



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:38 AM UTC

PDB ID : 8FUO / pdb_00008fu0
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

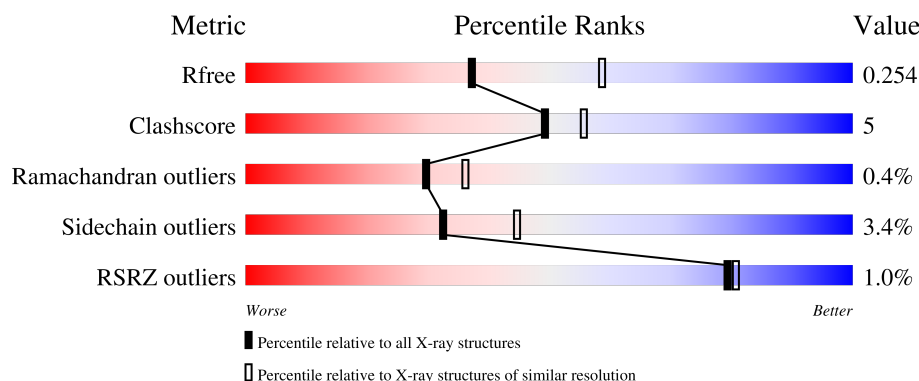
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (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	77% 12% 11%
1	C	392	2% 71% 17% 11%
2	B	378	% 81% 14% ..
2	D	378	2% 80% 16% ..

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
1	A	350	Total	C	N	O	S	0	1	0
			2803	1788	490	520	5			
1	C	350	Total	C	N	O	S	0	2	0
			2813	1795	494	519	5			

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

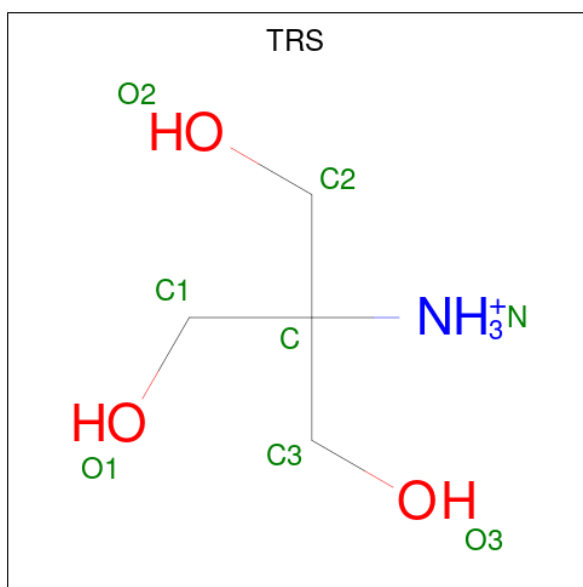
- Molecule 2 is a protein called Amidohydrolase.

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

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

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 5 is water.

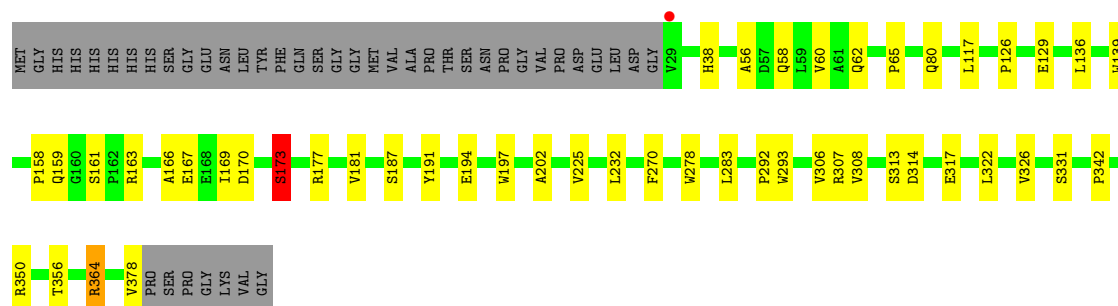
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	87	Total	O	0	0
			87	87		
5	C	30	Total	O	0	0
			30	30		
5	D	55	Total	O	0	0
			55	55		

3 Residue-property plots

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

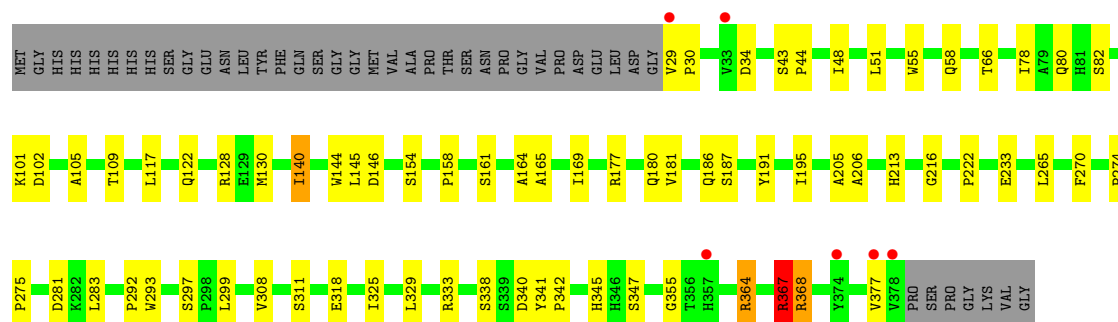
• Molecule 1: Amidohydrolase

Chain A: 



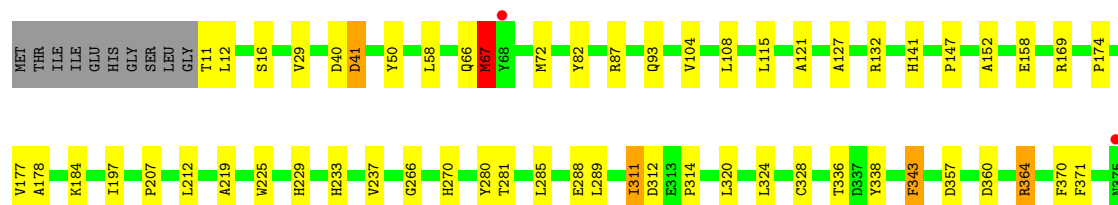
• Molecule 1: Amidohydrolase

Chain C: 



• Molecule 2: Amidohydrolase

Chain B: 



D360	P154
R364	V170
M368	L189
K369	F210
V373	H211
T374	L212
ASN	T226
GLN	S227
ALA	Y228
ASP	H229
	T230
	E231
	Y232
	H233
	H236
	V237
	S246
	F253
	N267
	F271
	I275
	V282
	L285
	E288
	K295
	H303
	P310
	F327
	C328
	N331
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	D345
	P346
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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)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.188 , 0.250 0.196 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: TRS, 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	0.50	1/2890 (0.0%)	0.60	1/3951 (0.0%)
1	C	0.43	3/2901 (0.1%)	0.56	1/3965 (0.0%)
2	B	0.49	0/2950	0.62	1/4035 (0.0%)
2	D	0.40	0/2966	0.59	0/4053
All	All	0.46	4/11707 (0.0%)	0.59	3/16004 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	SER	C-O	-5.33	1.17	1.24
1	C	206	ALA	N-CA	-5.12	1.40	1.46
1	C	205	ALA	C-O	-5.10	1.17	1.24
1	C	206	ALA	CA-C	-5.04	1.46	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ALA	N-CA-C	-7.20	101.82	113.19
2	B	67	MET	N-CA-C	5.79	118.46	111.40
1	A	177	ARG	N-CA-C	-5.28	106.34	112.89

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	27	0
1	C	2813	0	2707	41	0
2	B	2859	0	2715	39	0
2	D	2872	0	2747	32	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	120	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 (120) 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:HE1	1:C:128:ARG:NH1	1.28	1.41
2:B:67:MET:CE	1:C:128:ARG:NH1	2.08	1.16
1:A:170:ASP:O	1:A:173:SER:OG	1.81	0.98
2:B:67:MET:HE1	1:C:128:ARG:HH11	1.24	0.93
2:B:67:MET:CE	1:C:128:ARG:HH12	1.88	0.83
1:A:270:PHE:HB3	1:A:308:VAL:HG11	1.67	0.76
2:B:67:MET:HE1	1:C:128:ARG:HH12	1.43	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:67:MET:HE2	1:C:128:ARG:HH12	1.66	0.56
2:D:282:TRP:CZ3	2:D:295:LYS:HG3	2.41	0.55
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: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
2:D:67:MET:HE2	2:D:229:HIS:HB2	1.97	0.47
1:A:322:LEU:HD23	1:A:356:THR:HB	1.97	0.47
2:B:67:MET:CE	1:C:128:ARG:HH11	1.99	0.47
2:B:104:VAL:HG22	2:B:177:VAL:HG21	1.95	0.47
1:C:311[B]:SER:OG	1:C:338:SER:O	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:306:VAL:C	1:A:307:ARG:HD2	2.41	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
1:C:130:MET:HE2	1:C:164:ALA:HB2	2.00	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
2:B:72:MET:HE3	2:B:82:TYR:CE2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLN:HB3	1:C:216:GLY:HA3	2.00	0.42
2:B:66:GLN:H	2:B:66:GLN:CD	2.27	0.42
2:B:207:PRO:HB2	2:B:370:PHE:CZ	2.55	0.42
1:A:313:SER:OG	1:A:317:GLU:OE2	2.33	0.41
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
2:D:66:GLN:CD	2:D:66:GLN:H	2.28	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
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%)	21	25
2	B	365/378 (97%)	345 (94%)	18 (5%)	2 (0%)	24	29
2	D	365/378 (97%)	342 (94%)	21 (6%)	2 (0%)	24	29
All	All	1429/1540 (93%)	1351 (94%)	72 (5%)	6 (0%)	30	36

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 ⓘ

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%)	44 57
1	C	300/332 (90%)	286 (95%)	14 (5%)	23 33
2	B	302/318 (95%)	291 (96%)	11 (4%)	31 42
2	D	303/318 (95%)	294 (97%)	9 (3%)	36 48
All	All	1204/1300 (93%)	1163 (97%)	41 (3%)	32 45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	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	29	VAL
2	B	41	ASP
2	B	67	MET
2	B	197	ILE
2	B	212	LEU

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Mol	Chain	Res	Type
2	B	229	HIS
2	B	311	ILE
2	B	357	ASP
2	B	364	ARG
1	C	29	VAL
1	C	43	SER
1	C	48	ILE
1	C	58	GLN
1	C	82	SER
1	C	140	ILE
1	C	161	SER
1	C	195	ILE
1	C	299	LEU
1	C	347	SER
1	C	364	ARG
1	C	367	ARG
1	C	368	ARG
1	C	377	VAL
2	D	29	VAL
2	D	108	LEU
2	D	114	THR
2	D	115	LEU
2	D	132	ARG
2	D	170	VAL
2	D	229	HIS
2	D	237	VAL
2	D	357	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	346	HIS
2	B	241	GLN
2	D	124	GLN

5.3.3 RNA ⓘ

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 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	0.39	0	9,9,9	1.26	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	-	2/9/9/9	-

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	2.45	114.42	108.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	TRS	C2-C-C3-O3
4	B	401	TRS	C1-C-C3-O3

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%)	-0.43	1 (0%) 90 91	23, 43, 60, 76	1 (0%)
1	C	350/392 (89%)	0.25	6 (1%) 69 70	37, 63, 84, 92	2 (0%)
2	B	365/378 (96%)	-0.23	2 (0%) 87 89	25, 46, 71, 89	2 (0%)
2	D	364/378 (96%)	0.15	6 (1%) 70 72	26, 58, 84, 94	3 (0%)
All	All	1429/1540 (92%)	-0.06	15 (1%) 79 81	23, 51, 81, 94	8 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	115	LEU	3.4
1	C	357[A]	HIS	3.3
1	C	378	VAL	3.0
2	B	68	TYR	2.6
2	D	114	THR	2.6
2	D	355	PRO	2.5
2	D	368	MET	2.5
1	C	29	VAL	2.5
2	D	74	ALA	2.4
2	B	375	ASN	2.3
1	A	29	VAL	2.2
1	C	377	VAL	2.2
2	D	81	GLY	2.1
1	C	33	VAL	2.0
1	C	374	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

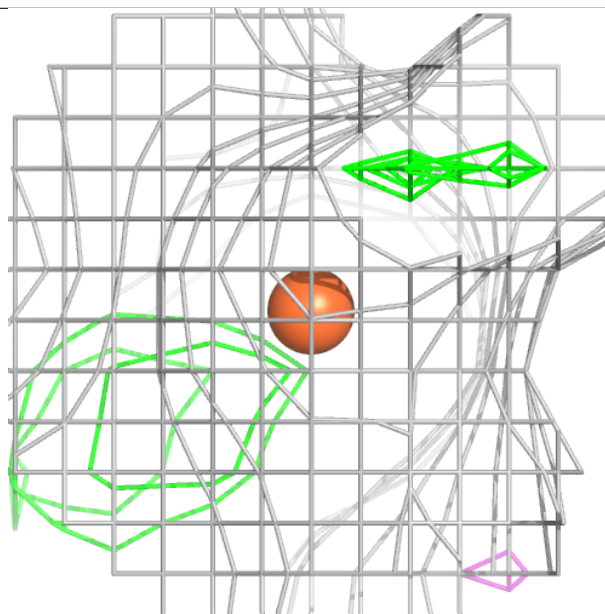
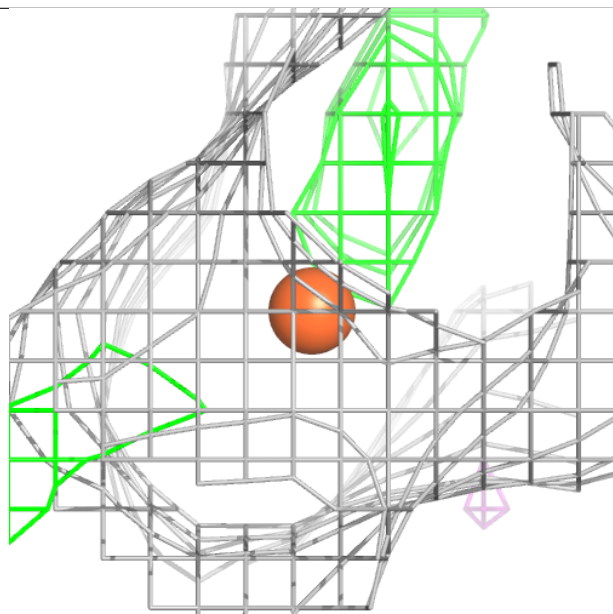
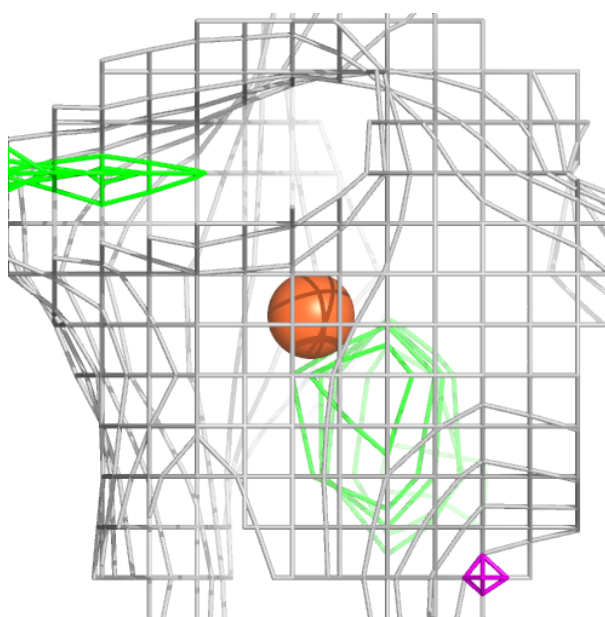
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TRS	B	401	8/8	0.92	0.10	44,51,57,59	0
3	FE	D	402	1/1	0.93	0.10	83,83,83,83	0
3	FE	B	402	1/1	0.96	0.12	65,65,65,65	0
3	FE	B	403	1/1	0.96	0.12	57,57,57,57	0
3	FE	C	401	1/1	0.98	0.08	77,77,77,77	0
3	FE	D	401	1/1	0.98	0.08	66,66,66,66	0
3	FE	A	401	1/1	1.00	0.08	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.

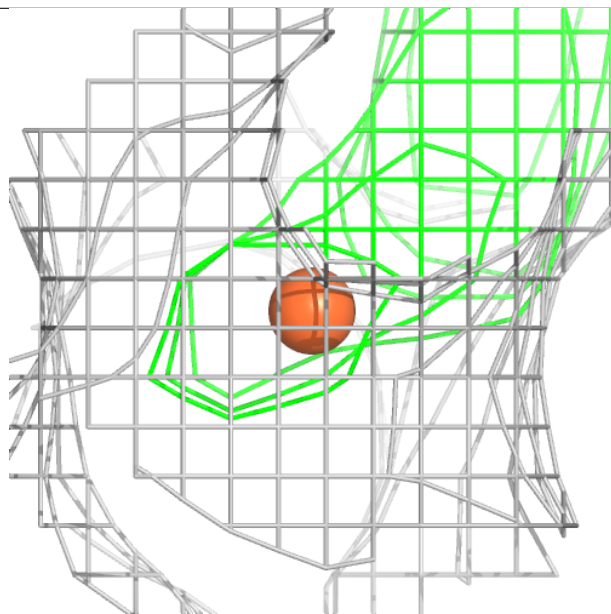
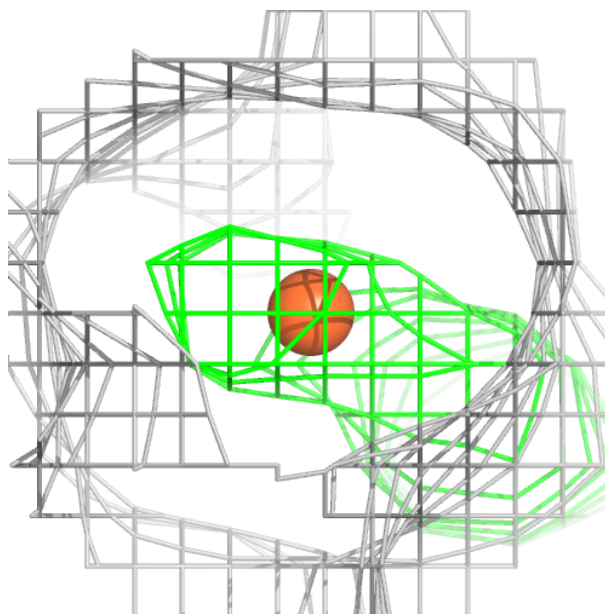
Electron density around FE D 402:

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



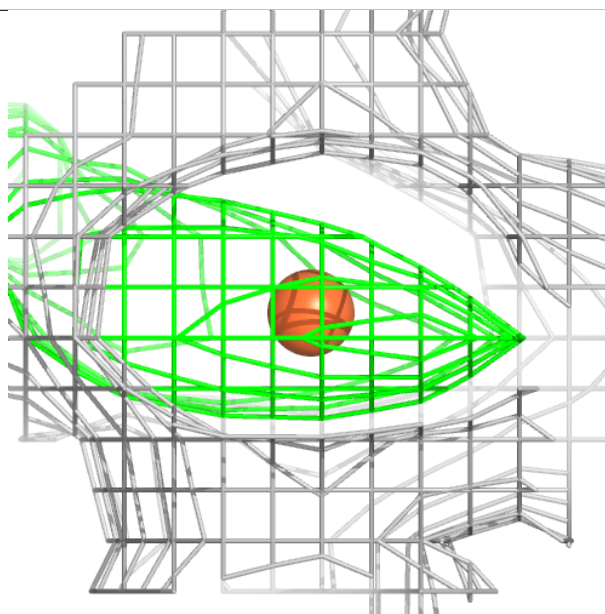
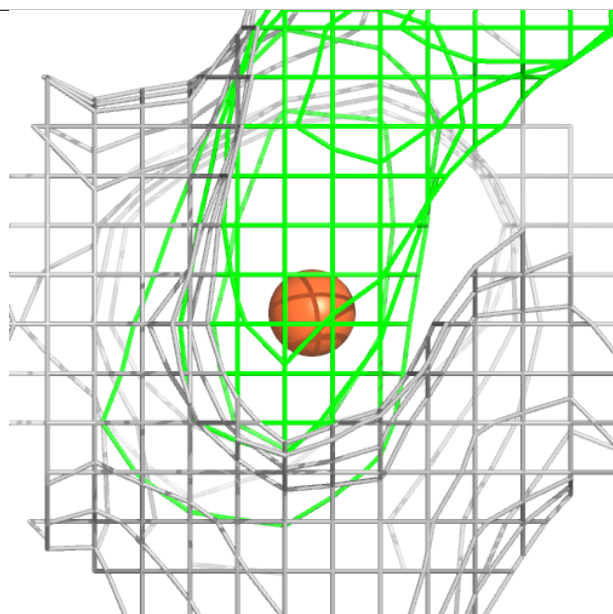
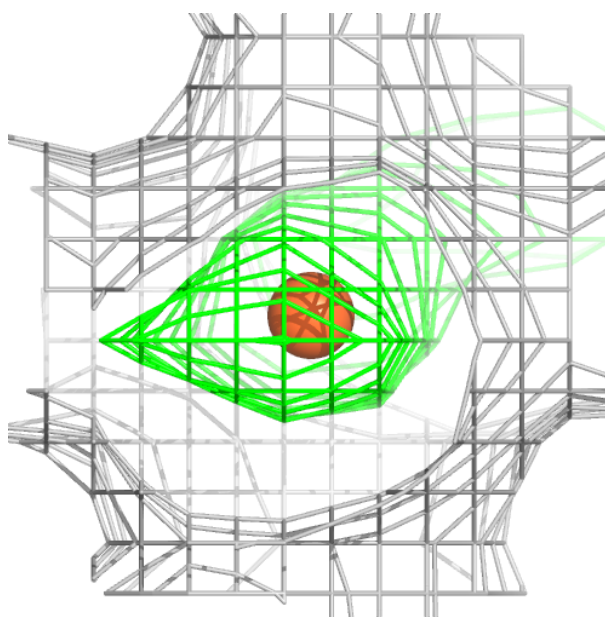
Electron density around FE B 402:

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



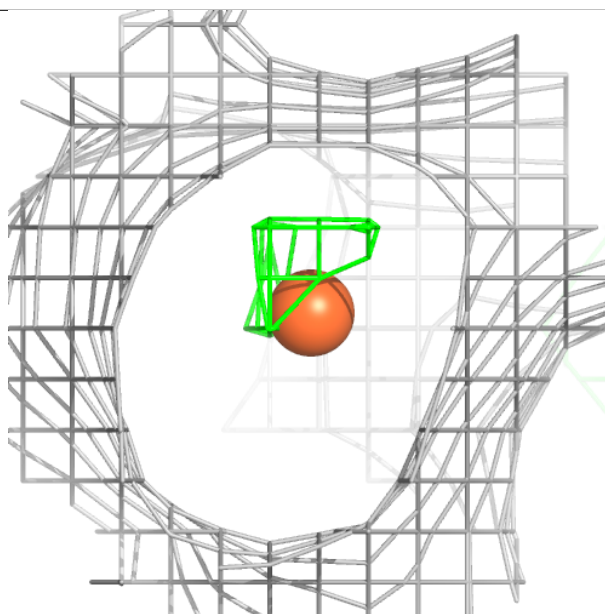
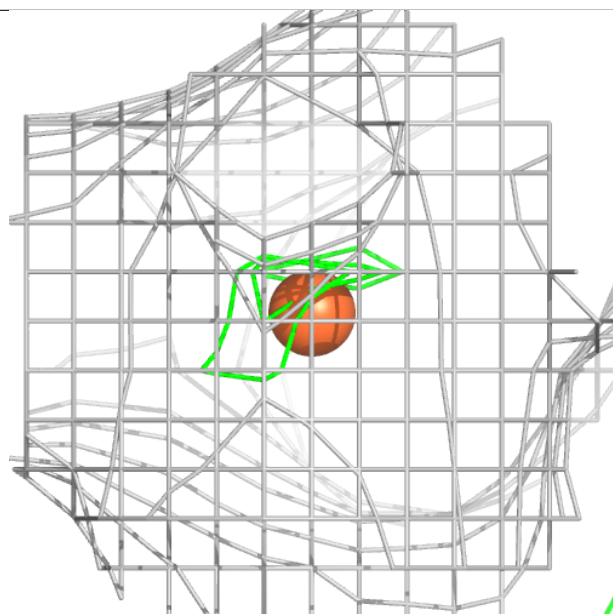
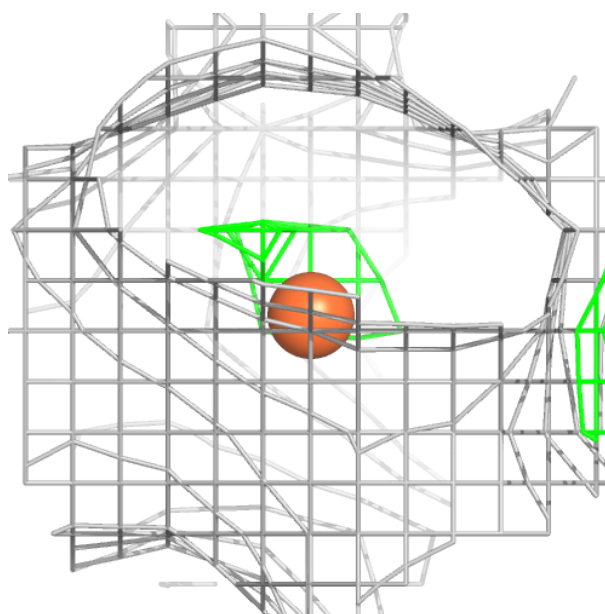
Electron density around FE B 403:

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



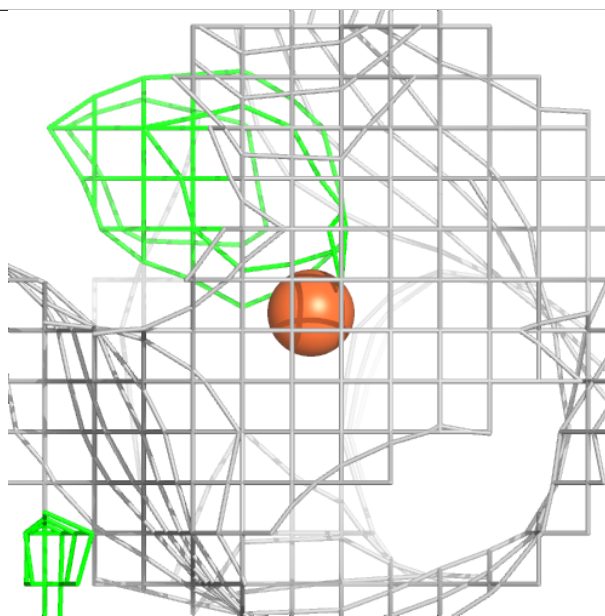
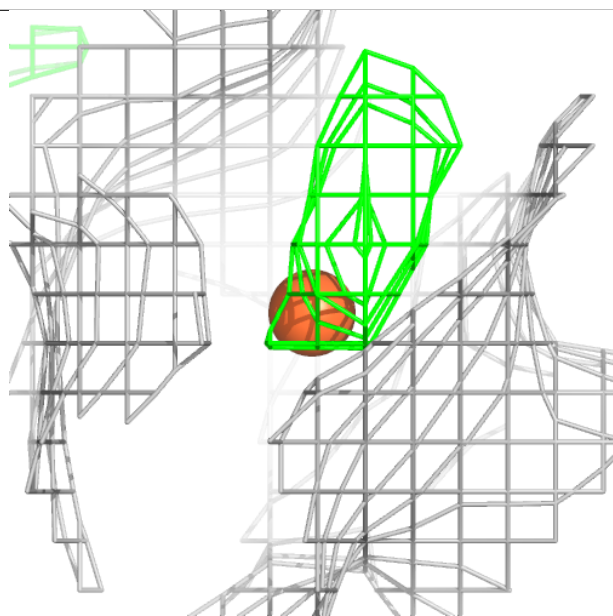
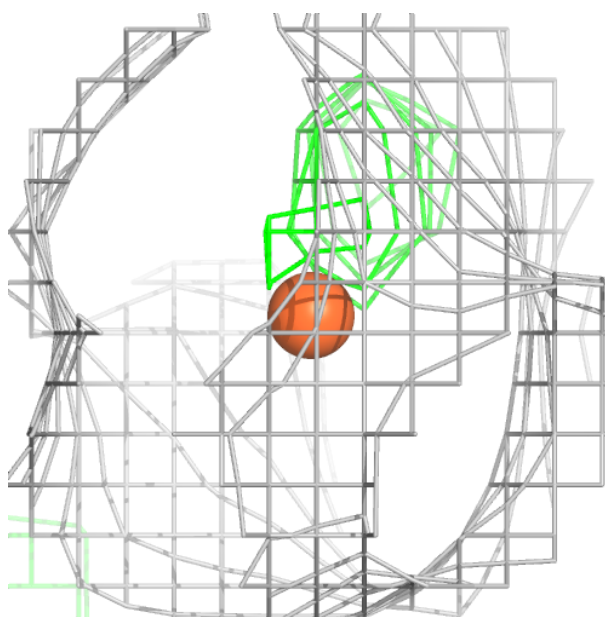
Electron density around FE C 401:

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



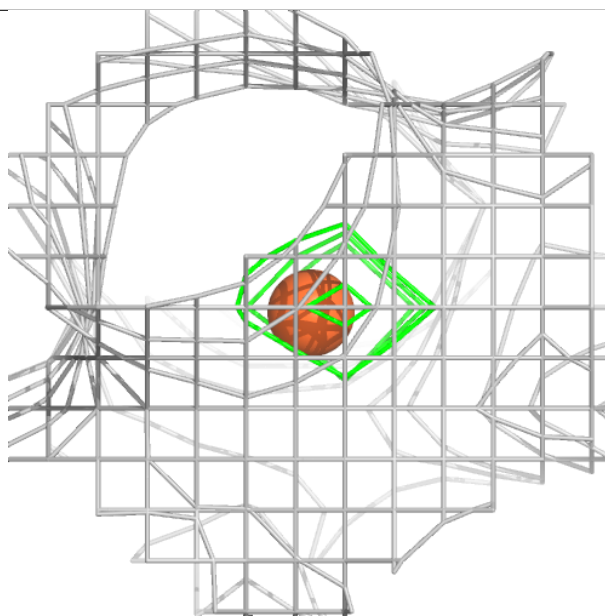
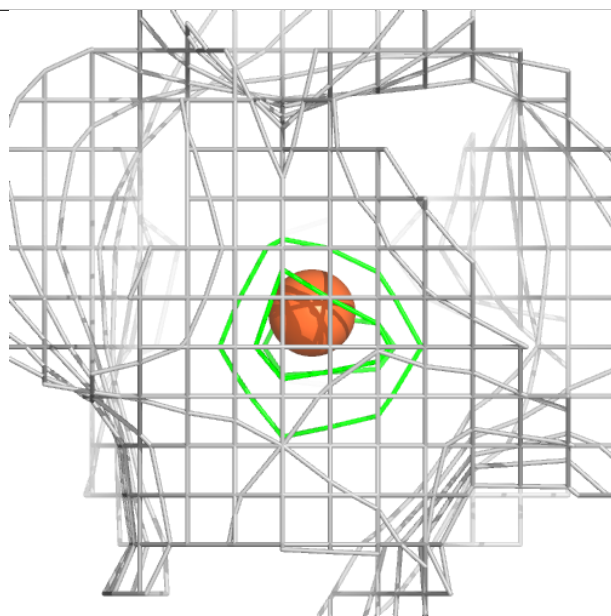
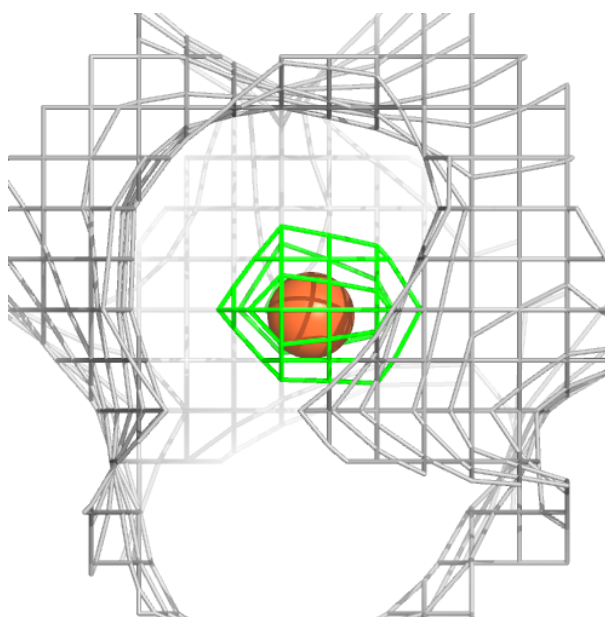
Electron density around FE D 401:

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



Electron density around FE A 401:

$2mF_o-DF_c$ (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.