



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 06:31 PM UTC

PDB ID : 6KXU / pdb_00006kxu
Title : BON1
Authors : Wang, Q.C.; Jiang, M.Q.; Isupov, M.N.; Sun, L.F.; Wu, Y.K.
Deposited on : 2019-09-12
Resolution : 2.83 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

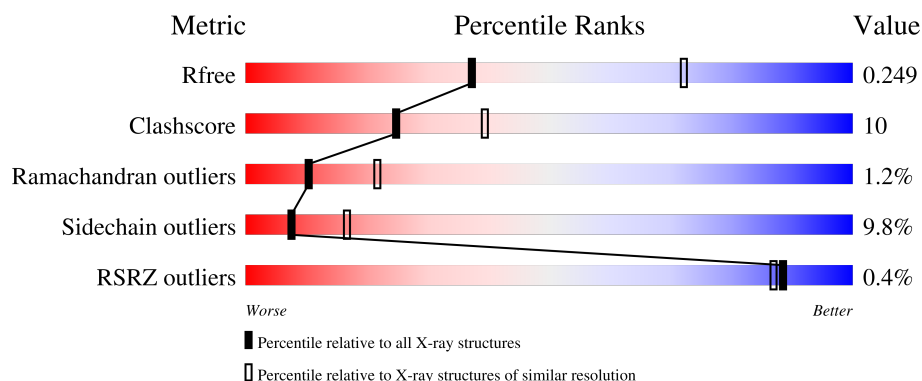
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	553	75% 21% • •
1	C	553	74% 22% •
1	D	553	% 72% 24% • •
1	F	553	% 74% 22% •
2	B	528	70% 22% • • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	548	73% 21%
4	G	526	2% 70% 23%
5	H	553	74% 20%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 33483 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 Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4242	2699	711	819	13			
1	C	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			
1	D	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			
1	F	553	Total	C	N	O	S	0	0	0
			4299	2735	719	832	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q941L3
A	-8	THR	-	expression tag	UNP Q941L3
A	-7	SER	-	expression tag	UNP Q941L3
A	-6	SER	-	expression tag	UNP Q941L3
A	-5	MET	-	expression tag	UNP Q941L3
A	-4	ALA	-	expression tag	UNP Q941L3
A	-3	ASP	-	expression tag	UNP Q941L3
A	-2	ILE	-	expression tag	UNP Q941L3
A	-1	GLY	-	expression tag	UNP Q941L3
A	0	SER	-	expression tag	UNP Q941L3
C	-9	GLY	-	expression tag	UNP Q941L3
C	-8	THR	-	expression tag	UNP Q941L3
C	-7	SER	-	expression tag	UNP Q941L3
C	-6	SER	-	expression tag	UNP Q941L3
C	-5	MET	-	expression tag	UNP Q941L3
C	-4	ALA	-	expression tag	UNP Q941L3
C	-3	ASP	-	expression tag	UNP Q941L3
C	-2	ILE	-	expression tag	UNP Q941L3
C	-1	GLY	-	expression tag	UNP Q941L3
C	0	SER	-	expression tag	UNP Q941L3
D	-9	GLY	-	expression tag	UNP Q941L3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	THR	-	expression tag	UNP Q941L3
D	-7	SER	-	expression tag	UNP Q941L3
D	-6	SER	-	expression tag	UNP Q941L3
D	-5	MET	-	expression tag	UNP Q941L3
D	-4	ALA	-	expression tag	UNP Q941L3
D	-3	ASP	-	expression tag	UNP Q941L3
D	-2	ILE	-	expression tag	UNP Q941L3
D	-1	GLY	-	expression tag	UNP Q941L3
D	0	SER	-	expression tag	UNP Q941L3
F	-9	GLY	-	expression tag	UNP Q941L3
F	-8	THR	-	expression tag	UNP Q941L3
F	-7	SER	-	expression tag	UNP Q941L3
F	-6	SER	-	expression tag	UNP Q941L3
F	-5	MET	-	expression tag	UNP Q941L3
F	-4	ALA	-	expression tag	UNP Q941L3
F	-3	ASP	-	expression tag	UNP Q941L3
F	-2	ILE	-	expression tag	UNP Q941L3
F	-1	GLY	-	expression tag	UNP Q941L3
F	0	SER	-	expression tag	UNP Q941L3

- Molecule 2 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3932	2507	660	753	12			

- Molecule 3 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	534	Total	C	N	O	S	0	0	0
			4158	2648	696	802	12			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	ALA	-	expression tag	UNP Q941L3
E	-3	ASP	-	expression tag	UNP Q941L3
E	-2	ILE	-	expression tag	UNP Q941L3
E	-1	GLY	-	expression tag	UNP Q941L3
E	0	SER	-	expression tag	UNP Q941L3

- Molecule 4 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	504	Total	C	N	O	S	0	0	0
			3930	2503	661	754	12			

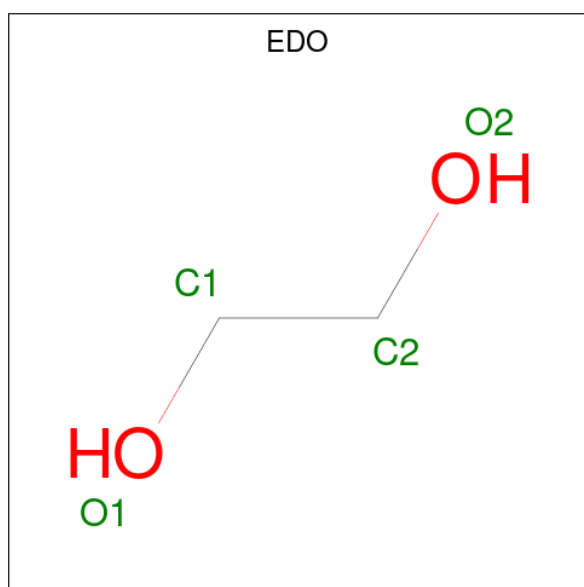
- Molecule 5 is a protein called Protein BONZAI 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	543	Total	C	N	O	S	0	0	0
			4227	2691	706	817	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	GLY	-	expression tag	UNP Q941L3
H	-8	THR	-	expression tag	UNP Q941L3
H	-7	SER	-	expression tag	UNP Q941L3
H	-6	SER	-	expression tag	UNP Q941L3
H	-5	MET	-	expression tag	UNP Q941L3
H	-4	ALA	-	expression tag	UNP Q941L3
H	-3	ASP	-	expression tag	UNP Q941L3
H	-2	ILE	-	expression tag	UNP Q941L3
H	-1	GLY	-	expression tag	UNP Q941L3
H	0	THR	-	expression tag	UNP Q941L3

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mn	0	0
			1	1		
8	B	1	Total	Mn	0	0
			1	1		
8	C	1	Total	Mn	0	0
			1	1		
8	D	2	Total	Mn	0	0
			2	2		
8	E	1	Total	Mn	0	0
			1	1		
8	F	2	Total	Mn	0	0
			2	2		
8	G	1	Total	Mn	0	0
			1	1		
8	H	1	Total	Mn	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Cl 1 1	0	0
9	D	1	Total Cl 1 1	0	0

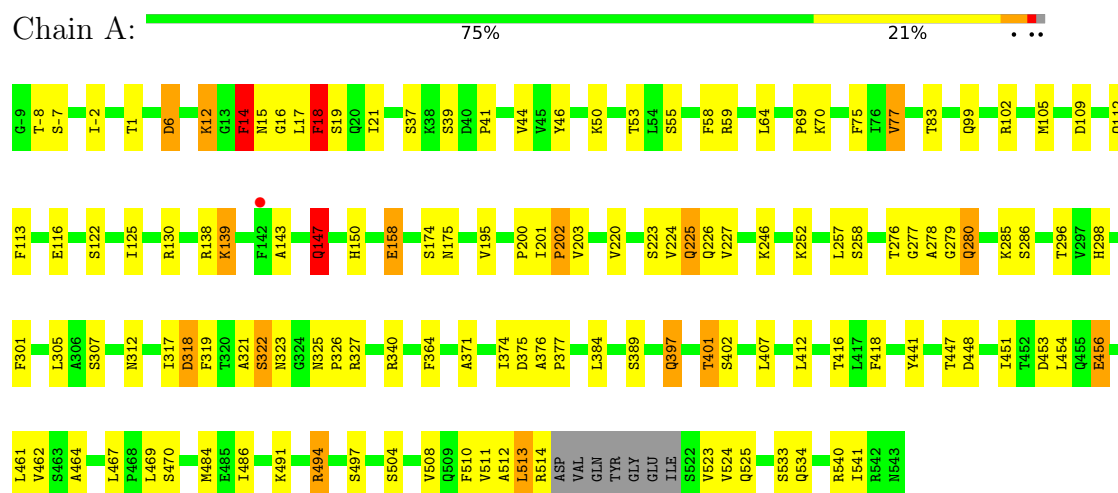
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total O 4 4	0	0
10	B	6	Total O 6 6	0	0
10	C	7	Total O 7 7	0	0
10	D	3	Total O 3 3	0	0
10	E	1	Total O 1 1	0	0
10	H	2	Total O 2 2	0	0

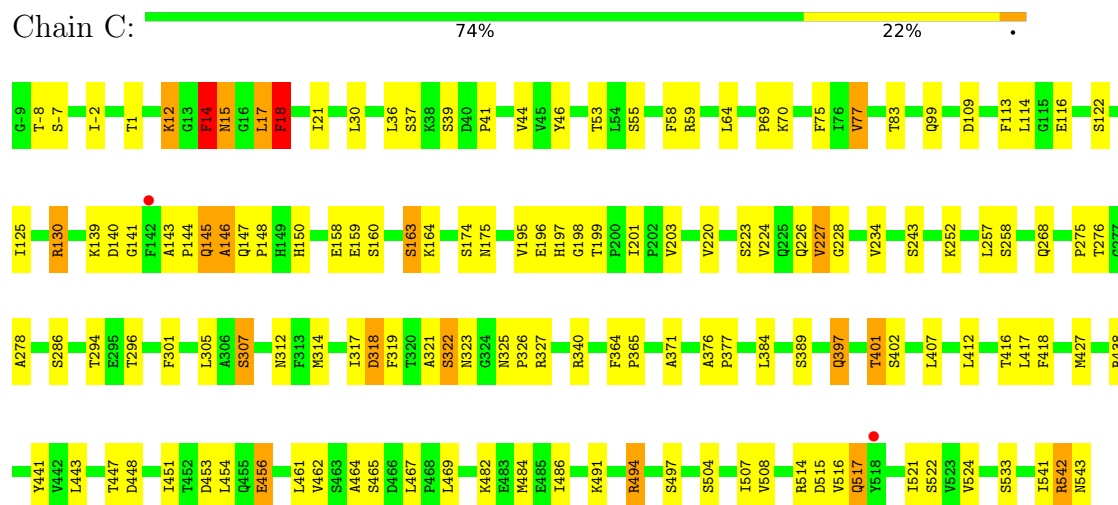
3 Residue-property plots

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

• Molecule 1: Protein BONZAI 1

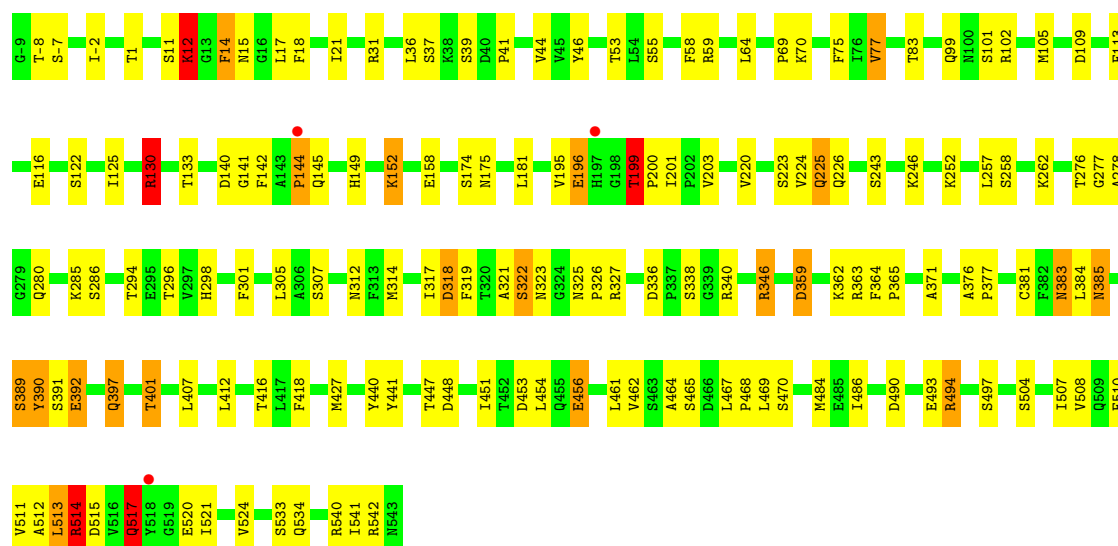


• Molecule 1: Protein BONZAI 1

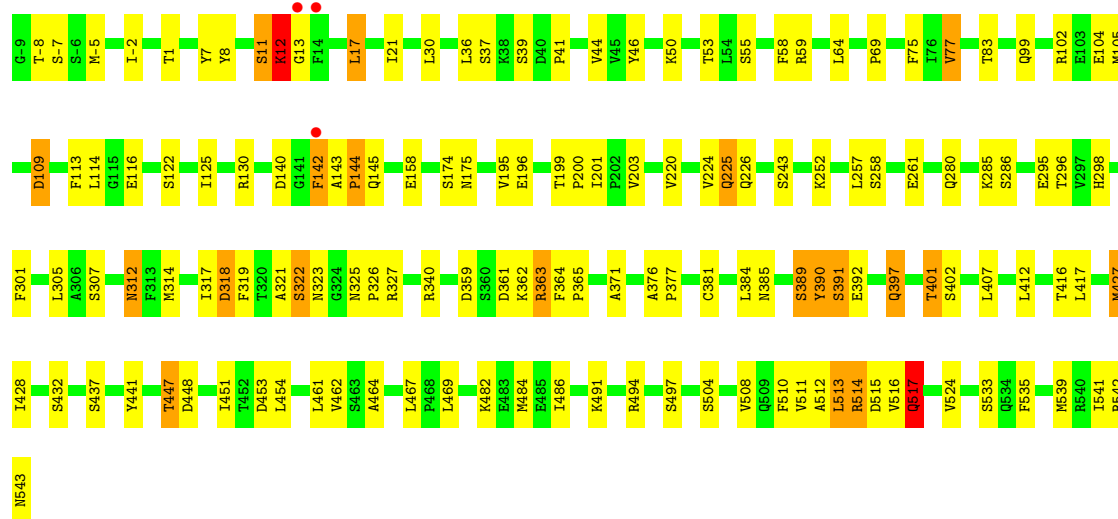
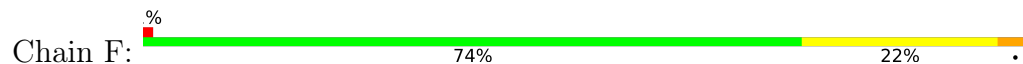


• Molecule 1: Protein BONZAI 1

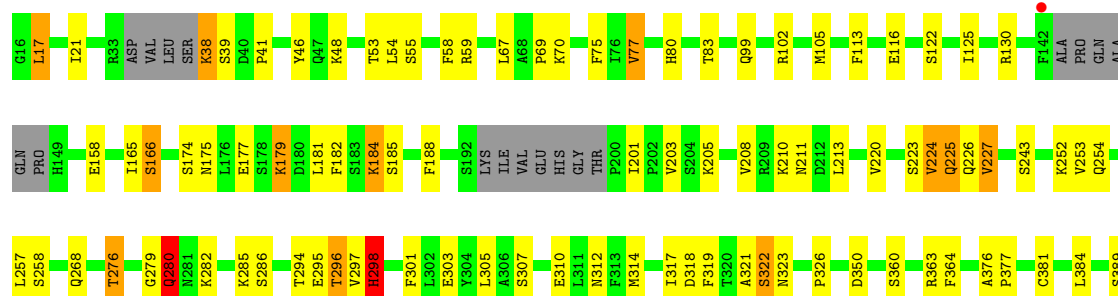


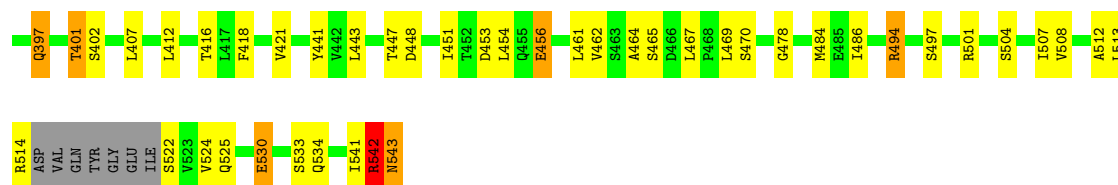


• Molecule 1: Protein BONZAI 1



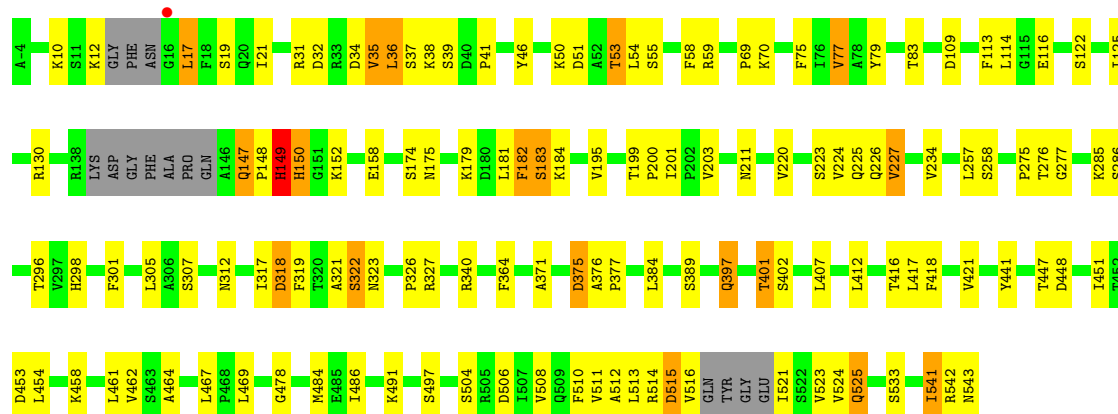
• Molecule 2: Protein BONZAI 1





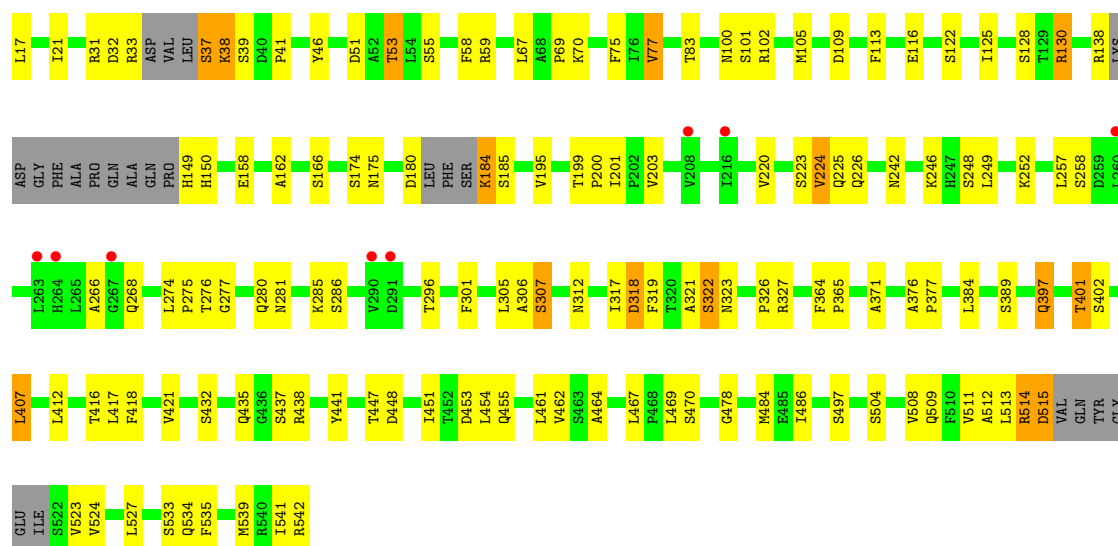
• Molecule 3: Protein BONZAI 1

Chain E: 73% 21%



• Molecule 4: Protein BONZAI 1

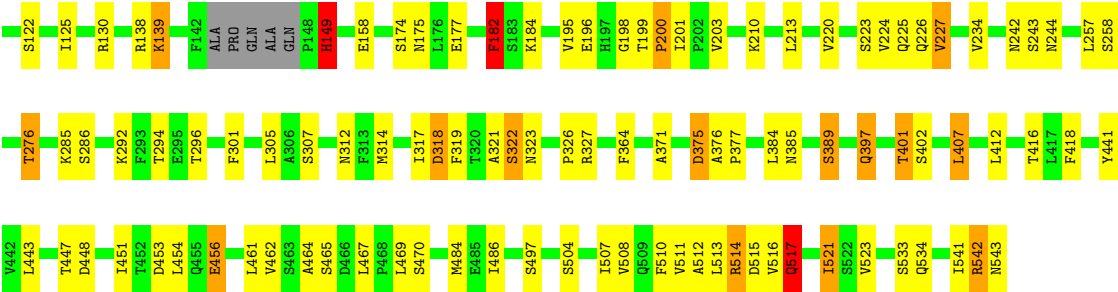
Chain G: 70% 23%



• Molecule 5: Protein BONZAI 1

Chain H: 74% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.41Å 118.70Å 222.32Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	82.31 – 2.83 82.31 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.31-2.83) 98.2 (82.31-2.83)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.204 , 0.249 0.203 , 0.249	Depositor DCC
R_{free} test set	7470 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.246 for h,-k,-l	Xtriage
Reported twinning fraction	0.733 for H, K, L 0.267 for -h,-k,l	Depositor
Outliers	7 of 148582 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33483	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1000e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, MN, EDO

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	0.55	0/4323	1.07	10/5847 (0.2%)
1	C	0.57	1/4382 (0.0%)	1.08	5/5929 (0.1%)
1	D	0.58	1/4382 (0.0%)	1.13	20/5929 (0.3%)
1	F	0.56	1/4382 (0.0%)	1.09	9/5929 (0.2%)
2	B	0.56	1/4004 (0.0%)	1.11	15/5408 (0.3%)
3	E	0.54	0/4234	1.08	10/5726 (0.2%)
4	G	0.56	0/4001	1.06	8/5408 (0.1%)
5	H	0.55	0/4305	1.09	11/5818 (0.2%)
All	All	0.56	4/34013 (0.0%)	1.09	88/45994 (0.2%)

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	1
1	D	0	1
1	F	0	1
2	B	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	HIS	CE1-NE2	7.71	1.40	1.32
1	F	447	THR	CB-OG1	6.17	1.53	1.43
2	B	80	HIS	CE1-NE2	6.10	1.38	1.32
1	D	392	GLU	CD-OE2	5.15	1.35	1.25

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	447	THR	CA-CB-OG1	14.00	130.59	109.60
2	B	38	LYS	CB-CA-C	11.43	131.82	110.10
1	F	447	THR	N-CA-CB	11.04	129.75	111.31
1	D	298	HIS	CB-CA-C	9.25	125.16	109.53
1	C	416	THR	CA-CB-OG1	9.10	123.25	109.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	PHE	Peptide
2	B	184	LYS	Peptide
2	B	296	THR	Peptide
1	D	12	LYS	Peptide
1	F	11	SER	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	4242	0	4246	79	0
1	C	4299	0	4297	81	0
1	D	4299	0	4298	93	0
1	F	4299	0	4295	101	0
2	B	3932	0	3944	77	0
3	E	4158	0	4172	76	0
4	G	3930	0	3945	90	0
5	H	4227	0	4233	82	0
6	A	12	0	18	0	0
6	B	4	0	6	0	0
6	C	16	0	24	0	0
6	D	4	0	6	1	0
6	F	8	0	12	0	0
6	G	4	0	6	1	0
6	H	8	0	12	0	0
7	A	6	0	8	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
8	D	2	0	0	0	0
8	E	1	0	0	0	0
8	F	2	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	4	0	0	0	0
10	B	6	0	0	0	0
10	C	7	0	0	1	0
10	D	3	0	0	0	0
10	E	1	0	0	0	0
10	H	2	0	0	1	0
All	All	33483	0	33522	655	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 10.

The worst 5 of 655 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:427:MET:HG3	4:G:184:LYS:N	1.61	1.15
1:F:318:ASP:OD2	1:F:447:THR:OG1	1.65	1.14
1:F:142:PHE:O	1:F:144:PRO:HD3	1.49	1.12
5:H:102:ARG:NH2	10:H:701:HOH:O	1.90	1.02
1:C:195:VAL:CG2	1:C:198:GLY:O	2.16	0.94

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	542/553 (98%)	504 (93%)	35 (6%)	3 (1%)	21	39
1	C	551/553 (100%)	503 (91%)	40 (7%)	8 (2%)	8	17
1	D	551/553 (100%)	510 (93%)	30 (5%)	11 (2%)	6	12
1	F	551/553 (100%)	510 (93%)	32 (6%)	9 (2%)	7	16
2	B	494/528 (94%)	463 (94%)	26 (5%)	5 (1%)	12	24
3	E	526/548 (96%)	487 (93%)	31 (6%)	8 (2%)	8	17
4	G	494/526 (94%)	465 (94%)	27 (6%)	2 (0%)	30	48
5	H	535/553 (97%)	494 (92%)	38 (7%)	3 (1%)	21	39
All	All	4244/4367 (97%)	3936 (93%)	259 (6%)	49 (1%)	10	22

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ALA
2	B	280	GLN
1	C	18	PHE
1	C	146	ALA
1	D	144	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	475/481 (99%)	427 (90%)	48 (10%)	7	15
1	C	481/481 (100%)	433 (90%)	48 (10%)	7	16
1	D	481/481 (100%)	434 (90%)	47 (10%)	7	17
1	F	481/481 (100%)	437 (91%)	44 (9%)	9	20
2	B	441/461 (96%)	393 (89%)	48 (11%)	6	12
3	E	467/477 (98%)	424 (91%)	43 (9%)	8	19
4	G	442/460 (96%)	400 (90%)	42 (10%)	8	18
5	H	474/481 (98%)	427 (90%)	47 (10%)	7	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3742/3803 (98%)	3375 (90%)	367 (10%)	7 17

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	525	GLN
4	G	122	SER
1	F	37	SER
1	F	307	SER
4	G	257	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	435	GLN
5	H	298	HIS
4	G	242	ASN
4	G	534	GLN
5	H	455	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	$\# Z > 2$
6	EDO	C	603	-	3,3,3	0.09	0	2,2,2	0.18	0
6	EDO	A	602	-	3,3,3	0.08	0	2,2,2	0.00	0
6	EDO	C	604	-	3,3,3	0.14	0	2,2,2	0.06	0
6	EDO	H	602	-	3,3,3	0.16	0	2,2,2	0.33	0
6	EDO	D	601	-	3,3,3	0.05	0	2,2,2	0.23	0
6	EDO	B	601	-	3,3,3	0.19	0	2,2,2	0.25	0
6	EDO	C	602	-	3,3,3	0.34	0	2,2,2	0.26	0
7	GOL	A	604	-	5,5,5	0.19	0	5,5,5	0.50	0
6	EDO	C	601	-	3,3,3	0.44	0	2,2,2	0.50	0
6	EDO	H	601	-	3,3,3	0.13	0	2,2,2	0.17	0
6	EDO	F	602	-	3,3,3	0.96	0	2,2,2	1.48	0
6	EDO	G	601	-	3,3,3	0.10	0	2,2,2	0.66	0
6	EDO	A	601	-	3,3,3	0.41	0	2,2,2	1.39	0
6	EDO	A	603	-	3,3,3	0.29	0	2,2,2	0.39	0
6	EDO	F	601	-	3,3,3	0.07	0	2,2,2	0.19	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
6	EDO	C	603	-	-	0/1/1/1	-
6	EDO	A	602	-	-	1/1/1/1	-
6	EDO	C	604	-	-	1/1/1/1	-
6	EDO	H	602	-	-	1/1/1/1	-
6	EDO	D	601	-	-	0/1/1/1	-
6	EDO	B	601	-	-	1/1/1/1	-
6	EDO	C	602	-	-	1/1/1/1	-
7	GOL	A	604	-	-	2/4/4/4	-
6	EDO	C	601	-	-	0/1/1/1	-
6	EDO	H	601	-	-	1/1/1/1	-
6	EDO	F	602	-	-	1/1/1/1	-
6	EDO	G	601	-	-	1/1/1/1	-
6	EDO	A	601	-	-	1/1/1/1	-
6	EDO	A	603	-	-	1/1/1/1	-
6	EDO	F	601	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	604	GOL	O1-C1-C2-C3
7	A	604	GOL	O1-C1-C2-O2
6	F	602	EDO	O1-C1-C2-O2
6	G	601	EDO	O1-C1-C2-O2
6	A	601	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	601	EDO	1	0
7	A	604	GOL	2	0
6	G	601	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	546/553 (98%)	-1.10	1 (0%) 91 91	44, 78, 129, 185	0
1	C	553/553 (100%)	-1.07	2 (0%) 88 87	29, 77, 141, 196	0
1	D	553/553 (100%)	-1.09	3 (0%) 87 85	25, 80, 147, 220	0
1	F	553/553 (100%)	-1.05	3 (0%) 87 85	46, 84, 156, 239	0
2	B	504/528 (95%)	-0.98	1 (0%) 91 91	38, 94, 167, 236	0
3	E	534/548 (97%)	-0.99	1 (0%) 91 91	50, 86, 162, 206	0
4	G	504/526 (95%)	-0.77	8 (1%) 70 64	37, 83, 208, 271	0
5	H	543/553 (98%)	-1.04	0 100 100	48, 87, 169, 235	0
All	All	4290/4367 (98%)	-1.02	19 (0%) 88 87	25, 83, 166, 271	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	267	GLY	11.1
4	G	208	VAL	4.4
1	A	142	PHE	3.9
1	F	142	PHE	3.8
1	F	14	PHE	3.0

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 ⓘ

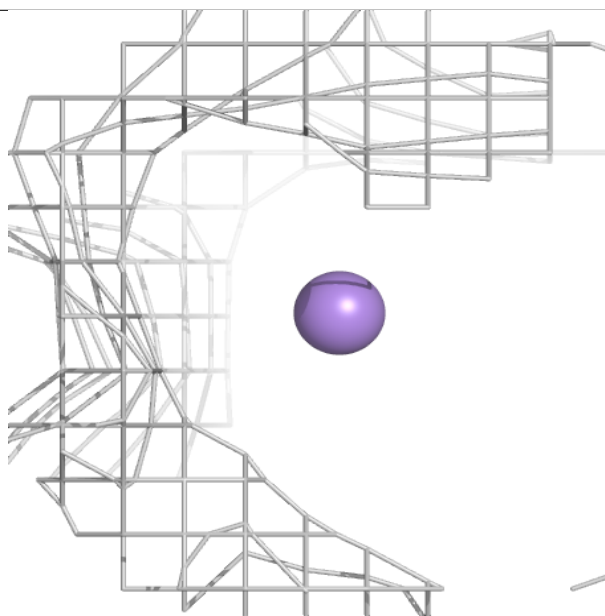
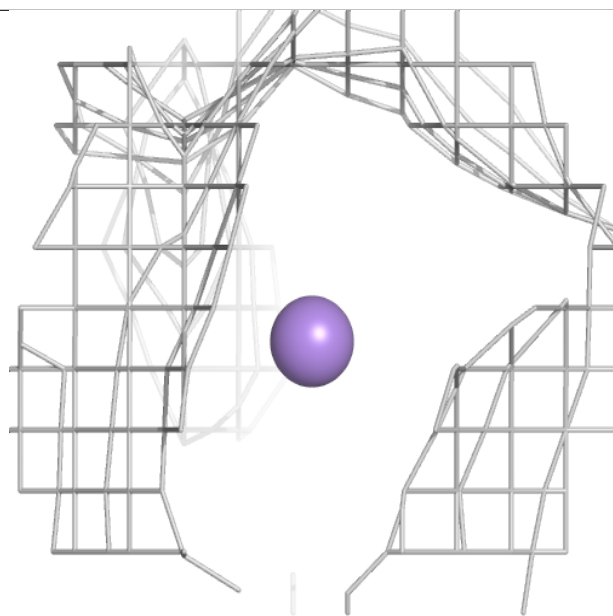
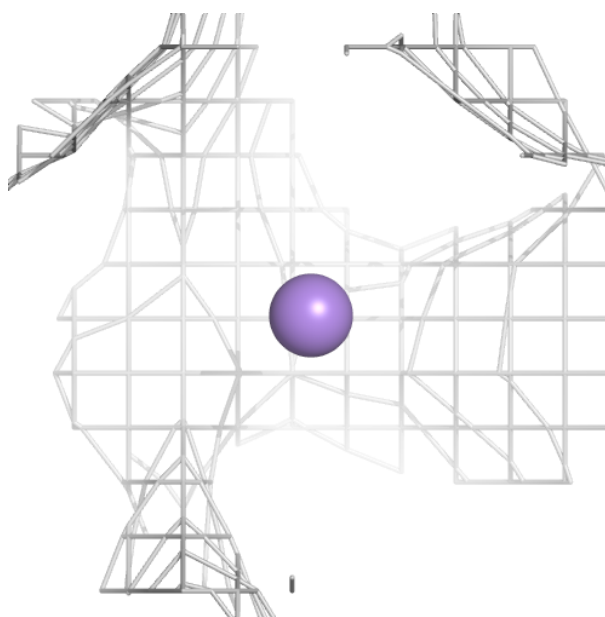
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	C	603	4/4	0.94	0.14	88,99,109,110	0
6	EDO	B	601	4/4	0.96	0.11	56,64,68,79	0
6	EDO	A	602	4/4	0.96	0.11	85,92,94,95	0
6	EDO	F	601	4/4	0.96	0.10	94,106,106,113	0
6	EDO	D	601	4/4	0.97	0.10	89,91,92,103	0
6	EDO	A	603	4/4	0.97	0.11	69,75,84,88	0
6	EDO	H	602	4/4	0.97	0.08	68,84,84,89	0
6	EDO	H	601	4/4	0.98	0.14	89,94,105,105	0
6	EDO	C	604	4/4	0.98	0.12	80,82,86,90	0
7	GOL	A	604	6/6	0.98	0.05	87,99,99,109	0
8	MN	B	602	1/1	0.98	0.03	141,141,141,141	1
8	MN	F	604	1/1	0.98	0.04	91,91,91,91	1
6	EDO	C	602	4/4	0.99	0.04	58,60,67,72	0
6	EDO	A	601	4/4	0.99	0.06	33,37,38,42	0
8	MN	A	605	1/1	0.99	0.04	133,133,133,133	1
6	EDO	G	601	4/4	0.99	0.05	60,68,71,71	0
8	MN	C	606	1/1	0.99	0.02	129,129,129,129	1
8	MN	D	603	1/1	0.99	0.02	164,164,164,164	1
8	MN	D	604	1/1	0.99	0.04	113,113,113,113	1
8	MN	E	601	1/1	0.99	0.03	117,117,117,117	1
6	EDO	C	601	4/4	0.99	0.07	67,78,83,84	0
8	MN	H	603	1/1	0.99	0.02	111,111,111,111	1
9	CL	C	605	1/1	0.99	0.04	76,76,76,76	0
9	CL	D	602	1/1	0.99	0.04	73,73,73,73	0
8	MN	F	603	1/1	1.00	0.04	127,127,127,127	1
6	EDO	F	602	4/4	1.00	0.06	21,29,30,31	0
8	MN	G	602	1/1	1.00	0.02	106,106,106,106	1

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.

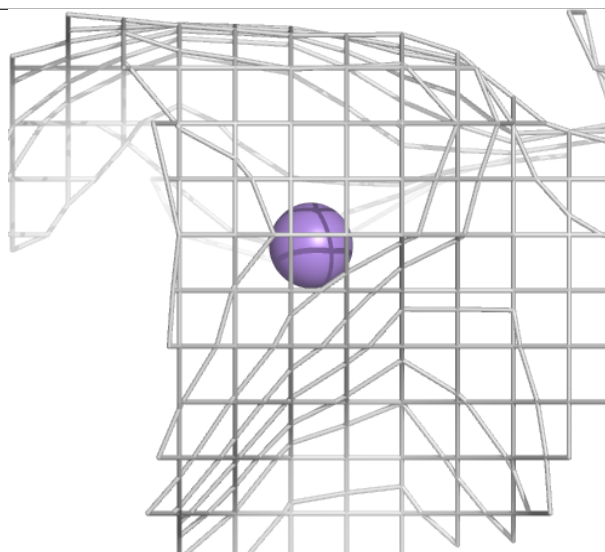
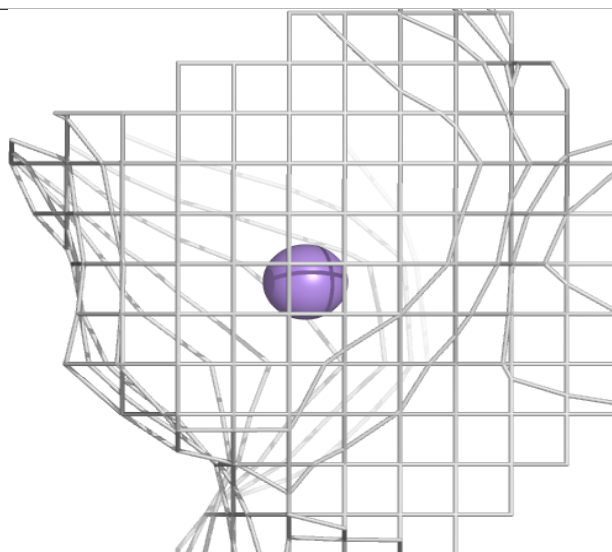
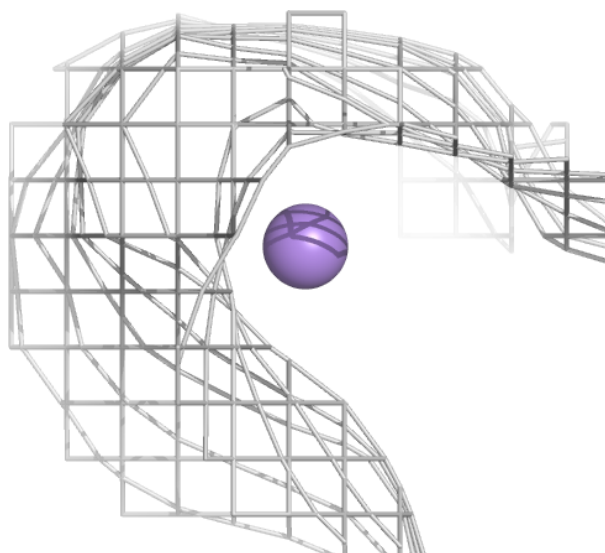
Electron density around MN B 602:

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



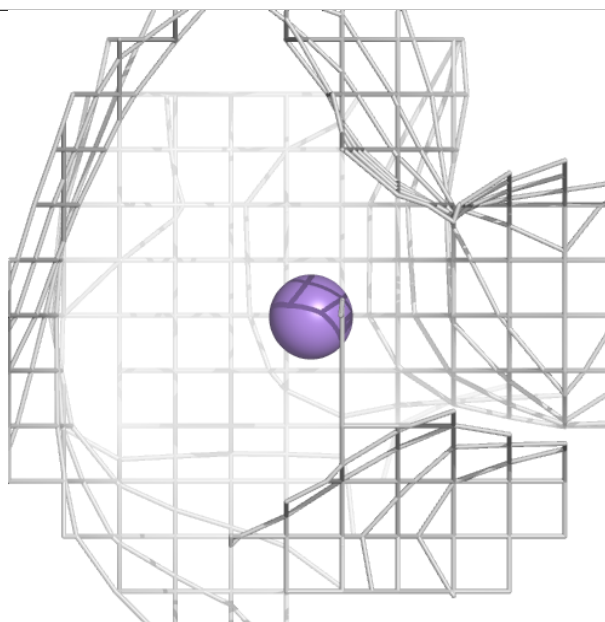
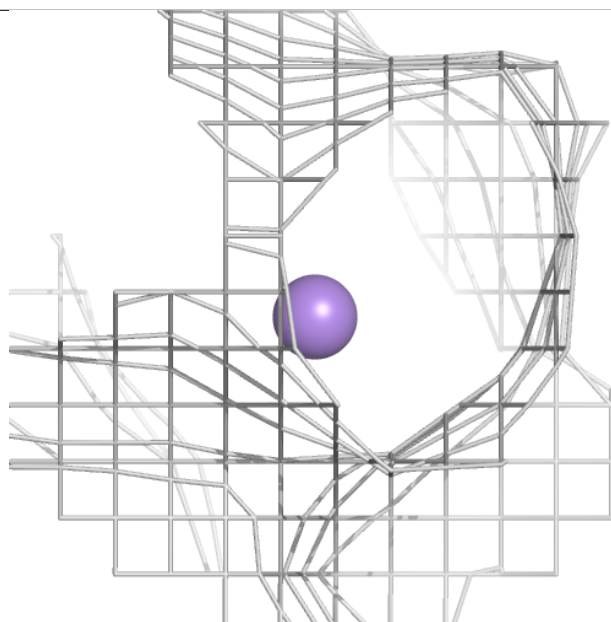
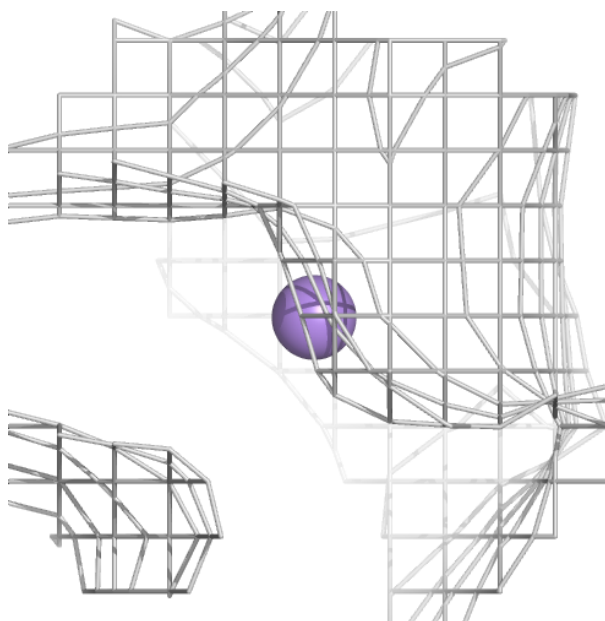
Electron density around MN F 604:

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



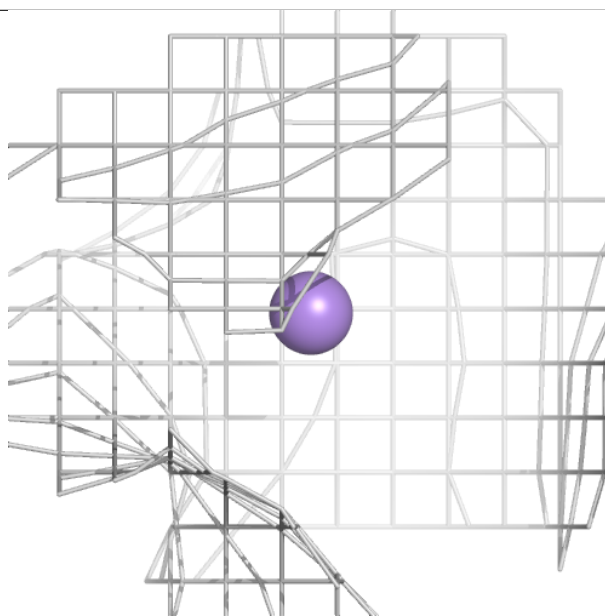
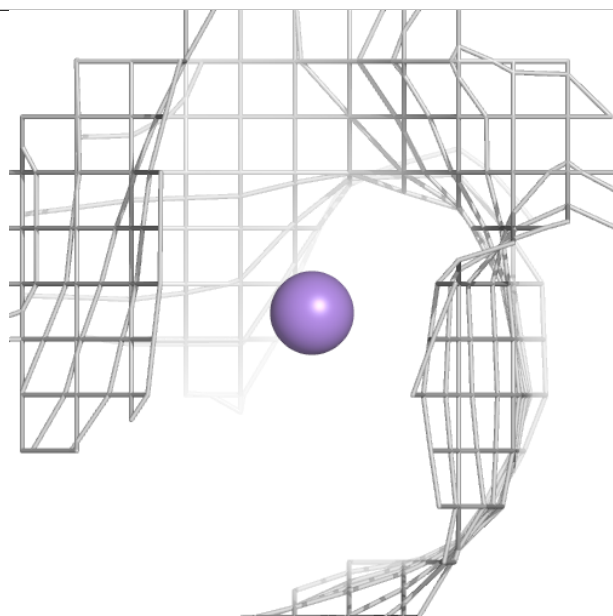
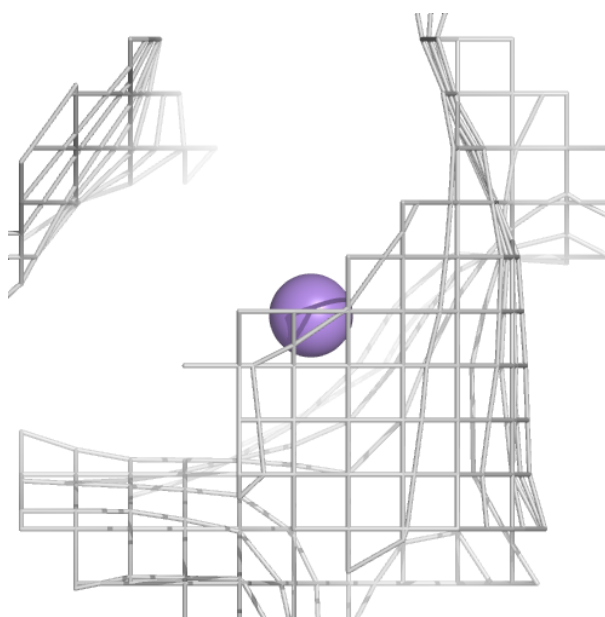
Electron density around MN A 605:

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



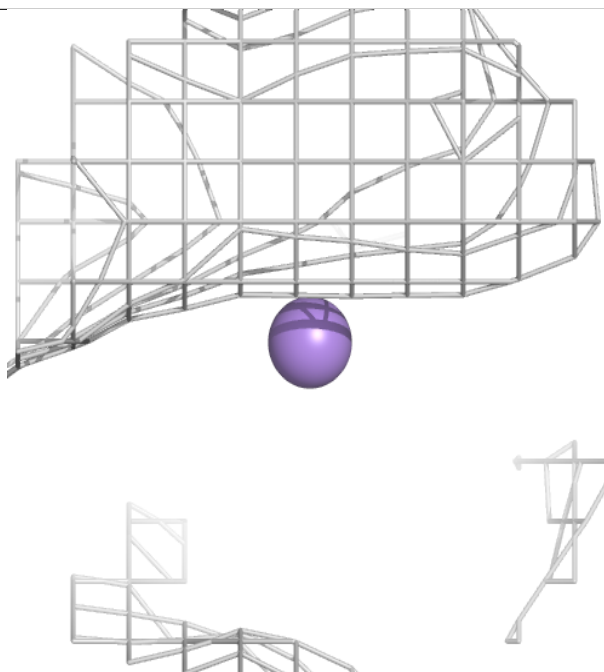
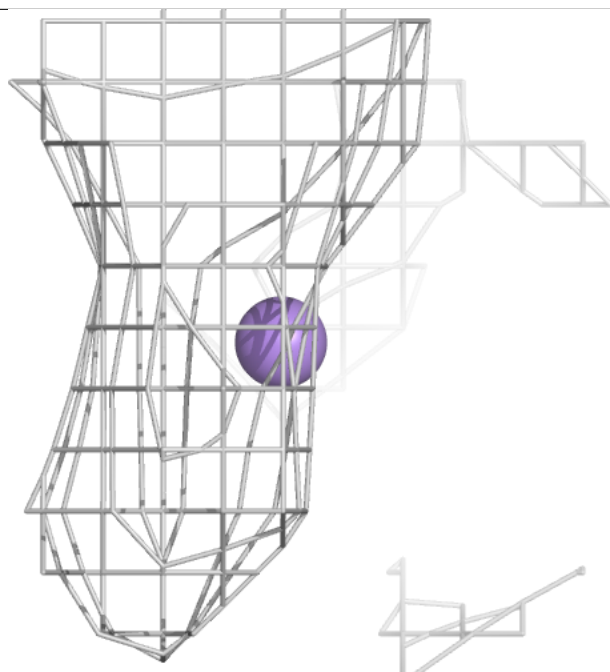
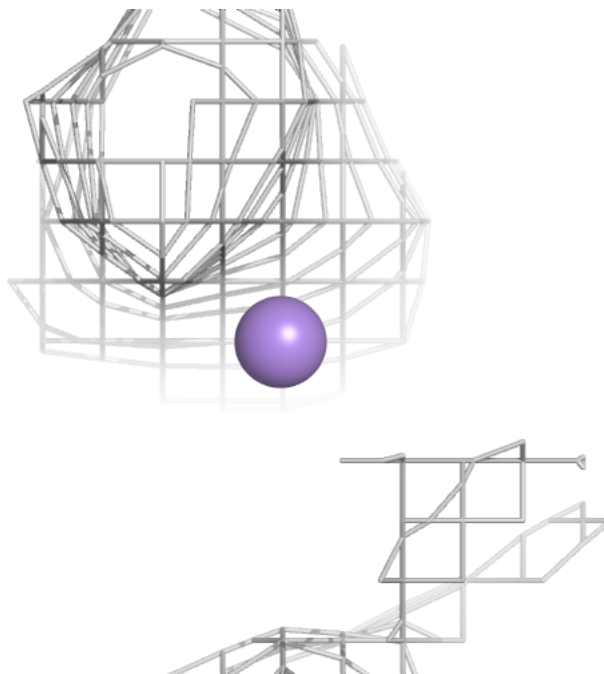
Electron density around MN C 606:

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



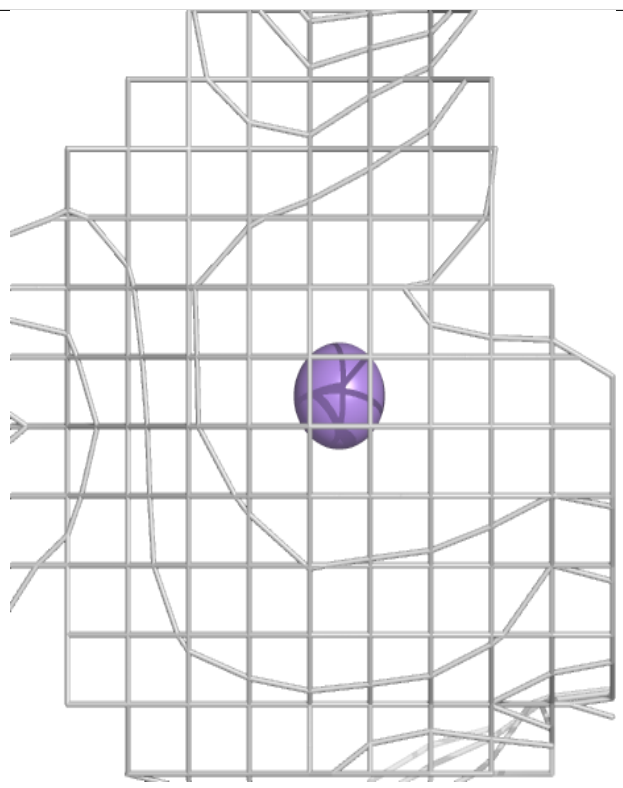
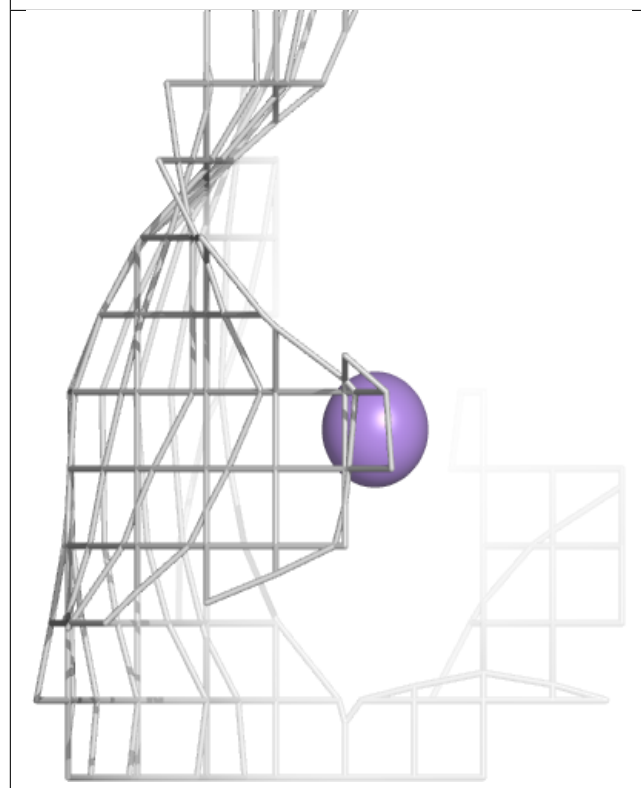
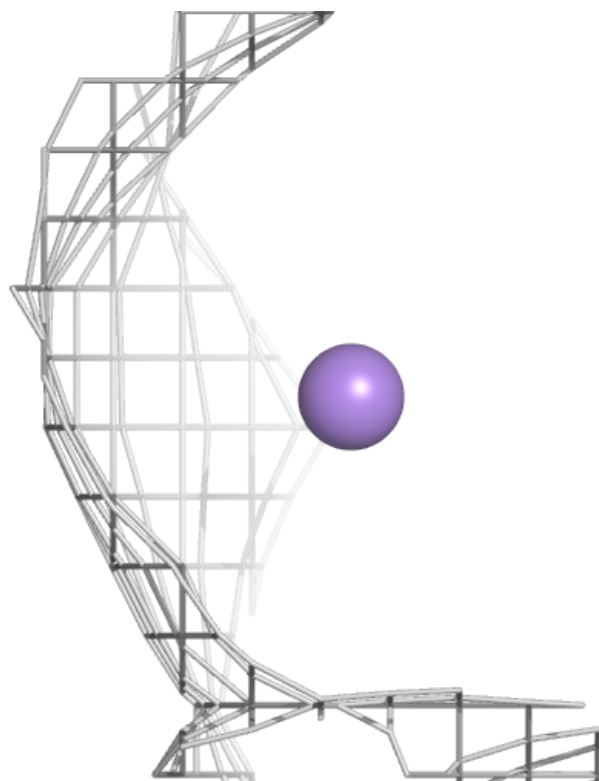
Electron density around MN D 603:

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



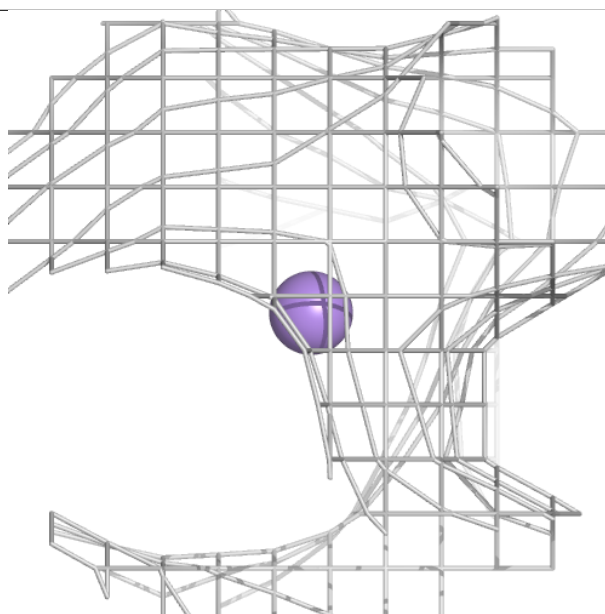
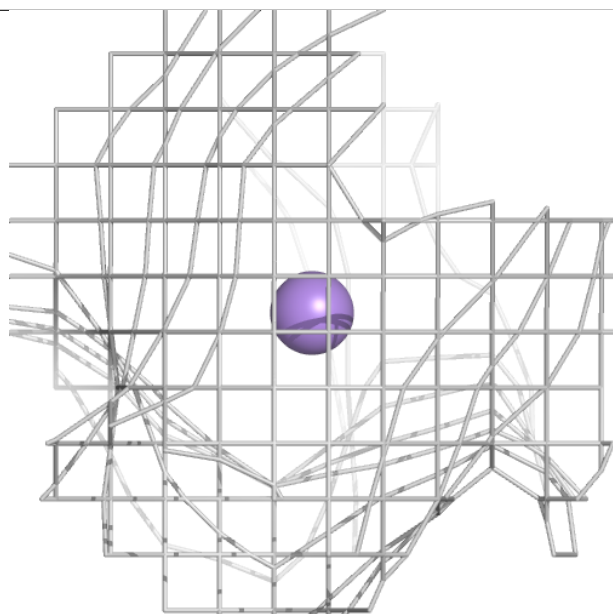
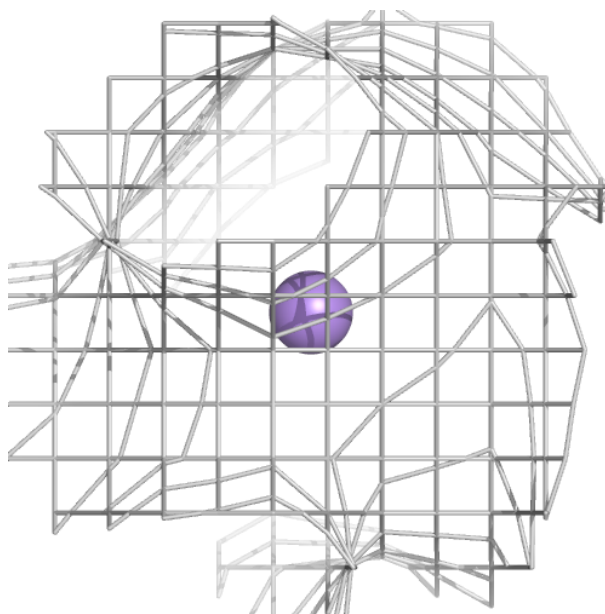
Electron density around MN D 604:

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



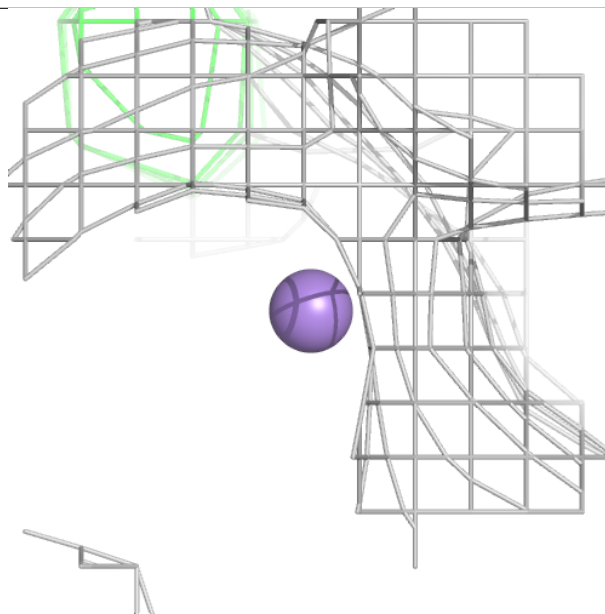
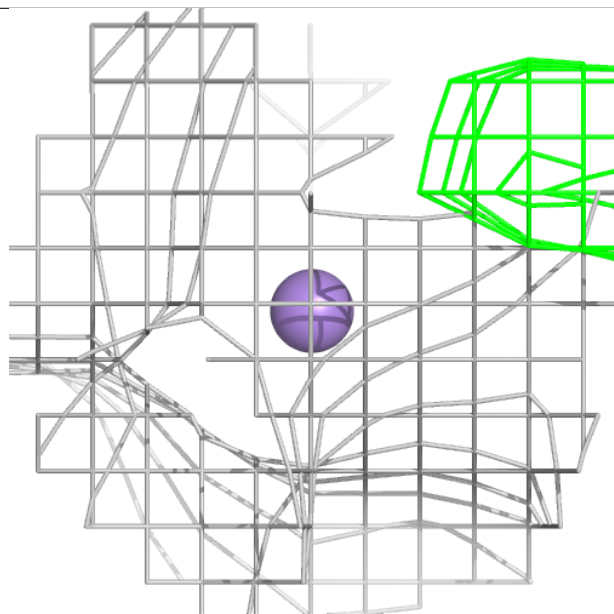
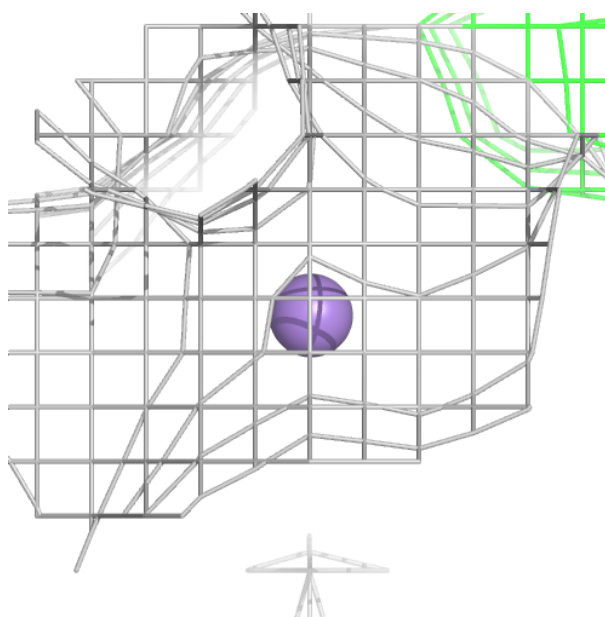
Electron density around MN E 601:

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



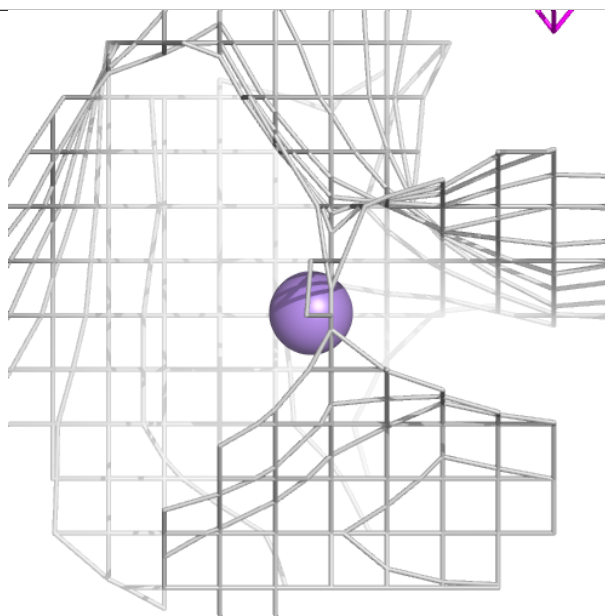
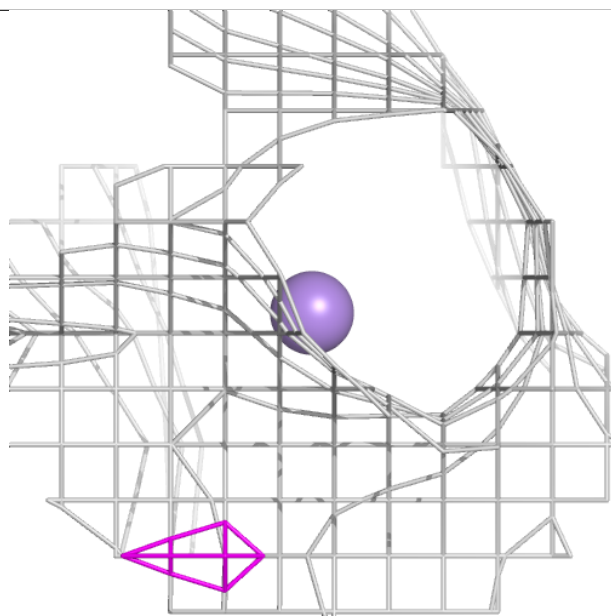
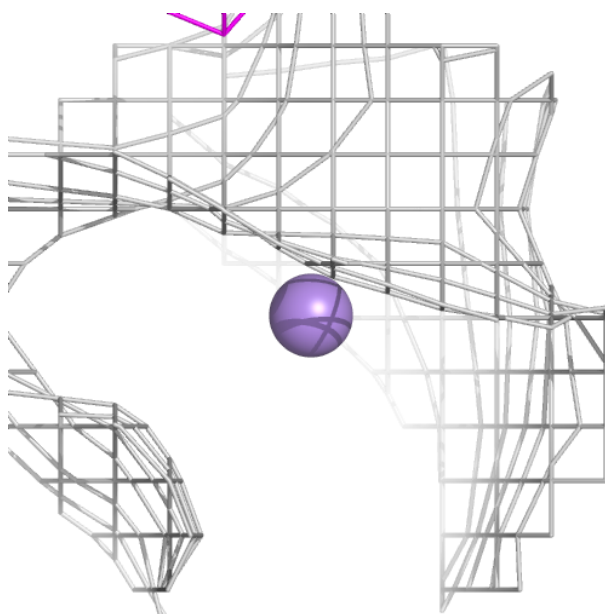
Electron density around MN H 603:

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



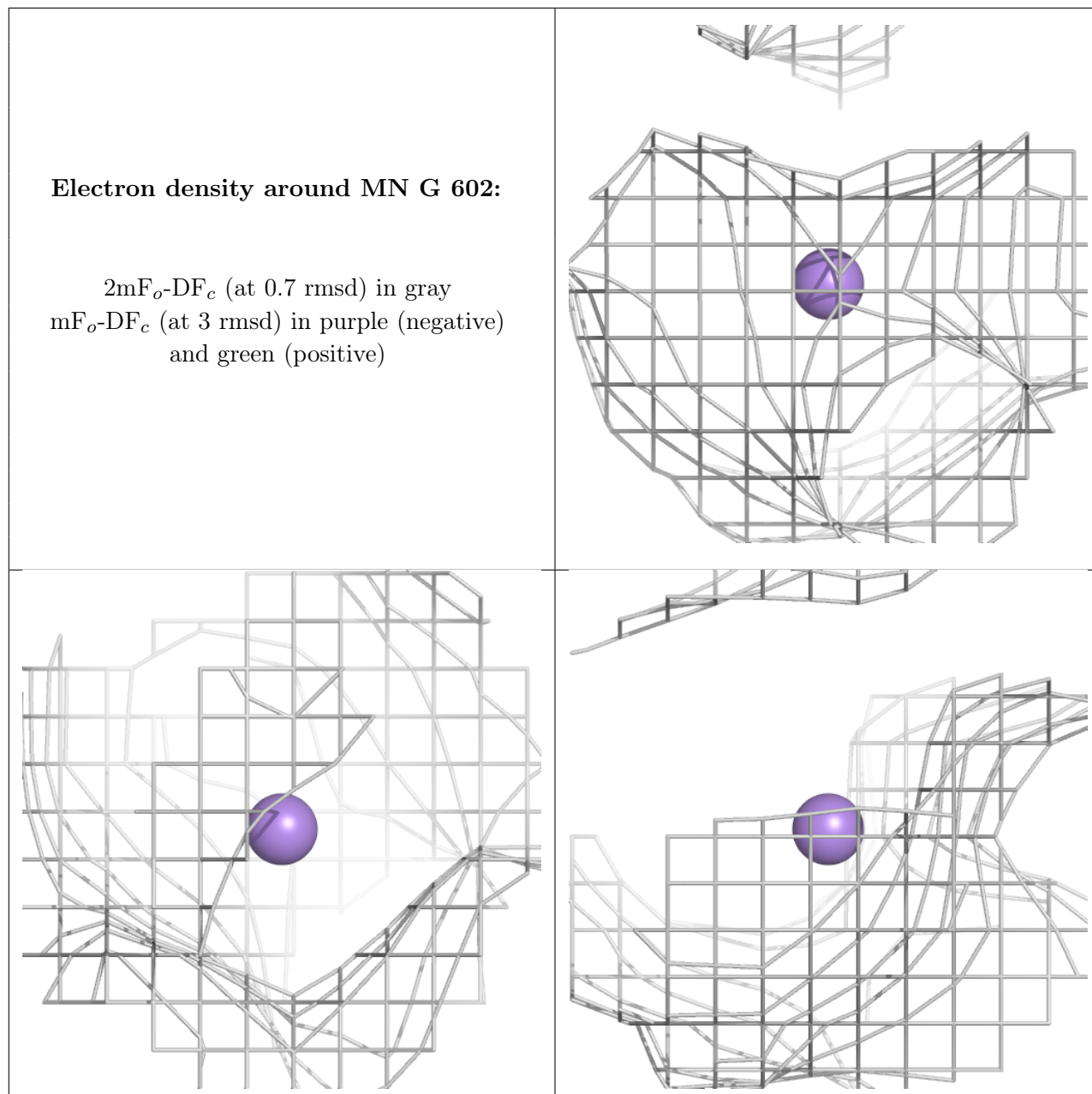
Electron density around MN F 603:

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



Electron density around MN G 602:

$2mF_o-DF_c$ (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.