Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 08:34 pm GMT

PDB ID	:	6YOM
Title	:	Crystal structure of tetrameric human D137N-SAMHD1 (residues 109-626) with XTP, dATP, dCMPNPP, Mn and Mg
Authors	:	Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.G.; Kelly, G.; Taylor, I.A.
Deposited on	:	2020-04-14
Resolution	:	3.25 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:

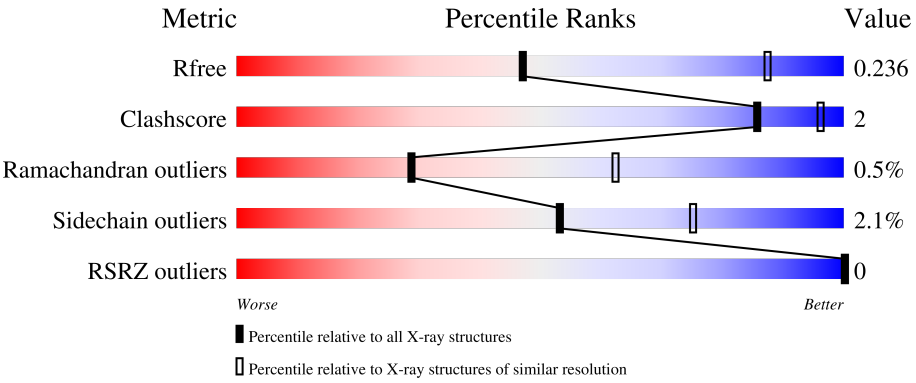
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 <=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	83% 8% 10%
1	B	520	84% 5% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7398 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	470	Total 3654	C 2343	N 630	O 661	S 20	0	0	0
1	B	466	Total 3556	C 2287	N 607	O 642	S 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 depositor).

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

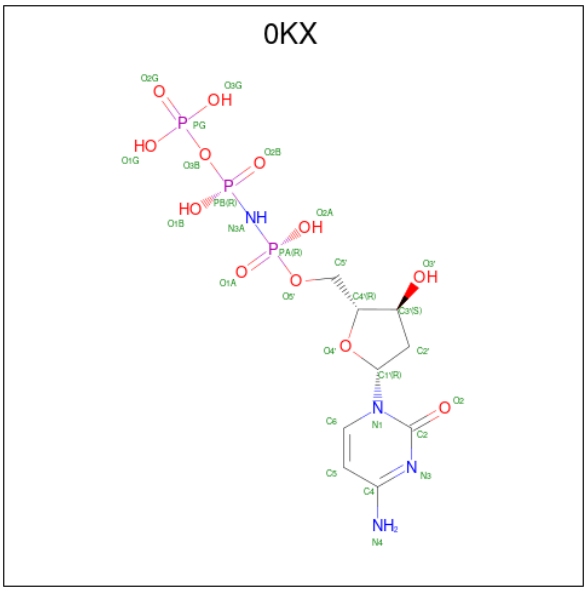
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0
3	B	1	Total 1	Mn 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

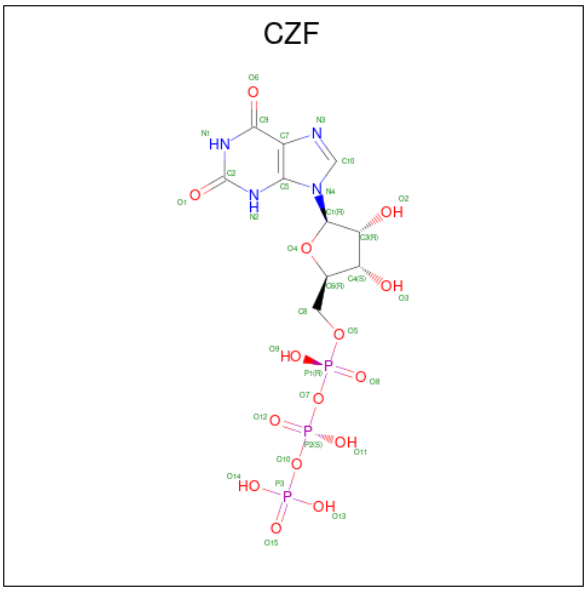
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0

- Molecule 5 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino} phosphoryl]cytidine (three-letter code: 0KX) (formula: $C_9H_{17}N_4O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



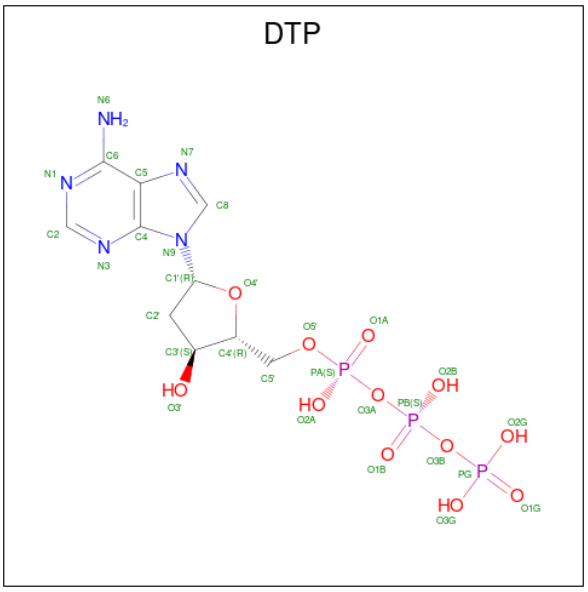
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 28 9 4 12 3	0	0
5	B	1	Total C N O P 28 9 4 12 3	0	0

- Molecule 6 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: $C_{10}H_{15}N_4O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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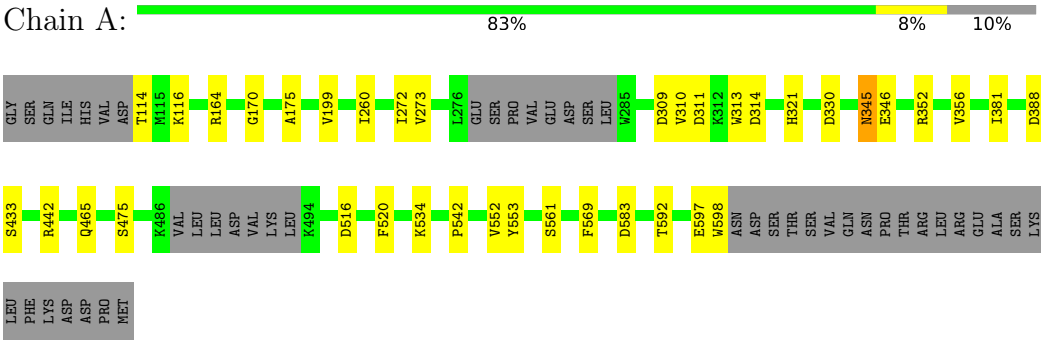
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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.

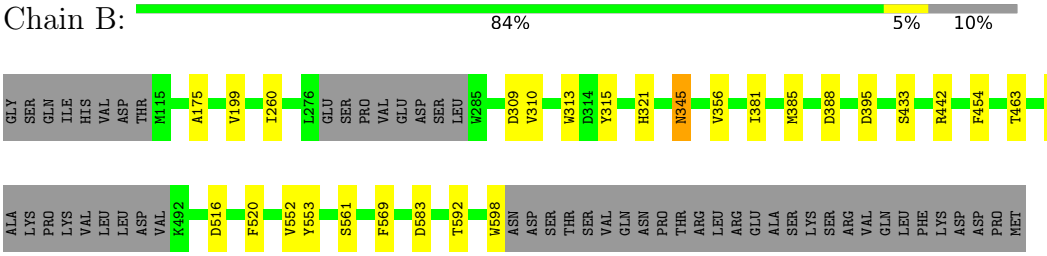
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.30Å 105.30Å 195.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.72 – 3.25 92.72 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.72-3.25) 100.0 (92.72-3.25)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.176 , 0.236 0.178 , 0.236	Depositor DCC
R_{free} test set	931 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	86.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7398	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 0KX, DTP, FE, MN, CZF, MG

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	0.74	0/3746	0.92	6/5098 (0.1%)
1	B	0.72	0/3647	0.89	1/4978 (0.0%)
All	All	0.73	0/7393	0.90	7/10076 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	B	583	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	330	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	164	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	352	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	583	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	311	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	3654	0	3442	17	0
1	B	3556	0	3287	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	28	0	15	0	0
5	B	28	0	15	2	0
6	A	32	0	0	2	0
6	B	32	0	0	0	0
7	A	30	0	12	0	0
7	B	30	0	12	1	0
All	All	7398	0	6783	31	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 2.

All (31) 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:534:LYS:HE3	1:A:542:PRO:O	1.99	0.63
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.83	0.60
1:A:321:HIS:CE1	1:B:321:HIS:CE1	2.90	0.59
1:B:592:THR:HG22	1:B:598:TRP:CZ3	2.38	0.59
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.87	0.57
1:A:592:THR:HG22	1:A:598:TRP:CZ3	2.40	0.56
1:B:592:THR:HG22	1:B:598:TRP:CE3	2.46	0.50
1:B:356:VAL:HG23	1:B:520:PHE:CZ	2.47	0.50
1:A:592:THR:HG22	1:A:598:TRP:CE3	2.47	0.49
1:B:381:ILE:HD13	1:B:553:TYR:CG	2.48	0.49
1:A:381:ILE:HD13	1:A:553:TYR:CG	2.48	0.48
1:A:381:ILE:HD13	1:A:553:TYR:CD2	2.49	0.48
1:A:356:VAL:HG23	1:A:520:PHE:CZ	2.50	0.47
1:B:381:ILE:HD13	1:B:553:TYR:CD2	2.49	0.47
1:B:315:TYR:CD1	5:B:706:0KX:H9	2.51	0.46
1:A:116:LYS:NZ	6:A:706:CZF:O1	2.46	0.45
1:A:310:VAL:HG12	1:A:313:TRP:CZ3	2.51	0.45
6:A:706:CZF:O12	7:B:701:DTP:O1G	2.36	0.44
1:B:310:VAL:HG12	1:B:313:TRP:CZ3	2.53	0.44
1:B:552:VAL:HG21	1:B:569:PHE:CD1	2.53	0.44
1:A:170:GLY:HA3	1:A:314:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ILE:HG22	1:B:260:ILE:O	2.19	0.43
1:A:552:VAL:HG21	1:A:569:PHE:CD1	2.55	0.42
1:A:272:ILE:HG22	1:A:273:VAL:HG23	2.01	0.42
1:A:433:SER:OG	1:A:442:ARG:NH1	2.50	0.42
1:A:260:ILE:HG22	1:A:260:ILE:O	2.19	0.42
1:B:385:MET:HG2	1:B:454:PHE:CE2	2.55	0.41
1:B:315:TYR:CG	5:B:706:0KX:H9	2.55	0.41
1:A:428:LEU:HD22	1:A:432:TYR:CZ	2.55	0.41
1:A:310:VAL:HG12	1:A:313:TRP:CE3	2.56	0.41
1:B:433:SER:OG	1:B:442:ARG:NH1	2.54	0.41

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	464/520 (89%)	435 (94%)	26 (6%)	3 (1%)	25	59
1	B	460/520 (88%)	429 (93%)	29 (6%)	2 (0%)	34	67
All	All	924/1040 (89%)	864 (94%)	55 (6%)	5 (0%)	29	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	ASP
1	A	597	GLU
1	A	345	ASN
1	B	345	ASN
1	B	516	ASP

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	371/464 (80%)	363 (98%)	8 (2%)	52 74
1	B	352/464 (76%)	345 (98%)	7 (2%)	55 76
All	All	723/928 (78%)	708 (98%)	15 (2%)	53 75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	309	ASP
1	A	345	ASN
1	A	346	GLU
1	A	388	ASP
1	A	465	GLN
1	A	475	SER
1	A	561	SER
1	B	309	ASP
1	B	345	ASN
1	B	388	ASP
1	B	395	ASP
1	B	463	THR
1	B	475	SER
1	B	561	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	321	HIS
1	A	328	ASN
1	A	345	ASN
1	A	364	HIS
1	A	375	GLN
1	A	380	ASN

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Mol	Chain	Res	Type
1	A	577	ASN
1	B	321	HIS
1	B	328	ASN
1	B	364	HIS
1	B	375	GLN
1	B	380	ASN
1	B	425	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 monosaccharides 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	$\#\|Z\| > 2$
6	CZF	B	707	4	24,34,34	0.90	1 (4%)	33,54,54	1.44	3 (9%)
7	DTP	A	707	4	26,32,32	0.95	1 (3%)	30,50,50	1.36	3 (10%)
6	CZF	A	706	4	24,34,34	0.91	2 (8%)	33,54,54	1.52	4 (12%)
5	0KX	A	705	3,4,2	28,29,29	1.06	2 (7%)	40,45,45	1.46	5 (12%)
5	0KX	B	706	3,4,2	28,29,29	1.10	3 (10%)	40,45,45	1.57	7 (17%)
7	DTP	B	701	4	26,32,32	1.10	2 (7%)	30,50,50	1.43	5 (16%)

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	CZF	B	707	4	-	3/18/38/38	0/3/3/3
7	DTP	A	707	4	-	3/18/34/34	0/3/3/3
6	CZF	A	706	4	-	6/18/38/38	0/3/3/3
5	0KX	A	705	3,4,2	-	1/19/34/34	0/2/2/2
5	0KX	B	706	3,4,2	-	2/19/34/34	0/2/2/2
7	DTP	B	701	4	-	3/18/34/34	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	706	0KX	PA-O1A	3.40	1.51	1.46
5	A	705	0KX	PA-O1A	3.32	1.51	1.46
7	B	701	DTP	C2-N3	3.23	1.37	1.32
6	B	707	CZF	C7-C9	-3.04	1.41	1.47
5	B	706	0KX	PB-O2B	3.03	1.51	1.46
6	A	706	CZF	C7-C9	-2.88	1.41	1.47
7	B	701	DTP	C5-C4	2.44	1.47	1.40
5	A	705	0KX	PB-O2B	2.41	1.50	1.46
6	A	706	CZF	C10-N3	-2.18	1.31	1.35
7	A	707	DTP	C2-N3	2.10	1.35	1.32
5	B	706	0KX	PA-O2A	-2.09	1.51	1.56

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	706	0KX	O1B-PB-O2B	5.23	120.88	109.92
6	A	706	CZF	C5-N2-C2	-4.76	120.67	128.11
6	B	707	CZF	C5-N2-C2	-4.72	120.74	128.11
5	A	705	0KX	O2A-PA-O1A	4.39	119.12	109.92
5	B	706	0KX	O2A-PA-O1A	4.03	118.38	109.92
6	B	707	CZF	N2-C2-N1	3.94	118.19	115.90
5	A	705	0KX	O3B-PB-N3A	-3.85	95.90	106.59
5	A	705	0KX	O1B-PB-O2B	3.82	117.94	109.92
6	A	706	CZF	N2-C2-N1	3.73	118.06	115.90
5	B	706	0KX	O1A-PA-N3A	3.68	117.19	111.77
7	A	707	DTP	N3-C2-N1	-3.48	123.25	128.68
5	B	706	0KX	O3B-PB-N3A	-3.08	98.06	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	706	0KX	O2B-PB-N3A	-3.06	107.26	111.77
7	B	701	DTP	O3G-PG-O2G	3.06	119.33	107.64
7	B	701	DTP	N3-C2-N1	-3.03	123.95	128.68
6	B	707	CZF	C9-N1-C2	-2.89	124.60	126.88
7	A	707	DTP	C2'-C1'-N9	2.81	120.75	114.27
5	A	705	0KX	O1B-PB-O3B	2.78	113.94	104.64
7	B	701	DTP	C5-C6-N6	-2.78	116.12	120.35
7	B	701	DTP	O3G-PG-O3B	-2.77	95.34	104.64
6	A	706	CZF	C9-N1-C2	-2.61	124.82	126.88
6	A	706	CZF	P2-O7-P1	-2.58	123.98	132.83
7	B	701	DTP	N6-C6-N1	2.23	123.21	118.57
5	B	706	0KX	O3G-PG-O1G	2.14	115.81	107.64
5	B	706	0KX	O2A-PA-O5'	2.06	112.32	106.75
5	A	705	0KX	PB-O3B-PG	-2.05	125.39	132.62
7	A	707	DTP	O3G-PG-O2G	2.01	115.33	107.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	0KX	PB-N3A-PA-O1A
5	B	706	0KX	PB-N3A-PA-O1A
6	A	706	CZF	P2-O10-P3-O14
6	B	707	CZF	P2-O10-P3-O13
6	B	707	CZF	P2-O10-P3-O14
7	A	707	DTP	PB-O3B-PG-O3G
7	B	701	DTP	PB-O3B-PG-O1G
7	A	707	DTP	PB-O3B-PG-O2G
6	A	706	CZF	C6-C8-O5-P1
6	A	706	CZF	P2-O7-P1-O9
5	B	706	0KX	C4'-C5'-O5'-PA
6	A	706	CZF	P2-O10-P3-O15
7	B	701	DTP	PB-O3B-PG-O2G
7	B	701	DTP	PB-O3B-PG-O3G
6	A	706	CZF	P2-O7-P1-O8
6	A	706	CZF	P3-O10-P2-O12
6	B	707	CZF	P2-O7-P1-O9
7	A	707	DTP	PB-O3B-PG-O1G

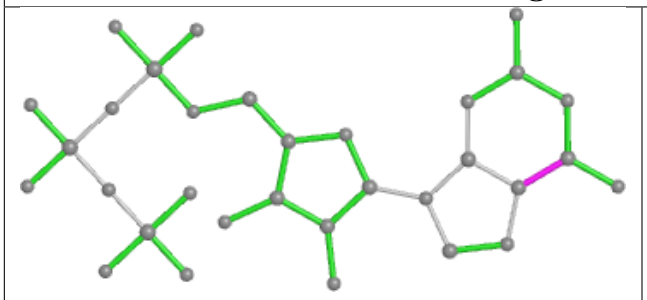
There are no ring outliers.

3 monomers are involved in 4 short contacts:

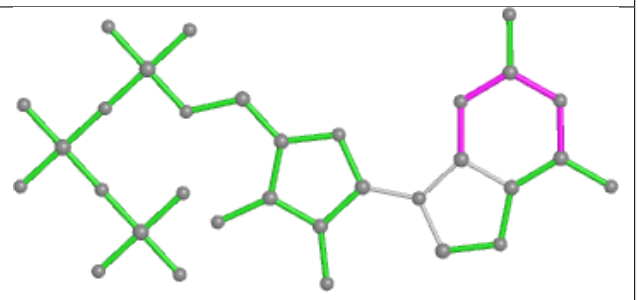
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	706	CZF	2	0
5	B	706	0KX	2	0
7	B	701	DTP	1	0

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 then 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.

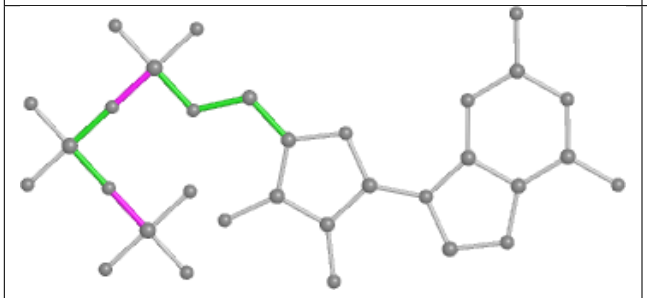
Ligand CZF B 707



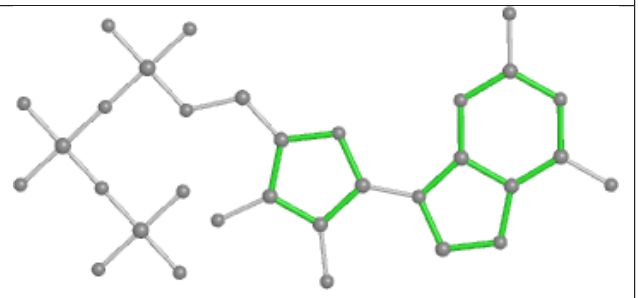
Bond lengths



Bond angles

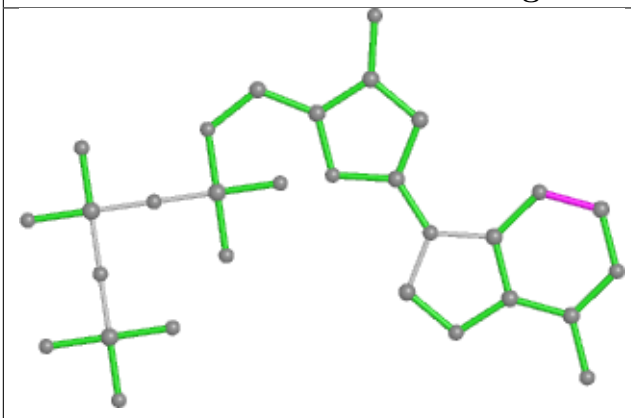


Torsions

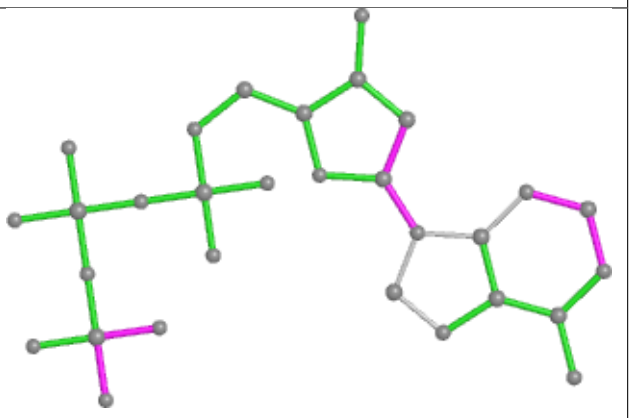


Rings

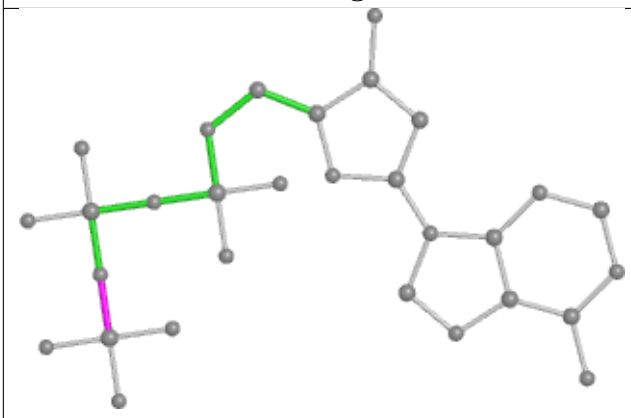
Ligand DTP A 707



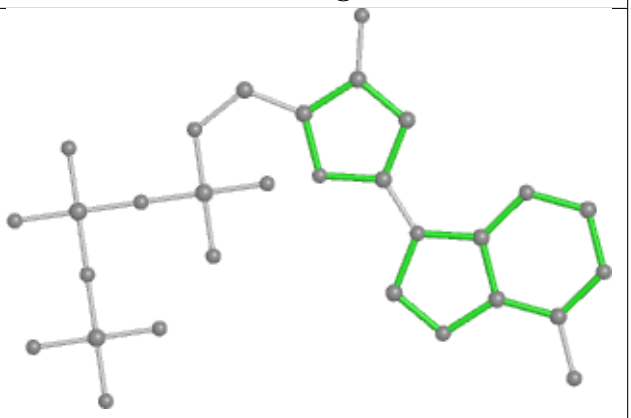
Bond lengths



Bond angles

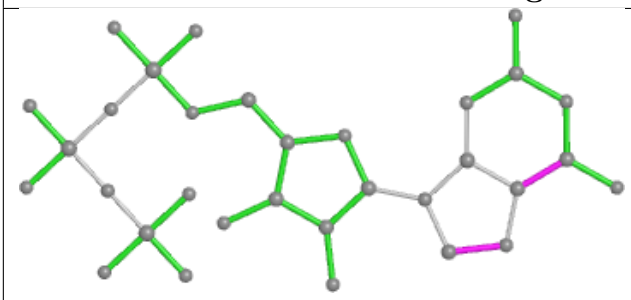


Torsions

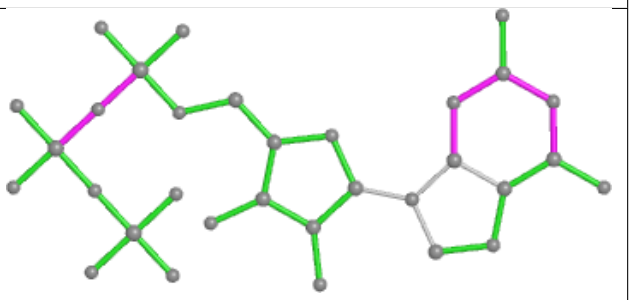


Rings

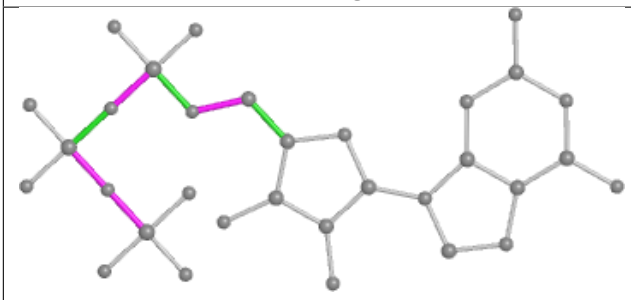
Ligand CZF A 706



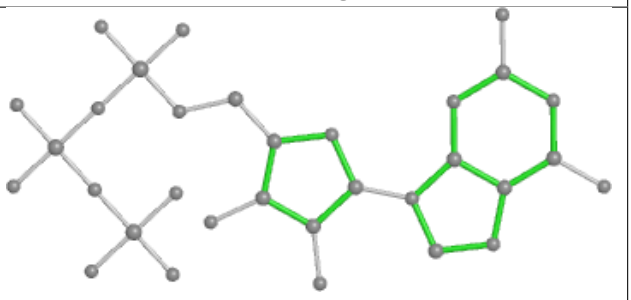
Bond lengths



Bond angles

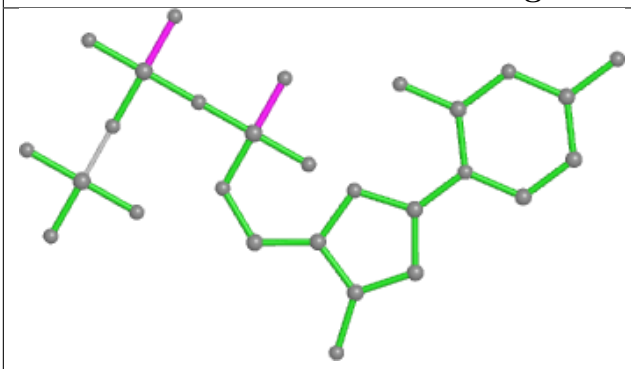


Torsions

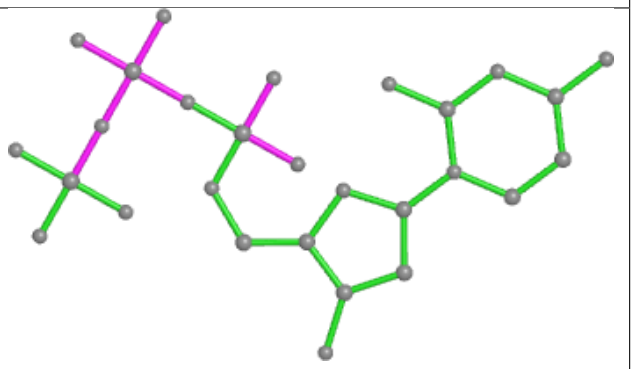


Rings

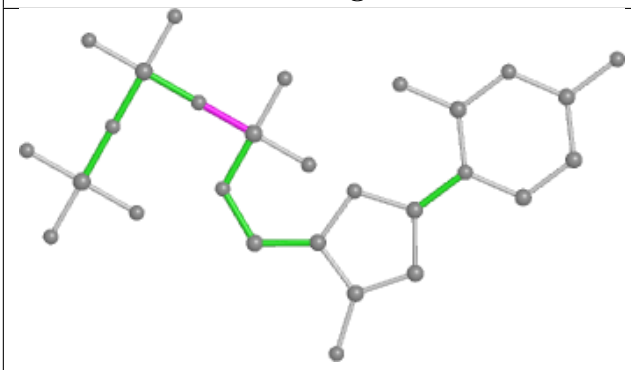
Ligand 0KX A 705



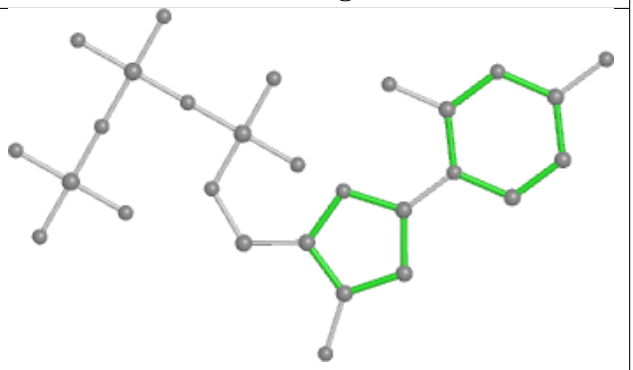
Bond lengths



Bond angles

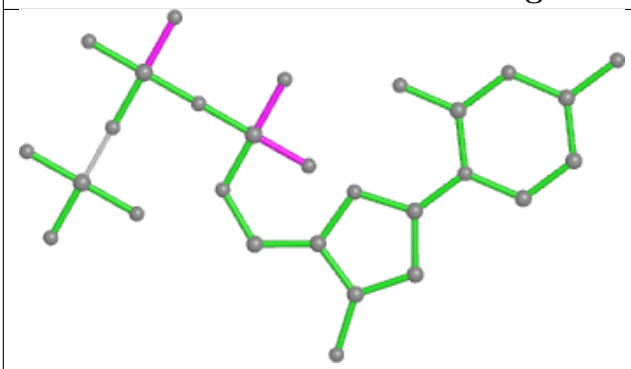


Torsions

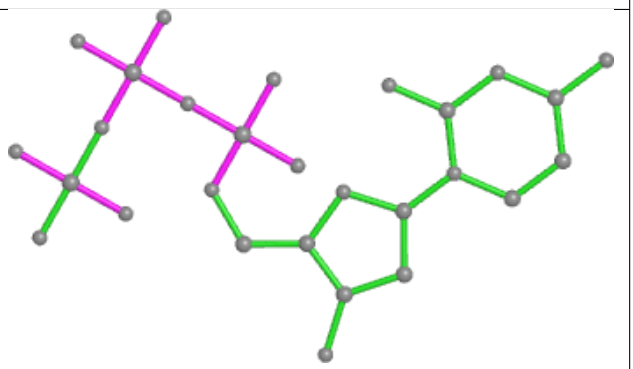


Rings

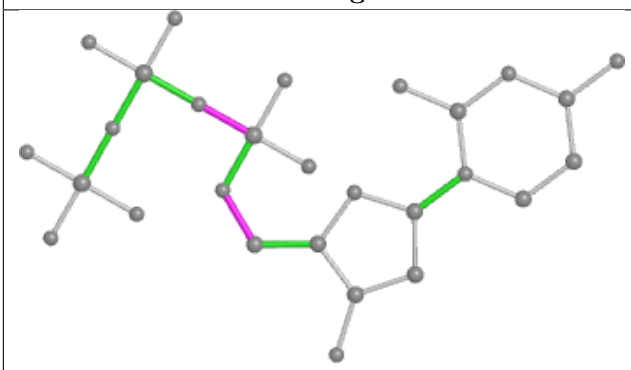
Ligand 0KX B 706



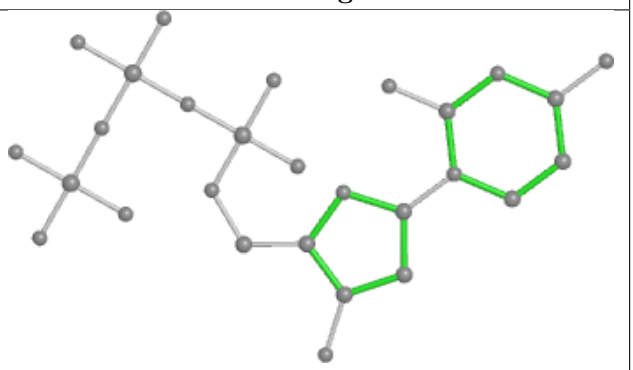
Bond lengths



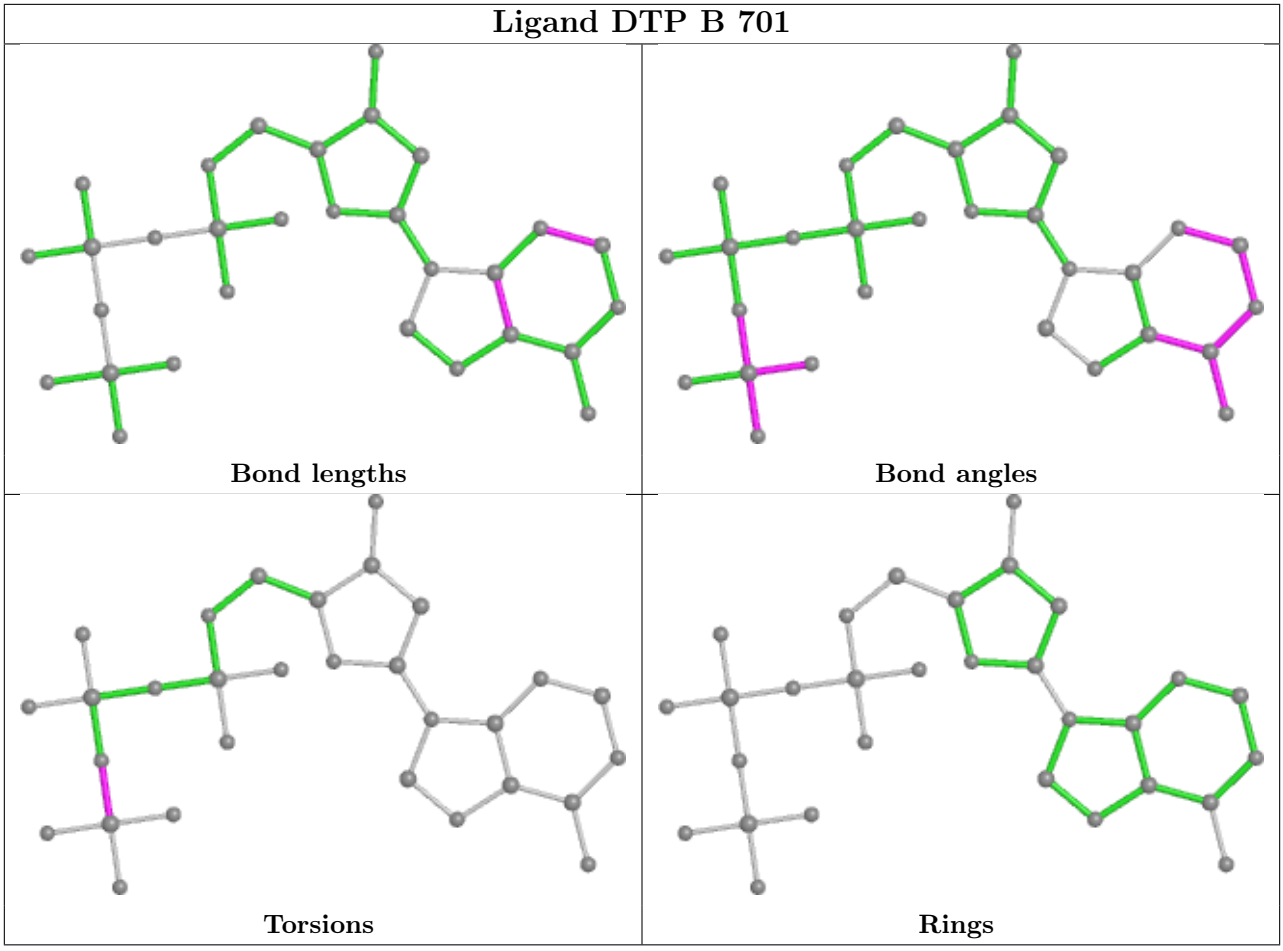
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	470/520 (90%)	0.01	0	100	100	48, 78, 115, 127	0
1	B	466/520 (89%)	0.03	0	100	100	52, 83, 111, 129	0
All	All	936/1040 (90%)	0.02	0	100	100	48, 81, 114, 129	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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, 95^{th} 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
4	MG	A	703	1/1	0.94	0.36	45,45,45,45	0
4	MG	A	704	1/1	0.95	0.12	45,45,45,45	0
4	MG	B	704	1/1	0.95	0.22	50,50,50,50	0
4	MG	B	705	1/1	0.95	0.13	58,58,58,58	0
5	0KX	B	706	28/28	0.96	0.19	57,68,75,78	0
6	CZF	A	706	32/32	0.96	0.17	53,60,69,72	0
6	CZF	B	707	32/32	0.96	0.17	55,60,74,77	0

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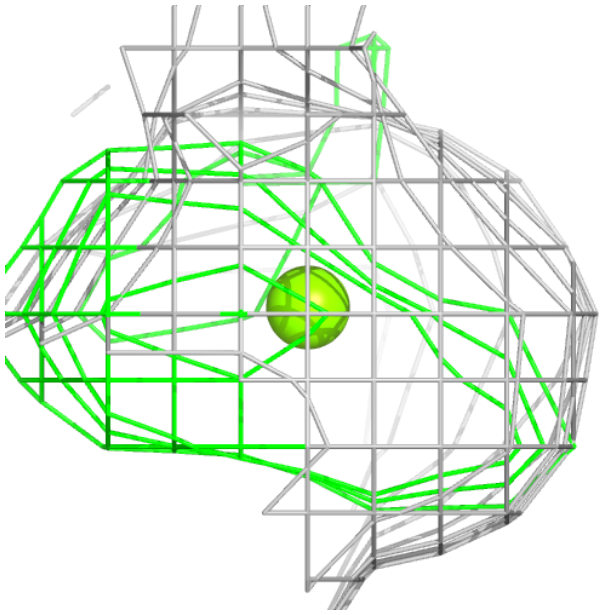
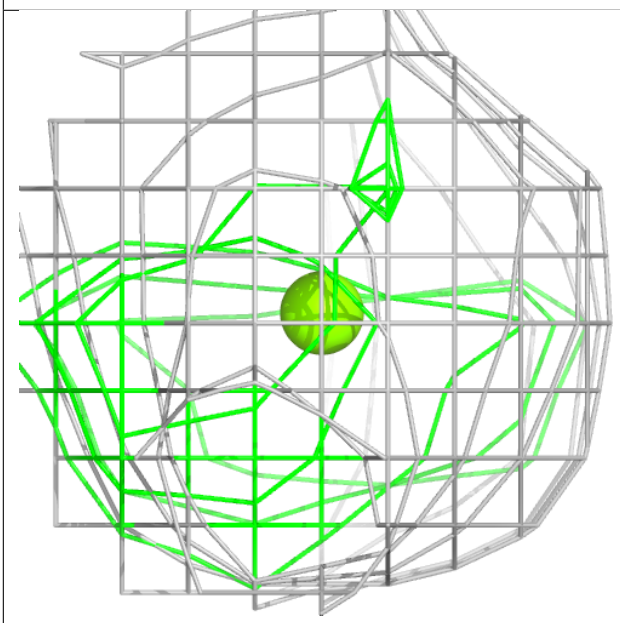
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	DTP	B	701	30/30	0.96	0.19	50,57,70,71	0
7	DTP	A	707	30/30	0.97	0.18	62,63,69,73	0
5	0KX	A	705	28/28	0.97	0.17	53,62,75,85	0
3	MN	A	702	1/1	0.98	0.06	57,57,57,57	0
3	MN	B	703	1/1	0.98	0.05	61,61,61,61	0
2	FE	A	701	1/1	0.99	0.10	53,53,53,53	0
2	FE	B	702	1/1	1.00	0.10	60,60,60,60	0

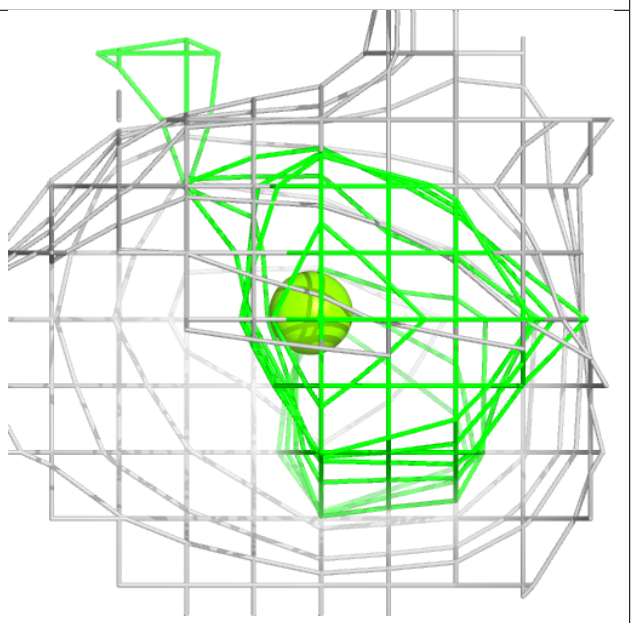
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MG 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)

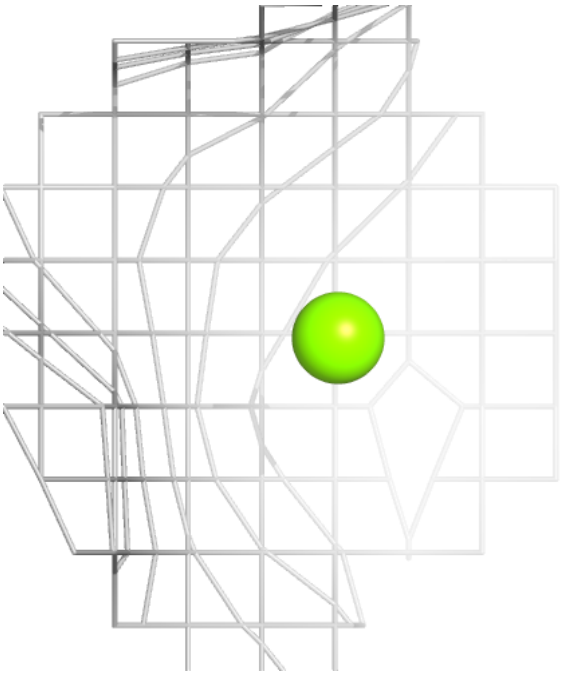


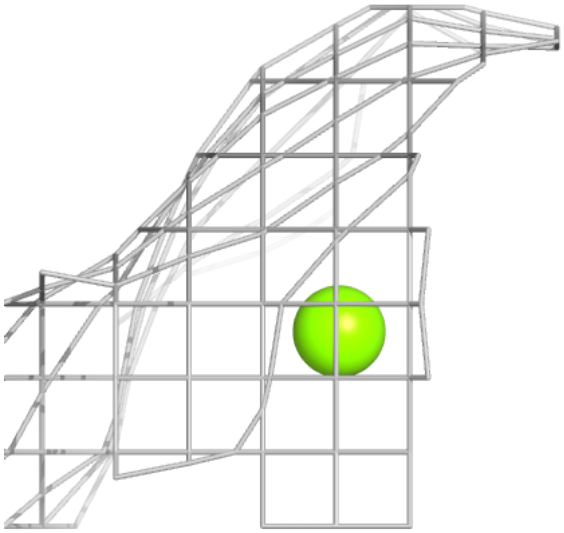


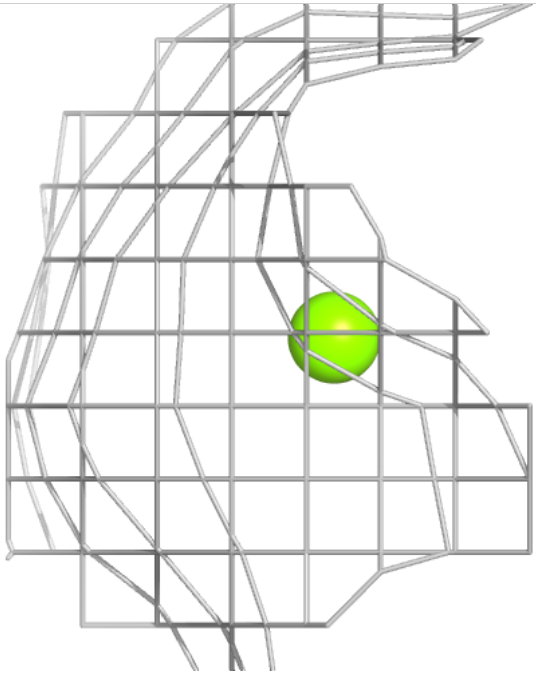


Electron density around MG A 704:

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

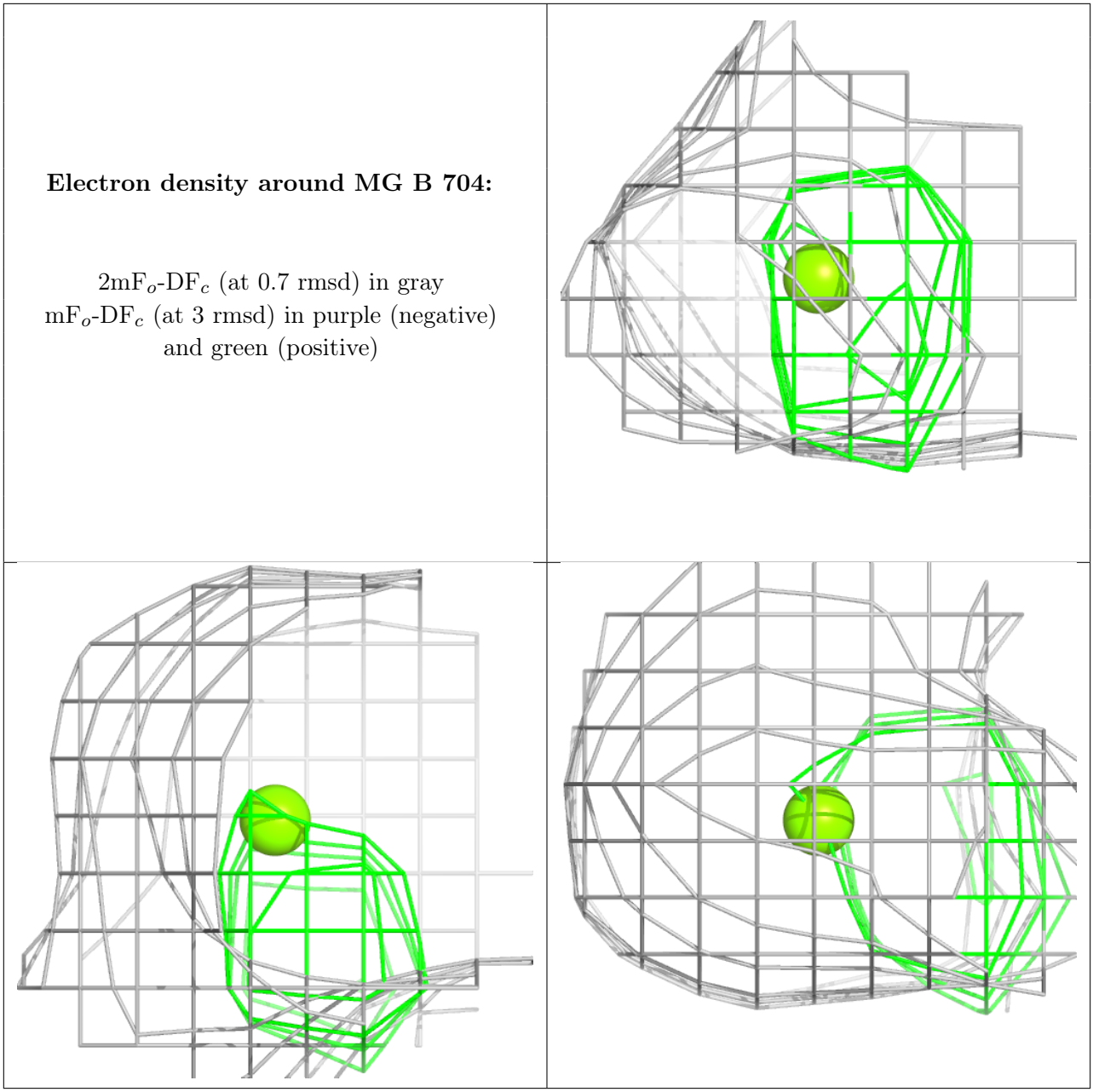






Electron density around MG B 704:

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



Electron density around MG B 705:

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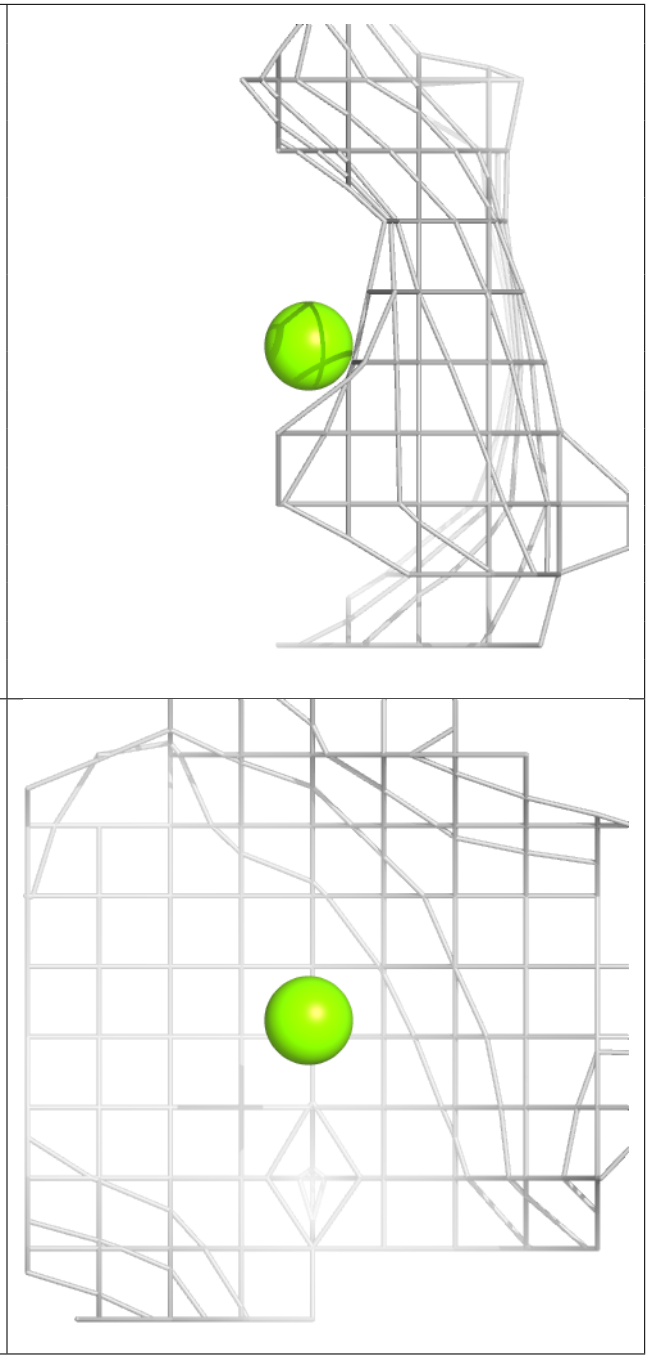
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 0KX B 706:

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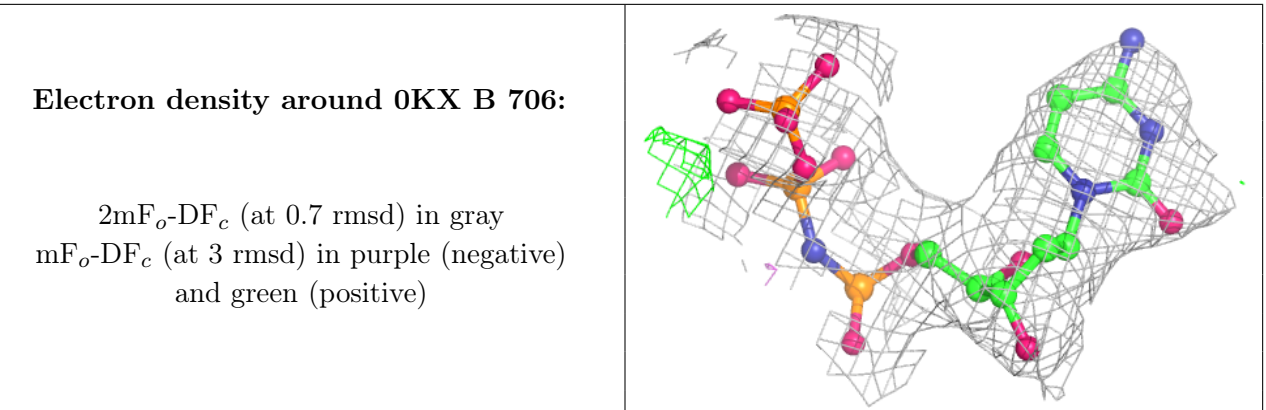
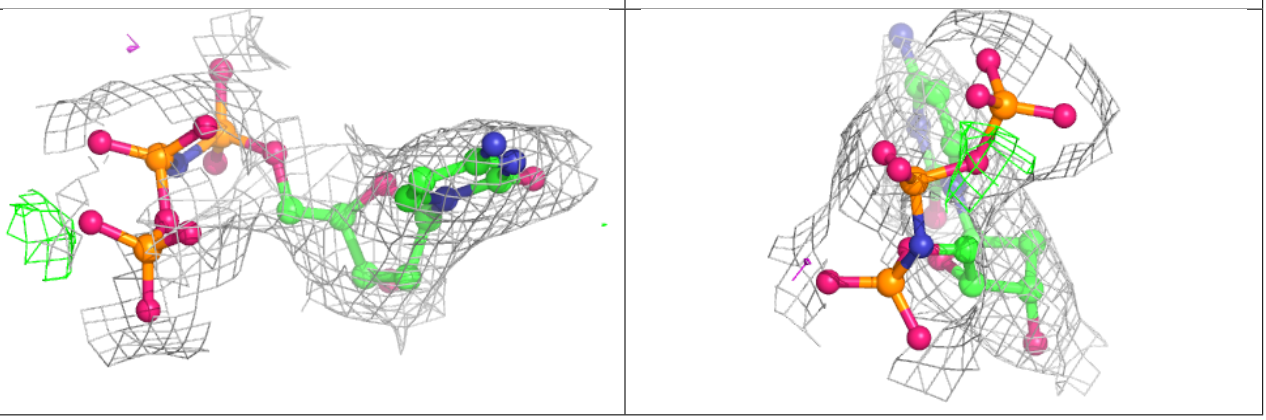
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around CZF A 706:

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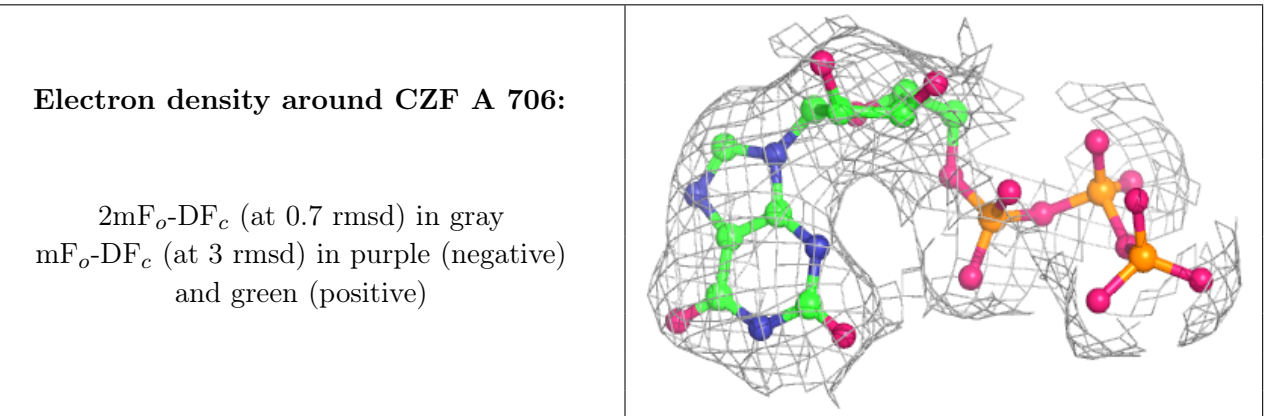
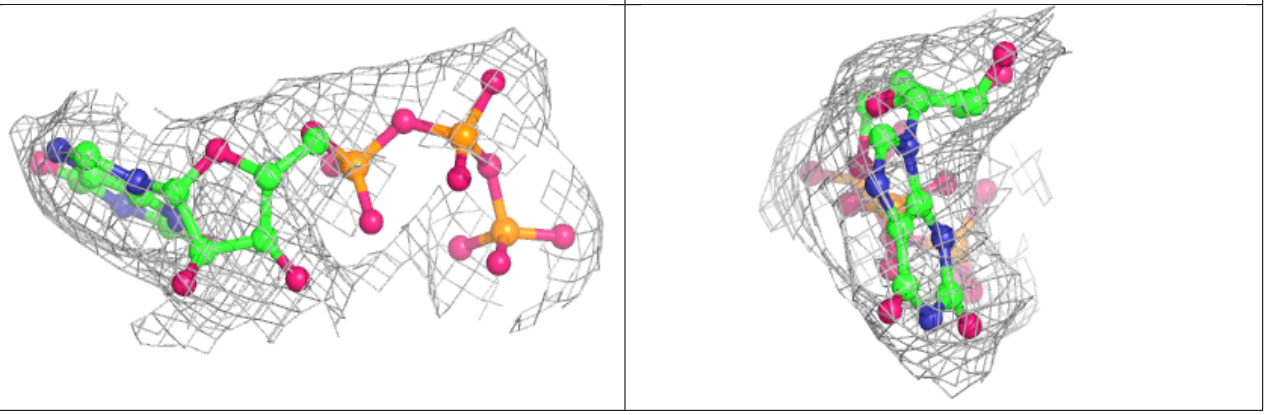
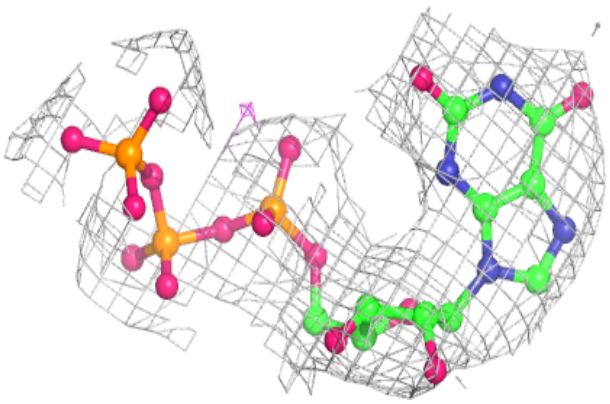
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

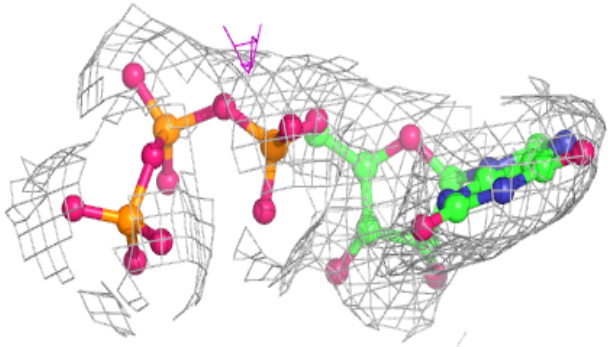


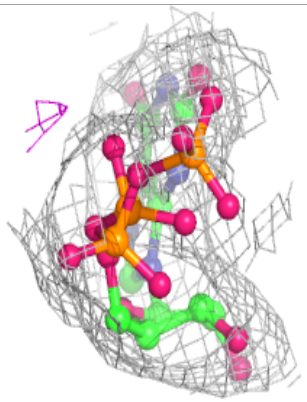


Electron density around CZF B 707:

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







Electron density around DTP B 701:

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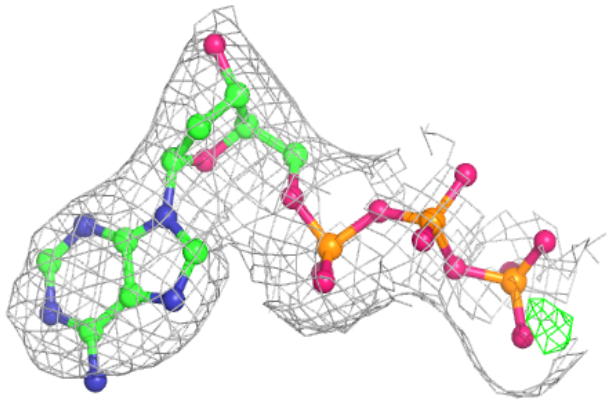
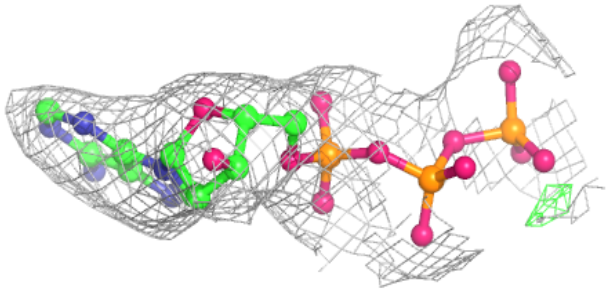
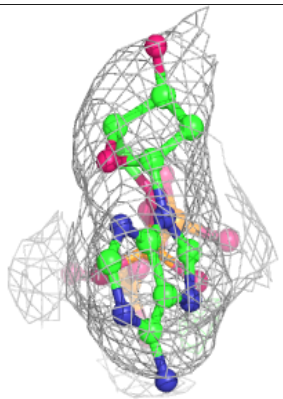
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

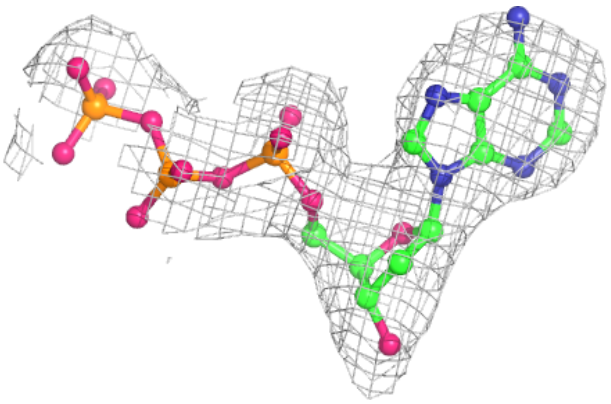


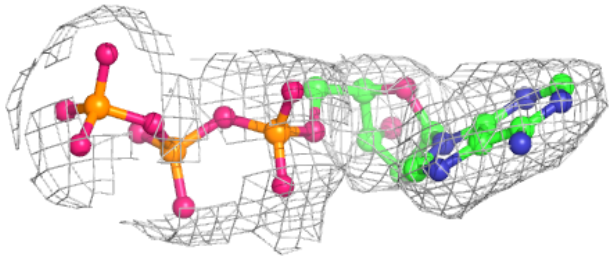


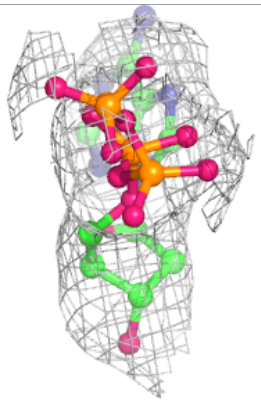


Electron density around DTP A 707:

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

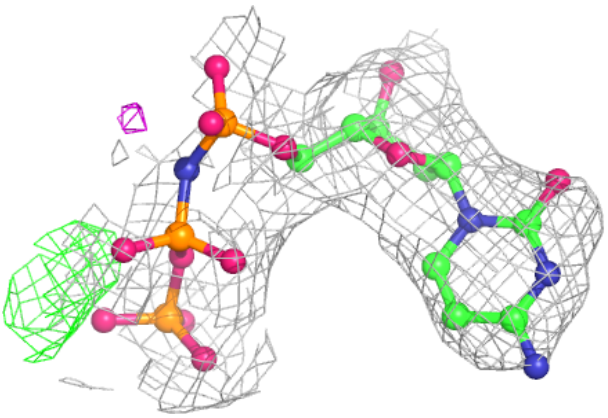


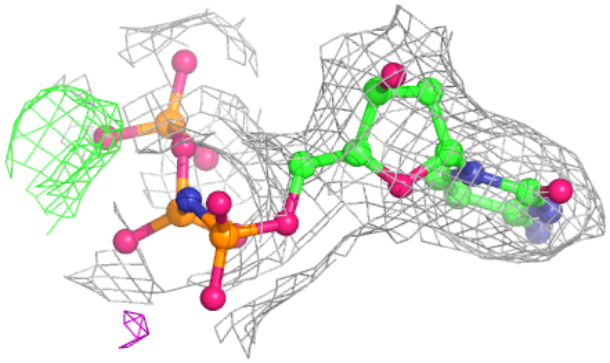


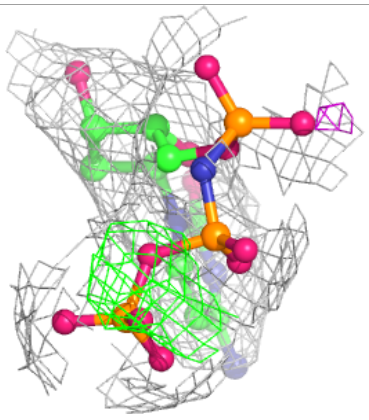


Electron density around 0KX A 705:

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

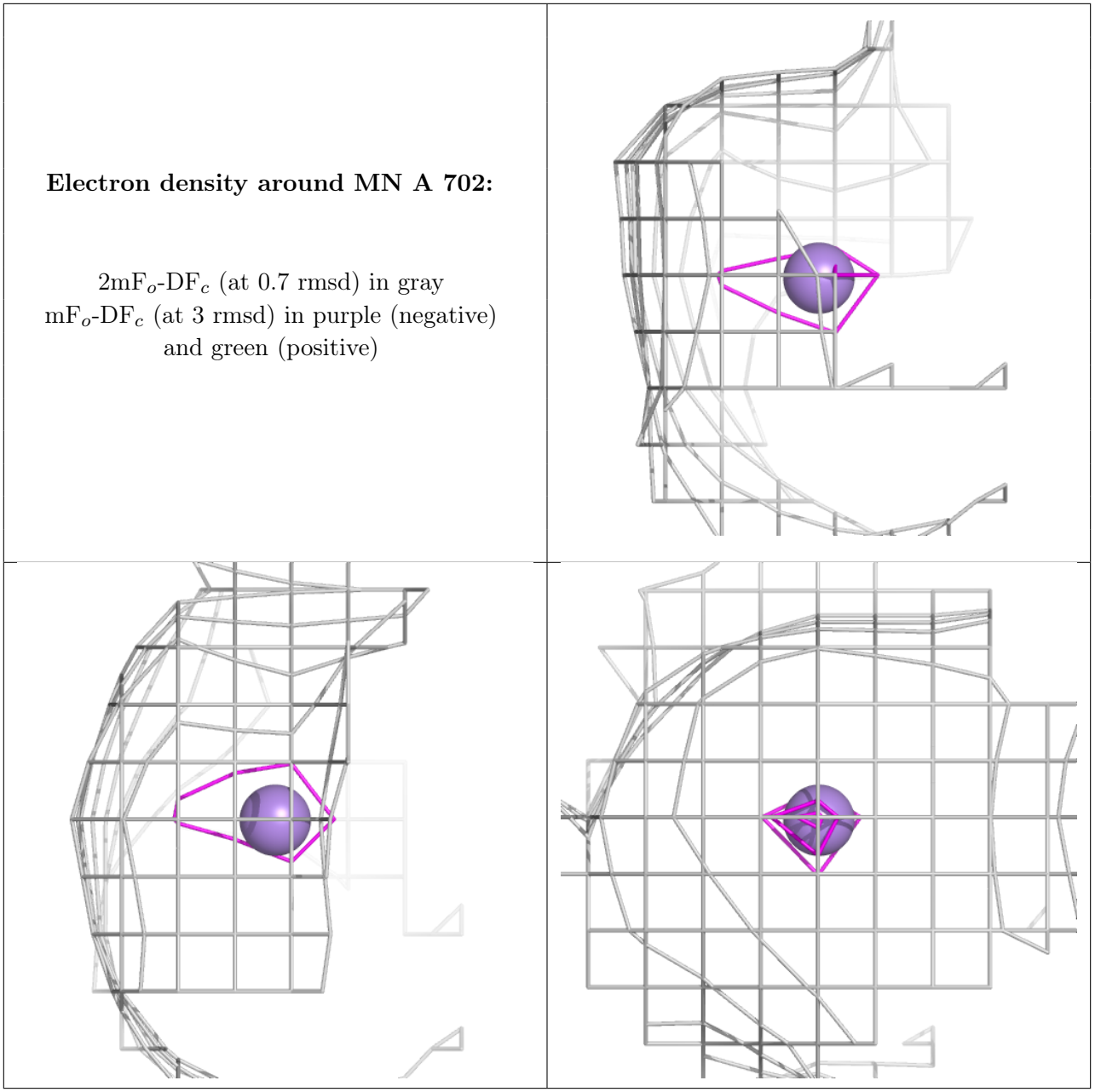






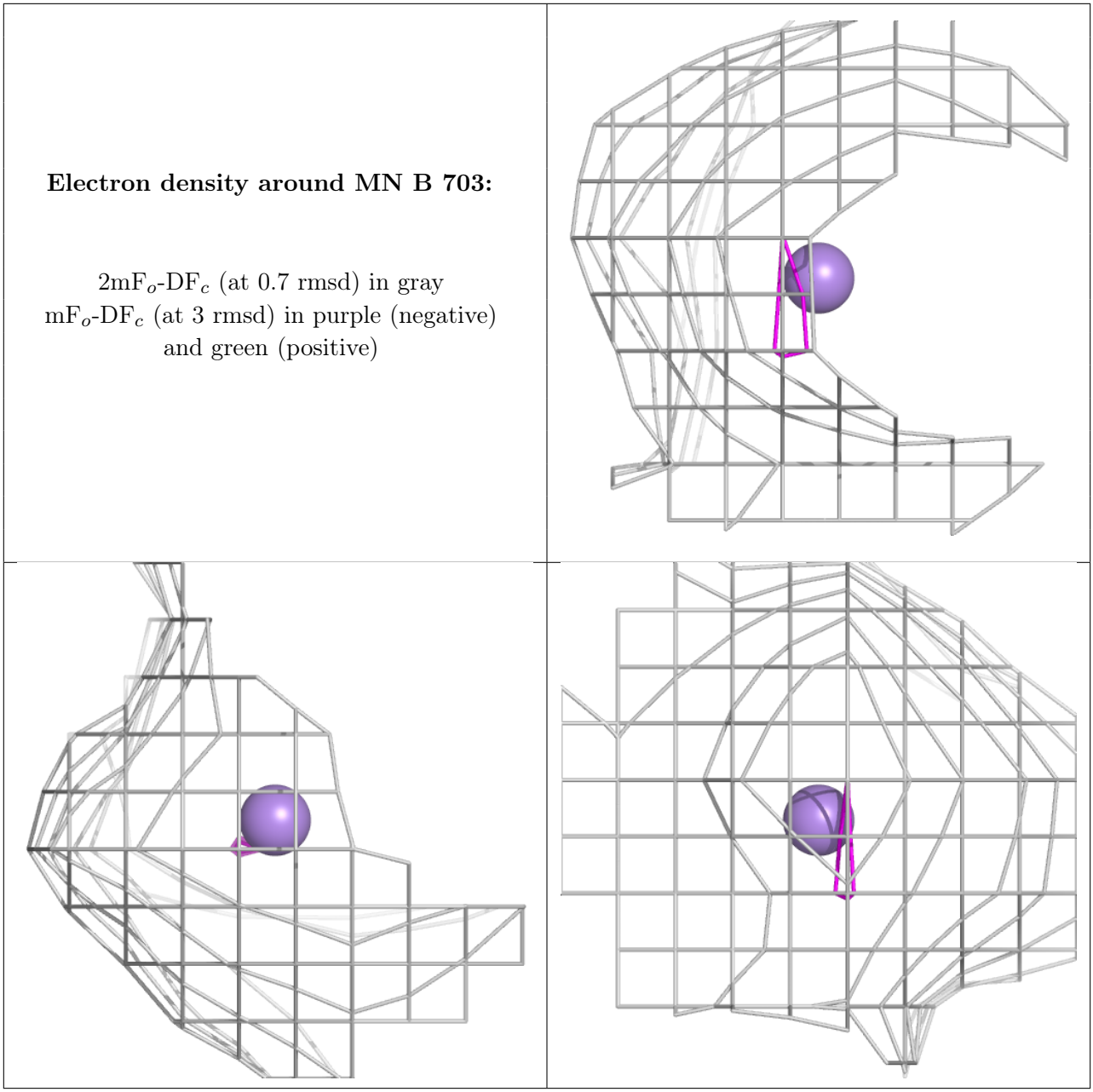
Electron density around MN A 702:

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



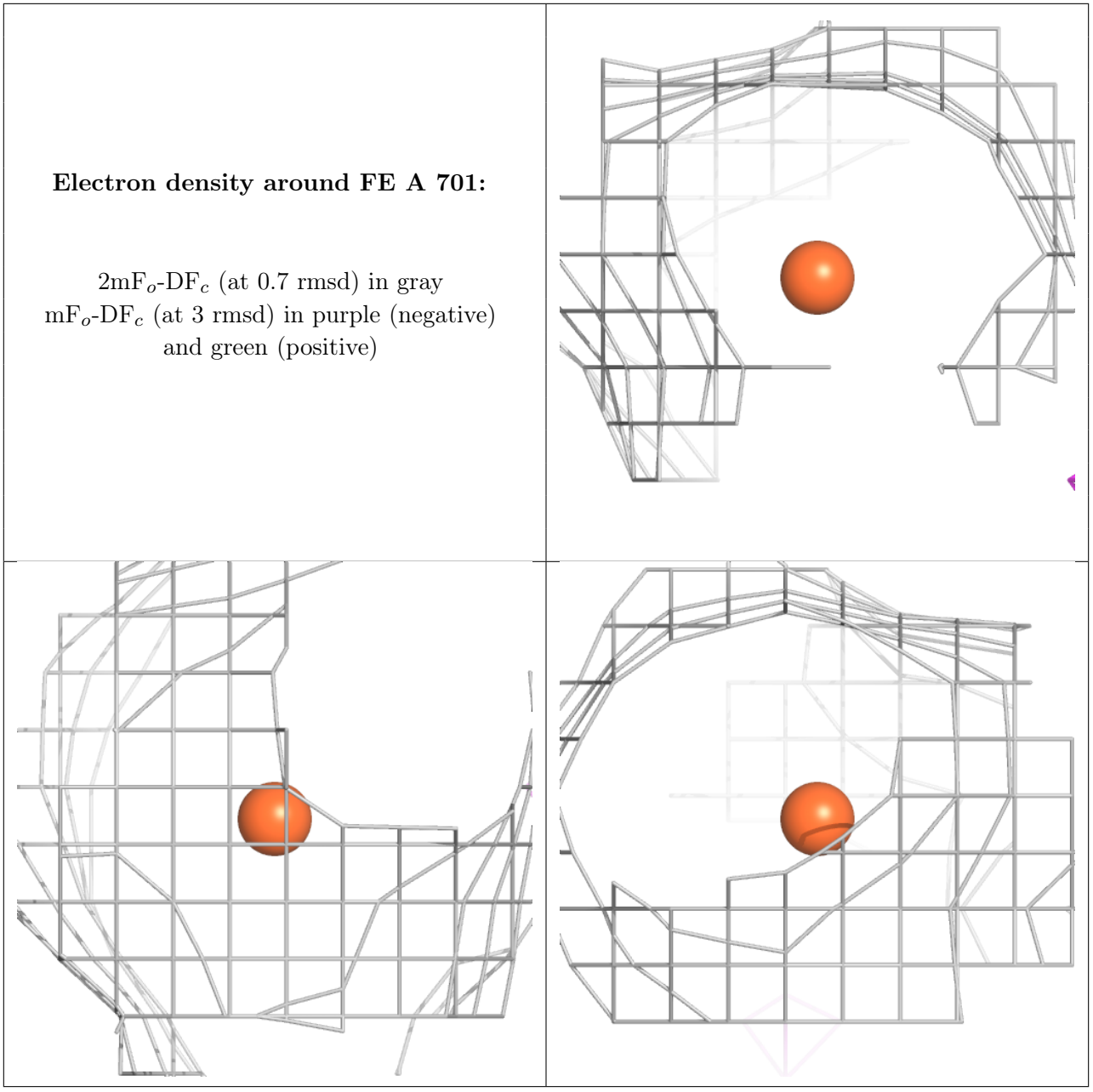
Electron density around MN B 703:

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



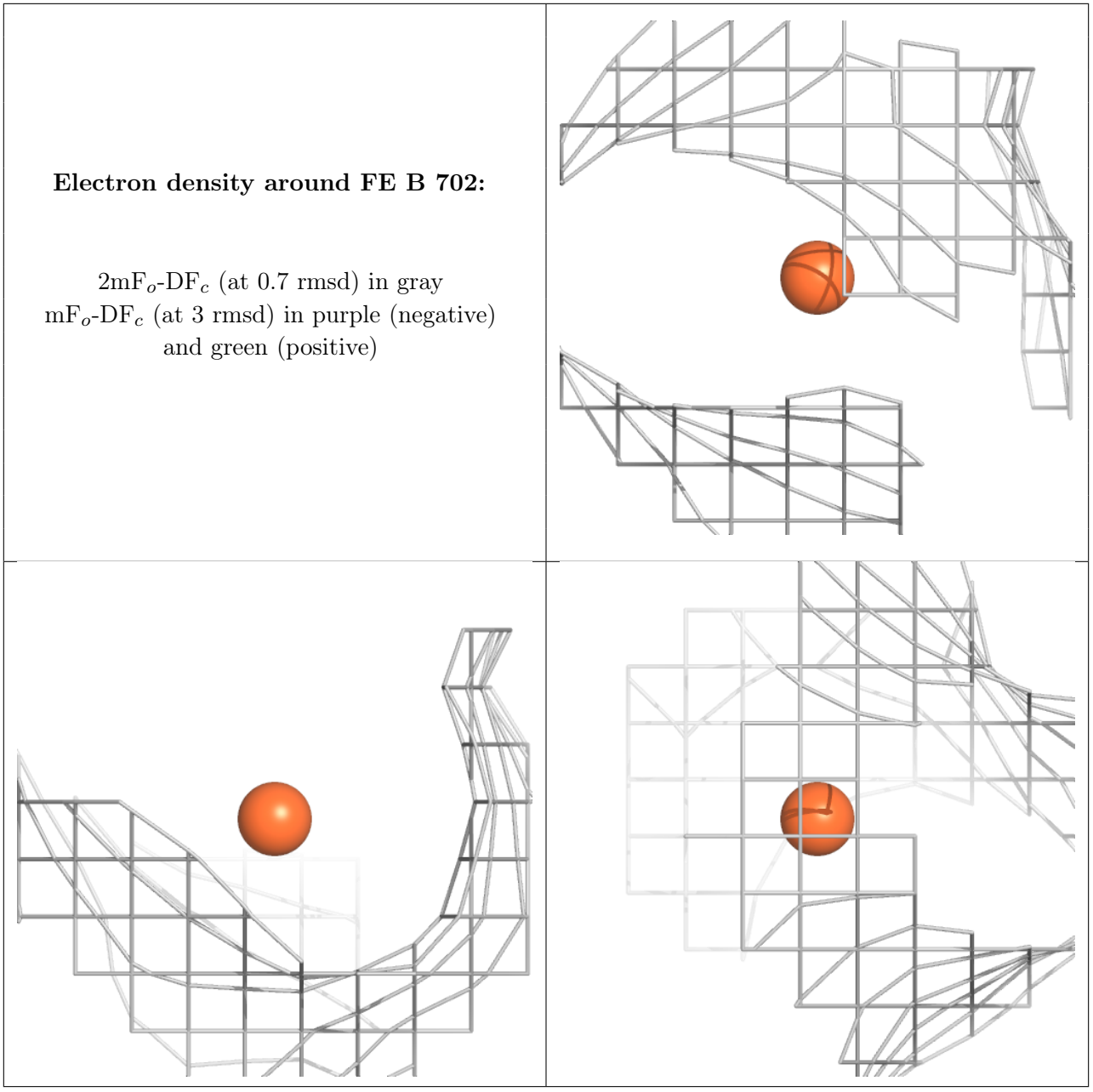
Electron density around FE A 701:

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



Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.