



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:37 PM UTC

PDB ID : 7FC0 / pdb\_00007fc0  
Title : Reconstitution of MbnABC complex from *Rugamonas rubra* ATCC-43154 (GroupIII)  
Authors : Chao, D.; Zhaolin, L.; Shoujie, L.; Li, Z.; Dan, Z.; Ying, J.; Wei, C.  
Deposited on : 2021-07-13  
Resolution : 2.64 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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

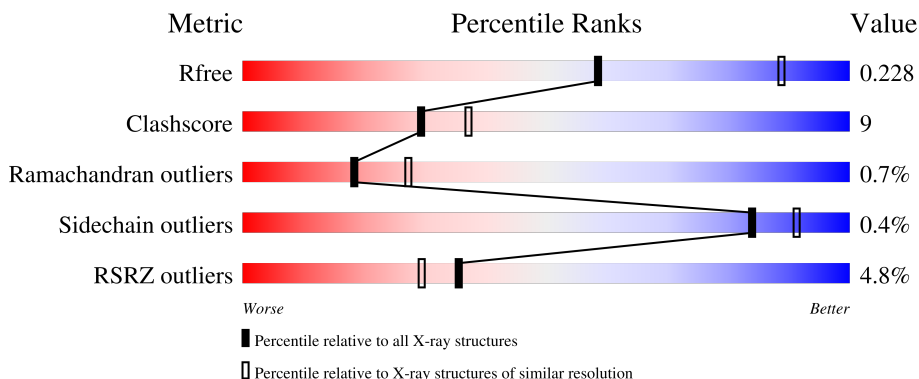
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 Å.

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



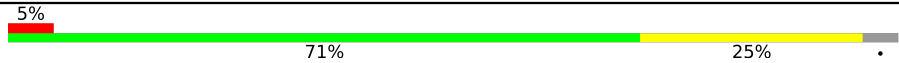
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	29	
1	D	29	
2	E	264	
3	B	263	
4	C	199	

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Mol	Chain	Length	Quality of chain
4	F	199	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '5%', a large green segment labeled '71%', a yellow segment labeled '25%', and a very small grey segment at the end. A small black dot is visible at the far right end of the bar.</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7715 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 RrMbnA precur peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	29	208	128	40	36	4	0	0	0
1	D	29	208	128	40	36	4	0	0	0

- Molecule 2 is a protein called Methanobactin biosynthesis cassette protein MbnB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	264	2092	1327	373	386	6	0	0	0

- Molecule 3 is a protein called Methanobactin biosynthesis cassette protein MbnB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	263	2088	1325	372	385	6	0	0	0

- Molecule 4 is a protein called Methanobactin biosynthesis cassette protein MbnC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	191	1503	962	272	264	5	0	0	0
4	C	191	1503	962	272	264	5	0	0	0

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	3	Total	Fe	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total 3	O 3	0	0

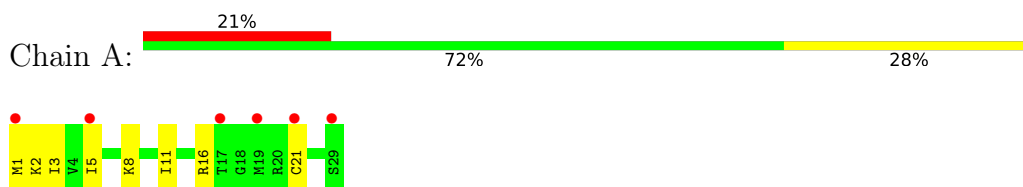
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total 4	O 4	0	0
6	E	34	Total 34	O 34	0	0
6	B	43	Total 43	O 43	0	0
6	F	7	Total 7	O 7	0	0
6	C	19	Total 19	O 19	0	0

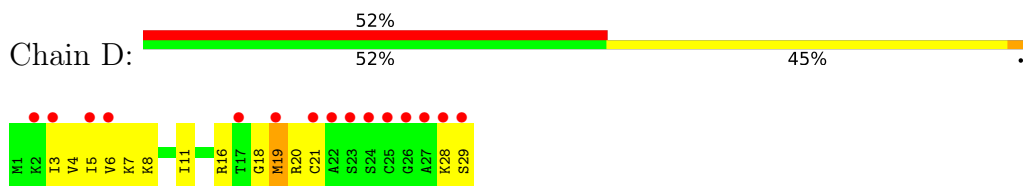
### 3 Residue-property plots [i](#)

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.

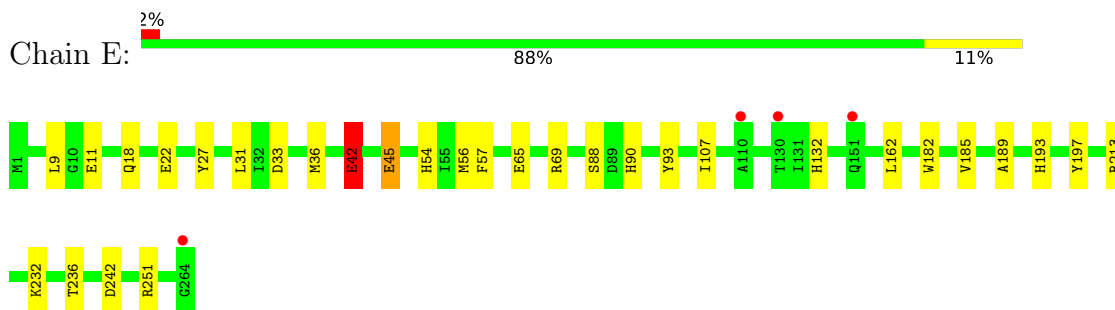
- Molecule 1: RrMbnA precusor peptide



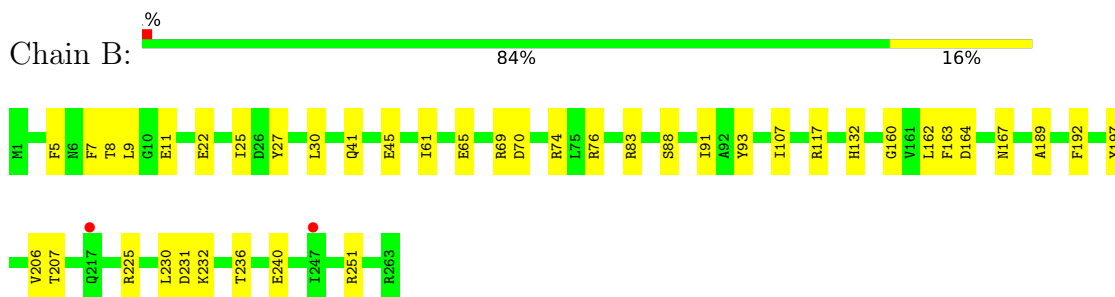
- Molecule 1: RrMbnA precusor peptide



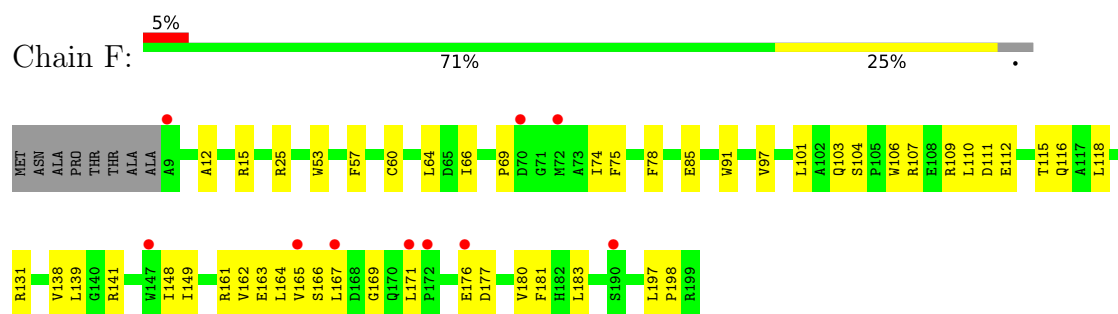
- Molecule 2: Methanobactin biosynthesis cassette protein MbnB



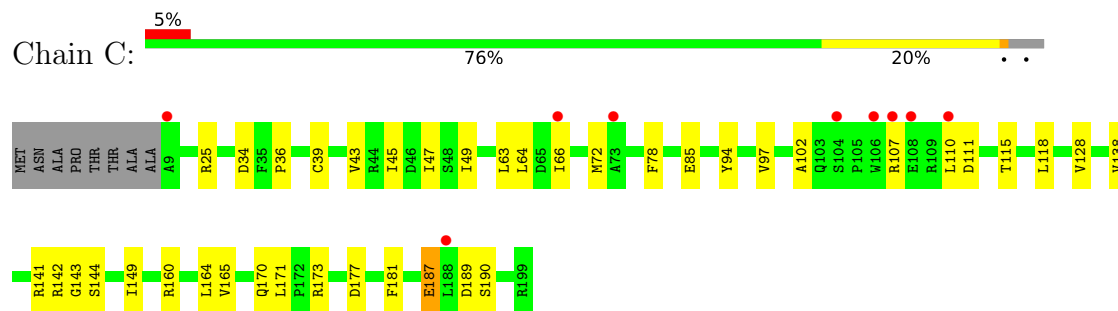
- Molecule 3: Methanobactin biosynthesis cassette protein MbnB



- Molecule 4: Methanobactin biosynthesis cassette protein MbnC



- Molecule 4: Methanobactin biosynthesis cassette protein MbnC



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.97Å 173.97Å 61.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.51 – 2.64 61.51 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.51-2.64) 91.5 (61.51-2.64)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.178 , 0.224 0.183 , 0.228	Depositor DCC
$R_{free}$ test set	2672 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.0	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 80.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: 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	0.51	0/207	0.84	0/272
1	D	0.52	0/207	0.94	0/272
2	E	0.41	0/2144	0.66	2/2912 (0.1%)
3	B	0.43	0/2140	0.67	0/2907
4	C	0.42	0/1548	0.70	0/2112
4	F	0.38	0/1548	0.69	0/2112
All	All	0.42	0/7794	0.69	2/10587 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	45	GLU	CA-CB-CG	5.96	126.01	114.10
2	E	42	GLU	N-CA-C	-5.57	98.94	110.80

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	208	0	236	10	0
1	D	208	0	236	11	0
2	E	2092	0	2003	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2088	0	2001	30	0
4	C	1503	0	1465	38	0
4	F	1503	0	1465	38	0
5	B	3	0	0	0	0
5	E	3	0	0	0	0
6	A	4	0	0	1	0
6	B	43	0	0	4	0
6	C	19	0	0	1	0
6	E	34	0	0	0	0
6	F	7	0	0	0	0
All	All	7715	0	7406	129	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 9.

All (129) 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)
3:B:225:ARG:NH1	6:B:401:HOH:O	1.99	0.96
4:C:141:ARG:NH2	4:C:142:ARG:HB3	1.85	0.89
1:A:1:MET:SD	1:A:2:LYS:HB2	2.14	0.88
3:B:206:VAL:HG21	4:C:43:VAL:HG11	1.56	0.86
4:F:197:LEU:HD12	4:F:198:PRO:HD2	1.58	0.85
4:F:104:SER:HG	4:F:106:TRP:HE3	1.27	0.83
4:F:167:LEU:HB2	1:D:4:VAL:HB	1.62	0.82
4:F:164:LEU:HB2	1:D:11:ILE:HD11	1.63	0.81
3:B:22:GLU:OE1	3:B:251:ARG:NH1	2.14	0.80
2:E:33:ASP:HA	2:E:36:MET:HG3	1.64	0.79
4:C:141:ARG:HH21	4:C:142:ARG:H	1.33	0.76
3:B:240:GLU:OE1	6:B:402:HOH:O	2.04	0.74
4:F:112:GLU:OE2	4:F:141:ARG:NH1	2.19	0.73
4:C:141:ARG:HD3	4:C:143:GLY:H	1.56	0.70
4:F:138:VAL:HG12	4:F:149:ILE:HG12	1.78	0.64
4:F:66:ILE:HD12	4:F:109:ARG:HB2	1.81	0.63
3:B:230:LEU:O	3:B:232:LYS:NZ	2.31	0.63
1:A:16:ARG:NH1	3:B:8:THR:OG1	2.27	0.63
3:B:93:TYR:CE2	3:B:107:ILE:HA	2.34	0.63
4:F:66:ILE:HG13	4:F:109:ARG:HD3	1.81	0.62
4:F:104:SER:OG	4:F:106:TRP:HE3	1.83	0.61
3:B:189:ALA:O	3:B:232:LYS:HE2	2.00	0.61
2:E:197:TYR:O	2:E:213:ARG:HD2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:138:VAL:HG21	4:F:181:PHE:CZ	2.36	0.60
4:F:161:ARG:NH2	4:F:163:GLU:OE1	2.33	0.60
2:E:18:GLN:O	2:E:22:GLU:HG2	2.02	0.59
2:E:93:TYR:CE2	2:E:107:ILE:HA	2.37	0.59
4:F:85:GLU:OE1	4:C:25:ARG:NH2	2.36	0.59
3:B:206:VAL:CG2	4:C:43:VAL:HG11	2.31	0.59
2:E:189:ALA:O	2:E:232:LYS:NZ	2.30	0.58
4:F:74:ILE:HD12	4:F:75:PHE:N	2.18	0.58
2:E:182:TRP:HE3	2:E:185:VAL:HG21	1.68	0.58
4:C:102:ALA:O	4:C:107:ARG:HG3	2.05	0.57
4:F:139:LEU:HD23	4:F:180:VAL:HG12	1.86	0.56
4:C:138:VAL:HG21	4:C:181:PHE:CZ	2.41	0.56
2:E:56:MET:HG2	2:E:57:PHE:CE2	2.41	0.56
4:F:91:TRP:HH2	4:F:180:VAL:HG11	1.71	0.56
4:C:141:ARG:HH22	4:C:142:ARG:HB3	1.68	0.56
4:F:60:CYS:SG	4:F:118:LEU:HD23	2.46	0.55
1:A:11:ILE:HD11	4:C:164:LEU:HB2	1.88	0.55
4:F:162:VAL:HG23	1:D:11:ILE:HB	1.87	0.55
4:C:107:ARG:HH11	4:C:107:ARG:HB3	1.72	0.53
2:E:65:GLU:O	2:E:69:ARG:HG3	2.08	0.53
3:B:70:ASP:OD2	3:B:74:ARG:NH1	2.39	0.53
4:F:165:VAL:HG12	1:D:8:LYS:HG2	1.91	0.53
4:C:107:ARG:HB3	4:C:107:ARG:NH1	2.24	0.53
1:D:18:GLY:O	1:D:19:MET:HB2	2.09	0.53
4:C:141:ARG:NH2	4:C:142:ARG:H	2.05	0.52
4:F:111:ASP:O	4:F:115:THR:HG23	2.10	0.52
4:F:107:ARG:O	4:F:110:LEU:HD12	2.10	0.52
4:C:72:MET:HE1	6:C:218:HOH:O	2.09	0.51
4:C:142:ARG:HB2	4:C:177:ASP:HA	1.92	0.51
2:E:162:LEU:HD21	2:E:193:HIS:CE1	2.45	0.51
4:F:25:ARG:HH22	4:C:85:GLU:HG2	1.75	0.50
1:A:1:MET:HE1	4:C:170:GLN:OE1	2.11	0.50
1:A:5:ILE:O	1:A:5:ILE:HD12	2.10	0.50
1:A:2:LYS:O	4:C:171:LEU:HD21	2.10	0.50
4:C:138:VAL:HG21	4:C:181:PHE:CE2	2.47	0.49
3:B:76:ARG:HD2	6:B:426:HOH:O	2.11	0.49
3:B:41:GLN:O	3:B:45:GLU:HG3	2.12	0.49
4:C:107:ARG:O	4:C:110:LEU:HD22	2.12	0.49
4:C:43:VAL:O	4:C:47:ILE:HG13	2.13	0.49
3:B:231:ASP:C	3:B:232:LYS:HG3	2.39	0.48
4:C:128:VAL:HG23	4:C:160:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:CYS:HA	3:B:9:LEU:HD21	1.96	0.48
3:B:117:ARG:NH1	6:B:404:HOH:O	2.43	0.48
2:E:42:GLU:HA	2:E:45:GLU:HG3	1.96	0.48
4:F:181:PHE:HE1	4:F:183:LEU:HD21	1.78	0.48
3:B:5:PHE:HB2	3:B:25:ILE:HG21	1.96	0.47
4:F:101:LEU:O	4:F:104:SER:HB3	2.14	0.47
1:A:3:ILE:HD11	4:C:190:SER:O	2.14	0.47
3:B:164:ASP:HB3	3:B:167:ASN:HB2	1.95	0.47
3:B:65:GLU:O	3:B:69:ARG:HG3	2.14	0.47
4:F:78:PHE:CZ	4:F:97:VAL:HG22	2.50	0.47
2:E:54:HIS:NE2	2:E:90:HIS:CE1	2.82	0.47
3:B:65:GLU:OE2	3:B:69:ARG:NH1	2.48	0.47
4:F:169:GLY:N	1:D:4:VAL:HG21	2.29	0.46
2:E:56:MET:HG2	2:E:57:PHE:CD2	2.51	0.46
4:C:78:PHE:CE2	4:C:97:VAL:HG12	2.51	0.46
2:E:56:MET:HB2	2:E:56:MET:HE2	1.53	0.45
4:F:66:ILE:CD1	4:F:109:ARG:HB2	2.47	0.45
3:B:132:HIS:CD2	3:B:160:GLY:HA3	2.51	0.45
4:C:144:SER:O	4:C:173:ARG:HD3	2.16	0.45
1:D:16:ARG:H	1:D:21:CYS:HB3	1.81	0.45
4:C:138:VAL:HG12	4:C:149:ILE:HG12	1.98	0.45
1:D:7:LYS:HG3	1:D:8:LYS:N	2.31	0.45
4:F:12:ALA:HB3	4:F:15:ARG:HG3	1.99	0.45
4:F:64:LEU:O	4:F:69:PRO:HA	2.17	0.44
2:E:31:LEU:HD12	2:E:31:LEU:HA	1.88	0.44
4:F:57:PHE:CE1	4:F:74:ILE:HD11	2.52	0.44
4:F:166:SER:O	1:D:6:VAL:HB	2.18	0.44
4:C:111:ASP:O	4:C:115:THR:HG23	2.17	0.44
4:C:36:PRO:HD2	4:C:39:CYS:SG	2.57	0.44
3:B:206:VAL:HG21	4:C:43:VAL:CG1	2.37	0.44
6:A:103:HOH:O	3:B:11:GLU:HB3	2.18	0.44
4:C:94:TYR:O	4:C:97:VAL:HG22	2.18	0.44
2:E:9:LEU:HB3	2:E:11:GLU:HG2	2.00	0.43
4:F:171:LEU:HD23	4:F:171:LEU:HA	1.75	0.43
2:E:93:TYR:CE1	2:E:107:ILE:HG22	2.52	0.43
3:B:27:TYR:CE1	3:B:236:THR:HB	2.53	0.43
3:B:88:SER:CB	3:B:162:LEU:HD13	2.48	0.43
4:C:25:ARG:NH1	4:C:34:ASP:OD2	2.51	0.43
4:C:64:LEU:HD12	4:C:64:LEU:HA	1.87	0.43
3:B:7:PHE:CD2	3:B:30:LEU:HD22	2.54	0.43
2:E:22:GLU:OE1	2:E:251:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:TYR:CZ	2:E:236:THR:HB	2.54	0.43
1:A:8:LYS:HG2	4:C:165:VAL:HG22	2.01	0.42
2:E:88:SER:HA	2:E:132:HIS:O	2.18	0.42
3:B:163:PHE:HB3	3:B:192:PHE:CD1	2.55	0.42
4:F:91:TRP:HZ3	4:F:139:LEU:HD21	1.85	0.42
2:E:242:ASP:O	1:D:16:ARG:NH1	2.35	0.42
4:C:187:GLU:H	4:C:187:GLU:HG3	1.76	0.42
4:F:111:ASP:OD1	4:F:111:ASP:N	2.51	0.42
4:F:116:GLN:HG2	4:F:148:ILE:HD11	2.01	0.42
1:D:28:LYS:HD3	1:D:29:SER:N	2.35	0.42
4:F:101:LEU:HA	4:F:104:SER:HB3	2.02	0.41
4:F:131:ARG:HD3	4:F:131:ARG:HA	1.92	0.41
3:B:197:TYR:CD1	3:B:207:THR:HG23	2.56	0.41
4:C:66:ILE:H	4:C:66:ILE:HG13	1.62	0.41
3:B:9:LEU:HD23	3:B:9:LEU:HA	1.88	0.41
3:B:61:ILE:HD11	3:B:91:ILE:HD13	2.03	0.41
3:B:83:ARG:HE	3:B:83:ARG:HB3	1.73	0.41
2:E:33:ASP:OD2	2:E:56:MET:O	2.38	0.41
4:F:53:TRP:CD2	4:F:57:PHE:HD2	2.39	0.40
4:C:78:PHE:CZ	4:C:97:VAL:HG12	2.56	0.40
4:C:45:ILE:O	4:C:49:ILE:HG12	2.21	0.40
4:F:109:ARG:HE	4:F:109:ARG:HB3	1.70	0.40
1:A:2:LYS:HA	1:A:2:LYS:HD2	1.78	0.40
4:C:63:LEU:HD11	4:C:118:LEU:HD21	2.04	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	27/29 (93%)	21 (78%)	6 (22%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	27/29 (93%)	21 (78%)	2 (7%)	4 (15%)	0	0
2	E	262/264 (99%)	257 (98%)	4 (2%)	1 (0%)	30	42
3	B	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
4	C	189/199 (95%)	184 (97%)	4 (2%)	1 (0%)	24	36
4	F	189/199 (95%)	184 (97%)	4 (2%)	1 (0%)	24	36
All	All	955/983 (97%)	922 (96%)	26 (3%)	7 (1%)	18	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	19	MET
4	F	177	ASP
1	D	3	ILE
1	D	20	ARG
4	C	189	ASP
2	E	42	GLU
1	D	5	ILE

### 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	23/23 (100%)	23 (100%)	0	100	100
1	D	23/23 (100%)	23 (100%)	0	100	100
2	E	210/210 (100%)	210 (100%)	0	100	100
3	B	210/210 (100%)	210 (100%)	0	100	100
4	C	149/154 (97%)	148 (99%)	1 (1%)	76	86
4	F	149/154 (97%)	147 (99%)	2 (1%)	61	76
All	All	764/774 (99%)	761 (100%)	3 (0%)	84	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	103	GLN
4	F	176	GLU
4	C	187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	67	GLN
3	B	34	ASN
3	B	37	GLN
3	B	67	GLN
3	B	96	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<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	29/29 (100%)	1.34	6 (20%) 2 2	82, 115, 163, 165	0
1	D	29/29 (100%)	2.11	15 (51%) 0 0	98, 137, 172, 186	0
2	E	264/264 (100%)	-0.09	4 (1%) 72 69	53, 78, 106, 132	0
3	B	263/263 (100%)	-0.15	2 (0%) 82 80	46, 76, 114, 136	0
4	C	191/199 (95%)	0.34	9 (4%) 36 30	56, 95, 150, 196	0
4	F	191/199 (95%)	0.33	10 (5%) 33 27	56, 99, 160, 214	0
All	All	967/983 (98%)	0.17	46 (4%) 35 29	46, 87, 148, 214	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	GLY	5.1
1	D	29	SER	5.1
1	D	22	ALA	4.7
1	D	27	ALA	4.7
4	C	110	LEU	4.3
4	C	66	ILE	4.3
4	F	72	MET	4.1
1	D	3	ILE	4.0
4	C	9	ALA	3.8
1	D	28	LYS	3.7
1	A	29	SER	3.5
2	E	110	ALA	3.3
1	A	19	MET	3.2
2	E	264	GLY	3.2
4	F	147	TRP	3.0
4	C	108	GLU	2.9
4	F	9	ALA	2.9
1	D	5	ILE	2.8
4	F	165	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	24	SER	2.7
4	F	172	PRO	2.7
1	D	21	CYS	2.7
3	B	247	ILE	2.7
1	D	23	SER	2.7
1	A	5	ILE	2.6
2	E	130	THR	2.6
4	F	70	ASP	2.6
1	D	19	MET	2.6
4	F	171	LEU	2.5
4	C	107	ARG	2.5
3	B	217	GLN	2.5
4	C	73	ALA	2.4
1	A	21	CYS	2.4
4	F	176	GLU	2.4
2	E	151	GLN	2.4
1	A	17	THR	2.3
1	D	17	THR	2.3
1	D	2	LYS	2.1
1	A	1	MET	2.1
1	D	6	VAL	2.1
4	C	104	SER	2.1
1	D	25	CYS	2.1
4	C	106	TRP	2.1
4	F	167	LEU	2.1
4	C	188	LEU	2.1
4	F	190	SER	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 oligosaccharides in this entry.

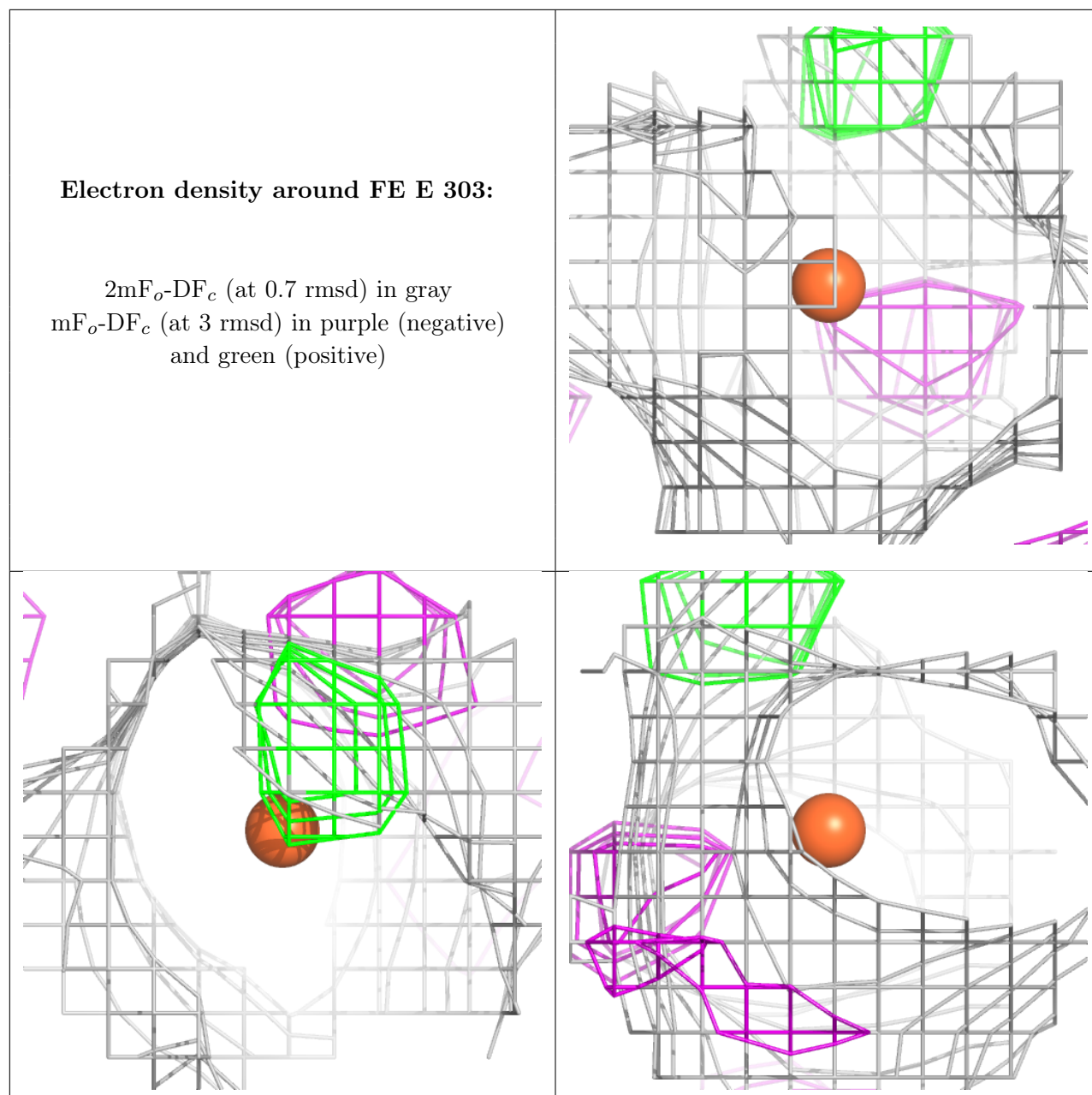
## 6.4 Ligands [i](#)

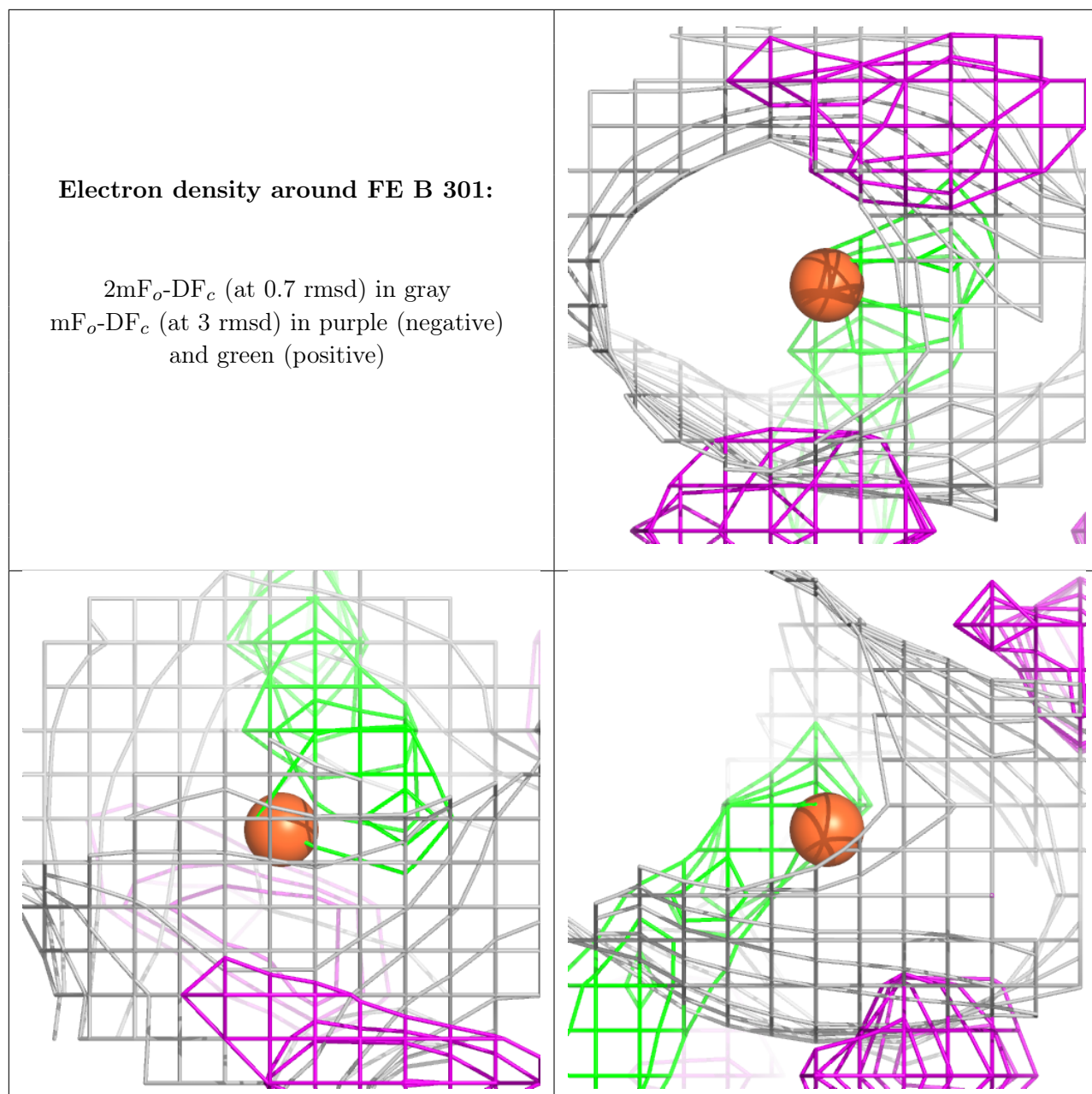
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
5	FE	E	303	1/1	0.98	0.04	78,78,78,78	0
5	FE	B	301	1/1	0.98	0.06	81,81,81,81	0
5	FE	B	303	1/1	0.99	0.03	61,61,61,61	0
5	FE	E	302	1/1	1.00	0.02	60,60,60,60	0
5	FE	B	302	1/1	1.00	0.02	64,64,64,64	0
5	FE	E	301	1/1	1.00	0.02	76,76,76,76	0

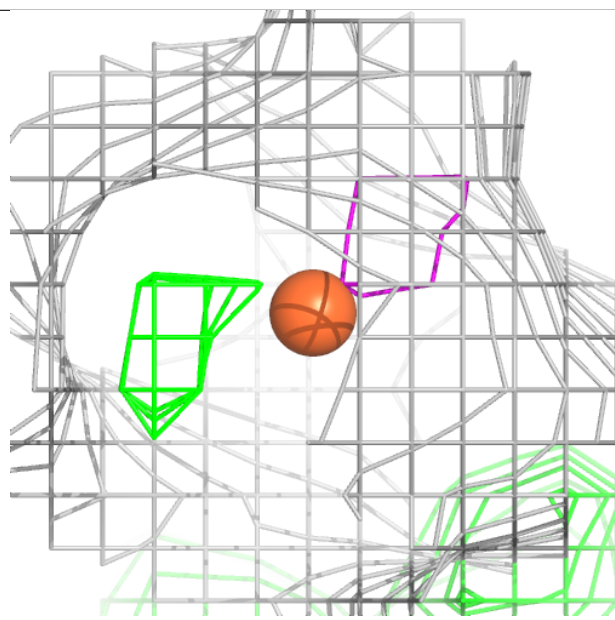
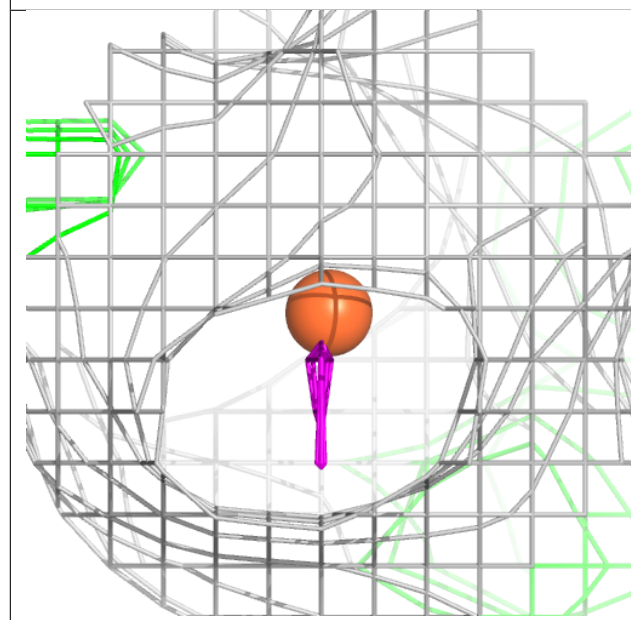
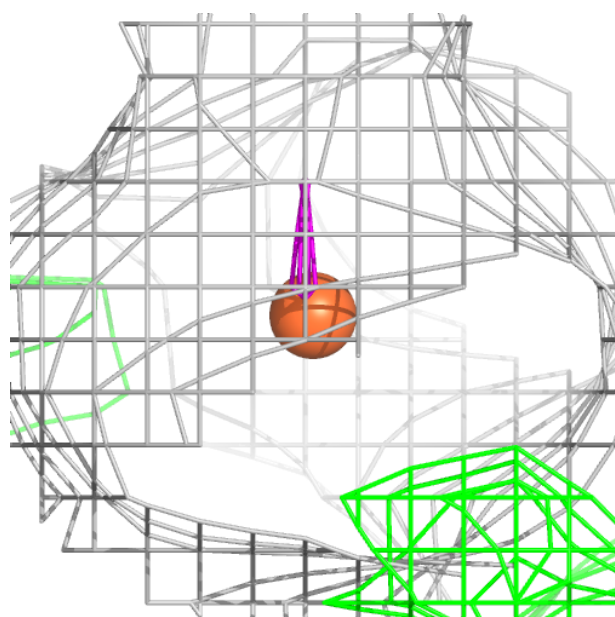
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

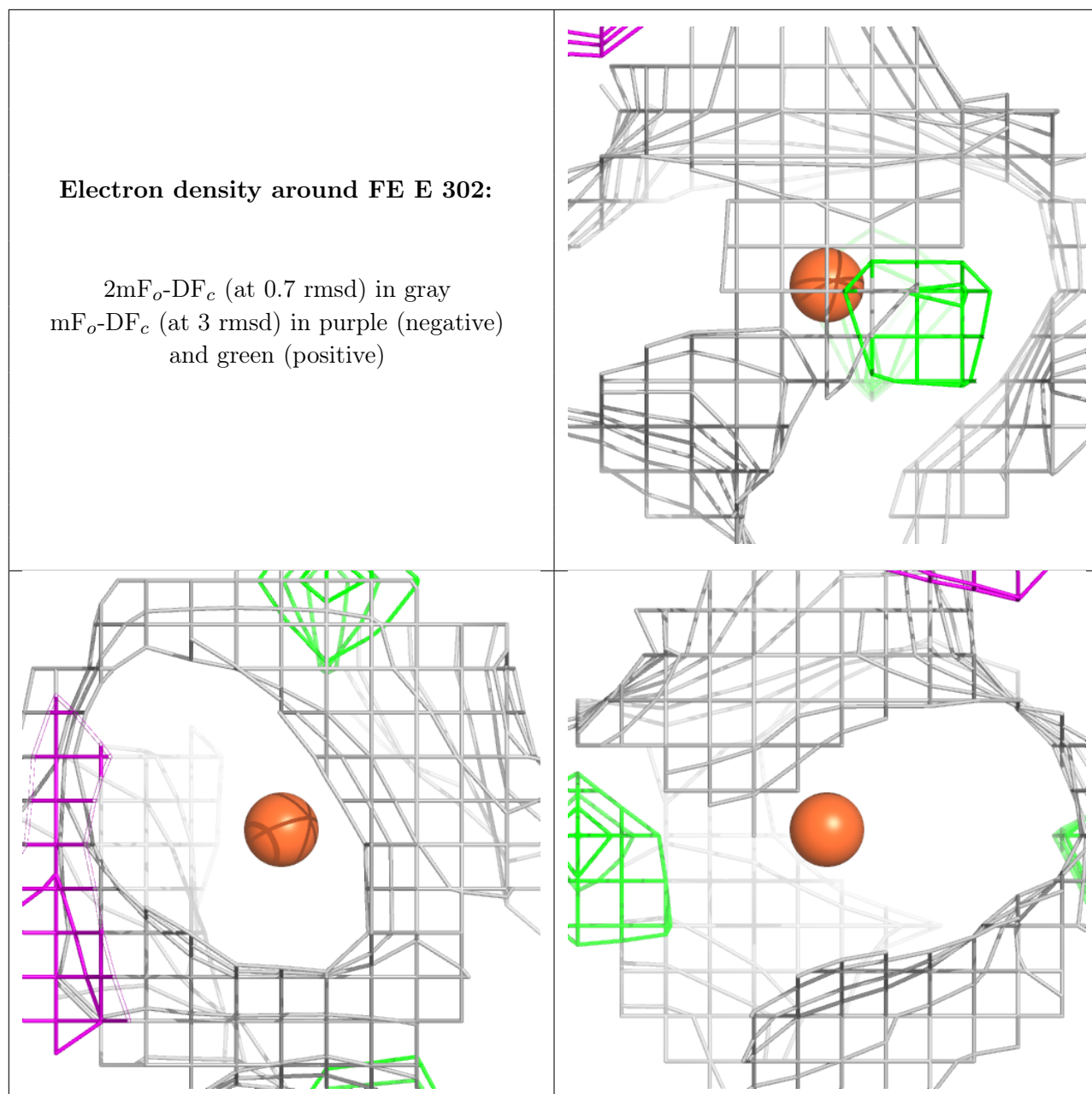


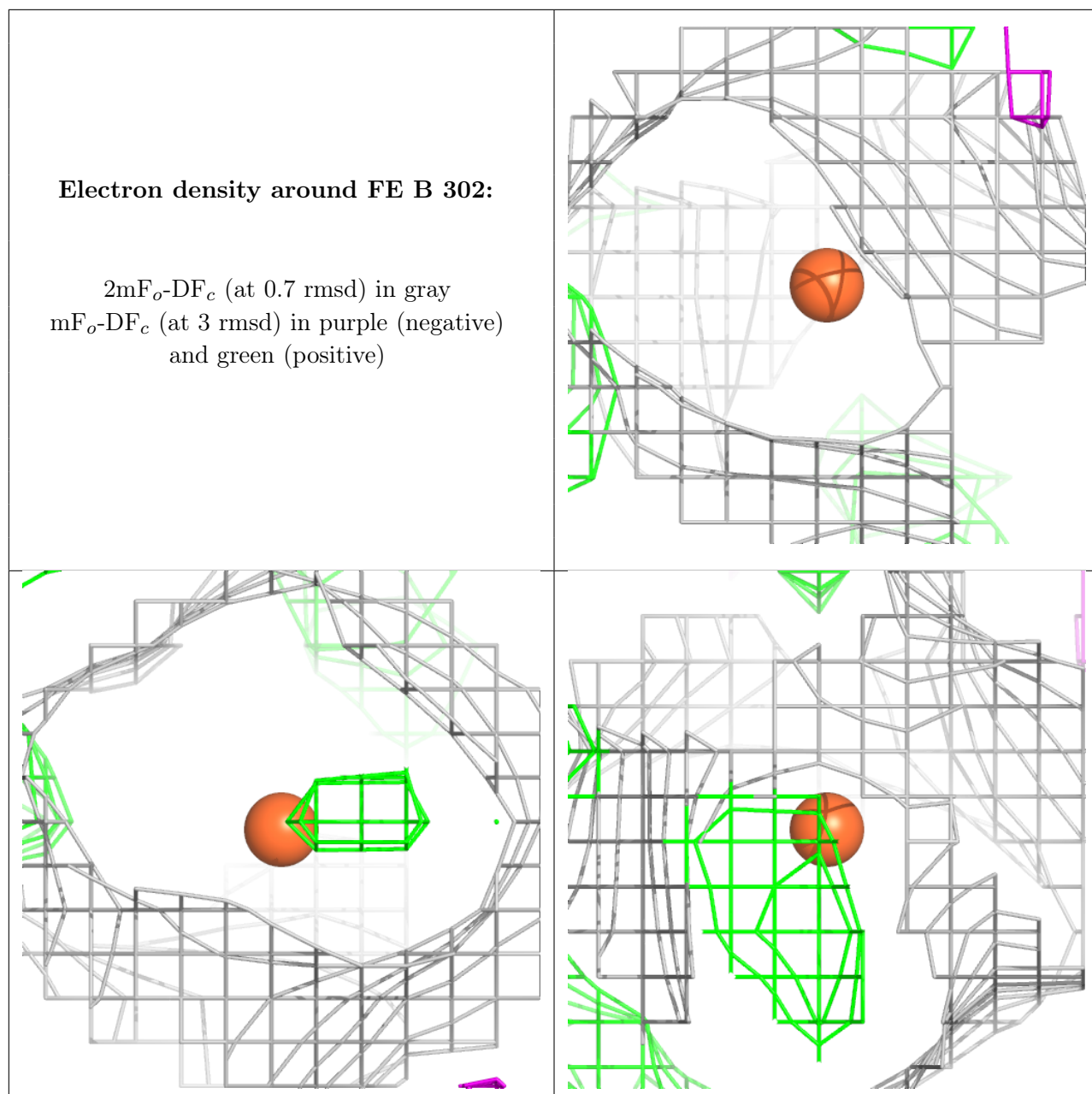


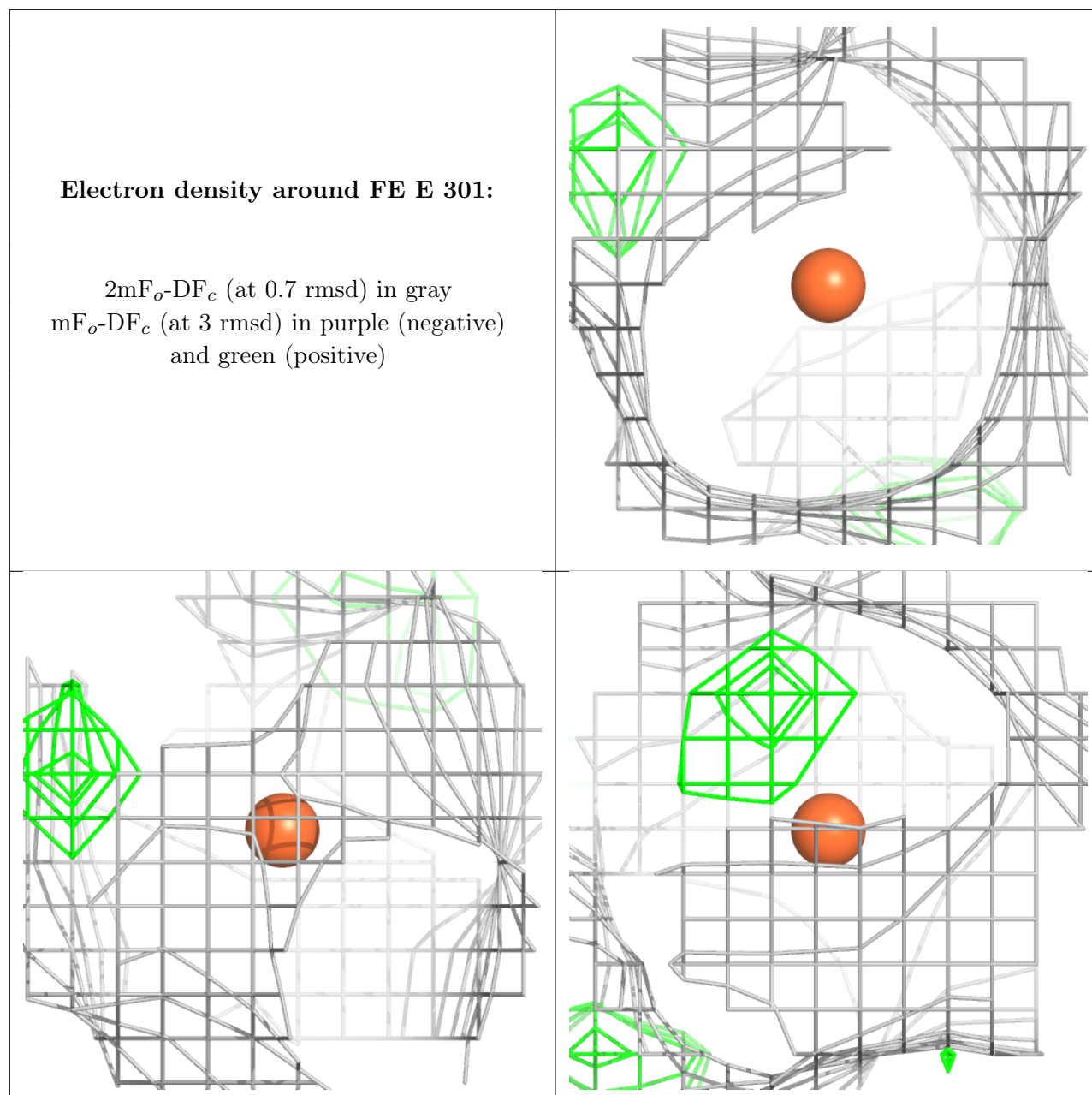
**Electron density around FE B 303:**

$2mF_o-DF_c$  (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.