



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:33 PM UTC

PDB ID : 8JZG / pdb_00008jzg
Title : C. glutamicum S-adenosylmethionine synthase co-crystallized with Adenosine, triphosphate, and SAM
Authors : Lee, S.; Kim, K.J.
Deposited on : 2023-07-05
Resolution : 2.39 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

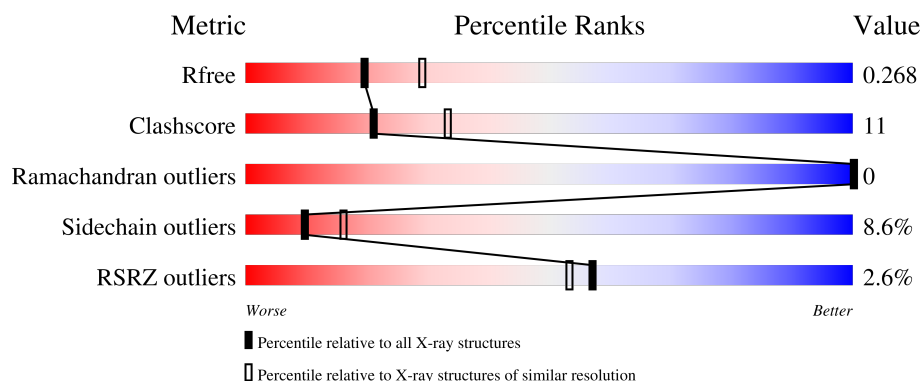
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	407	0% 70% 22% • 5%
1	B	407	3% 71% 22% • •
1	C	407	4% 66% 24% • 5%
1	D	407	3% 72% 20% • 5%

2 Entry composition [i](#)

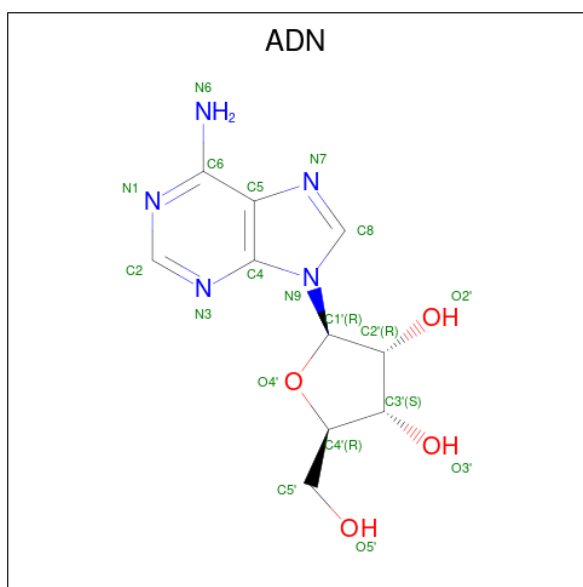
There are 9 unique types of molecules in this entry. The entry contains 12405 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2948	1848	517	576	7			
1	B	390	Total	C	N	O	S	0	0	0
			2984	1869	523	585	7			
1	C	386	Total	C	N	O	S	0	0	0
			2957	1853	518	579	7			
1	D	387	Total	C	N	O	S	0	0	0
			2964	1858	519	580	7			

- Molecule 2 is ADENOSINE (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄) (labeled as "Ligand of Interest" by depositor).



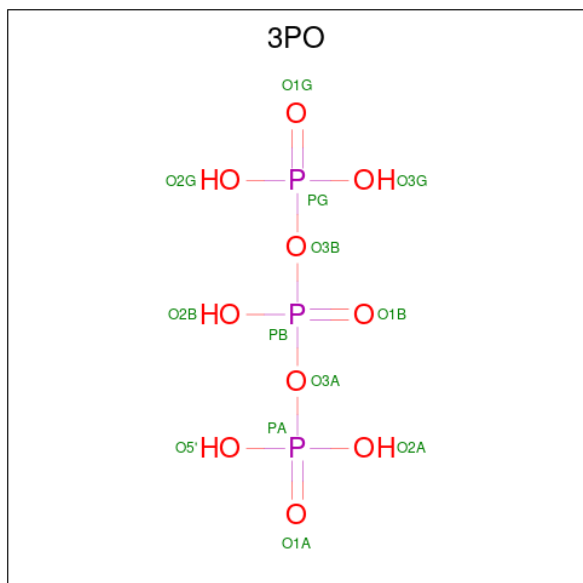
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

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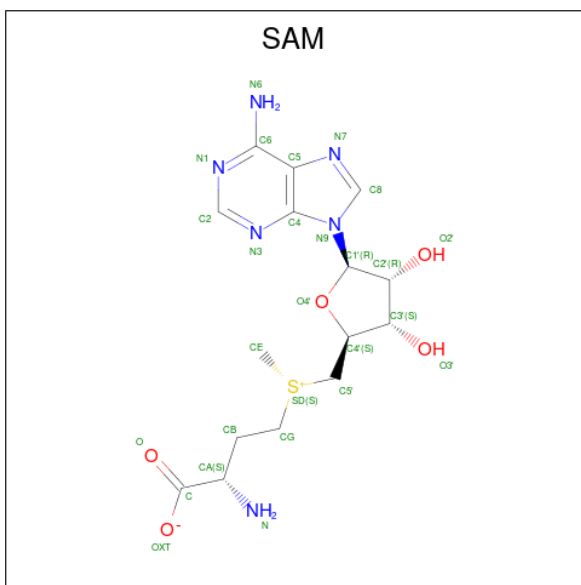
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			19	10	5	4		
2	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is TRIPHOSPHATE (CCD ID: 3PO) (formula: $\text{H}_5\text{O}_{10}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



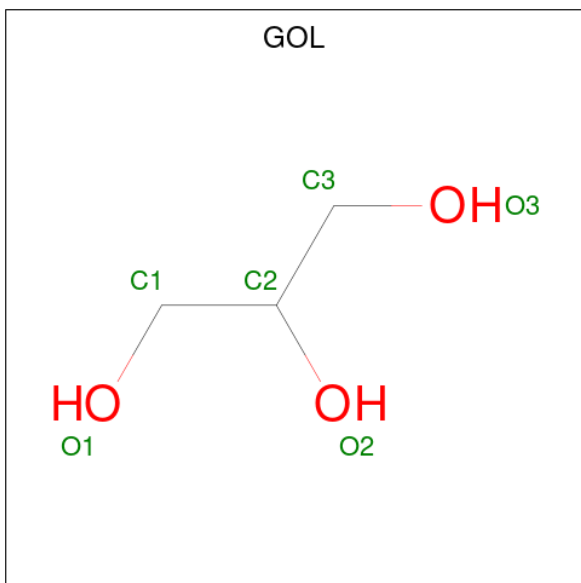
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			13	10	3		
3	B	1	Total	O	P	0	0
			13	10	3		
3	C	1	Total	O	P	0	0
			13	10	3		
3	D	1	Total	O	P	0	0
			13	10	3		

- Molecule 4 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $\text{C}_{15}\text{H}_{22}\text{N}_6\text{O}_5\text{S}$) (labeled as "Ligand of Interest" by depositor).



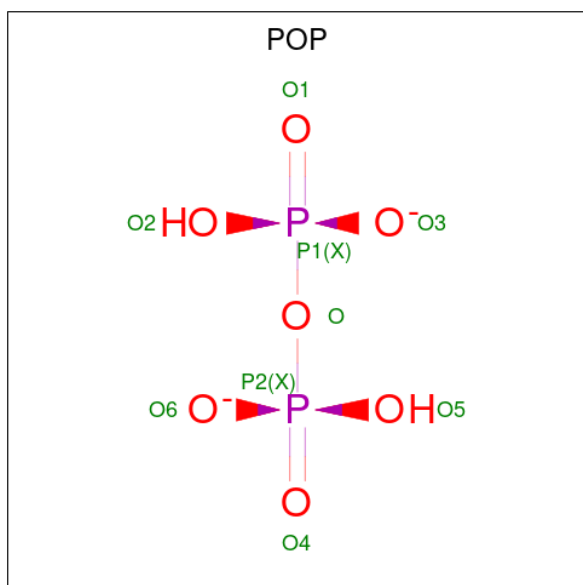
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 15	N 6	O 5	S 1	0	0
4	B	1	Total 27	C 15	N 6	O 5	S 1	0	0
4	C	1	Total 27	C 15	N 6	O 5	S 1	0	0
4	D	1	Total 27	C 15	N 6	O 5	S 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		
7	B	2	Total	Mg	0	0
			2	2		
7	C	2	Total	Mg	0	0
			2	2		
7	D	2	Total	Mg	0	0
			2	2		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total 2	K 2	0	0
8	C	1	Total 1	K 1	0	0
8	D	1	Total 1	K 1	0	0

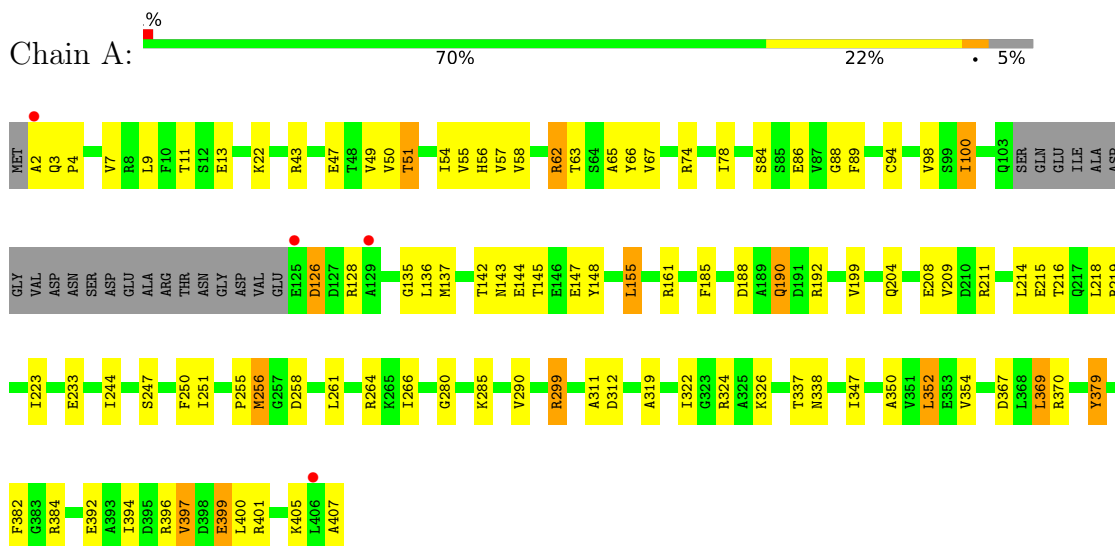
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	92	Total 92	O 92	0	0
9	B	91	Total 91	O 91	0	0
9	C	55	Total 55	O 55	0	0
9	D	45	Total 45	O 45	0	0

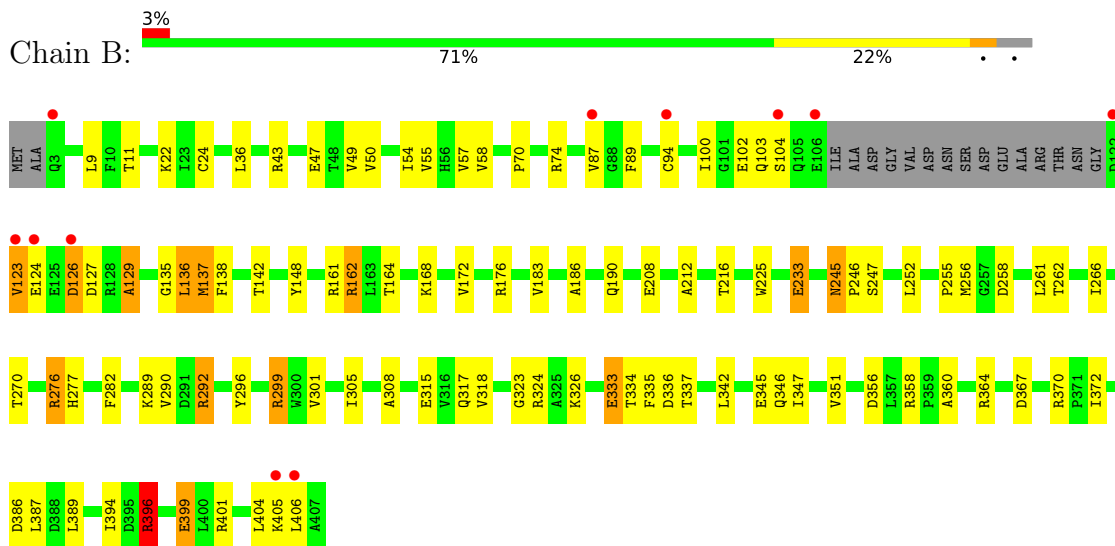
3 Residue-property plots [i](#)

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: S-adenosylmethionine synthase

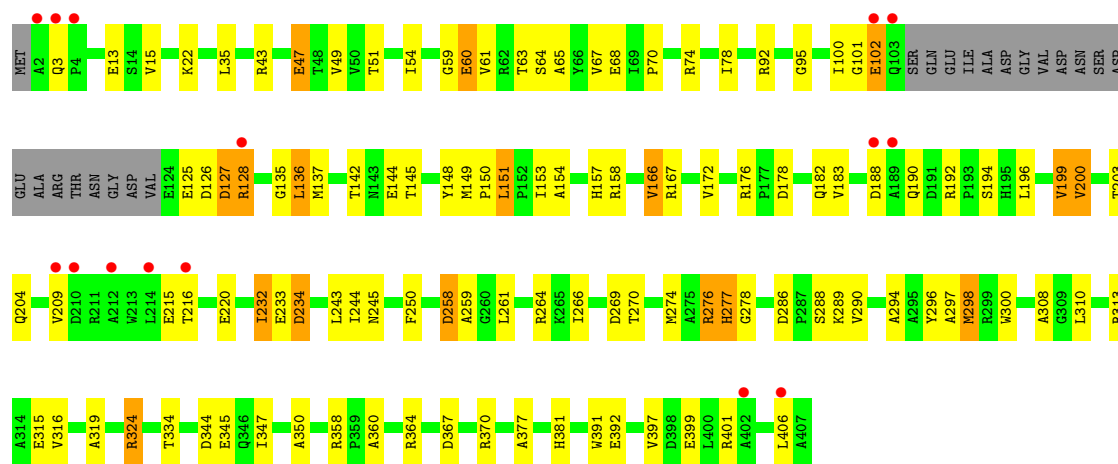


- Molecule 1: S-adenosylmethionine synthase

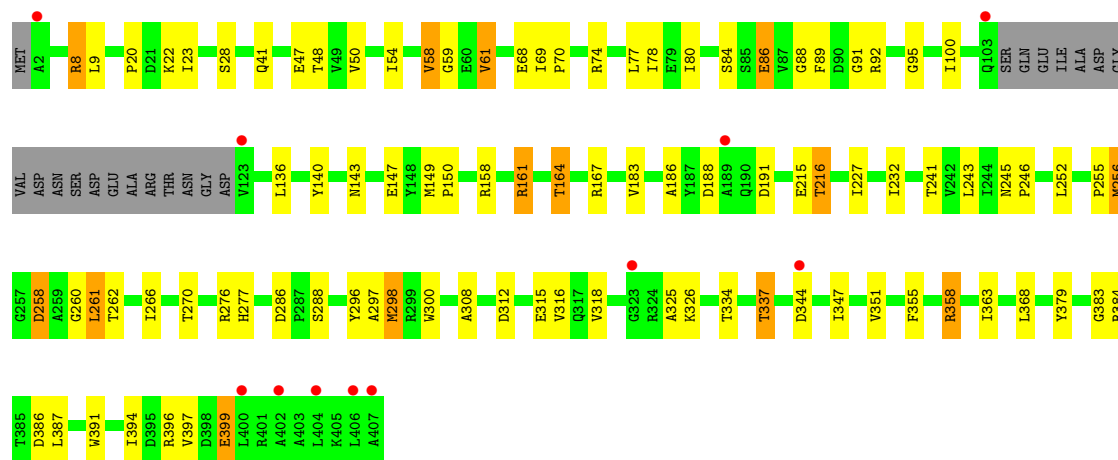


- Molecule 1: S-adenosylmethionine synthase





• Molecule 1: S-adenosylmethionine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.31Å 116.81Å 116.31Å 90.00° 103.31° 90.00°	Depositor
Resolution (Å)	32.63 – 2.39 32.63 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (32.63-2.39) 98.9 (32.63-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.260 0.198 , 0.268	Depositor DCC
R_{free} test set	3194 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12405	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: SAM, K, ADN, POP, 3PO, MG, GOL

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	1.08	0/3000	1.43	8/4075 (0.2%)
1	B	0.97	1/3036 (0.0%)	1.33	11/4124 (0.3%)
1	C	1.06	0/3009	1.47	15/4087 (0.4%)
1	D	1.06	0/3016	1.41	2/4097 (0.0%)
All	All	1.05	1/12061 (0.0%)	1.41	36/16383 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	VAL	N-CA	5.04	1.49	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	GLU	N-CA-C	-12.25	94.75	111.28
1	D	337	THR	N-CA-C	-6.64	103.57	112.94
1	C	178	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	102	GLU	CB-CA-C	-6.36	102.83	112.11
1	A	379	TYR	N-CA-C	-6.30	102.54	111.56
1	B	11	THR	CA-CB-OG1	-6.30	100.14	109.60
1	D	216	THR	CB-CA-C	6.26	119.89	109.56
1	A	126	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	396	ARG	CA-C-N	5.58	127.67	120.70
1	B	396	ARG	C-N-CA	5.58	127.67	120.70
1	C	128	ARG	N-CA-C	-5.55	106.36	113.02
1	C	64	SER	N-CA-C	-5.52	106.22	113.17
1	C	234	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	127	ASP	N-CA-C	-5.46	106.62	113.72
1	B	245	ASN	CB-CA-C	5.44	115.83	110.71
1	B	129	ALA	CA-C-N	5.42	126.08	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ALA	C-N-CA	5.42	126.08	120.60
1	C	324	ARG	CA-C-N	5.39	127.51	120.28
1	C	324	ARG	C-N-CA	5.39	127.51	120.28
1	A	251	ILE	N-CA-C	-5.29	106.53	111.45
1	B	386	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	277	HIS	CA-C-N	5.24	126.94	120.34
1	C	277	HIS	C-N-CA	5.24	126.94	120.34
1	C	176	ARG	CB-CA-C	5.19	117.10	109.22
1	C	60	GLU	CB-CG-CD	5.18	121.41	112.60
1	C	259	ALA	CA-C-N	5.13	125.72	122.18
1	C	259	ALA	C-N-CA	5.13	125.72	122.18
1	A	84	SER	CA-C-N	5.08	128.73	120.60
1	A	84	SER	C-N-CA	5.08	128.73	120.60
1	B	176	ARG	CB-CA-C	5.05	116.80	109.08
1	B	372	ILE	CA-C-O	-5.04	115.39	119.97
1	B	36	LEU	CA-C-N	5.04	127.03	120.28
1	B	36	LEU	C-N-CA	5.04	127.03	120.28
1	A	219	ARG	CA-C-N	5.02	127.45	120.63
1	A	219	ARG	C-N-CA	5.02	127.45	120.63
1	A	219	ARG	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

There are no planarity outliers.

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	2948	0	2917	71	1
1	B	2984	0	2944	72	0
1	C	2957	0	2923	70	1
1	D	2964	0	2932	67	0
2	A	19	0	13	0	0
2	B	19	0	13	0	0
2	C	19	0	13	1	0
2	D	19	0	13	1	0
3	A	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	0	2	0
3	C	13	0	0	0	0
3	D	13	0	0	0	0
4	A	27	0	22	2	0
4	B	27	0	22	1	0
4	C	27	0	22	0	0
4	D	27	0	22	4	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	9	0	0	2	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
8	A	2	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	92	0	0	1	0
9	B	91	0	0	2	0
9	C	55	0	0	0	0
9	D	45	0	0	1	0
All	All	12405	0	11872	263	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 11.

All (263) 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:D:50:VAL:HG12	1:D:255:PRO:HB3	1.44	0.99
1:D:260:GLY:C	1:D:261:LEU:HD23	1.90	0.96
1:B:333:GLU:OE2	9:B:601:HOH:O	1.91	0.88
1:C:61:VAL:O	1:C:102:GLU:O	1.91	0.87
1:C:63:THR:HG22	1:C:65:ALA:H	1.39	0.86
1:D:50:VAL:CG1	1:D:255:PRO:HB3	2.06	0.85
1:B:252:LEU:HD13	1:B:256:MET:HE3	1.59	0.84
1:D:48:THR:H	1:D:262:THR:HG23	1.44	0.82
1:D:358:ARG:HH11	1:D:358:ARG:HG3	1.48	0.77
1:A:11:THR:HG22	1:B:136:LEU:HD12	1.69	0.73
1:B:89:PHE:CD1	1:B:255:PRO:HG2	2.23	0.73
1:C:68:GLU:H	1:C:68:GLU:CD	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:SER:OG	1:D:262:THR:HG21	1.89	0.71
1:B:127:ASP:HA	1:B:360:ALA:HB3	1.73	0.71
1:C:188:ASP:HB2	1:C:192:ARG:HG3	1.72	0.71
1:B:136:LEU:HD22	1:B:136:LEU:H	1.56	0.71
1:D:261:LEU:HD23	1:D:261:LEU:N	2.04	0.71
1:D:363:ILE:HA	1:D:368:LEU:HD12	1.72	0.71
1:A:299:ARG:HG3	1:A:382:PHE:CD1	2.27	0.69
1:D:358:ARG:HH11	1:D:358:ARG:CG	2.06	0.68
1:A:190:GLN:HB2	1:A:192:ARG:HD3	1.76	0.68
1:C:266:ILE:HD11	1:D:266:ILE:HD11	1.74	0.68
1:A:51:THR:HG22	1:A:54:ILE:HG23	1.76	0.68
1:D:48:THR:H	1:D:262:THR:CG2	2.05	0.68
1:C:154:ALA:O	1:C:158:ARG:HG3	1.95	0.66
1:C:182:GLN:HB3	1:C:200:VAL:HG13	1.76	0.65
1:A:65:ALA:O	4:A:503:SAM:HE2	1.97	0.65
1:A:397:VAL:O	1:A:401:ARG:HG3	1.98	0.64
1:A:56:HIS:CE1	6:A:505:POP:O1	2.50	0.63
1:C:286:ASP:OD1	1:C:288:SER:OG	2.11	0.63
1:A:88:GLY:O	1:A:256:MET:HG3	1.99	0.63
1:C:142:THR:OG1	1:C:144:GLU:HG3	1.99	0.63
1:A:57:VAL:HG12	1:A:100:ILE:HD11	1.80	0.62
1:C:204:GLN:HA	1:C:250:PHE:O	1.98	0.62
1:C:196:LEU:HD21	1:C:199:VAL:HG12	1.80	0.62
1:C:308:ALA:HB3	1:C:310:LEU:HG	1.83	0.61
1:B:404:LEU:O	1:B:406:LEU:HG	2.01	0.61
1:D:227:ILE:HG23	1:D:232:ILE:HG13	1.82	0.61
1:A:401:ARG:HB3	1:A:401:ARG:NH1	2.15	0.60
1:A:49:VAL:HG13	1:A:261:LEU:HD23	1.82	0.60
1:D:74:ARG:HD3	1:D:91:GLY:O	2.02	0.60
1:B:396:ARG:O	1:B:399:GLU:HG2	2.01	0.60
1:D:143:ASN:ND2	1:D:312:ASP:OD1	2.35	0.60
1:D:252:LEU:HD13	1:D:256:MET:HG3	1.82	0.60
1:D:276:ARG:NH1	1:D:315:GLU:OE1	2.32	0.60
1:B:356:ASP:OD1	1:B:358:ARG:HD3	2.02	0.59
1:A:74:ARG:NH1	1:A:94:CYS:O	2.33	0.59
1:A:63:THR:HG22	4:A:503:SAM:H3'	1.85	0.59
1:C:298:MET:HG3	1:C:316:VAL:HB	1.84	0.59
1:A:401:ARG:HB3	1:A:401:ARG:HH11	1.67	0.58
1:B:43:ARG:NH1	1:B:124:GLU:HG2	2.18	0.58
1:D:325:ALA:HB1	1:D:358:ARG:HD2	1.86	0.57
1:A:379:TYR:O	1:A:384:ARG:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:OD2	1:A:192:ARG:HB2	2.04	0.57
1:D:298:MET:HA	1:D:298:MET:CE	2.35	0.57
1:A:247:SER:HB2	1:B:323:GLY:HA3	1.87	0.57
1:C:142:THR:O	1:C:148:TYR:HA	2.05	0.56
1:B:103:GLN:HB3	4:B:503:SAM:H4'	1.87	0.56
1:B:137:MET:CE	1:B:318:VAL:HG13	2.35	0.56
1:D:9:LEU:HD23	1:D:186:ALA:HA	1.88	0.56
1:B:142:THR:O	1:B:148:TYR:HA	2.06	0.55
1:D:384:ARG:HG2	1:D:387:LEU:HD12	1.88	0.55
1:C:264:ARG:NH2	1:D:47:GLU:OE2	2.39	0.55
1:D:399:GLU:CD	1:D:399:GLU:H	2.13	0.55
1:B:70:PRO:O	1:B:74:ARG:HG3	2.07	0.55
1:B:282:PHE:HA	1:B:292:ARG:HG3	1.88	0.55
1:C:188:ASP:OD1	1:C:194:SER:HB2	2.07	0.55
1:C:150:PRO:HB3	1:C:274:MET:HG3	1.89	0.54
1:B:127:ASP:OD2	1:B:364:ARG:NH2	2.41	0.54
1:B:333:GLU:OE1	1:B:335:PHE:N	2.32	0.54
1:C:35:LEU:HD22	1:C:63:THR:HG21	1.90	0.54
1:B:123:VAL:HG22	1:B:129:ALA:CB	2.38	0.53
1:C:47:GLU:HG3	1:D:261:LEU:HD11	1.90	0.53
1:D:84:SER:OG	1:D:86:GLU:HB2	2.08	0.53
1:C:367:ASP:O	1:C:370:ARG:HD3	2.09	0.53
1:D:308:ALA:HA	1:D:397:VAL:HG13	1.90	0.53
1:A:367:ASP:O	1:A:370:ARG:HD3	2.08	0.53
1:B:367:ASP:O	1:B:370:ARG:NH1	2.41	0.53
1:D:270:THR:HG21	1:D:277:HIS:CD2	2.43	0.53
1:C:51:THR:HG21	1:D:58:VAL:HG13	1.91	0.52
1:D:358:ARG:HG3	1:D:358:ARG:NH1	2.21	0.52
1:A:299:ARG:NH1	1:A:392:GLU:OE1	2.43	0.52
1:C:125:GLU:HA	1:C:128:ARG:HB3	1.89	0.52
1:D:312:ASP:HB2	1:D:337:THR:HB	1.91	0.52
1:C:286:ASP:OD2	1:C:289:LYS:NZ	2.42	0.52
1:D:164:THR:HG21	1:D:379:TYR:OH	2.08	0.52
1:D:243:LEU:HB3	1:D:246:PRO:HG3	1.92	0.51
1:A:396:ARG:O	1:A:399:GLU:HG2	2.10	0.51
1:A:47:GLU:HG3	1:B:261:LEU:HD11	1.92	0.51
1:C:137:MET:SD	1:C:137:MET:N	2.84	0.51
1:D:59:GLY:O	1:D:100:ILE:HA	2.10	0.51
1:B:299:ARG:HD2	1:B:299:ARG:O	2.11	0.51
1:A:3:GLN:N	1:A:4:PRO:CD	2.74	0.51
1:C:397:VAL:O	1:C:401:ARG:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:VAL:HG13	1:B:261:LEU:CD2	2.41	0.50
1:D:347:ILE:O	1:D:351:VAL:HG23	2.11	0.50
1:B:9:LEU:HD23	1:B:186:ALA:HA	1.93	0.50
1:A:56:HIS:ND1	6:A:505:POP:O1	2.44	0.50
1:A:261:LEU:HD11	1:B:47:GLU:CG	2.41	0.50
1:B:342:LEU:HA	1:B:346:GLN:OE1	2.11	0.50
1:C:127:ASP:HB3	1:C:358:ARG:CZ	2.41	0.50
1:D:54:ILE:HD12	1:D:95:GLY:C	2.37	0.50
1:B:292:ARG:HD3	1:B:296:TYR:CZ	2.47	0.50
1:B:308:ALA:HA	1:B:401:ARG:HH21	1.76	0.50
1:C:401:ARG:NH1	1:C:406:LEU:HD13	2.27	0.50
1:D:80:ILE:O	1:D:167:ARG:NH1	2.45	0.50
1:D:88:GLY:O	1:D:256:MET:HG2	2.12	0.49
1:D:355:PHE:CE1	1:D:396:ARG:HG2	2.47	0.49
1:B:49:VAL:HG13	1:B:261:LEU:HD21	1.93	0.49
1:D:20:PRO:HA	1:D:23:ILE:HD12	1.94	0.49
1:A:261:LEU:HD11	1:B:47:GLU:HG2	1.93	0.49
1:C:136:LEU:O	1:C:278:GLY:HA3	2.13	0.49
1:B:50:VAL:HG12	1:B:55:VAL:HG22	1.94	0.49
1:B:212:ALA:O	1:B:216:THR:HG23	2.13	0.49
1:A:142:THR:O	1:A:148:TYR:HA	2.12	0.49
1:A:199:VAL:HG11	1:A:223:ILE:HD13	1.95	0.49
1:A:143:ASN:ND2	1:A:312:ASP:OD1	2.46	0.49
1:A:142:THR:OG1	1:A:144:GLU:HG3	2.13	0.48
1:B:136:LEU:HD22	1:B:136:LEU:N	2.25	0.48
1:B:136:LEU:N	1:B:136:LEU:HD13	2.28	0.48
1:A:2:ALA:HA	1:B:405:LYS:HD2	1.96	0.48
1:B:396:ARG:HG3	1:B:399:GLU:HG3	1.95	0.48
1:D:89:PHE:CD2	1:D:255:PRO:HG2	2.48	0.48
1:C:203:THR:O	1:C:250:PHE:HB3	2.14	0.48
1:B:394:ILE:O	1:B:394:ILE:HG22	2.14	0.48
1:D:149:MET:CG	1:D:383:GLY:HA3	2.43	0.48
1:C:296:TYR:CE2	1:C:391:TRP:CH2	3.01	0.48
1:D:100:ILE:HD11	4:D:503:SAM:N7	2.29	0.48
1:C:166:VAL:HG13	1:C:172:VAL:HB	1.96	0.47
1:A:401:ARG:NH1	1:A:407:ALA:O	2.47	0.47
1:B:292:ARG:HD3	1:B:296:TYR:OH	2.14	0.47
1:A:266:ILE:HD11	1:B:266:ILE:HD11	1.96	0.47
1:C:188:ASP:HB2	1:C:192:ARG:CG	2.41	0.47
1:A:49:VAL:HG13	1:A:261:LEU:CD2	2.44	0.47
1:A:66:TYR:CE2	4:D:503:SAM:HE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLY:C	1:B:136:LEU:HD13	2.40	0.47
1:B:282:PHE:CA	1:B:292:ARG:HG3	2.44	0.47
1:D:8:ARG:NH2	1:D:191:ASP:OD1	2.40	0.47
1:B:123:VAL:HG22	1:B:129:ALA:HB1	1.96	0.47
1:C:54:ILE:HD12	1:C:95:GLY:C	2.40	0.47
1:D:245:ASN:N	1:D:246:PRO:HD3	2.30	0.47
1:D:161:ARG:NH1	1:D:386:ASP:OD2	2.48	0.46
1:B:138:PHE:CE1	1:B:317:GLN:HB2	2.50	0.46
1:A:51:THR:HG22	1:A:54:ILE:CG2	2.43	0.46
1:C:51:THR:HG21	1:D:58:VAL:CG1	2.45	0.46
1:C:308:ALA:HA	1:C:397:VAL:HG13	1.97	0.46
1:D:89:PHE:CD2	1:D:255:PRO:CG	2.98	0.46
1:A:135:GLY:O	1:A:319:ALA:HA	2.16	0.46
1:A:369:LEU:C	1:A:370:ARG:HG3	2.41	0.46
1:B:270:THR:HG21	1:B:277:HIS:CD2	2.51	0.46
1:D:143:ASN:ND2	1:D:312:ASP:HA	2.31	0.46
1:A:285:LYS:NZ	3:B:502:3PO:O3G	2.46	0.46
1:B:124:GLU:HA	9:B:668:HOH:O	2.16	0.46
1:D:286:ASP:OD1	1:D:288:SER:OG	2.15	0.46
1:A:394:ILE:HG12	9:A:648:HOH:O	2.16	0.46
1:A:137:MET:HE2	1:A:290:VAL:HG13	1.98	0.45
1:A:347:ILE:O	1:A:350:ALA:HB3	2.15	0.45
1:B:126:ASP:OD1	1:B:126:ASP:N	2.49	0.45
1:B:127:ASP:HA	1:B:360:ALA:CB	2.45	0.45
1:C:270:THR:HG21	1:C:277:HIS:CD2	2.51	0.45
1:C:296:TYR:CD2	1:C:391:TRP:CZ3	3.04	0.45
1:A:379:TYR:O	1:A:384:ARG:NH1	2.49	0.45
1:B:137:MET:HE2	1:B:318:VAL:HG13	1.97	0.45
1:A:322:ILE:HG12	1:B:247:SER:CB	2.46	0.45
1:C:258:ASP:OD2	2:C:501:ADN:H5'1	2.16	0.45
1:C:269:ASP:HB3	1:C:381:HIS:CD2	2.51	0.45
1:A:50:VAL:HG12	1:A:55:VAL:HG22	1.99	0.45
1:C:70:PRO:O	1:C:74:ARG:HG3	2.17	0.45
1:C:101:GLY:O	1:C:102:GLU:HB2	2.16	0.45
1:D:261:LEU:N	1:D:261:LEU:CD2	2.76	0.45
1:A:47:GLU:CG	1:B:261:LEU:HD11	2.47	0.45
1:C:297:ALA:O	1:C:300:TRP:HB3	2.17	0.45
1:D:334:THR:OG1	1:D:344:ASP:OD1	2.35	0.45
1:A:43:ARG:HB2	1:A:62:ARG:HB3	1.99	0.45
1:A:145:THR:HB	1:A:147:GLU:OE2	2.17	0.45
1:D:140:TYR:CE2	1:D:150:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ARG:HD3	1:D:315:GLU:OE2	2.16	0.45
1:C:137:MET:HE2	1:C:290:VAL:HG13	2.00	0.44
1:C:276:ARG:HD3	1:C:315:GLU:OE1	2.18	0.44
1:A:215:GLU:HA	1:A:244:ILE:HD12	1.98	0.44
1:B:57:VAL:HG12	1:B:100:ILE:HD11	2.00	0.44
1:B:266:ILE:HD12	1:B:277:HIS:CE1	2.52	0.44
1:D:296:TYR:CD2	1:D:391:TRP:CZ3	3.05	0.44
1:C:59:GLY:O	1:C:100:ILE:HA	2.18	0.44
1:C:136:LEU:C	1:C:137:MET:SD	3.01	0.44
1:C:153:ILE:HG13	1:C:157:HIS:CD2	2.53	0.44
1:D:78:ILE:HD11	1:D:92:ARG:HG3	2.00	0.44
1:A:98:VAL:HG13	1:A:100:ILE:HD13	2.00	0.44
1:C:15:VAL:HG23	1:C:22:LYS:HG3	1.99	0.44
1:A:74:ARG:O	1:A:78:ILE:HG13	2.18	0.43
1:A:311:ALA:HB1	1:A:337:THR:OG1	2.18	0.43
1:D:69:ILE:N	1:D:70:PRO:CD	2.81	0.43
1:A:354:VAL:HG21	1:A:400:LEU:HD23	2.00	0.43
1:D:149:MET:HG3	1:D:383:GLY:HA3	2.00	0.43
1:B:233:GLU:CD	1:B:233:GLU:H	2.26	0.43
1:D:161:ARG:HG2	1:D:379:TYR:CG	2.53	0.43
1:A:190:GLN:HB2	1:A:192:ARG:CD	2.47	0.43
1:A:264:ARG:NH2	1:B:262:THR:O	2.49	0.43
1:C:22:LYS:HD3	1:C:377:ALA:O	2.18	0.43
1:A:299:ARG:HH11	1:A:392:GLU:CD	2.26	0.43
1:B:334:THR:O	1:B:337:THR:OG1	2.34	0.43
1:D:260:GLY:O	1:D:261:LEU:HD23	2.14	0.43
1:B:347:ILE:O	1:B:351:VAL:HG23	2.18	0.43
1:C:128:ARG:HD3	1:C:128:ARG:HA	1.77	0.43
1:A:155:LEU:HD12	1:A:185:PHE:CE2	2.53	0.43
1:C:360:ALA:O	1:C:364:ARG:HG3	2.18	0.43
1:D:298:MET:SD	1:D:318:VAL:HB	2.58	0.43
1:A:369:LEU:O	1:A:370:ARG:HG3	2.19	0.43
1:C:43:ARG:O	1:C:61:VAL:HA	2.18	0.43
1:A:188:ASP:CG	1:A:190:GLN:HG2	2.44	0.43
1:A:280:GLY:HA2	3:B:502:3PO:O1G	2.19	0.43
1:C:215:GLU:HG2	1:C:244:ILE:HB	2.01	0.43
1:C:298:MET:HG2	1:C:316:VAL:O	2.18	0.43
1:C:151:LEU:HD11	1:C:232:ILE:HD11	2.01	0.42
1:A:13:GLU:HG2	1:B:136:LEU:HD21	2.02	0.42
1:A:188:ASP:OD1	1:A:190:GLN:HG2	2.18	0.42
1:D:77:LEU:HD13	1:D:89:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ASP:OD1	1:D:188:ASP:C	2.62	0.42
1:A:66:TYR:CD2	4:D:503:SAM:HE3	2.55	0.42
1:B:252:LEU:HD13	1:B:256:MET:CE	2.40	0.42
1:B:301:VAL:O	1:B:305:ILE:HG13	2.18	0.42
1:A:204:GLN:HA	1:A:250:PHE:O	2.20	0.42
1:D:297:ALA:O	1:D:300:TRP:HB3	2.19	0.42
1:D:298:MET:HA	1:D:298:MET:HE2	2.02	0.42
1:D:158:ARG:NH1	9:D:602:HOH:O	2.51	0.42
1:A:401:ARG:HH12	1:A:407:ALA:N	2.18	0.42
1:B:387:LEU:HD12	1:B:389:LEU:HD11	2.02	0.42
1:B:399:GLU:CD	1:B:399:GLU:H	2.28	0.42
1:A:89:PHE:CE2	1:A:255:PRO:HG2	2.54	0.42
1:B:24:CYS:SG	1:B:50:VAL:HG22	2.60	0.42
1:C:334:THR:OG1	1:C:344:ASP:OD1	2.38	0.42
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.96	0.42
1:C:126:ASP:O	1:C:364:ARG:NH2	2.53	0.42
1:C:137:MET:HG2	1:C:294:ALA:HB3	2.01	0.41
1:A:215:GLU:HA	1:A:244:ILE:CD1	2.50	0.41
1:B:103:GLN:O	1:B:104:SER:HB2	2.20	0.41
1:D:258:ASP:OD2	2:D:501:ADN:H5'2	2.20	0.41
1:C:298:MET:HA	1:C:298:MET:HE2	2.02	0.41
1:A:190:GLN:CD	1:A:190:GLN:N	2.78	0.41
1:B:74:ARG:NH2	1:B:94:CYS:O	2.49	0.41
1:C:347:ILE:O	1:C:350:ALA:HB3	2.20	0.41
1:C:135:GLY:O	1:C:319:ALA:HA	2.21	0.41
1:D:61:VAL:HG22	4:D:503:SAM:H2'	2.03	0.41
1:B:123:VAL:HG13	1:B:129:ALA:HB1	2.02	0.41
1:C:290:VAL:HG22	1:C:294:ALA:HB2	2.03	0.41
1:B:245:ASN:N	1:B:246:PRO:CD	2.84	0.41
1:B:162:ARG:HG3	1:B:225:TRP:CE3	2.56	0.41
1:B:299:ARG:HD2	1:B:299:ARG:C	2.45	0.41
1:C:49:VAL:HG13	1:C:261:LEU:CD2	2.50	0.41
1:C:78:ILE:HD11	1:C:92:ARG:HG3	2.02	0.41
1:C:49:VAL:HG13	1:C:261:LEU:HD23	2.03	0.41
1:A:47:GLU:HG3	1:B:261:LEU:CD1	2.50	0.40
1:B:276:ARG:HD3	1:B:315:GLU:OE1	2.21	0.40
1:C:298:MET:HA	1:C:298:MET:CE	2.51	0.40
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.95	0.40
1:A:214:LEU:O	1:A:218:LEU:HG	2.20	0.40
1:C:145:THR:OG1	1:C:149:MET:N	2.44	0.40
1:B:123:VAL:HG22	1:B:129:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:THR:HG22	1:B:168:LYS:HD2	2.04	0.40
1:C:244:ILE:O	1:C:245:ASN:C	2.65	0.40
1:C:127:ASP:OD1	1:C:364:ARG:NE	2.48	0.40
1:C:216:THR:O	1:C:220:GLU:HG3	2.22	0.40
1:D:8:ARG:HG3	1:D:8:ARG:HH11	1.86	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:405:LYS:O	1:C:190:GLN:NE2[1_554]	1.77	0.43

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	381/407 (94%)	366 (96%)	15 (4%)	0	100	100
1	B	386/407 (95%)	371 (96%)	15 (4%)	0	100	100
1	C	382/407 (94%)	357 (94%)	25 (6%)	0	100	100
1	D	383/407 (94%)	357 (93%)	26 (7%)	0	100	100
All	All	1532/1628 (94%)	1451 (95%)	81 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	310/328 (94%)	280 (90%)	30 (10%)	8	12
1	B	314/328 (96%)	286 (91%)	28 (9%)	9	15
1	C	311/328 (95%)	286 (92%)	25 (8%)	11	19
1	D	312/328 (95%)	288 (92%)	24 (8%)	12	20
All	All	1247/1312 (95%)	1140 (91%)	107 (9%)	10	16

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	9	LEU
1	A	22	LYS
1	A	51	THR
1	A	58	VAL
1	A	62	ARG
1	A	67	VAL
1	A	86	GLU
1	A	100	ILE
1	A	126	ASP
1	A	128	ARG
1	A	136	LEU
1	A	155	LEU
1	A	161	ARG
1	A	190	GLN
1	A	208	GLU
1	A	209	VAL
1	A	211	ARG
1	A	216	THR
1	A	233	GLU
1	A	256	MET
1	A	258	ASP
1	A	299	ARG
1	A	324	ARG
1	A	326	LYS
1	A	338	ASN
1	A	352	LEU
1	A	369	LEU
1	A	397	VAL
1	A	399	GLU

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Mol	Chain	Res	Type
1	B	22	LYS
1	B	54	ILE
1	B	58	VAL
1	B	87	VAL
1	B	102	GLU
1	B	123	VAL
1	B	126	ASP
1	B	136	LEU
1	B	137	MET
1	B	161	ARG
1	B	162	ARG
1	B	183	VAL
1	B	190	GLN
1	B	208	GLU
1	B	233	GLU
1	B	258	ASP
1	B	276	ARG
1	B	289	LYS
1	B	290	VAL
1	B	292	ARG
1	B	299	ARG
1	B	324	ARG
1	B	326	LYS
1	B	333	GLU
1	B	336	ASP
1	B	345	GLU
1	B	396	ARG
1	B	399	GLU
1	C	3	GLN
1	C	13	GLU
1	C	47	GLU
1	C	60	GLU
1	C	67	VAL
1	C	136	LEU
1	C	151	LEU
1	C	166	VAL
1	C	167	ARG
1	C	183	VAL
1	C	199	VAL
1	C	200	VAL
1	C	209	VAL
1	C	232	ILE

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Mol	Chain	Res	Type
1	C	233	GLU
1	C	234	ASP
1	C	243	LEU
1	C	258	ASP
1	C	276	ARG
1	C	298	MET
1	C	313	ARG
1	C	324	ARG
1	C	345	GLU
1	C	392	GLU
1	C	399	GLU
1	D	8	ARG
1	D	22	LYS
1	D	41	GLN
1	D	58	VAL
1	D	61	VAL
1	D	68	GLU
1	D	86	GLU
1	D	136	LEU
1	D	147	GLU
1	D	161	ARG
1	D	164	THR
1	D	183	VAL
1	D	215	GLU
1	D	216	THR
1	D	241	THR
1	D	256	MET
1	D	258	ASP
1	D	261	LEU
1	D	298	MET
1	D	316	VAL
1	D	326	LYS
1	D	358	ARG
1	D	394	ILE
1	D	399	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	B	56	HIS
1	B	134	GLN

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Mol	Chain	Res	Type
1	C	3	GLN
1	C	56	HIS
1	C	83	ASN
1	D	3	GLN
1	D	103	GLN
1	D	205	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	SAM	A	503	-	27,29,29	0.55	1 (3%)	34,42,42	1.05	4 (11%)
3	3PO	B	502	7	10,12,12	3.62	2 (20%)	17,20,20	2.94	7 (41%)
4	SAM	B	503	-	27,29,29	0.49	1 (3%)	34,42,42	0.86	1 (2%)
4	SAM	C	503	-	27,29,29	0.50	1 (3%)	34,42,42	0.81	1 (2%)
3	3PO	D	502	7	10,12,12	2.57	1 (10%)	17,20,20	1.63	2 (11%)
6	POP	A	505	-	6,8,8	0.52	0	12,13,13	1.02	0
2	ADN	B	501	-	21,21,21	0.44	0	31,31,31	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	504	-	5,5,5	0.10	0	5,5,5	0.48	0
3	3PO	C	502	8,7	10,12,12	3.33	1 (10%)	17,20,20	2.56	6 (35%)
2	ADN	C	501	-	21,21,21	0.37	0	31,31,31	0.69	1 (3%)
2	ADN	D	501	-	21,21,21	0.33	0	31,31,31	0.52	0
2	ADN	A	501	-	21,21,21	0.36	0	31,31,31	0.54	0
3	3PO	A	502	8,7	10,12,12	2.39	3 (30%)	17,20,20	1.47	3 (17%)
4	SAM	D	503	-	27,29,29	0.47	0	34,42,42	1.12	1 (2%)
5	GOL	B	504	-	5,5,5	0.11	0	5,5,5	0.31	0

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	SAM	A	503	-	-	4/17/33/33	0/3/3/3
3	3PO	B	502	7	-	0/12/12/12	-
4	SAM	B	503	-	-	6/17/33/33	0/3/3/3
4	SAM	C	503	-	-	3/17/33/33	0/3/3/3
3	3PO	D	502	7	-	2/12/12/12	-
6	POP	A	505	-	-	0/6/6/6	-
2	ADN	B	501	-	-	3/6/22/22	0/3/3/3
5	GOL	A	504	-	-	2/4/4/4	-
3	3PO	C	502	8,7	-	1/12/12/12	-
2	ADN	C	501	-	-	3/6/22/22	0/3/3/3
2	ADN	D	501	-	-	5/6/22/22	0/3/3/3
2	ADN	A	501	-	-	3/6/22/22	0/3/3/3
3	3PO	A	502	8,7	-	2/12/12/12	-
4	SAM	D	503	-	-	1/17/33/33	0/3/3/3
5	GOL	B	504	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	3PO	PB-O3B	10.62	1.71	1.59
3	C	502	3PO	PB-O3B	10.07	1.70	1.59
3	D	502	3PO	PB-O3B	7.49	1.67	1.59
3	A	502	3PO	PB-O3A	6.35	1.66	1.59
3	A	502	3PO	PB-O3B	2.50	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	SAM	OXT-C	-2.30	1.23	1.30
3	B	502	3PO	PG-O2G	-2.27	1.46	1.54
4	C	503	SAM	OXT-C	-2.24	1.23	1.30
4	B	503	SAM	OXT-C	-2.21	1.23	1.30
3	A	502	3PO	PA-O5'	-2.08	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	3PO	O2B-PB-O3B	8.49	130.22	107.27
3	C	502	3PO	O2B-PB-O3B	6.49	124.82	107.27
3	B	502	3PO	O2B-PB-O3A	-5.08	93.55	107.27
4	D	503	SAM	OXT-C-O	-5.05	112.63	124.08
3	D	502	3PO	O2B-PB-O3B	4.65	119.83	107.27
3	B	502	3PO	O2G-PG-O3B	4.43	119.47	104.64
3	C	502	3PO	O2B-PB-O3A	-4.41	95.35	107.27
3	C	502	3PO	O3G-PG-O3B	3.97	117.93	104.64
3	C	502	3PO	O2G-PG-O3B	3.86	117.58	104.64
4	C	503	SAM	OXT-C-O	-3.13	116.97	124.08
4	A	503	SAM	O3'-C3'-C4'	-2.96	102.58	111.08
4	B	503	SAM	OXT-C-O	-2.89	117.53	124.08
3	A	502	3PO	O3B-PB-O1B	-2.78	102.33	110.70
4	A	503	SAM	O3'-C3'-C2'	2.72	120.52	111.82
3	B	502	3PO	O3B-PB-O1B	-2.66	102.71	110.70
3	C	502	3PO	O3B-PG-O1G	-2.64	97.12	111.04
3	D	502	3PO	O2B-PB-O3A	-2.61	100.23	107.27
4	A	503	SAM	OXT-C-O	-2.52	118.37	124.08
3	B	502	3PO	O3G-PG-O3B	2.43	112.78	104.64
4	A	503	SAM	O4'-C4'-C5'	2.42	114.99	108.88
3	B	502	3PO	O3A-PA-O1A	-2.23	99.29	111.04
3	A	502	3PO	O2G-PG-O3B	2.16	111.88	104.64
3	B	502	3PO	O5'-PA-O3A	2.15	111.85	104.64
3	C	502	3PO	O3B-PB-O1B	-2.12	104.34	110.70
2	C	501	ADN	C2'-C3'-C4'	2.10	106.67	102.61
3	A	502	3PO	O3A-PA-O1A	-2.02	100.43	111.04

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	3PO	PB-O3A-PA-O2A
3	D	502	3PO	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	A	503	SAM	N-CA-CB-CG
4	A	503	SAM	O4'-C4'-C5'-SD
4	A	503	SAM	C3'-C4'-C5'-SD
4	B	503	SAM	O-C-CA-N
4	B	503	SAM	CB-CG-SD-CE
4	D	503	SAM	CB-CG-SD-CE
5	B	504	GOL	C1-C2-C3-O3
5	B	504	GOL	O2-C2-C3-O3
2	D	501	ADN	O4'-C4'-C5'-O5'
2	D	501	ADN	C3'-C4'-C5'-O5'
4	B	503	SAM	OXT-C-CA-N
5	A	504	GOL	O1-C1-C2-C3
4	C	503	SAM	OXT-C-CA-N
5	A	504	GOL	O1-C1-C2-O2
4	C	503	SAM	O-C-CA-N
2	B	501	ADN	C2'-C1'-N9-C8
3	C	502	3PO	PB-O3B-PG-O2G
2	A	501	ADN	C2'-C1'-N9-C8
2	C	501	ADN	C2'-C1'-N9-C8
2	D	501	ADN	C2'-C1'-N9-C8
4	A	503	SAM	CA-CB-CG-SD
2	C	501	ADN	C2'-C1'-N9-C4
2	B	501	ADN	C2'-C1'-N9-C4
2	D	501	ADN	C2'-C1'-N9-C4
2	D	501	ADN	O4'-C1'-N9-C8
4	B	503	SAM	O-C-CA-CB
2	B	501	ADN	O4'-C1'-N9-C8
4	B	503	SAM	OXT-C-CA-CB
3	A	502	3PO	PB-O3A-PA-O5'
2	A	501	ADN	O4'-C1'-N9-C8
2	C	501	ADN	O4'-C1'-N9-C8
4	C	503	SAM	O4'-C1'-N9-C8
2	A	501	ADN	C2'-C1'-N9-C4
4	B	503	SAM	O4'-C1'-N9-C8
3	D	502	3PO	PG-O3B-PB-O2B

There are no ring outliers.

7 monomers are involved in 13 short contacts:

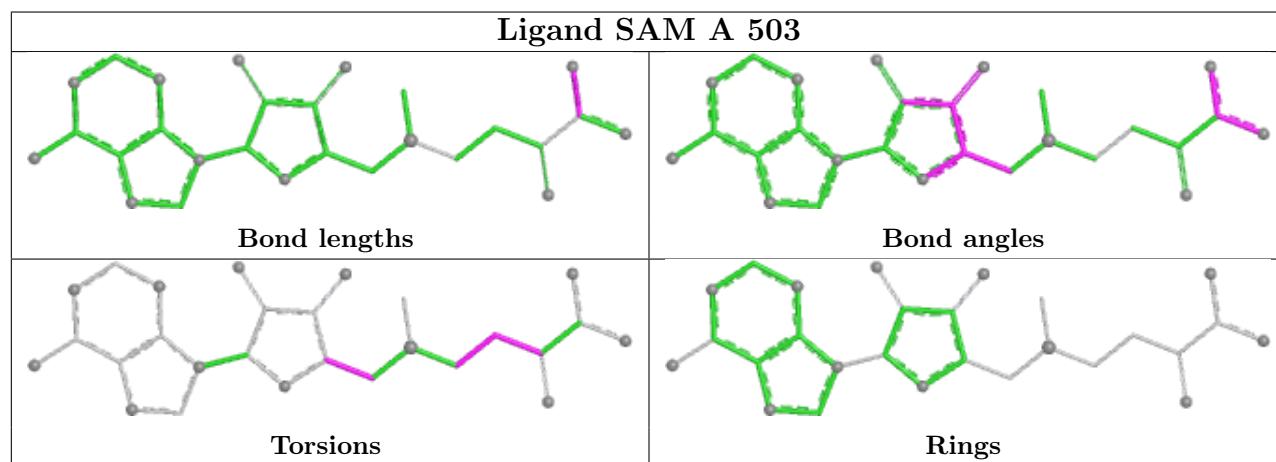
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	SAM	2	0
3	B	502	3PO	2	0

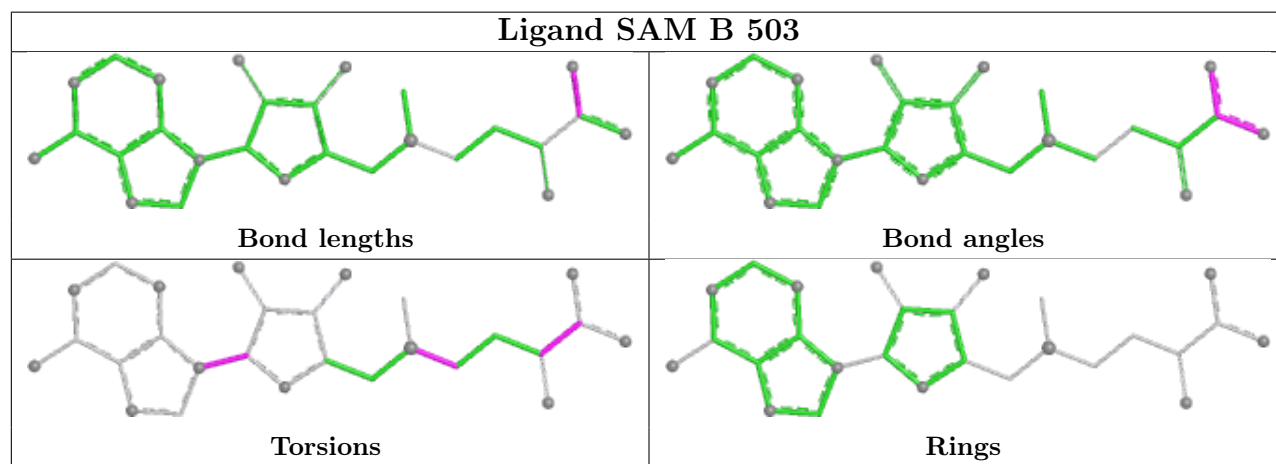
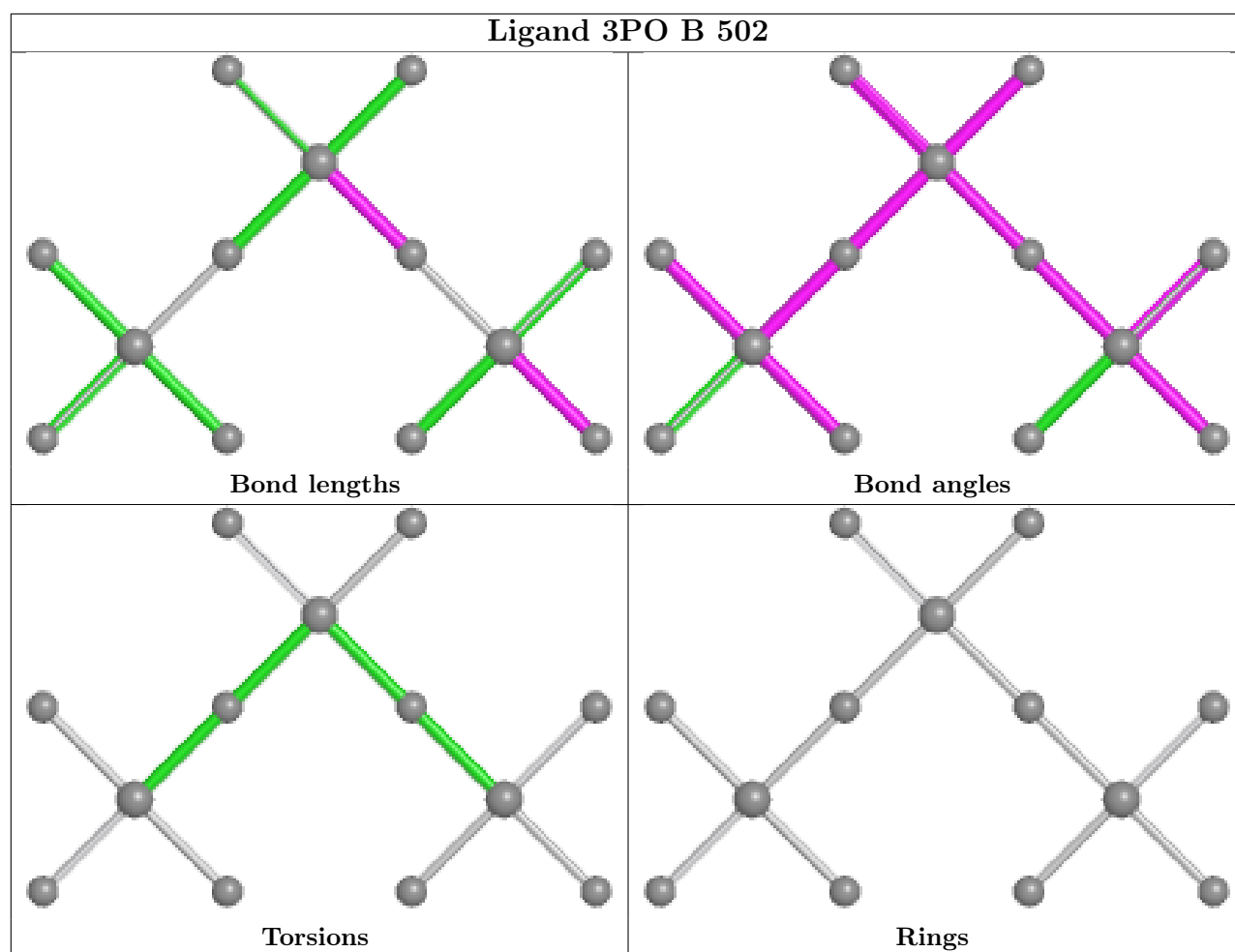
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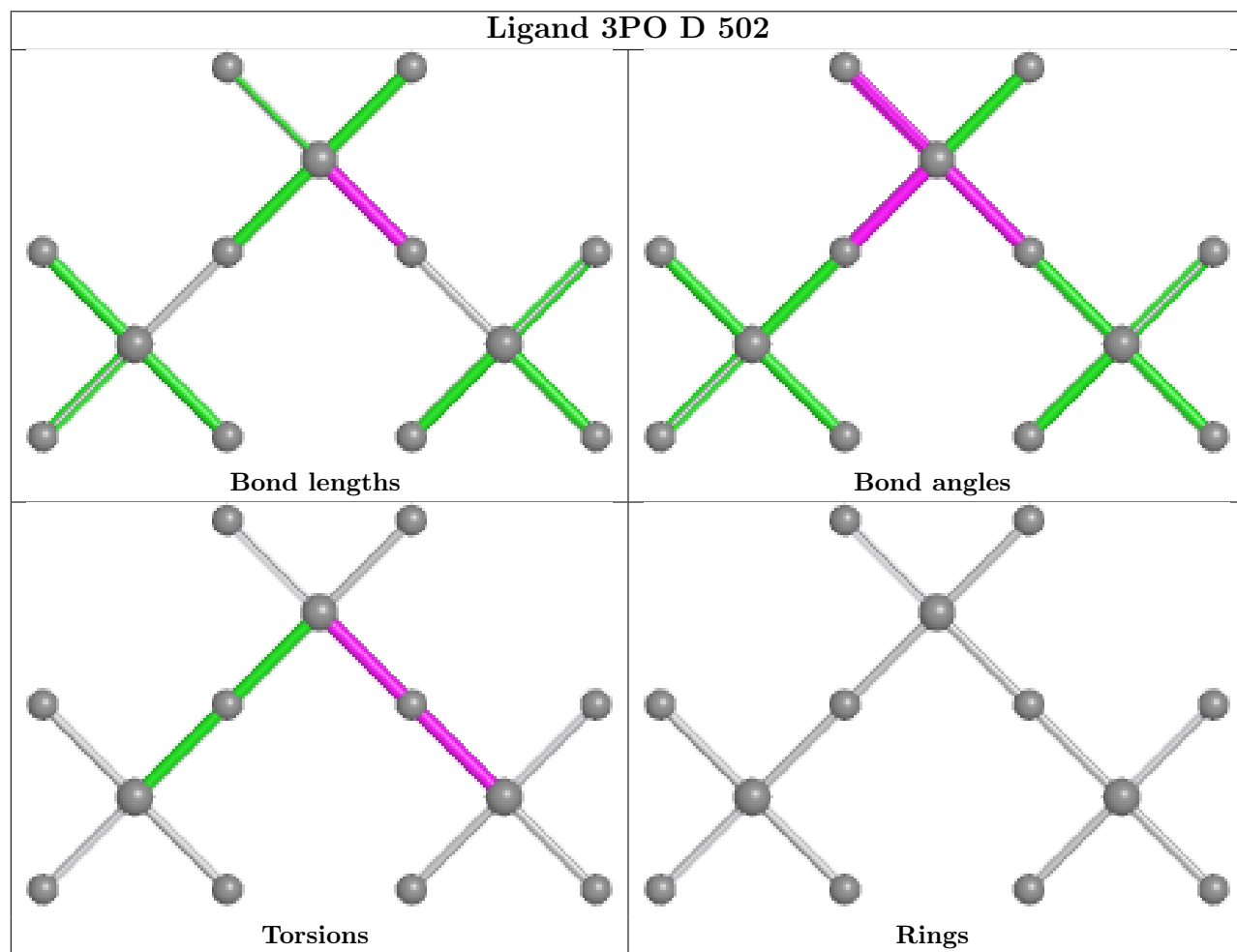
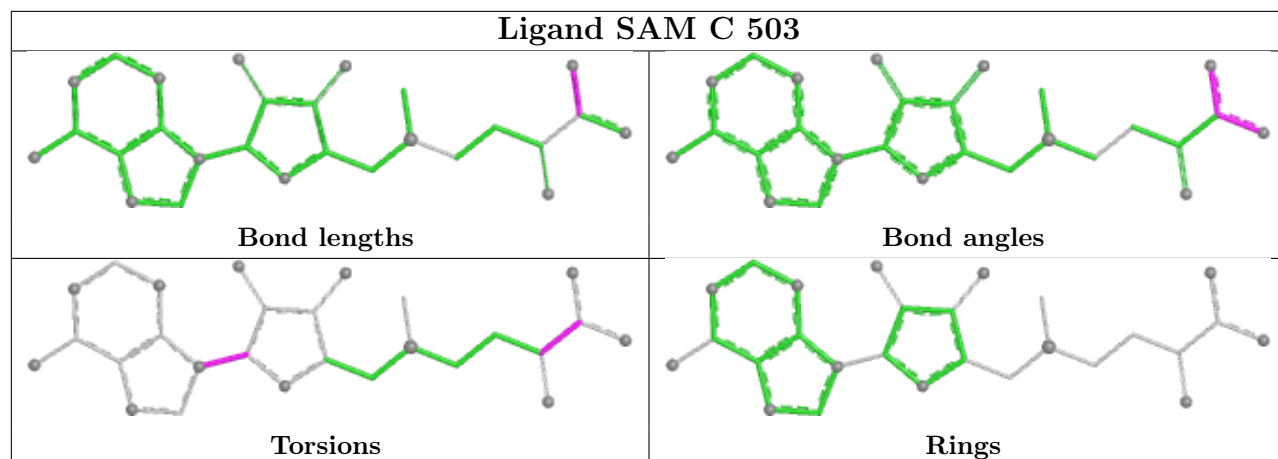
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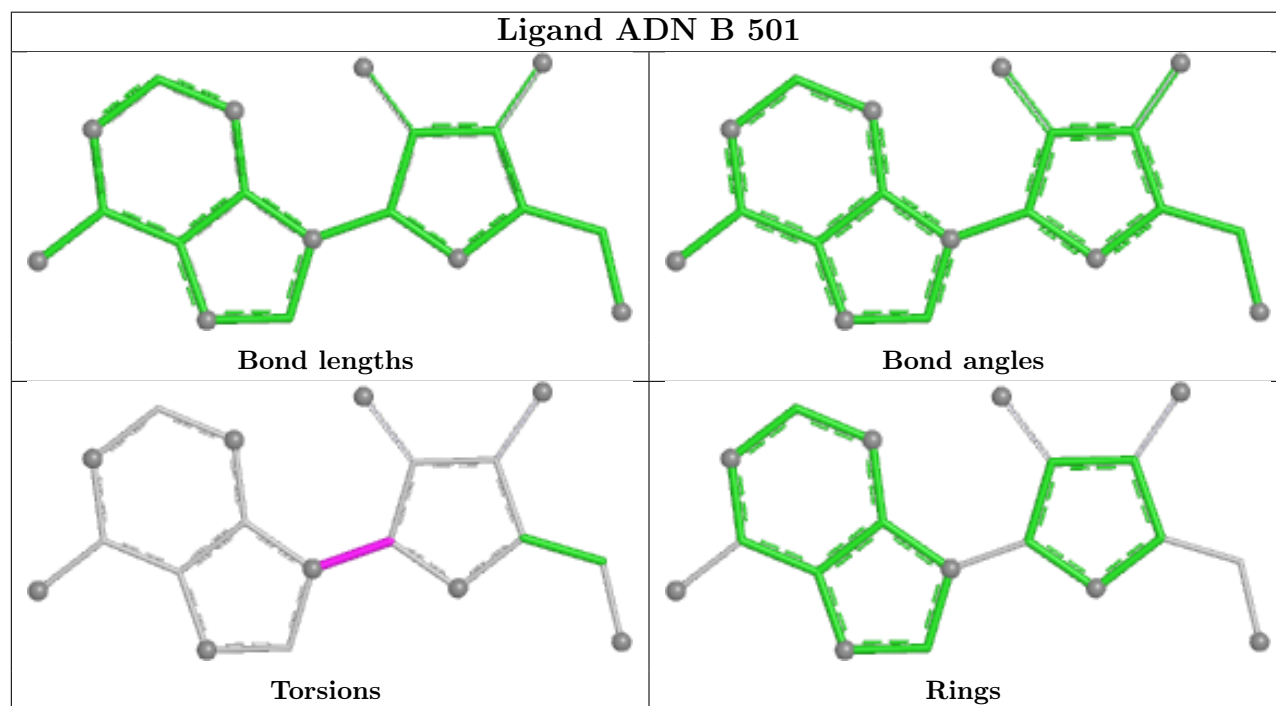
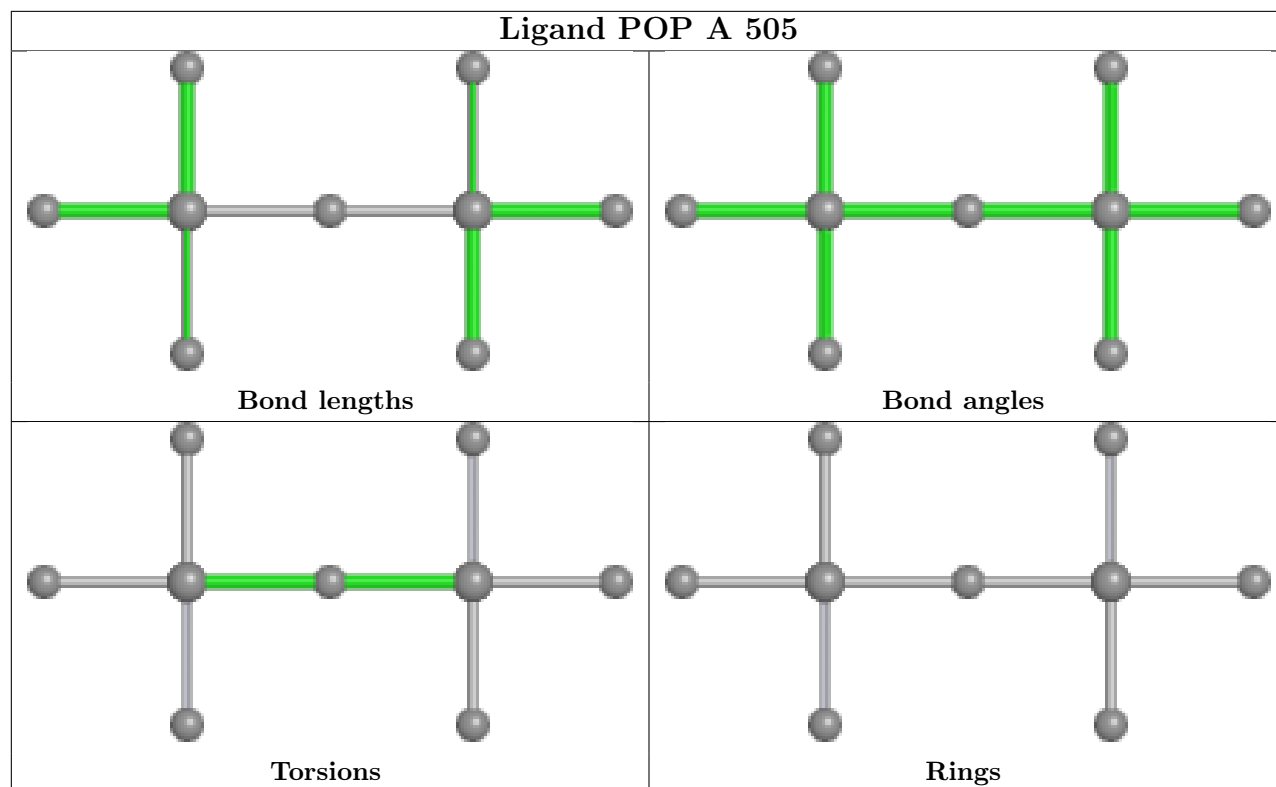
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	SAM	1	0
6	A	505	POP	2	0
2	C	501	ADN	1	0
2	D	501	ADN	1	0
4	D	503	SAM	4	0

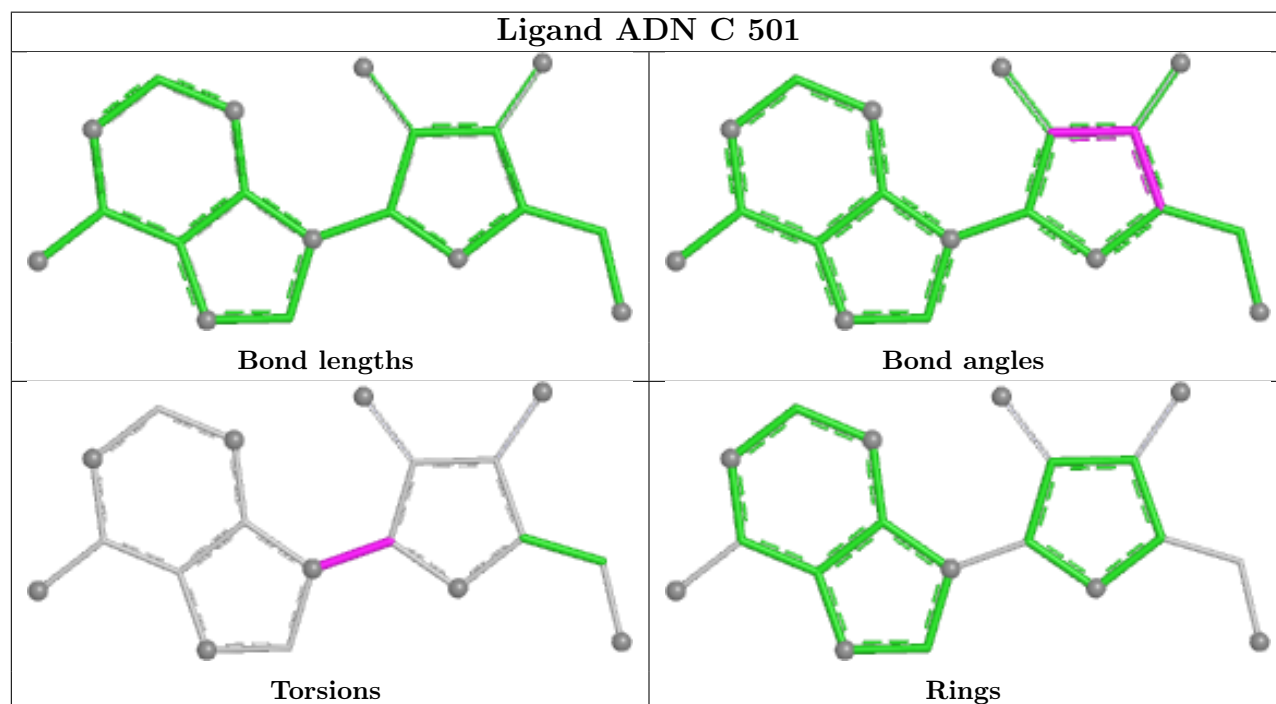
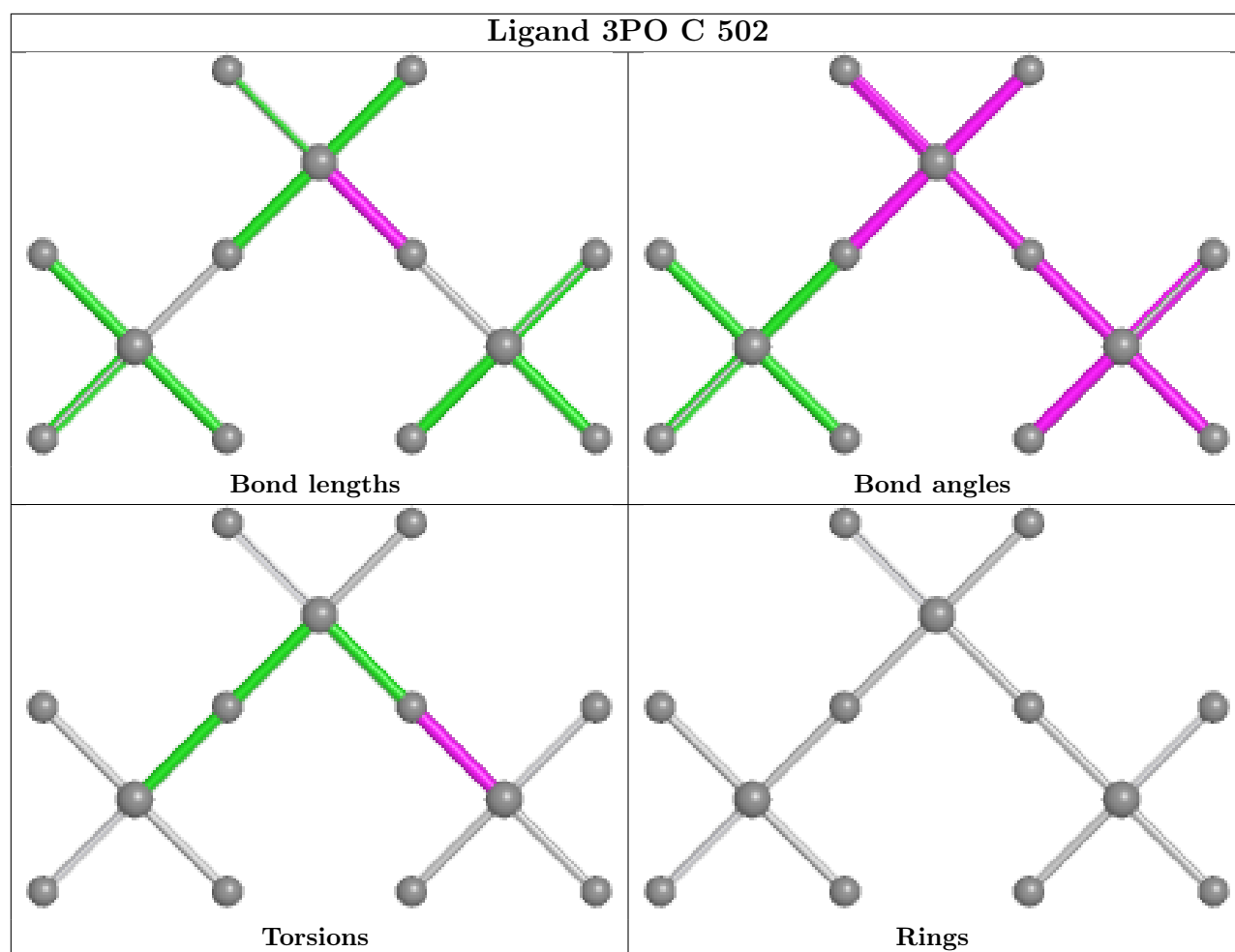
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

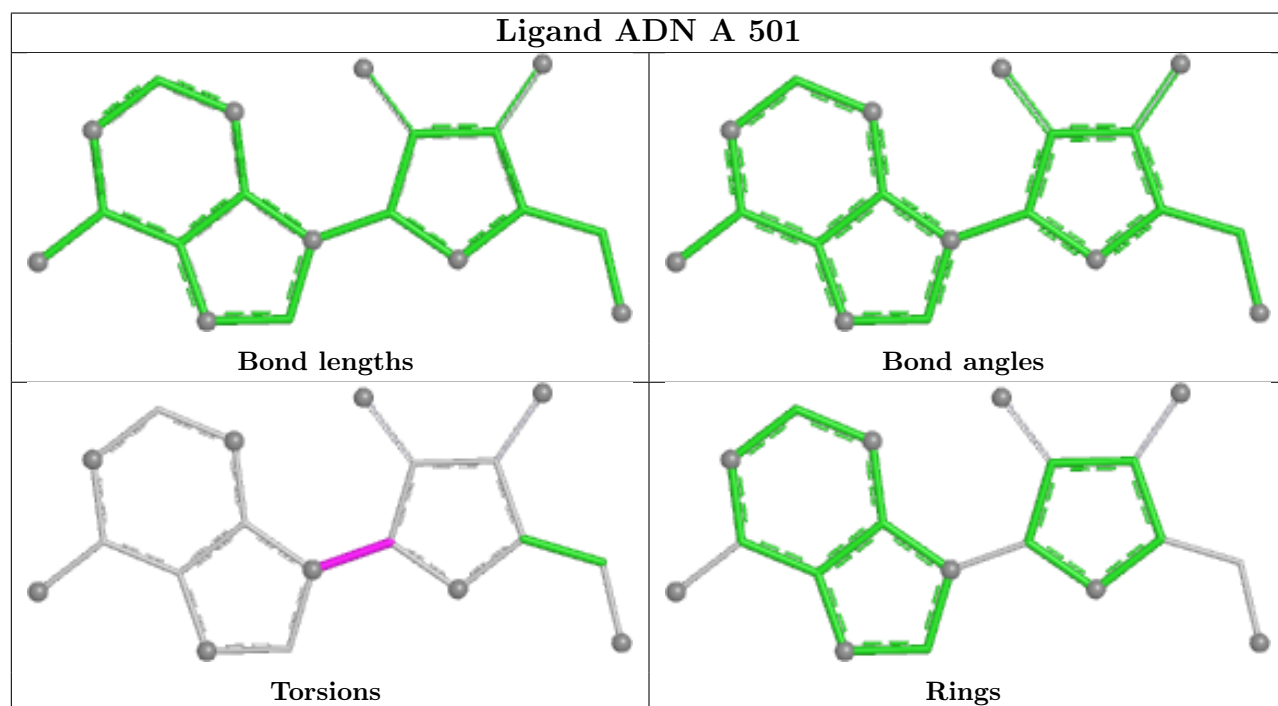
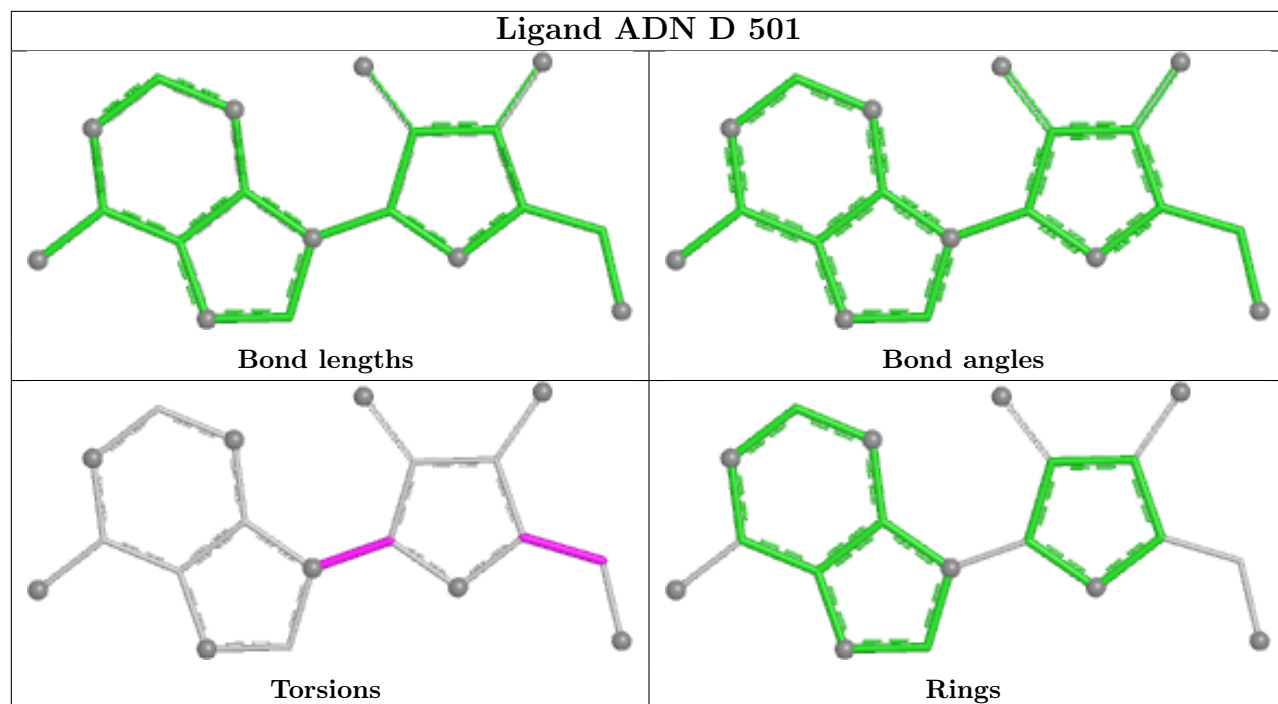


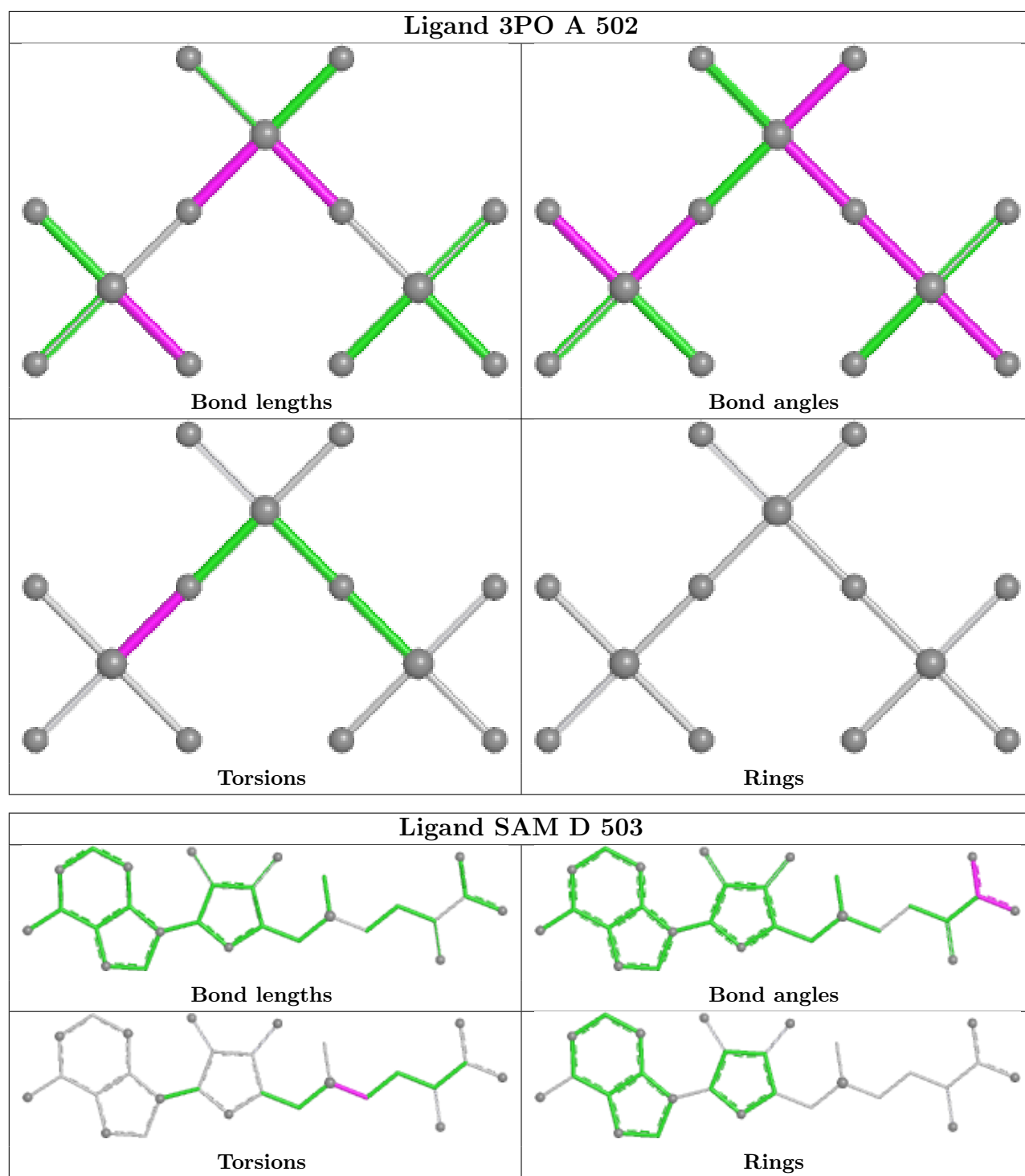












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	385/407 (94%)	-0.00	4 (1%) 79 76	16, 35, 62, 110	0
1	B	390/407 (95%)	0.10	11 (2%) 55 51	19, 35, 70, 124	0
1	C	386/407 (94%)	0.30	15 (3%) 43 39	25, 45, 76, 122	0
1	D	387/407 (95%)	0.27	11 (2%) 55 51	25, 47, 73, 105	0
All	All	1548/1628 (95%)	0.17	41 (2%) 57 53	16, 40, 73, 124	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	VAL	4.9
1	A	125	GLU	4.6
1	B	122	ASP	4.2
1	B	126	ASP	3.9
1	A	129	ALA	3.4
1	D	123	VAL	3.3
1	C	103	GLN	3.0
1	A	406	LEU	3.0
1	B	406	LEU	2.9
1	C	209	VAL	2.9
1	D	344	ASP	2.6
1	B	3	GLN	2.5
1	C	4	PRO	2.5
1	C	214	LEU	2.5
1	A	2	ALA	2.5
1	B	124	GLU	2.5
1	C	189	ALA	2.5
1	D	323	GLY	2.5
1	C	102	GLU	2.4
1	B	106	GLU	2.4
1	B	87	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	2	ALA	2.4
1	C	406	LEU	2.4
1	C	216	THR	2.3
1	C	3	GLN	2.3
1	D	103	GLN	2.3
1	C	212	ALA	2.3
1	D	404	LEU	2.2
1	C	210	ASP	2.2
1	D	407	ALA	2.2
1	B	405	LYS	2.2
1	B	104	SER	2.2
1	D	400	LEU	2.1
1	D	406	LEU	2.1
1	C	188	ASP	2.1
1	B	94	CYS	2.1
1	C	2	ALA	2.1
1	D	402	ALA	2.1
1	C	128	ARG	2.1
1	C	402	ALA	2.0
1	D	189	ALA	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
6	POP	A	505	9/9	0.81	0.11	72,79,90,100	0
7	MG	B	506	1/1	0.82	0.17	31,31,31,31	0
2	ADN	D	501	19/19	0.87	0.11	33,41,44,47	0

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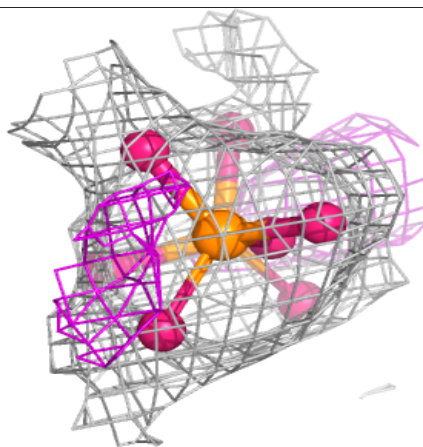
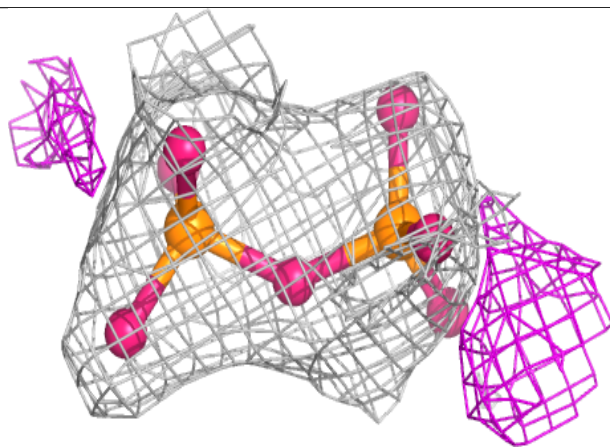
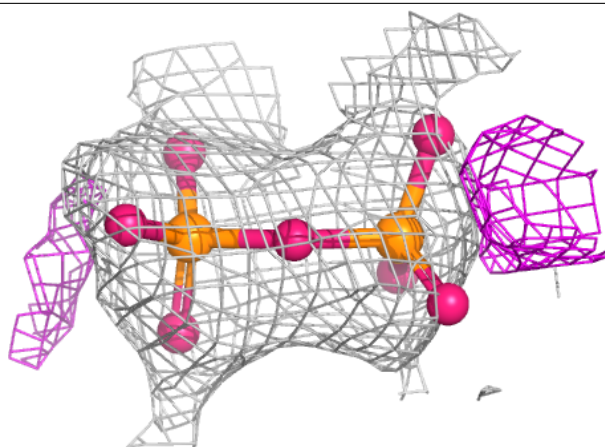
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SAM	A	503	27/27	0.87	0.10	35,42,64,66	0
2	ADN	A	501	19/19	0.88	0.09	28,37,41,42	0
2	ADN	C	501	19/19	0.88	0.10	35,51,61,61	0
3	3PO	B	502	13/13	0.89	0.10	27,32,47,54	0
2	ADN	B	501	19/19	0.89	0.09	30,39,48,48	0
3	3PO	C	502	13/13	0.90	0.09	29,40,49,50	0
8	K	A	508	1/1	0.90	0.09	60,60,60,60	0
7	MG	B	505	1/1	0.91	0.07	41,41,41,41	0
8	K	C	506	1/1	0.91	0.09	68,68,68,68	0
8	K	A	509	1/1	0.92	0.11	64,64,64,64	0
7	MG	A	507	1/1	0.92	0.05	33,33,33,33	0
8	K	D	506	1/1	0.92	0.08	69,69,69,69	0
7	MG	C	504	1/1	0.93	0.09	33,33,33,33	0
7	MG	C	505	1/1	0.93	0.06	43,43,43,43	0
7	MG	D	504	1/1	0.94	0.07	43,43,43,43	0
7	MG	D	505	1/1	0.94	0.06	26,26,26,26	0
4	SAM	D	503	27/27	0.94	0.08	33,37,61,62	0
5	GOL	A	504	6/6	0.94	0.10	36,41,45,46	0
4	SAM	B	503	27/27	0.94	0.08	31,40,72,78	0
4	SAM	C	503	27/27	0.94	0.07	35,43,55,61	0
7	MG	A	506	1/1	0.95	0.07	29,29,29,29	0
3	3PO	D	502	13/13	0.95	0.07	30,37,52,53	0
5	GOL	B	504	6/6	0.96	0.07	32,37,39,40	0
3	3PO	A	502	13/13	0.96	0.07	28,32,45,51	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.

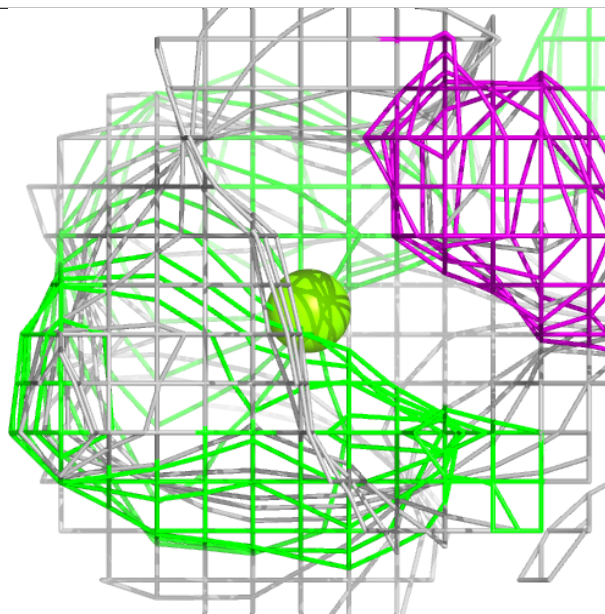
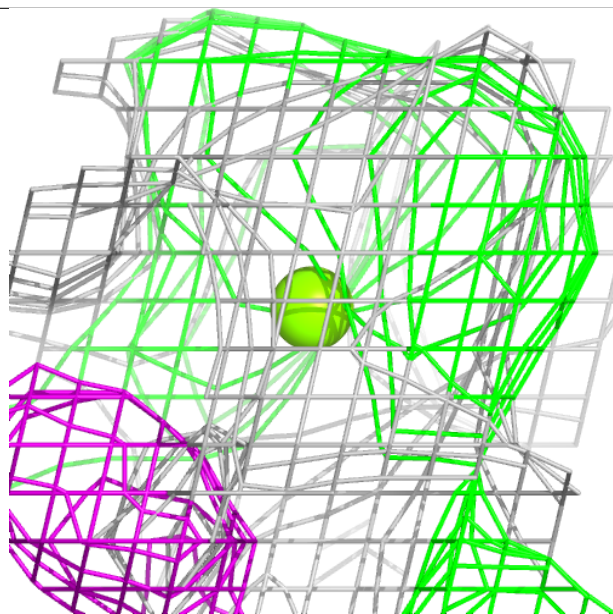
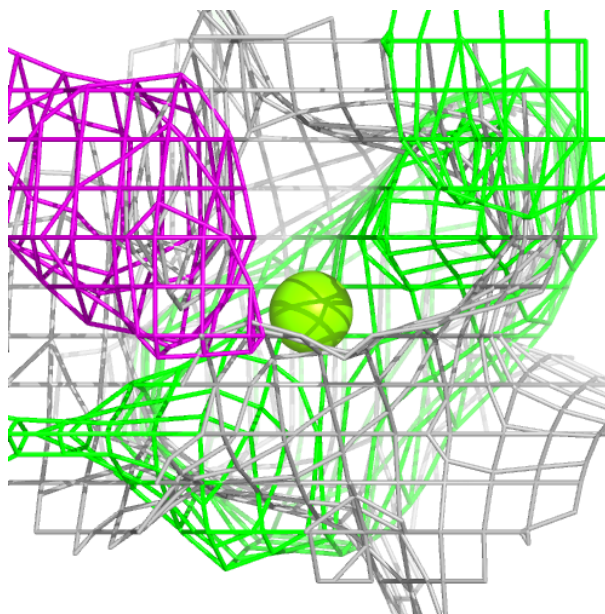
Electron density around POP A 505:

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



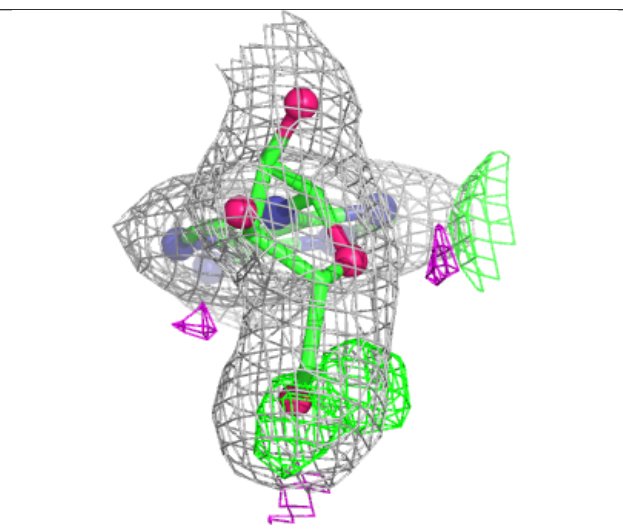
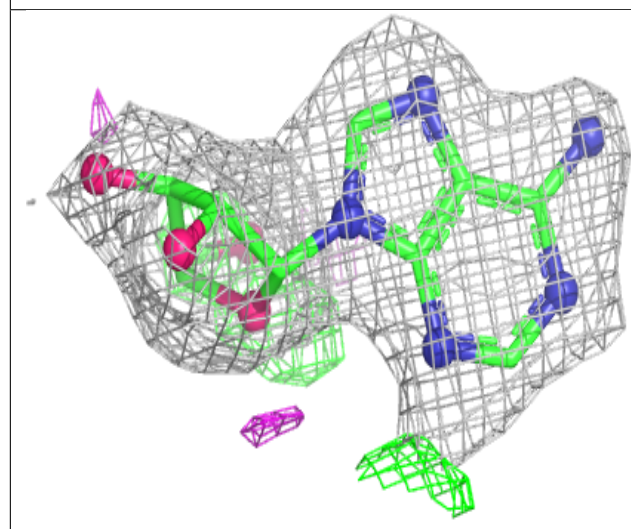
Electron density around MG B 506:

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



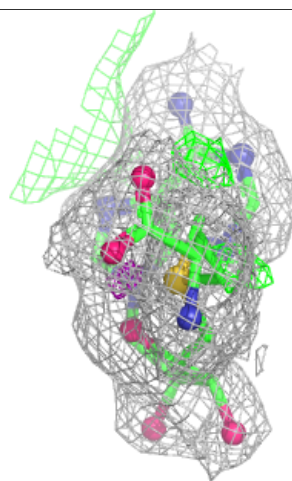
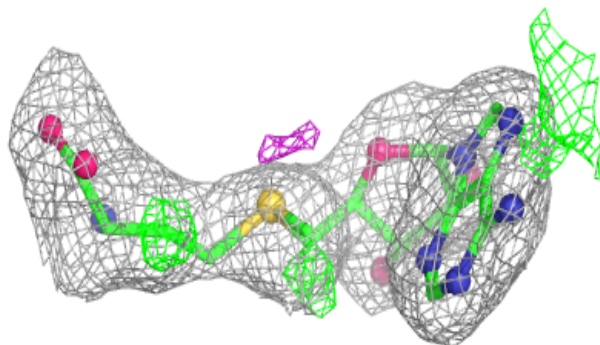
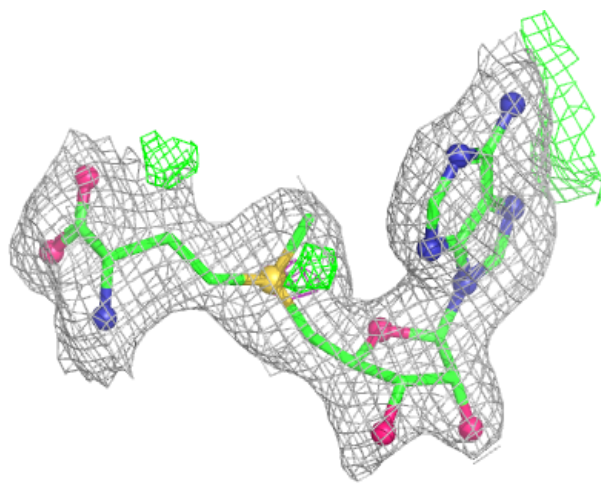
Electron density around ADN D 501:

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



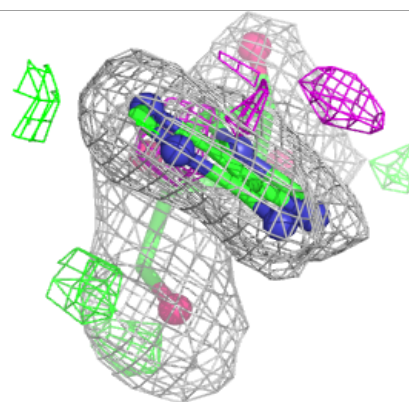
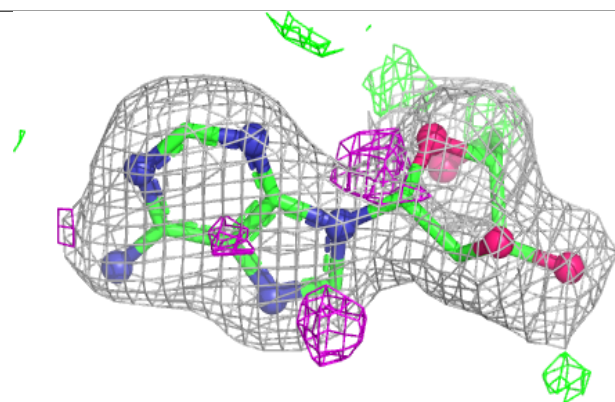
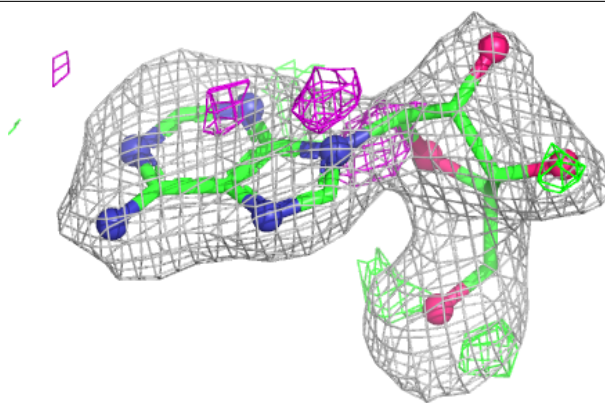
Electron density around SAM A 503:

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



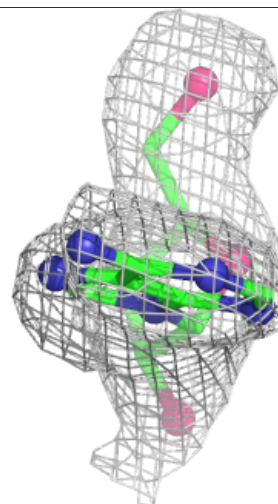
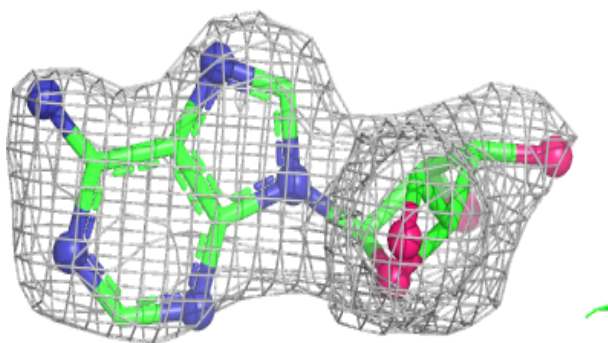
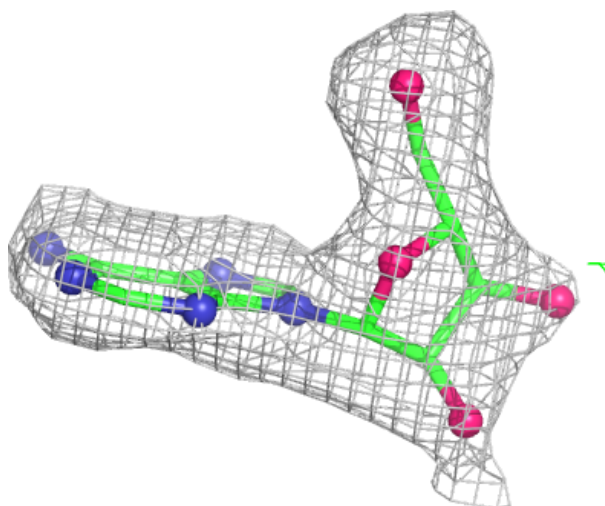
Electron density around ADN A 501:

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



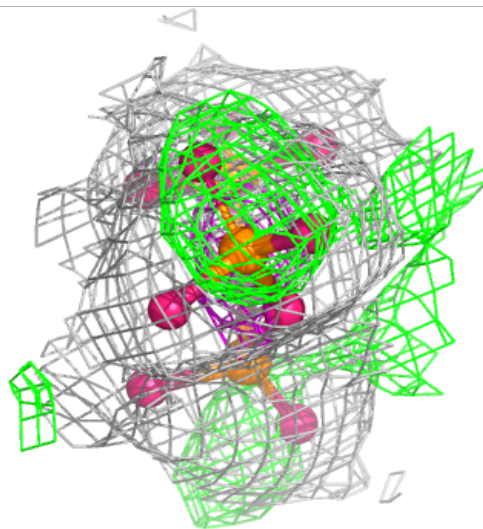
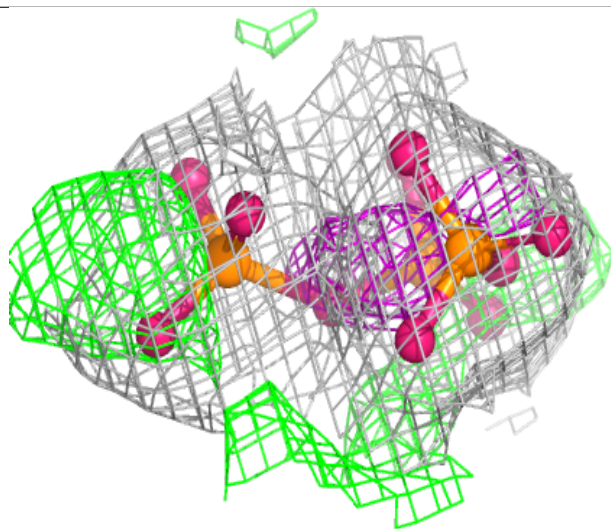
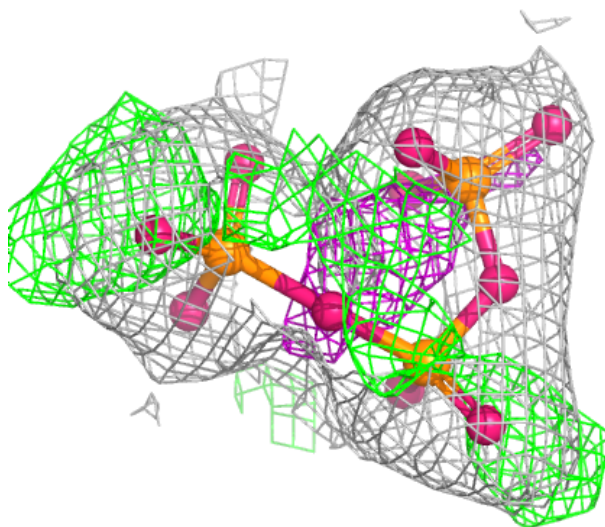
Electron density around ADN C 501:

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



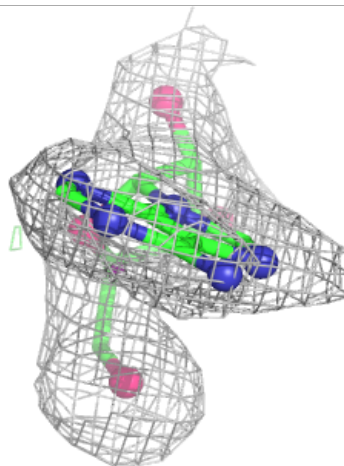
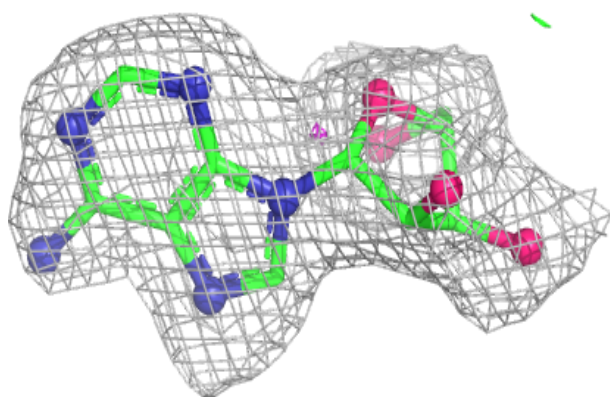
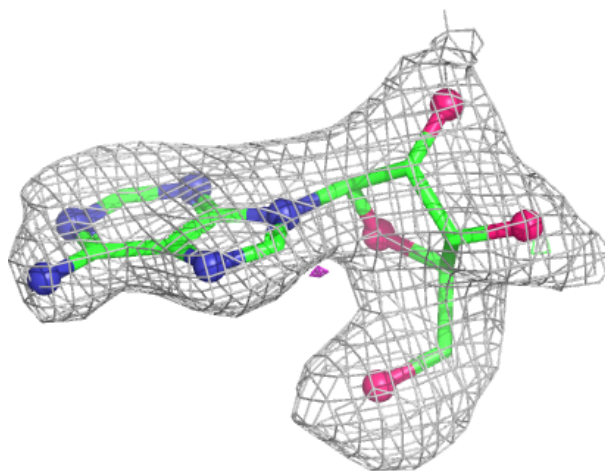
Electron density around 3PO B 502:

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



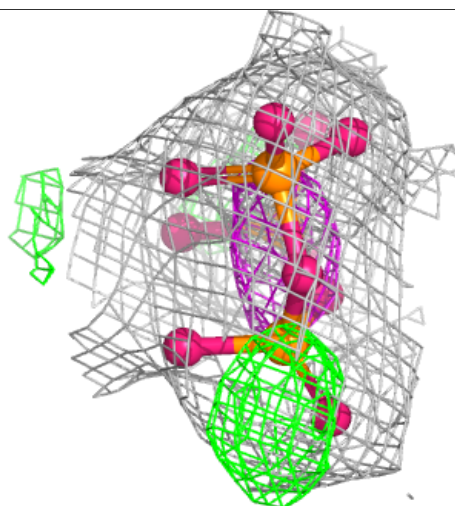
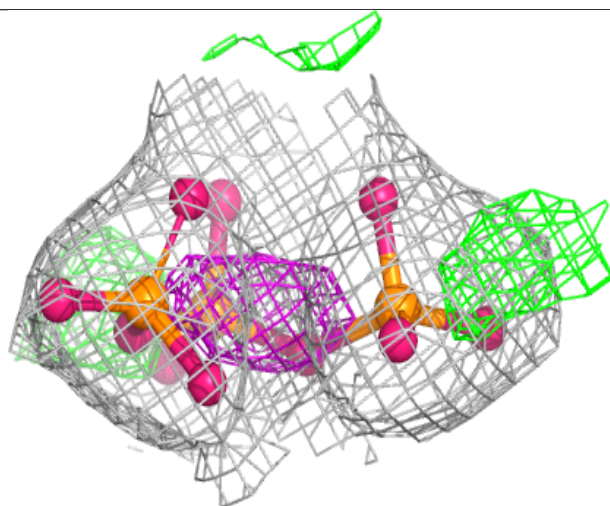
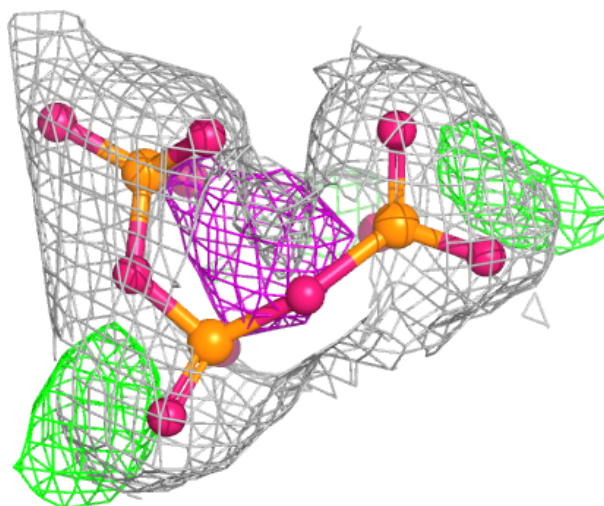
Electron density around ADN B 501:

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



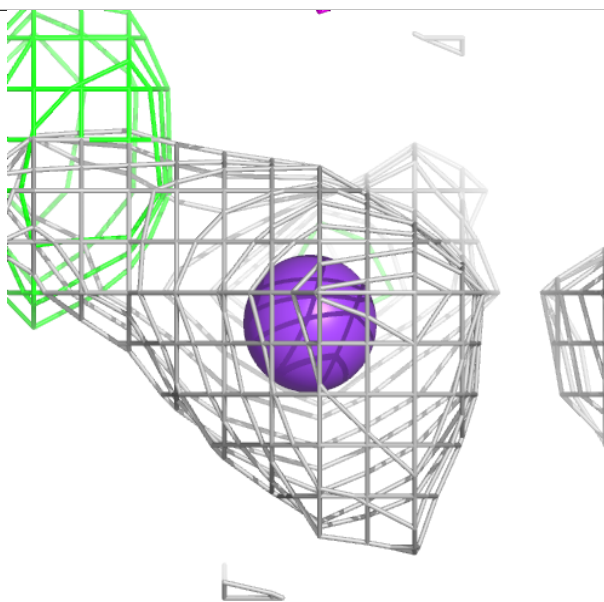
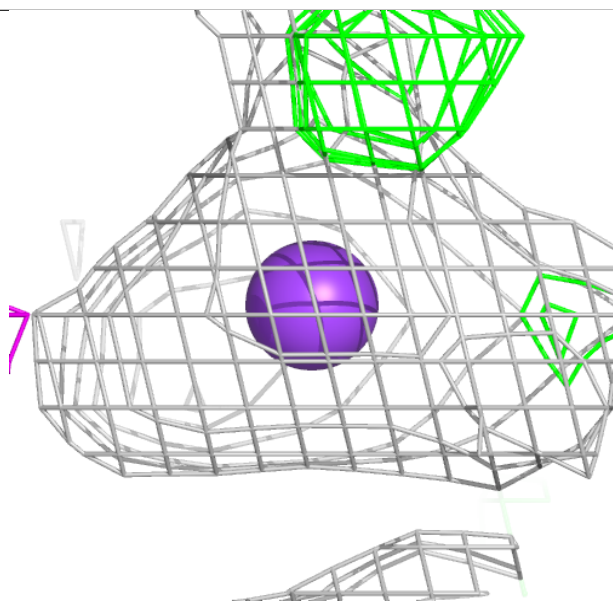
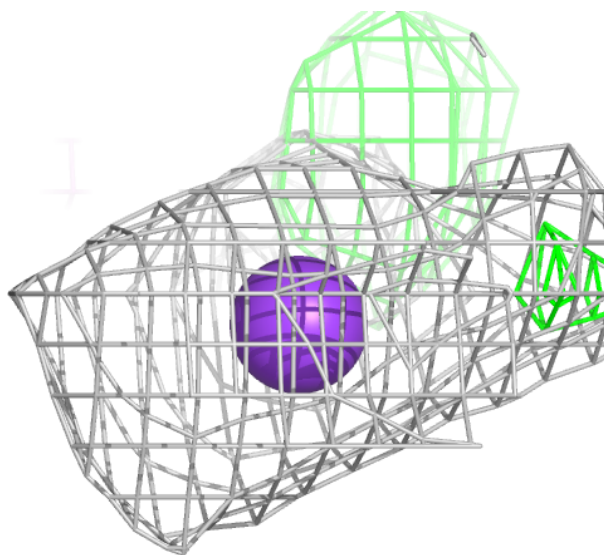
Electron density around 3PO C 502:

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



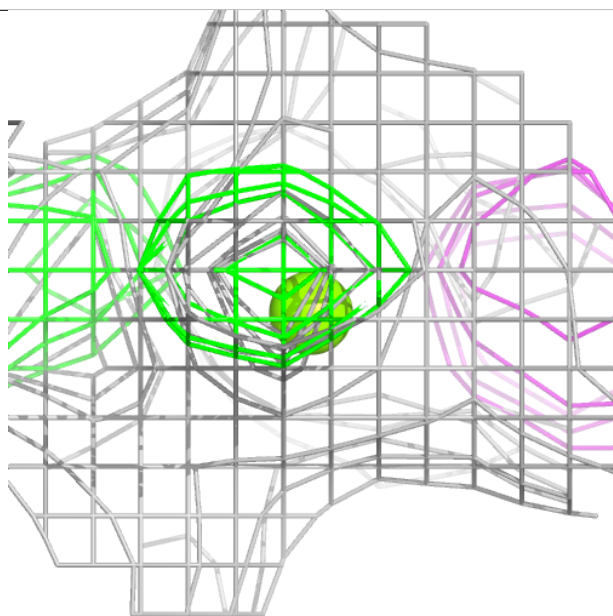
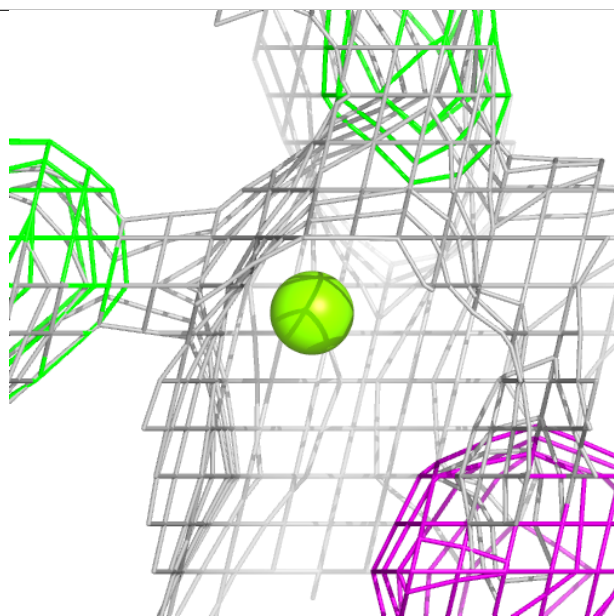
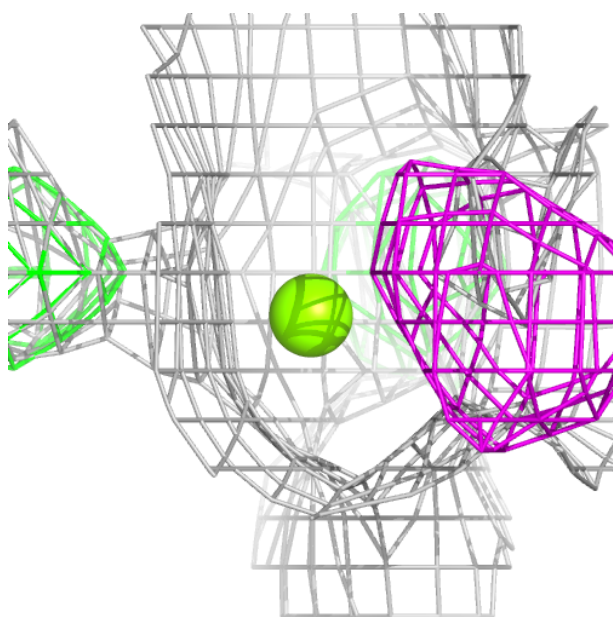
Electron density around K A 508:

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



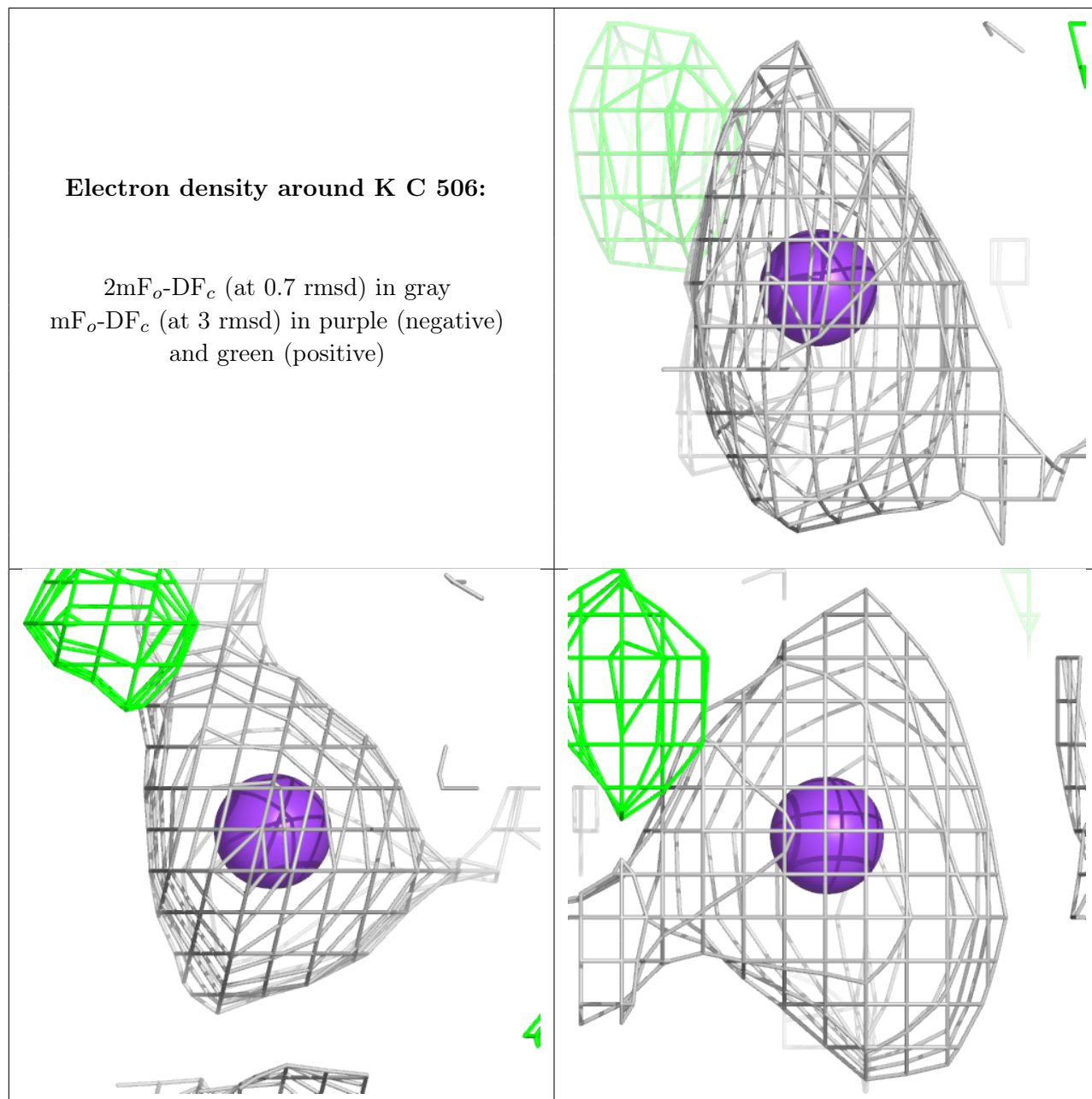
Electron density around MG B 505:

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



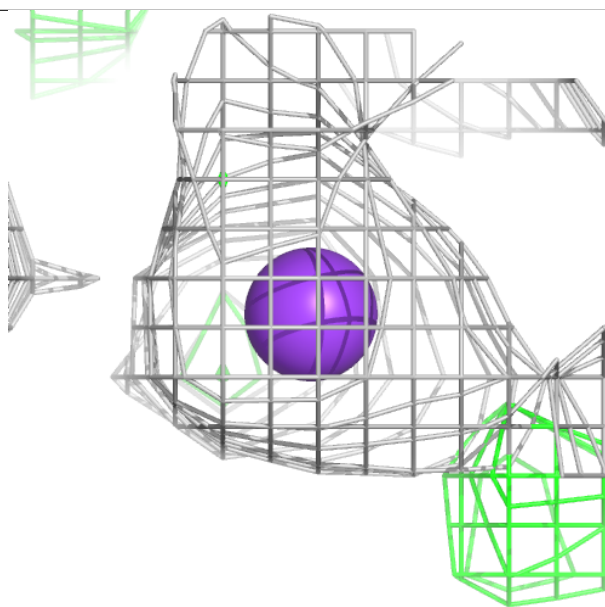
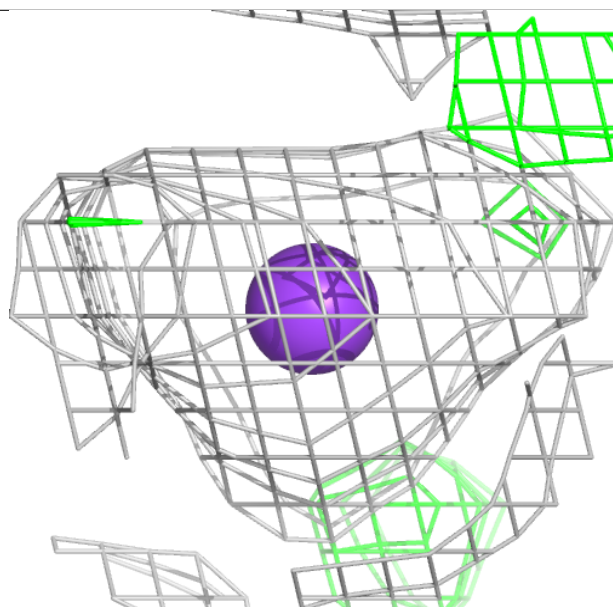
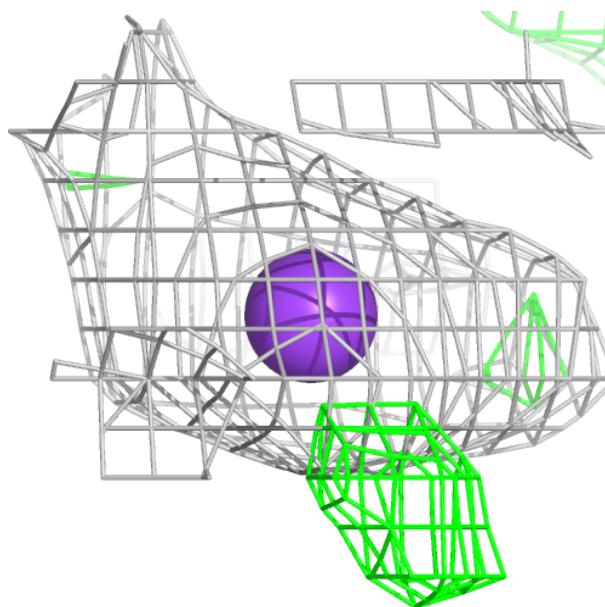
Electron density around K C 506:

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



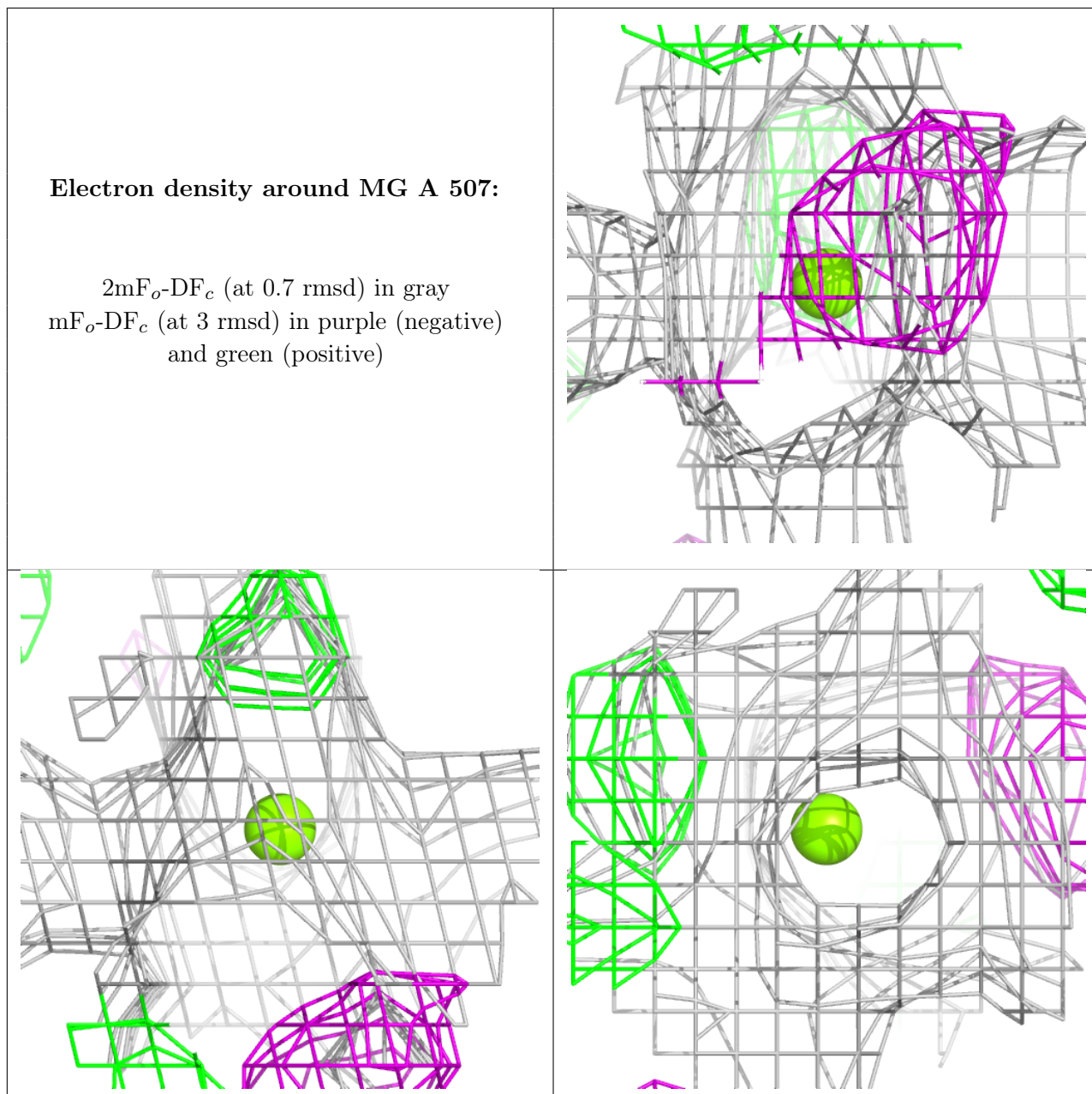
Electron density around K A 509:

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



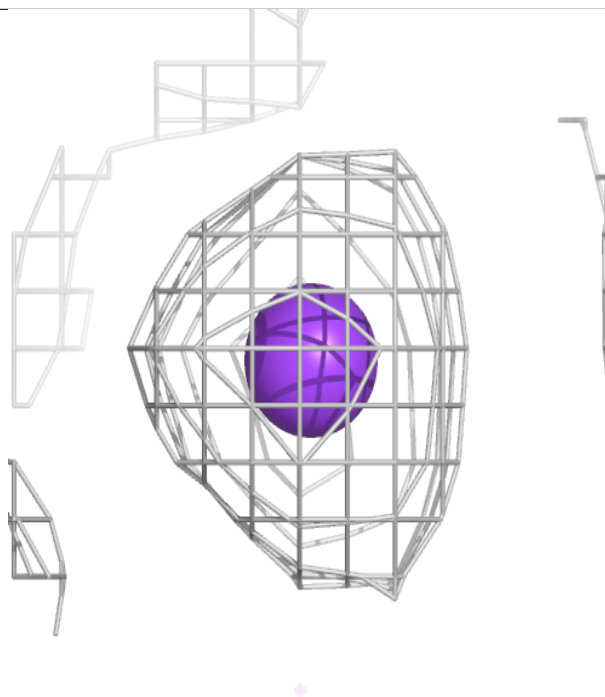
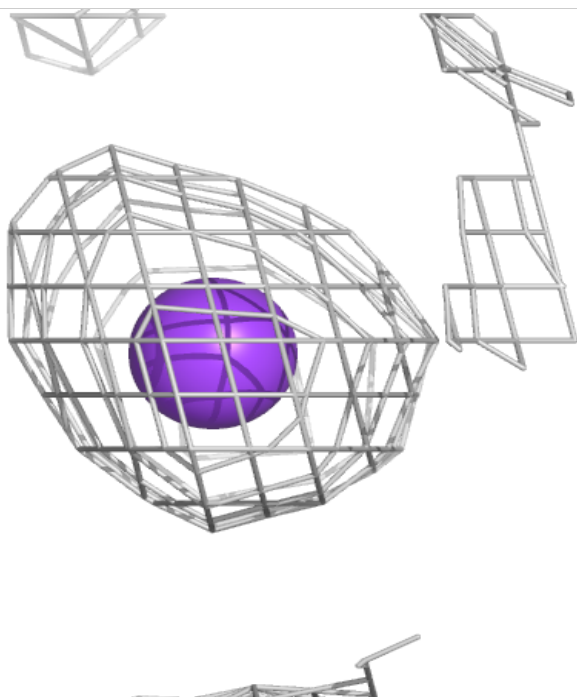
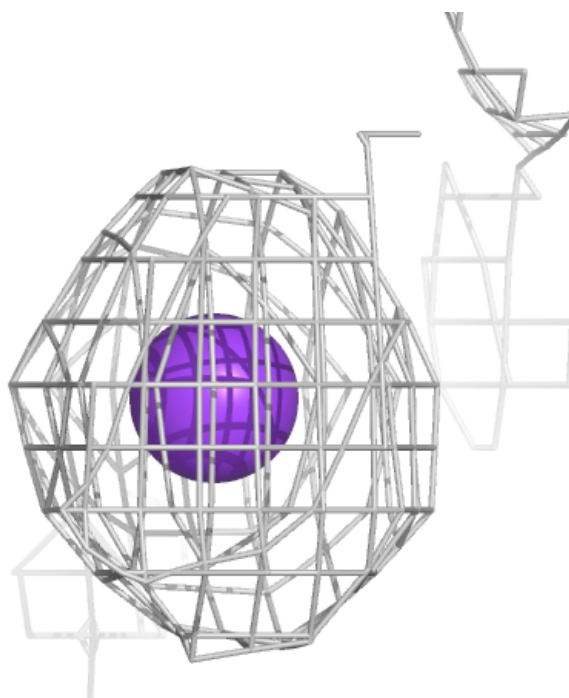
Electron density around MG A 507:

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



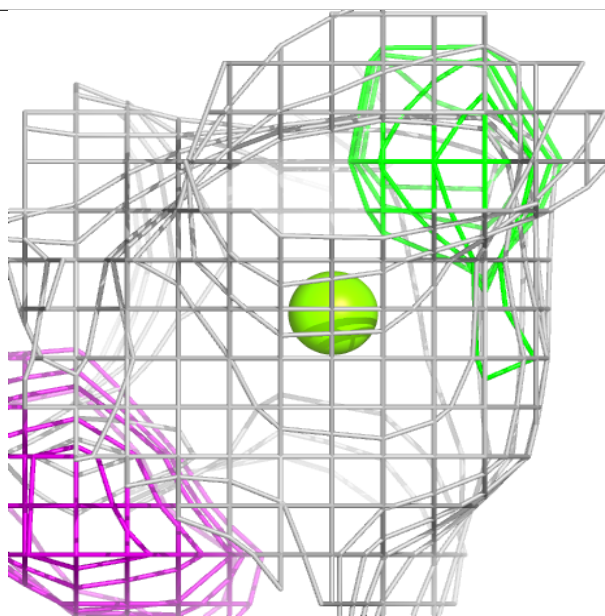
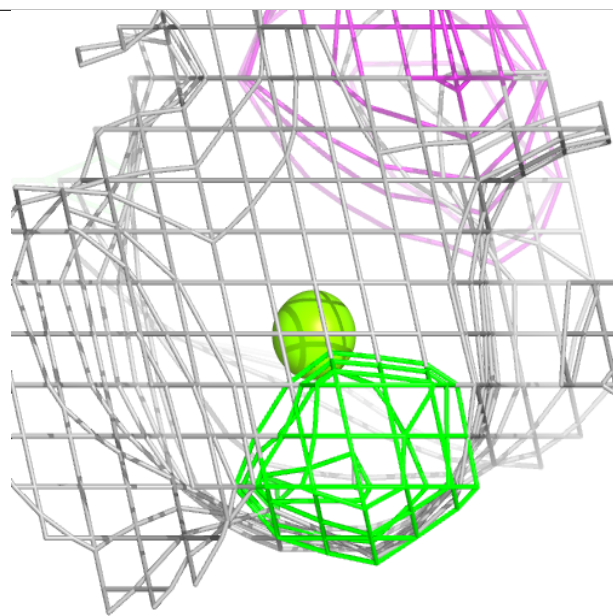
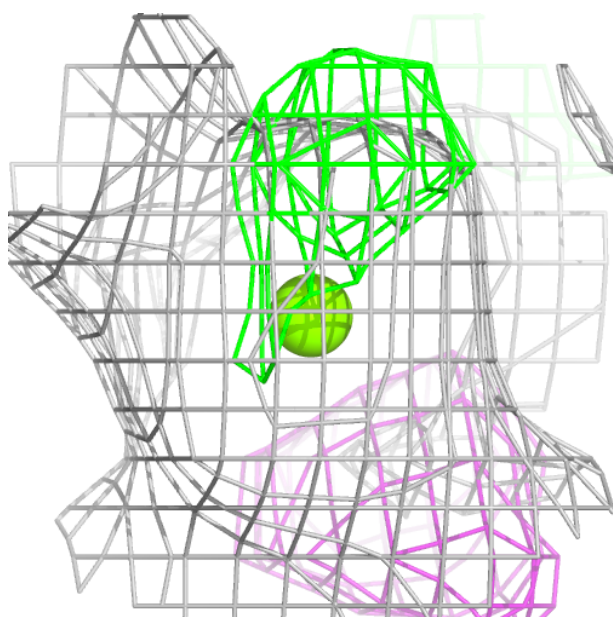
Electron density around K D 506:

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



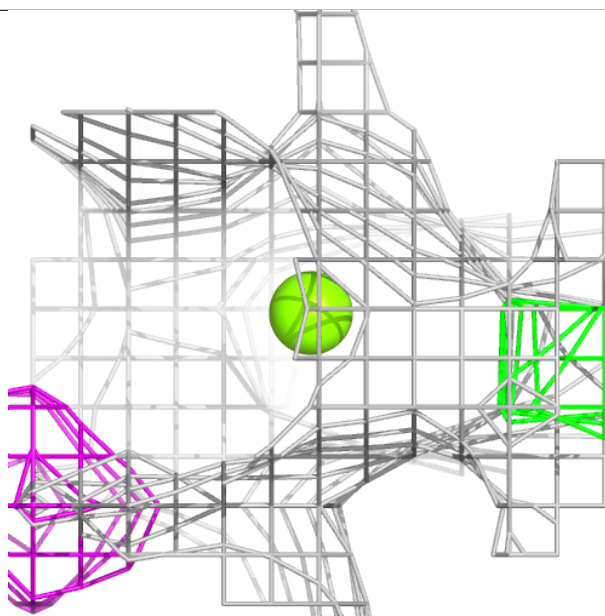
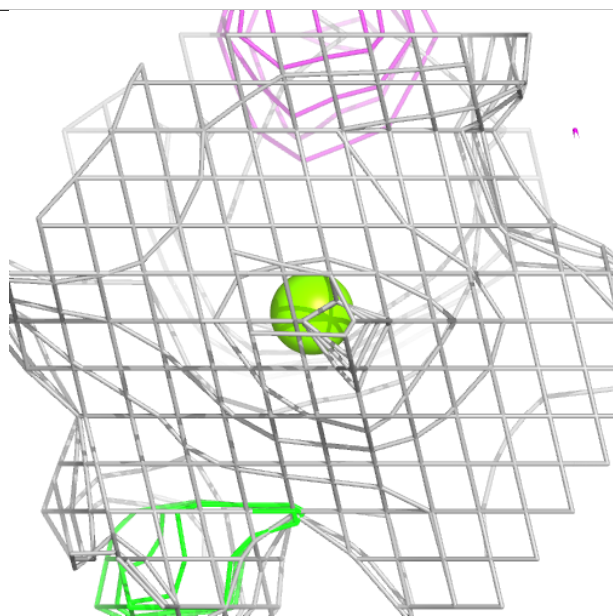
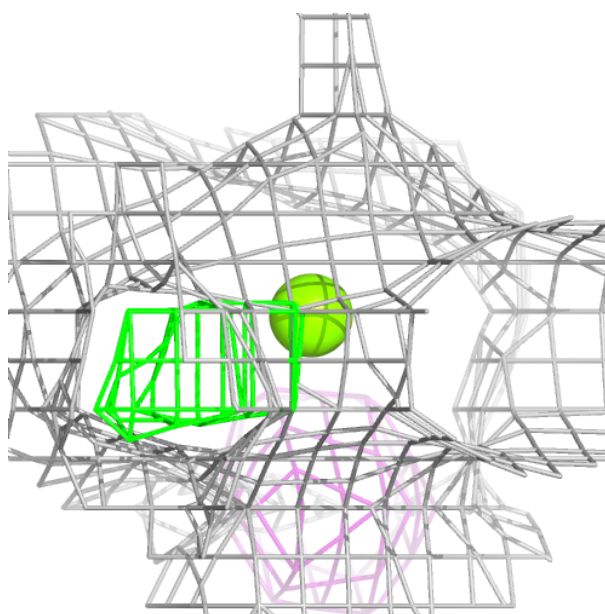
Electron density around MG C 504:

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



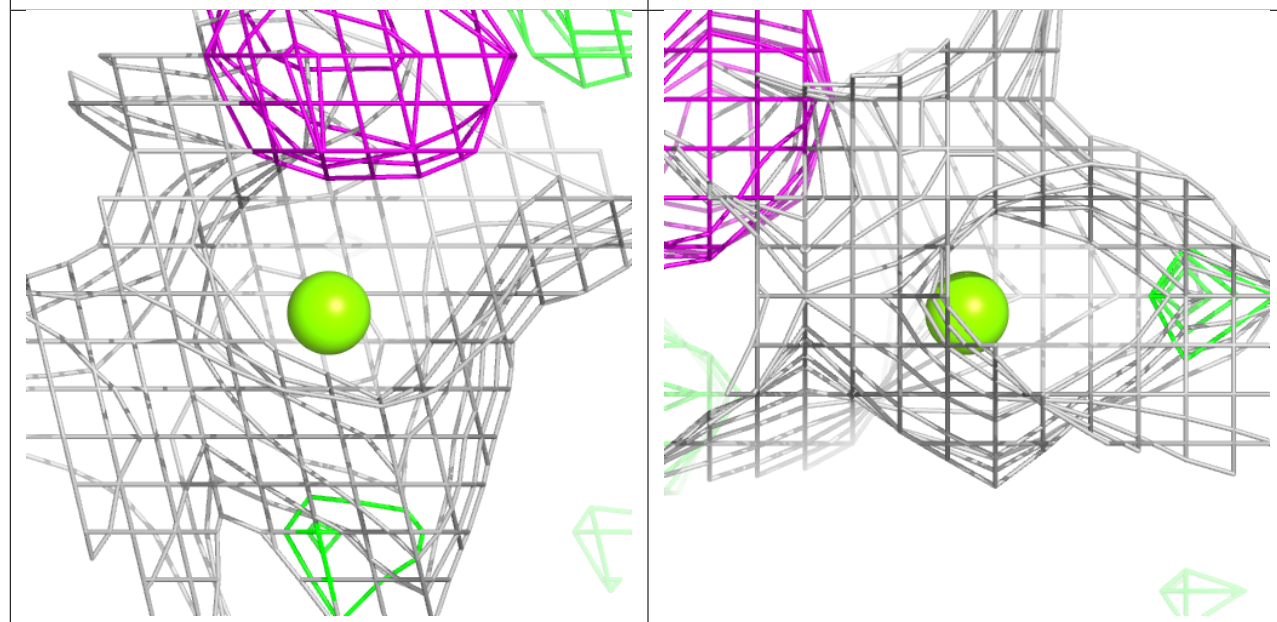
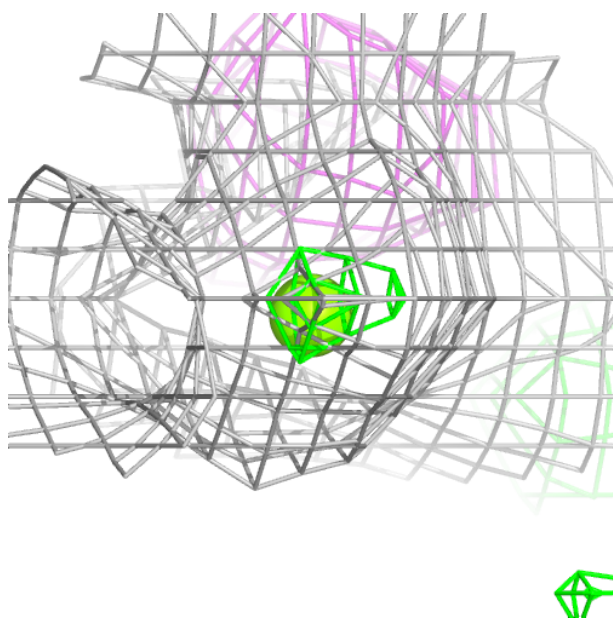
Electron density around MG C 505:

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



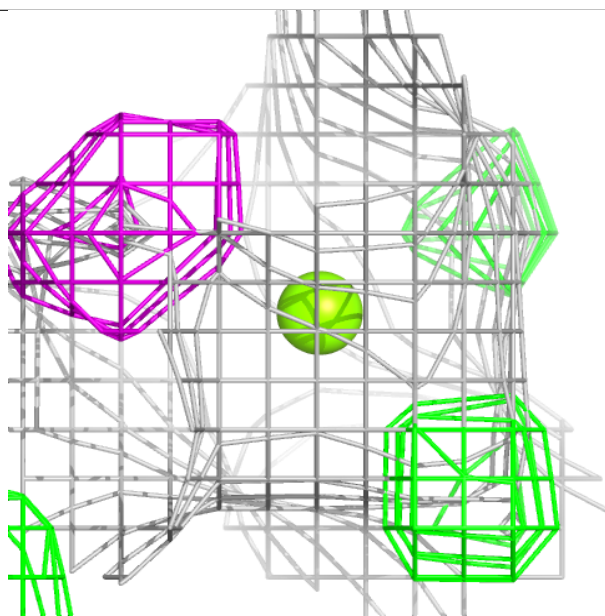
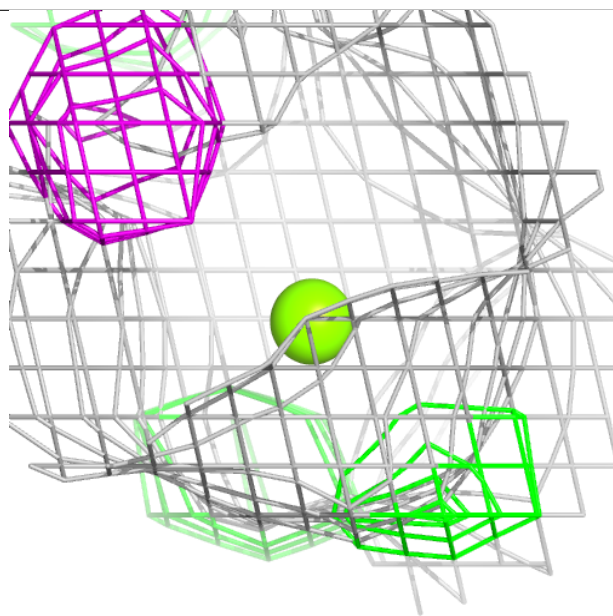
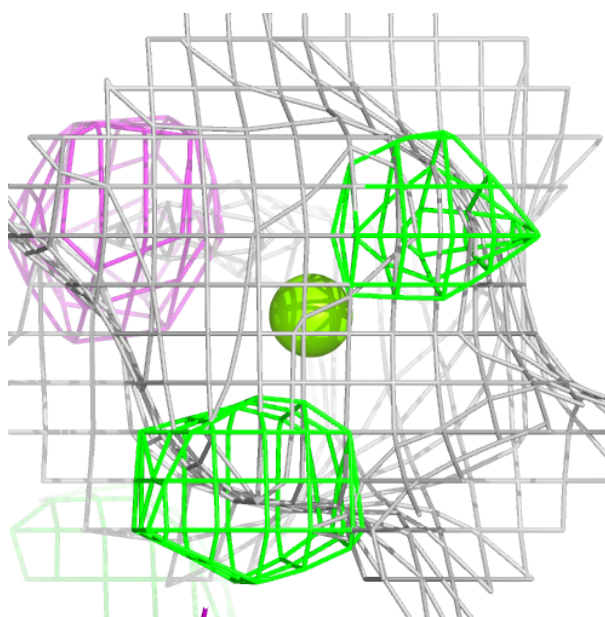
Electron density around MG D 504:

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



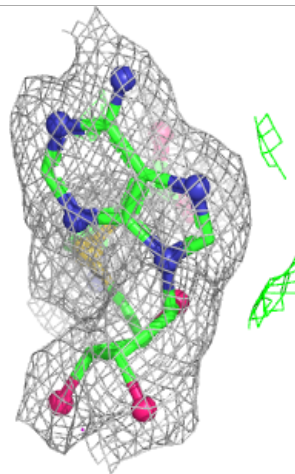
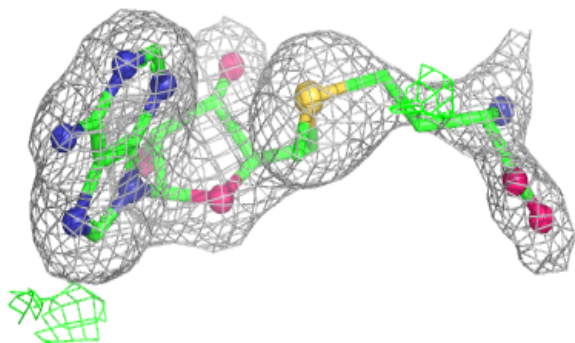
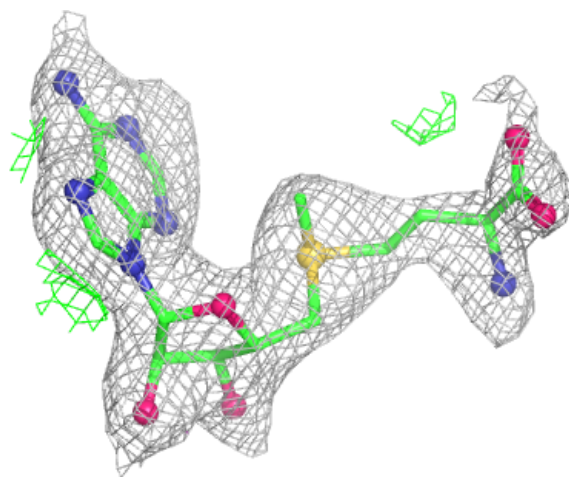
Electron density around MG D 505:

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



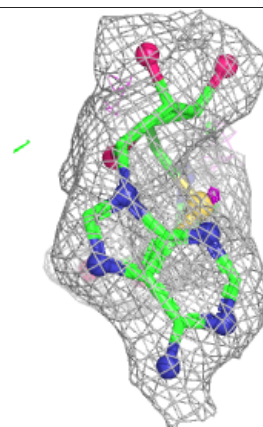
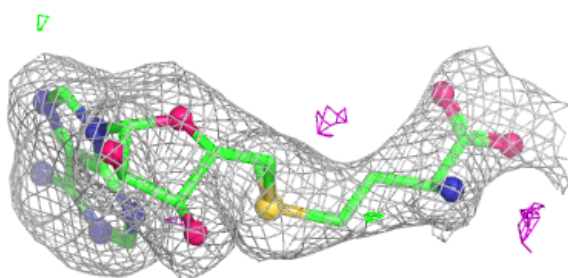
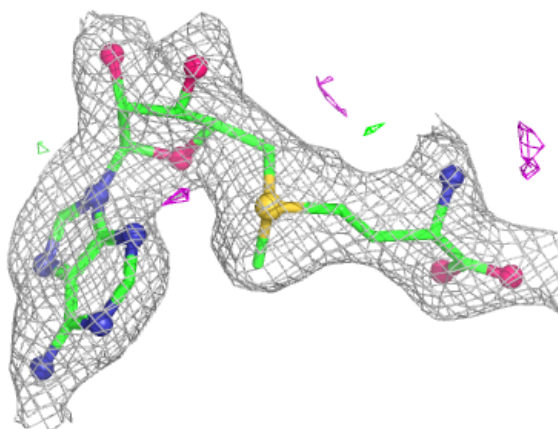
Electron density around SAM D 503:

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



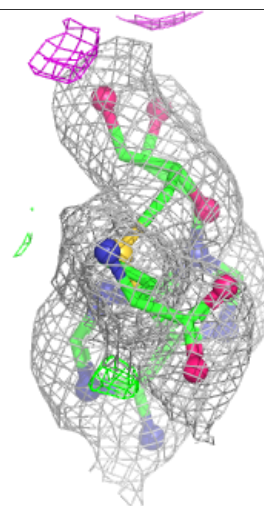
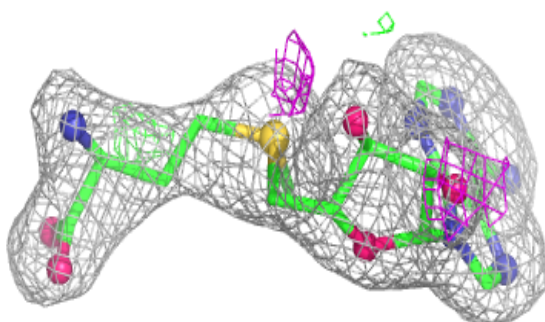
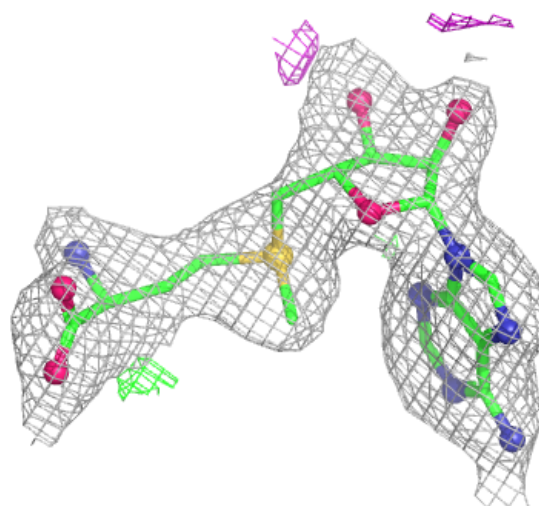
Electron density around SAM B 503:

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



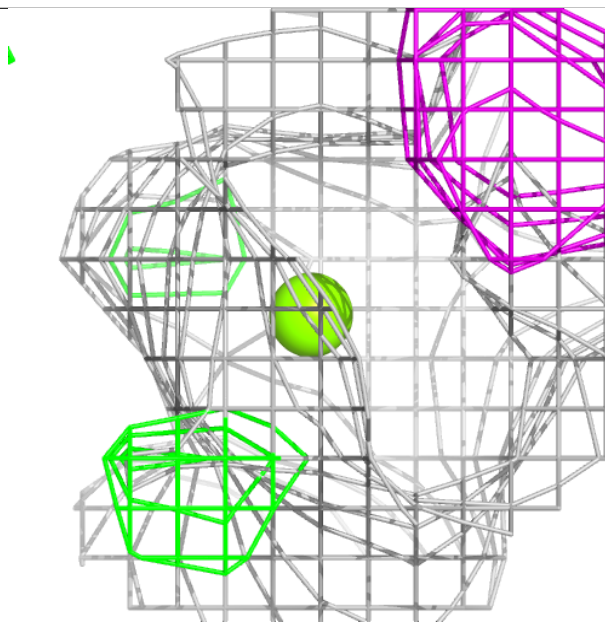
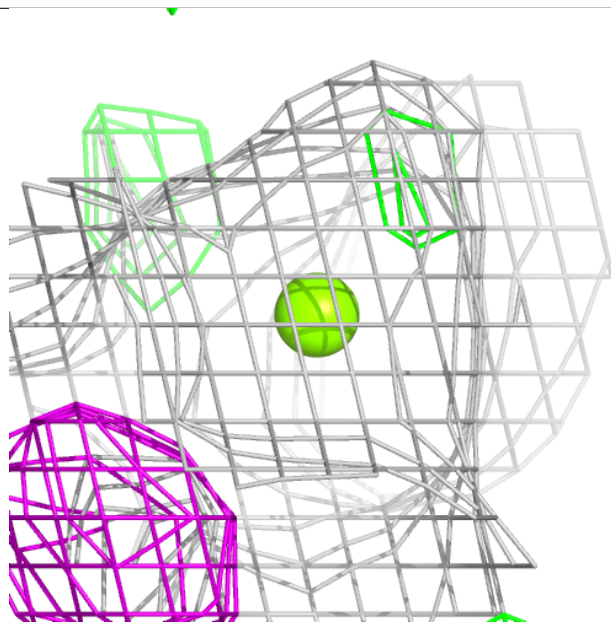
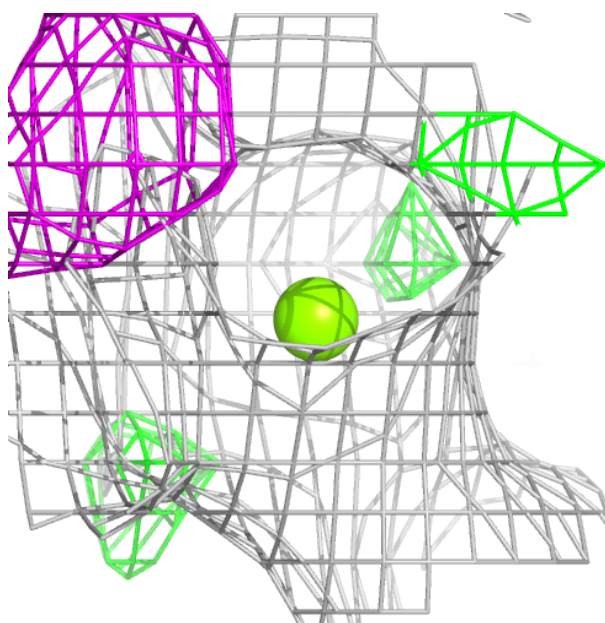
Electron density around SAM C 503:

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



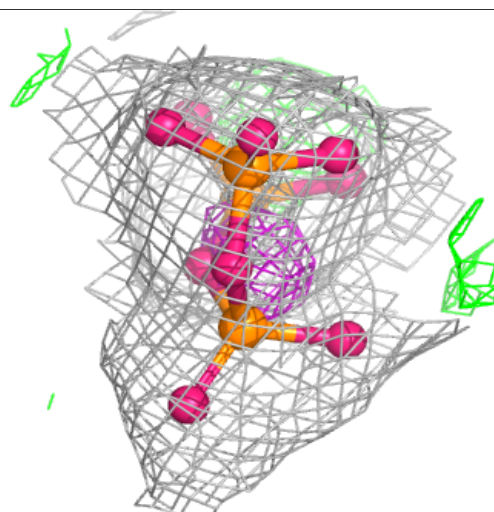
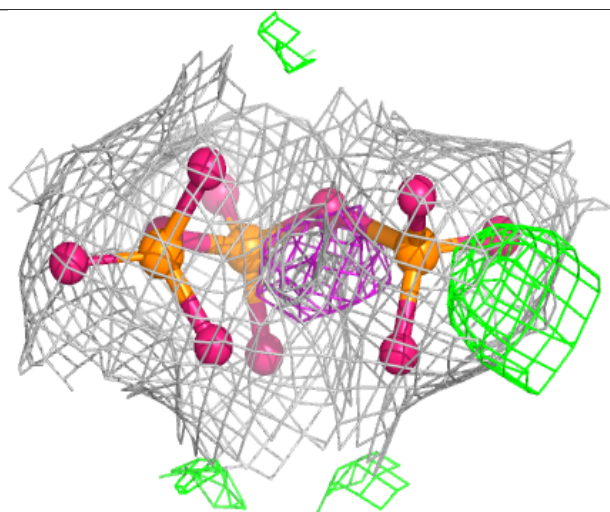
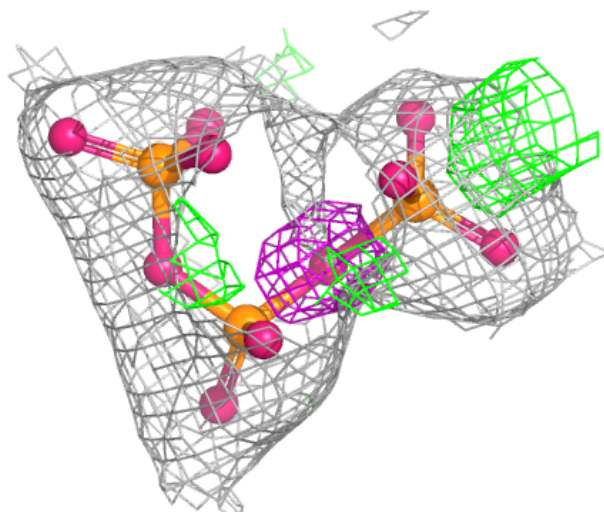
Electron density around MG A 506:

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



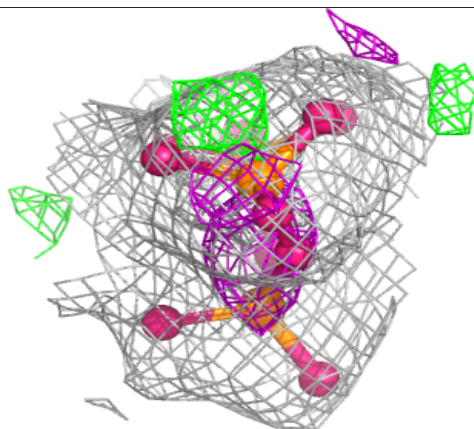
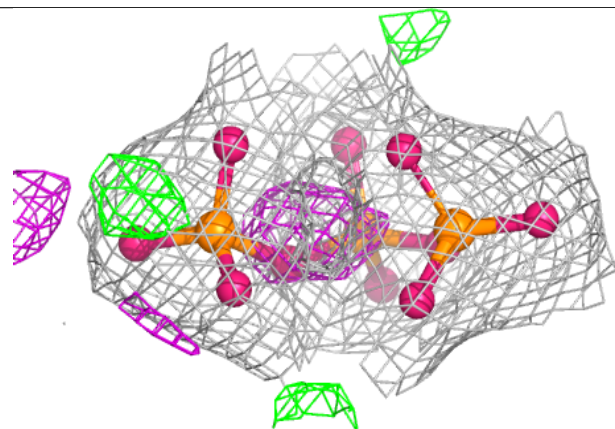
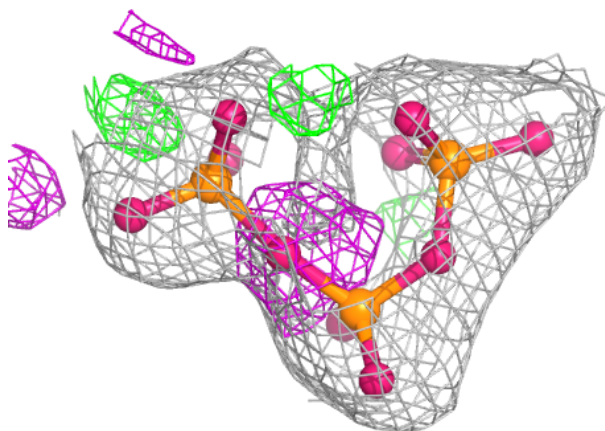
Electron density around 3PO D 502:

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



Electron density around 3PO A 502:

$2mF_o - DF_c$ (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.