



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:24 AM UTC

PDB ID : 7B2C / pdb_00007b2c
Title : Crystal structure of the ethyl-coenzyme M reductase from Candidatus
Ethanoperedens thermophilum gassed with xenon
Authors : Wagner, T.; Lemaire, O.N.; Engilberge, S.
Deposited on : 2020-11-26
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

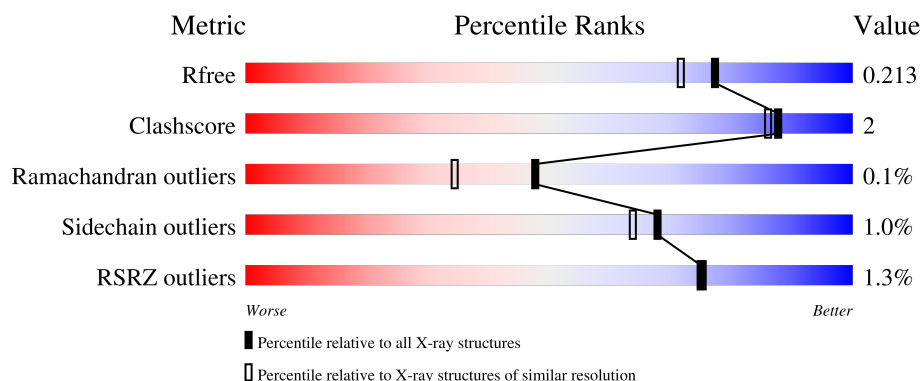
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

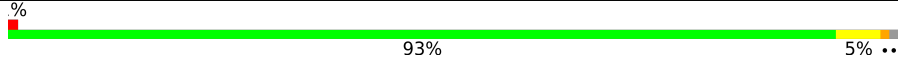
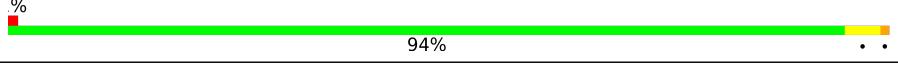
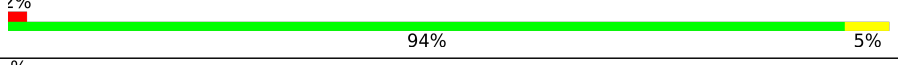
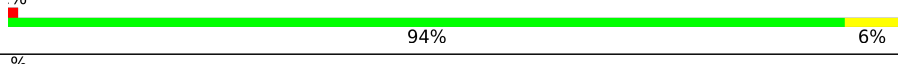
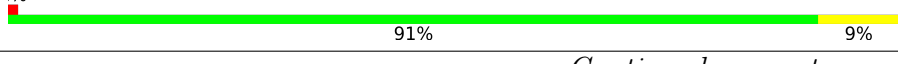
The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	
1	D	595	
2	B	467	
2	E	467	
3	C	266	

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Mol	Chain	Length	Quality of chain
3	F	266	% 92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	XE	B	511[B]	-	-	X	-
10	XE	F	1106[A]	-	-	X	-
4	USN	A	1201	X	-	-	-
4	USN	F	1101	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23280 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 Ethyl-Coenzyme M reductase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	5	0
			4669	2933	816	891	29			
1	D	593	Total	C	N	O	S	0	4	0
			4675	2942	816	888	29			

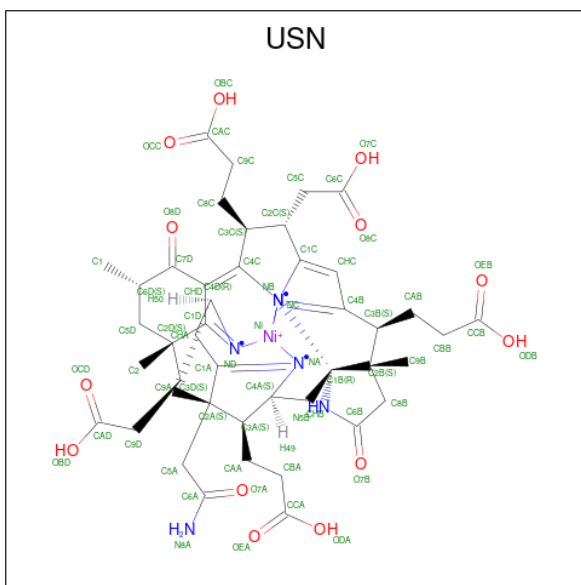
- Molecule 2 is a protein called Ethyl-Coenzyme M reductase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	0	2	0
			3517	2222	609	670	16			
2	E	466	Total	C	N	O	S	0	1	0
			3503	2215	604	668	16			

- Molecule 3 is a protein called Ethyl-Coenzyme M reductase gamma subunit.

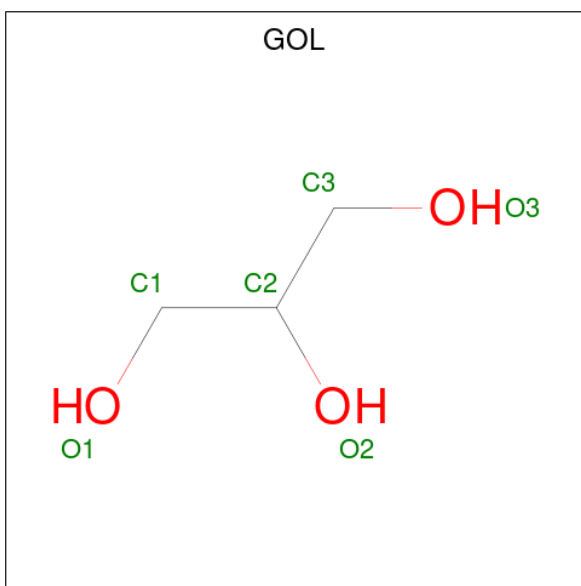
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	2	0
			2134	1322	387	408	17			
3	F	265	Total	C	N	O	S	0	3	0
			2140	1325	388	410	17			

- Molecule 4 is Dimethylated-F430 cofactor (CCD ID: USN) (formula: C₄₄H₅₅N₆NiO₁₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 64	C 44	N 6	Ni 1	O 13	0	0
4	F	1	Total 64	C 44	N 6	Ni 1	O 13	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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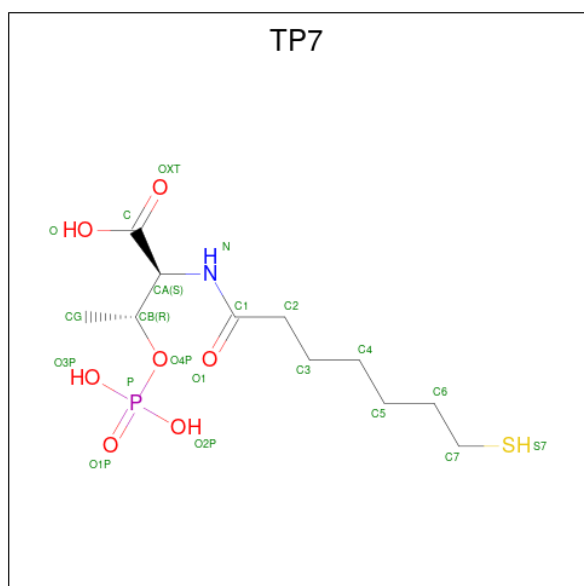
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

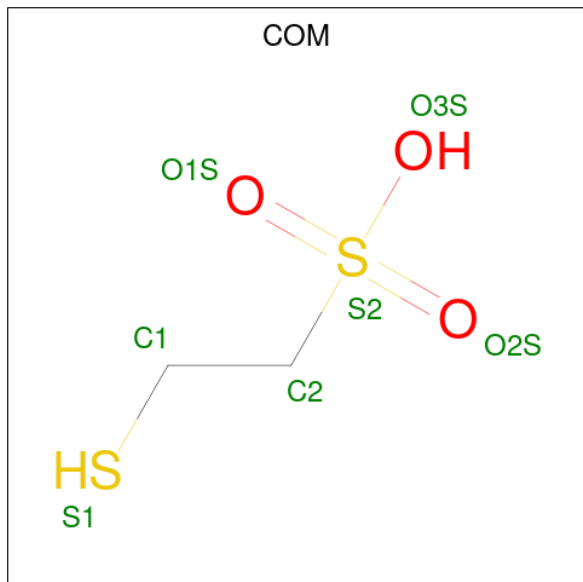
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		
6	D	3	Total	Na	0	0
			3	3		

- Molecule 7 is Coenzyme B (CCD ID: TP7) (formula: C₁₁H₂₂NO₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
7	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0

- Molecule 8 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	S	0	0
			7	2	3	2		
8	F	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	K	0	0
			2	2		
9	B	5	Total	K	0	0
			5	5		
9	C	1	Total	K	0	0
			1	1		
9	D	1	Total	K	0	0
			1	1		
9	E	7	Total	K	0	0
			7	7		
9	F	1	Total	K	0	0
			1	1		

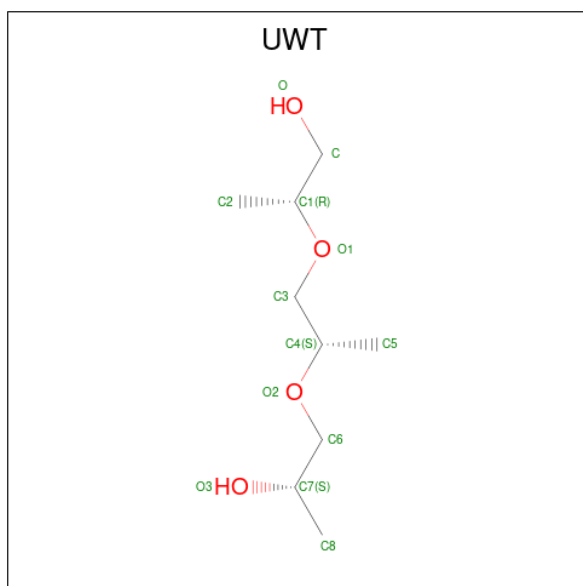
- Molecule 10 is XENON (CCD ID: XE) (formula: Xe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total 3	Xe 3	0	0
10	B	3	Total 3	Xe 3	0	1
10	C	2	Total 2	Xe 2	0	1
10	D	3	Total 3	Xe 3	0	0
10	E	3	Total 3	Xe 3	0	1
10	F	2	Total 2	Xe 2	0	1

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	2	Total 2	Cl 2	0	0
11	E	3	Total 3	Cl 3	0	0

- Molecule 12 is (2R)-2-[(2S)-2-[(2S)-2-oxidanylpropoxy]propoxy]propan-1-ol (CCD ID: UWT) (formula: C₉H₂₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total 11	C 8	O 3	0	0

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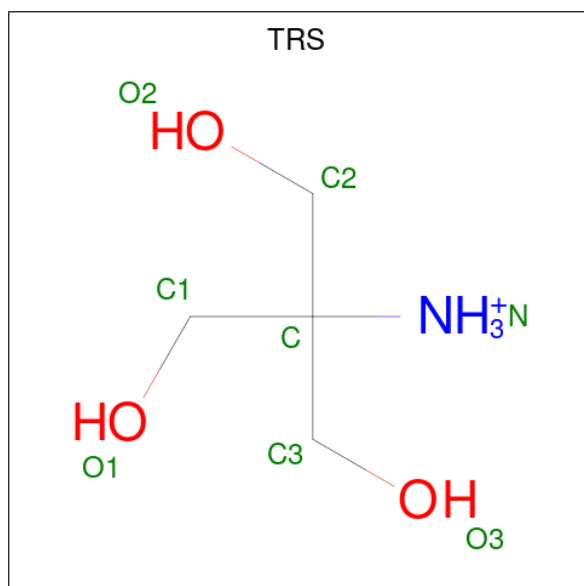
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	F	1	Total	C	O	0	0
			13	9	4		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	1	Total	Mg	0	0
			1	1		

- Molecule 14 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	E	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	498	Total	O	0	4
			498	498		
15	B	406	Total	O	0	7
			406	406		
15	C	248	Total	O	0	2
			248	248		

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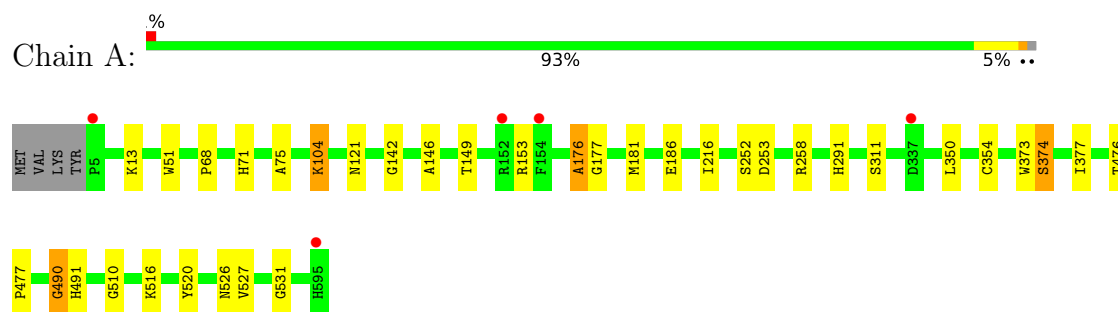
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	D	479	Total 479	O 479	0	5
15	E	436	Total 436	O 436	0	3
15	F	279	Total 279	O 279	0	2

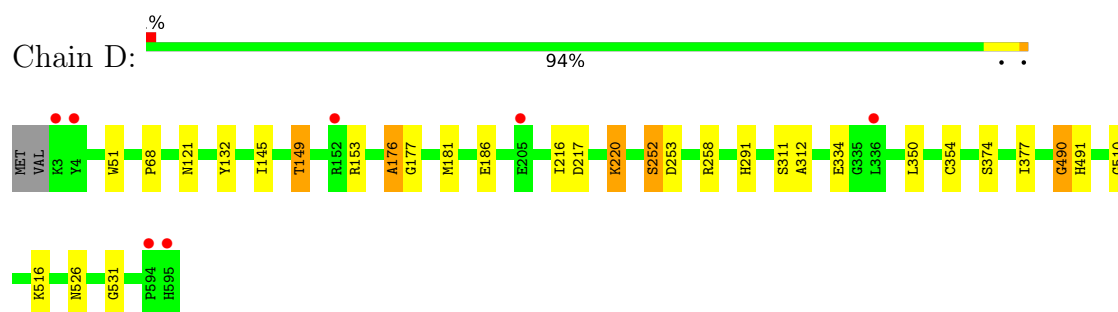
3 Residue-property plots [i](#)

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

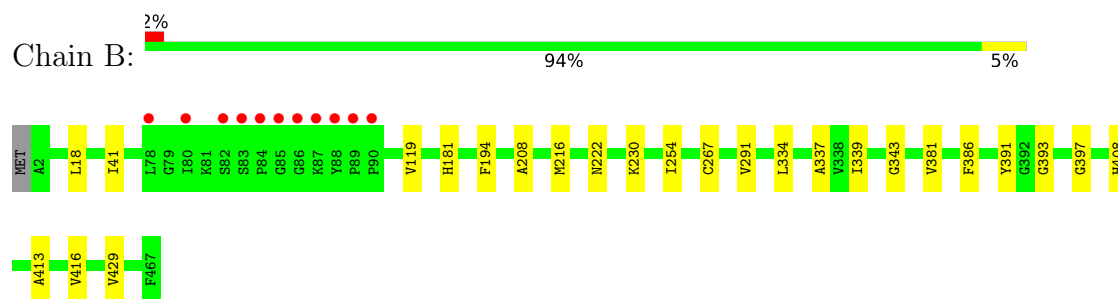
- Molecule 1: Ethyl-Coenzyme M reductase alpha subunit



- Molecule 1: Ethyl-Coenzyme M reductase alpha subunit



- Molecule 2: Ethyl-Coenzyme M reductase beta subunit

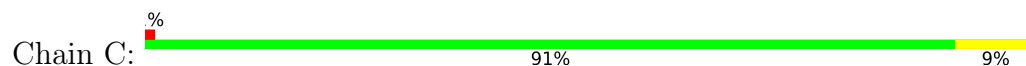


- Molecule 2: Ethyl-Coenzyme M reductase beta subunit

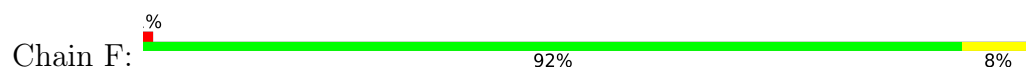




- Molecule 3: Ethyl-Coenzyme M reductase gamma subunit



- Molecule 3: Ethyl-Coenzyme M reductase gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.79Å 147.19Å 113.38Å 90.00° 107.20° 90.00°	Depositor
Resolution (Å)	35.90 – 1.80 35.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (35.90-1.80) 96.1 (35.90-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.80Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.174 , 0.201 0.188 , 0.213	Depositor DCC
R_{free} test set	11695 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23280	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: I2M, MG, K, HIC, CL, TRS, TP7, NA, GL3, XE, USN, AGM, COM, MGN, SMC, UWT, GOL, MHS

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	0.68	0/4713	0.98	10/6373 (0.2%)
1	D	0.68	1/4723 (0.0%)	0.99	9/6388 (0.1%)
2	B	0.69	0/3589	0.99	6/4872 (0.1%)
2	E	0.69	0/3578	0.98	5/4857 (0.1%)
3	C	0.66	0/2178	0.95	4/2944 (0.1%)
3	F	0.66	0/2184	0.95	2/2952 (0.1%)
All	All	0.68	1/20965 (0.0%)	0.98	36/28386 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	220	LYS	C-O	-5.05	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	PHE	N-CA-C	-7.13	100.77	110.68
1	D	176	ALA	N-CA-C	7.08	122.09	112.68
1	A	177	GLY	N-CA-C	7.07	124.94	112.64
2	E	194	PHE	N-CA-C	-6.93	101.05	110.68
2	B	391	TYR	N-CA-C	6.70	119.59	111.82
2	E	208	ALA	N-CA-C	6.67	121.43	113.16
2	E	391	TYR	N-CA-C	6.66	119.55	111.82
2	B	208	ALA	N-CA-C	6.49	121.21	113.16
1	A	176	ALA	N-CA-C	6.30	121.31	112.93
2	B	408	HIS	N-CA-C	6.23	117.74	111.07
1	A	216	ILE	N-CA-C	-6.16	98.12	107.73
1	D	526	ASN	N-CA-C	6.06	119.34	109.59
2	E	408	HIS	N-CA-C	5.99	117.48	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	SER	N-CA-C	-5.91	101.26	110.42
1	A	311	SER	N-CA-C	-5.90	101.27	110.42
1	A	526	ASN	N-CA-C	5.86	119.26	109.95
2	B	18	LEU	N-CA-C	-5.85	104.90	112.68
1	D	216	ILE	N-CA-C	-5.75	98.94	107.51
2	E	18	LEU	N-CA-C	-5.71	105.08	112.68
1	D	177	GLY	N-CA-C	5.68	120.65	112.81
3	C	116	ASP	N-CA-C	-5.48	100.09	109.24
3	F	258	MET	N-CA-C	-5.46	104.20	111.24
1	D	176	ALA	CA-C-N	-5.41	117.06	122.69
1	D	176	ALA	C-N-CA	-5.41	117.06	122.69
3	C	258	MET	N-CA-C	-5.38	104.30	111.24
1	A	520	TYR	N-CA-C	-5.37	100.18	109.58
2	B	119	VAL	N-CA-C	-5.35	106.59	111.67
3	F	157	THR	N-CA-C	-5.32	104.10	111.28
1	A	374	SER	N-CA-C	5.29	116.73	111.07
1	A	516	LYS	N-CA-C	-5.27	103.65	110.19
1	D	181	MET	N-CA-C	5.22	118.58	110.17
1	A	181	MET	N-CA-C	5.12	118.42	110.17
1	A	142	GLY	N-CA-C	-5.11	103.62	111.64
3	C	157	THR	N-CA-C	-5.08	104.42	111.28
3	C	215	THR	N-CA-C	5.08	117.27	110.35
1	D	516	LYS	N-CA-C	-5.03	104.22	110.41

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	4669	0	4445	16	0
1	D	4675	0	4464	20	0
2	B	3517	0	3485	14	0
2	E	3503	0	3473	18	0
3	C	2134	0	2088	8	0
3	F	2140	0	2092	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	64	0	0	0	0
4	F	64	0	0	1	0
5	A	12	0	16	2	0
5	B	6	0	8	1	0
5	D	12	0	16	0	0
5	F	6	0	8	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
7	A	21	0	19	0	0
7	D	21	0	19	0	0
8	A	7	0	5	0	0
8	F	7	0	5	1	0
9	A	2	0	0	0	0
9	B	5	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	7	0	0	0	0
9	F	1	0	0	0	0
10	A	3	0	0	0	0
10	B	3	0	0	3	0
10	C	2	0	0	1	0
10	D	3	0	0	1	0
10	E	3	0	0	1	0
10	F	2	0	0	2	0
11	B	2	0	0	0	0
11	E	3	0	0	0	0
12	C	11	0	0	0	0
12	F	13	0	0	0	0
13	D	1	0	0	0	0
14	E	8	0	12	1	0
15	A	498	0	0	1	0
15	B	406	0	0	2	0
15	C	248	0	0	1	0
15	D	479	0	0	2	0
15	E	436	0	0	2	0
15	F	279	0	0	5	0
All	All	23280	0	20155	81	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 (81) 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)
2:B:267:CYS:SG	10:B:510:XE:XE	3.15	0.82
2:B:429:VAL:HG21	1:D:149[B]:THR:HG22	1.66	0.78
2:E:267:CYS:SG	10:E:513:XE:XE	3.20	0.77
10:B:511[B]:XE:XE	1:D:153:ARG:HG3	2.72	0.68
2:E:413:ALA:O	2:E:416:VAL:HG22	1.98	0.64
2:B:429:VAL:CG2	1:D:149[B]:THR:HG22	2.32	0.60
3:F:202:MET:HE2	10:F:1106[A]:XE:XE	2.81	0.57
1:D:149[B]:THR:O	1:D:153:ARG:HB2	2.06	0.56
3:C:168:ASP:HB3	3:C:180:MET:HE2	1.88	0.55
3:F:255:LEU:HD12	3:F:266:MET:HE1	1.88	0.55
2:B:413:ALA:O	2:B:416:VAL:HG22	2.06	0.54
2:B:334:LEU:HG	2:B:416:VAL:HG11	1.89	0.53
1:A:104:LYS:HG2	15:A:1537:HOH:O	2.09	0.53
1:A:350:LEU:HD12	1:A:350:LEU:C	2.34	0.52
1:D:350:LEU:C	1:D:350:LEU:HD12	2.34	0.52
2:B:291:VAL:HG21	2:B:337:ALA:HA	1.92	0.52
2:E:291:VAL:HG21	2:E:337:ALA:HA	1.93	0.51
2:E:81:LYS:HD2	2:E:86:GLY:HA3	1.92	0.51
2:E:127:VAL:O	14:E:501:TRS:H32	2.11	0.50
10:B:511[B]:XE:XE	1:D:153:ARG:CG	3.36	0.50
3:C:202:MET:HE2	10:C:305[A]:XE:XE	2.90	0.50
1:D:217:ASP:CG	1:D:220:LYS:HG3	2.37	0.49
2:E:43:LYS:HE3	15:E:871:HOH:O	2.12	0.49
1:D:217:ASP:OD2	1:D:220:LYS:HG3	2.12	0.49
1:D:149[A]:THR:O	1:D:153:ARG:HB2	2.11	0.49
2:B:429:VAL:HG21	1:D:149[B]:THR:CG2	2.40	0.48
2:E:334:LEU:HG	2:E:416:VAL:HG11	1.96	0.48
5:B:501:GOL:H2	15:B:808:HOH:O	2.13	0.48
1:D:490:GL3:HA2	2:E:381:VAL:CG1	2.44	0.47
2:B:230:LYS:NZ	15:B:601:HOH:O	2.31	0.47
3:F:211:LEU:HD11	15:F:1205:HOH:O	2.15	0.47
2:E:81:LYS:HD2	2:E:86:GLY:CA	2.45	0.47
1:A:121:ASN:HA	1:A:374:SER:OG	2.16	0.46
10:D:710:XE:XE	3:F:249:ILE:HG21	2.94	0.46
1:A:146:ALA:O	1:A:149:THR:HG22	2.16	0.45
2:E:43:LYS:NZ	15:E:609:HOH:O	2.49	0.45
3:C:255:LEU:HD12	3:C:266:MET:HE1	1.99	0.45
3:F:202:MET:CE	10:F:1106[A]:XE:XE	3.43	0.45
4:F:1101:USN:C1C	8:F:1102:COM:H12	2.46	0.44
1:A:149:THR:OG1	1:A:153:ARG:HD3	2.17	0.44
2:E:230:LYS:HE3	15:F:1308:HOH:O	2.16	0.44
3:C:231:ASP:N	3:C:232:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ASN:HA	1:D:374:SER:OG	2.17	0.44
2:B:222:ASN:OD1	2:B:397:GLY:HA3	2.18	0.44
3:C:89:ILE:HG12	3:C:125:THR:HG22	2.00	0.43
3:C:101:HIS:HB3	3:C:119:VAL:HG13	1.99	0.43
2:B:429:VAL:HG11	1:D:145:ILE:HG23	1.99	0.43
3:F:66:GLU:HG2	15:F:1431:HOH:O	2.19	0.43
1:D:176:ALA:O	1:D:186:GLU:HB3	2.19	0.43
3:F:89:ILE:HG12	3:F:125:THR:HG22	2.00	0.43
3:F:101:HIS:HB3	3:F:119:VAL:HG13	2.01	0.43
2:B:386:PHE:O	2:B:393:GLY:HA3	2.19	0.43
2:E:386:PHE:O	2:E:393:GLY:HA3	2.19	0.43
1:D:252[B]:SER:OG	1:D:253:ASP:N	2.51	0.42
2:E:220:MET:HE2	2:E:223:HIS:CE1	2.54	0.42
2:E:339:ILE:O	2:E:343:GLY:HA3	2.18	0.42
1:A:510:GLY:O	2:E:181:HIS:CE1	2.72	0.42
2:E:220:MET:CE	2:E:223:HIS:CE1	3.03	0.42
1:D:51:TRP:CE2	1:D:68:PRO:HD2	2.55	0.42
1:A:13:LYS:NZ	5:A:1202:GOL:H2	2.34	0.42
1:A:51:TRP:CE2	1:A:68:PRO:HD2	2.55	0.42
1:D:354:SMC:SG	1:D:531:GLY:HA3	2.59	0.42
1:A:176:ALA:O	1:A:186:GLU:HB3	2.20	0.42
3:C:205:PRO:HB2	15:C:416:HOH:O	2.19	0.42
3:C:175:ILE:O	3:C:175:ILE:HG22	2.20	0.42
1:D:217:ASP:HB3	15:D:1177:HOH:O	2.19	0.42
1:A:476:THR:HB	1:A:477:PRO:CD	2.49	0.41
2:E:230:LYS:CE	15:F:1308:HOH:O	2.67	0.41
1:A:373:TRP:CE3	1:A:527:VAL:HG11	2.55	0.41
3:F:175:ILE:O	3:F:175:ILE:HG22	2.21	0.41
2:B:339:ILE:O	2:B:343:GLY:HA3	2.19	0.41
2:E:222:ASN:OD1	2:E:397:GLY:HA3	2.20	0.41
1:A:71:HIS:ND1	1:A:75:ALA:O	2.54	0.41
1:A:354:SMC:SG	1:A:531:GLY:HA3	2.60	0.41
1:A:490:GL3:HA2	2:B:381:VAL:CG1	2.50	0.41
3:F:170:MET:HE3	3:F:170:MET:HB3	1.94	0.41
1:A:253:ASP:HB3	15:D:1108:HOH:O	2.20	0.41
2:B:181:HIS:CE1	1:D:510:GLY:O	2.74	0.41
1:A:13:LYS:HZ2	5:A:1202:GOL:H2	1.85	0.41
1:D:132:TYR:CE1	1:D:312:ALA:HB2	2.56	0.41
3:F:37:LYS:CE	15:F:1202:HOH:O	2.69	0.41

There are no symmetry-related clashes.

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	587/595 (99%)	563 (96%)	22 (4%)	2 (0%)	36	25
1	D	588/595 (99%)	568 (97%)	18 (3%)	2 (0%)	36	25
2	B	466/467 (100%)	455 (98%)	11 (2%)	0	100	100
2	E	465/467 (100%)	457 (98%)	8 (2%)	0	100	100
3	C	264/266 (99%)	257 (97%)	7 (3%)	0	100	100
3	F	265/266 (100%)	258 (97%)	7 (3%)	0	100	100
All	All	2635/2656 (99%)	2558 (97%)	73 (3%)	4 (0%)	48	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252[A]	SER
1	A	252[B]	SER
1	D	252[A]	SER
1	D	252[B]	SER

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	471/470 (100%)	469 (100%)	2 (0%)	84	83
1	D	472/470 (100%)	468 (99%)	4 (1%)	73	70
2	B	365/364 (100%)	362 (99%)	3 (1%)	73	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	364/364 (100%)	362 (100%)	2 (0%)	81	80
3	C	236/236 (100%)	230 (98%)	6 (2%)	42	30
3	F	237/236 (100%)	232 (98%)	5 (2%)	47	36
All	All	2145/2140 (100%)	2123 (99%)	22 (1%)	68	64

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	258	ARG
2	B	41	ILE
2	B	216	MET
2	B	254	ILE
3	C	29	GLU
3	C	69	ILE
3	C	103	THR
3	C	117	ASN
3	C	178	CYS
3	C	222	ARG
1	D	149[A]	THR
1	D	149[B]	THR
1	D	258	ARG
1	D	334	GLU
2	E	216	MET
2	E	254	ILE
3	F	29	GLU
3	F	69	ILE
3	F	103	THR
3	F	117	ASN
3	F	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	65	ASN
1	A	79	GLN
1	A	141	ASN
1	A	240	GLN
1	A	427	GLN

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Mol	Chain	Res	Type
1	A	450	GLN
1	A	475	ASN
2	B	120	ASN
2	B	160	GLN
2	B	321	ASN
3	C	47	HIS
3	C	184	ASN
1	D	65	ASN
1	D	79	GLN
1	D	240	GLN
1	D	427	GLN
1	D	450	GLN
2	E	31	GLN
2	E	160	GLN
3	F	4	GLN
3	F	47	HIS
3	F	184	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	I2M	D	377	1	7,8,9	1.04	1 (14%)	6,11,13	1.49	1 (16%)
1	SMC	D	354	1	5,6,7	0.75	0	3,6,8	0.19	0
1	MHS	A	291	1	10,11,12	1.27	1 (10%)	5,14,16	3.23	2 (40%)
1	MHS	D	291	1	10,11,12	1.25	1 (10%)	5,14,16	3.20	2 (40%)
1	AGM	A	305	1	10,11,12	0.46	0	7,13,15	0.77	0
1	AGM	D	305	1	10,11,12	0.48	0	7,13,15	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	I2M	A	377	1	7,8,9	1.08	1 (14%)	6,11,13	1.44	1 (16%)
1	MGN	A	445	1	6,9,10	0.75	0	7,12,14	0.74	0
1	HIC	D	491	1	10,11,12	0.99	0	9,14,16	3.75	2 (22%)
1	MGN	D	445	1	6,9,10	0.72	0	7,12,14	0.62	0
1	GL3	D	490	1	2,3,4	4.63	1 (50%)	1,2,4	0.34	0
1	SMC	A	354	1	5,6,7	0.75	0	3,6,8	0.32	0
1	HIC	A	491	1	10,11,12	1.01	0	9,14,16	3.50	2 (22%)
1	GL3	A	490	1	2,3,4	4.00	1 (50%)	1,2,4	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	I2M	D	377	1	-	0/7/11/13	-
1	SMC	D	354	1	-	0/3/5/7	-
1	MHS	A	291	1	-	0/5/6/8	0/1/1/1
1	MHS	D	291	1	-	0/5/6/8	0/1/1/1
1	AGM	A	305	1	-	1/10/11/13	-
1	AGM	D	305	1	-	1/10/11/13	-
1	I2M	A	377	1	-	0/7/11/13	-
1	MGN	A	445	1	-	0/7/9/12	-
1	HIC	D	491	1	-	2/5/6/8	0/1/1/1
1	MGN	D	445	1	-	0/7/9/12	-
1	GL3	D	490	1	-	0/1/1/2	-
1	SMC	A	354	1	-	0/3/5/7	-
1	HIC	A	491	1	-	2/5/6/8	0/1/1/1
1	GL3	A	490	1	-	0/1/1/2	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	490	GL3	C-S	-6.54	1.54	1.80
1	A	490	GL3	C-S	-5.66	1.57	1.80
1	A	377	I2M	CB-CA	-2.49	1.53	1.57
1	D	377	I2M	CB-CA	-2.38	1.53	1.57
1	D	291	MHS	CD2-CG	2.31	1.39	1.36
1	A	291	MHS	CD2-CG	2.08	1.39	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	491	HIC	NE2-CE1-ND1	-10.12	108.79	112.66
1	A	491	HIC	NE2-CE1-ND1	-9.68	108.96	112.66
1	A	291	MHS	ND1-CE1-NE2	-6.60	109.01	112.94
1	D	291	MHS	ND1-CE1-NE2	-6.51	109.06	112.94
1	D	491	HIC	CD2-NE2-CE1	3.98	108.28	106.71
1	A	491	HIC	CD2-NE2-CE1	3.32	108.02	106.71
1	A	377	I2M	C-CA-N	2.99	114.88	110.34
1	D	377	I2M	C-CA-N	2.84	114.65	110.34
1	A	291	MHS	CD2-NE2-CE1	2.41	108.40	105.24
1	D	291	MHS	CD2-NE2-CE1	2.29	108.24	105.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	491	HIC	CA-CB-CG-CD2
1	D	491	HIC	CA-CB-CG-CD2
1	A	491	HIC	CA-CB-CG-ND1
1	D	491	HIC	CA-CB-CG-ND1
1	A	305	AGM	NE1-CD-CG-CB
1	D	305	AGM	CE2-CD-NE1-CZ

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	354	SMC	1	0
1	D	490	GL3	1	0
1	A	354	SMC	1	0
1	A	490	GL3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 59 ligands modelled in this entry, 44 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	USN	A	1201	8	63,73,73	2.66	21 (33%)	76,123,123	2.19	26 (34%)
12	UWT	F	1103	-	12,12,12	0.60	0	14,14,14	0.85	0
8	COM	F	1102	4	6,6,6	1.18	0	8,8,8	2.08	3 (37%)
4	USN	F	1101	8	63,73,73	2.95	25 (39%)	76,123,123	2.16	25 (32%)
7	TP7	A	1204	-	19,20,20	0.76	0	24,26,26	0.91	0
5	GOL	A	1202	-	5,5,5	0.30	0	5,5,5	0.23	0
5	GOL	B	501	-	5,5,5	0.22	0	5,5,5	0.36	0
14	TRS	E	501	-	7,7,7	0.16	0	9,9,9	0.39	0
5	GOL	A	1211	-	5,5,5	0.08	0	5,5,5	0.31	0
5	GOL	D	703	-	5,5,5	0.29	0	5,5,5	0.35	0
8	COM	A	1205	4	6,6,6	1.50	2 (33%)	8,8,8	1.99	4 (50%)
7	TP7	D	701	-	19,20,20	0.85	1 (5%)	24,26,26	1.00	0
5	GOL	F	1107	-	5,5,5	0.09	0	5,5,5	0.31	0
5	GOL	D	702	-	5,5,5	0.24	0	5,5,5	0.34	0
12	UWT	C	301	-	10,10,12	0.54	0	11,11,14	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	USN	A	1201	8	1/1/31/33	2/28/193/193	-
12	UWT	F	1103	-	-	4/12/12/12	-
8	COM	F	1102	4	-	0/4/4/4	-
4	USN	F	1101	8	1/1/31/33	2/28/193/193	-
7	TP7	A	1204	-	-	1/24/24/24	-
5	GOL	A	1202	-	-	2/4/4/4	-
5	GOL	B	501	-	-	0/4/4/4	-
14	TRS	E	501	-	-	6/9/9/9	-
5	GOL	A	1211	-	-	2/4/4/4	-
5	GOL	D	703	-	-	2/4/4/4	-
8	COM	A	1205	4	-	0/4/4/4	-
7	TP7	D	701	-	-	1/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	F	1107	-	-	2/4/4/4	-
5	GOL	D	702	-	-	0/4/4/4	-
12	UWT	C	301	-	-	1/9/9/12	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1101	USN	NI-NA	10.43	2.14	1.89
4	A	1201	USN	NI-NA	9.19	2.11	1.89
4	A	1201	USN	NI-ND	7.68	2.08	1.89
4	F	1101	USN	CHD-C1D	-7.62	1.32	1.43
4	A	1201	USN	CHB-C4A	7.47	1.62	1.51
4	F	1101	USN	NI-NB	7.44	2.07	1.89
4	F	1101	USN	O8D-C7D	5.98	1.32	1.22
4	A	1201	USN	NI-NB	5.97	2.03	1.89
4	F	1101	USN	NI-ND	5.82	2.03	1.89
4	F	1101	USN	CHA-C4D	5.19	1.58	1.53
4	F	1101	USN	C9B-C2B	5.04	1.63	1.54
4	A	1201	USN	CHD-C1D	-4.71	1.36	1.43
4	F	1101	USN	CHB-C1B	4.58	1.56	1.53
4	A	1201	USN	C4D-ND	-4.44	1.42	1.49
4	F	1101	USN	O8C-C6C	4.06	1.35	1.22
4	F	1101	USN	C3A-C4A	3.87	1.60	1.53
4	F	1101	USN	OBD-CAD	-3.61	1.18	1.30
4	F	1101	USN	CHB-C4A	3.36	1.56	1.51
4	A	1201	USN	C2A-C3A	3.35	1.60	1.54
4	F	1101	USN	C4A-NA	3.22	1.54	1.49
4	F	1101	USN	CHC-C4B	3.21	1.48	1.39
4	A	1201	USN	CHC-C1C	-3.14	1.30	1.36
4	A	1201	USN	OBC-CAC	-3.07	1.20	1.30
4	A	1201	USN	OCC-CAC	3.05	1.32	1.22
4	A	1201	USN	CHC-C4B	3.03	1.47	1.39
4	A	1201	USN	CAB-C3B	2.95	1.61	1.54
4	A	1201	USN	OEA-CCA	2.88	1.31	1.22
4	A	1201	USN	C5D-C6D	2.87	1.58	1.53
4	F	1101	USN	C2-C2D	2.78	1.59	1.54
4	F	1101	USN	CBB-CCB	-2.70	1.44	1.50
4	F	1101	USN	CHC-C1C	-2.61	1.31	1.36
4	F	1101	USN	CAB-C3B	2.58	1.60	1.54
4	A	1201	USN	C2B-C3B	-2.46	1.50	1.57
8	A	1205	COM	O2S-S2	2.43	1.52	1.45
4	A	1201	USN	C4A-NA	-2.42	1.45	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1201	USN	OBD-CAD	-2.40	1.22	1.30
4	F	1101	USN	CAA-CBA	2.39	1.60	1.52
4	F	1101	USN	O7B-C6B	2.38	1.28	1.23
4	A	1201	USN	C4B-NB	-2.36	1.25	1.30
8	A	1205	COM	O1S-S2	2.31	1.51	1.45
4	F	1101	USN	C9A-C2A	-2.30	1.50	1.54
4	A	1201	USN	CHD-C7D	2.28	1.51	1.44
4	F	1101	USN	C4D-ND	-2.27	1.45	1.49
7	D	701	TP7	P-O4P	2.24	1.63	1.59
4	A	1201	USN	C3A-C4A	2.22	1.57	1.53
4	F	1101	USN	C8B-C2B	-2.15	1.51	1.54
4	F	1101	USN	C5D-C2D	2.10	1.57	1.54
4	F	1101	USN	CAA-C3A	2.03	1.57	1.53
4	A	1201	USN	O7A-C6A	2.02	1.30	1.23

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1201	USN	C9A-C2A-C3A	5.88	121.42	112.99
4	F	1101	USN	CAA-CBA-CCA	-5.78	97.08	112.49
4	F	1101	USN	C9A-C2A-C3A	5.17	120.41	112.99
4	A	1201	USN	C9B-C2B-C8B	-5.07	97.86	110.61
4	A	1201	USN	O7B-C6B-C8B	-4.94	117.00	126.92
4	A	1201	USN	C6D-C7D-CHD	4.82	122.56	115.54
4	A	1201	USN	C3A-C4A-NA	4.52	109.17	102.30
4	F	1101	USN	C3A-C2A-C1A	4.48	104.46	99.97
4	F	1101	USN	C1-C6D-C5D	-4.39	102.82	111.99
4	A	1201	USN	C2C-C5C-C6C	-4.08	106.32	113.95
4	F	1101	USN	C2A-C3A-C4A	-4.07	96.20	102.36
4	F	1101	USN	CAB-C3B-C2B	-3.97	110.25	119.00
8	A	1205	COM	O1S-S2-C2	3.80	112.47	106.73
4	A	1201	USN	C9D-C3D-C4D	-3.78	104.75	114.64
4	A	1201	USN	C4B-CHC-C1C	3.75	131.90	125.84
4	F	1101	USN	C2B-C1B-NB	3.68	107.32	101.86
8	F	1102	COM	O2S-S2-O1S	-3.67	101.87	113.82
4	F	1101	USN	C2D-C3D-C4D	-3.56	96.97	102.36
4	F	1101	USN	C3D-C4D-ND	3.48	107.60	102.30
4	A	1201	USN	C2B-C1B-NB	3.40	106.91	101.86
4	F	1101	USN	CBA-CAA-C3A	-3.34	105.86	114.08
4	A	1201	USN	C1-C6D-C5D	-3.34	105.02	111.99
4	F	1101	USN	OEB-CCB-CBB	-3.31	112.60	123.09
4	A	1201	USN	C2C-C3C-C4C	3.30	108.22	102.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1101	USN	ODB-CCB-CBB	3.13	123.88	114.00
8	F	1102	COM	O1S-S2-C2	3.11	111.42	106.73
4	A	1201	USN	O7C-C6C-O8C	-3.05	115.48	123.33
8	F	1102	COM	O2S-S2-C2	3.03	111.30	106.73
4	A	1201	USN	C8C-C3C-C2C	-3.02	104.83	113.07
4	F	1101	USN	C8B-C2B-C1B	2.97	109.01	102.21
4	F	1101	USN	C6D-C7D-CHD	2.96	119.85	115.54
4	A	1201	USN	ODB-CCB-CBB	2.89	123.12	114.00
4	A	1201	USN	OBD-CAD- OCD	-2.84	116.02	123.33
4	A	1201	USN	C5C-C2C-C3C	-2.84	108.05	115.05
4	F	1101	USN	CHD-C1D-ND	2.80	128.97	124.51
4	F	1101	USN	C5D-C2D-C3D	-2.75	109.58	114.05
4	F	1101	USN	ODA-CCA-CBA	2.70	122.53	114.00
4	F	1101	USN	C3A-C4A-NA	2.68	106.38	102.30
4	A	1201	USN	C8C-C9C-CAC	-2.63	105.47	112.49
4	F	1101	USN	CHA-C4D-C3D	-2.58	110.26	117.74
4	A	1201	USN	C4D-ND-C1D	2.56	112.30	108.46
4	A	1201	USN	CAB-C3B-C2B	-2.55	113.37	119.00
4	F	1101	USN	CHC-C1C-NC	2.53	128.47	124.39
4	A	1201	USN	O7C-C6C-C5C	2.50	121.77	114.00
4	A	1201	USN	C9B-C2B-C1B	2.46	118.18	113.03
4	A	1201	USN	CHD-C1D-ND	2.44	128.39	124.51
8	A	1205	COM	O3S-S2-O1S	-2.42	105.34	111.40
4	F	1101	USN	C2B-C1B-N5B	-2.26	98.34	105.72
4	A	1201	USN	C8B-C6B-N5B	2.26	114.86	109.41
4	F	1101	USN	OEA-CCA-CBA	-2.23	116.01	123.09
4	A	1201	USN	C3D-C4D-ND	2.22	105.67	102.30
4	F	1101	USN	C3B-C4B-CHC	-2.21	118.61	123.33
4	F	1101	USN	C3D-C2D-C1D	2.13	103.26	100.69
8	A	1205	COM	O3S-S2-C2	2.11	110.13	106.00
4	A	1201	USN	C9B-C2B-C3B	2.10	118.24	112.91
4	F	1101	USN	O7C-C6C-C5C	2.10	120.51	114.00
4	A	1201	USN	OEB-CCB-CBB	-2.04	116.61	123.09
8	A	1205	COM	C2-C1-S1	-2.03	107.95	113.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1201	USN	NC
4	F	1101	USN	NC

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1202	GOL	O1-C1-C2-C3
5	D	703	GOL	O1-C1-C2-C3
5	F	1107	GOL	C1-C2-C3-O3
12	F	1103	UWT	O1-C3-C4-O2
12	F	1103	UWT	C2-C1-O1-C3
14	E	501	TRS	C2-C-C1-O1
5	A	1211	GOL	O1-C1-C2-C3
5	A	1202	GOL	O1-C1-C2-O2
5	A	1211	GOL	O1-C1-C2-O2
5	D	703	GOL	O1-C1-C2-O2
5	F	1107	GOL	O2-C2-C3-O3
14	E	501	TRS	C3-C-C1-O1
14	E	501	TRS	C2-C-C3-O3
14	E	501	TRS	N-C-C3-O3
12	C	301	UWT	C5-C4-O2-C6
12	F	1103	UWT	C4-C3-O1-C1
12	F	1103	UWT	O1-C3-C4-C5
14	E	501	TRS	N-C-C1-O1
4	A	1201	USN	CAA-CBA-CCA-OEA
7	D	701	TP7	C3-C4-C5-C6
4	A	1201	USN	CAA-CBA-CCA-ODA
4	F	1101	USN	CAA-CBA-CCA-OEA
4	F	1101	USN	CAA-CBA-CCA-ODA
7	A	1204	TP7	C3-C4-C5-C6
14	E	501	TRS	C1-C-C3-O3

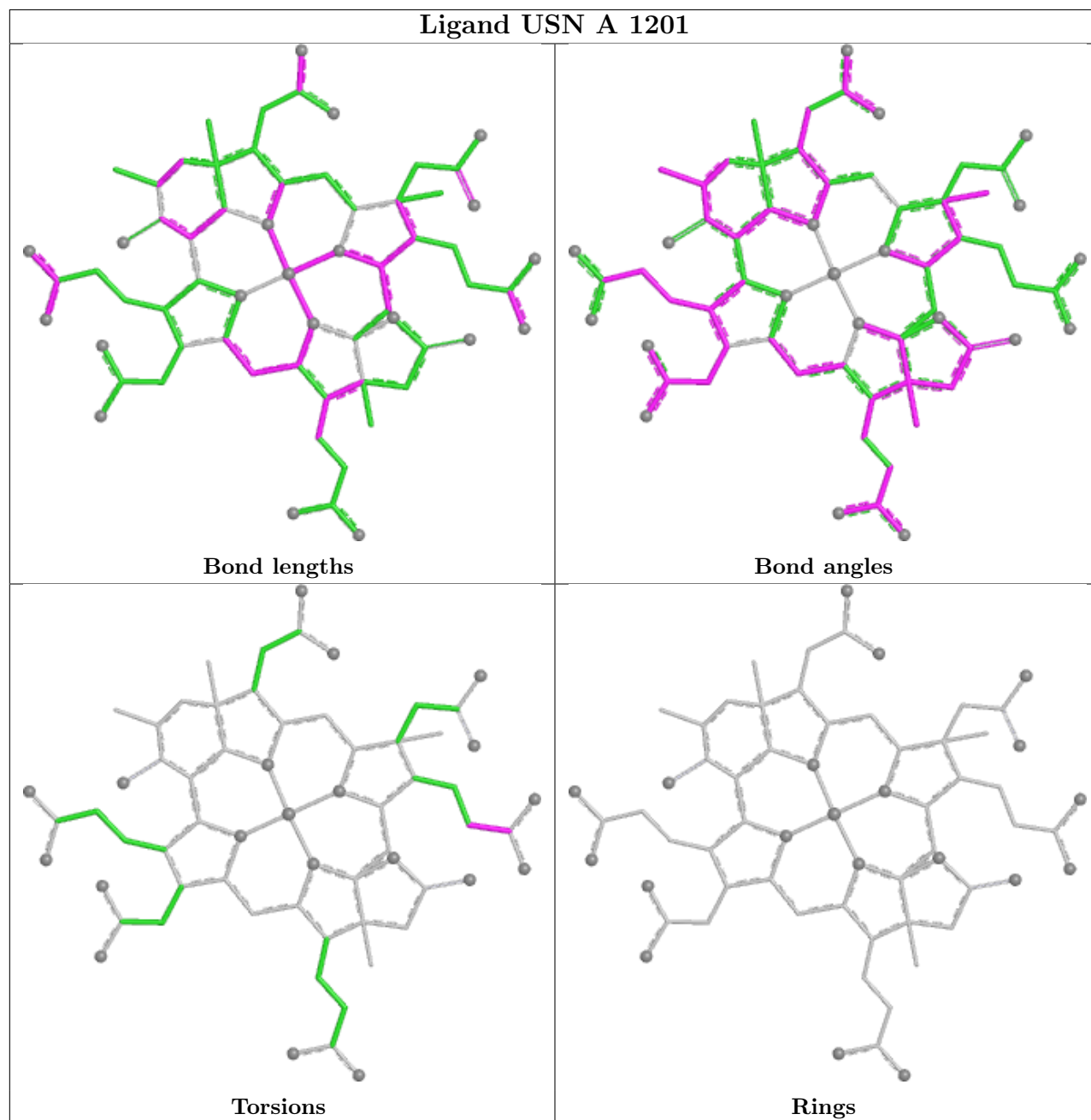
There are no ring outliers.

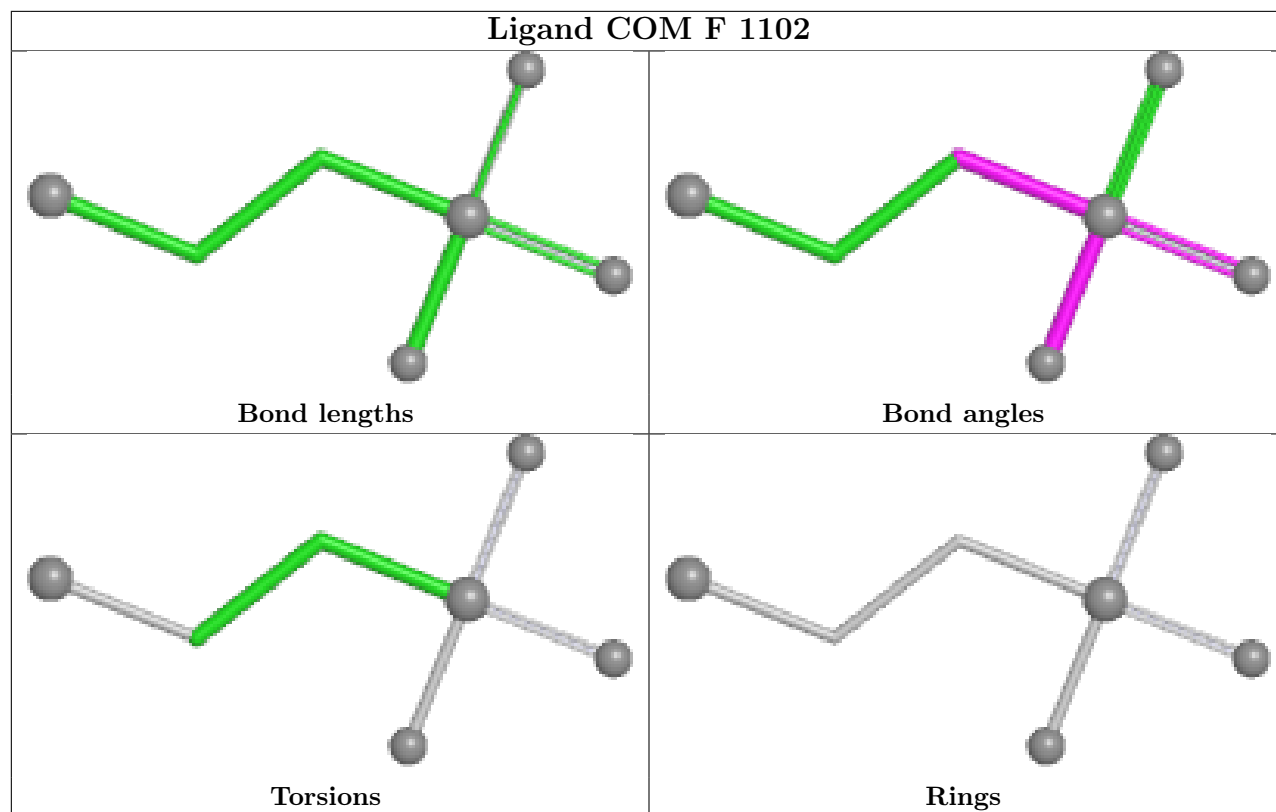
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	1102	COM	1	0
4	F	1101	USN	1	0
5	A	1202	GOL	2	0
5	B	501	GOL	1	0
14	E	501	TRS	1	0

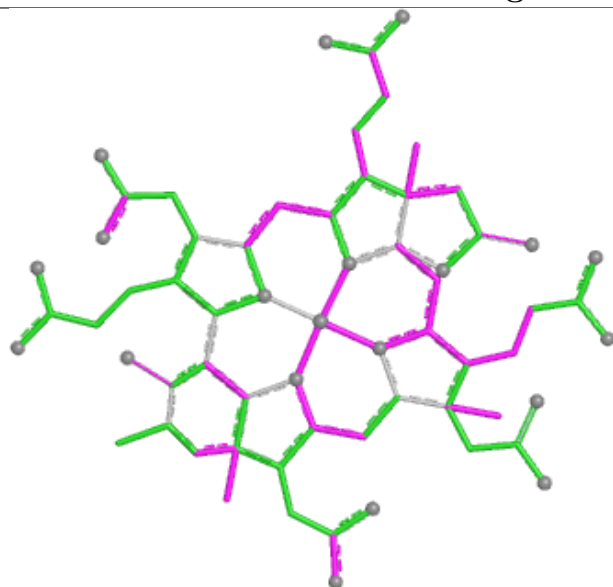
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

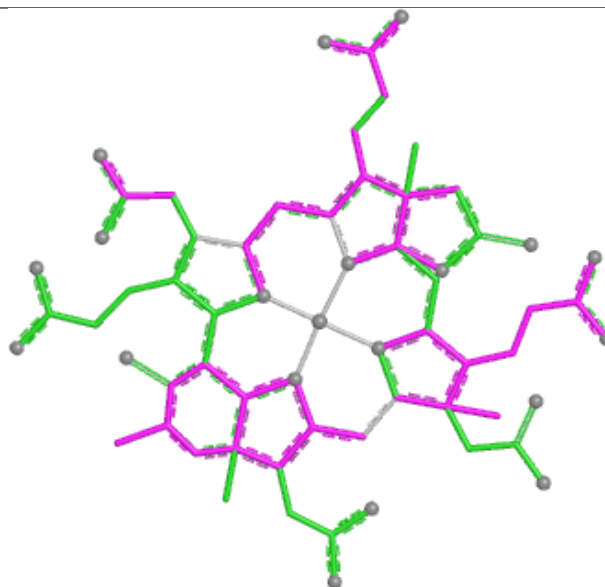




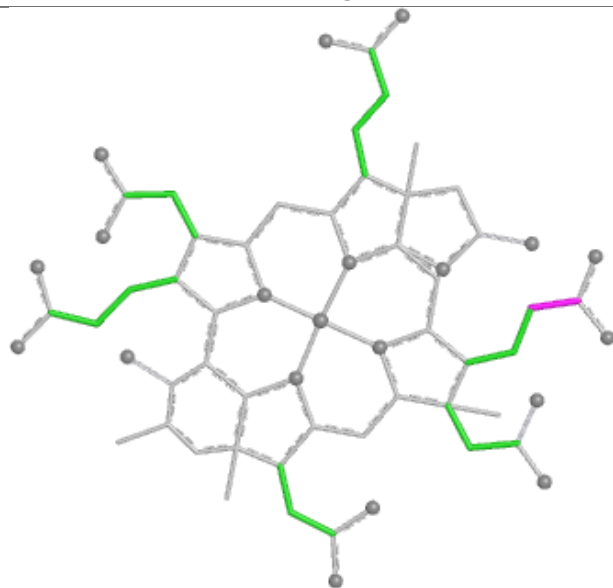
Ligand USN F 1101



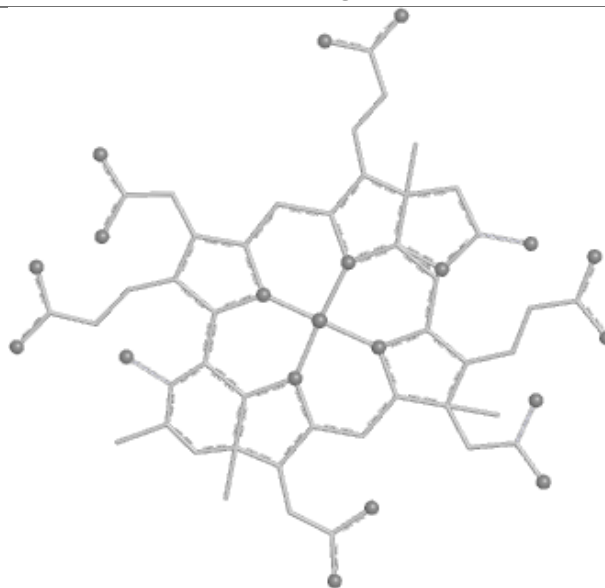
Bond lengths



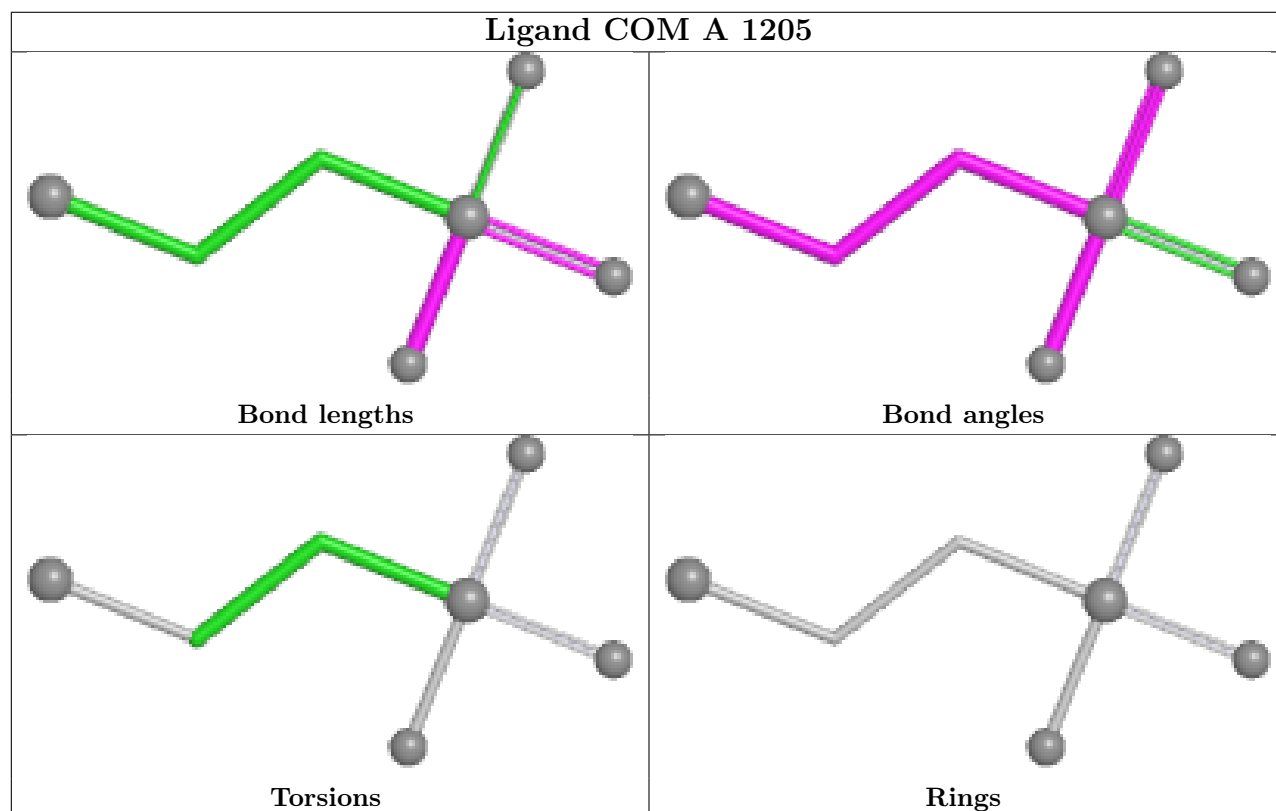
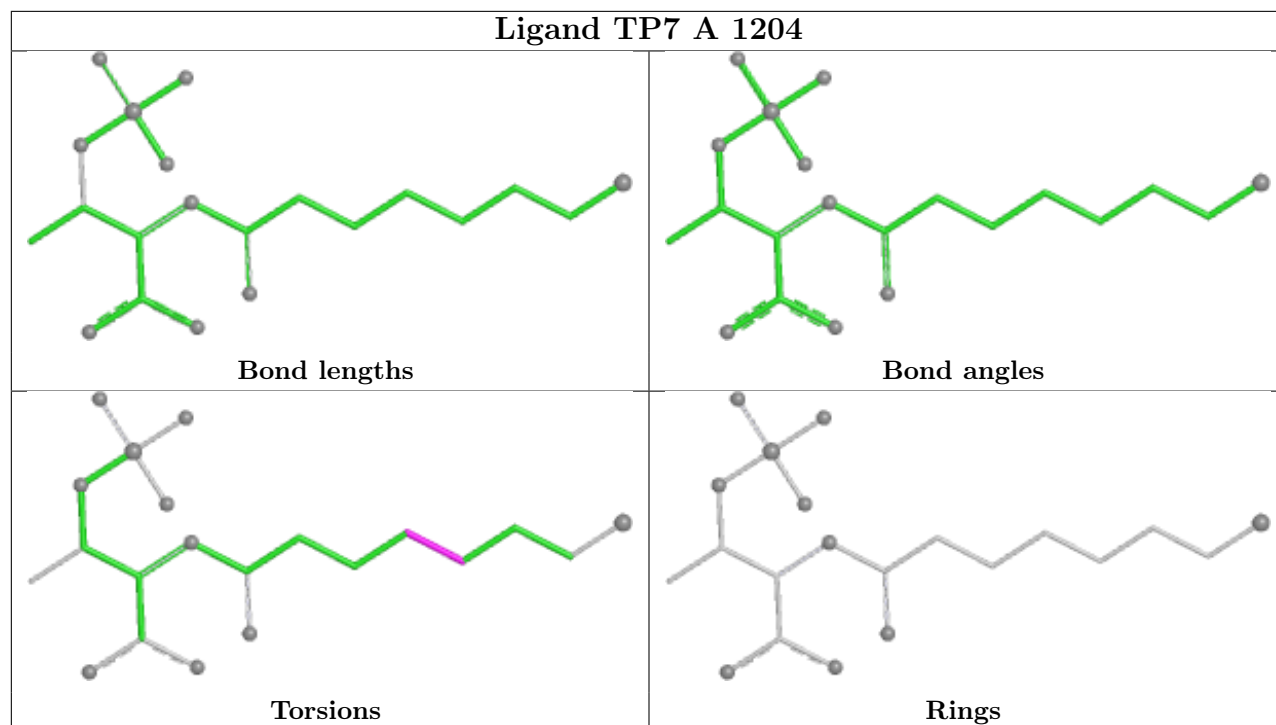
Bond angles

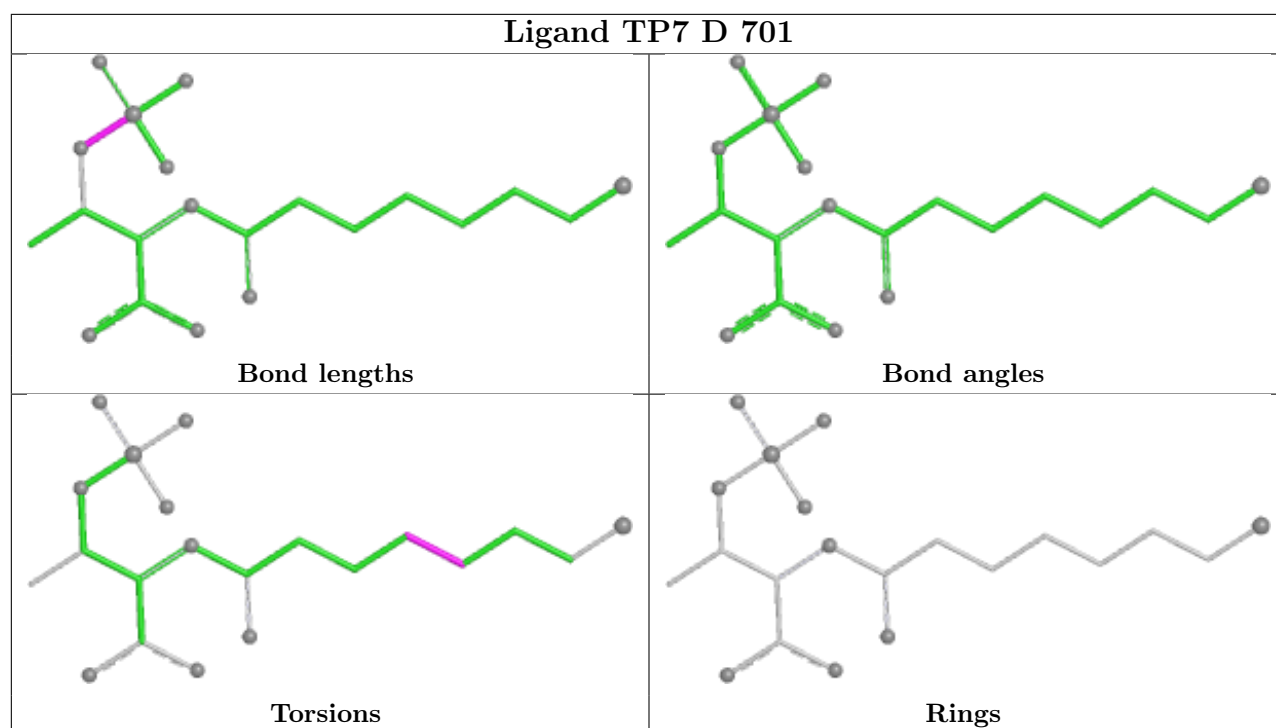


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	584/595 (98%)	-0.27	5 (0%) 81 81	4, 12, 25, 46	5 (0%)
1	D	586/595 (98%)	-0.30	7 (1%) 76 77	4, 13, 26, 52	4 (0%)
2	B	466/467 (99%)	-0.14	11 (2%) 59 60	7, 13, 32, 75	2 (0%)
2	E	466/467 (99%)	-0.21	5 (1%) 78 78	8, 13, 28, 45	1 (0%)
3	C	265/266 (99%)	-0.03	2 (0%) 82 83	9, 19, 35, 47	1 (0%)
3	F	265/266 (99%)	-0.13	3 (1%) 78 78	9, 17, 31, 44	2 (0%)
All	All	2632/2656 (99%)	-0.21	33 (1%) 75 75	4, 14, 29, 75	15 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TYR	5.9
2	B	84	PRO	4.9
2	B	80	ILE	4.8
2	B	85	GLY	4.7
2	B	87	LYS	4.5
1	D	3	LYS	4.3
2	B	82	SER	4.3
3	C	2	VAL	4.2
2	B	89	PRO	4.0
1	D	595	HIS	3.7
3	F	2	VAL	3.7
2	B	83	SER	3.4
2	E	89	PRO	3.3
1	A	154	PHE	2.9
2	B	86	GLY	2.9
1	D	594	PRO	2.8
1	D	4	TYR	2.7
1	A	337	ASP	2.6
3	C	179	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	595	HIS	2.5
1	A	5	PRO	2.5
2	B	78	LEU	2.5
2	E	88	TYR	2.4
1	D	152[A]	ARG	2.4
2	B	90	PRO	2.3
2	E	84	PRO	2.3
1	D	205	GLU	2.2
1	D	336	LEU	2.1
3	F	66	GLU	2.1
3	F	179	ILE	2.1
2	E	122	ASP	2.1
2	E	79	GLY	2.0
1	A	152[A]	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MHS	A	291	11/12	0.92	0.07	8,10,13,14	0
1	MGN	A	445	10/11	0.94	0.07	9,10,12,12	0
1	I2M	A	377	9/10	0.95	0.07	8,9,10,10	0
1	HIC	D	491	11/12	0.95	0.06	8,8,9,10	0
1	AGM	D	305	12/13	0.96	0.05	7,9,10,11	0
1	HIC	A	491	11/12	0.96	0.06	7,9,10,10	0
1	AGM	A	305	12/13	0.96	0.06	6,8,9,11	0
1	SMC	A	354	7/8	0.97	0.07	7,7,9,11	0
1	MGN	D	445	10/11	0.97	0.05	8,9,11,12	0
1	MHS	D	291	11/12	0.97	0.05	10,12,13,16	0
1	I2M	D	377	9/10	0.97	0.06	8,9,12,12	0
1	SMC	D	354	7/8	0.98	0.05	8,8,10,10	0
1	GL3	A	490	4/5	0.99	0.04	8,8,8,9	0
1	GL3	D	490	4/5	0.99	0.04	8,8,9,9	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	F	1107	6/6	0.59	0.24	45,45,45,45	0
5	GOL	A	1211	6/6	0.63	0.21	50,50,50,50	0
5	GOL	A	1202	6/6	0.77	0.16	46,47,48,48	0
5	GOL	D	703	6/6	0.83	0.17	46,48,48,49	0
12	UWT	C	301	11/13	0.84	0.14	23,29,36,37	0
12	UWT	F	1103	13/13	0.84	0.13	21,29,40,41	0
14	TRS	E	501	8/8	0.84	0.14	33,35,37,38	0
9	K	E	510	1/1	0.85	0.13	57,57,57,57	0
13	MG	D	711	1/1	0.86	0.18	38,38,38,38	0
9	K	E	508	1/1	0.87	0.15	68,68,68,68	0
5	GOL	B	501	6/6	0.89	0.14	23,25,26,28	0
5	GOL	D	702	6/6	0.89	0.14	52,53,53,53	0
11	CL	E	504	1/1	0.91	0.22	42,42,42,42	0
9	K	E	507	1/1	0.92	0.09	32,32,32,32	0
9	K	B	503	1/1	0.92	0.09	29,29,29,29	0
9	K	C	303	1/1	0.92	0.11	41,41,41,41	0
9	K	E	502	1/1	0.92	0.13	42,42,42,42	0
9	K	D	707	1/1	0.93	0.10	42,42,42,42	0
9	K	B	502	1/1	0.93	0.06	32,32,32,32	0
10	XE	B	510	1/1	0.94	0.08	46,46,46,46	1
10	XE	E	513	1/1	0.94	0.08	47,47,47,47	1
10	XE	E	514[B]	1/1	0.94	0.12	46,46,46,46	1
9	K	A	1206	1/1	0.94	0.11	38,38,38,38	0
10	XE	C	305[A]	1/1	0.95	0.10	34,34,34,34	1
10	XE	A	1210	1/1	0.95	0.09	32,32,32,32	1
9	K	F	1104	1/1	0.96	0.12	26,26,26,26	0
6	NA	D	704	1/1	0.96	0.04	9,9,9,9	0
6	NA	D	705	1/1	0.96	0.05	14,14,14,14	0
10	XE	B	511[B]	1/1	0.96	0.14	41,41,41,41	1
9	K	E	509	1/1	0.96	0.07	33,33,33,33	0
7	TP7	A	1204	21/21	0.96	0.07	7,10,14,16	0
8	COM	F	1102	7/7	0.97	0.07	8,9,10,11	0
10	XE	C	304	1/1	0.97	0.05	18,18,18,18	1
9	K	E	506	1/1	0.97	0.14	31,31,31,31	0
10	XE	D	710	1/1	0.97	0.05	25,25,25,25	1
6	NA	C	302	1/1	0.97	0.05	10,10,10,10	0
4	USN	A	1201	64/64	0.97	0.06	7,10,14,16	0

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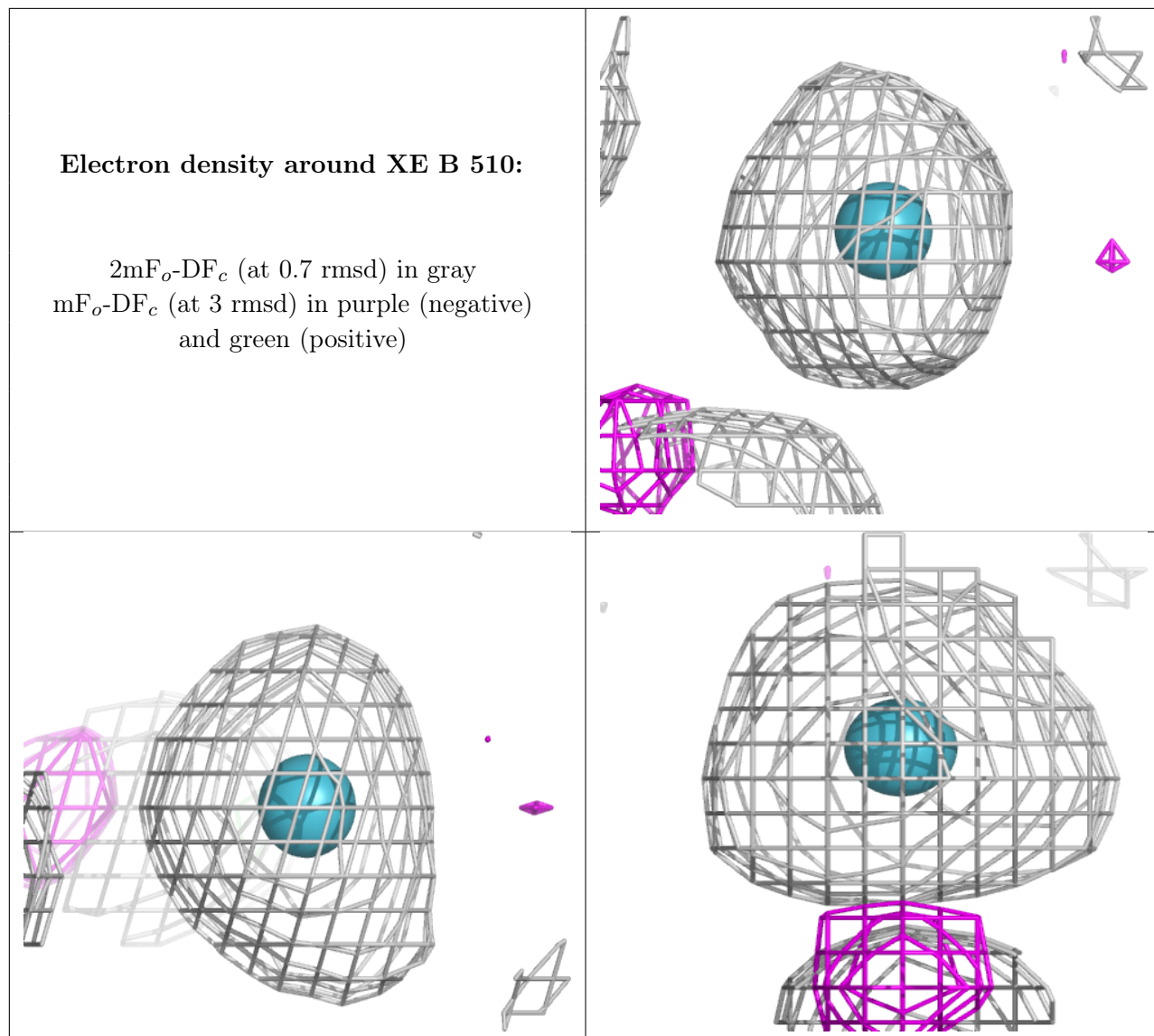
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	XE	F	1106[A]	1/1	0.97	0.08	30,30,30,30	1
11	CL	B	505	1/1	0.97	0.08	26,26,26,26	0
4	USN	F	1101	64/64	0.97	0.06	8,9,13,15	0
9	K	B	506	1/1	0.97	0.05	25,25,25,25	0
9	K	B	508	1/1	0.97	0.06	20,20,20,20	0
6	NA	A	1203	1/1	0.97	0.04	15,15,15,15	0
7	TP7	D	701	21/21	0.97	0.06	7,10,14,17	0
11	CL	E	505	1/1	0.98	0.10	22,22,22,22	0
10	XE	F	1105	1/1	0.98	0.05	15,15,15,15	1
9	K	A	1207	1/1	0.98	0.08	23,23,23,23	0
6	NA	D	706	1/1	0.98	0.03	18,18,18,18	0
9	K	B	507	1/1	0.98	0.06	32,32,32,32	0
9	K	E	511	1/1	0.99	0.04	19,19,19,19	0
11	CL	B	504	1/1	0.99	0.08	19,19,19,19	0
10	XE	D	708	1/1	0.99	0.02	10,10,10,10	1
11	CL	E	503	1/1	0.99	0.04	16,16,16,16	0
10	XE	D	709	1/1	0.99	0.02	13,13,13,13	1
10	XE	B	509	1/1	0.99	0.02	12,12,12,12	1
10	XE	E	512	1/1	0.99	0.02	13,13,13,13	1
8	COM	A	1205	7/7	0.99	0.05	7,8,9,9	0
10	XE	A	1208	1/1	0.99	0.03	13,13,13,13	1
10	XE	A	1209	1/1	0.99	0.03	11,11,11,11	1

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

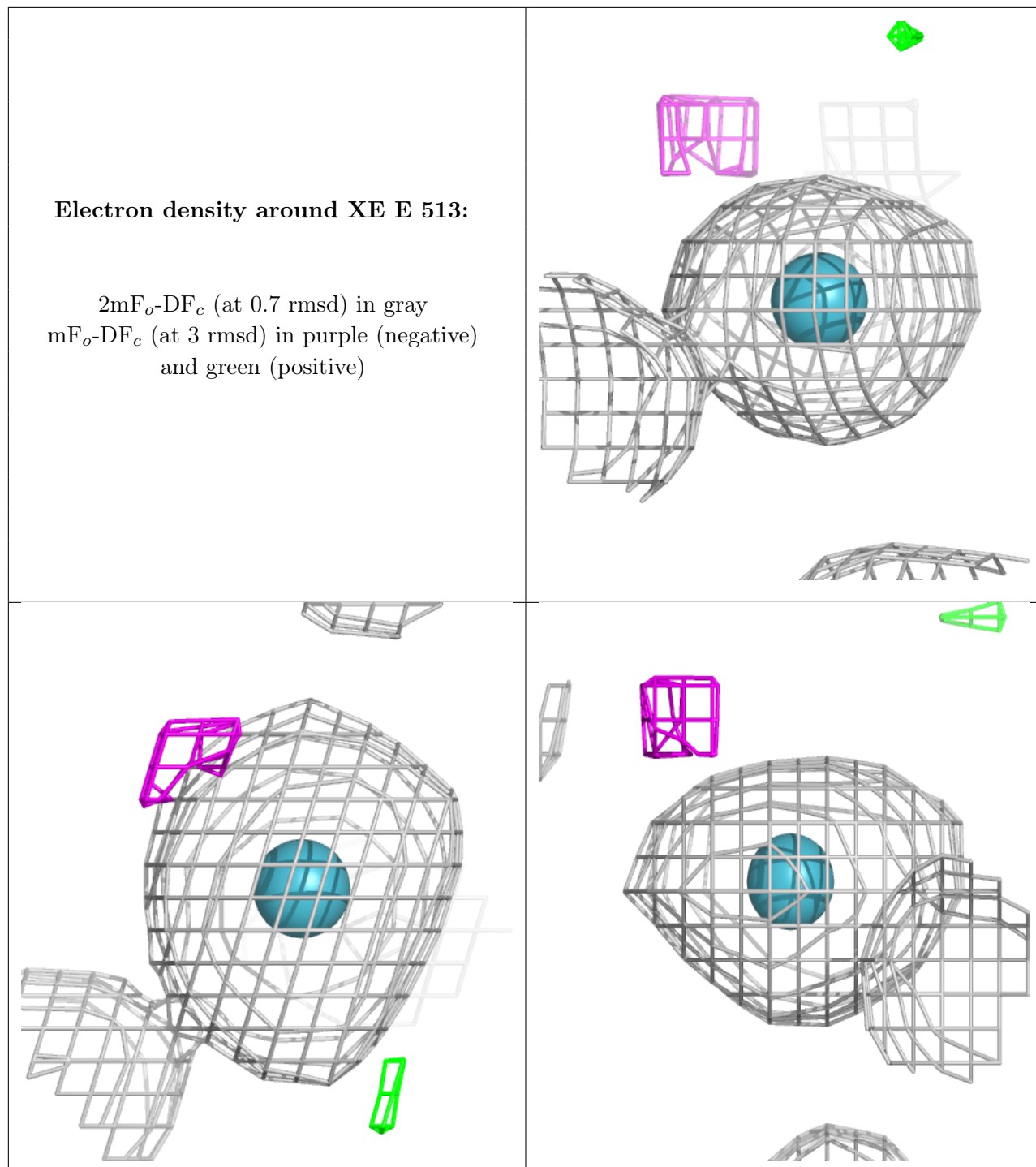
Electron density around XE B 510:

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



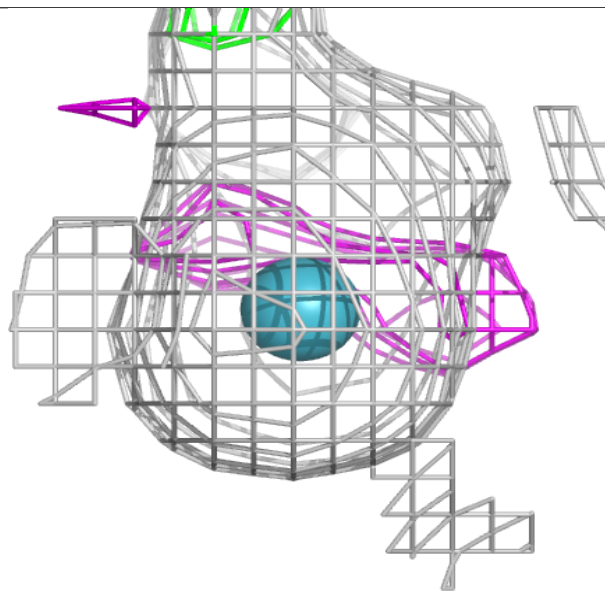
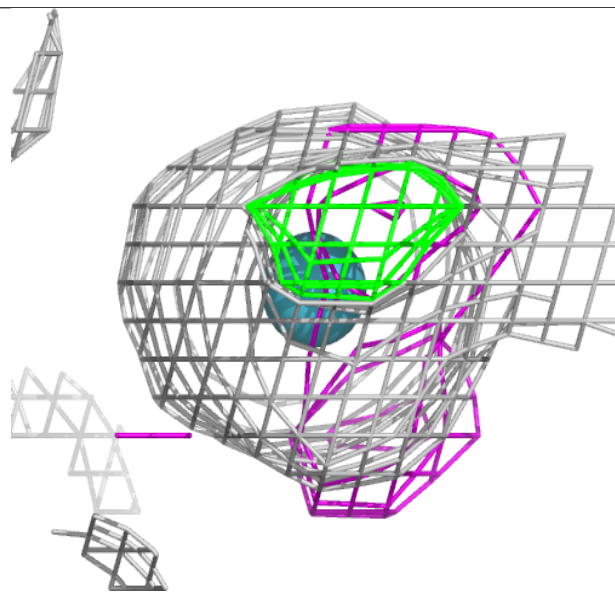
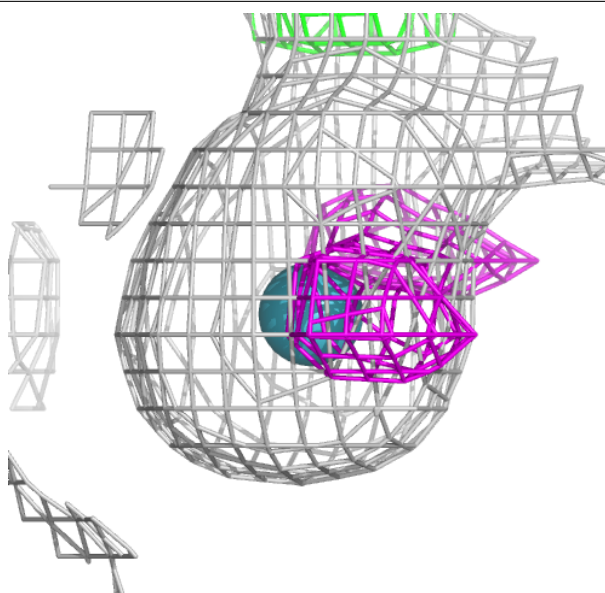
Electron density around XE E 513:

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



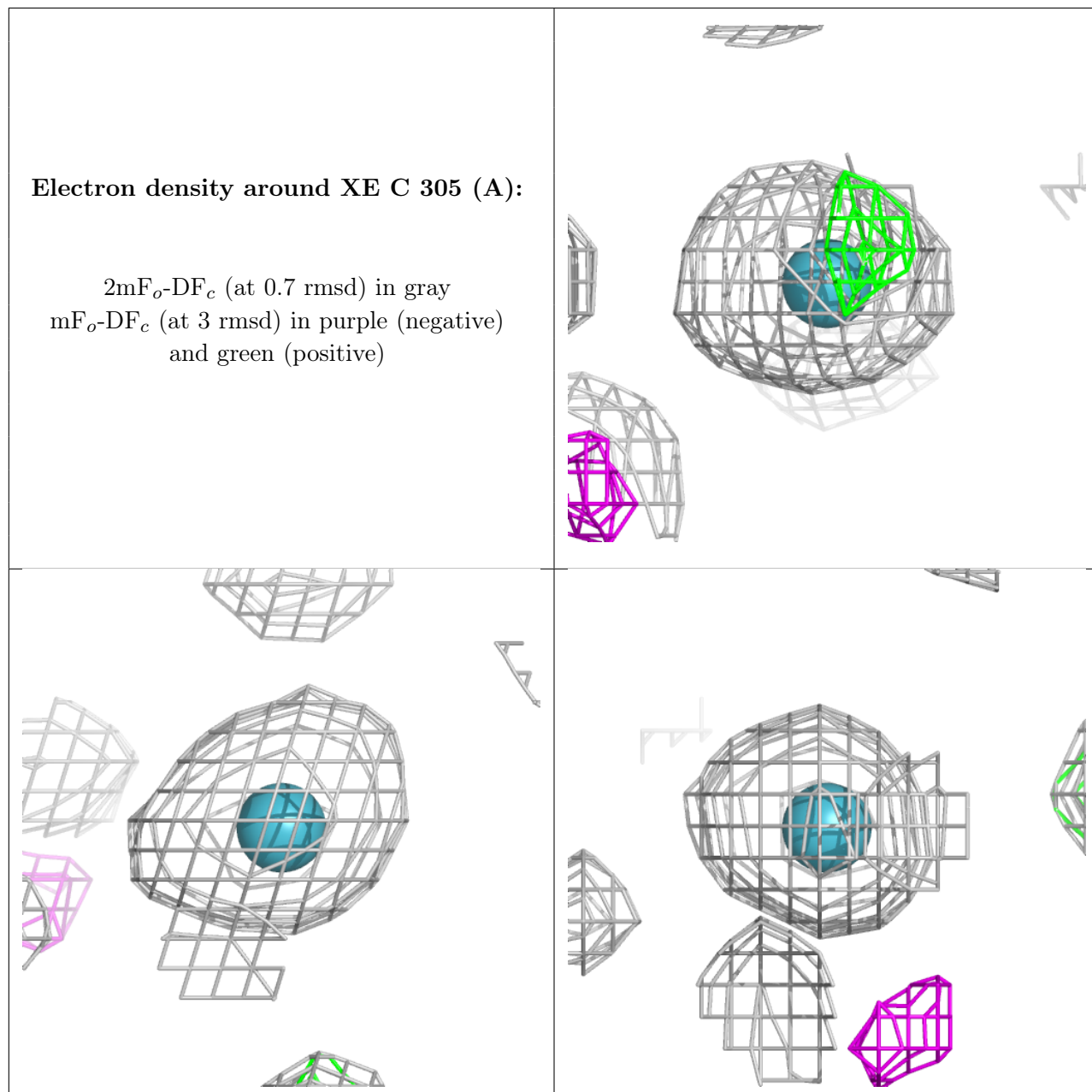
Electron density around XE E 514 (B):

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



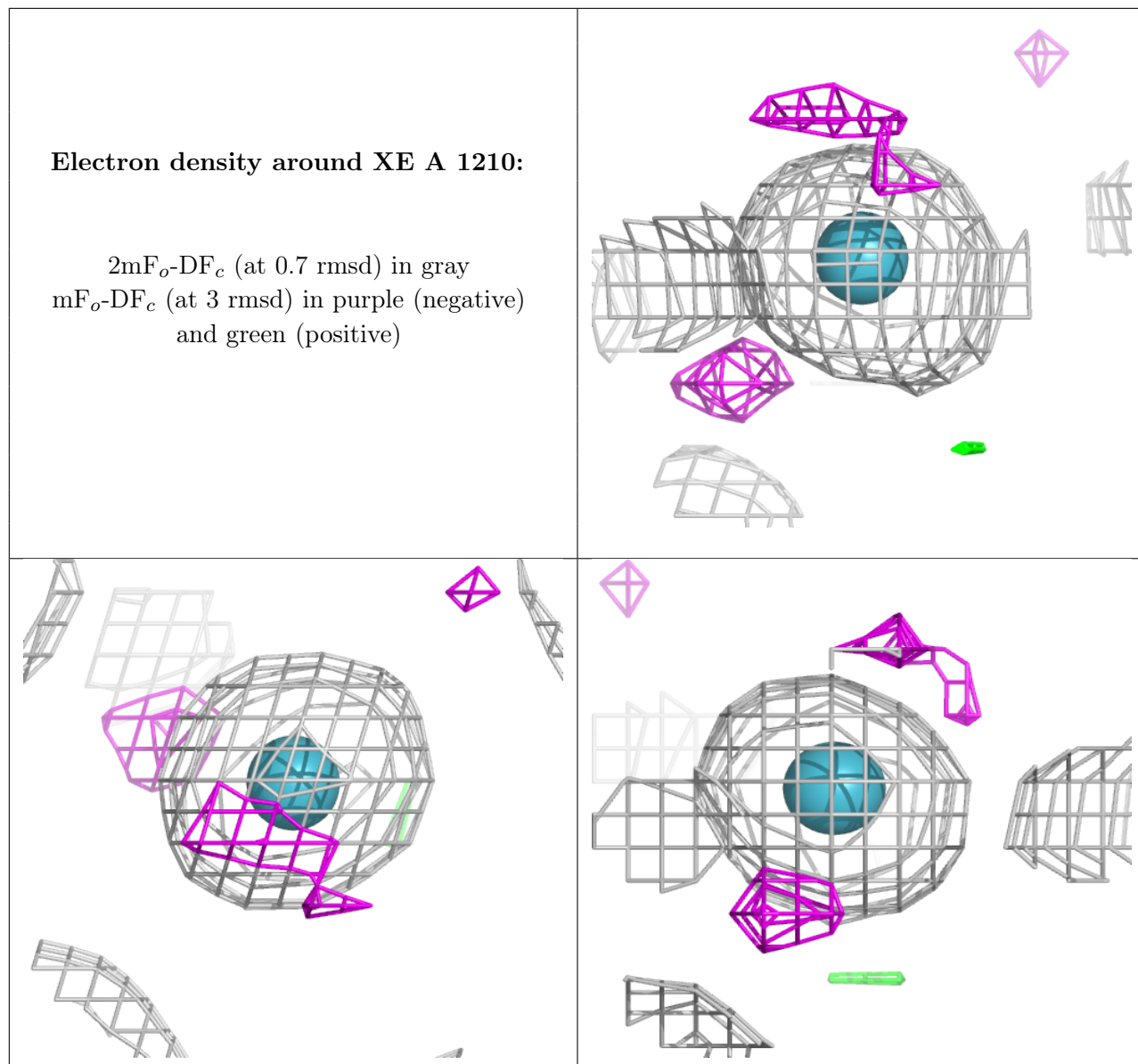
Electron density around XE C 305 (A):

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



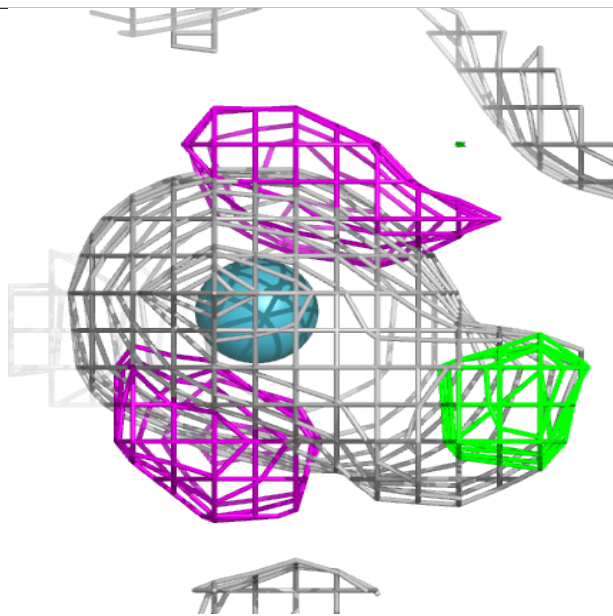
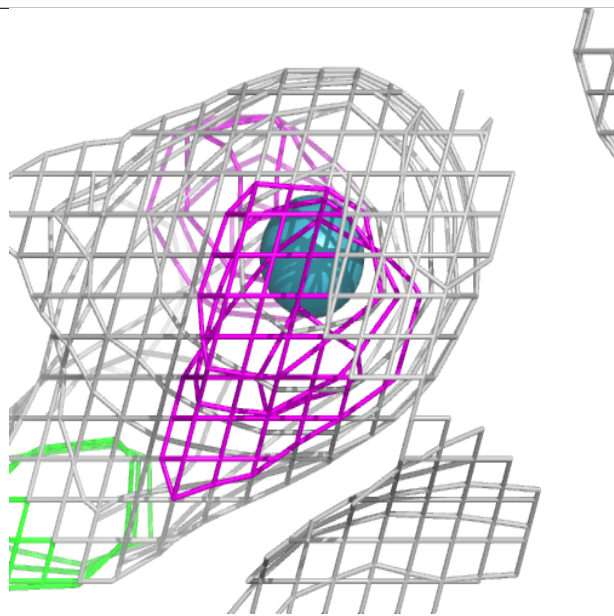
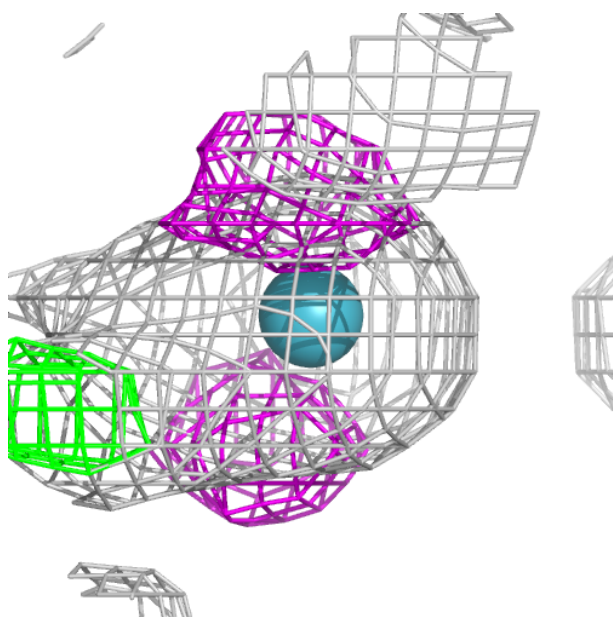
Electron density around XE A 1210:

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



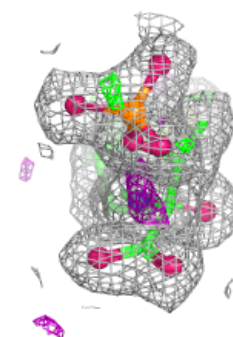
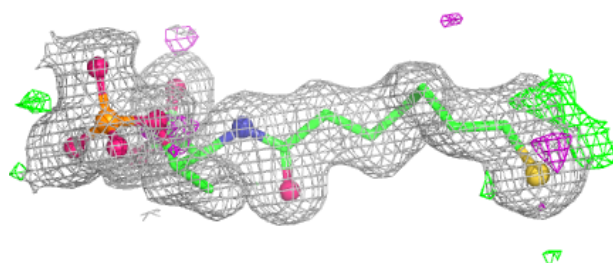
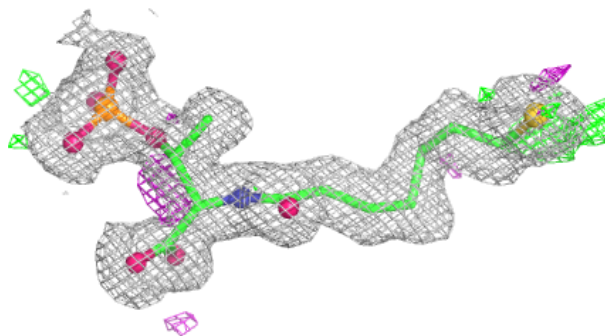
Electron density around XE B 511 (B):

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

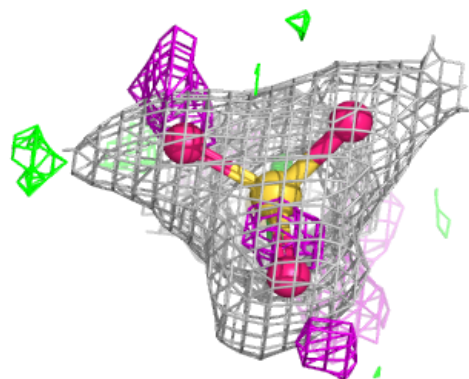
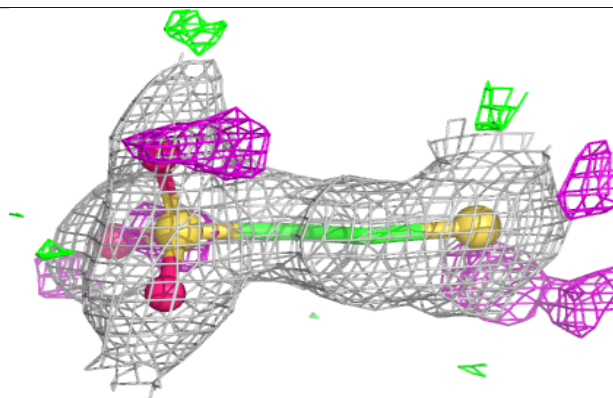
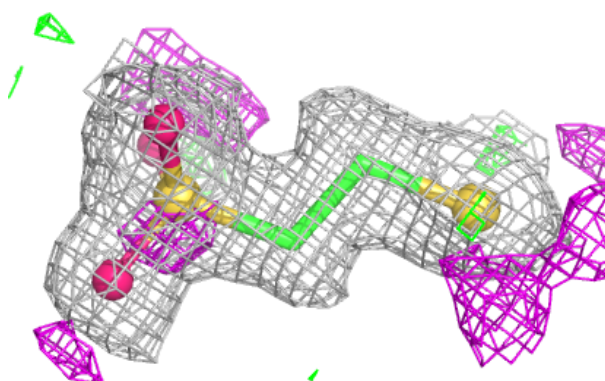


Electron density around TP7 A 1204:

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

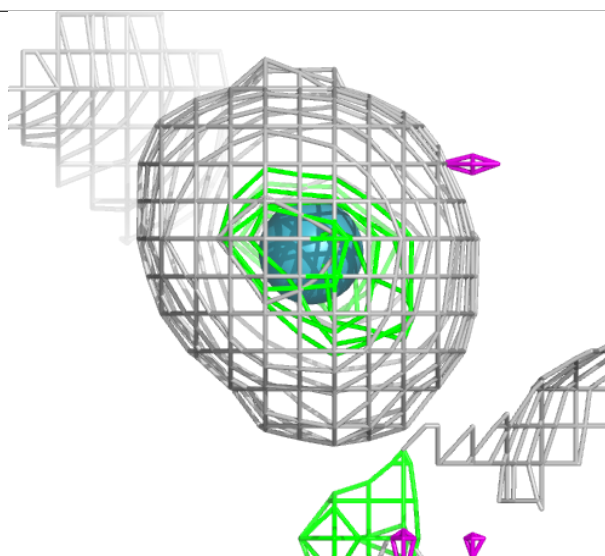
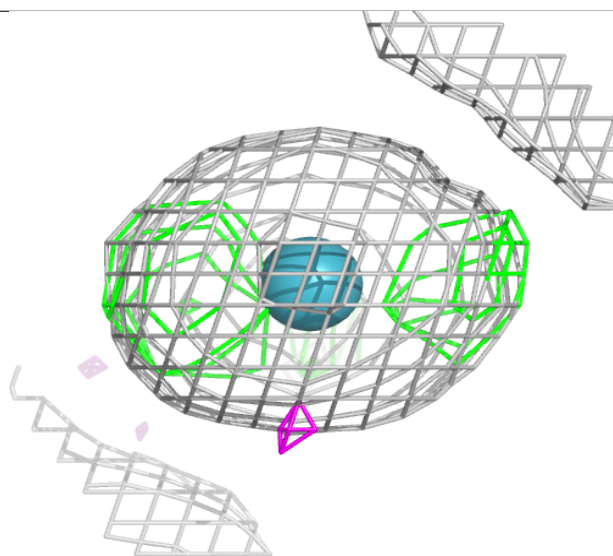
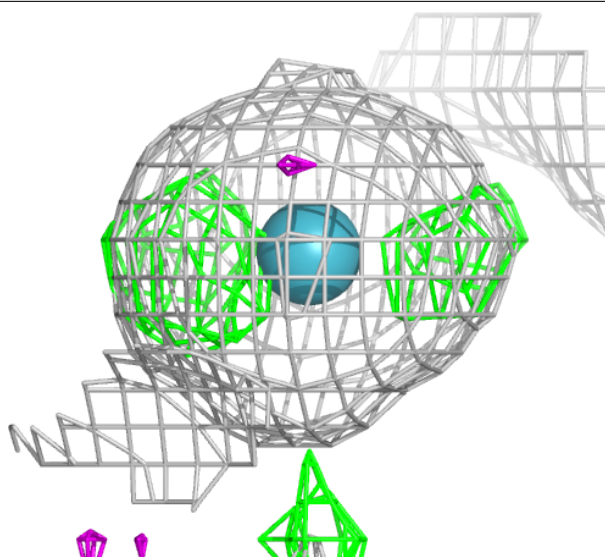
**Electron density around COM F 1102:**

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



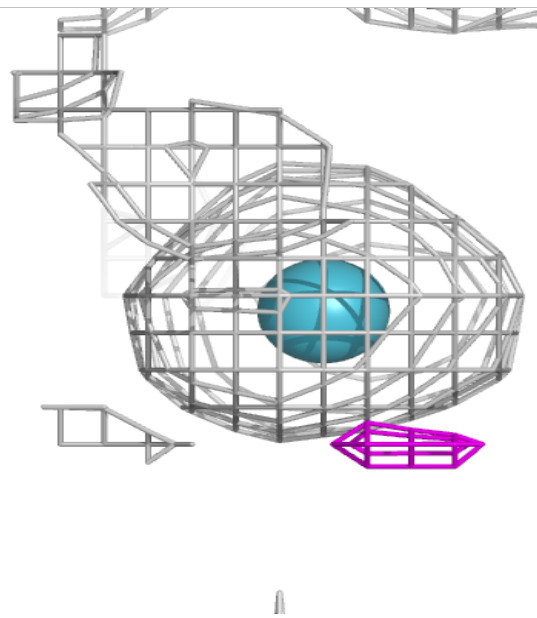
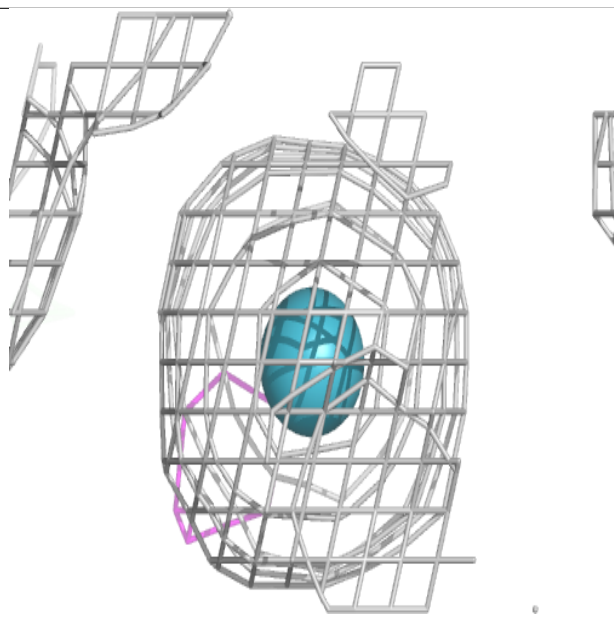
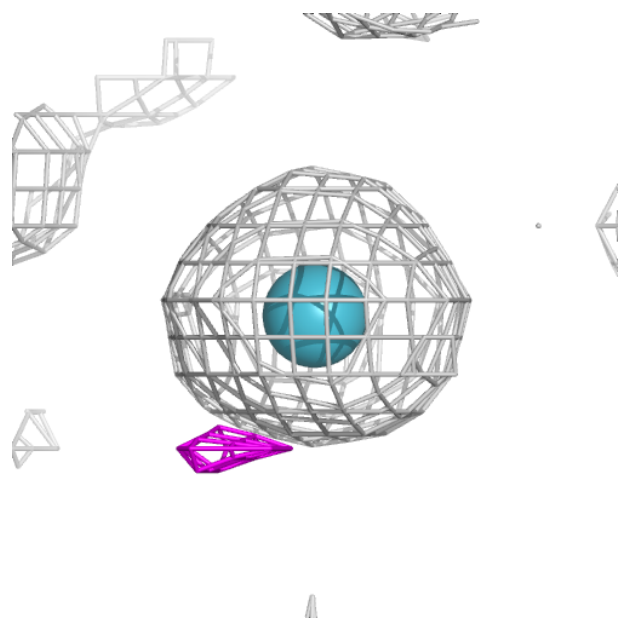
Electron density around XE C 304:

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



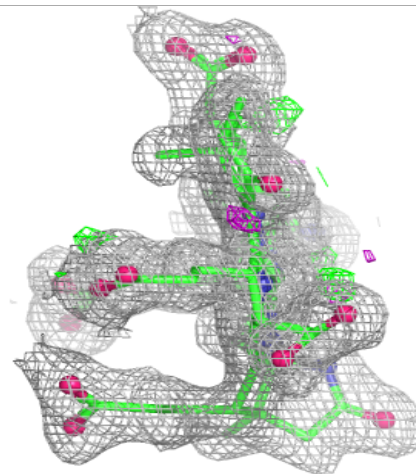
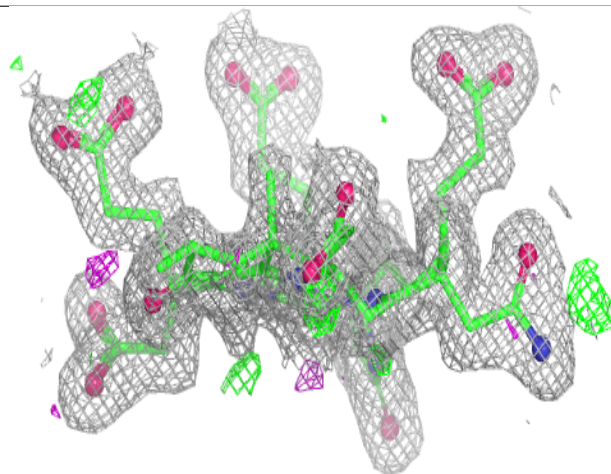
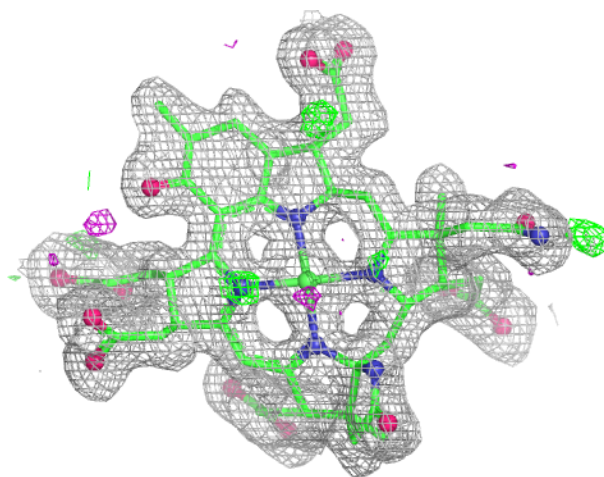
Electron density around XE D 710:

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



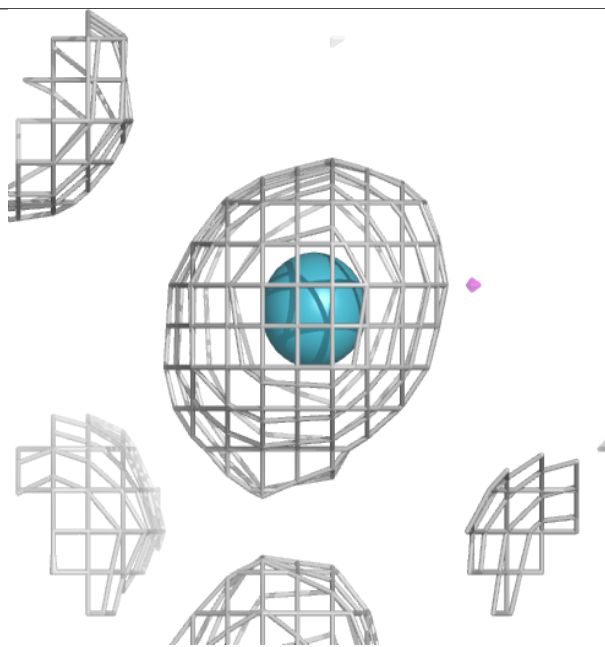
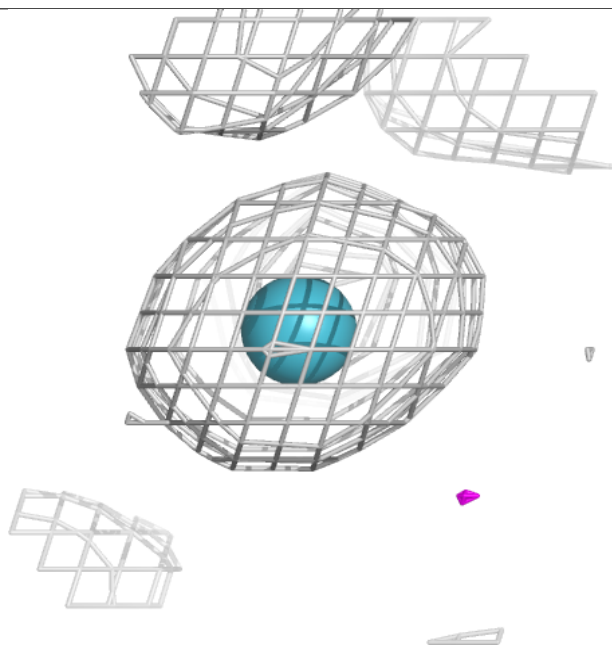
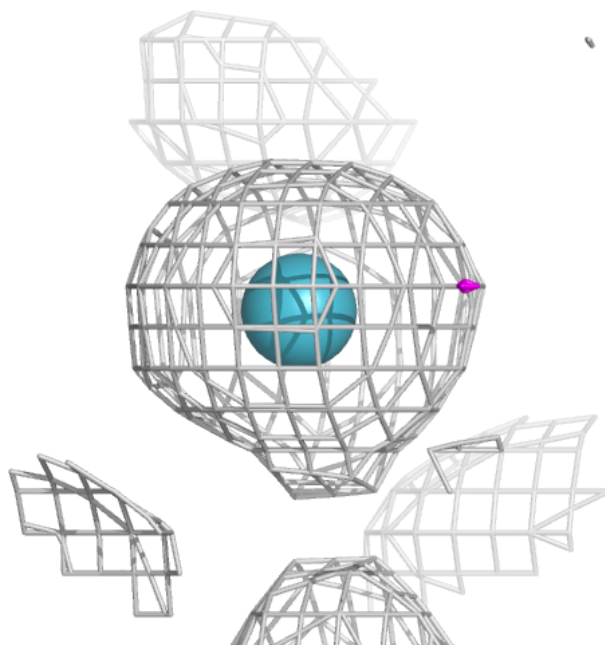
Electron density around USN A 1201:

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



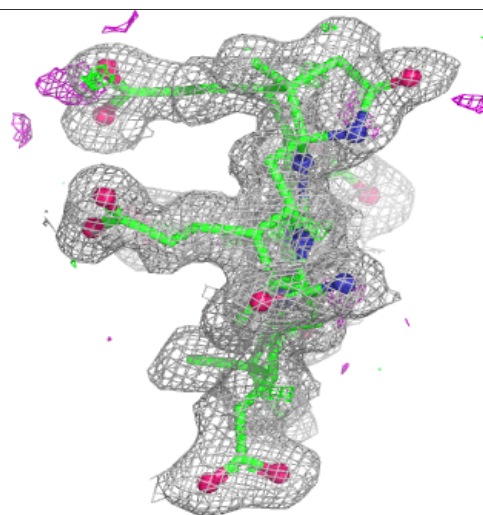
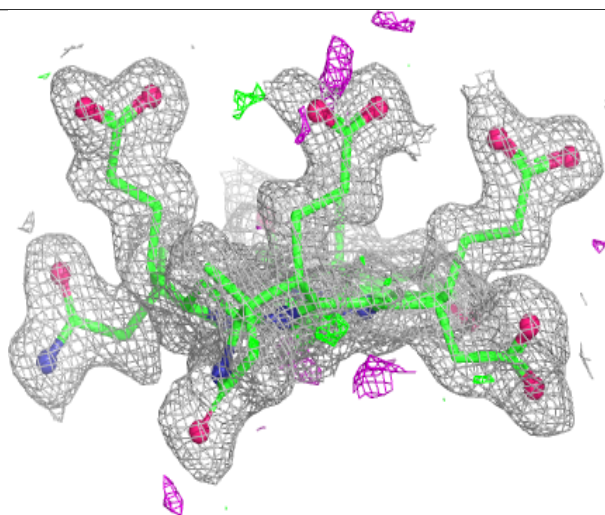
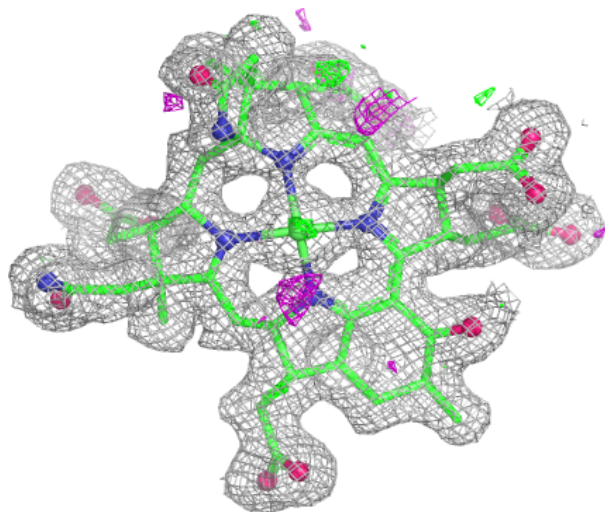
Electron density around XE F 1106 (A):

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



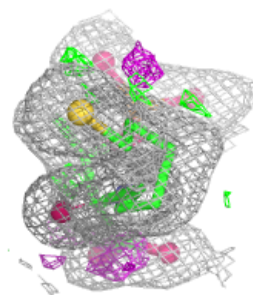
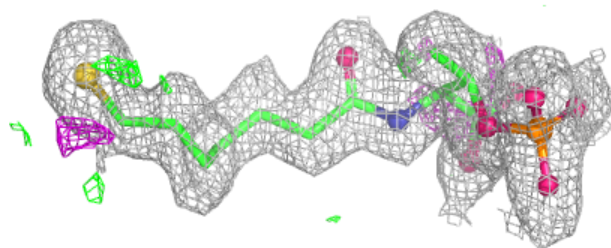
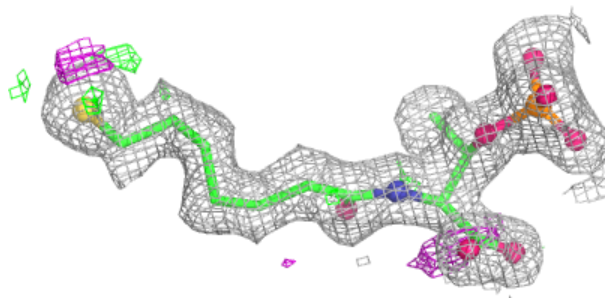
Electron density around USN F 1101:

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



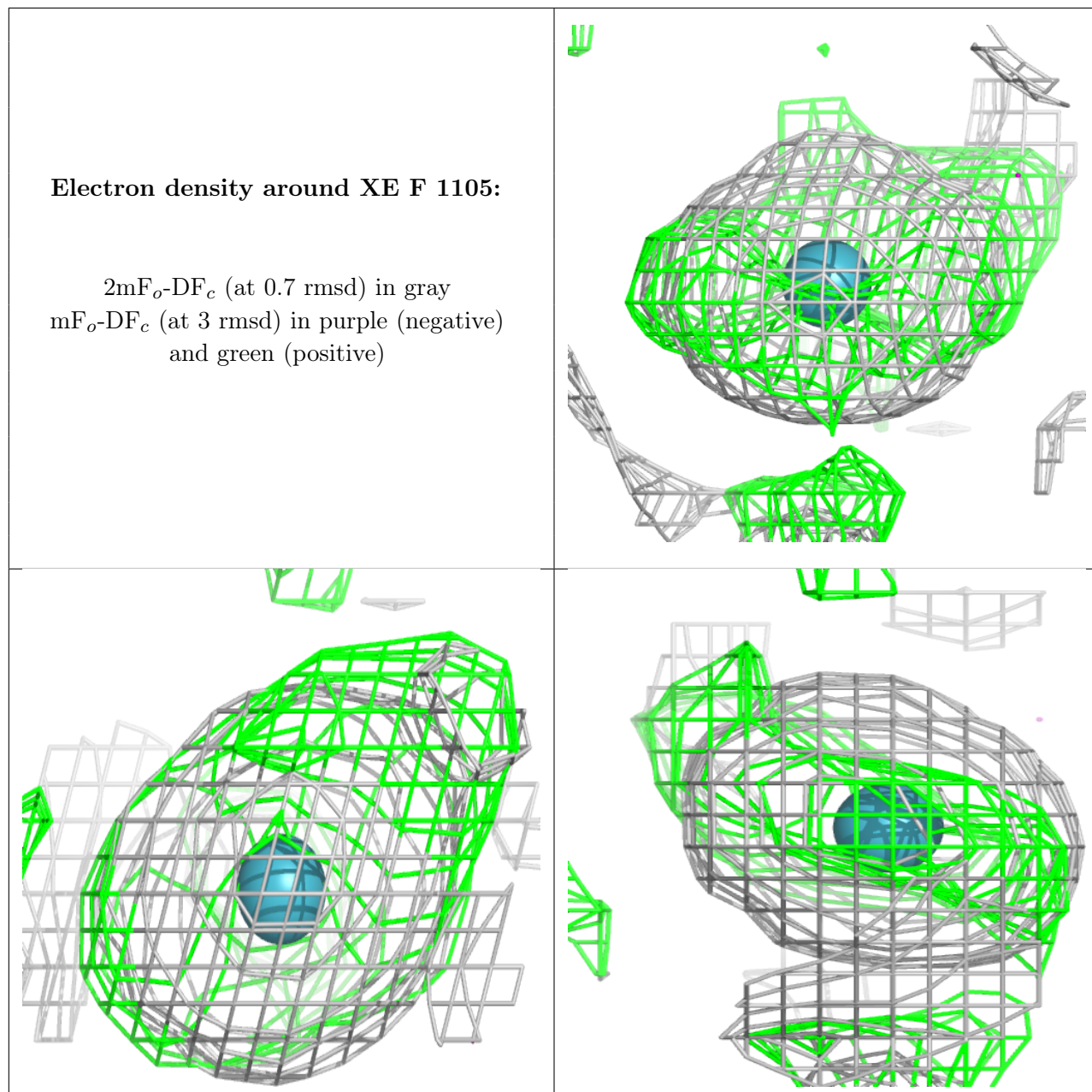
Electron density around TP7 D 701:

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



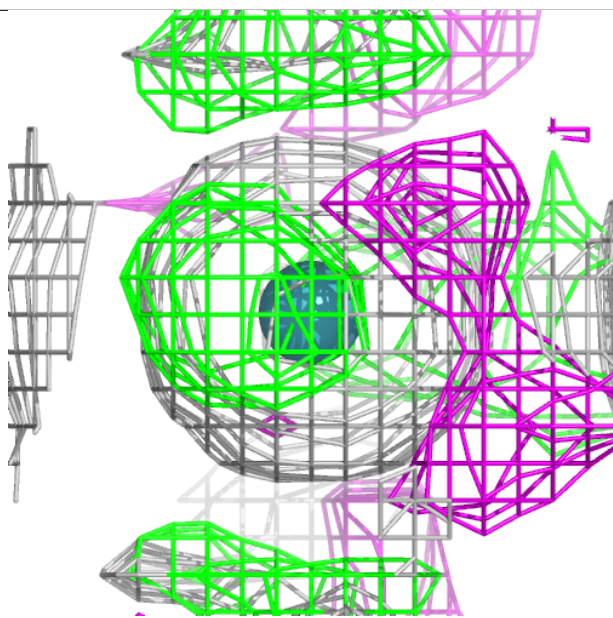
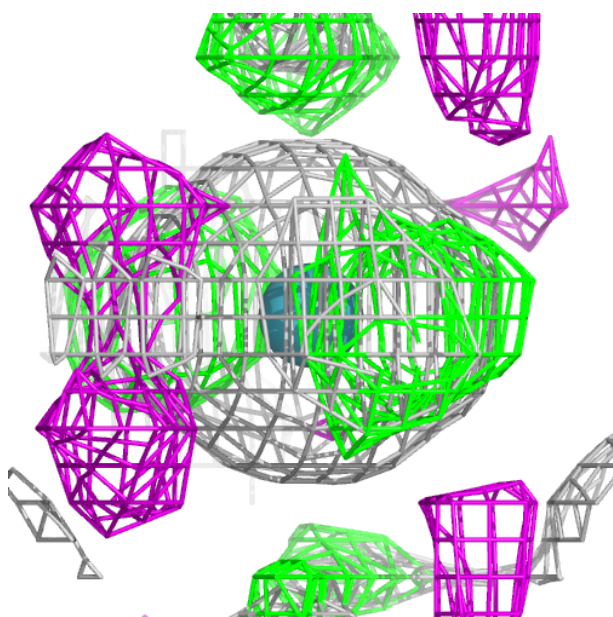
Electron density around XE F 1105:

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



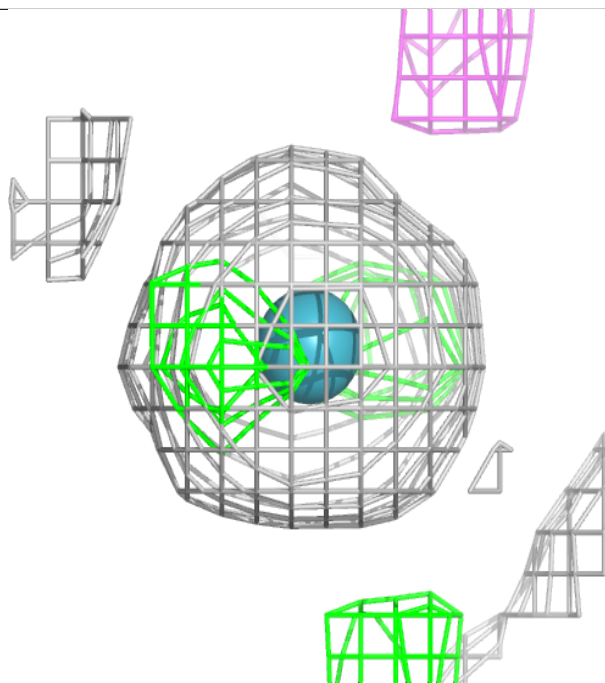
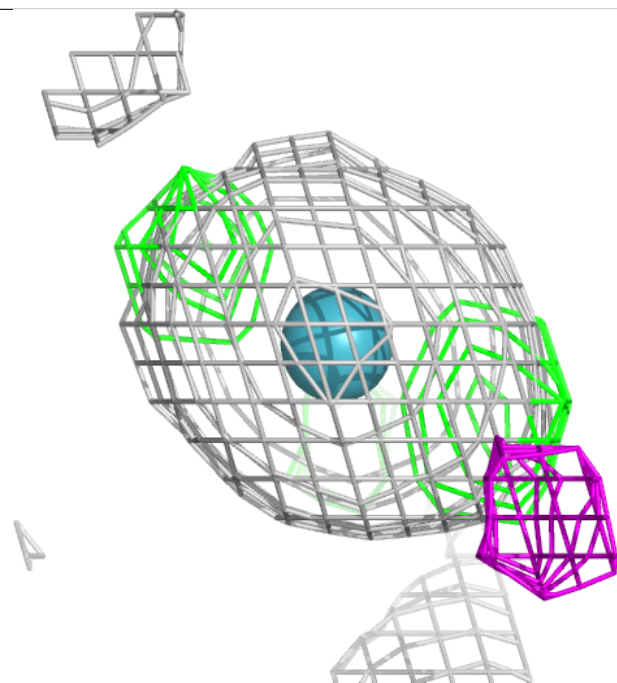
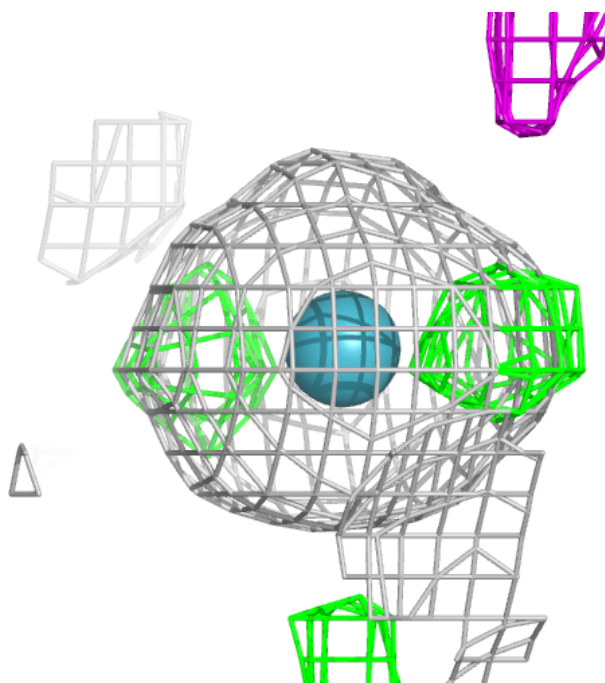
Electron density around XE D 708:

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



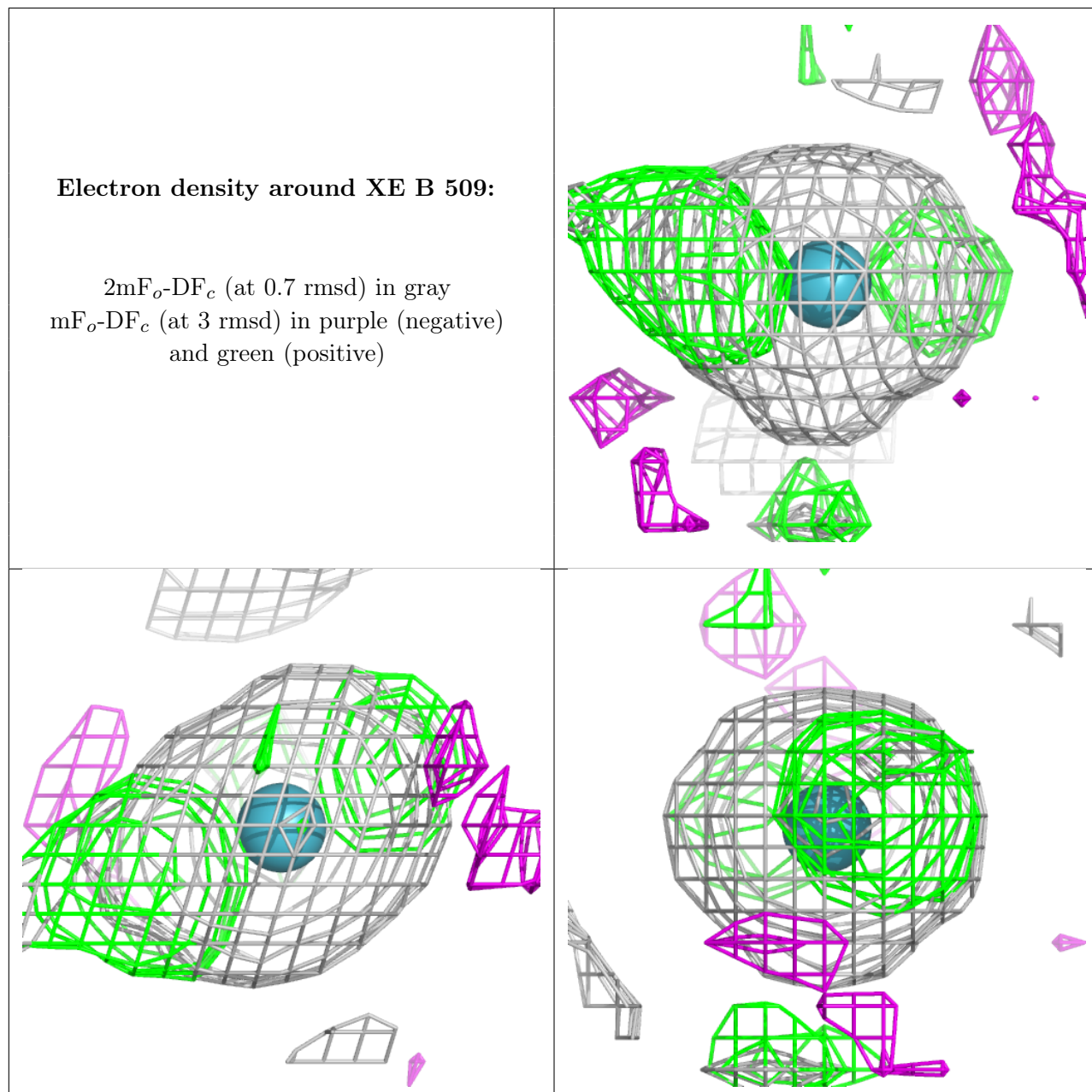
Electron density around XE D 709:

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



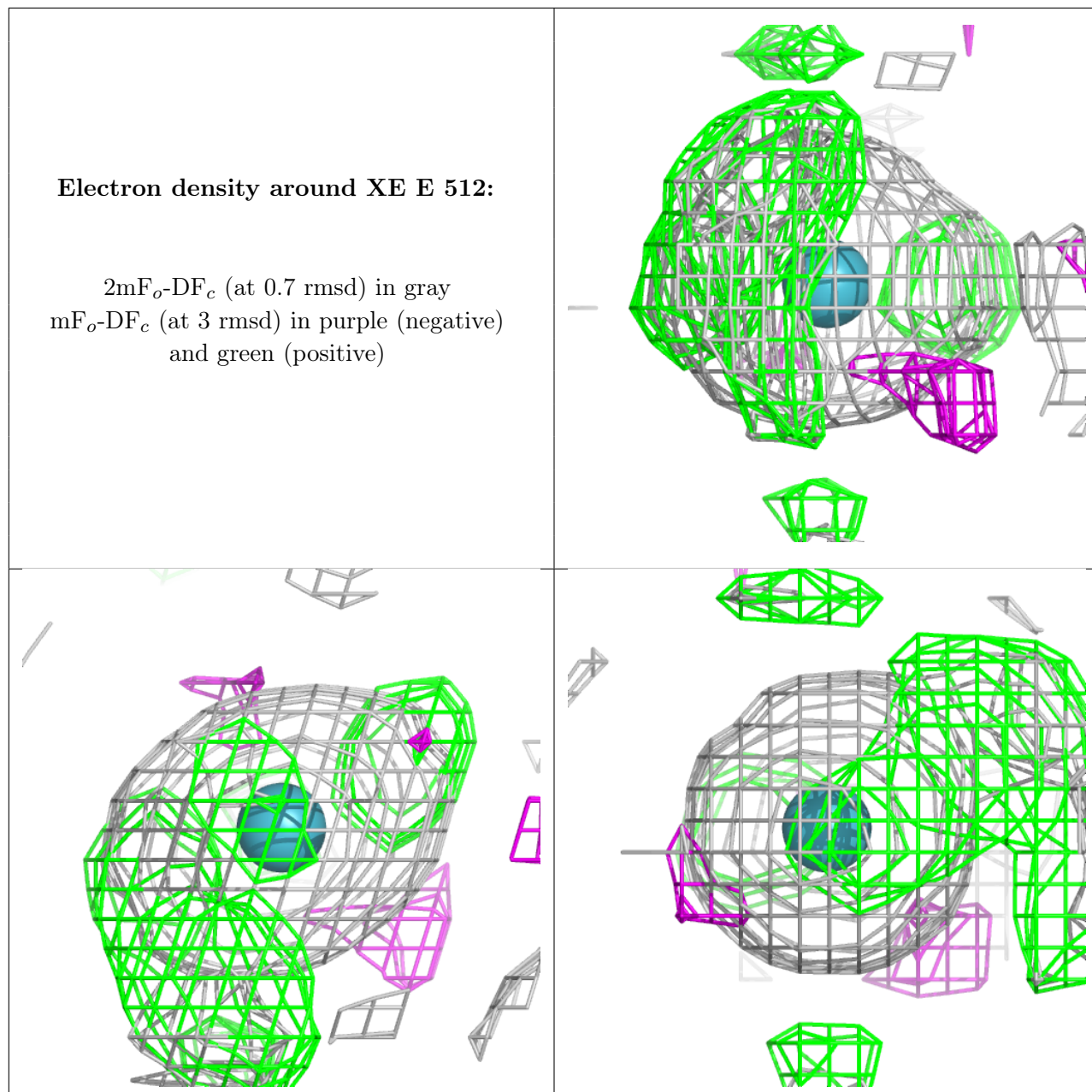
Electron density around XE B 509:

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



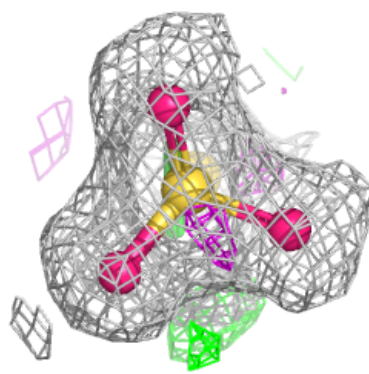
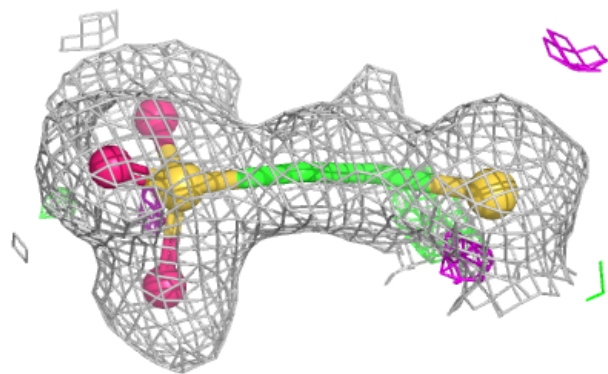
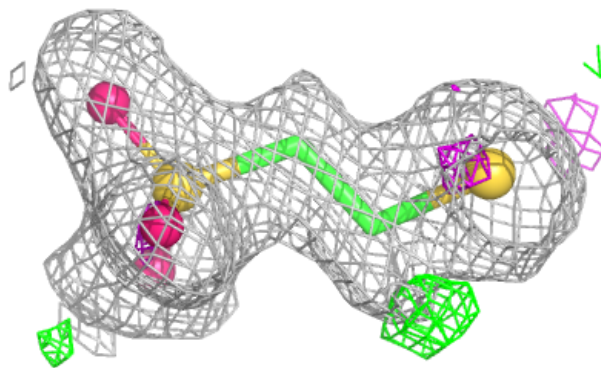
Electron density around XE E 512:

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



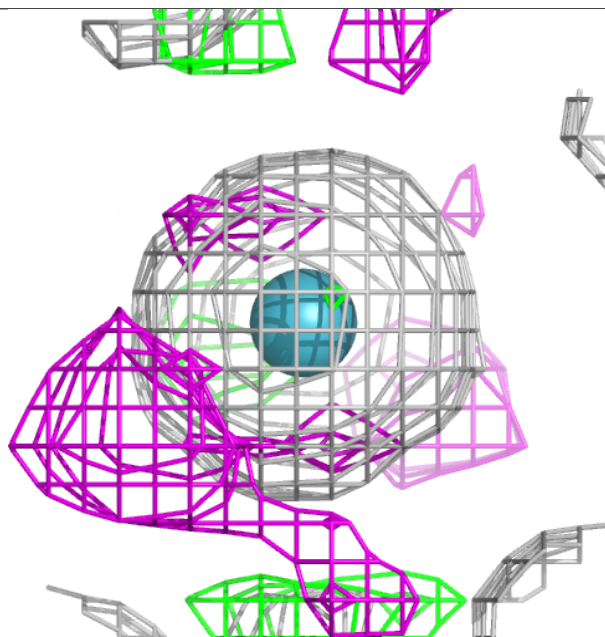
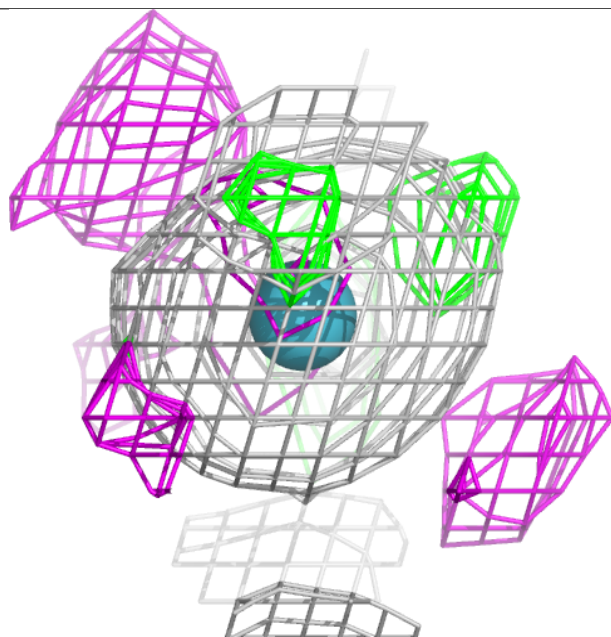
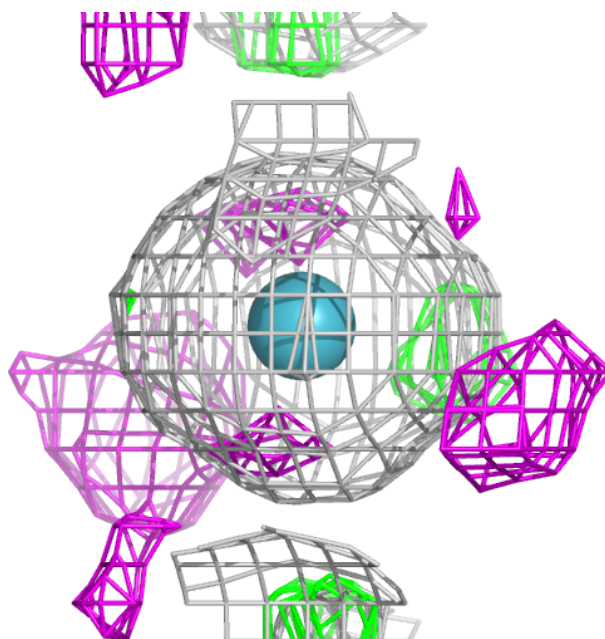
Electron density around COM A 1205:

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



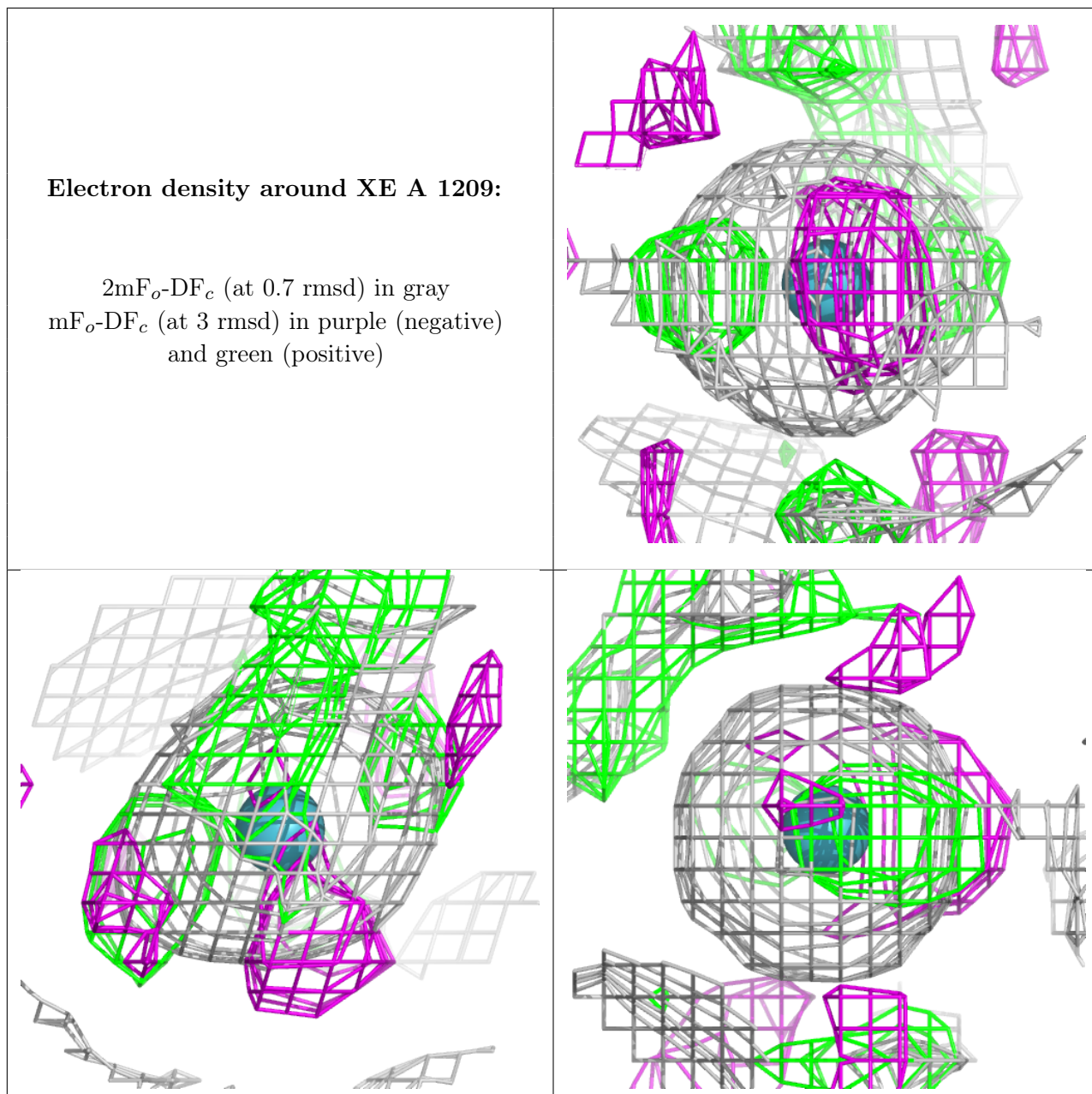
Electron density around XE A 1208:

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



Electron density around XE A 1209:

$2mF_o-DF_c$ (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.