



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 10:38 PM JST

PDB ID : 7DT0  
Title : Proline hydroxylase H11-N101I mutant  
Authors : Gong, W.G.; Yang, L.Y.  
Deposited on : 2021-01-04  
Resolution : 2.43 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36



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Mol	Chain	Length	Quality of chain
1	G	266	
1	H	266	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AKG	B	501	-	X	-	-
2	AKG	E	501	-	X	-	-
2	AKG	G	501	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15768 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.

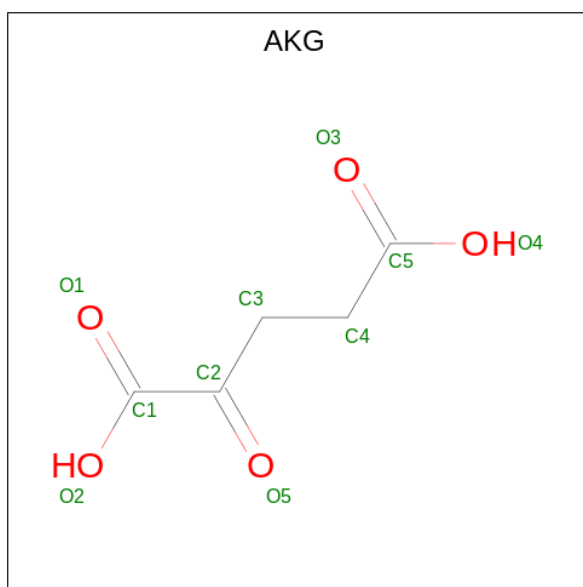
- Molecule 1 is a protein called Phytanoyl-CoA dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	Total 1983	C 1265	N 350	O 363	S 5	0	0	0
1	B	244	Total 1919	C 1226	N 340	O 348	S 5	0	0	0
1	C	242	Total 1900	C 1211	N 336	O 348	S 5	0	0	0
1	D	243	Total 1896	C 1213	N 333	O 345	S 5	0	0	0
1	E	246	Total 1919	C 1223	N 341	O 350	S 5	0	0	0
1	F	245	Total 1910	C 1218	N 336	O 351	S 5	0	0	0
1	G	244	Total 1899	C 1211	N 335	O 348	S 5	0	0	0
1	H	241	Total 1897	C 1211	N 336	O 346	S 4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ILE	ASN	engineered mutation	UNP S5TUM1
B	101	ILE	ASN	engineered mutation	UNP S5TUM1
C	101	ILE	ASN	engineered mutation	UNP S5TUM1
D	101	ILE	ASN	engineered mutation	UNP S5TUM1
E	101	ILE	ASN	engineered mutation	UNP S5TUM1
F	101	ILE	ASN	engineered mutation	UNP S5TUM1
G	101	ILE	ASN	engineered mutation	UNP S5TUM1
H	101	ILE	ASN	engineered mutation	UNP S5TUM1

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	D	1	Total C O 10 5 5	0	0
2	E	1	Total C O 10 5 5	0	0
2	F	1	Total C O 10 5 5	0	0
2	G	1	Total C O 10 5 5	0	0
2	H	1	Total C O 10 5 5	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

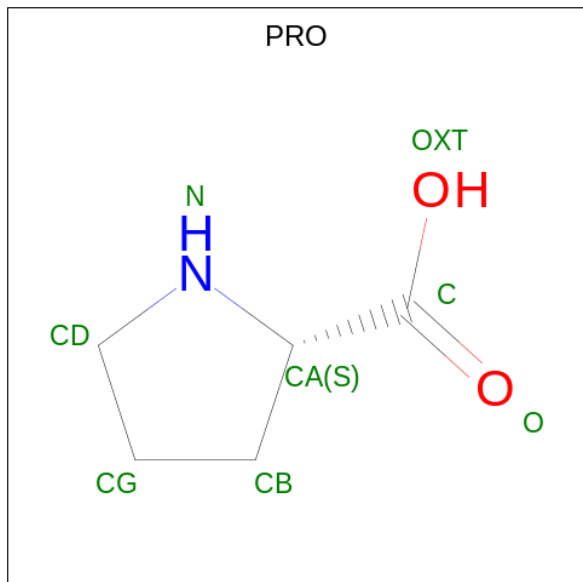
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Fe 1 1	0	0
3	E	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0
3	G	1	Total Fe 1 1	0	0
3	H	1	Total Fe 1 1	0	0

- Molecule 4 is PROLINE (three-letter code: PRO) (formula:  $C_5H_9NO_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 5 1 2	0	0
4	B	1	Total C N O 8 5 1 2	0	0
4	C	1	Total C N O 8 5 1 2	0	0
4	D	1	Total C N O 8 5 1 2	0	0
4	E	1	Total C N O 8 5 1 2	0	0
4	F	1	Total C N O 8 5 1 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			8	5	1	2		
4	H	1	Total	C	N	O	0	0
			8	5	1	2		

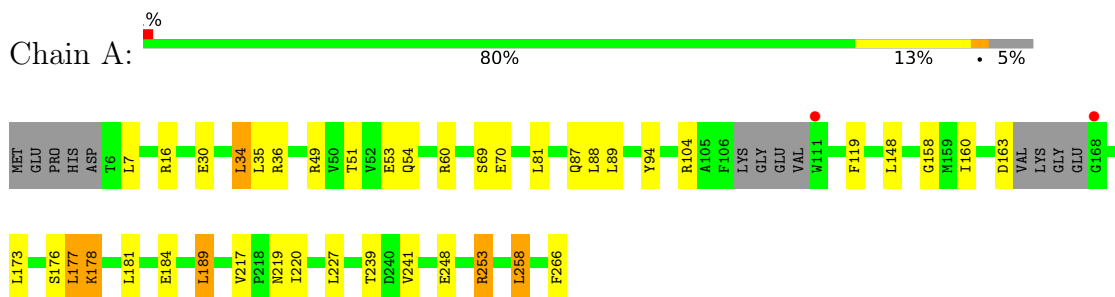
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	60	Total	O	0	0
			60	60		
5	C	34	Total	O	0	0
			34	34		
5	D	43	Total	O	0	0
			43	43		
5	E	39	Total	O	0	0
			39	39		
5	F	31	Total	O	0	0
			31	31		
5	G	23	Total	O	0	0
			23	23		
5	H	20	Total	O	0	0
			20	20		

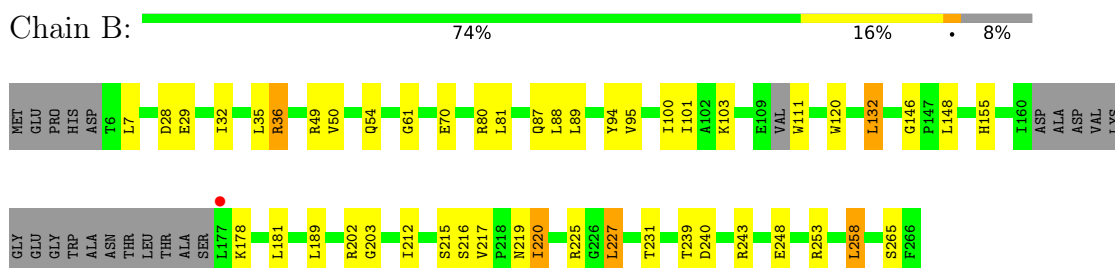
### 3 Residue-property plots

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.

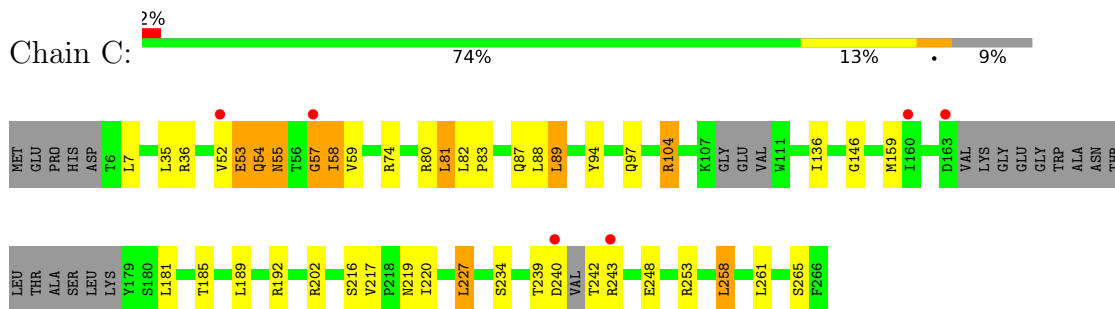
- Molecule 1: Phytanoyl-CoA dioxygenase



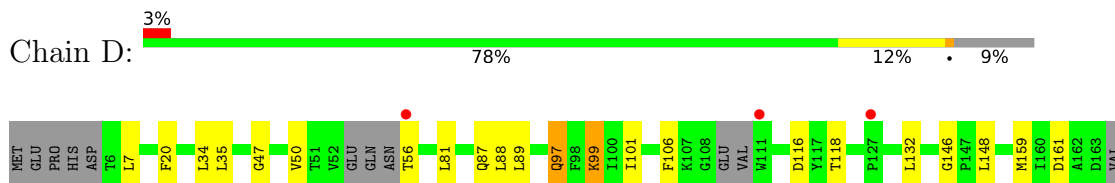
- Molecule 1: Phytanoyl-CoA dioxygenase



- Molecule 1: Phytanoyl-CoA dioxygenase



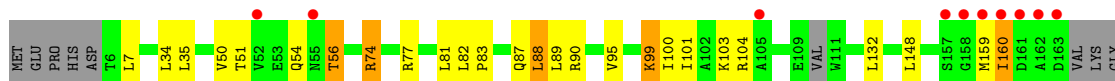
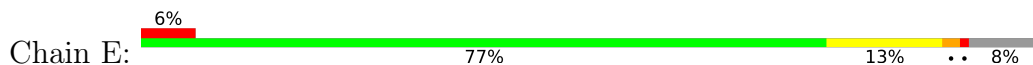
- Molecule 1: Phytanoyl-CoA dioxygenase







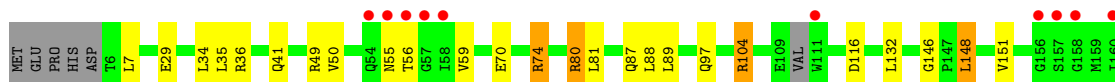
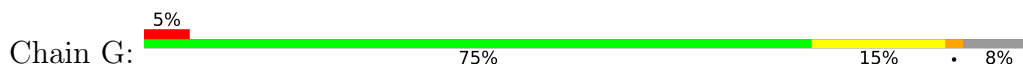
- Molecule 1: Phytanoyl-CoA dioxygenase



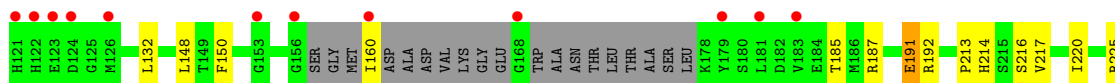
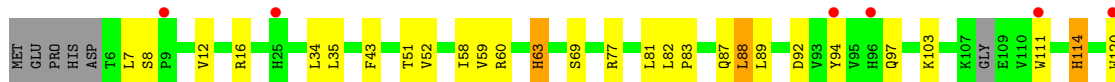
- Molecule 1: Phytanoyl-CoA dioxygenase



- Molecule 1: Phytanoyl-CoA dioxygenase



- Molecule 1: Phytanoyl-CoA dioxygenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.91Å 138.64Å 152.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.60 – 2.43 47.62 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.9 (102.60-2.43) 99.9 (47.62-2.43)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	50.00 (at 2.42Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.201 , 0.270 0.207 , 0.270	Depositor DCC
$R_{free}$ test set	4950 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AKG, FE

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	0.85	0/2035	1.00	5/2769 (0.2%)
1	B	0.90	1/1969 (0.1%)	1.06	11/2675 (0.4%)
1	C	0.79	0/1949	0.94	4/2647 (0.2%)
1	D	0.78	0/1945	0.91	1/2644 (0.0%)
1	E	0.76	0/1969	0.93	6/2677 (0.2%)
1	F	0.76	0/1960	0.88	2/2667 (0.1%)
1	G	0.74	1/1948 (0.1%)	0.94	6/2651 (0.2%)
1	H	0.75	0/1945	0.93	2/2641 (0.1%)
All	All	0.79	2/15720 (0.0%)	0.95	37/21371 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	GLU	CG-CD	6.45	1.61	1.51
1	G	29	GLU	CG-CD	6.03	1.60	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	B	253	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	A	253	ARG	NE-CZ-NH1	8.85	124.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	227	LEU	CA-CB-CG	8.05	133.81	115.30
1	G	227	LEU	CA-CB-CG	7.40	132.32	115.30
1	G	80	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	B	225	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	D	116	ASP	CB-CG-OD1	6.91	124.52	118.30
1	G	49	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	28	ASP	CB-CG-OD2	-6.62	112.35	118.30
1	B	49	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	240	ASP	CB-CG-OD1	6.15	123.83	118.30
1	H	77	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	E	77	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	28	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	88	LEU	CB-CG-CD1	5.91	121.05	111.00
1	H	225	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	E	90	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	B	36	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	89	LEU	CB-CG-CD1	5.56	120.45	111.00
1	A	49	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	16	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	G	116	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	54	GLN	N-CA-C	5.46	125.74	111.00
1	B	243	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	227	LEU	CA-CB-CG	5.33	127.57	115.30
1	E	258	LEU	CA-CB-CG	5.32	127.54	115.30
1	B	29	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	F	49	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	227	LEU	CA-CB-CG	5.21	127.28	115.30
1	G	74	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	G	148	LEU	CA-CB-CG	5.12	127.09	115.30
1	E	77	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	49	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	265	SER	N-CA-C	-5.09	97.25	111.00
1	C	265	SER	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1983	0	1909	13	1
1	B	1919	0	1857	19	1
1	C	1900	0	1815	20	0
1	D	1896	0	1823	11	1
1	E	1919	0	1835	13	0
1	F	1910	0	1822	23	1
1	G	1899	0	1814	12	0
1	H	1897	0	1821	15	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
2	G	10	0	4	0	0
2	H	10	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	7	0	0
4	B	8	0	7	0	0
4	C	8	0	7	0	0
4	D	8	0	7	0	0
4	E	8	0	7	0	0
4	F	8	0	7	0	0
4	G	8	0	7	0	0
4	H	8	0	7	1	0
5	A	43	0	0	0	0
5	B	60	0	0	0	0
5	C	34	0	0	0	0
5	D	43	0	0	1	0
5	E	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	31	0	0	1	0
5	G	23	0	0	1	0
5	H	20	0	0	1	0
All	All	15768	0	14784	122	2

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 (122) 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:C:54:GLN:N	1:C:55:ASN:CB	1.84	1.41
1:C:54:GLN:H	1:C:55:ASN:CB	1.49	1.12
1:C:53:GLU:O	1:C:55:ASN:O	1.85	0.92
1:C:53:GLU:C	1:C:55:ASN:O	2.07	0.92
1:A:7:LEU:H	1:A:87:GLN:HE22	1.16	0.91
1:C:54:GLN:CA	1:C:55:ASN:CB	2.49	0.90
1:C:7:LEU:H	1:C:87:GLN:HE22	1.27	0.81
1:B:7:LEU:H	1:B:87:GLN:HE22	1.29	0.79
1:F:105:ALA:HB1	1:F:222:PRO:HA	1.64	0.78
1:B:111:TRP:HB2	1:B:216:SER:O	1.83	0.77
1:E:160:ILE:HD11	1:E:189:LEU:HD21	1.65	0.77
1:D:118:THR:HG23	1:D:159:MET:HE2	1.66	0.77
1:B:111:TRP:O	1:B:215:SER:OG	2.03	0.76
1:C:57:GLY:O	1:C:58:ILE:O	2.05	0.74
1:C:59:VAL:O	1:C:104:ARG:NH2	2.19	0.74
1:D:7:LEU:H	1:D:87:GLN:HE22	1.33	0.74
1:E:7:LEU:H	1:E:87:GLN:HE22	1.37	0.73
1:D:161:ASP:CB	5:F:627:HOH:O	2.35	0.73
1:H:7:LEU:H	1:H:87:GLN:HE22	1.39	0.69
1:F:94:TYR:HA	1:F:258:LEU:HD22	1.75	0.69
1:A:176:SER:C	1:A:177:LEU:HD22	2.14	0.68
1:C:239:THR:O	1:C:239:THR:HG23	1.94	0.68
1:D:146:GLY:HA2	1:D:217:VAL:HG23	1.76	0.66
1:G:146:GLY:HA2	1:G:217:VAL:HG23	1.77	0.65
1:H:103:LYS:NZ	1:H:217:VAL:O	2.29	0.64
1:B:32:ILE:HD11	1:B:203:GLY:HA2	1.80	0.63
1:E:99:LYS:HE2	1:E:101:ILE:HD11	1.82	0.61
1:C:52:VAL:HG12	1:C:59:VAL:HG12	1.84	0.60
1:C:240:ASP:C	1:C:242:THR:N	2.55	0.60
1:B:103:LYS:NZ	1:B:217:VAL:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:VAL:HG11	1:G:189:LEU:HG	1.86	0.58
1:A:7:LEU:N	1:A:87:GLN:HE22	1.96	0.57
1:C:53:GLU:C	1:C:55:ASN:CB	2.71	0.57
1:F:254:ASP:OD1	1:F:254:ASP:C	2.42	0.57
1:G:7:LEU:H	1:G:87:GLN:HE22	1.53	0.56
1:D:99:LYS:HD2	1:D:101:ILE:HD11	1.87	0.56
1:H:150:PHE:CD1	1:H:214:HIS:HB3	2.41	0.56
1:C:53:GLU:HG3	1:C:55:ASN:CB	2.36	0.56
1:D:262:GLN:CB	5:D:638:HOH:O	2.53	0.56
1:E:74:ARG:HG3	1:E:263:ALA:HB1	1.88	0.56
1:F:7:LEU:HG	1:F:84:ILE:HG12	1.88	0.55
1:A:30:GLU:O	1:A:34:LEU:HD22	2.07	0.54
1:H:120:TRP:CH2	1:H:231:THR:HG21	2.42	0.54
1:E:192:ARG:CZ	1:E:192:ARG:HB2	2.37	0.54
1:A:53:GLU:OE1	1:A:60:ARG:NH2	2.40	0.54
1:E:217:VAL:HG12	1:E:218:PRO:HD2	1.90	0.53
1:C:146:GLY:HA2	1:C:217:VAL:HG23	1.89	0.53
1:H:92:ASP:O	1:H:235:VAL:HG23	2.09	0.53
1:A:177:LEU:CD2	1:A:177:LEU:N	2.73	0.52
1:B:94:TYR:HA	1:B:258:LEU:HD22	1.92	0.52
1:D:262:GLN:CB	1:D:264:THR:HG23	2.39	0.52
1:H:94:TYR:HE1	1:H:252:ALA:HB3	1.73	0.52
1:H:120:TRP:NE1	4:H:503:PRO:OXT	2.34	0.51
1:C:94:TYR:HA	1:C:258:LEU:HD22	1.93	0.51
1:B:61:GLY:HA2	1:B:100:ILE:O	2.10	0.50
1:H:16:ARG:NH2	1:H:88:LEU:O	2.44	0.50
1:H:43:PHE:CD1	1:H:59:VAL:HG11	2.46	0.50
1:D:118:THR:HG23	1:D:159:MET:CE	2.38	0.50
1:B:146:GLY:HA2	1:B:217:VAL:HG23	1.94	0.49
1:G:262:GLN:HA	1:G:263:ALA:HB2	1.94	0.49
1:F:97:GLN:HG3	1:F:231:THR:HB	1.94	0.49
1:F:220:ILE:HG21	1:G:217:VAL:HG12	1.94	0.48
1:B:120:TRP:CH2	1:B:231:THR:HG21	2.48	0.48
1:H:114:HIS:CE1	5:H:601:HOH:O	2.67	0.48
1:H:8:SER:O	1:H:12:VAL:HG23	2.13	0.48
1:E:104:ARG:NH2	1:E:224:ASP:OD2	2.47	0.47
1:F:132:LEU:O	1:F:132:LEU:HD12	2.14	0.47
1:B:7:LEU:N	1:B:87:GLN:HE22	2.07	0.47
1:E:95:VAL:HG23	1:E:258:LEU:HD21	1.96	0.47
1:C:82:LEU:HB3	1:C:83:PRO:HD3	1.96	0.47
1:A:241:VAL:HG12	1:A:253:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG21	1:E:217:VAL:HG13	1.96	0.47
1:G:74:ARG:HH11	1:G:261:LEU:HD13	1.81	0.46
1:E:100:ILE:HG12	1:E:228:VAL:HG22	1.97	0.46
1:F:56:THR:HG21	1:F:58:ILE:HD12	1.97	0.46
1:B:101:ILE:HD12	1:B:227:LEU:HD12	1.97	0.46
1:C:239:THR:O	1:C:239:THR:CG2	2.64	0.46
1:F:74:ARG:O	1:F:75:LEU:C	2.55	0.45
1:F:235:VAL:O	1:F:238:LYS:HB3	2.16	0.45
1:G:209:ASP:O	1:G:212:ILE:HG22	2.16	0.45
1:A:177:LEU:HD22	1:A:177:LEU:N	2.31	0.45
1:B:111:TRP:CD1	1:B:111:TRP:C	2.89	0.45
1:G:223:PHE:HB2	5:G:615:HOH:O	2.15	0.45
1:G:59:VAL:O	1:G:104:ARG:NH2	2.47	0.45
1:B:36:ARG:NH2	1:B:202:ARG:NH2	2.65	0.45
1:B:111:TRP:O	1:B:111:TRP:CD1	2.70	0.44
1:G:225:ARG:HH21	1:G:227:LEU:HD23	1.82	0.44
1:D:97:GLN:HG3	1:D:231:THR:HB	2.00	0.44
1:F:132:LEU:HD12	1:F:132:LEU:C	2.38	0.44
1:F:212:ILE:HG23	1:F:212:ILE:O	2.18	0.43
1:G:254:ASP:OD1	1:G:254:ASP:C	2.55	0.43
1:A:94:TYR:HA	1:A:258:LEU:HD22	2.00	0.43
1:F:56:THR:CG2	1:F:58:ILE:HD12	2.47	0.43
1:F:145:ASN:HA	1:F:219:ASN:ND2	2.33	0.43
1:E:82:LEU:HB3	1:E:83:PRO:HD3	2.01	0.43
1:C:217:VAL:HG12	1:D:220:ILE:HG21	2.01	0.43
1:F:262:GLN:O	1:F:264:THR:HG23	2.18	0.43
1:B:95:VAL:HG23	1:B:258:LEU:HD21	2.01	0.43
1:A:176:SER:C	1:A:177:LEU:CD2	2.86	0.43
1:B:220:ILE:CG2	1:E:217:VAL:HG13	2.48	0.43
1:F:56:THR:HG23	1:F:58:ILE:HG13	2.00	0.43
1:G:70:GLU:O	1:G:74:ARG:HG3	2.19	0.43
1:F:58:ILE:HG21	1:F:104:ARG:HD3	2.00	0.43
1:A:176:SER:O	1:A:177:LEU:HD22	2.20	0.42
1:B:132:LEU:C	1:B:132:LEU:HD12	2.39	0.42
1:H:187:ARG:O	1:H:191:GLU:HG3	2.18	0.42
1:F:53:GLU:HB2	1:F:56:THR:HG22	2.01	0.42
1:E:103:LYS:NZ	1:E:217:VAL:O	2.53	0.42
1:F:106:PHE:CD1	1:F:106:PHE:N	2.86	0.42
1:A:160:ILE:HD11	1:A:189:LEU:HD21	2.01	0.42
1:F:49:ARG:HG2	1:F:249:TRP:CD2	2.54	0.42
1:F:151:VAL:HG11	1:F:189:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:HB3	1:H:83:PRO:HD3	2.02	0.42
1:H:114:HIS:O	1:H:213:PRO:HA	2.20	0.42
1:B:155:HIS:HB3	1:B:212:ILE:HA	2.02	0.41
1:C:146:GLY:HA2	1:C:217:VAL:CG2	2.50	0.41
1:D:20:PHE:HA	1:D:207:TRP:O	2.20	0.41
1:C:81:LEU:HD21	1:C:136:ILE:HD11	2.02	0.41
1:H:63:HIS:CD2	1:H:63:HIS:N	2.88	0.41
1:A:119:PHE:CE2	1:A:178:LYS:HE3	2.55	0.41
1:F:7:LEU:HB2	1:F:87:GLN:HE22	1.85	0.41
1:F:261:LEU:O	1:F:263:ALA:N	2.54	0.41

All (2) 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:54:GLN:O	1:F:47:GLY:O[4_445]	1.97	0.23
1:B:54:GLN:O	1:D:47:GLY:O[3_545]	2.03	0.17

## 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	247/266 (93%)	239 (97%)	7 (3%)	1 (0%)	34 41
1	B	238/266 (90%)	227 (95%)	11 (5%)	0	100 100
1	C	234/266 (88%)	220 (94%)	11 (5%)	3 (1%)	12 11
1	D	235/266 (88%)	226 (96%)	9 (4%)	0	100 100
1	E	240/266 (90%)	226 (94%)	11 (5%)	3 (1%)	12 11
1	F	239/266 (90%)	214 (90%)	21 (9%)	4 (2%)	9 7
1	G	238/266 (90%)	229 (96%)	8 (3%)	1 (0%)	34 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	233/266 (88%)	213 (91%)	19 (8%)	1 (0%)	34	41
All	All	1904/2128 (90%)	1794 (94%)	97 (5%)	13 (1%)	22	26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	LYS
1	C	58	ILE
1	C	55	ASN
1	E	54	GLN
1	F	162	ALA
1	E	56	THR
1	F	262	GLN
1	H	238	LYS
1	E	217	VAL
1	G	55	ASN
1	F	129	PRO
1	C	57	GLY
1	F	127	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/223 (92%)	182 (88%)	24 (12%)	5	4
1	B	200/223 (90%)	182 (91%)	18 (9%)	9	10
1	C	196/223 (88%)	170 (87%)	26 (13%)	4	3
1	D	196/223 (88%)	176 (90%)	20 (10%)	7	7
1	E	197/223 (88%)	173 (88%)	24 (12%)	5	4
1	F	197/223 (88%)	174 (88%)	23 (12%)	5	4
1	G	195/223 (87%)	172 (88%)	23 (12%)	5	4
1	H	197/223 (88%)	166 (84%)	31 (16%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1584/1784 (89%)	1395 (88%)	189 (12%)	5 4

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	LEU
1	A	36	ARG
1	A	51	THR
1	A	69	SER
1	A	70	GLU
1	A	81	LEU
1	A	88	LEU
1	A	89	LEU
1	A	104	ARG
1	A	148	LEU
1	A	163	ASP
1	A	173	LEU
1	A	177	LEU
1	A	181	LEU
1	A	184	GLU
1	A	189	LEU
1	A	217	VAL
1	A	219	ASN
1	A	220	ILE
1	A	239	THR
1	A	248	GLU
1	A	258	LEU
1	A	266	PHE
1	B	35	LEU
1	B	50	VAL
1	B	70	GLU
1	B	80	ARG
1	B	81	LEU
1	B	88	LEU
1	B	89	LEU
1	B	132	LEU
1	B	148	LEU
1	B	178	LYS
1	B	181	LEU
1	B	189	LEU
1	B	219	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	220	ILE
1	B	239	THR
1	B	248	GLU
1	B	258	LEU
1	B	265	SER
1	C	35	LEU
1	C	36	ARG
1	C	53	GLU
1	C	74	ARG
1	C	80	ARG
1	C	81	LEU
1	C	88	LEU
1	C	89	LEU
1	C	97	GLN
1	C	104	ARG
1	C	159	MET
1	C	181	LEU
1	C	185	THR
1	C	189	LEU
1	C	192	ARG
1	C	202	ARG
1	C	216	SER
1	C	219	ASN
1	C	220	ILE
1	C	227	LEU
1	C	234	SER
1	C	243	ARG
1	C	248	GLU
1	C	253	ARG
1	C	258	LEU
1	C	261	LEU
1	D	34	LEU
1	D	35	LEU
1	D	50	VAL
1	D	56	THR
1	D	81	LEU
1	D	88	LEU
1	D	89	LEU
1	D	97	GLN
1	D	99	LYS
1	D	106	PHE
1	D	132	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	148	LEU
1	D	178	LYS
1	D	181	LEU
1	D	189	LEU
1	D	192	ARG
1	D	219	ASN
1	D	220	ILE
1	D	234	SER
1	D	258	LEU
1	E	34	LEU
1	E	35	LEU
1	E	50	VAL
1	E	51	THR
1	E	56	THR
1	E	74	ARG
1	E	81	LEU
1	E	88	LEU
1	E	89	LEU
1	E	99	LYS
1	E	132	LEU
1	E	148	LEU
1	E	159	MET
1	E	160	ILE
1	E	181	LEU
1	E	192	ARG
1	E	217	VAL
1	E	219	ASN
1	E	220	ILE
1	E	234	SER
1	E	239	THR
1	E	248	GLU
1	E	253	ARG
1	E	258	LEU
1	F	34	LEU
1	F	56	THR
1	F	59	VAL
1	F	70	GLU
1	F	81	LEU
1	F	88	LEU
1	F	89	LEU
1	F	97	GLN
1	F	148	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	159	MET
1	F	163	ASP
1	F	180	SER
1	F	181	LEU
1	F	214	HIS
1	F	219	ASN
1	F	220	ILE
1	F	221	SER
1	F	224	ASP
1	F	239	THR
1	F	242	THR
1	F	248	GLU
1	F	254	ASP
1	F	258	LEU
1	G	34	LEU
1	G	35	LEU
1	G	36	ARG
1	G	41	GLN
1	G	50	VAL
1	G	56	THR
1	G	80	ARG
1	G	81	LEU
1	G	88	LEU
1	G	89	LEU
1	G	97	GLN
1	G	104	ARG
1	G	132	LEU
1	G	148	LEU
1	G	181	LEU
1	G	182	ASP
1	G	219	ASN
1	G	220	ILE
1	G	227	LEU
1	G	238	LYS
1	G	239	THR
1	G	243	ARG
1	G	248	GLU
1	H	34	LEU
1	H	35	LEU
1	H	51	THR
1	H	52	VAL
1	H	58	ILE

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Mol	Chain	Res	Type
1	H	60	ARG
1	H	63	HIS
1	H	69	SER
1	H	81	LEU
1	H	88	LEU
1	H	89	LEU
1	H	97	GLN
1	H	111	TRP
1	H	114	HIS
1	H	132	LEU
1	H	148	LEU
1	H	160	ILE
1	H	185	THR
1	H	191	GLU
1	H	192	ARG
1	H	216	SER
1	H	220	ILE
1	H	234	SER
1	H	240	ASP
1	H	242	THR
1	H	245	THR
1	H	249	TRP
1	H	253	ARG
1	H	259	THR
1	H	264	THR
1	H	266	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	87	GLN
1	A	171	ASN
1	A	219	ASN
1	B	87	GLN
1	B	155	HIS
1	B	219	ASN
1	C	63	HIS
1	C	87	GLN
1	C	97	GLN
1	C	219	ASN
1	D	87	GLN

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Mol	Chain	Res	Type
1	D	193	ASN
1	D	219	ASN
1	E	87	GLN
1	E	219	ASN
1	F	87	GLN
1	F	214	HIS
1	F	219	ASN
1	G	87	GLN
1	G	219	ASN
1	H	55	ASN
1	H	63	HIS
1	H	87	GLN
1	H	121	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	AKG	A	501	3	9,9,9	1.48	2 (22%)	11,11,11	1.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AKG	G	501	3	9,9,9	1.58	1 (11%)	11,11,11	2.19	3 (27%)
4	PRO	E	503	-	8,8,8	0.69	0	10,10,10	1.55	3 (30%)
4	PRO	C	503	-	8,8,8	0.80	0	10,10,10	1.28	1 (10%)
2	AKG	F	501	3	9,9,9	1.63	2 (22%)	11,11,11	1.31	2 (18%)
4	PRO	B	502	-	8,8,8	0.86	0	10,10,10	0.85	0
4	PRO	A	503	-	8,8,8	0.66	0	10,10,10	1.66	2 (20%)
2	AKG	E	501	3	9,9,9	2.24	2 (22%)	11,11,11	2.78	6 (54%)
2	AKG	B	501	3	9,9,9	1.72	2 (22%)	11,11,11	2.42	6 (54%)
4	PRO	D	503	-	8,8,8	0.69	0	10,10,10	1.70	3 (30%)
2	AKG	C	501	3	9,9,9	1.78	2 (22%)	11,11,11	1.78	2 (18%)
2	AKG	H	501	3	9,9,9	1.60	1 (11%)	11,11,11	2.17	5 (45%)
4	PRO	H	503	-	8,8,8	0.65	0	10,10,10	1.50	2 (20%)
4	PRO	F	503	-	8,8,8	0.92	1 (12%)	10,10,10	1.65	1 (10%)
4	PRO	G	503	-	8,8,8	0.74	0	10,10,10	1.55	2 (20%)
2	AKG	D	501	3	9,9,9	1.58	2 (22%)	11,11,11	1.33	2 (18%)

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	AKG	A	501	3	-	6/9/9/9	-
2	AKG	G	501	3	-	8/9/9/9	-
4	PRO	E	503	-	-	0/4/11/11	0/1/1/1
4	PRO	C	503	-	-	2/4/11/11	0/1/1/1
2	AKG	F	501	3	-	4/9/9/9	-
4	PRO	B	502	-	-	2/4/11/11	0/1/1/1
4	PRO	A	503	-	-	0/4/11/11	0/1/1/1
2	AKG	E	501	3	-	6/9/9/9	-
2	AKG	B	501	3	-	9/9/9/9	-
4	PRO	D	503	-	-	0/4/11/11	0/1/1/1
2	AKG	C	501	3	-	5/9/9/9	-
2	AKG	H	501	3	-	5/9/9/9	-
4	PRO	H	503	-	-	0/4/11/11	0/1/1/1
4	PRO	F	503	-	-	2/4/11/11	0/1/1/1
4	PRO	G	503	-	-	0/4/11/11	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AKG	D	501	3	-	5/9/9/9	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	AKG	C2-C1	-5.47	1.46	1.53
2	B	501	AKG	O1-C1	3.67	1.32	1.22
2	G	501	AKG	C2-C1	-3.08	1.49	1.53
2	F	501	AKG	C2-C1	-2.95	1.49	1.53
2	C	501	AKG	C2-C1	-2.80	1.49	1.53
2	H	501	AKG	C2-C1	-2.77	1.49	1.53
2	E	501	AKG	O1-C1	2.73	1.29	1.22
2	D	501	AKG	O1-C1	2.63	1.29	1.22
2	D	501	AKG	C2-C1	-2.60	1.50	1.53
2	F	501	AKG	O1-C1	2.41	1.29	1.22
2	C	501	AKG	C3-C2	2.41	1.53	1.51
2	A	501	AKG	C2-C1	-2.39	1.50	1.53
2	B	501	AKG	O5-C2	2.30	1.27	1.23
4	F	503	PRO	OXT-C	-2.22	1.23	1.30
2	A	501	AKG	O1-C1	2.16	1.28	1.22

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	AKG	O1-C1-C2	-4.62	115.56	121.72
2	G	501	AKG	O1-C1-C2	-4.59	115.60	121.72
2	E	501	AKG	C3-C2-C1	4.41	124.16	115.97
2	E	501	AKG	O5-C2-C1	-4.12	113.45	119.43
2	B	501	AKG	O5-C2-C1	3.99	125.22	119.43
2	H	501	AKG	C3-C2-C1	3.92	123.26	115.97
4	F	503	PRO	OXT-C-O	-3.77	115.52	124.09
2	E	501	AKG	C4-C3-C2	-3.62	106.20	113.03
2	G	501	AKG	O2-C1-C2	3.56	123.72	113.97
2	C	501	AKG	C3-C4-C5	3.46	121.04	113.60
2	B	501	AKG	O1-C1-C2	-3.36	117.23	121.72
2	B	501	AKG	C4-C3-C2	-3.34	106.74	113.03
2	C	501	AKG	C3-C2-C1	3.25	122.00	115.97
2	G	501	AKG	C3-C2-C1	3.23	121.97	115.97
4	D	503	PRO	OXT-C-CA	3.15	123.86	113.40
4	A	503	PRO	OXT-C-CA	3.13	123.80	113.40
4	G	503	PRO	OXT-C-CA	3.06	123.57	113.40
4	E	503	PRO	OXT-C-CA	2.98	123.32	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	PRO	OXT-C-O	-2.90	117.51	124.09
2	H	501	AKG	O2-C1-C2	2.87	121.83	113.97
2	B	501	AKG	O5-C2-C3	-2.80	115.00	121.20
4	D	503	PRO	OXT-C-O	-2.78	117.77	124.09
4	H	503	PRO	OXT-C-CA	2.77	122.62	113.40
2	H	501	AKG	C3-C4-C5	2.56	119.11	113.60
4	H	503	PRO	OXT-C-O	-2.49	118.43	124.09
4	G	503	PRO	OXT-C-O	-2.45	118.53	124.09
2	B	501	AKG	O4-C5-C4	2.38	121.67	114.03
2	F	501	AKG	C3-C2-C1	2.31	120.27	115.97
4	D	503	PRO	CD-N-CA	2.31	113.44	107.08
2	D	501	AKG	C4-C3-C2	-2.30	108.70	113.03
2	H	501	AKG	O1-C1-C2	-2.26	118.70	121.72
2	E	501	AKG	O2-C1-O1	2.26	128.78	123.61
2	B	501	AKG	O3-C5-C4	-2.25	115.85	123.08
2	E	501	AKG	C3-C4-C5	2.25	118.44	113.60
2	H	501	AKG	O4-C5-C4	2.23	121.20	114.03
2	D	501	AKG	C3-C2-C1	2.19	120.04	115.97
2	F	501	AKG	O1-C1-C2	-2.16	118.84	121.72
4	E	503	PRO	OXT-C-O	-2.09	119.35	124.09
4	C	503	PRO	OXT-C-CA	2.08	120.31	113.40
4	E	503	PRO	CD-N-CA	2.02	112.64	107.08

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AKG	O2-C1-C2-O5
2	A	501	AKG	O2-C1-C2-C3
2	B	501	AKG	O1-C1-C2-O5
2	B	501	AKG	O1-C1-C2-C3
2	B	501	AKG	O2-C1-C2-O5
2	B	501	AKG	O2-C1-C2-C3
2	B	501	AKG	C1-C2-C3-C4
2	B	501	AKG	C2-C3-C4-C5
2	C	501	AKG	O1-C1-C2-C3
2	C	501	AKG	O2-C1-C2-C3
2	D	501	AKG	O1-C1-C2-C3
2	D	501	AKG	O2-C1-C2-C3
2	E	501	AKG	O1-C1-C2-O5
2	E	501	AKG	O1-C1-C2-C3
2	E	501	AKG	O2-C1-C2-O5

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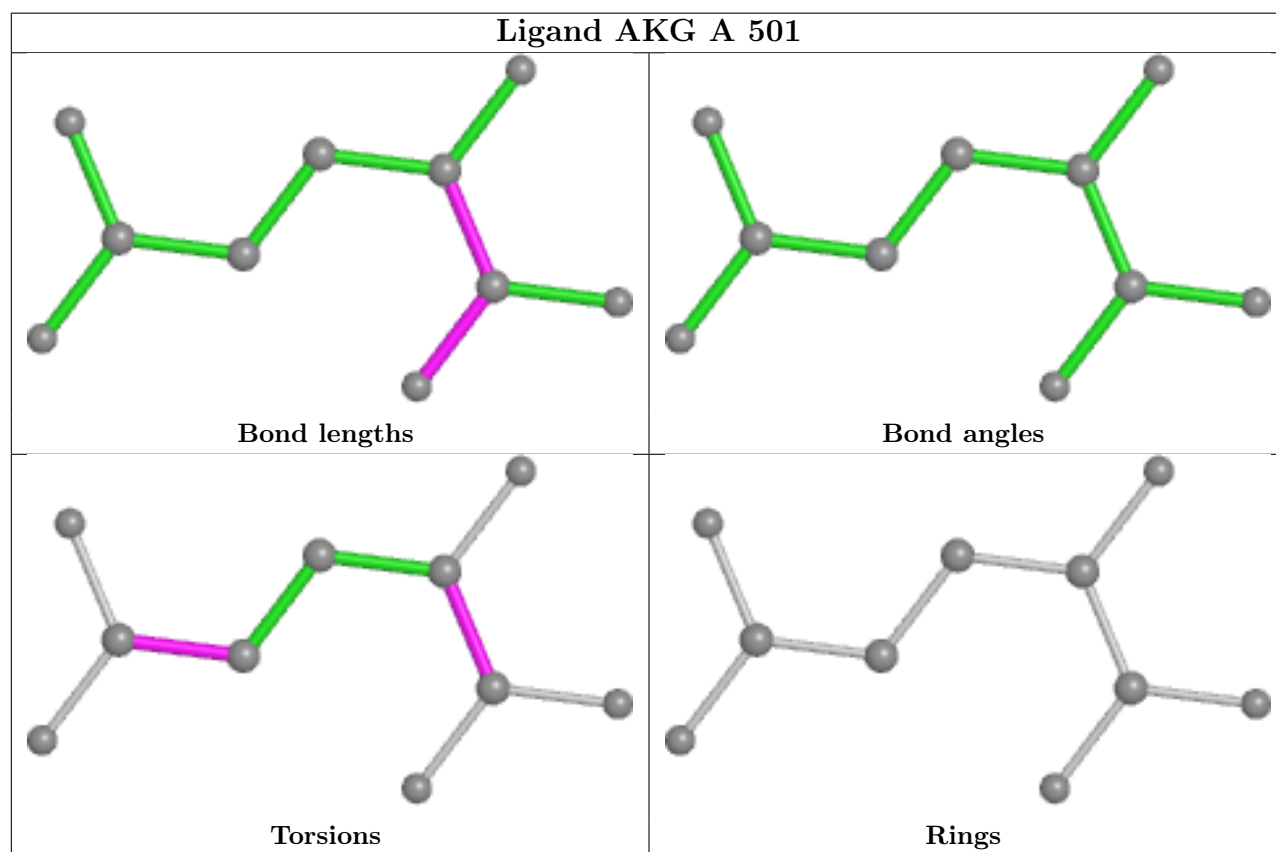
Mol	Chain	Res	Type	Atoms
2	E	501	AKG	O2-C1-C2-C3
2	F	501	AKG	O1-C1-C2-C3
2	F	501	AKG	O2-C1-C2-C3
2	F	501	AKG	C2-C3-C4-C5
2	G	501	AKG	O1-C1-C2-O5
2	G	501	AKG	O1-C1-C2-C3
2	G	501	AKG	O2-C1-C2-O5
2	G	501	AKG	O2-C1-C2-C3
2	H	501	AKG	O2-C1-C2-O5
2	H	501	AKG	O2-C1-C2-C3
2	G	501	AKG	C2-C3-C4-C5
4	B	502	PRO	O-C-CA-CB
4	C	503	PRO	O-C-CA-CB
2	A	501	AKG	O1-C1-C2-O5
2	C	501	AKG	O1-C1-C2-O5
2	D	501	AKG	O1-C1-C2-O5
2	F	501	AKG	O1-C1-C2-O5
2	H	501	AKG	O1-C1-C2-O5
2	A	501	AKG	O1-C1-C2-C3
2	H	501	AKG	O1-C1-C2-C3
4	B	502	PRO	OXT-C-CA-CB
4	C	503	PRO	OXT-C-CA-CB
2	D	501	AKG	C3-C4-C5-O3
2	A	501	AKG	C3-C4-C5-O3
2	B	501	AKG	C3-C4-C5-O3
2	A	501	AKG	C3-C4-C5-O4
2	D	501	AKG	C3-C4-C5-O4
2	B	501	AKG	O5-C2-C3-C4
4	F	503	PRO	O-C-CA-CB
2	E	501	AKG	C3-C4-C5-O4
2	B	501	AKG	C3-C4-C5-O4
2	E	501	AKG	C3-C4-C5-O3
2	G	501	AKG	C3-C4-C5-O4
2	G	501	AKG	C3-C4-C5-O3
4	F	503	PRO	OXT-C-CA-CB
2	G	501	AKG	C1-C2-C3-C4
2	C	501	AKG	C3-C4-C5-O4
2	C	501	AKG	C3-C4-C5-O3
2	H	501	AKG	C3-C4-C5-O4

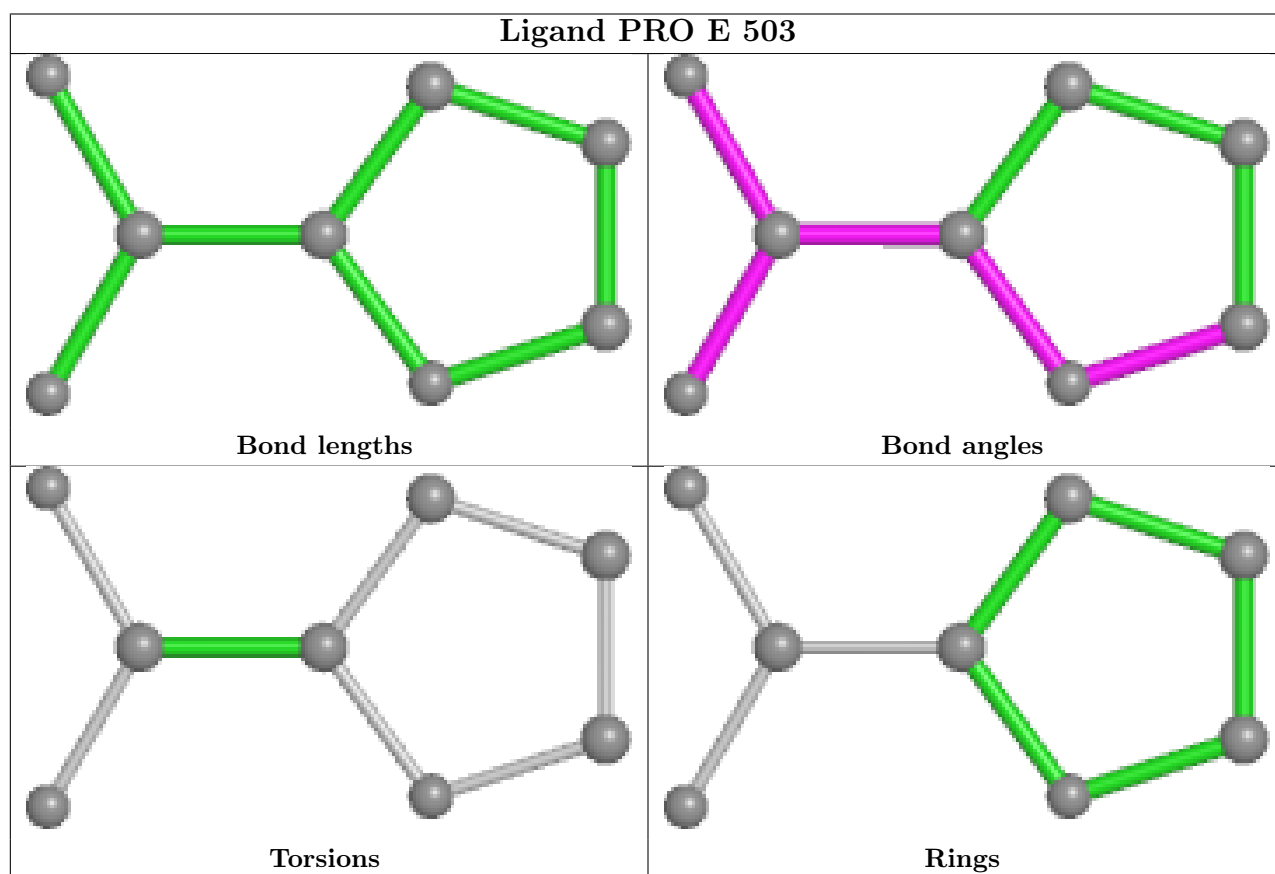
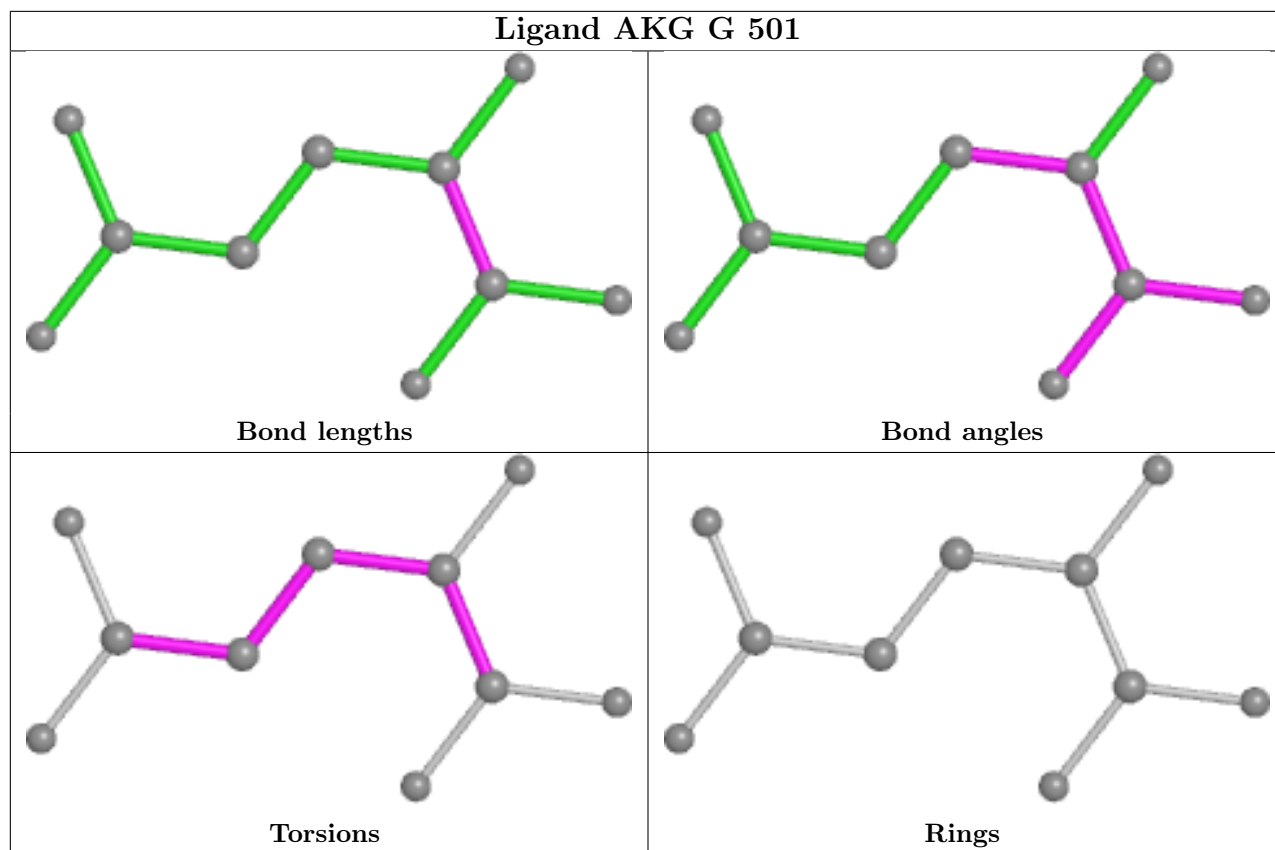
There are no ring outliers.

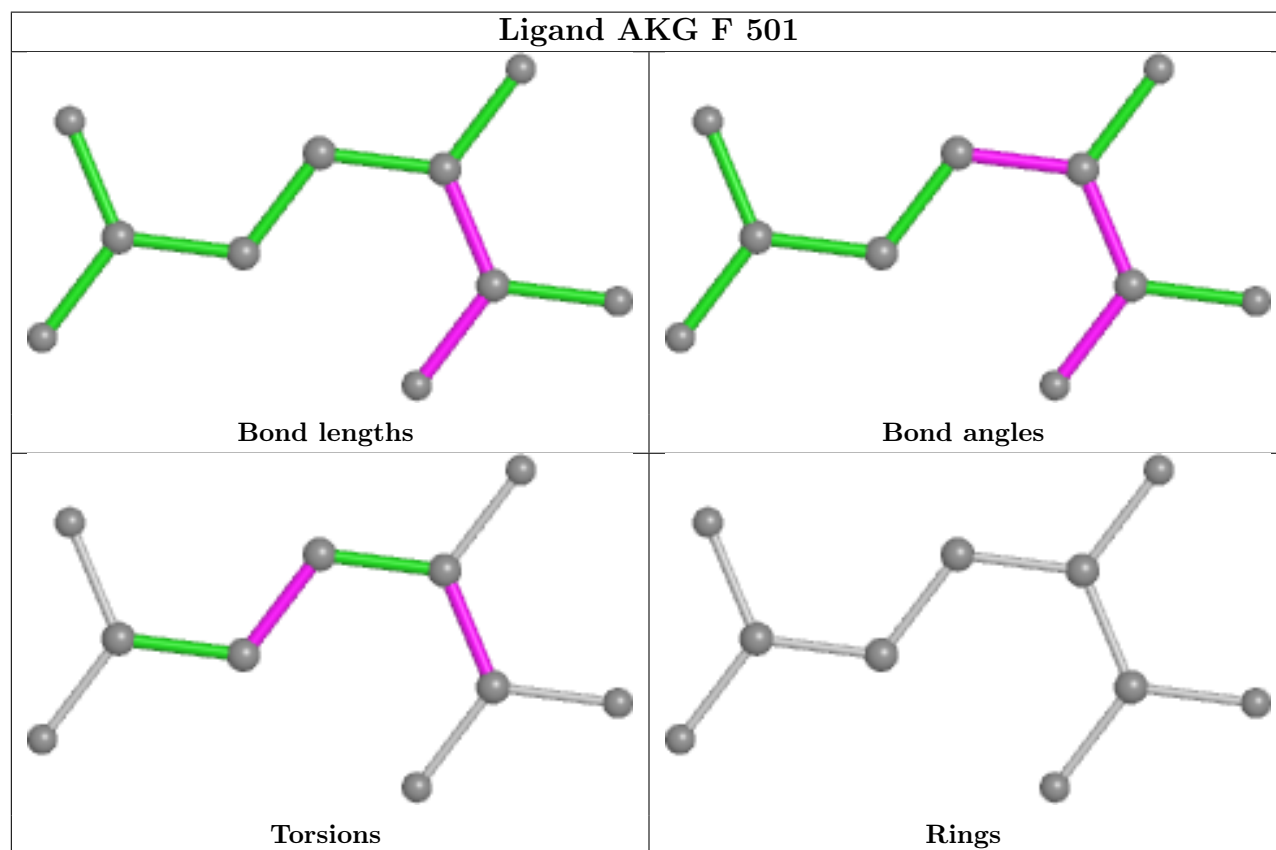
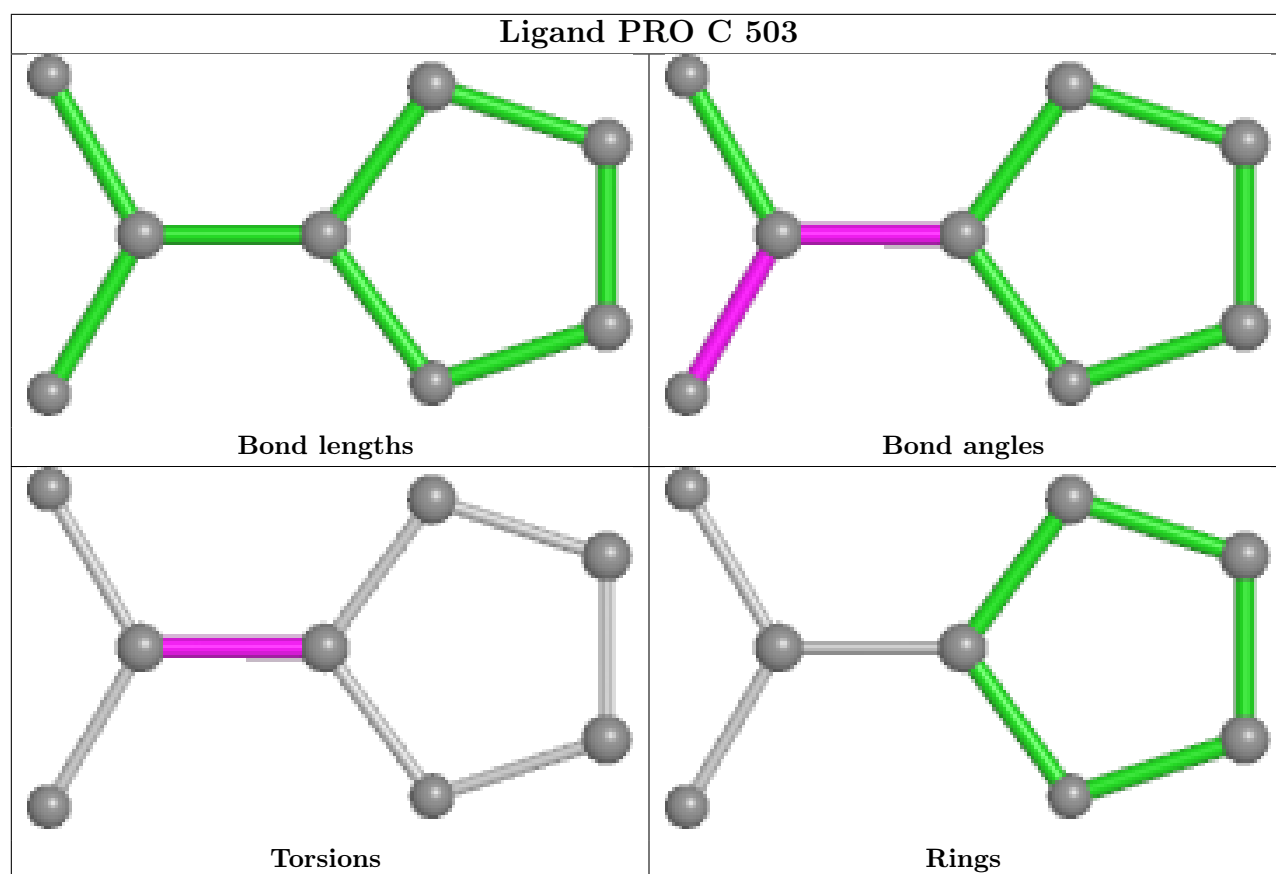
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	503	PRO	1	0

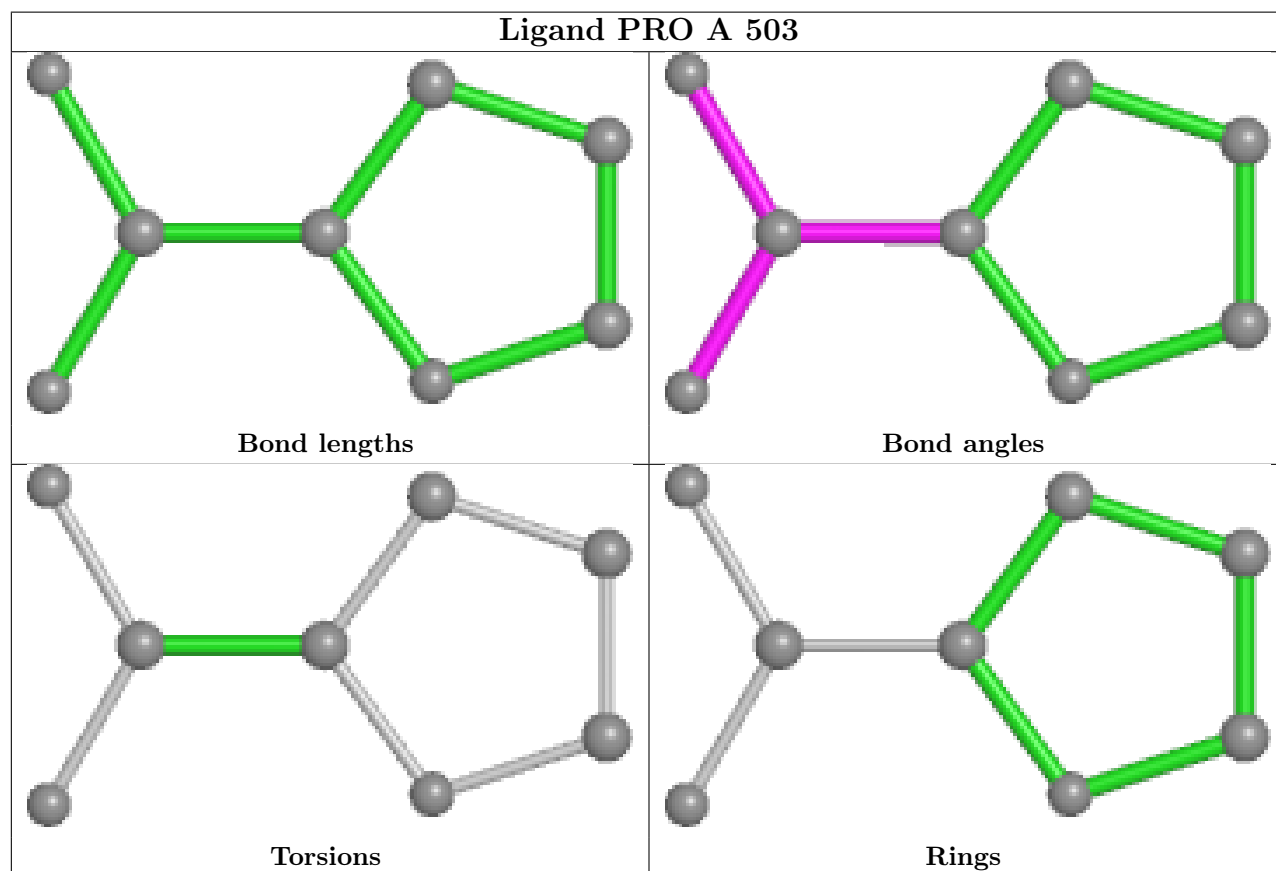
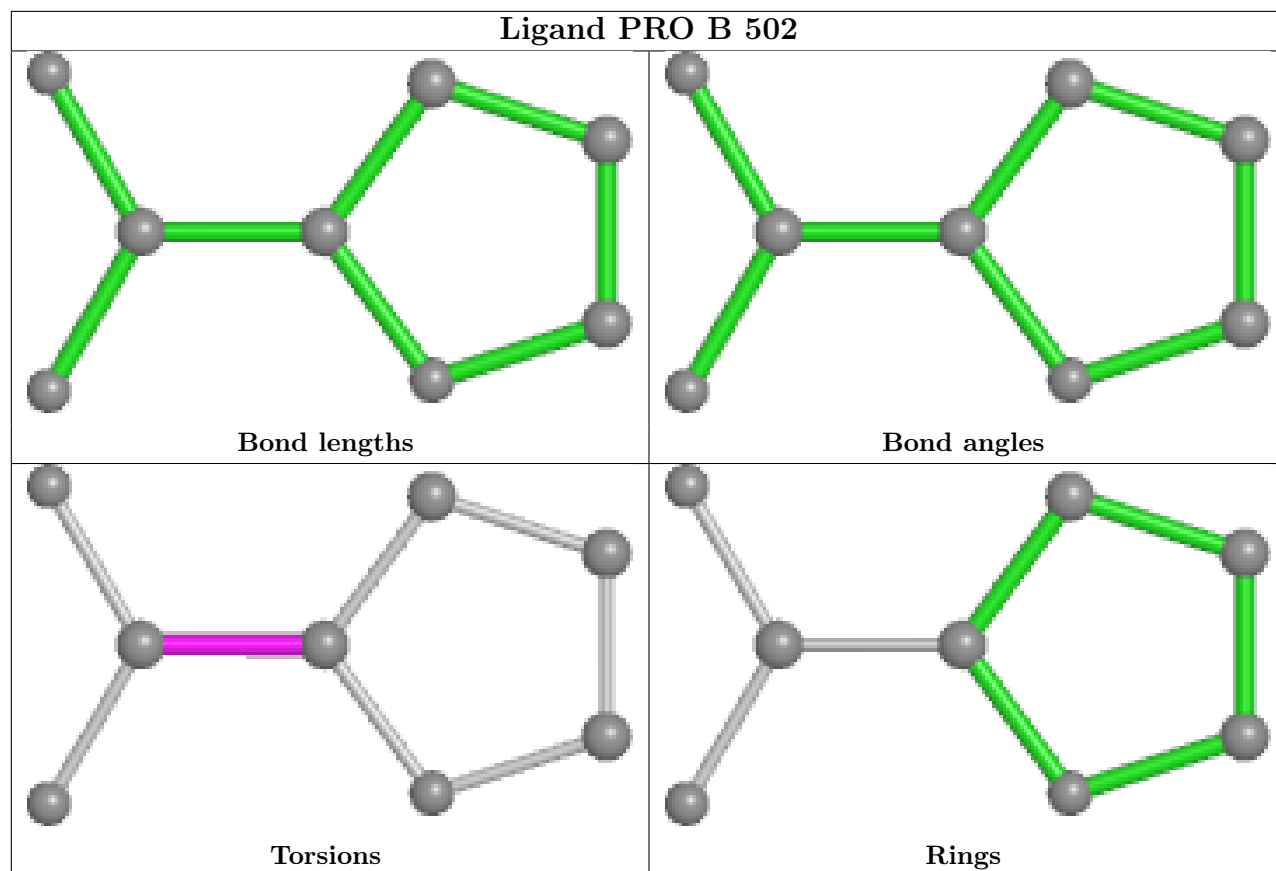
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

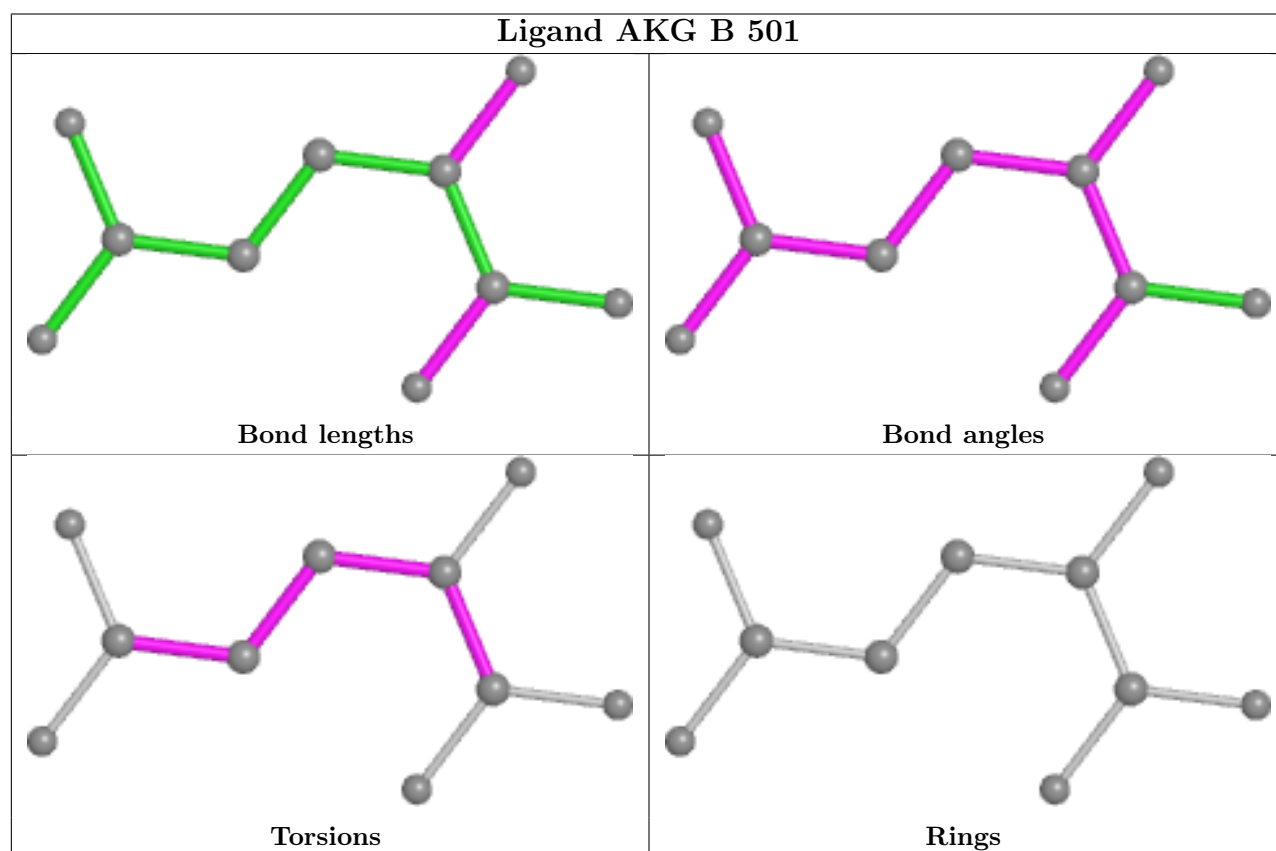
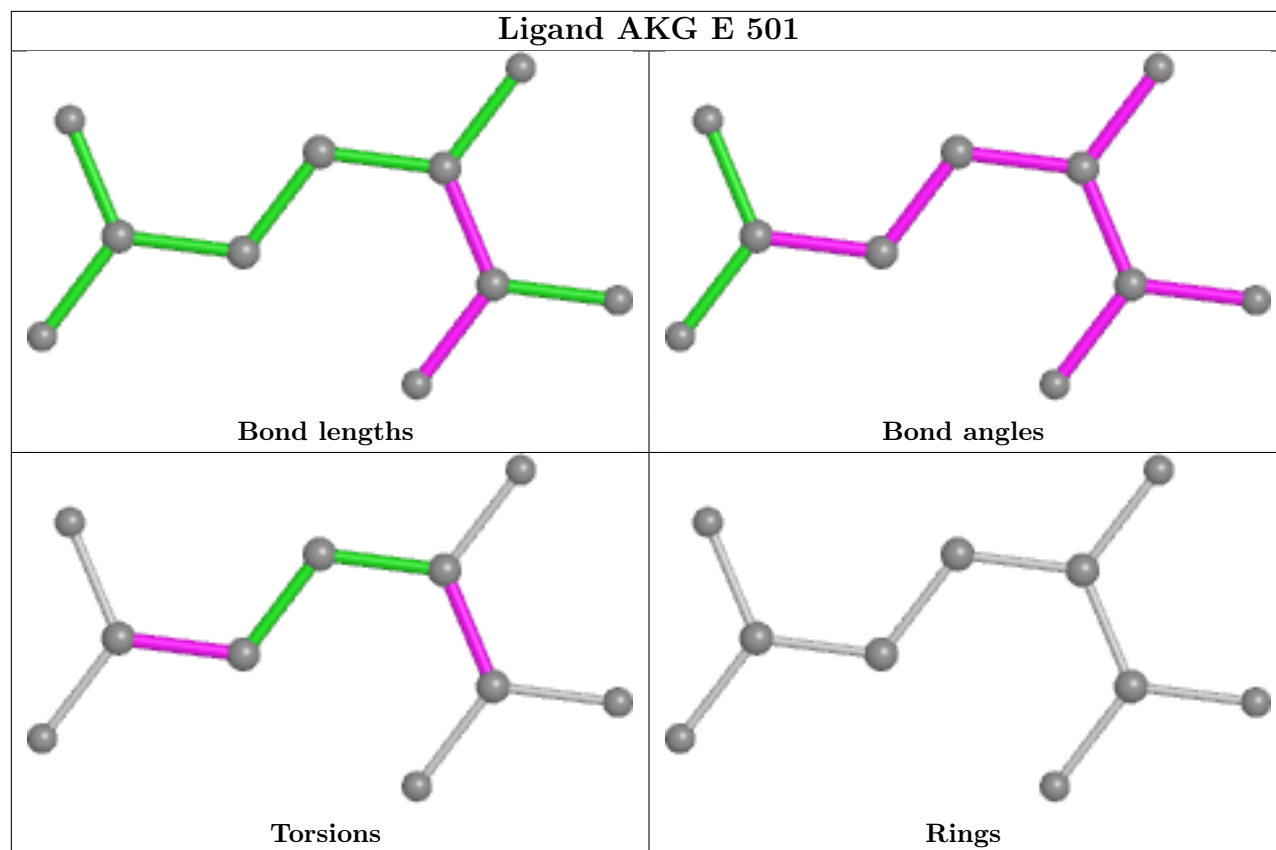


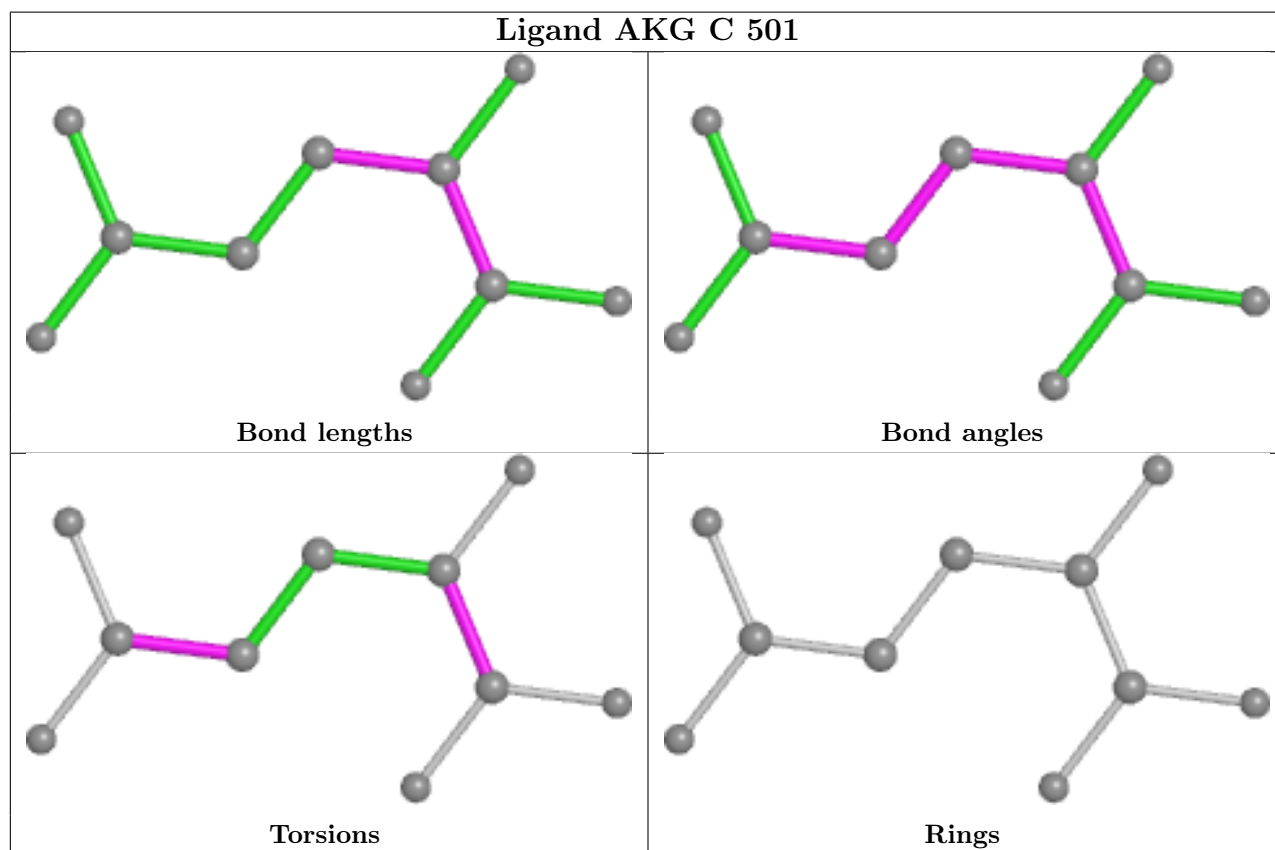
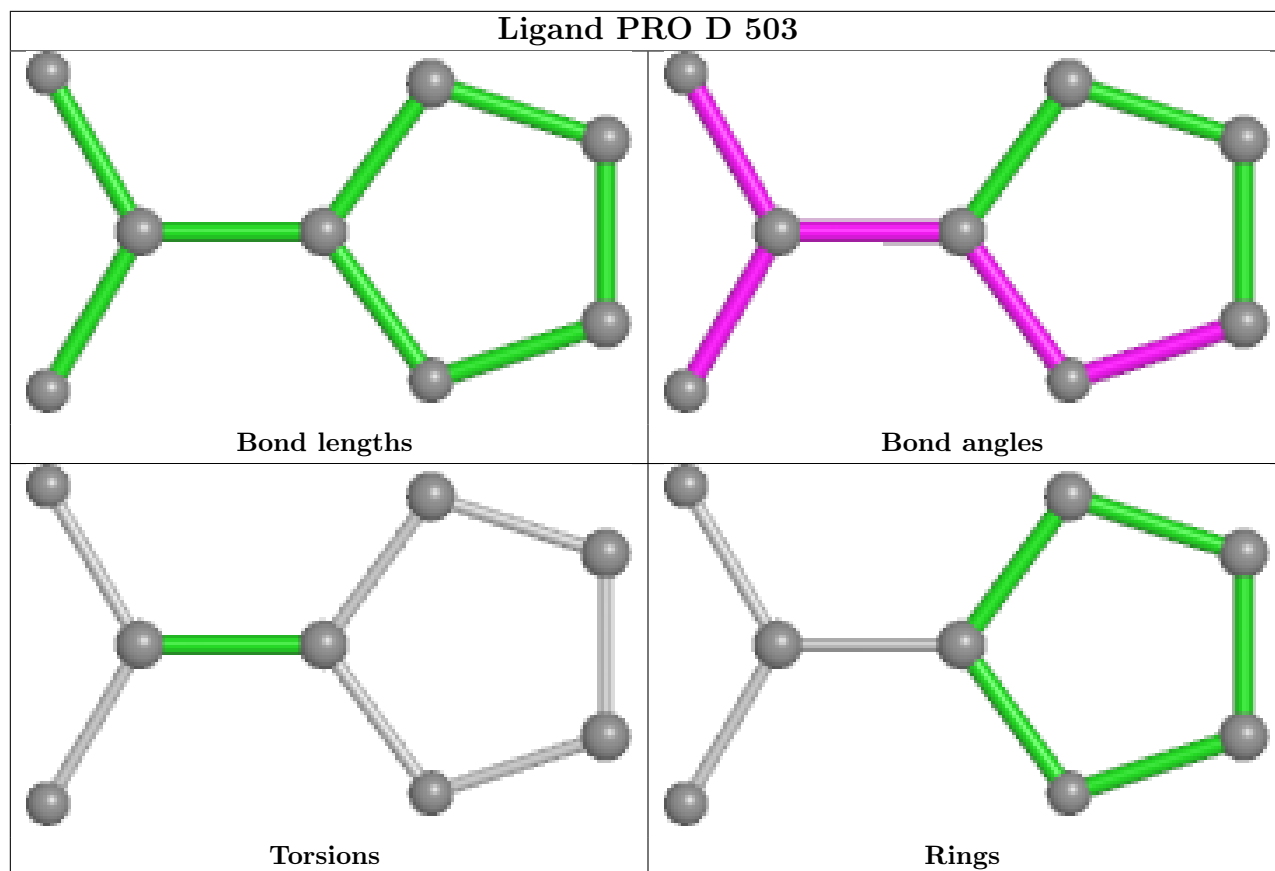


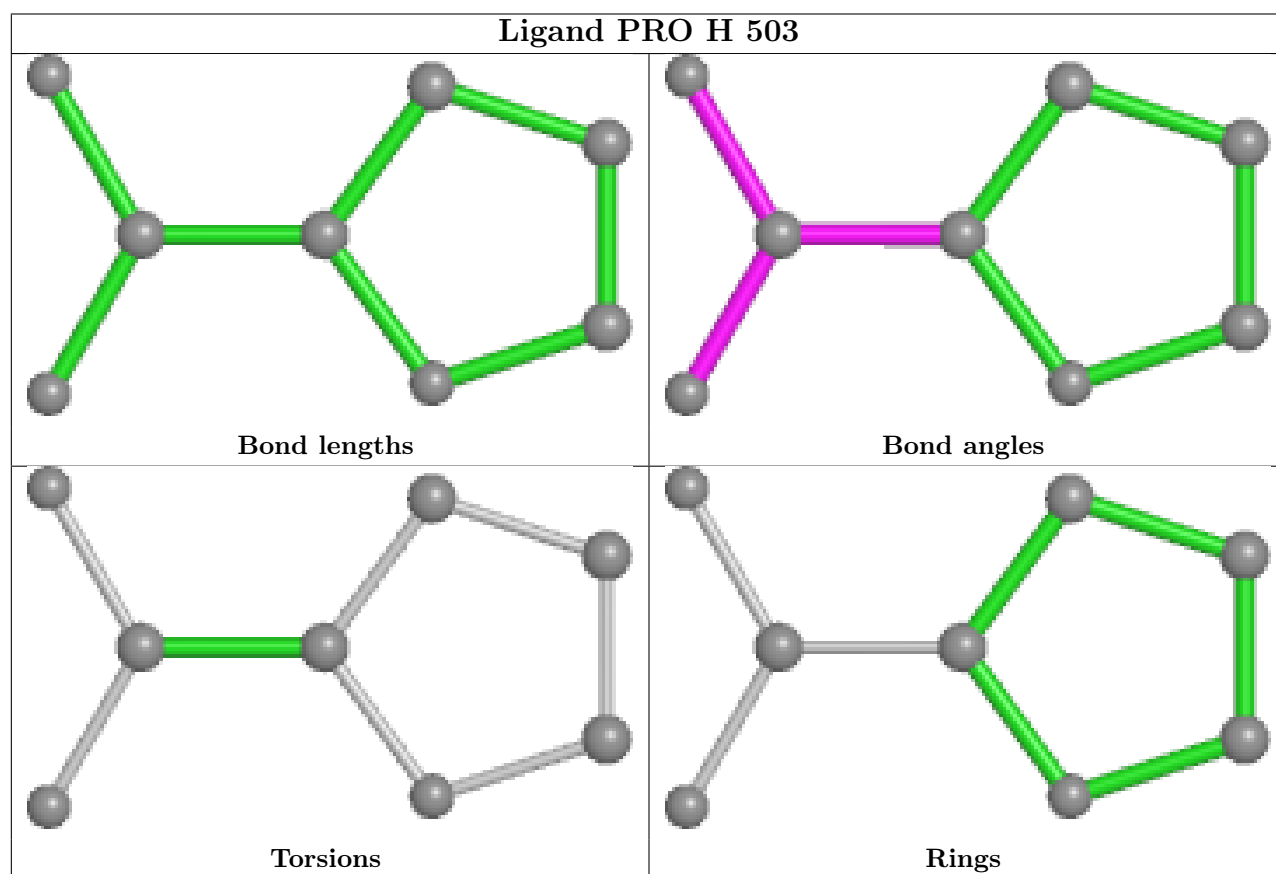
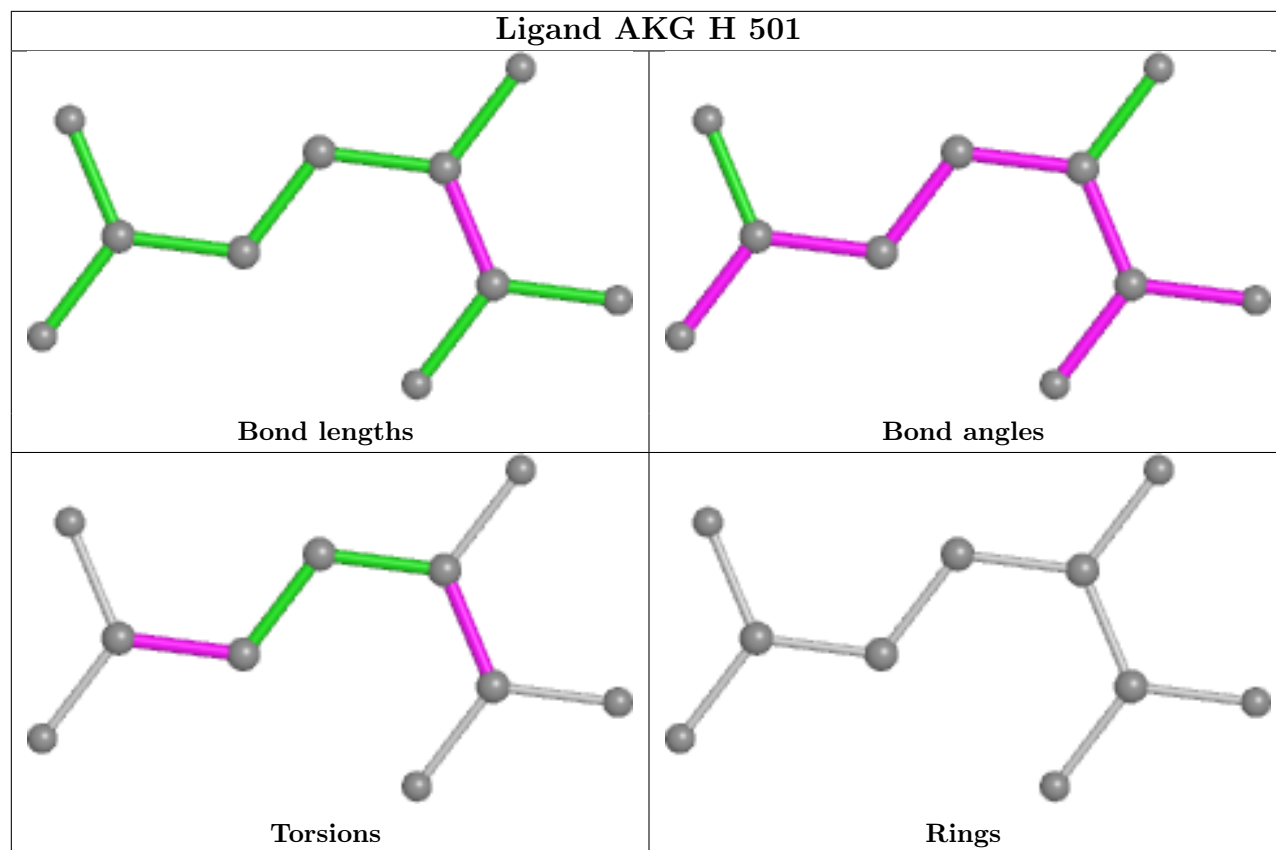


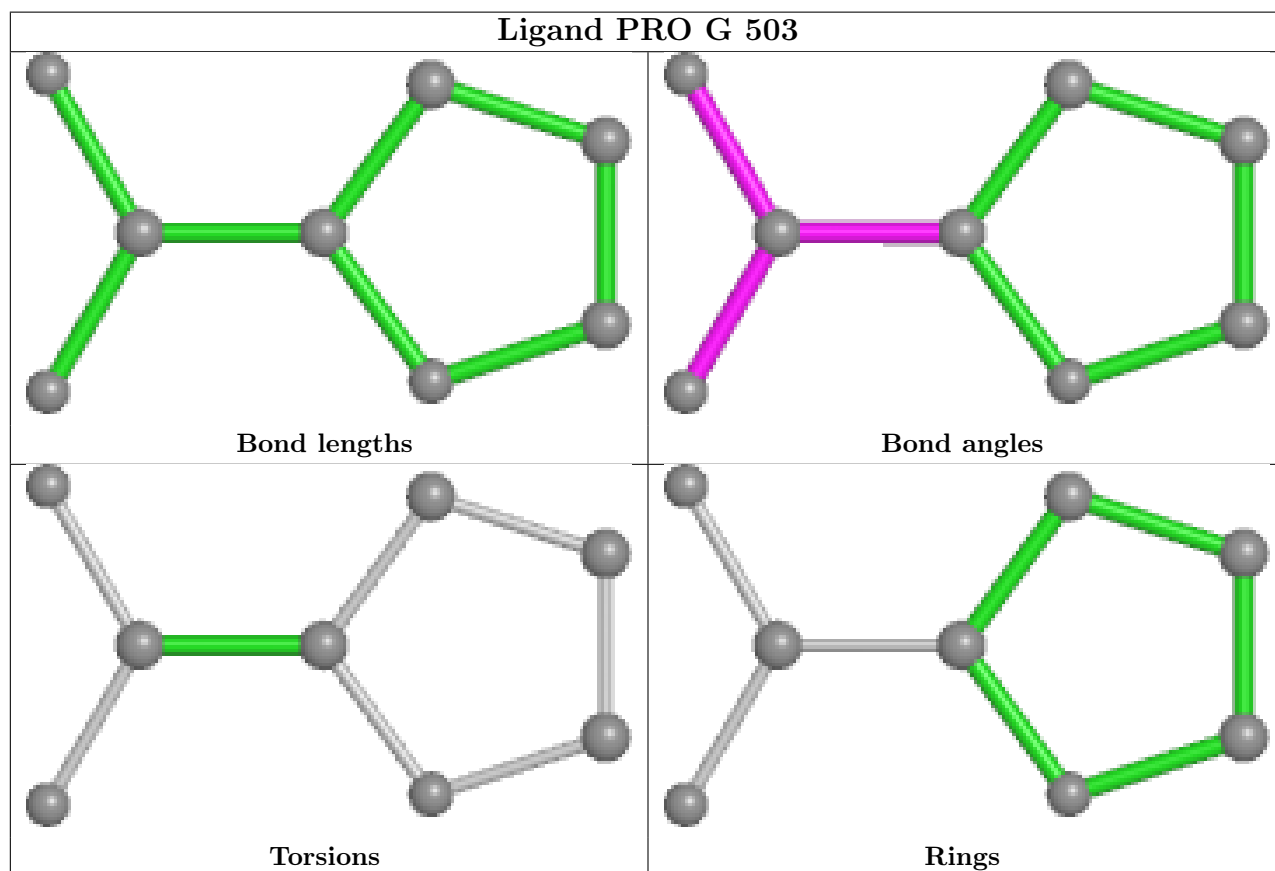
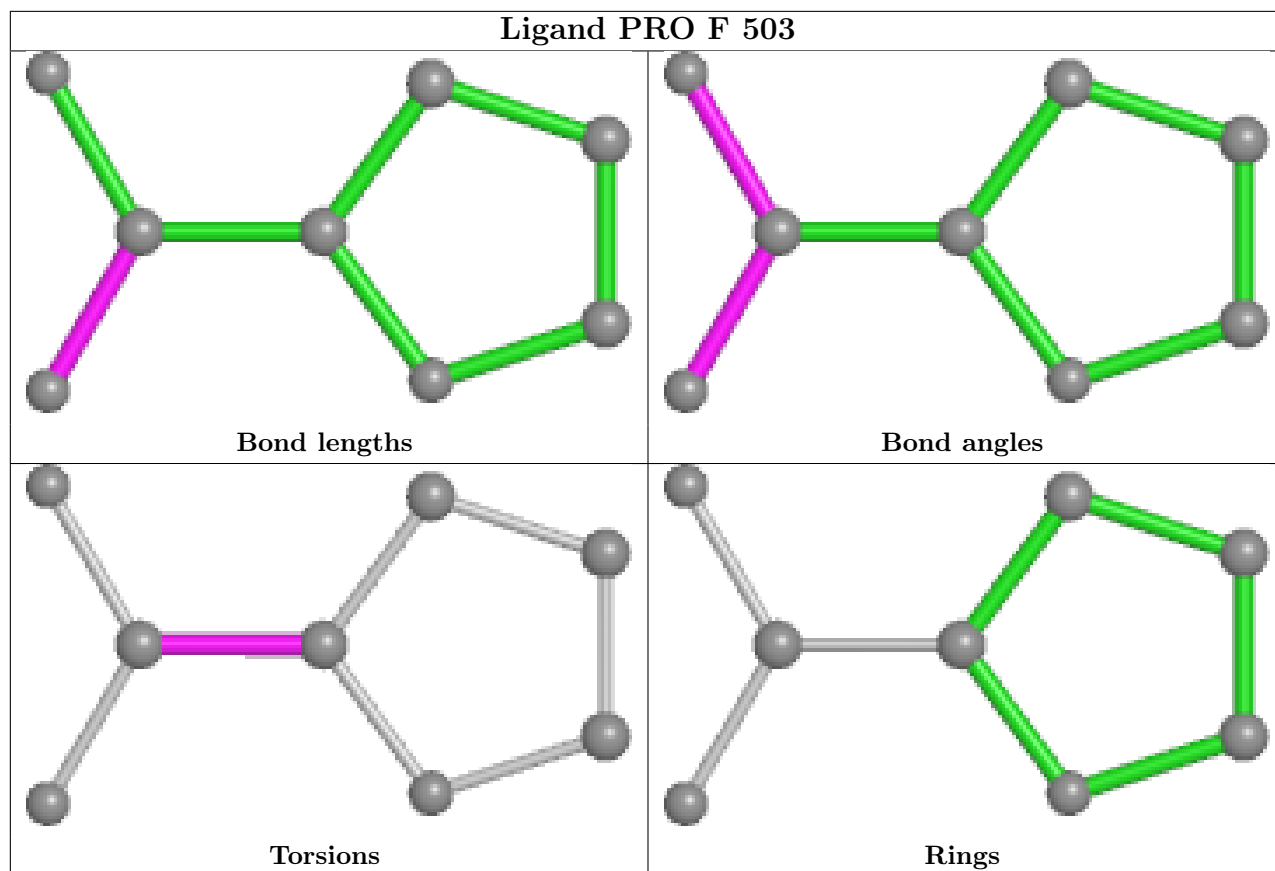


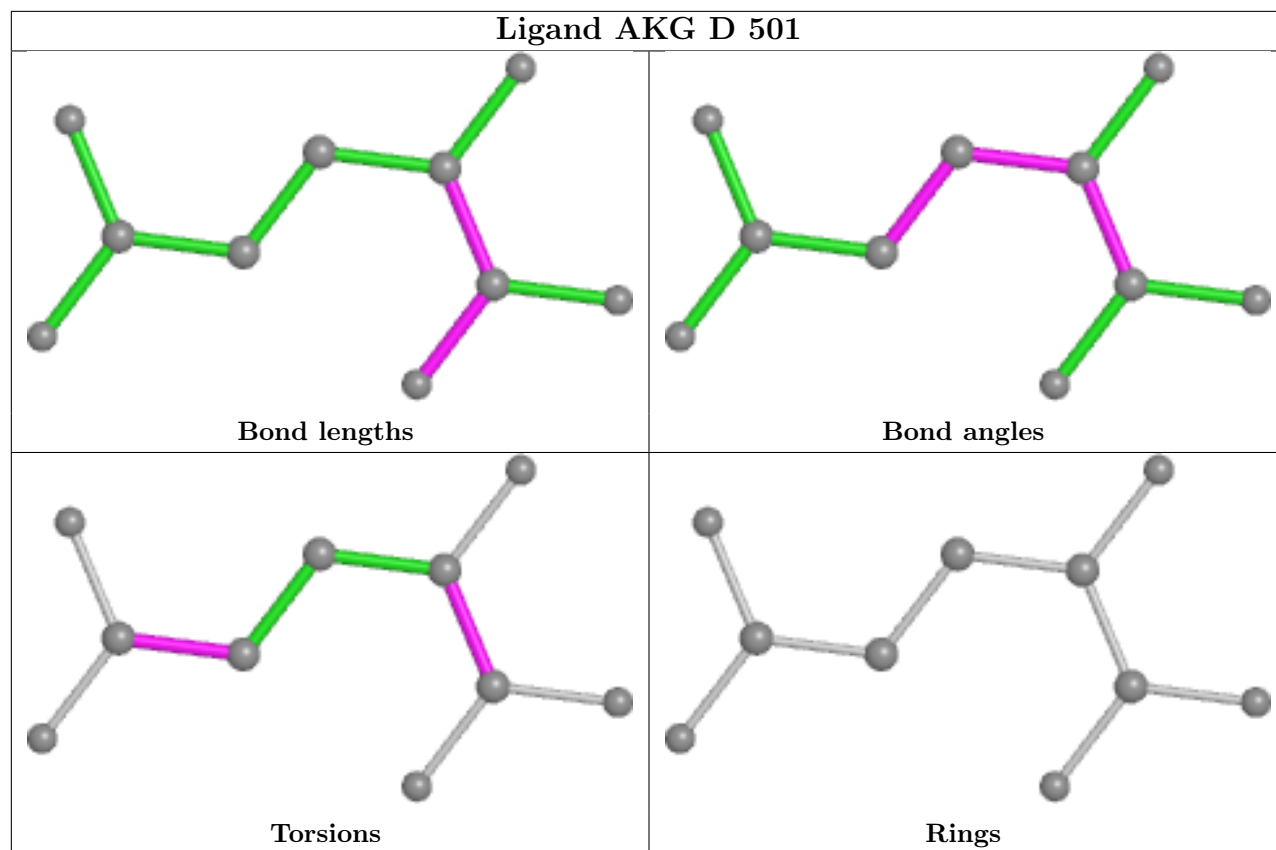












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	253/266 (95%)	-0.11	2 (0%) 86 85	22, 37, 70, 101	0
1	B	244/266 (91%)	-0.08	1 (0%) 92 92	21, 33, 62, 99	0
1	C	242/266 (90%)	-0.07	6 (2%) 57 53	27, 45, 88, 122	0
1	D	243/266 (91%)	0.08	8 (3%) 46 43	30, 44, 85, 110	0
1	E	246/266 (92%)	0.27	17 (6%) 16 13	28, 47, 118, 157	0
1	F	245/266 (92%)	0.18	13 (5%) 26 23	31, 52, 99, 181	0
1	G	244/266 (91%)	0.07	13 (5%) 26 23	31, 51, 103, 144	0
1	H	241/266 (90%)	0.56	30 (12%) 4 2	30, 58, 101, 126	0
All	All	1958/2128 (92%)	0.11	90 (4%) 32 30	21, 46, 95, 181	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	162	ALA	9.1
1	E	163	ASP	8.2
1	E	158	GLY	7.0
1	F	162	ALA	5.9
1	G	54	GLN	5.8
1	H	243	ARG	5.4
1	H	111	TRP	5.3
1	F	157	SER	5.3
1	D	263	ALA	5.3
1	E	160	ILE	5.2
1	H	168	GLY	5.2
1	H	253	ARG	5.2
1	H	241	VAL	5.1
1	C	163	ASP	4.9
1	E	178	LYS	4.7
1	E	161	ASP	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	263	ALA	4.6
1	C	243	ARG	4.3
1	H	160	ILE	4.2
1	F	161	ASP	4.1
1	G	57	GLY	4.1
1	H	179	TYR	4.0
1	G	160	ILE	3.9
1	H	121	HIS	3.8
1	E	159	MET	3.7
1	H	120	TRP	3.6
1	F	108	GLY	3.6
1	G	158	GLY	3.6
1	E	52	VAL	3.4
1	E	179	TYR	3.4
1	H	122	HIS	3.4
1	F	158	GLY	3.3
1	H	181	LEU	3.3
1	G	58	ILE	3.3
1	F	160	ILE	3.2
1	H	94	TYR	3.2
1	B	177	LEU	3.2
1	H	237	ASN	3.0
1	F	245	THR	3.0
1	G	177	LEU	3.0
1	H	242	THR	2.9
1	C	57	GLY	2.9
1	F	243	ARG	2.9
1	H	126	MET	2.8
1	C	160	ILE	2.8
1	D	111	TRP	2.8
1	D	177	LEU	2.7
1	H	25	HIS	2.7
1	E	241	VAL	2.7
1	E	244	GLY	2.6
1	G	163	ASP	2.6
1	E	243	ARG	2.6
1	F	163	ASP	2.6
1	G	161	ASP	2.6
1	H	233	ASN	2.5
1	E	157	SER	2.5
1	H	252	ALA	2.5
1	H	124	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	242	THR	2.4
1	F	111	TRP	2.4
1	H	245	THR	2.4
1	H	153	GLY	2.3
1	H	9	PRO	2.3
1	G	156	GLY	2.3
1	C	240	ASP	2.3
1	G	157	SER	2.3
1	H	251	ALA	2.3
1	F	119	PHE	2.3
1	E	55	ASN	2.2
1	F	240	ASP	2.2
1	H	96	HIS	2.2
1	D	127	PRO	2.2
1	G	111	TRP	2.2
1	D	235	VAL	2.2
1	D	241	VAL	2.2
1	G	55	ASN	2.2
1	E	253	ARG	2.2
1	E	245	THR	2.1
1	H	240	ASP	2.1
1	H	183	VAL	2.1
1	F	242	THR	2.1
1	G	56	THR	2.1
1	H	156	GLY	2.1
1	E	105	ALA	2.1
1	H	239	THR	2.1
1	H	123	GLU	2.1
1	A	111	TRP	2.1
1	C	52	VAL	2.0
1	A	168	GLY	2.0
1	D	56	THR	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 monosaccharides in this entry.

## 6.4 Ligands

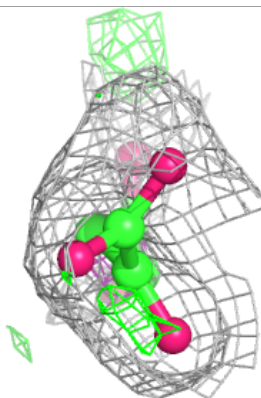
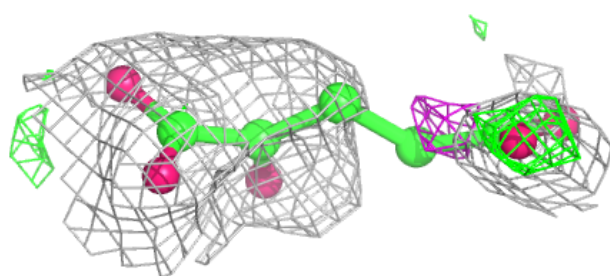
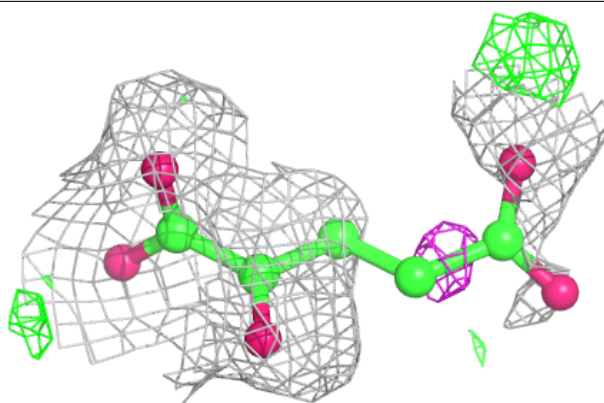
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AKG	C	501	10/10	0.77	0.27	56,79,99,99	0
2	AKG	H	501	10/10	0.79	0.27	61,78,94,95	0
4	PRO	H	503	8/8	0.82	0.43	62,69,78,78	0
2	AKG	B	501	10/10	0.84	0.25	38,60,80,80	0
4	PRO	G	503	8/8	0.87	0.24	72,78,79,85	0
4	PRO	F	503	8/8	0.88	0.26	54,67,70,72	0
4	PRO	D	503	8/8	0.89	0.17	50,54,59,60	0
4	PRO	C	503	8/8	0.91	0.29	75,85,93,94	0
2	AKG	D	501	10/10	0.91	0.20	30,60,81,85	0
2	AKG	F	501	10/10	0.91	0.26	34,61,98,102	0
2	AKG	A	501	10/10	0.91	0.20	42,58,69,73	0
4	PRO	B	502	8/8	0.91	0.21	36,39,43,46	0
4	PRO	E	503	8/8	0.92	0.34	71,74,75,76	0
4	PRO	A	503	8/8	0.93	0.16	44,47,49,50	0
2	AKG	G	501	10/10	0.93	0.21	52,72,107,109	0
2	AKG	E	501	10/10	0.94	0.24	42,65,101,117	0
3	FE	B	503	1/1	0.97	0.46	55,55,55,55	0
3	FE	H	502	1/1	0.98	0.15	51,51,51,51	0
3	FE	C	502	1/1	0.98	0.17	42,42,42,42	0
3	FE	F	502	1/1	0.98	0.15	42,42,42,42	0
3	FE	E	502	1/1	0.99	0.15	35,35,35,35	0
3	FE	A	502	1/1	0.99	0.18	29,29,29,29	0
3	FE	G	502	1/1	0.99	0.19	41,41,41,41	0
3	FE	D	502	1/1	0.99	0.19	35,35,35,35	0

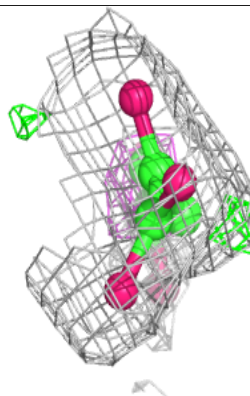
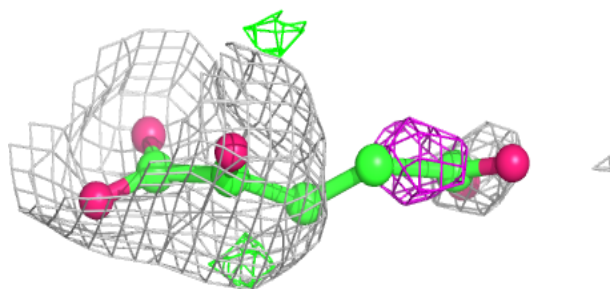
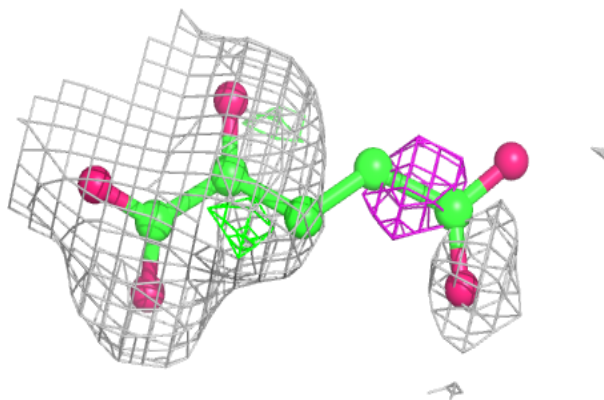
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AKG 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)

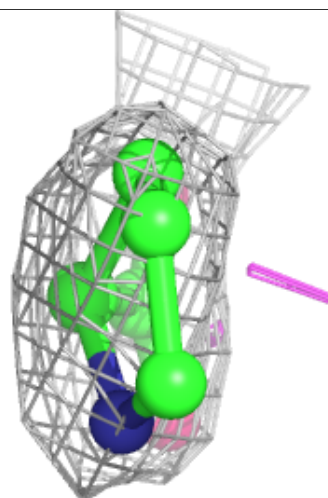
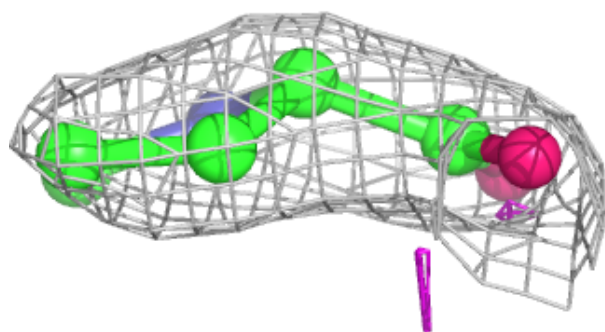
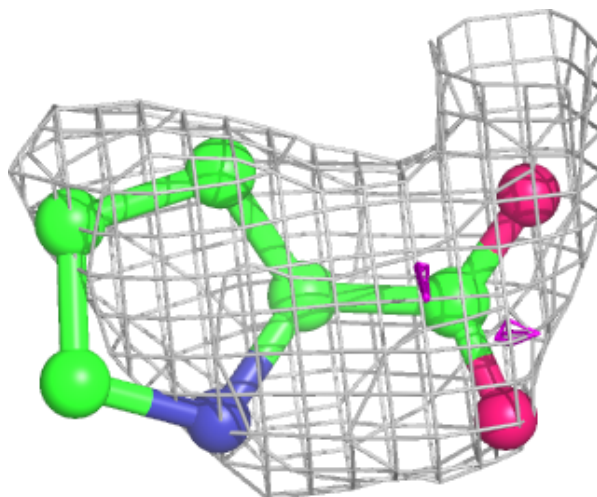
**Electron density around AKG H 501:**

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



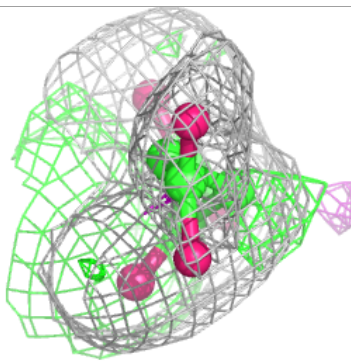
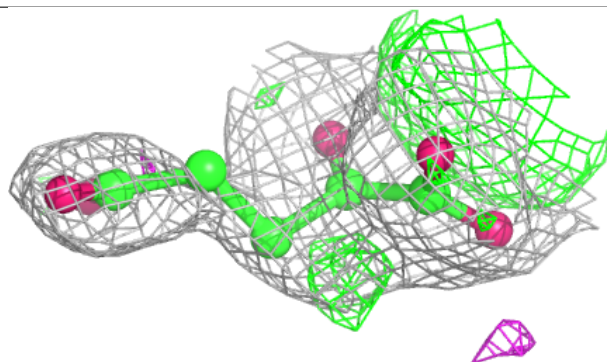
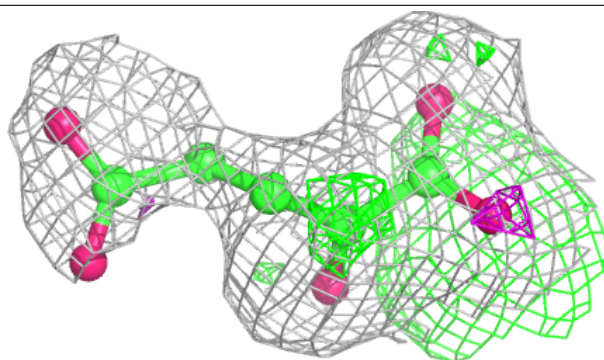
**Electron density around PRO H 503:**

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

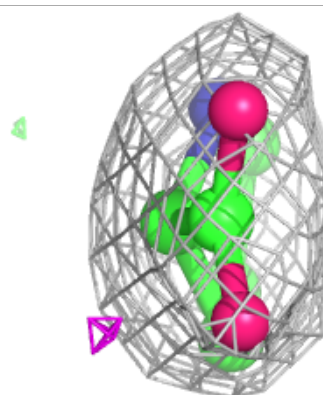
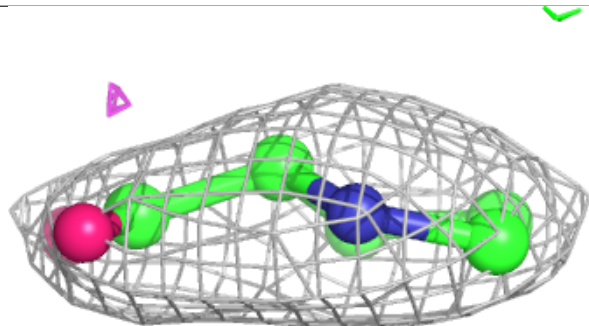
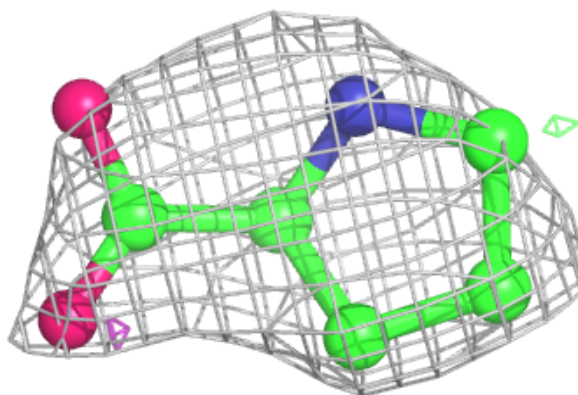


**Electron density around AKG B 501:**

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

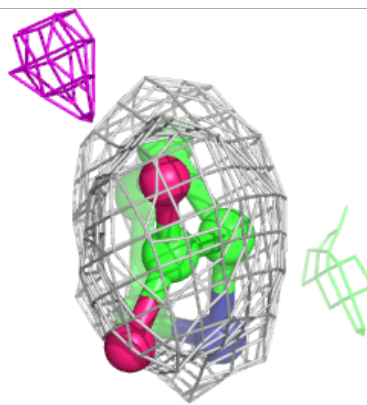
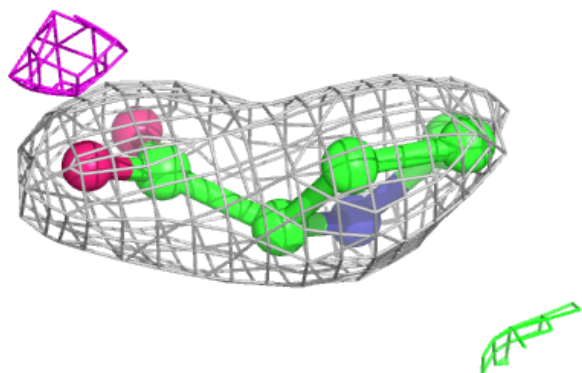
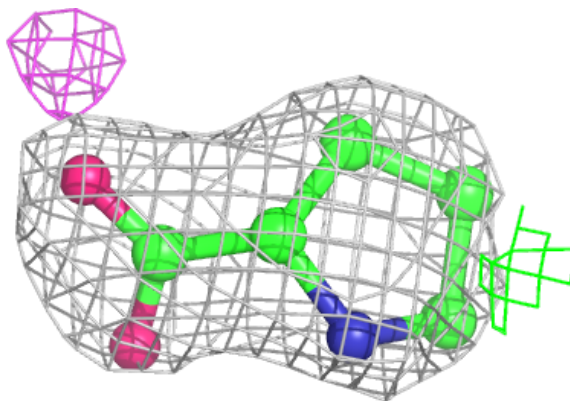
**Electron density around PRO G 503:**

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

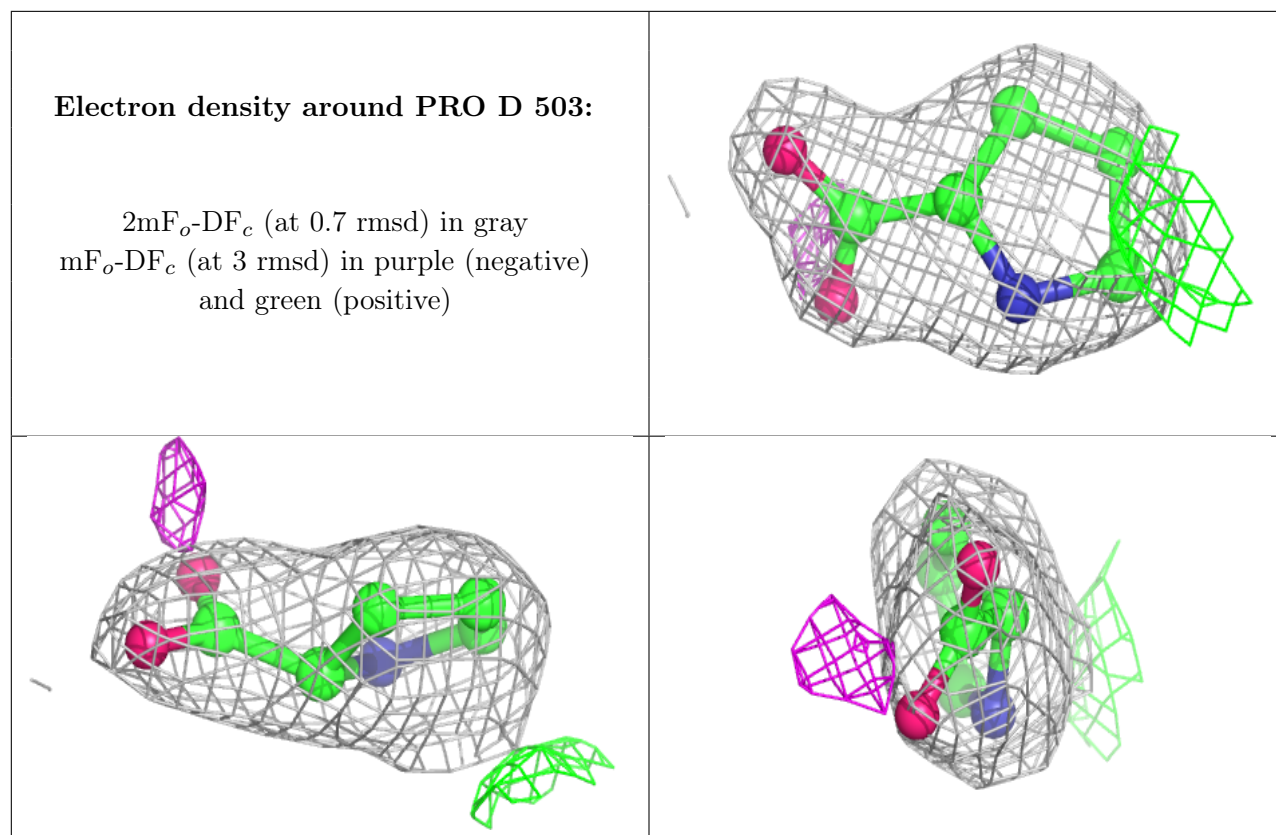


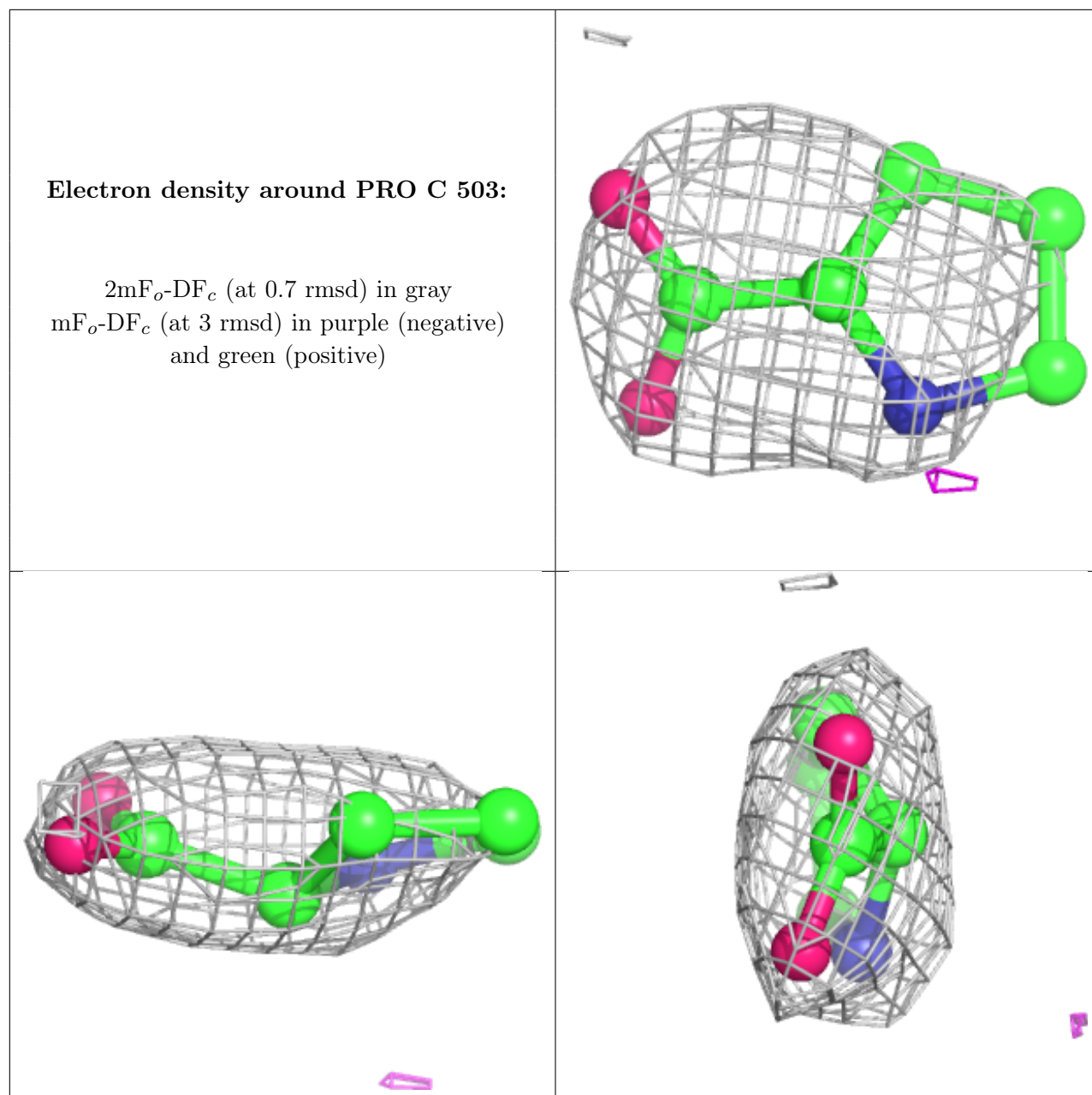
**Electron density around PRO F 503:**

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





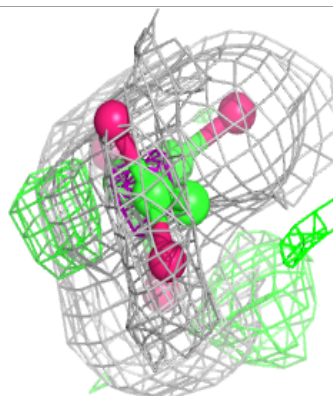
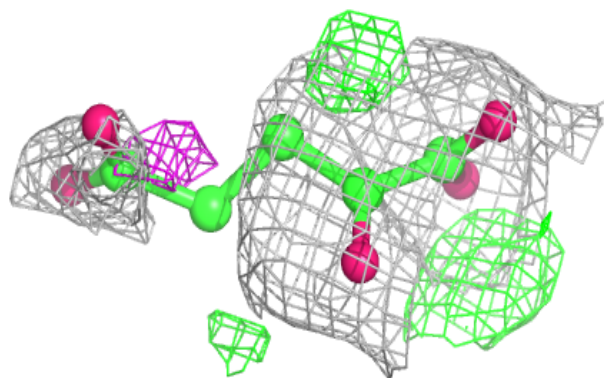
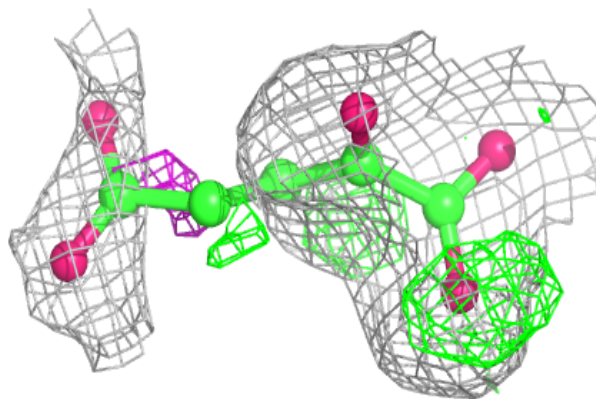




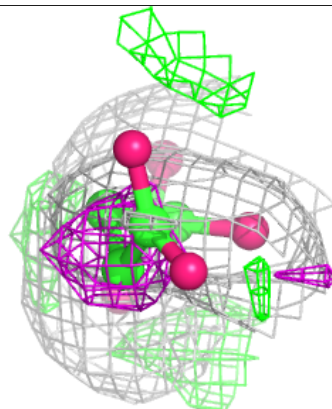
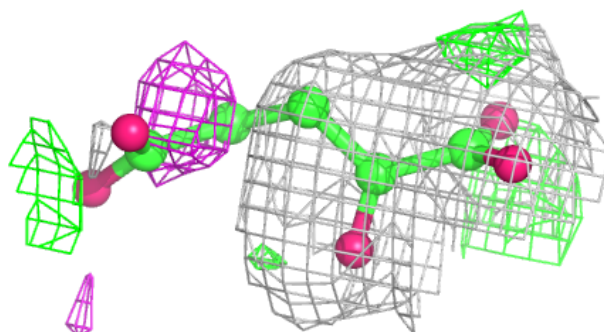
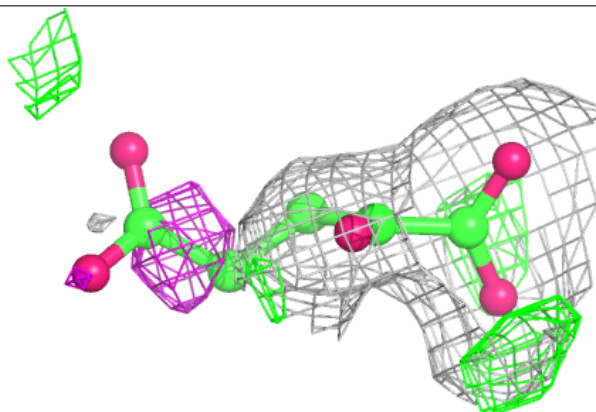


**Electron density around AKG D 501:**

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

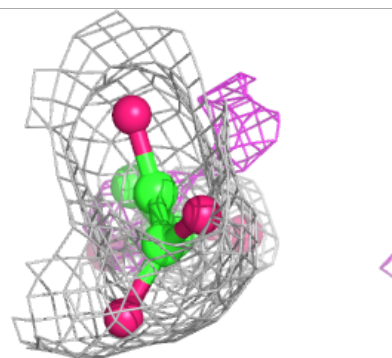
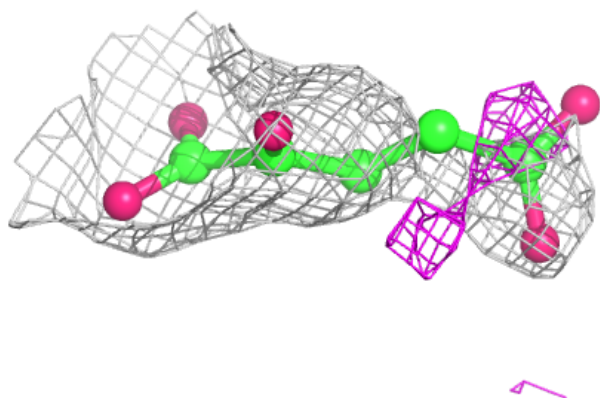
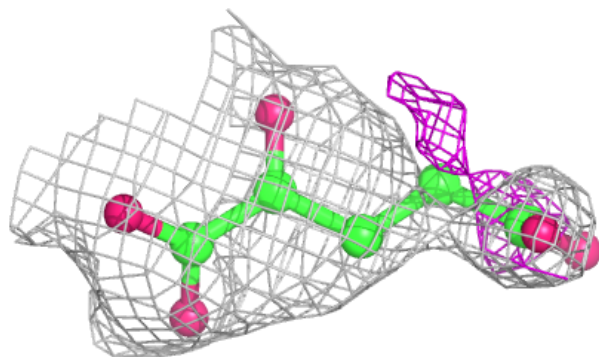
**Electron density around AKG F 501:**

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



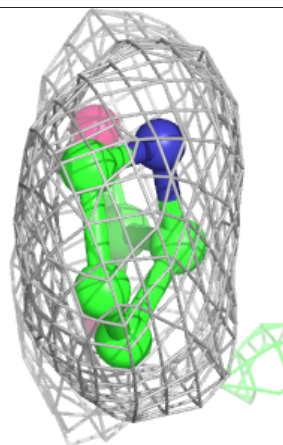
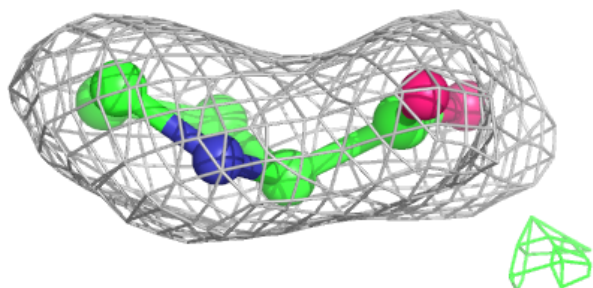
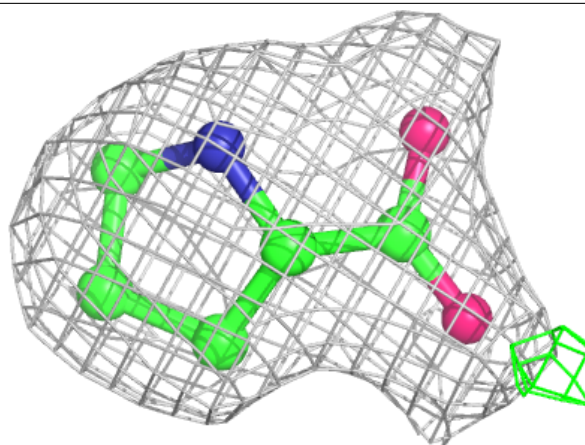
**Electron density around AKG A 501:**

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

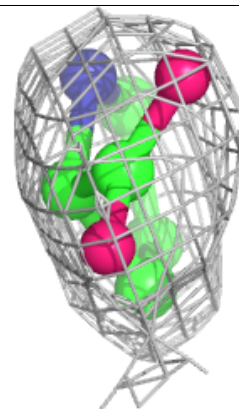
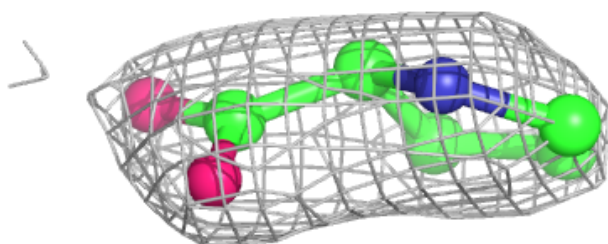
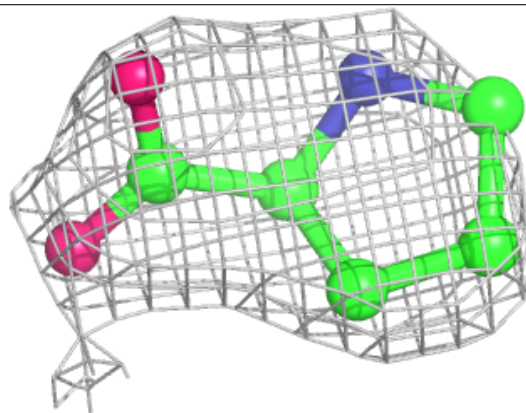


**Electron density around PRO B 502:**

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

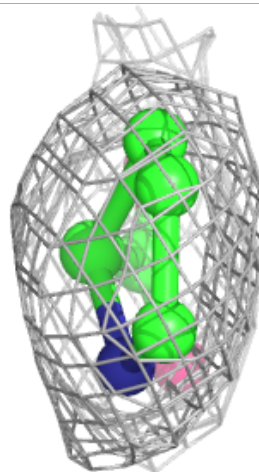
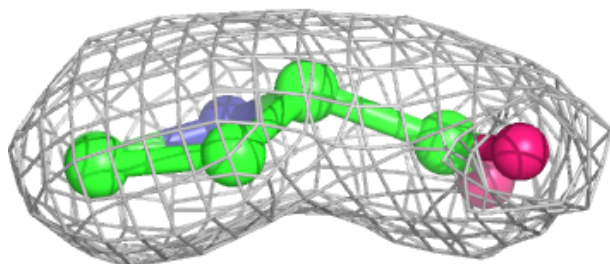
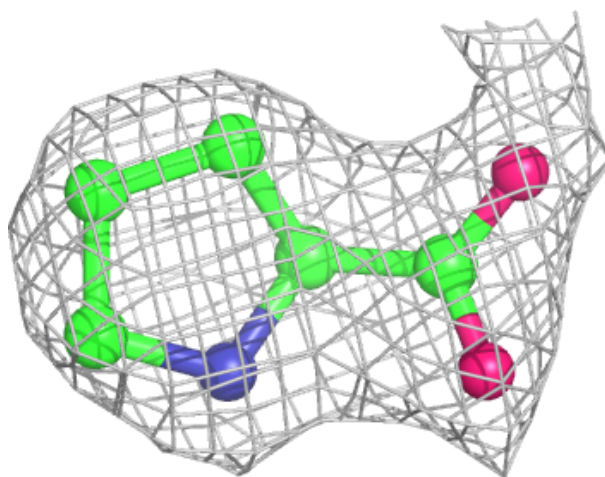
**Electron density around PRO E 503:**

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



**Electron density around PRO A 503:**

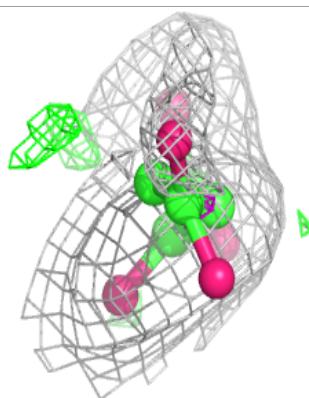
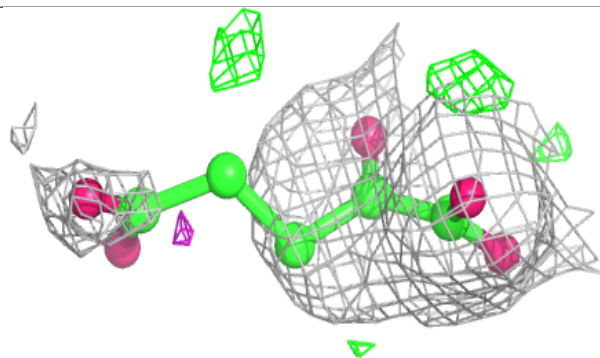
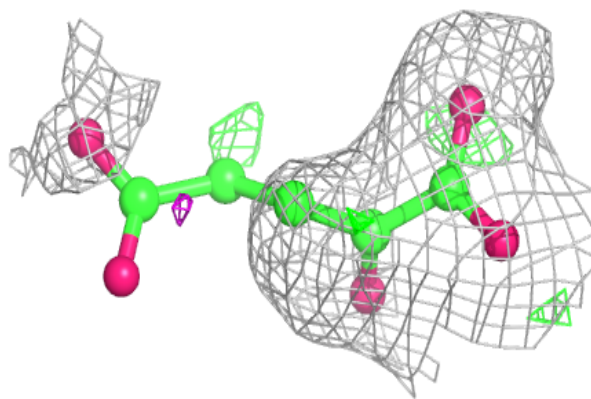
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



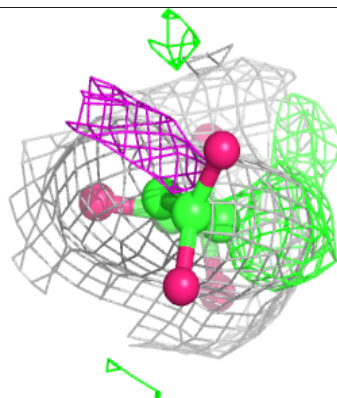
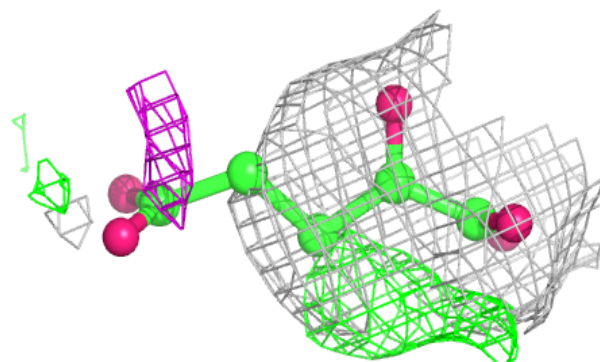
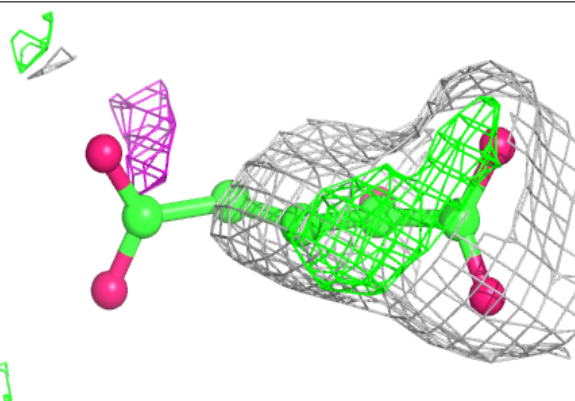


**Electron density around AKG G 501:**

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

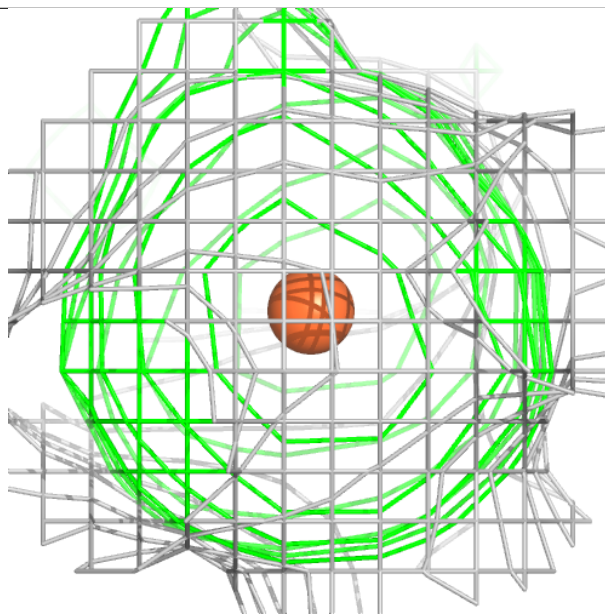
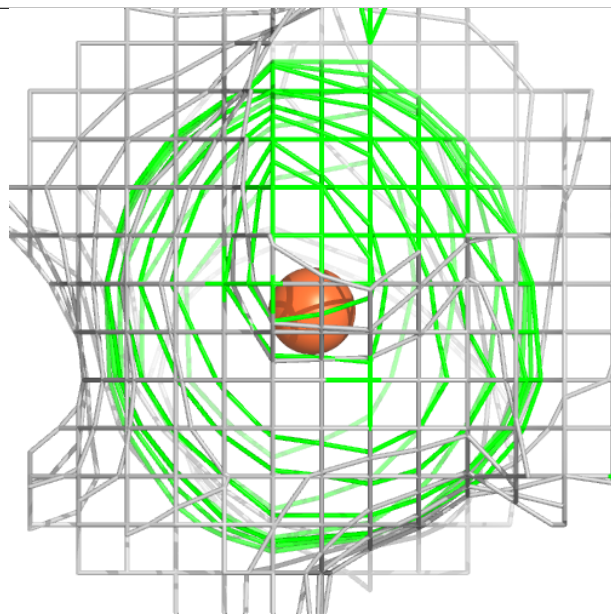
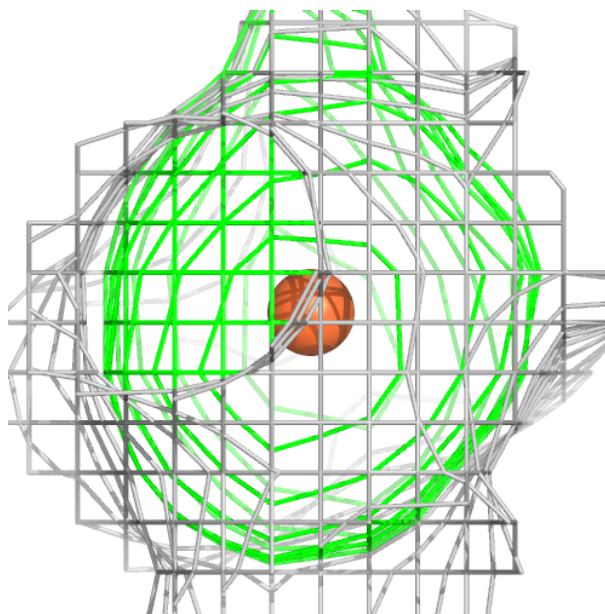
**Electron density around AKG E 501:**

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



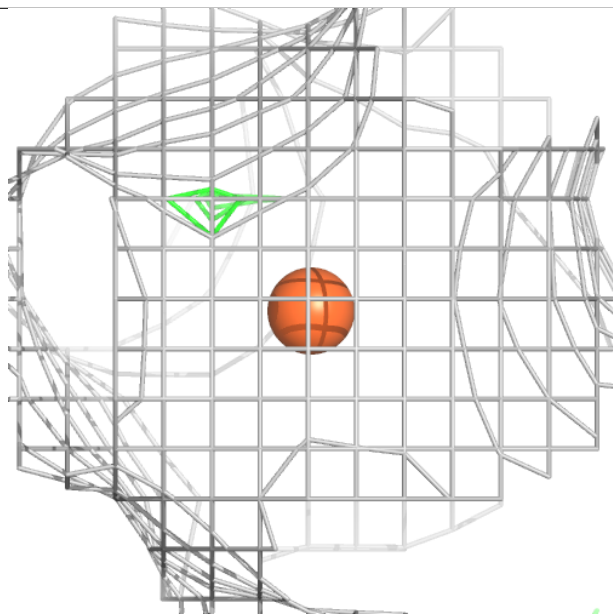
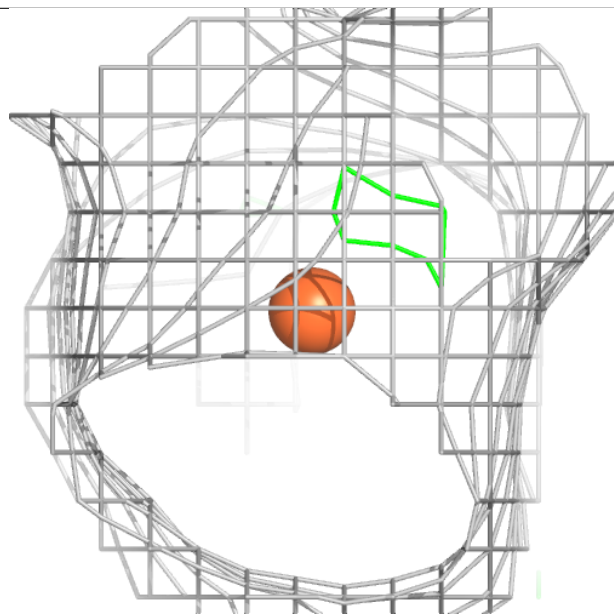
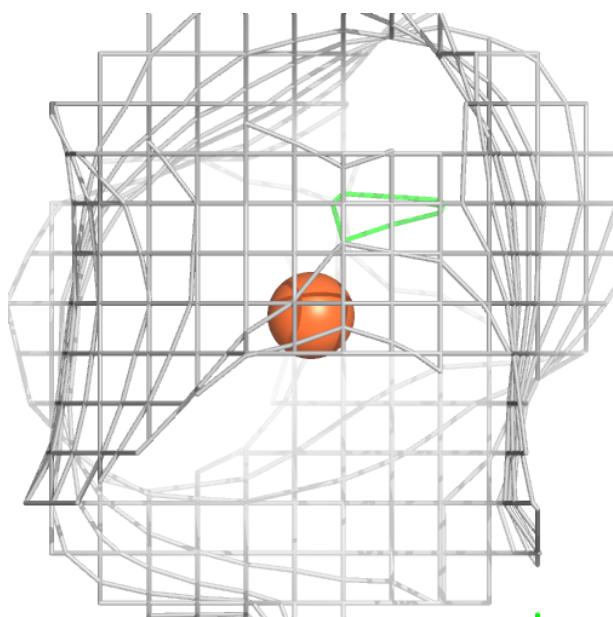
**Electron density around FE B 503:**

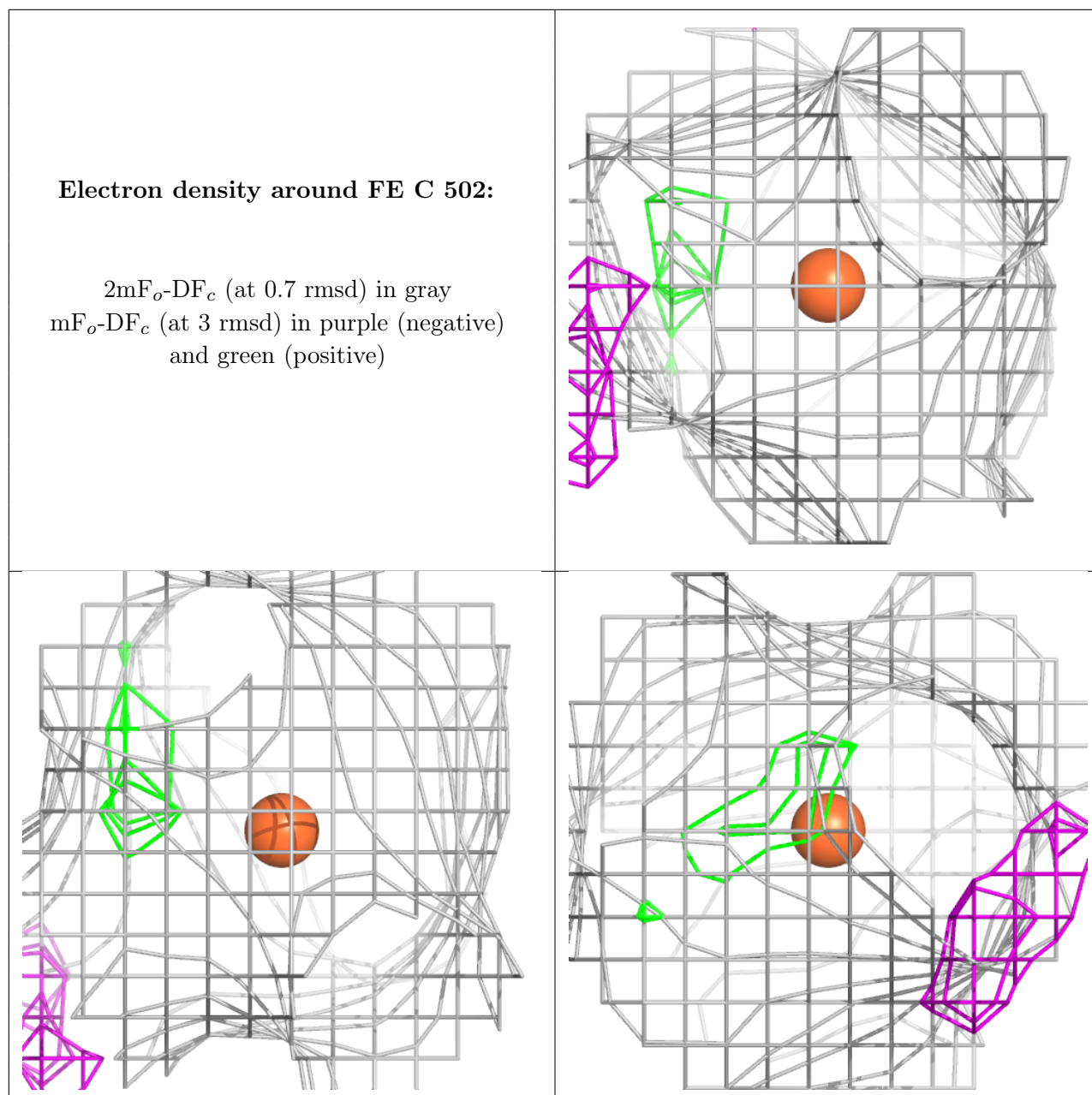
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



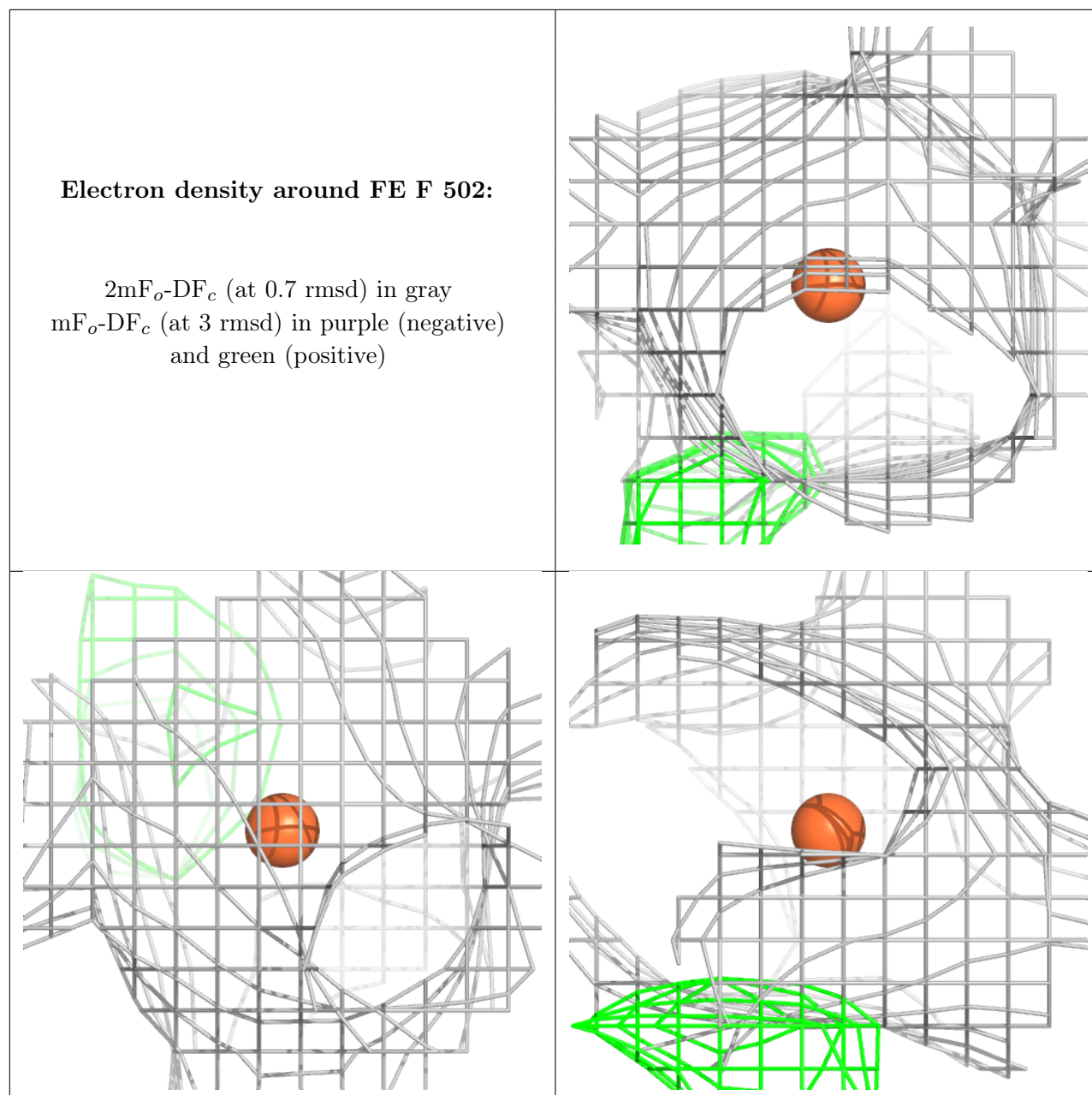
**Electron density around FE H 502:**

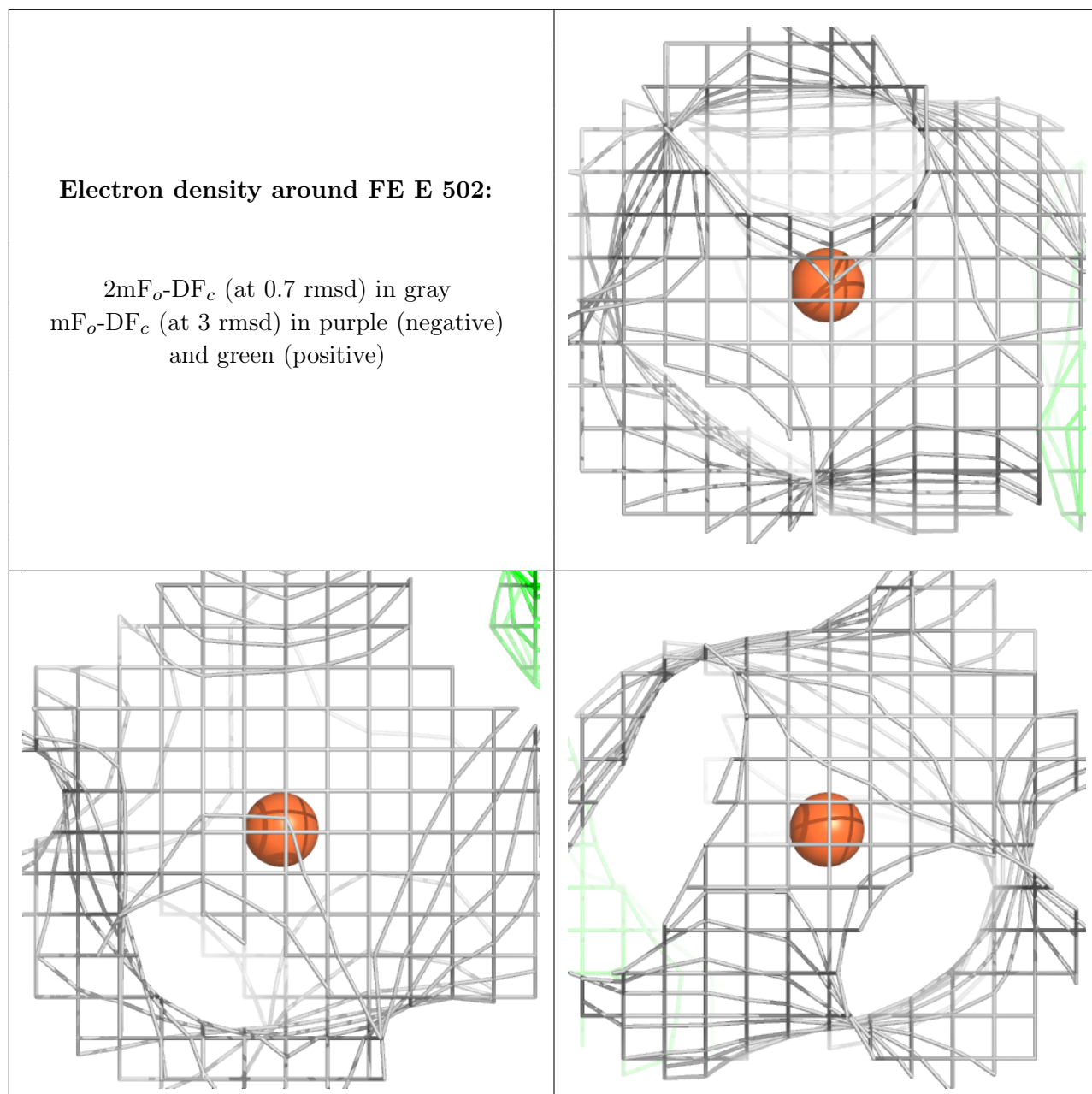
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





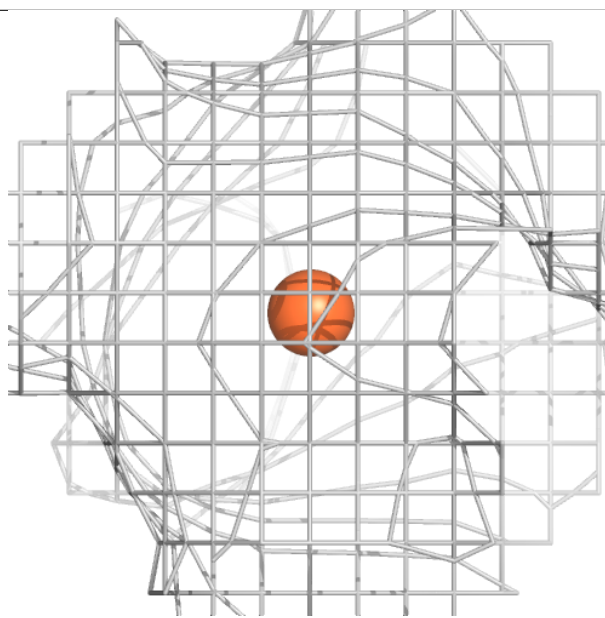
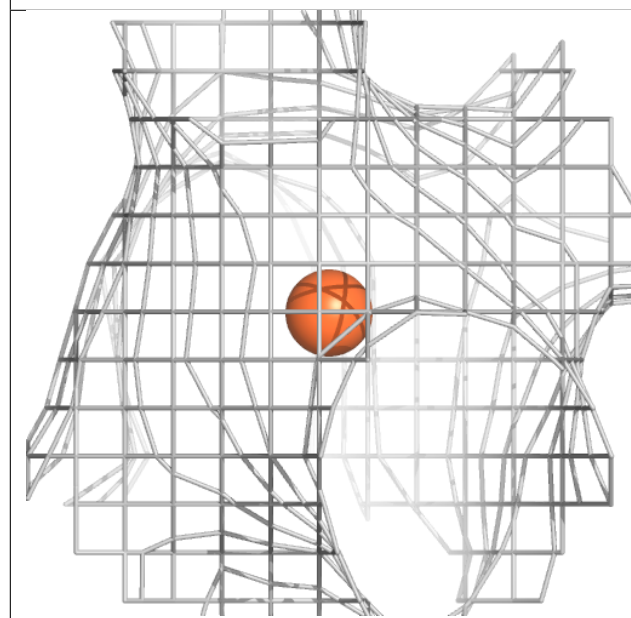
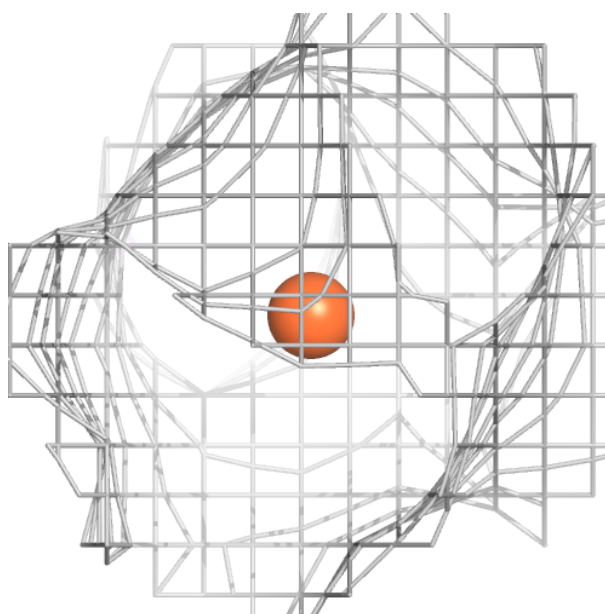






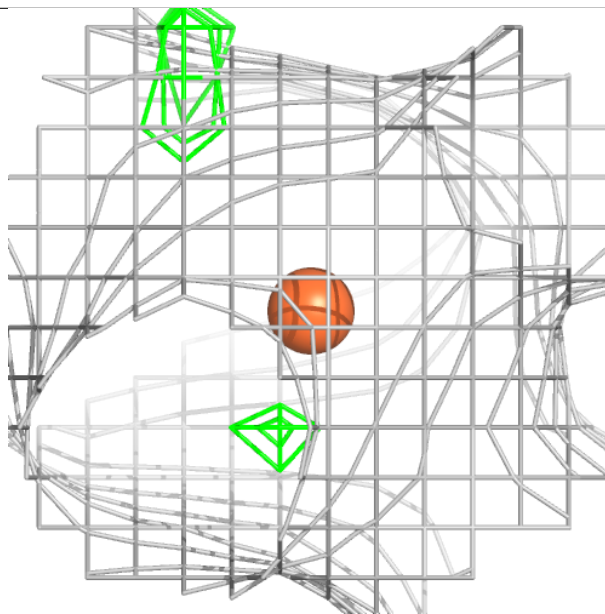
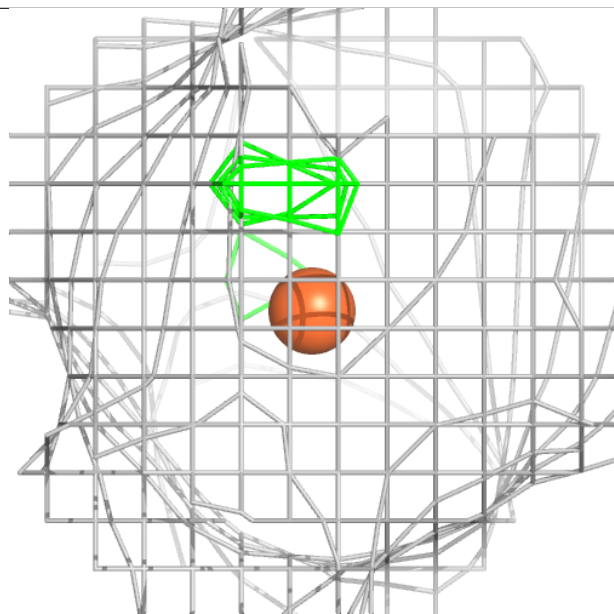
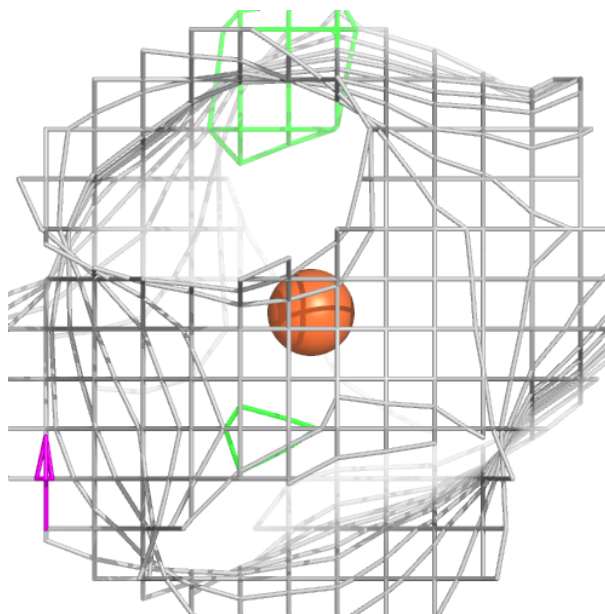
**Electron density around FE A 502:**

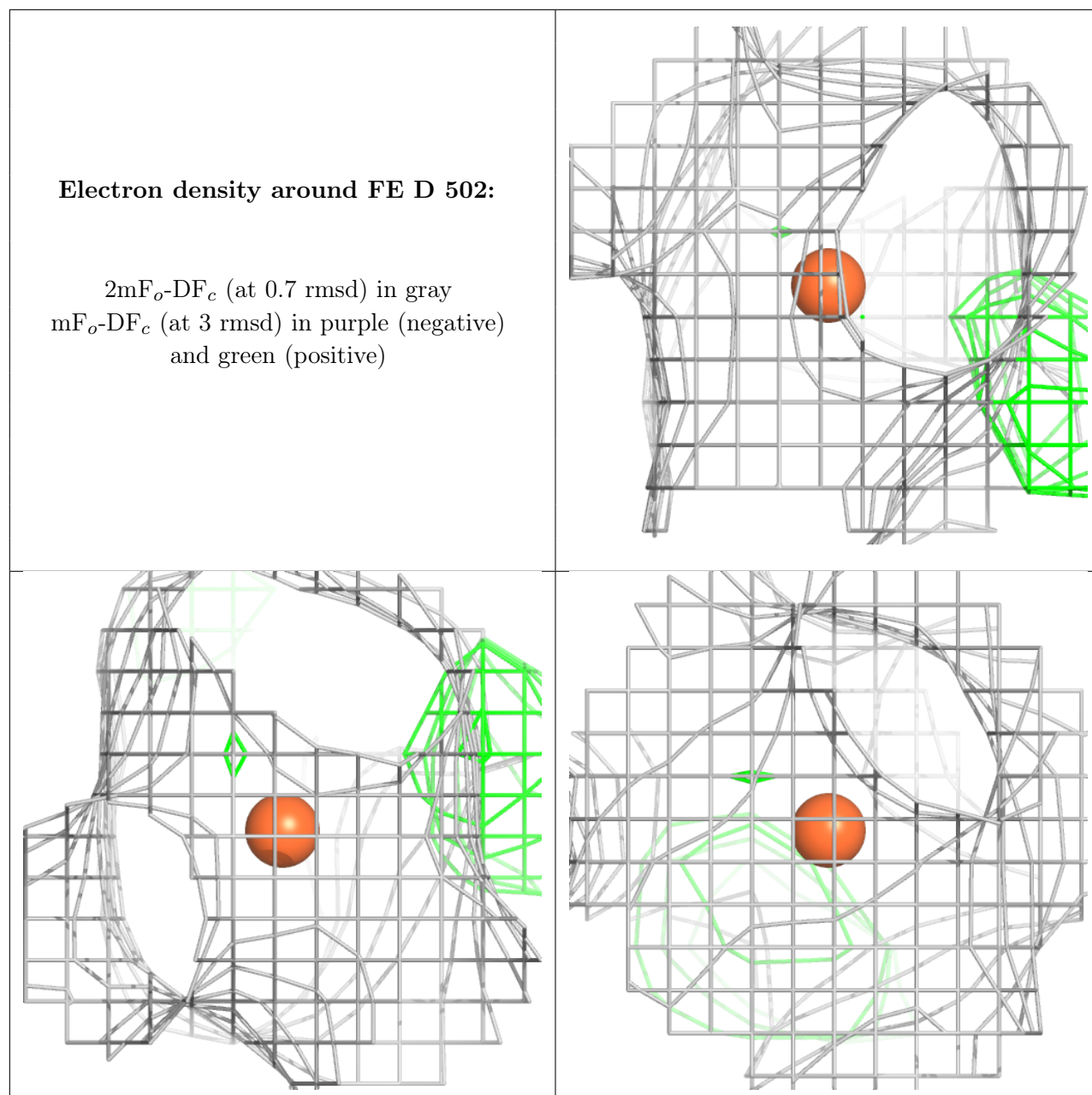
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE G 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.