



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:31 AM UTC

PDB ID : 6TXF / pdb_00006txf
Title : Crystal structure of tetrameric human D137N-SAMHD1 (residues 109-626) with XTP, dAMPNPP and Mn
Authors : Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.G.; Kelly, G.; Taylor, I.A.
Deposited on : 2020-01-14
Resolution : 2.25 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

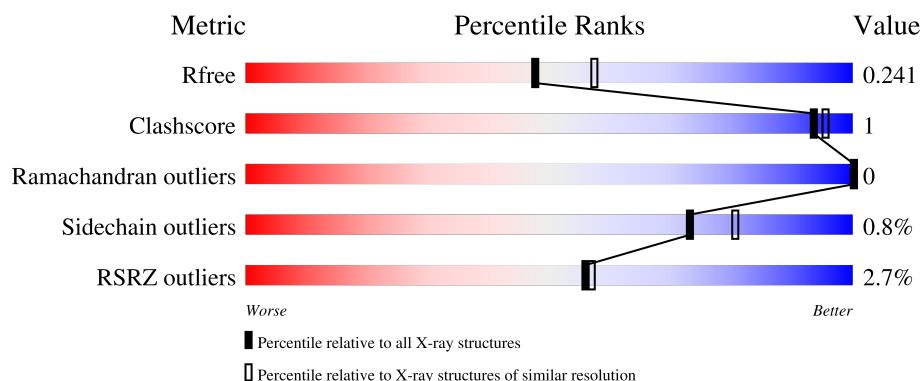
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

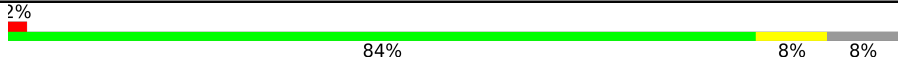
The reported resolution of this entry is 2.25 Å.

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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	520	
1	B	520	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8030 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3879	2483	675	701	20			
1	B	479	Total	C	N	O	S	0	0	0
			3869	2477	670	702	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	SER	-	expression tag	UNP Q9Y3Z3
A	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
B	137	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

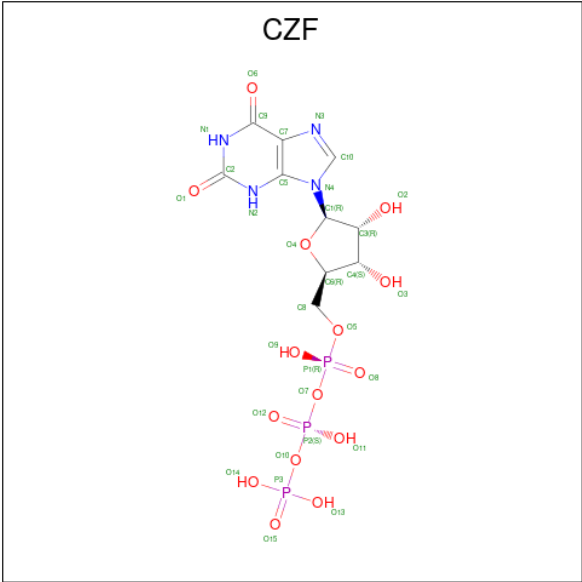
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mn	0	0
			3	3		
3	B	3	Total	Mn	0	0
			3	3		

- # DZ4

- Molecule 5 is [[(2 {R},3 {S},4 {R},5 {R})-5-[2,6-bis(oxidanylidene)-3 {H}-purin-9-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: CZF) (formula: C₁₀H₁₅N₄O₁₅P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	4	15	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	4	15	3		

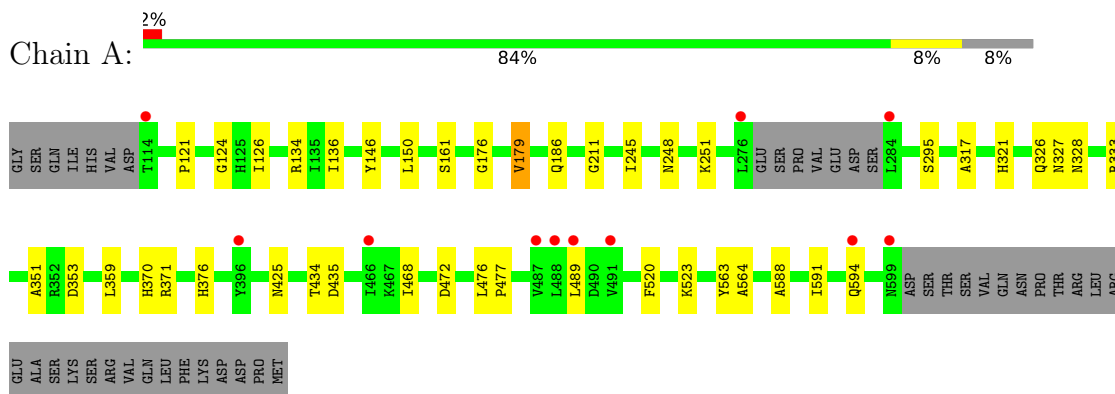
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total	O	0	0
			51	51		
6	B	39	Total	O	0	0
			39	39		

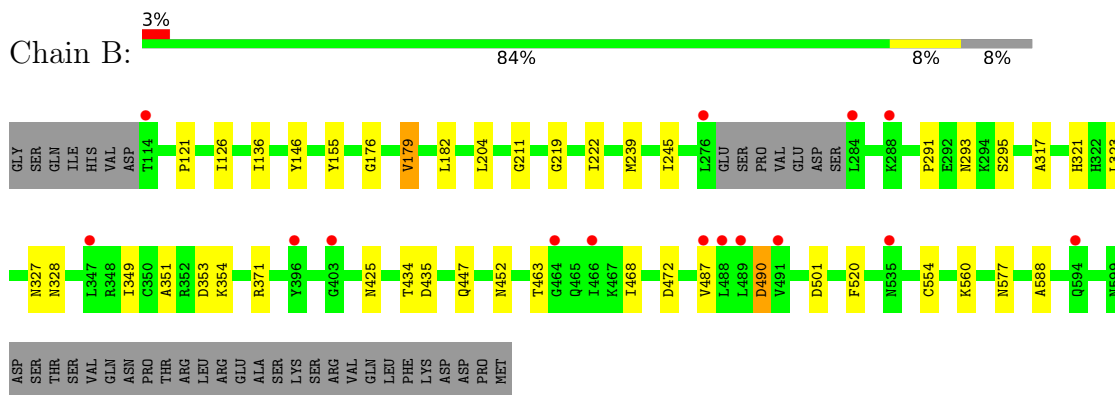
3 Residue-property plots

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: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.98Å 104.98Å 195.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.51 – 2.25 71.51 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.4 (71.51-2.25) 97.4 (71.51-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.195 , 0.239 0.200 , 0.241	Depositor DCC
R_{free} test set	2575 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8030	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: CZF, DZ4, FE, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.41	18/3972 (0.5%)	1.27	13/5373 (0.2%)
1	B	1.36	16/3962 (0.4%)	1.23	14/5362 (0.3%)
All	All	1.39	34/7934 (0.4%)	1.25	27/10735 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	LYS	C-O	-7.71	1.14	1.24
1	A	371	ARG	C-O	-6.85	1.16	1.24
1	A	327	ASN	C-O	-6.83	1.15	1.24
1	B	323	LEU	C-O	6.78	1.32	1.24
1	A	121	PRO	C-O	-6.77	1.15	1.24
1	B	371	ARG	C-O	-6.23	1.16	1.24
1	A	134	ARG	C-O	-6.23	1.16	1.24
1	B	327	ASN	CA-CB	6.19	1.62	1.53
1	A	327	ASN	CA-CB	6.06	1.62	1.53
1	A	328	ASN	CG-OD1	6.04	1.35	1.23
1	A	124	GLY	C-O	6.03	1.32	1.23
1	B	317	ALA	N-CA	-5.99	1.39	1.46
1	A	161	SER	CB-OG	5.92	1.53	1.42
1	B	554	CYS	C-O	-5.90	1.16	1.24
1	A	126	ILE	N-CA	-5.88	1.39	1.46
1	B	447	GLN	CA-C	5.79	1.60	1.52
1	B	353	ASP	C-O	-5.67	1.17	1.24
1	A	150	LEU	C-O	-5.63	1.16	1.24
1	B	146	TYR	CA-CB	5.62	1.61	1.53
1	B	219	GLY	N-CA	5.60	1.52	1.45
1	A	186	GLN	CA-C	5.57	1.59	1.52
1	A	353	ASP	C-O	-5.53	1.17	1.24
1	A	370	HIS	CA-CB	5.44	1.61	1.53
1	B	204	LEU	CA-C	-5.36	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	ALA	C-O	5.35	1.30	1.24
1	A	333	ARG	CZ-NH2	-5.24	1.26	1.33
1	B	452	ASN	CA-C	-5.16	1.48	1.53
1	B	222	ILE	CA-CB	5.14	1.57	1.53
1	A	248	ASN	N-CA	5.13	1.51	1.46
1	A	359	LEU	C-O	-5.13	1.17	1.24
1	B	501	ASP	C-O	-5.10	1.18	1.24
1	B	349	ILE	C-O	-5.04	1.18	1.24
1	A	328	ASN	CG-ND2	5.01	1.43	1.33
1	B	121	PRO	C-O	-5.01	1.18	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASN	N-CA-C	6.74	120.81	112.59
1	B	588	ALA	CA-C-N	6.42	126.35	119.28
1	B	588	ALA	C-N-CA	6.42	126.35	119.28
1	A	588	ALA	CA-C-N	6.33	126.24	119.28
1	A	588	ALA	C-N-CA	6.33	126.24	119.28
1	A	136	ILE	N-CA-C	6.21	116.96	110.62
1	A	211	GLY	CA-C-N	6.15	126.51	119.93
1	A	211	GLY	C-N-CA	6.15	126.51	119.93
1	B	245	ILE	CB-CA-C	-5.95	104.36	111.97
1	B	328	ASN	N-CA-C	5.77	119.63	112.59
1	B	211	GLY	CA-C-N	5.74	126.07	119.93
1	B	211	GLY	C-N-CA	5.74	126.07	119.93
1	B	136	ILE	N-CA-C	5.66	116.39	110.62
1	A	376	HIS	N-CA-C	-5.63	101.70	110.10
1	A	251	LYS	CA-C-N	-5.49	113.38	119.19
1	A	251	LYS	C-N-CA	-5.49	113.38	119.19
1	A	245	ILE	CB-CA-C	-5.42	105.03	111.97
1	B	472	ASP	N-CA-C	5.38	119.33	112.87
1	A	472	ASP	N-CA-C	5.30	119.23	112.87
1	B	182	LEU	CA-C-N	5.26	125.82	119.98
1	B	182	LEU	C-N-CA	5.26	125.82	119.98
1	A	179	VAL	CA-C-O	-5.19	115.67	121.17
1	B	126	ILE	N-CA-C	5.14	115.88	108.48
1	B	447	GLN	CB-CA-C	5.13	119.30	110.79
1	B	239	MET	CG-SD-CE	5.10	112.13	100.90
1	B	179	VAL	CA-C-O	-5.10	115.77	121.17
1	A	523	LYS	CG-CD-CE	5.07	122.96	111.30

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	3879	0	3820	15	0
1	B	3869	0	3796	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	60	0	26	1	0
4	B	60	0	26	0	0
5	A	32	0	0	0	0
5	B	32	0	0	0	0
6	A	51	0	0	1	2
6	B	39	0	0	0	2
All	All	8030	0	7668	22	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 1.

All (22) 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:489:LEU:HD11	1:A:563:TYR:CD2	2.12	0.84
1:A:425:ASN:OD1	1:B:425:ASN:ND2	2.22	0.73
1:A:489:LEU:HD12	1:A:564:ALA:HA	1.81	0.63
1:A:489:LEU:HD11	1:A:563:TYR:HD2	1.68	0.56
1:A:489:LEU:HD21	1:A:563:TYR:HE2	1.71	0.54
1:A:489:LEU:HD21	1:A:563:TYR:CE2	2.42	0.53
1:B:490:ASP:HB2	1:B:560:LYS:HE2	1.91	0.53
1:B:463:THR:HG22	1:B:577:ASN:O	2.09	0.51
1:A:321:HIS:CE1	1:B:321:HIS:CE1	3.01	0.49
1:A:146:TYR:HH	1:B:155:TYR:HH	1.63	0.47
1:B:176:GLY:HA2	1:B:179:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ALA:O	1:B:520:PHE:HA	2.15	0.46
4:A:705:DZ4:PA	6:A:814:HOH:O	2.74	0.45
1:A:176:GLY:HA2	1:A:179:VAL:HG12	1.98	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.18	0.44
1:B:434:THR:O	1:B:435:ASP:C	2.61	0.43
1:A:591:ILE:O	1:A:594:GLN:HG2	2.19	0.42
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.79	0.41
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.21	0.41
1:A:434:THR:O	1:A:435:ASP:C	2.63	0.40
1:A:146:TYR:OH	1:B:155:TYR:OH	2.37	0.40
1:A:476:LEU:N	1:A:477:PRO:HD2	2.37	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)
6:A:850:HOH:O	6:B:839:HOH:O[7_555]	1.90	0.30
6:A:851:HOH:O	6:B:835:HOH:O[7_555]	2.09	0.11

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	475/520 (91%)	465 (98%)	10 (2%)	0	100	100
1	B	475/520 (91%)	463 (98%)	12 (2%)	0	100	100
All	All	950/1040 (91%)	928 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	416/464 (90%)	413 (99%)	3 (1%)	76	82
1	B	414/464 (89%)	410 (99%)	4 (1%)	68	77
All	All	830/928 (89%)	823 (99%)	7 (1%)	73	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	A	326	GLN
1	A	468	ILE
1	B	295	SER
1	B	468	ILE
1	B	487	VAL
1	B	490	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	ASN
1	A	425	ASN
1	A	447	GLN
1	A	452	ASN
1	A	571	GLN
1	B	248	ASN
1	B	364	HIS
1	B	425	ASN
1	B	447	GLN
1	B	452	ASN
1	B	567	GLN
1	B	571	GLN
1	B	599	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	DZ4	A	707	3	31,32,32	1.16	2 (6%)	44,50,50	1.18	6 (13%)
4	DZ4	B	706	2,3	31,32,32	1.41	3 (9%)	44,50,50	1.38	4 (9%)
5	CZF	A	706	3	33,34,34	1.18	2 (6%)	45,54,54	1.12	2 (4%)
4	DZ4	A	705	2,3	31,32,32	1.49	4 (12%)	44,50,50	1.40	6 (13%)
4	DZ4	B	701	3	31,32,32	1.08	3 (9%)	44,50,50	1.66	8 (18%)
5	CZF	B	707	3	33,34,34	0.86	1 (3%)	45,54,54	1.40	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DZ4	A	707	3	-	8/19/34/34	0/3/3/3
4	DZ4	B	706	2,3	-	1/19/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CZF	A	706	3	-	6/22/38/38	0/3/3/3
4	DZ4	A	705	2,3	-	1/19/34/34	0/3/3/3
4	DZ4	B	701	3	-	3/19/34/34	0/3/3/3
5	CZF	B	707	3	-	12/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	DZ4	PB-O1B	5.03	1.53	1.46
4	A	705	DZ4	PB-O1B	4.90	1.53	1.46
5	A	706	CZF	P2-O7	4.01	1.63	1.59
4	A	705	DZ4	PG-O3G	-3.89	1.40	1.54
4	B	706	DZ4	PB-O2B	-3.53	1.47	1.56
4	A	705	DZ4	PA-O1A	3.48	1.51	1.46
4	B	706	DZ4	PA-O1A	3.40	1.51	1.46
4	A	707	DZ4	PA-O1A	3.30	1.51	1.46
4	B	701	DZ4	PB-O1B	3.00	1.50	1.46
4	A	707	DZ4	PA-O2A	-2.93	1.49	1.56
4	B	701	DZ4	PB-O2B	-2.85	1.49	1.56
4	B	701	DZ4	PA-O1A	2.51	1.50	1.46
5	A	706	CZF	C5-N4	2.51	1.39	1.37
4	A	705	DZ4	PB-O2B	-2.30	1.50	1.56
5	B	707	CZF	P1-O7	2.20	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	DZ4	O2B-PB-O1B	6.02	122.77	109.87
5	B	707	CZF	P1-O5-C8	5.12	150.71	121.35
4	A	705	DZ4	O2B-PB-O1B	4.52	119.56	109.87
4	B	701	DZ4	O2A-PA-O1A	4.31	119.12	109.87
4	B	701	DZ4	O1B-PB-N3A	-4.26	105.50	111.77
4	B	706	DZ4	O2A-PA-O1A	4.19	118.85	109.87
4	A	705	DZ4	O2A-PA-O1A	4.07	118.59	109.87
4	B	706	DZ4	O2A-PA-O5'	-4.00	96.05	106.69
4	B	706	DZ4	O3B-PB-N3A	-3.37	97.25	106.59
4	B	706	DZ4	O2B-PB-O1B	3.30	116.94	109.87
4	A	705	DZ4	O5'-PA-O1A	-3.20	104.78	114.27
4	A	707	DZ4	O2A-PA-O1A	3.05	116.41	109.87
4	A	707	DZ4	O2B-PB-O1B	2.96	116.21	109.87
4	A	707	DZ4	O3G-PG-O2G	2.84	118.46	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	705	DZ4	O1A-PA-N3A	-2.67	107.83	111.77
4	A	707	DZ4	O2A-PA-O5'	-2.65	99.63	106.69
5	B	707	CZF	O5-P1-O8	2.63	119.36	108.94
4	B	701	DZ4	O3G-PG-O2G	2.42	116.86	107.80
4	A	705	DZ4	O3'-C3'-C2'	2.41	119.25	110.88
4	B	701	DZ4	O1A-PA-N3A	-2.34	108.32	111.77
5	A	706	CZF	O3-C4-C6	-2.32	104.43	111.08
5	B	707	CZF	O9-P1-O7	2.29	113.47	107.27
4	A	707	DZ4	O1A-PA-N3A	-2.23	108.49	111.77
5	B	707	CZF	N2-C2-N1	2.22	119.24	115.74
4	A	705	DZ4	O1B-PB-N3A	-2.20	108.53	111.77
4	A	707	DZ4	O1B-PB-N3A	-2.20	108.54	111.77
5	B	707	CZF	O13-P3-O10	-2.15	97.43	104.64
4	B	701	DZ4	O2A-PA-O5'	-2.11	101.08	106.69
5	B	707	CZF	O4-C1-N4	-2.10	103.59	108.36
4	B	701	DZ4	O2B-PB-O3B	-2.06	97.78	104.64
5	A	706	CZF	P1-O5-C8	2.05	133.09	121.35
4	B	701	DZ4	O3'-C3'-C4'	2.03	117.78	110.07

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	DZ4	PA-N3A-PB-O1B
4	A	707	DZ4	PB-N3A-PA-O1A
4	A	707	DZ4	PA-N3A-PB-O1B
4	A	707	DZ4	PG-O3B-PB-O2B
4	A	707	DZ4	PB-O3B-PG-O2G
4	B	701	DZ4	PB-N3A-PA-O1A
4	B	706	DZ4	PA-N3A-PB-O1B
5	A	706	CZF	P2-O10-P3-O14
5	B	707	CZF	C8-O5-P1-O8
5	B	707	CZF	O4-C6-C8-O5
5	B	707	CZF	C4-C6-C8-O5
5	B	707	CZF	P2-O10-P3-O15
5	A	706	CZF	P2-O10-P3-O15
5	B	707	CZF	P2-O10-P3-O14
5	A	706	CZF	P2-O7-P1-O9
5	B	707	CZF	P2-O7-P1-O9
4	B	701	DZ4	PA-N3A-PB-O3B
5	B	707	CZF	C8-O5-P1-O7
5	B	707	CZF	C8-O5-P1-O9

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Mol	Chain	Res	Type	Atoms
5	A	706	CZF	C6-C8-O5-P1
4	A	707	DZ4	PB-O3B-PG-O3G
5	A	706	CZF	P2-O7-P1-O8
5	B	707	CZF	P2-O7-P1-O8
4	A	707	DZ4	PG-O3B-PB-O1B
4	B	701	DZ4	PG-O3B-PB-O1B
5	B	707	CZF	C6-C8-O5-P1
4	A	707	DZ4	PB-O3B-PG-O1G
4	A	707	DZ4	PA-N3A-PB-O3B
5	B	707	CZF	C3-C1-N4-C5
5	A	706	CZF	P3-O10-P2-O11
5	B	707	CZF	P3-O10-P2-O11

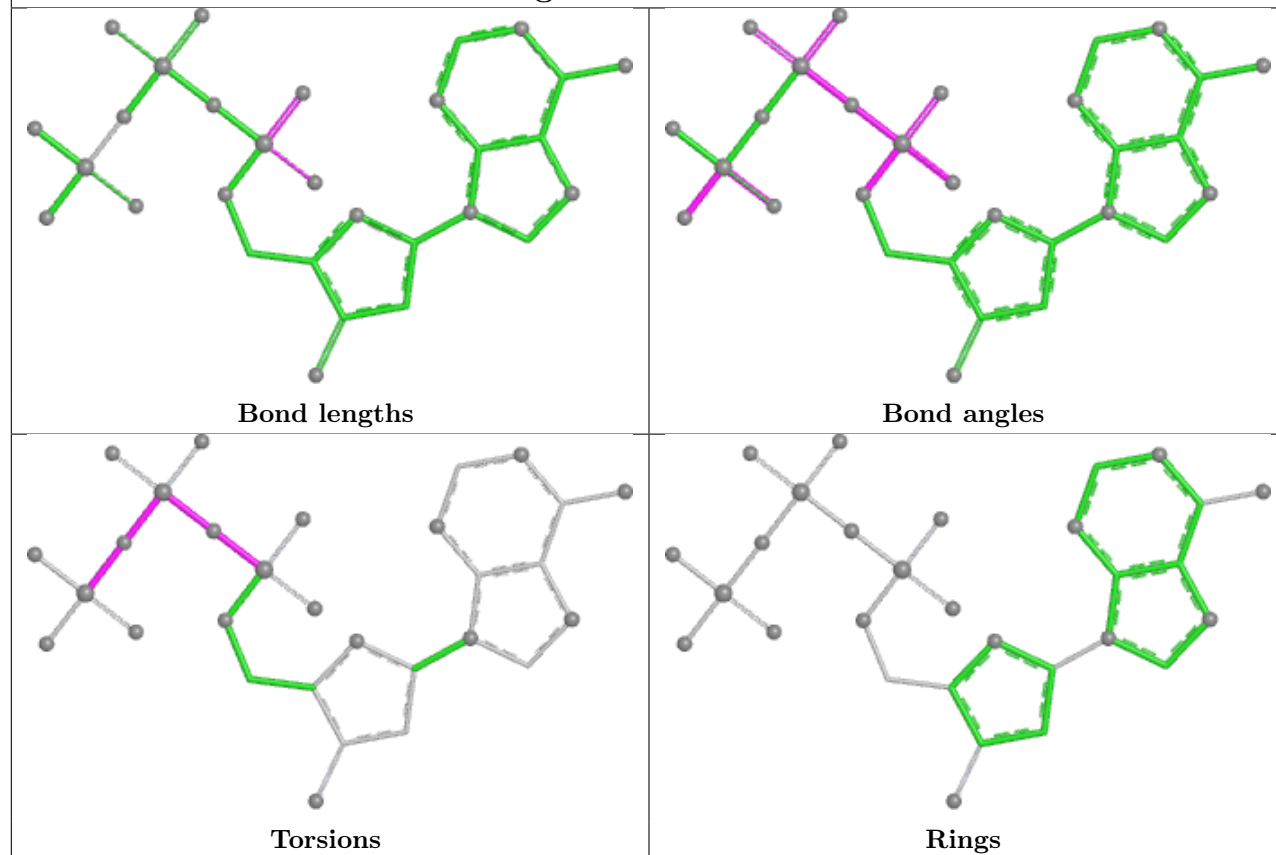
There are no ring outliers.

1 monomer is involved in 1 short contact:

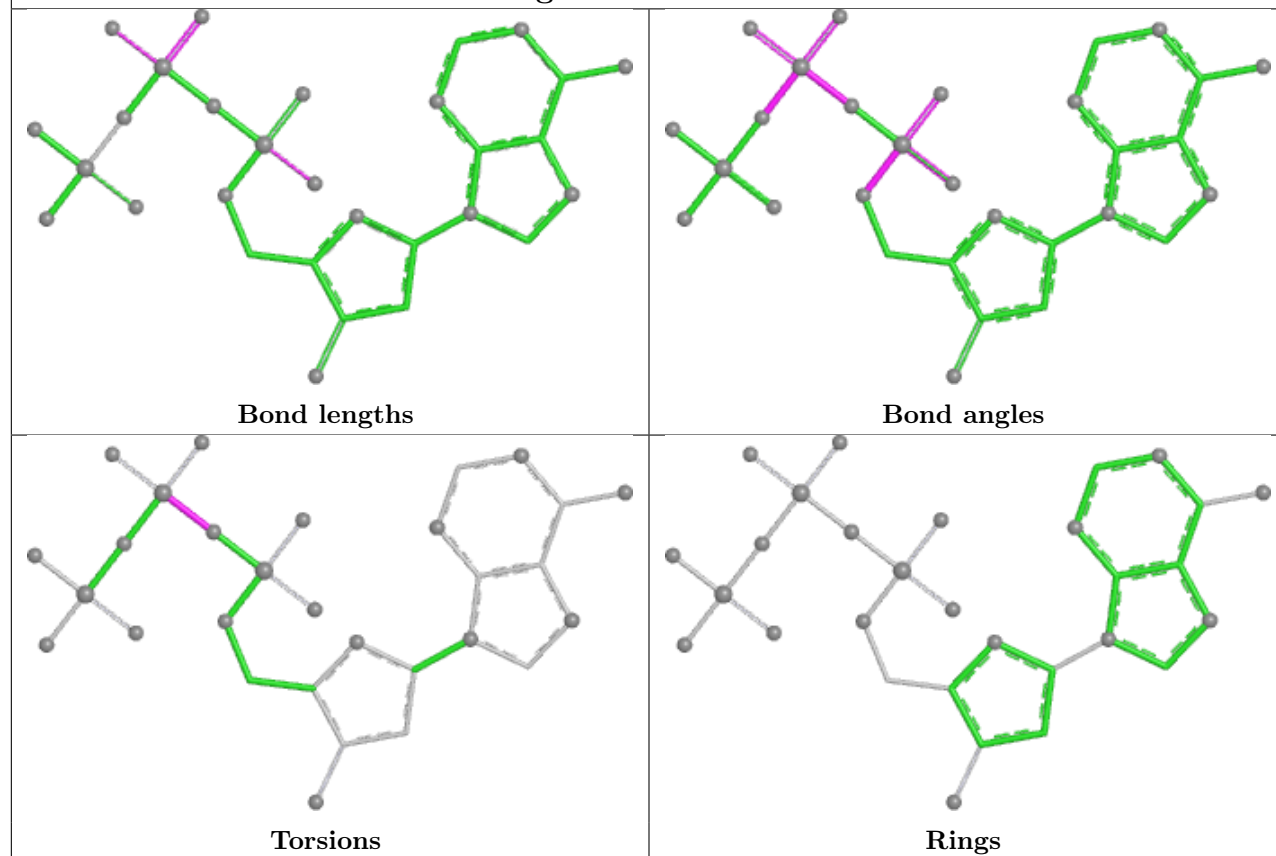
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	DZ4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

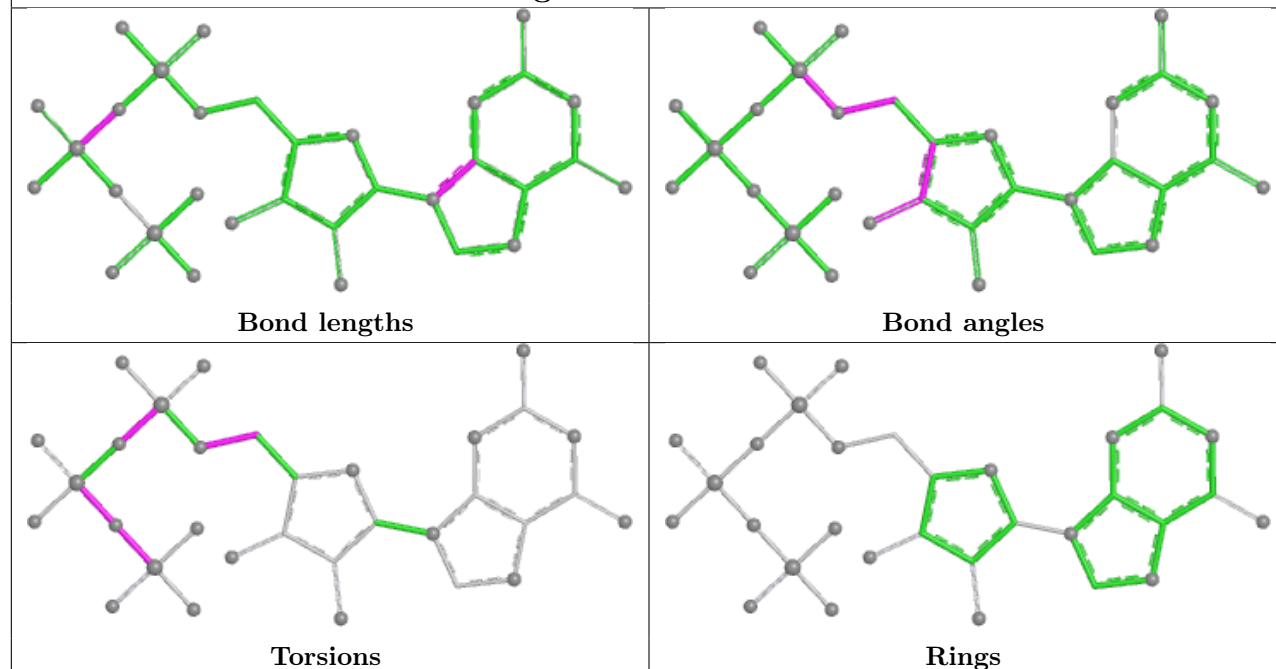
Ligand DZ4 A 707



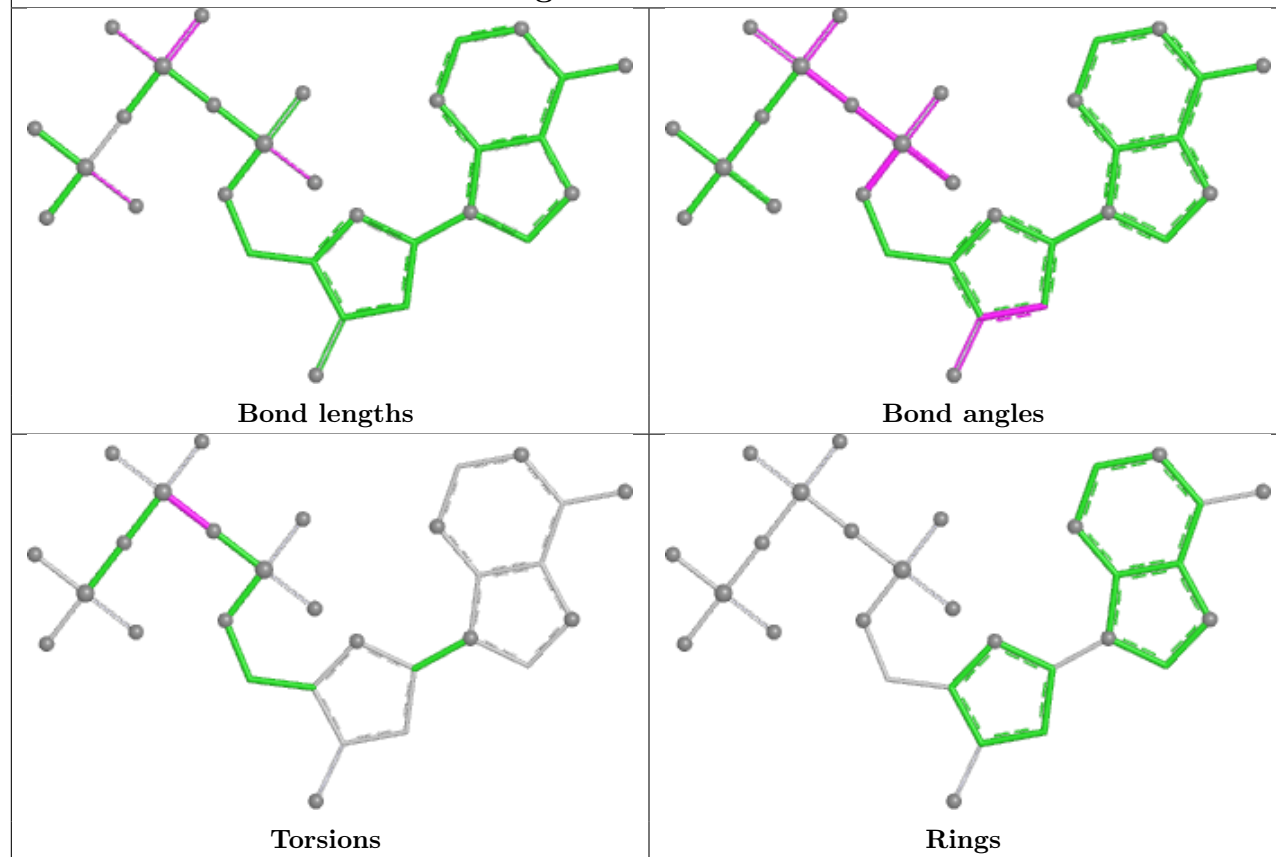
Ligand DZ4 B 706

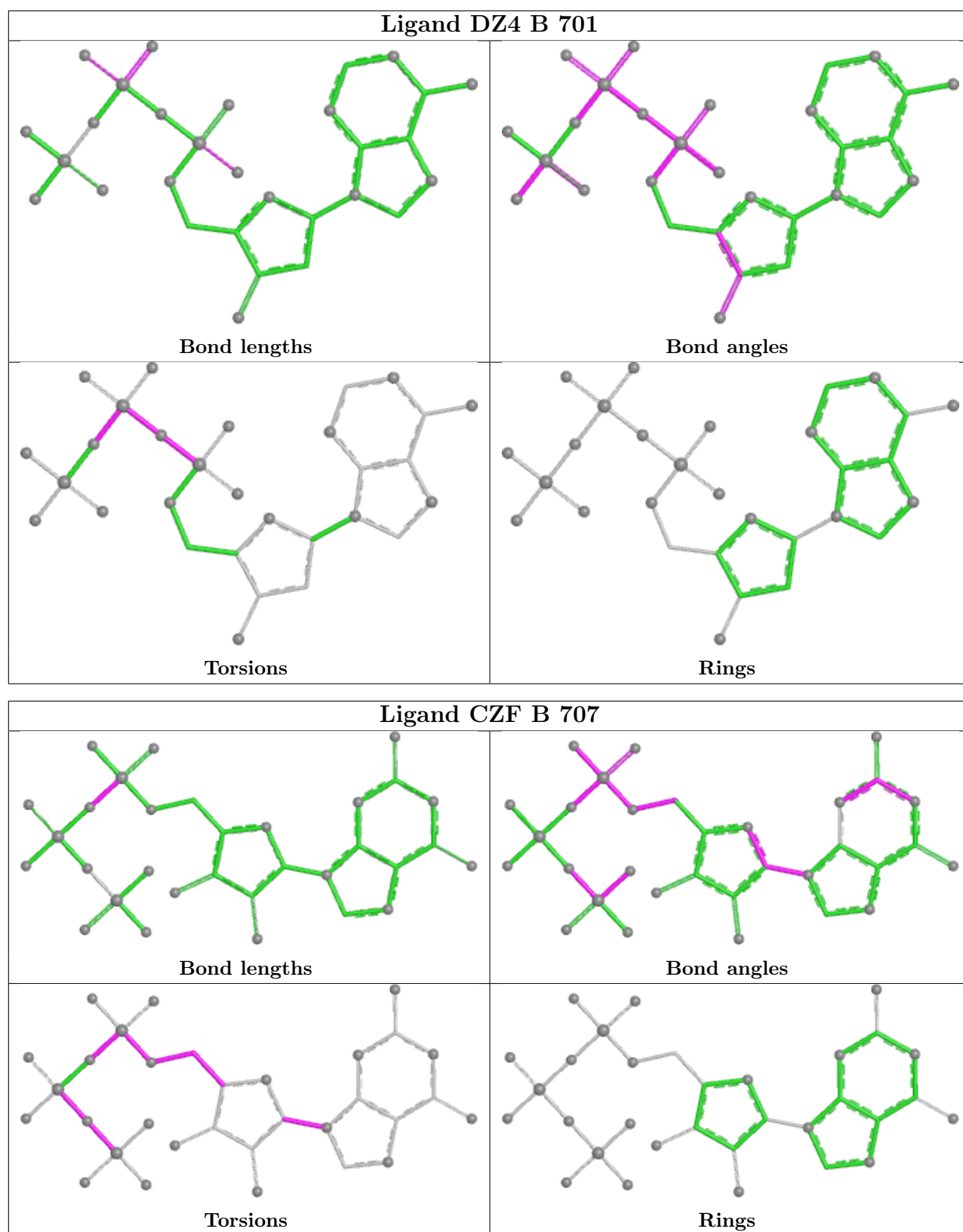


Ligand CZF A 706



Ligand DZ4 A 705





5.7 Other polymers [i](#)

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	479/520 (92%)	-0.00	11 (2%) 61 61	23, 42, 80, 136	0
1	B	479/520 (92%)	0.14	15 (3%) 51 51	27, 47, 80, 139	0
All	All	958/1040 (92%)	0.07	26 (2%) 56 57	23, 45, 80, 139	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	VAL	5.4
1	A	284	LEU	5.1
1	A	466	ILE	4.2
1	B	488	LEU	4.2
1	B	114	THR	4.2
1	B	276	LEU	4.1
1	B	491	VAL	3.9
1	A	488	LEU	3.8
1	A	489	LEU	3.6
1	A	487	VAL	3.4
1	B	284	LEU	3.3
1	B	535	ASN	2.8
1	B	489	LEU	2.8
1	A	114	THR	2.7
1	B	288	LYS	2.7
1	B	464	GLY	2.6
1	B	403	GLY	2.5
1	A	599	ASN	2.4
1	B	466	ILE	2.4
1	A	594	GLN	2.4
1	B	594	GLN	2.3
1	A	276	LEU	2.3
1	A	396	TYR	2.2
1	A	491	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	347	LEU	2.1
1	B	396	TYR	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](#)

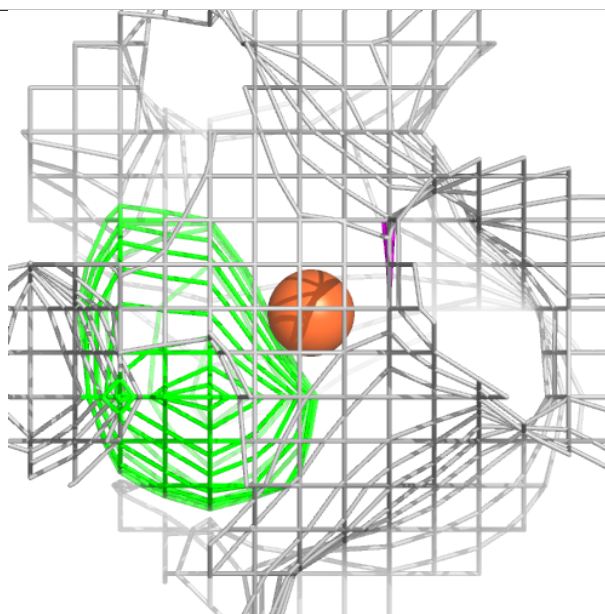
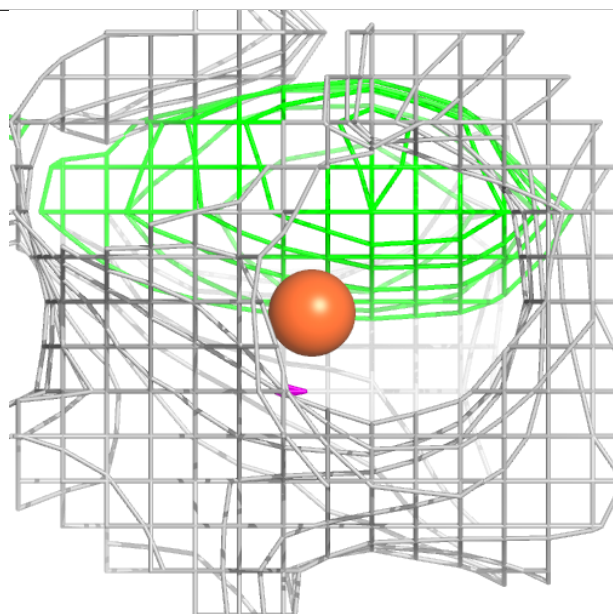
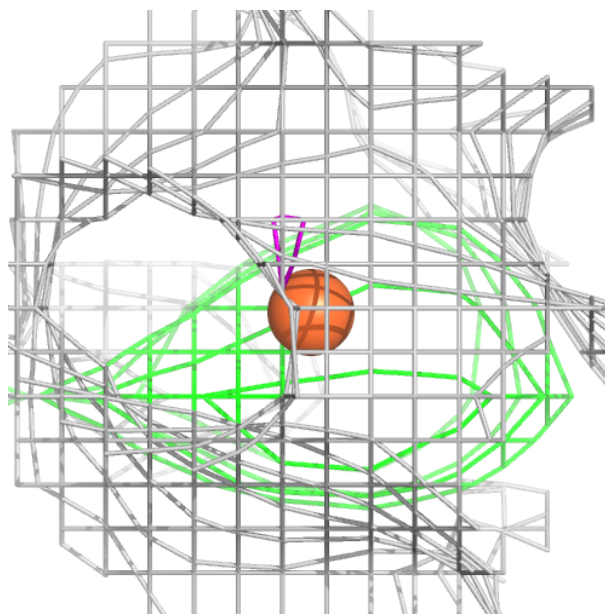
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	FE	B	702	1/1	0.91	0.06	34,34,34,34	0
3	MN	B	705	1/1	0.93	0.07	45,45,45,45	0
3	MN	B	703	1/1	0.94	0.06	41,41,41,41	0
4	DZ4	B	706	30/30	0.97	0.06	30,33,36,39	0
5	CZF	B	707	32/32	0.97	0.05	31,35,44,47	0
4	DZ4	B	701	30/30	0.98	0.04	23,25,33,36	0
4	DZ4	A	705	30/30	0.98	0.05	28,31,38,39	0
5	CZF	A	706	32/32	0.98	0.04	23,26,37,39	0
4	DZ4	A	707	30/30	0.98	0.05	25,31,39,41	0
3	MN	A	704	1/1	0.99	0.03	33,33,33,33	0
3	MN	B	704	1/1	1.00	0.02	39,39,39,39	0
3	MN	A	703	1/1	1.00	0.01	31,31,31,31	0
2	FE	A	701	1/1	1.00	0.01	26,26,26,26	0
3	MN	A	702	1/1	1.00	0.01	30,30,30,30	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.

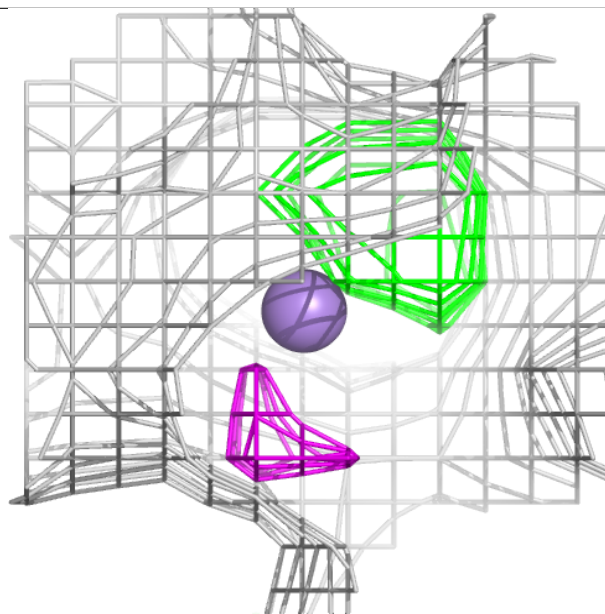
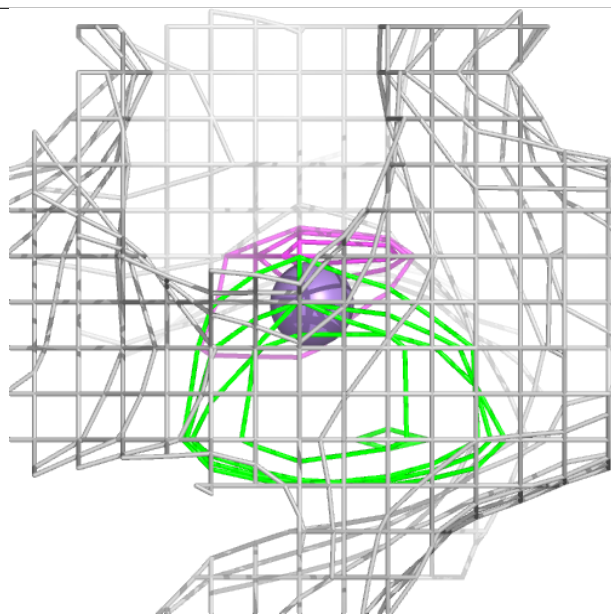
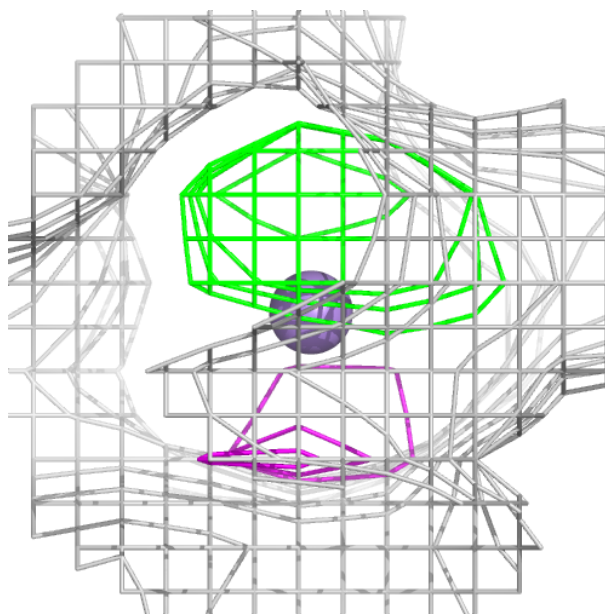
Electron density around FE B 702:

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



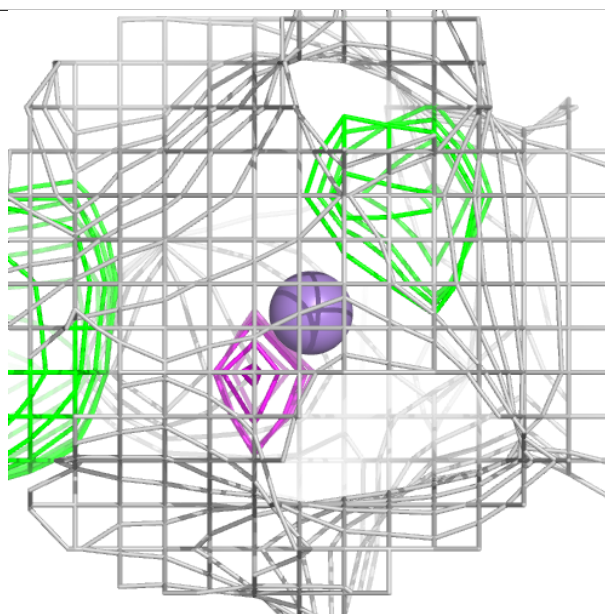
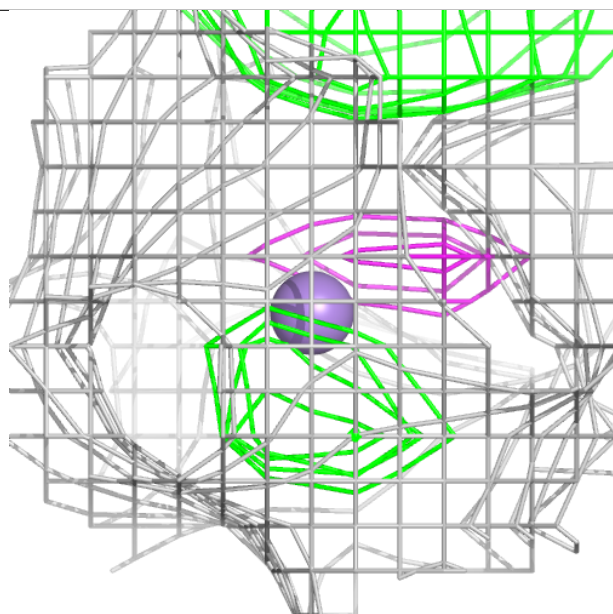
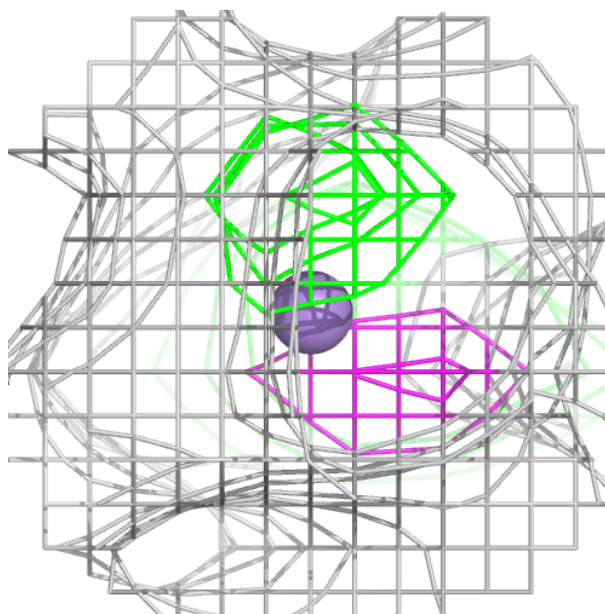
Electron density around MN B 705:

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



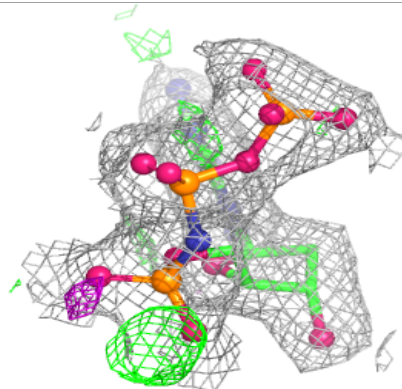
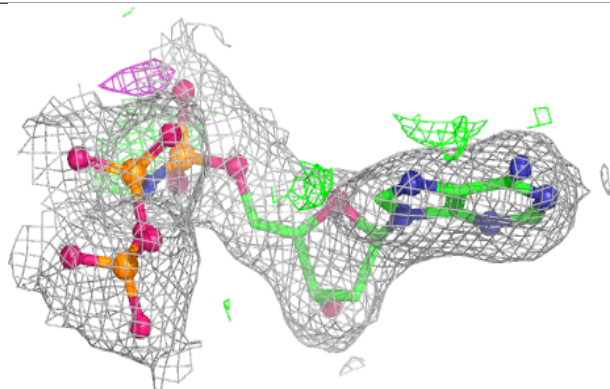
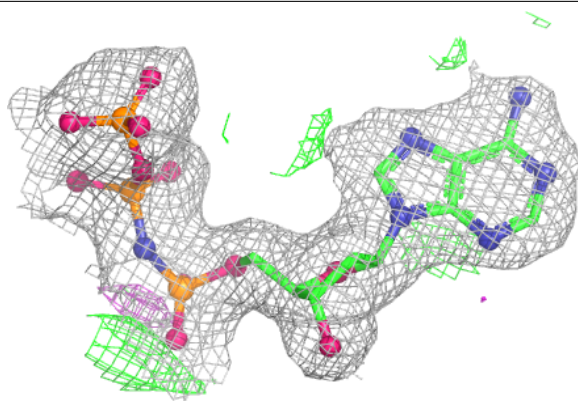
Electron density around MN B 703:

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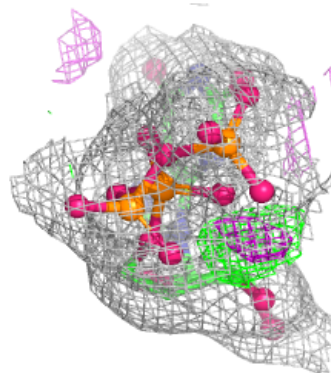
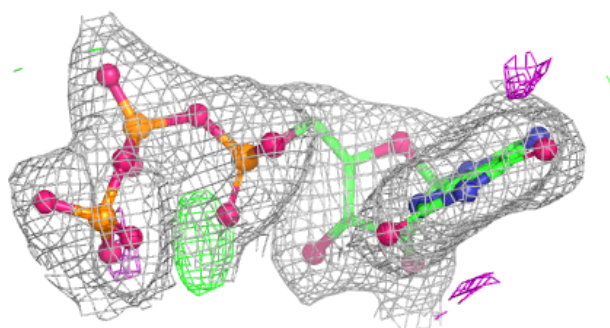
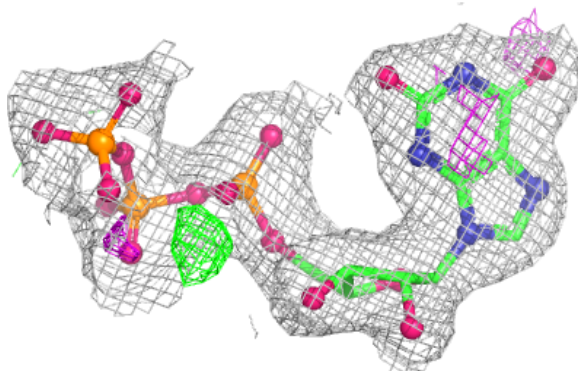


Electron density around DZ4 B 706:

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

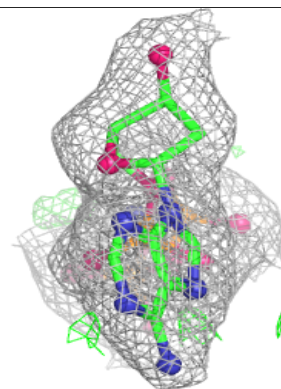
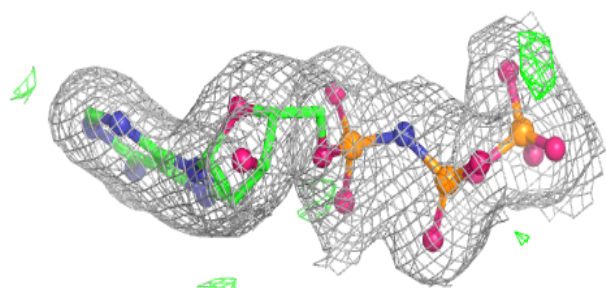
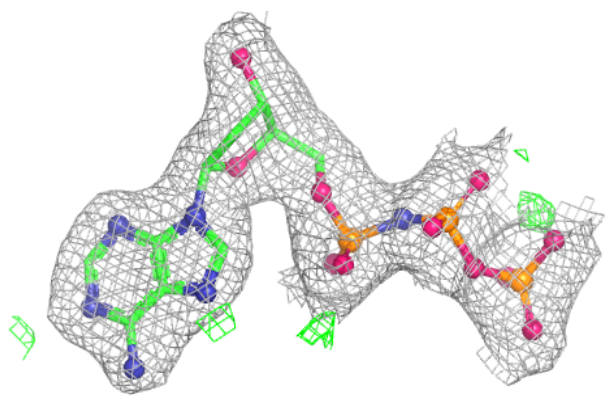
**Electron density around CZF B 707:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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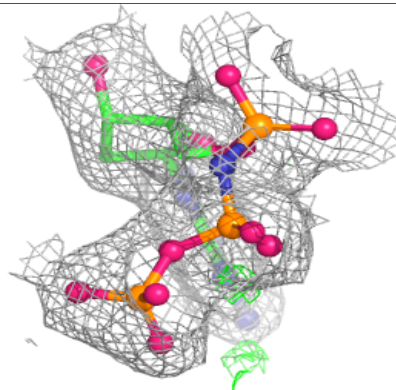
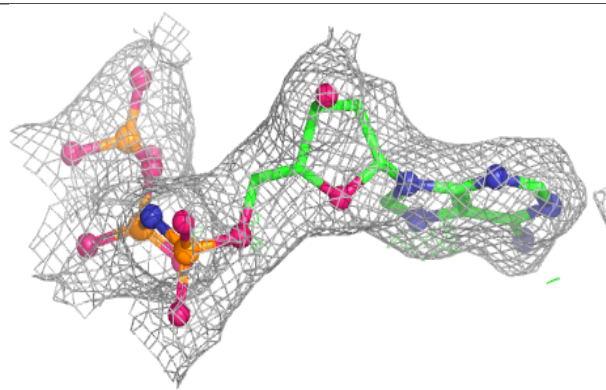
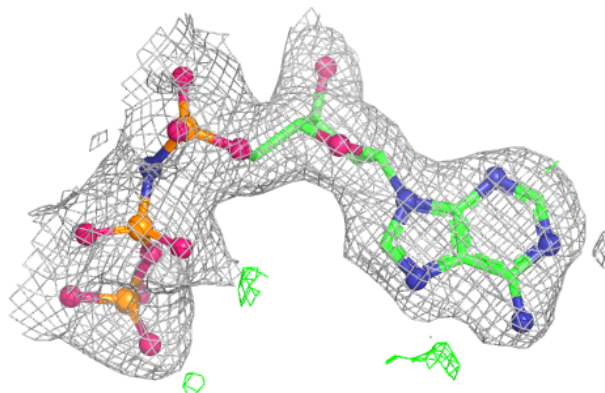


Electron density around DZ4 B 701:

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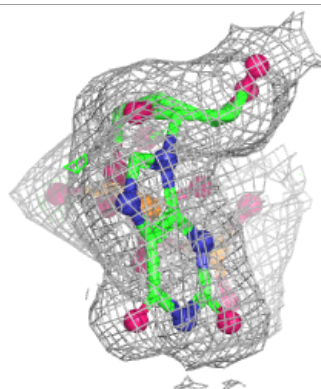
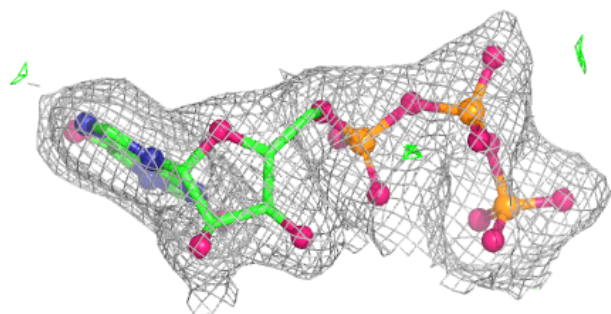
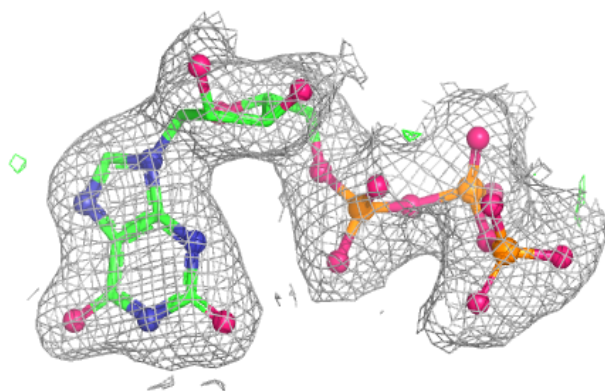
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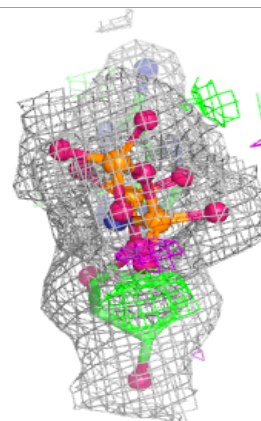
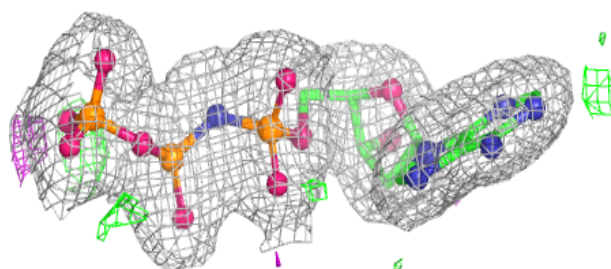
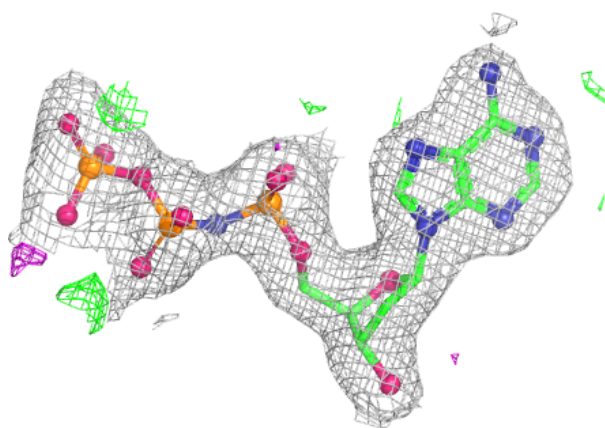


Electron density around CZF A 706:

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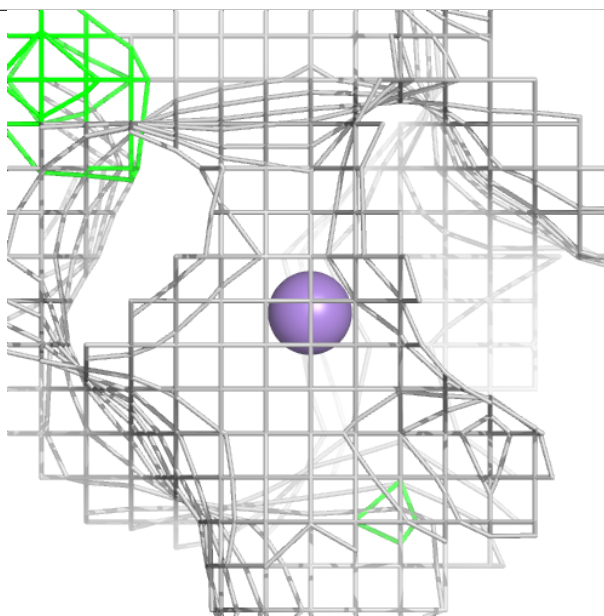
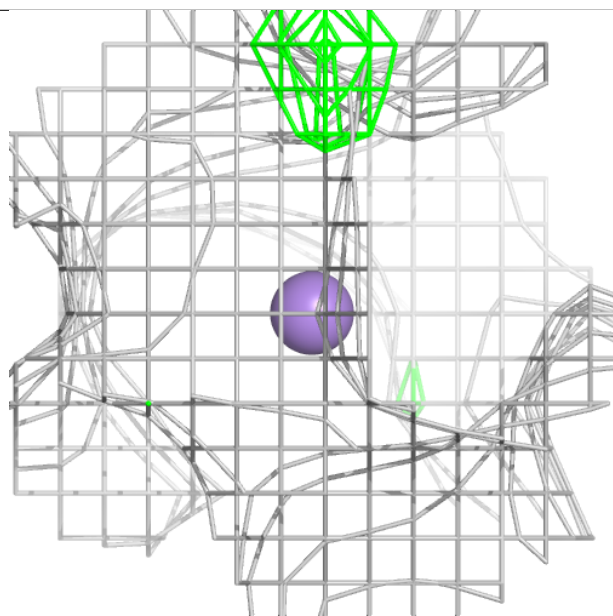
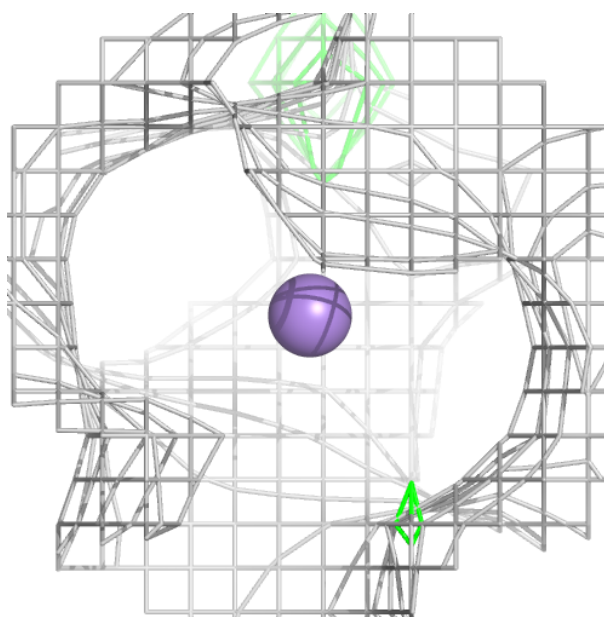
**Electron density around DZ4 A 707:**

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and green (positive)



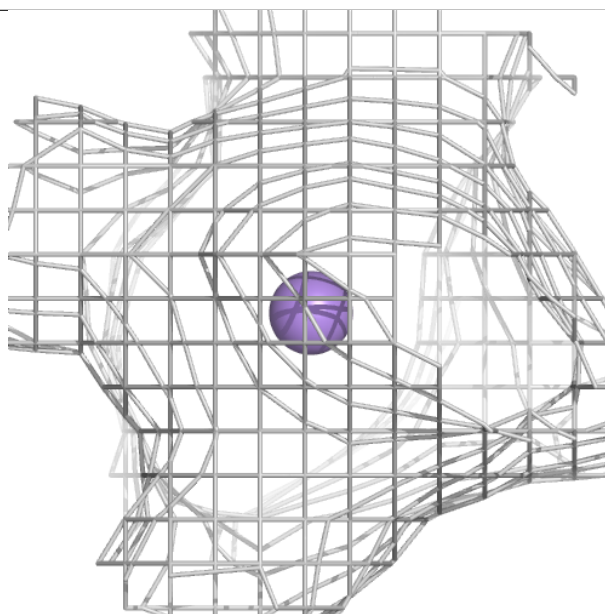
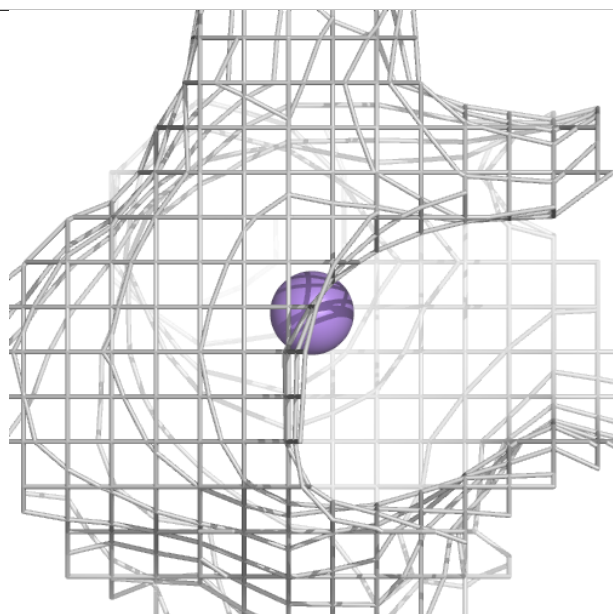
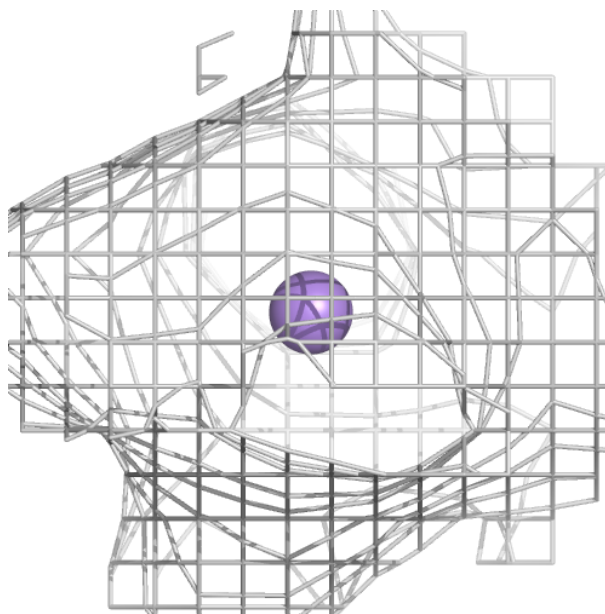
Electron density around MN A 704:

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and green (positive)



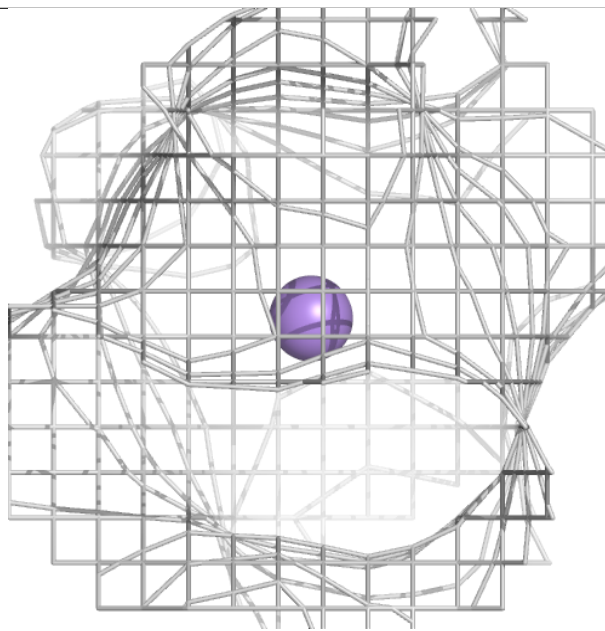
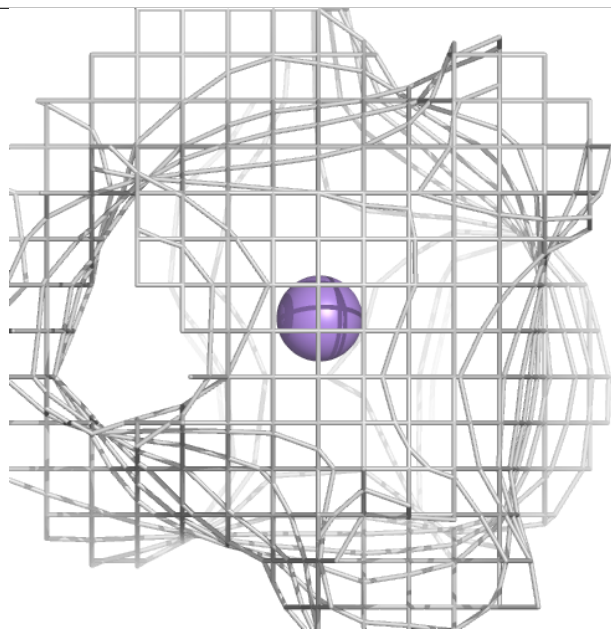
Electron density around MN B 704:

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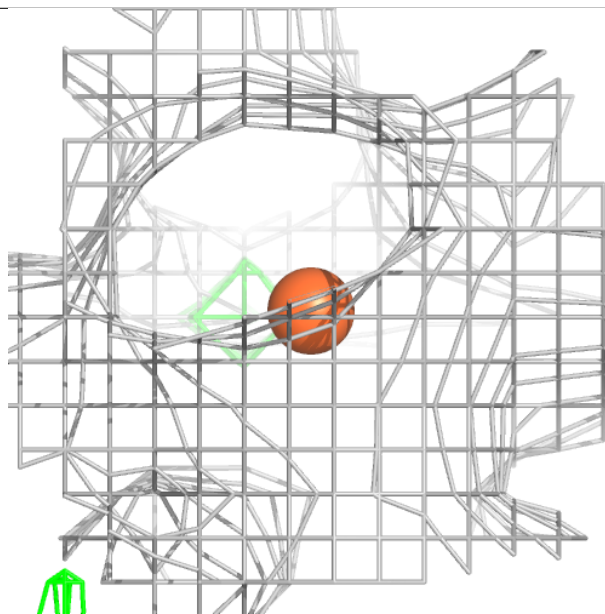
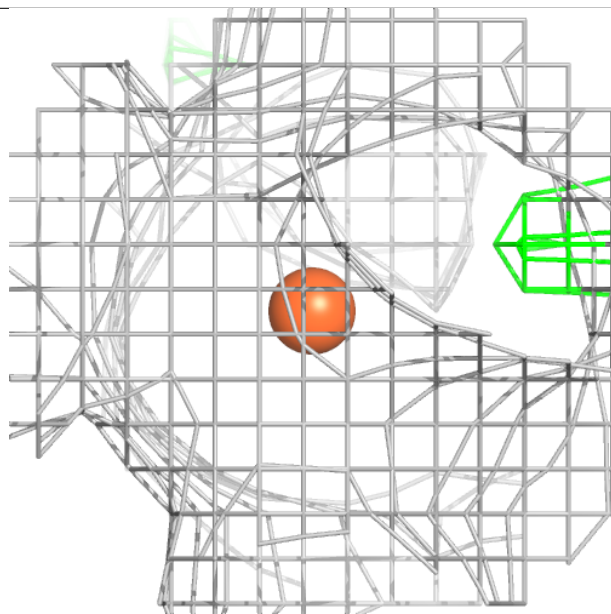
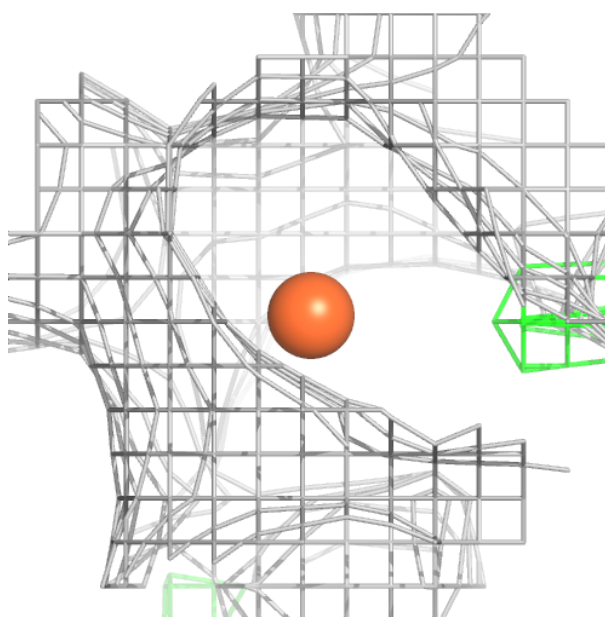
Electron density around MN A 703:

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



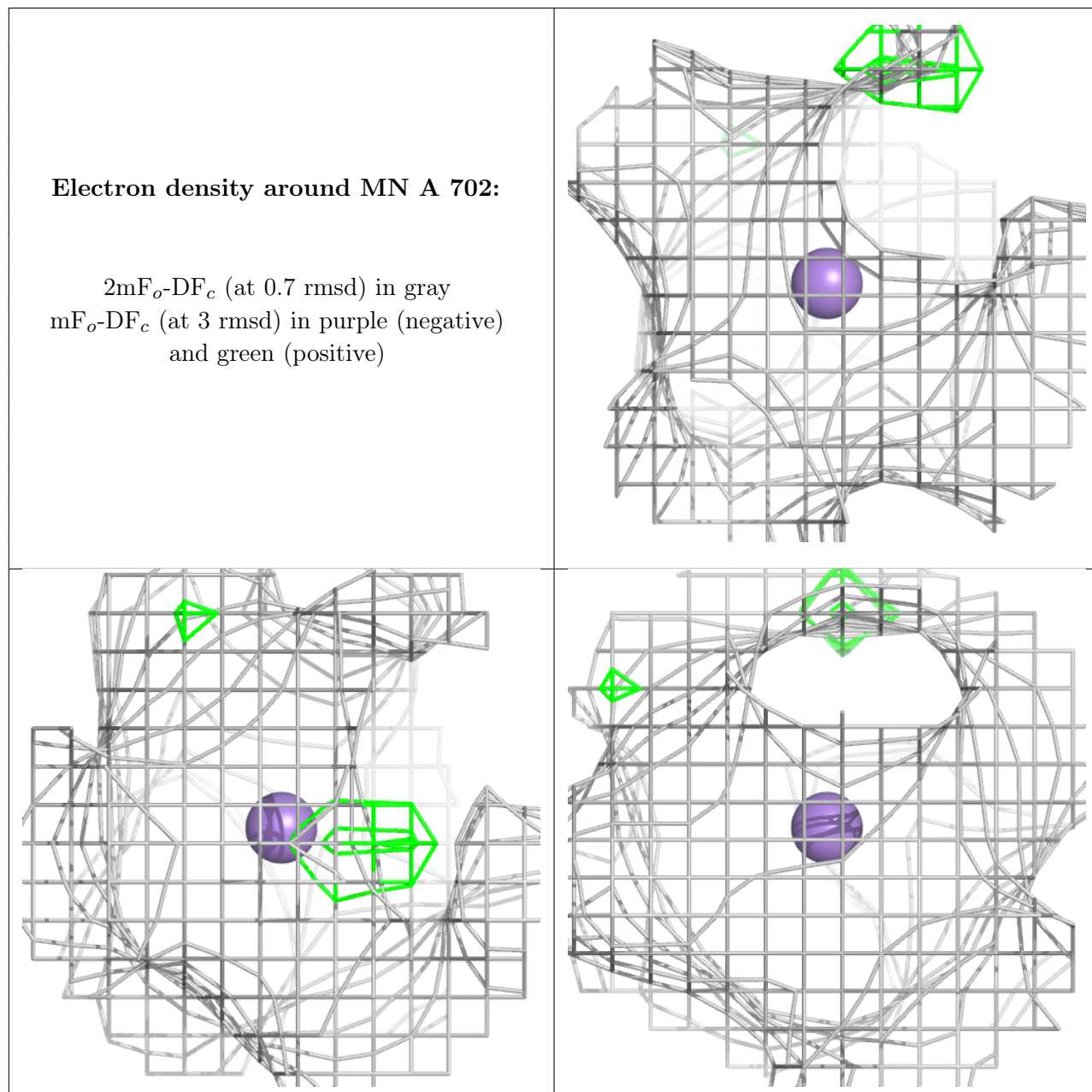
Electron density around FE A 701:

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



Electron density around MN A 702:

$2mF_o-DF_c$ (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.