



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 04:01 pm GMT

PDB ID : 4Z3X
Title : Active site complex BamBC of Benzoyl Coenzyme A reductase in complex with 1-Monoenoyl-CoA
Authors : Weinert, T.; Kung, J.W.; Weidenweber, S.; Huwiler, S.G.; Boll, M.; Ermler, U.
Deposited on : 2015-04-01
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

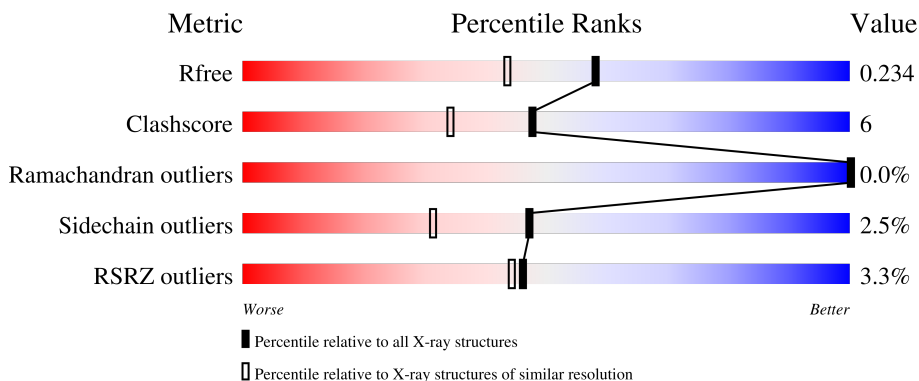
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	653	
1	B	653	
1	C	653	
1	D	653	

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Mol	Chain	Length	Quality of chain
2	E	179	<p>2% 75% 17% • 7%</p>
2	F	179	<p>81% 14% 5%</p>
2	G	179	<p>75% 18% • 6%</p>
2	H	179	<p>% 77% 12% • 10%</p>

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
3	SF4	H	1003	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27713 atoms, of which 60 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 Benzoyl-CoA reductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	653	5187	3312	875	966	34	0	1	0
1	B	653	5185	3311	876	964	34	0	0	0
1	C	653	5181	3309	876	962	34	0	0	0
1	D	652	5181	3309	875	963	34	0	0	0

- Molecule 2 is a protein called Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	166	1260	784	223	239	14	0	0	0
2	F	170	1317	816	226	261	14	0	1	0
2	G	169	1315	814	228	259	14	0	2	0
2	H	161	1221	758	213	236	14	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



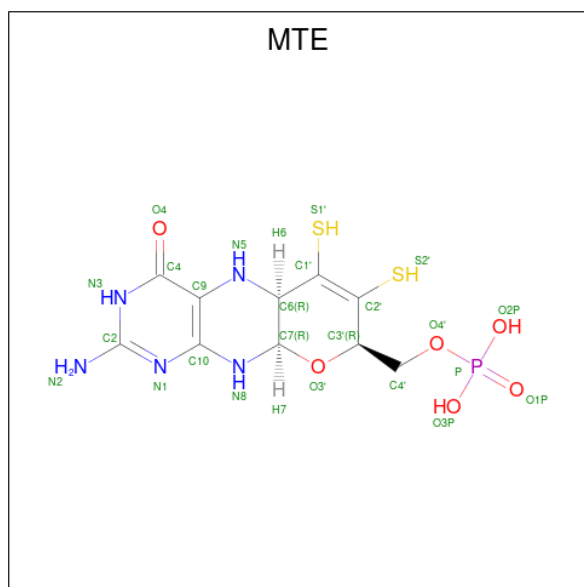
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	H	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	Fe	S	0	0
			8	4	4		
3	H	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 5 is TUNGSTEN ION (three-letter code: W) (formula: W).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total W 1 1	0	0
5	B	1	Total W 1 1	0	0
5	C	1	Total W 1 1	0	0
5	D	1	Total W 1 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

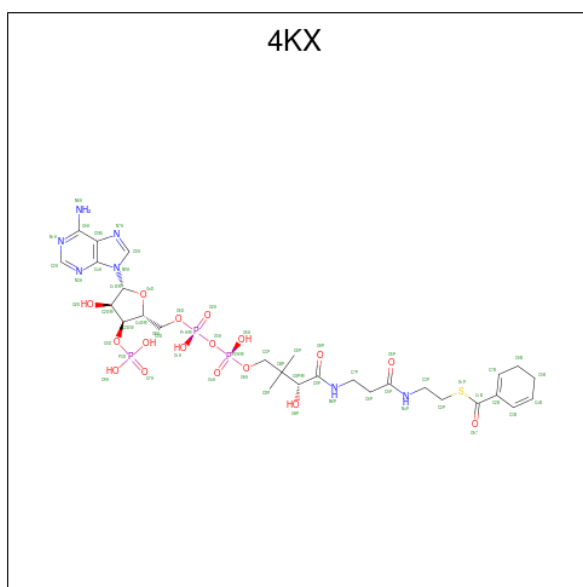
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total X 1 1	0	0
7	B	1	Total X 1 1	0	0
7	C	1	Total X 1 1	0	0
7	D	1	Total X 1 1	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	A	1	24	6	14	4	0	0
8	A	1	24	6	14	4	0	0
8	D	1	24	6	14	4	0	0

- Molecule 9 is 1,5 Dienoyl-CoA (three-letter code: 4KX) (formula: $C_{28}H_{42}N_7O_{17}P_3S$).



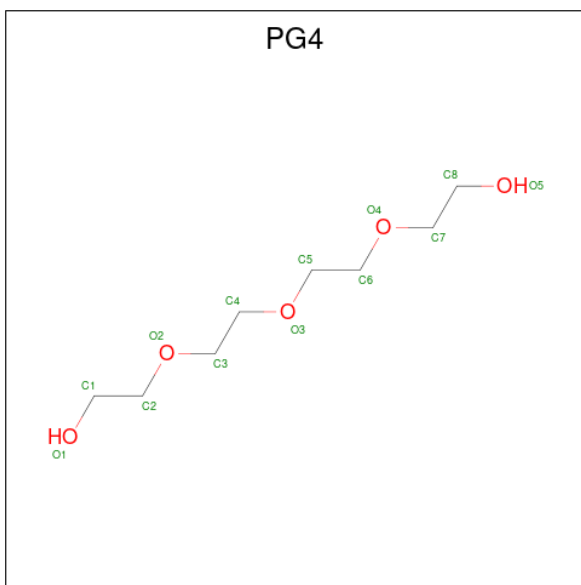
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
9	A	1	56	28	7	17	3	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
9	B	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		
9	C	1	Total	C	N	O	P	S	0	1
			112	56	14	34	6	2		
9	D	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
10	D	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	261	Total	O	0	0
			261	261		
11	B	118	Total	O	0	0
			118	118		
11	C	226	Total	O	0	0
			226	226		
11	D	230	Total	O	0	0
			230	230		
11	E	90	Total	O	0	0
			90	90		

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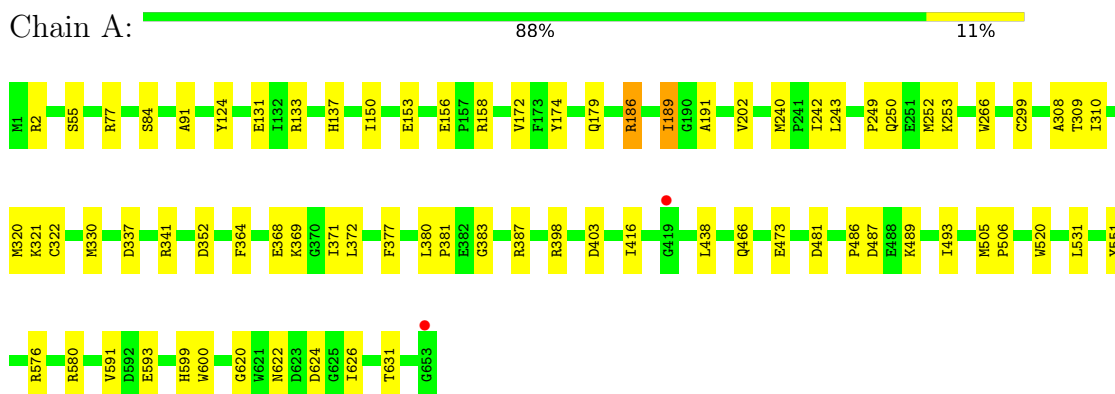
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	90	Total O 90 90	0	0
11	G	71	Total O 71 71	0	0
11	H	65	Total O 65 65	0	0

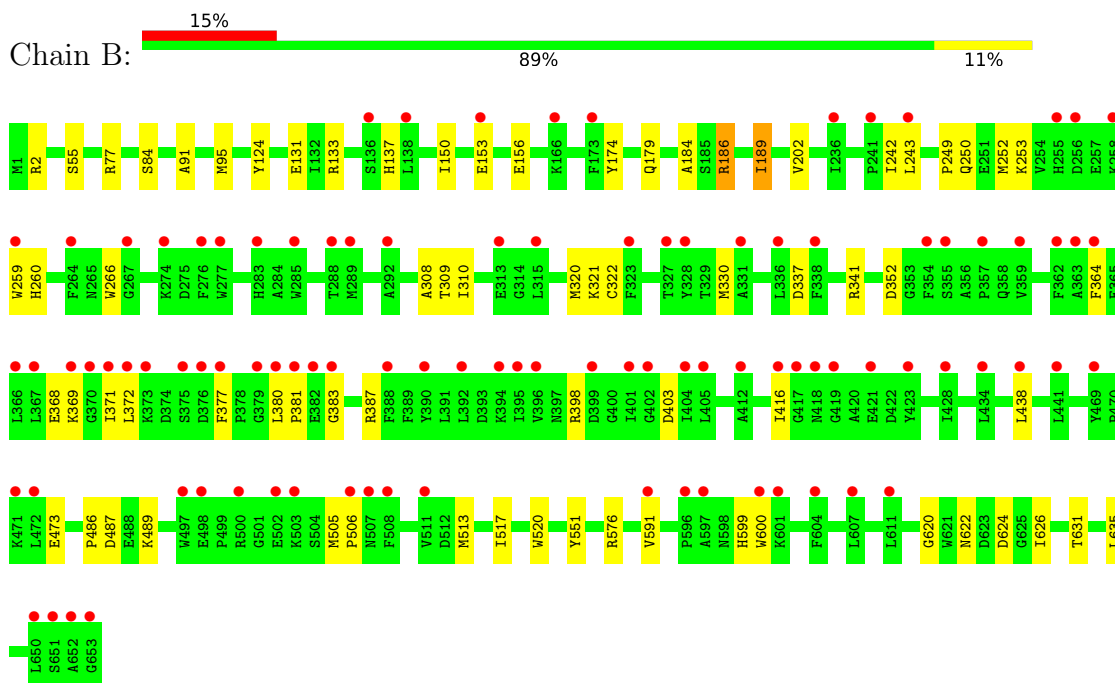
3 Residue-property plots [i](#)

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

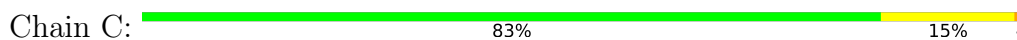
- Molecule 1: Benzoyl-CoA reductase, putative

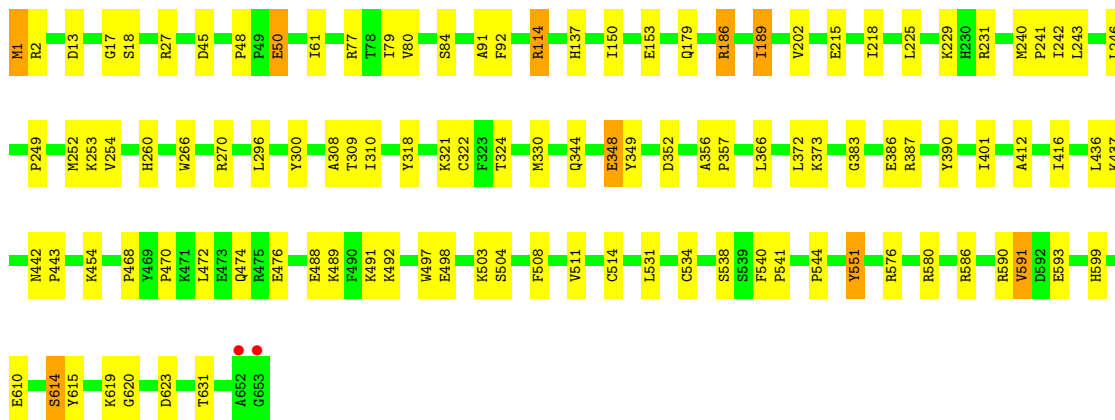


- Molecule 1: Benzoyl-CoA reductase, putative



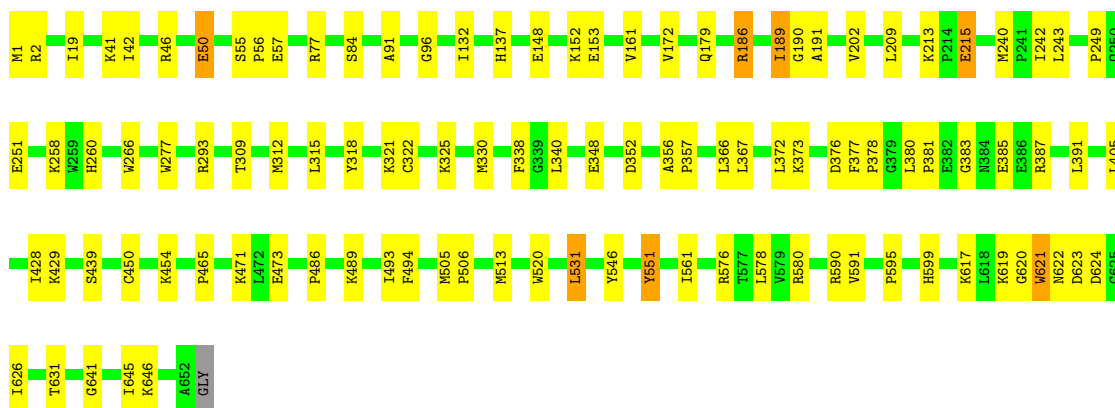
- Molecule 1: Benzoyl-CoA reductase, putative





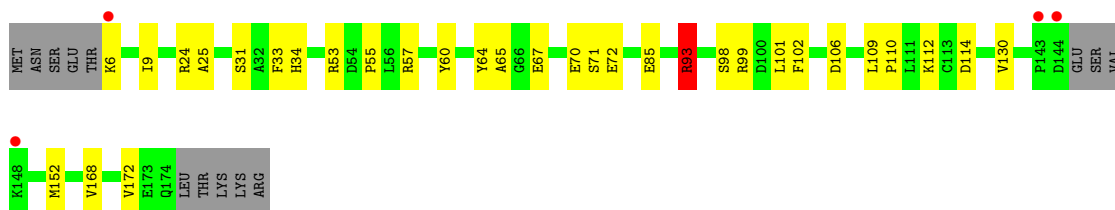
- Molecule 1: Benzoyl-CoA reductase, putative

Chain D: 83% 15%



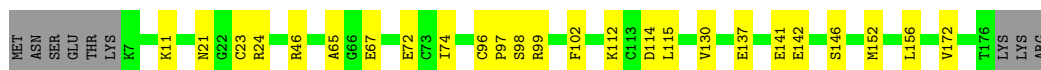
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain E: 75% 17% 2%



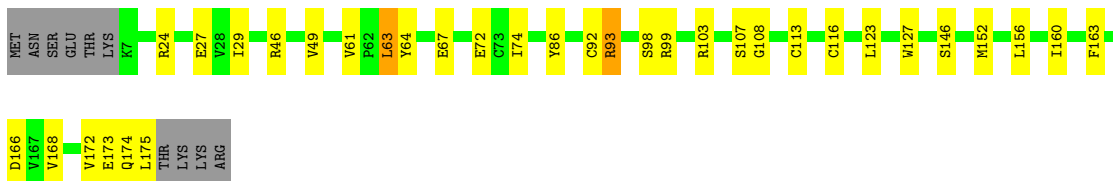
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain F: 81% 14% 5%




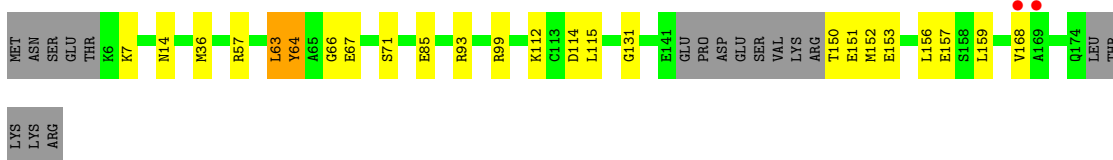
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain G:  75% 18% • 6%



- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain H:  77% 12% • 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.77Å 116.26Å 143.97Å 90.00° 110.43° 90.00°	Depositor
Resolution (Å)	88.07 – 1.85 88.07 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.8 (88.07-1.85) 92.8 (88.07-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.84Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.186 , 0.233 0.189 , 0.234	Depositor DCC
R_{free} test set	4088 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.238	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27713	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, W, 4KX, UNL, PG4, MTE, PGE

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	0.75	0/5316	0.73	3/7187 (0.0%)
1	B	0.65	0/5311	0.70	3/7179 (0.0%)
1	C	0.84	2/5307 (0.0%)	0.80	5/7174 (0.1%)
1	D	0.93	4/5307 (0.1%)	0.88	7/7174 (0.1%)
2	E	0.96	4/1282 (0.3%)	1.03	7/1734 (0.4%)
2	F	0.95	0/1343	0.95	3/1819 (0.2%)
2	G	0.91	3/1344 (0.2%)	0.89	4/1819 (0.2%)
2	H	0.85	1/1242 (0.1%)	0.84	2/1681 (0.1%)
All	All	0.83	14/26452 (0.1%)	0.81	34/35767 (0.1%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	546	TYR	CD2-CE2	6.91	1.49	1.39
2	G	86	TYR	CE1-CZ	6.81	1.47	1.38
1	D	546	TYR	CD1-CE1	6.75	1.49	1.39
2	E	130	VAL	CB-CG2	6.52	1.66	1.52
2	E	25	ALA	CA-CB	6.20	1.65	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	186	ARG	NE-CZ-NH1	17.61	129.10	120.30
1	D	186	ARG	NE-CZ-NH2	-14.24	113.18	120.30
1	A	186	ARG	NE-CZ-NH2	-12.21	114.20	120.30
2	E	93	ARG	NE-CZ-NH1	-11.98	114.31	120.30
1	A	186	ARG	NE-CZ-NH1	11.54	126.07	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5187	0	5113	51	0
1	B	5185	0	5118	49	0
1	C	5181	0	5114	81	0
1	D	5181	0	5115	63	0
2	E	1260	0	1209	17	0
2	F	1317	0	1266	15	0
2	G	1315	0	1263	28	0
2	H	1221	0	1158	21	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
3	E	24	0	0	0	0
3	F	24	0	0	1	0
3	G	24	0	0	0	0
3	H	24	0	0	3	0
4	A	48	0	20	2	0
4	B	48	0	20	5	0
4	C	48	0	20	1	0
4	D	48	0	20	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	20	28	28	2	0
8	D	10	14	14	1	0
9	A	56	0	38	4	0
9	B	56	0	38	4	0
9	C	112	0	76	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	56	0	38	4	0
10	D	13	18	18	1	0
11	A	261	0	0	3	1
11	B	118	0	0	2	0
11	C	226	0	0	6	0
11	D	230	0	0	4	0
11	E	90	0	0	2	0
11	F	90	0	0	0	0
11	G	71	0	0	0	0
11	H	65	0	0	4	0
All	All	27653	60	25686	318	1

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 6.

The worst 5 of 318 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:C:1:MET:SD	1:C:2:ARG:N	2.35	1.00
2:G:152:MET:HE2	2:H:168:VAL:HA	1.55	0.88
1:D:84:SER:HB2	1:D:91:ALA:HB2	1.57	0.86
1:D:137:HIS:NE2	1:D:153:GLU:OE2	2.10	0.84
2:G:64:TYR:O	2:G:93:ARG:HD2	1.78	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:968:HOH:O	11:A:1030:HOH:O[2_645]	2.17	0.03

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	652/653 (100%)	628 (96%)	24 (4%)	0	100	100
1	B	651/653 (100%)	627 (96%)	24 (4%)	0	100	100
1	C	651/653 (100%)	629 (97%)	22 (3%)	0	100	100
1	D	650/653 (100%)	623 (96%)	27 (4%)	0	100	100
2	E	162/179 (90%)	157 (97%)	5 (3%)	0	100	100
2	F	169/179 (94%)	167 (99%)	2 (1%)	0	100	100
2	G	169/179 (94%)	166 (98%)	2 (1%)	1 (1%)	25	12
2	H	157/179 (88%)	155 (99%)	2 (1%)	0	100	100
All	All	3261/3328 (98%)	3152 (97%)	108 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	174	GLN

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	547/548 (100%)	535 (98%)	12 (2%)	52	36
1	B	547/548 (100%)	536 (98%)	11 (2%)	55	40
1	C	546/548 (100%)	529 (97%)	17 (3%)	40	23
1	D	547/548 (100%)	534 (98%)	13 (2%)	49	33
2	E	136/159 (86%)	131 (96%)	5 (4%)	34	17
2	F	148/159 (93%)	145 (98%)	3 (2%)	55	40
2	G	147/159 (92%)	143 (97%)	4 (3%)	44	29
2	H	132/159 (83%)	129 (98%)	3 (2%)	50	34
All	All	2750/2828 (97%)	2682 (98%)	68 (2%)	47	31

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	152	MET
2	F	152	MET
2	H	36	MET
1	C	45	ASP
1	C	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 8 are monoatomic and 4 are unknown - leaving 33 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	$\# Z > 2$
10	PG4	D	708	-	12,12,12	0.66	0	11,11,11	0.57	0
3	SF4	B	701	1	0,12,12	-	-	-		
3	SF4	H	1003	2	0,12,12	-	-	-		
8	PGE	A	708	-	9,9,9	0.82	0	8,8,8	0.83	0
4	MTE	C	702	5,6	21,26,26	2.33	6 (28%)	21,40,40	2.59	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	H	1002	2	0,12,12	-	-	-	-	-
3	SF4	F	1002	2	0,12,12	-	-	-	-	-
3	SF4	C	701	1	0,12,12	-	-	-	-	-
3	SF4	D	702	1	0,12,12	-	-	-	-	-
4	MTE	D	704	5,6	21,26,26	2.32	5 (23%)	21,40,40	3.21	9 (42%)
4	MTE	B	702	5,6	21,26,26	2.83	11 (52%)	21,40,40	2.29	8 (38%)
8	PGE	A	707	-	9,9,9	0.55	0	8,8,8	0.61	0
4	MTE	A	703	5,6	21,26,26	2.95	8 (38%)	21,40,40	3.18	10 (47%)
9	4KX	C	707[A]	-	49,59,59	1.27	2 (4%)	58,87,87	1.07	4 (6%)
4	MTE	C	703	5,6	21,26,26	2.54	7 (33%)	21,40,40	2.61	9 (42%)
4	MTE	D	703	5,6	21,26,26	2.47	8 (38%)	21,40,40	2.64	6 (28%)
4	MTE	A	702	5,6	21,26,26	2.59	13 (61%)	21,40,40	2.70	9 (42%)
3	SF4	A	701	1	0,12,12	-	-	-	-	-
8	PGE	D	707	-	9,9,9	0.45	0	8,8,8	0.53	0
3	SF4	E	1003	2	0,12,12	-	-	-	-	-
3	SF4	G	1002	2	0,12,12	-	-	-	-	-
4	MTE	B	703	5,6	21,26,26	2.44	8 (38%)	21,40,40	2.83	5 (23%)
9	4KX	C	707[B]	-	49,59,59	1.31	2 (4%)	58,87,87	1.12	4 (6%)
9	4KX	B	707	-	49,59,59	1.29	3 (6%)	58,87,87	1.19	4 (6%)
3	SF4	E	1001	2	0,12,12	-	-	-	-	-
3	SF4	F	1003	2	0,12,12	-	-	-	-	-
3	SF4	G	1003	2	0,12,12	-	-	-	-	-
3	SF4	H	1001	2	0,12,12	-	-	-	-	-
3	SF4	F	1001	2	0,12,12	-	-	-	-	-
9	4KX	A	709	-	49,59,59	1.31	2 (4%)	58,87,87	1.08	4 (6%)
3	SF4	E	1002	2	0,12,12	-	-	-	-	-
3	SF4	G	1001	2	0,12,12	-	-	-	-	-
9	4KX	D	709	-	49,59,59	1.31	2 (4%)	58,87,87	1.12	5 (8%)

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
10	PG4	D	708	-	-	6/10/10/10	-
3	SF4	B	701	1	-	-	0/6/5/5
3	SF4	H	1003	2	-	-	0/6/5/5
8	PGE	A	708	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MTE	C	702	5,6	-	0/6/34/34	0/3/3/3
3	SF4	H	1002	2	-	-	0/6/5/5
3	SF4	F	1002	2	-	-	0/6/5/5
3	SF4	C	701	1	-	-	0/6/5/5
4	MTE	D	704	5,6	-	0/6/34/34	0/3/3/3
3	SF4	D	702	1	-	-	0/6/5/5
4	MTE	B	702	5,6	-	0/6/34/34	0/3/3/3
8	PGE	A	707	-	-	3/7/7/7	-
4	MTE	A	703	5,6	-	0/6/34/34	0/3/3/3
9	4KX	C	707[A]	-	-	3/48/79/79	0/4/4/4
4	MTE	D	703	5,6	-	0/6/34/34	0/3/3/3
4	MTE	C	703	5,6	-	0/6/34/34	0/3/3/3
4	MTE	A	702	5,6	-	1/6/34/34	0/3/3/3
3	SF4	A	701	1	-	-	0/6/5/5
8	PGE	D	707	-	-	2/7/7/7	-
3	SF4	E	1003	2	-	-	0/6/5/5
4	MTE	B	703	5,6	-	2/6/34/34	0/3/3/3
3	SF4	G	1002	2	-	-	0/6/5/5
9	4KX	C	707[B]	-	-	22/48/79/79	0/4/4/4
9	4KX	B	707	-	-	5/48/79/79	0/4/4/4
3	SF4	E	1001	2	-	-	0/6/5/5
3	SF4	F	1003	2	-	-	0/6/5/5
3	SF4	G	1003	2	-	-	0/6/5/5
3	SF4	H	1001	2	-	-	0/6/5/5
3	SF4	F	1001	2	-	-	0/6/5/5
9	4KX	A	709	-	-	2/48/79/79	0/4/4/4
3	SF4	E	1002	2	-	-	0/6/5/5
3	SF4	G	1001	2	-	-	0/6/5/5
9	4KX	D	709	-	-	4/48/79/79	0/4/4/4

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	707[A]	4KX	C3B-C4B	7.29	1.52	1.33
9	C	707[B]	4KX	C3B-C4B	7.29	1.52	1.33
9	B	707	4KX	C3B-C4B	7.16	1.52	1.33
9	A	709	4KX	C3B-C4B	7.08	1.52	1.33
4	A	703	MTE	C9-C4	6.79	1.50	1.41

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	704	MTE	O3'-C7-N8	-7.88	100.46	108.57
4	B	703	MTE	C10-C9-C4	7.86	121.55	114.57
4	D	704	MTE	C10-C9-C4	7.65	121.37	114.57
4	A	702	MTE	C9-C10-N8	7.29	124.80	118.13
4	A	703	MTE	O3'-C7-N8	-7.00	101.37	108.57

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	MTE	C4'-O4'-P-O2P
4	B	703	MTE	C4'-O4'-P-O3P
9	B	707	4KX	N8P-C9P-CAP-OAP
9	C	707[B]	4KX	C5D-O5D-P1A-O1A
9	C	707[B]	4KX	CCP-O6A-P2A-O4A

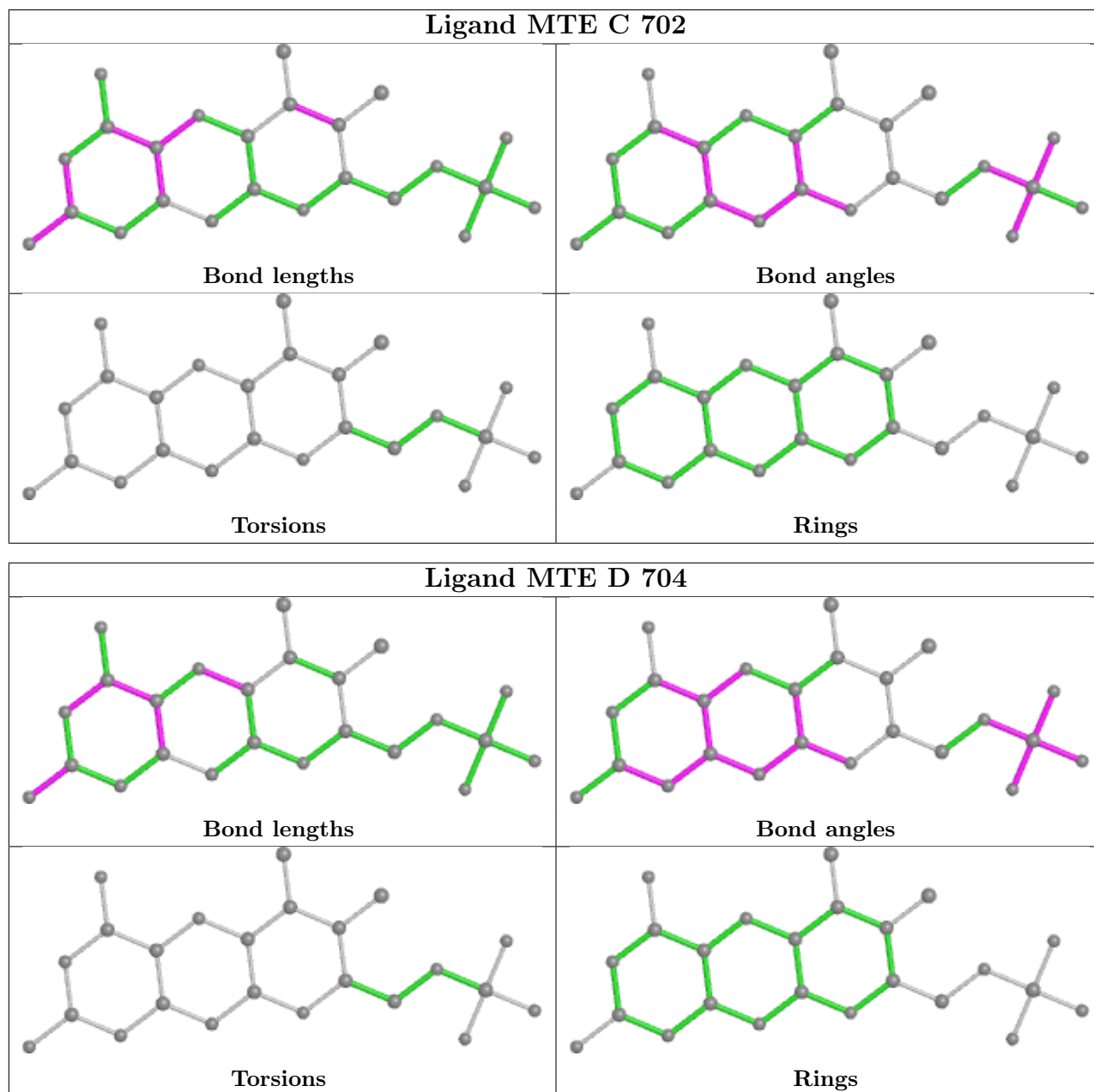
There are no ring outliers.

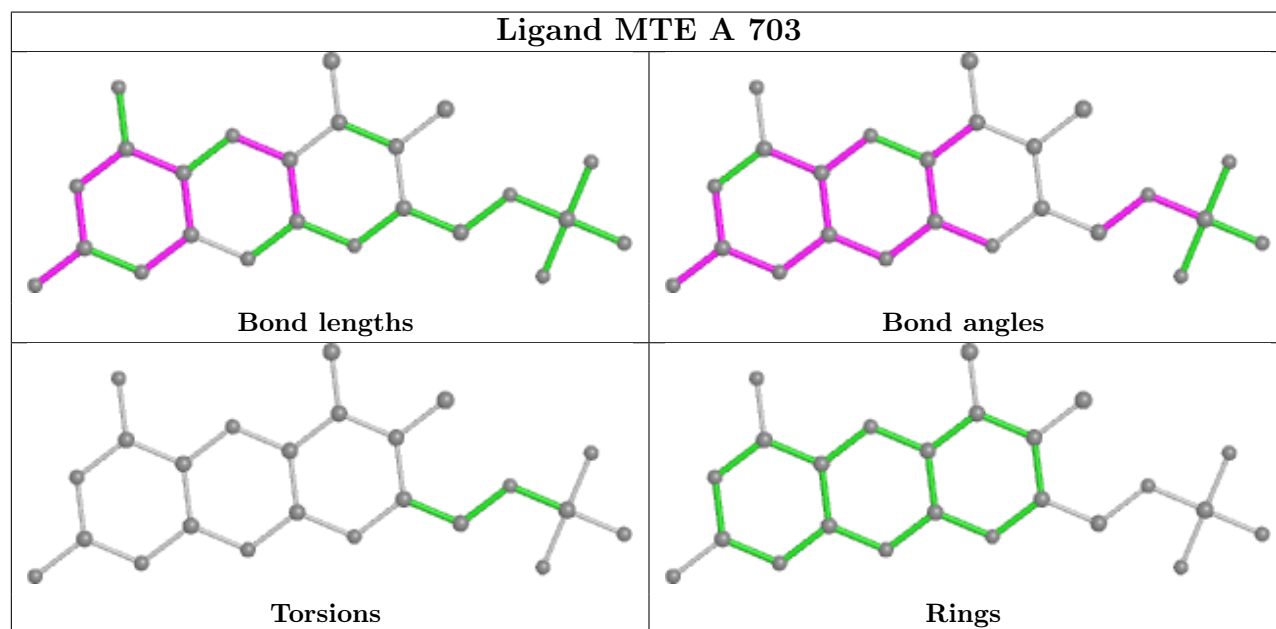
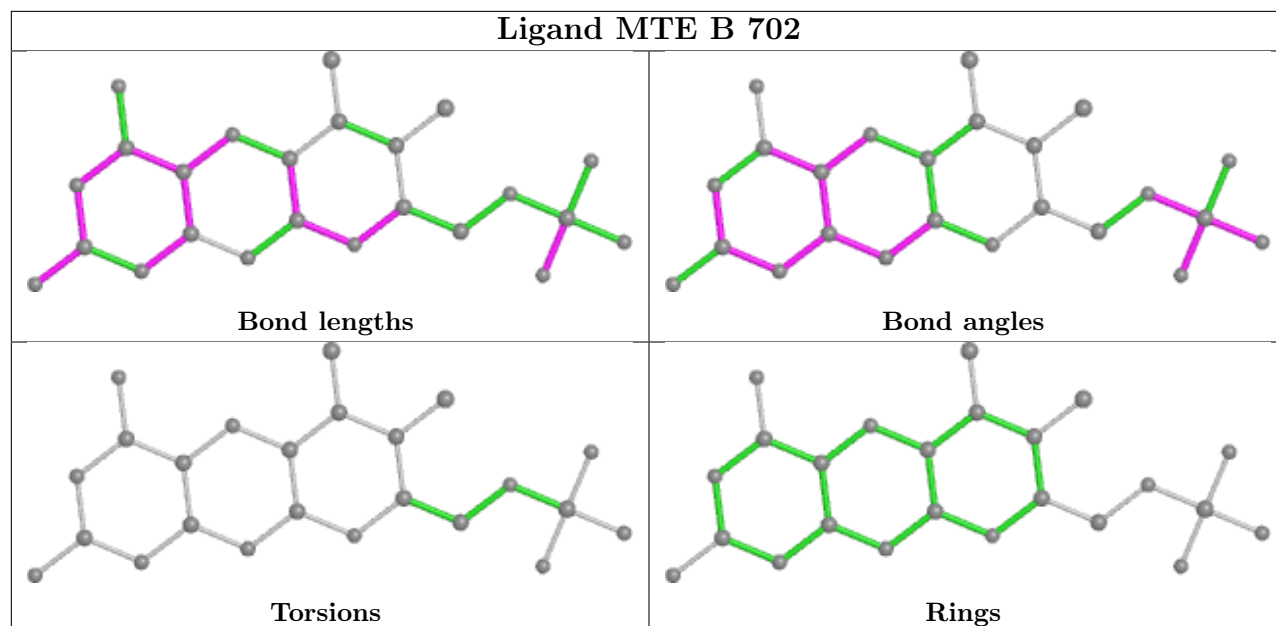
17 monomers are involved in 40 short contacts:

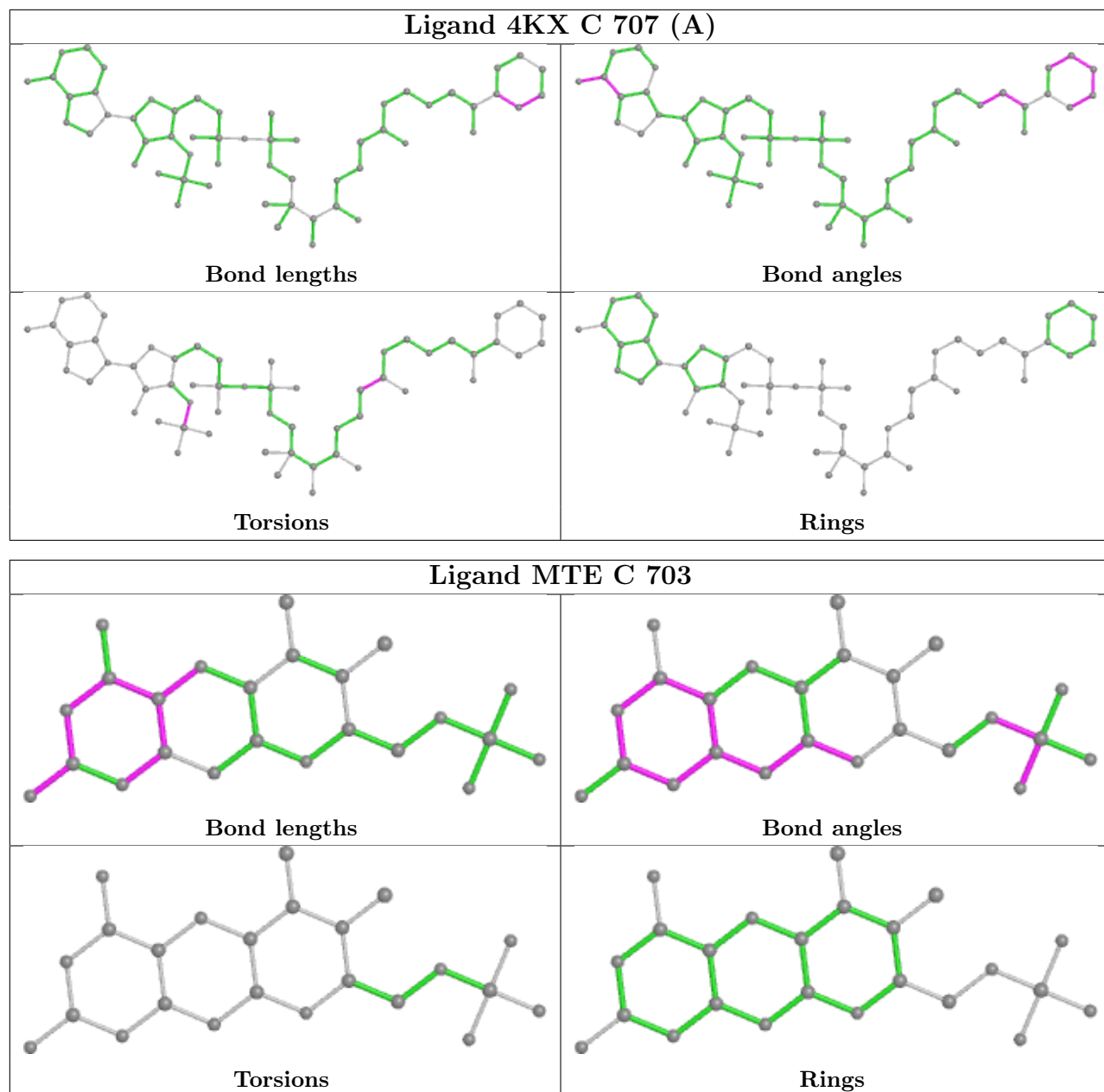
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	708	PG4	1	0
3	H	1003	SF4	2	0
8	A	708	PGE	2	0
3	H	1002	SF4	1	0
3	F	1002	SF4	1	0
4	B	702	MTE	2	0
9	C	707[A]	4KX	4	0
4	C	703	MTE	1	0
4	D	703	MTE	2	0
4	A	702	MTE	2	0
3	A	701	SF4	1	0
8	D	707	PGE	1	0
4	B	703	MTE	3	0
9	C	707[B]	4KX	5	0
9	B	707	4KX	4	0
9	A	709	4KX	4	0
9	D	709	4KX	4	0

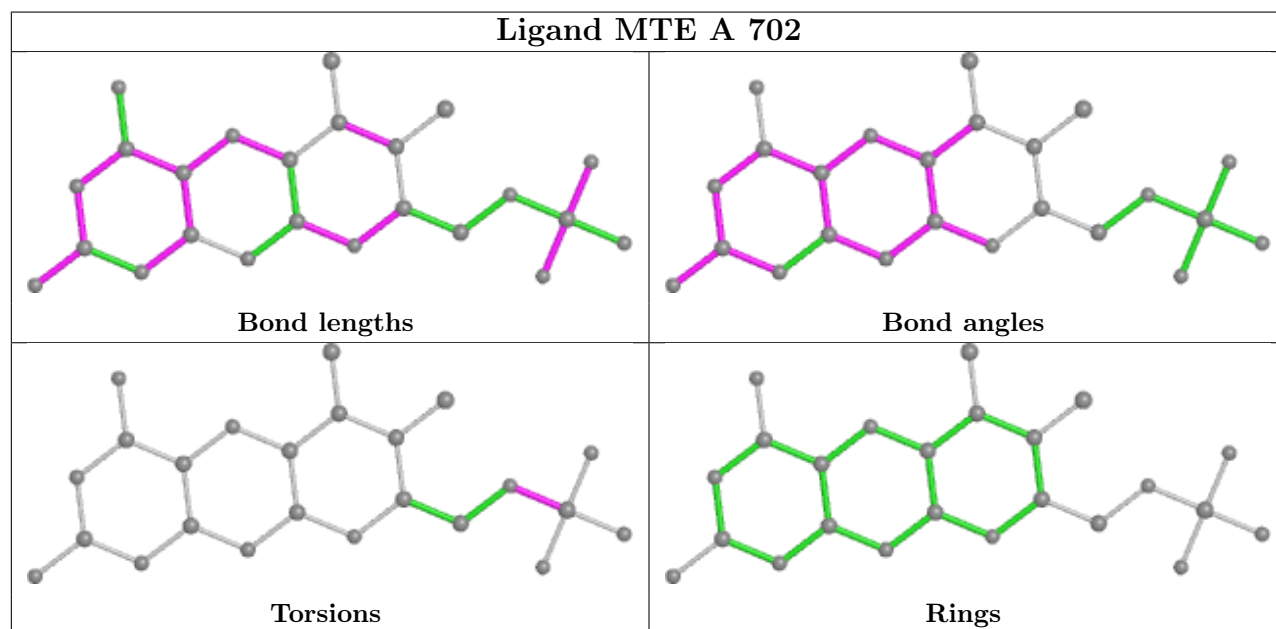
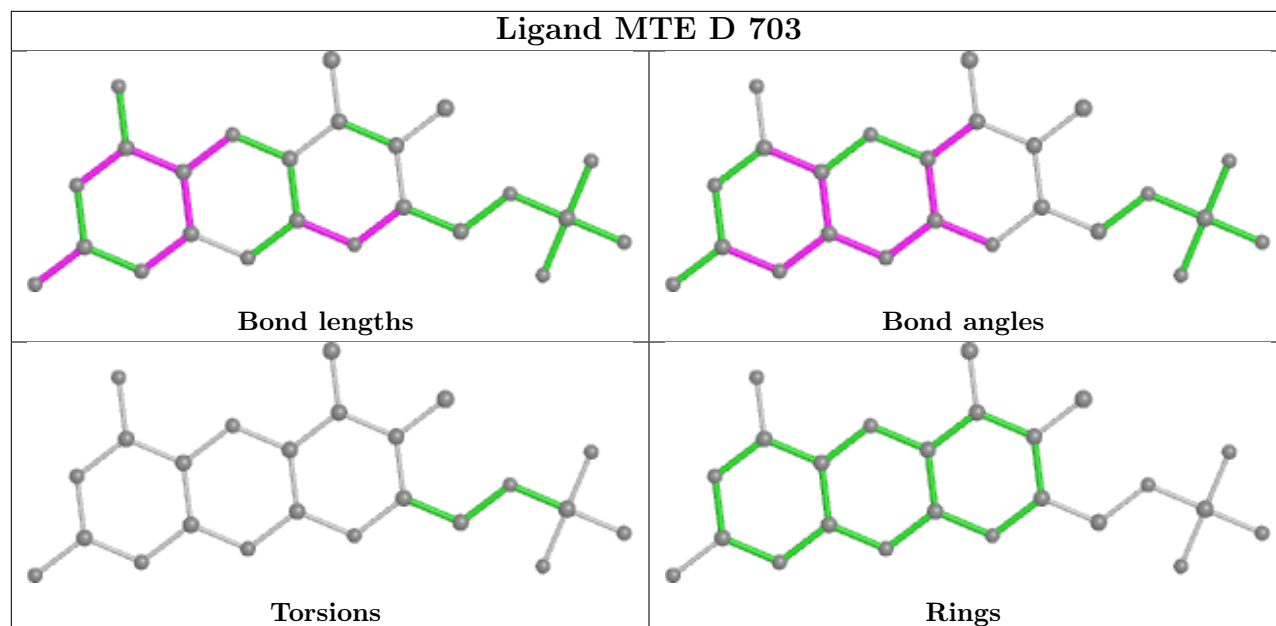
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

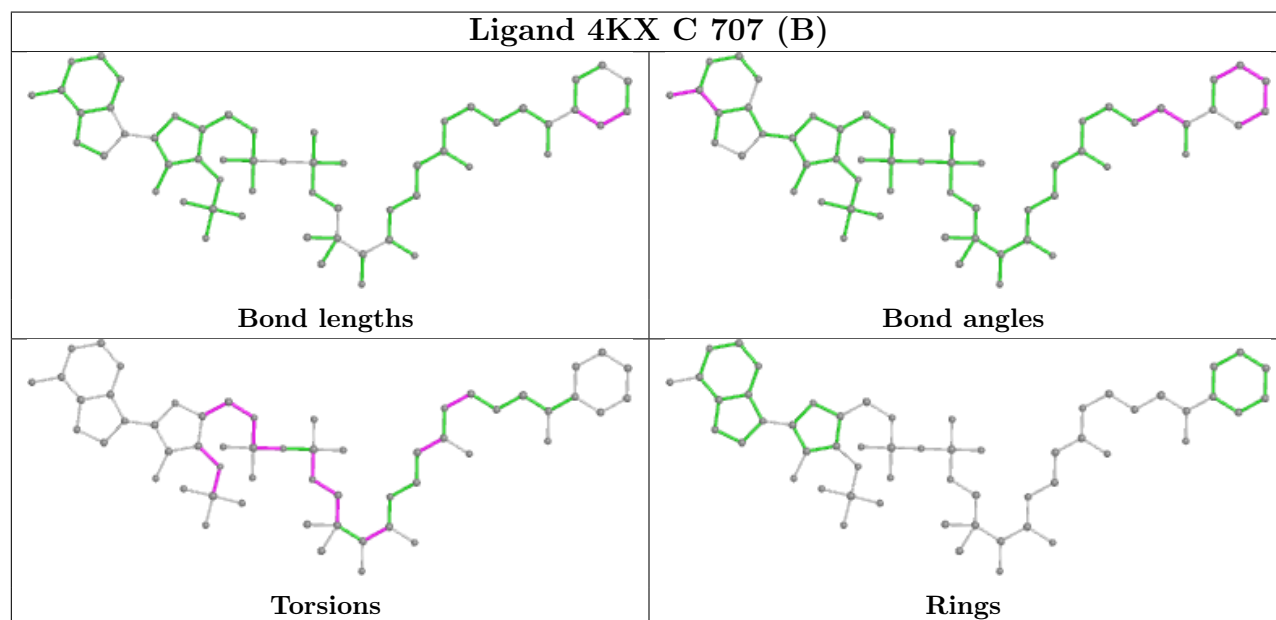
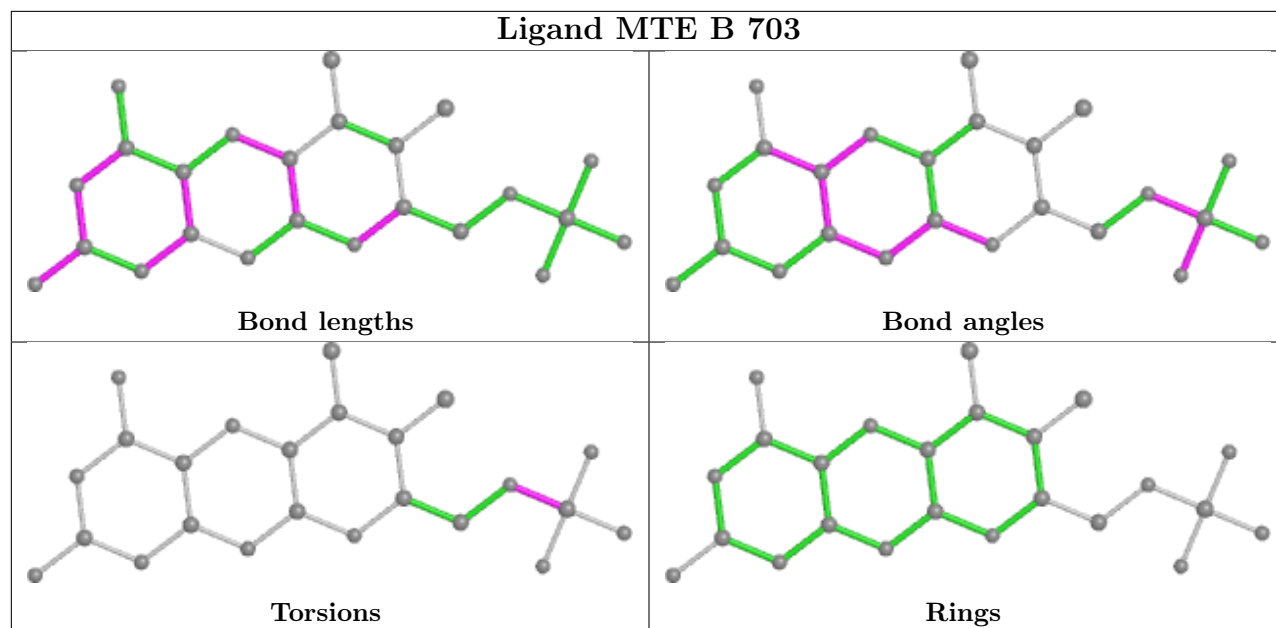
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

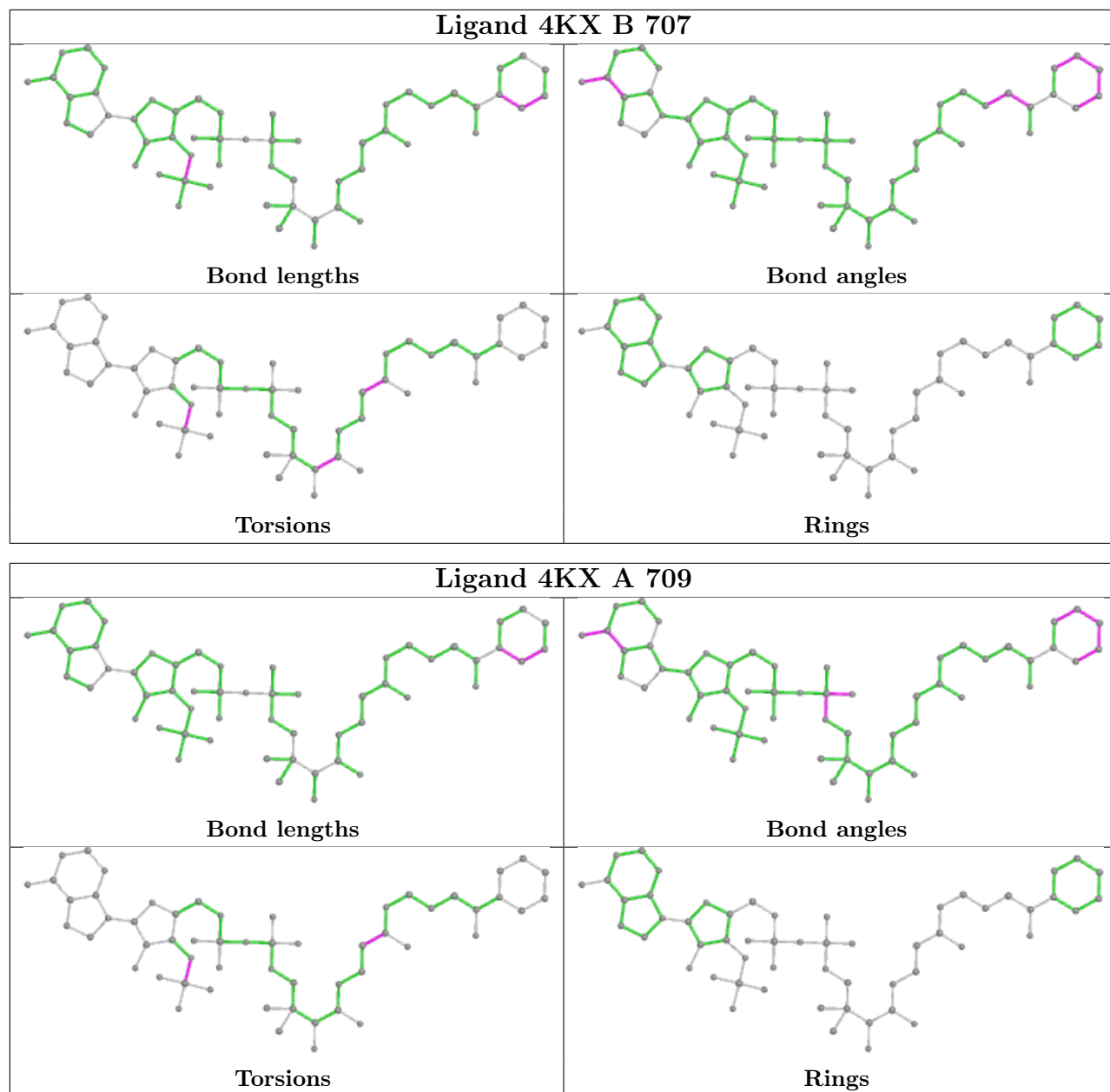


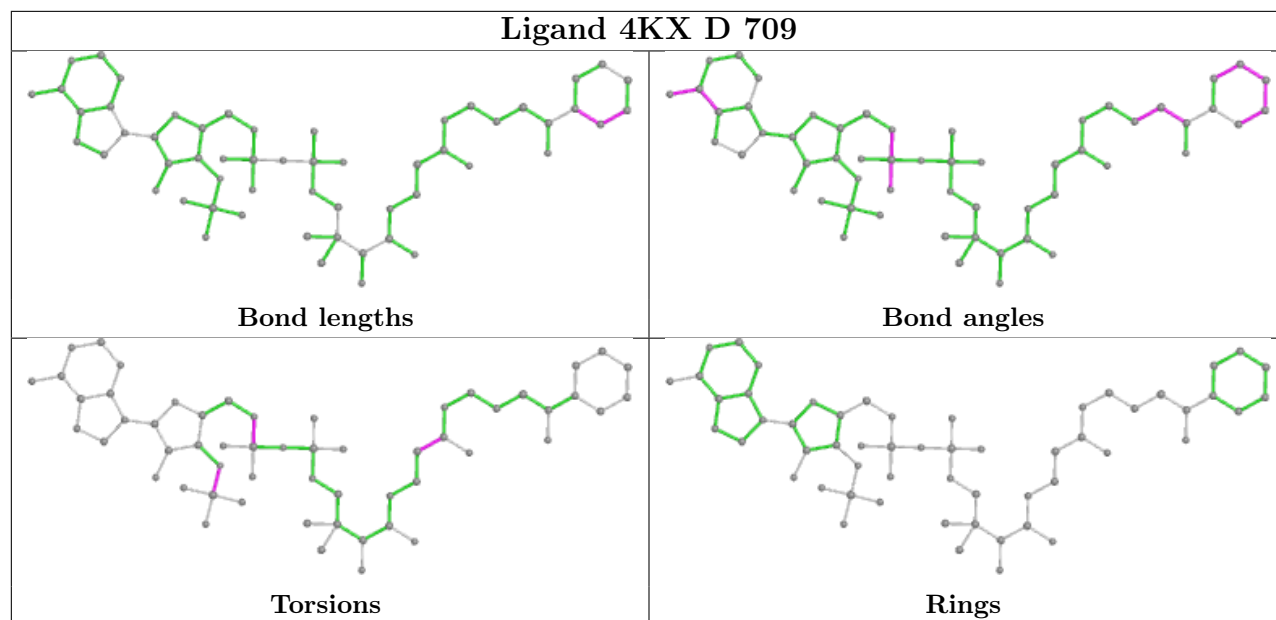












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	653/653 (100%)	-0.18	2 (0%) 94 93	27, 45, 73, 123	0
1	B	653/653 (100%)	0.80	98 (15%) 2 2	36, 82, 128, 169	0
1	C	653/653 (100%)	-0.22	2 (0%) 94 93	31, 48, 80, 136	0
1	D	652/653 (99%)	-0.29	0 100 100	26, 48, 75, 99	0
2	E	166/179 (92%)	-0.23	4 (2%) 59 57	31, 43, 77, 140	0
2	F	170/179 (94%)	-0.32	0 100 100	30, 42, 68, 86	0
2	G	169/179 (94%)	-0.18	0 100 100	31, 46, 99, 130	0
2	H	161/179 (89%)	-0.30	2 (1%) 79 79	30, 46, 99, 116	0
All	All	3277/3328 (98%)	-0.03	108 (3%) 46 44	26, 50, 101, 169	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	PHE	8.3
1	B	416	ILE	7.6
1	B	366	LEU	7.2
1	B	405	LEU	6.8
2	E	143	PRO	6.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

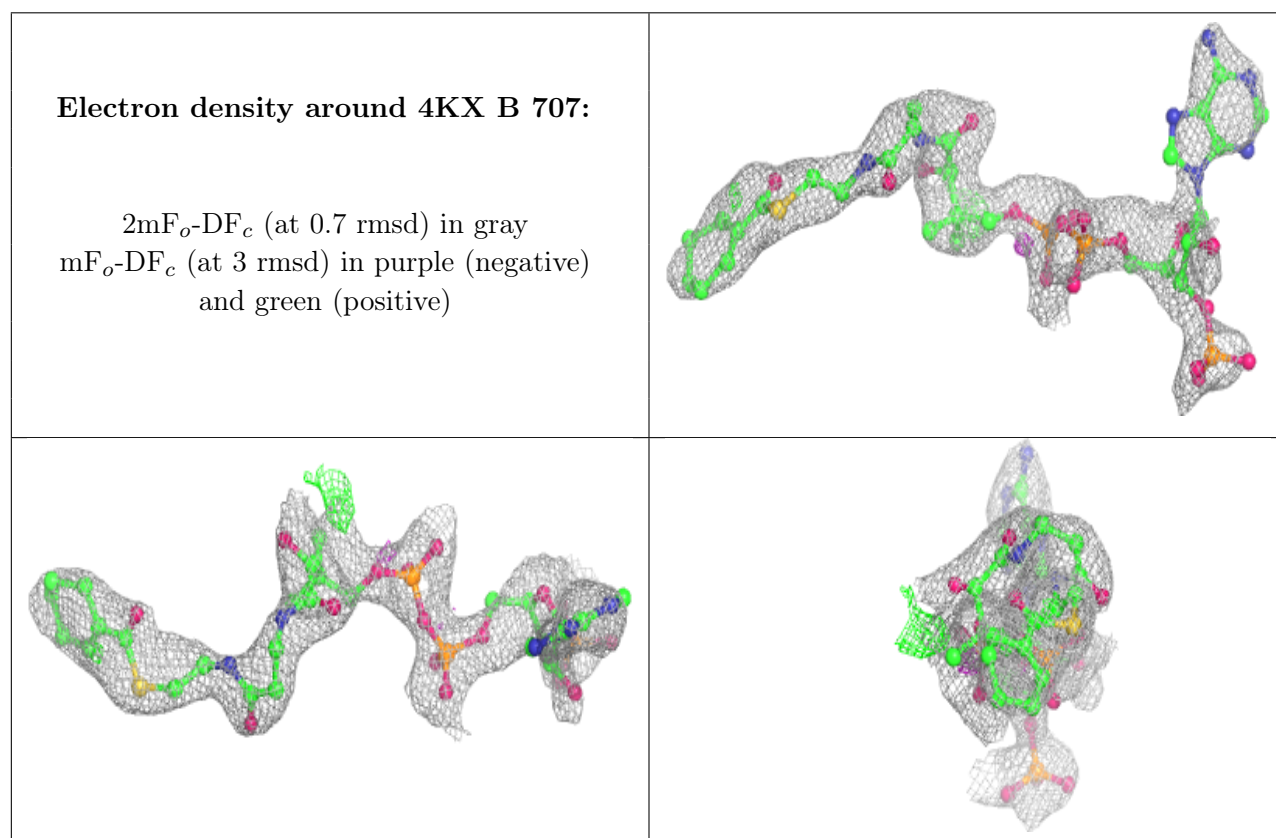
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	PGE	A	707	10/10	0.69	0.14	70,92,111,112	0
9	4KX	B	707	56/56	0.79	0.19	65,100,129,156	56
9	4KX	C	707[A]	56/56	0.80	0.20	57,67,87,90	56
9	4KX	C	707[B]	56/56	0.80	0.20	42,68,80,84	56
8	PGE	D	707	10/10	0.85	0.11	64,80,91,102	0
10	PG4	D	708	13/13	0.85	0.12	51,66,80,81	0
8	PGE	A	708	10/10	0.87	0.10	48,66,84,85	0
7	UNL	C	705	1/-	0.89	0.44	46,46,46,46	0
6	MG	B	706	1/1	0.90	0.10	44,44,44,44	0
4	MTE	B	702	24/24	0.91	0.11	34,49,58,86	0
7	UNL	A	706	1/-	0.93	0.39	33,33,33,33	0
4	MTE	B	703	24/24	0.94	0.11	38,52,64,74	0
9	4KX	A	709	56/56	0.94	0.11	27,40,81,100	56
7	UNL	D	701	1/-	0.94	0.32	32,32,32,32	0
9	4KX	D	709	56/56	0.95	0.09	29,41,64,81	0
4	MTE	C	703	24/24	0.95	0.09	29,37,42,44	0
7	UNL	B	705	1/-	0.96	0.29	30,30,30,30	0
6	MG	C	704	1/1	0.96	0.13	33,33,33,33	0
4	MTE	D	704	24/24	0.97	0.09	21,31,36,37	0
5	W	B	704	1/1	0.97	0.06	58,58,58,58	0
6	MG	A	705	1/1	0.97	0.07	28,28,28,28	0
3	SF4	A	701	8/8	0.97	0.10	25,31,34,38	0
3	SF4	B	701	8/8	0.97	0.06	39,46,46,56	0
4	MTE	A	703	24/24	0.97	0.10	19,29,32,35	0
4	MTE	C	702	24/24	0.98	0.12	28,34,37,38	0
3	SF4	F	1001	8/8	0.98	0.11	29,34,36,37	0
4	MTE	D	703	24/24	0.98	0.09	24,29,32,33	0
3	SF4	G	1002	8/8	0.98	0.12	33,37,38,39	0
3	SF4	H	1002	8/8	0.98	0.11	39,41,44,46	0
3	SF4	H	1003	8/8	0.98	0.11	39,41,41,42	0
4	MTE	A	702	24/24	0.98	0.11	16,27,33,35	0
3	SF4	C	701	8/8	0.98	0.10	30,34,41,45	0
6	MG	D	706	1/1	0.98	0.10	32,32,32,32	0
3	SF4	D	702	8/8	0.98	0.10	28,31,37,39	0
3	SF4	E	1002	8/8	0.98	0.11	36,37,39,40	0
3	SF4	G	1003	8/8	0.99	0.11	39,41,42,44	0
3	SF4	H	1001	8/8	0.99	0.12	30,33,35,36	0

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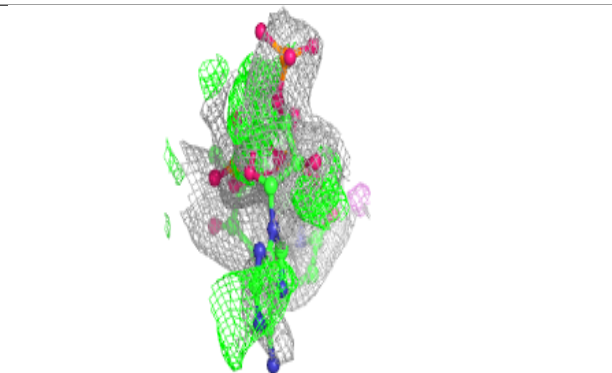
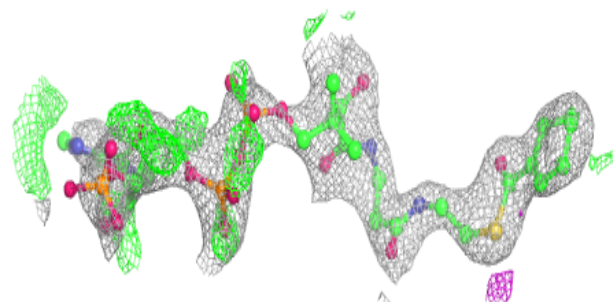
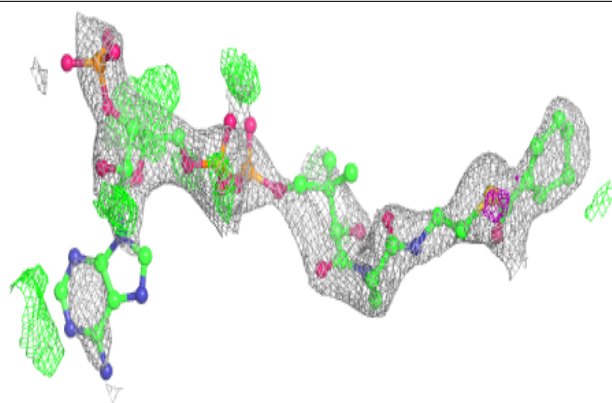
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SF4	E	1001	8/8	0.99	0.11	32,34,36,37	0
3	SF4	F	1002	8/8	0.99	0.13	30,31,33,33	0
3	SF4	F	1003	8/8	0.99	0.11	29,36,39,39	0
3	SF4	G	1001	8/8	0.99	0.13	33,36,38,40	0
5	W	C	706	1/1	0.99	0.16	44,44,44,44	0
3	SF4	E	1003	8/8	0.99	0.11	34,34,36,36	0
5	W	D	705	1/1	1.00	0.17	35,35,35,35	0
5	W	A	704	1/1	1.00	0.16	33,33,33,33	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.

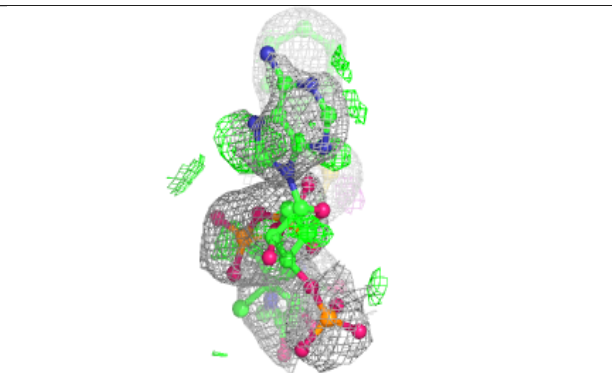
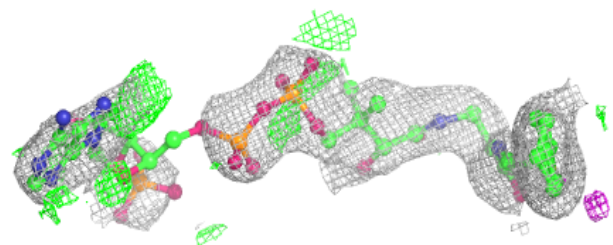
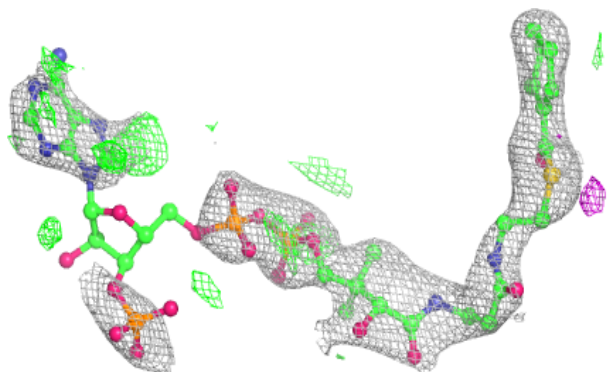


Electron density around 4KX C 707 (A):

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

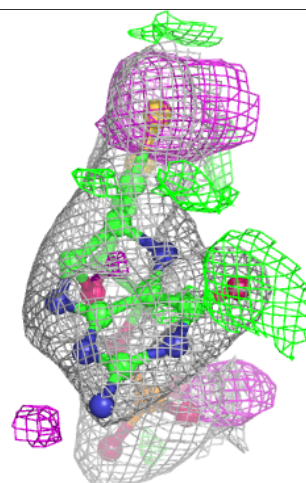
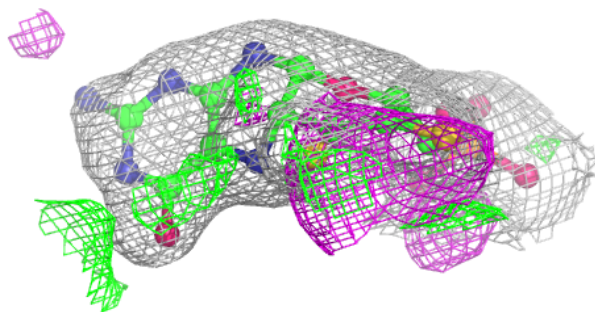
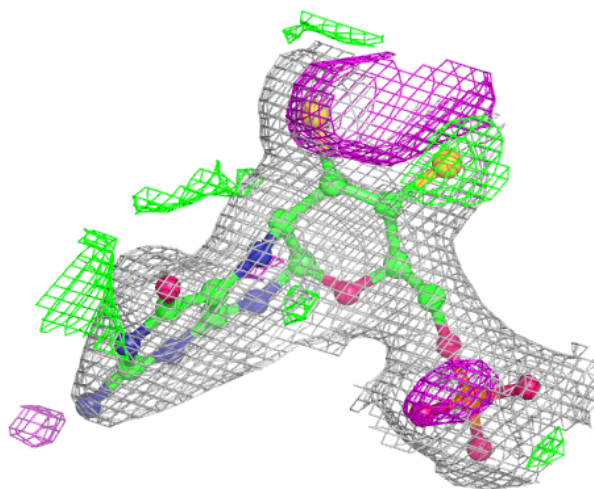
**Electron density around 4KX C 707 (B):**

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



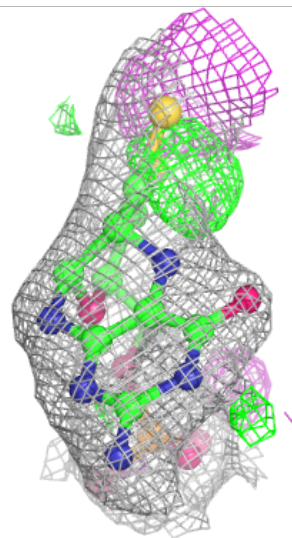
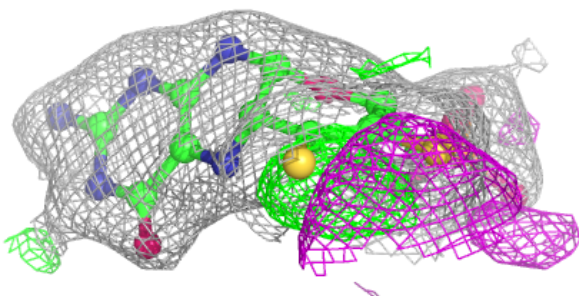
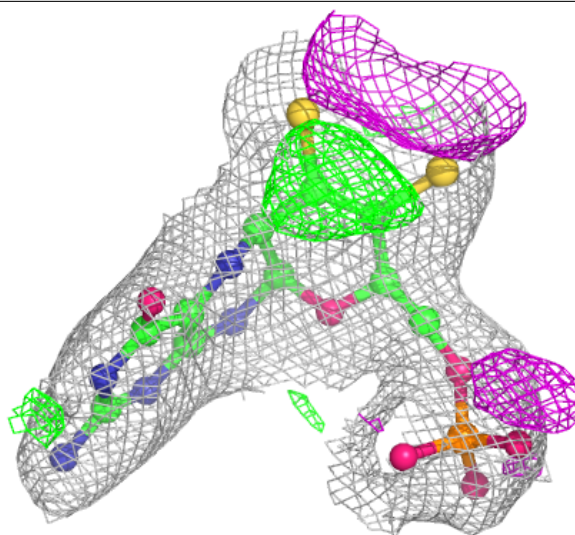
Electron density around MTE B 702:

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



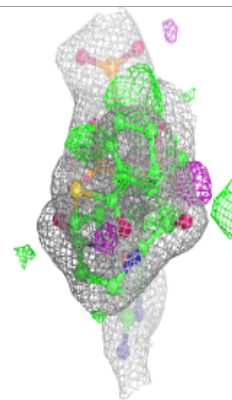
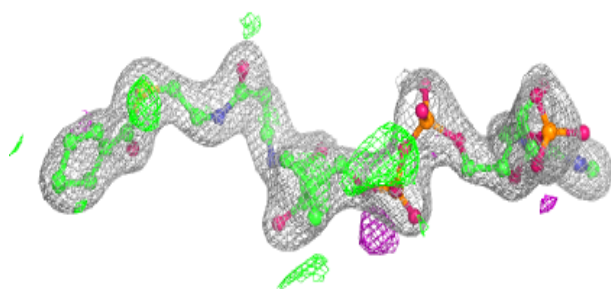
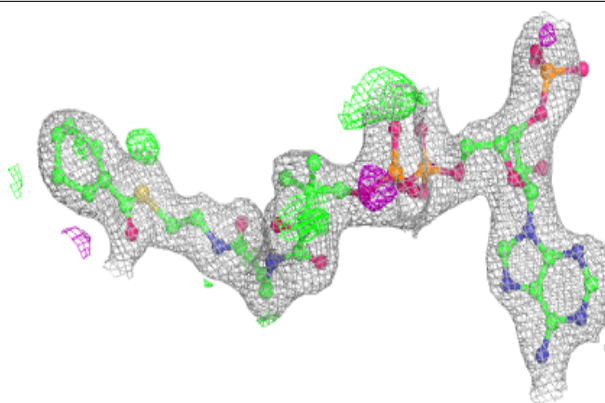
Electron density around MTE B 703:

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

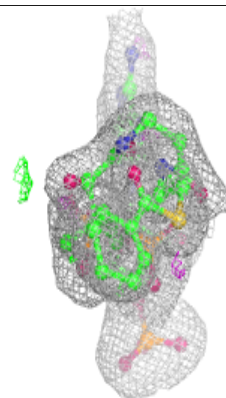
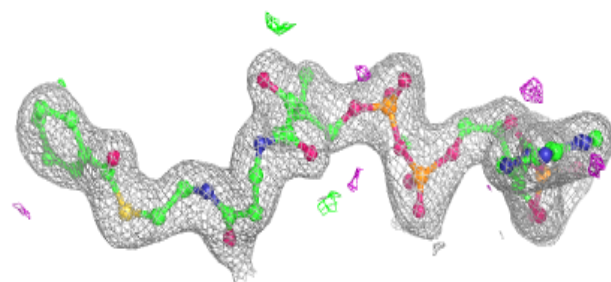
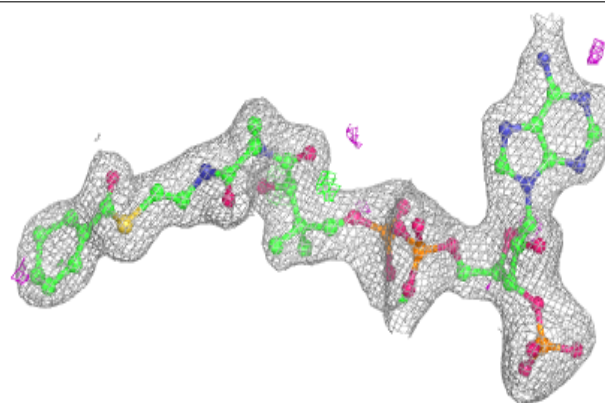


Electron density around 4KX A 709:

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

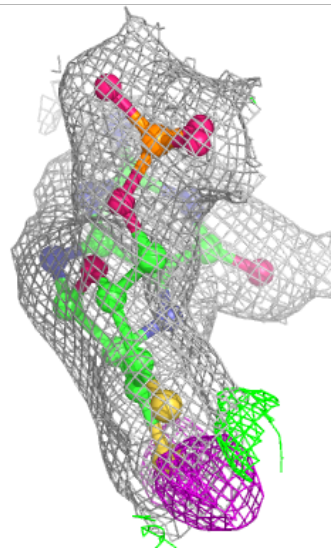
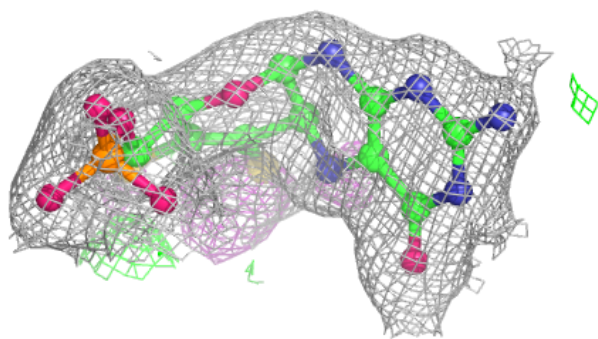
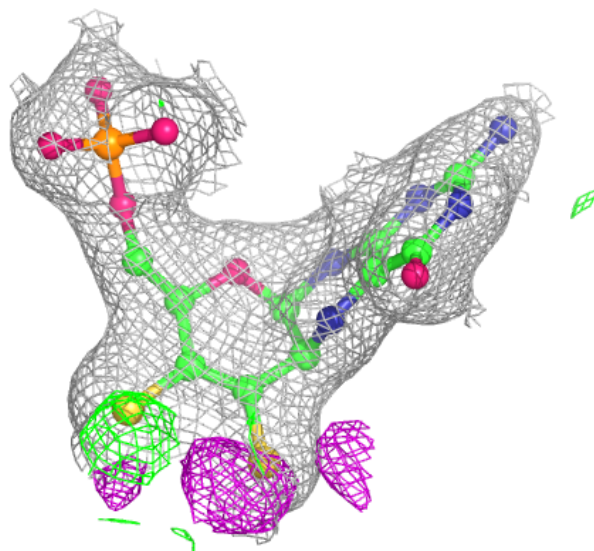
**Electron density around 4KX D 709:**

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



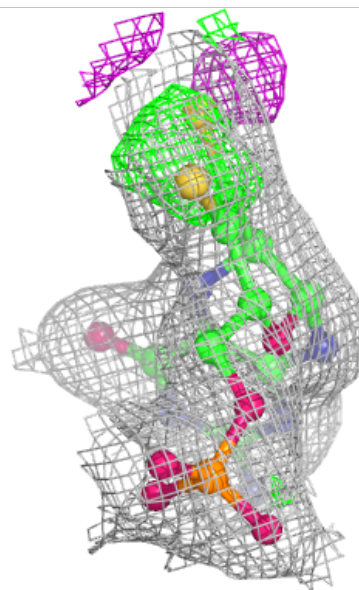
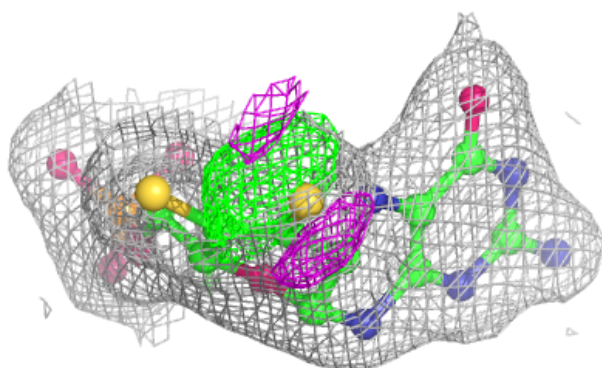
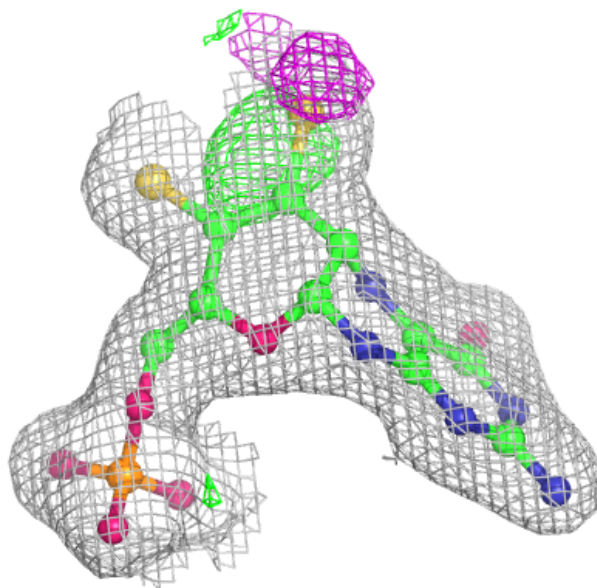
Electron density around MTE C 703:

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



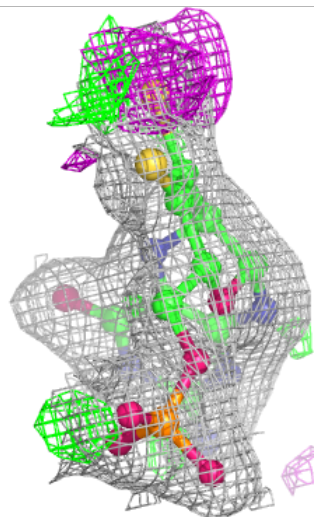
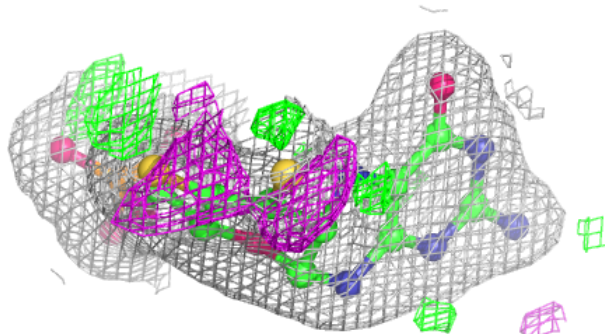
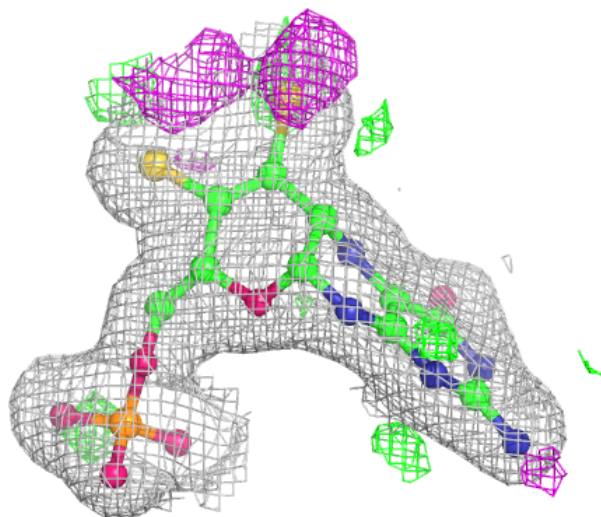
Electron density around MTE D 704:

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



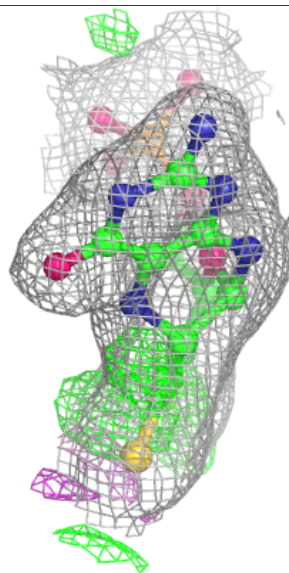
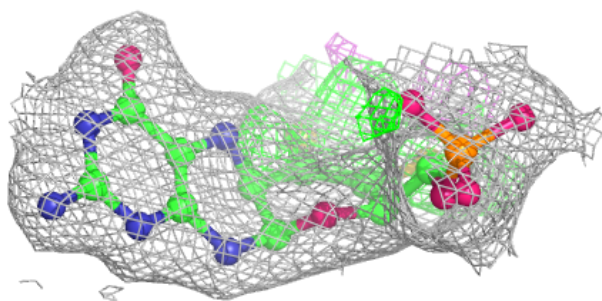
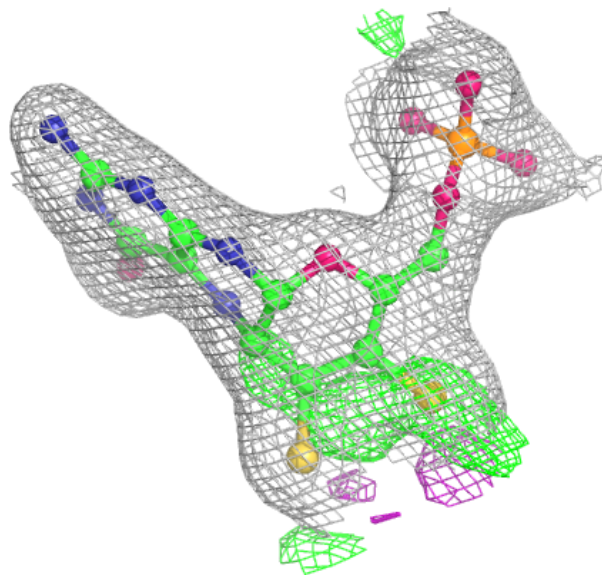
Electron density around MTE A 703:

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



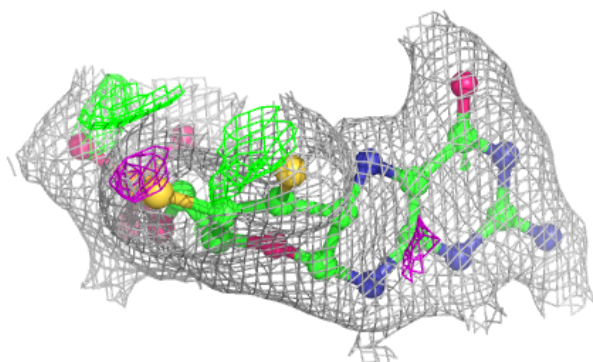
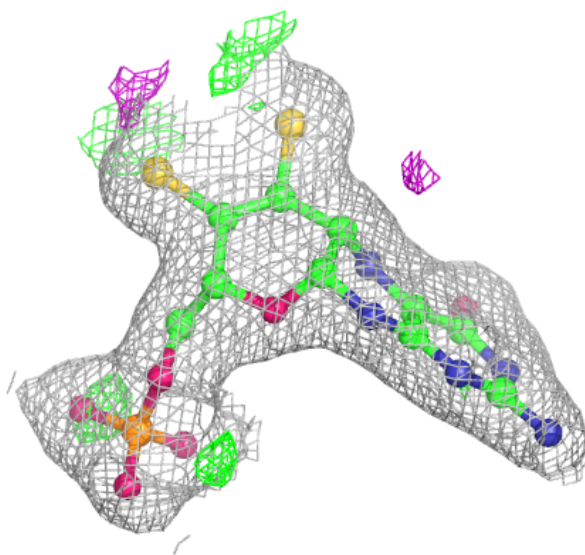
Electron density around MTE C 702:

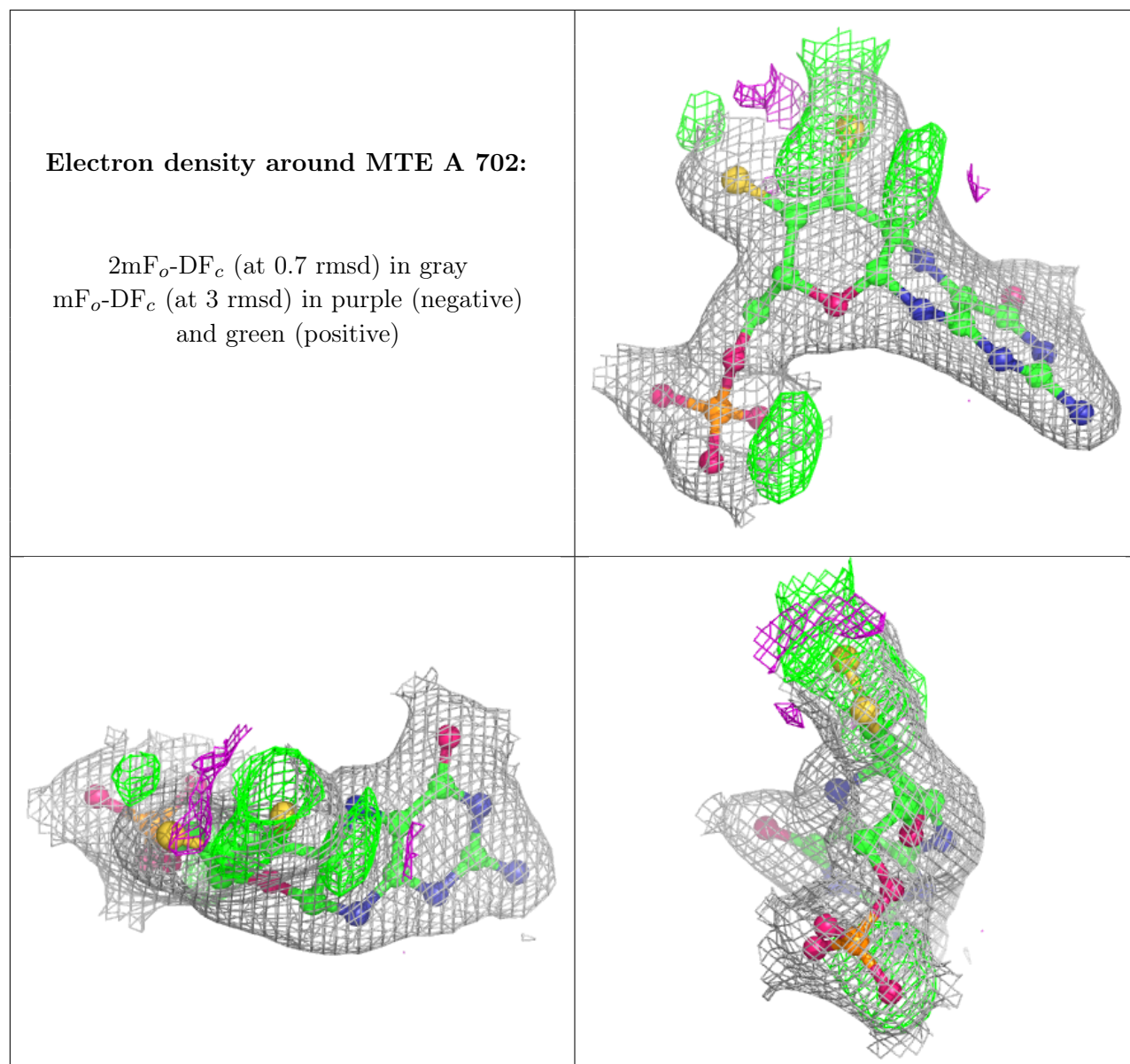
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MTE D 703:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.