



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 09:54 AM JST

PDB ID : 6LL1  
Title : Oxygen-exposed reduced terminal oxygenase in carbazole 1,9a-dioxygenase  
Authors : Wang, Y.X.; Suzuki-Minakuchi, C.; Nojiri, H.  
Deposited on : 2019-12-21  
Resolution : 2.15 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

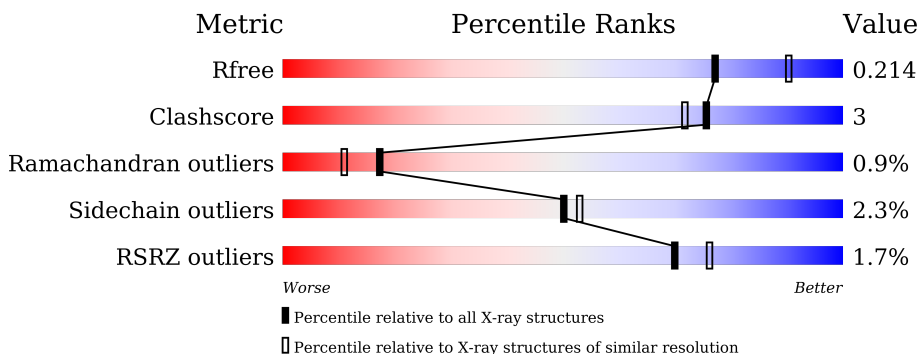
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	 2% 86% 11% .
1	B	392	 2% 87% 9% ...
1	C	392	 2% 86% 11% ..

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9852 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 Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	3081	1970	523	575	13	0	0	0
1	B	383	3084	1972	523	576	13	0	1	0
1	C	383	3081	1970	523	575	13	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

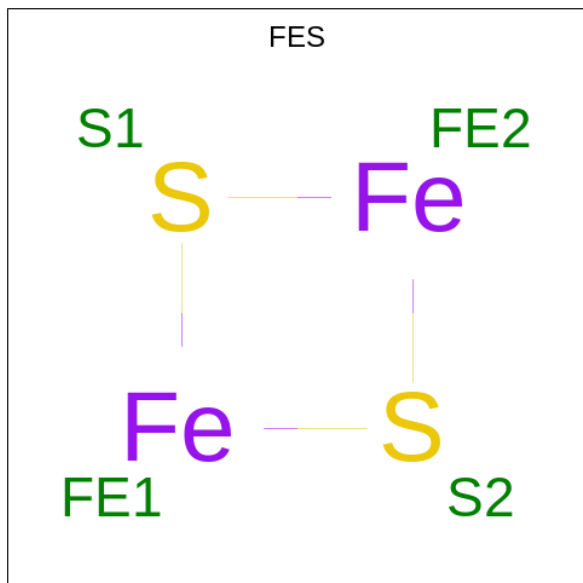
Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP Q84II6
A	386	GLU	-	expression tag	UNP Q84II6
A	387	HIS	-	expression tag	UNP Q84II6
A	388	HIS	-	expression tag	UNP Q84II6
A	389	HIS	-	expression tag	UNP Q84II6
A	390	HIS	-	expression tag	UNP Q84II6
A	391	HIS	-	expression tag	UNP Q84II6
A	392	HIS	-	expression tag	UNP Q84II6
B	385	LEU	-	expression tag	UNP Q84II6
B	386	GLU	-	expression tag	UNP Q84II6
B	387	HIS	-	expression tag	UNP Q84II6
B	388	HIS	-	expression tag	UNP Q84II6
B	389	HIS	-	expression tag	UNP Q84II6
B	390	HIS	-	expression tag	UNP Q84II6
B	391	HIS	-	expression tag	UNP Q84II6
B	392	HIS	-	expression tag	UNP Q84II6
C	385	LEU	-	expression tag	UNP Q84II6
C	386	GLU	-	expression tag	UNP Q84II6
C	387	HIS	-	expression tag	UNP Q84II6
C	388	HIS	-	expression tag	UNP Q84II6
C	389	HIS	-	expression tag	UNP Q84II6
C	390	HIS	-	expression tag	UNP Q84II6
C	391	HIS	-	expression tag	UNP Q84II6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP Q84II6

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0
2	C	1	4	2	2	0	0

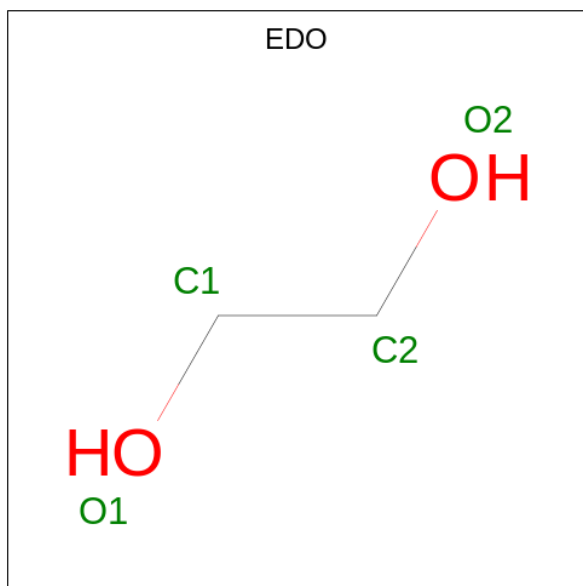
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



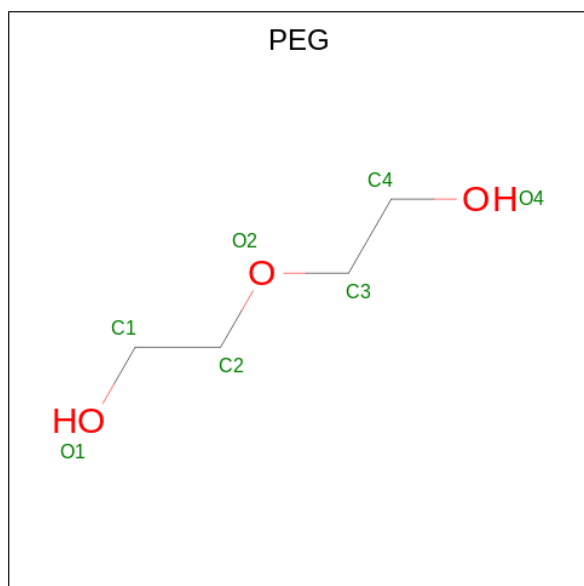
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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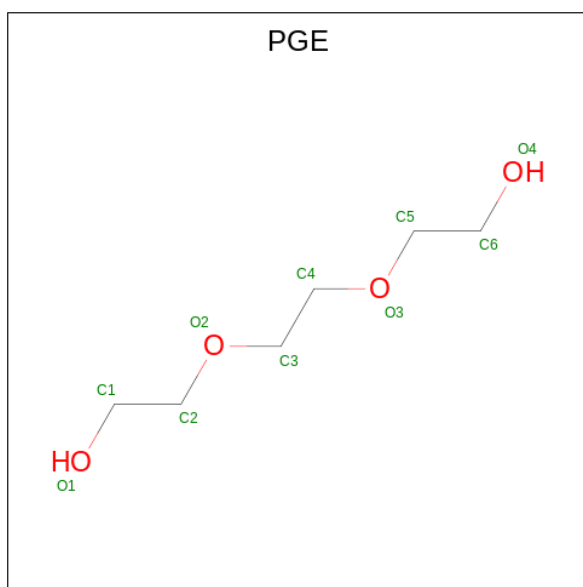
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



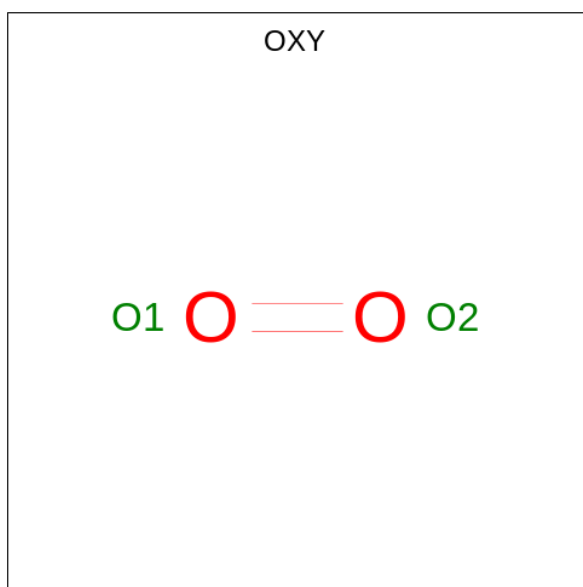
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



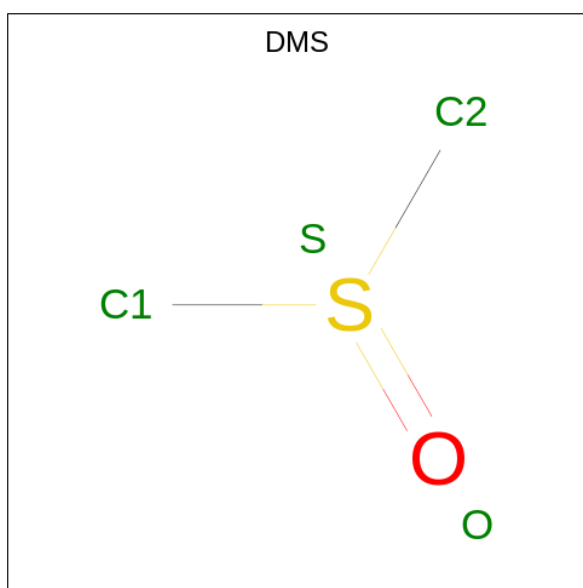
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0
7	B	1	Total C O 10 6 4	0	0
7	B	1	Total C O 10 6 4	0	0
7	C	1	Total C O 10 6 4	0	0
7	C	1	Total C O 10 6 4	0	0

- Molecule 8 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O 2 2	0	0
8	C	1	Total O 2 2	0	0

- Molecule 9 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O S 4 2 1 1	0	0

- Molecule 10 is water.

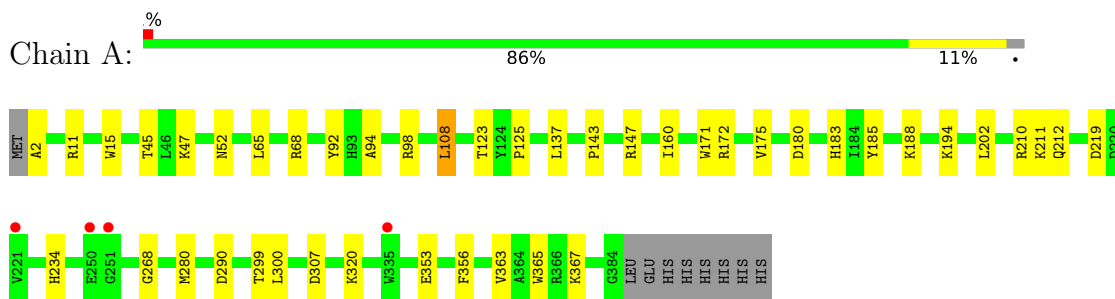


<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
10	A	135	Total 135	O 135	0	0
10	B	170	Total 170	O 170	0	0
10	C	143	Total 143	O 143	0	0

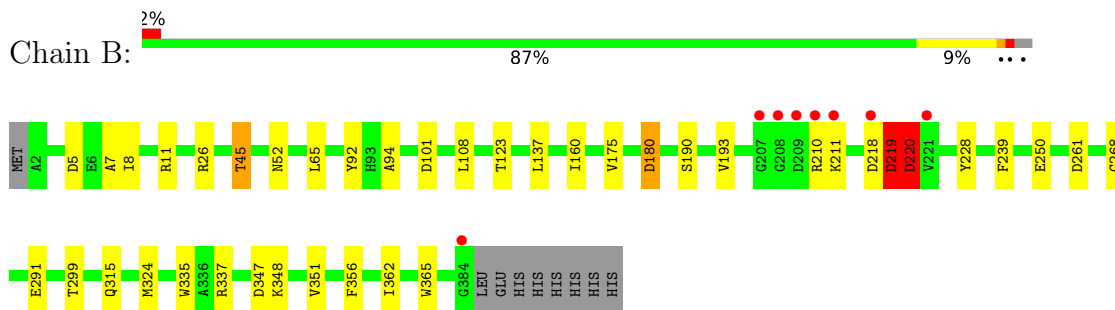
### 3 Residue-property plots [i](#)

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

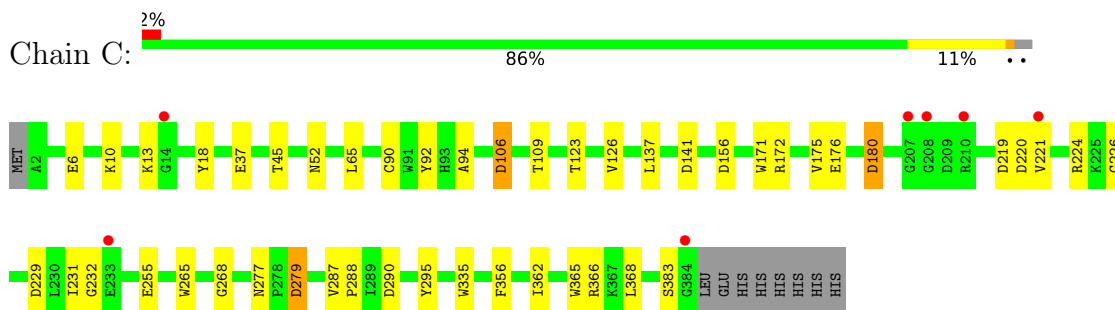
- Molecule 1: Terminal oxygenase component of carbazole



- Molecule 1: Terminal oxygenase component of carbazole



- Molecule 1: Terminal oxygenase component of carbazole



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.74Å 91.74Å 240.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.45 – 2.15 45.05 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (79.45-2.15) 98.3 (45.05-2.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.80 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.153 , 0.209 0.162 , 0.214	Depositor DCC
$R_{free}$ test set	3074 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: FES, DMS, PEG, PGE, FE2, OXY, MG, EDO

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	0.82	1/3163 (0.0%)	0.89	5/4294 (0.1%)
1	B	0.93	2/3169 (0.1%)	0.94	6/4302 (0.1%)
1	C	0.83	1/3163 (0.0%)	0.91	9/4294 (0.2%)
All	All	0.86	4/9495 (0.0%)	0.92	20/12890 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	TRP	CB-CG	-10.51	1.31	1.50
1	C	335	TRP	CB-CG	-6.90	1.37	1.50
1	B	291	GLU	CD-OE1	5.23	1.31	1.25
1	A	353	GLU	CD-OE1	5.21	1.31	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	A	290	ASP	CB-CG-OD1	7.92	125.42	118.30
1	B	180	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	B	337	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	324	MET	CG-SD-CE	6.49	110.58	100.20
1	A	68	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	290	ASP	CB-CG-OD1	6.42	124.07	118.30
1	C	229	ASP	CB-CG-OD1	6.27	123.95	118.30
1	C	106	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	101	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	98	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	C	106	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	224	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	219	ASP	CB-CG-OD1	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	68	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	126	VAL	CB-CA-C	-5.27	101.39	111.40
1	C	279	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	180	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	220	ASP	N-CA-C	-5.01	97.46	111.00

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	3081	0	2992	20	0
1	B	3084	0	2997	20	0
1	C	3081	0	2992	19	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	28	0	42	2	0
5	B	8	0	12	1	0
5	C	4	0	6	0	0
6	A	14	0	20	0	0
6	B	14	0	20	1	0
6	C	14	0	20	1	0
7	A	10	0	14	0	0
7	B	20	0	28	0	0
7	C	20	0	28	1	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	4	0	6	1	0
10	A	135	0	0	1	0
10	B	170	0	0	2	0
10	C	143	0	0	1	0
All	All	9852	0	9177	58	0

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

All (58) 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:45:THR:OG1	10:C:501:HOH:O	1.83	0.92
1:B:45:THR:OG1	10:B:501:HOH:O	1.76	0.81
1:C:255:GLU:OE1	9:C:410:DMS:S	2.52	0.67
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.82	0.62
1:A:2:ALA:N	10:A:505:HOH:O	2.36	0.58
1:A:185:TYR:CZ	1:A:188:LYS:HE3	2.38	0.58
1:A:194:LYS:O	5:A:410:EDO:C1	2.56	0.54
1:B:210:ARG:O	1:B:210:ARG:HD3	2.07	0.53
1:B:348:LYS:O	1:B:351:VAL:HG22	2.08	0.53
1:C:52:ASN:HD21	6:C:406:PEG:H31	1.74	0.53
1:A:47:LYS:HE3	1:A:52:ASN:HD21	1.74	0.52
1:C:226:GLY:HA3	1:C:265:TRP:CE3	2.46	0.50
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.92	0.50
1:A:175:VAL:HG11	1:A:365:TRP:CE2	2.47	0.50
1:B:7:ALA:O	1:B:11:ARG:HG3	2.11	0.50
1:B:65:LEU:HD23	1:B:123:THR:HG22	1.92	0.49
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.94	0.49
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.94	0.48
1:B:52:ASN:HD21	6:B:407:PEG:H12	1.77	0.48
1:A:15:TRP:CZ3	1:A:363:VAL:HG13	2.48	0.48
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.50	0.47
1:C:231:ILE:HG23	1:C:232:GLY:N	2.30	0.47
1:A:47:LYS:HE3	1:A:52:ASN:ND2	2.30	0.47
1:B:175:VAL:HG11	1:B:365:TRP:CE2	2.50	0.47
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.96	0.46
1:C:277:ASN:HB3	1:C:279:ASP:OD1	2.16	0.46
1:A:202:LEU:O	1:C:109:THR:HG22	2.16	0.46
1:B:218:ASP:C	1:B:219:ASP:O	2.53	0.45
1:A:160:ILE:HG23	1:A:299:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:TYR:HE2	1:B:261:ASP:OD1	2.00	0.44
1:A:180:ASP:HB3	1:A:183:HIS:HB3	1.99	0.44
1:C:37:GLU:HB3	7:C:408:PGE:H6	2.00	0.44
1:B:219:ASP:O	1:B:220:ASP:CB	2.66	0.43
1:C:18:TYR:CE2	1:C:366:ARG:HG2	2.53	0.43
1:B:190[B]:SER:OG	1:B:193:VAL:HG23	2.18	0.43
1:B:160:ILE:HG23	1:B:299:THR:HB	1.99	0.43
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.48	0.42
1:C:171:TRP:CG	1:C:288:PRO:HG3	2.54	0.42
1:B:210:ARG:NH1	5:B:406:EDO:O1	2.45	0.42
1:C:175:VAL:HG11	1:C:365:TRP:CE2	2.55	0.42
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.54	0.42
1:C:180:ASP:HB2	1:C:362:ILE:HD11	2.01	0.42
1:C:279:ASP:OD1	1:C:279:ASP:N	2.31	0.42
1:B:5:ASP:OD2	1:B:7:ALA:HB3	2.19	0.41
1:B:8:ILE:HD13	1:B:347:ASP:HB2	2.01	0.41
1:A:125:PRO:HA	5:A:408:EDO:C2	2.51	0.41
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.51	0.41
1:B:315:GLN:NE2	10:B:513:HOH:O	2.49	0.41
1:A:212:GLN:OE1	1:A:234:HIS:NE2	2.54	0.41
1:C:176:GLU:O	1:C:180:ASP:HB2	2.21	0.41
1:C:90:CYS:O	1:C:94:ALA:HA	2.21	0.40
1:A:280:MET:CE	1:A:300:LEU:HD13	2.51	0.40
1:B:218:ASP:C	1:B:218:ASP:OD1	2.59	0.40
1:A:185:TYR:CE1	1:A:188:LYS:HE3	2.56	0.40
1:A:363:VAL:HG12	1:A:367:LYS:HE2	2.03	0.40
1:B:180:ASP:HB2	1:B:362:ILE:HD11	2.04	0.40
1:B:239:PHE:O	1:B:250:GLU:HA	2.20	0.40
1:C:6:GLU:O	1:C:10:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/392 (97%)	365 (96%)	15 (4%)	1 (0%)	41	37
1	B	382/392 (97%)	356 (93%)	22 (6%)	4 (1%)	15	9
1	C	381/392 (97%)	362 (95%)	14 (4%)	5 (1%)	12	6
All	All	1144/1176 (97%)	1083 (95%)	51 (4%)	10 (1%)	17	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	ASP
1	B	220	ASP
1	C	13	LYS
1	A	268	GLY
1	C	221	VAL
1	C	268	GLY
1	B	211	LYS
1	B	268	GLY
1	C	219	ASP
1	C	220	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	330/339 (97%)	320 (97%)	10 (3%)	41	40
1	B	331/339 (98%)	326 (98%)	5 (2%)	65	69
1	C	330/339 (97%)	322 (98%)	8 (2%)	49	51
All	All	991/1017 (97%)	968 (98%)	23 (2%)	50	53

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

Mol	Chain	Res	Type
1	A	11	ARG
1	A	45	THR
1	A	92	TYR

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	137	LEU
1	A	210	ARG
1	A	211	LYS
1	A	307	ASP
1	A	320	LYS
1	A	356	PHE
1	B	45	THR
1	B	92	TYR
1	B	137	LEU
1	B	219	ASP
1	B	356	PHE
1	C	92	TYR
1	C	106	ASP
1	C	137	LEU
1	C	141	ASP
1	C	156	ASP
1	C	356	PHE
1	C	368	LEU
1	C	383	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 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
5	EDO	A	409	-	3,3,3	0.40	0	2,2,2	0.40	0
5	EDO	C	405	-	3,3,3	0.42	0	2,2,2	0.44	0
2	FES	B	401	1	0,4,4	-	-	-	-	-
5	EDO	A	408	-	3,3,3	0.53	0	2,2,2	0.68	0
7	PGE	C	408	-	9,9,9	0.51	0	8,8,8	0.40	0
6	PEG	C	406	-	6,6,6	0.39	0	5,5,5	1.11	0
5	EDO	A	407	-	3,3,3	0.52	0	2,2,2	0.24	0
8	OXY	B	404	4	1,1,1	0.03	0	-	-	-
5	EDO	A	404	-	3,3,3	0.34	0	2,2,2	0.52	0
5	EDO	A	406	-	3,3,3	0.38	0	2,2,2	0.36	0
7	PGE	A	413	-	9,9,9	0.63	0	8,8,8	0.78	0
2	FES	A	401	1	0,4,4	-	-	-	-	-
5	EDO	B	405	-	3,3,3	0.39	0	2,2,2	0.77	0
8	OXY	C	404	4	1,1,1	0.18	0	-	-	-
9	DMS	C	410	-	3,3,3	0.48	0	3,3,3	0.85	0
7	PGE	C	409	-	9,9,9	0.78	0	8,8,8	0.78	0
6	PEG	C	407	-	6,6,6	0.50	0	5,5,5	0.59	0
6	PEG	A	412	-	6,6,6	0.53	0	5,5,5	1.06	0
7	PGE	B	409	-	9,9,9	0.57	0	8,8,8	0.65	0
2	FES	C	401	1	0,4,4	-	-	-	-	-
5	EDO	B	406	-	3,3,3	0.37	0	2,2,2	0.72	0
5	EDO	A	410	-	3,3,3	0.41	0	2,2,2	0.28	0
7	PGE	B	410	-	9,9,9	0.96	0	8,8,8	0.98	0
6	PEG	A	411	-	6,6,6	0.43	0	5,5,5	0.51	0
6	PEG	B	408	-	6,6,6	0.36	0	5,5,5	0.80	0
6	PEG	B	407	-	6,6,6	0.53	0	5,5,5	1.42	1 (20%)
5	EDO	A	405	-	3,3,3	0.55	0	2,2,2	0.14	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
5	EDO	A	409	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	405	-	-	0/1/1/1	-
7	PGE	C	408	-	-	2/7/7/7	-
5	EDO	A	408	-	-	1/1/1/1	-
2	FES	B	401	1	-	-	0/1/1/1
6	PEG	C	406	-	-	3/4/4/4	-
5	EDO	A	407	-	-	0/1/1/1	-
5	EDO	A	404	-	-	0/1/1/1	-
5	EDO	A	406	-	-	1/1/1/1	-
7	PGE	A	413	-	-	2/7/7/7	-
2	FES	A	401	1	-	-	0/1/1/1
5	EDO	B	405	-	-	0/1/1/1	-
7	PGE	C	409	-	-	3/7/7/7	-
6	PEG	C	407	-	-	2/4/4/4	-
6	PEG	A	412	-	-	3/4/4/4	-
7	PGE	B	409	-	-	5/7/7/7	-
2	FES	C	401	1	-	-	0/1/1/1
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	A	410	-	-	0/1/1/1	-
7	PGE	B	410	-	-	3/7/7/7	-
6	PEG	A	411	-	-	2/4/4/4	-
6	PEG	B	408	-	-	1/4/4/4	-
6	PEG	B	407	-	-	2/4/4/4	-
5	EDO	A	405	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	407	PEG	C3-O2-C2	2.73	125.12	113.29

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	412	PEG	C4-C3-O2-C2
6	B	407	PEG	C1-C2-O2-C3
6	A	412	PEG	O1-C1-C2-O2
6	C	406	PEG	O1-C1-C2-O2
6	B	408	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	C	409	PGE	O3-C5-C6-O4
6	A	411	PEG	O1-C1-C2-O2
7	A	413	PGE	O2-C3-C4-O3
6	A	411	PEG	O2-C3-C4-O4
6	A	412	PEG	O2-C3-C4-O4
7	A	413	PGE	O1-C1-C2-O2
7	B	409	PGE	O2-C3-C4-O3
5	A	409	EDO	O1-C1-C2-O2
7	B	409	PGE	C1-C2-O2-C3
7	B	409	PGE	C6-C5-O3-C4
6	C	407	PEG	C1-C2-O2-C3
7	C	408	PGE	C3-C4-O3-C5
7	C	409	PGE	C4-C3-O2-C2
6	C	406	PEG	C1-C2-O2-C3
7	B	410	PGE	C4-C3-O2-C2
7	C	409	PGE	C1-C2-O2-C3
6	B	407	PEG	C4-C3-O2-C2
5	A	408	EDO	O1-C1-C2-O2
5	B	406	EDO	O1-C1-C2-O2
6	C	407	PEG	O2-C3-C4-O4
7	B	409	PGE	O3-C5-C6-O4
7	B	409	PGE	O1-C1-C2-O2
6	C	406	PEG	C4-C3-O2-C2
7	B	410	PGE	O2-C3-C4-O3
7	C	408	PGE	C4-C3-O2-C2
5	A	406	EDO	O1-C1-C2-O2
7	B	410	PGE	O1-C1-C2-O2

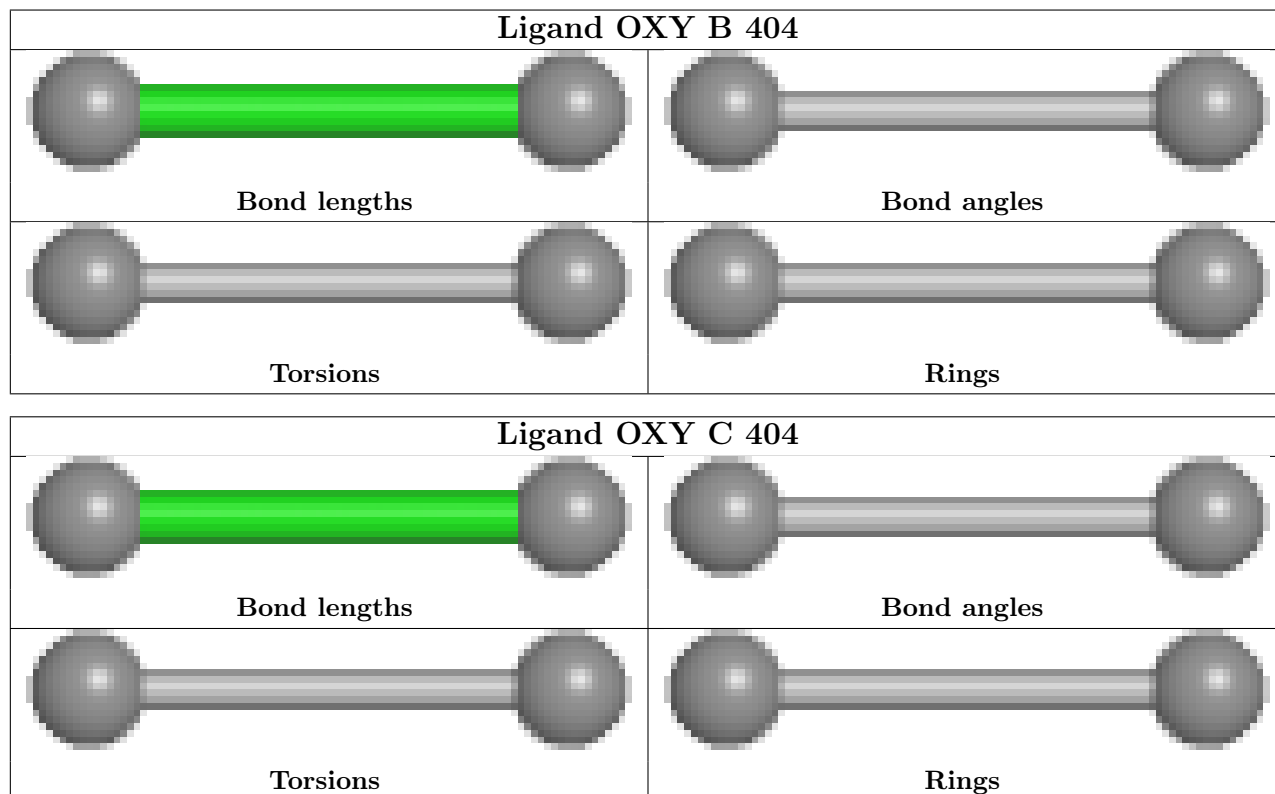
There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	EDO	1	0
7	C	408	PGE	1	0
6	C	406	PEG	1	0
9	C	410	DMS	1	0
5	B	406	EDO	1	0
5	A	410	EDO	1	0
6	B	407	PEG	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	383/392 (97%)	-0.24	4 (1%) 82 86	12, 27, 58, 85	0
1	B	383/392 (97%)	-0.35	8 (2%) 63 71	12, 21, 47, 103	0
1	C	383/392 (97%)	-0.27	7 (1%) 68 75	15, 27, 57, 75	0
All	All	1149/1176 (97%)	-0.28	19 (1%) 70 76	12, 25, 57, 103	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	384	GLY	6.8
1	B	207	GLY	4.8
1	A	251	GLY	4.6
1	C	221	VAL	3.5
1	B	218	ASP	3.4
1	A	335	TRP	3.2
1	C	384	GLY	3.2
1	B	210	ARG	3.2
1	B	209	ASP	3.0
1	C	210	ARG	2.9
1	C	208	GLY	2.8
1	A	221	VAL	2.7
1	C	207	GLY	2.7
1	B	208	GLY	2.6
1	B	221	VAL	2.6
1	C	14	GLY	2.4
1	C	233	GLU	2.3
1	A	250	GLU	2.2
1	B	211	LYS	2.2

## 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<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.

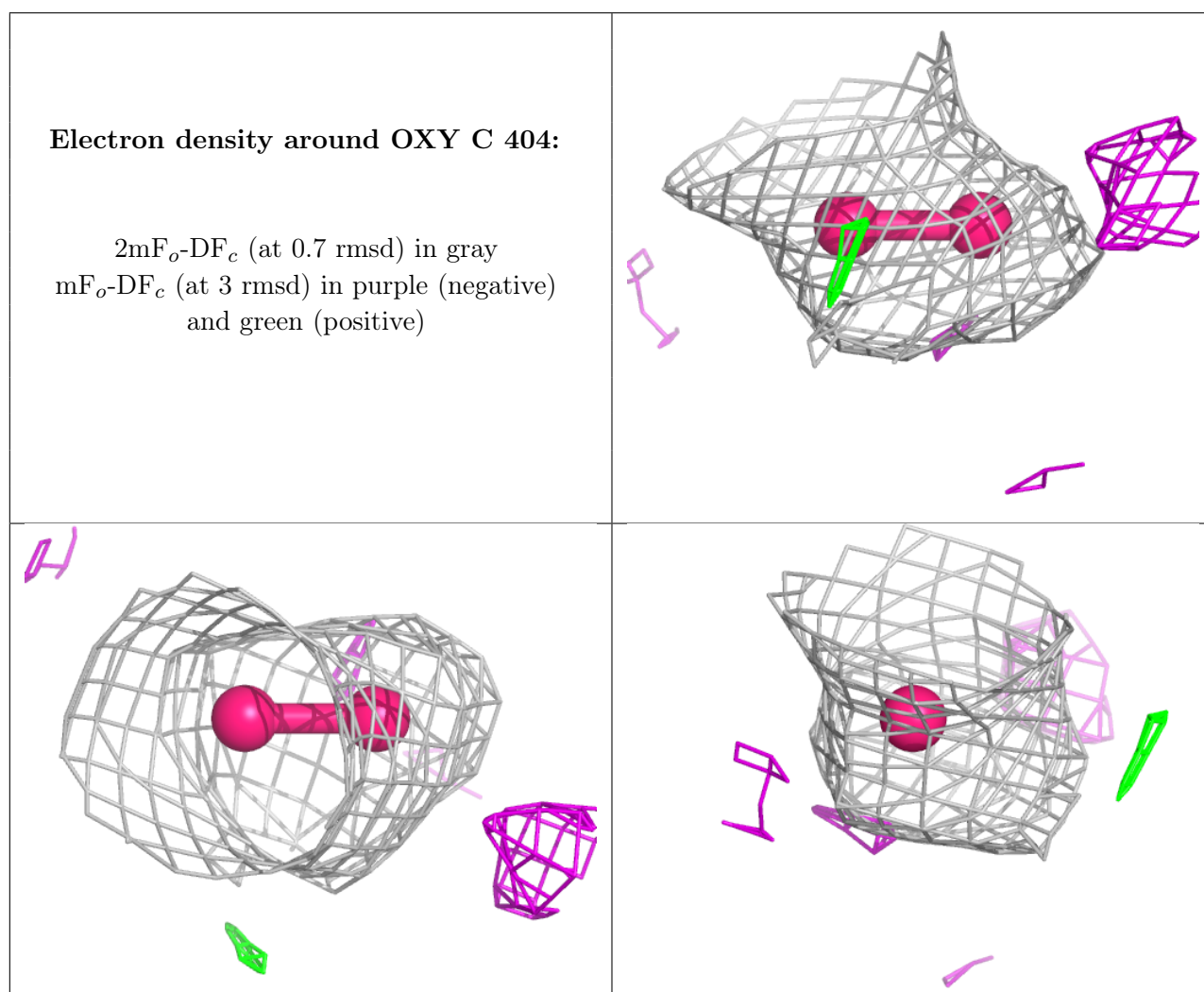
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PEG	C	407	7/7	0.70	0.22	57,62,64,67	0
7	PGE	C	409	10/10	0.72	0.37	35,53,56,58	0
7	PGE	A	413	10/10	0.74	0.17	53,56,59,61	0
7	PGE	B	410	10/10	0.76	0.23	41,47,50,59	0
5	EDO	A	410	4/4	0.78	0.16	57,59,62,65	0
7	PGE	C	408	10/10	0.85	0.15	46,52,54,54	0
5	EDO	A	407	4/4	0.86	0.18	48,48,52,53	0
5	EDO	A	405	4/4	0.86	0.17	50,53,54,56	0
6	PEG	B	407	7/7	0.86	0.14	31,34,46,50	0
6	PEG	B	408	7/7	0.86	0.15	41,43,47,50	0
6	PEG	C	406	7/7	0.86	0.15	33,38,45,50	0
9	DMS	C	410	4/4	0.86	0.20	72,72,78,79	0
5	EDO	A	408	4/4	0.87	0.18	27,29,33,38	0
6	PEG	A	411	7/7	0.88	0.18	31,36,48,52	0
5	EDO	B	405	4/4	0.90	0.24	31,33,39,43	0
5	EDO	C	405	4/4	0.90	0.18	35,39,41,51	0
5	EDO	A	406	4/4	0.91	0.35	42,45,46,47	0
3	MG	C	402	1/1	0.91	0.04	40,40,40,40	0
5	EDO	B	406	4/4	0.92	0.17	41,42,45,47	0
7	PGE	B	409	10/10	0.92	0.19	44,47,49,50	0
6	PEG	A	412	7/7	0.93	0.14	41,43,48,54	0
3	MG	B	402	1/1	0.94	0.07	36,36,36,36	0
5	EDO	A	409	4/4	0.94	0.32	49,51,51,53	0
5	EDO	A	404	4/4	0.97	0.09	23,28,30,34	0
3	MG	A	402	1/1	0.97	0.11	26,26,26,26	0
8	OXY	C	404	2/2	0.98	0.11	28,28,28,30	0
8	OXY	B	404	2/2	0.99	0.11	30,30,30,37	0

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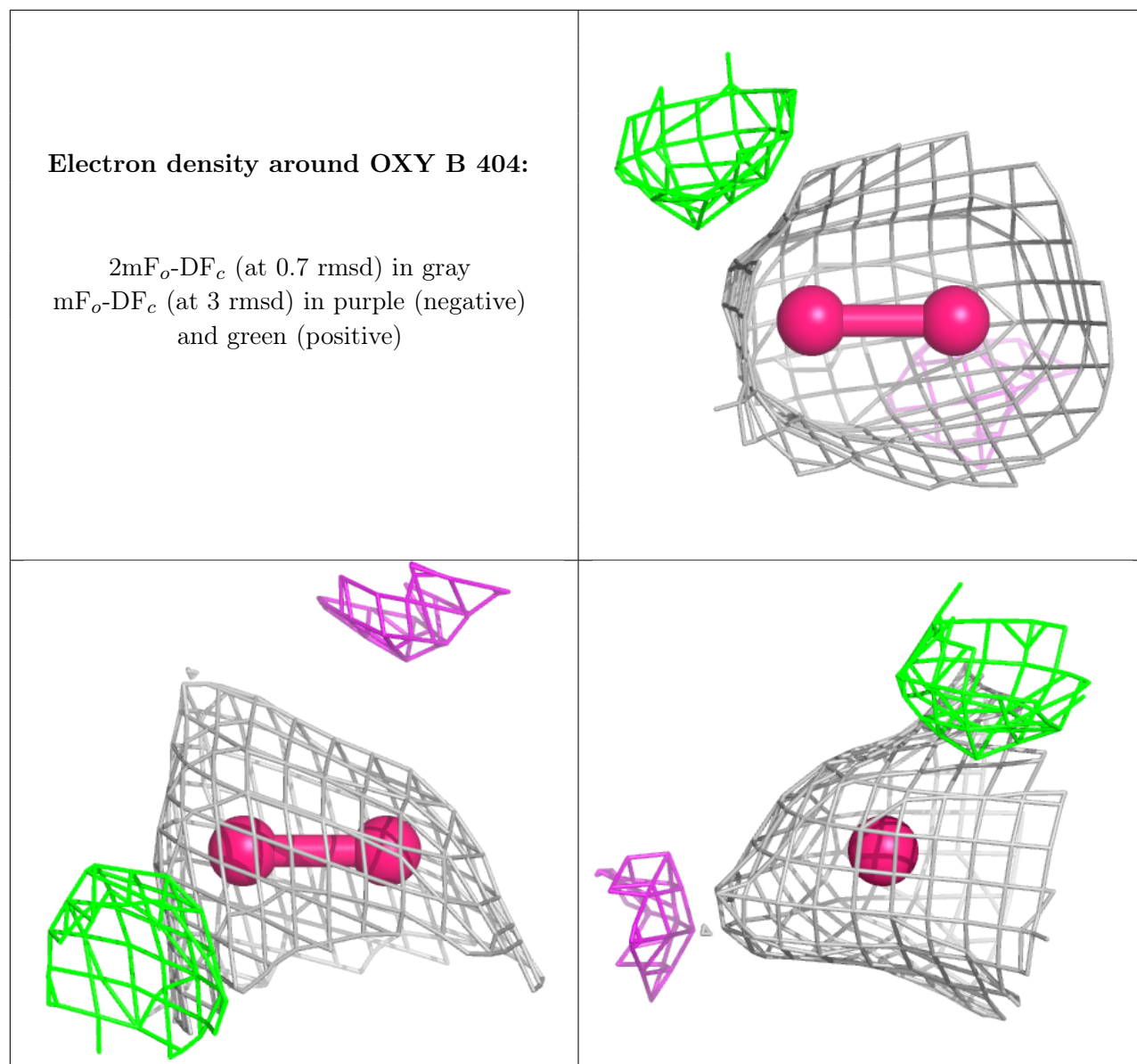
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FES	B	401	4/4	0.99	0.07	14,15,16,16	0
2	FES	C	401	4/4	0.99	0.05	20,22,23,24	0
2	FES	A	401	4/4	1.00	0.08	12,12,14,14	0
4	FE2	A	403	1/1	1.00	0.08	25,25,25,25	0
4	FE2	B	403	1/1	1.00	0.08	16,16,16,16	0
4	FE2	C	403	1/1	1.00	0.06	19,19,19,19	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.

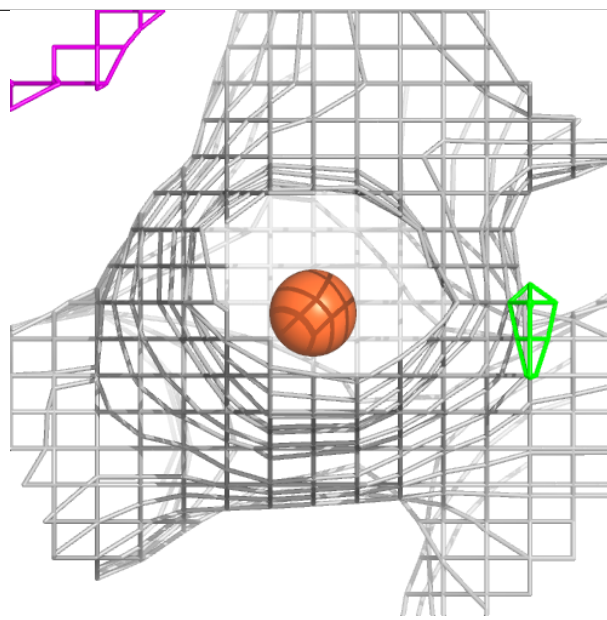
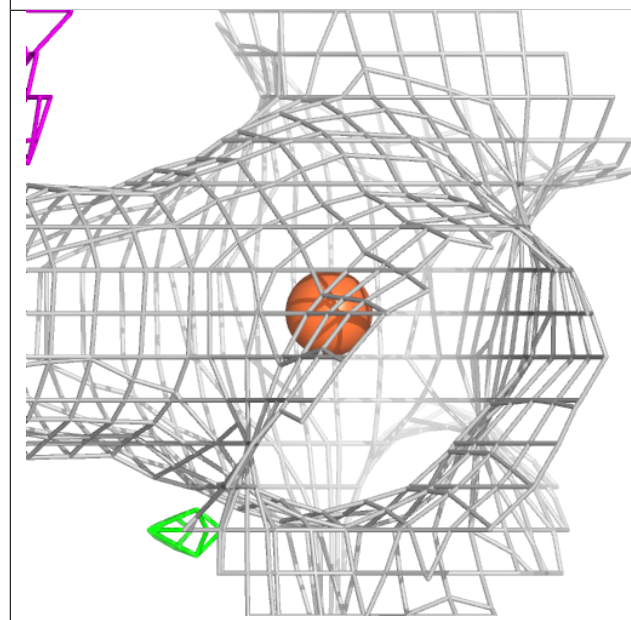
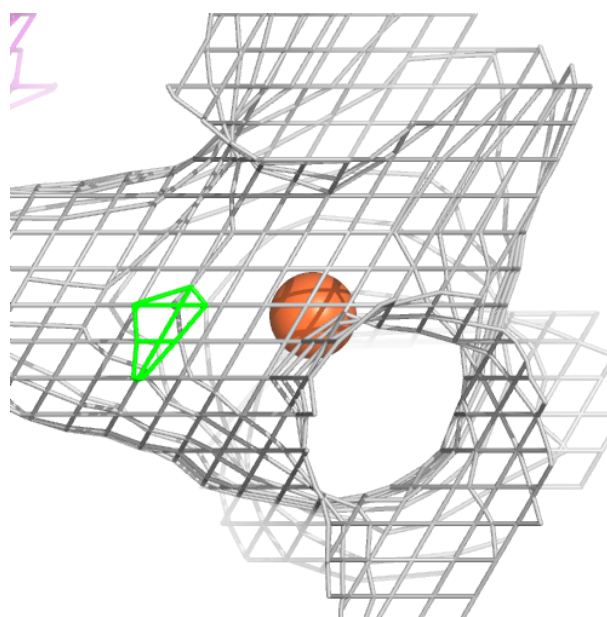






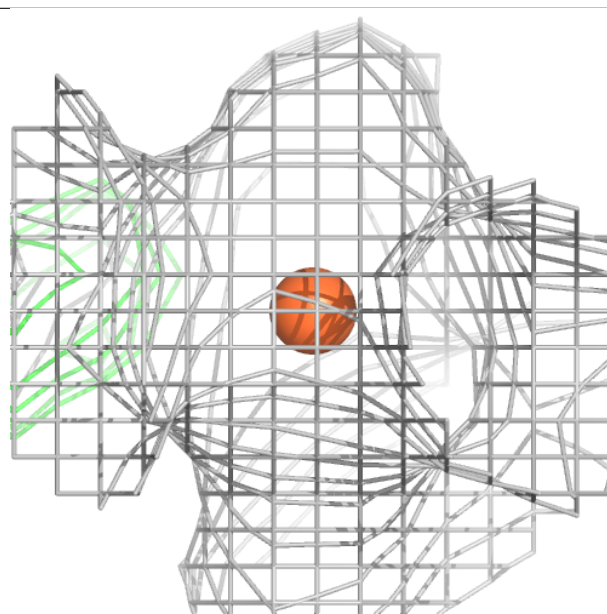
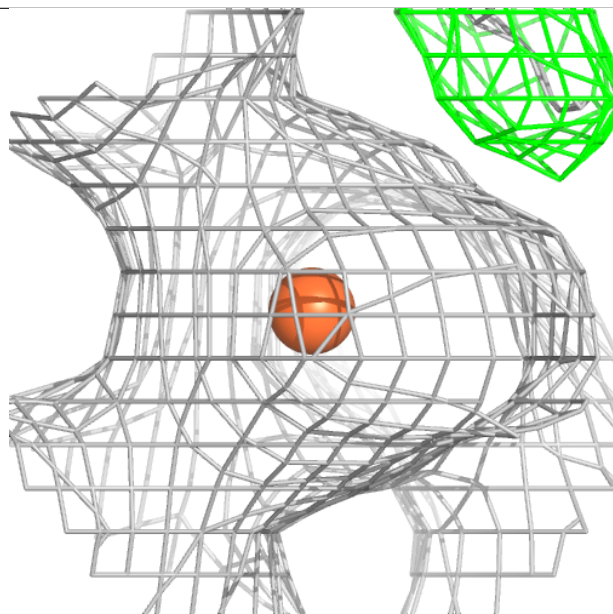
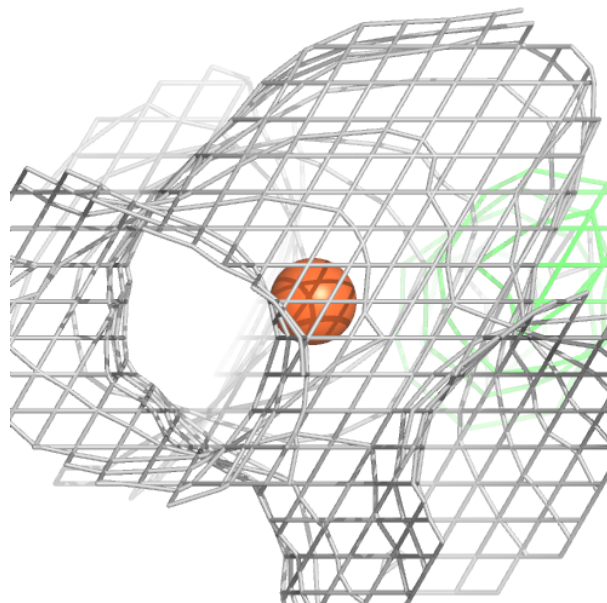
**Electron density around FE2 A 403:**

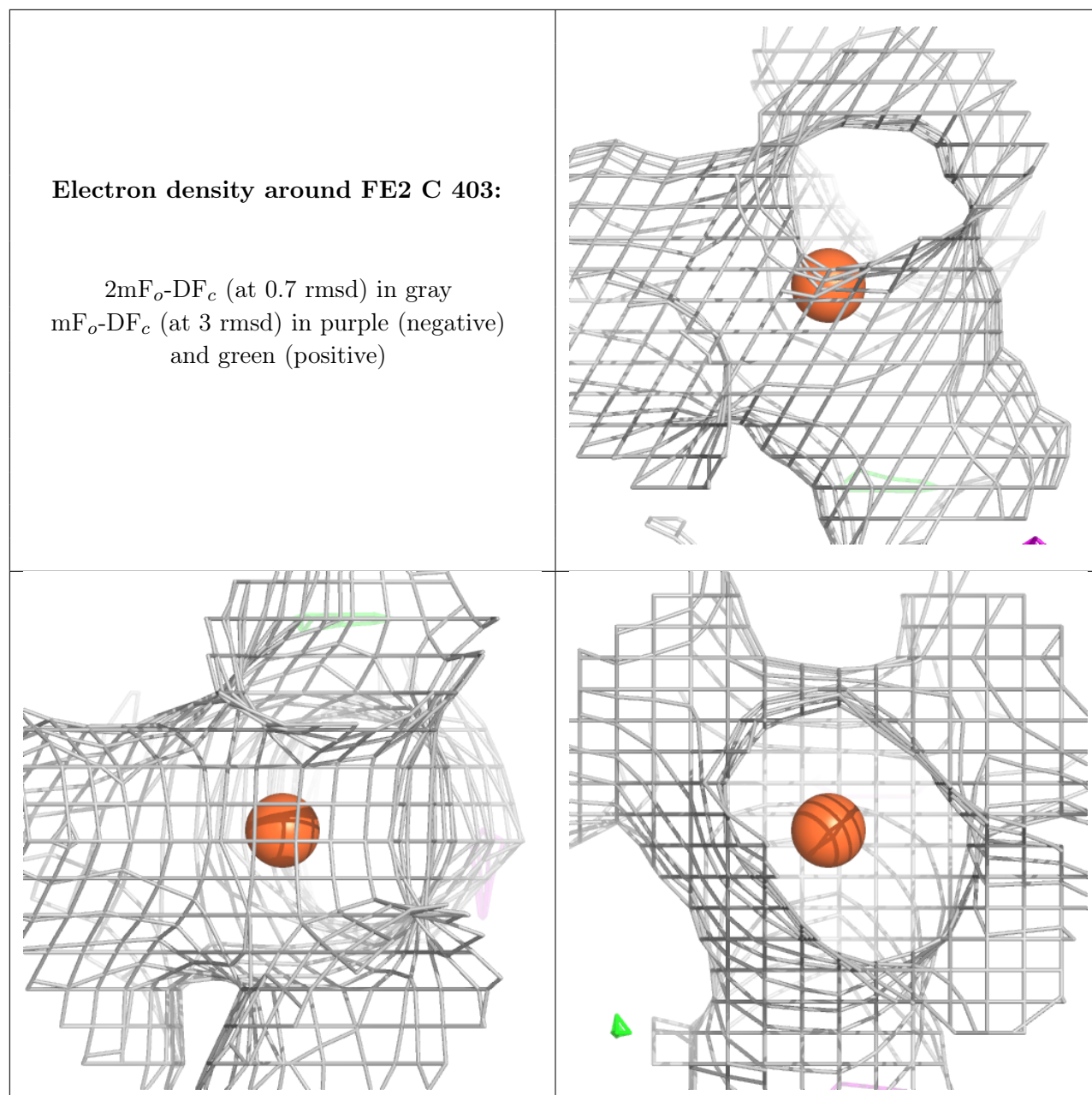
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE2 B 403:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.