expression tag	UNP O33336
B	-6	LEU	-	expression tag	UNP O33336
B	-5	VAL	-	expression tag	UNP O33336
B	-4	PRO	-	expression tag	UNP O33336
B	-3	ARG	-	expression tag	UNP O33336
B	-2	GLY	-	expression tag	UNP O33336
B	-1	SER	-	expression tag	UNP O33336
B	0	HIS	-	expression tag	UNP O33336
C	-19	MET	-	initiating methionine	UNP O33336
C	-18	GLY	-	expression tag	UNP O33336
C	-17	SER	-	expression tag	UNP O33336
C	-16	SER	-	expression tag	UNP O33336
C	-15	HIS	-	expression tag	UNP O33336
C	-14	HIS	-	expression tag	UNP O33336
C	-13	HIS	-	expression tag	UNP O33336
C	-12	HIS	-	expression tag	UNP O33336
C	-11	HIS	-	expression tag	UNP O33336
C	-10	HIS	-	expression tag	UNP O33336
C	-9	SER	-	expression tag	UNP O33336
C	-8	SER	-	expression tag	UNP O33336
C	-7	GLY	-	expression tag	UNP O33336
C	-6	LEU	-	expression tag	UNP O33336
C	-5	VAL	-	expression tag	UNP O33336
C	-4	PRO	-	expression tag	UNP O33336
C	-3	ARG	-	expression tag	UNP O33336
C	-2	GLY	-	expression tag	UNP O33336
C	-1	SER	-	expression tag	UNP O33336
C	0	HIS	-	expression tag	UNP O33336
D	-19	MET	-	initiating methionine	UNP O33336
D	-18	GLY	-	expression tag	UNP O33336
D	-17	SER	-	expression tag	UNP O33336

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O33336
D	-15	HIS	-	expression tag	UNP O33336
D	-14	HIS	-	expression tag	UNP O33336
D	-13	HIS	-	expression tag	UNP O33336
D	-12	HIS	-	expression tag	UNP O33336
D	-11	HIS	-	expression tag	UNP O33336
D	-10	HIS	-	expression tag	UNP O33336
D	-9	SER	-	expression tag	UNP O33336
D	-8	SER	-	expression tag	UNP O33336
D	-7	GLY	-	expression tag	UNP O33336
D	-6	LEU	-	expression tag	UNP O33336
D	-5	VAL	-	expression tag	UNP O33336
D	-4	PRO	-	expression tag	UNP O33336
D	-3	ARG	-	expression tag	UNP O33336
D	-2	GLY	-	expression tag	UNP O33336
D	-1	SER	-	expression tag	UNP O33336
D	0	HIS	-	expression tag	UNP O33336

- Molecule 2 is a protein called Phenolphthiocerol/phthiocerol polyketide synthase subunit C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	86	Total	C	N	O	S	Se	0	0	0
			644	404	113	124	1	2			
2	F	88	Total	C	N	O	S	Se	0	0	0
			654	409	118	124	1	2			

There are 50 discrepancies between the modelled and reference sequences:

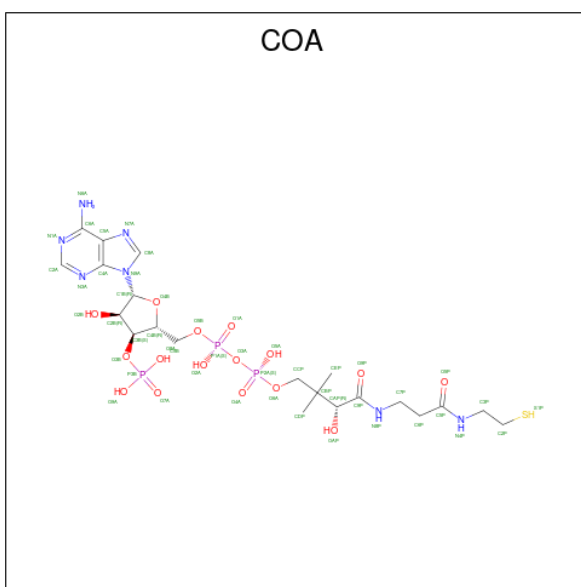
Chain	Residue	Modelled	Actual	Comment	Reference
E	2021	MSE	-	initiating methionine	UNP P96202
E	2022	GLY	-	expression tag	UNP P96202
E	2023	SER	-	expression tag	UNP P96202
E	2024	SER	-	expression tag	UNP P96202
E	2025	HIS	-	expression tag	UNP P96202
E	2026	HIS	-	expression tag	UNP P96202
E	2027	HIS	-	expression tag	UNP P96202
E	2028	HIS	-	expression tag	UNP P96202
E	2029	HIS	-	expression tag	UNP P96202
E	2030	HIS	-	expression tag	UNP P96202
E	2031	SER	-	expression tag	UNP P96202
E	2032	SER	-	expression tag	UNP P96202
E	2033	GLY	-	expression tag	UNP P96202

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2034	LEU	-	expression tag	UNP P96202
E	2035	VAL	-	expression tag	UNP P96202
E	2036	PRO	-	expression tag	UNP P96202
E	2037	ARG	-	expression tag	UNP P96202
E	2038	GLY	-	expression tag	UNP P96202
E	2039	SER	-	expression tag	UNP P96202
E	2040	HIS	-	expression tag	UNP P96202
E	2041	MSE	-	expression tag	UNP P96202
E	2189	THR	-	expression tag	UNP P96202
E	2190	SER	-	expression tag	UNP P96202
E	2191	GLY	-	expression tag	UNP P96202
E	2192	SER	-	expression tag	UNP P96202
F	2021	MSE	-	initiating methionine	UNP P96202
F	2022	GLY	-	expression tag	UNP P96202
F	2023	SER	-	expression tag	UNP P96202
F	2024	SER	-	expression tag	UNP P96202
F	2025	HIS	-	expression tag	UNP P96202
F	2026	HIS	-	expression tag	UNP P96202
F	2027	HIS	-	expression tag	UNP P96202
F	2028	HIS	-	expression tag	UNP P96202
F	2029	HIS	-	expression tag	UNP P96202
F	2030	HIS	-	expression tag	UNP P96202
F	2031	SER	-	expression tag	UNP P96202
F	2032	SER	-	expression tag	UNP P96202
F	2033	GLY	-	expression tag	UNP P96202
F	2034	LEU	-	expression tag	UNP P96202
F	2035	VAL	-	expression tag	UNP P96202
F	2036	PRO	-	expression tag	UNP P96202
F	2037	ARG	-	expression tag	UNP P96202
F	2038	GLY	-	expression tag	UNP P96202
F	2039	SER	-	expression tag	UNP P96202
F	2040	HIS	-	expression tag	UNP P96202
F	2041	MSE	-	expression tag	UNP P96202
F	2189	THR	-	expression tag	UNP P96202
F	2190	SER	-	expression tag	UNP P96202
F	2191	GLY	-	expression tag	UNP P96202
F	2192	SER	-	expression tag	UNP P96202

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).

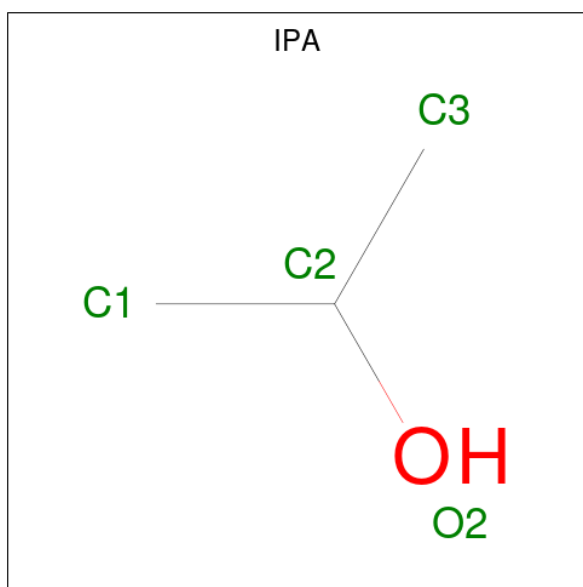


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0	
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0	
3	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3		0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	B	2	Total	Mn	0	0
			2	2		
4	C	2	Total	Mn	0	0
			2	2		
4	D	2	Total	Mn	0	0
			2	2		

- Molecule 5 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			12	3	8	1		
5	E	1	Total	C	H	O	0	0
			12	3	8	1		

- Molecule 6 is water.

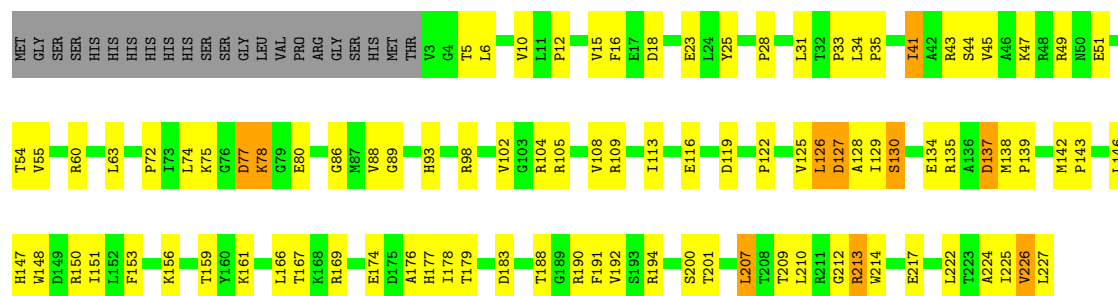
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	8	Total	O	0	0
			8	8		
6	C	15	Total	O	0	0
			15	15		
6	D	12	Total	O	0	0
			12	12		
6	E	4	Total	O	0	0
			4	4		
6	F	2	Total	O	0	0
			2	2		

3 Residue-property plots

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

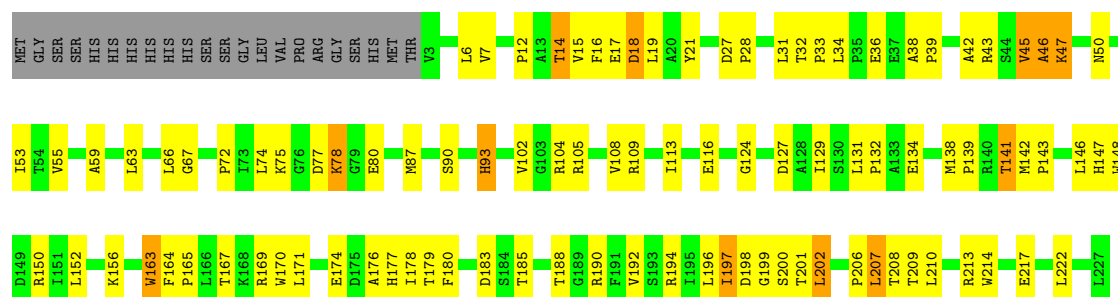
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain A: 



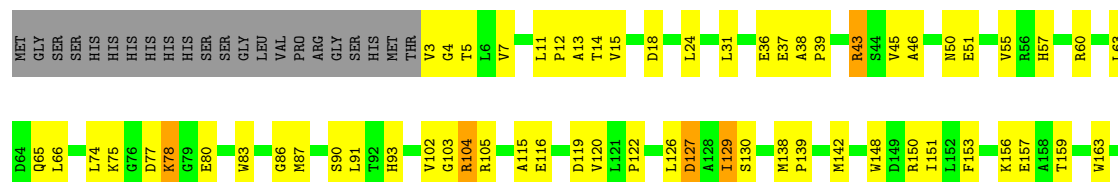
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

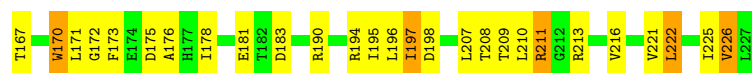
Chain B: 



• Molecule 1: 4'-phosphopantetheinyl transferase PptT

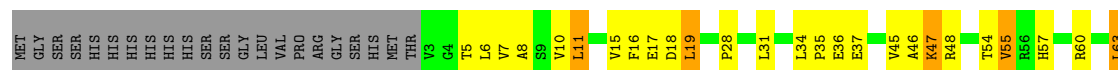
Chain C: 





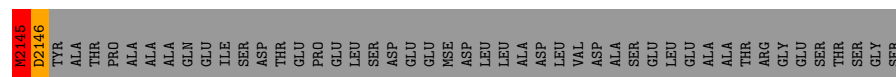
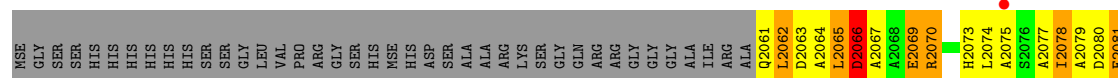
- Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain D: 51% 34% 7% 9%



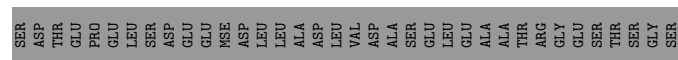
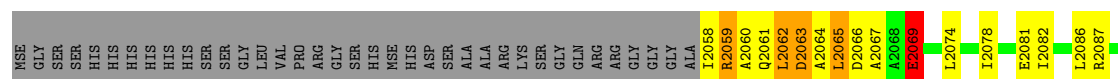
- Molecule 2: Phenolphthiocerol/phthiocerol polyketide synthase subunit C

Chain E: 15% 22% 12% 50%



- Molecule 2: Phenolphthiocerol/phthiocerol polyketide synthase subunit C

Chain F: 19% 20% 11% 49%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.34Å 280.84Å 47.34Å 90.00° 92.83° 90.00°	Depositor
Resolution (Å)	47.28 – 2.50 47.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.28-2.50) 91.1 (47.28-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, R_{free}	0.196 , 0.241 0.198 , 0.247	Depositor DCC
R_{free} test set	1984 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.050 for l,k,-h 0.066 for h,-k,-l 0.449 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8405	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: COA, MN, IPA

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	0.38	0/1766	0.57	0/2414
1	B	0.35	0/1766	0.55	0/2414
1	C	0.36	0/1766	0.54	0/2414
1	D	0.38	0/1781	0.59	0/2433
2	E	0.31	0/652	0.56	0/887
2	F	0.30	0/661	0.62	0/898
All	All	0.36	0/8392	0.57	0/11460

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	F	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PRO	Peptide
2	F	2069	GLU	Peptide
2	F	2136	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	0	1724	99	1
1	B	1720	0	1724	82	0
1	C	1720	0	1724	82	0
1	D	1732	0	1741	97	1
2	E	644	0	639	95	0
2	F	654	0	660	88	0
3	A	27	0	11	3	0
3	B	27	0	11	4	0
3	C	48	0	32	9	0
3	D	31	0	10	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	C	4	8	8	0	0
5	E	4	8	8	0	0
6	A	9	0	0	7	0
6	B	8	0	0	2	0
6	C	15	0	0	5	0
6	D	12	0	0	5	0
6	E	4	0	0	1	0
6	F	2	0	0	0	0
All	All	8389	16	8292	532	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 32.

The worst 5 of 532 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:HE2	1:A:146:LEU:HD13	1.24	1.10
2:F:2063:ASP:HB2	2:F:2066:ASP:HB3	1.27	1.07
1:A:125:VAL:O	6:A:401:HOH:O	1.73	1.03
1:C:18:ASP:HB3	1:C:104:ARG:HB2	1.42	1.00
1:D:18:ASP:OD2	1:D:104:ARG:NH1	1.96	0.98

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:190:ARG:NH1	1:D:64:ASP:O[2_455]	1.88	0.32

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/247 (90%)	203 (91%)	18 (8%)	2 (1%)	14	27
1	B	223/247 (90%)	208 (93%)	14 (6%)	1 (0%)	30	49
1	C	223/247 (90%)	205 (92%)	17 (8%)	1 (0%)	30	49
1	D	224/247 (91%)	211 (94%)	12 (5%)	1 (0%)	30	49
2	E	84/172 (49%)	68 (81%)	12 (14%)	4 (5%)	2	2
2	F	86/172 (50%)	70 (81%)	14 (16%)	2 (2%)	5	8
All	All	1063/1332 (80%)	965 (91%)	87 (8%)	11 (1%)	12	24

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	2066	ASP
1	A	33	PRO
2	E	2064	ALA
2	E	2145	MSE
1	A	78	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/201 (90%)	165 (91%)	16 (9%)	9	20
1	B	181/201 (90%)	161 (89%)	20 (11%)	6	13
1	C	181/201 (90%)	166 (92%)	15 (8%)	10	22
1	D	183/201 (91%)	159 (87%)	24 (13%)	4	8
2	E	66/129 (51%)	41 (62%)	25 (38%)	0	0
2	F	67/129 (52%)	46 (69%)	21 (31%)	0	0
All	All	859/1062 (81%)	738 (86%)	121 (14%)	3	7

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	55	VAL
2	F	2121	ILE
1	D	182	THR
2	F	2119	LEU
2	F	2142	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	C	50	ASN
1	C	65	GLN
2	F	2073	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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$
3	COA	A	301	4	29,29,50	3.33	8 (27%)	44,45,75	1.54	8 (18%)
5	IPA	C	304	-	3,3,3	0.62	0	3,3,3	0.57	0
5	IPA	E	2201	-	3,3,3	0.63	0	3,3,3	0.38	0
3	COA	D	301	4	32,33,50	3.51	10 (31%)	50,52,75	1.58	12 (24%)
3	COA	C	301	4	47,50,50	2.79	8 (17%)	69,75,75	1.65	19 (27%)
3	COA	B	301	4	29,29,50	3.26	7 (24%)	44,45,75	1.53	9 (20%)

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
3	COA	C	301	4	-	12/48/64/64	0/3/3/3
3	COA	B	301	4	-	3/15/31/64	0/3/3/3
3	COA	D	301	4	-	9/21/37/64	0/3/3/3
3	COA	A	301	4	-	0/15/31/64	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	COA	P3B-O3B	16.85	1.89	1.59
3	B	301	COA	P3B-O3B	15.41	1.86	1.59
3	A	301	COA	P3B-O3B	15.22	1.86	1.59
3	C	301	COA	P3B-O3B	15.19	1.86	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	COA	P1A-O3A	6.36	1.66	1.59

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	COA	O3A-P1A-O1A	-4.61	96.85	110.70
3	C	301	COA	O3B-P3B-O7A	-3.85	95.62	109.33
3	C	301	COA	P3B-O3B-C3B	-3.80	113.29	123.43
3	B	301	COA	P3B-O3B-C3B	-3.77	113.37	123.43
3	A	301	COA	P3B-O3B-C3B	-3.72	113.49	123.43

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

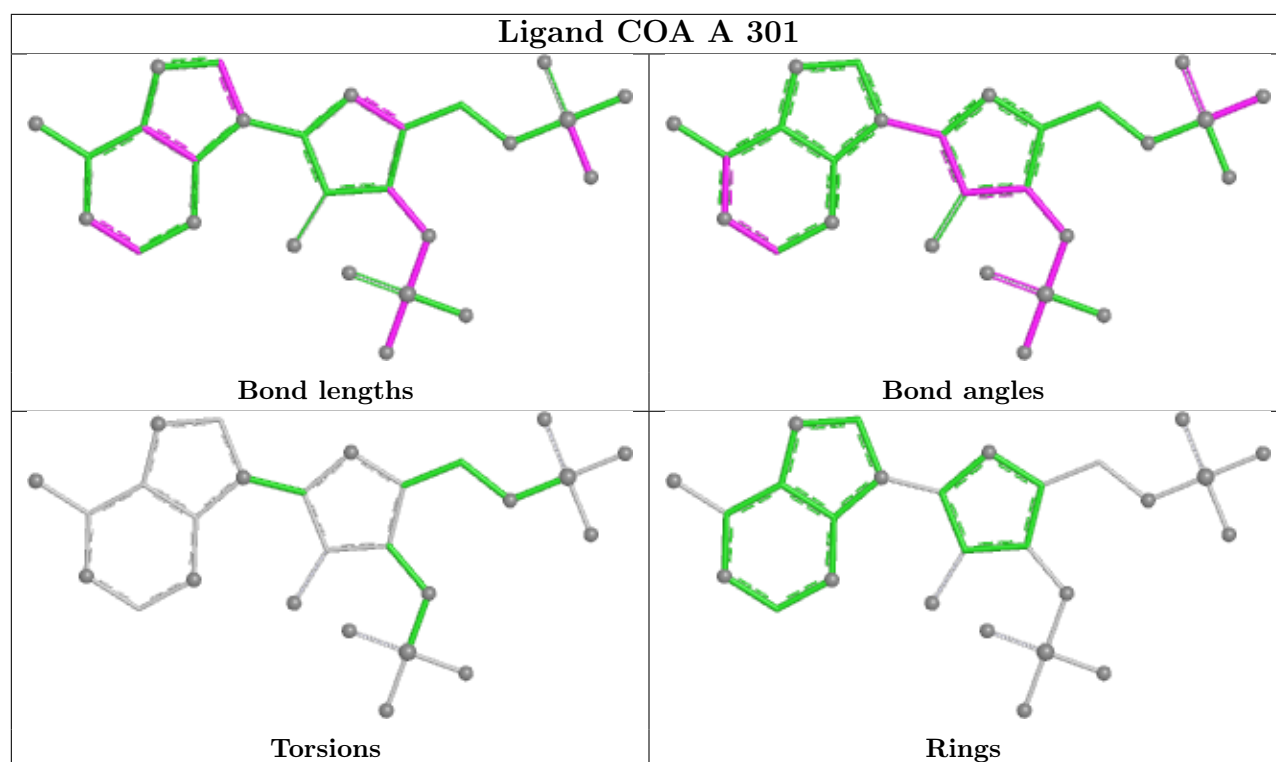
Mol	Chain	Res	Type	Atoms
3	C	301	COA	CCP-O6A-P2A-O4A
3	C	301	COA	O9P-C9P-CAP-OAP
3	C	301	COA	S1P-C2P-C3P-N4P
3	D	301	COA	C5B-O5B-P1A-O1A
3	D	301	COA	C5B-O5B-P1A-O2A

There are no ring outliers.

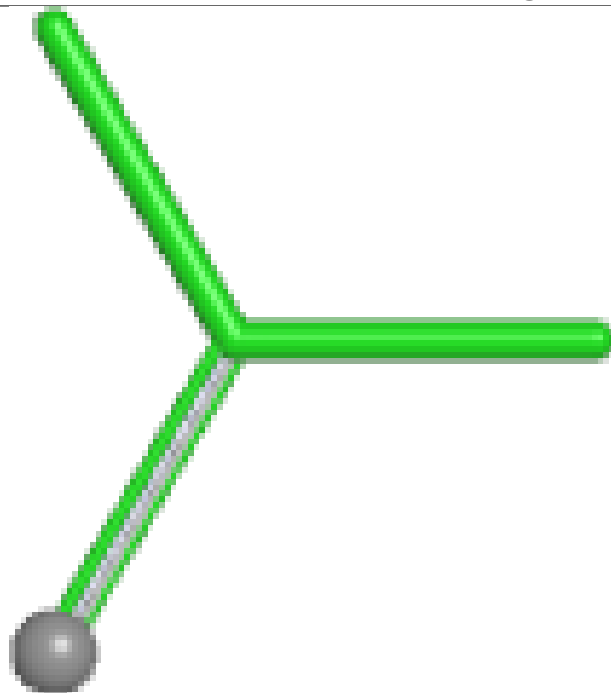
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	COA	3	0
3	D	301	COA	4	0
3	C	301	COA	9	0
3	B	301	COA	4	0

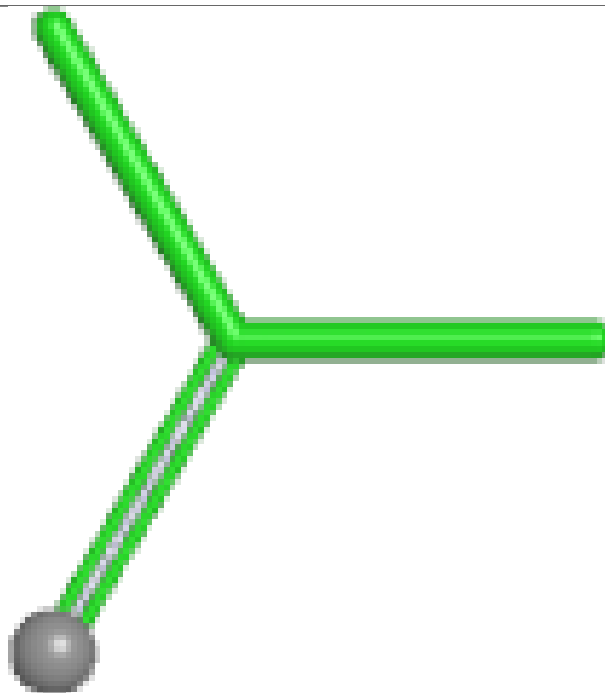
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



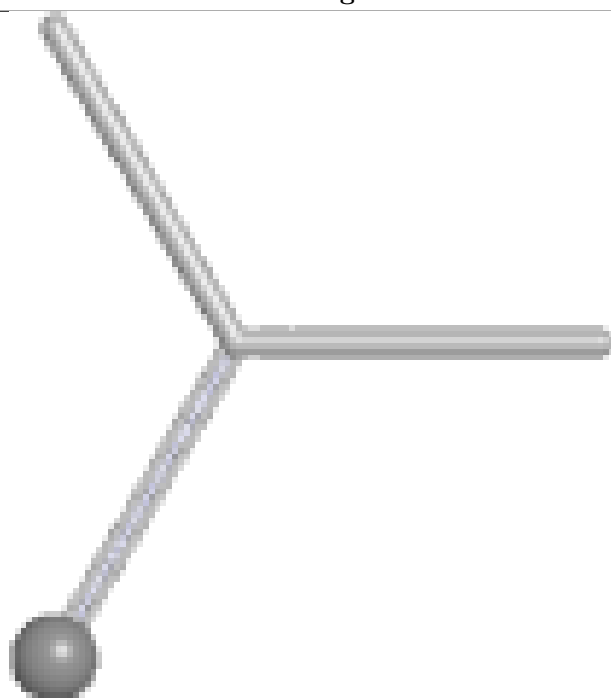
Ligand IPA C 304



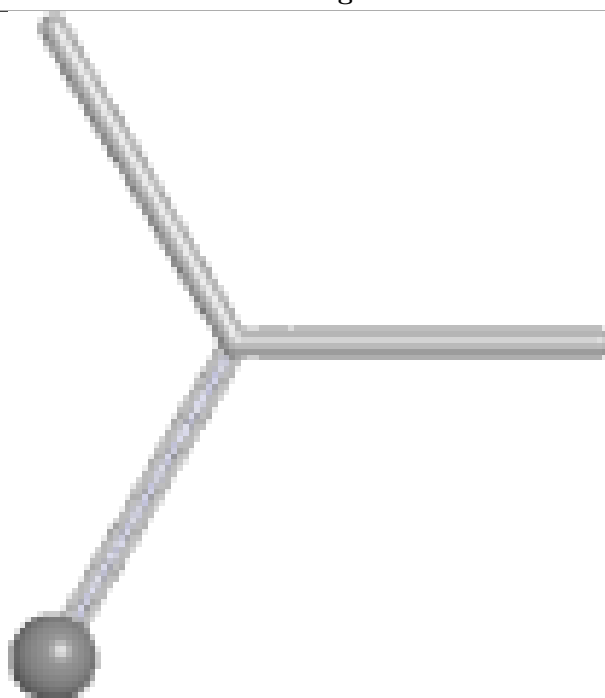
Bond lengths



Bond angles

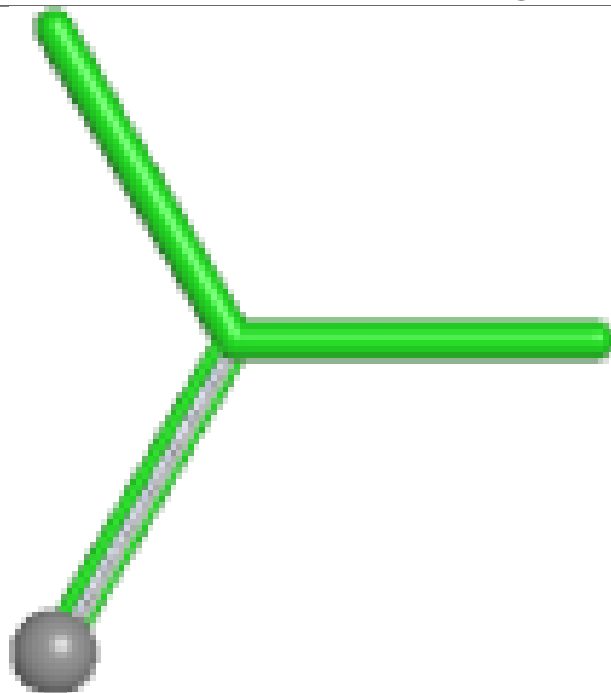


Torsions

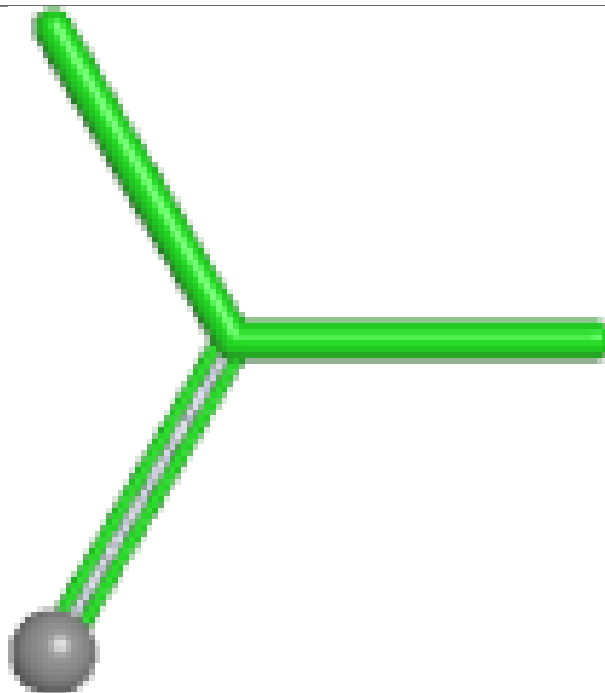


Rings

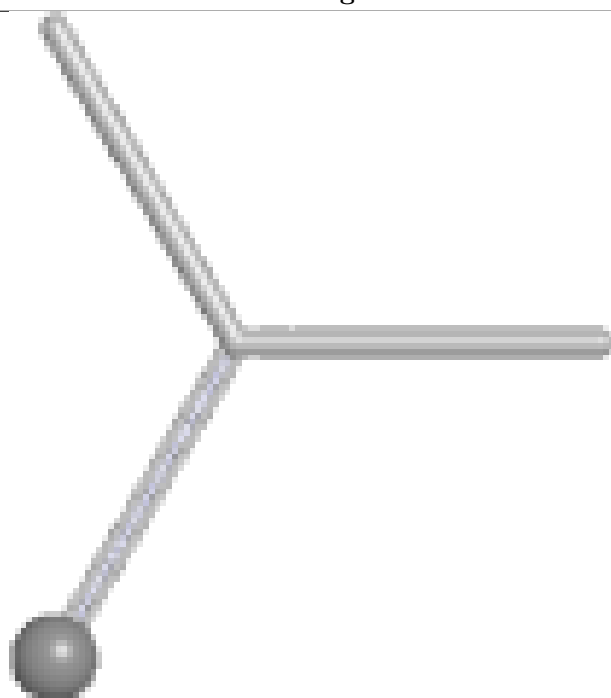
Ligand IPA E 2201



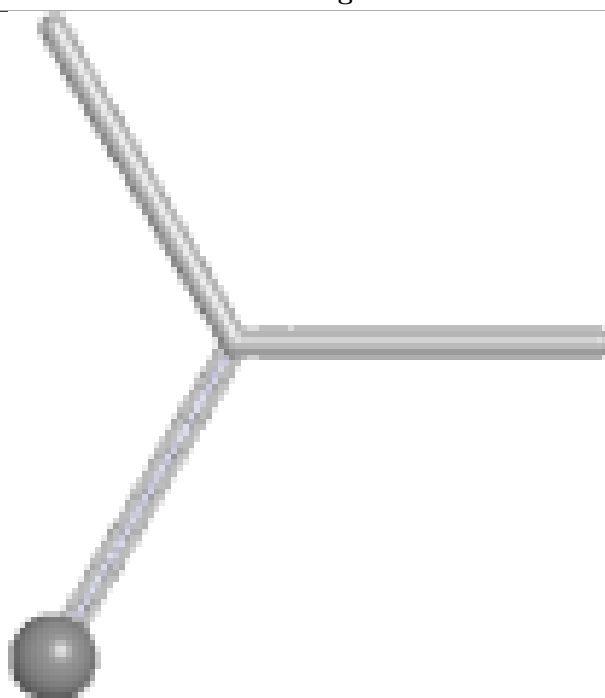
Bond lengths



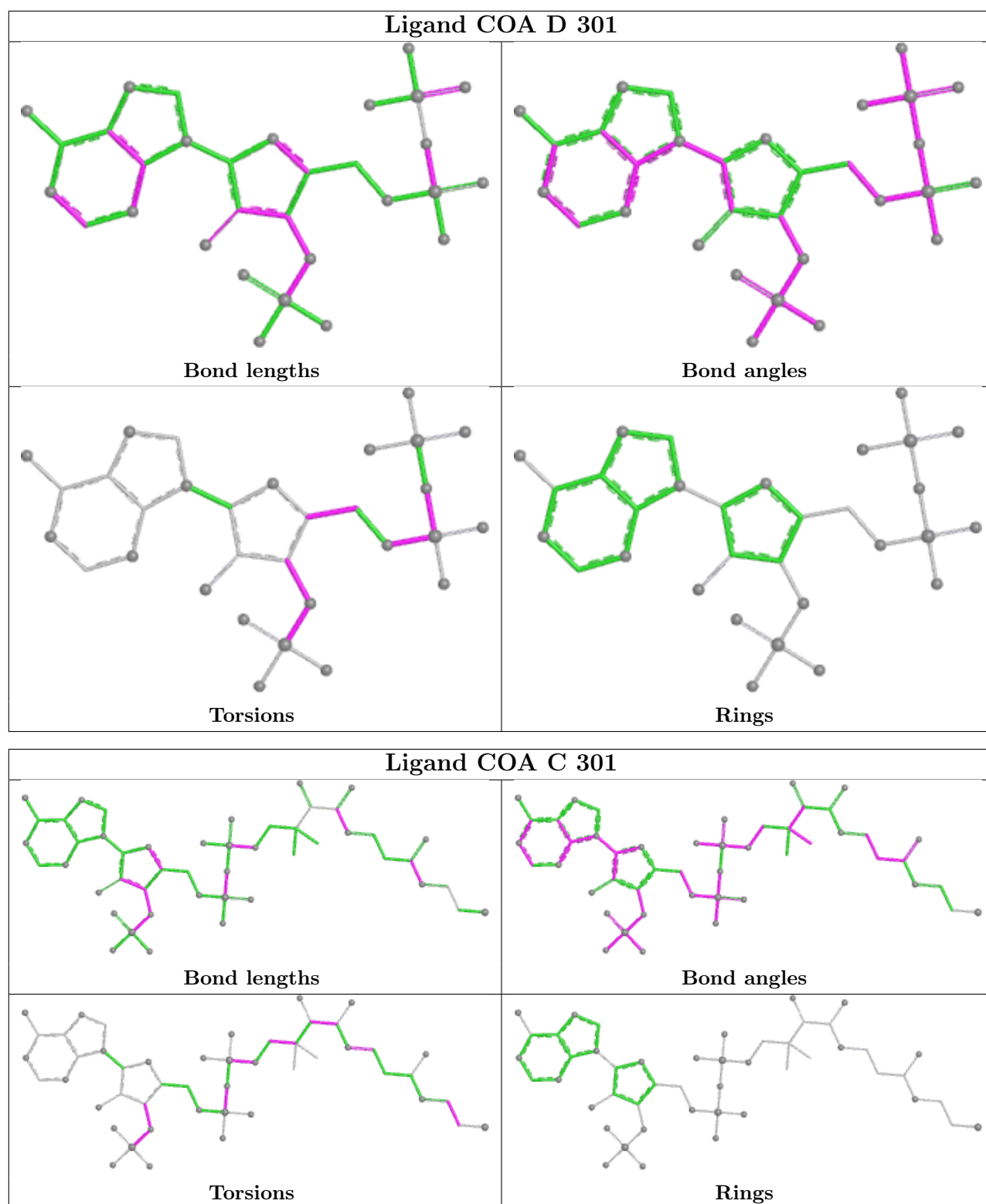
Bond angles

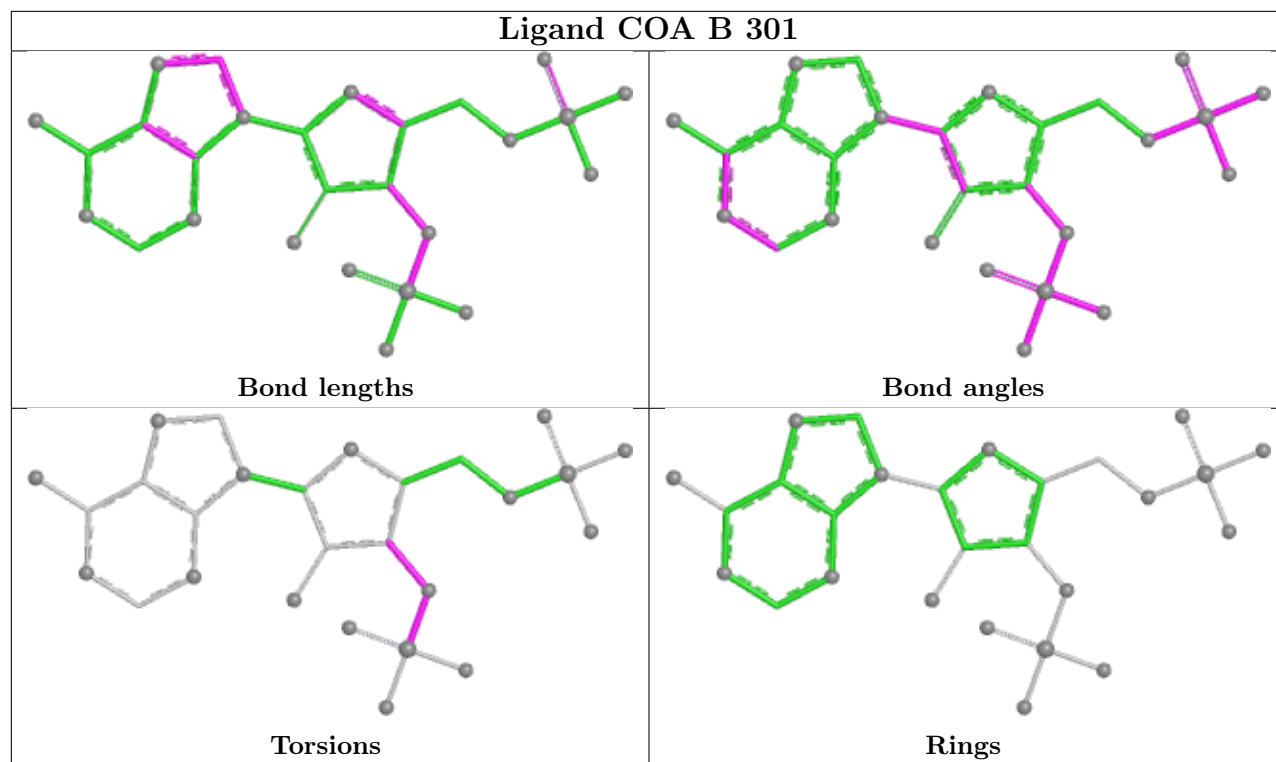


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	225/247 (91%)	-0.67	0	100	100	44, 78, 123, 168	0
1	B	225/247 (91%)	-0.72	0	100	100	47, 79, 125, 153	0
1	C	225/247 (91%)	-0.62	0	100	100	44, 79, 132, 154	0
1	D	225/247 (91%)	-0.64	0	100	100	44, 78, 132, 188	1 (0%)
2	E	84/172 (48%)	-0.41	1 (1%)	76	73	86, 118, 158, 176	0
2	F	86/172 (50%)	-0.28	0	100	100	88, 127, 176, 206	0
All	All	1070/1332 (80%)	-0.61	1 (0%)	92	90	44, 83, 144, 206	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2075	ALA	2.7

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](#)

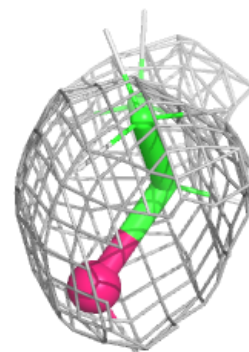
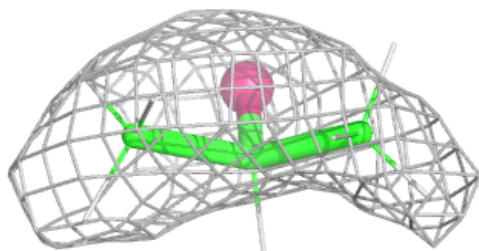
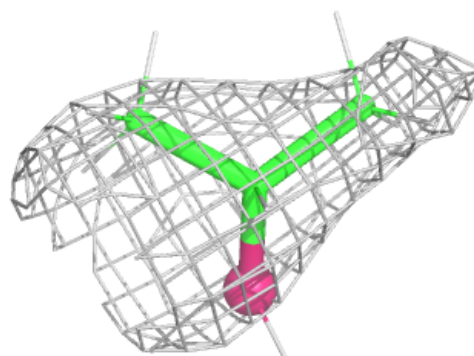
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IPA	C	304	4/4	0.94	0.09	82,99,104,104	0
5	IPA	E	2201	4/4	0.95	0.06	86,104,116,121	0
3	COA	C	301	48/48	0.99	0.05	36,72,138,140	0
3	COA	D	301	31/48	0.99	0.05	31,58,95,105	0
4	MN	B	302	1/1	0.99	0.02	66,66,66,66	0
3	COA	A	301	27/48	0.99	0.04	28,49,73,73	0
3	COA	B	301	27/48	0.99	0.04	32,53,65,69	0
4	MN	B	303	1/1	1.00	0.01	54,54,54,54	0
4	MN	C	302	1/1	1.00	0.01	67,67,67,67	0
4	MN	C	303	1/1	1.00	0.01	47,47,47,47	0
4	MN	D	302	1/1	1.00	0.02	62,62,62,62	0
4	MN	D	303	1/1	1.00	0.04	43,43,43,43	0
4	MN	A	303	1/1	1.00	0.03	61,61,61,61	0
4	MN	A	302	1/1	1.00	0.03	59,59,59,59	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.

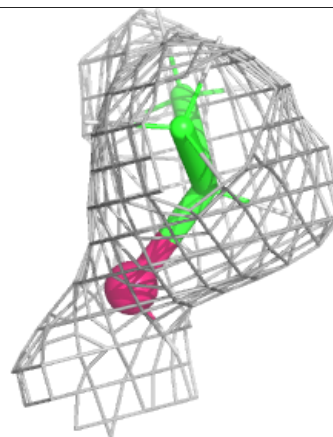
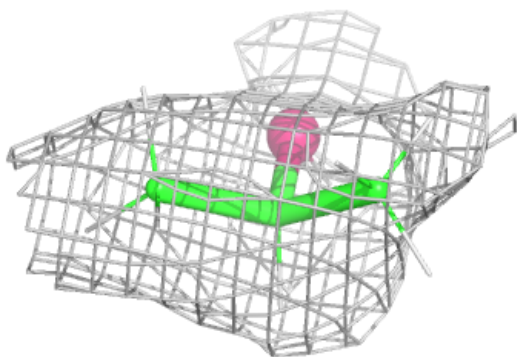
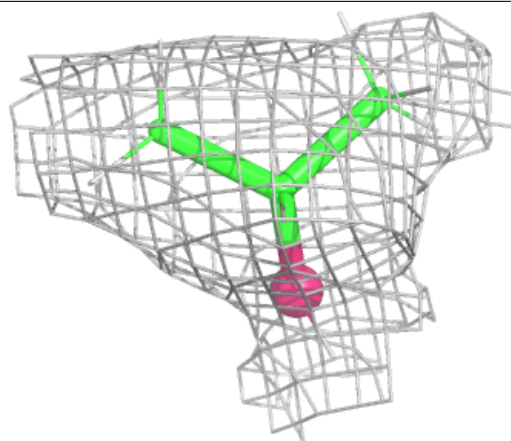
Electron density around IPA C 304:

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



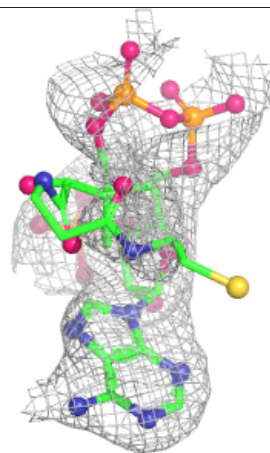
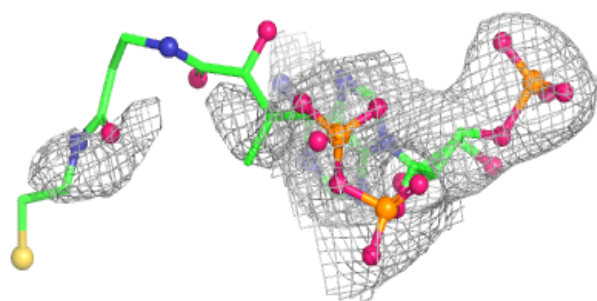
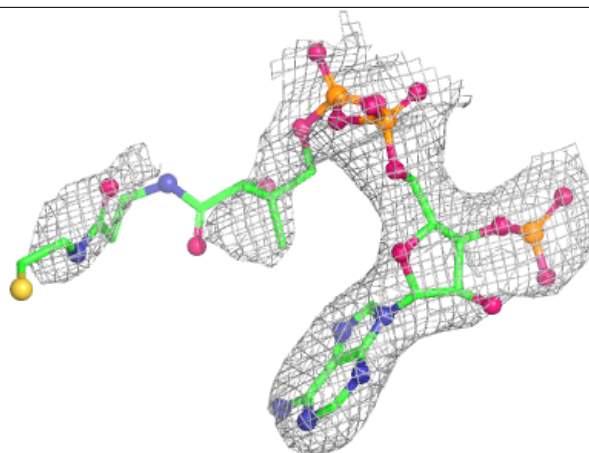
Electron density around IPA E 2201:

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and green (positive)



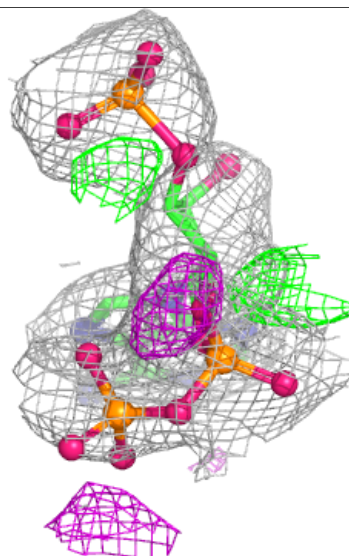
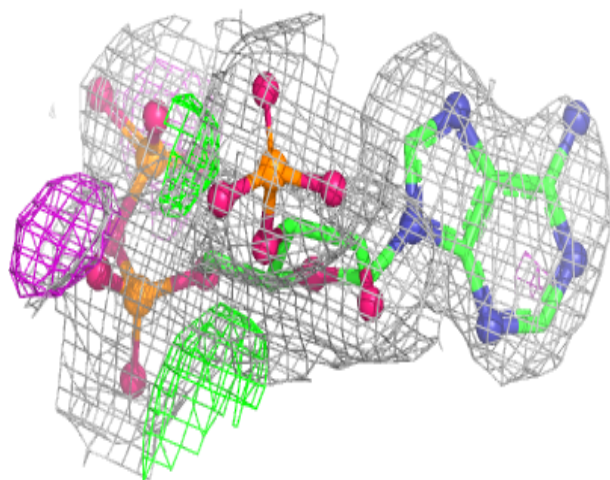
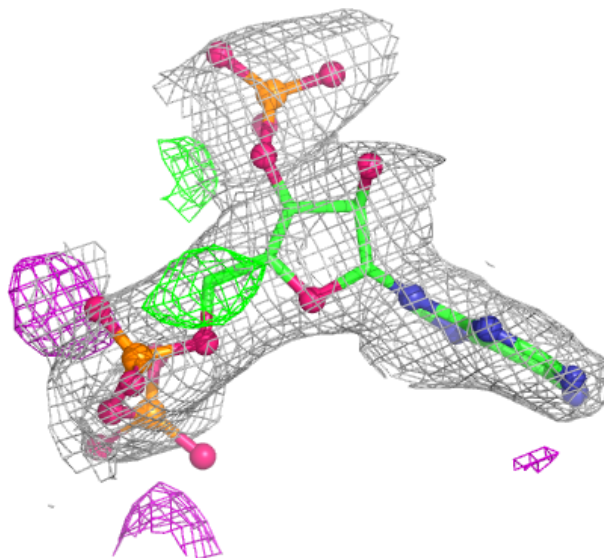
Electron density around COA C 301:

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



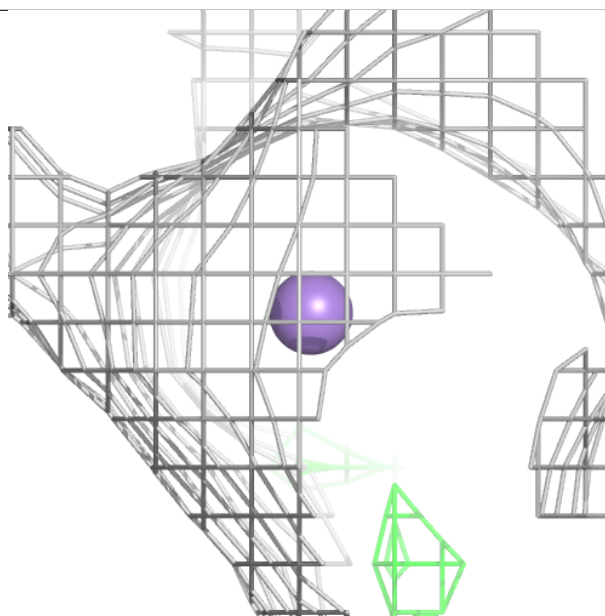
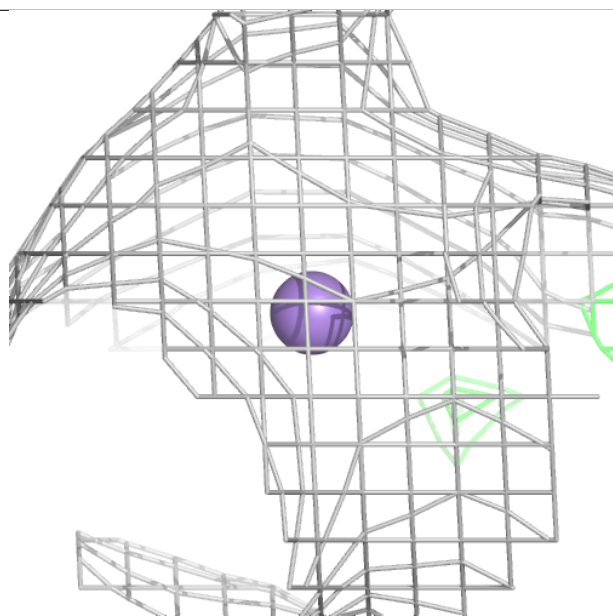
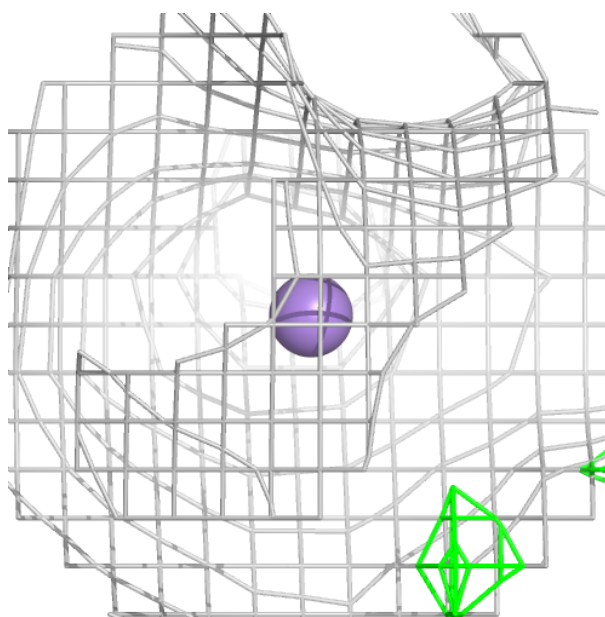
Electron density around COA D 301:

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



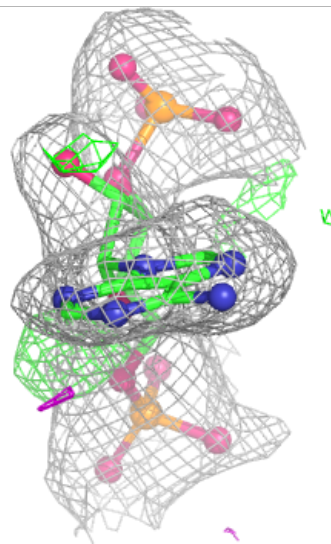
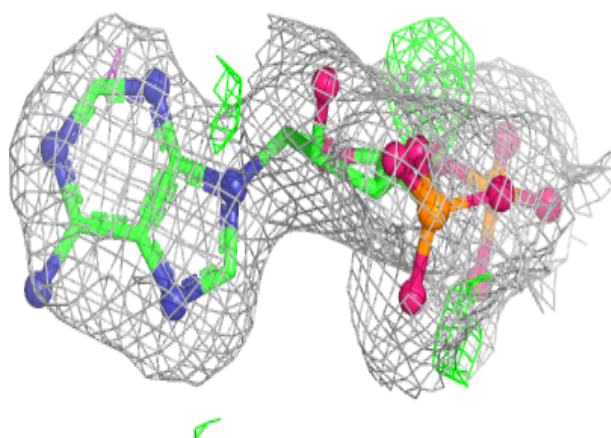
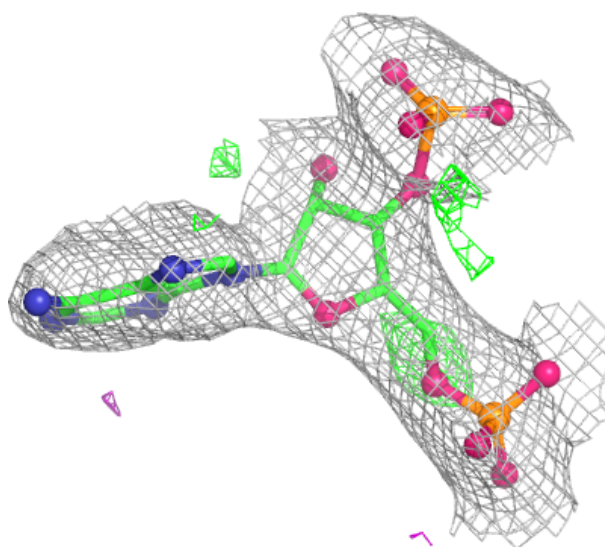
Electron density around MN B 302:

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and green (positive)



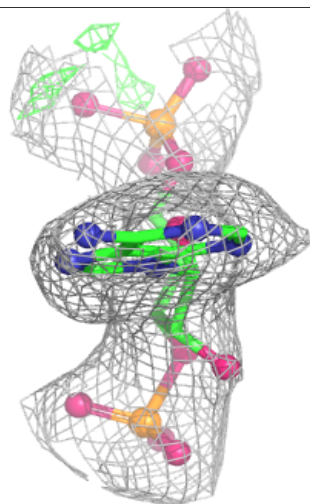
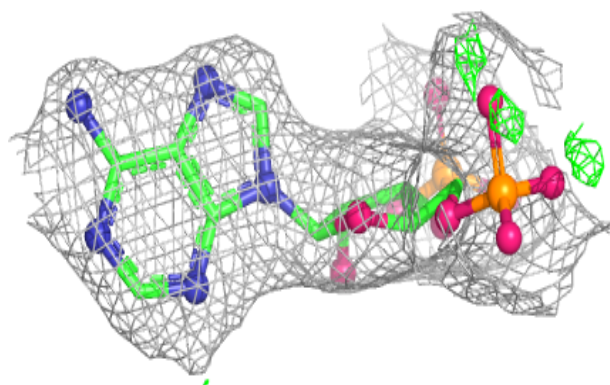
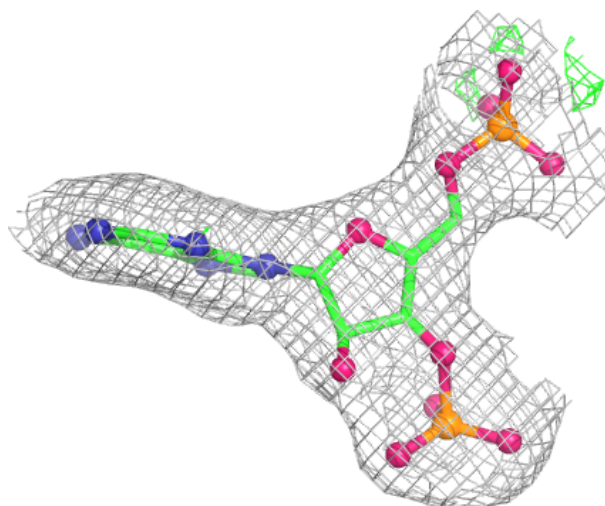
Electron density around COA A 301:

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and green (positive)



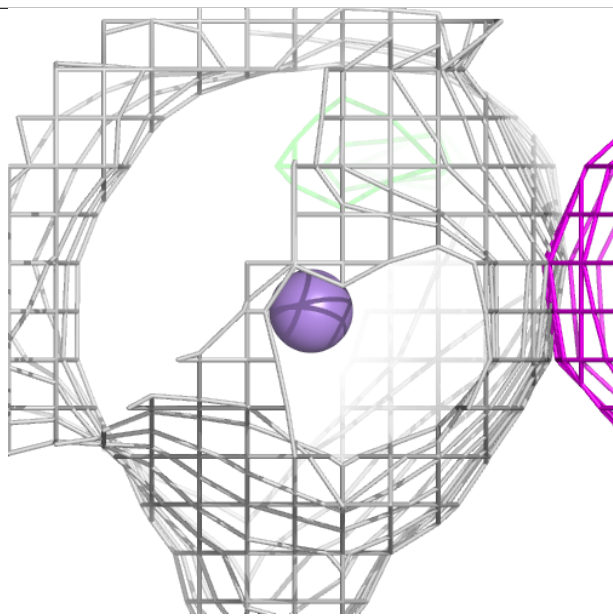
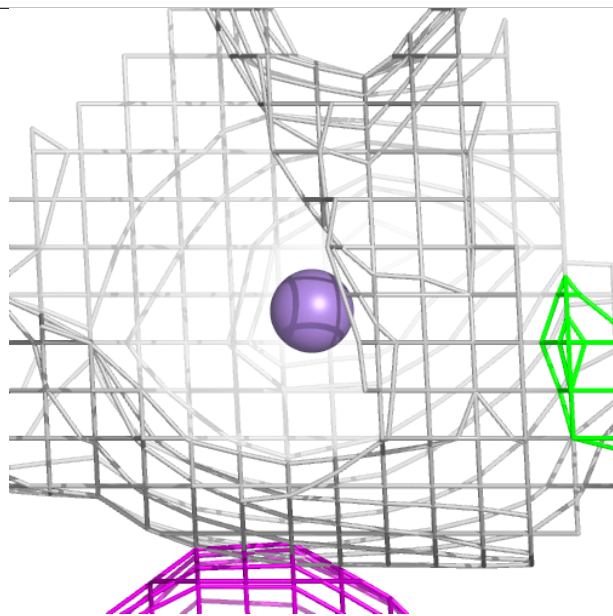
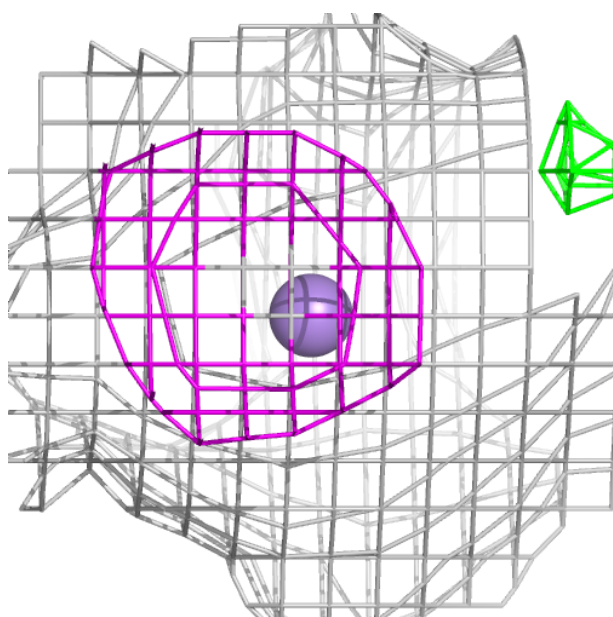
Electron density around COA B 301:

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and green (positive)



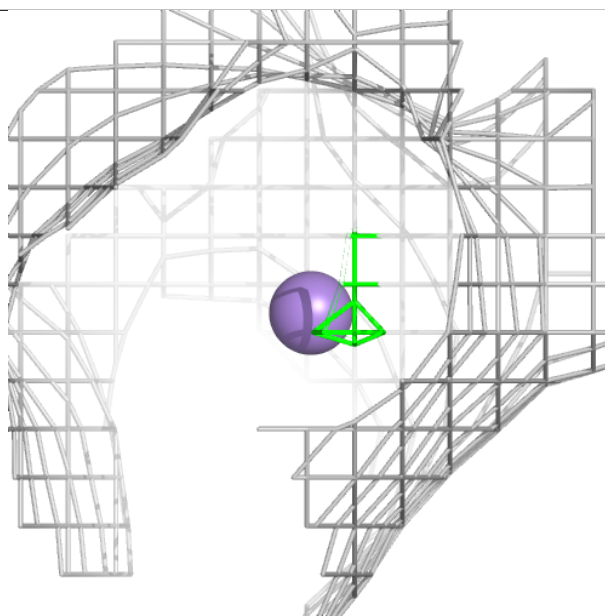
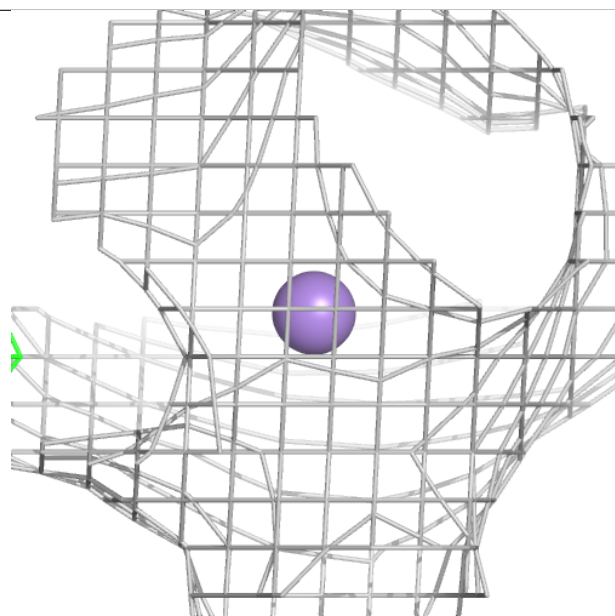
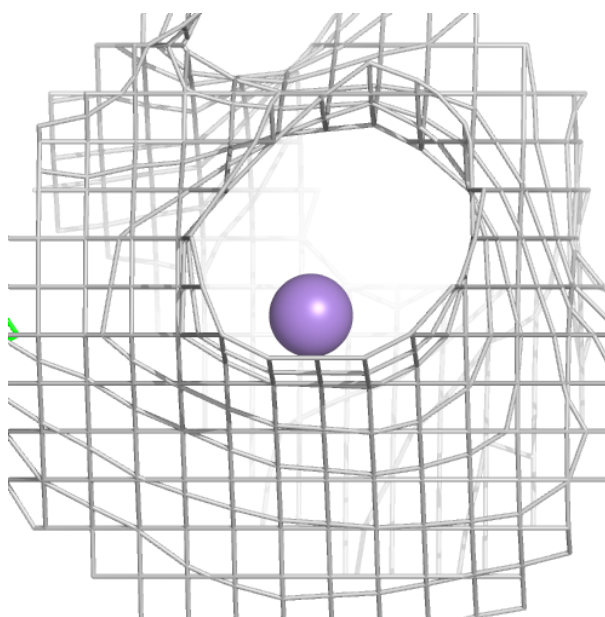
Electron density around MN B 303:

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and green (positive)



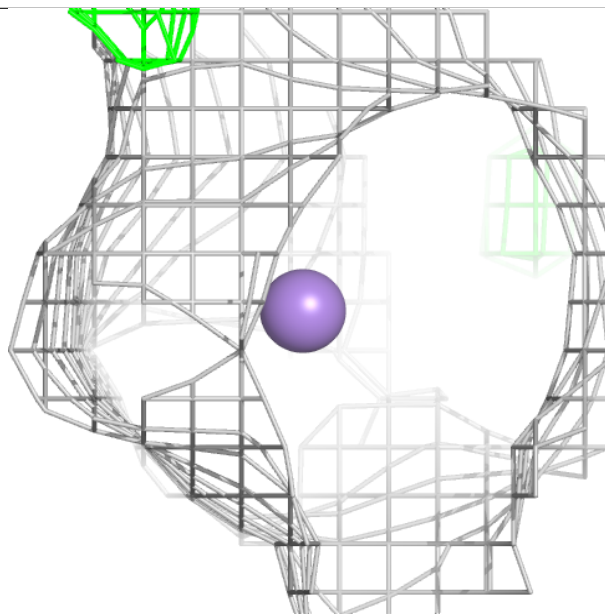
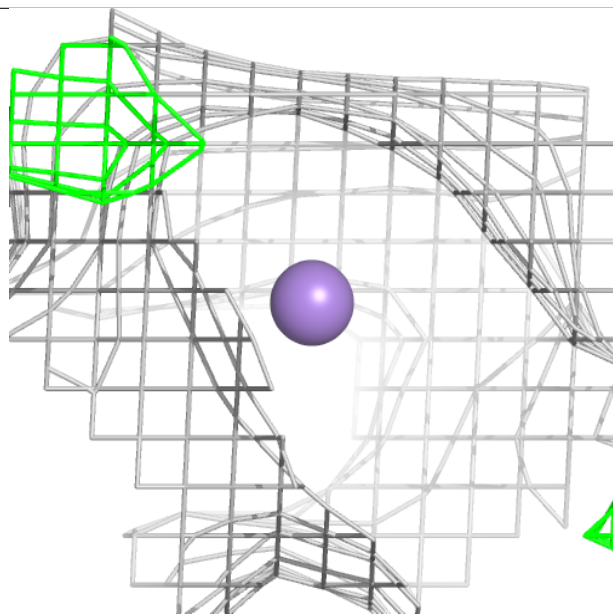
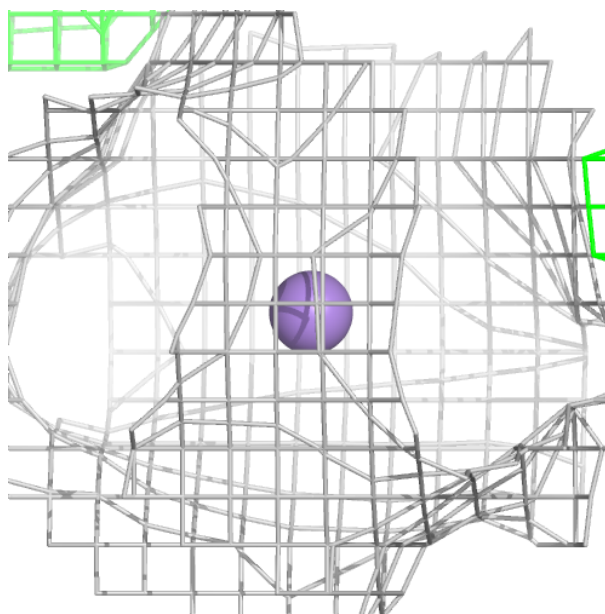
Electron density around MN C 302:

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and green (positive)



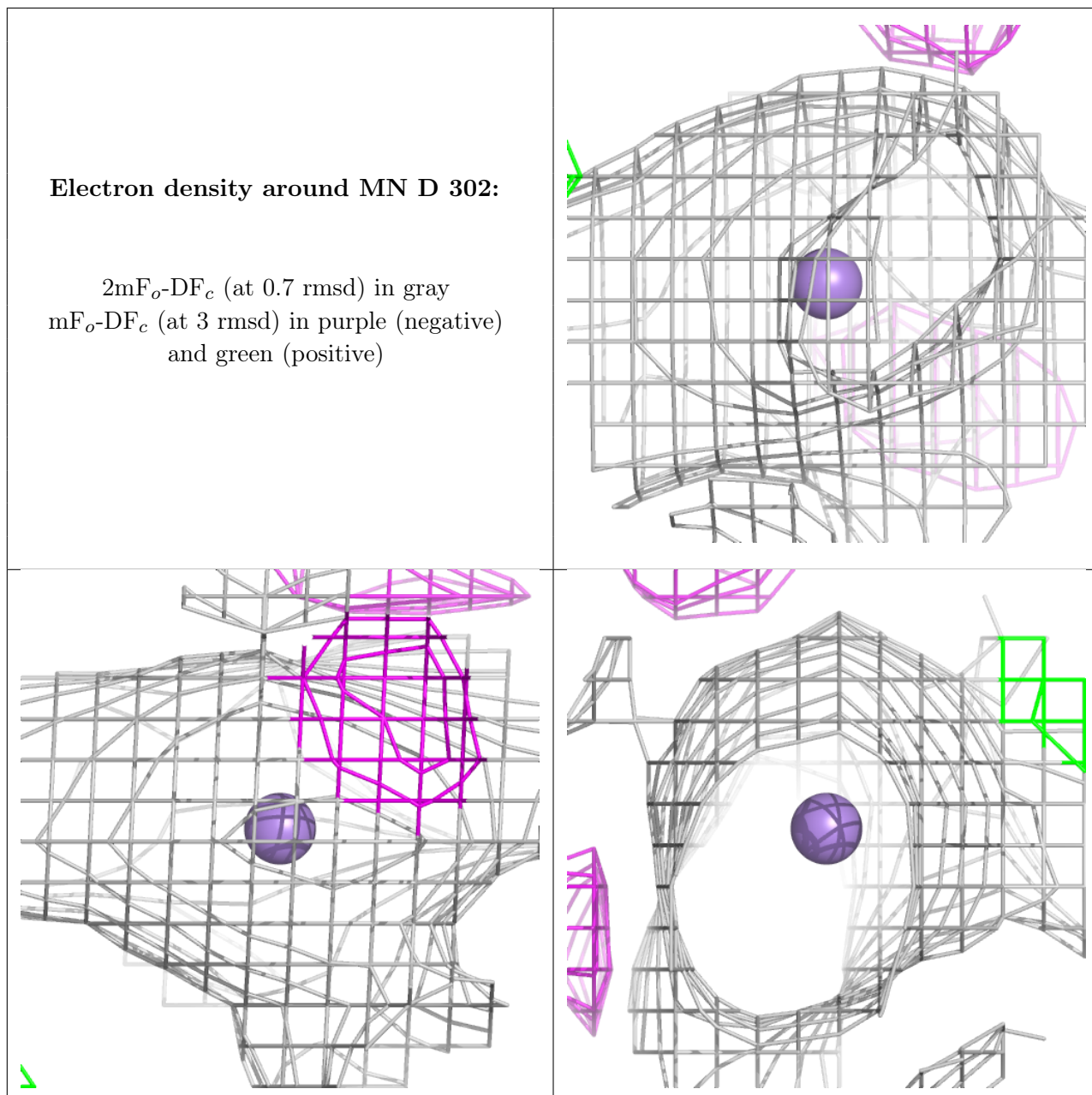
Electron density around MN C 303:

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and green (positive)



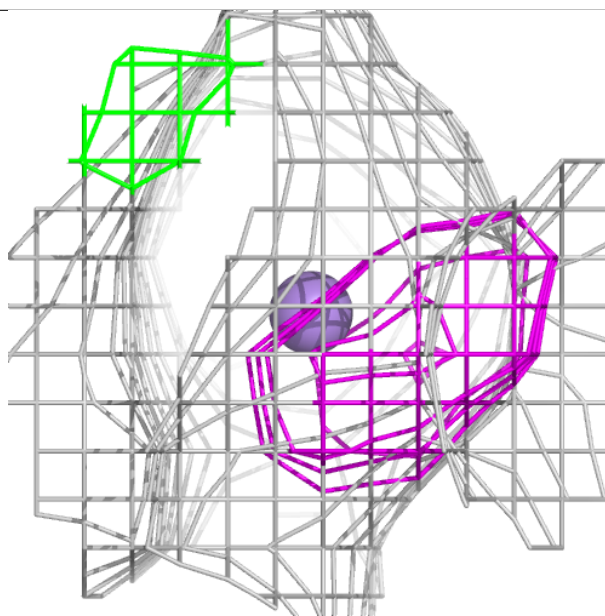
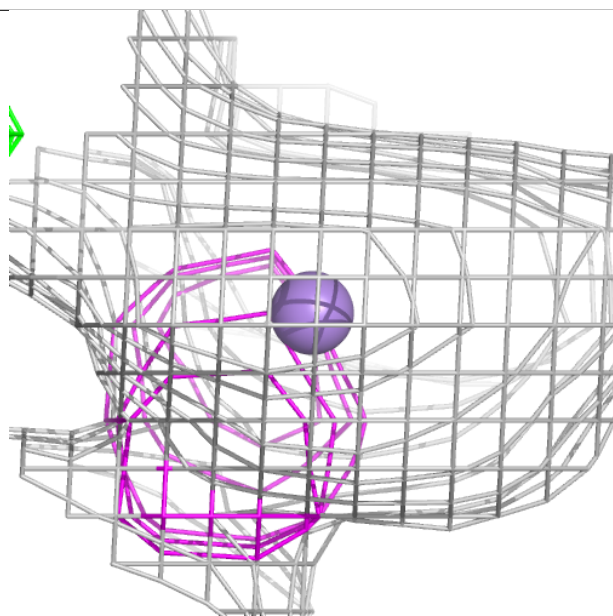
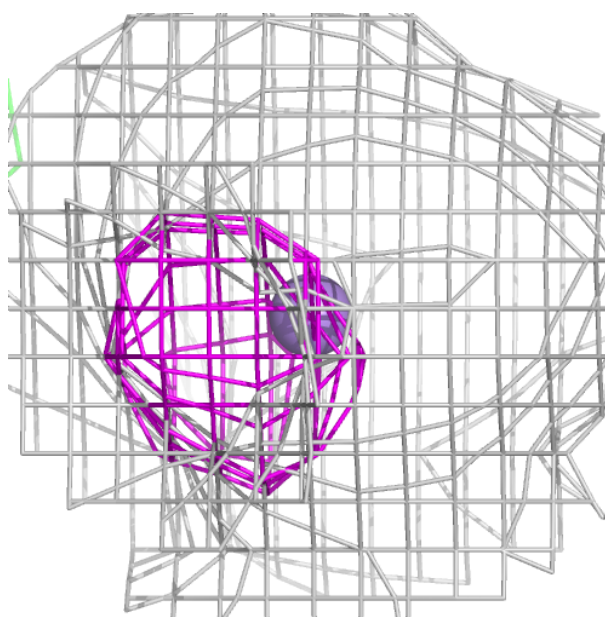
Electron density around MN D 302:

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



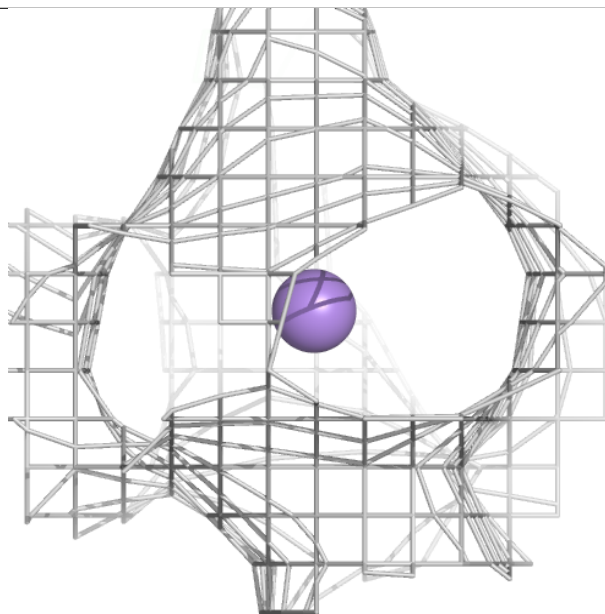
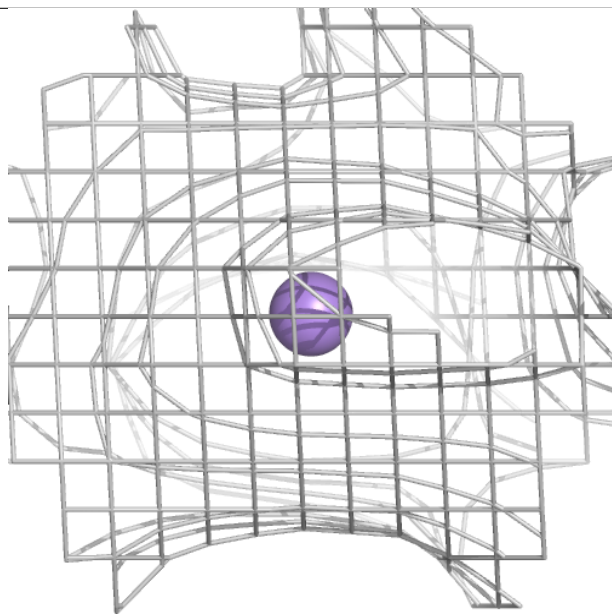
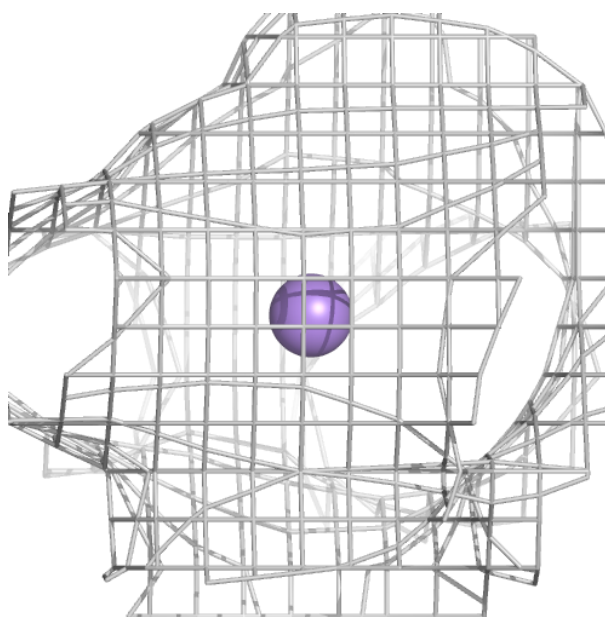
Electron density around MN D 303:

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



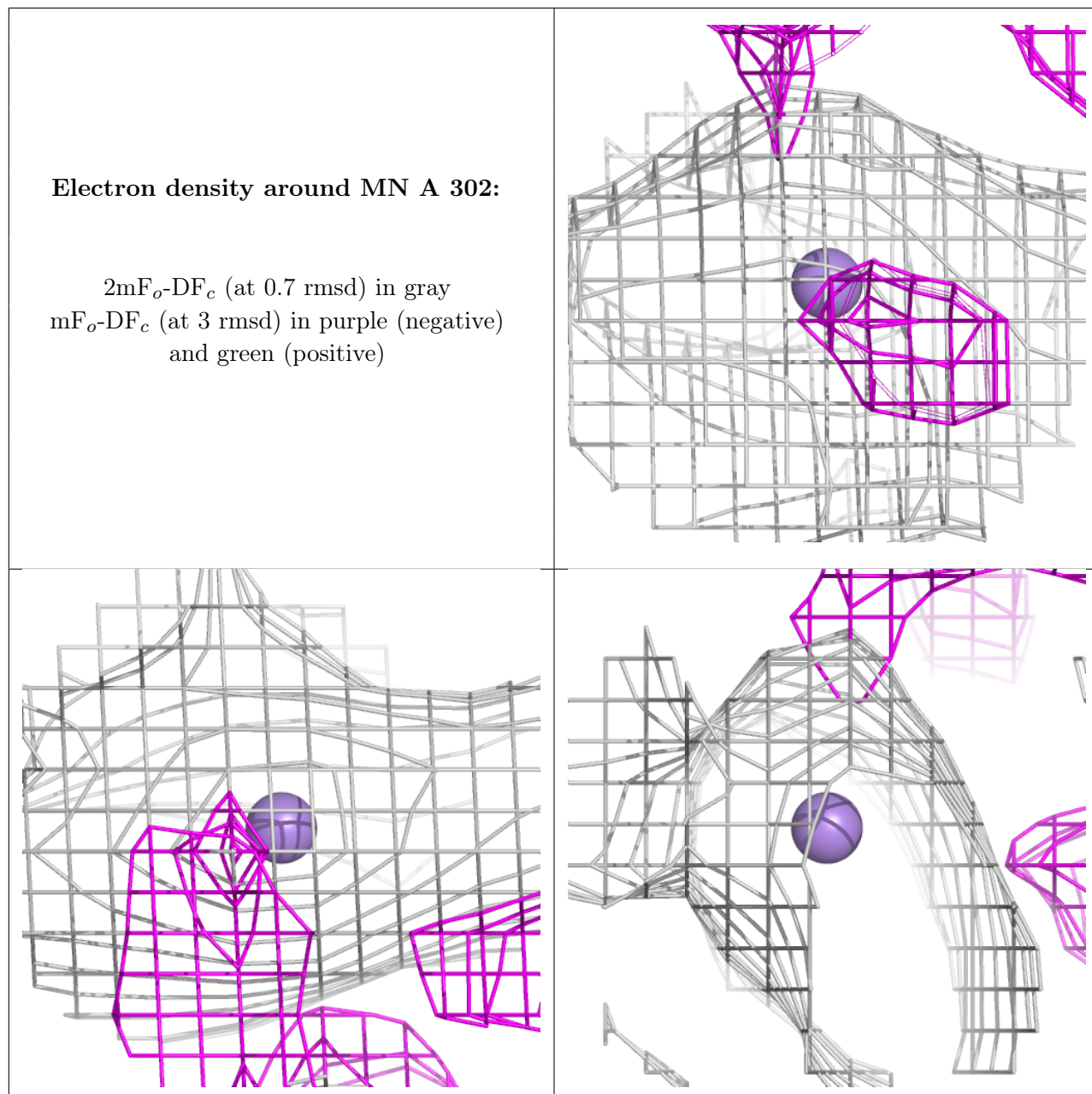
Electron density around MN A 303:

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



Electron density around MN A 302:

$2mF_o-DF_c$ (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.