



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 8HBB / pdb_00008hbb
Title : Crystal structure of Caenorhabditis elegans NMAD-1 in complex with ligand III
Authors : Shang, G.; Chen, Z.
Deposited on : 2022-10-27
Resolution : 3.09 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

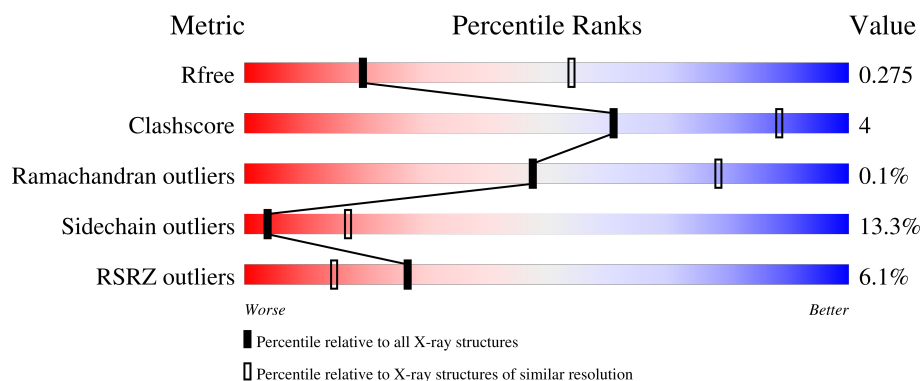
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	286	3% 72% 16% • 11%
1	B	286	5% 71% 16% • 11%
1	C	286	7% 72% 15% • 11%
1	D	286	7% 74% 13% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7693 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 DNA N6-methyl adenine demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1973	1240	341	376	16			
1	B	255	Total	C	N	O	S	0	0	0
			1957	1228	338	375	16			
1	C	254	Total	C	N	O	S	0	0	0
			1882	1182	324	363	13			
1	D	255	Total	C	N	O	S	0	0	0
			1863	1167	323	358	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	HIS	-	expression tag	UNP Q8MNT9
A	7	HIS	-	expression tag	UNP Q8MNT9
A	8	HIS	-	expression tag	UNP Q8MNT9
A	9	HIS	-	expression tag	UNP Q8MNT9
A	10	HIS	-	expression tag	UNP Q8MNT9
A	11	HIS	-	expression tag	UNP Q8MNT9
A	12	GLU	-	expression tag	UNP Q8MNT9
A	13	ASN	-	expression tag	UNP Q8MNT9
A	14	LEU	-	expression tag	UNP Q8MNT9
A	15	TYR	-	expression tag	UNP Q8MNT9
A	16	PHE	-	expression tag	UNP Q8MNT9
A	17	GLN	-	expression tag	UNP Q8MNT9
A	18	GLY	-	expression tag	UNP Q8MNT9
A	19	SER	-	expression tag	UNP Q8MNT9
A	20	MET	-	expression tag	UNP Q8MNT9
A	109	LYS	GLU	engineered mutation	UNP Q8MNT9
A	112	LYS	GLN	engineered mutation	UNP Q8MNT9
A	114	LYS	GLN	engineered mutation	UNP Q8MNT9
B	6	HIS	-	expression tag	UNP Q8MNT9
B	7	HIS	-	expression tag	UNP Q8MNT9
B	8	HIS	-	expression tag	UNP Q8MNT9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	expression tag	UNP Q8MNT9
B	10	HIS	-	expression tag	UNP Q8MNT9
B	11	HIS	-	expression tag	UNP Q8MNT9
B	12	GLU	-	expression tag	UNP Q8MNT9
B	13	ASN	-	expression tag	UNP Q8MNT9
B	14	LEU	-	expression tag	UNP Q8MNT9
B	15	TYR	-	expression tag	UNP Q8MNT9
B	16	PHE	-	expression tag	UNP Q8MNT9
B	17	GLN	-	expression tag	UNP Q8MNT9
B	18	GLY	-	expression tag	UNP Q8MNT9
B	19	SER	-	expression tag	UNP Q8MNT9
B	20	MET	-	expression tag	UNP Q8MNT9
B	109	LYS	GLU	engineered mutation	UNP Q8MNT9
B	112	LYS	GLN	engineered mutation	UNP Q8MNT9
B	114	LYS	GLN	engineered mutation	UNP Q8MNT9
C	6	HIS	-	expression tag	UNP Q8MNT9
C	7	HIS	-	expression tag	UNP Q8MNT9
C	8	HIS	-	expression tag	UNP Q8MNT9
C	9	HIS	-	expression tag	UNP Q8MNT9
C	10	HIS	-	expression tag	UNP Q8MNT9
C	11	HIS	-	expression tag	UNP Q8MNT9
C	12	GLU	-	expression tag	UNP Q8MNT9
C	13	ASN	-	expression tag	UNP Q8MNT9
C	14	LEU	-	expression tag	UNP Q8MNT9
C	15	TYR	-	expression tag	UNP Q8MNT9
C	16	PHE	-	expression tag	UNP Q8MNT9
C	17	GLN	-	expression tag	UNP Q8MNT9
C	18	GLY	-	expression tag	UNP Q8MNT9
C	19	SER	-	expression tag	UNP Q8MNT9
C	20	MET	-	expression tag	UNP Q8MNT9
C	109	LYS	GLU	engineered mutation	UNP Q8MNT9
C	112	LYS	GLN	engineered mutation	UNP Q8MNT9
C	114	LYS	GLN	engineered mutation	UNP Q8MNT9
D	6	HIS	-	expression tag	UNP Q8MNT9
D	7	HIS	-	expression tag	UNP Q8MNT9
D	8	HIS	-	expression tag	UNP Q8MNT9
D	9	HIS	-	expression tag	UNP Q8MNT9
D	10	HIS	-	expression tag	UNP Q8MNT9
D	11	HIS	-	expression tag	UNP Q8MNT9
D	12	GLU	-	expression tag	UNP Q8MNT9
D	13	ASN	-	expression tag	UNP Q8MNT9
D	14	LEU	-	expression tag	UNP Q8MNT9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	15	TYR	-	expression tag	UNP Q8MNT9
D	16	PHE	-	expression tag	UNP Q8MNT9
D	17	GLN	-	expression tag	UNP Q8MNT9
D	18	GLY	-	expression tag	UNP Q8MNT9
D	19	SER	-	expression tag	UNP Q8MNT9
D	20	MET	-	expression tag	UNP Q8MNT9
D	109	LYS	GLU	engineered mutation	UNP Q8MNT9
D	112	LYS	GLN	engineered mutation	UNP Q8MNT9
D	114	LYS	GLN	engineered mutation	UNP Q8MNT9

- 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	1	Total Mn 1 1	0	0
2	B	2	Total Mn 2 2	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	C	2	Total O 2 2	0	0

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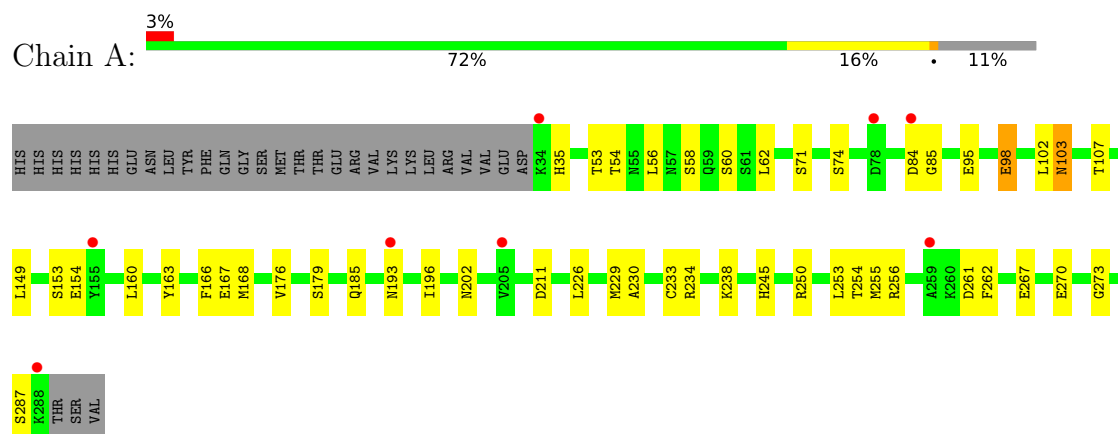
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total	O	0	0
			4	4		

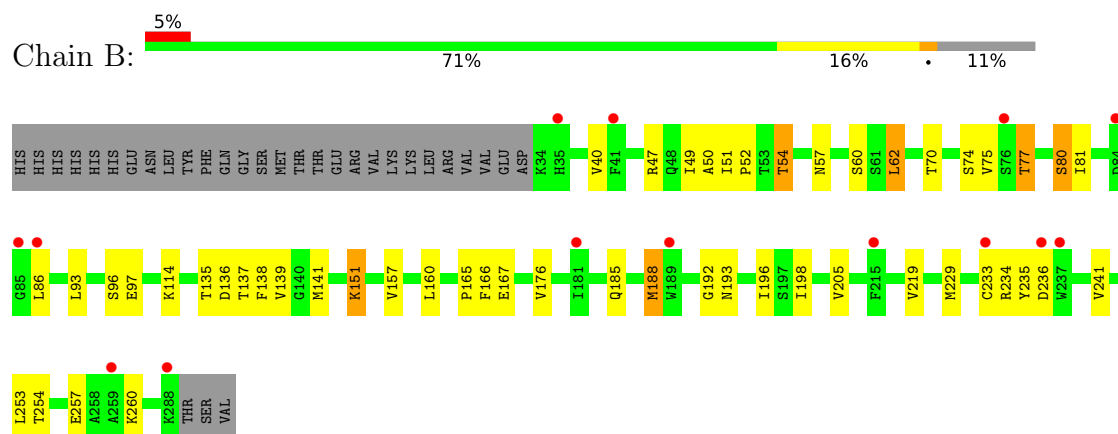
3 Residue-property plots [i](#)

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.

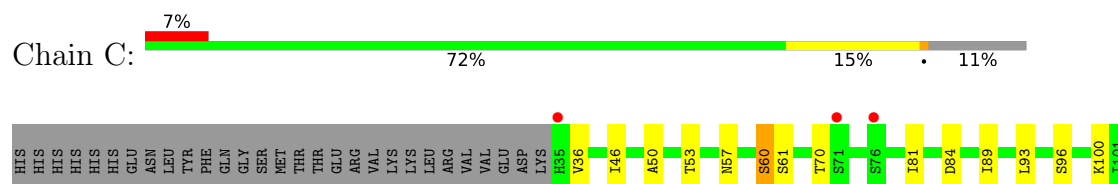
- Molecule 1: DNA N6-methyl adenine demethylase

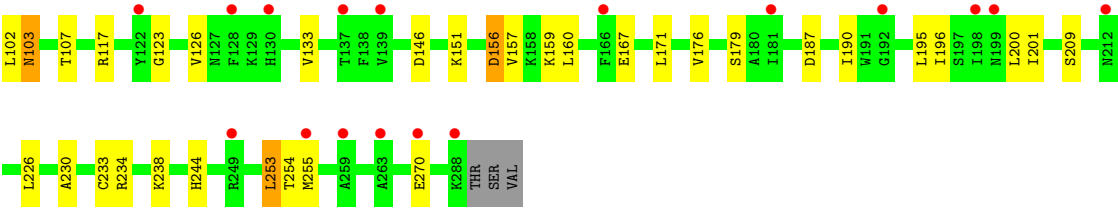


- Molecule 1: DNA N6-methyl adenine demethylase

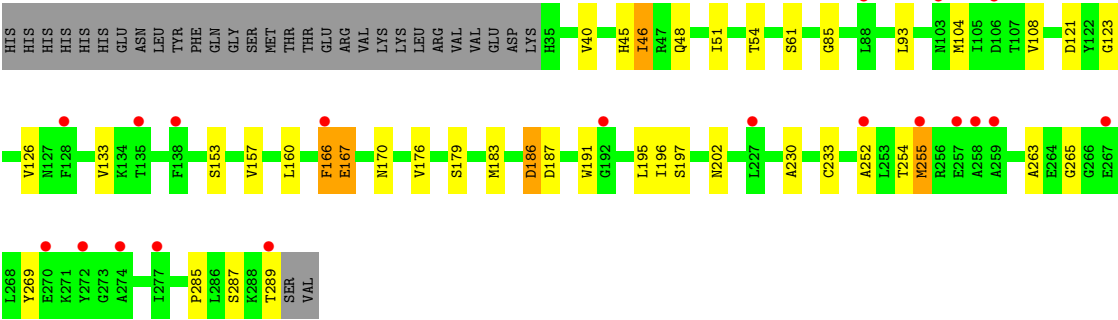


- Molecule 1: DNA N6-methyl adenine demethylase





● Molecule 1: DNA N6-methyl adenine demethylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.18Å 75.33Å 118.18Å 90.00° 113.19° 90.00°	Depositor
Resolution (Å)	47.18 – 3.09 47.18 – 3.09	Depositor EDS
% Data completeness (in resolution range)	67.8 (47.18-3.09) 81.1 (47.18-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.63 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.260 , 0.282 0.269 , 0.275	Depositor DCC
R_{free} test set	1125 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7693	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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: CL, 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	0.86	0/2013	1.26	0/2727
1	B	0.87	0/1996	1.28	1/2705 (0.0%)
1	C	0.87	0/1917	1.25	0/2606
1	D	0.89	0/1901	1.29	2/2592 (0.1%)
All	All	0.87	0/7827	1.27	3/10630 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	THR	N-CA-C	-5.25	106.92	113.38
1	D	285	PRO	CB-CA-C	-5.25	106.62	111.40
1	D	265	GLY	N-CA-C	-5.13	108.53	115.36

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	1973	0	1851	14	2
1	B	1957	0	1814	19	1
1	C	1882	0	1714	16	0
1	D	1863	0	1640	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	3	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
All	All	7693	0	7019	61	2

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 (61) 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:D:123:GLY:HA3	1:D:167:GLU:HG2	1.69	0.74
1:C:123:GLY:HA3	1:C:167:GLU:HG3	1.83	0.60
1:B:141:MET:HE3	1:B:165:PRO:HB2	1.83	0.59
1:A:103:ASN:O	1:A:107:THR:HG23	2.02	0.58
1:C:156:ASP:HB3	1:C:159:LYS:HB2	1.86	0.58
1:B:188:MET:HB3	1:B:235:TYR:HE1	1.68	0.57
1:B:50:ALA:HB3	1:B:81:ILE:HG13	1.91	0.53
1:C:126:VAL:HG22	1:C:133:VAL:HG13	1.90	0.53
1:B:192:GLY:HA3	1:B:257:GLU:HG3	1.91	0.52
1:C:89:ILE:HD12	1:C:226:LEU:HD22	1.91	0.52
1:C:107:THR:HG22	1:D:202:ASN:HD21	1.75	0.51
1:C:126:VAL:HG13	1:C:133:VAL:HG22	1.92	0.51
1:C:230:ALA:HA	1:C:234:ARG:HB2	1.92	0.51
1:D:263:ALA:O	1:D:269:TYR:HB2	2.10	0.51
1:A:98:GLU:HG3	1:A:102:LEU:HD12	1.92	0.51
1:A:193:ASN:O	1:A:234:ARG:HD3	2.11	0.50
1:C:103:ASN:O	1:C:107:THR:HG23	2.11	0.50
1:B:49:ILE:HD12	1:B:80:SER:HB2	1.94	0.50
1:C:57:ASN:H	1:C:60:SER:HB2	1.77	0.49
1:D:170:ASN:HA	1:D:252:ALA:O	2.12	0.49
1:B:93:LEU:HD22	1:B:97:GLU:HB3	1.94	0.48
1:C:126:VAL:HG21	1:C:190:ILE:HD13	1.95	0.48
1:A:262:PHE:O	1:A:273:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:HB3	1:A:256:ARG:HG3	1.96	0.48
1:B:47:ARG:HB3	1:B:49:ILE:HG12	1.94	0.48
1:B:193:ASN:O	1:B:234:ARG:HD3	2.13	0.48
1:D:186:ASP:HB2	1:D:195:LEU:HD11	1.95	0.47
1:A:185:GLN:HG2	1:A:238:LYS:HG2	1.95	0.47
1:B:77:THR:O	1:B:80:SER:HB3	2.15	0.47
1:B:86:LEU:HD21	1:B:219:VAL:HG21	1.95	0.47
1:B:62:LEU:HD12	1:B:205:VAL:HG23	1.96	0.46
1:A:168:MET:HE3	1:A:168:MET:HB2	1.75	0.46
1:D:255:MET:HE3	1:D:255:MET:HB2	1.73	0.45
1:D:126:VAL:HG13	1:D:133:VAL:HG22	1.98	0.45
1:A:196:ILE:HB	1:A:255:MET:HB2	1.98	0.45
1:D:104:MET:O	1:D:108:VAL:HG23	2.16	0.45
1:B:229:MET:HE3	1:B:229:MET:HB2	1.68	0.44
1:A:202:ASN:O	1:A:250:ARG:HG3	2.18	0.44
1:D:187:ASP:O	1:D:191:TRP:HB2	2.18	0.44
1:D:85:GLY:HA3	1:D:230:ALA:O	2.18	0.43
1:B:47:ARG:HH11	1:B:49:ILE:HD11	1.82	0.43
1:C:102:LEU:HD23	1:C:102:LEU:HA	1.92	0.43
1:B:138:PHE:HZ	1:B:141:MET:HE2	1.84	0.43
1:C:93:LEU:HD23	1:C:151:LYS:HE2	2.01	0.43
1:C:50:ALA:HB3	1:C:81:ILE:HG13	2.00	0.43
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.88	0.43
1:C:117:ARG:HH11	1:C:171:LEU:HD22	1.84	0.43
1:A:149:LEU:HD22	1:A:163:TYR:HB3	2.02	0.42
1:B:51:ILE:HA	1:B:52:PRO:HD3	1.93	0.42
1:B:114:LYS:H	1:B:114:LYS:HG2	1.47	0.42
1:B:138:PHE:CZ	1:B:141:MET:HE2	2.55	0.42
1:B:151:LYS:HB2	1:B:151:LYS:HE3	1.88	0.42
1:A:85:GLY:HA3	1:A:230:ALA:O	2.20	0.41
1:C:200:LEU:HD11	1:C:253:LEU:HD12	2.02	0.41
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.87	0.41
1:B:188:MET:H	1:B:188:MET:HG2	1.49	0.41
1:A:229:MET:HB2	1:A:229:MET:HE3	1.77	0.41
1:A:62:LEU:HB2	1:A:245:HIS:HA	2.03	0.41
1:D:166:PHE:HB3	1:D:191:TRP:HZ3	1.86	0.41
1:C:187:ASP:OD1	1:C:190:ILE:HG22	2.22	0.40
1:D:46:ILE:H	1:D:46:ILE:HG12	1.71	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:OE1	1:B:236:ASP:OD2[1_565]	1.69	0.51
1:A:154:GLU:OE1	1:D:45:HIS:NE2[4_545]	2.15	0.05

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	253/286 (88%)	250 (99%)	3 (1%)	0	100	100
1	B	253/286 (88%)	249 (98%)	4 (2%)	0	100	100
1	C	252/286 (88%)	246 (98%)	5 (2%)	1 (0%)	30	61
1	D	253/286 (88%)	246 (97%)	7 (3%)	0	100	100
All	All	1011/1144 (88%)	991 (98%)	19 (2%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/260 (80%)	183 (88%)	24 (12%)	5	22
1	B	202/260 (78%)	172 (85%)	30 (15%)	3	13
1	C	187/260 (72%)	161 (86%)	26 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	180/260 (69%)	157 (87%)	23 (13%)	4	18
All	All	776/1040 (75%)	673 (87%)	103 (13%)	4	17

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	53	THR
1	A	54	THR
1	A	58	SER
1	A	60	SER
1	A	71	SER
1	A	74	SER
1	A	84	ASP
1	A	95	GLU
1	A	98	GLU
1	A	103	ASN
1	A	153	SER
1	A	160	LEU
1	A	166	PHE
1	A	176	VAL
1	A	179	SER
1	A	211	ASP
1	A	226	LEU
1	A	233	CYS
1	A	253	LEU
1	A	254	THR
1	A	261	ASP
1	A	267	GLU
1	A	287	SER
1	B	40	VAL
1	B	54	THR
1	B	57	ASN
1	B	60	SER
1	B	62	LEU
1	B	70	THR
1	B	74	SER
1	B	75	VAL
1	B	77	THR
1	B	80	SER
1	B	96	SER
1	B	135	THR

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Mol	Chain	Res	Type
1	B	136	ASP
1	B	137	THR
1	B	139	VAL
1	B	151	LYS
1	B	157	VAL
1	B	160	LEU
1	B	166	PHE
1	B	167	GLU
1	B	176	VAL
1	B	185	GLN
1	B	188	MET
1	B	196	ILE
1	B	198	ILE
1	B	233	CYS
1	B	241	VAL
1	B	253	LEU
1	B	254	THR
1	B	260	LYS
1	C	36	VAL
1	C	46	ILE
1	C	53	THR
1	C	60	SER
1	C	61	SER
1	C	70	THR
1	C	84	ASP
1	C	96	SER
1	C	100	LYS
1	C	103	ASN
1	C	146	ASP
1	C	156	ASP
1	C	157	VAL
1	C	160	LEU
1	C	176	VAL
1	C	179	SER
1	C	195	LEU
1	C	196	ILE
1	C	209	SER
1	C	233	CYS
1	C	238	LYS
1	C	244	HIS
1	C	253	LEU
1	C	254	THR

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Mol	Chain	Res	Type
1	C	255	MET
1	C	270	GLU
1	D	40	VAL
1	D	46	ILE
1	D	48	GLN
1	D	51	ILE
1	D	54	THR
1	D	61	SER
1	D	121	ASP
1	D	153	SER
1	D	157	VAL
1	D	160	LEU
1	D	166	PHE
1	D	167	GLU
1	D	176	VAL
1	D	179	SER
1	D	183	MET
1	D	186	ASP
1	D	196	ILE
1	D	197	SER
1	D	233	CYS
1	D	254	THR
1	D	255	MET
1	D	287	SER
1	D	289	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	170	ASN
1	A	223	HIS
1	B	223	HIS
1	C	57	ASN
1	C	90	HIS
1	C	91	ASN
1	C	170	ASN
1	C	199	ASN
1	D	202	ASN

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, 9 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	255/286 (89%)	0.55	8 (3%)	51 30	37, 41, 48, 55	0
1	B	255/286 (89%)	0.68	14 (5%)	30 16	40, 45, 51, 61	0
1	C	254/286 (88%)	0.86	20 (7%)	18 10	47, 55, 68, 73	0
1	D	255/286 (89%)	0.87	20 (7%)	19 10	43, 55, 71, 75	0
All	All	1019/1144 (89%)	0.74	62 (6%)	27 15	37, 48, 67, 75	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	288	LYS	4.3
1	B	233	CYS	4.1
1	B	84	ASP	3.5
1	B	288	LYS	3.4
1	B	35	HIS	3.3
1	D	270	GLU	3.1
1	C	255	MET	3.1
1	D	103	ASN	2.9
1	A	193	ASN	2.9
1	A	78	ASP	2.9
1	B	259	ALA	2.8
1	C	128	PHE	2.8
1	D	192	GLY	2.8
1	C	76	SER	2.8
1	C	270	GLU	2.7
1	D	267	GLU	2.6
1	D	135	THR	2.6
1	D	259	ALA	2.6
1	A	34	LYS	2.6
1	C	212	ASN	2.5
1	C	181	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	215	PHE	2.5
1	C	139	VAL	2.5
1	D	128	PHE	2.5
1	C	259	ALA	2.4
1	B	236	ASP	2.4
1	B	181	ILE	2.4
1	C	199	ASN	2.4
1	D	289	THR	2.4
1	C	198	ILE	2.3
1	B	41	PHE	2.3
1	B	85	GLY	2.3
1	C	192	GLY	2.3
1	D	255	MET	2.3
1	D	272	TYR	2.3
1	D	106	ASP	2.3
1	B	237	TRP	2.2
1	D	166	PHE	2.2
1	C	122	TYR	2.2
1	C	249	ARG	2.2
1	D	257	GLU	2.2
1	A	84	ASP	2.2
1	C	166	PHE	2.2
1	B	189	TRP	2.2
1	C	35	HIS	2.2
1	A	205	VAL	2.2
1	D	88	LEU	2.2
1	A	288	LYS	2.2
1	D	274	ALA	2.2
1	C	263	ALA	2.1
1	A	155	TYR	2.1
1	B	76	SER	2.1
1	B	86	LEU	2.1
1	C	137	THR	2.1
1	C	71	SER	2.1
1	C	130	HIS	2.1
1	D	258	ALA	2.1
1	D	252	ALA	2.0
1	D	138	PHE	2.0
1	D	277	ILE	2.0
1	A	259	ALA	2.0
1	D	227	LEU	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](#)

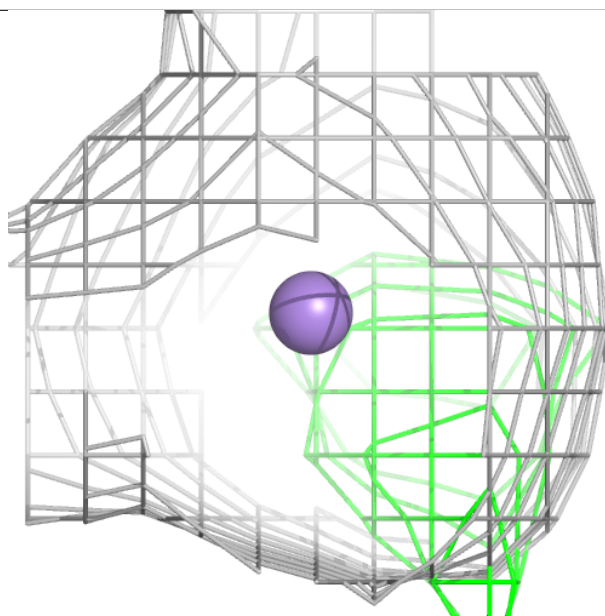
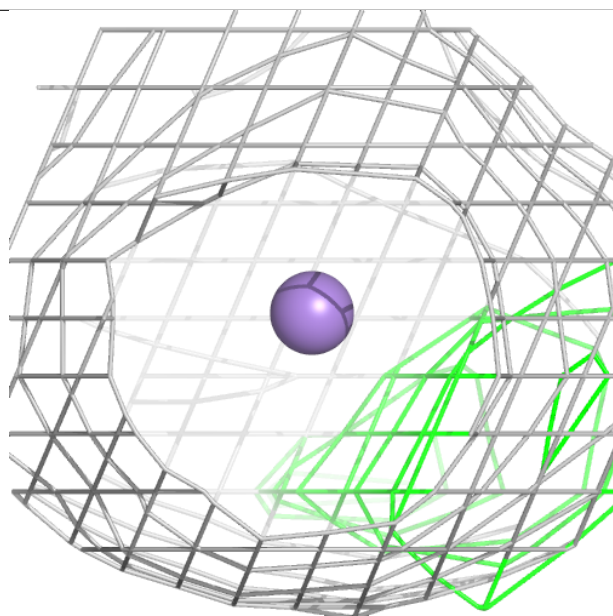
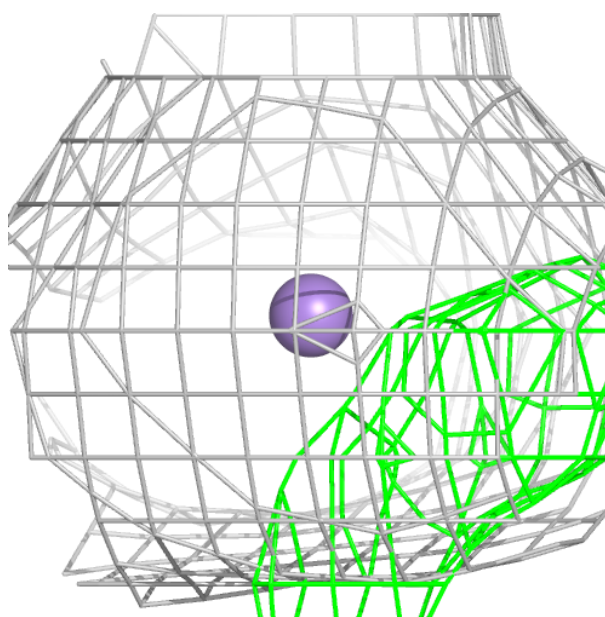
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MN	D	301	1/1	0.87	0.07	57,57,57,57	0
2	MN	C	301	1/1	0.91	0.08	56,56,56,56	0
2	MN	B	301	1/1	0.91	0.07	51,51,51,51	0
3	CL	A	303	1/1	0.91	0.12	37,37,37,37	0
3	CL	B	302	1/1	0.93	0.11	42,42,42,42	0
3	CL	C	302	1/1	0.94	0.13	47,47,47,47	0
2	MN	B	303	1/1	0.95	0.14	49,49,49,49	0
3	CL	A	302	1/1	0.98	0.14	37,37,37,37	0
2	MN	A	301	1/1	0.98	0.07	38,38,38,38	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.

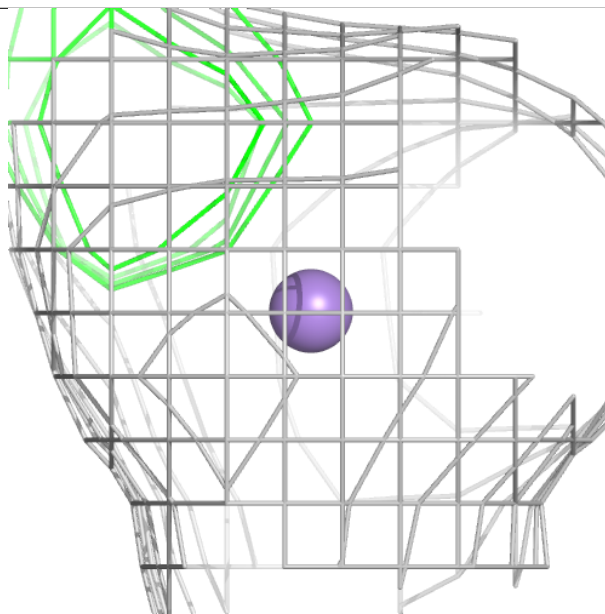
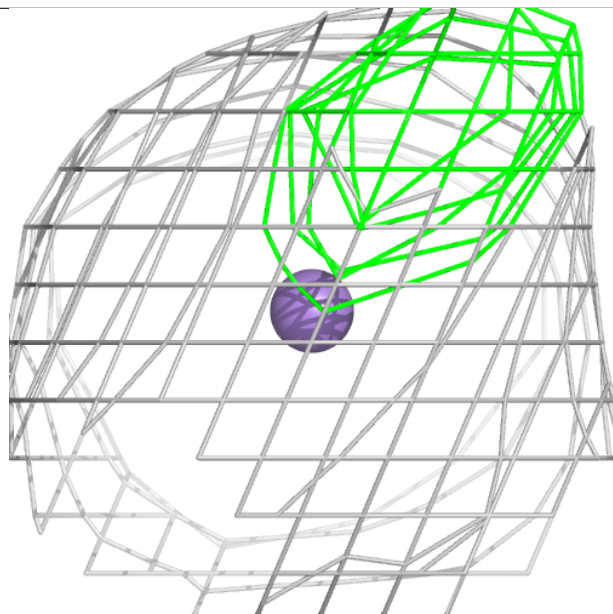
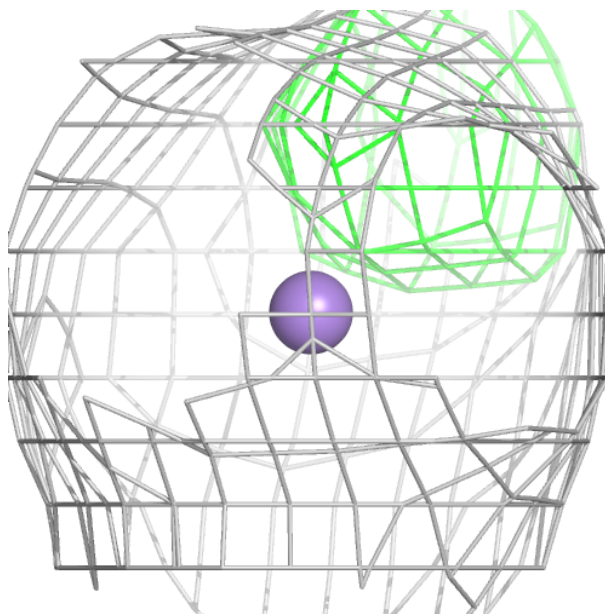
Electron density around MN D 301:

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



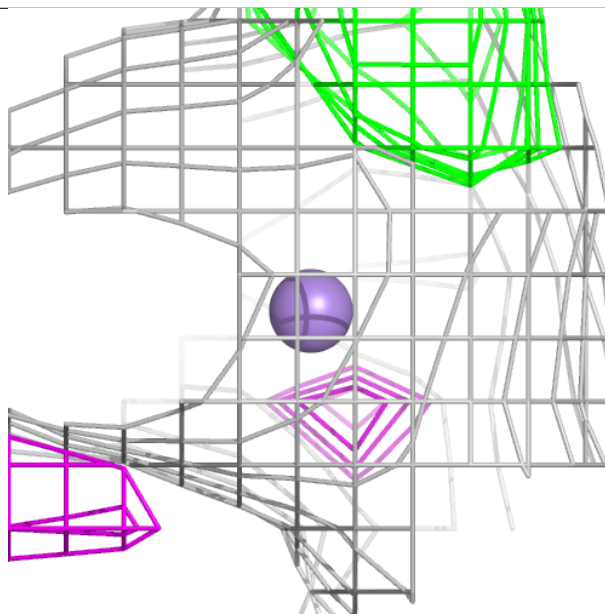
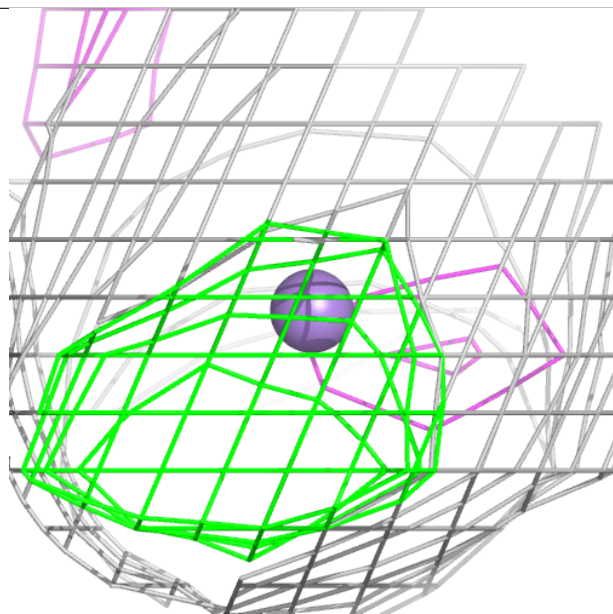
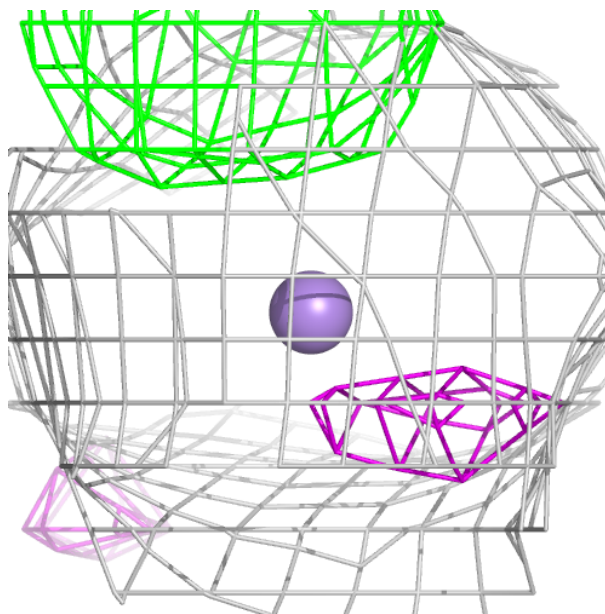
Electron density around MN C 301:

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



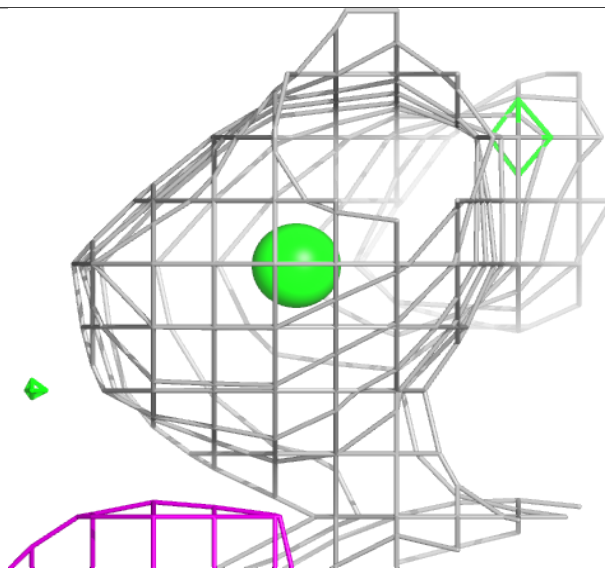
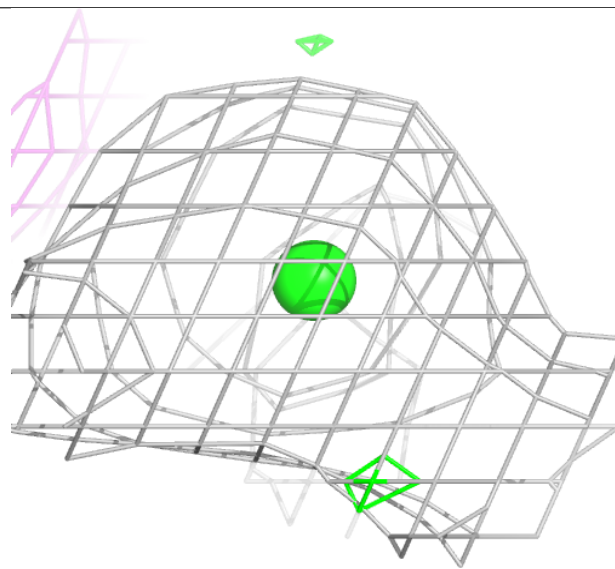
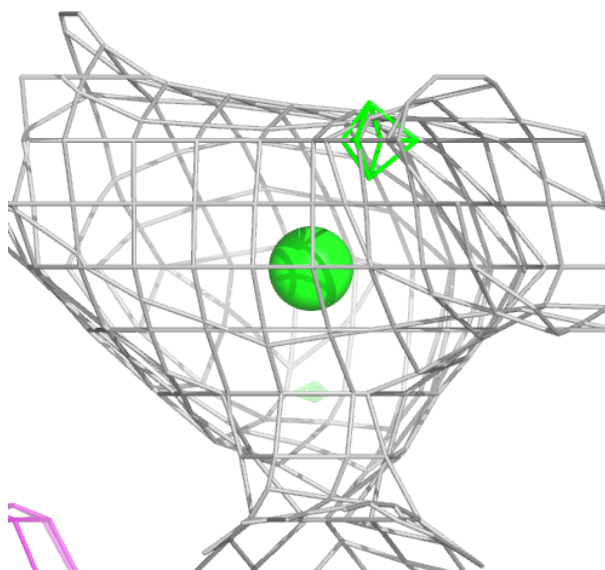
Electron density around MN B 301:

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



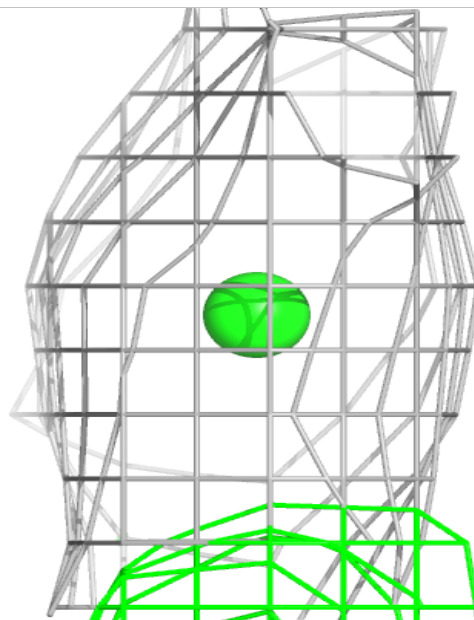
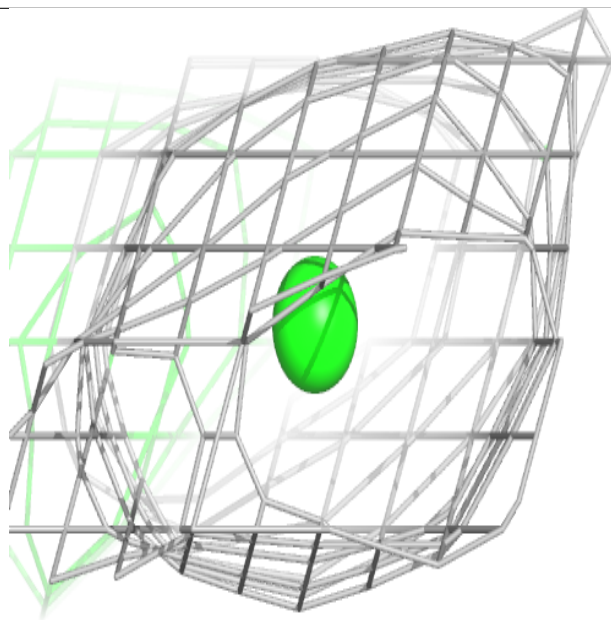
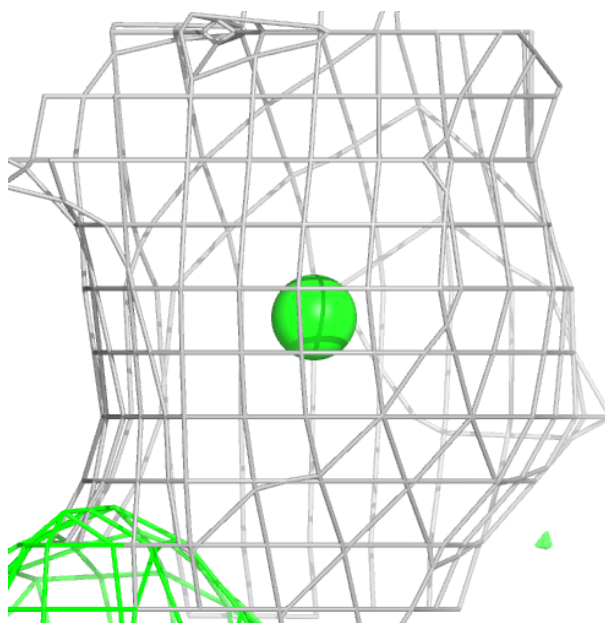
Electron density around CL A 303:

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



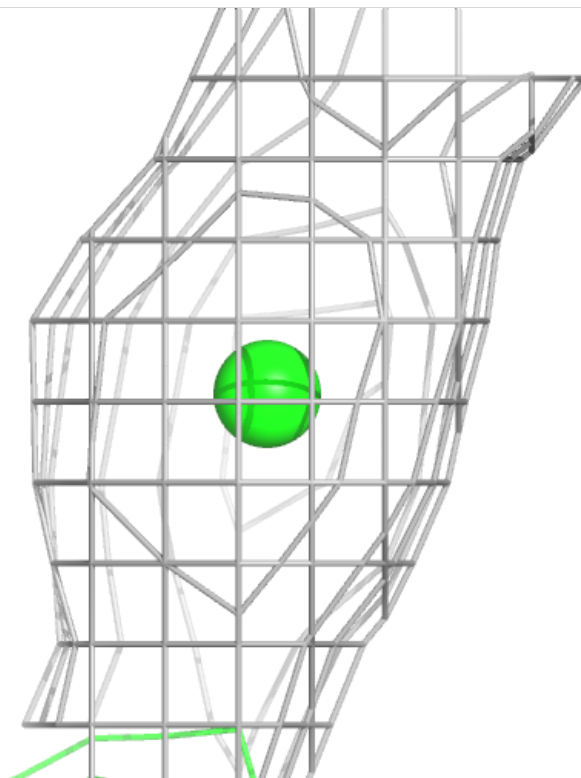
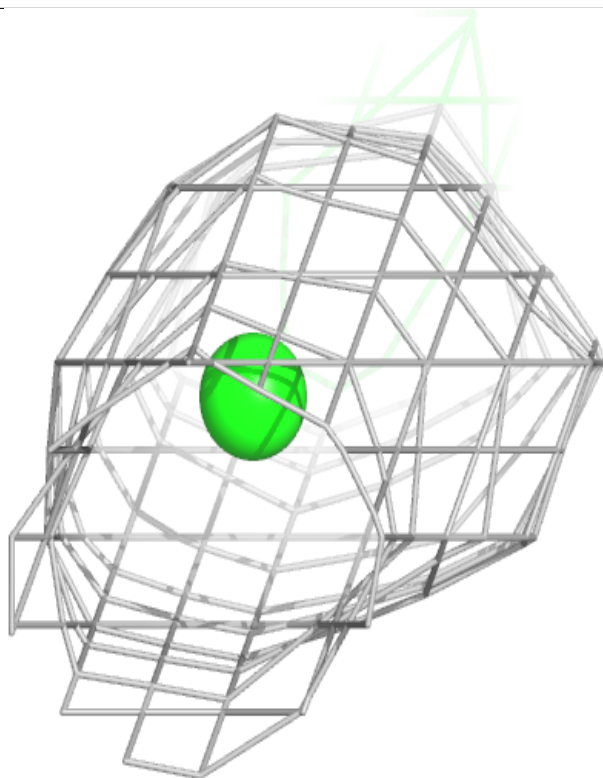
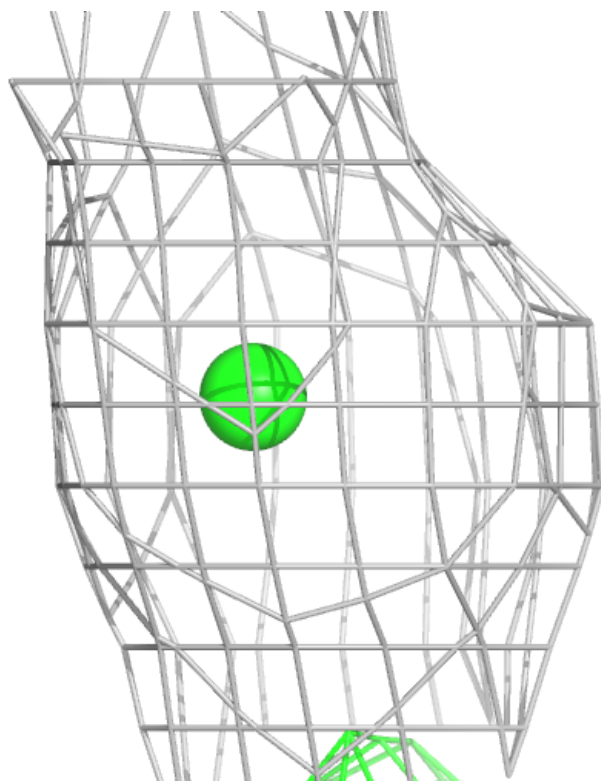
Electron density around CL B 302:

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



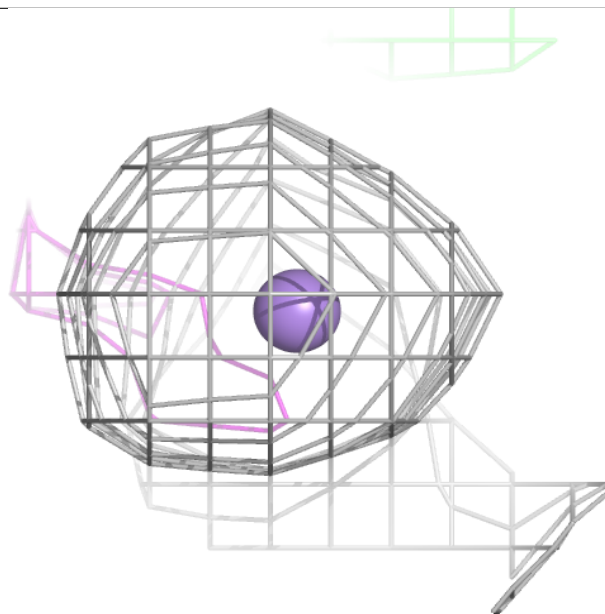
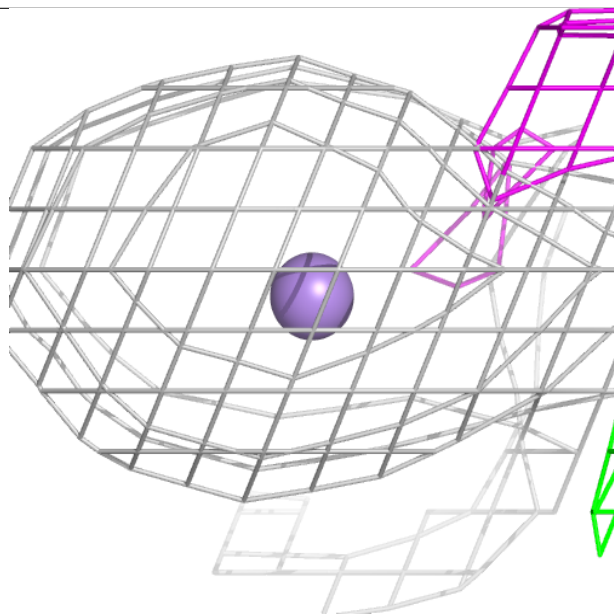
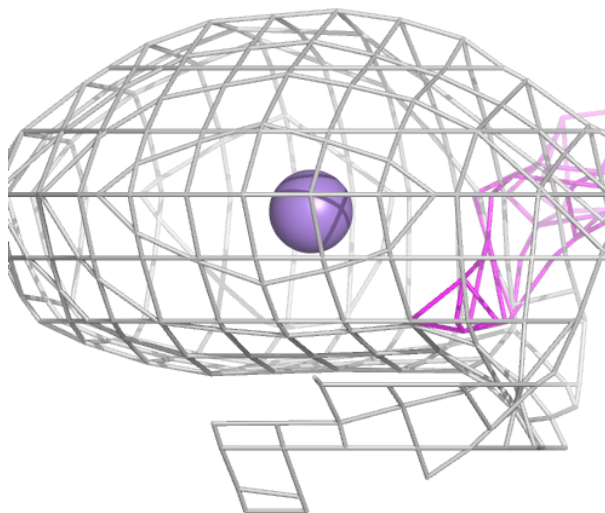
Electron density around CL C 302:

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



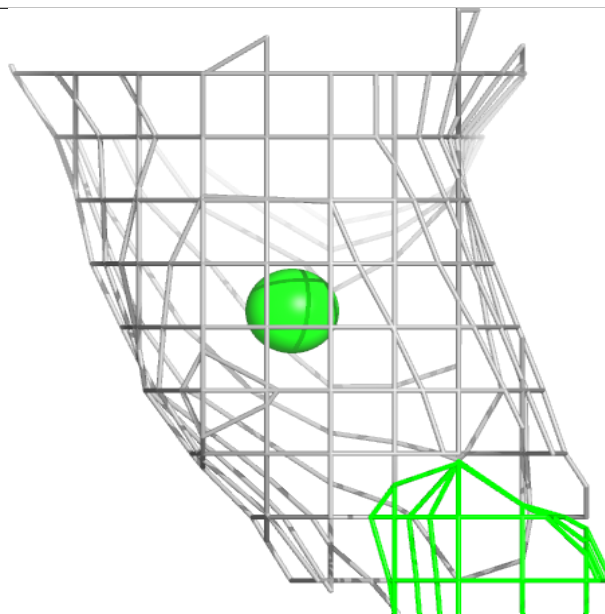
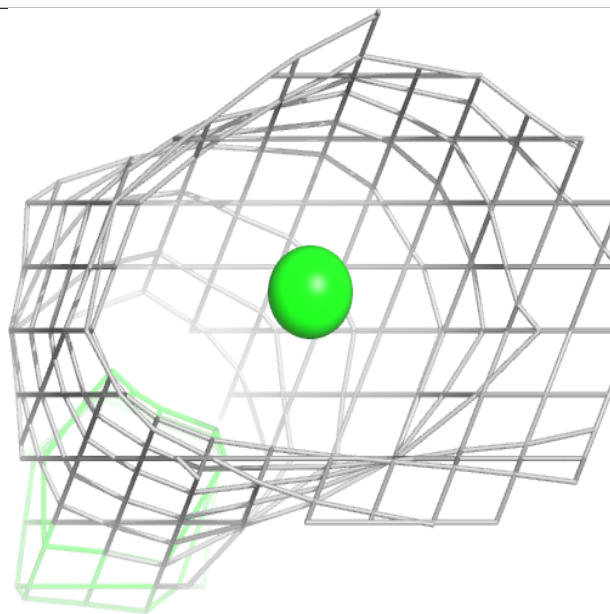
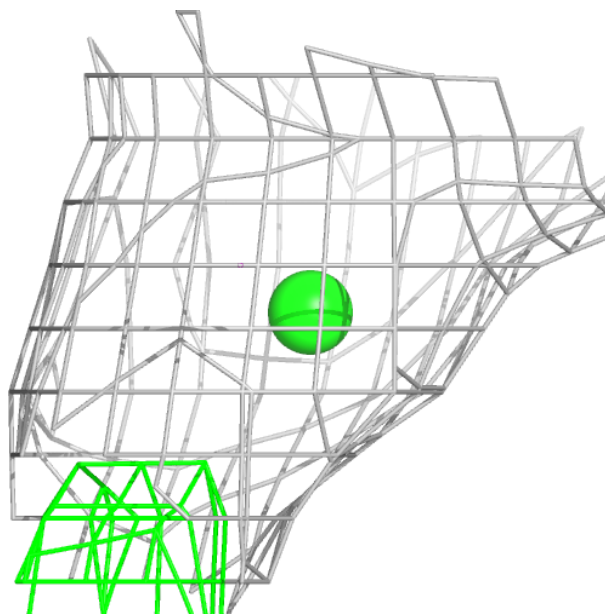
Electron density around MN B 303:

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



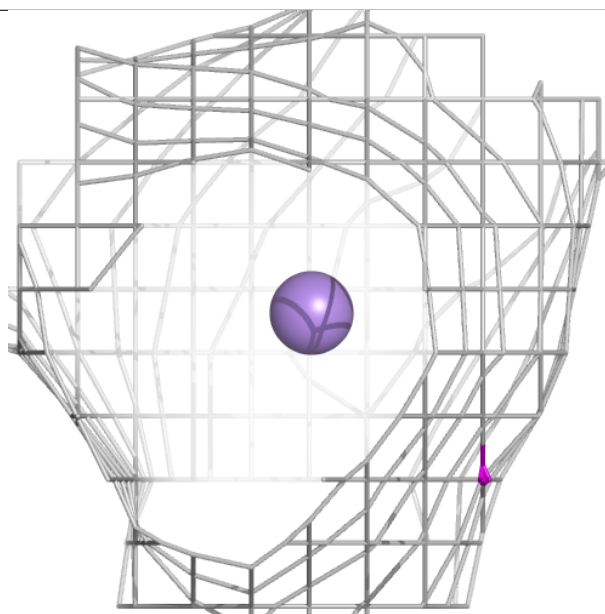
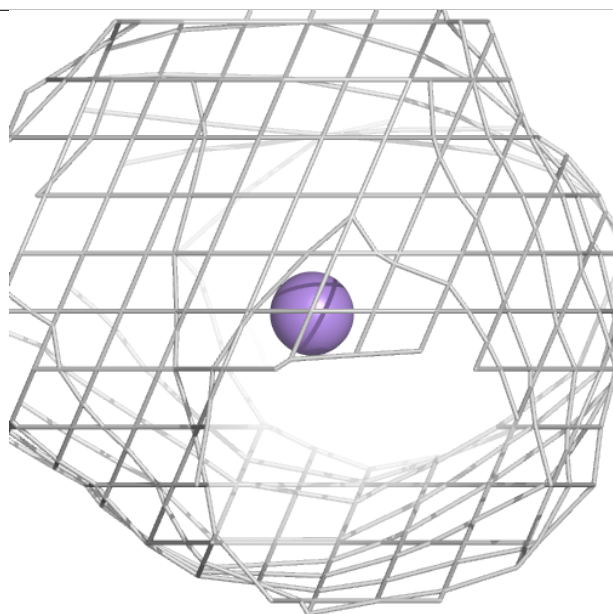
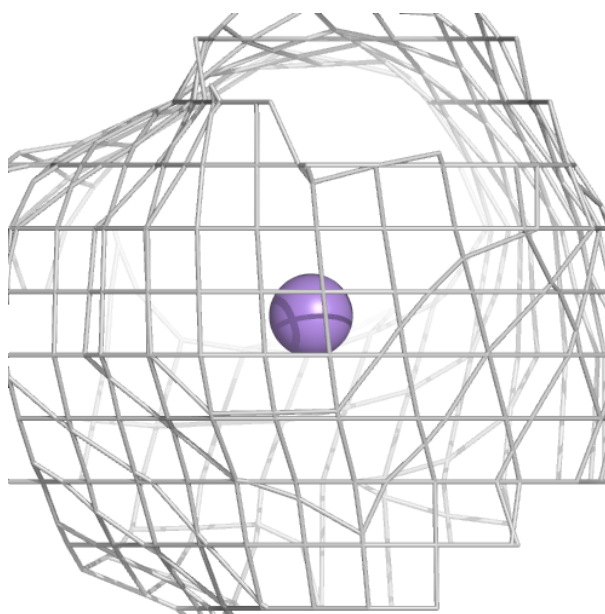
Electron density around CL A 302:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.