



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:11 PM UTC

PDB ID : 8FUN / pdb\_00008fun  
Title : Enzymatically Active, Mn/Fe Metallated Form of AibH1H2  
Authors : Powell, M.M.; Rittle, J.  
Deposited on : 2023-01-17  
Resolution : 2.24 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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

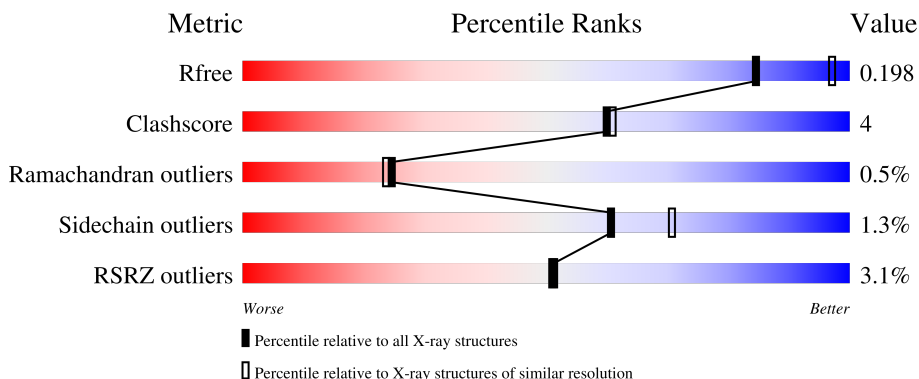
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


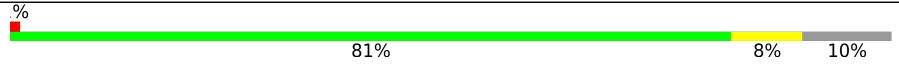
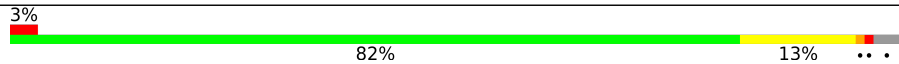

The reported resolution of this entry is 2.24 Å.

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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	 83% 5% 11%
1	C	392	 81% 8% 10%
2	B	378	 82% 13% 3%
2	D	378	 80% 15% 7%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 12070 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	2807	1791	491	520	5	0	1	0
1	C	351	2817	1797	495	520	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 2883	C 1836	N 492	O 546	S 9	0	2	0
2	D	370	Total 2926	C 1864	N 504	O 549	S 9	0	3	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
6	B	1	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	164	164	164	0	0
7	B	161	161	161	0	0
7	C	156	156	156	0	0

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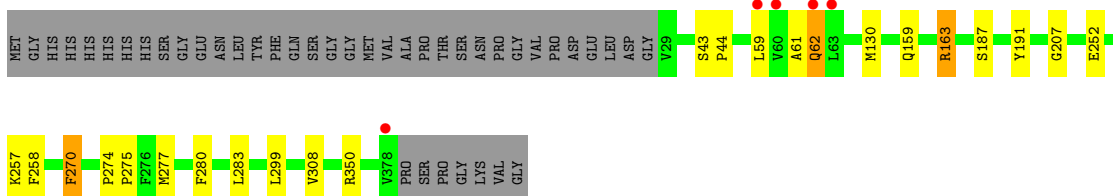
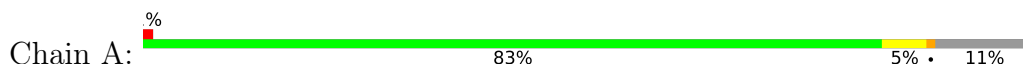
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	D	140	Total	O	0	0
			140	140		

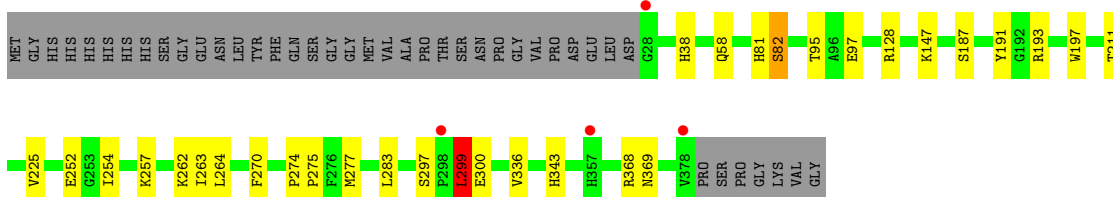
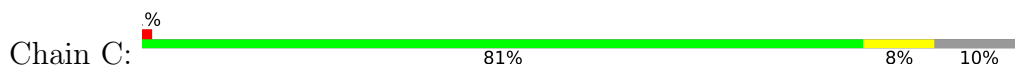
### 3 Residue-property plots [i](#)

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.

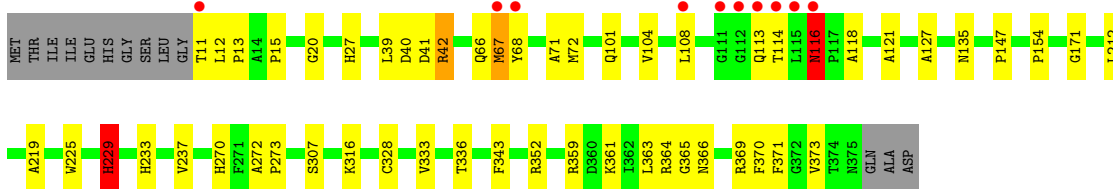
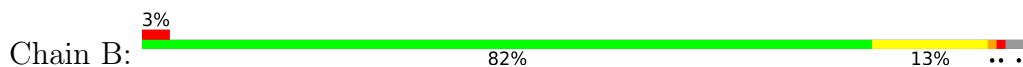
- Molecule 1: Amidohydrolase



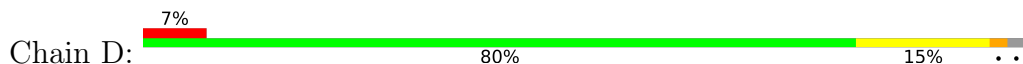
- Molecule 1: Amidohydrolase

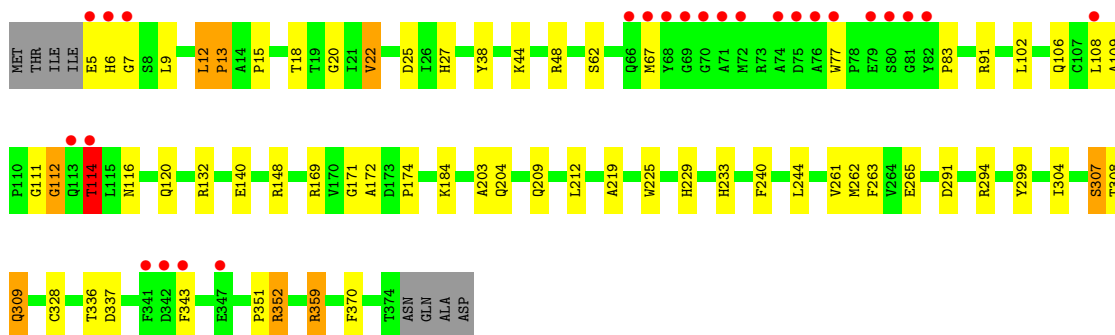


- Molecule 2: Amidohydrolase



- Molecule 2: Amidohydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.14Å 148.92Å 234.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.24 48.56 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.56-2.24) 99.3 (48.56-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.177 , 0.198 0.178 , 0.198	Depositor DCC
$R_{free}$ test set	2000 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: TRS, MG, FE, MN

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	0.53	4/2894 (0.1%)	0.64	2/3955 (0.1%)
1	C	0.64	7/2905 (0.2%)	0.64	2/3970 (0.1%)
2	B	0.76	10/2974 (0.3%)	0.73	5/4063 (0.1%)
2	D	0.79	13/3021 (0.4%)	0.73	3/4125 (0.1%)
All	All	0.69	34/11794 (0.3%)	0.69	12/16113 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	ILE	C-O	-7.38	1.16	1.24
1	A	280	PHE	C-O	-6.78	1.16	1.24
2	B	364	ARG	C-O	-6.71	1.15	1.24
2	D	22	VAL	C-O	-6.51	1.16	1.24
1	C	300	GLU	C-O	-6.49	1.16	1.24
2	D	308	THR	C-O	-6.20	1.16	1.24
2	B	229	HIS	C-O	-6.16	1.17	1.24
1	C	262	LYS	C-O	-6.12	1.16	1.24
2	B	39	LEU	C-O	-6.07	1.16	1.24
2	B	370	PHE	C-O	-6.04	1.17	1.24
1	C	82	SER	C-O	-5.95	1.16	1.24
1	C	81	HIS	C-O	-5.92	1.16	1.23
1	A	163	ARG	C-O	-5.90	1.17	1.24
2	D	9	LEU	C-O	-5.78	1.17	1.24
2	D	351	PRO	C-O	-5.77	1.17	1.23
2	B	369	ARG	C-O	-5.72	1.16	1.24
2	D	359	ARG	C-O	-5.68	1.17	1.24
1	A	252	GLU	C-O	-5.65	1.16	1.24
2	D	7	GLY	C-O	-5.65	1.16	1.23
2	B	118	ALA	N-CA	-5.59	1.39	1.46
1	C	299	LEU	C-O	-5.58	1.17	1.24
2	D	12	LEU	C-O	-5.57	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	SER	C-O	-5.55	1.16	1.23
2	B	68	TYR	C-O	-5.48	1.17	1.23
2	D	120	GLN	C-O	-5.38	1.16	1.24
2	B	71	ALA	C-O	-5.36	1.16	1.23
2	D	20	GLY	C-O	-5.34	1.18	1.23
1	A	59	LEU	C-O	-5.33	1.17	1.24
2	D	13	PRO	C-O	-5.32	1.17	1.23
2	B	316	LYS	C-O	-5.28	1.17	1.24
2	D	109	ALA	C-O	-5.21	1.17	1.24
2	D	18	THR	C-O	-5.07	1.17	1.24
2	B	118	ALA	C-O	-5.05	1.18	1.24
2	D	307	SER	C-O	-5.01	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	308	THR	N-CA-C	7.31	120.68	111.69
2	B	116	ASN	CA-C-N	6.64	127.00	119.83
2	B	116	ASN	C-N-CA	6.64	127.00	119.83
2	D	111	GLY	N-CA-C	6.45	120.82	112.18
2	D	114	THR	N-CA-C	6.21	118.89	108.02
1	A	159	GLN	N-CA-C	6.20	120.45	113.01
2	B	229	HIS	N-CA-C	6.04	117.86	111.28
2	B	352	ARG	N-CA-C	5.91	118.47	111.33
1	C	368	ARG	N-CA-C	5.63	117.42	111.28
1	A	61	ALA	N-CA-C	5.59	119.72	113.01
2	B	365	GLY	N-CA-C	5.31	119.11	112.73
1	C	82	SER	N-CA-C	5.01	117.47	111.71

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	2807	0	2705	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2817	0	2710	15	0
2	B	2883	0	2756	29	0
2	D	2926	0	2806	47	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	B	8	0	12	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	1	0	0	0	0
7	A	164	0	0	2	0
7	B	161	0	0	1	0
7	C	156	0	0	0	0
7	D	140	0	0	4	0
All	All	12070	0	10989	96	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 4.

All (96) 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:D:352:ARG:HH11	2:D:352:ARG:HG3	1.10	1.07
2:B:113:GLN:CB	2:B:116:ASN:HD21	1.84	0.91
2:D:6:HIS:ND1	2:D:6:HIS:O	2.06	0.88
1:A:270:PHE:HB3	1:A:308:VAL:HG11	1.56	0.87
2:D:352:ARG:HG3	2:D:352:ARG:NH1	1.88	0.85
2:B:42:ARG:NH2	2:D:291:ASP:OD2	2.17	0.78
2:D:6:HIS:HB3	2:D:203:ALA:O	1.86	0.74
2:D:5:GLU:HB2	2:D:172:ALA:HA	1.70	0.72
2:B:359:ARG:HD2	2:B:363:LEU:HD12	1.72	0.71
2:B:72:MET:HE2	2:B:114:THR:OG1	1.90	0.71
2:B:116:ASN:OD1	2:B:116:ASN:N	2.23	0.70
2:B:113:GLN:CB	2:B:116:ASN:ND2	2.54	0.70
2:D:307:SER:OG	7:D:501:HOH:O	1.96	0.65
2:D:15:PRO:HB3	7:D:584:HOH:O	1.96	0.64
2:B:359:ARG:HD2	2:B:363:LEU:CD1	2.32	0.60
2:D:67:MET:HG3	2:D:229:HIS:CG	2.36	0.60
2:B:15:PRO:HG2	2:B:373:VAL:HG22	1.83	0.60
1:C:58:GLN:NE2	1:C:128:ARG:HH11	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:HA2	7:A:654:HOH:O	2.02	0.59
2:D:5:GLU:HB3	2:D:204:GLN:O	2.03	0.58
1:C:95:THR:HB	1:C:97:GLU:OE1	2.04	0.57
1:A:277:MET:HB3	1:A:299:LEU:HD23	1.87	0.57
2:D:62:SER:HB3	2:D:116:ASN:HD21	1.69	0.56
2:B:40:ASP:HB2	7:B:647:HOH:O	2.06	0.56
2:B:66:GLN:H	2:B:66:GLN:CD	2.14	0.56
2:D:5:GLU:HG2	2:D:171:GLY:O	2.06	0.56
1:C:193:ARG:HA	1:C:252:GLU:OE1	2.07	0.54
2:D:6:HIS:CB	2:D:203:ALA:O	2.54	0.53
1:A:283:LEU:HD13	2:B:233:HIS:HB3	1.89	0.53
2:B:20:GLY:HA3	2:B:101:GLN:HG3	1.91	0.53
2:B:12:LEU:HD11	2:B:147:PRO:HB3	1.89	0.53
2:B:104:VAL:HG21	2:B:371:PHE:CZ	2.44	0.53
2:D:38:TYR:OH	2:D:140:GLU:OE1	2.22	0.52
2:B:27:HIS:CE1	2:B:108:LEU:HD11	2.44	0.52
2:B:171:GLY:O	4:B:501:TRS:O2	2.28	0.52
1:C:274:PRO:HB2	1:C:275:PRO:HD3	1.91	0.52
1:C:97:GLU:CD	1:C:97:GLU:H	2.18	0.51
2:D:359:ARG:NH2	7:D:504:HOH:O	2.44	0.50
2:D:106:GLN:NE2	2:D:209:GLN:OE1	2.45	0.50
2:D:336:THR:HB	2:D:343:PHE:CE2	2.47	0.50
2:D:12:LEU:HD12	2:D:13:PRO:HD2	1.93	0.49
2:B:272:ALA:HB3	2:B:273:PRO:HD3	1.94	0.49
2:D:294:ARG:HB2	2:D:299:TYR:CE2	2.48	0.49
1:A:187:SER:HB3	1:A:191:TYR:CZ	2.48	0.48
2:D:48:ARG:HD3	7:D:575:HOH:O	2.12	0.48
2:D:5:GLU:N	2:D:5:GLU:OE1	2.47	0.48
1:C:187:SER:HB3	1:C:191:TYR:CZ	2.49	0.47
2:D:219:ALA:HA	2:D:225:TRP:CZ2	2.49	0.47
1:C:283:LEU:HD13	2:D:233:HIS:HB3	1.96	0.47
1:A:62:GLN:HA	2:D:67:MET:O	2.14	0.47
1:A:274:PRO:HB2	1:A:275:PRO:HD3	1.97	0.47
2:D:67:MET:CG	2:D:229:HIS:CD2	2.98	0.47
2:B:307:SER:HA	2:B:333:VAL:O	2.16	0.46
2:D:309:GLN:NE2	2:D:309:GLN:C	2.73	0.46
1:C:58:GLN:HE22	1:C:128:ARG:HH11	1.64	0.46
2:B:121:ALA:HB3	2:B:127:ALA:HB2	1.97	0.46
2:D:240:PHE:CD1	2:D:263:PHE:HB3	2.50	0.45
2:D:91:ARG:HG3	2:D:148:ARG:NH1	2.31	0.45
1:A:257:LYS:HD3	1:A:258:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:HG12	2:D:184:LYS:HA	1.99	0.45
2:B:67:MET:HG3	2:B:229:HIS:CE1	2.52	0.44
1:C:38:HIS:CD2	1:C:343:HIS:CE1	3.05	0.44
2:B:336:THR:HB	2:B:343:PHE:CE2	2.53	0.44
2:D:261[A]:VAL:CG2	2:D:304:ILE:HD13	2.47	0.44
1:A:43:SER:HB2	1:A:44:PRO:HD2	1.99	0.44
2:D:62:SER:HB3	2:D:116:ASN:ND2	2.32	0.44
2:B:67:MET:HG3	2:B:229:HIS:CG	2.53	0.44
2:D:22:VAL:HG22	2:D:102:LEU:HB3	1.99	0.44
2:D:309:GLN:C	2:D:309:GLN:HE21	2.26	0.43
2:B:12:LEU:HA	2:B:13:PRO:HD3	1.74	0.43
1:A:130:MET:HG3	7:A:506:HOH:O	2.18	0.43
2:D:6:HIS:ND1	2:D:6:HIS:C	2.72	0.43
2:D:77:TRP:CE3	2:D:83:PRO:HD3	2.53	0.43
2:B:361:LYS:O	2:B:366:ASN:HB2	2.19	0.43
2:D:25:ASP:HA	2:D:106:GLN:HG3	2.00	0.43
2:D:44:LYS:O	2:D:48:ARG:HG3	2.18	0.43
2:B:135:ASN:OD1	2:B:154:PRO:HD2	2.19	0.43
2:D:265:GLU:HG3	2:D:309:GLN:HE22	1.83	0.43
2:B:237:VAL:HG13	2:B:270:HIS:CE1	2.54	0.42
2:D:67:MET:HG2	2:D:229:HIS:CD2	2.54	0.42
2:D:294:ARG:HB2	2:D:299:TYR:CZ	2.54	0.42
2:D:27:HIS:CD2	2:D:337:ASP:OD1	2.72	0.42
2:D:132:ARG:HG3	2:D:169:ARG:NH2	2.34	0.42
2:D:112:GLY:C	2:D:114:THR:H	2.28	0.42
2:B:66:GLN:CD	2:B:66:GLN:N	2.76	0.42
1:C:211:THR:HA	1:C:264:LEU:O	2.19	0.42
1:C:277:MET:HB3	1:C:299:LEU:HD12	2.02	0.42
2:B:219:ALA:HA	2:B:225:TRP:CZ2	2.55	0.42
1:C:336:VAL:HG12	1:C:369:ASN:HB3	2.02	0.41
1:C:197:TRP:CD1	1:C:254:ILE:HD11	2.56	0.41
2:D:244:LEU:C	2:D:244:LEU:HD23	2.46	0.41
2:D:106:GLN:HE22	2:D:209:GLN:CD	2.29	0.41
2:D:12:LEU:HB3	2:D:174:PRO:HG2	2.03	0.41
2:D:262:MET:HB2	2:D:370:PHE:CZ	2.56	0.40
2:B:113:GLN:CB	2:B:116:ASN:OD1	2.69	0.40
1:C:147:LYS:HA	1:C:147:LYS:HD3	1.81	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%)	345 (99%)	3 (1%)	1 (0%)	36	38
1	C	351/392 (90%)	346 (99%)	4 (1%)	1 (0%)	36	38
2	B	365/378 (97%)	342 (94%)	21 (6%)	2 (0%)	24	23
2	D	371/378 (98%)	345 (93%)	23 (6%)	3 (1%)	16	13
All	All	1436/1540 (93%)	1378 (96%)	51 (4%)	7 (0%)	24	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	328	CYS
2	D	112	GLY
2	D	328	CYS
1	C	270	PHE
1	A	270	PHE
2	D	212	LEU
2	B	212	LEU

### 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	300/332 (90%)	297 (99%)	3 (1%)	68	76
1	C	300/332 (90%)	297 (99%)	3 (1%)	68	76
2	B	307/318 (96%)	301 (98%)	6 (2%)	48	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	310/318 (98%)	306 (99%)	4 (1%)	61	71
All	All	1217/1300 (94%)	1201 (99%)	16 (1%)	61	71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	163	ARG
1	A	350	ARG
2	B	11	THR
2	B	41	ASP
2	B	42	ARG
2	B	67	MET
2	B	116	ASN
2	B	229	HIS
1	C	82	SER
1	C	257	LYS
1	C	299	LEU
2	D	108	LEU
2	D	114	THR
2	D	309	GLN
2	D	352	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	357	HIS
2	B	31	GLN
2	B	241	GLN
1	C	256	GLN
1	C	375	ASN
2	D	59	GLN
2	D	106	GLN
2	D	116	ASN
2	D	124	GLN
2	D	241	GLN
2	D	309	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 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	501	-	7,7,7	0.48	0	9,9,9	0.73	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
4	TRS	B	501	-	-	5/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	TRS	N-C-C1-O1
4	B	501	TRS	C3-C-C1-O1
4	B	501	TRS	C3-C-C2-O2
4	B	501	TRS	C1-C-C2-O2
4	B	501	TRS	N-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	TRS	1	0

## 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	350/392 (89%)	-0.55	5 (1%) 73 75	13, 23, 38, 68	1 (0%)
1	C	351/392 (89%)	-0.47	4 (1%) 78 79	14, 25, 38, 67	2 (0%)
2	B	365/378 (96%)	-0.34	10 (2%) 56 57	12, 23, 44, 72	2 (0%)
2	D	370/378 (97%)	-0.10	25 (6%) 23 21	14, 26, 67, 98	3 (0%)
All	All	1436/1540 (93%)	-0.36	44 (3%) 51 51	12, 24, 50, 98	8 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	80	SER	4.2
2	D	82	TYR	4.2
2	D	70	GLY	4.0
2	D	68	TYR	3.8
2	D	81	GLY	3.7
2	D	67	MET	3.6
2	B	114	THR	3.6
2	D	341	PHE	3.5
2	D	66	GLN	3.5
2	B	111	GLY	3.3
1	A	60	VAL	3.3
2	D	77	TRP	3.2
2	D	69	GLY	3.1
2	B	115	LEU	3.1
2	B	68	TYR	3.0
2	B	11	THR	2.9
2	D	6	HIS	2.9
1	C	357[A]	HIS	2.9
2	D	76	ALA	2.8
2	D	79	GLU	2.8
1	A	59	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	71	ALA	2.8
2	D	7	GLY	2.8
2	D	113	GLN	2.8
2	D	74	ALA	2.7
2	D	108	LEU	2.7
2	D	114	THR	2.7
2	D	75	ASP	2.6
1	A	63	LEU	2.6
2	B	112	GLY	2.6
2	B	116	ASN	2.5
2	B	113	GLN	2.5
2	D	343	PHE	2.4
2	B	108	LEU	2.4
2	D	347	GLU	2.4
1	A	378	VAL	2.3
2	D	5	GLU	2.3
2	D	342	ASP	2.3
1	A	62	GLN	2.3
2	D	72	MET	2.2
1	C	28	GLY	2.1
1	C	298	PRO	2.1
1	C	378	VAL	2.1
2	B	67	MET	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, 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.

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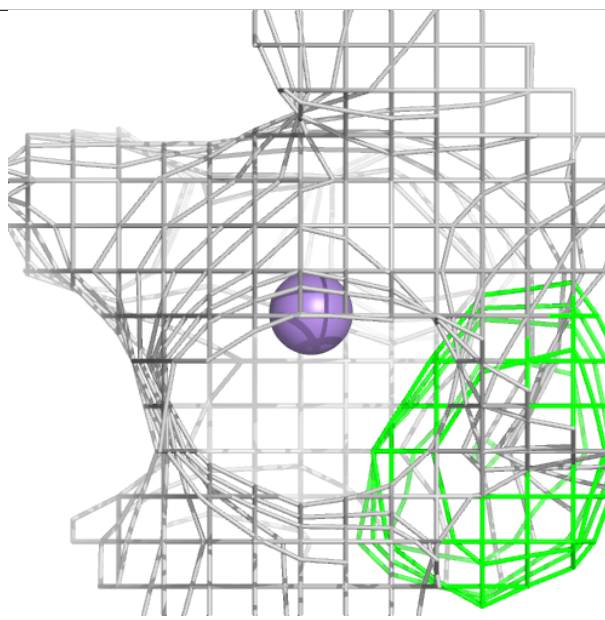
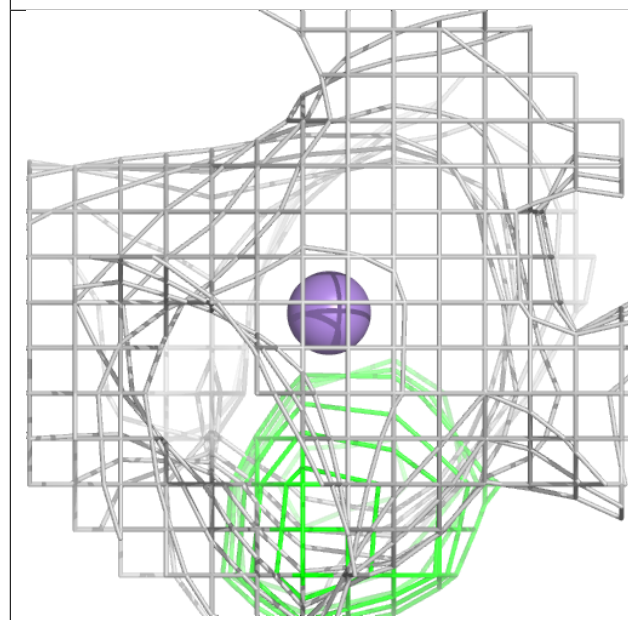
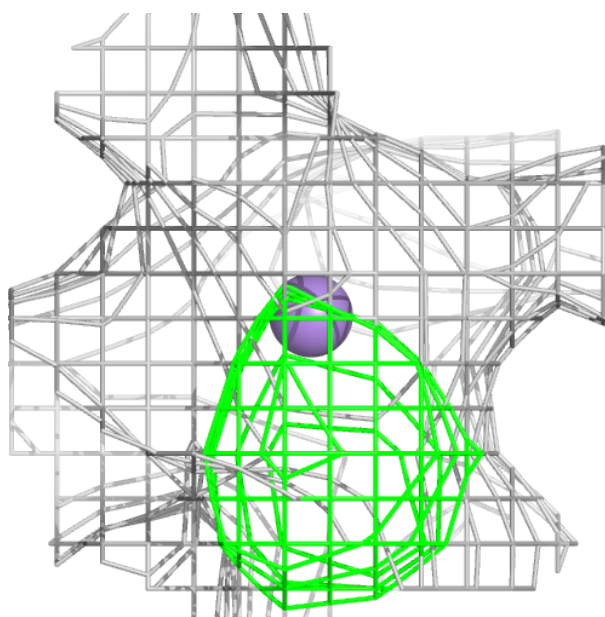
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	TRS	B	501	8/8	0.78	0.16	35,42,48,56	0
5	MG	C	402	1/1	0.88	0.14	35,35,35,35	0
3	MN	D	402	1/1	0.90	0.06	46,46,46,46	1
5	MG	B	503	1/1	0.92	0.09	36,36,36,36	1
3	MN	D	401	1/1	0.96	0.05	35,35,35,35	0
3	MN	B	502	1/1	0.98	0.04	36,36,36,36	0
3	MN	A	401	1/1	0.99	0.02	24,24,24,24	0
6	FE	B	504	1/1	0.99	0.06	33,33,33,33	0
3	MN	C	401	1/1	1.00	0.01	25,25,25,25	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.

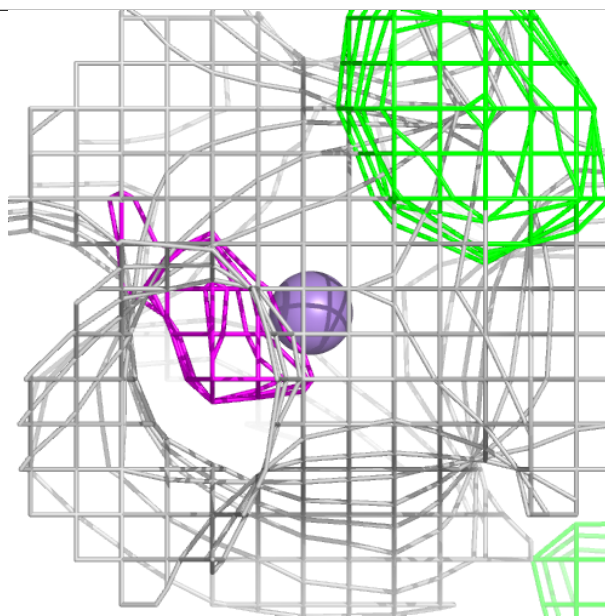
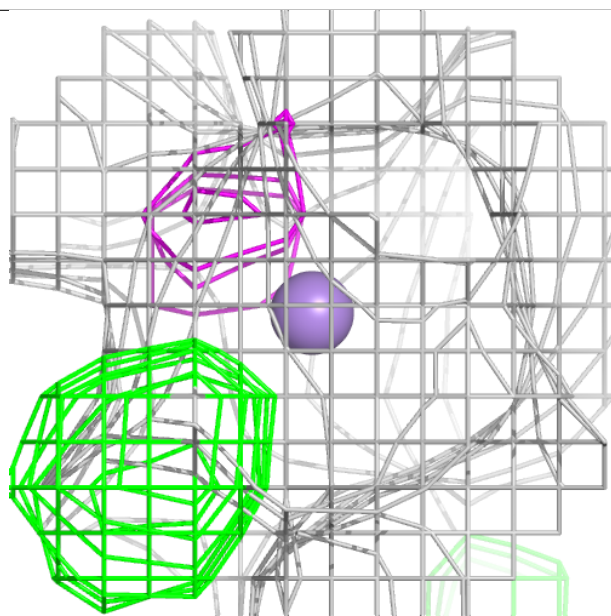
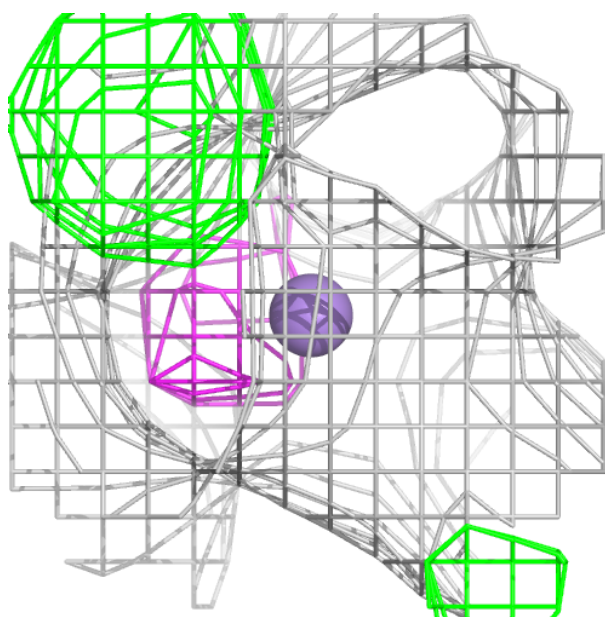
**Electron density around MN D 402:**

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



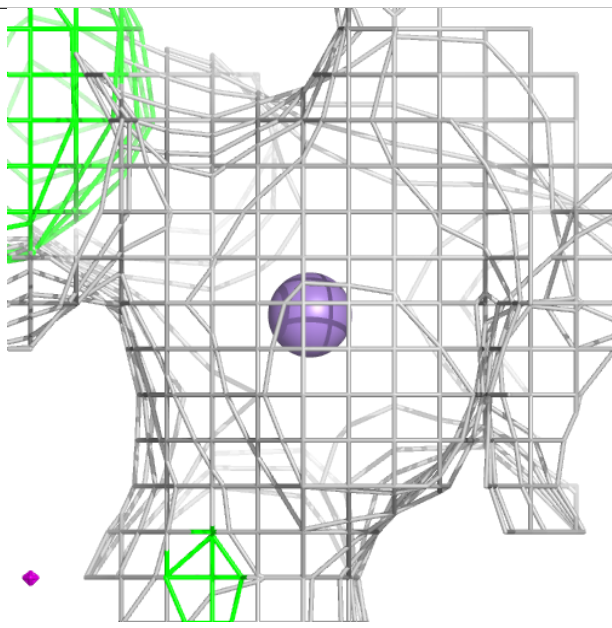
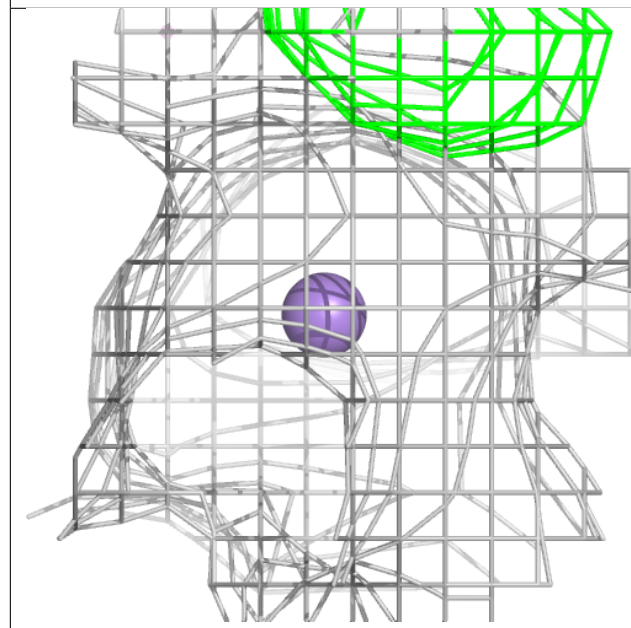
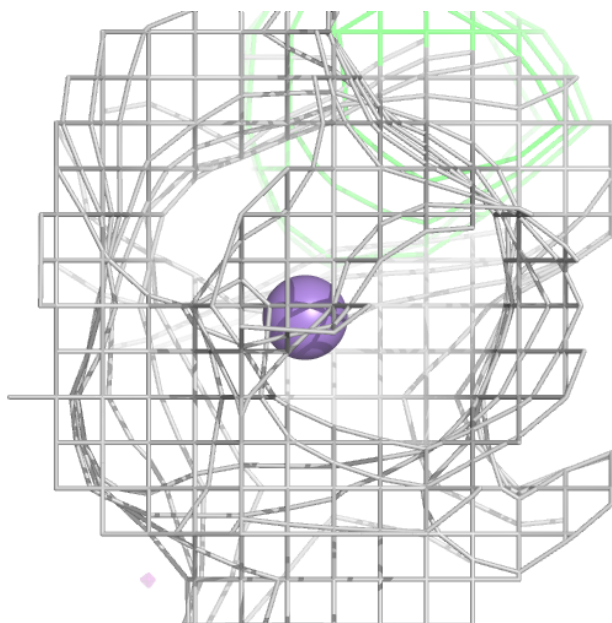
**Electron density around MN D 401:**

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



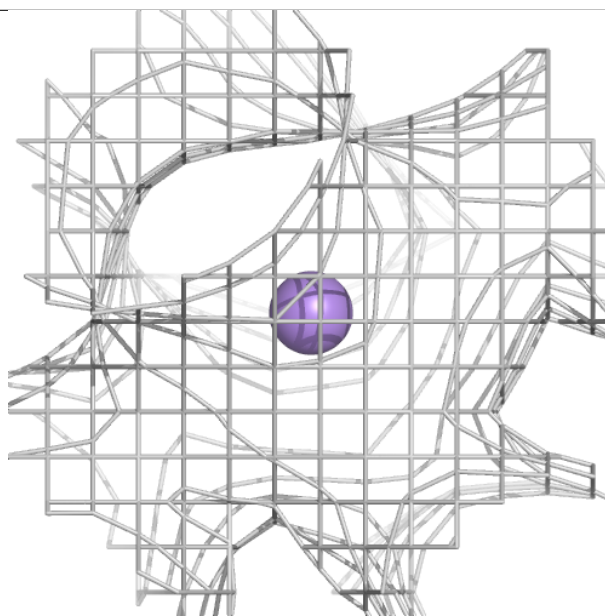
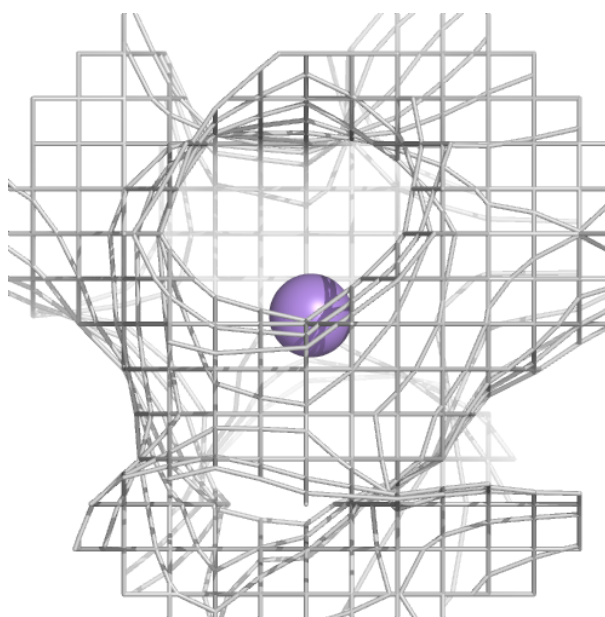
**Electron density around MN B 502:**

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



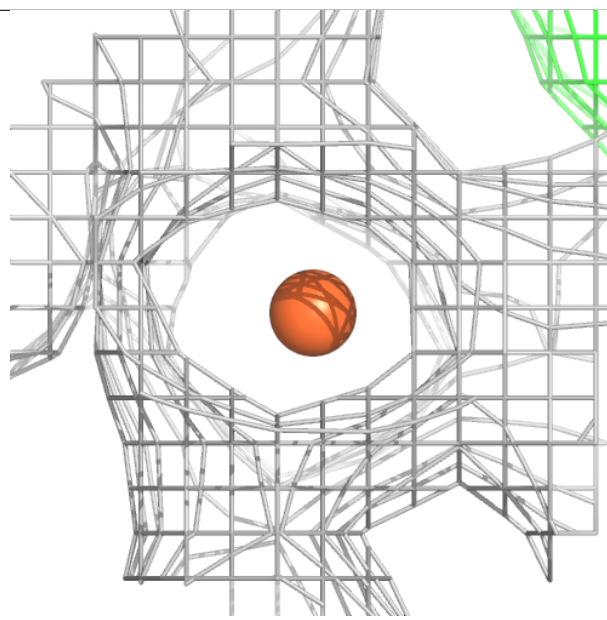
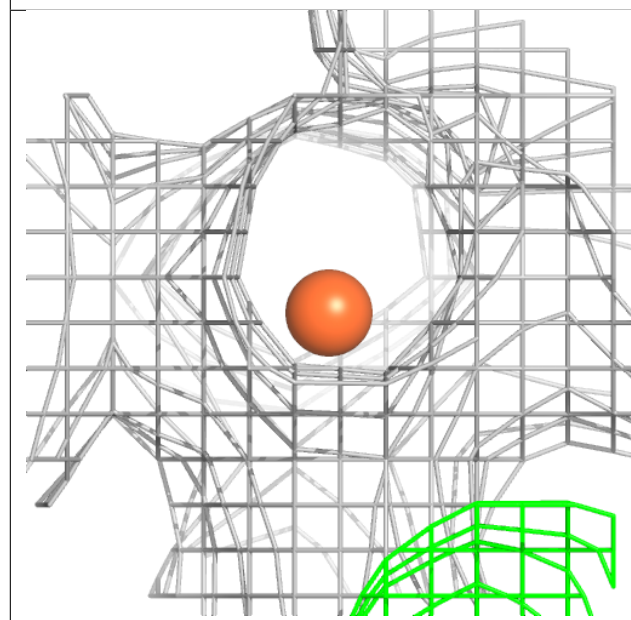
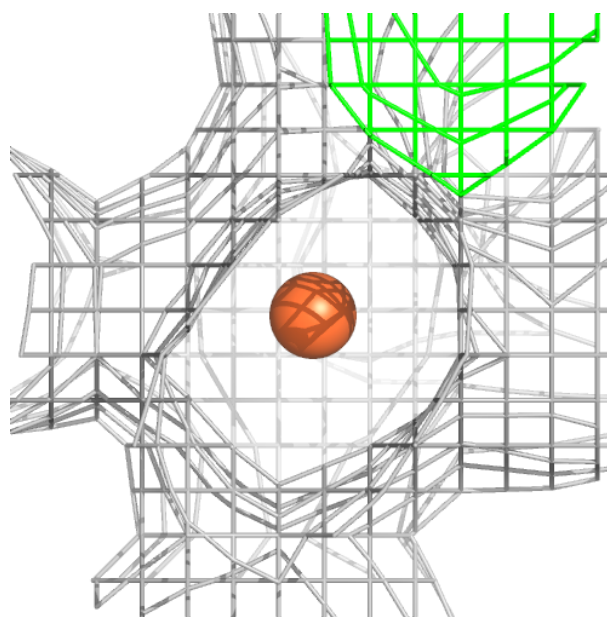
**Electron density around MN A 401:**

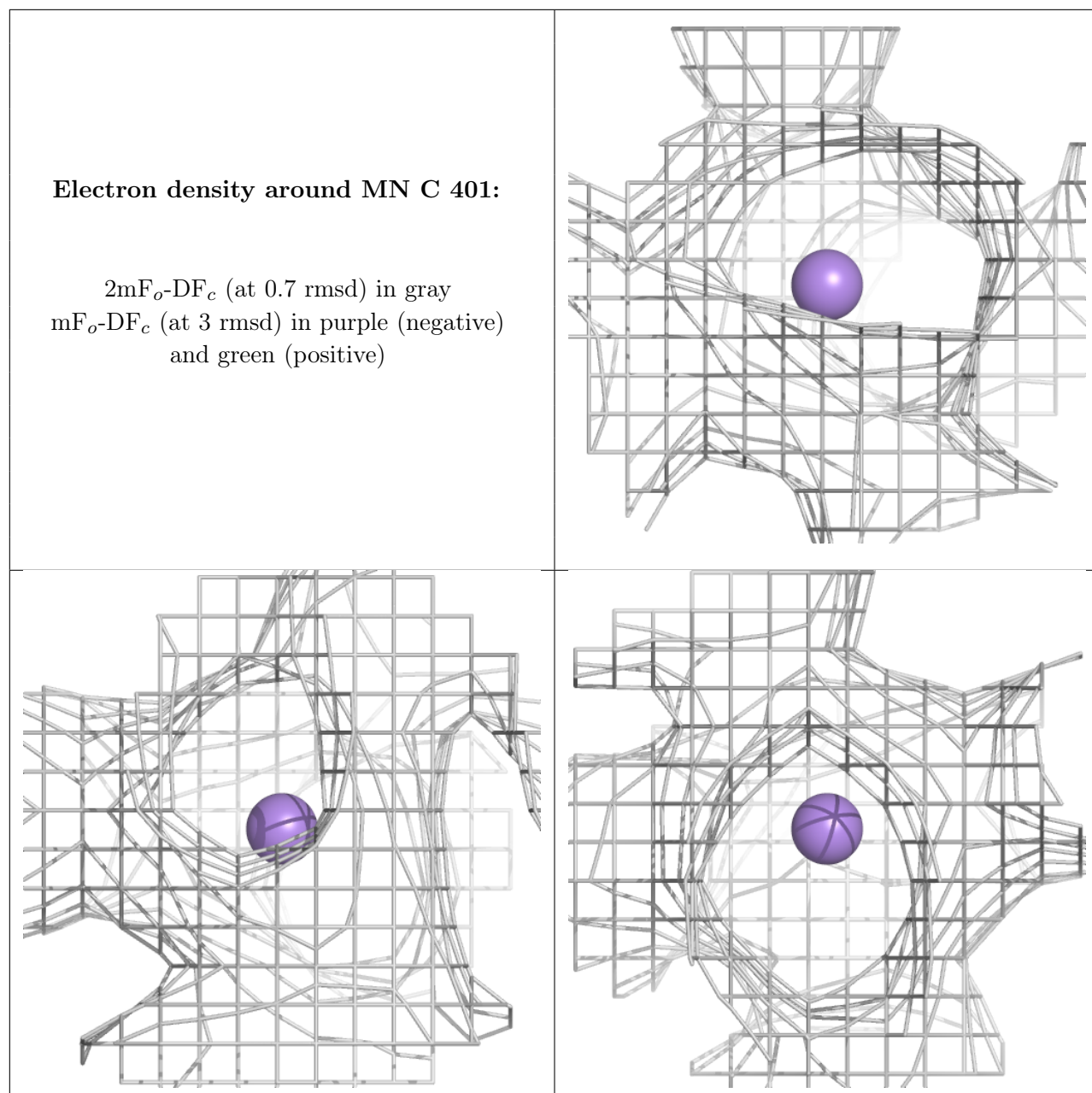
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE B 504:**

$2mF_o-DF_c$  (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.