

Full wwPDB X-ray Structure Validation Report (i)

Jan 11, 2022 – 09:14 pm GMT

PDB ID : 7PTM

Title: Crystal Structure of Two-Domain Laccase mutant M199G/R240H from Strep-

tomyces griseoflavus

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Deposited on : 2021-09-27

Resolution : 1.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

 $Xtriage\ (Phenix) \quad : \quad 1.13$

EDS : 2.24

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

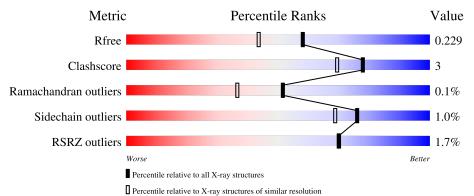
Validation Pipeline (wwPDB-VP) : 2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\mathring{A}))$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	284	92%	6%	-
1	В	284	92%	6%	-
1	С	284	90%	7%	-
1	D	284	89%	9%	-
1	Е	284	92%	6%	•



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$\operatorname{ol} \mid \operatorname{C}$	Chain	Length	Quality of chain	
	E	201	2%	 _
	${ m F}$	284	88%	8%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13699 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 Two-domain laccase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	278	Total	С	N	Ο	S	0	4	0
1	A	210	2158	1347	392	407	12	U	4	
1	В	278	Total	С	N	О	S	0	1	0
1	Ъ	210	2133	1331	389	402	11	U	1	
1	С	275	Total	С	N	О	S	0	3	0
1		210	2130	1328	389	402	11	U		
1	D	277	Total	С	N	О	S	0	5	0
1	ט	211	2160	1348	392	407	13	U	3	
1	Е	279	Total	С	N	О	S	0	3	0
1	l Li	219	2156	1345	395	405	11	U	3	
1	F	275	Total	С	N	О	S	0	2	0
1	I.	210	2122	1324	387	400	11	0		

There are 12 discrepancies between the modelled and reference sequences:

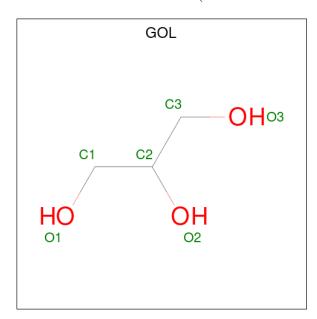
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
A	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
В	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
В	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
С	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
С	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
D	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
D	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
Е	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
Е	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81
F	199	GLY	MET	engineered mutation	UNP A0A0M4FJ81
F	240	HIS	ARG	engineered mutation	UNP A0A0M4FJ81

• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cu 4 4	0	0
2	В	4	Total Cu 4 4	0	0
2	С	4	Total Cu 4 4	0	0
2	D	5	Total Cu 5 5	0	0
2	E	4	Total Cu 4 4	0	0
2	F	3	Total Cu 3 3	0	0

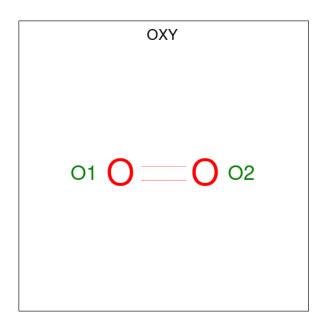
• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

• Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	В	1	Total O 2 2	0	0
4	С	1	Total O 2 2	0	0
4	D	1	Total O 2 2	0	0
4	D	1	Total O 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total O 131 131	0	0
5	В	144	Total O 144 144	0	0
5	С	129	Total O 129 129	0	0
5	D	135	Total O 135 135	0	0
5	Е	114	Total O 114 114	0	0
5	F	147	Total O 147 147	0	0

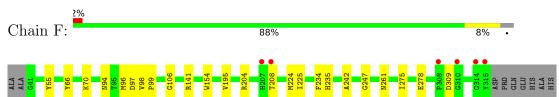


3 Residue-property plots (i)

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



 \bullet Molecule 1: Two-domain laccase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	74.06Å 93.73Å 119.23Å	Depositor
a, b, c, α , β , γ	90.00° 91.30° 90.00°	Depositor
Resolution (Å)	24.68 - 1.85	Depositor
resolution (A)	24.68 - 1.85	EDS
% Data completeness	99.2 (24.68-1.85)	Depositor
(in resolution range)	99.2 (24.68-1.85)	EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.53 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0230, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.183 , 0.224	Depositor
it, it _{free}	0.188 , 0.229	DCC
R_{free} test set	6895 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13699	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: OXY, GOL, CU

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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.40	0/2221	0.68	0/3018
1	В	0.41	0/2196	0.67	0/2985
1	С	0.40	0/2192	0.65	0/2978
1	D	0.40	0/2223	0.65	0/3020
1	Е	0.38	0/2219	0.65	0/3016
1	F	0.41	0/2184	0.67	0/2967
All	All	0.40	0/13235	0.66	0/17984

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2158	0	2022	15	0
1	В	2133	0	1999	12	0
1	С	2130	0	1993	11	0
1	D	2160	0	2023	20	0
1	Е	2156	0	2024	10	0
1	F	2122	0	1988	14	0
2	A	4	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	4	0	0	0	0
2	С	4	0	0	0	0
2	D	5	0	0	0	0
2	Ε	4	0	0	0	0
2	F	3	0	0	0	0
3	A	6	0	8	1	0
4	A	2	0	0	0	0
4	В	2	0	0	0	0
4	С	2	0	0	1	0
4	D	4	0	0	0	0
5	A	131	0	0	2	0
5	В	144	0	0	3	0
5	С	129	0	0	2	0
5	D	135	0	0	3	0
5	Ε	114	0	0	1	0
5	F	147	0	0	2	0
All	All	13699	0	12057	72	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 3.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:297:MET:HE1	1:D:198:ASP:HB3	1.57	0.86
5:B:594:HOH:O	1:D:171:ARG:HD2	1.91	0.71
1:D:94:ASN:OD1	1:D:96:MET:HB2	1.89	0.70
1:A:64:MET:HG2	1:A:96:MET:SD	2.33	0.68
1:D:118:GLN:HE22	1:E:302:LEU:HD21	1.59	0.67
1:A:229:GLU:OE2	1:B:293:SER:N	2.27	0.65
1:A:51:ARG:HH11	1:A:51:ARG:HG3	1.64	0.63
1:A:55:TYR:OH	1:A:70:LYS:HE3	1.99	0.63
1:A:94:ASN:OD1	1:A:96:MET:HB2	2.00	0.62
1:B:117:LYS:HE2	1:F:97:ASP:OD2	2.00	0.61
1:C:57:GLU:OE2	1:C:71:GLY:N	2.30	0.60
1:D:257:GLN:HG3	5:D:609:HOH:O	2.02	0.59
1:D:293:SER:O	1:D:297[A]:MET:HG2	2.03	0.59
1:D:257:GLN:CG	5:D:609:HOH:O	2.50	0.58
1:D:248:MET:HE1	1:F:141:ARG:HH12	1.68	0.58
1:E:294:HIS:O	1:E:299:MET:HB2	2.04	0.57
1:D:293:SER:O	1:D:297[B]:MET:HG2	2.04	0.57



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Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance} (\mathring{\rm A})$	overlap(Å)	
1:D:118:GLN:NE2	1:E:302:LEU:HD21	2.20	0.57	
1:A:165:HIS:HD2	5:B:512:HOH:O	1.88	0.56	
1:D:45:ALA:HB2	1:D:183:LYS:HD2	1.89	0.55	
1:B:237:HIS:CE1	1:B:286:MET:HE2	2.43	0.53	
1:A:51:ARG:HG3	1:A:51:ARG:NH1	2.23	0.53	
1:C:236:MET:HE2	1:C:239:HIS:HB2	1.90	0.53	
1:E:237:HIS:CE1	1:E:286:MET:HE2	2.45	0.52	
1:C:160:VAL:HG12	5:C:501:HOH:O	2.11	0.50	
1:E:51:ARG:NH1	1:E:91:GLU:OE2	2.44	0.50	
1:D:257:GLN:HA	5:D:609:HOH:O	2.11	0.49	
1:C:234:PHE:O	1:C:261:ASN:HA	2.12	0.49	
1:C:45:ALA:HB2	1:C:183:LYS:HD2	1.95	0.48	
1:F:235:HIS:HB2	1:F:261:ASN:OD1	2.13	0.48	
1:F:70:LYS:HE2	5:F:557:HOH:O	2.13	0.48	
1:A:165:HIS:HE1	5:A:627:HOH:O	1.97	0.48	
1:D:159:HIS:CE1	1:E:286:MET:HE1	2.49	0.48	
1:D:204:ARG:HD3	1:D:210:PRO:HD3	1.95	0.47	
1:B:207:HIS:HE1	5:B:594:HOH:O	1.97	0.47	
1:B:98:VAL:HG12	1:F:99:PRO:HD2	1.95	0.47	
1:C:242:ALA:O	1:C:247:GLY:HA2	2.14	0.46	
1:F:204:ARG:NH2	1:F:208:THR:O	2.44	0.46	
1:A:159:HIS:CE1	1:B:286:MET:HE1	2.51	0.46	
1:F:94:ASN:OD1	1:F:96:MET:HB2	2.15	0.46	
1:D:300[A]:VAL:HG13	5:F:560:HOH:O	2.15	0.45	
1:E:106:GLY:HA3	1:E:154:TRP:CD2	2.52	0.45	
1:A:306:LYS:HE3	1:A:306:LYS:HB2	1.83	0.44	
1:C:117:LYS:HB2	1:C:117:LYS:HE2	1.54	0.43	
1:D:52:VAL:HG21	1:D:68:LEU:HD13	2.00	0.43	
1:A:182:ARG:HD2	5:A:503:HOH:O	2.17	0.43	
1:C:290:HIS:NE2	4:C:405:OXY:O1	2.51	0.43	
1:D:195:VAL:HG22	1:D:225:ILE:HB	2.00	0.43	
1:E:128:THR:HB	5:E:565:HOH:O	2.17	0.43	
1:A:246:THR:HG22	3:A:403:GOL:H11	2.01	0.42	
1:F:275:ILE:HB	1:F:278:GLU:HB2	2.00	0.42	
1:B:106:GLY:HA3	1:B:154:TRP:CD2	2.55	0.42	
1:B:242:ALA:O	1:B:247:GLY:HA2	2.19	0.42	
1:E:195:VAL:HA	1:E:225:ILE:O	2.20	0.42	
1:F:97:ASP:OD1	1:F:98:VAL:HG13	2.20	0.42	
1:F:106:GLY:HA3	1:F:154:TRP:CD2	2.54	0.42	
1:D:289:CYS:O	1:D:295:SER:HB3	2.19	0.42	
1:E:275:ILE:HB	1:E:278:GLU:HB2	2.02	0.42	



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\left(\operatorname{\mathring{A}} ight)$	overlap (Å)
1:C:275:ILE:HB	1:C:278:GLU:HB2	2.02	0.42
1:F:195:VAL:HA	1:F:225:ILE:O	2.20	0.42
1:C:175:TYR:HB2	5:C:504:HOH:O	2.18	0.41
1:B:233:THR:O	1:B:289:CYS:HA	2.19	0.41
1:F:242:ALA:O	1:F:247:GLY:HA2	2.20	0.41
1:C:156:TYR:CZ	1:C:176:GLY:HA3	2.56	0.41
1:F:234:PHE:O	1:F:261:ASN:HA	2.20	0.41
1:F:55:TYR:O	1:F:66:TYR:HA	2.21	0.41
1:D:52:VAL:CG2	1:D:68:LEU:HD13	2.51	0.41
1:A:70:LYS:HD2	1:A:70:LYS:H	1.85	0.41
1:A:234:PHE:O	1:A:261:ASN:HA	2.21	0.41
1:D:106:GLY:HA3	1:D:154:TRP:CD2	2.56	0.40
1:A:111[B]:ILE:HG21	1:B:283:GLY:HA3	2.03	0.40
1:B:286:MET:HE2	1:B:286:MET:HB2	1.89	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	Perce	ntiles
1	A	280/284~(99%)	271 (97%)	9 (3%)	0	100	100
1	В	277/284 (98%)	273 (99%)	4 (1%)	0	100	100
1	С	276/284 (97%)	270 (98%)	6 (2%)	0	100	100
1	D	280/284 (99%)	276 (99%)	4 (1%)	0	100	100
1	E	280/284 (99%)	272 (97%)	7 (2%)	1 (0%)	34	19
1	F	275/284 (97%)	271 (98%)	4 (2%)	0	100	100
All	All	1668/1704 (98%)	1633 (98%)	34 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type	
1	${ m E}$	143	ASP	

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	$222/222 \ (100\%)$	221 (100%)	1 (0%)	88 86
1	В	219/222 (99%)	215 (98%)	4 (2%)	59 45
1	С	219/222 (99%)	217 (99%)	2 (1%)	78 72
1	D	223/222 (100%)	221 (99%)	2 (1%)	78 72
1	Е	221/222 (100%)	219 (99%)	2 (1%)	78 72
1	F	218/222 (98%)	216 (99%)	2 (1%)	78 72
All	All	1322/1332 (99%)	1309 (99%)	13 (1%)	76 69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	MET
1	В	118	GLN
1	В	224	MET
1	В	240	HIS
1	В	316	ASP
1	С	224	MET
1	С	297	MET
1	D	72	LYS
1	D	224	MET
1	Е	117	LYS
1	Е	224	MET
1	F	224	MET
1	F	309	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:



Mol	Chain	Res	Type
1	В	207	HIS
1	D	118	GLN

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 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Trme	Chain	Res	Link Bond lengths			В	ond ang	gles	
Mol	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	OXY	A	404	2	1,1,1	0.13	0	-		
3	GOL	A	403	-	5,5,5	0.91	0	5,5,5	1.31	0
4	OXY	С	405	2	1,1,1	0.15	0	-		
4	OXY	D	404	2	1,1,1	0.20	0	-		
4	OXY	В	403	2	1,1,1	0.18	0	-		
4	OXY	D	407	2	1,1,1	0.13	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	403	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	A	403	GOL	O1-C1-C2-O2

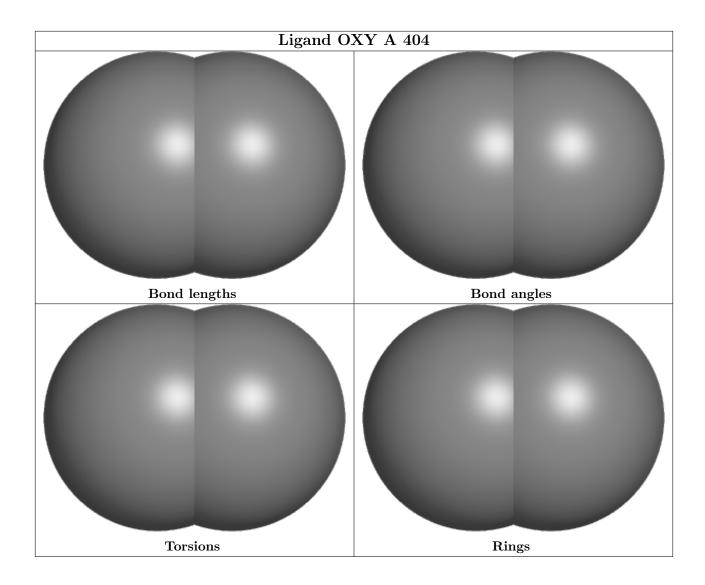
There are no ring outliers.

2 monomers are involved in 2 short contacts:

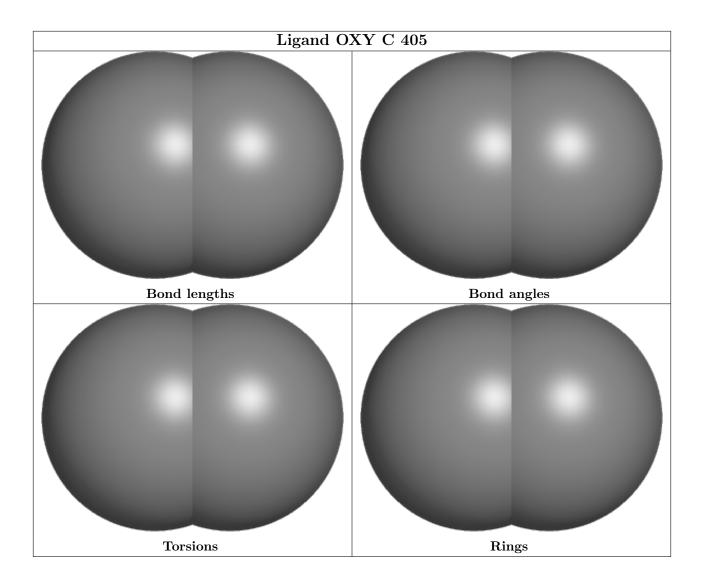
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	GOL	1	0
4	С	405	OXY	1	0

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 then 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.

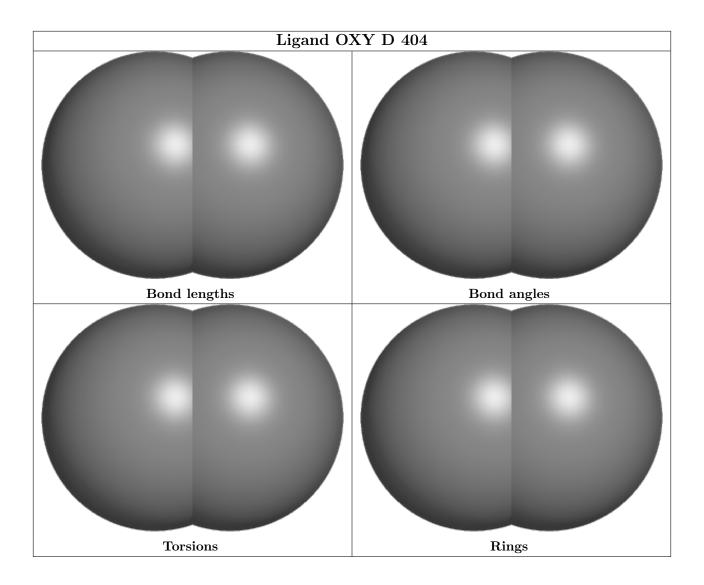




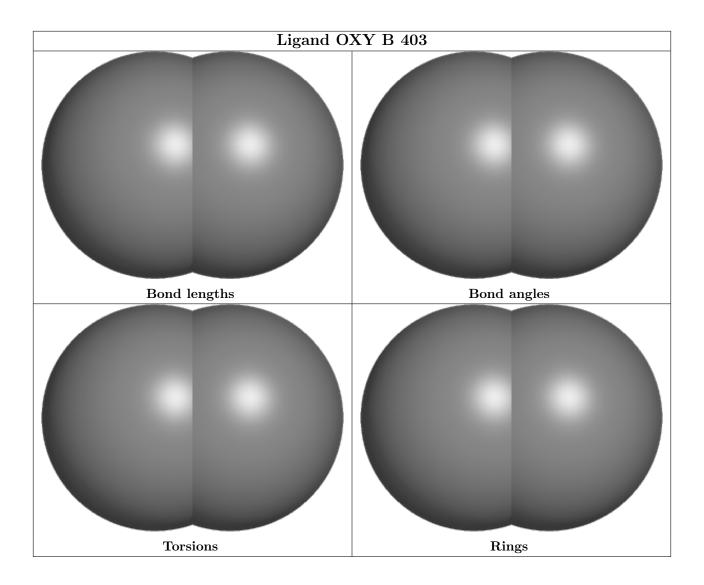




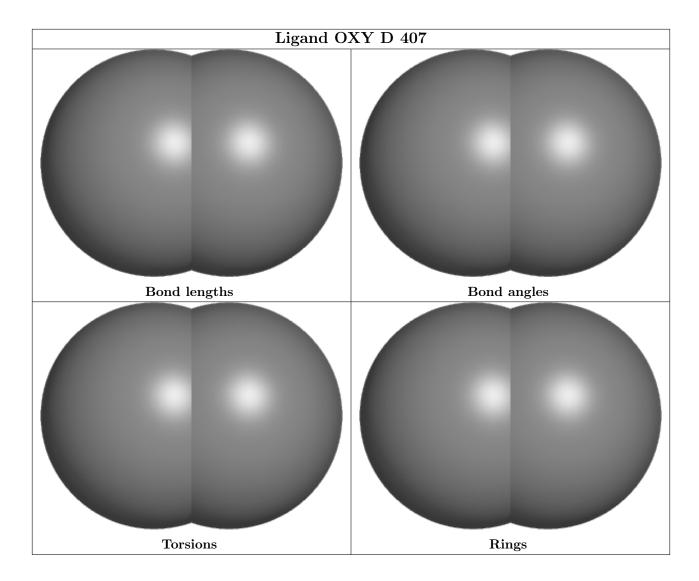












5.7 Other polymers (i)

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 (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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	278/284 (97%)	-0.24	3 (1%) 80 81	8, 15, 30, 46	0
1	В	278/284 (97%)	-0.20	6 (2%) 62 61	8, 14, 28, 67	0
1	С	275/284 (96%)	-0.18	2 (0%) 87 88	8, 17, 30, 38	1 (0%)
1	D	277/284 (97%)	-0.19	4 (1%) 75 76	7, 16, 30, 44	0
1	E	279/284 (98%)	0.02	8 (2%) 51 50	9, 18, 33, 66	1 (0%)
1	F	275/284 (96%)	-0.25	6 (2%) 62 61	7, 14, 28, 44	2 (0%)
All	All	1662/1704 (97%)	-0.17	29 (1%) 70 70	7, 16, 30, 67	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	39	ALA	12.7
1	Е	40	ALA	10.1
1	В	317	PRO	7.8
1	В	40	ALA	6.4
1	Е	317	PRO	5.6
1	В	316	ASP	4.3
1	Е	142	ALA	4.2
1	Е	316	ASP	4.1
1	A	40	ALA	4.0
1	Е	41	GLY	2.9
1	A	142	ALA	2.9
1	С	314	GLY	2.8
1	F	314	GLY	2.7
1	F	208	THR	2.7
1	В	142	ALA	2.6
1	D	142	ALA	2.6
1	A	308	PRO	2.6
1	D	144	GLY	2.6
1	В	208	THR	2.6



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Mol	Chain	Res	Type	RSRZ
1	F	207	HIS	2.6
1	F	310	GLY	2.5
1	В	314	GLY	2.4
1	D	51	ARG	2.4
1	С	61	GLY	2.4
1	Е	119	ASN	2.2
1	Е	313	PRO	2.1
1	D	143	ASP	2.1
1	F	308	PRO	2.1
1	F	315	TYR	2.1

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 (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, 95^{th} 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	$\operatorname{B-factors}({\rm \AA}^2)$	Q<0.9
2	CU	В	405	1/1	0.88	0.32	15,15,15,15	1
3	GOL	A	403	6/6	0.91	0.13	18,21,27,31	0
2	CU	D	403	1/1	0.93	0.54	8,8,8,8	1
2	CU	Ε	403	1/1	0.94	0.13	14,14,14,14	1
2	CU	D	406	1/1	0.94	0.13	19,19,19,19	1
2	CU	В	404	1/1	0.95	0.12	12,12,12,12	1
4	OXY	A	404	2/2	0.95	0.10	23,23,23,25	0
4	OXY	D	404	2/2	0.95	0.10	13,13,13,18	0
4	OXY	D	407	2/2	0.95	0.12	22,22,22,26	0
2	CU	A	406	1/1	0.96	0.18	17,17,17,17	1
2	CU	Е	404	1/1	0.96	0.18	19,19,19,19	1
4	OXY	В	403	2/2	0.97	0.11	19,19,19,21	0
4	OXY	С	405	2/2	0.97	0.14	16,16,16,26	0

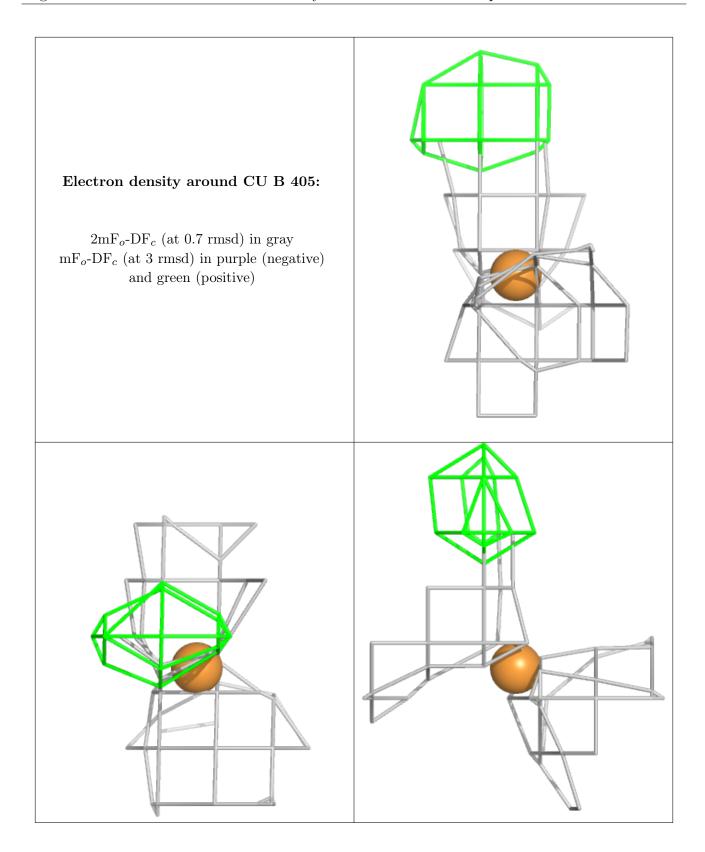


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Mol	\mathbf{Type}	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	CU	A	405	1/1	0.97	0.11	16,16,16,16	1
2	CU	С	402	1/1	0.97	0.27	16,16,16,16	1
2	CU	D	405	1/1	0.98	0.10	19,19,19,19	1
2	CU	F	401	1/1	0.98	0.18	15,15,15,15	1
2	CU	A	402	1/1	0.99	0.05	18,18,18,18	1
2	CU	E	402	1/1	0.99	0.07	22,22,22,22	1
2	CU	С	404	1/1	0.99	0.04	14,14,14,14	0
2	CU	В	402	1/1	0.99	0.05	19,19,19,19	1
2	CU	С	401	1/1	0.99	0.09	21,21,21,21	1
2	CU	F	403	1/1	0.99	0.03	16,16,16,16	1
2	CU	В	401	1/1	1.00	0.03	13,13,13,13	0
2	CU	Е	401	1/1	1.00	0.04	11,11,11,11	1
2	CU	D	401	1/1	1.00	0.04	10,10,10,10	1
2	CU	D	402	1/1	1.00	0.05	14,14,14,14	0
2	CU	A	401	1/1	1.00	0.04	11,11,11,11	0
2	CU	С	403	1/1	1.00	0.04	11,11,11,11	0
2	CU	F	402	1/1	1.00	0.03	12,12,12,12	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.

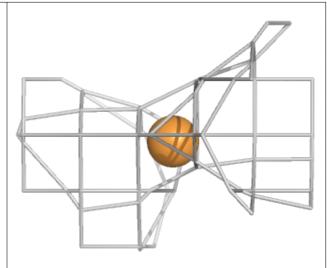


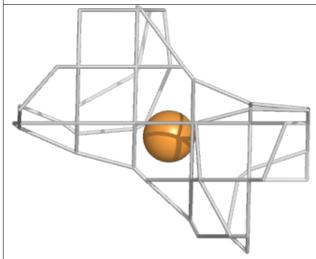


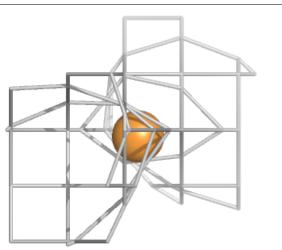


Electron density around CU D 403:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)







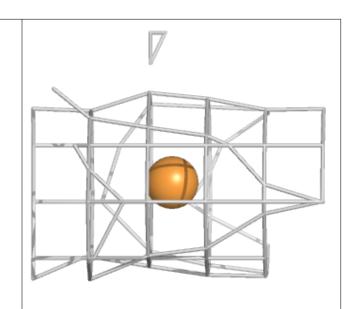


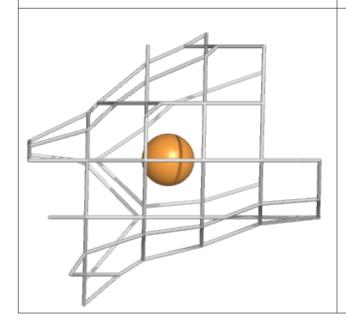
Electron density around CU E 403: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

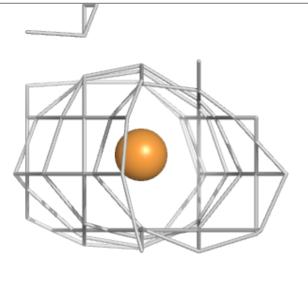


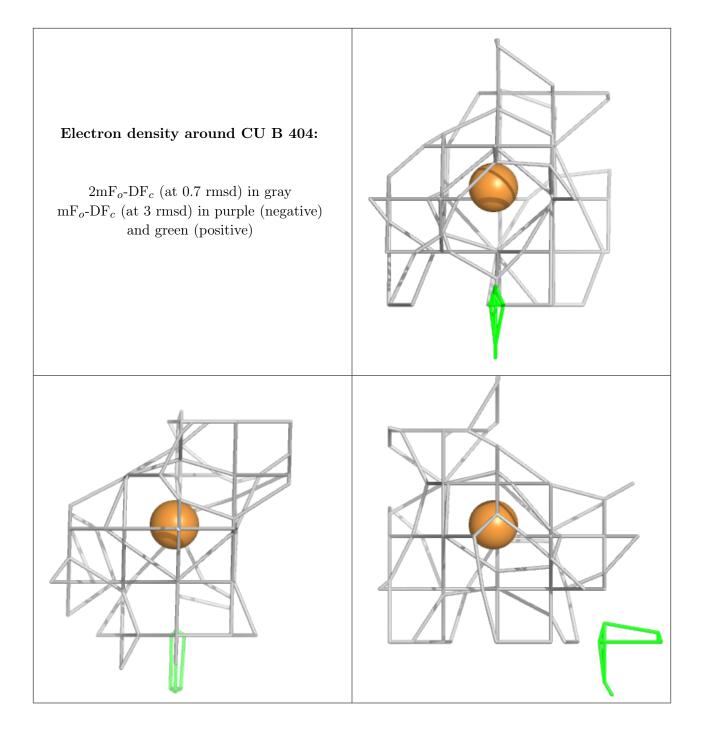
Electron density around CU D 406:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









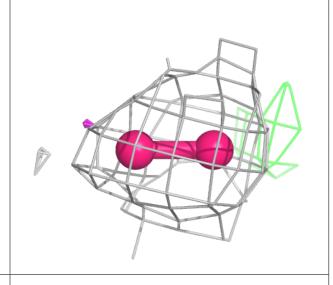


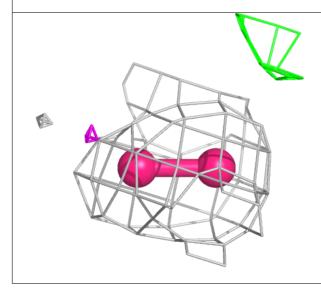
Electron density around OXY A 404: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

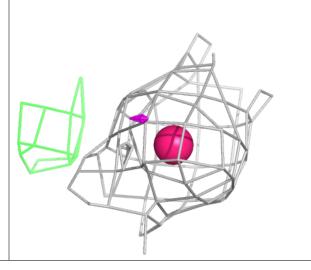


Electron density around OXY D 404:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

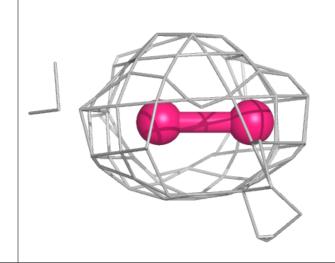


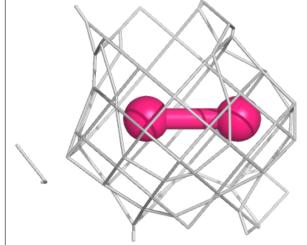


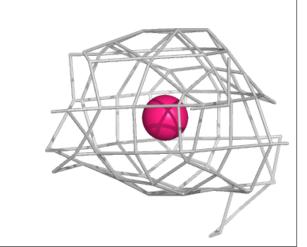


Electron density around OXY D 407:

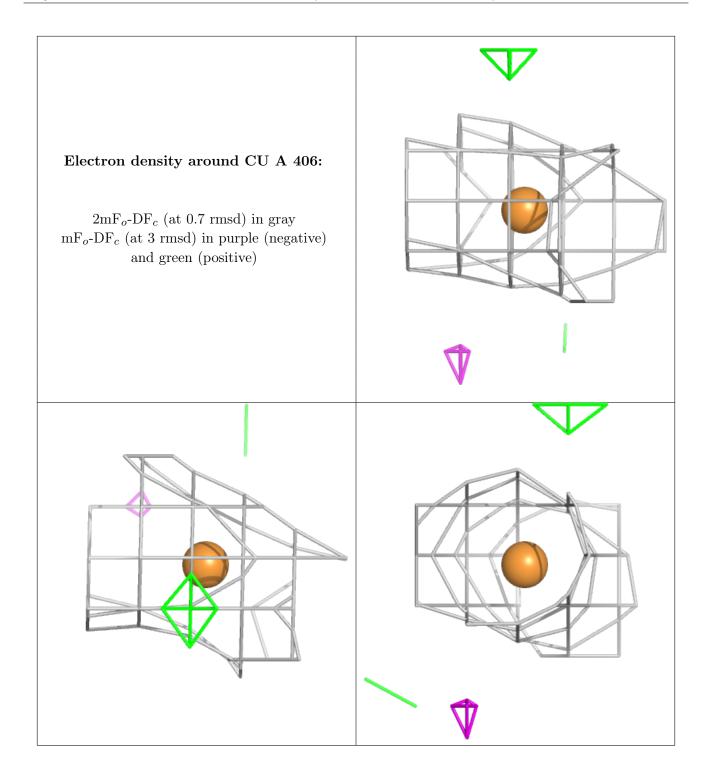
 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



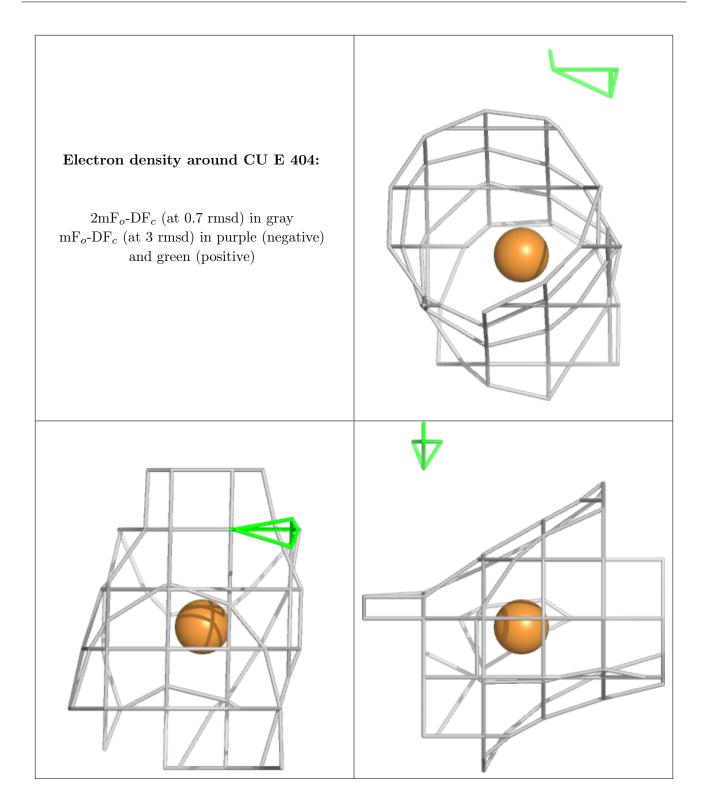






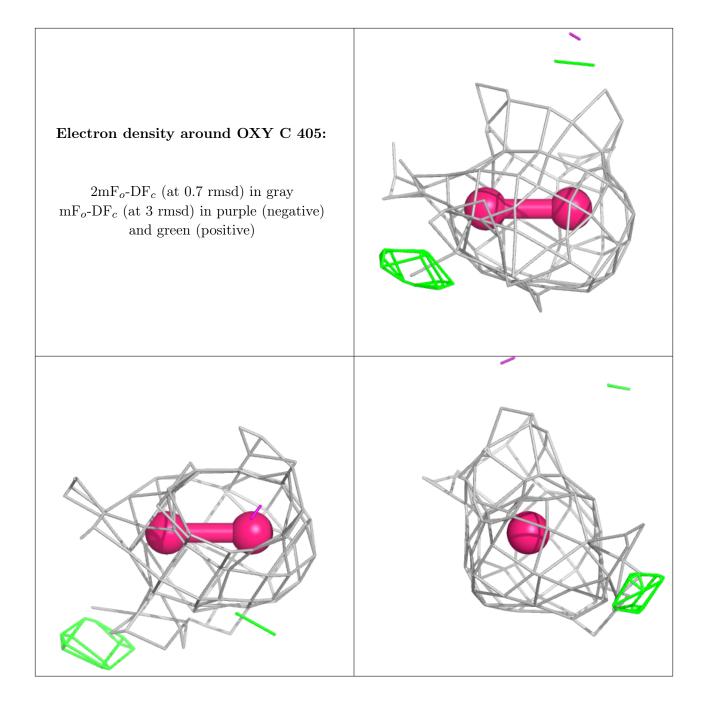




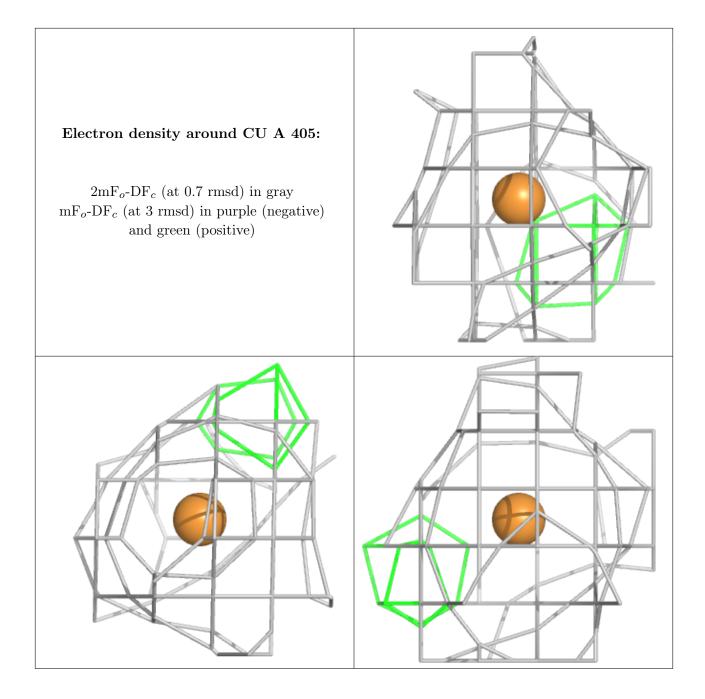








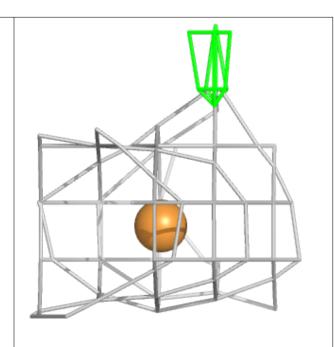


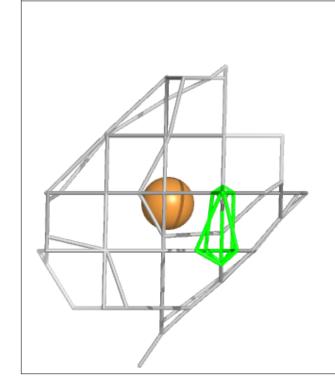


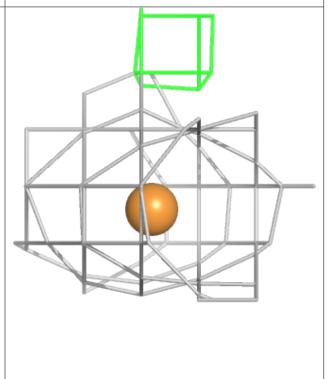


Electron density around CU C 402:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



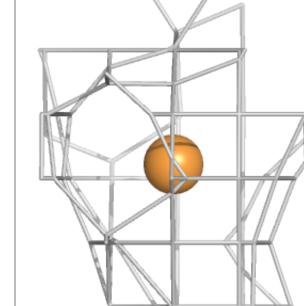


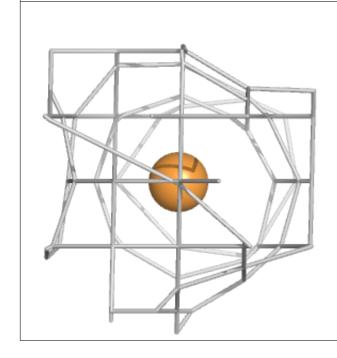


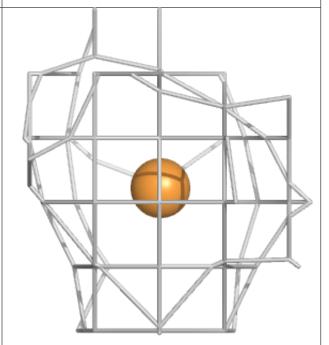


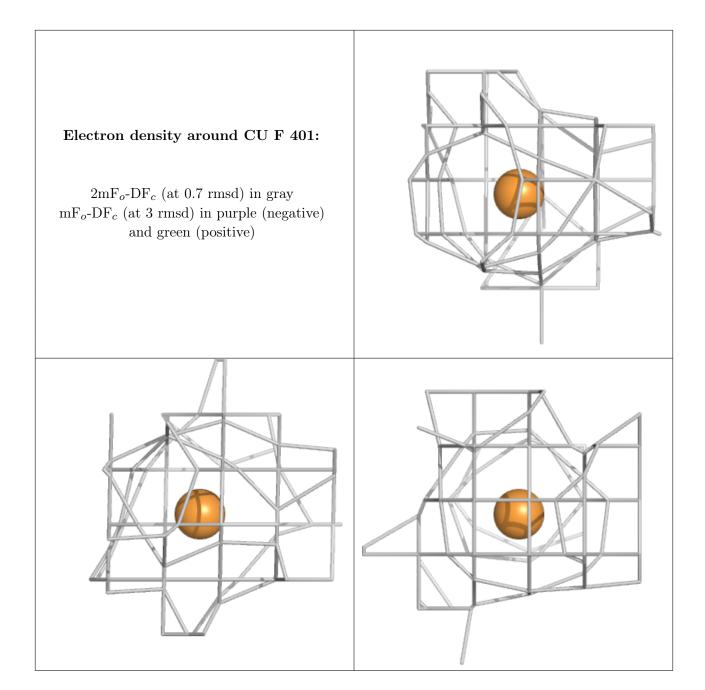
Electron density around CU D 405: $2 {\rm mF}_o\text{-DF}_c \ ({\rm at}\ 0.7\ {\rm rmsd})\ {\rm in\ gray}$ ${\rm mF}_o\text{-DF}_c \ ({\rm at}\ 3\ {\rm rmsd})\ {\rm in\ purple}\ ({\rm negative})$

and green (positive)





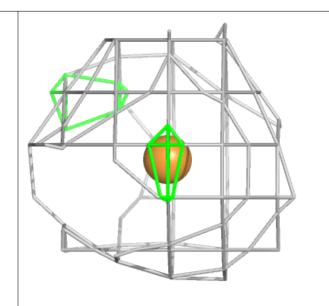


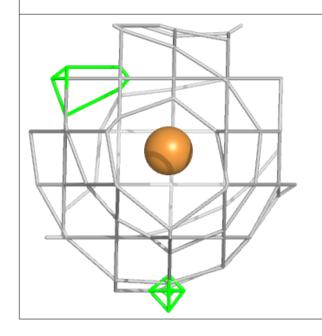


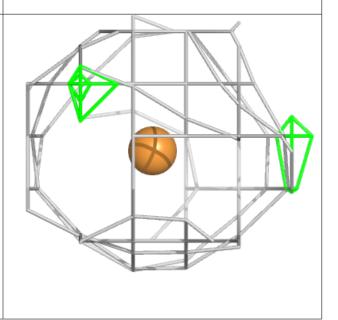


Electron density around CU A 402:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)







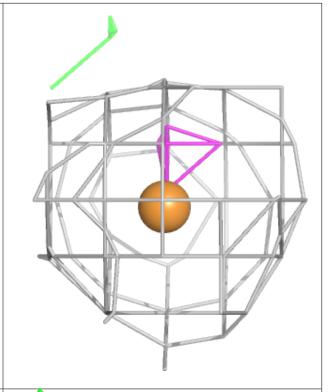


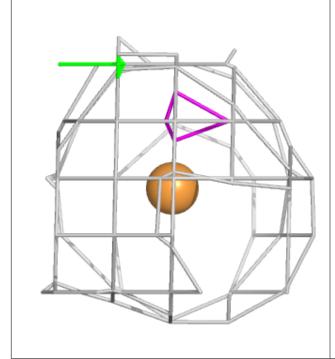
Electron density around CU E 402: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

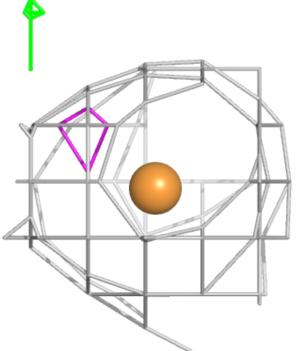


Electron density around CU C 404:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

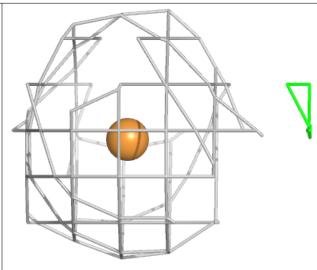


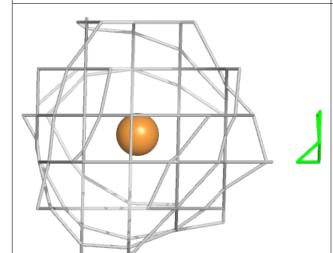


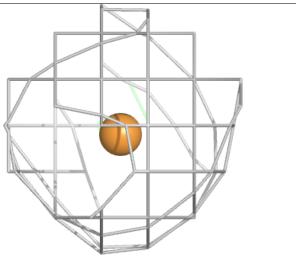


Electron density around CU B 402:

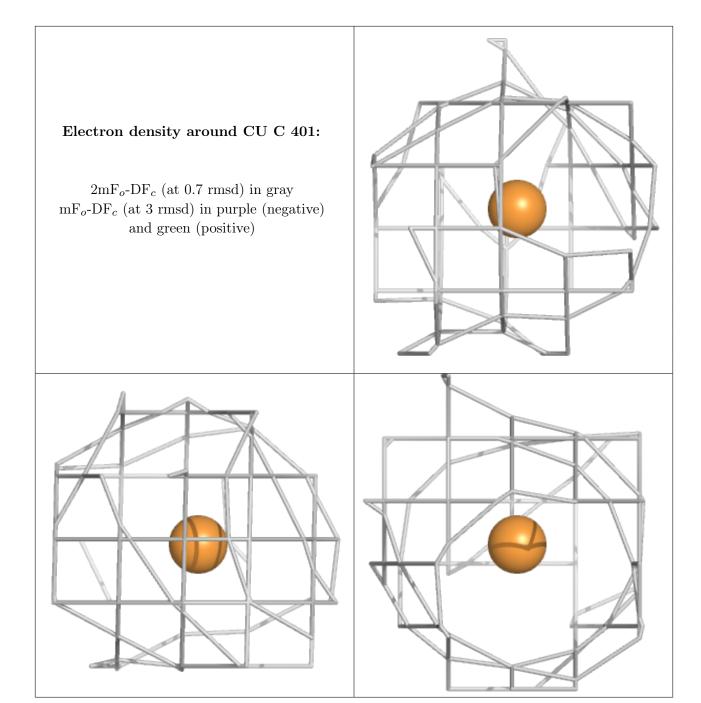
 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









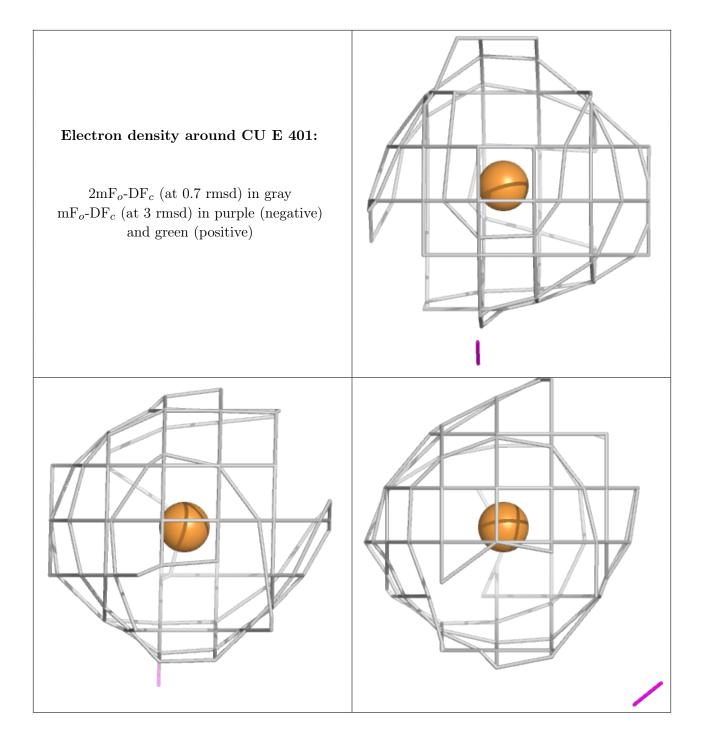




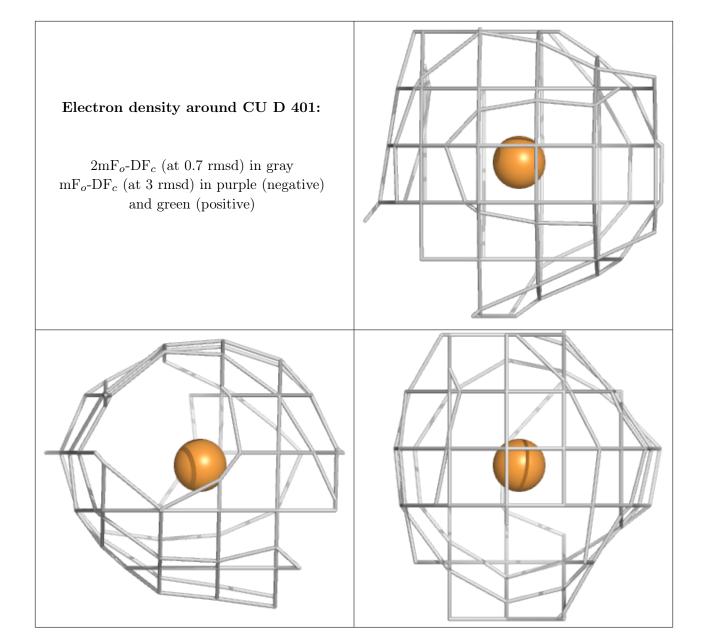


Electron density around CU B 401: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

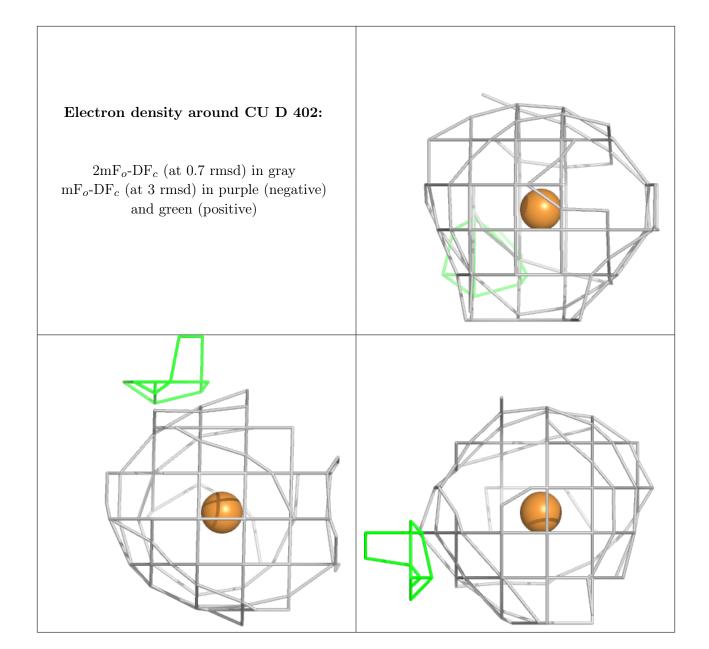




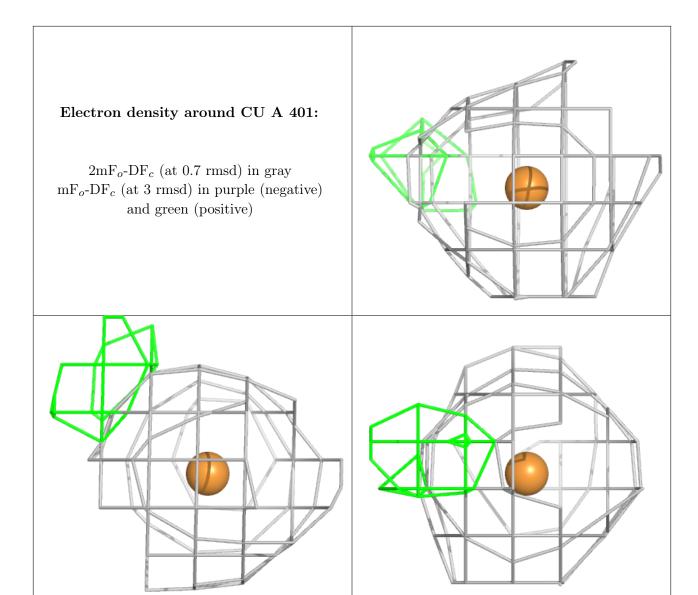








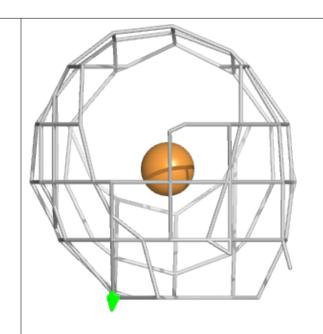


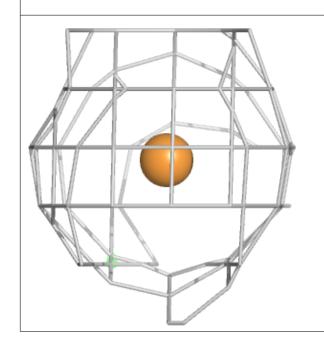


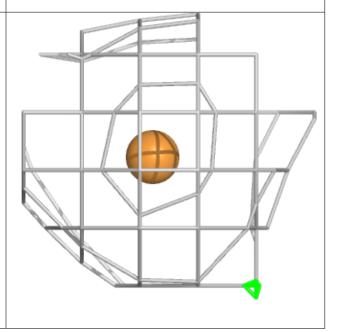


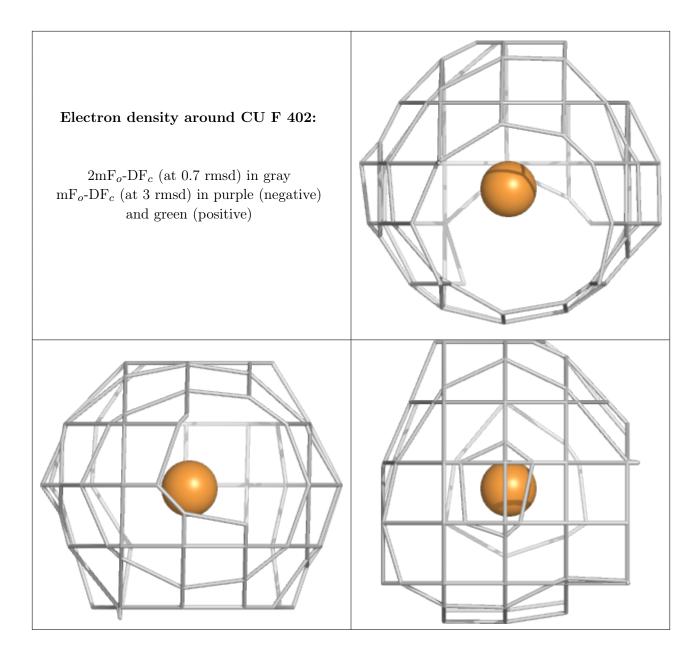
Electron density around CU C 403:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

