



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:08 AM UTC

PDB ID : 8HMO / pdb_00008hmo
Title : Crystal Structure of metal-dependent hydrolase complexed with manganese from *Bacillus smithii*
Authors : Yoneda, K.; Sakuraba, H.; Ohshima, T.
Deposited on : 2022-12-05
Resolution : 2.53 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:

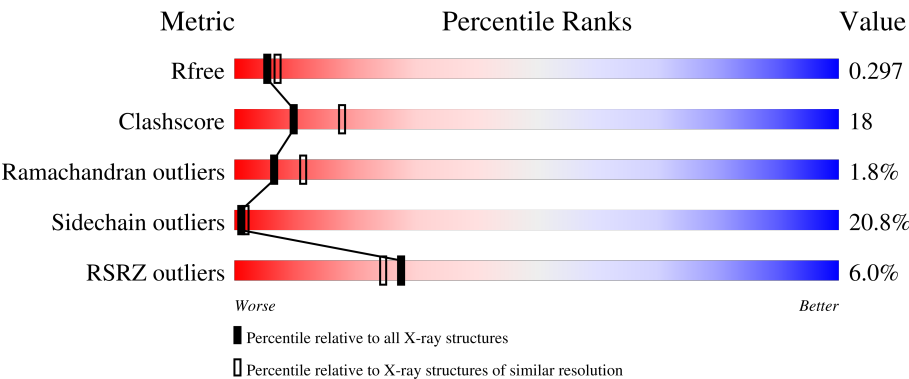
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	213	5% 57%31%7% . .
1	B	213	5% 62%29% . . .
1	C	213	5% 54%36%5%5%
1	D	213	6% 53%32%8% . 6%
1	E	213	7% 59%31%6% .

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Mol	Chain	Length	Quality of chain
1	F	213	7% 57% 32% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9914 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 Metal-dependent hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1608	1018	269	312	9			
1	B	205	Total	C	N	O	S	0	0	0
			1608	1018	269	312	9			
1	C	203	Total	C	N	O	S	0	0	0
			1585	1001	265	310	9			
1	D	201	Total	C	N	O	S	0	0	0
			1569	993	262	305	9			
1	E	204	Total	C	N	O	S	0	0	0
			1600	1014	267	310	9			
1	F	204	Total	C	N	O	S	0	0	0
			1603	1015	268	311	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	LEU	-	expression tag	UNP A0A0H4P0S7
A	207	GLU	-	expression tag	UNP A0A0H4P0S7
A	208	HIS	-	expression tag	UNP A0A0H4P0S7
A	209	HIS	-	expression tag	UNP A0A0H4P0S7
A	210	HIS	-	expression tag	UNP A0A0H4P0S7
A	211	HIS	-	expression tag	UNP A0A0H4P0S7
A	212	HIS	-	expression tag	UNP A0A0H4P0S7
A	213	HIS	-	expression tag	UNP A0A0H4P0S7
B	206	LEU	-	expression tag	UNP A0A0H4P0S7
B	207	GLU	-	expression tag	UNP A0A0H4P0S7
B	208	HIS	-	expression tag	UNP A0A0H4P0S7
B	209	HIS	-	expression tag	UNP A0A0H4P0S7
B	210	HIS	-	expression tag	UNP A0A0H4P0S7
B	211	HIS	-	expression tag	UNP A0A0H4P0S7
B	212	HIS	-	expression tag	UNP A0A0H4P0S7
B	213	HIS	-	expression tag	UNP A0A0H4P0S7
C	206	LEU	-	expression tag	UNP A0A0H4P0S7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	207	GLU	-	expression tag	UNP A0A0H4P0S7
C	208	HIS	-	expression tag	UNP A0A0H4P0S7
C	209	HIS	-	expression tag	UNP A0A0H4P0S7
C	210	HIS	-	expression tag	UNP A0A0H4P0S7
C	211	HIS	-	expression tag	UNP A0A0H4P0S7
C	212	HIS	-	expression tag	UNP A0A0H4P0S7
C	213	HIS	-	expression tag	UNP A0A0H4P0S7
D	206	LEU	-	expression tag	UNP A0A0H4P0S7
D	207	GLU	-	expression tag	UNP A0A0H4P0S7
D	208	HIS	-	expression tag	UNP A0A0H4P0S7
D	209	HIS	-	expression tag	UNP A0A0H4P0S7
D	210	HIS	-	expression tag	UNP A0A0H4P0S7
D	211	HIS	-	expression tag	UNP A0A0H4P0S7
D	212	HIS	-	expression tag	UNP A0A0H4P0S7
D	213	HIS	-	expression tag	UNP A0A0H4P0S7
E	206	LEU	-	expression tag	UNP A0A0H4P0S7
E	207	GLU	-	expression tag	UNP A0A0H4P0S7
E	208	HIS	-	expression tag	UNP A0A0H4P0S7
E	209	HIS	-	expression tag	UNP A0A0H4P0S7
E	210	HIS	-	expression tag	UNP A0A0H4P0S7
E	211	HIS	-	expression tag	UNP A0A0H4P0S7
E	212	HIS	-	expression tag	UNP A0A0H4P0S7
E	213	HIS	-	expression tag	UNP A0A0H4P0S7
F	206	LEU	-	expression tag	UNP A0A0H4P0S7
F	207	GLU	-	expression tag	UNP A0A0H4P0S7
F	208	HIS	-	expression tag	UNP A0A0H4P0S7
F	209	HIS	-	expression tag	UNP A0A0H4P0S7
F	210	HIS	-	expression tag	UNP A0A0H4P0S7
F	211	HIS	-	expression tag	UNP A0A0H4P0S7
F	212	HIS	-	expression tag	UNP A0A0H4P0S7
F	213	HIS	-	expression tag	UNP A0A0H4P0S7

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

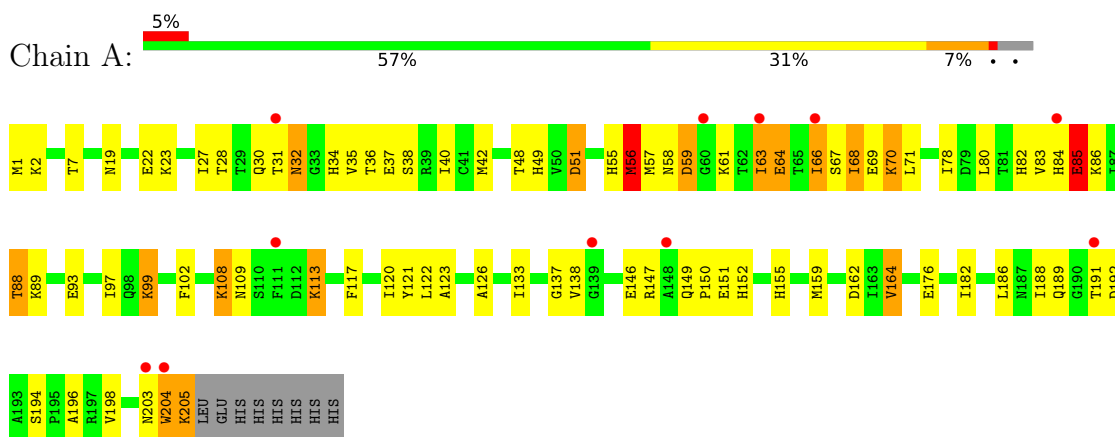
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total 62	O 62	0	0
3	B	56	Total 56	O 56	0	0
3	C	54	Total 54	O 54	0	0
3	D	63	Total 63	O 63	0	0
3	E	47	Total 47	O 47	0	0
3	F	47	Total 47	O 47	0	0

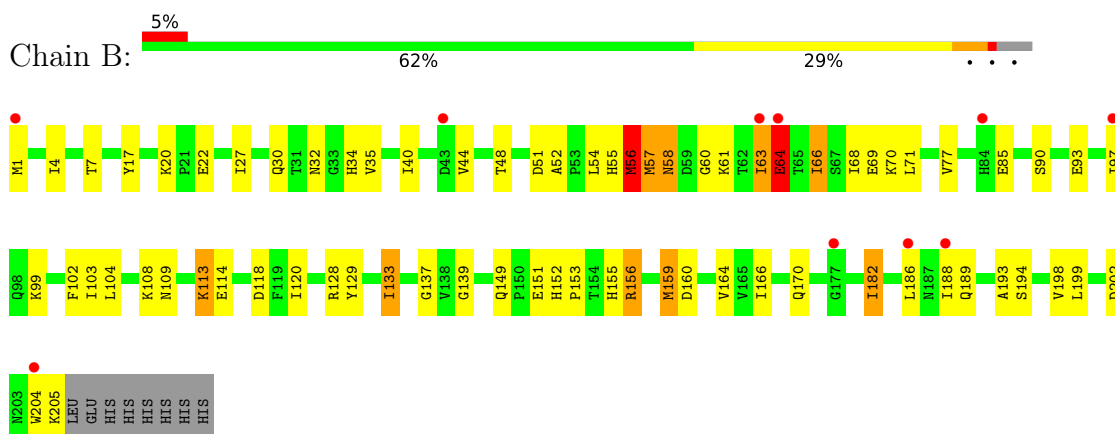
3 Residue-property plots [i](#)

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.

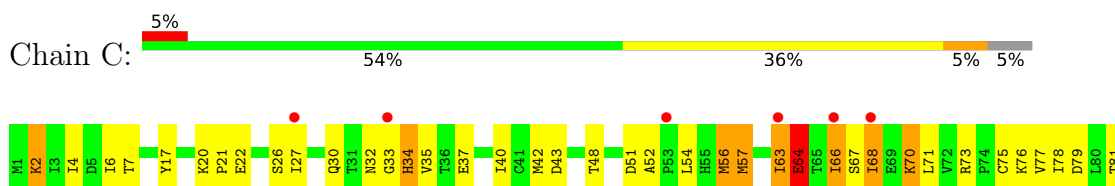
- Molecule 1: Metal-dependent hydrolase

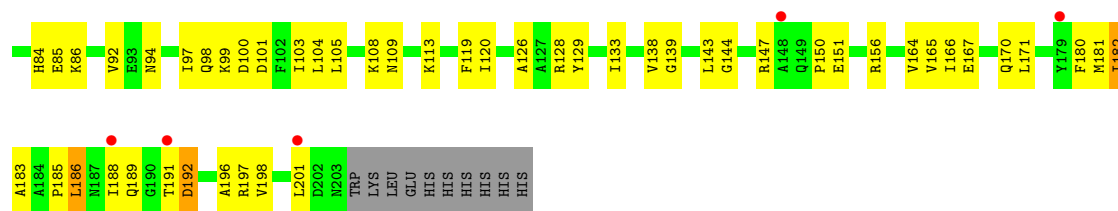


- Molecule 1: Metal-dependent hydrolase

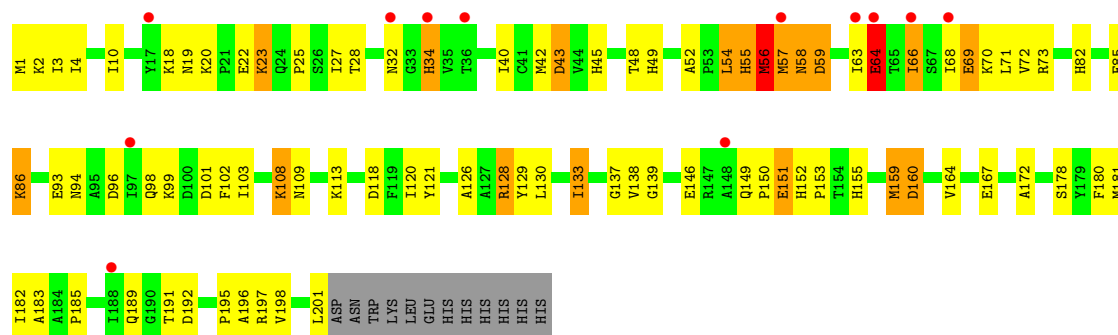


- Molecule 1: Metal-dependent hydrolase

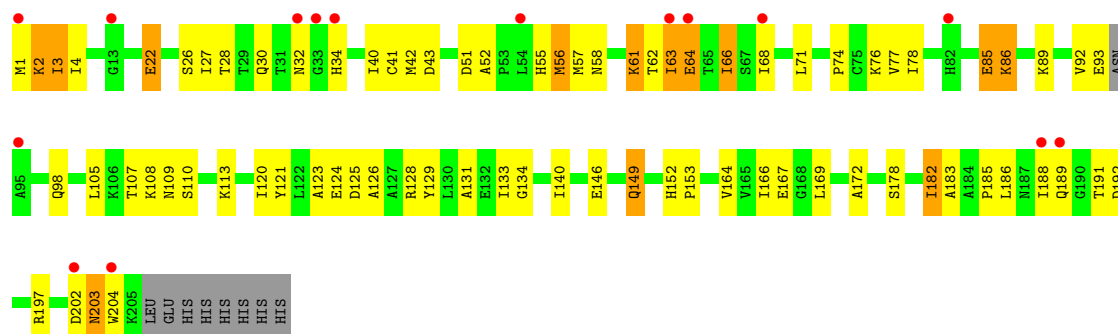




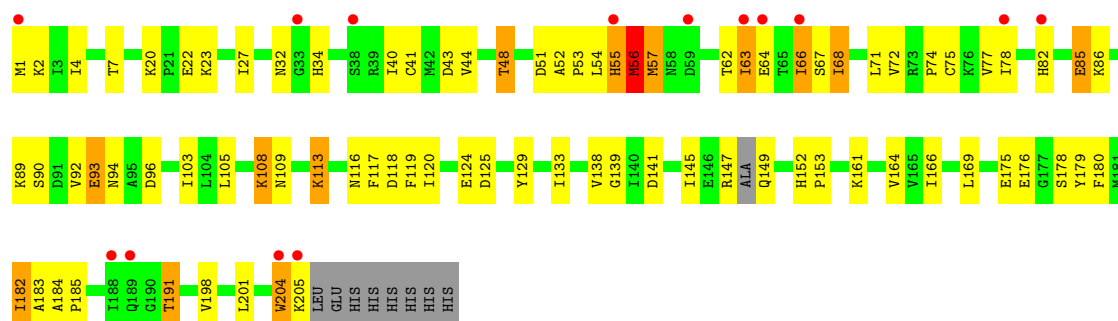
• Molecule 1: Metal-dependent hydrolase



• Molecule 1: Metal-dependent hydrolase



• Molecule 1: Metal-dependent hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.21Å 70.20Å 104.84Å 90.00° 105.77° 90.00°	Depositor
Resolution (Å)	43.45 – 2.53 43.45 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.3 (43.45-2.53) 97.3 (43.45-2.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.250 , 0.299 0.255 , 0.297	Depositor DCC
R_{free} test set	2065 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9914	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.04	0/1638	1.39	5/2220 (0.2%)
1	B	1.04	0/1638	1.35	3/2220 (0.1%)
1	C	1.04	0/1613	1.39	2/2186 (0.1%)
1	D	1.05	0/1597	1.41	1/2164 (0.0%)
1	E	1.03	0/1629	1.37	1/2206 (0.0%)
1	F	1.02	0/1632	1.40	2/2210 (0.1%)
All	All	1.04	0/9747	1.39	14/13206 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ASP	CA-CB-CG	8.59	121.19	112.60
1	C	48	THR	CB-CA-C	6.02	119.30	110.26
1	F	125	ASP	CA-CB-CG	5.96	118.56	112.60
1	E	51	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	59	ASP	N-CA-C	-5.76	105.44	112.88
1	F	51	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	51	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	51	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	59	ASP	CA-C-N	5.26	125.91	120.60
1	A	59	ASP	C-N-CA	5.26	125.91	120.60
1	B	151	GLU	CA-C-N	5.08	128.32	122.83
1	B	151	GLU	C-N-CA	5.08	128.32	122.83
1	A	123	ALA	CA-C-N	5.03	126.98	120.44
1	A	123	ALA	C-N-CA	5.03	126.98	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1608	0	1610	58	0
1	B	1608	0	1610	47	0
1	C	1585	0	1587	66	0
1	D	1569	0	1577	71	0
1	E	1600	0	1603	57	0
1	F	1603	0	1604	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	62	0	0	28	0
3	B	56	0	0	26	0
3	C	54	0	0	42	0
3	D	63	0	0	35	0
3	E	47	0	0	35	0
3	F	47	0	0	30	0
All	All	9914	0	9591	337	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 18.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:VAL:HG22	3:F:413:HOH:O	1.38	1.22
1:A:83:VAL:HG23	3:A:422:HOH:O	1.46	1.14
1:D:133:ILE:HG13	3:D:420:HOH:O	1.56	1.06
1:C:81:THR:HG23	3:C:416:HOH:O	1.55	1.04
1:E:78:ILE:HG13	3:E:423:HOH:O	1.56	1.04
3:C:413:HOH:O	1:D:55:HIS:HA	1.56	1.04
1:E:120:ILE:HG22	3:E:401:HOH:O	1.60	1.00
1:C:150:PRO:HA	3:C:412:HOH:O	1.61	0.99
1:A:137:GLY:HA3	3:A:406:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HB2	3:A:403:HOH:O	1.74	0.87
1:A:68:ILE:HD13	3:A:453:HOH:O	1.76	0.85
1:C:52:ALA:HB2	1:C:63:ILE:HG12	1.58	0.83
1:A:164:VAL:HG22	3:A:406:HOH:O	1.75	0.83
1:F:82:HIS:HB3	3:F:444:HOH:O	1.78	0.82
1:F:75:CYS:SG	3:F:410:HOH:O	2.37	0.82
1:C:92:VAL:HG21	3:C:401:HOH:O	1.78	0.82
1:D:129:TYR:CD2	3:D:420:HOH:O	2.33	0.81
1:A:68:ILE:HG22	3:A:425:HOH:O	1.81	0.81
1:D:98:GLN:HG2	3:D:425:HOH:O	1.80	0.80
1:C:92:VAL:CG2	3:C:401:HOH:O	2.28	0.79
1:B:133:ILE:HG13	3:B:410:HOH:O	1.83	0.79
1:D:63:ILE:O	1:D:64:GLU:HB2	1.82	0.79
1:C:170:GLN:C	3:C:409:HOH:O	2.24	0.79
1:C:6:ILE:HB	3:C:409:HOH:O	1.83	0.78
1:C:126:ALA:HA	3:C:401:HOH:O	1.84	0.77
1:D:52:ALA:HB2	1:D:63:ILE:HG12	1.64	0.76
1:B:57:MET:C	3:B:401:HOH:O	2.29	0.76
1:A:64:GLU:HG3	1:A:189:GLN:OE1	1.86	0.75
1:C:77:VAL:N	3:C:402:HOH:O	2.21	0.74
1:B:129:TYR:CD2	3:B:410:HOH:O	2.41	0.74
1:E:182:ILE:HG21	1:F:182:ILE:HG21	1.70	0.73
1:B:109:ASN:HD21	1:B:120:ILE:H	1.37	0.73
1:D:73:ARG:HG2	3:D:401:HOH:O	1.88	0.73
1:E:182:ILE:HD12	1:F:182:ILE:HD12	1.70	0.72
1:B:170:GLN:HG3	3:B:429:HOH:O	1.90	0.72
1:D:129:TYR:CE2	3:D:442:HOH:O	2.41	0.72
1:A:80:LEU:HA	3:A:422:HOH:O	1.90	0.71
1:C:35:VAL:HA	3:C:413:HOH:O	1.88	0.71
1:A:204:TRP:HB2	3:A:455:HOH:O	1.90	0.71
1:C:167:GLU:HG3	3:C:411:HOH:O	1.90	0.71
1:B:54:LEU:HA	3:B:401:HOH:O	1.91	0.70
1:A:122:LEU:C	3:A:401:HOH:O	2.34	0.70
1:F:129:TYR:HD2	3:F:406:HOH:O	1.75	0.70
1:B:55:HIS:O	1:B:56:MET:HB2	1.91	0.70
1:C:76:LYS:C	3:C:402:HOH:O	2.34	0.69
1:C:186:LEU:HD12	3:D:447:HOH:O	1.92	0.69
1:E:121:TYR:N	3:E:401:HOH:O	2.24	0.69
1:A:68:ILE:CG2	3:B:456:HOH:O	2.41	0.69
1:E:62:THR:HG23	3:E:417:HOH:O	1.94	0.68
1:C:171:LEU:HG	3:C:409:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:LYS:HG3	3:F:415:HOH:O	1.93	0.67
1:A:102:PHE:CZ	3:A:406:HOH:O	2.48	0.67
1:C:17:TYR:CD1	3:C:407:HOH:O	2.48	0.67
1:B:52:ALA:HB2	1:B:63:ILE:HG12	1.77	0.67
1:C:186:LEU:CD1	3:D:447:HOH:O	2.41	0.67
1:E:189:GLN:HG2	3:E:430:HOH:O	1.95	0.66
1:E:2:LYS:HA	3:E:429:HOH:O	1.94	0.66
1:F:145:ILE:HD12	3:F:412:HOH:O	1.94	0.66
1:C:57:MET:SD	3:C:448:HOH:O	2.52	0.66
1:E:41:CYS:CB	1:F:41:CYS:SG	2.84	0.66
1:B:60:GLY:HA3	3:B:401:HOH:O	1.96	0.65
1:A:159:MET:HA	3:A:408:HOH:O	1.96	0.64
1:C:143:LEU:C	3:C:407:HOH:O	2.39	0.64
1:B:129:TYR:C	3:B:410:HOH:O	2.40	0.64
1:D:10:ILE:HG22	3:D:439:HOH:O	1.98	0.63
1:F:74:PRO:HD2	3:F:431:HOH:O	1.97	0.63
1:F:48:THR:HG21	3:F:408:HOH:O	1.97	0.63
1:C:109:ASN:HD21	1:C:120:ILE:H	1.47	0.62
1:A:63:ILE:HD12	1:A:194:SER:HB3	1.82	0.62
1:E:169:LEU:HG	3:E:408:HOH:O	1.97	0.62
1:B:63:ILE:O	1:B:64:GLU:HB2	2.00	0.62
1:C:104:LEU:HB2	3:C:402:HOH:O	2.00	0.62
1:E:110:SER:C	3:E:414:HOH:O	2.42	0.62
1:D:101:ASP:HB3	3:D:421:HOH:O	2.00	0.61
1:D:55:HIS:O	1:D:56:MET:HB2	2.00	0.61
1:D:155:HIS:O	1:D:159:MET:HG3	2.01	0.61
1:C:77:VAL:CA	3:C:402:HOH:O	2.49	0.61
1:D:109:ASN:HD21	1:D:120:ILE:H	1.49	0.61
1:F:52:ALA:HB2	1:F:63:ILE:HG12	1.83	0.61
1:F:55:HIS:O	1:F:56:MET:HB2	2.00	0.61
1:E:107:THR:HG22	3:E:407:HOH:O	2.01	0.60
1:E:126:ALA:HA	3:E:405:HOH:O	2.00	0.60
1:D:72:VAL:N	3:D:401:HOH:O	2.34	0.60
1:F:78:ILE:HD12	3:F:405:HOH:O	2.01	0.60
1:D:63:ILE:HD13	1:D:66:ILE:HD12	1.82	0.60
1:E:66:ILE:HD11	1:E:71:LEU:HD11	1.83	0.60
1:D:70:LYS:C	3:D:401:HOH:O	2.44	0.60
1:B:133:ILE:HB	3:B:410:HOH:O	2.01	0.60
1:A:49:HIS:C	3:A:413:HOH:O	2.44	0.60
1:E:129:TYR:HD2	3:E:403:HOH:O	1.84	0.59
1:A:196:ALA:HB3	3:A:413:HOH:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ALA:O	1:F:185:PRO:HD3	2.02	0.59
1:F:57:MET:HB3	3:F:414:HOH:O	2.02	0.59
1:F:43:ASP:HB2	3:F:402:HOH:O	2.03	0.59
1:E:52:ALA:HB2	1:E:63:ILE:HG12	1.85	0.59
1:B:58:ASN:N	3:B:401:HOH:O	2.34	0.59
1:E:89:LYS:HG3	3:E:405:HOH:O	2.03	0.58
1:C:32:ASN:HA	3:C:421:HOH:O	2.03	0.58
3:C:445:HOH:O	1:D:43:ASP:HB2	2.03	0.58
1:E:121:TYR:HB2	1:E:146:GLU:HA	1.86	0.58
1:D:150:PRO:O	1:D:151:GLU:HB2	2.04	0.58
1:D:66:ILE:HB	3:D:459:HOH:O	2.04	0.57
1:E:77:VAL:C	3:E:423:HOH:O	2.46	0.57
1:C:54:LEU:HG	1:C:54:LEU:O	2.03	0.57
1:F:198:VAL:HB	3:F:408:HOH:O	2.04	0.57
1:A:80:LEU:CA	3:A:422:HOH:O	2.50	0.56
1:E:107:THR:CG2	3:E:407:HOH:O	2.52	0.56
1:D:93:GLU:CG	3:D:442:HOH:O	2.54	0.55
1:C:97:ILE:HG12	1:C:103:ILE:HG21	1.88	0.55
1:C:165:VAL:CG1	3:C:411:HOH:O	2.54	0.55
1:A:155:HIS:O	1:A:159:MET:HG3	2.07	0.55
1:C:77:VAL:HA	3:C:402:HOH:O	2.07	0.55
1:A:182:ILE:HG21	1:B:182:ILE:HG21	1.89	0.54
1:C:128:ARG:NH1	3:C:408:HOH:O	2.40	0.54
1:B:113:LYS:NZ	3:B:403:HOH:O	2.40	0.54
1:A:182:ILE:O	1:A:198:VAL:HA	2.08	0.54
1:B:56:MET:HE2	1:B:152:HIS:CG	2.43	0.54
1:C:144:GLY:N	3:C:407:HOH:O	2.40	0.54
1:B:20:LYS:HD2	3:B:433:HOH:O	2.08	0.53
1:B:66:ILE:HD11	1:B:71:LEU:HD11	1.88	0.53
1:F:23:LYS:HA	3:F:402:HOH:O	2.07	0.53
1:C:79:ASP:HA	3:C:416:HOH:O	2.08	0.53
1:C:129:TYR:HB3	3:C:401:HOH:O	2.09	0.53
1:C:182:ILE:HG21	1:D:182:ILE:HG21	1.90	0.53
1:E:166:ILE:HG22	3:E:408:HOH:O	2.09	0.53
1:A:63:ILE:HD13	1:A:66:ILE:HD11	1.90	0.52
1:A:108:LYS:HG3	3:A:402:HOH:O	2.09	0.52
1:E:92:VAL:HG21	3:E:403:HOH:O	2.10	0.52
1:A:113:LYS:HB3	3:A:447:HOH:O	2.10	0.52
1:B:149:GLN:HB3	1:B:153:PRO:HD2	1.91	0.52
1:B:189:GLN:HG2	3:B:424:HOH:O	2.08	0.52
1:B:103:ILE:HG23	3:B:417:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ILE:C	3:C:411:HOH:O	2.52	0.52
1:F:169:LEU:HG	3:F:401:HOH:O	2.10	0.52
1:E:166:ILE:C	3:E:408:HOH:O	2.53	0.52
1:F:109:ASN:HD21	1:F:120:ILE:H	1.58	0.52
1:C:165:VAL:HG12	3:C:411:HOH:O	2.10	0.52
1:D:54:LEU:O	1:D:55:HIS:C	2.53	0.52
1:D:196:ALA:HA	3:D:447:HOH:O	2.10	0.52
1:A:19:ASN:ND2	3:A:404:HOH:O	2.32	0.51
1:A:122:LEU:HG	3:A:401:HOH:O	2.10	0.51
1:D:96:ASP:C	3:D:425:HOH:O	2.53	0.51
1:D:126:ALA:O	1:D:130:LEU:HG	2.10	0.51
1:D:129:TYR:C	3:D:420:HOH:O	2.53	0.51
1:B:189:GLN:CG	3:B:424:HOH:O	2.58	0.51
1:D:20:LYS:NZ	3:D:408:HOH:O	2.42	0.51
1:C:192:ASP:OD2	1:C:192:ASP:N	2.43	0.51
1:D:183:ALA:O	1:D:185:PRO:HD3	2.11	0.51
1:E:74:PRO:HD2	3:E:424:HOH:O	2.11	0.51
1:A:51:ASP:HB3	1:A:159:MET:HE1	1.93	0.51
1:B:57:MET:CB	3:B:401:HOH:O	2.57	0.51
1:C:98:GLN:HA	3:C:451:HOH:O	2.10	0.51
1:C:32:ASN:CA	3:C:421:HOH:O	2.59	0.51
1:C:66:ILE:HG12	1:C:71:LEU:HD11	1.92	0.51
1:C:186:LEU:HD11	1:D:195:PRO:HB2	1.93	0.51
1:A:162:ASP:HA	3:A:408:HOH:O	2.10	0.50
1:E:109:ASN:HD21	1:E:120:ILE:H	1.59	0.50
1:E:129:TYR:HB3	3:E:403:HOH:O	2.11	0.50
1:D:66:ILE:O	1:D:66:ILE:HG12	2.10	0.50
1:A:55:HIS:O	1:A:56:MET:HB2	2.10	0.50
1:C:63:ILE:O	1:C:64:GLU:HB2	2.10	0.50
1:B:7:THR:HG23	1:B:48:THR:HB	1.92	0.50
1:A:68:ILE:HG22	3:B:456:HOH:O	2.07	0.50
1:D:128:ARG:NH1	3:D:409:HOH:O	2.44	0.50
1:E:61:LYS:HA	3:E:417:HOH:O	2.11	0.50
1:E:108:LYS:HG3	3:E:402:HOH:O	2.11	0.50
1:F:7:THR:HA	3:F:408:HOH:O	2.12	0.50
1:B:17:TYR:HD2	3:B:433:HOH:O	1.94	0.49
1:D:4:ILE:HG12	3:D:443:HOH:O	2.12	0.49
1:D:149:GLN:HB3	1:D:153:PRO:HD2	1.94	0.49
1:A:37:GLU:HG2	3:A:434:HOH:O	2.11	0.49
1:E:131:ALA:HB3	3:E:409:HOH:O	2.12	0.49
1:D:109:ASN:HD21	1:D:120:ILE:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:CYS:HB3	1:C:181:MET:HB2	1.95	0.49
1:A:63:ILE:HG21	1:A:194:SER:HB2	1.95	0.48
1:D:66:ILE:CG1	3:D:459:HOH:O	2.61	0.48
1:D:108:LYS:HG3	3:D:412:HOH:O	2.12	0.48
1:B:202:ASP:HB3	3:B:455:HOH:O	2.13	0.48
1:F:23:LYS:HG2	3:F:402:HOH:O	2.13	0.48
1:D:45:HIS:HA	1:D:49:HIS:CD2	2.49	0.48
1:E:63:ILE:O	1:E:64:GLU:HB2	2.13	0.48
1:C:35:VAL:HG22	1:D:56:MET:HE3	1.96	0.48
1:D:54:LEU:O	1:D:57:MET:N	2.46	0.48
1:A:56:MET:HE2	1:A:152:HIS:CG	2.49	0.47
1:B:63:ILE:HG21	1:B:194:SER:HB2	1.96	0.47
1:B:182:ILE:O	1:B:198:VAL:HA	2.13	0.47
1:A:35:VAL:HG22	1:B:56:MET:HE3	1.96	0.47
1:F:182:ILE:HA	3:F:413:HOH:O	2.14	0.47
1:D:71:LEU:N	3:D:401:HOH:O	2.48	0.47
1:A:80:LEU:HB3	3:A:422:HOH:O	2.14	0.47
1:A:97:ILE:HB	3:A:415:HOH:O	2.14	0.47
1:B:128:ARG:HA	3:B:423:HOH:O	2.14	0.47
1:E:85:GLU:O	1:E:120:ILE:HA	2.14	0.47
3:C:405:HOH:O	1:D:34:HIS:CE1	2.68	0.47
1:A:117:PHE:HB2	3:A:457:HOH:O	2.14	0.47
1:C:139:GLY:HA2	1:C:166:ILE:O	2.14	0.47
1:D:72:VAL:HG22	3:D:407:HOH:O	2.15	0.47
1:E:92:VAL:CG2	3:E:403:HOH:O	2.63	0.47
1:F:179:TYR:HB2	3:F:410:HOH:O	2.15	0.47
1:E:128:ARG:HG2	3:E:433:HOH:O	2.13	0.47
1:D:103:ILE:O	1:D:138:VAL:HA	2.15	0.47
1:A:36:THR:O	1:B:55:HIS:HD2	1.98	0.47
1:A:150:PRO:O	1:A:151:GLU:HB2	2.15	0.47
1:B:156:ARG:O	1:B:160:ASP:HB2	2.15	0.47
1:D:56:MET:HE2	1:D:152:HIS:CG	2.50	0.47
1:E:125:ASP:C	3:E:405:HOH:O	2.58	0.47
1:F:139:GLY:HA2	1:F:166:ILE:O	2.14	0.47
1:F:103:ILE:HD12	1:F:105:LEU:HD21	1.97	0.46
1:A:32:ASN:N	1:A:32:ASN:HD22	2.11	0.46
1:F:68:ILE:HG12	3:F:427:HOH:O	2.14	0.46
1:F:113:LYS:HA	1:F:113:LYS:HD3	1.64	0.46
1:A:80:LEU:CB	3:A:422:HOH:O	2.63	0.46
1:A:205:LYS:HB3	1:A:205:LYS:HE2	1.80	0.46
1:C:34:HIS:N	3:C:404:HOH:O	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ALA:CB	3:E:414:HOH:O	2.63	0.46
1:A:70:LYS:HB2	1:A:70:LYS:HE2	1.76	0.46
1:E:86:LYS:HB3	1:E:121:TYR:CE2	2.51	0.46
1:F:116:ASN:HB3	3:F:404:HOH:O	2.15	0.46
1:E:110:SER:HB3	3:E:414:HOH:O	2.16	0.45
1:A:7:THR:HG23	1:A:48:THR:HB	1.98	0.45
3:C:413:HOH:O	1:D:56:MET:N	2.49	0.45
1:D:172:ALA:N	3:D:417:HOH:O	2.50	0.45
1:F:52:ALA:HB2	1:F:63:ILE:CG1	2.45	0.45
1:F:54:LEU:HD22	1:F:62:THR:HG22	1.99	0.45
1:E:197:ARG:HB3	1:F:184:ALA:HB1	1.99	0.45
1:F:180:PHE:HB3	1:F:201:LEU:HB2	1.98	0.45
1:F:119:PHE:CZ	1:F:147:ARG:HB3	2.52	0.45
1:F:139:GLY:C	3:F:412:HOH:O	2.60	0.45
1:B:199:LEU:HD11	3:B:456:HOH:O	2.16	0.45
1:A:99:LYS:HD3	3:A:452:HOH:O	2.16	0.45
1:F:103:ILE:O	1:F:138:VAL:HA	2.17	0.45
1:F:205:LYS:NZ	3:F:411:HOH:O	2.49	0.45
1:C:185:PRO:O	1:D:197:ARG:HD3	2.17	0.44
1:E:172:ALA:HA	3:E:414:HOH:O	2.16	0.44
1:C:126:ALA:O	3:C:401:HOH:O	2.21	0.44
1:E:202:ASP:O	1:E:203:ASN:C	2.60	0.44
1:C:2:LYS:HB3	1:C:2:LYS:HE2	1.59	0.44
1:C:151:GLU:N	3:C:412:HOH:O	2.45	0.44
1:E:120:ILE:C	3:E:401:HOH:O	2.60	0.44
1:C:119:PHE:CZ	1:C:147:ARG:HB3	2.53	0.44
1:D:69:GLU:O	3:D:401:HOH:O	2.21	0.44
1:D:129:TYR:CD2	3:D:442:HOH:O	2.68	0.44
1:D:66:ILE:CB	3:D:459:HOH:O	2.62	0.44
1:D:139:GLY:HA3	3:D:456:HOH:O	2.17	0.44
1:E:3:ILE:HB	3:F:427:HOH:O	2.16	0.44
1:D:48:THR:HG23	3:D:419:HOH:O	2.18	0.44
1:F:116:ASN:CB	3:F:404:HOH:O	2.65	0.44
1:E:134:GLY:HA3	3:E:436:HOH:O	2.17	0.43
1:F:66:ILE:HG12	1:F:71:LEU:HD11	1.99	0.43
1:F:68:ILE:CG1	3:F:427:HOH:O	2.65	0.43
1:D:71:LEU:HB3	1:D:183:ALA:HB3	1.99	0.43
1:A:88:THR:C	1:A:126:ALA:HB2	2.43	0.43
1:A:162:ASP:CA	3:A:408:HOH:O	2.65	0.43
1:B:64:GLU:HB2	3:B:407:HOH:O	2.18	0.43
1:B:58:ASN:HD22	1:B:58:ASN:HA	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:LYS:HB2	1:F:23:LYS:HD2	2.00	0.43
1:C:34:HIS:CD2	1:D:58:ASN:HB2	2.54	0.43
1:C:66:ILE:HG12	1:C:66:ILE:O	2.17	0.43
1:D:182:ILE:O	1:D:198:VAL:HA	2.17	0.43
1:C:103:ILE:HD12	1:C:105:LEU:HD21	2.00	0.43
1:C:171:LEU:N	3:C:409:HOH:O	2.50	0.43
1:C:180:PHE:HB3	1:C:201:LEU:HB2	2.00	0.43
1:D:18:LYS:NZ	3:D:413:HOH:O	2.48	0.43
1:D:121:TYR:HB2	1:D:146:GLU:HA	2.01	0.43
1:E:86:LYS:HD2	1:E:123:ALA:HB2	2.00	0.43
1:A:121:TYR:CD2	1:A:147:ARG:HG2	2.53	0.43
1:C:7:THR:HG21	1:C:197:ARG:HD2	2.00	0.43
1:C:56:MET:HB3	3:C:448:HOH:O	2.18	0.43
1:A:56:MET:HE3	1:B:35:VAL:HG22	2.00	0.43
1:A:68:ILE:HG21	3:B:456:HOH:O	2.10	0.43
1:B:129:TYR:CG	3:B:410:HOH:O	2.67	0.43
1:D:66:ILE:O	1:D:66:ILE:CG1	2.66	0.43
1:F:43:ASP:CB	3:F:402:HOH:O	2.62	0.43
1:C:156:ARG:CD	3:C:427:HOH:O	2.67	0.43
1:F:54:LEU:O	1:F:57:MET:O	2.37	0.43
1:E:105:LEU:C	3:E:407:HOH:O	2.62	0.42
1:A:186:LEU:HD12	3:B:430:HOH:O	2.18	0.42
1:E:22:GLU:H	1:E:22:GLU:HG3	1.48	0.42
1:C:70:LYS:HB3	1:C:70:LYS:HE3	1.81	0.42
1:D:86:LYS:HB3	1:D:121:TYR:CE2	2.54	0.42
1:E:41:CYS:HB3	1:F:41:CYS:SG	2.58	0.42
1:F:44:VAL:HG11	1:F:191:THR:HG21	2.02	0.42
1:F:89:LYS:HG2	1:F:93:GLU:HG3	2.00	0.42
1:A:66:ILE:HG12	1:A:71:LEU:HD11	2.02	0.42
1:B:44:VAL:HG23	1:B:193:ALA:HB3	2.02	0.42
1:B:102:PHE:CE1	1:B:137:GLY:HA3	2.55	0.42
1:E:76:LYS:C	3:E:423:HOH:O	2.62	0.42
1:D:160:ASP:HB3	3:D:424:HOH:O	2.20	0.42
1:A:82:HIS:CE1	3:A:422:HOH:O	2.72	0.42
1:A:182:ILE:HD12	1:B:182:ILE:HD12	2.02	0.42
1:B:133:ILE:CG1	3:B:410:HOH:O	2.56	0.42
1:C:37:GLU:HA	1:D:192:ASP:OD1	2.20	0.42
1:D:93:GLU:HG3	3:D:442:HOH:O	2.16	0.42
1:E:172:ALA:HB2	3:E:414:HOH:O	2.18	0.42
1:C:68:ILE:H	1:C:68:ILE:HG13	1.44	0.41
1:E:124:GLU:O	1:E:125:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ILE:HG22	1:B:133:ILE:HG21	2.03	0.41
1:C:186:LEU:HD12	1:C:186:LEU:HA	1.83	0.41
1:D:128:ARG:HE	1:D:128:ARG:HB3	1.33	0.41
1:E:56:MET:HE2	1:E:152:HIS:CG	2.54	0.41
3:C:445:HOH:O	1:D:23:LYS:HA	2.20	0.41
1:F:43:ASP:CG	3:F:402:HOH:O	2.63	0.41
1:B:155:HIS:O	1:B:159:MET:HG3	2.21	0.41
1:F:166:ILE:C	3:F:401:HOH:O	2.62	0.41
1:B:102:PHE:HA	1:B:137:GLY:O	2.21	0.41
1:E:55:HIS:HB2	1:E:192:ASP:HB2	2.02	0.41
1:F:67:SER:HA	3:F:442:HOH:O	2.20	0.41
1:B:139:GLY:HA2	1:B:166:ILE:O	2.20	0.41
1:C:165:VAL:HG13	3:C:411:HOH:O	2.17	0.41
1:D:180:PHE:HB3	1:D:201:LEU:HB2	2.02	0.41
1:E:183:ALA:O	1:E:185:PRO:HD3	2.20	0.41
1:A:83:VAL:CG2	3:A:422:HOH:O	2.30	0.41
1:A:85:GLU:O	1:A:120:ILE:HA	2.21	0.41
1:C:185:PRO:HA	1:C:196:ALA:HA	2.02	0.41
1:D:82:HIS:CD2	1:D:82:HIS:H	2.39	0.41
1:E:121:TYR:C	3:E:401:HOH:O	2.63	0.41
1:E:149:GLN:HB3	1:E:153:PRO:HD2	2.03	0.41
1:F:77:VAL:O	1:F:176:GLU:HG3	2.21	0.41
1:F:124:GLU:CD	1:F:153:PRO:HB2	2.46	0.41
1:B:77:VAL:HA	1:B:104:LEU:O	2.21	0.41
1:A:205:LYS:HE3	1:B:205:LYS:HE3	2.03	0.40
1:C:32:ASN:C	3:C:421:HOH:O	2.63	0.40
1:E:140:ILE:HG22	1:E:167:GLU:HA	2.03	0.40
1:A:121:TYR:HB2	1:A:146:GLU:HA	2.04	0.40
1:C:183:ALA:HA	1:C:198:VAL:HG22	2.03	0.40
1:D:52:ALA:O	1:D:54:LEU:N	2.55	0.40
1:D:102:PHE:CE1	1:D:137:GLY:HA3	2.57	0.40
1:F:52:ALA:O	1:F:54:LEU:N	2.55	0.40
1:A:109:ASN:HD21	1:A:120:ILE:H	1.69	0.40
1:C:17:TYR:CE1	3:C:407:HOH:O	2.71	0.40
1:D:25:PRO:HG3	3:D:439:HOH:O	2.21	0.40
1:D:73:ARG:HB3	3:D:401:HOH:O	2.21	0.40
1:D:129:TYR:CE2	3:D:420:HOH:O	2.68	0.40
1:F:56:MET:HE2	1:F:152:HIS:CG	2.56	0.40
1:C:20:LYS:HA	1:C:21:PRO:HD3	1.94	0.40
1:E:105:LEU:HB3	3:E:407:HOH:O	2.21	0.40
1:F:117:PHE:N	3:F:404:HOH:O	2.54	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	203/213 (95%)	186 (92%)	15 (7%)	2 (1%)	12	23
1	B	203/213 (95%)	179 (88%)	22 (11%)	2 (1%)	12	23
1	C	201/213 (94%)	185 (92%)	13 (6%)	3 (2%)	8	15
1	D	199/213 (93%)	180 (90%)	14 (7%)	5 (2%)	4	6
1	E	200/213 (94%)	184 (92%)	13 (6%)	3 (2%)	8	15
1	F	200/213 (94%)	179 (90%)	14 (7%)	7 (4%)	3	3
All	All	1206/1278 (94%)	1093 (91%)	91 (8%)	22 (2%)	6	11

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	19	ASN
1	D	64	GLU
1	E	64	GLU
1	F	64	GLU
1	F	96	ASP
1	B	64	GLU
1	C	64	GLU
1	D	54	LEU
1	D	55	HIS
1	D	56	MET
1	F	56	MET
1	A	56	MET
1	E	85	GLU
1	E	203	ASN
1	B	56	MET
1	C	85	GLU
1	F	85	GLU

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Mol	Chain	Res	Type
1	A	85	GLU
1	F	55	HIS
1	F	204	TRP
1	C	33	GLY
1	F	53	PRO

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	179/187 (96%)	133 (74%)	46 (26%)	0	1
1	B	179/187 (96%)	145 (81%)	34 (19%)	1	2
1	C	177/187 (95%)	140 (79%)	37 (21%)	1	2
1	D	175/187 (94%)	137 (78%)	38 (22%)	1	1
1	E	178/187 (95%)	144 (81%)	34 (19%)	1	2
1	F	179/187 (96%)	146 (82%)	33 (18%)	1	3
All	All	1067/1122 (95%)	845 (79%)	222 (21%)	1	2

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	22	GLU
1	A	23	LYS
1	A	27	ILE
1	A	28	THR
1	A	30	GLN
1	A	31	THR
1	A	32	ASN
1	A	34	HIS
1	A	38	SER
1	A	40	ILE
1	A	42	MET

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Mol	Chain	Res	Type
1	A	56	MET
1	A	57	MET
1	A	58	ASN
1	A	59	ASP
1	A	61	LYS
1	A	63	ILE
1	A	64	GLU
1	A	66	ILE
1	A	67	SER
1	A	68	ILE
1	A	69	GLU
1	A	70	LYS
1	A	78	ILE
1	A	84	HIS
1	A	85	GLU
1	A	86	LYS
1	A	88	THR
1	A	89	LYS
1	A	93	GLU
1	A	99	LYS
1	A	108	LYS
1	A	113	LYS
1	A	133	ILE
1	A	138	VAL
1	A	149	GLN
1	A	164	VAL
1	A	176	GLU
1	A	188	ILE
1	A	191	THR
1	A	192	ASP
1	A	203	ASN
1	A	204	TRP
1	A	205	LYS
1	B	1	MET
1	B	4	ILE
1	B	22	GLU
1	B	27	ILE
1	B	30	GLN
1	B	32	ASN
1	B	34	HIS
1	B	40	ILE
1	B	56	MET

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Mol	Chain	Res	Type
1	B	57	MET
1	B	58	ASN
1	B	61	LYS
1	B	63	ILE
1	B	64	GLU
1	B	66	ILE
1	B	68	ILE
1	B	69	GLU
1	B	70	LYS
1	B	85	GLU
1	B	90	SER
1	B	93	GLU
1	B	99	LYS
1	B	108	LYS
1	B	113	LYS
1	B	114	GLU
1	B	118	ASP
1	B	133	ILE
1	B	156	ARG
1	B	159	MET
1	B	164	VAL
1	B	182	ILE
1	B	186	LEU
1	B	188	ILE
1	B	204	TRP
1	C	2	LYS
1	C	4	ILE
1	C	22	GLU
1	C	26	SER
1	C	27	ILE
1	C	30	GLN
1	C	34	HIS
1	C	40	ILE
1	C	42	MET
1	C	43	ASP
1	C	56	MET
1	C	57	MET
1	C	63	ILE
1	C	64	GLU
1	C	66	ILE
1	C	67	SER
1	C	68	ILE

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Mol	Chain	Res	Type
1	C	70	LYS
1	C	73	ARG
1	C	78	ILE
1	C	84	HIS
1	C	86	LYS
1	C	94	ASN
1	C	99	LYS
1	C	100	ASP
1	C	101	ASP
1	C	108	LYS
1	C	113	LYS
1	C	133	ILE
1	C	138	VAL
1	C	164	VAL
1	C	182	ILE
1	C	186	LEU
1	C	188	ILE
1	C	189	GLN
1	C	191	THR
1	C	192	ASP
1	D	1	MET
1	D	2	LYS
1	D	3	ILE
1	D	22	GLU
1	D	23	LYS
1	D	27	ILE
1	D	28	THR
1	D	32	ASN
1	D	34	HIS
1	D	40	ILE
1	D	42	MET
1	D	43	ASP
1	D	56	MET
1	D	57	MET
1	D	58	ASN
1	D	59	ASP
1	D	64	GLU
1	D	66	ILE
1	D	68	ILE
1	D	69	GLU
1	D	85	GLU
1	D	86	LYS

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Mol	Chain	Res	Type
1	D	94	ASN
1	D	99	LYS
1	D	108	LYS
1	D	113	LYS
1	D	118	ASP
1	D	128	ARG
1	D	133	ILE
1	D	151	GLU
1	D	159	MET
1	D	160	ASP
1	D	164	VAL
1	D	167	GLU
1	D	178	SER
1	D	181	MET
1	D	189	GLN
1	D	191	THR
1	E	1	MET
1	E	2	LYS
1	E	3	ILE
1	E	4	ILE
1	E	22	GLU
1	E	26	SER
1	E	27	ILE
1	E	28	THR
1	E	30	GLN
1	E	32	ASN
1	E	34	HIS
1	E	40	ILE
1	E	42	MET
1	E	43	ASP
1	E	56	MET
1	E	57	MET
1	E	58	ASN
1	E	61	LYS
1	E	63	ILE
1	E	66	ILE
1	E	68	ILE
1	E	86	LYS
1	E	93	GLU
1	E	98	GLN
1	E	113	LYS
1	E	133	ILE

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Mol	Chain	Res	Type
1	E	149	GLN
1	E	164	VAL
1	E	178	SER
1	E	182	ILE
1	E	186	LEU
1	E	188	ILE
1	E	191	THR
1	E	204	TRP
1	F	1	MET
1	F	2	LYS
1	F	4	ILE
1	F	22	GLU
1	F	27	ILE
1	F	32	ASN
1	F	34	HIS
1	F	40	ILE
1	F	48	THR
1	F	56	MET
1	F	57	MET
1	F	63	ILE
1	F	66	ILE
1	F	68	ILE
1	F	85	GLU
1	F	86	LYS
1	F	90	SER
1	F	92	VAL
1	F	93	GLU
1	F	94	ASN
1	F	108	LYS
1	F	113	LYS
1	F	118	ASP
1	F	133	ILE
1	F	141	ASP
1	F	149	GLN
1	F	161	LYS
1	F	164	VAL
1	F	175	GLU
1	F	178	SER
1	F	182	ILE
1	F	191	THR
1	F	204	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	58	ASN
1	A	82	HIS
1	A	84	HIS
1	A	109	ASN
1	A	203	ASN
1	B	34	HIS
1	B	55	HIS
1	B	58	ASN
1	B	82	HIS
1	B	109	ASN
1	B	116	ASN
1	C	19	ASN
1	C	30	GLN
1	C	55	HIS
1	C	58	ASN
1	C	109	ASN
1	D	34	HIS
1	D	82	HIS
1	D	109	ASN
1	D	116	ASN
1	D	189	GLN
1	E	19	ASN
1	E	30	GLN
1	E	55	HIS
1	E	58	ASN
1	E	82	HIS
1	E	109	ASN
1	F	34	HIS
1	F	82	HIS
1	F	84	HIS
1	F	109	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 12 ligands modelled in this entry, 12 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	205/213 (96%)	0.45	11 (5%) 31 28	33, 52, 78, 94	0
1	B	205/213 (96%)	0.45	10 (4%) 35 31	36, 55, 92, 123	0
1	C	203/213 (95%)	0.56	11 (5%) 31 28	33, 57, 80, 112	0
1	D	201/213 (94%)	0.57	12 (5%) 27 24	37, 57, 86, 103	0
1	E	204/213 (95%)	0.75	15 (7%) 20 18	40, 64, 92, 136	0
1	F	204/213 (95%)	0.83	14 (6%) 23 20	42, 66, 94, 137	0
All	All	1222/1278 (95%)	0.60	73 (5%) 27 24	33, 58, 89, 137	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	TRP	3.9
1	A	139	GLY	3.6
1	C	63	ILE	3.6
1	D	188	ILE	3.5
1	F	64	GLU	3.4
1	E	33	GLY	3.3
1	A	191	THR	3.2
1	F	82	HIS	3.2
1	F	63	ILE	3.2
1	C	191	THR	3.2
1	E	95	ALA	3.1
1	F	188	ILE	3.1
1	F	204	TRP	3.0
1	F	66	ILE	3.0
1	E	82	HIS	3.0
1	A	60	GLY	2.9
1	B	188	ILE	2.9
1	B	64	GLU	2.9
1	E	204	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	57	MET	2.8
1	D	63	ILE	2.7
1	C	148	ALA	2.7
1	D	97	ILE	2.7
1	C	68	ILE	2.6
1	F	205	LYS	2.6
1	E	189	GLN	2.6
1	B	1	MET	2.6
1	B	204	TRP	2.5
1	E	188	ILE	2.5
1	D	17	TYR	2.5
1	A	66	ILE	2.5
1	A	31	THR	2.5
1	C	33	GLY	2.5
1	F	59	ASP	2.5
1	D	36	THR	2.5
1	D	34	HIS	2.4
1	D	64	GLU	2.4
1	D	66	ILE	2.4
1	F	78	ILE	2.4
1	D	32	ASN	2.4
1	C	66	ILE	2.4
1	E	68	ILE	2.4
1	F	1	MET	2.4
1	E	13	GLY	2.3
1	B	43	ASP	2.3
1	E	54	LEU	2.3
1	E	63	ILE	2.3
1	A	203	ASN	2.3
1	F	38	SER	2.3
1	E	1	MET	2.3
1	B	97	ILE	2.2
1	A	111	PHE	2.2
1	A	84	HIS	2.2
1	F	189	GLN	2.2
1	E	64	GLU	2.2
1	C	53	PRO	2.2
1	E	34	HIS	2.2
1	A	63	ILE	2.2
1	C	188	ILE	2.2
1	B	177	GLY	2.2
1	C	179	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	63	ILE	2.2
1	A	148	ALA	2.1
1	B	84	HIS	2.1
1	E	202	ASP	2.1
1	C	201	LEU	2.1
1	E	32	ASN	2.1
1	D	68	ILE	2.1
1	D	148	ALA	2.1
1	B	186	LEU	2.1
1	F	33	GLY	2.1
1	F	55	HIS	2.0
1	C	27	ILE	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(Å ²)	Q<0.9
2	MN	D	301	1/1	0.57	0.16	53,53,53,53	0
2	MN	B	301	1/1	0.59	0.18	53,53,53,53	0
2	MN	F	302	1/1	0.69	0.14	53,53,53,53	0
2	MN	D	302	1/1	0.73	0.14	50,50,50,50	0
2	MN	B	302	1/1	0.76	0.14	61,61,61,61	0
2	MN	E	302	1/1	0.83	0.10	70,70,70,70	0
2	MN	F	301	1/1	0.88	0.10	57,57,57,57	0
2	MN	E	301	1/1	0.95	0.08	61,61,61,61	0
2	MN	A	302	1/1	0.97	0.03	44,44,44,44	0
2	MN	A	301	1/1	0.98	0.09	42,42,42,42	0
2	MN	C	301	1/1	0.98	0.07	49,49,49,49	0

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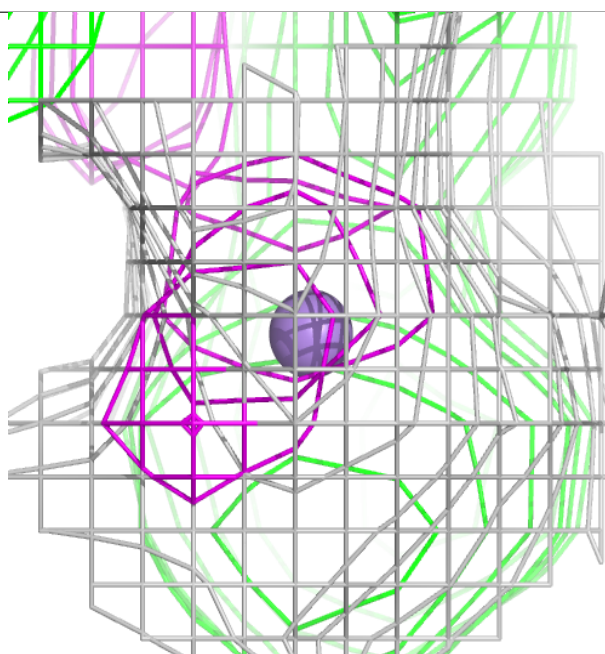
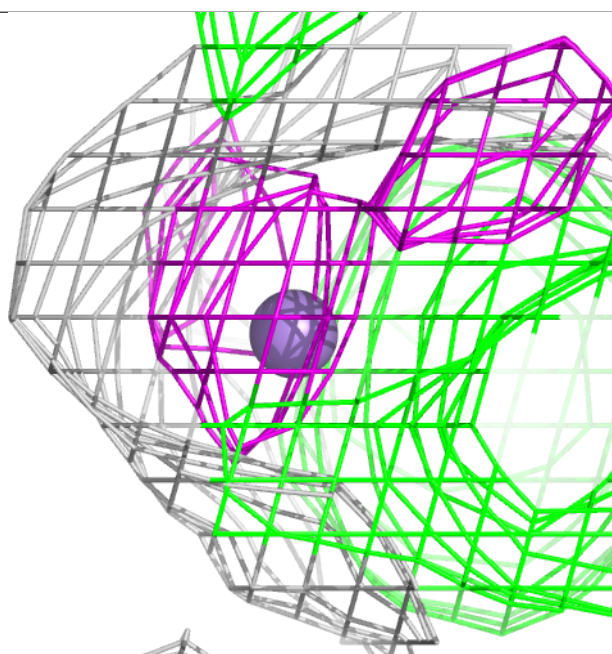
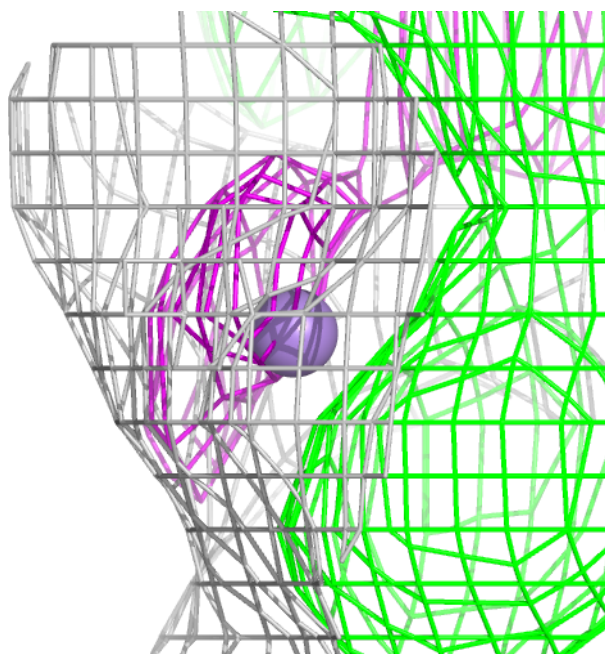
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	C	302	1/1	0.98	0.05	52,52,52,52	0

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.

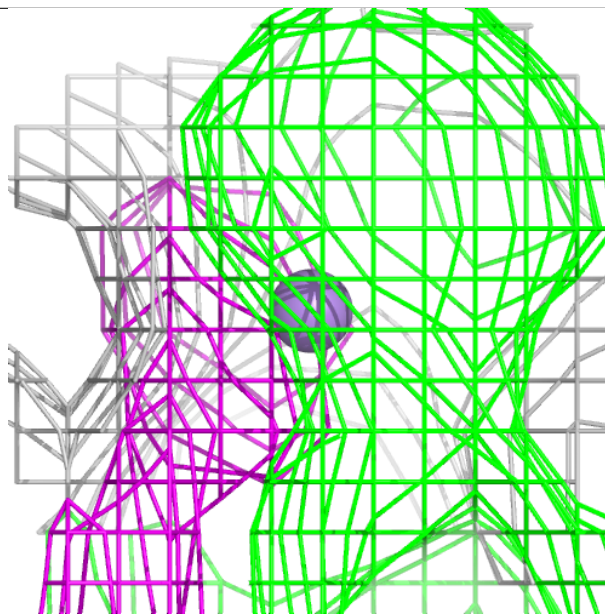
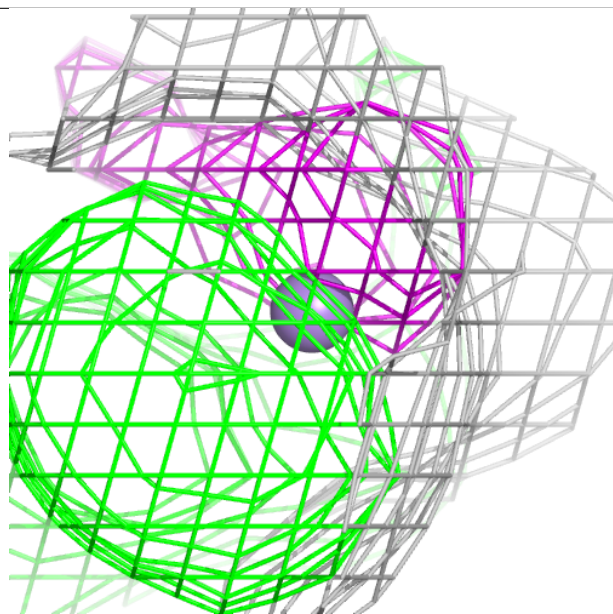
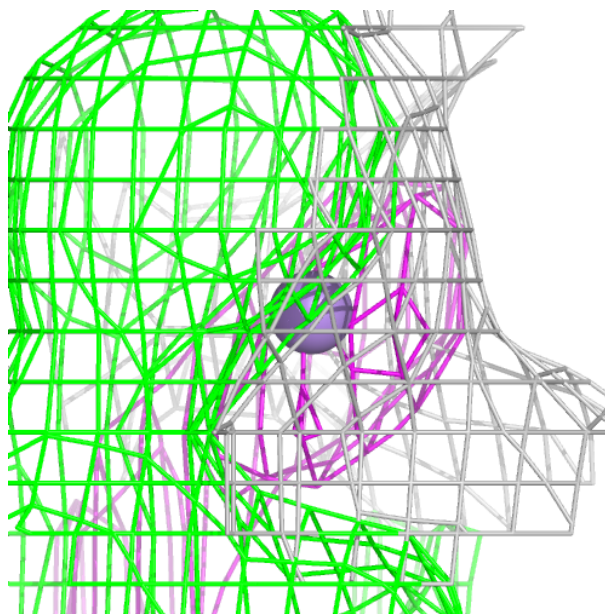
Electron density around MN D 301:

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



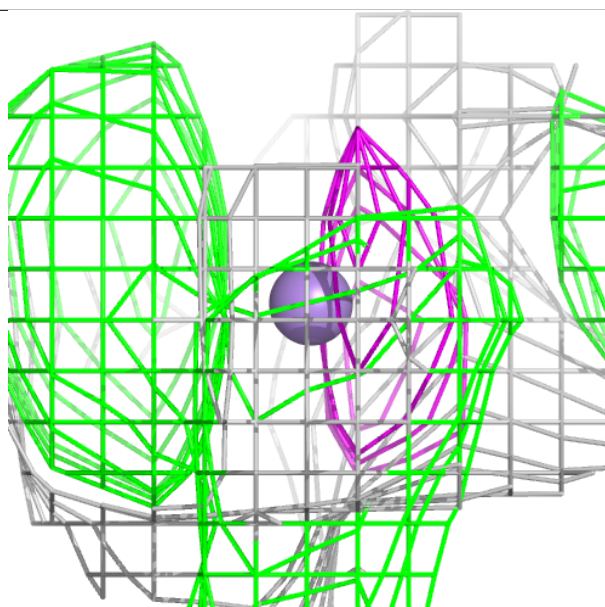
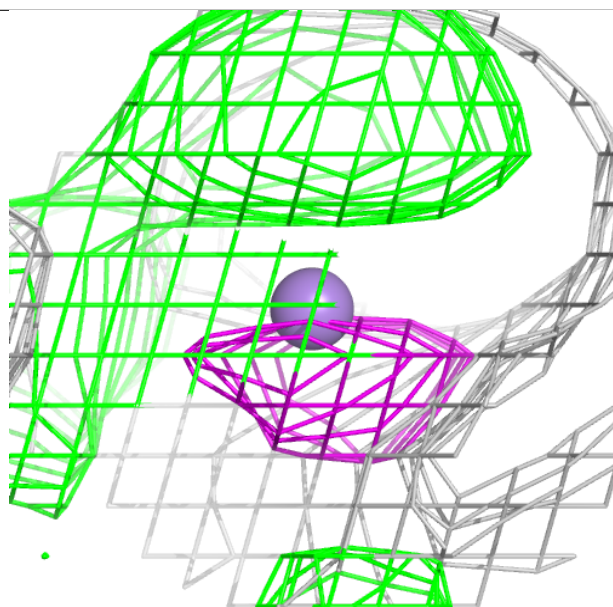
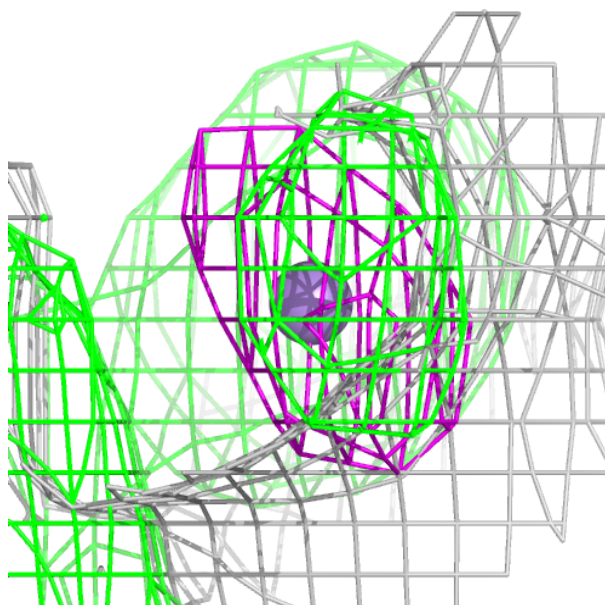
Electron density around MN B 301:

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



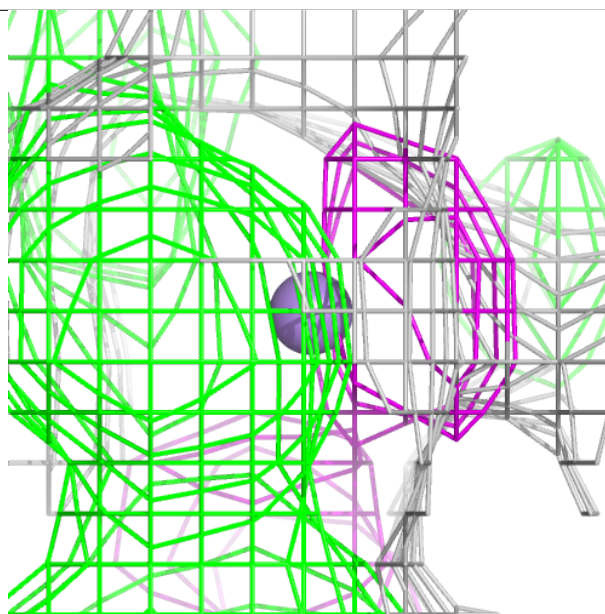
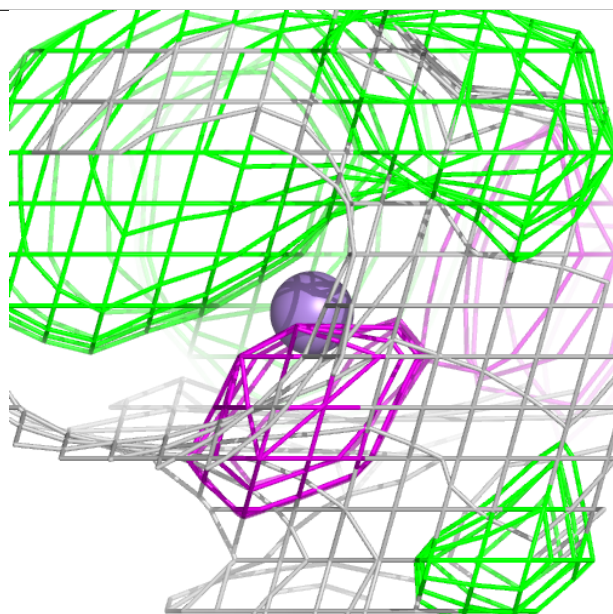
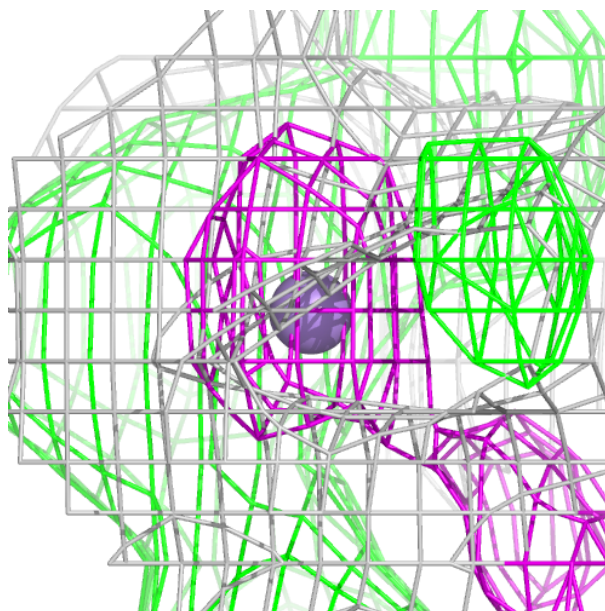
Electron density around MN F 302:

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



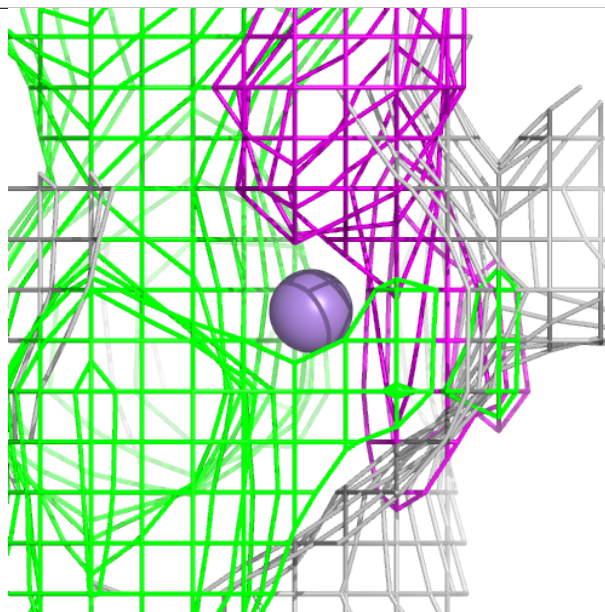
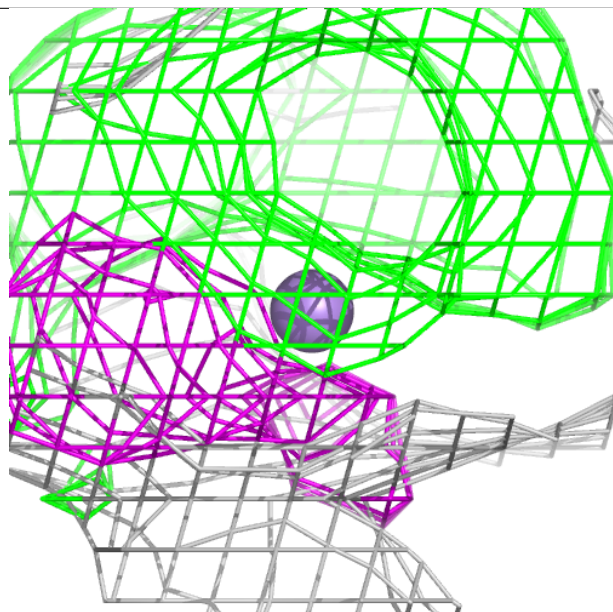
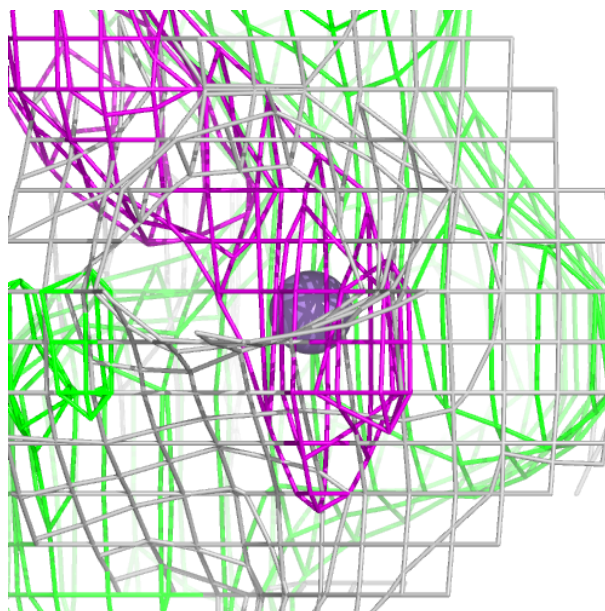
Electron density around MN D 302:

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



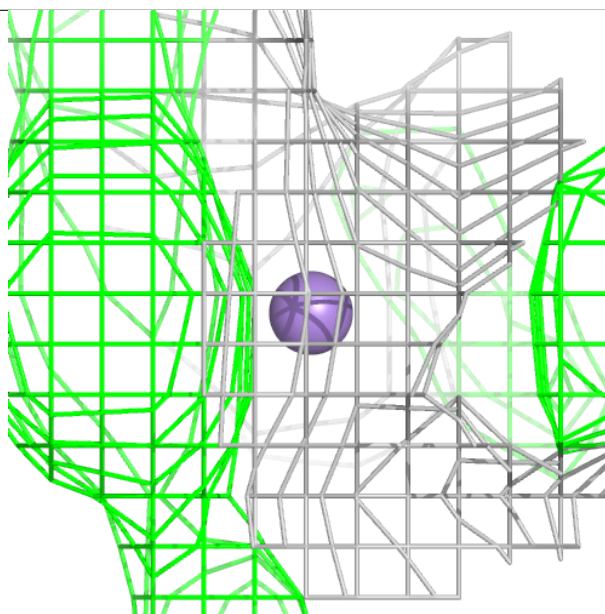
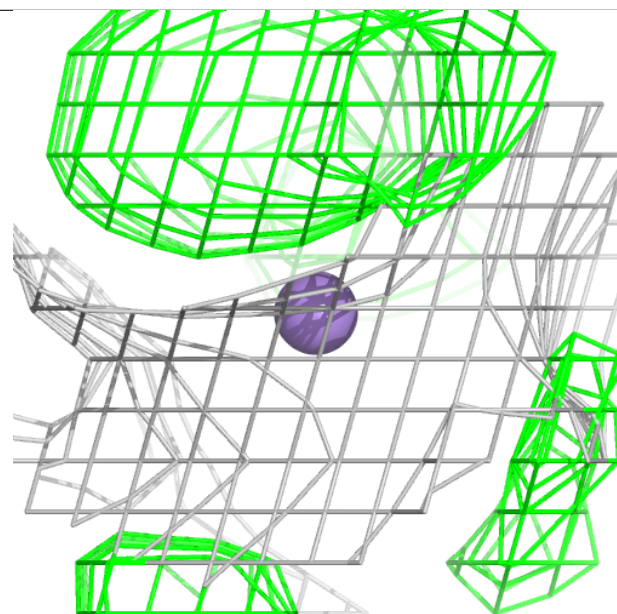
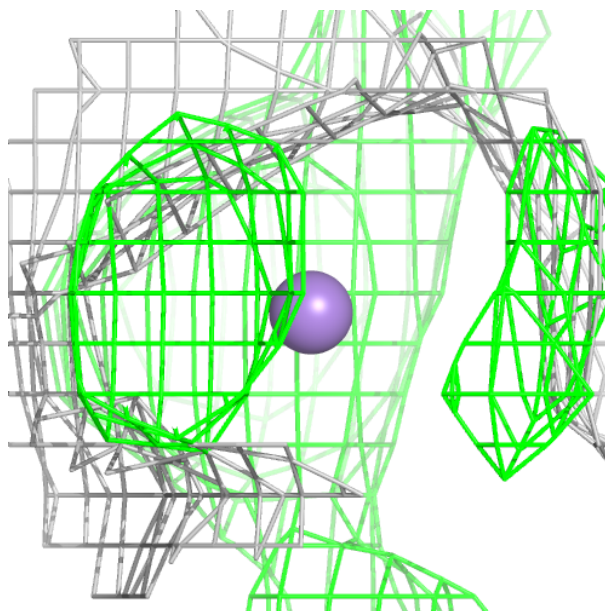
Electron density around MN B 302:

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



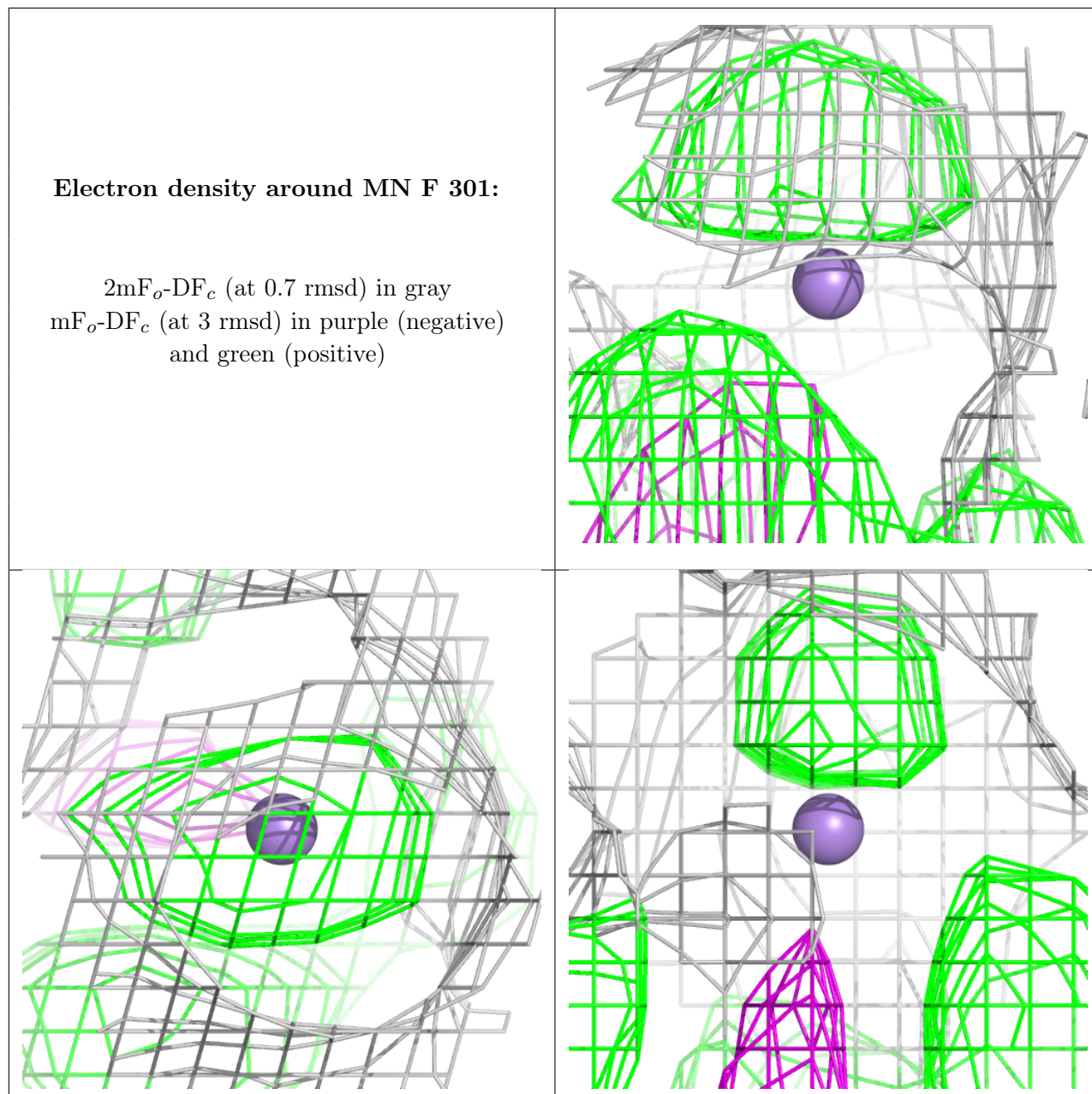
Electron density around MN E 302:

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



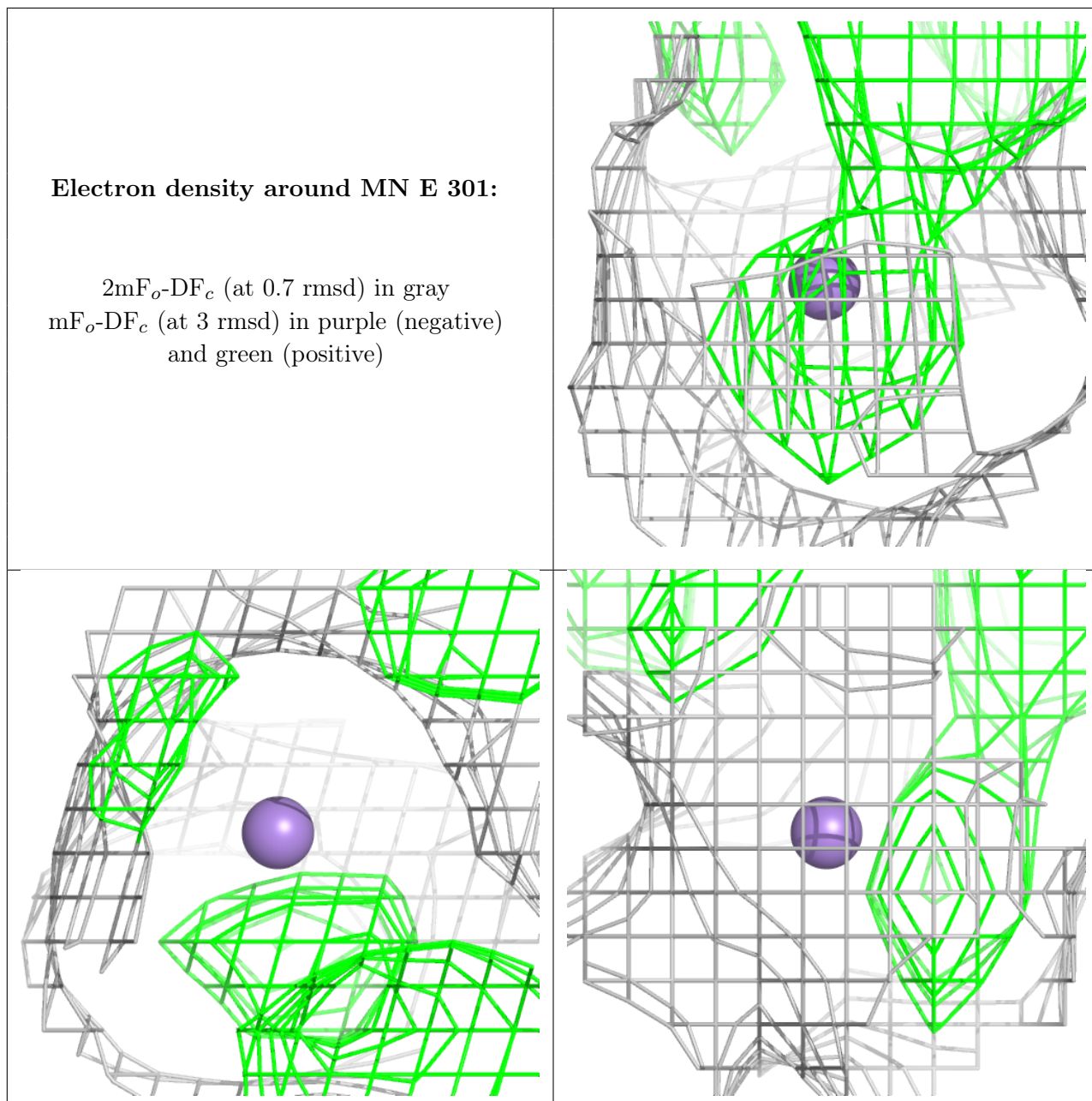
Electron density around MN F 301:

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



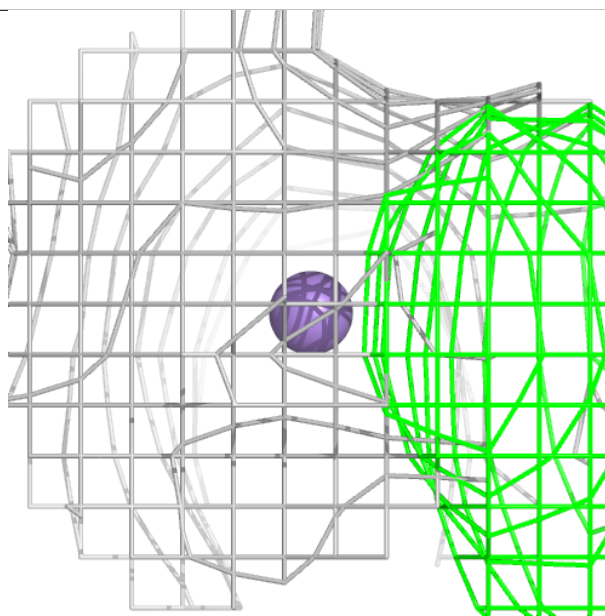
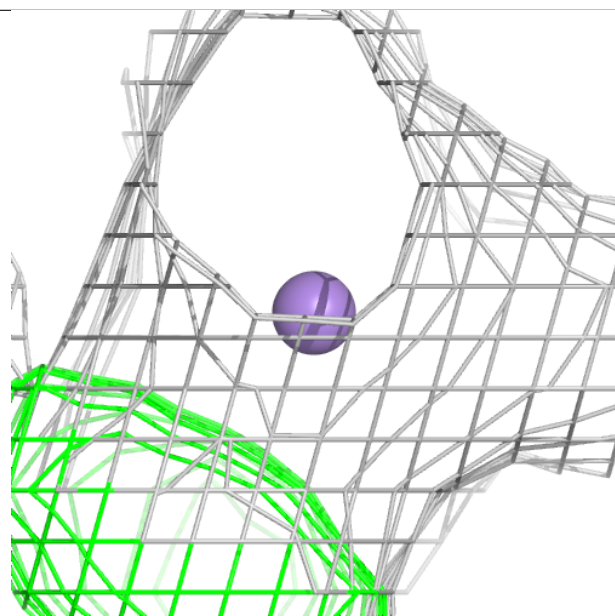
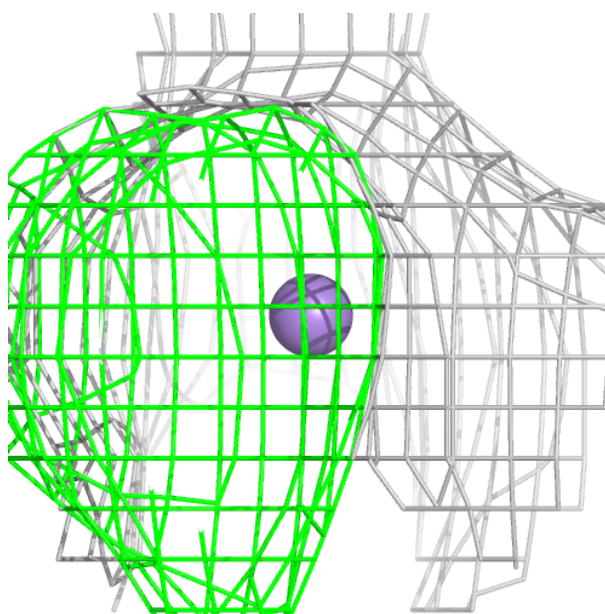
Electron density around MN E 301:

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



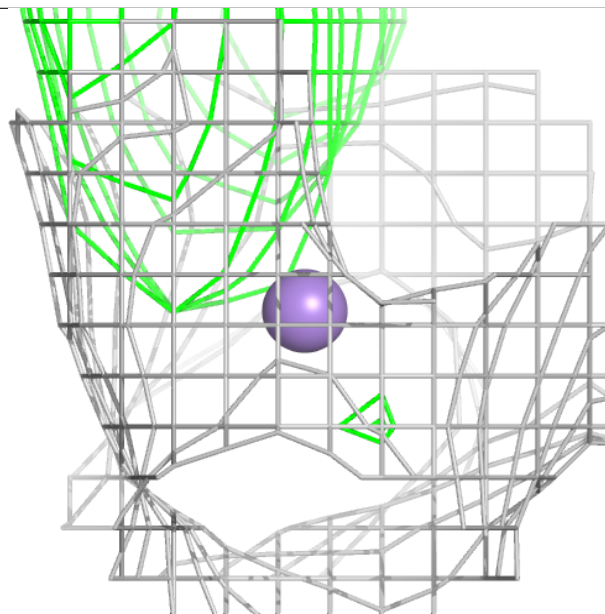
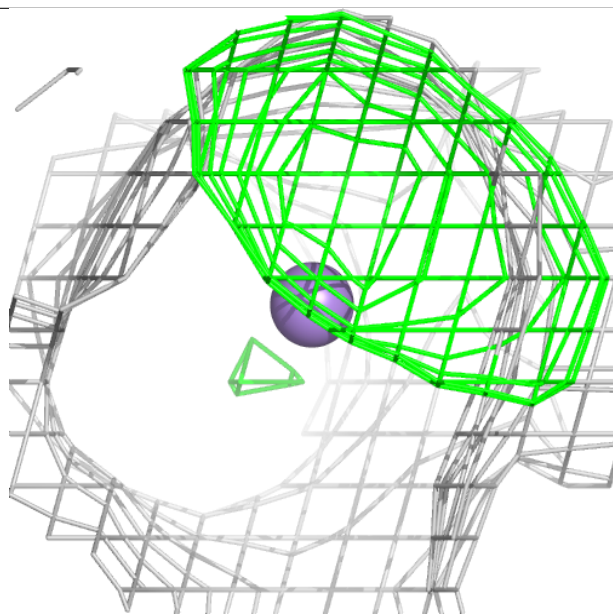
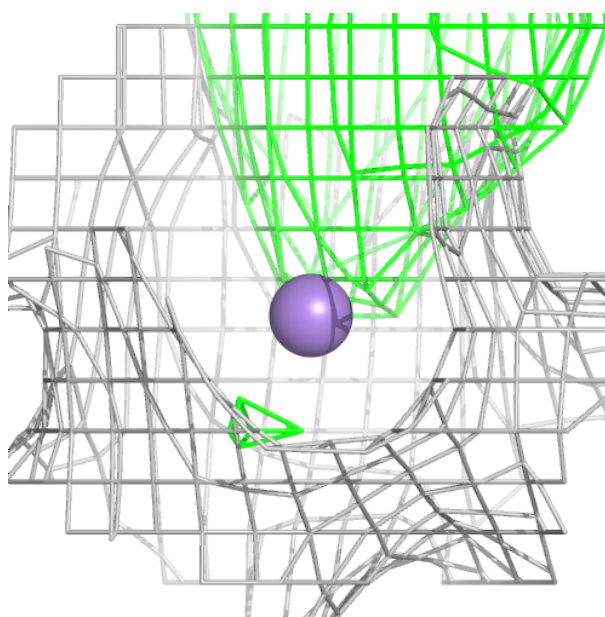
Electron density around MN A 302:

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



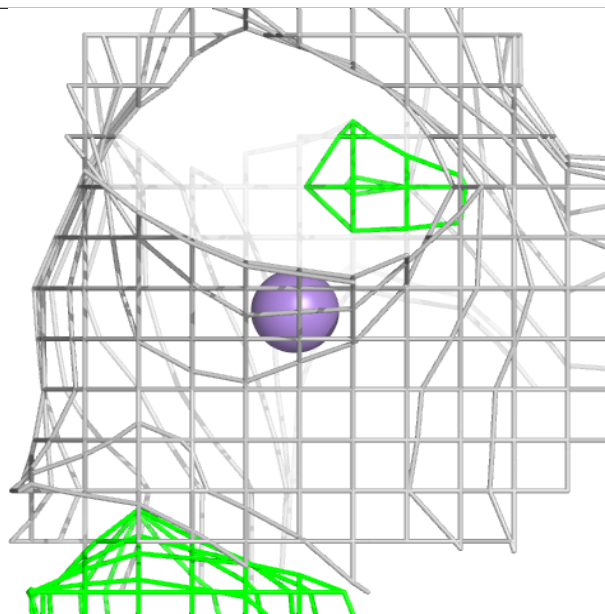
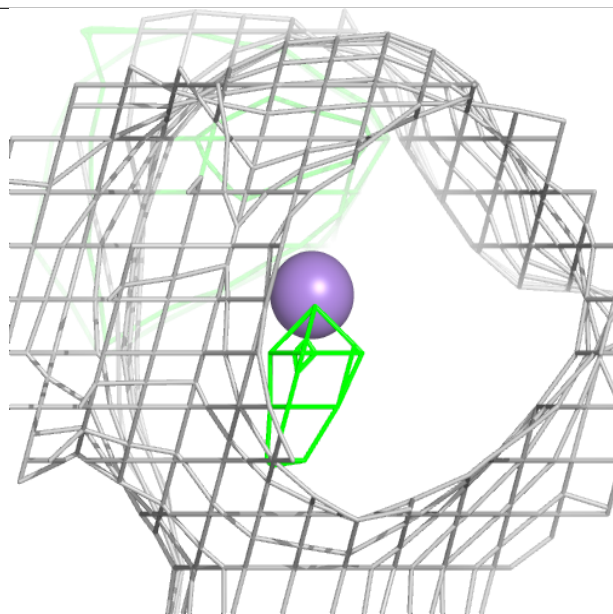
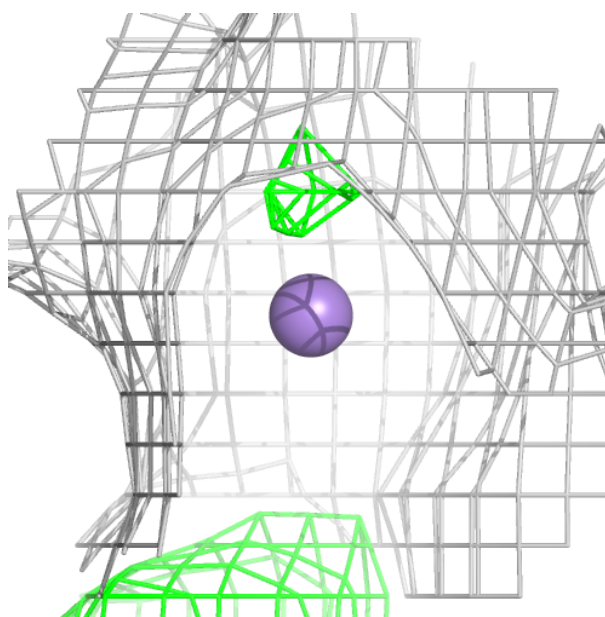
Electron density around MN A 301:

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



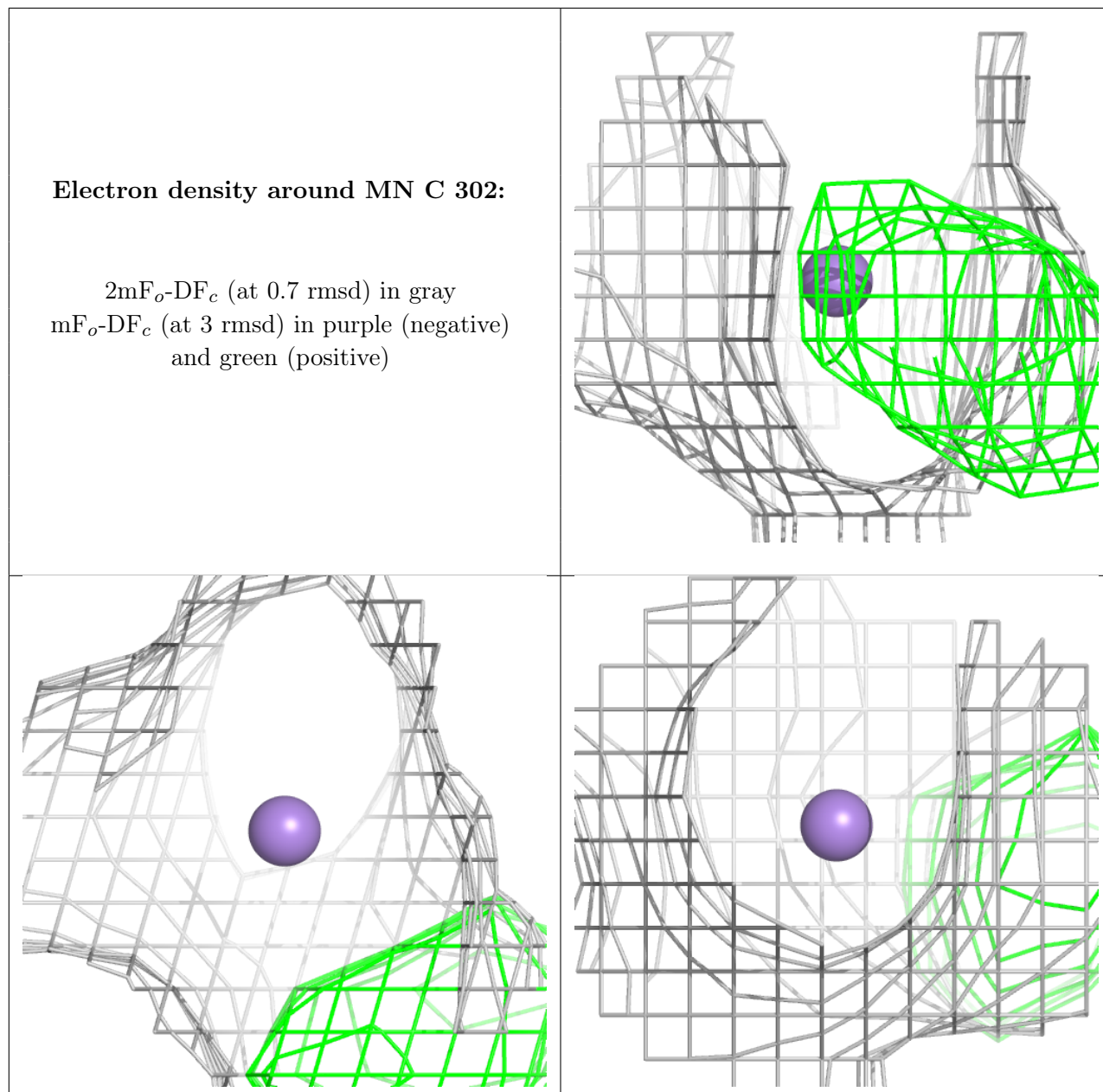
Electron density around MN C 301:

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



Electron density around MN C 302:

$2mF_o-DF_c$ (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.