



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:56 PM UTC

PDB ID : 9KUN / pdb_00009kun
Title : Crystal structure of ligand-free trypanosome alternative oxidase
Authors : Ebiloma, G.U.; Balogun, E.O.; Dardonville, C.; Shiba, T.; De Koning, H.P.
Deposited on : 2024-12-04
Resolution : 2.70 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

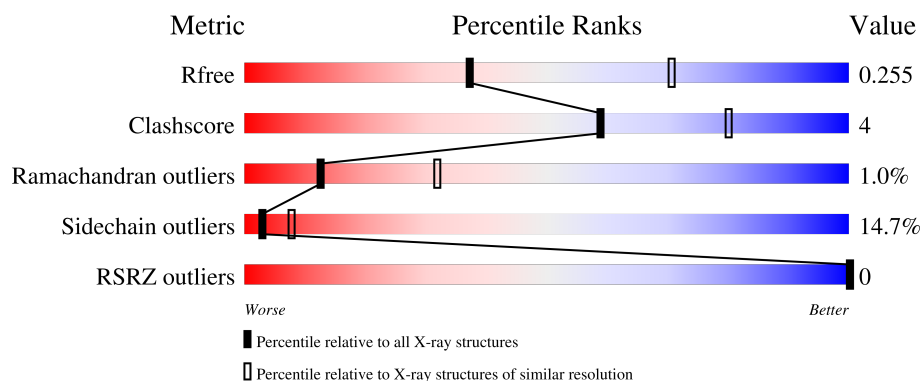
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	
1	B	271	
1	C	271	
1	D	271	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8788 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.

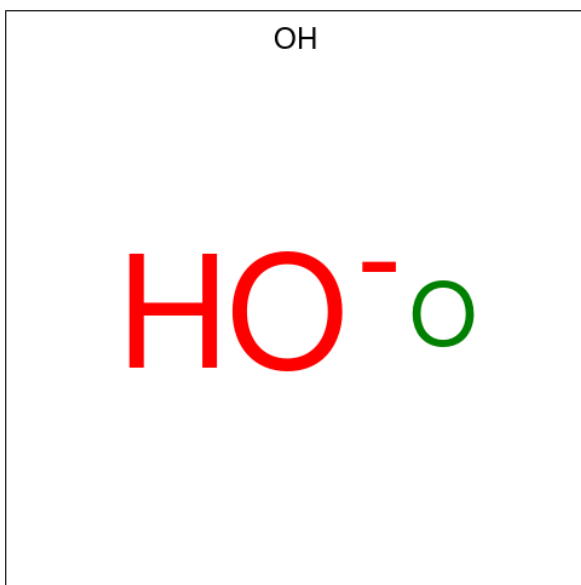
- Molecule 1 is a protein called Alternative oxidase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2146	1375	381	380	10			
1	B	268	Total	C	N	O	S	0	1	0
			2188	1401	391	386	10			
1	C	266	Total	C	N	O	S	0	0	0
			2160	1384	383	383	10			
1	D	270	Total	C	N	O	S	0	0	0
			2195	1405	389	391	10			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

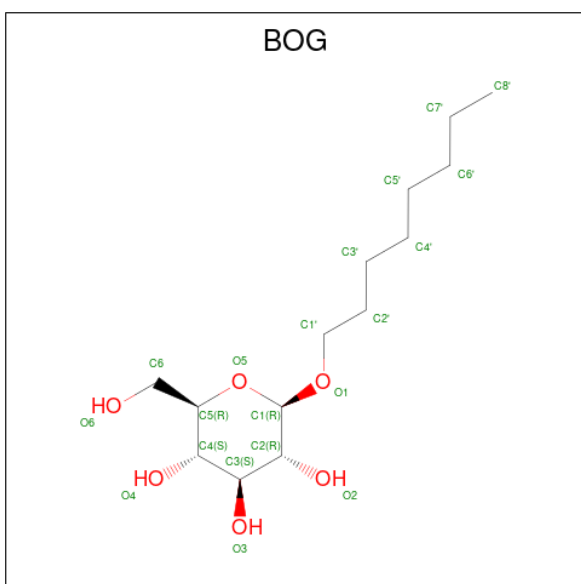
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

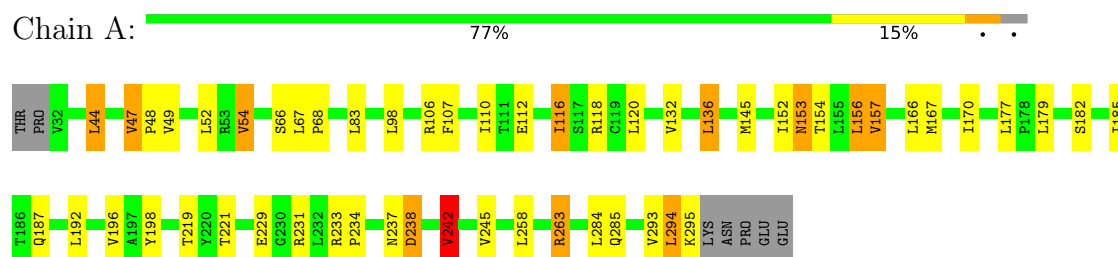
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	15	Total	O	0	0
			15	15		
5	C	11	Total	O	0	0
			11	11		
5	D	10	Total	O	0	0
			10	10		

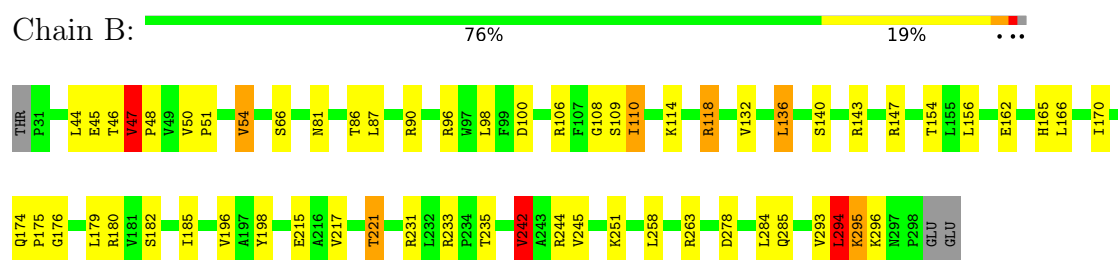
3 Residue-property plots

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

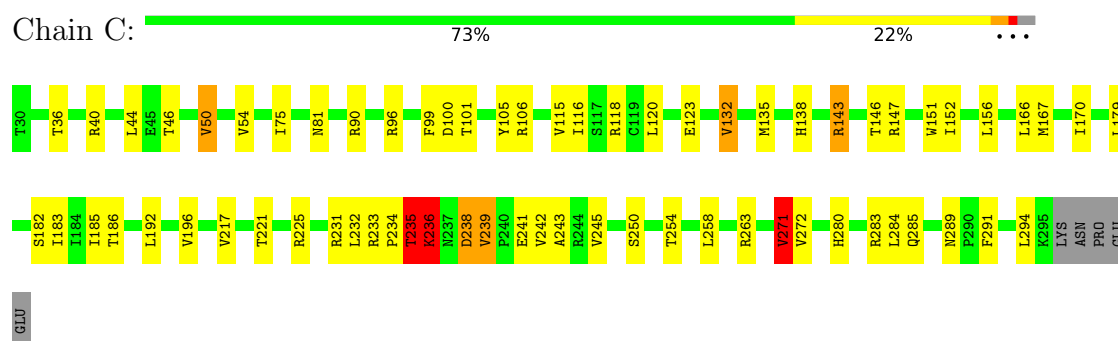
- Molecule 1: Alternative oxidase, mitochondrial



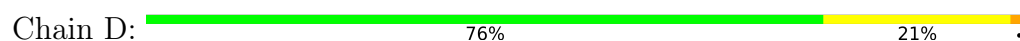
- Molecule 1: Alternative oxidase, mitochondrial

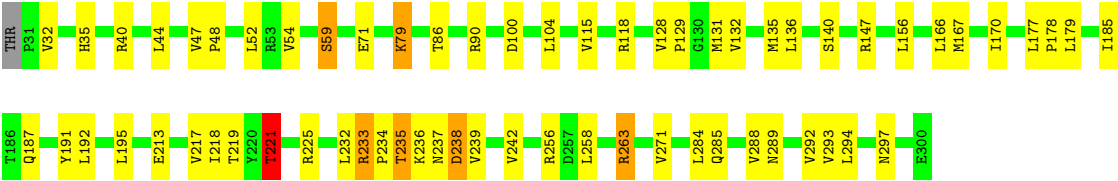


- Molecule 1: Alternative oxidase, mitochondrial



- Molecule 1: Alternative oxidase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.42Å 223.01Å 62.86Å 90.00° 115.28° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (20.00-2.70) 85.8 (20.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.204 , 0.258 0.205 , 0.255	Depositor DCC
R_{free} test set	2110 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.449 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8788	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, BOG, OH

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	0.98	1/2195 (0.0%)	1.13	3/2982 (0.1%)
1	B	0.99	2/2239 (0.1%)	1.17	3/3041 (0.1%)
1	C	0.92	1/2210 (0.0%)	1.12	9/3004 (0.3%)
1	D	0.88	1/2246 (0.0%)	1.06	2/3051 (0.1%)
All	All	0.94	5/8890 (0.1%)	1.12	17/12078 (0.1%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	LEU	CA-C	8.08	1.63	1.52
1	B	47	VAL	CA-CB	8.01	1.59	1.53
1	B	294	LEU	CA-C	7.73	1.63	1.52
1	C	238	ASP	CA-C	5.77	1.60	1.53
1	D	238	ASP	CA-C	5.12	1.59	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	VAL	N-CA-CB	10.91	117.37	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	ASP	CA-C-N	10.28	132.27	123.33
1	C	238	ASP	C-N-CA	10.28	132.27	123.33
1	C	271	VAL	CB-CA-C	-7.11	102.55	112.14
1	B	108	GLY	N-CA-C	-6.70	103.81	111.85
1	A	242	VAL	CB-CA-C	-6.31	103.81	111.88
1	A	242	VAL	N-CA-CB	6.28	117.47	110.51
1	C	132	VAL	N-CA-CB	5.85	118.06	110.57
1	B	242	VAL	CB-CA-C	-5.72	104.41	112.14
1	A	238	ASP	N-CA-C	-5.71	98.65	110.80
1	D	221	THR	N-CA-CB	5.52	118.42	110.20
1	C	96	ARG	N-CA-C	-5.47	104.19	111.24
1	C	183	ILE	N-CA-C	5.46	115.91	110.23
1	D	239	VAL	N-CA-CB	-5.42	104.41	109.99
1	C	239	VAL	N-CA-CB	-5.35	106.70	112.37
1	C	236	LYS	N-CA-C	-5.22	99.69	110.80
1	C	238	ASP	CB-CA-C	5.13	120.04	111.83

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	294	LEU	Peptide
1	C	233	ARG	Peptide
1	D	237	ASN	Peptide

5.2 Too-close contacts [i](#)

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	2146	0	2175	19	0
1	B	2188	0	2221	22	0
1	C	2160	0	2189	25	0
1	D	2195	0	2221	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0
5	A	11	0	0	0	0
5	B	15	0	0	0	0
5	C	11	0	0	1	0
5	D	10	0	0	1	0
All	All	8788	0	8862	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (78) 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:B:221:THR:HG22	1:B:263:ARG:HE	1.34	0.92
1:C:234:PRO:O	1:C:236:LYS:N	2.02	0.91
1:C:217:VAL:O	1:C:221:THR:HG22	1.80	0.80
1:C:167:MET:HE2	1:D:147:ARG:HD3	1.72	0.71
1:C:75:ILE:HD11	1:C:221:THR:HG21	1.74	0.69
1:D:217:VAL:O	1:D:221:THR:HG23	1.96	0.65
1:B:96:ARG:NH1	1:B:215:GLU:OE1	2.31	0.64
1:B:100:ASP:OD1	1:B:118:ARG:NH2	2.31	0.64
1:B:217:VAL:O	1:B:221:THR:HG23	1.98	0.63
1:C:50:VAL:HG23	1:D:293:VAL:HG21	1.83	0.61
1:B:54:VAL:HG22	1:B:242:VAL:HG13	1.81	0.61
1:A:234:PRO:HG2	1:A:237:ASN:HD21	1.66	0.60
1:D:288:VAL:HG12	5:D:604:HOH:O	2.04	0.58
1:C:235:THR:OG1	1:C:238:ASP:HB2	2.06	0.56
1:C:234:PRO:C	1:C:236:LYS:N	2.64	0.55
1:A:221:THR:HG22	1:A:263:ARG:HH21	1.73	0.54
1:C:234:PRO:C	1:C:236:LYS:H	2.17	0.53
1:C:75:ILE:HD11	1:C:221:THR:CG2	2.36	0.53
1:D:289:ASN:O	1:D:292:VAL:HG22	2.08	0.53
1:A:44:LEU:HG	1:B:278:ASP:HB3	1.92	0.52
1:D:221:THR:HG22	1:D:263:ARG:HE	1.74	0.52
1:D:233:ARG:O	1:D:235:THR:N	2.45	0.50
1:D:79:LYS:H	1:D:79:LYS:CE	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ARG:HA	1:C:285:GLN:HE22	1.77	0.49
1:A:229:GLU:OE1	1:A:231:ARG:NH2	2.46	0.49
1:B:221:THR:HG22	1:B:263:ARG:NE	2.16	0.49
1:C:138:HIS:CG	1:D:131:MET:HE3	2.49	0.47
1:D:221:THR:O	1:D:225:ARG:HG2	2.15	0.47
1:C:135:MET:HE2	1:D:135:MET:SD	2.54	0.47
1:A:145:MET:HE1	1:B:175:PRO:CG	2.44	0.47
1:B:176:GLY:O	1:B:180[B]:ARG:HG3	2.14	0.46
1:C:143:ARG:HB3	1:D:187:GLN:OE1	2.15	0.46
1:D:191:TYR:CE1	1:D:195:LEU:HD22	2.51	0.46
1:D:71:GLU:OE1	1:D:256:ARG:NH2	2.44	0.45
1:C:272:VAL:HA	1:C:291:PHE:CE2	2.51	0.45
1:B:136:LEU:HD23	1:B:198:TYR:CD1	2.52	0.45
1:B:293:VAL:O	1:B:295:LYS:N	2.50	0.45
1:B:54:VAL:HG22	1:B:242:VAL:CG1	2.46	0.44
1:A:67:LEU:N	1:A:68:PRO:HD2	2.33	0.44
1:A:187:GLN:NE2	1:B:143:ARG:HH11	2.16	0.44
1:A:221:THR:HG22	1:A:263:ARG:NH2	2.33	0.44
1:A:54:VAL:HG22	1:A:242:VAL:HG12	1.99	0.44
1:C:147:ARG:HD3	1:D:167:MET:HE2	2.00	0.44
1:A:152:ILE:HG22	1:A:156:LEU:HD22	2.00	0.44
1:C:147:ARG:CD	1:D:167:MET:HE2	2.48	0.44
1:C:243:ALA:HB1	1:C:258:LEU:HD11	2.00	0.44
1:B:86:THR:HG22	1:B:90:ARG:HD3	1.99	0.43
1:C:271:VAL:HG13	1:D:40:ARG:O	2.18	0.43
1:A:167:MET:HE2	1:B:147:ARG:HD3	2.00	0.43
1:D:79:LYS:H	1:D:79:LYS:HE3	1.83	0.43
1:D:86:THR:HG22	1:D:90:ARG:HD2	2.00	0.43
1:A:145:MET:HE1	1:B:175:PRO:HG2	2.01	0.43
1:D:79:LYS:N	1:D:79:LYS:HE2	2.34	0.43
1:C:151:TRP:O	1:C:152:ILE:C	2.61	0.42
1:A:136:LEU:HD23	1:A:198:TYR:HB3	2.01	0.42
1:A:293:VAL:O	1:A:295:LYS:N	2.52	0.42
1:D:47:VAL:N	1:D:48:PRO:CD	2.82	0.42
1:B:110:ILE:O	1:B:110:ILE:HG23	2.20	0.42
1:D:236:LYS:HA	1:D:238:ASP:OD1	2.19	0.42
1:A:293:VAL:HG21	1:B:51:PRO:HD2	2.02	0.42
1:C:101:THR:HG22	1:C:106:ARG:HG2	2.02	0.42
1:C:151:TRP:CD1	1:C:289:ASN:HB2	2.54	0.42
1:D:128:VAL:HB	1:D:129:PRO:HD3	2.02	0.42
1:D:177:LEU:N	1:D:178:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HD23	1:B:198:TYR:HD1	1.85	0.41
1:C:182:SER:O	1:C:186:THR:OG1	2.30	0.41
1:C:40:ARG:O	1:D:271:VAL:HG12	2.21	0.41
1:C:272:VAL:HA	1:C:291:PHE:CZ	2.55	0.41
1:B:47:VAL:N	1:B:48:PRO:CD	2.83	0.41
1:D:35:HIS:CD2	1:D:35:HIS:C	2.99	0.41
1:A:112:GLU:O	1:A:116:ILE:HD12	2.21	0.41
1:B:86:THR:HG23	5:C:603:HOH:O	2.20	0.41
1:B:162:GLU:O	1:B:165:HIS:HB2	2.21	0.41
1:A:47:VAL:N	1:A:48:PRO:CD	2.84	0.41
1:A:153:ASN:O	1:A:157:VAL:HG13	2.21	0.40
1:D:218:ILE:O	1:D:219:THR:C	2.62	0.40
1:A:54:VAL:HG22	1:A:242:VAL:CG1	2.52	0.40
1:C:280:HIS:HA	1:C:285:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/271 (97%)	249 (95%)	10 (4%)	3 (1%)	11	29
1	B	267/271 (98%)	248 (93%)	15 (6%)	4 (2%)	8	22
1	C	264/271 (97%)	244 (92%)	18 (7%)	2 (1%)	16	37
1	D	268/271 (99%)	255 (95%)	11 (4%)	2 (1%)	18	41
All	All	1061/1084 (98%)	996 (94%)	54 (5%)	11 (1%)	12	32

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	LEU

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Mol	Chain	Res	Type
1	B	110	ILE
1	B	294	LEU
1	C	235	THR
1	C	236	LYS
1	B	251	LYS
1	D	234	PRO
1	B	81	ASN
1	A	110	ILE
1	D	59	SER
1	A	238	ASP

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	239/246 (97%)	204 (85%)	35 (15%)	3	8
1	B	244/246 (99%)	207 (85%)	37 (15%)	3	7
1	C	241/246 (98%)	202 (84%)	39 (16%)	2	6
1	D	245/246 (100%)	214 (87%)	31 (13%)	4	11
All	All	969/984 (98%)	827 (85%)	142 (15%)	3	8

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	47	VAL
1	A	49	VAL
1	A	52	LEU
1	A	54	VAL
1	A	66	SER
1	A	83	LEU
1	A	98	LEU
1	A	106	ARG
1	A	107	PHE
1	A	116	ILE

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Mol	Chain	Res	Type
1	A	118	ARG
1	A	120	LEU
1	A	132	VAL
1	A	136	LEU
1	A	153	ASN
1	A	154	THR
1	A	156	LEU
1	A	157	VAL
1	A	166	LEU
1	A	170	ILE
1	A	177	LEU
1	A	179	LEU
1	A	182	SER
1	A	185	ILE
1	A	192	LEU
1	A	196	VAL
1	A	219	THR
1	A	233	ARG
1	A	242	VAL
1	A	245	VAL
1	A	258	LEU
1	A	263	ARG
1	A	284	LEU
1	A	285	GLN
1	B	44	LEU
1	B	45	GLU
1	B	46	THR
1	B	47	VAL
1	B	50	VAL
1	B	54	VAL
1	B	66	SER
1	B	87	LEU
1	B	98	LEU
1	B	106	ARG
1	B	109	SER
1	B	114	LYS
1	B	118	ARG
1	B	132	VAL
1	B	136	LEU
1	B	140	SER
1	B	154	THR
1	B	156	LEU

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Mol	Chain	Res	Type
1	B	166	LEU
1	B	170	ILE
1	B	174	GLN
1	B	179	LEU
1	B	182	SER
1	B	185	ILE
1	B	196	VAL
1	B	221	THR
1	B	231	ARG
1	B	233	ARG
1	B	235	THR
1	B	242	VAL
1	B	244	ARG
1	B	245	VAL
1	B	258	LEU
1	B	284	LEU
1	B	285	GLN
1	B	295	LYS
1	B	296	LYS
1	C	36	THR
1	C	44	LEU
1	C	46	THR
1	C	50	VAL
1	C	54	VAL
1	C	81	ASN
1	C	90	ARG
1	C	99	PHE
1	C	100	ASP
1	C	105	TYR
1	C	115	VAL
1	C	116	ILE
1	C	118	ARG
1	C	120	LEU
1	C	123	GLU
1	C	132	VAL
1	C	143	ARG
1	C	146	THR
1	C	156	LEU
1	C	166	LEU
1	C	170	ILE
1	C	179	LEU
1	C	185	ILE

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Mol	Chain	Res	Type
1	C	192	LEU
1	C	196	VAL
1	C	225	ARG
1	C	231	ARG
1	C	232	LEU
1	C	235	THR
1	C	239	VAL
1	C	241	GLU
1	C	242	VAL
1	C	245	VAL
1	C	250	SER
1	C	254	THR
1	C	263	ARG
1	C	271	VAL
1	C	284	LEU
1	C	294	LEU
1	D	32	VAL
1	D	44	LEU
1	D	52	LEU
1	D	54	VAL
1	D	59	SER
1	D	79	LYS
1	D	100	ASP
1	D	104	LEU
1	D	115	VAL
1	D	118	ARG
1	D	132	VAL
1	D	136	LEU
1	D	140	SER
1	D	156	LEU
1	D	166	LEU
1	D	170	ILE
1	D	179	LEU
1	D	185	ILE
1	D	192	LEU
1	D	213	GLU
1	D	221	THR
1	D	232	LEU
1	D	233	ARG
1	D	235	THR
1	D	242	VAL
1	D	258	LEU

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Mol	Chain	Res	Type
1	D	263	ARG
1	D	284	LEU
1	D	285	GLN
1	D	294	LEU
1	D	297	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	237	ASN
1	A	260	ASN
1	A	269	HIS
1	A	273	ASN
1	A	274	HIS
1	B	81	ASN
1	B	174	GLN
1	B	187	GLN
1	B	237	ASN
1	B	260	ASN
1	B	269	HIS
1	B	273	ASN
1	B	285	GLN
1	C	72	ASN
1	C	81	ASN
1	C	187	GLN
1	C	248	ASN
1	C	260	ASN
1	C	269	HIS
1	C	273	ASN
1	C	274	HIS
1	C	285	GLN
1	D	81	ASN
1	D	248	ASN
1	D	260	ASN
1	D	269	HIS
1	D	273	ASN
1	D	274	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 14 ligands modelled in this entry, 8 are monoatomic and 4 are modelled with single atom - leaving 2 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	BOG	B	504	-	20,20,20	0.95	1 (5%)	25,25,25	1.45	3 (12%)
4	BOG	A	504	-	20,20,20	1.04	1 (5%)	25,25,25	2.29	4 (16%)

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	BOG	B	504	-	-	6/11/31/31	0/1/1/1
4	BOG	A	504	-	-	9/11/31/31	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	BOG	O1-C1	3.18	1.45	1.40
4	A	504	BOG	O1-C1	2.91	1.45	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	BOG	O1-C1-C2	8.43	121.08	108.27
4	B	504	BOG	C1-O5-C5	4.38	122.28	113.72
4	A	504	BOG	O5-C1-C2	4.23	119.07	110.37
4	A	504	BOG	C4-C3-C2	3.86	117.61	110.83
4	A	504	BOG	O5-C1-O1	3.23	117.67	110.04
4	B	504	BOG	C1-C2-C3	2.47	115.20	110.01
4	B	504	BOG	O5-C1-C2	2.41	115.33	110.37

There are no chirality outliers.

All (15) torsion outliers are listed below:

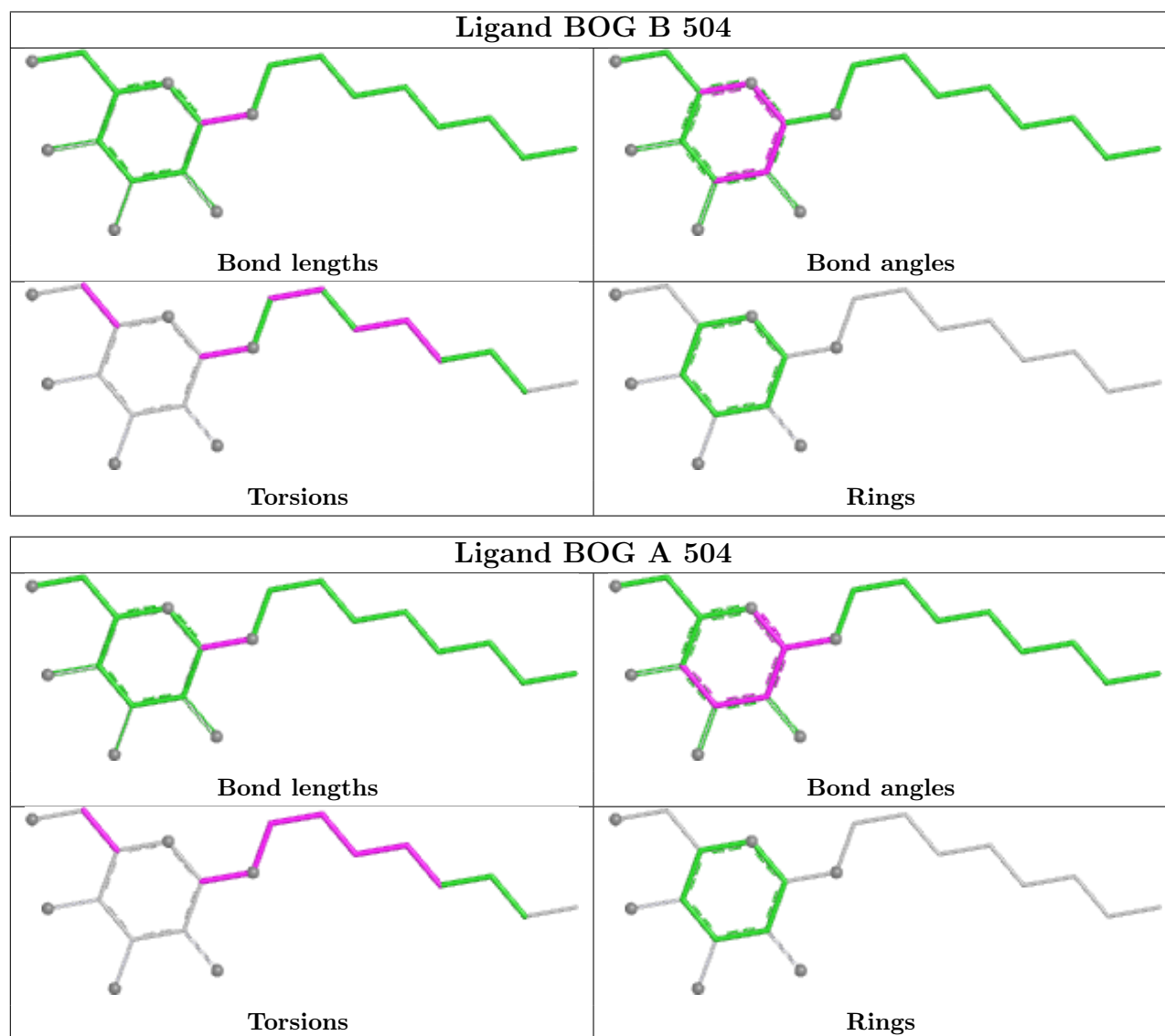
Mol	Chain	Res	Type	Atoms
4	A	504	BOG	O5-C1-O1-C1'
4	B	504	BOG	O5-C5-C6-O6
4	A	504	BOG	O5-C5-C6-O6
4	B	504	BOG	C4-C5-C6-O6
4	A	504	BOG	C4-C5-C6-O6
4	A	504	BOG	O1-C1'-C2'-C3'
4	B	504	BOG	O1-C1'-C2'-C3'
4	A	504	BOG	C2'-C3'-C4'-C5'
4	B	504	BOG	C3'-C4'-C5'-C6'
4	B	504	BOG	C2'-C3'-C4'-C5'
4	A	504	BOG	C2-C1-O1-C1'
4	B	504	BOG	O5-C1-O1-C1'
4	A	504	BOG	C2'-C1'-O1-C1
4	A	504	BOG	C3'-C4'-C5'-C6'
4	A	504	BOG	C1'-C2'-C3'-C4'

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	264/271 (97%)	-1.54	0 100 100	22, 37, 70, 106	0
1	B	268/271 (98%)	-1.55	0 100 100	18, 38, 80, 132	1 (0%)
1	C	266/271 (98%)	-1.47	0 100 100	29, 49, 102, 142	0
1	D	270/271 (99%)	-1.50	0 100 100	28, 49, 99, 144	0
All	All	1068/1084 (98%)	-1.51	0 100 100	18, 43, 89, 144	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

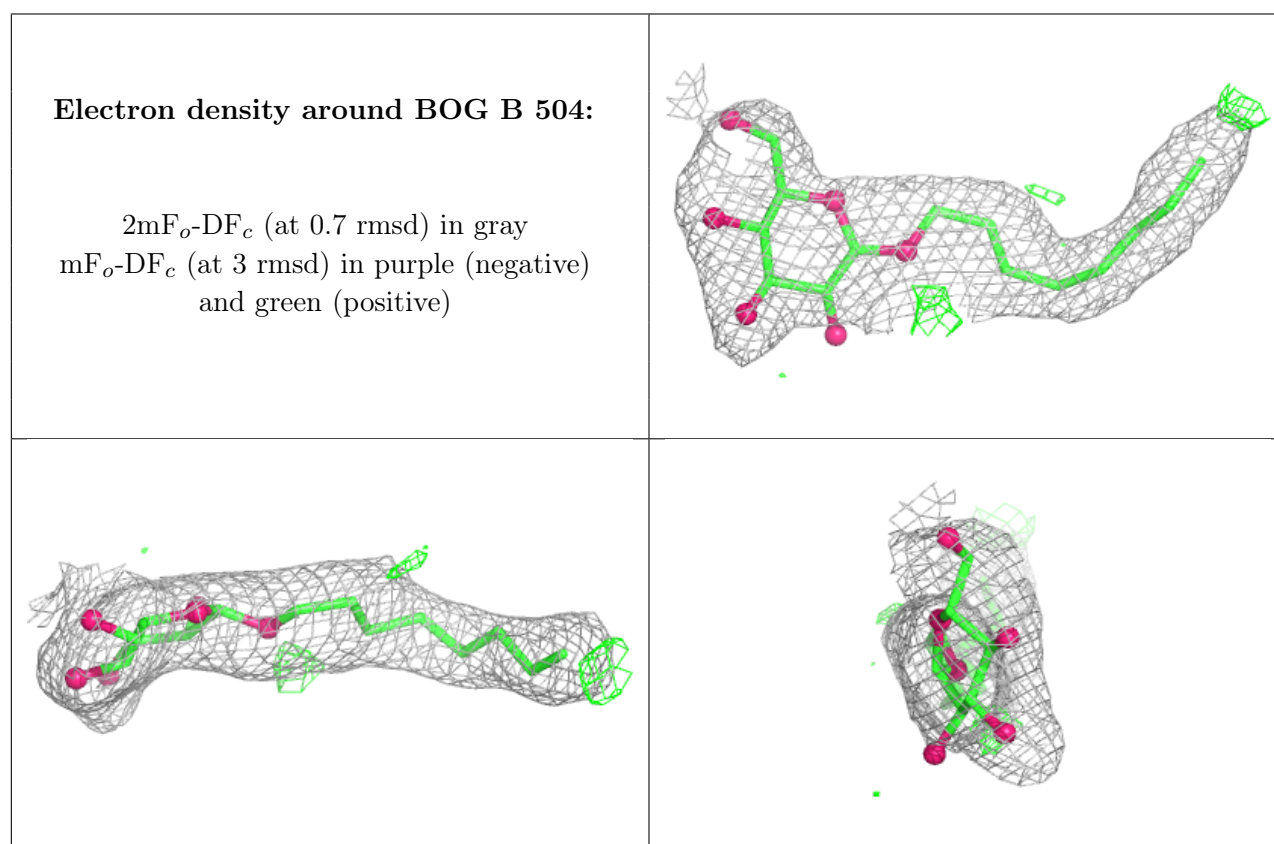
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BOG	B	504	20/20	0.98	0.04	38,61,77,81	0
3	OH	B	503	1/1	0.99	0.05	32,32,32,32	0
4	BOG	A	504	20/20	0.99	0.03	38,56,68,72	0
3	OH	A	503	1/1	0.99	0.03	17,17,17,17	0

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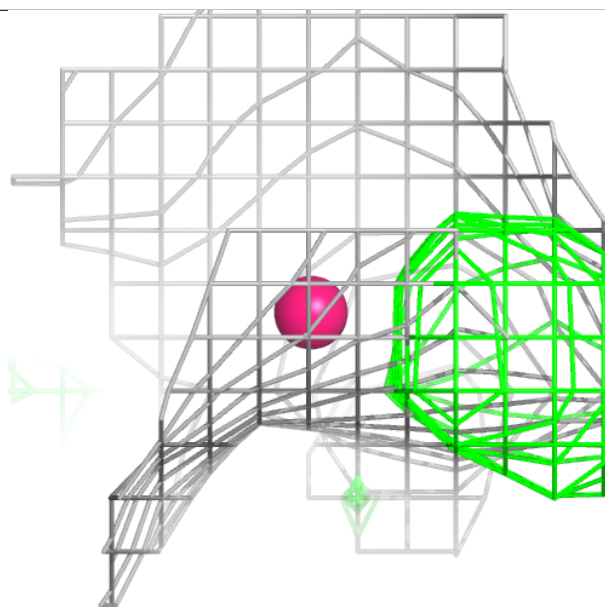
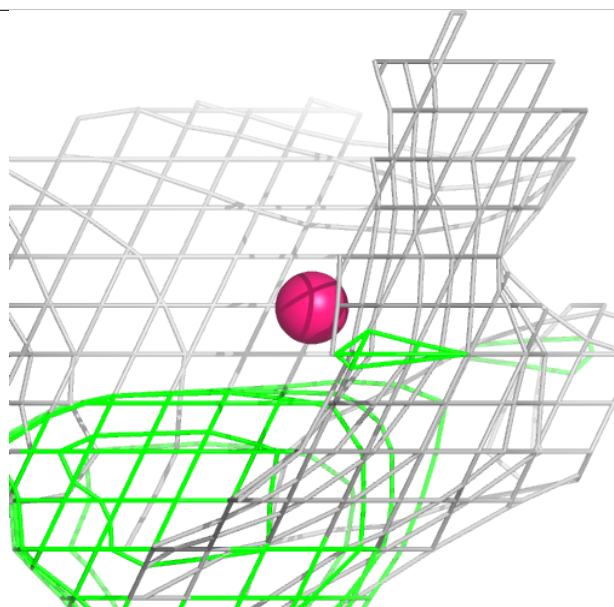
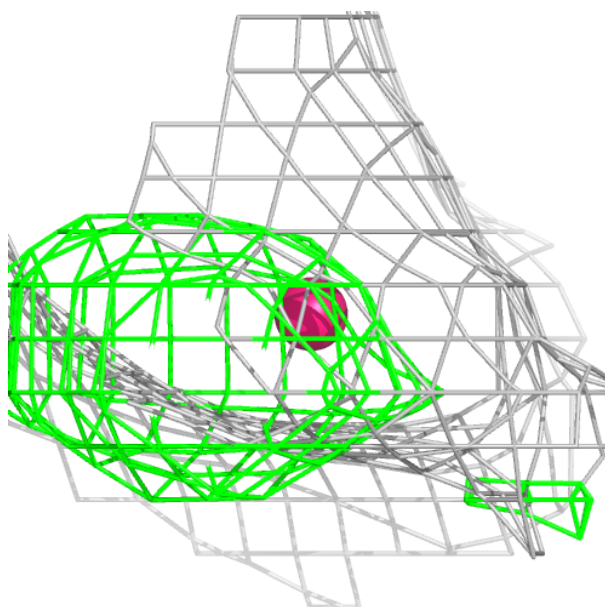
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	C	501	1/1	1.00	0.01	45,45,45,45	0
2	FE	C	502	1/1	1.00	0.01	39,39,39,39	0
2	FE	D	501	1/1	1.00	0.01	32,32,32,32	0
2	FE	D	502	1/1	1.00	0.01	41,41,41,41	0
2	FE	A	501	1/1	1.00	0.02	34,34,34,34	0
2	FE	A	502	1/1	1.00	0.01	34,34,34,34	0
3	OH	C	503	1/1	1.00	0.03	18,18,18,18	0
3	OH	D	503	1/1	1.00	0.05	33,33,33,33	0
2	FE	B	501	1/1	1.00	0.01	42,42,42,42	0
2	FE	B	502	1/1	1.00	0.01	34,34,34,34	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.



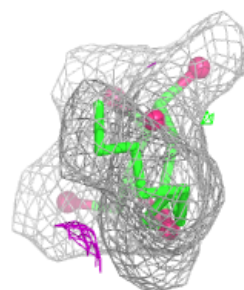
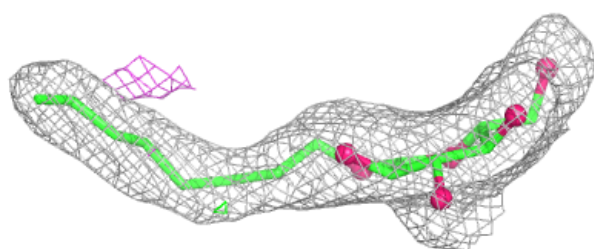
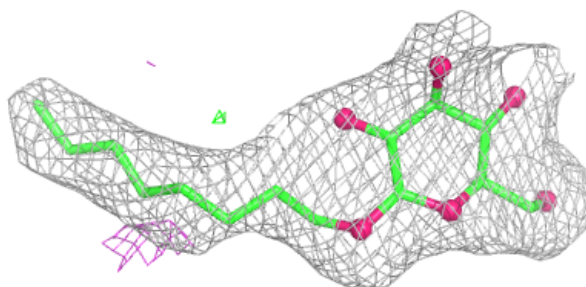
Electron density around OH B 503:

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



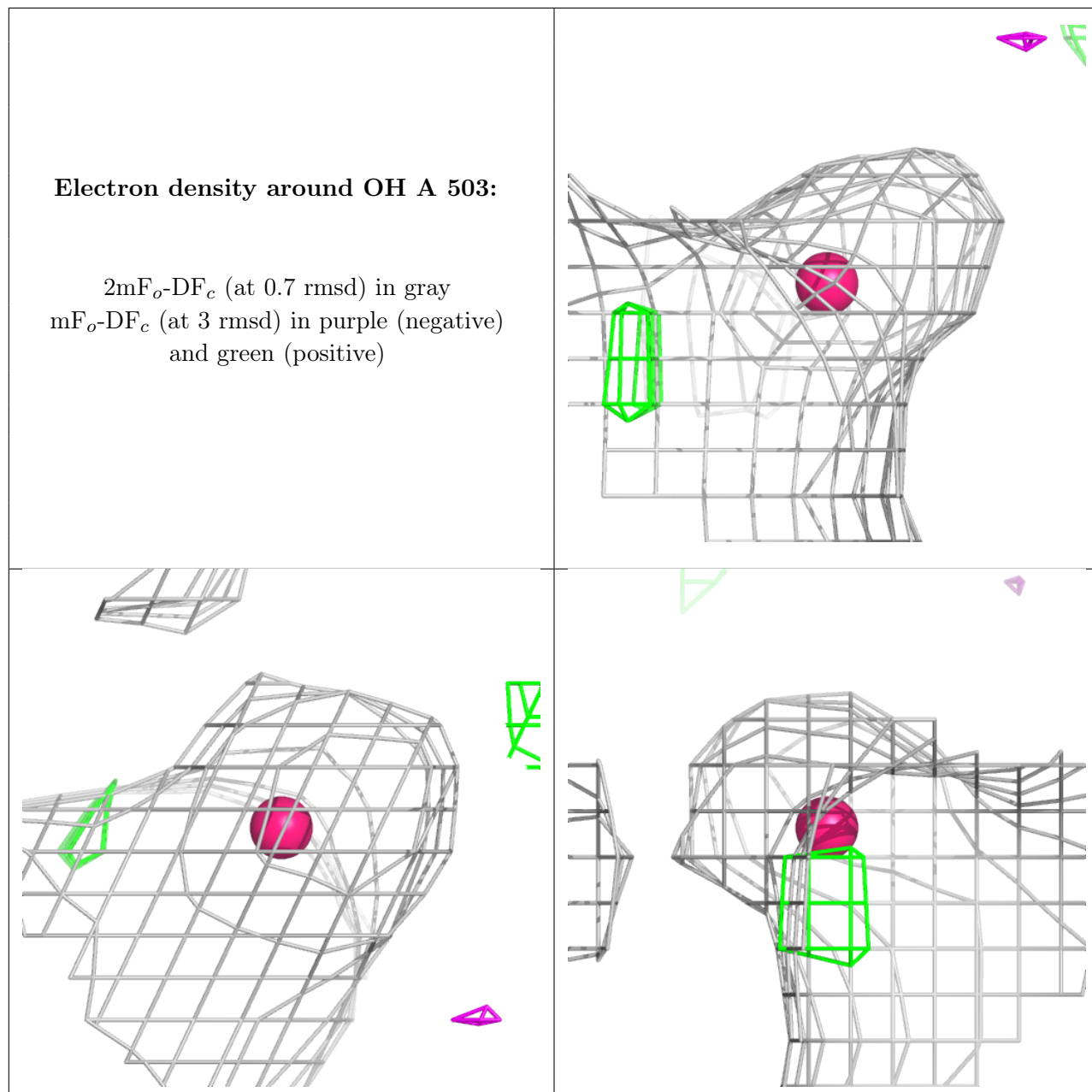
Electron density around BOG A 504:

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



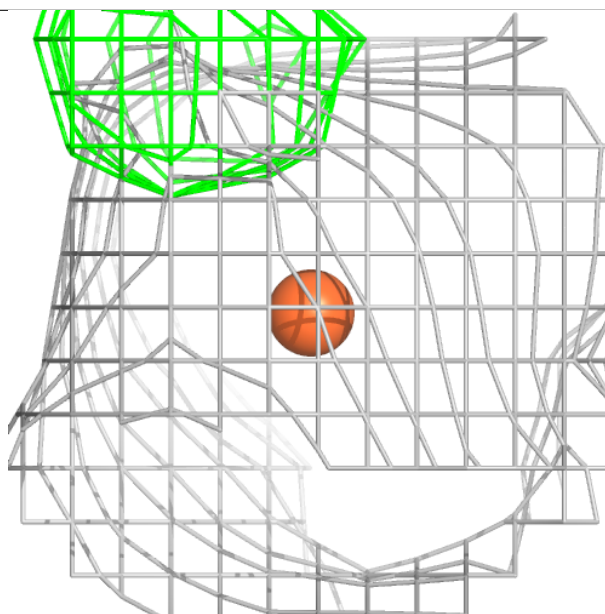
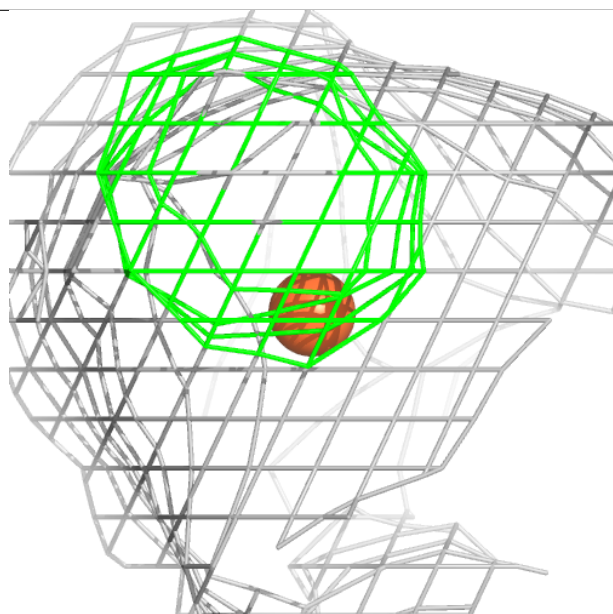
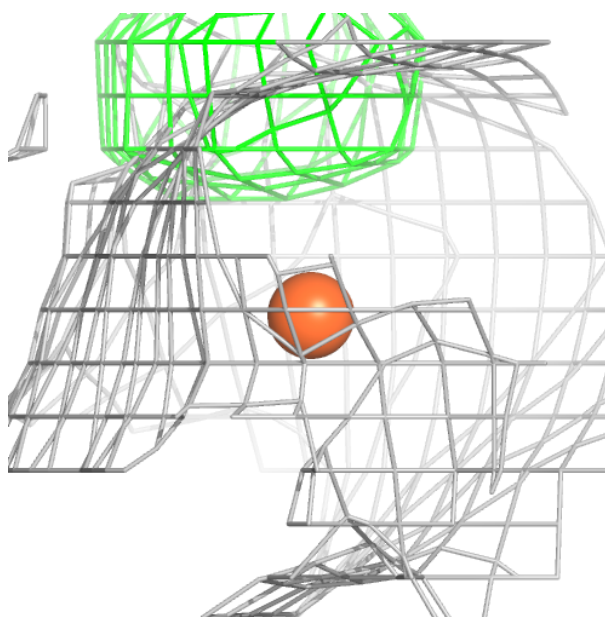
Electron density around OH A 503:

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



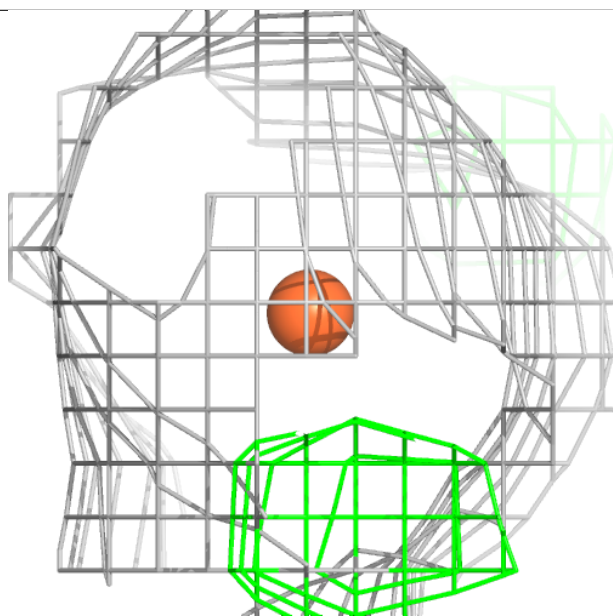
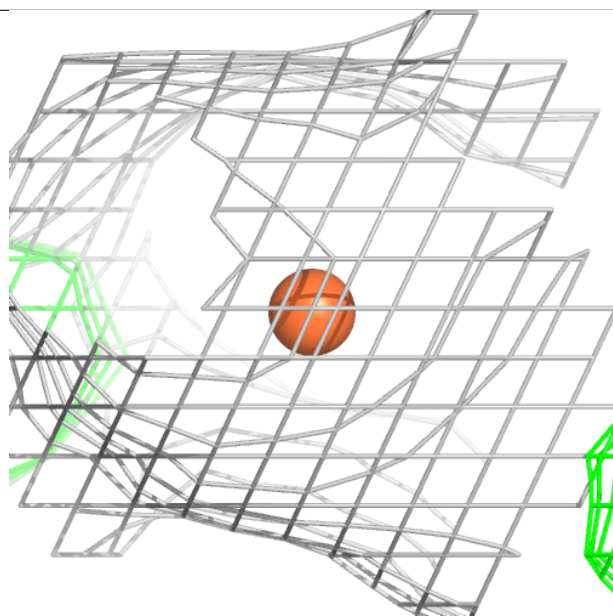
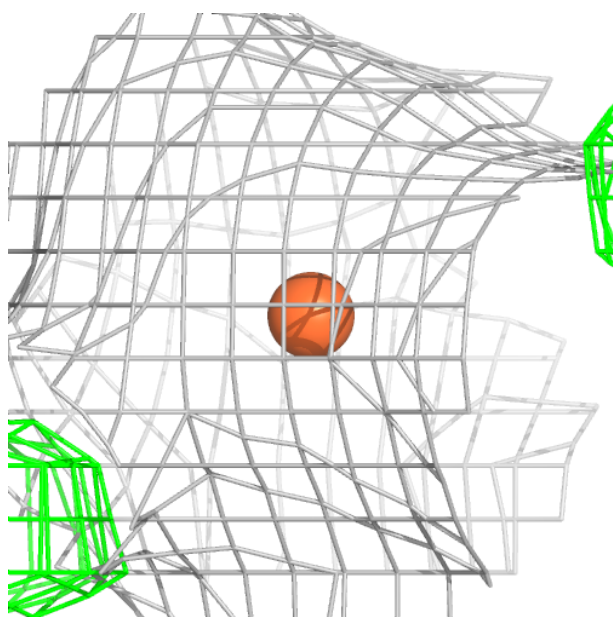
Electron density around FE C 501:

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



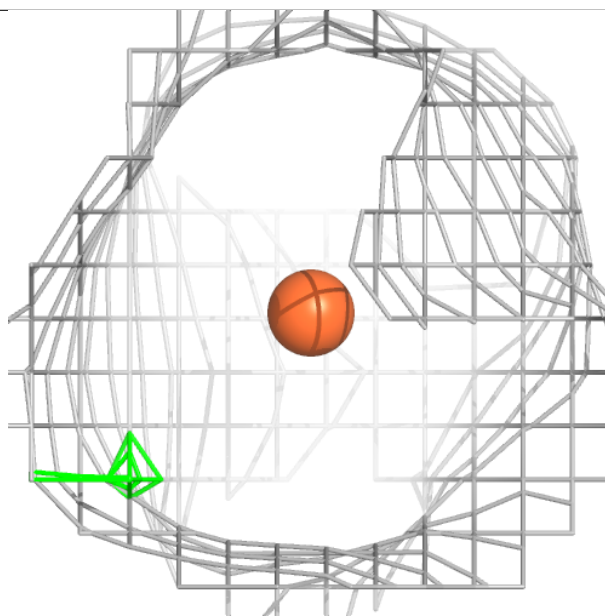
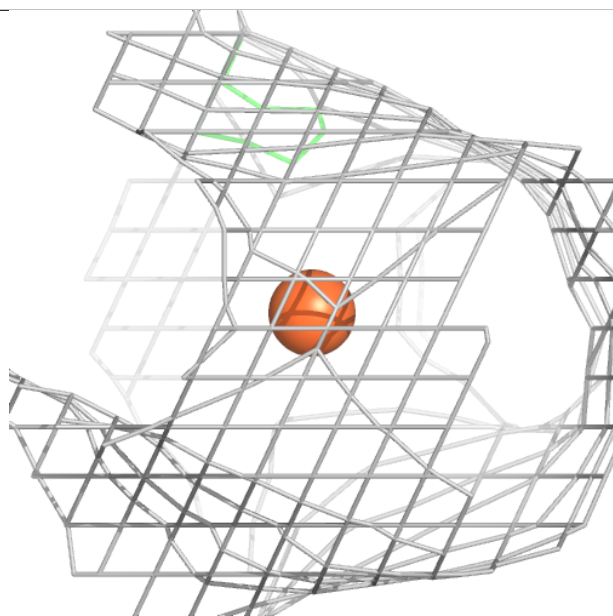
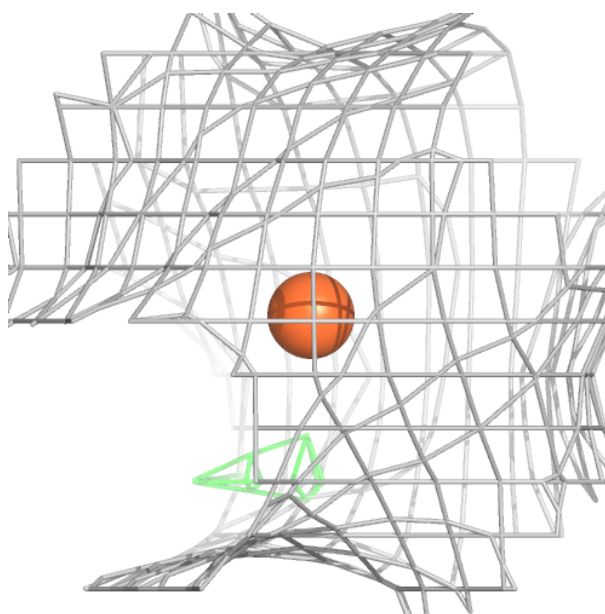
Electron density around FE C 502:

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



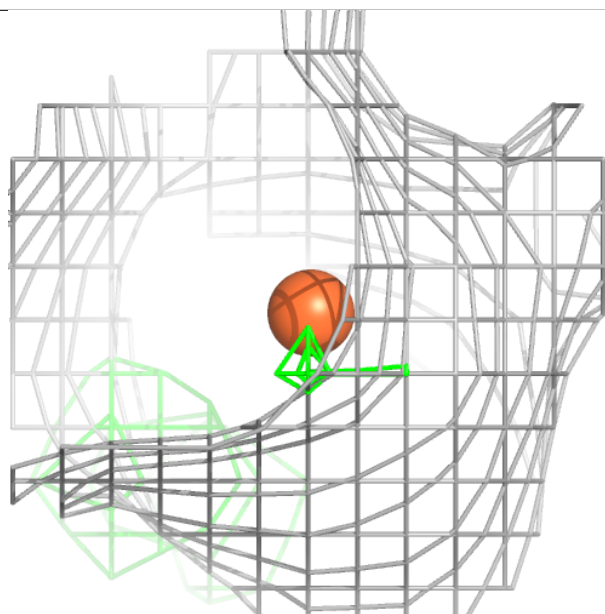
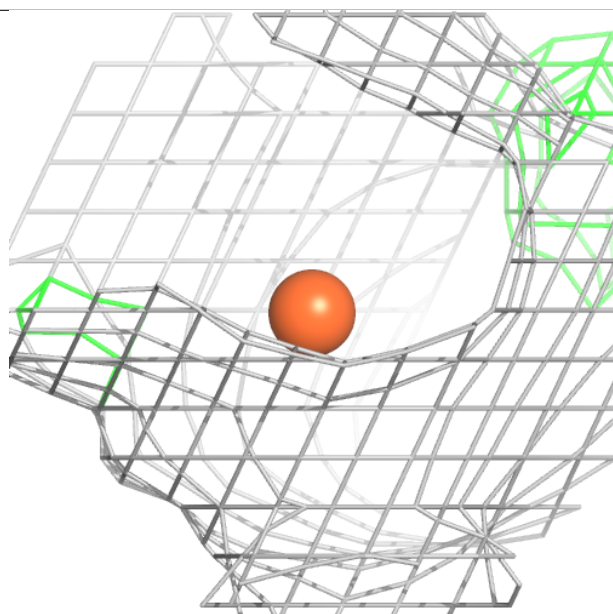
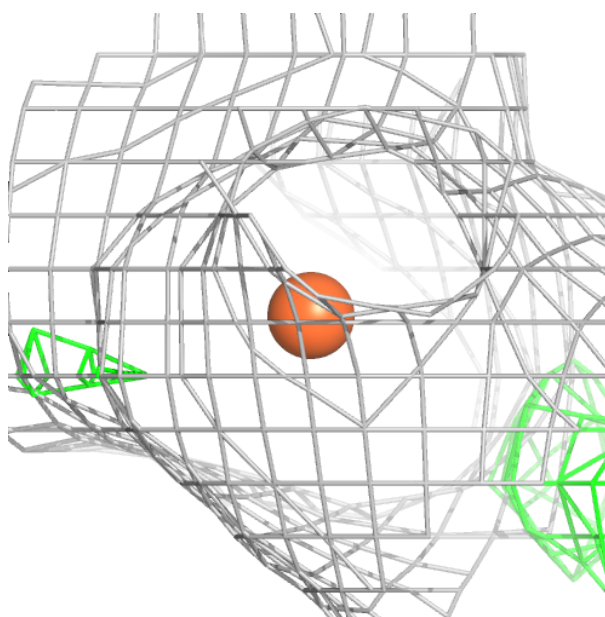
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and green (positive)



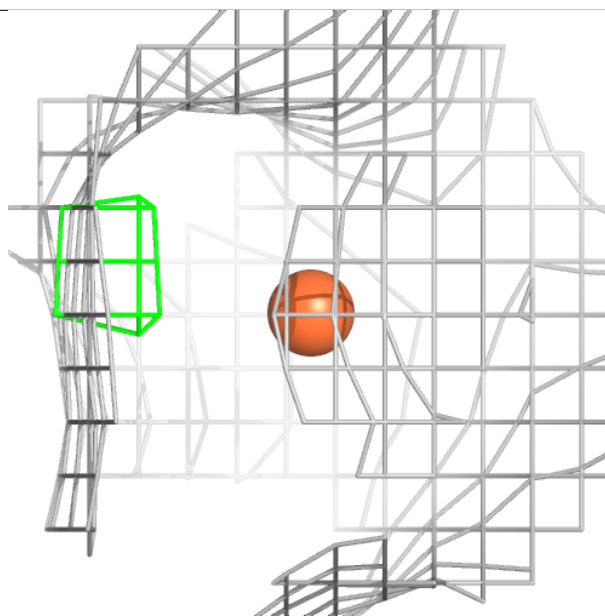
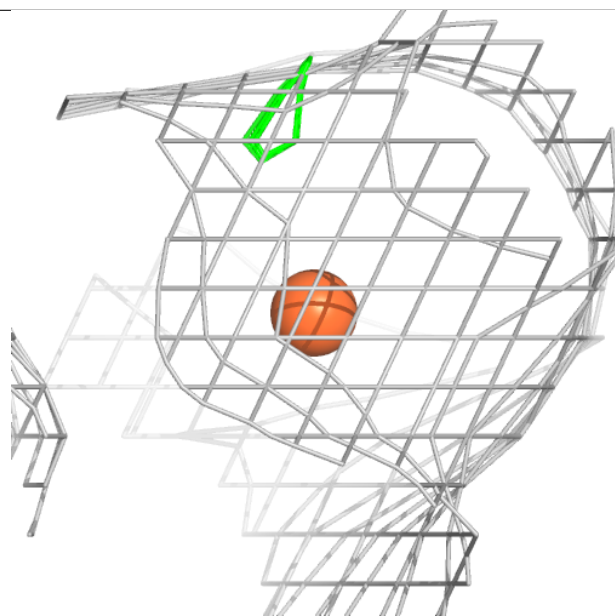
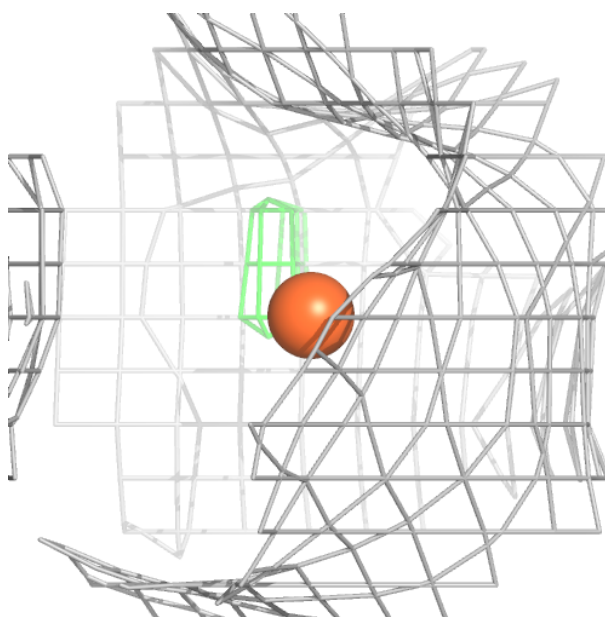
Electron density around FE D 502:

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and green (positive)



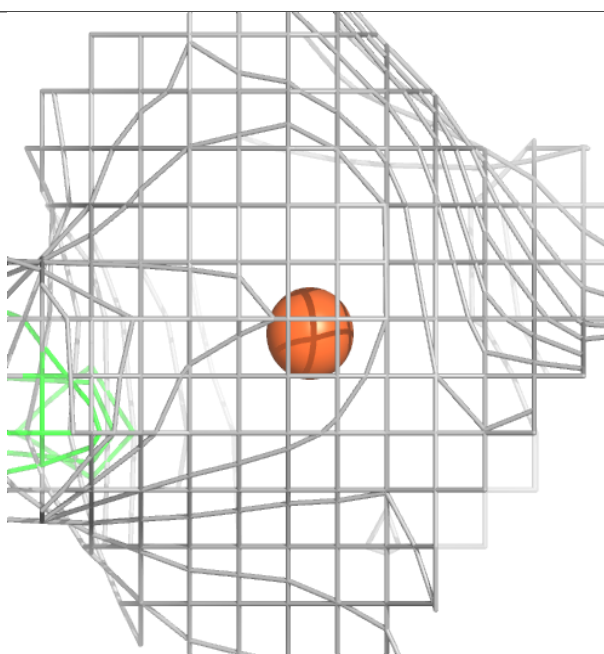
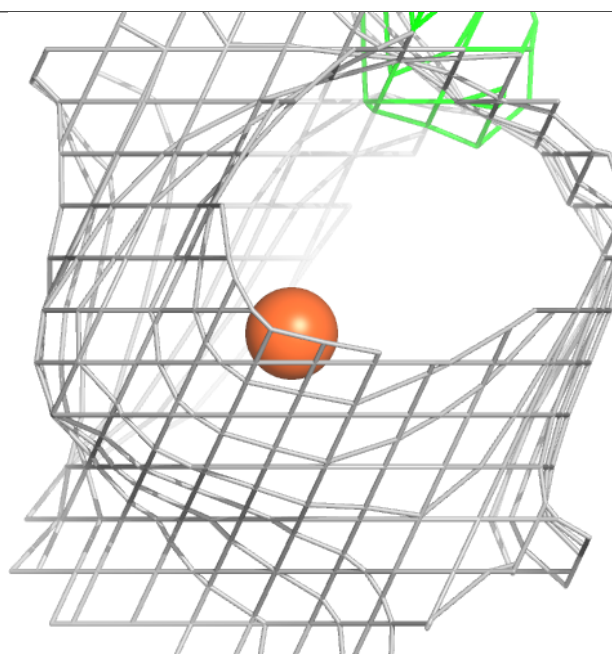
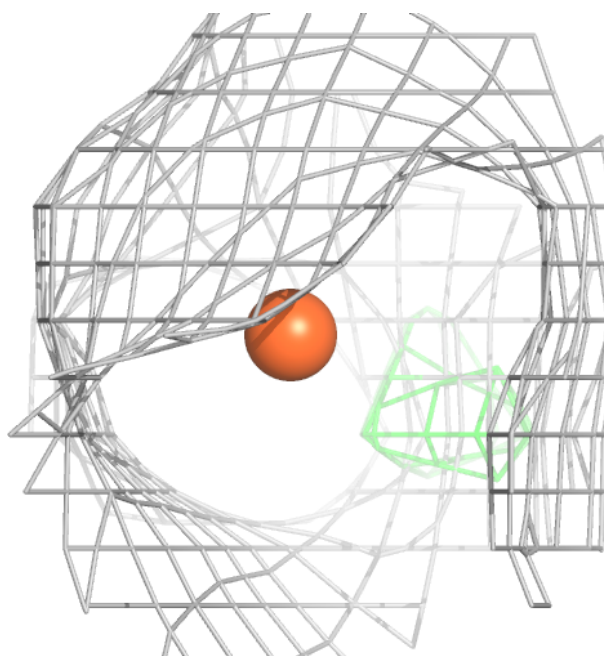
Electron density around FE A 501:

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and green (positive)



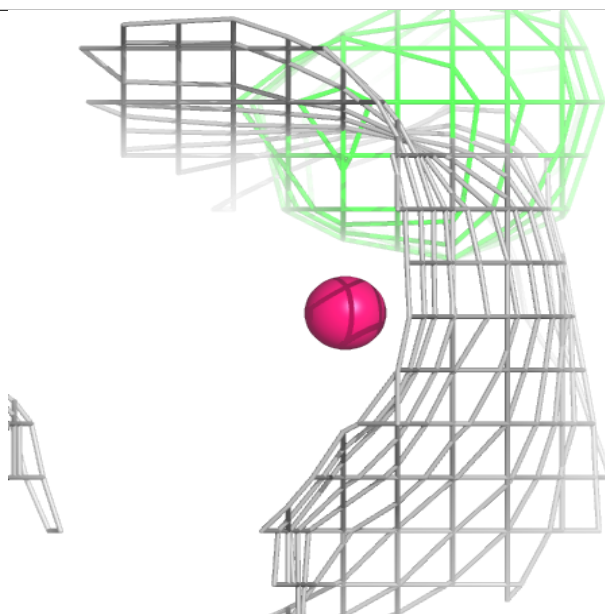
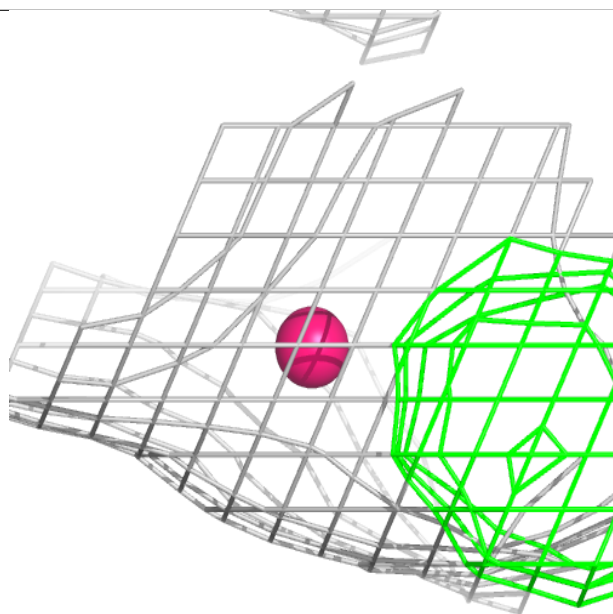
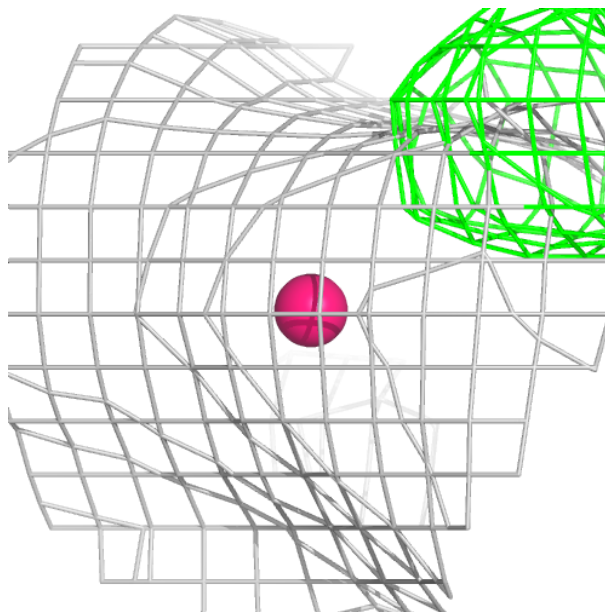
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and green (positive)



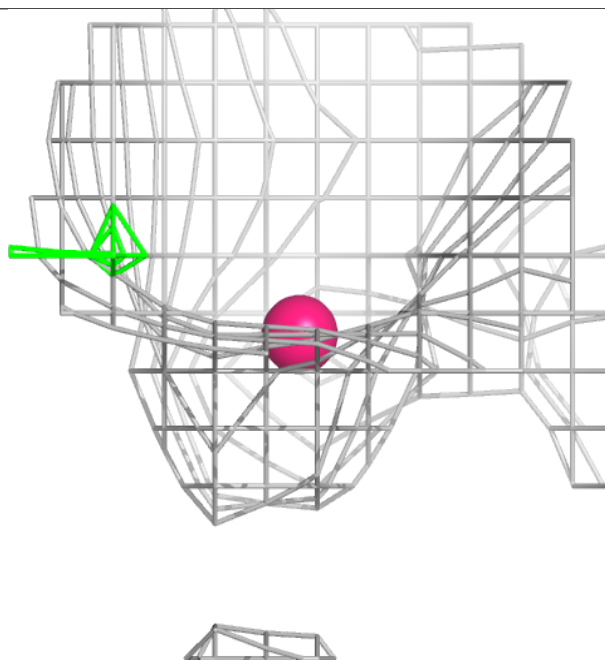
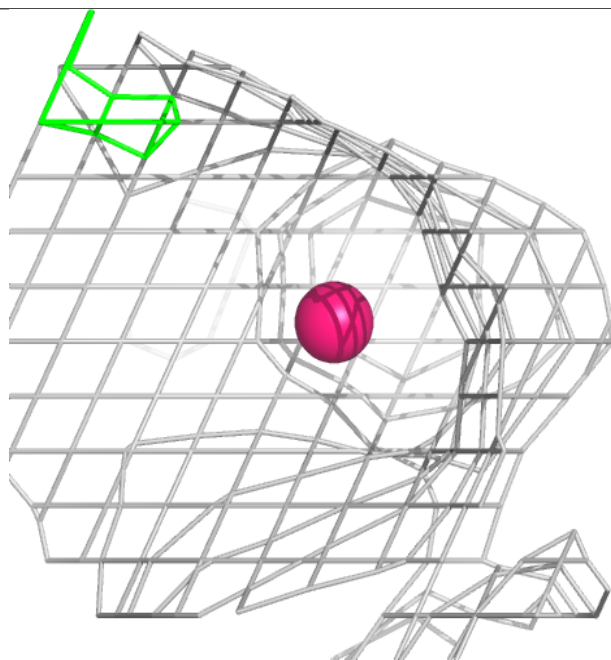
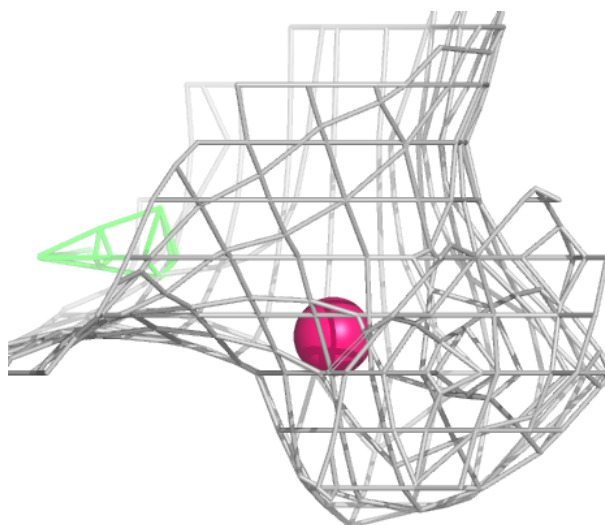
Electron density around OH C 503:

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and green (positive)



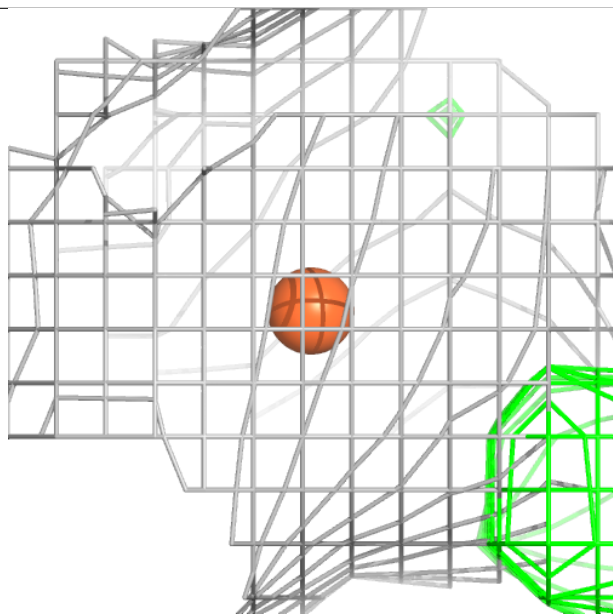
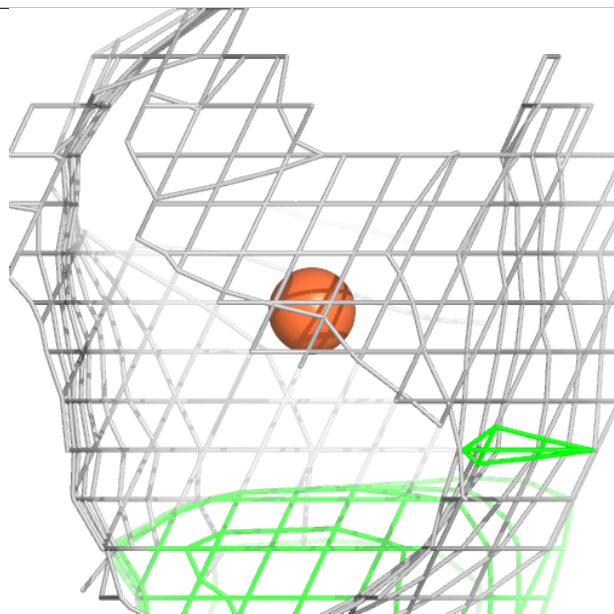
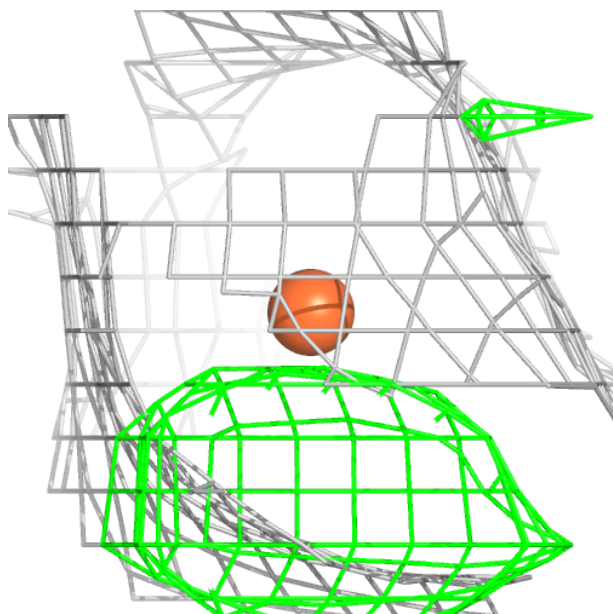
Electron density around OH D 503:

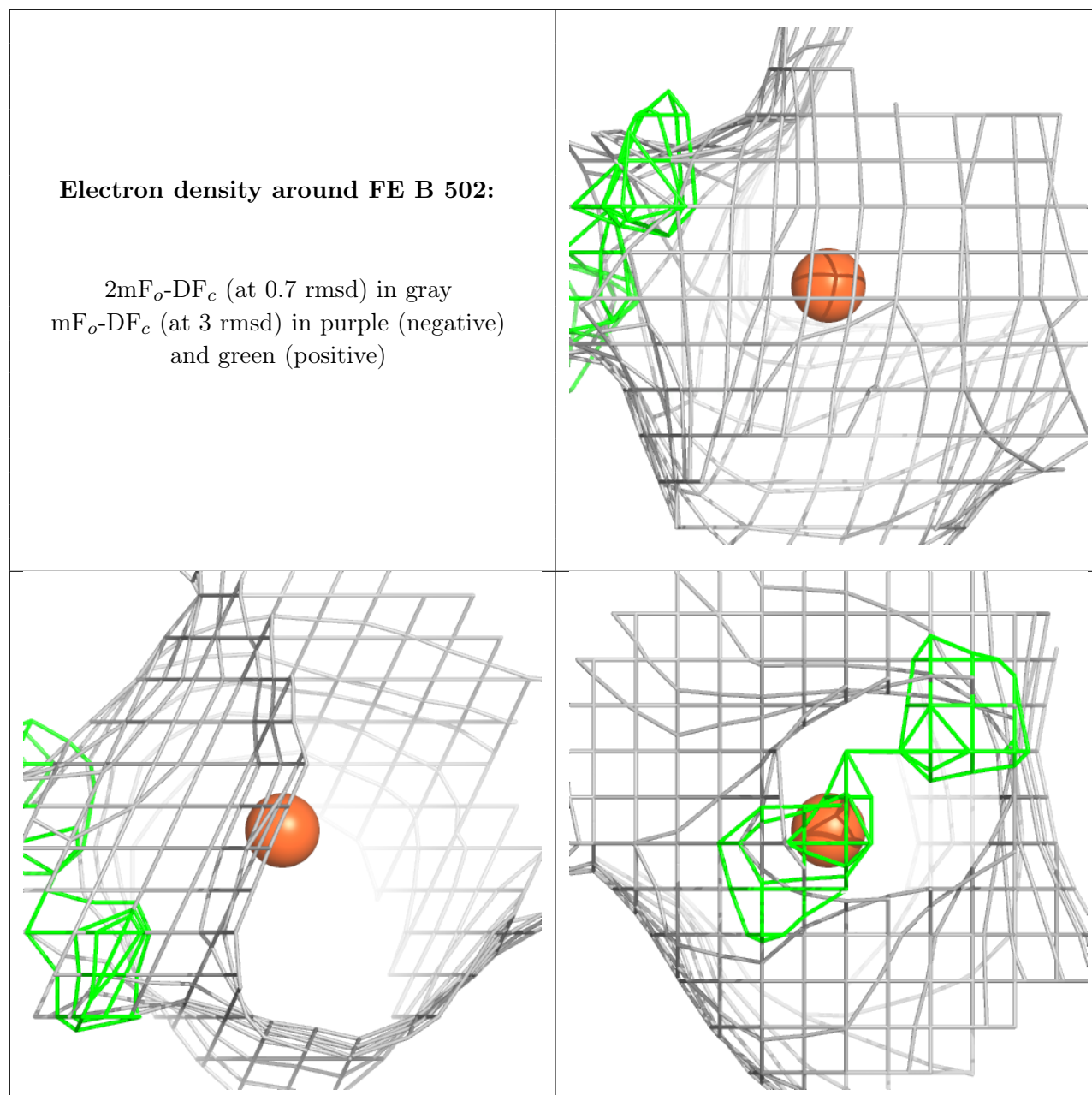
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.