



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:21 PM UTC

PDB ID : 6TVV / pdb_00006tvv
Title : Crystal structure of 3'-5' RecJ exonuclease from M. Jannaschii
Authors : De March, M.; Medagli, B.; Krastanova, I.; Saha, I.; Pisani, F.; Onesti, S.
Deposited on : 2020-01-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

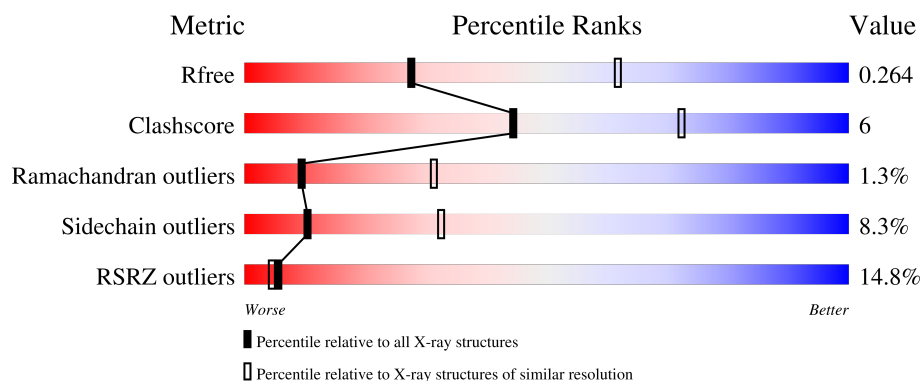
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	432	5% 78% 18% ...
1	B	432	25% 86% 12% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6373 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.

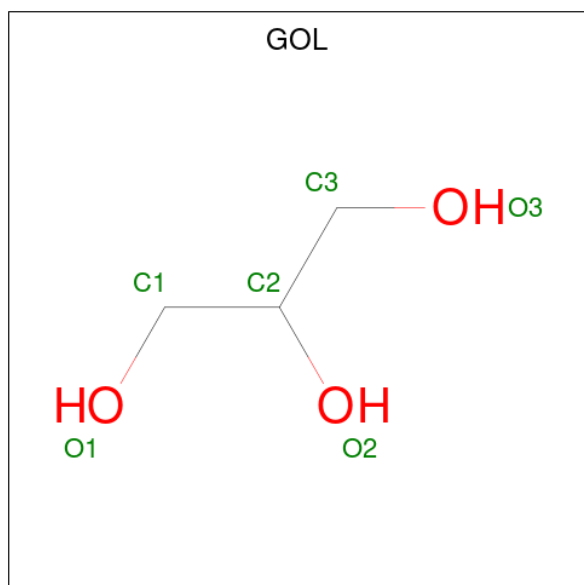
- Molecule 1 is a protein called MjaRecJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3279	2129	541	595	14			
1	B	428	Total	C	N	O	S	0	0	0
			3059	1972	516	558	13			

- 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	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

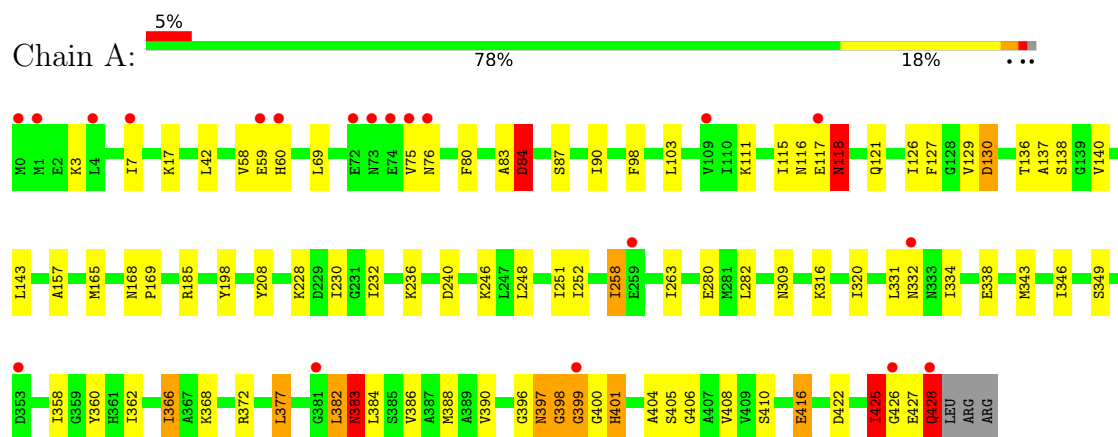
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	2	Total	O	0	0
			2	2		

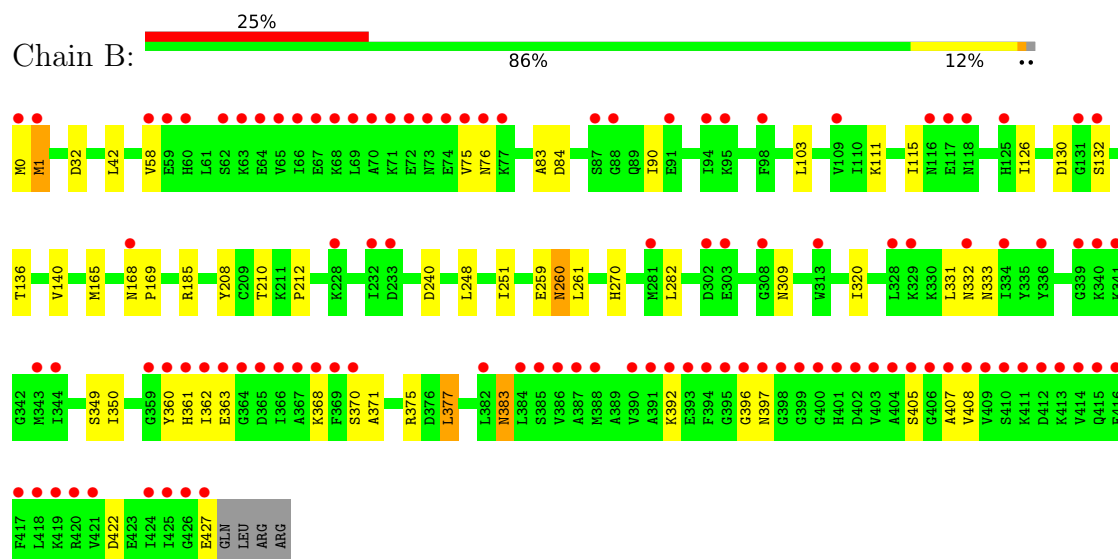
3 Residue-property plots [i](#)

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: MjaRecJ



• Molecule 1: MjaRecJ



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.07Å 92.07Å 275.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.33 – 2.80 87.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (87.33-2.80) 99.8 (87.33-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.264 0.214 , 0.264	Depositor DCC
R_{free} test set	1478 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: GOL, 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	1.07	0/3338	1.49	10/4518 (0.2%)
1	B	1.09	1/3114 (0.0%)	1.49	3/4244 (0.1%)
All	All	1.08	1/6452 (0.0%)	1.49	13/8762 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	HIS	CE1-NE2	5.67	1.38	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ASN	CB-CA-C	8.27	123.10	110.62
1	A	84	ASP	CB-CA-C	7.41	123.18	111.91
1	A	84	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	425	ILE	CA-C-N	6.29	128.27	120.34
1	A	425	ILE	C-N-CA	6.29	128.27	120.34
1	A	240	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	240	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	84	ASP	CA-CB-CG	5.40	118.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	GLN	CA-C-O	5.24	129.71	120.80
1	A	398	GLY	CA-C-N	5.13	127.35	122.27
1	A	398	GLY	C-N-CA	5.13	127.35	122.27
1	B	32	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	399	GLY	CA-C-O	-5.04	117.24	122.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASN	Peptide
1	A	398	GLY	Peptide
1	B	168	ASN	Peptide

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	3279	0	3257	49	0
1	B	3059	0	2791	25	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	18	0	24	0	0
4	A	11	0	0	0	0
4	B	2	0	0	0	0
All	All	6373	0	6072	74	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 6.

All (74) 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:A:129:VAL:O	1:A:130:ASP:CB	2.32	0.77
1:A:383:ASN:HD21	1:A:386:VAL:HG23	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:O	1:B:1:MET:HG3	1.95	0.66
1:A:115:ILE:O	1:A:116:ASN:CG	2.39	0.65
1:A:383:ASN:HD21	1:A:386:VAL:CG2	2.10	0.64
1:B:260:ASN:HD22	1:B:260:ASN:N	1.95	0.64
1:A:280:GLU:OE2	1:A:316:LYS:HE2	2.00	0.62
1:A:117:GLU:O	1:A:118:ASN:ND2	2.33	0.61
1:B:361:HIS:O	1:B:361:HIS:CG	2.54	0.60
1:A:129:VAL:O	1:A:130:ASP:HB2	2.03	0.59
1:A:426:GLY:O	1:A:428:GLN:N	2.34	0.59
1:B:75:VAL:O	1:B:75:VAL:HG23	2.01	0.59
1:B:1:MET:O	1:B:1:MET:CG	2.52	0.58
1:A:75:VAL:HG23	1:A:75:VAL:O	2.04	0.58
1:B:383:ASN:ND2	1:B:427:GLU:O	2.38	0.56
1:A:426:GLY:C	1:A:428:GLN:H	2.14	0.55
1:A:129:VAL:O	1:A:130:ASP:HB3	2.07	0.55
1:A:17:LYS:HE3	1:A:118:ASN:HA	1.88	0.54
1:A:252:ILE:HD12	1:A:258:ILE:HG12	1.89	0.54
1:B:259:GLU:HG2	1:B:260:ASN:HD22	1.74	0.53
1:A:84:ASP:HB2	1:A:137:ALA:CB	2.38	0.53
1:A:383:ASN:ND2	1:A:386:VAL:HG23	2.20	0.53
1:A:118:ASN:C	1:A:118:ASN:HD22	2.16	0.53
1:A:90:ILE:HD11	1:A:115:ILE:CD1	2.39	0.52
1:B:392:LYS:HA	1:B:396:GLY:O	2.11	0.51
1:B:361:HIS:O	1:B:363:GLU:N	2.44	0.50
1:A:360:TYR:HA	1:A:368:LYS:O	2.12	0.50
1:A:400:GLY:O	1:A:405:SER:HB3	2.12	0.49
1:A:7:ILE:HD13	1:A:127:PHE:CD2	2.47	0.49
1:B:130:ASP:OD2	1:B:132:SER:OG	2.31	0.49
1:A:83:ALA:O	1:A:103:LEU:O	2.30	0.49
1:A:397:ASN:N	1:A:397:ASN:ND2	2.61	0.49
1:A:3:LYS:O	1:A:7:ILE:HG12	2.13	0.48
1:B:360:TYR:HA	1:B:368:LYS:O	2.13	0.48
1:A:377:LEU:HB3	1:A:382:LEU:HD12	1.96	0.47
1:A:388:MET:HG3	1:A:405:SER:OG	2.15	0.46
1:B:248:LEU:HA	1:B:251:ILE:HG22	1.97	0.46
1:B:371:ALA:H	1:B:405:SER:CB	2.28	0.46
1:A:208:TYR:HA	1:A:320:ILE:HG13	1.98	0.46
1:A:397:ASN:N	1:A:397:ASN:HD22	2.14	0.46
1:A:377:LEU:O	1:A:382:LEU:HB2	2.16	0.45
1:B:83:ALA:O	1:B:103:LEU:O	2.34	0.45
1:A:248:LEU:HA	1:A:251:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:HIS:HB2	1:A:404:ALA:O	2.17	0.44
1:A:416:GLU:CD	1:A:416:GLU:N	2.76	0.44
1:A:400:GLY:O	1:A:405:SER:CB	2.65	0.44
1:B:397:ASN:O	1:B:407:ALA:O	2.36	0.44
1:A:90:ILE:HD11	1:A:115:ILE:HD13	1.99	0.44
1:A:331:LEU:O	1:A:422:ASP:CG	2.61	0.44
1:B:136:THR:O	1:B:140:VAL:HG23	2.18	0.44
1:A:396:GLY:C	1:A:397:ASN:ND2	2.77	0.43
1:B:331:LEU:O	1:B:422:ASP:CG	2.61	0.43
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.81	0.43
1:A:366:ILE:CD1	1:A:408:VAL:CG1	2.98	0.42
1:B:210:THR:OG1	1:B:350:ILE:HD13	2.19	0.42
1:B:370:SER:HA	1:B:405:SER:CB	2.50	0.42
1:B:259:GLU:HG2	1:B:260:ASN:ND2	2.34	0.42
1:A:383:ASN:ND2	1:A:386:VAL:CG2	2.79	0.42
1:A:7:ILE:HG21	1:A:143:LEU:HD13	2.02	0.42
1:A:136:THR:O	1:A:140:VAL:HG23	2.19	0.41
1:A:87:SER:OG	1:A:121:GLN:NE2	2.50	0.41
1:B:111:LYS:HA	1:B:126:ILE:HG12	2.03	0.41
1:A:7:ILE:CD1	1:A:127:PHE:CD2	3.03	0.41
1:A:338:GLU:HB2	1:A:360:TYR:CZ	2.55	0.41
1:A:198:TYR:CE1	1:A:316:LYS:HE3	2.56	0.41
1:B:90:ILE:HD11	1:B:115:ILE:CD1	2.51	0.41
1:A:111:LYS:HA	1:A:126:ILE:HG12	2.03	0.41
1:B:212:PRO:CD	1:B:261:LEU:HD23	2.50	0.41
1:A:168:ASN:HA	1:A:169:PRO:HA	1.83	0.40
1:A:75:VAL:O	1:A:75:VAL:CG2	2.69	0.40
1:A:138:SER:HB2	1:A:157:ALA:HA	2.02	0.40
1:A:80:PHE:CD1	1:A:98:PHE:HD1	2.39	0.40
1:B:208:TYR:HA	1:B:320:ILE:HG13	2.03	0.40
1:A:399:GLY:N	1:A:406:GLY: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	427/432 (99%)	406 (95%)	15 (4%)	6 (1%)	9	30
1	B	426/432 (99%)	400 (94%)	21 (5%)	5 (1%)	10	34
All	All	853/864 (99%)	806 (94%)	36 (4%)	11 (1%)	9	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	A	427	GLU
1	B	76	ASN
1	B	362	ILE
1	A	76	ASN
1	A	332	ASN
1	A	401	HIS
1	B	332	ASN
1	B	169	PRO
1	B	408	VAL
1	A	425	ILE

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	333/373 (89%)	297 (89%)	36 (11%)	6	21
1	B	266/373 (71%)	252 (95%)	14 (5%)	20	52
All	All	599/746 (80%)	549 (92%)	50 (8%)	10	32

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	58	VAL

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Mol	Chain	Res	Type
1	A	59	GLU
1	A	60	HIS
1	A	69	LEU
1	A	84	ASP
1	A	118	ASN
1	A	165	MET
1	A	185	ARG
1	A	228	LYS
1	A	230	ILE
1	A	232	ILE
1	A	236	LYS
1	A	246	LYS
1	A	258	ILE
1	A	263	ILE
1	A	282	LEU
1	A	309	ASN
1	A	334	ILE
1	A	343	MET
1	A	346	ILE
1	A	349	SER
1	A	358	ILE
1	A	362	ILE
1	A	366	ILE
1	A	372	ARG
1	A	377	LEU
1	A	382	LEU
1	A	383	ASN
1	A	384	LEU
1	A	390	VAL
1	A	397	ASN
1	A	410	SER
1	A	416	GLU
1	A	425	ILE
1	A	428	GLN
1	B	0	MET
1	B	1	MET
1	B	42	LEU
1	B	58	VAL
1	B	165	MET
1	B	185	ARG
1	B	260	ASN
1	B	282	LEU

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Mol	Chain	Res	Type
1	B	309	ASN
1	B	333	ASN
1	B	349	SER
1	B	375	ARG
1	B	377	LEU
1	B	383	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	97	ASN
1	A	118	ASN
1	A	121	GLN
1	A	238	GLN
1	A	288	ASN
1	A	361	HIS
1	A	383	ASN
1	A	397	ASN
1	B	118	ASN
1	B	121	GLN
1	B	235	ASN
1	B	238	GLN
1	B	260	ASN
1	B	288	ASN
1	B	310	GLN
1	B	361	HIS

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

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
3	GOL	A	504	-	5,5,5	0.13	0	5,5,5	0.30	0
3	GOL	A	503	-	5,5,5	0.07	0	5,5,5	0.26	0
3	GOL	A	505	-	5,5,5	0.18	0	5,5,5	0.47	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
3	GOL	A	504	-	-	3/4/4/4	-
3	GOL	A	503	-	-	3/4/4/4	-
3	GOL	A	505	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	GOL	C1-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
3	A	505	GOL	O2-C2-C3-O3
3	A	503	GOL	C1-C2-C3-O3
3	A	505	GOL	C1-C2-C3-O3
3	A	503	GOL	O2-C2-C3-O3
3	A	504	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	429/432 (99%)	-0.06	20 (4%) 36 29	33, 49, 69, 114	23 (5%)
1	B	428/432 (99%)	1.42	107 (25%) 2 1	32, 57, 80, 126	115 (26%)
All	All	857/864 (99%)	0.68	127 (14%) 5 4	32, 53, 77, 126	138 (16%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	ASN	10.3
1	B	72	GLU	9.2
1	A	75	VAL	8.6
1	B	402	ASP	8.6
1	B	401	HIS	8.2
1	B	394	PHE	7.6
1	B	362	ILE	7.5
1	B	403	VAL	7.2
1	B	75	VAL	7.1
1	B	361	HIS	7.0
1	B	73	ASN	6.9
1	B	410	SER	6.9
1	B	417	PHE	6.7
1	B	76	ASN	6.6
1	B	368	LYS	6.6
1	B	408	VAL	6.5
1	B	407	ALA	6.4
1	B	405	SER	6.4
1	B	64	GLU	6.3
1	B	426	GLY	6.2
1	B	391	ALA	6.2
1	B	390	VAL	6.1
1	B	409	VAL	6.1
1	B	396	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	399	GLY	5.9
1	B	406	GLY	5.9
1	B	395	GLY	5.9
1	B	328	LEU	5.9
1	A	73	ASN	5.8
1	B	400	GLY	5.8
1	B	393	GLU	5.7
1	B	71	LYS	5.6
1	B	398	GLY	5.5
1	B	340	LYS	5.4
1	B	365	ASP	5.4
1	B	420	ARG	5.3
1	B	385	SER	5.3
1	B	69	LEU	5.2
1	B	366	ILE	5.2
1	B	232	ILE	5.2
1	B	404	ALA	5.2
1	B	91	GLU	5.1
1	B	416	GLU	5.0
1	B	367	ALA	5.0
1	B	392	LYS	4.9
1	B	341	LYS	4.8
1	B	382	LEU	4.7
1	B	413	LYS	4.7
1	B	418	LEU	4.7
1	B	67	GLU	4.7
1	B	70	ALA	4.6
1	A	74	GLU	4.6
1	B	421	VAL	4.5
1	B	131	GLY	4.5
1	B	74	GLU	4.5
1	B	369	PHE	4.5
1	B	63	LYS	4.5
1	B	370	SER	4.5
1	B	344	ILE	4.5
1	B	66	ILE	4.4
1	B	414	VAL	4.3
1	A	60	HIS	4.3
1	A	72	GLU	4.2
1	B	363	GLU	4.2
1	B	424	ILE	4.2
1	B	387	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	59	GLU	4.1
1	B	62	SER	4.1
1	B	118	ASN	4.1
1	B	412	ASP	4.0
1	B	388	MET	4.0
1	B	360	TYR	4.0
1	A	76	ASN	3.9
1	B	411	LYS	3.7
1	B	65	VAL	3.4
1	B	116	ASN	3.4
1	A	353	ASP	3.4
1	A	428	GLN	3.3
1	B	332	ASN	3.3
1	B	60	HIS	3.3
1	B	68	LYS	3.2
1	B	132	SER	3.2
1	B	302	ASP	3.2
1	B	95	LYS	3.2
1	B	109	VAL	3.2
1	B	415	GLN	3.2
1	B	228	LYS	3.1
1	B	427	GLU	3.1
1	B	329	LYS	3.1
1	A	426	GLY	3.0
1	A	117	GLU	3.0
1	B	313	TRP	2.8
1	B	1	MET	2.8
1	B	94	ILE	2.8
1	B	303	GLU	2.8
1	B	339	GLY	2.8
1	B	364	GLY	2.8
1	B	98	PHE	2.8
1	B	425	ILE	2.8
1	B	117	GLU	2.7
1	B	386	VAL	2.7
1	A	1	MET	2.7
1	B	58	VAL	2.7
1	B	308	GLY	2.7
1	A	0	MET	2.6
1	B	343	MET	2.6
1	A	4	LEU	2.5
1	B	88	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	0	MET	2.5
1	A	259	GLU	2.5
1	B	168	ASN	2.5
1	B	87	SER	2.3
1	B	334	ILE	2.3
1	A	7	ILE	2.3
1	B	77	LYS	2.2
1	B	336	TYR	2.2
1	B	384	LEU	2.2
1	B	281	MET	2.1
1	A	59	GLU	2.1
1	B	125	HIS	2.1
1	B	359	GLY	2.1
1	A	332	ASN	2.1
1	B	419	LYS	2.0
1	A	381	GLY	2.0
1	A	399	GLY	2.0
1	B	233	ASP	2.0
1	A	109	VAL	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	A	502	1/1	0.72	0.24	73,73,73,73	1
3	GOL	A	504	6/6	0.76	0.32	83,87,90,91	5
3	GOL	A	503	6/6	0.88	0.16	80,89,90,93	4
3	GOL	A	505	6/6	0.89	0.18	65,71,75,76	0

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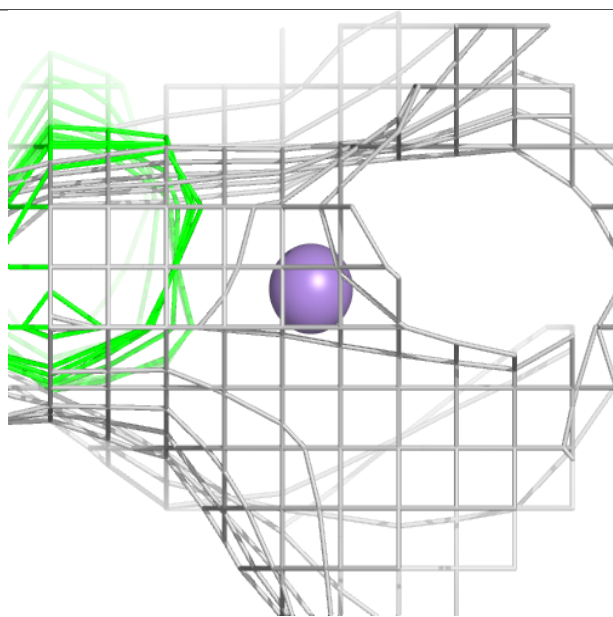
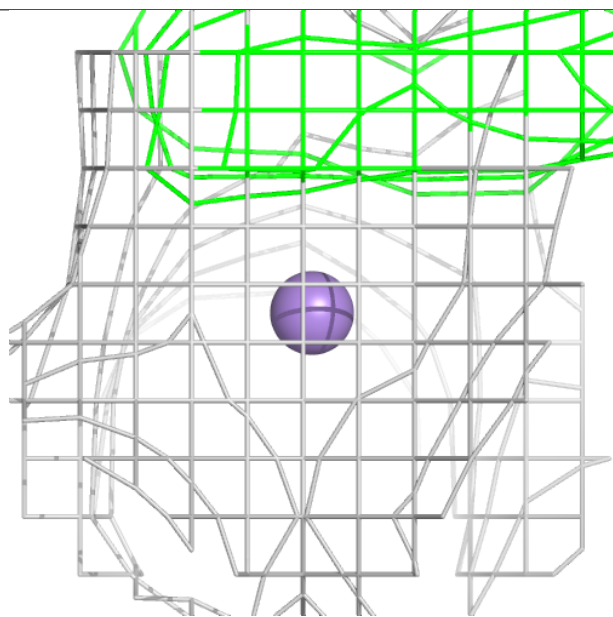
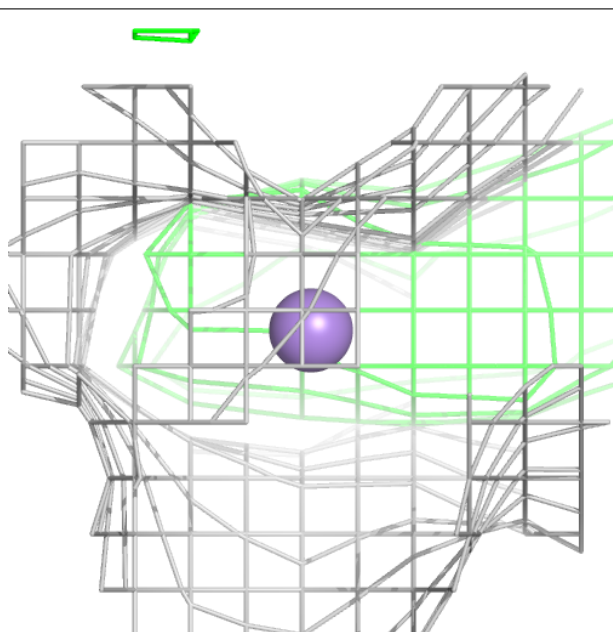
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	502	1/1	0.93	0.10	54,54,54,54	1
2	MN	A	501	1/1	0.93	0.10	57,57,57,57	0
2	MN	B	501	1/1	0.97	0.04	59,59,59,59	0

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.

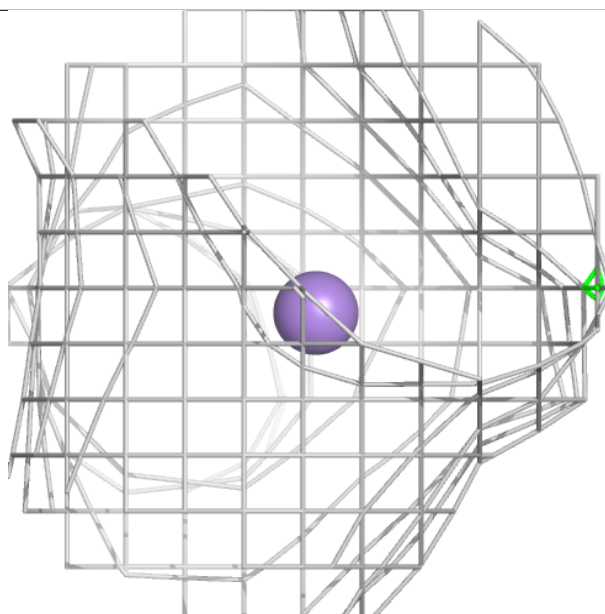
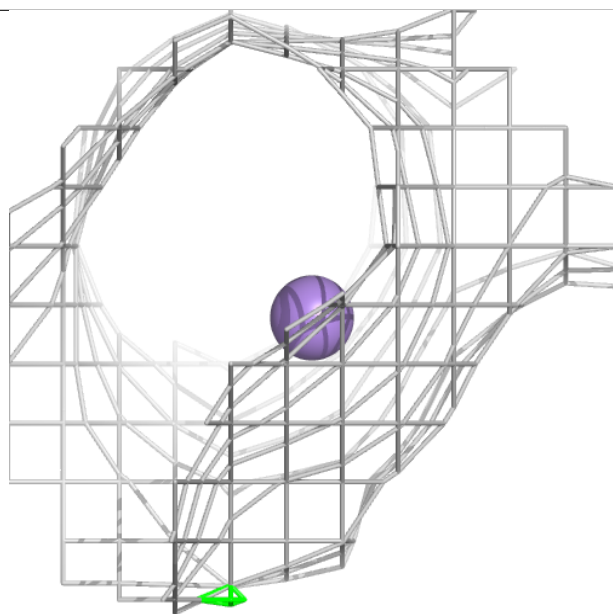
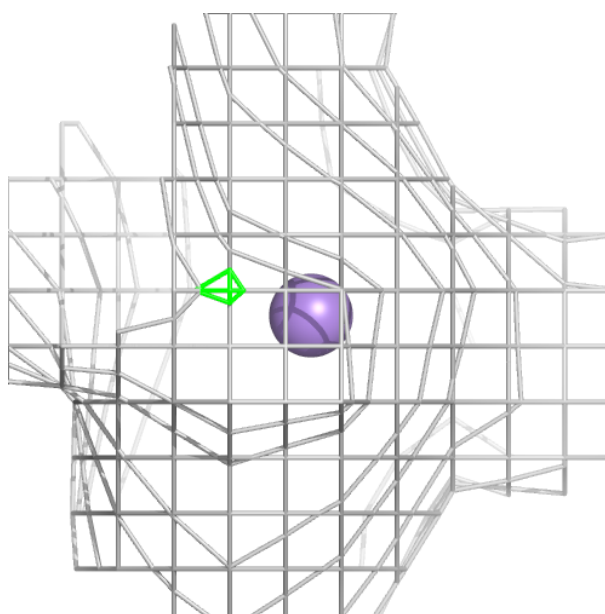
Electron density around MN A 502:

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



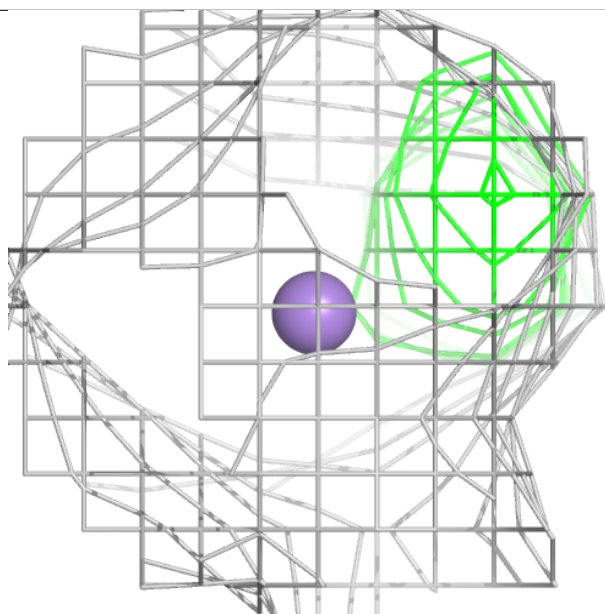
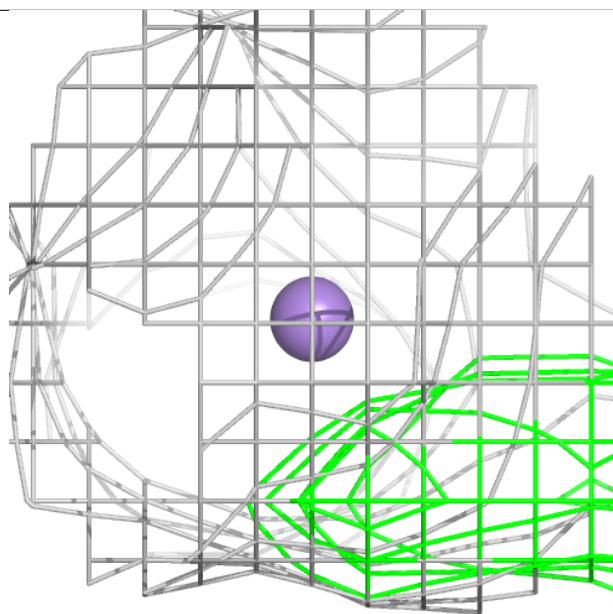
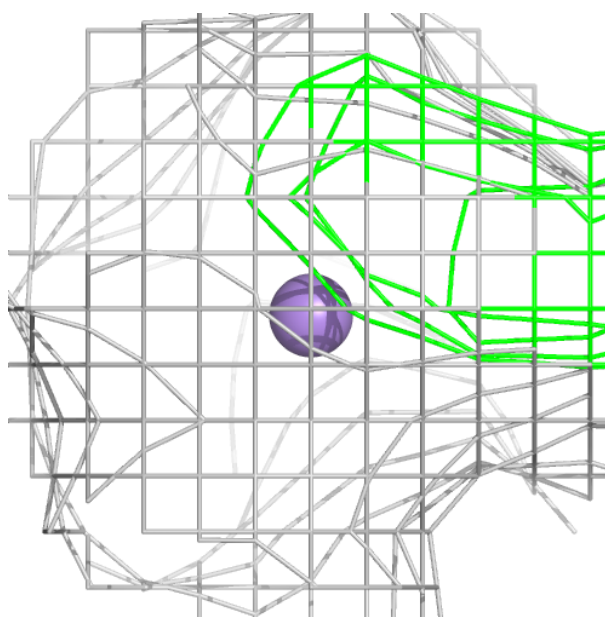
Electron density around MN B 502:

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



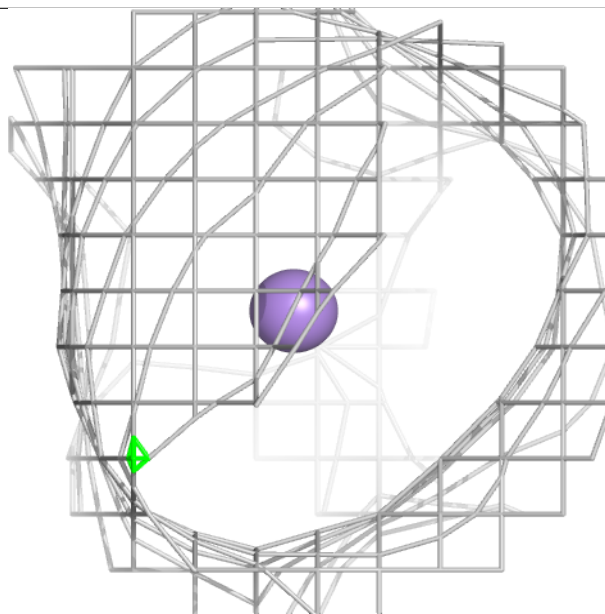
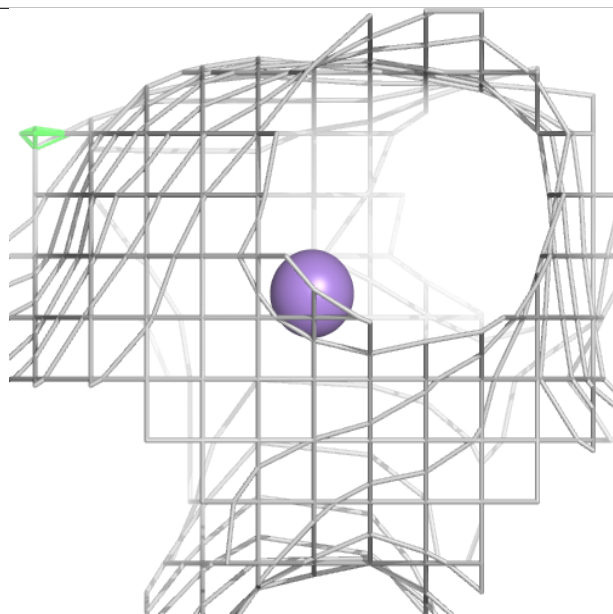
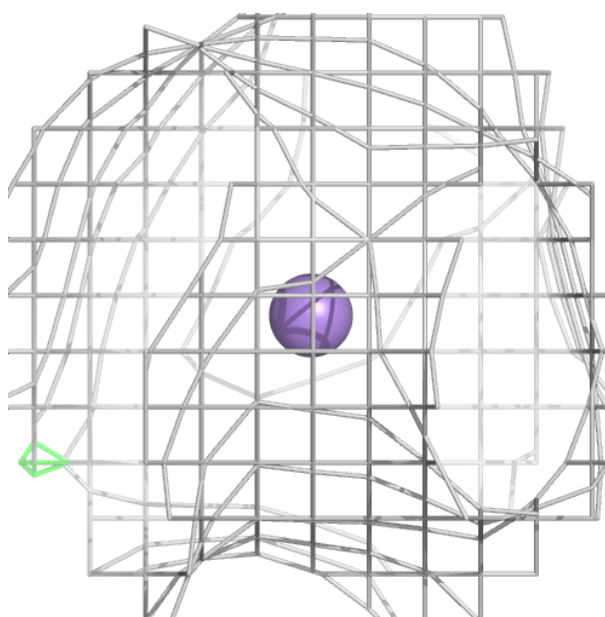
Electron density around MN A 501:

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



Electron density around MN B 501:

$2mF_o-DF_c$ (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.