



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2023 – 03:23 PM EDT

PDB ID : 8FUO
Title : Fe-bound AibH1H2
Authors : Powell, M.M.; Rittle, J.
Deposited on : 2023-01-17
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.2
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) : 2.32.2

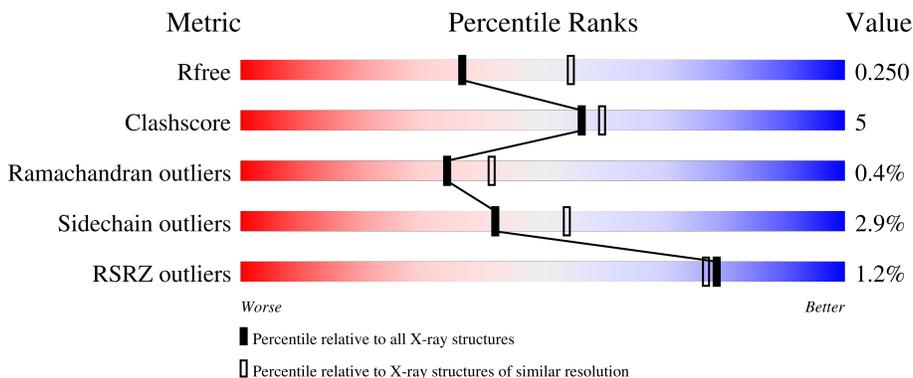
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	392	
1	C	392	
2	B	378	
2	D	378	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11658 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 Amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2803	1788	490	520	5	0	1	0
1	C	350	2813	1795	494	519	5	0	2	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP A0A402C2V4
A	-5	GLY	-	expression tag	UNP A0A402C2V4
A	-4	HIS	-	expression tag	UNP A0A402C2V4
A	-3	HIS	-	expression tag	UNP A0A402C2V4
A	-2	HIS	-	expression tag	UNP A0A402C2V4
A	-1	HIS	-	expression tag	UNP A0A402C2V4
A	0	HIS	-	expression tag	UNP A0A402C2V4
A	1	HIS	-	expression tag	UNP A0A402C2V4
A	2	SER	-	expression tag	UNP A0A402C2V4
A	3	GLY	-	expression tag	UNP A0A402C2V4
A	4	GLU	-	expression tag	UNP A0A402C2V4
A	5	ASN	-	expression tag	UNP A0A402C2V4
A	6	LEU	-	expression tag	UNP A0A402C2V4
A	7	TYR	-	expression tag	UNP A0A402C2V4
A	8	PHE	-	expression tag	UNP A0A402C2V4
A	9	GLN	-	expression tag	UNP A0A402C2V4
A	10	SER	-	expression tag	UNP A0A402C2V4
A	11	GLY	-	expression tag	UNP A0A402C2V4
A	12	GLY	-	expression tag	UNP A0A402C2V4
C	-6	MET	-	expression tag	UNP A0A402C2V4
C	-5	GLY	-	expression tag	UNP A0A402C2V4
C	-4	HIS	-	expression tag	UNP A0A402C2V4
C	-3	HIS	-	expression tag	UNP A0A402C2V4
C	-2	HIS	-	expression tag	UNP A0A402C2V4
C	-1	HIS	-	expression tag	UNP A0A402C2V4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A0A402C2V4
C	1	HIS	-	expression tag	UNP A0A402C2V4
C	2	SER	-	expression tag	UNP A0A402C2V4
C	3	GLY	-	expression tag	UNP A0A402C2V4
C	4	GLU	-	expression tag	UNP A0A402C2V4
C	5	ASN	-	expression tag	UNP A0A402C2V4
C	6	LEU	-	expression tag	UNP A0A402C2V4
C	7	TYR	-	expression tag	UNP A0A402C2V4
C	8	PHE	-	expression tag	UNP A0A402C2V4
C	9	GLN	-	expression tag	UNP A0A402C2V4
C	10	SER	-	expression tag	UNP A0A402C2V4
C	11	GLY	-	expression tag	UNP A0A402C2V4
C	12	GLY	-	expression tag	UNP A0A402C2V4

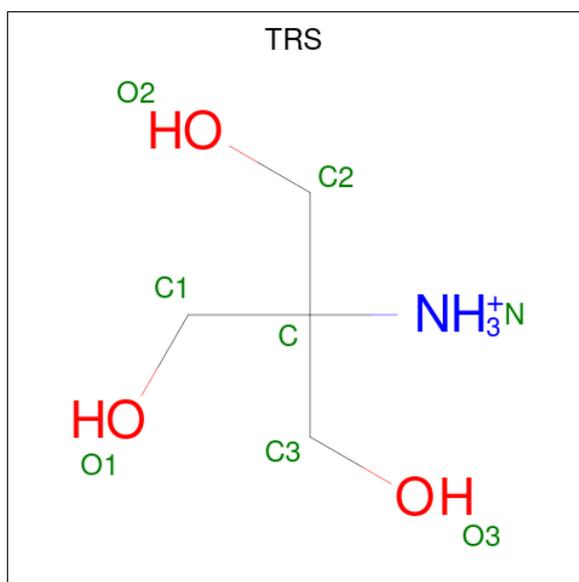
- Molecule 2 is a protein called Amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	365	Total 2859	C 1823	N 485	O 542	S 9	0	2	0
2	D	364	Total 2872	C 1832	N 493	O 538	S 9	0	3	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Fe 1	0	0
3	B	2	Total 2	Fe 2	0	0
3	C	1	Total 1	Fe 1	0	0
3	D	2	Total 2	Fe 2	0	0

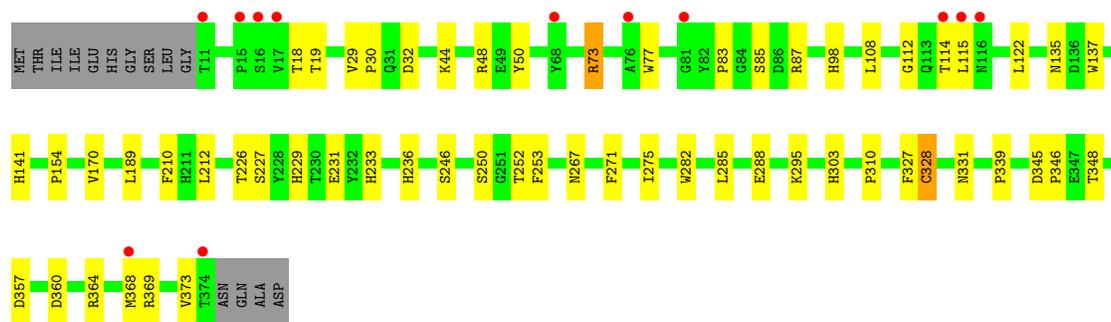
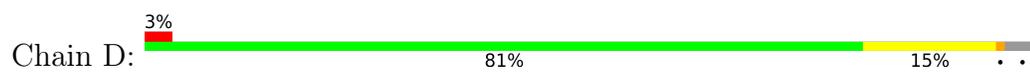
- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	8	4	1	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	87	Total	O	0	0
			87	87		
5	C	30	Total	O	0	0
			30	30		
5	D	55	Total	O	0	0
			55	55		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.78Å 150.57Å 234.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.74 – 2.43 79.74 – 2.43	Depositor EDS
% Data completeness (in resolution range)	96.7 (79.74-2.43) 94.9 (79.74-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.188 , 0.250 0.188 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11658	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	1/2890 (0.0%)	0.60	0/3951
1	C	0.43	0/2901	0.54	0/3965
2	B	0.50	0/2950	0.61	1/4035 (0.0%)
2	D	0.43	0/2966	0.59	0/4053
All	All	0.47	1/11707 (0.0%)	0.59	1/16004 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	ASP	CB-CG	-5.45	1.40	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	212	LEU	CA-CB-CG	5.76	128.55	115.30

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	2803	0	2694	25	0
1	C	2813	0	2707	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2859	0	2715	36	0
2	D	2872	0	2747	31	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	B	8	0	11	0	0
5	A	125	0	0	0	0
5	B	87	0	0	0	0
5	C	30	0	0	0	0
5	D	55	0	0	0	0
All	All	11658	0	10874	112	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 5.

All (112) 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)
2:B:67:MET:CE	1:C:128:ARG:NH1	2.08	1.16
2:B:67:MET:HE1	1:C:128:ARG:NH1	1.68	1.06
2:B:67:MET:HE2	1:C:128:ARG:HH12	1.19	1.06
1:A:170:ASP:O	1:A:173:SER:OG	1.81	0.98
2:B:67:MET:HE2	1:C:128:ARG:NH1	1.75	0.89
2:B:67:MET:HE1	1:C:128:ARG:HH11	1.40	0.86
1:A:270:PHE:HB3	1:A:308:VAL:HG11	1.67	0.76
2:D:267:ASN:ND2	2:D:310:PRO:O	2.26	0.68
1:C:154:SER:HB3	1:C:180:GLN:HG3	1.76	0.67
1:C:265:LEU:HB2	1:C:308:VAL:HG12	1.78	0.65
2:D:98:HIS:HB3	2:D:346:PRO:HG3	1.79	0.64
2:B:360[A]:ASP:OD1	2:B:364:ARG:NH2	2.31	0.64
2:B:12:LEU:HD11	2:B:147:PRO:HB3	1.80	0.63
1:A:283:LEU:HD13	2:B:233:HIS:HB3	1.81	0.62
1:C:158:PRO:HD2	1:C:165:ALA:HA	1.82	0.61
1:C:78:ILE:HG22	2:D:285:LEU:HD21	1.82	0.61
1:C:102:ASP:OD2	1:C:341:TYR:OH	2.16	0.60
2:D:135:ASN:OD1	2:D:154:PRO:HD2	2.01	0.60
2:D:18:THR:OG1	2:D:19:THR:N	2.35	0.57
2:B:108:LEU:HD13	2:B:115:LEU:HD13	1.87	0.56
1:A:163:ARG:NH1	1:A:167:GLU:OE1	2.38	0.56
2:D:282:TRP:CZ3	2:D:295:LYS:HG3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PRO:HD3	2:D:227:SER:HB3	1.90	0.54
2:D:32:ASP:OD1	2:D:112:GLY:HA2	2.08	0.53
2:B:67:MET:CE	1:C:128:ARG:HH11	1.99	0.53
2:D:77:TRP:CE3	2:D:83:PRO:HD3	2.44	0.52
1:C:281:ASP:OD1	1:C:297:SER:OG	2.22	0.52
2:B:311:ILE:HG13	2:B:312:ASP:N	2.25	0.52
1:C:186:GLN:NE2	1:C:222:PRO:HA	2.24	0.52
1:C:283:LEU:HD13	2:D:233:HIS:HB3	1.91	0.52
1:A:225:VAL:HG12	2:B:184:LYS:HA	1.92	0.52
2:D:360[A]:ASP:OD1	2:D:364:ARG:NH1	2.44	0.51
1:A:326:VAL:HG13	1:A:331:SER:O	2.11	0.51
1:A:80:GLN:HA	1:A:342:PRO:O	2.09	0.51
1:C:117:LEU:HD11	1:C:213:HIS:CE1	2.46	0.51
2:B:288:GLU:HB2	2:D:50:TYR:CZ	2.45	0.51
2:B:320:LEU:O	2:B:324:LEU:HG	2.11	0.51
1:C:318:GLU:O	1:C:355:GLY:HA2	2.11	0.50
2:B:87:ARG:NH1	2:B:141:HIS:O	2.39	0.50
2:B:50:TYR:CZ	2:D:288:GLU:HB2	2.47	0.50
2:B:93:GLN:OE1	2:B:338:TYR:OH	2.19	0.50
1:A:169:ILE:HD11	1:A:181:VAL:HG11	1.92	0.50
1:C:364:ARG:HA	1:C:368:ARG:HB2	1.94	0.50
1:C:292:PRO:HD2	1:C:293:TRP:CZ3	2.46	0.49
1:C:34:ASP:HB2	1:C:109:THR:HG21	1.93	0.49
2:D:345:ASP:HB3	2:D:348:THR:OG1	2.13	0.49
1:C:274:PRO:HB2	1:C:275:PRO:HD3	1.94	0.49
2:B:104:VAL:HG21	2:B:371:PHE:CZ	2.48	0.48
2:B:152:ALA:HA	2:B:178:ALA:O	2.13	0.48
1:A:292:PRO:HD2	1:A:293:TRP:CZ3	2.49	0.48
1:C:80:GLN:HA	1:C:342:PRO:O	2.13	0.48
1:A:187:SER:HB3	1:A:191:TYR:CZ	2.48	0.47
1:C:146:ASP:OD1	1:C:177:ARG:NH1	2.32	0.47
1:A:322:LEU:HD23	1:A:356:THR:HB	1.97	0.47
2:B:104:VAL:HG22	2:B:177:VAL:HG21	1.95	0.47
2:D:189:LEU:HD13	2:D:210:PHE:CZ	2.49	0.47
1:C:101:LYS:O	1:C:105:ALA:HB2	2.15	0.47
1:C:233:GLU:OE1	2:D:246:SER:HB2	2.15	0.47
2:B:219:ALA:HA	2:B:225:TRP:CZ2	2.50	0.47
1:A:314:ASP:HA	2:B:280:TYR:CG	2.50	0.46
2:B:121:ALA:HB3	2:B:127:ALA:HB2	1.97	0.46
1:C:30:PRO:O	1:C:367:ARG:HG3	2.16	0.46
1:C:51:LEU:HD22	1:C:55:TRP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:HA	1:A:197:TRP:CE2	2.50	0.46
2:D:73:ARG:HG2	2:D:339:PRO:O	2.16	0.46
2:D:29:VAL:HG13	2:D:85:SER:HB3	1.98	0.45
2:B:237:VAL:HG13	2:B:270:HIS:CE1	2.51	0.45
2:D:364:ARG:O	2:D:368:MET:HG3	2.16	0.45
2:D:44:LYS:O	2:D:48:ARG:HG3	2.16	0.45
1:C:325:ILE:O	1:C:329:LEU:HG	2.16	0.45
2:B:132:ARG:HG3	2:B:169:ARG:CZ	2.47	0.45
2:D:368:MET:HB3	2:D:373:VAL:HB	1.98	0.45
2:D:122:LEU:HD23	2:D:122:LEU:HA	1.86	0.45
2:D:331:ASN:OD1	2:D:369:ARG:NH2	2.47	0.44
2:B:40:ASP:OD2	2:B:41:ASP:N	2.50	0.44
1:C:140:ILE:O	1:C:144:TRP:HB2	2.17	0.44
2:D:250:SER:HG	2:D:252:THR:HG1	1.65	0.44
1:A:129:GLU:HG2	1:A:158:PRO:HB3	1.99	0.44
2:D:253:PHE:CE1	2:D:303:HIS:HB3	2.53	0.43
2:B:58:LEU:HG	1:C:122:GLN:OE1	2.18	0.43
2:B:336:THR:HB	2:B:343:PHE:CE2	2.54	0.43
1:A:38:HIS:CE1	1:A:117:LEU:HD11	2.54	0.43
2:D:212:LEU:HD21	2:D:236:HIS:NE2	2.33	0.43
2:B:158:GLU:HA	2:B:158:GLU:OE1	2.18	0.43
1:C:44:PRO:HG3	1:C:66:THR:HA	2.01	0.43
1:A:364:ARG:HE	1:A:364:ARG:HB3	1.72	0.43
2:D:30:PRO:HA	2:D:137:TRP:CZ2	2.54	0.43
1:A:194:GLU:HA	1:A:197:TRP:CD2	2.53	0.43
1:C:145:LEU:HB3	1:C:177:ARG:HD2	2.00	0.42
2:D:189:LEU:HD13	2:D:210:PHE:CE2	2.54	0.42
1:C:274:PRO:HG3	1:C:329:LEU:HD23	2.02	0.42
2:D:87:ARG:HD3	2:D:141:HIS:O	2.20	0.42
2:B:12:LEU:HB3	2:B:174:PRO:HG2	2.01	0.42
2:B:177:VAL:O	2:B:207:PRO:HD2	2.20	0.42
2:D:226:THR:HB	2:D:231:GLU:HB3	2.01	0.42
1:A:283:LEU:HA	1:A:283:LEU:HD23	1.62	0.42
1:C:186:GLN:HB3	1:C:216:GLY:HA3	2.00	0.42
2:B:207:PRO:HB2	2:B:370:PHE:CZ	2.55	0.42
1:A:62:GLN:O	1:A:65:PRO:HD3	2.20	0.41
1:C:169:ILE:HD11	1:C:181:VAL:HG11	2.01	0.41
1:A:136:LEU:O	1:A:139:TRP:HB3	2.21	0.41
1:C:340:ASP:OD2	1:C:345:HIS:NE2	2.49	0.41
1:A:232:LEU:HD23	2:B:289:LEU:HD12	2.02	0.41
1:A:278:TRP:CZ2	2:B:314:PRO:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:ILE:HA	1:C:325:ILE:HD12	1.83	0.41
2:B:281:THR:HG22	2:B:285:LEU:HD12	2.02	0.40
1:A:56:ALA:O	1:A:60:VAL:HG23	2.20	0.40
1:A:166:ALA:HB1	1:A:202:ALA:HB2	2.02	0.40
2:B:237:VAL:HG22	2:B:266:GLY:O	2.21	0.40
1:C:333:ARG:HA	1:C:333:ARG:HD3	1.92	0.40
1:C:187:SER:HB3	1:C:191:TYR:CZ	2.57	0.40
2:D:271:PHE:O	2:D:275:ILE:HG13	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	349/392 (89%)	338 (97%)	11 (3%)	0	100	100
1	C	350/392 (89%)	326 (93%)	22 (6%)	2 (1%)	25	29
2	B	365/378 (97%)	345 (94%)	18 (5%)	2 (0%)	29	34
2	D	365/378 (97%)	342 (94%)	21 (6%)	2 (0%)	29	34
All	All	1429/1540 (93%)	1351 (94%)	72 (5%)	6 (0%)	34	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	328	CYS
1	C	270	PHE
2	B	343	PHE
1	C	367	ARG
2	D	327	PHE
2	D	328	CYS

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	299/332 (90%)	292 (98%)	7 (2%)	50	63
1	C	300/332 (90%)	288 (96%)	12 (4%)	31	41
2	B	302/318 (95%)	294 (97%)	8 (3%)	46	58
2	D	303/318 (95%)	295 (97%)	8 (3%)	46	58
All	All	1204/1300 (93%)	1169 (97%)	35 (3%)	42	54

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	159	GLN
1	A	161	SER
1	A	173	SER
1	A	350	ARG
1	A	364	ARG
1	A	378	VAL
2	B	11	THR
2	B	16	SER
2	B	41	ASP
2	B	67	MET
2	B	82	TYR
2	B	229	HIS
2	B	311	ILE
2	B	357	ASP
1	C	29	VAL
1	C	43	SER
1	C	58	GLN
1	C	82	SER
1	C	125	GLN
1	C	127	ARG
1	C	161	SER
1	C	347	SER
1	C	364	ARG

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Mol	Chain	Res	Type
1	C	367	ARG
1	C	368	ARG
1	C	377	VAL
2	D	73	ARG
2	D	108	LEU
2	D	114	THR
2	D	115	LEU
2	D	170	VAL
2	D	229	HIS
2	D	328	CYS
2	D	357	ASP

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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRS	B	401	3	7,7,7	0.36	0	9,9,9	1.09	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	B	401	3	-	0/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	TRS	C3-C-N	2.16	114.42	107.98

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/392 (89%)	-0.61	0 100 100	27, 43, 60, 76	0
1	C	350/392 (89%)	-0.24	4 (1%) 80 79	37, 63, 84, 92	0
2	B	365/378 (96%)	-0.53	1 (0%) 94 94	26, 46, 71, 89	0
2	D	364/378 (96%)	-0.19	12 (3%) 46 43	31, 58, 84, 94	0
All	All	1429/1540 (92%)	-0.39	17 (1%) 79 77	26, 51, 81, 94	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	TYR	3.9
1	C	377	VAL	3.1
2	D	16	SER	3.0
2	D	114	THR	2.8
2	D	68	TYR	2.7
2	D	368	MET	2.7
2	D	81	GLY	2.7
2	B	68	TYR	2.7
1	C	260	LYS	2.6
1	C	378	VAL	2.5
2	D	374	THR	2.4
2	D	116	ASN	2.2
2	D	11	THR	2.2
2	D	76	ALA	2.2
2	D	115	LEU	2.2
2	D	17	VAL	2.2
2	D	15	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

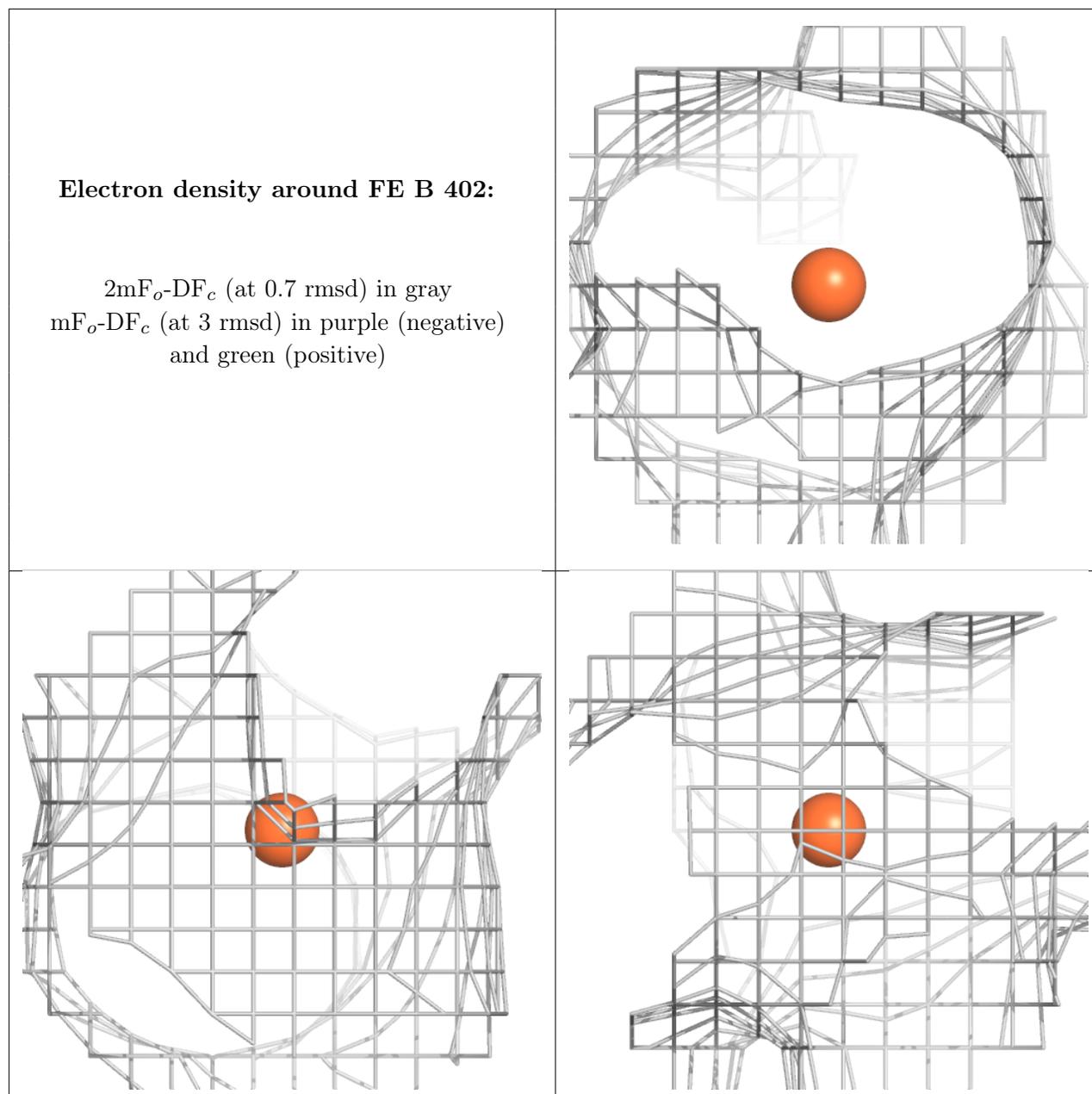
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

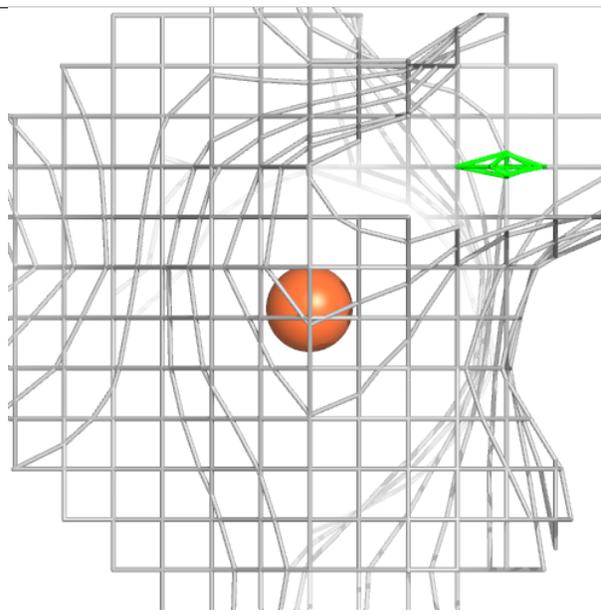
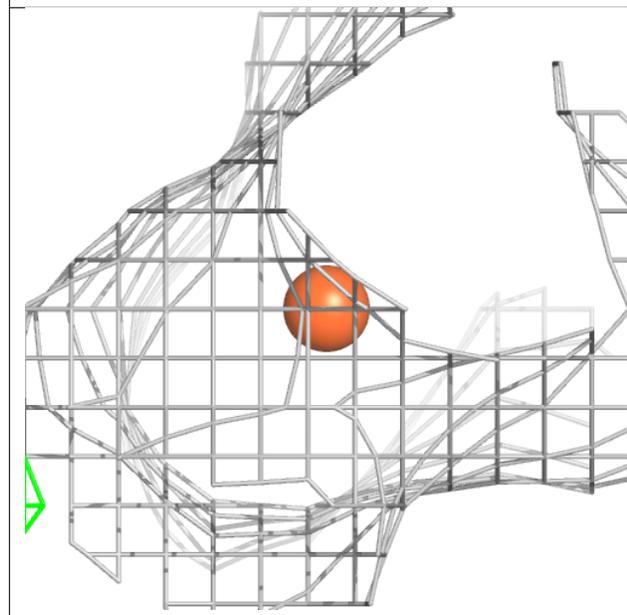
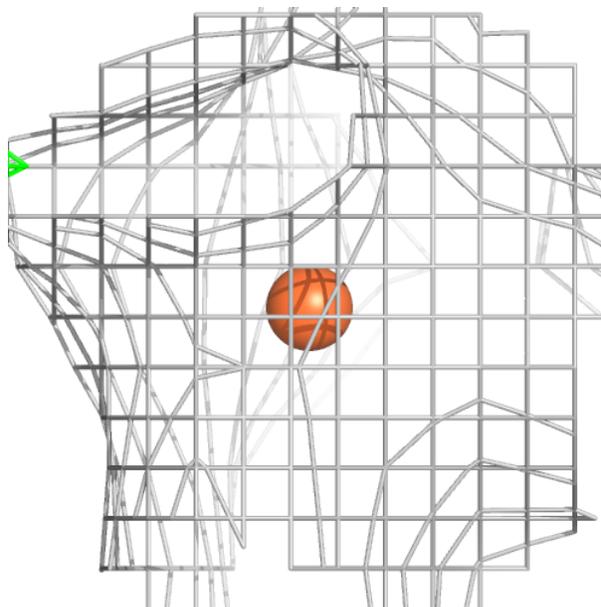
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FE	B	402	1/1	0.95	0.08	65,65,65,65	0
3	FE	D	402	1/1	0.95	0.05	83,83,83,83	0
4	TRS	B	401	8/8	0.95	0.10	44,51,57,59	0
3	FE	C	401	1/1	0.96	0.06	77,77,77,77	0
3	FE	D	401	1/1	0.96	0.06	66,66,66,66	0
3	FE	B	403	1/1	0.98	0.10	57,57,57,57	0
3	FE	A	401	1/1	0.99	0.06	52,52,52,52	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.



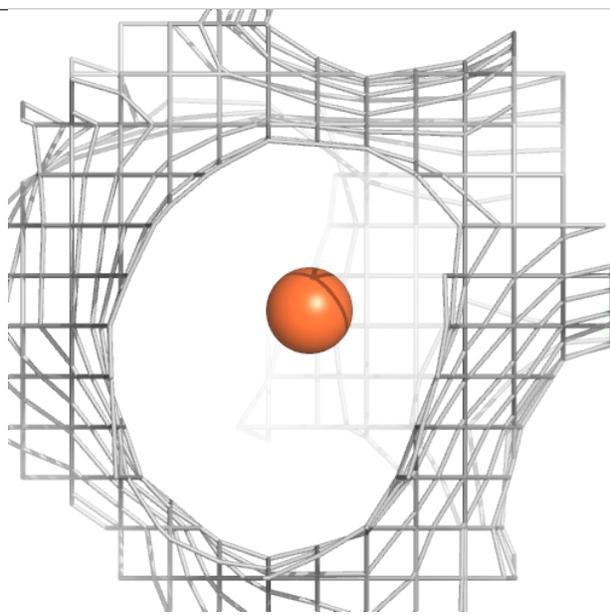
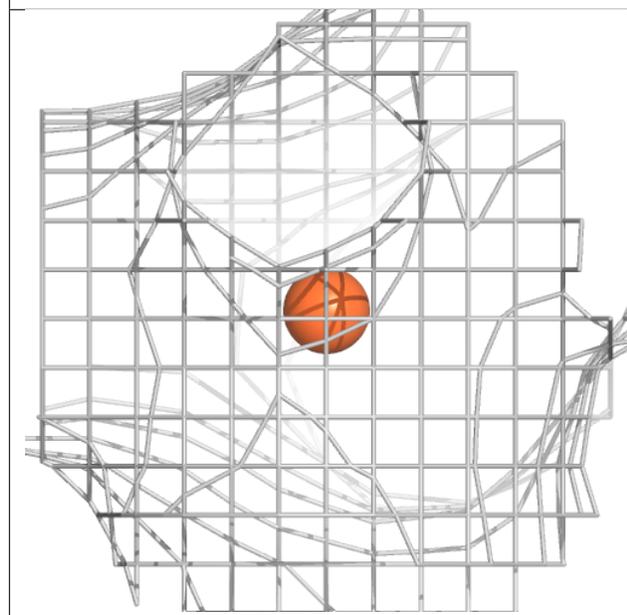
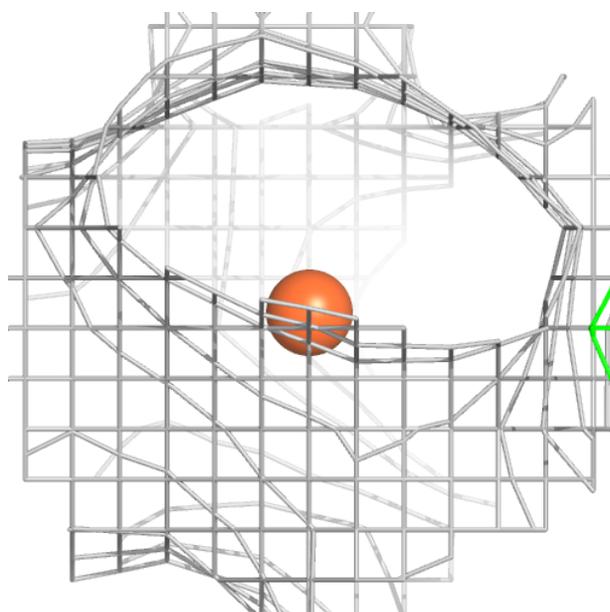
Electron density around FE D 402:

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



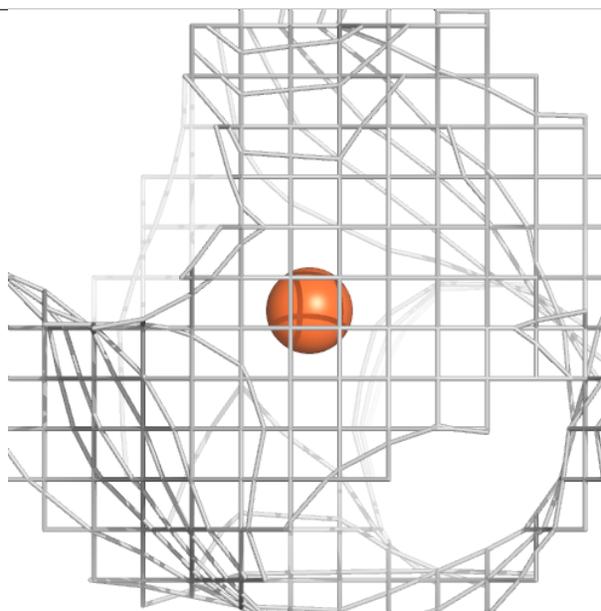
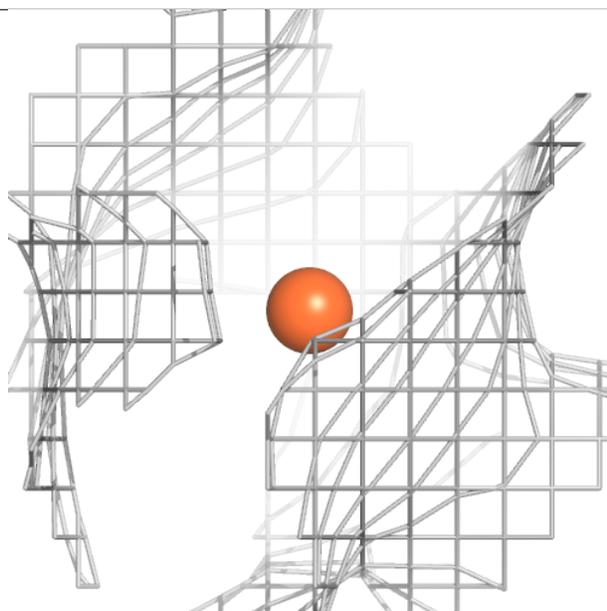
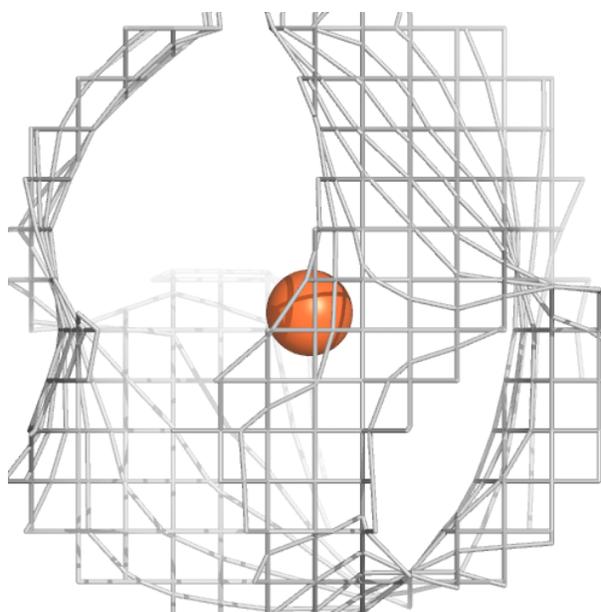
Electron density around FE C 401:

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



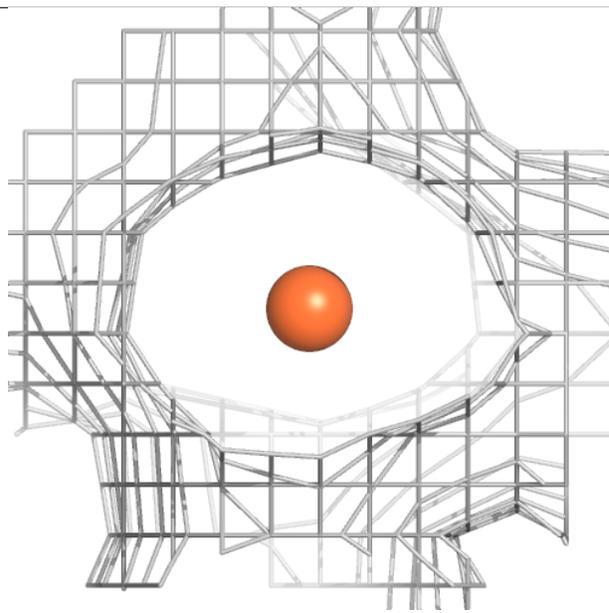
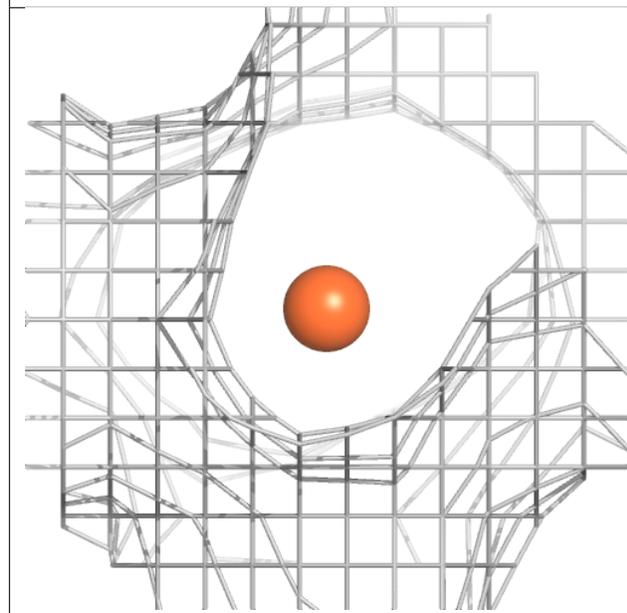
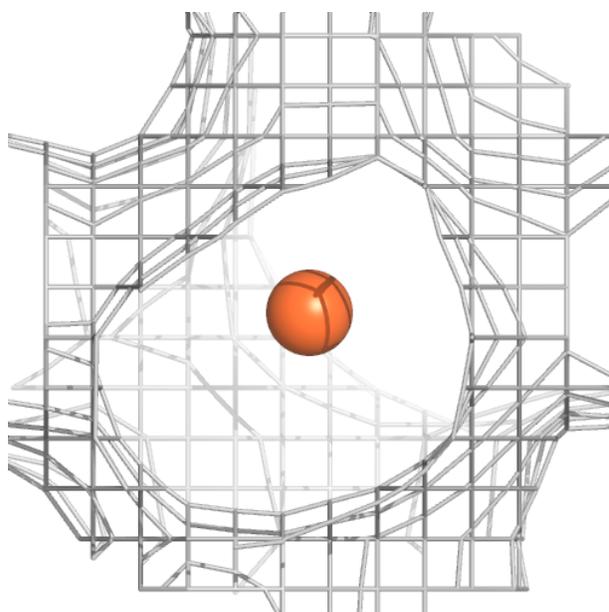
Electron density around FE D 401:

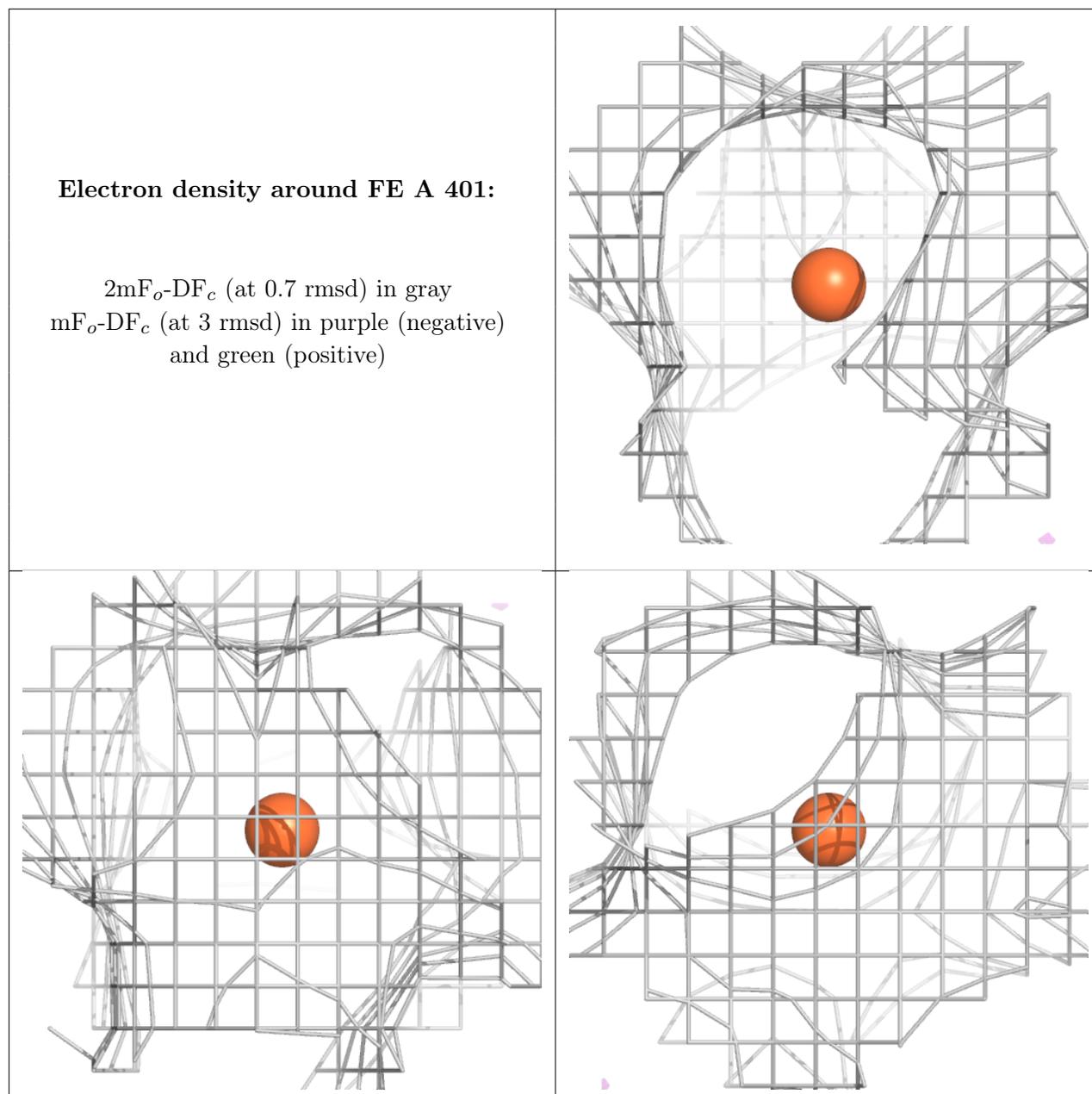
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE B 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.