



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:23 AM BST

PDB ID : 6TXF
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

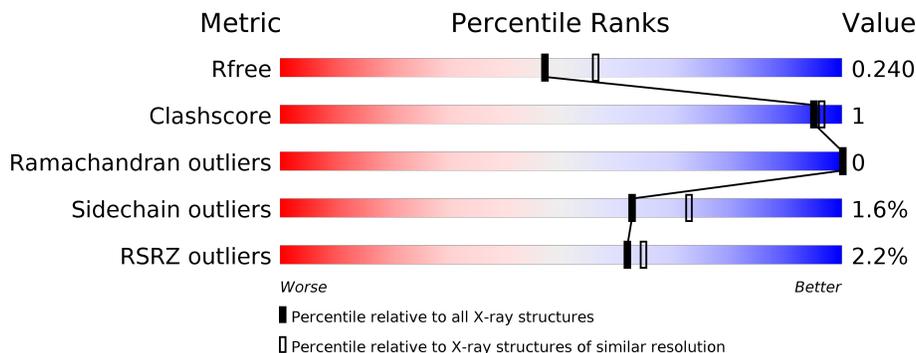
1 Overall quality at a glance

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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 on 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	 3% 86% 6% 8%
1	B	520	 % 87% 5% 8%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	479	3879	2483	675	701	20	0	0	0
1	B	479	3869	2477	670	702	20	0	0	0

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

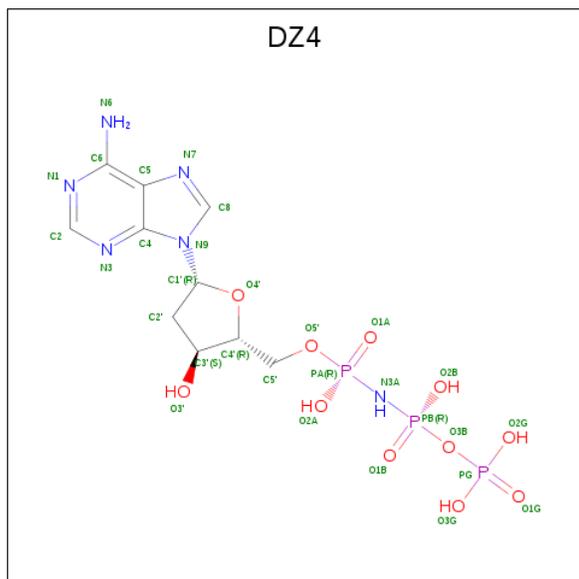
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

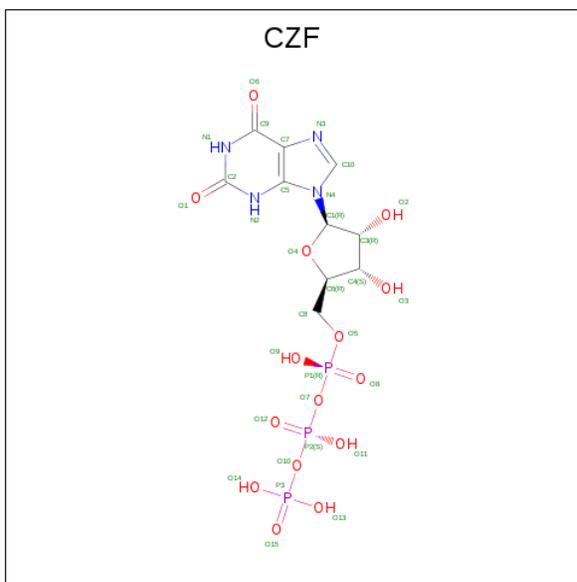
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mn	0	0
			3	3		
3	A	3	Total	Mn	0	0
			3	3		

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonoxy)phosphoryl]amino}phosphoryl]adenosine (three-letter code: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	A	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	6	11	3		

- 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 (three-letter code: CZF) (formula: C₁₀H₁₅N₄O₁₅P₃) (labeled as "Ligand of Interest" by author).



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

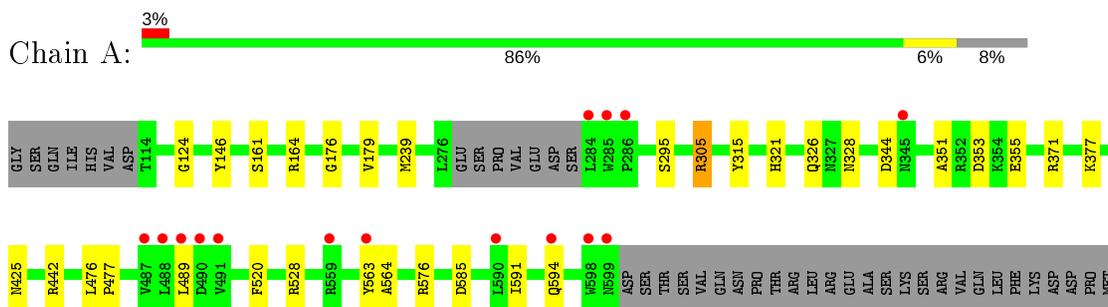
- Molecule 6 is water.

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

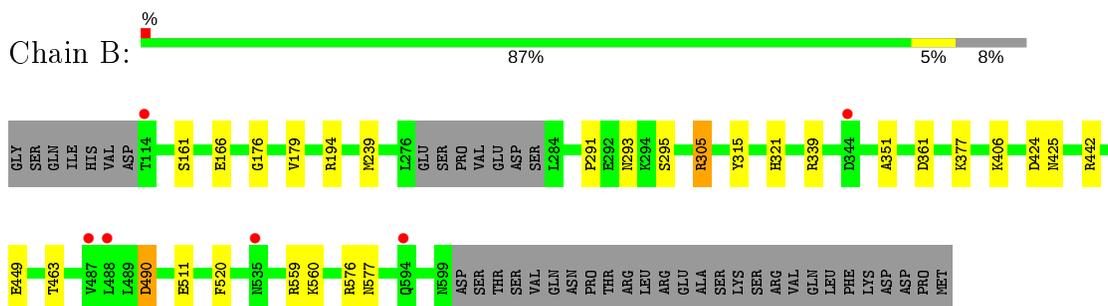
3 Residue-property plots [i](#)

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

- Molecule 1: 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 71.54 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.4 (71.51-2.25) 97.2 (71.54-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.25Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.195 , 0.239 0.200 , 0.240	Depositor DCC
R_{free} test set	2570 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8030	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CZF, FE, DZ4

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	1.10	5/3972 (0.1%)	1.05	11/5373 (0.2%)
1	B	1.05	5/3962 (0.1%)	1.04	10/5362 (0.2%)
All	All	1.08	10/7934 (0.1%)	1.05	21/10735 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	SER	CB-OG	9.03	1.53	1.42
1	B	449	GLU	CD-OE1	6.82	1.33	1.25
1	A	355	GLU	CD-OE1	6.78	1.33	1.25
1	B	161	SER	CB-OG	6.72	1.50	1.42
1	B	166	GLU	CD-OE2	5.70	1.31	1.25
1	B	166	GLU	CG-CD	5.64	1.60	1.51
1	A	146	TYR	CG-CD1	-5.47	1.32	1.39
1	A	124	GLY	C-O	5.41	1.32	1.23
1	B	449	GLU	CD-OE2	5.17	1.31	1.25
1	A	328	ASN	CG-OD1	5.04	1.35	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	B	239	MET	CG-SD-CE	7.46	112.13	100.20
1	B	576	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	164	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	576	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	239	MET	CG-SD-CE	6.44	110.50	100.20
1	B	559	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	B	442	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	449	GLU	OE1-CD-OE2	6.00	130.50	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	585	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	344	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	371	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	353	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	305	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	339	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	361	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	424	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	305	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	559	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	528	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	164	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	12	0
1	B	3869	0	3796	7	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	18	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 (18) 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:B:176:GLY:HA2	1:B:179:VAL:HG12	1.97	0.46
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:A:591:ILE:O	1:A:594:GLN:HG2	2.19	0.42
1:A:489:LEU:HA	1:A:489:LEU:HD23	1.79	0.41
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.21	0.41
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 [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	475/520 (91%)	465 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	416/464 (90%)	411 (99%)	5 (1%)	71	80
1	B	414/464 (89%)	406 (98%)	8 (2%)	57	66
All	All	830/928 (89%)	817 (98%)	13 (2%)	62	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	A	305	ARG
1	A	315	TYR
1	A	326	GLN
1	A	377	LYS
1	B	194	ARG
1	B	295	SER
1	B	305	ARG
1	B	315	TYR
1	B	377	LYS
1	B	406	LYS
1	B	490	ASP
1	B	511	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	GLN
1	A	380	ASN
1	A	425	ASN
1	B	328	ASN
1	B	364	HIS
1	B	375	GLN
1	B	380	ASN
1	B	425	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	29,32,32	1.25	2 (6%)	33,50,50	1.37	6 (18%)
5	CZF	B	707	3	25,34,34	1.02	1 (4%)	29,54,54	3.06	5 (17%)
4	DZ4	A	705	3,2	29,32,32	1.47	4 (13%)	33,50,50	1.61	7 (21%)
4	DZ4	B	701	3	29,32,32	1.07	3 (10%)	33,50,50	1.91	8 (24%)
5	CZF	A	706	3	25,34,34	1.25	3 (12%)	29,54,54	2.98	4 (13%)
4	DZ4	B	706	3,2	29,32,32	1.41	3 (10%)	33,50,50	1.64	5 (15%)

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	-	7/15/34/34	0/3/3/3
5	CZF	B	707	3	-	10/18/38/38	0/3/3/3
4	DZ4	A	705	3,2	-	1/15/34/34	0/3/3/3
4	DZ4	B	701	3	-	2/15/34/34	0/3/3/3
5	CZF	A	706	3	-	5/18/38/38	0/3/3/3
4	DZ4	B	706	3,2	-	2/15/34/34	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	DZ4	PB-O1B	4.82	1.53	1.46
4	A	705	DZ4	PB-O1B	4.69	1.53	1.46
5	A	706	CZF	C9-N1	3.85	1.39	1.33
4	A	705	DZ4	PG-O3G	-3.76	1.40	1.54
5	B	707	CZF	C9-N1	3.71	1.39	1.33
4	B	706	DZ4	PB-O2B	-3.47	1.47	1.56
4	A	705	DZ4	PA-O1A	3.34	1.51	1.46
4	B	706	DZ4	PA-O1A	3.27	1.51	1.46
4	A	707	DZ4	PA-O1A	3.17	1.51	1.46
4	B	701	DZ4	PB-O1B	2.88	1.50	1.46
4	A	707	DZ4	PA-O2A	-2.87	1.49	1.56
4	B	701	DZ4	PB-O2B	-2.79	1.49	1.56
4	B	701	DZ4	PA-O1A	2.42	1.50	1.46
5	A	706	CZF	C5-N2	2.27	1.36	1.33
4	A	705	DZ4	PB-O2B	-2.25	1.50	1.56
5	A	706	CZF	C10-N3	-2.08	1.31	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	706	CZF	C9-N1-C2	12.39	125.60	115.14
5	B	707	CZF	C9-N1-C2	12.20	125.44	115.14
5	B	707	CZF	C7-C9-N1	-7.61	113.03	123.43
5	A	706	CZF	C7-C9-N1	-7.31	113.44	123.43
4	B	701	DZ4	O2B-PB-O1B	6.13	122.77	109.92
5	B	707	CZF	P1-O5-C8	4.95	150.71	121.68
4	A	705	DZ4	O2B-PB-O1B	4.60	119.56	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	DZ4	O2A-PA-O1A	4.39	119.12	109.92
4	B	701	DZ4	O1B-PB-N3A	-4.26	105.50	111.77
4	B	706	DZ4	O2A-PA-O1A	4.26	118.85	109.92
4	A	705	DZ4	O2A-PA-O1A	4.14	118.59	109.92
4	B	706	DZ4	O2A-PA-O5'	-3.95	96.05	106.75
4	B	706	DZ4	O3B-PB-N3A	-3.37	97.25	106.59
4	B	706	DZ4	O2B-PB-O1B	3.35	116.94	109.92
4	B	706	DZ4	C5-C6-N6	3.18	125.18	120.35
4	A	707	DZ4	O2A-PA-O1A	3.09	116.41	109.92
4	A	707	DZ4	O2B-PB-O1B	3.00	116.21	109.92
4	A	707	DZ4	O3G-PG-O2G	2.83	118.46	107.64
5	A	706	CZF	C1-N4-C5	2.83	131.61	126.64
4	A	705	DZ4	O1A-PA-N3A	-2.67	107.83	111.77
4	A	705	DZ4	C5-C6-N6	2.66	124.40	120.35
5	B	707	CZF	O5-P1-O8	2.63	119.36	109.07
4	A	707	DZ4	O2A-PA-O5'	-2.62	99.63	106.75
4	A	705	DZ4	O5'-PA-O1A	-2.46	104.78	114.24
4	B	701	DZ4	O3G-PG-O2G	2.41	116.86	107.64
4	B	701	DZ4	O1A-PA-N3A	-2.34	108.32	111.77
4	A	705	DZ4	O3'-C3'-C2'	2.34	119.25	110.90
5	A	706	CZF	O3-C4-C6	-2.29	104.43	111.05
4	A	707	DZ4	O1A-PA-N3A	-2.23	108.49	111.77
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'	-2.09	101.08	106.75
4	B	701	DZ4	O2B-PB-O3B	-2.06	97.78	104.64
4	B	701	DZ4	O3'-C3'-C4'	2.01	117.78	110.10

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

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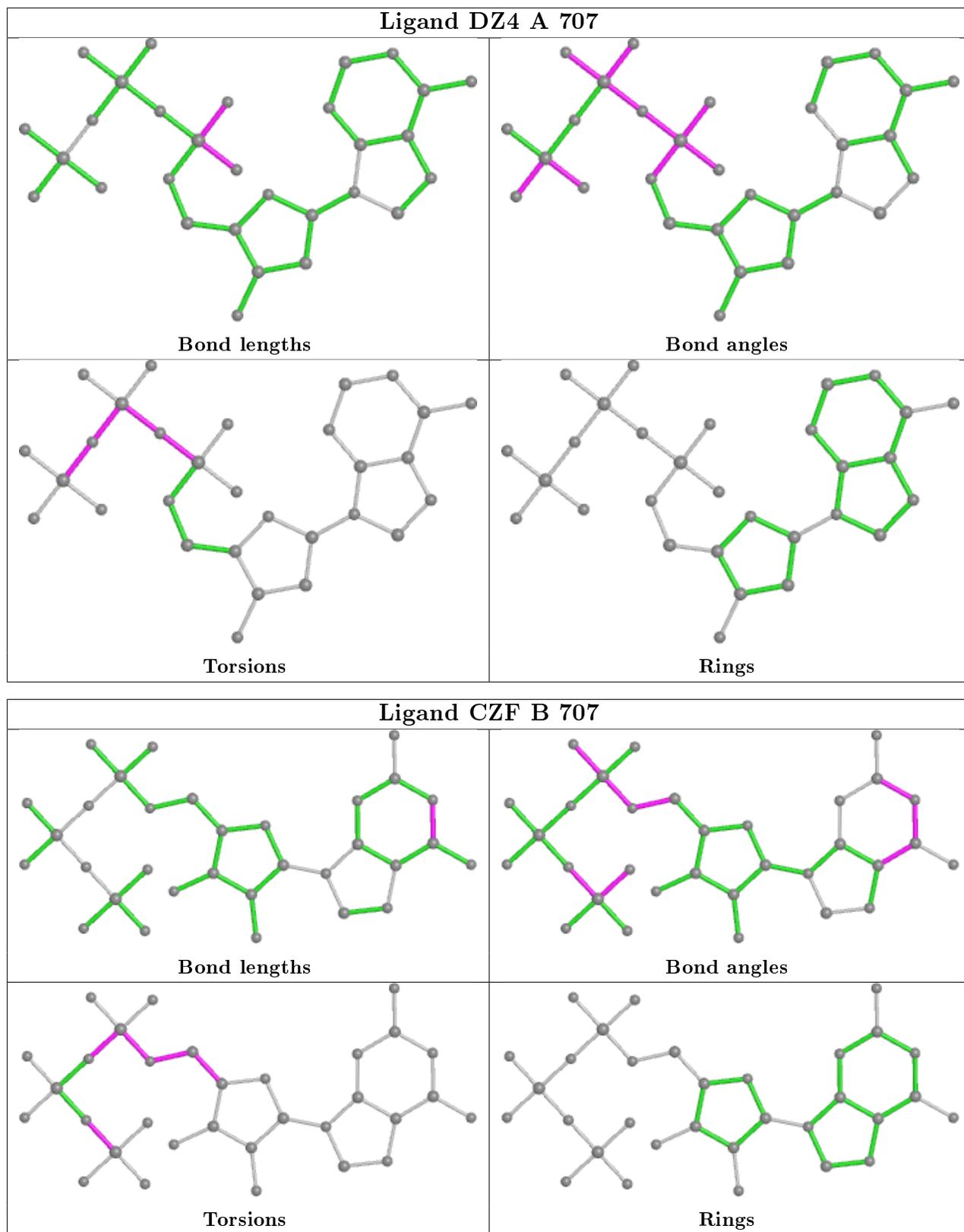
Mol	Chain	Res	Type	Atoms
4	B	701	DZ4	PB-N3A-PA-O1A
5	B	707	CZF	O4-C6-C8-O5
5	B	707	CZF	C4-C6-C8-O5
5	B	707	CZF	P2-O10-P3-O15
5	A	706	CZF	P2-O10-P3-O15
5	B	707	CZF	P2-O10-P3-O14
5	B	707	CZF	C8-O5-P1-O7
5	A	706	CZF	P2-O7-P1-O9
5	B	707	CZF	P2-O7-P1-O9
5	A	706	CZF	C6-C8-O5-P1
5	B	707	CZF	C8-O5-P1-O9
4	B	701	DZ4	PA-N3A-PB-O3B
4	B	706	DZ4	C4'-C5'-O5'-PA
4	A	707	DZ4	PB-O3B-PG-O3G
5	A	706	CZF	P2-O7-P1-O8
5	B	707	CZF	P2-O7-P1-O8
5	B	707	CZF	C6-C8-O5-P1
4	A	707	DZ4	PA-N3A-PB-O3B

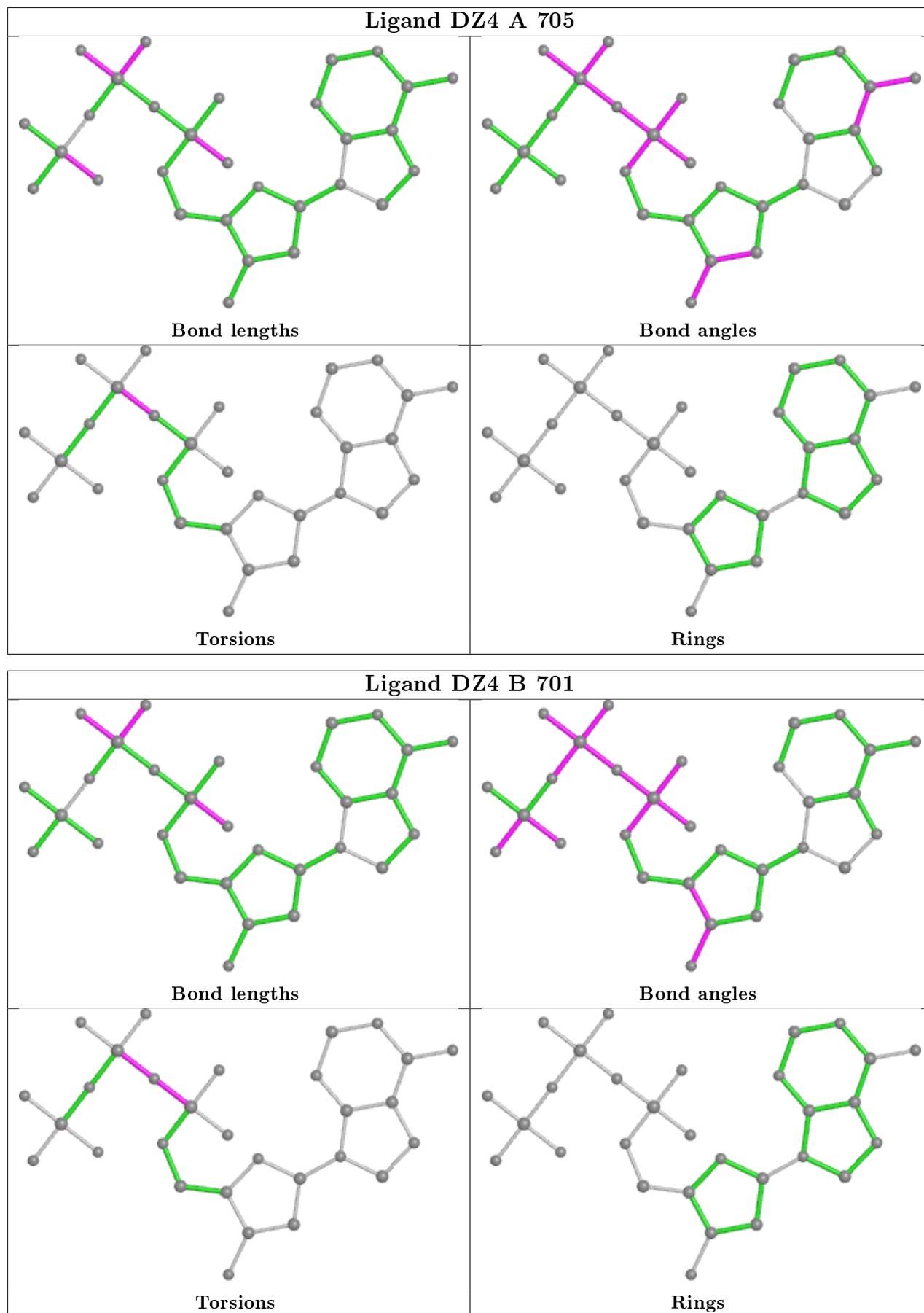
There are no ring outliers.

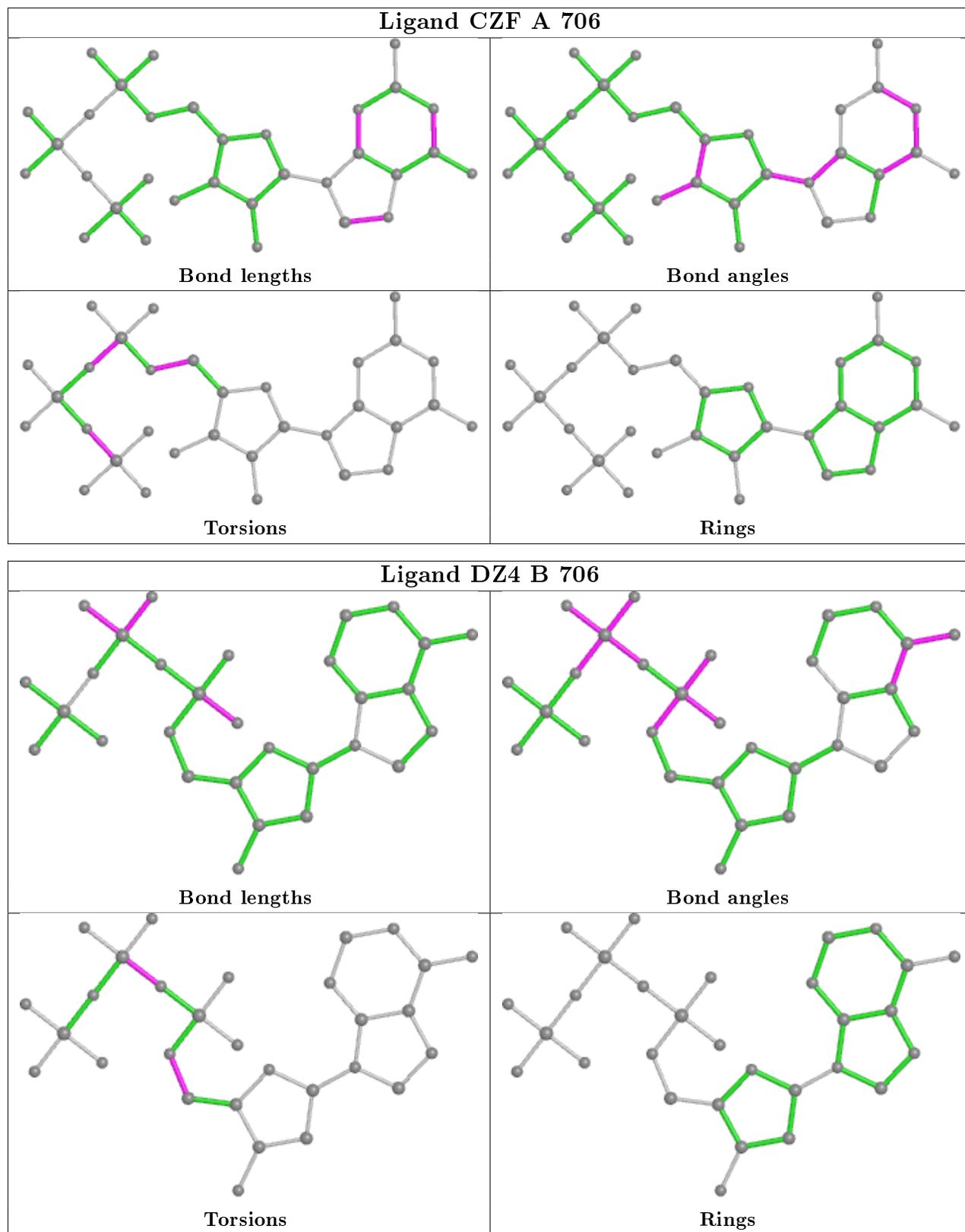
1 monomer is involved in 1 short contact:

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.







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%)	-0.33	15 (3%) 49 52	23, 42, 81, 136	0
1	B	479/520 (92%)	-0.23	6 (1%) 77 79	27, 47, 80, 139	0
All	All	958/1040 (92%)	-0.28	21 (2%) 62 65	23, 45, 80, 139	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	8.9
1	A	488	LEU	6.1
1	A	490	ASP	5.4
1	B	488	LEU	4.8
1	A	559	ARG	4.3
1	A	487	VAL	4.0
1	B	487	VAL	3.9
1	A	594	GLN	3.3
1	A	284	LEU	2.9
1	A	599	ASN	2.7
1	B	114	THR	2.7
1	A	345	ASN	2.6
1	A	563	TYR	2.6
1	A	598	TRP	2.4
1	B	594	GLN	2.3
1	A	285	TRP	2.2
1	B	535	ASN	2.1
1	A	491	VAL	2.1
1	A	590	LEU	2.1
1	B	344	ASP	2.0
1	A	286	PRO	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](#)

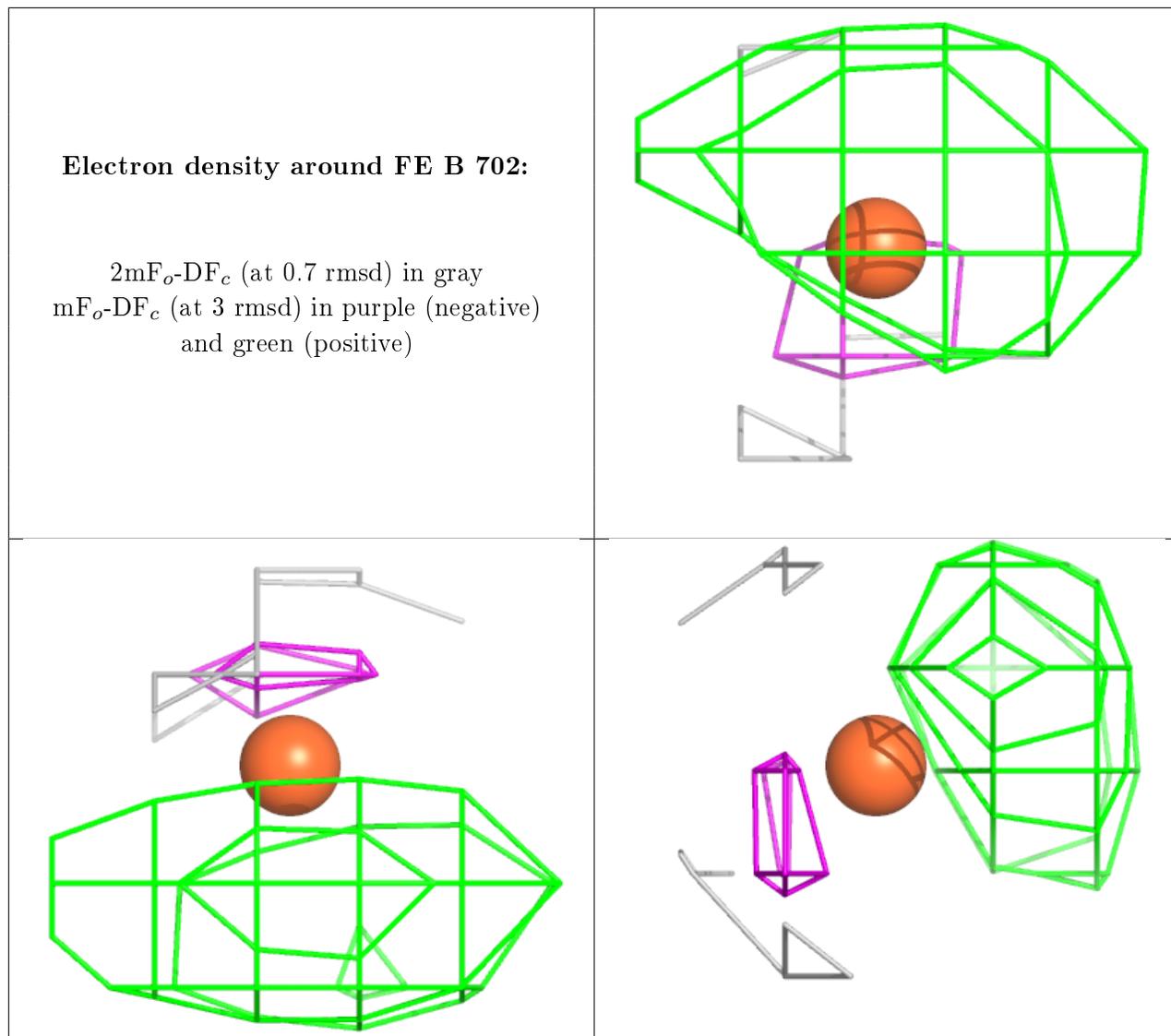
There are no monosaccharides in this entry.

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.

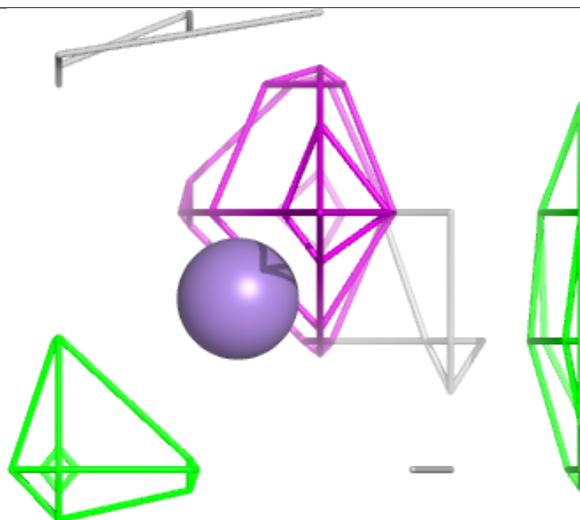
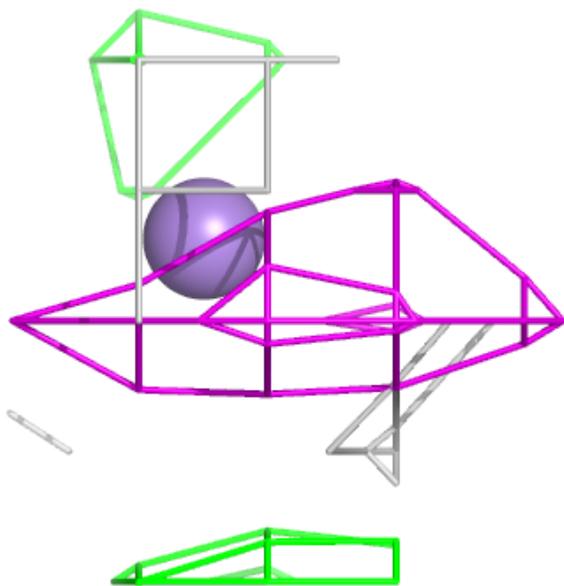
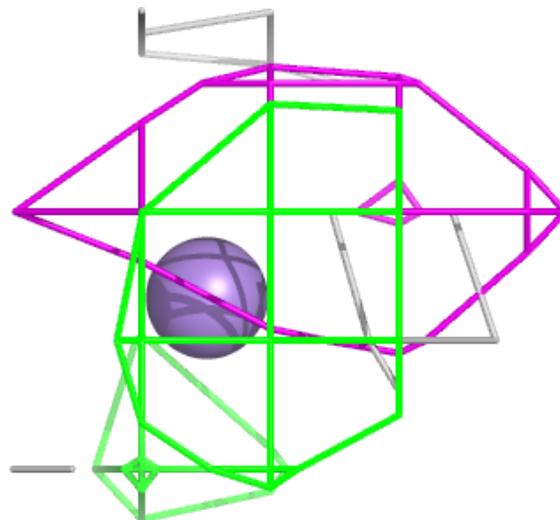
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	B	702	1/1	0.86	0.14	34,34,34,34	0
3	MN	B	703	1/1	0.90	0.14	41,41,41,41	0
3	MN	B	705	1/1	0.91	0.14	45,45,45,45	0
5	CZF	B	707	32/32	0.97	0.09	31,35,44,47	0
4	DZ4	B	706	30/30	0.98	0.10	30,33,36,39	0
4	DZ4	A	705	30/30	0.98	0.10	28,31,38,39	0
4	DZ4	B	701	30/30	0.98	0.12	23,25,33,36	0
4	DZ4	A	707	30/30	0.98	0.08	25,31,39,41	0
5	CZF	A	706	32/32	0.99	0.12	23,26,37,39	0
3	MN	A	702	1/1	0.99	0.11	30,30,30,30	0
3	MN	A	704	1/1	0.99	0.15	33,33,33,33	0
3	MN	B	704	1/1	0.99	0.10	39,39,39,39	0
2	FE	A	701	1/1	1.00	0.11	26,26,26,26	0
3	MN	A	703	1/1	1.00	0.09	31,31,31,31	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.



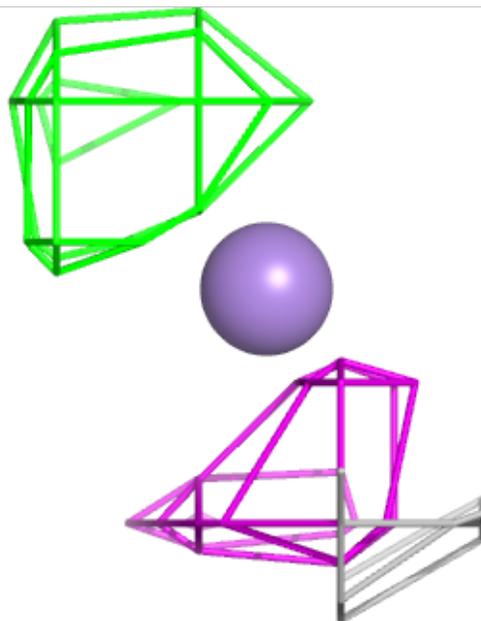
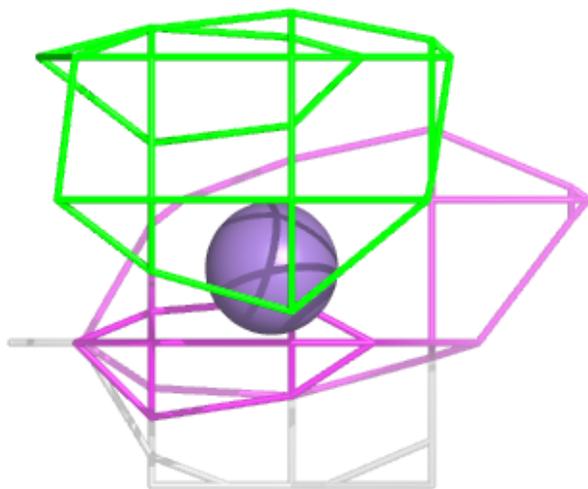
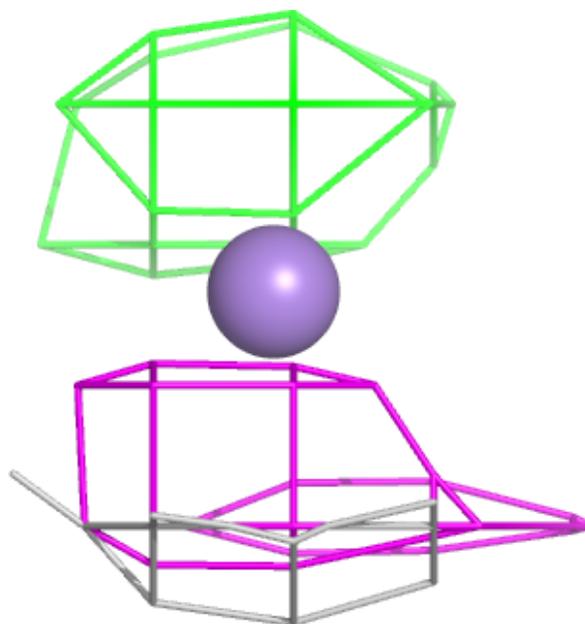
Electron density around MN B 703:

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



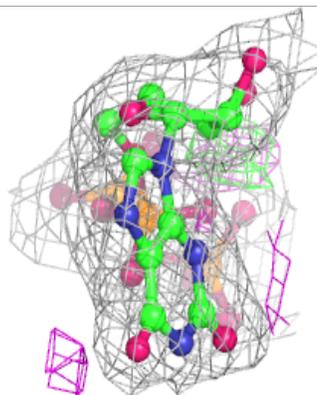
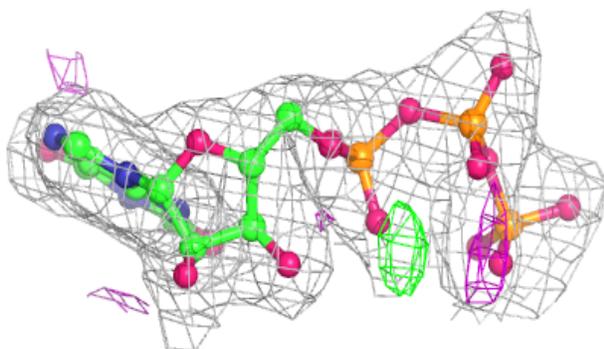
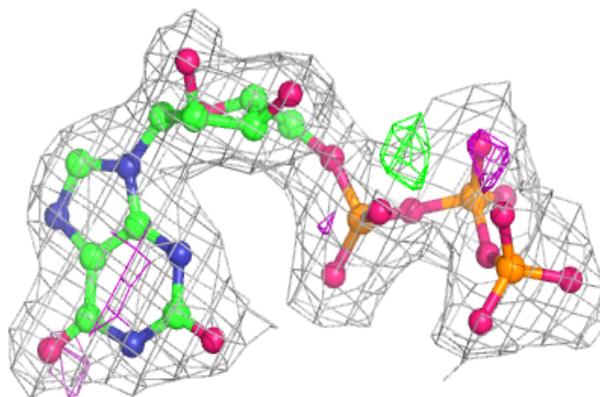
Electron density around MN B 705:

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and green (positive)

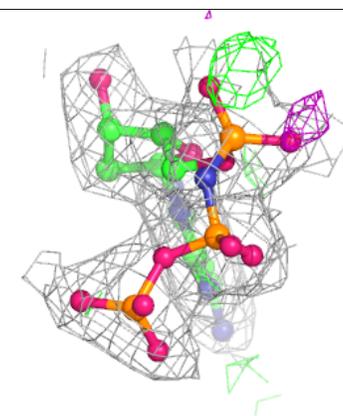
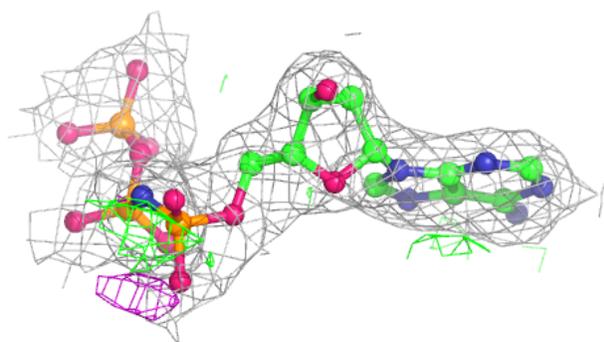
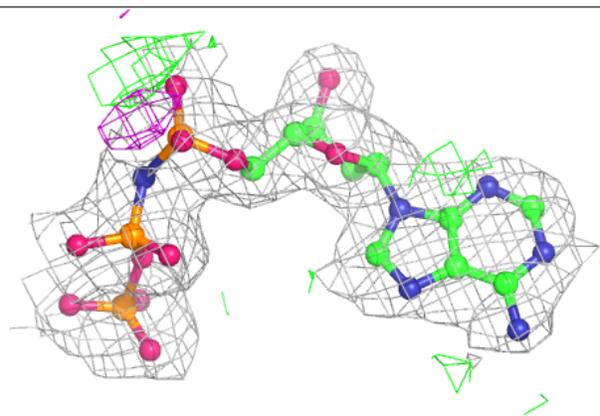


Electron density around CZF B 707:

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

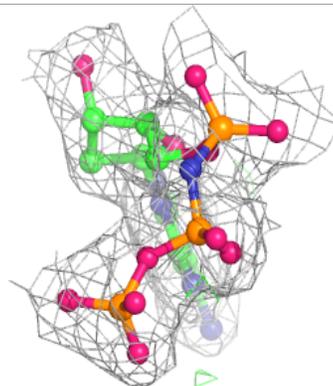
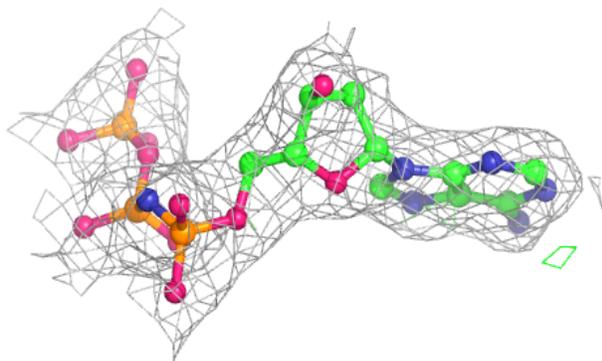
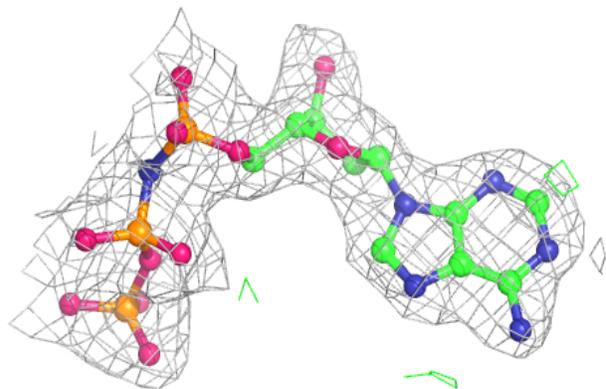
**Electron density around DZ4 B 706:**

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

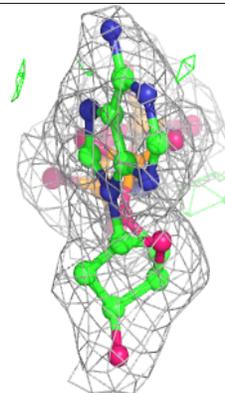
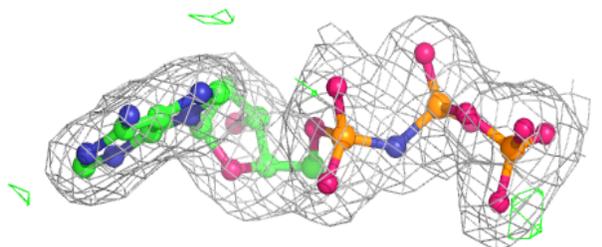
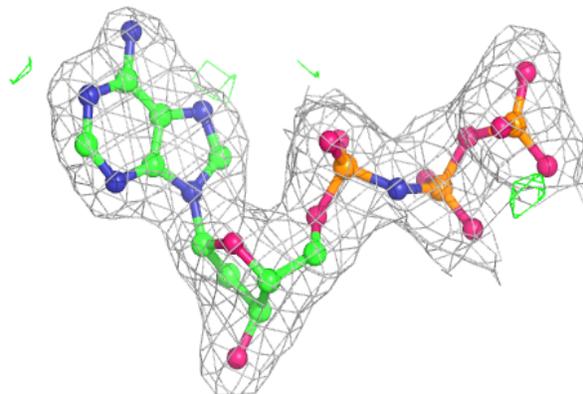


Electron density around DZ4 A 705:

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and green (positive)

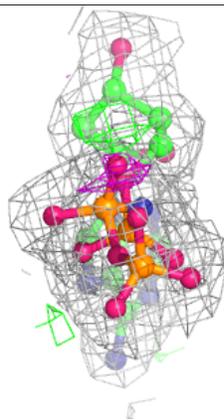
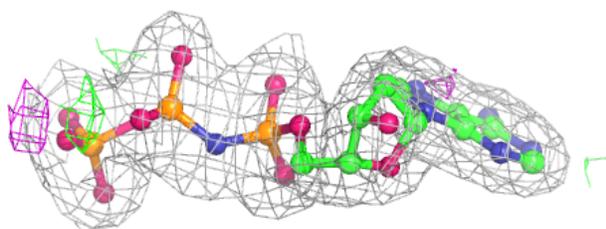
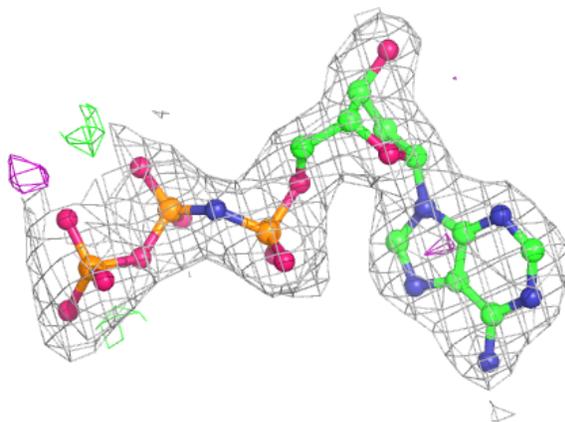
**Electron density around DZ4 B 701:**

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and green (positive)

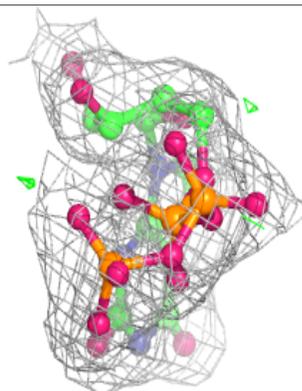
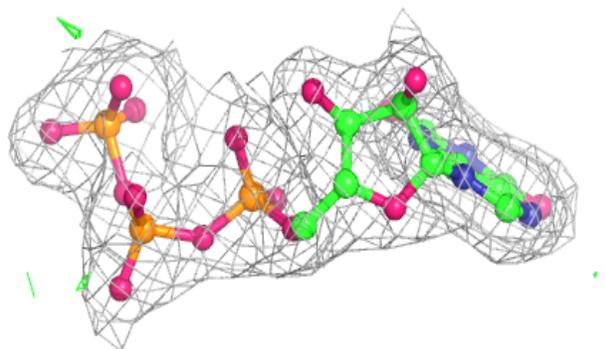
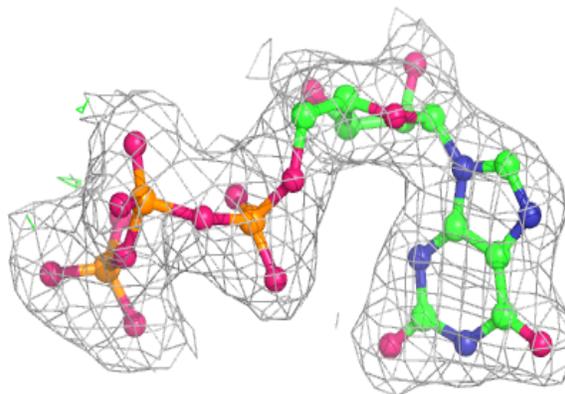


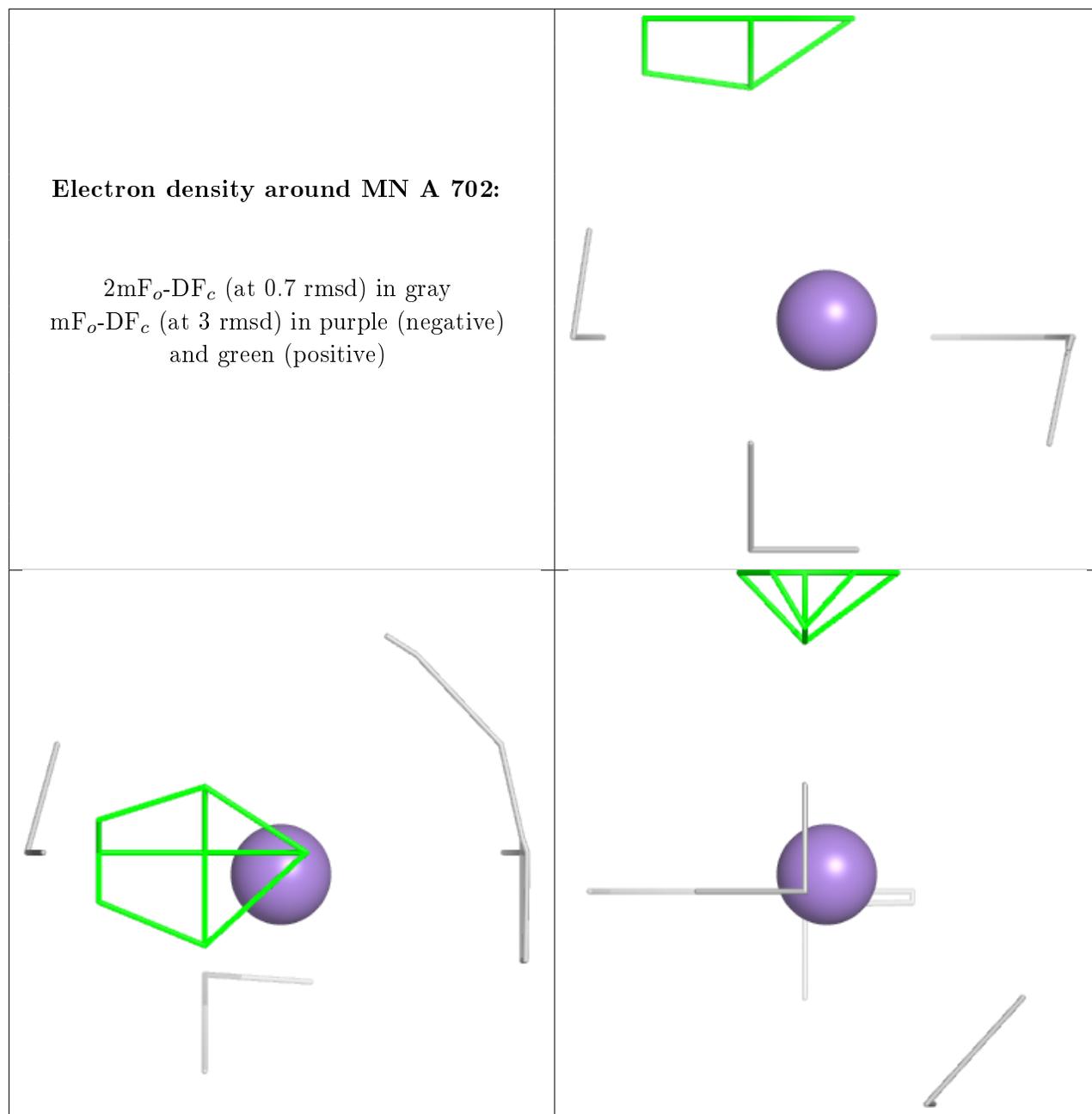
Electron density around DZ4 A 707:

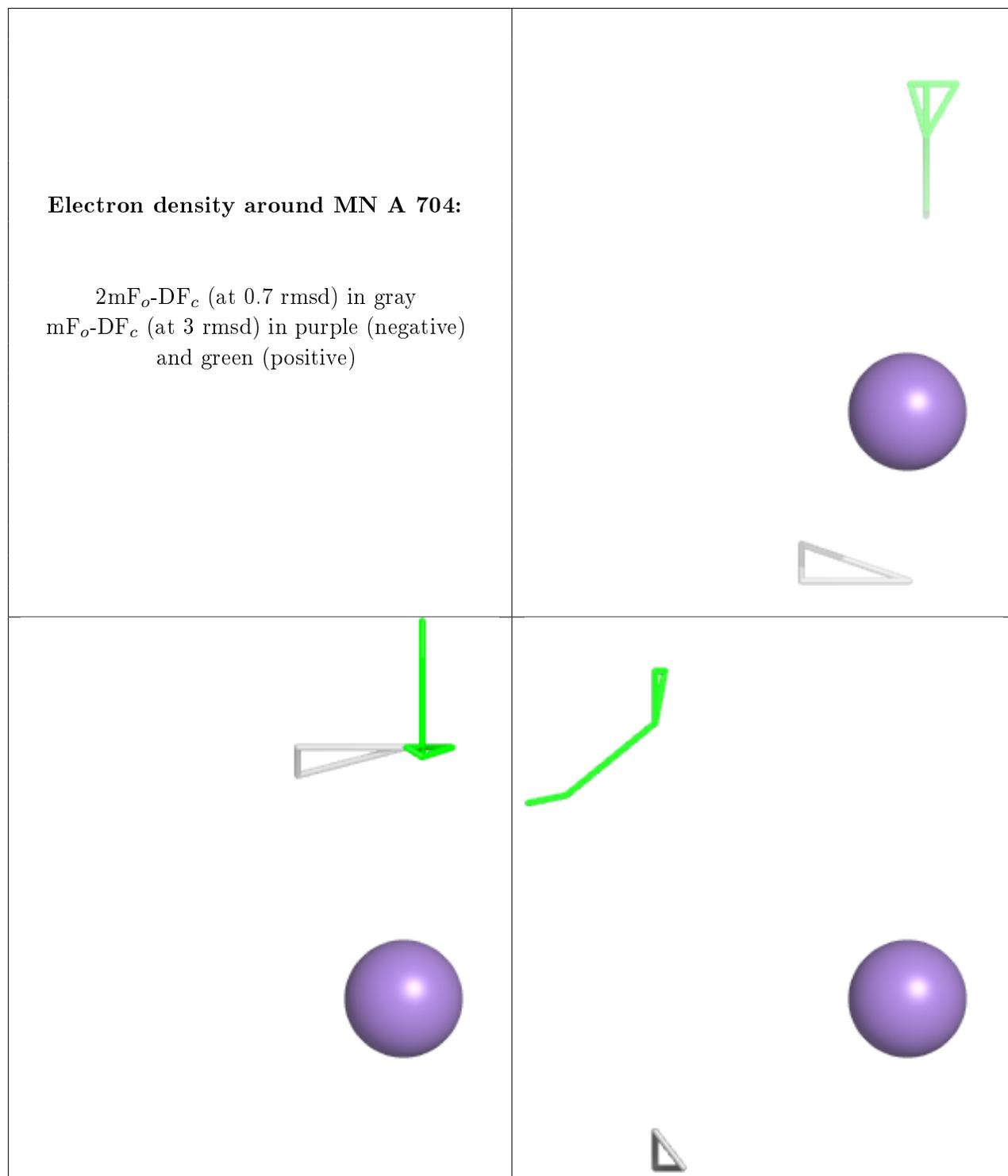
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

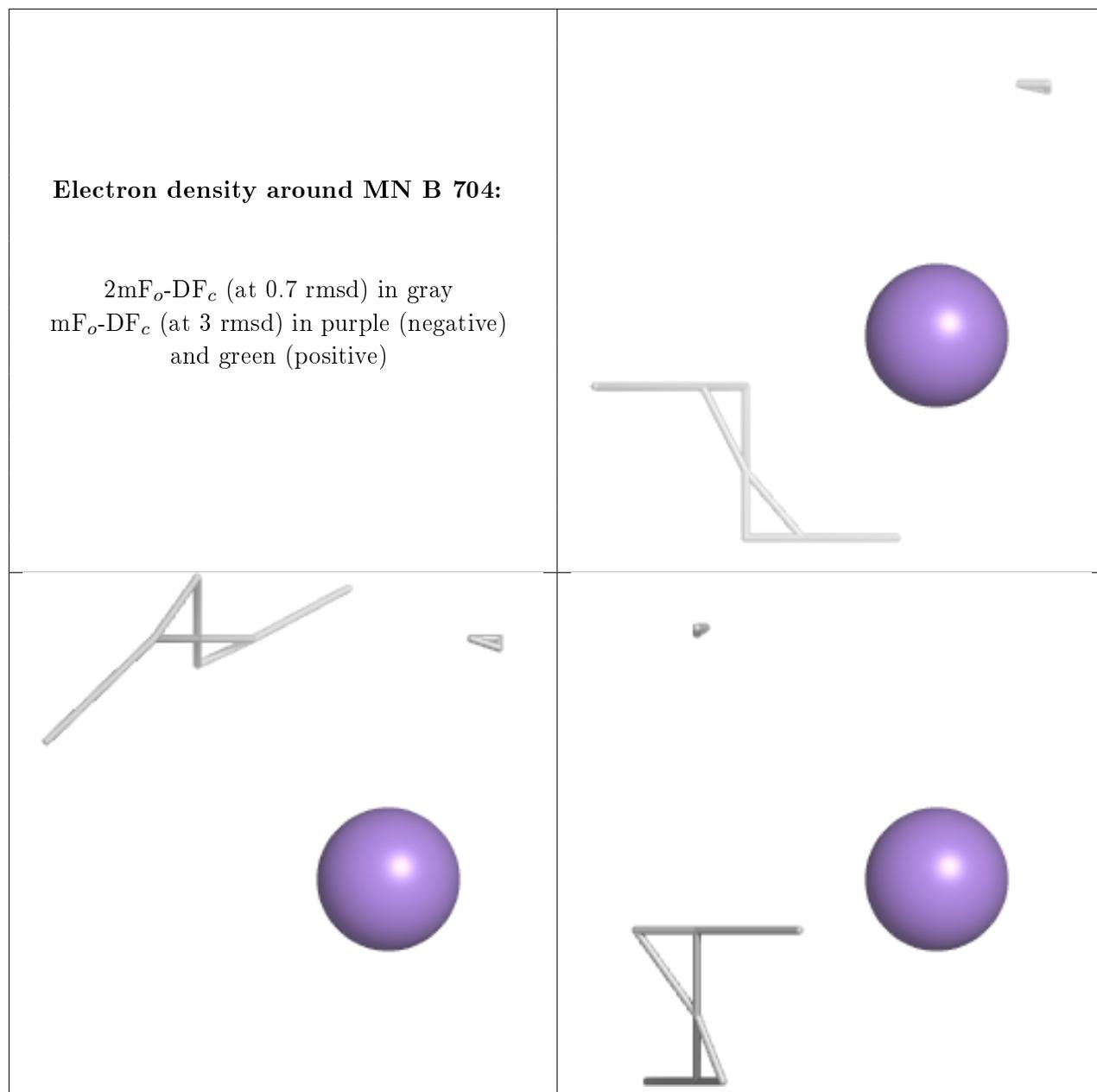
**Electron density around CZF A 706:**

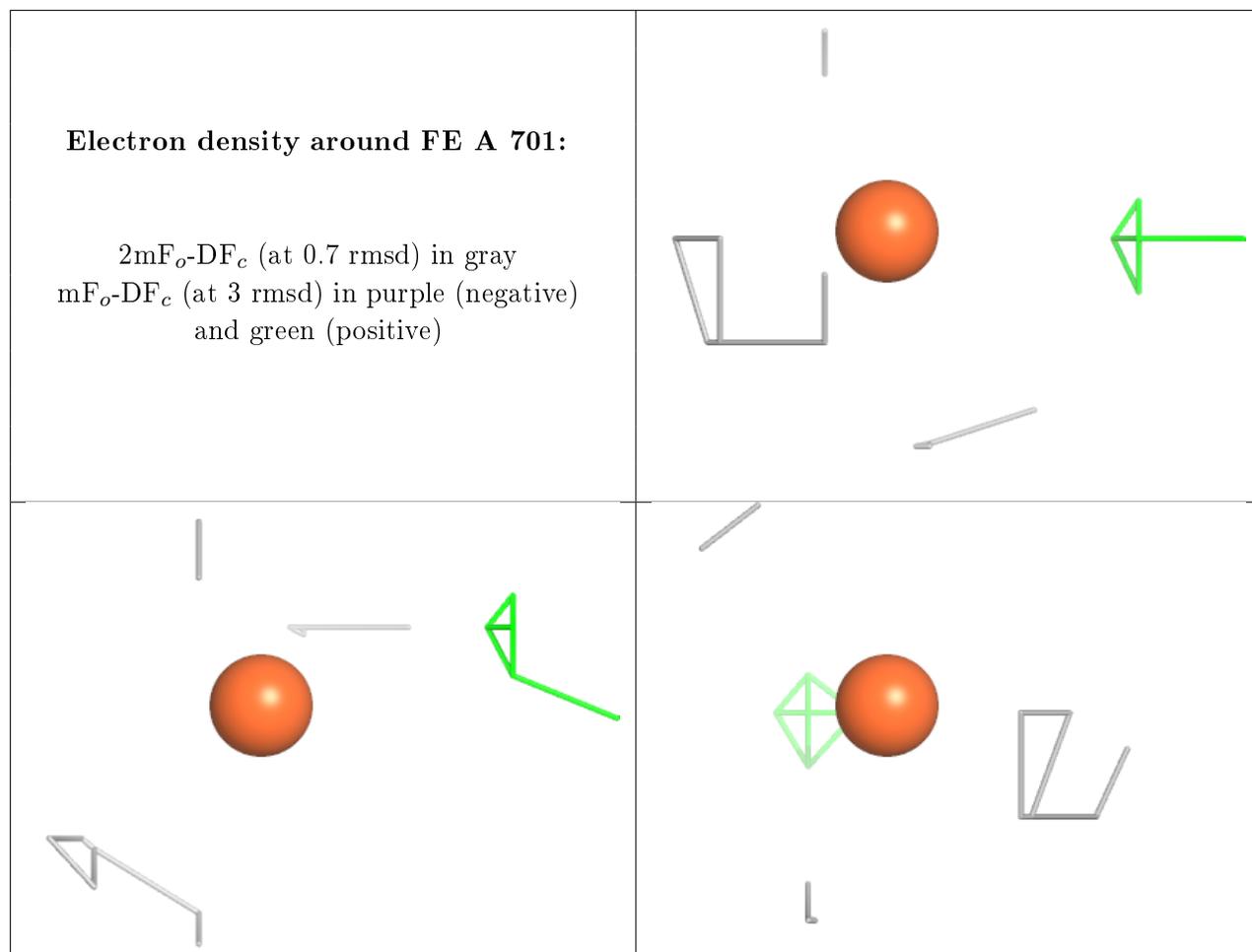
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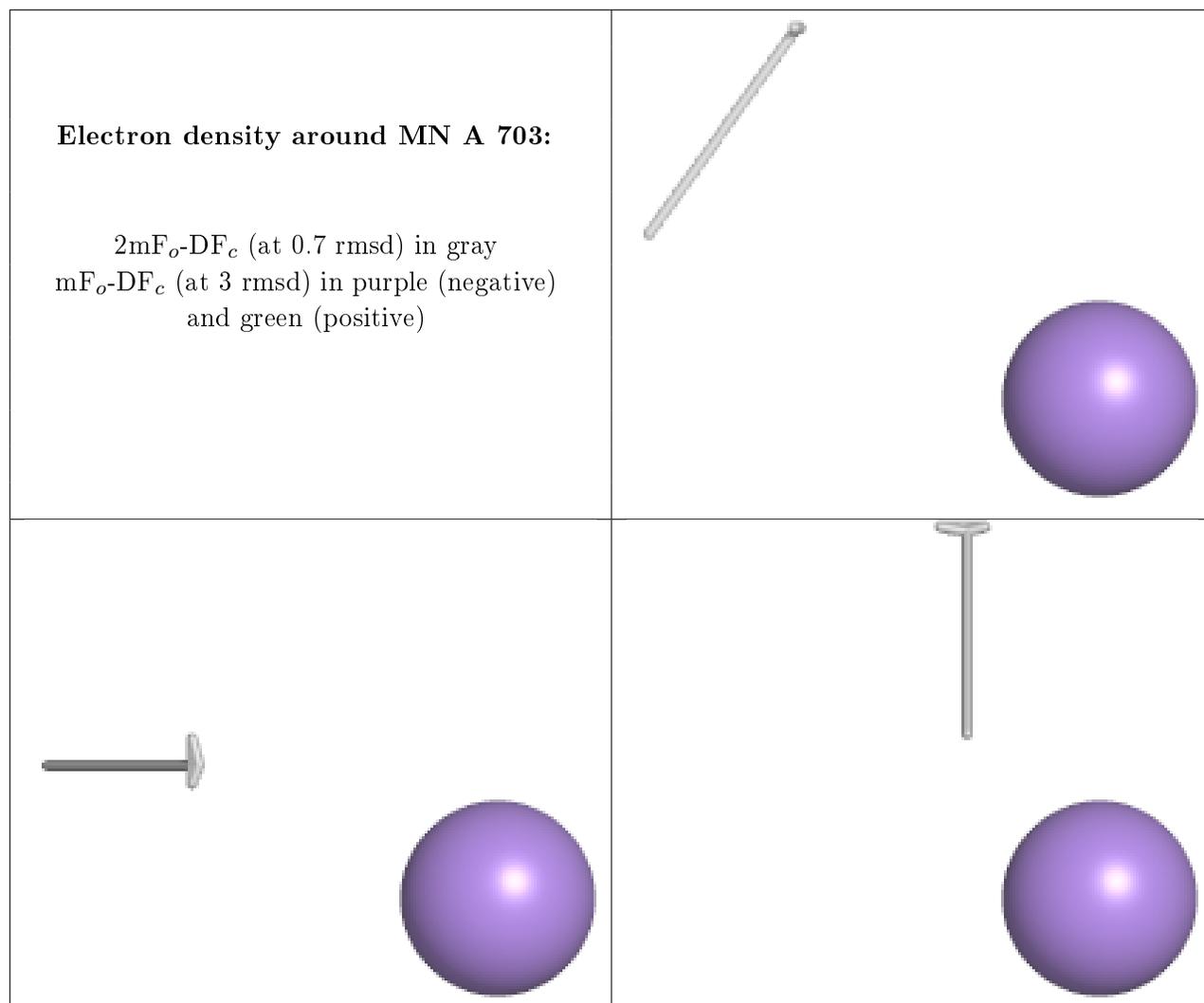












6.5 Other polymers [i](#)

There are no such residues in this entry.