



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:28 AM UTC

PDB ID : 9QUR / pdb_00009qur
Title : Crystal structure of gamma-Glutamyl-Methylamide Synthetase from Methylovorus mays (MmGmaS) in complex with ATPgS
Authors : Vascon, F.; Loprete, G.; Bergantino, E.; Cendron, L.
Deposited on : 2025-04-11
Resolution : 2.65 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

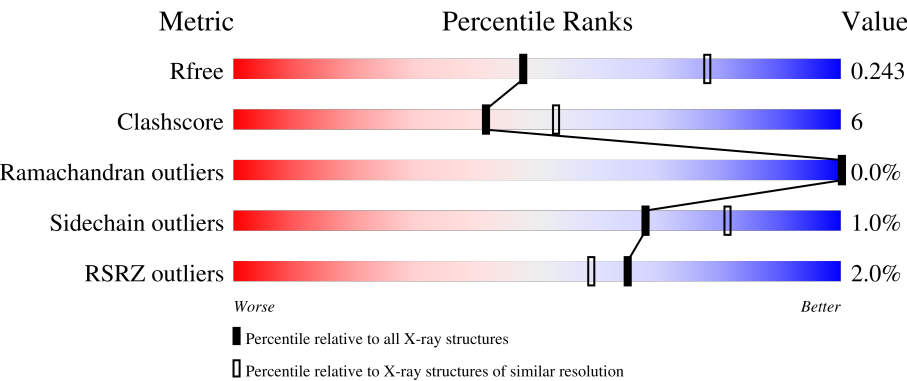
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	447	3% 81% 17% .
1	B	447	% 84% 15%
1	C	447	% 81% 17% .
1	D	447	2% 85% 13% ..
1	E	447	3% 84% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	447	2%85%14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21045 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 Glutamate--methylamine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3463	2206	580	659	18			
1	B	446	Total	C	N	O	S	0	0	0
			3463	2206	580	659	18			
1	C	446	Total	C	N	O	S	0	1	0
			3471	2211	581	660	19			
1	D	443	Total	C	N	O	S	0	1	0
			3447	2197	578	655	17			
1	E	444	Total	C	N	O	S	0	0	0
			3447	2197	576	656	18			
1	F	444	Total	C	N	O	S	0	0	0
			3447	2197	576	656	18			

There are 30 discrepancies between the modelled and reference sequences:

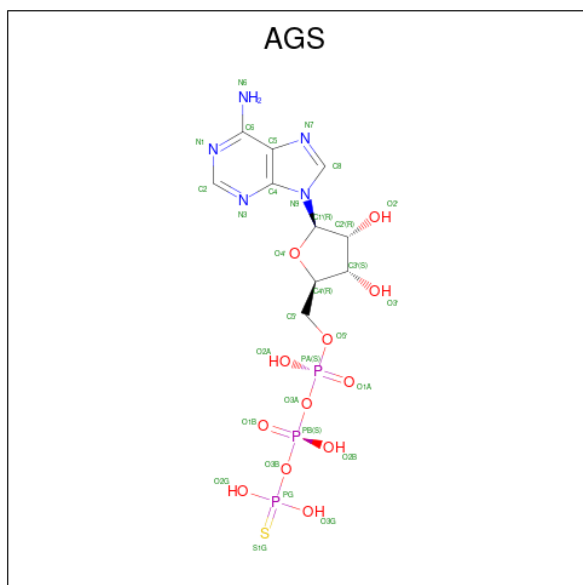
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A9ZPH9
A	-1	SER	-	expression tag	UNP A9ZPH9
A	0	HIS	-	expression tag	UNP A9ZPH9
A	1	MET	-	expression tag	UNP A9ZPH9
A	2	GLU	-	expression tag	UNP A9ZPH9
B	-2	GLY	-	expression tag	UNP A9ZPH9
B	-1	SER	-	expression tag	UNP A9ZPH9
B	0	HIS	-	expression tag	UNP A9ZPH9
B	1	MET	-	expression tag	UNP A9ZPH9
B	2	GLU	-	expression tag	UNP A9ZPH9
C	-2	GLY	-	expression tag	UNP A9ZPH9
C	-1	SER	-	expression tag	UNP A9ZPH9
C	0	HIS	-	expression tag	UNP A9ZPH9
C	1	MET	-	expression tag	UNP A9ZPH9
C	2	GLU	-	expression tag	UNP A9ZPH9
D	-2	GLY	-	expression tag	UNP A9ZPH9
D	-1	SER	-	expression tag	UNP A9ZPH9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A9ZPH9
D	1	MET	-	expression tag	UNP A9ZPH9
D	2	GLU	-	expression tag	UNP A9ZPH9
E	-2	GLY	-	expression tag	UNP A9ZPH9
E	-1	SER	-	expression tag	UNP A9ZPH9
E	0	HIS	-	expression tag	UNP A9ZPH9
E	1	MET	-	expression tag	UNP A9ZPH9
E	2	GLU	-	expression tag	UNP A9ZPH9
F	-2	GLY	-	expression tag	UNP A9ZPH9
F	-1	SER	-	expression tag	UNP A9ZPH9
F	0	HIS	-	expression tag	UNP A9ZPH9
F	1	MET	-	expression tag	UNP A9ZPH9
F	2	GLU	-	expression tag	UNP A9ZPH9

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		
3	D	3	Total	Mg	0	0
			3	3		
3	E	3	Total	Mg	0	0
			3	3		
3	F	3	Total	Mg	0	0
			3	3		

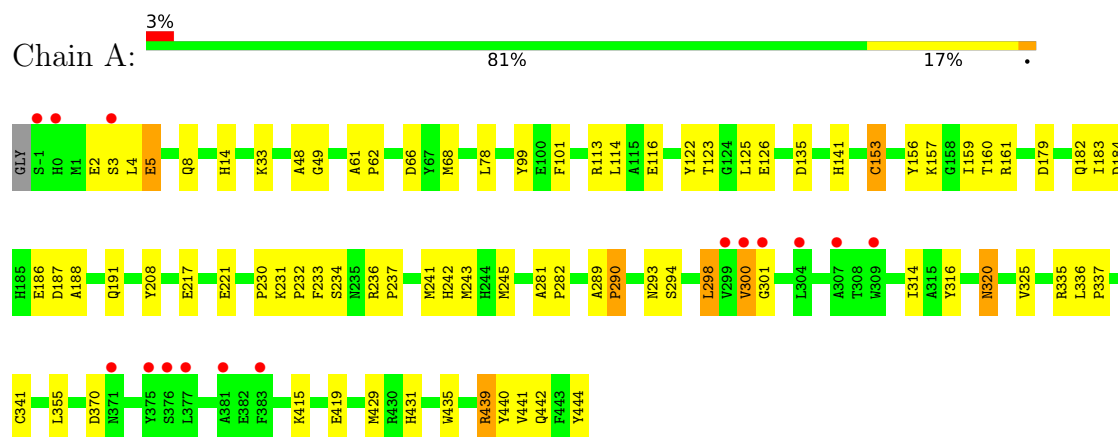
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	20	Total	O	0	0
			20	20		
4	C	19	Total	O	0	0
			19	19		
4	D	18	Total	O	0	0
			18	18		
4	E	16	Total	O	0	0
			16	16		
4	F	17	Total	O	0	0
			17	17		

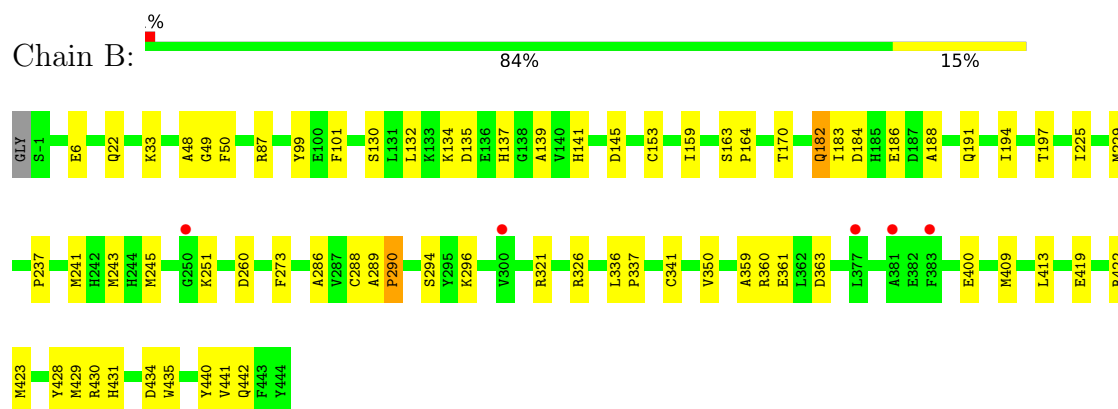
3 Residue-property plots [i](#)

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.

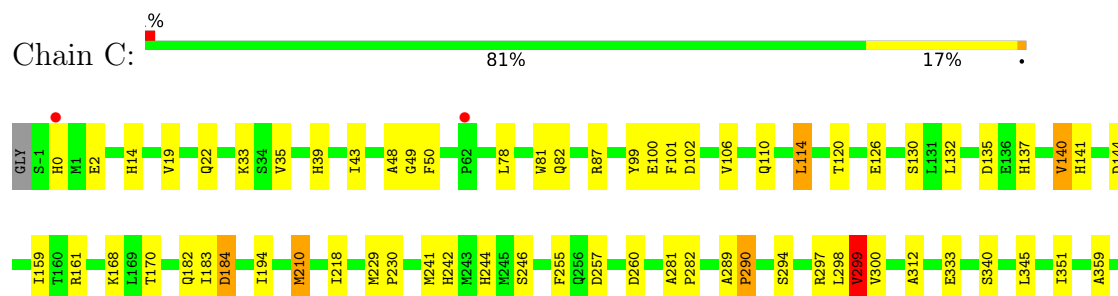
• Molecule 1: Glutamate--methylamine ligase



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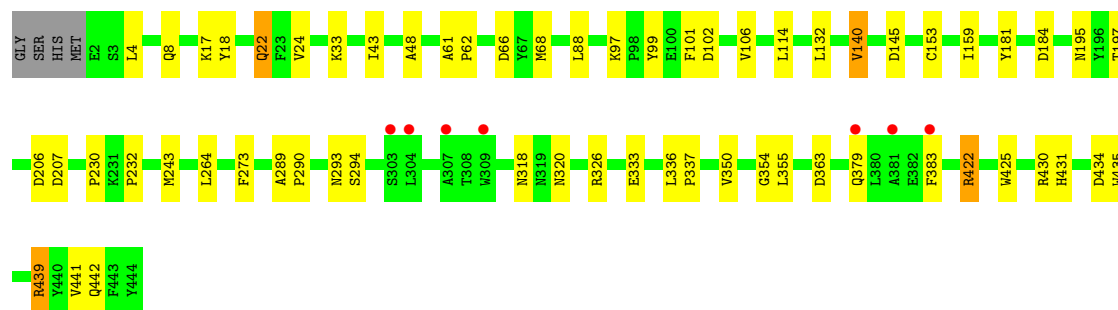
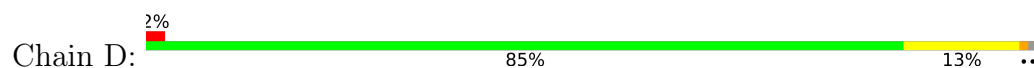


• Molecule 1: Glutamate--methylamine ligase

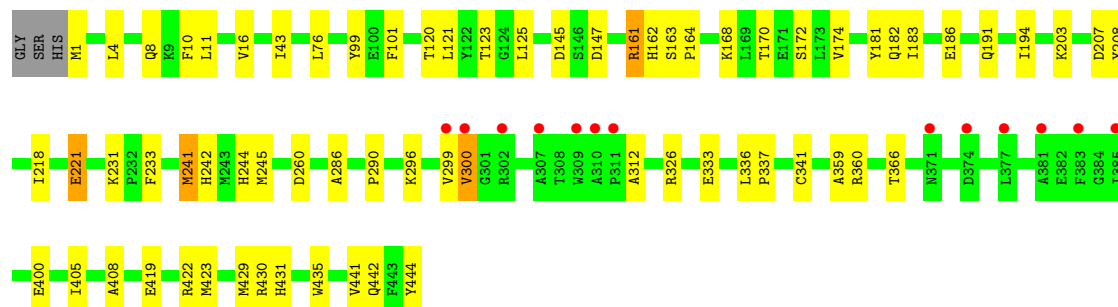
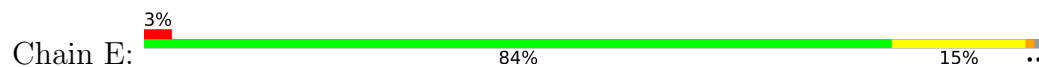




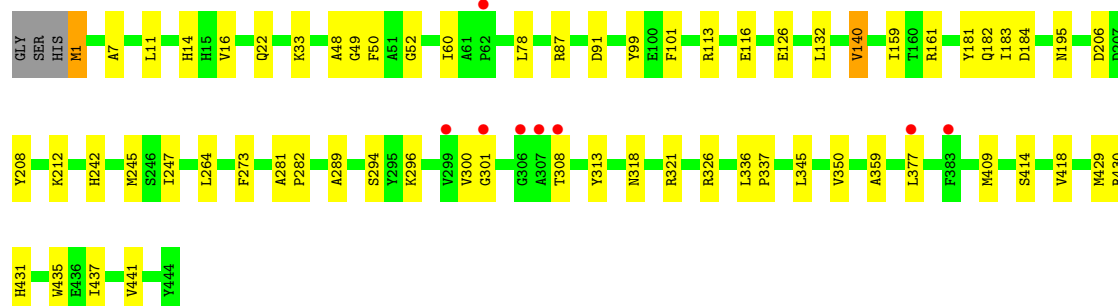
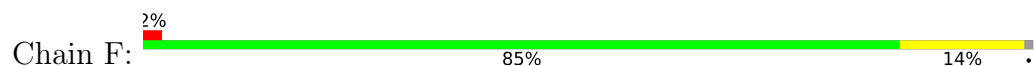
• Molecule 1: Glutamate--methylamine ligase



• Molecule 1: Glutamate--methylamine ligase



• Molecule 1: Glutamate--methylamine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.74Å 246.92Å 105.76Å 90.00° 111.17° 90.00°	Depositor
Resolution (Å)	90.89 – 2.65 90.89 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (90.89-2.65) 98.7 (90.89-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.225 , 0.260 (Not available) , 0.243	Depositor DCC
R_{free} test set	2031 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21045	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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: MG, AGS

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	0.58	1/3550 (0.0%)	1.14	6/4818 (0.1%)
1	B	0.53	0/3550	1.15	9/4818 (0.2%)
1	C	0.60	1/3558 (0.0%)	1.14	11/4828 (0.2%)
1	D	0.57	2/3536 (0.1%)	1.16	10/4799 (0.2%)
1	E	0.53	0/3533	1.14	8/4795 (0.2%)
1	F	0.53	0/3533	1.13	2/4795 (0.0%)
All	All	0.56	4/21260 (0.0%)	1.14	46/28853 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	1
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	PRO	N-CD	-16.28	1.25	1.47
1	A	290	PRO	N-CD	-14.58	1.27	1.47
1	D	422[A]	ARG	C-O	6.87	1.32	1.24
1	D	422[B]	ARG	C-O	6.87	1.32	1.24

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	422[A]	ARG	CA-C-O	8.53	129.46	120.42
1	D	422[B]	ARG	CA-C-O	8.53	129.46	120.42
1	C	299	VAL	N-CA-CB	-8.46	102.42	112.07
1	D	206	ASP	CA-CB-CG	7.52	120.12	112.60
1	C	366	THR	CA-CB-OG1	-6.85	99.32	109.60
1	C	290	PRO	N-CA-CB	-6.73	96.18	103.25
1	A	290	PRO	N-CA-CB	-6.71	96.21	103.25
1	C	290	PRO	CA-N-CD	6.54	121.16	112.00
1	B	170	THR	CA-CB-OG1	-6.40	100.00	109.60
1	F	206	ASP	CA-CB-CG	6.32	118.92	112.60
1	B	145	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	290	PRO	CA-N-CD	6.02	120.42	112.00
1	E	120	THR	CA-CB-OG1	-5.93	100.70	109.60
1	C	120	THR	CA-CB-OG1	-5.90	100.75	109.60
1	C	260	ASP	CA-CB-CG	5.84	118.44	112.60
1	E	145	ASP	CA-CB-CG	5.83	118.43	112.60
1	E	241	MET	CB-CA-C	-5.76	103.59	111.95
1	E	221	GLU	CB-CG-CD	5.73	122.34	112.60
1	D	439	ARG	CB-CA-C	-5.71	99.49	109.07
1	A	320	ASN	CB-CA-C	5.70	119.74	110.22
1	D	434	ASP	CA-CB-CG	5.59	118.19	112.60
1	F	91	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	444	TYR	CB-CA-C	5.49	120.54	110.10
1	E	366	THR	CA-CB-OG1	-5.46	101.41	109.60
1	D	290	PRO	N-CA-CB	-5.44	97.54	103.25
1	C	257	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	363	ASP	CB-CA-C	5.43	116.04	109.85
1	E	147	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	182	GLN	N-CA-CB	-5.34	101.47	110.49
1	D	197	THR	CA-CB-OG1	-5.31	101.64	109.60
1	B	197	THR	CA-CB-OG1	-5.25	101.73	109.60
1	E	444	TYR	CB-CA-C	5.24	120.06	110.10
1	D	363	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	290	PRO	N-CA-CB	-5.20	97.79	103.25
1	E	260	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	260	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	187	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	184	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	434	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	144	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	145	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	207	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	100	GLU	CB-CG-CD	5.07	121.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	THR	CA-CB-OG1	-5.07	102.00	109.60
1	B	428	TYR	CB-CA-C	5.03	118.78	110.88
1	B	6	GLU	CB-CG-CD	5.02	121.13	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	B	326	ARG	Sidechain
1	C	161	ARG	Sidechain
1	D	422[A]	ARG	Sidechain
1	D	422[B]	ARG	Sidechain
1	D	439	ARG	Sidechain
1	E	161	ARG	Sidechain
1	F	161	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3463	0	3360	63	1
1	B	3463	0	3360	49	0
1	C	3471	0	3368	57	0
1	D	3447	0	3349	40	0
1	E	3447	0	3348	42	1
1	F	3447	0	3348	44	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	3	0
2	E	31	0	12	4	0
2	F	31	0	12	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	13	0	0	5	0
4	B	20	0	0	2	0
4	C	19	0	0	4	0
4	D	18	0	0	4	0
4	E	16	0	0	2	0
4	F	17	0	0	0	0
All	All	21045	0	20205	265	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 6.

All (265) 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)
2:E:501:AGS:H2'	4:E:604:HOH:O	1.17	1.30
1:C:35:VAL:HG21	1:C:43:ILE:HD11	1.09	1.07
1:A:230:PRO:HD2	1:A:293:ASN:HD22	1.31	0.93
1:F:182:GLN:HE21	1:F:195:ASN:HD22	1.23	0.87
1:A:231:LYS:H	1:A:293:ASN:HD21	1.24	0.85
1:C:19:VAL:O	1:C:35:VAL:HG22	1.80	0.81
1:B:441:VAL:HA	1:C:229:MET:HE2	1.62	0.81
1:A:231:LYS:N	1:A:293:ASN:HD21	1.79	0.81
1:D:441:VAL:HG13	1:D:442:GLN:HG2	1.61	0.80
1:C:437:ILE:O	1:C:441:VAL:HG23	1.83	0.79
1:A:300:VAL:HG22	1:D:430:ARG:NH2	2.00	0.76
1:C:35:VAL:CG2	1:C:43:ILE:HD11	2.04	0.74
1:A:230:PRO:CD	1:A:293:ASN:HD22	2.00	0.74
1:C:33:LYS:HD2	1:C:48:ALA:HB1	1.70	0.73
1:F:301:GLY:HA3	1:F:308:THR:HG21	1.71	0.73
1:C:35:VAL:HG21	1:C:43:ILE:CD1	2.04	0.73
1:E:429:MET:O	1:F:296:LYS:HD2	1.87	0.73
1:F:14:HIS:CD2	1:F:78:LEU:HD11	2.24	0.72
1:D:243:MET:HE1	1:D:350:VAL:HG21	1.72	0.72
1:A:232:PRO:HD2	4:A:606:HOH:O	1.89	0.72
1:E:168:LYS:O	1:E:172:SER:OG	2.06	0.72
1:A:99:TYR:CE2	1:A:101:PHE:HB2	2.26	0.70
1:E:441:VAL:HG13	1:E:442:GLN:HG3	1.73	0.70
1:B:359:ALA:HB1	1:E:359:ALA:HB1	1.72	0.70
1:F:33:LYS:HD2	1:F:48:ALA:HB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LYS:HE3	1:F:49:GLY:O	1.94	0.68
1:B:229:MET:HE2	1:C:441:VAL:HA	1.75	0.67
1:F:301:GLY:CA	1:F:308:THR:HG21	2.27	0.65
1:A:159:ILE:HD13	1:A:184:ASP:HA	1.78	0.65
1:B:360:ARG:HD3	1:E:360:ARG:HD3	1.79	0.65
1:E:1:MET:HE1	1:E:10:PHE:CG	2.32	0.64
1:A:243:MET:HE2	1:A:245:MET:CE	2.28	0.64
1:F:245:MET:HE1	1:F:350:VAL:CG1	2.28	0.64
1:B:245:MET:HE1	1:B:350:VAL:CG1	2.28	0.63
1:E:121:LEU:HD11	1:E:245:MET:HG2	1.80	0.63
1:D:326:ARG:NH2	2:D:501:AGS:O1B	2.25	0.63
1:A:335:ARG:HD3	4:A:604:HOH:O	1.99	0.63
1:A:157:LYS:HE2	4:A:605:HOH:O	1.99	0.62
1:C:99:TYR:CE2	1:C:101:PHE:HB2	2.34	0.62
1:F:245:MET:HE1	1:F:350:VAL:HG12	1.80	0.62
1:E:296:LYS:HE3	1:F:429:MET:O	2.00	0.62
1:E:241:MET:HE1	1:E:341:CYS:SG	2.41	0.61
1:F:33:LYS:CE	1:F:49:GLY:O	2.48	0.61
1:C:297:ARG:C	1:C:299:VAL:H	2.09	0.61
1:C:126:GLU:OE1	1:C:242:HIS:HB2	2.02	0.60
1:A:182:GLN:OE1	1:C:33:LYS:HD3	2.01	0.60
1:A:243:MET:HE2	1:A:245:MET:HE2	1.85	0.59
1:E:430:ARG:HH22	1:F:301:GLY:HA2	1.65	0.59
1:D:114:LEU:HD23	1:D:355:LEU:HD21	1.84	0.59
1:A:335:ARG:NH2	4:A:601:HOH:O	2.15	0.59
1:E:99:TYR:CE2	1:E:101:PHE:HB2	2.38	0.59
1:C:141:HIS:HD2	4:C:618:HOH:O	1.85	0.58
1:F:113:ARG:O	1:F:116:GLU:HG2	2.03	0.58
1:D:24:VAL:HG13	4:D:603:HOH:O	2.02	0.58
1:C:300:VAL:HG23	1:C:312:ALA:HB2	1.86	0.58
1:B:440:TYR:HE1	4:C:611:HOH:O	1.87	0.58
1:F:377:LEU:HD12	1:F:377:LEU:H	1.68	0.58
1:E:431:HIS:CD2	1:F:435:TRP:HB2	2.39	0.58
1:E:4:LEU:O	1:E:8:GLN:HG3	2.03	0.57
1:C:183:ILE:HG23	1:C:194:ILE:HG12	1.86	0.57
1:A:320:ASN:ND2	1:A:370:ASP:O	2.37	0.57
1:A:231:LYS:H	1:A:293:ASN:ND2	2.00	0.57
1:B:251:LYS:HE2	1:B:251:LYS:HA	1.87	0.57
1:A:135:ASP:OD2	1:A:141:HIS:HE1	1.88	0.57
1:A:435:TRP:HB2	1:D:431:HIS:CD2	2.40	0.56
1:B:137:HIS:HD2	1:C:137:HIS:HD2	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:MET:HE1	1:B:341:CYS:SG	2.46	0.56
1:B:153:CYS:HB2	4:B:608:HOH:O	2.06	0.56
1:E:181:TYR:CD1	1:E:182:GLN:HB2	2.41	0.56
1:F:181:TYR:OH	2:F:501:AGS:H3'	2.04	0.56
2:E:501:AGS:H8	4:E:604:HOH:O	2.07	0.55
1:A:300:VAL:HG22	1:D:430:ARG:HH21	1.70	0.55
1:E:400:GLU:OE1	1:E:422:ARG:NH2	2.39	0.55
1:F:208:TYR:CE2	1:F:212:LYS:HD2	2.41	0.55
1:A:217:GLU:O	1:A:221:GLU:HG3	2.07	0.55
1:B:188:ALA:HB2	1:B:237:PRO:HB2	1.89	0.55
1:D:379:GLN:HG2	1:D:383:PHE:CE2	2.42	0.55
1:F:182:GLN:C	1:F:183:ILE:HG13	2.31	0.55
1:F:289:ALA:HB1	1:F:294:SER:HB3	1.89	0.55
1:D:114:LEU:CD2	1:D:355:LEU:HD21	2.36	0.54
1:A:301:GLY:H	1:D:430:ARG:HH22	1.55	0.54
1:D:61:ALA:HB1	1:D:62:PRO:HD2	1.89	0.54
1:B:186:GLU:HB2	1:B:191:GLN:HG2	1.89	0.54
1:B:135:ASP:OD2	1:B:141:HIS:HE1	1.89	0.54
1:D:22:GLN:NE2	4:D:603:HOH:O	2.40	0.54
1:F:1:MET:HE2	1:F:7:ALA:HA	1.90	0.54
1:E:218:ILE:O	1:E:221:GLU:HG2	2.07	0.54
1:A:66:ASP:HB3	1:A:68:MET:HE2	1.90	0.53
1:B:441:VAL:HG13	1:B:442:GLN:HG3	1.91	0.53
1:A:3:SER:HB3	1:A:5:GLU:HG2	1.89	0.53
1:E:326:ARG:NH2	2:E:501:AGS:O1B	2.25	0.53
1:E:186:GLU:HB2	1:E:191:GLN:HG2	1.91	0.53
1:A:33:LYS:HD2	1:A:48:ALA:HB1	1.90	0.53
1:B:435:TRP:HB2	1:C:431:HIS:CD2	2.44	0.53
1:E:4:LEU:HG	1:E:8:GLN:HE21	1.73	0.53
1:E:1:MET:HE1	1:E:10:PHE:CD2	2.44	0.53
1:A:431:HIS:CD2	1:D:435:TRP:HB2	2.43	0.52
1:C:289:ALA:N	1:C:290:PRO:HD3	2.25	0.52
1:C:281:ALA:HB3	1:C:282:PRO:HD3	1.91	0.52
1:B:289:ALA:HB1	1:B:294:SER:HB3	1.90	0.52
1:B:409:MET:HE2	1:B:413:LEU:HG	1.91	0.52
1:A:153:CYS:HB2	4:C:606:HOH:O	2.08	0.52
1:F:33:LYS:HG3	1:F:50:PHE:CE2	2.44	0.52
1:C:130:SER:HB3	1:C:132:LEU:HD21	1.92	0.52
1:B:400:GLU:OE1	1:B:422:ARG:NH2	2.44	0.51
1:C:359:ALA:HB1	1:F:359:ALA:HB1	1.92	0.51
1:B:431:HIS:CD2	1:C:435:TRP:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:VAL:HG11	1:F:430:ARG:HG2	1.91	0.51
1:A:336:LEU:HB3	1:A:337:PRO:HD3	1.93	0.51
1:C:378:GLU:O	1:C:382:GLU:HG3	2.09	0.51
1:A:4:LEU:O	1:A:8:GLN:HG3	2.11	0.51
1:D:326:ARG:NE	1:D:333:GLU:OE1	2.43	0.51
1:F:22:GLN:OE1	1:F:87:ARG:NH1	2.43	0.51
1:E:1:MET:HE3	1:E:76:LEU:HD23	1.93	0.51
1:A:5:GLU:CD	1:A:5:GLU:H	2.18	0.51
1:B:33:LYS:HD2	1:B:48:ALA:HB1	1.93	0.51
1:C:168:LYS:HD3	1:C:218:ILE:HG23	1.92	0.50
1:D:379:GLN:HG2	1:D:383:PHE:HE2	1.74	0.50
1:C:400:GLU:CD	1:C:422:ARG:HH21	2.20	0.50
1:F:182:GLN:NE2	2:F:501:AGS:O2A	2.44	0.50
1:A:125:LEU:HD13	1:A:241:MET:CE	2.41	0.50
1:A:439:ARG:HG3	1:A:439:ARG:HH11	1.76	0.50
1:A:14:HIS:CD2	1:A:78:LEU:HD11	2.46	0.50
1:A:289:ALA:N	1:A:290:PRO:HD3	2.25	0.50
1:F:414:SER:O	1:F:418:VAL:HG23	2.12	0.50
1:C:33:LYS:HE3	1:C:49:GLY:O	2.12	0.50
1:A:439:ARG:NH2	4:A:602:HOH:O	2.32	0.50
1:F:377:LEU:HD12	1:F:377:LEU:N	2.26	0.50
1:A:179:ASP:OD1	1:C:39:HIS:HE1	1.95	0.49
1:B:33:LYS:CE	1:B:49:GLY:O	2.60	0.49
1:F:345:LEU:HD22	1:F:409:MET:HE2	1.94	0.49
1:D:159:ILE:HD12	1:D:184:ASP:HA	1.94	0.49
1:D:243:MET:HE1	1:D:350:VAL:HG11	1.94	0.49
1:B:183:ILE:HG23	1:B:194:ILE:HG12	1.95	0.49
1:D:132:LEU:HD13	1:D:140:VAL:HG11	1.94	0.49
1:A:186:GLU:HB2	1:A:191:GLN:HG2	1.94	0.48
1:D:230:PRO:HD2	1:D:293:ASN:OD1	2.12	0.48
1:A:231:LYS:N	1:A:293:ASN:ND2	2.55	0.48
1:F:52:GLY:HA3	1:F:60:ILE:HD12	1.95	0.48
1:B:130:SER:HB3	1:B:132:LEU:HD21	1.95	0.48
1:A:61:ALA:HB1	1:A:62:PRO:HD2	1.95	0.48
1:B:430:ARG:HG2	1:C:299:VAL:HG21	1.94	0.48
1:A:113:ARG:O	1:A:116:GLU:HG2	2.13	0.48
1:D:99:TYR:CE2	1:D:101:PHE:HB2	2.48	0.48
1:A:290:PRO:HG3	1:A:341:CYS:HA	1.95	0.48
1:D:102:ASP:O	1:D:106:VAL:HG23	2.13	0.48
1:F:159:ILE:HD12	1:F:184:ASP:HA	1.96	0.48
1:A:114:LEU:HD23	1:A:355:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:PHE:CZ	1:D:354:GLY:HA3	2.48	0.47
1:D:289:ALA:HB1	1:D:294:SER:HB3	1.96	0.47
1:E:241:MET:CE	1:E:341:CYS:SG	3.01	0.47
1:C:170:THR:HG21	1:C:183:ILE:HD11	1.96	0.47
1:C:246:SER:HA	1:C:255:PHE:CD2	2.49	0.47
1:F:11:LEU:HD22	1:F:16:VAL:HG11	1.95	0.47
1:A:230:PRO:HD2	1:A:293:ASN:ND2	2.14	0.47
1:A:439:ARG:HD3	1:A:440:TYR:CE1	2.49	0.47
1:B:243:MET:CE	1:B:350:VAL:HG11	2.45	0.47
1:A:156:TYR:OH	1:C:82:GLN:NE2	2.48	0.47
1:B:33:LYS:HG3	1:B:50:PHE:CE1	2.50	0.47
1:D:264:LEU:HD21	1:D:318:ASN:HB2	1.97	0.47
1:A:125:LEU:HD13	1:A:241:MET:HE2	1.96	0.47
1:C:439:ARG:HD3	1:C:440:TYR:CE1	2.50	0.47
1:B:184:ASP:OD2	1:D:33:LYS:HE2	2.16	0.46
1:E:286:ALA:O	1:E:290:PRO:HB3	2.15	0.46
1:C:81:TRP:HH2	1:C:210[A]:MET:SD	2.39	0.46
1:F:99:TYR:CE2	1:F:101:PHE:HB2	2.50	0.46
1:F:300:VAL:HG21	1:F:313:TYR:OH	2.15	0.46
1:A:208:TYR:CD1	1:A:241:MET:HE3	2.51	0.46
1:A:429:MET:HE1	1:D:425:TRP:HH2	1.81	0.46
1:A:66:ASP:CB	1:A:68:MET:HE2	2.45	0.46
1:D:132:LEU:HD13	1:D:140:VAL:CG1	2.45	0.46
1:D:181:TYR:OH	2:D:501:AGS:H3'	2.16	0.46
1:C:159:ILE:HD12	1:C:184:ASP:HA	1.97	0.46
1:D:4:LEU:O	1:D:8:GLN:HG3	2.15	0.45
1:E:326:ARG:NE	1:E:333:GLU:OE1	2.49	0.45
1:B:225:ILE:HG23	1:C:442:GLN:HG2	1.98	0.45
1:F:247:ILE:HD11	1:F:273:PHE:CE2	2.52	0.45
1:F:437:ILE:HG23	1:F:441:VAL:HG21	1.98	0.45
1:A:114:LEU:CD2	1:A:355:LEU:HD21	2.47	0.45
1:B:163:SER:N	1:B:164:PRO:CD	2.79	0.45
1:B:182:GLN:C	1:B:183:ILE:HG13	2.40	0.45
1:B:336:LEU:N	1:B:337:PRO:CD	2.80	0.45
1:C:22:GLN:OE1	1:C:87:ARG:NH1	2.48	0.45
1:C:33:LYS:CE	1:C:49:GLY:O	2.65	0.45
1:E:11:LEU:HD22	1:E:16:VAL:HG11	1.98	0.45
1:C:102:ASP:O	1:C:106:VAL:HG23	2.16	0.45
1:A:126:GLU:OE1	1:A:242:HIS:HB2	2.16	0.45
1:C:110:GLN:O	1:C:114:LEU:HD12	2.17	0.45
1:B:296:LYS:NZ	1:C:429:MET:O	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASP:HB3	1:D:68:MET:HE2	1.99	0.45
1:D:320:ASN:N	1:D:326:ARG:HG3	2.31	0.45
1:D:43:ILE:HG21	1:D:88:LEU:HD23	1.99	0.44
1:E:203:LYS:NZ	1:E:207:ASP:OD2	2.43	0.44
1:B:22:GLN:OE1	1:B:87:ARG:NH1	2.50	0.44
1:B:245:MET:HE2	1:B:273:PHE:CE1	2.52	0.44
1:B:296:LYS:HE3	1:C:436:GLU:OE2	2.17	0.44
1:C:230:PRO:HD3	1:C:340:SER:HB3	1.99	0.44
1:A:316:TYR:HA	1:A:325:VAL:O	2.18	0.44
1:B:229:MET:HE1	1:C:441:VAL:HG22	2.00	0.43
1:E:123:THR:HA	1:E:244:HIS:O	2.18	0.43
1:E:435:TRP:HB2	1:F:431:HIS:CD2	2.52	0.43
1:E:419:GLU:O	1:E:423:MET:HG3	2.18	0.43
1:A:233:PHE:HB2	1:A:236:ARG:HB2	2.00	0.43
1:C:141:HIS:CD2	4:C:618:HOH:O	2.66	0.43
1:B:241:MET:CE	1:B:341:CYS:SG	3.07	0.43
1:C:0:HIS:O	1:C:2:GLU:HG3	2.17	0.43
1:B:430:ARG:NH2	1:C:300:VAL:O	2.52	0.43
1:D:195:ASN:ND2	2:D:501:AGS:O2A	2.51	0.43
1:C:289:ALA:HB1	1:C:294:SER:HB3	2.00	0.43
1:C:14:HIS:CD2	1:C:78:LEU:HD11	2.54	0.43
1:C:114:LEU:HD11	1:C:351:ILE:CG2	2.48	0.43
1:C:135:ASP:OD2	1:C:141:HIS:HE1	2.02	0.43
1:F:321:ARG:NH2	1:F:326:ARG:HH12	2.17	0.43
1:B:134:LYS:HA	1:B:139:ALA:O	2.19	0.43
1:B:321:ARG:HH22	1:D:66:ASP:CG	2.27	0.43
1:E:231:LYS:HE3	1:E:233:PHE:O	2.18	0.43
1:E:244:HIS:CD2	1:E:333:GLU:HG3	2.54	0.43
1:C:396:LEU:HD13	1:C:422:ARG:HG2	2.00	0.42
1:F:126:GLU:OE1	1:F:242:HIS:HB2	2.19	0.42
1:A:188:ALA:HB2	1:A:237:PRO:HB2	2.01	0.42
1:D:336:LEU:HB3	1:D:337:PRO:HD3	2.01	0.42
1:A:182:GLN:C	1:A:183:ILE:HG13	2.45	0.42
1:B:288:CYS:O	1:B:341:CYS:HB3	2.20	0.42
1:B:99:TYR:CE2	1:B:101:PHE:HB2	2.55	0.42
1:B:186:GLU:OE1	4:B:601:HOH:O	2.22	0.42
1:E:183:ILE:HG23	1:E:194:ILE:HG12	2.01	0.42
1:E:336:LEU:N	1:E:337:PRO:CD	2.83	0.42
1:A:122:TYR:O	1:A:245:MET:HA	2.20	0.42
1:D:232:PRO:HD2	4:D:610:HOH:O	2.19	0.42
1:B:286:ALA:O	1:B:290:PRO:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:HE1	1:B:350:VAL:HG11	2.02	0.42
1:B:419:GLU:O	1:B:423:MET:HG3	2.20	0.42
1:E:170:THR:O	1:E:174:VAL:HG23	2.20	0.41
1:E:125:LEU:HD12	1:E:208:TYR:HB2	2.02	0.41
1:C:297:ARG:C	1:C:299:VAL:N	2.76	0.41
1:C:345:LEU:HD22	1:C:409:MET:HE2	2.02	0.41
1:E:405:ILE:O	1:E:408:ALA:HB3	2.21	0.41
1:F:336:LEU:N	1:F:337:PRO:CD	2.83	0.41
1:A:281:ALA:HB3	1:A:314:ILE:HD13	2.01	0.41
1:D:33:LYS:HD2	1:D:48:ALA:HB1	2.02	0.41
1:A:441:VAL:HG13	1:A:442:GLN:HG3	2.02	0.41
1:B:429:MET:HE2	1:C:391:ASN:HB3	2.02	0.41
1:D:17:LYS:HG3	1:D:18:TYR:CE2	2.54	0.41
1:F:264:LEU:HD21	1:F:318:ASN:HB2	2.03	0.41
1:E:245:MET:HE3	1:E:245:MET:HB2	1.71	0.41
1:D:153:CYS:HB2	4:D:604:HOH:O	2.20	0.41
1:F:377:LEU:H	1:F:377:LEU:CD1	2.32	0.41
1:A:415:LYS:O	1:A:419:GLU:HG3	2.21	0.41
1:A:294:SER:O	1:A:298:LEU:HD22	2.21	0.41
1:C:132:LEU:HD13	1:C:140:VAL:HG11	2.02	0.41
1:F:126:GLU:CD	2:F:501:AGS:O2B	2.64	0.41
1:F:132:LEU:HD13	1:F:140:VAL:CG1	2.51	0.41
1:A:125:LEU:HB3	1:A:241:MET:HE2	2.02	0.41
1:E:4:LEU:HG	1:E:8:GLN:NE2	2.35	0.41
1:E:300:VAL:HG23	1:E:312:ALA:HB2	2.02	0.41
1:A:157:LYS:O	1:A:160:THR:HG22	2.21	0.40
1:E:163:SER:N	1:E:164:PRO:CD	2.84	0.40
1:E:242:HIS:CE1	2:E:501:AGS:O2G	2.72	0.40
1:A:33:LYS:CE	1:A:49:GLY:O	2.69	0.40
1:A:281:ALA:HB3	1:A:282:PRO:HD3	2.02	0.40
1:C:33:LYS:HG3	1:C:50:PHE:CE2	2.56	0.40
1:C:244:HIS:CD2	1:C:333:GLU:HG3	2.56	0.40
1:B:245:MET:HE1	1:B:350:VAL:HG12	2.00	0.40
1:F:281:ALA:HB3	1:F:282:PRO:HD3	2.03	0.40
1:B:360:ARG:O	1:B:361:GLU:C	2.64	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:217:GLU:OE2	1:E:161:ARG:NH1[4_546]	2.19	0.01

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	444/447 (99%)	433 (98%)	11 (2%)	0	100	100
1	B	444/447 (99%)	432 (97%)	12 (3%)	0	100	100
1	C	445/447 (100%)	429 (96%)	15 (3%)	1 (0%)	43	60
1	D	442/447 (99%)	430 (97%)	12 (3%)	0	100	100
1	E	442/447 (99%)	428 (97%)	14 (3%)	0	100	100
1	F	442/447 (99%)	433 (98%)	9 (2%)	0	100	100
All	All	2659/2682 (99%)	2585 (97%)	73 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	298	LEU

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	364/364 (100%)	357 (98%)	7 (2%)	50	71
1	B	364/364 (100%)	362 (100%)	2 (0%)	81	91
1	C	365/364 (100%)	359 (98%)	6 (2%)	55	74
1	D	362/364 (100%)	359 (99%)	3 (1%)	73	85
1	E	362/364 (100%)	359 (99%)	3 (1%)	73	85
1	F	362/364 (100%)	360 (99%)	2 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2179/2184 (100%)	2156 (99%)	23 (1%)	68 80

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	5	GLU
1	A	153	CYS
1	A	234	SER
1	A	298	LEU
1	A	300	VAL
1	A	439	ARG
1	B	159	ILE
1	B	182	GLN
1	C	114	LEU
1	C	140	VAL
1	C	210[A]	MET
1	C	210[B]	MET
1	C	241	MET
1	C	299	VAL
1	D	22	GLN
1	D	97	LYS
1	D	140	VAL
1	E	43	ILE
1	E	162	HIS
1	E	300	VAL
1	F	1	MET
1	F	140	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	14	HIS
1	A	27	HIS
1	A	95	ASN
1	A	141	HIS
1	A	293	ASN
1	A	379	GLN
1	A	390	GLN
1	A	438	ASN

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Mol	Chain	Res	Type
1	B	8	GLN
1	B	27	HIS
1	B	137	HIS
1	B	141	HIS
1	B	244	HIS
1	B	390	GLN
1	B	438	ASN
1	C	27	HIS
1	C	39	HIS
1	C	82	GLN
1	C	95	ASN
1	C	137	HIS
1	C	141	HIS
1	C	390	GLN
1	C	403	GLN
1	C	438	ASN
1	D	8	GLN
1	D	82	GLN
1	D	95	ASN
1	D	182	GLN
1	D	195	ASN
1	E	8	GLN
1	E	27	HIS
1	E	41	ASN
1	E	95	ASN
1	E	182	GLN
1	E	195	ASN
1	E	390	GLN
1	E	438	ASN
1	F	8	GLN
1	F	182	GLN
1	F	319	ASN
1	F	379	GLN
1	F	403	GLN

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 24 ligands modelled in this entry, 18 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	$\# Z > 2$
2	AGS	C	501	3	32,33,33	0.85	2 (6%)	45,52,52	0.81	1 (2%)
2	AGS	F	501	3	32,33,33	1.01	2 (6%)	45,52,52	0.79	1 (2%)
2	AGS	D	501	3	32,33,33	0.83	2 (6%)	45,52,52	0.75	1 (2%)
2	AGS	B	501	3	32,33,33	0.77	1 (3%)	45,52,52	0.63	0
2	AGS	E	501	3	32,33,33	0.85	2 (6%)	45,52,52	0.69	1 (2%)
2	AGS	A	501	3	32,33,33	0.77	1 (3%)	45,52,52	0.77	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
2	AGS	C	501	3	-	11/21/38/38	0/3/3/3
2	AGS	F	501	3	-	6/21/38/38	0/3/3/3
2	AGS	D	501	3	-	4/21/38/38	0/3/3/3
2	AGS	B	501	3	-	5/21/38/38	0/3/3/3
2	AGS	E	501	3	-	3/21/38/38	0/3/3/3
2	AGS	A	501	3	-	3/21/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	AGS	PA-O3A	3.61	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	AGS	PA-O3A	2.57	1.62	1.59
2	F	501	AGS	PB-O3B	2.49	1.62	1.59
2	C	501	AGS	PA-O3A	2.47	1.62	1.59
2	C	501	AGS	PB-O3B	2.30	1.62	1.59
2	E	501	AGS	PB-O3B	2.29	1.62	1.59
2	D	501	AGS	PB-O3B	2.26	1.61	1.59
2	D	501	AGS	PA-O3A	2.17	1.61	1.59
2	A	501	AGS	PA-O3A	2.09	1.61	1.59
2	B	501	AGS	PA-O3A	2.02	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	AGS	PB-O3B-PG	2.71	143.07	133.17
2	C	501	AGS	C3'-C2'-C1'	-2.43	96.87	101.46
2	E	501	AGS	PB-O3B-PG	2.11	140.89	133.17
2	F	501	AGS	O2'-C2'-C3'	2.05	118.39	111.82

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AGS	C5'-O5'-PA-O1A
2	A	501	AGS	C5'-O5'-PA-O2A
2	A	501	AGS	C5'-O5'-PA-O3A
2	C	501	AGS	PB-O3B-PG-O3G
2	C	501	AGS	C5'-O5'-PA-O1A
2	C	501	AGS	C5'-O5'-PA-O2A
2	C	501	AGS	C5'-O5'-PA-O3A
2	F	501	AGS	C5'-O5'-PA-O1A
2	F	501	AGS	O4'-C4'-C5'-O5'
2	B	501	AGS	PA-O3A-PB-O1B
2	B	501	AGS	O4'-C4'-C5'-O5'
2	F	501	AGS	C3'-C4'-C5'-O5'
2	F	501	AGS	PB-O3A-PA-O5'
2	C	501	AGS	C3'-C4'-C5'-O5'
2	C	501	AGS	O4'-C4'-C5'-O5'
2	C	501	AGS	C2'-C1'-N9-C8
2	F	501	AGS	C5'-O5'-PA-O2A
2	F	501	AGS	C5'-O5'-PA-O3A
2	B	501	AGS	PA-O3A-PB-O2B
2	D	501	AGS	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	E	501	AGS	PA-O3A-PB-O2B
2	B	501	AGS	C3'-C4'-C5'-O5'
2	C	501	AGS	PB-O3A-PA-O1A
2	C	501	AGS	PB-O3B-PG-O2G
2	E	501	AGS	O4'-C4'-C5'-O5'
2	D	501	AGS	PG-O3B-PB-O1B
2	D	501	AGS	PG-O3B-PB-O2B
2	C	501	AGS	PB-O3A-PA-O2A
2	B	501	AGS	C2'-C1'-N9-C8
2	D	501	AGS	C2'-C1'-N9-C8
2	C	501	AGS	O4'-C1'-N9-C8
2	E	501	AGS	C2'-C1'-N9-C8

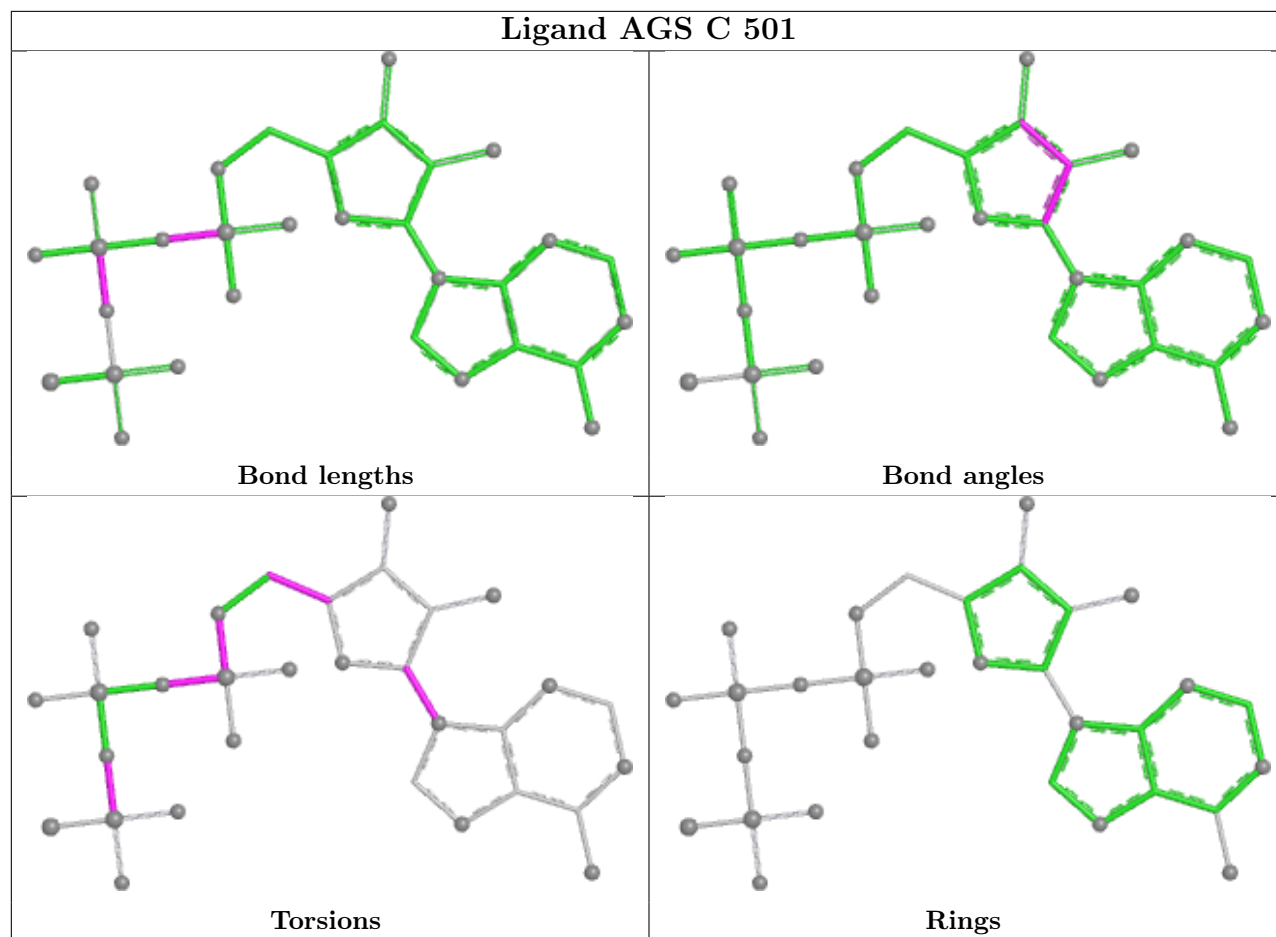
There are no ring outliers.

3 monomers are involved in 10 short contacts:

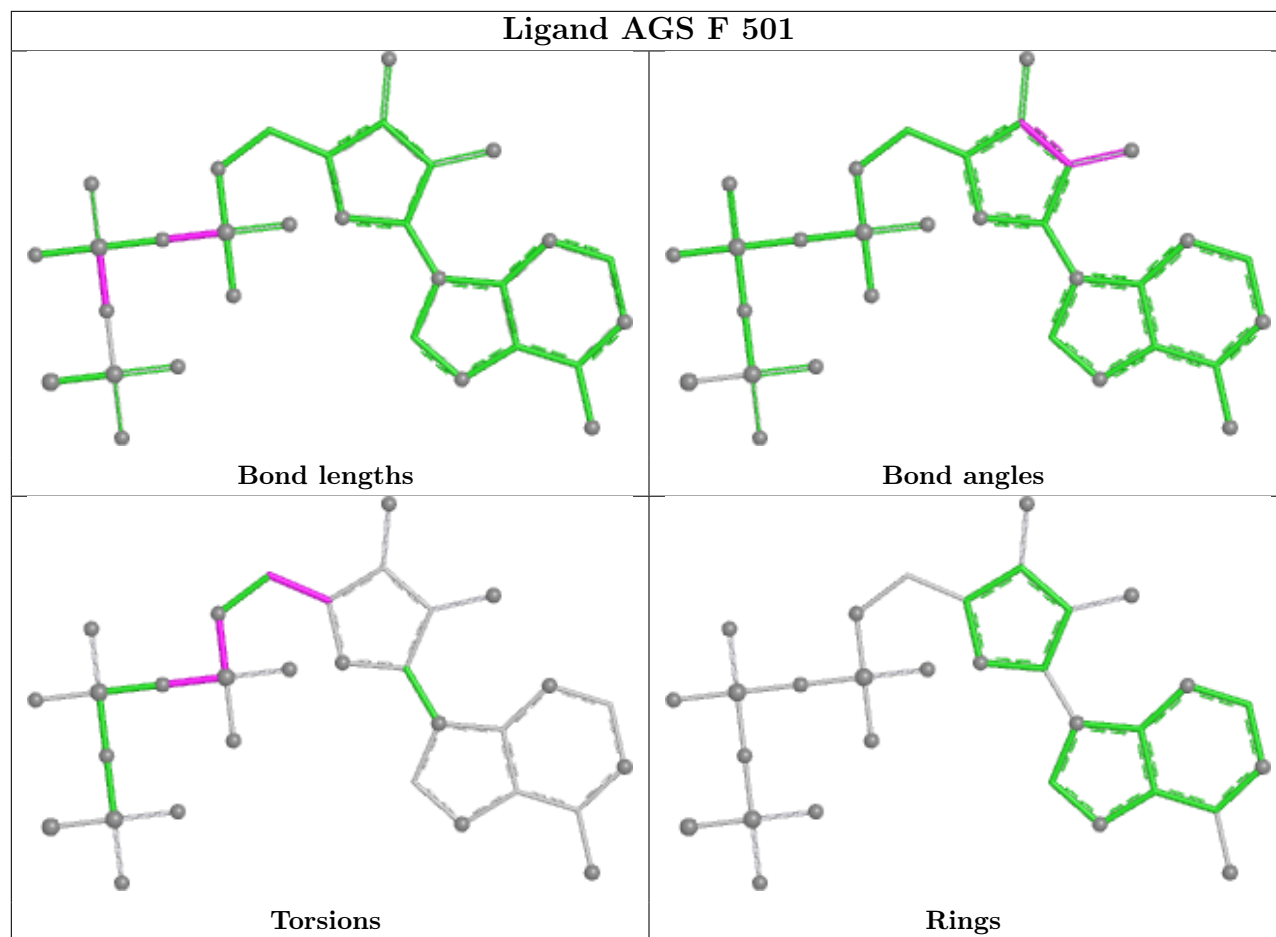
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	AGS	3	0
2	D	501	AGS	3	0
2	E	501	AGS	4	0

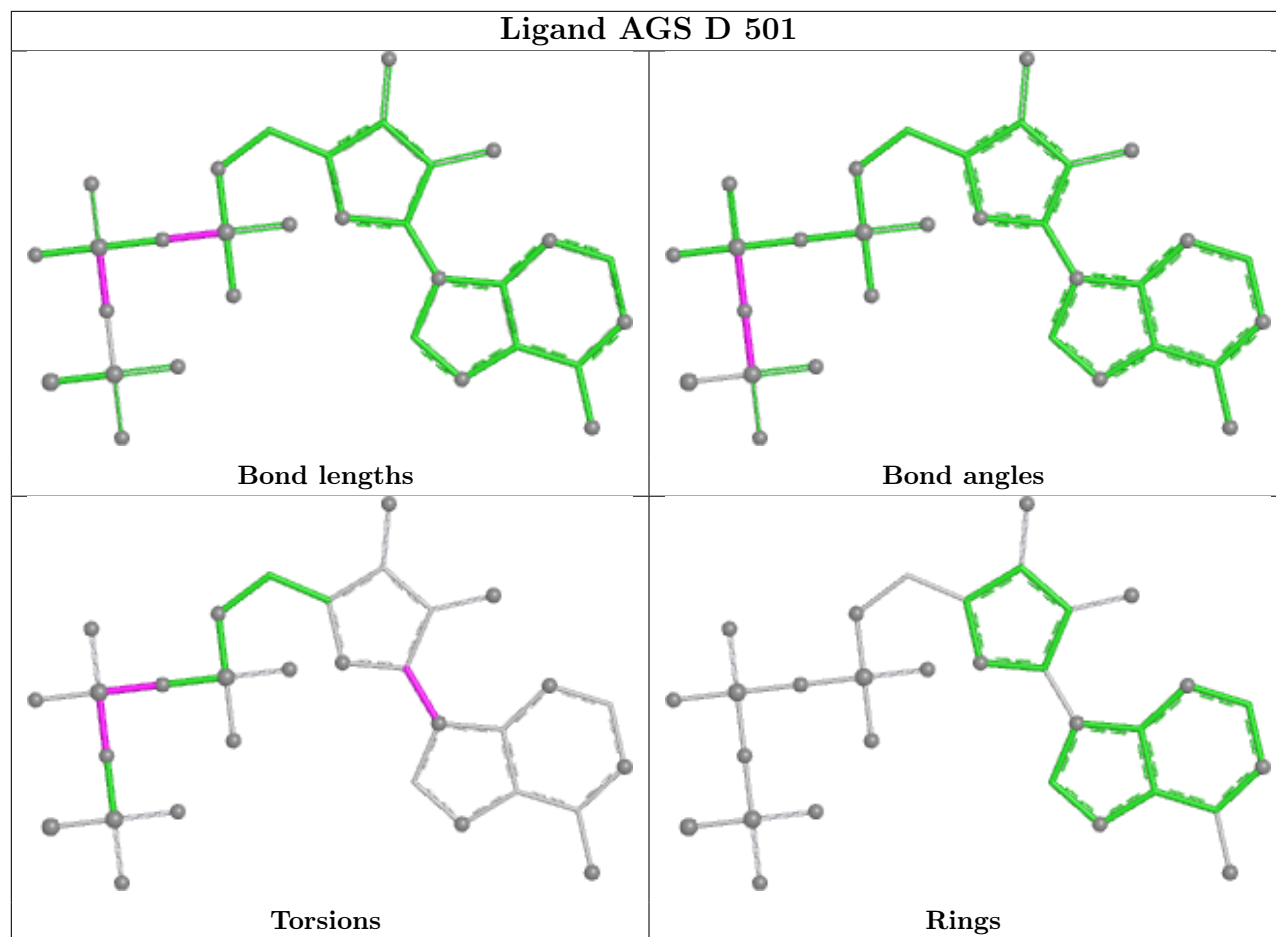
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

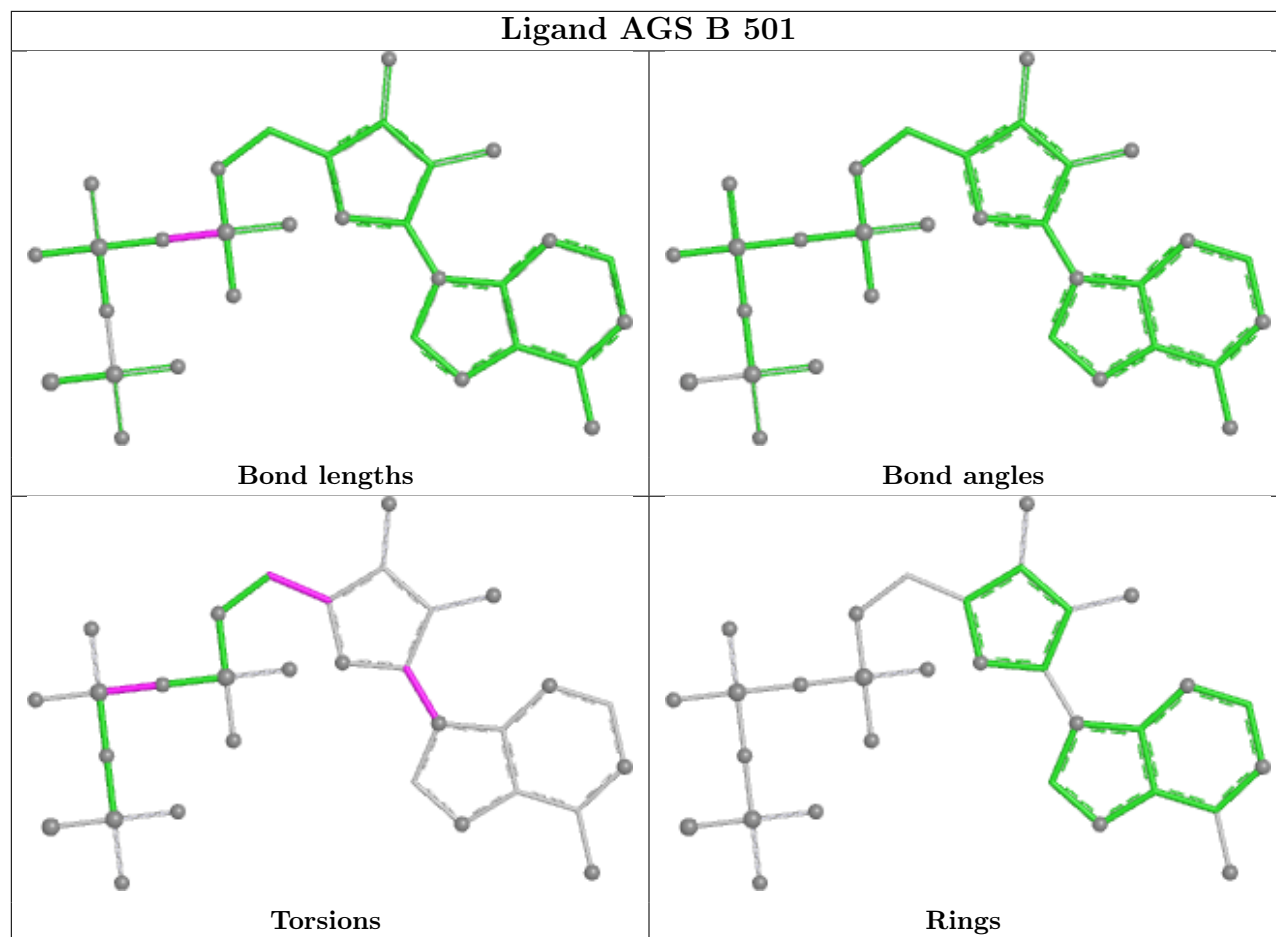
Ligand AGS C 501



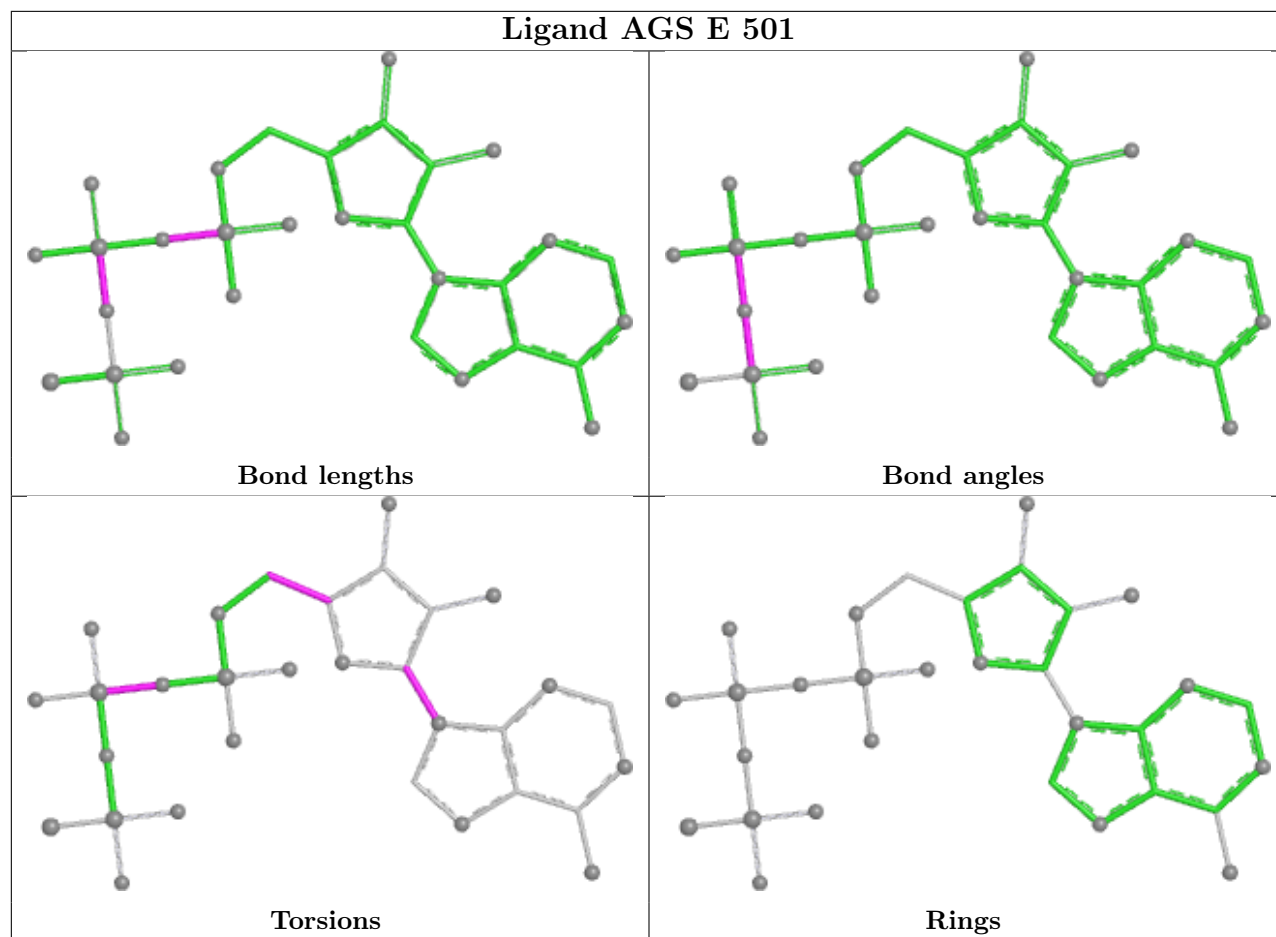
Ligand AGS F 501

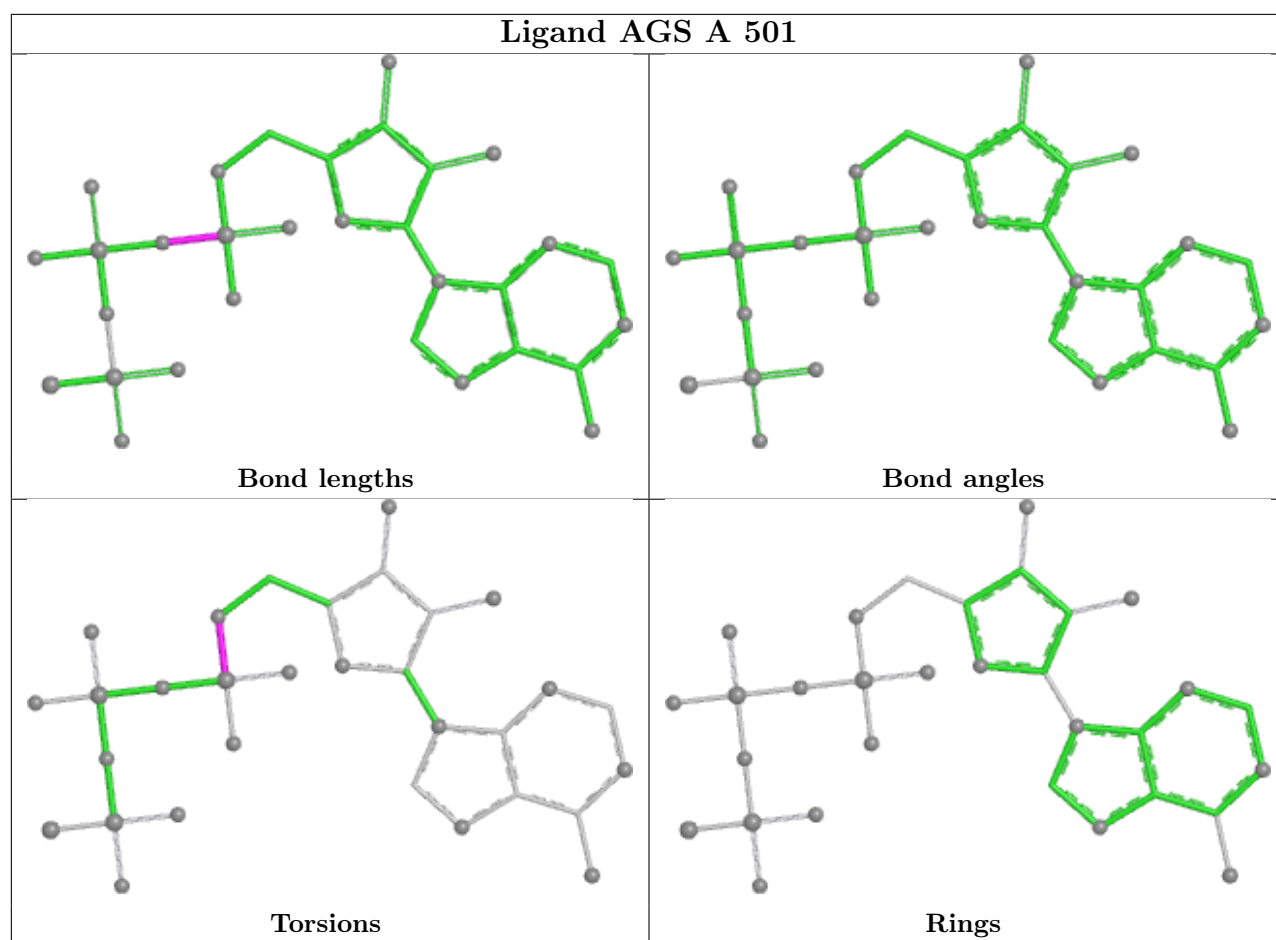






Ligand AGS E 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	446/447 (99%)	-0.11	15 (3%)	48 40	20, 34, 70, 104	0
1	B	446/447 (99%)	-0.22	5 (1%)	78 75	19, 32, 64, 103	0
1	C	446/447 (99%)	-0.14	6 (1%)	75 71	14, 34, 66, 110	1 (0%)
1	D	443/447 (99%)	-0.16	7 (1%)	70 66	13, 33, 65, 105	1 (0%)
1	E	444/447 (99%)	-0.15	13 (2%)	53 46	21, 34, 67, 111	0
1	F	444/447 (99%)	-0.22	8 (1%)	67 63	20, 34, 62, 95	0
All	All	2669/2682 (99%)	-0.17	54 (2%)	65 59	13, 34, 67, 111	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	PHE	4.2
1	F	377	LEU	3.8
1	B	381	ALA	3.6
1	B	300	VAL	3.6
1	A	0	HIS	3.5
1	A	300	VAL	3.5
1	D	383	PHE	3.5
1	A	377	LEU	3.3
1	F	383	PHE	3.2
1	C	0	HIS	3.2
1	A	371	ASN	3.2
1	B	377	LEU	3.1
1	A	383	PHE	3.1
1	A	307	ALA	3.0
1	E	383	PHE	3.0
1	E	307	ALA	2.9
1	C	383	PHE	2.9
1	E	311	PRO	2.8
1	C	377	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	381	ALA	2.8
1	A	299	VAL	2.8
1	E	302	ARG	2.8
1	D	304	LEU	2.8
1	B	250	GLY	2.8
1	A	301	GLY	2.7
1	D	381	ALA	2.6
1	D	309	TRP	2.5
1	A	381	ALA	2.5
1	A	-1	SER	2.5
1	A	375	TYR	2.4
1	D	307	ALA	2.4
1	E	310	ALA	2.4
1	F	62	PRO	2.4
1	C	62	PRO	2.4
1	E	371	ASN	2.4
1	A	309	TRP	2.4
1	E	300	VAL	2.4
1	E	377	LEU	2.3
1	A	3	SER	2.3
1	F	301	GLY	2.3
1	E	299	VAL	2.3
1	A	376	SER	2.3
1	F	299	VAL	2.3
1	C	372	LEU	2.3
1	E	374	ASP	2.2
1	F	306	GLY	2.2
1	D	379	GLN	2.1
1	A	304	LEU	2.1
1	E	385	ILE	2.1
1	D	303	SER	2.1
1	F	307	ALA	2.1
1	E	309	TRP	2.1
1	F	308	THR	2.0
1	C	371	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

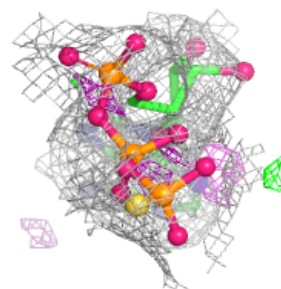
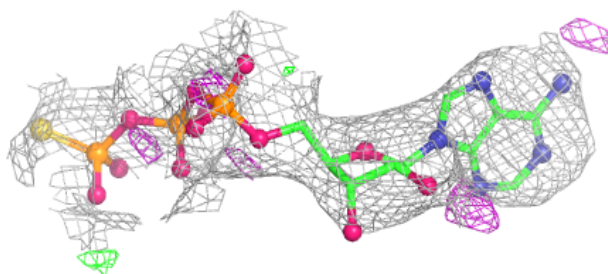
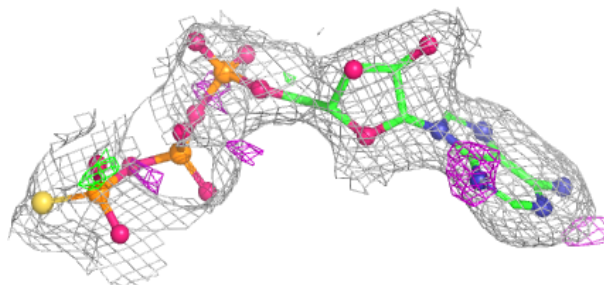
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AGS	F	501	31/31	0.87	0.13	39,56,101,114	0
2	AGS	C	501	31/31	0.88	0.12	44,51,106,107	0
2	AGS	A	501	31/31	0.88	0.12	35,52,96,96	0
2	AGS	E	501	31/31	0.89	0.11	48,54,89,92	0
2	AGS	B	501	31/31	0.89	0.11	49,60,92,95	0
2	AGS	D	501	31/31	0.90	0.11	43,54,89,93	0
3	MG	B	502	1/1	0.94	0.08	18,18,18,18	0
3	MG	A	504	1/1	0.97	0.06	40,40,40,40	0
3	MG	A	503	1/1	0.97	0.06	29,29,29,29	0
3	MG	B	504	1/1	0.98	0.05	41,41,41,41	0
3	MG	C	504	1/1	0.98	0.04	39,39,39,39	0
3	MG	D	504	1/1	0.98	0.04	41,41,41,41	0
3	MG	E	503	1/1	0.98	0.03	32,32,32,32	0
3	MG	E	504	1/1	0.98	0.03	35,35,35,35	0
3	MG	F	504	1/1	0.98	0.05	41,41,41,41	0
3	MG	D	502	1/1	0.99	0.07	16,16,16,16	0
3	MG	D	503	1/1	0.99	0.02	30,30,30,30	0
3	MG	A	502	1/1	0.99	0.06	10,10,10,10	0
3	MG	E	502	1/1	0.99	0.04	11,11,11,11	0
3	MG	C	502	1/1	0.99	0.06	13,13,13,13	0
3	MG	C	503	1/1	0.99	0.02	20,20,20,20	0
3	MG	F	503	1/1	0.99	0.02	21,21,21,21	0
3	MG	B	503	1/1	0.99	0.02	31,31,31,31	0
3	MG	F	502	1/1	1.00	0.03	9,9,9,9	0

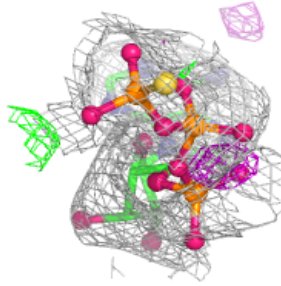
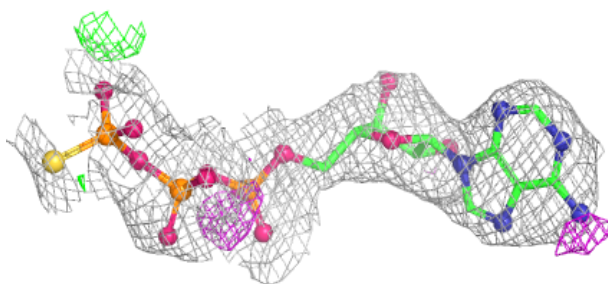
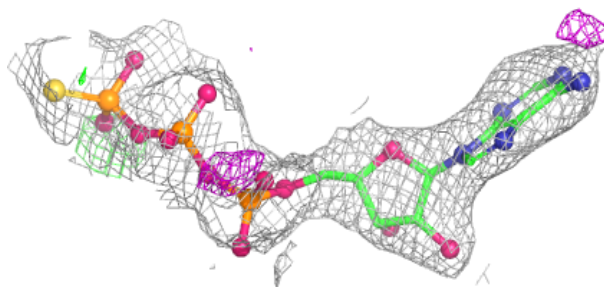
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS F 501:

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

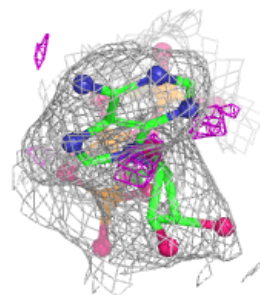
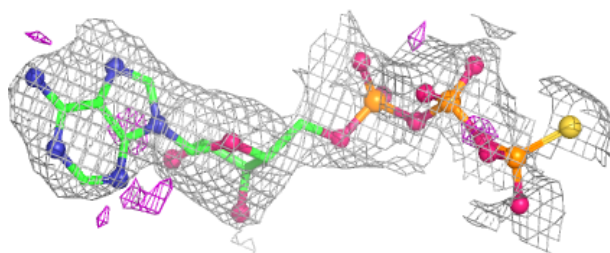
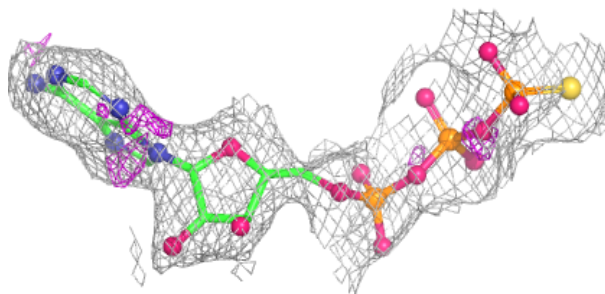
**Electron density around AGS C 501:**

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

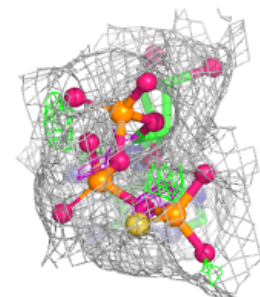
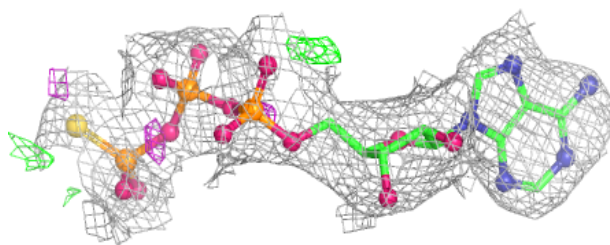
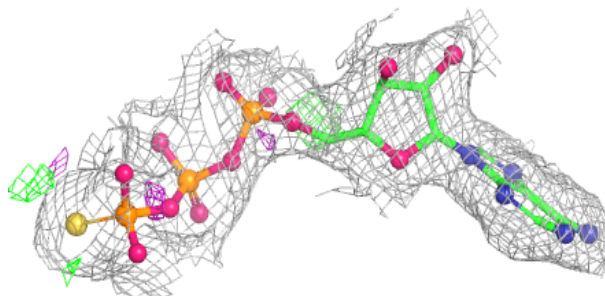


Electron density around AGS A 501:

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

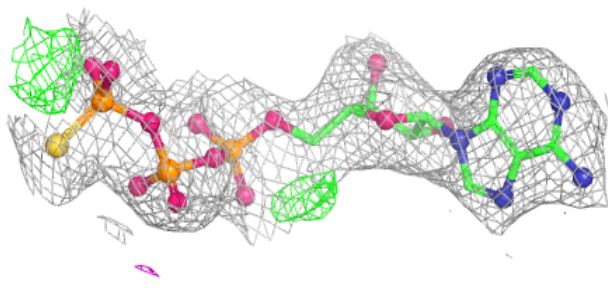
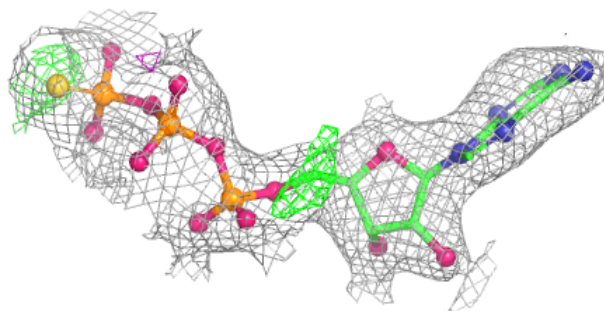
**Electron density around AGS E 501:**

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

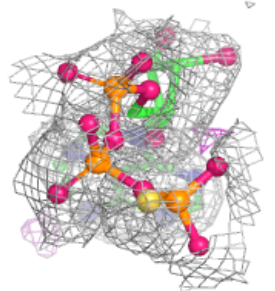
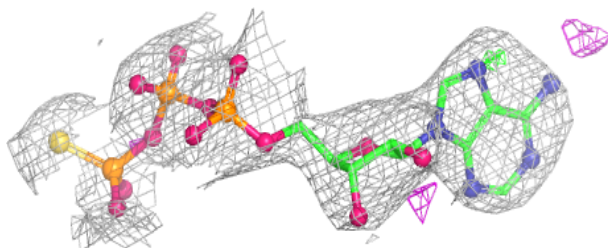
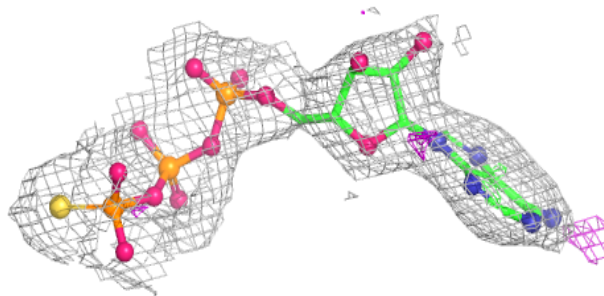


Electron density around AGS B 501:

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

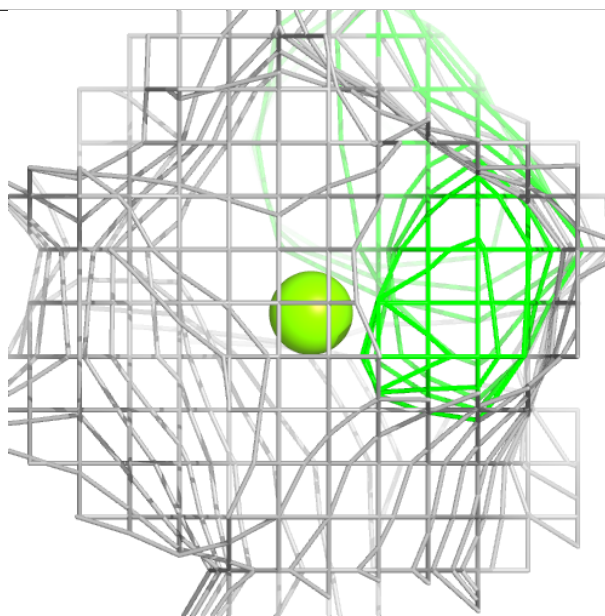
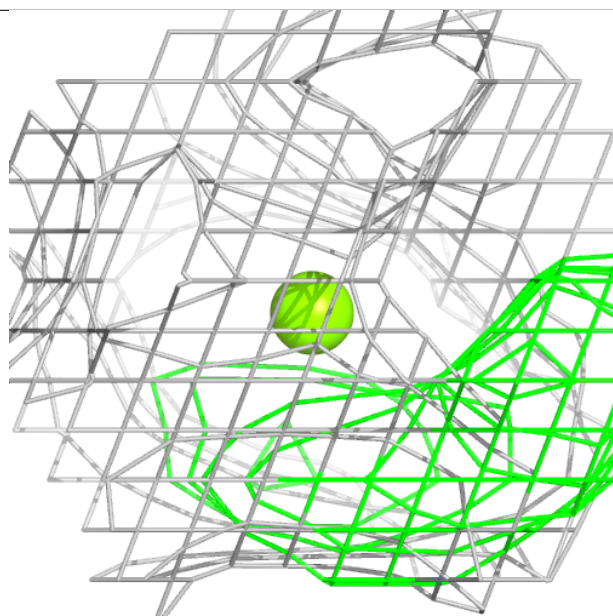
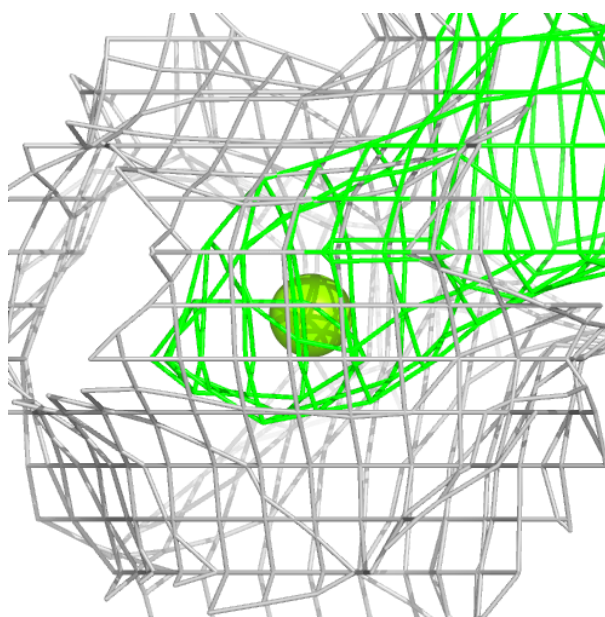
**Electron density around AGS D 501:**

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



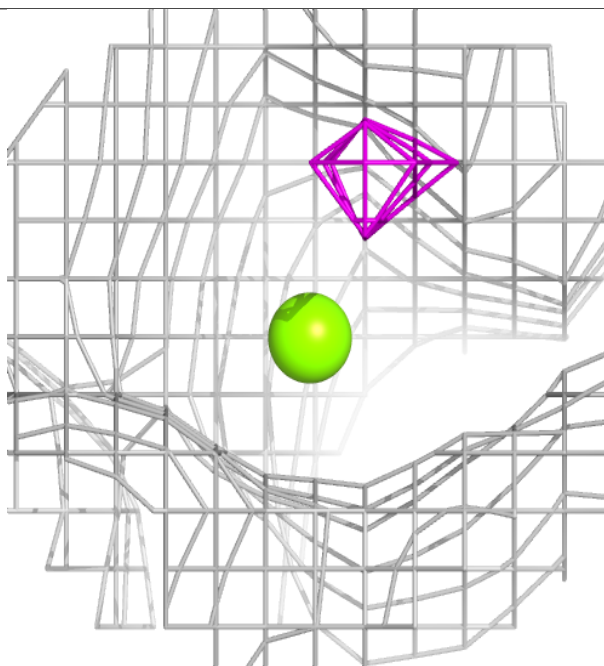
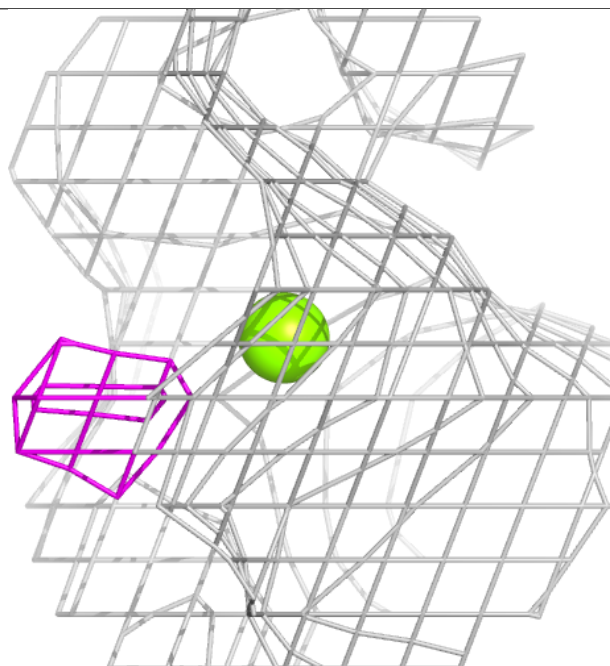
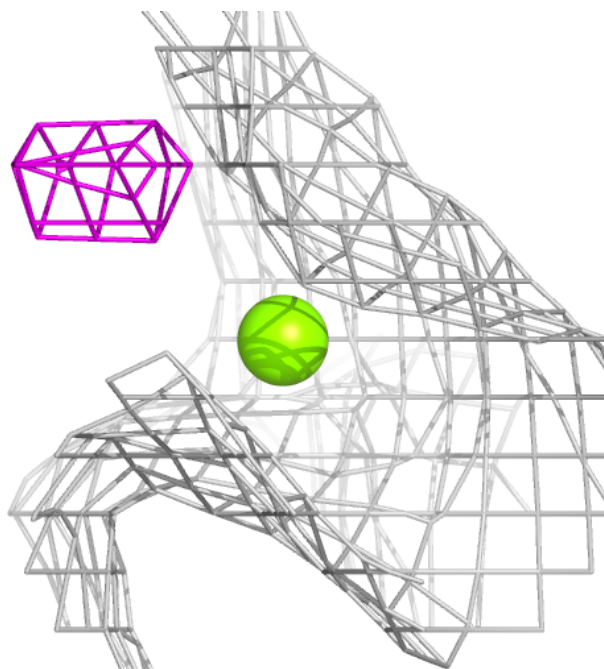
Electron density around MG B 502:

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



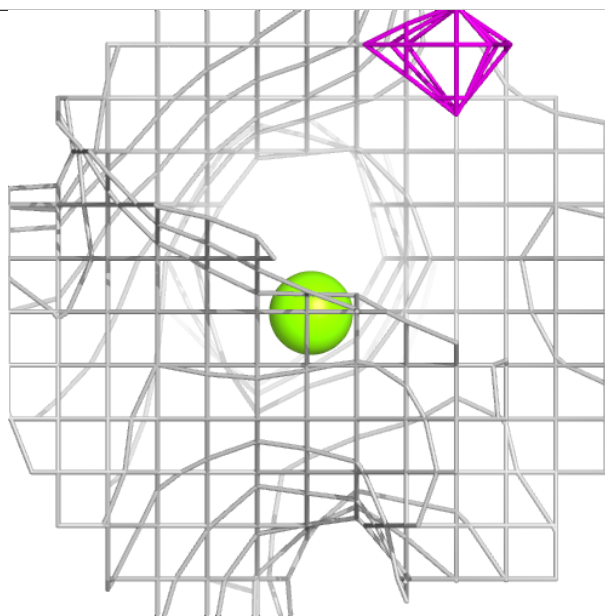
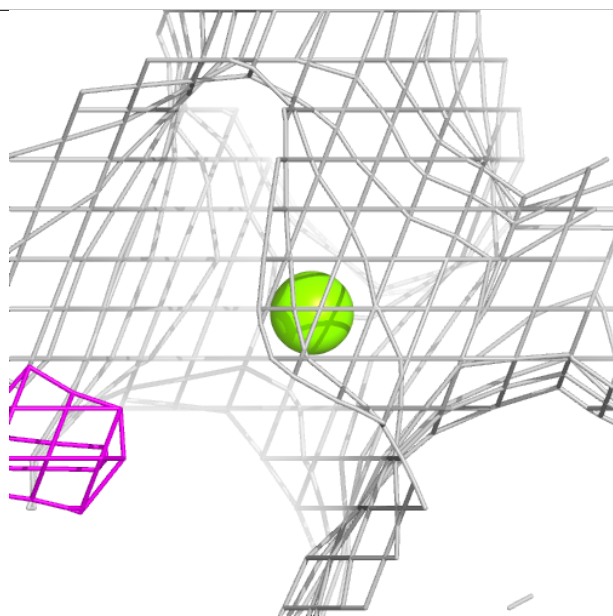
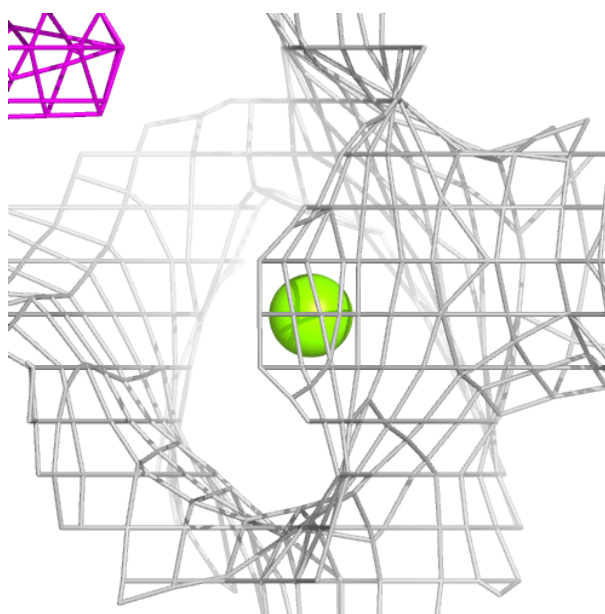
Electron density around MG A 504:

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



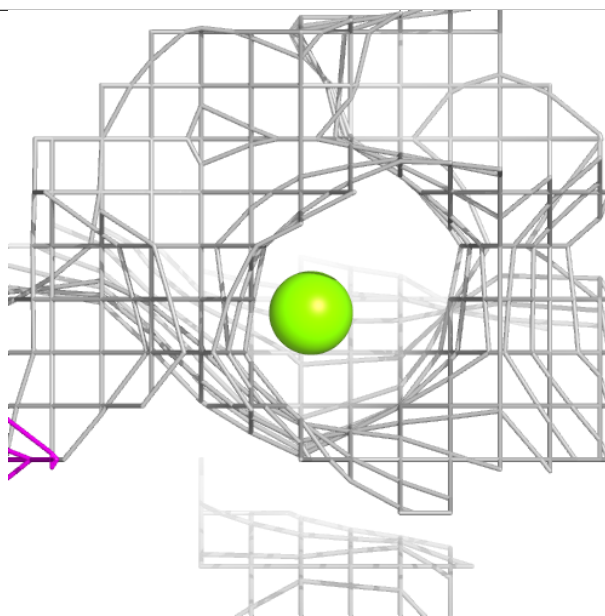
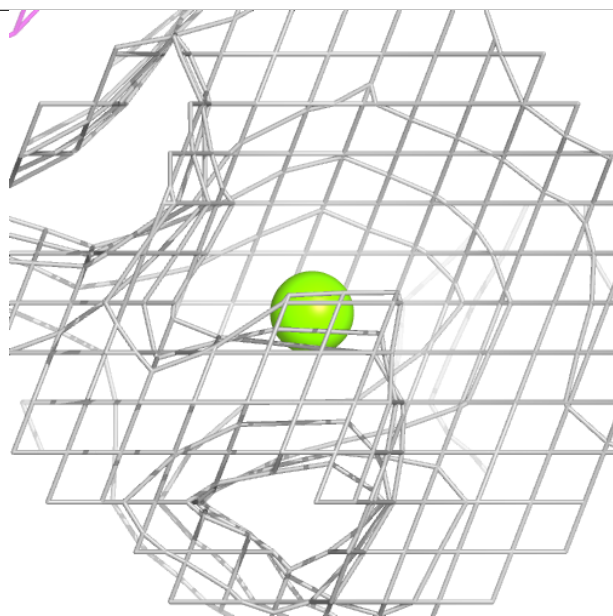
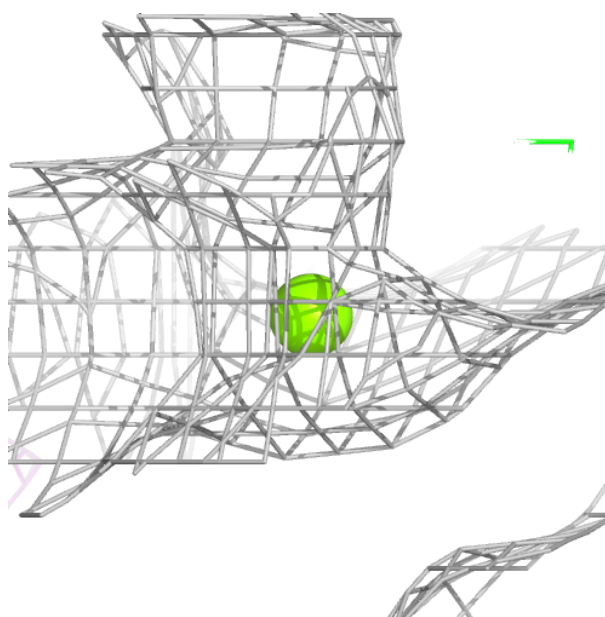
Electron density around MG A 503:

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



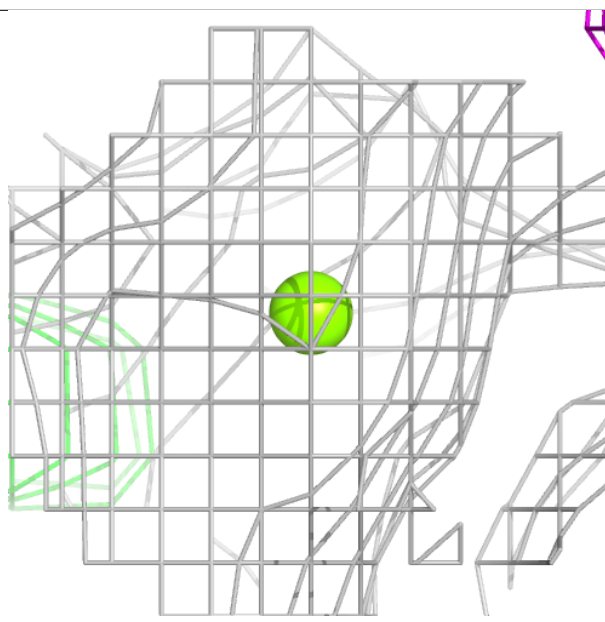
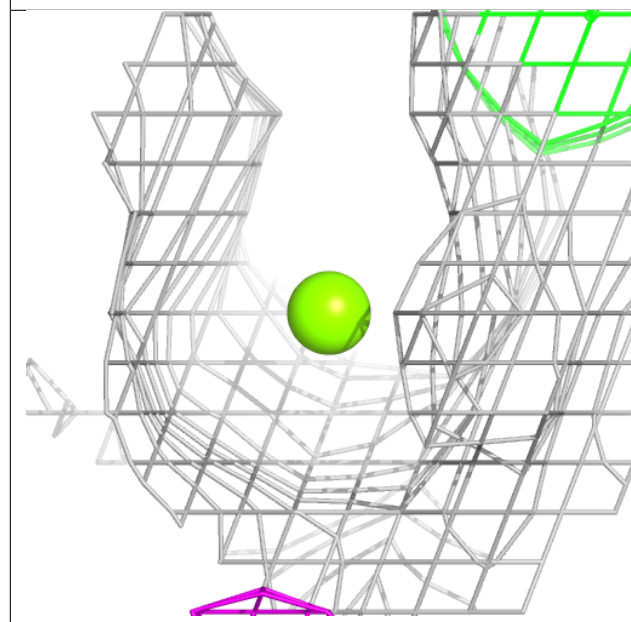
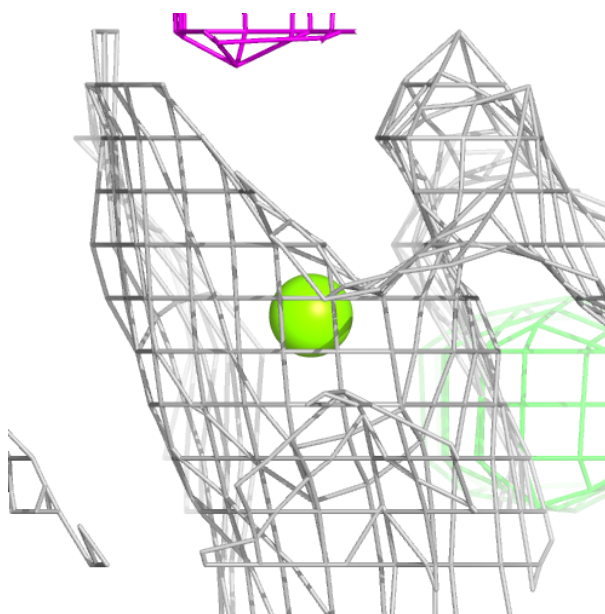
Electron density around MG B 504:

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



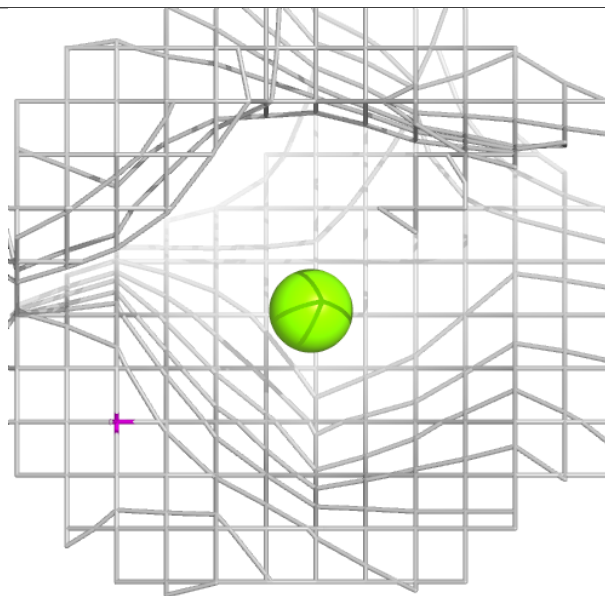
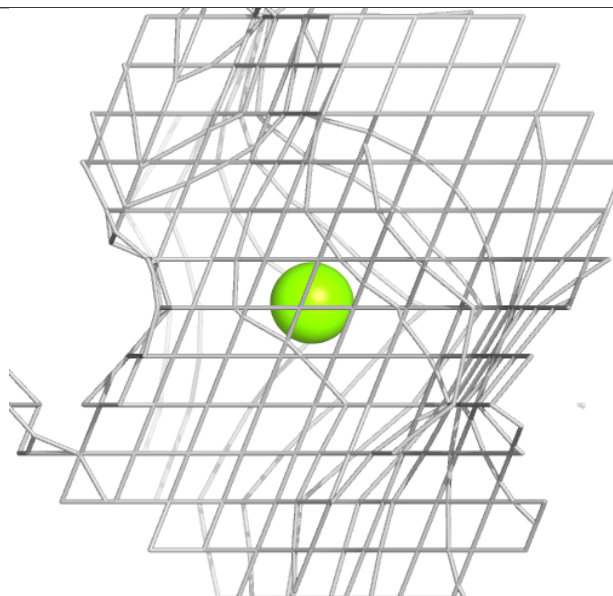
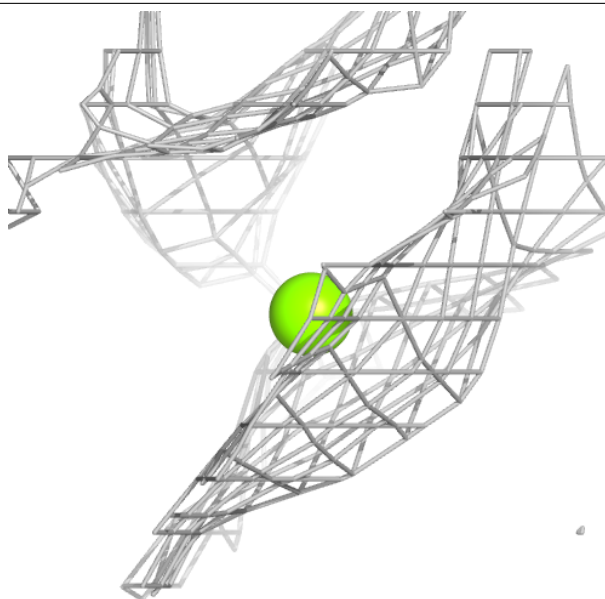
Electron density around MG C 504:

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



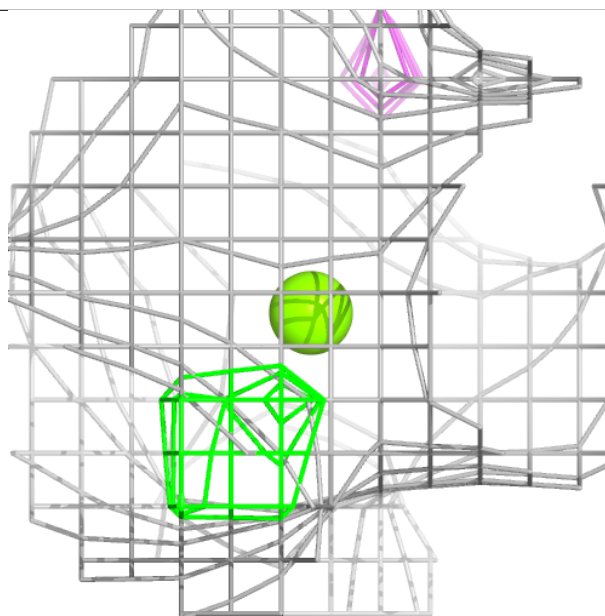
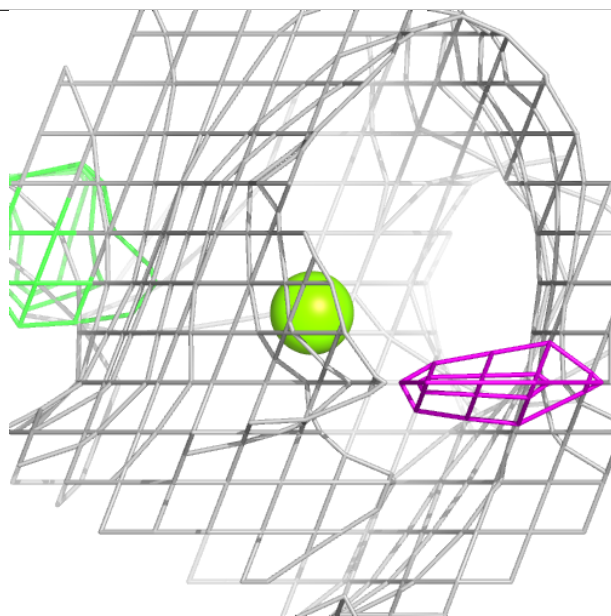
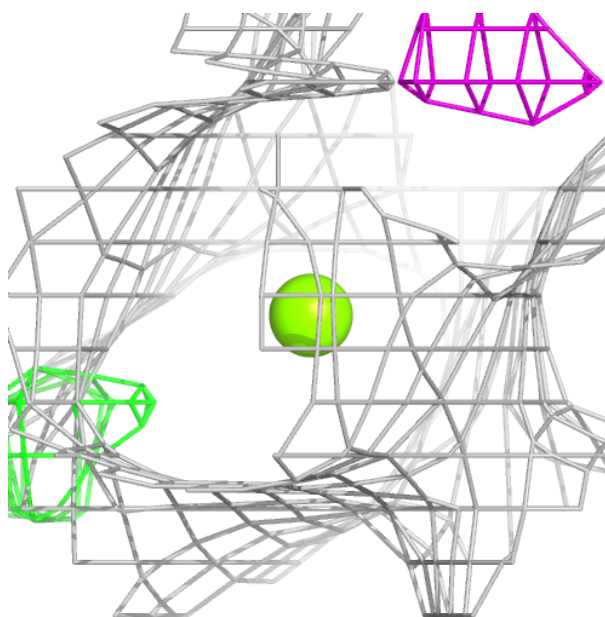
Electron density around MG D 504:

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



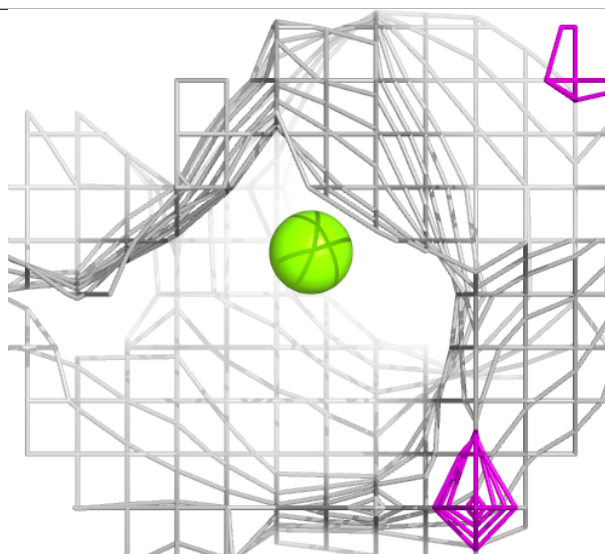
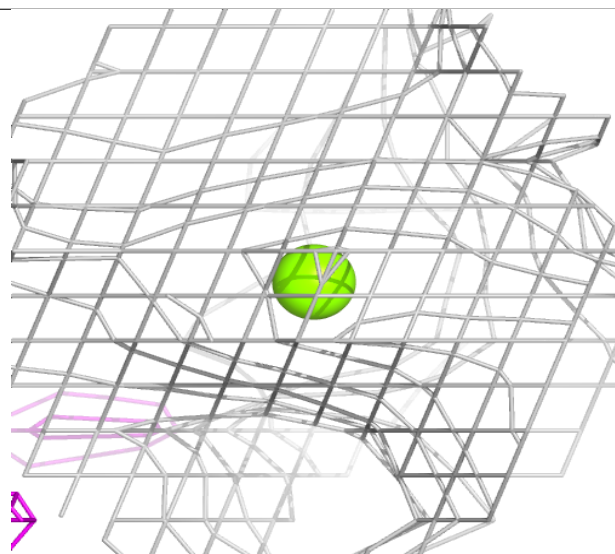
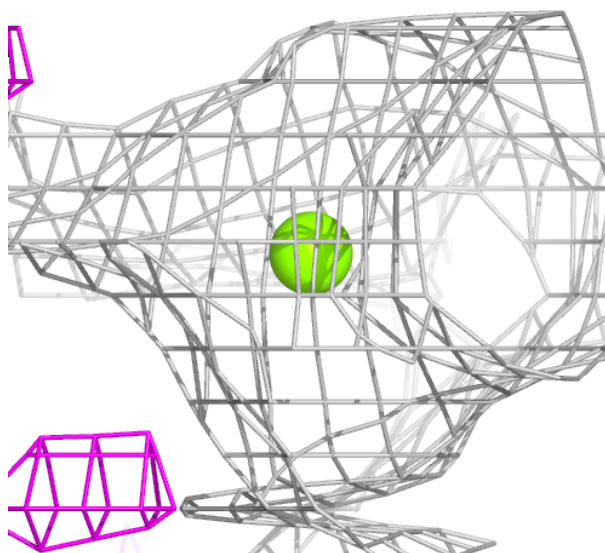
Electron density around MG E 503:

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



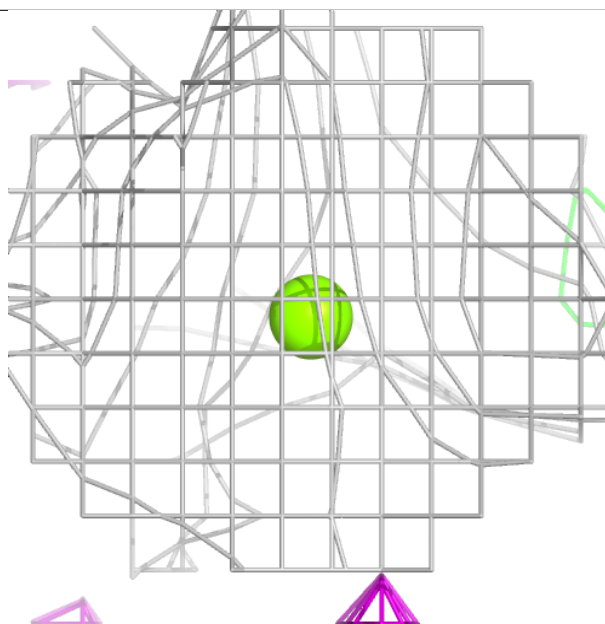
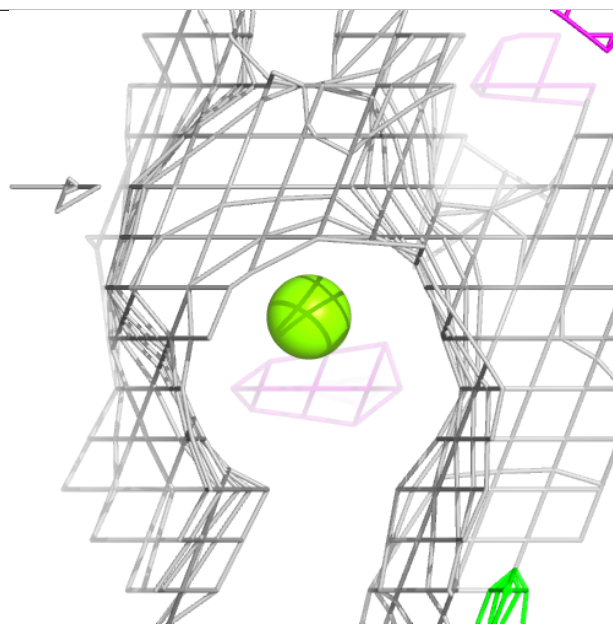
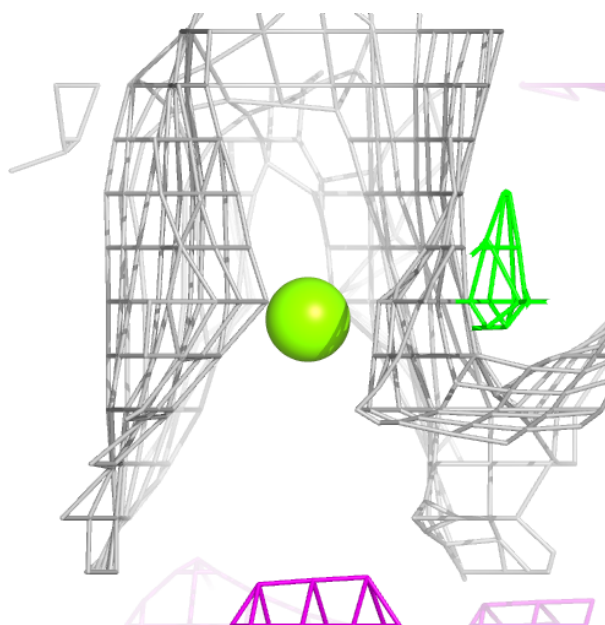
Electron density around MG E 504:

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



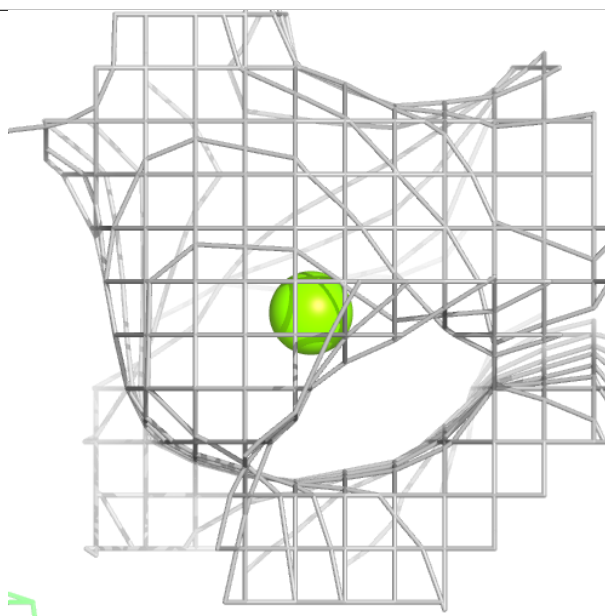
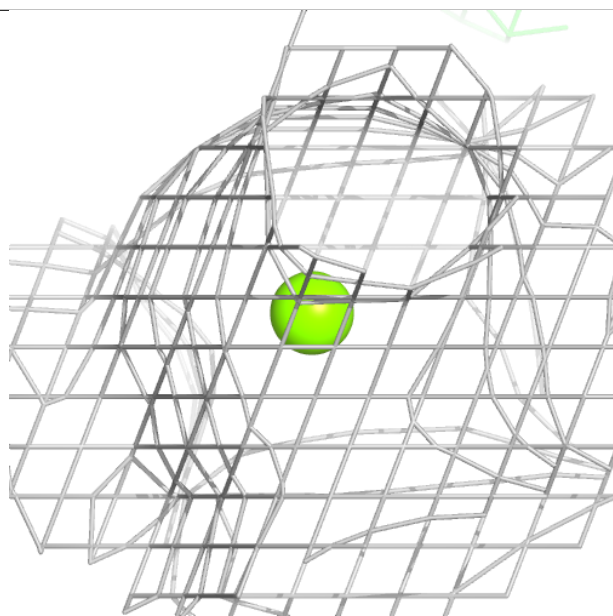
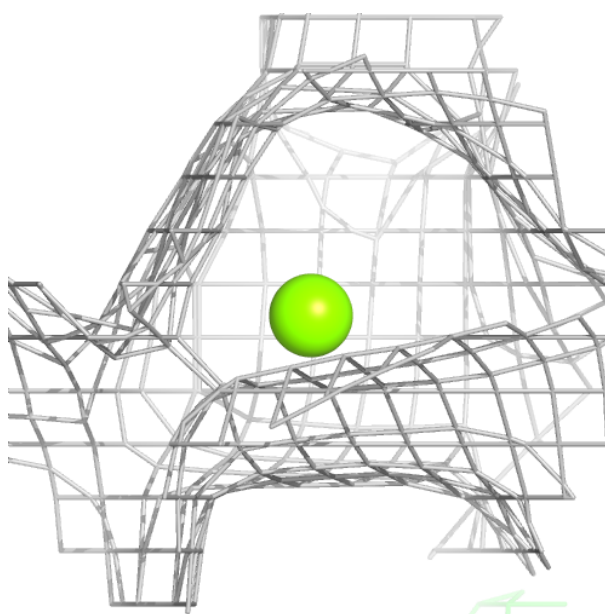
Electron density around MG F 504:

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



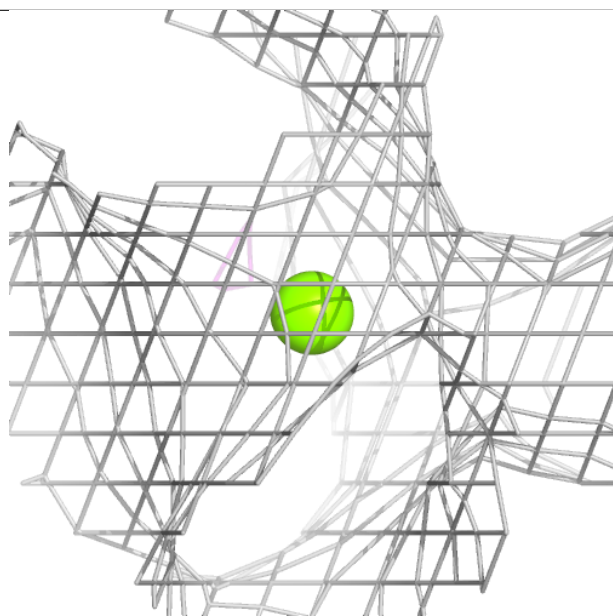
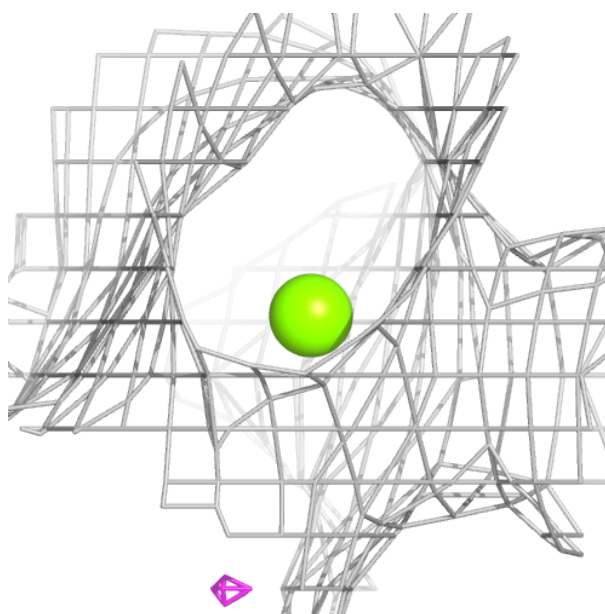
Electron density around MG D 502:

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



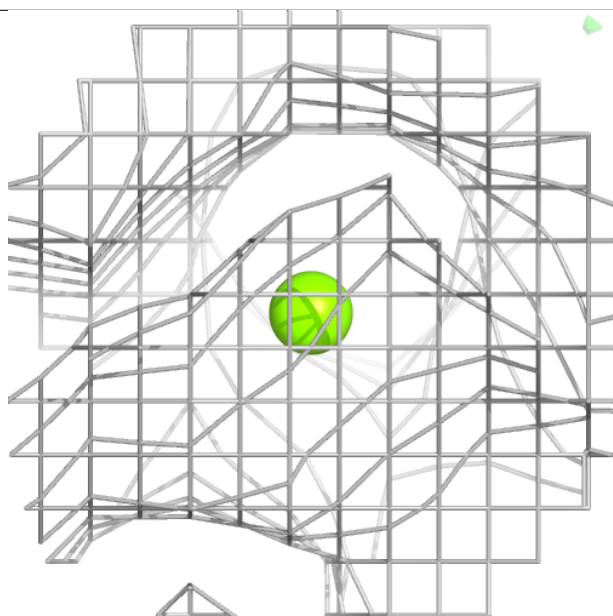
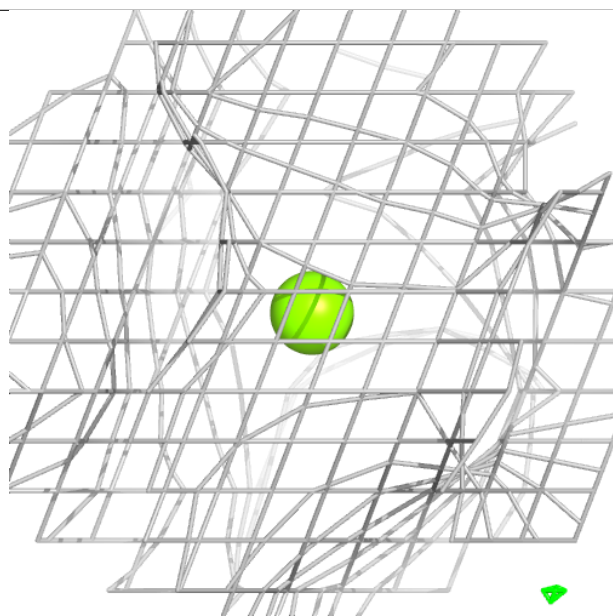
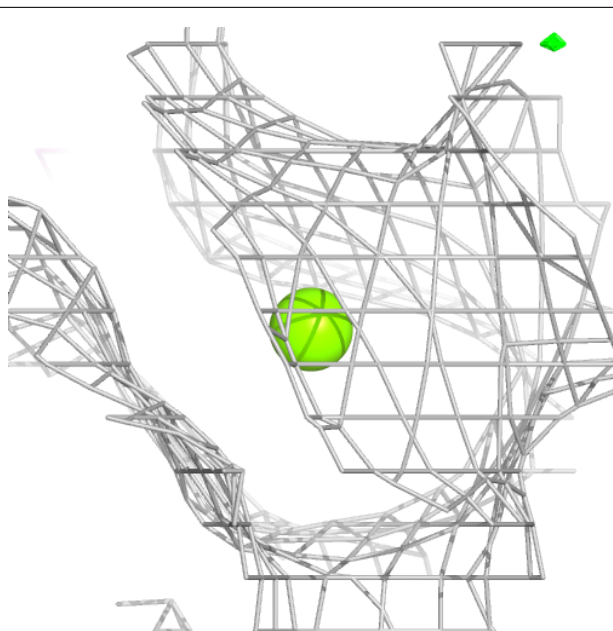
Electron density around MG D 503:

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



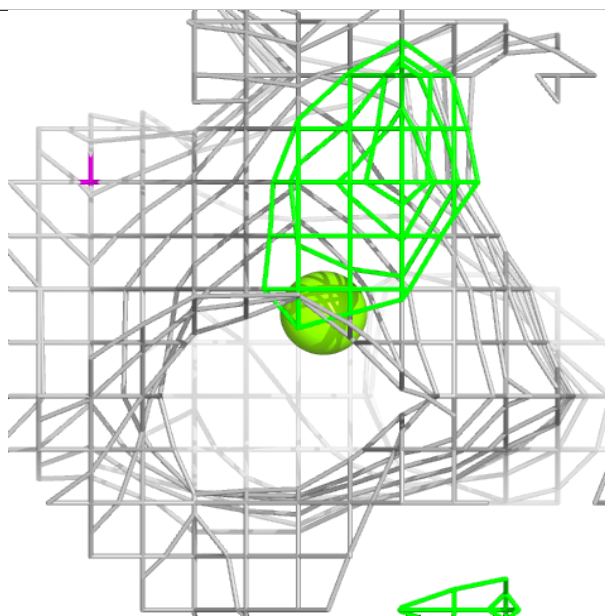
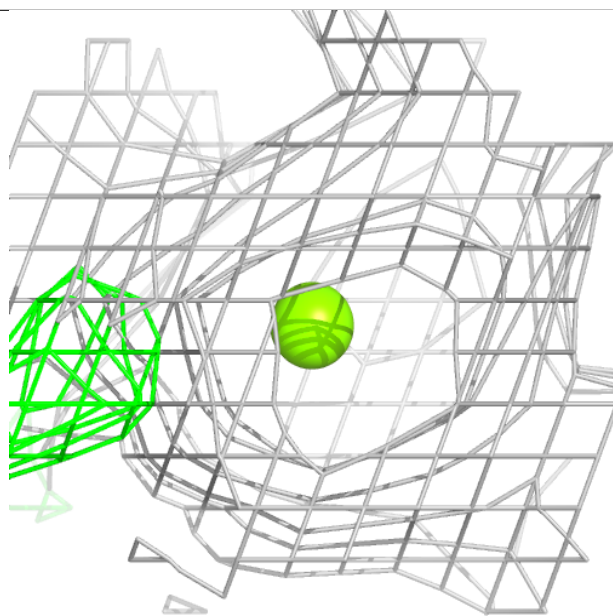
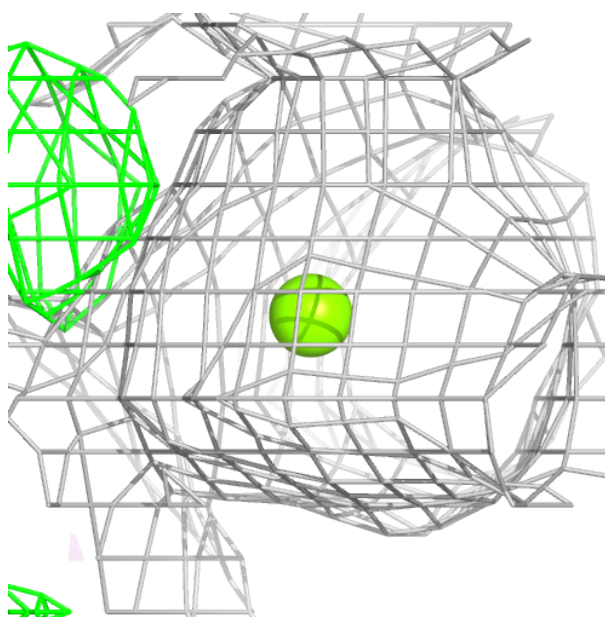
Electron density around MG A 502:

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



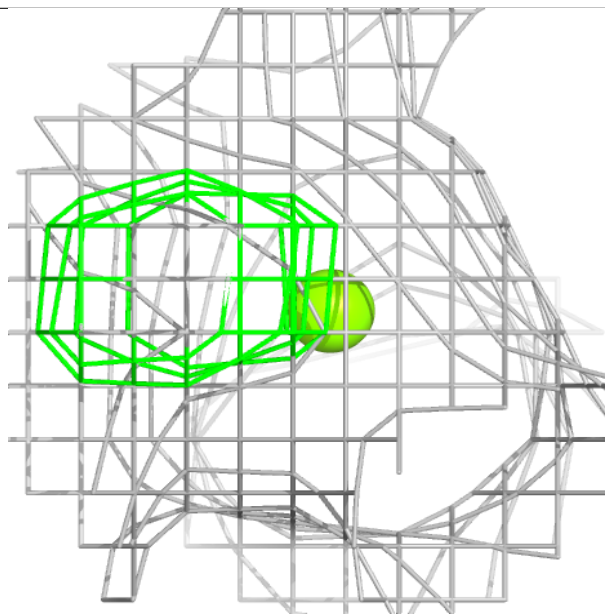
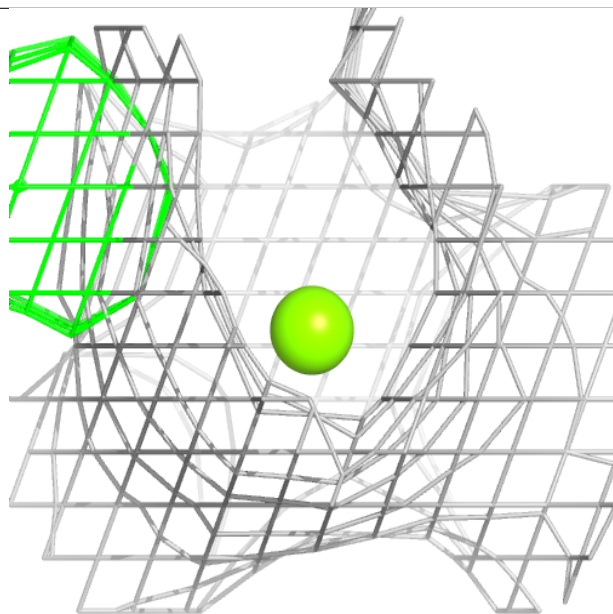
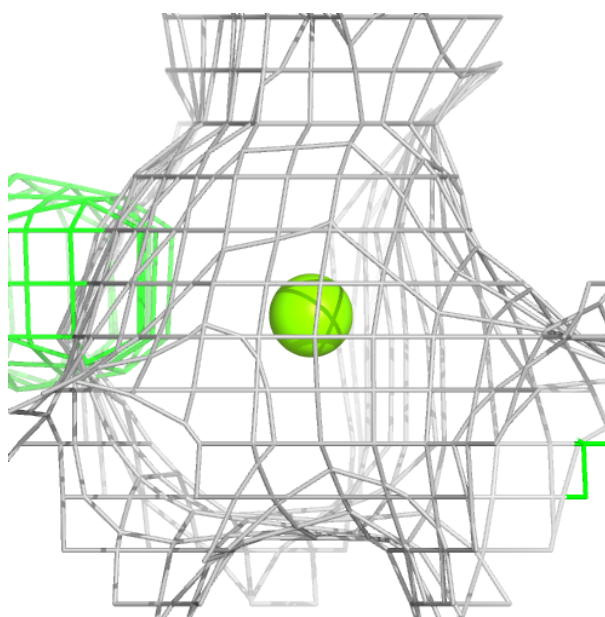
Electron density around MG E 502:

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



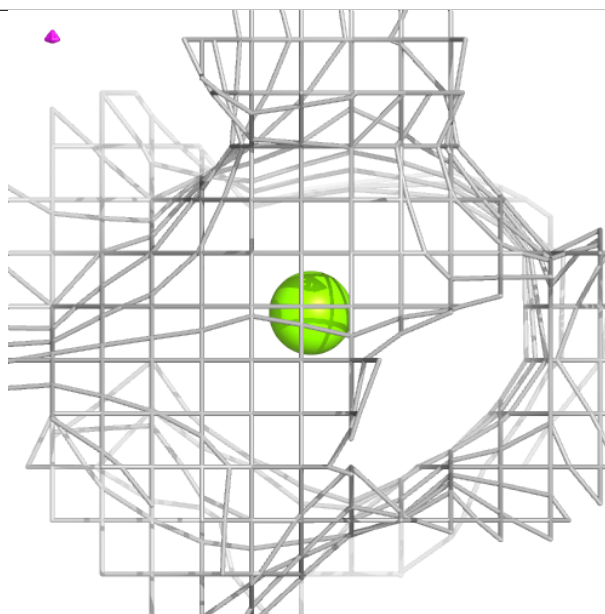
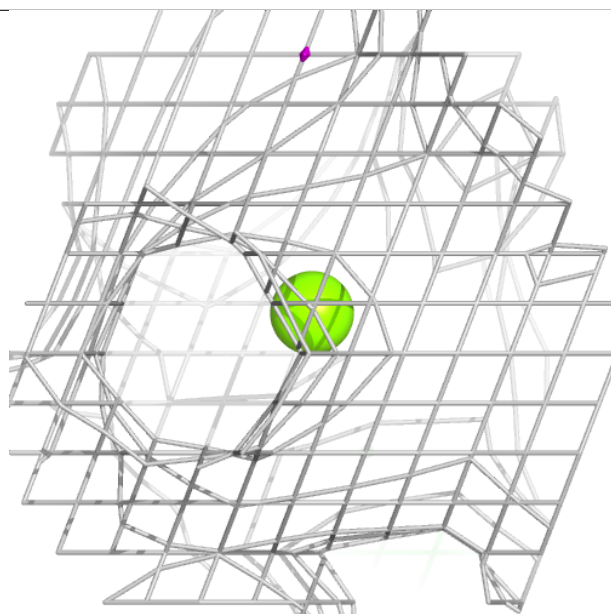
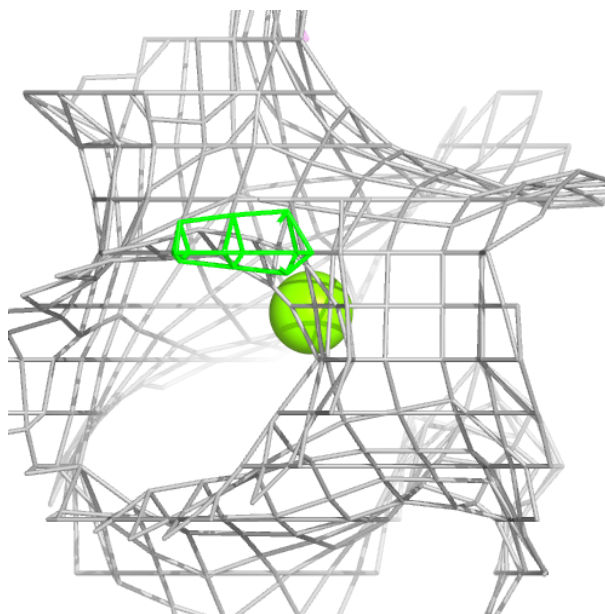
Electron density around MG C 502:

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



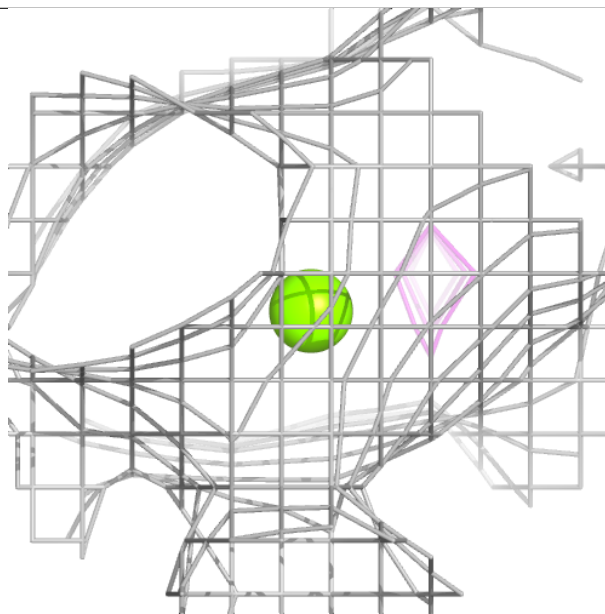
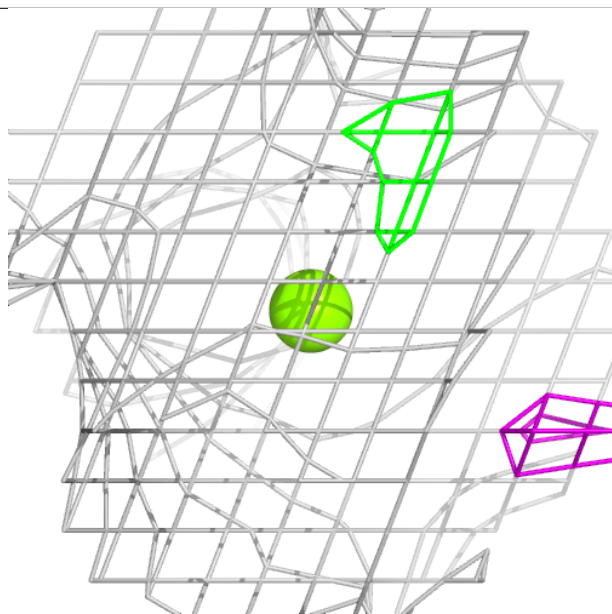
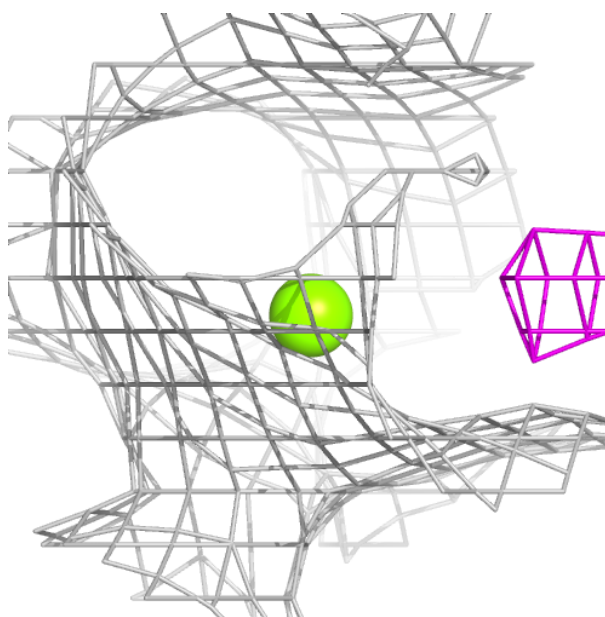
Electron density around MG C 503:

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



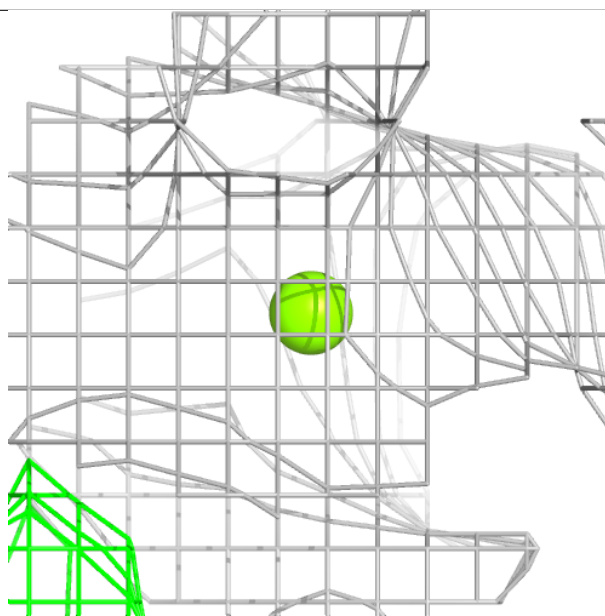
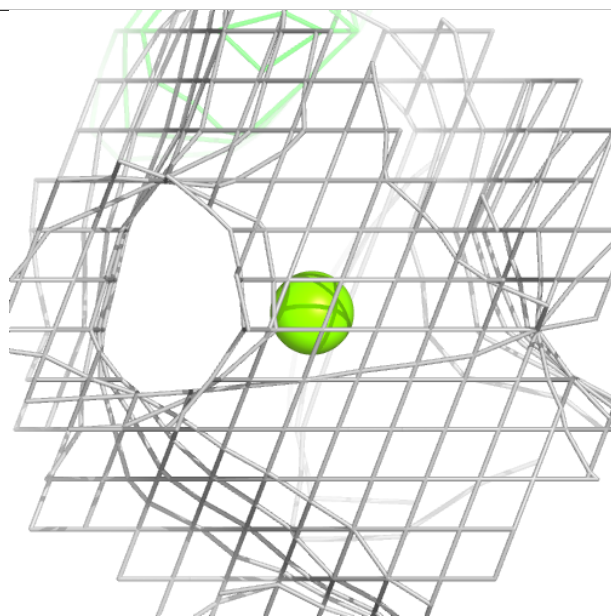
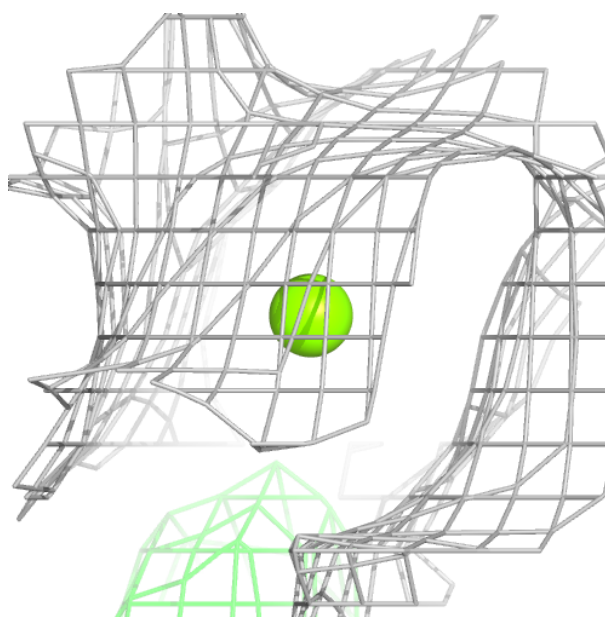
Electron density around MG F 503:

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



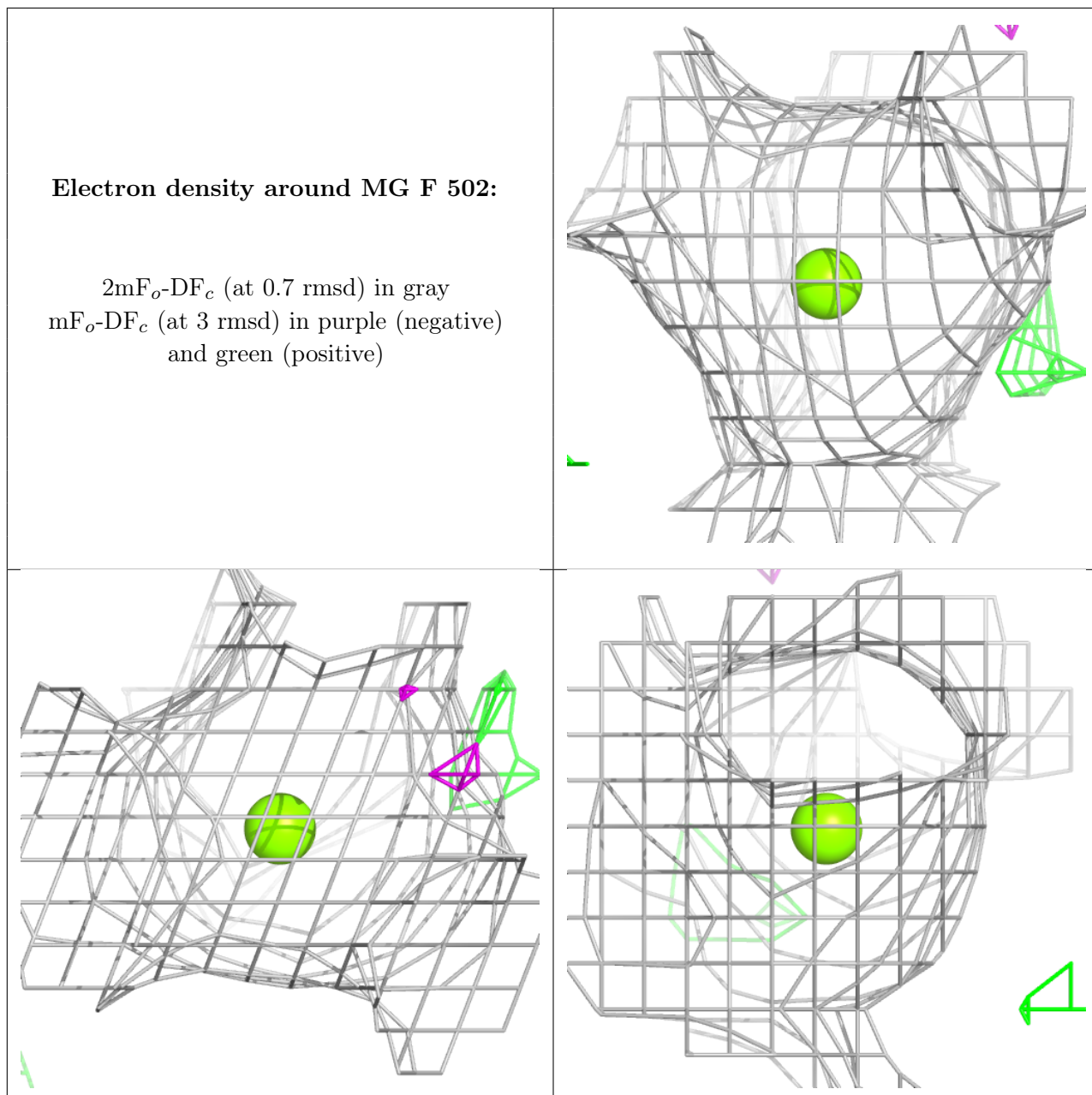
Electron density around MG B 503:

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



Electron density around MG F 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** ⓘ

There are no such residues in this entry.