wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 07:22 pm GMT

PDB ID	:	4Z40
Title	:	Active site complex BamBC of Benzoyl Coenzyme A reductase as isolated
Authors	:	Weinert, T.; Kung, J.W.; Weidenweber, S.; Huwiler, S.G.; Boll, M.; Ermler, U.
Deposited on	:	2015-04-01
Resolution	:	2.35 Å(reported)

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

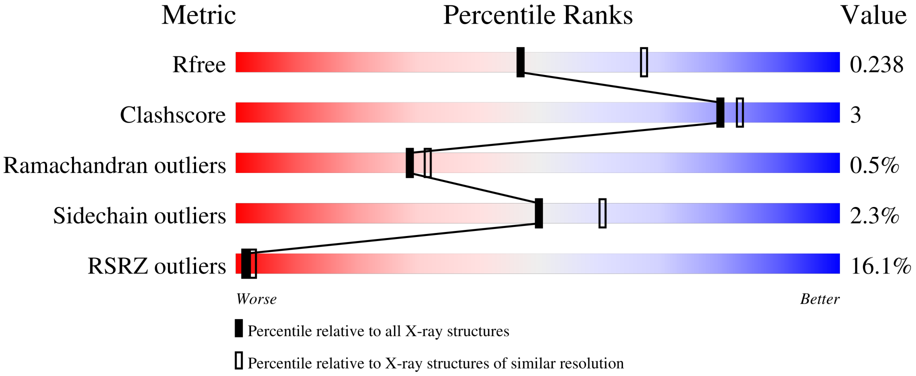
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

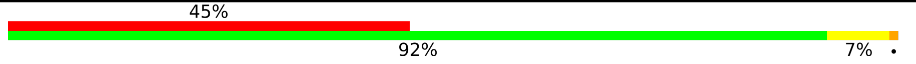
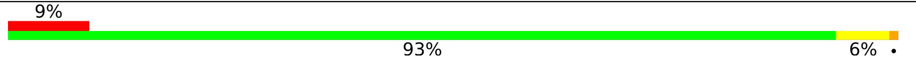
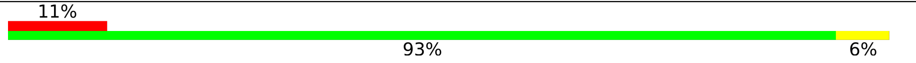
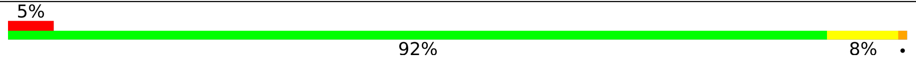
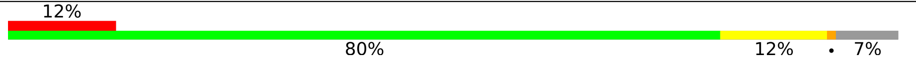
The reported resolution of this entry is 2.35 Å.

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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	653	
1	B	653	
1	C	653	
1	D	653	
2	E	179	

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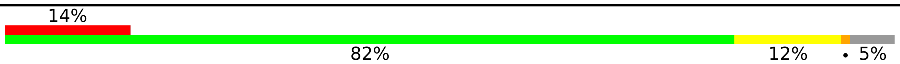
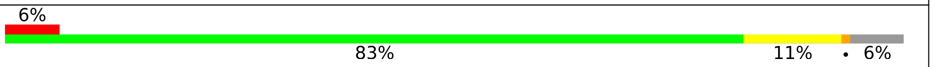
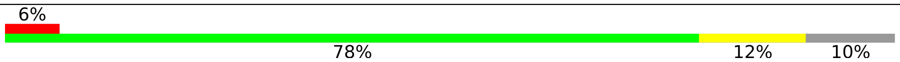
Mol	Chain	Length	Quality of chain
2	F	179	
2	G	179	
2	H	179	

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	UNL	A	701	-	-	X	-
3	UNL	D	701	-	-	X	-
4	SF4	F	1002	-	-	X	-
4	SF4	G	1002	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26313 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 Benzoyl-CoA reductase, putative.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	652	Total C N O S 5180 3308 875 963 34	0	0	0
1	B	652	Total C N O S 5180 3308 875 963 34	0	0	0
1	C	652	Total C N O S 5185 3311 875 965 34	0	0	0
1	D	652	Total C N O S 5180 3308 875 963 34	0	0	0

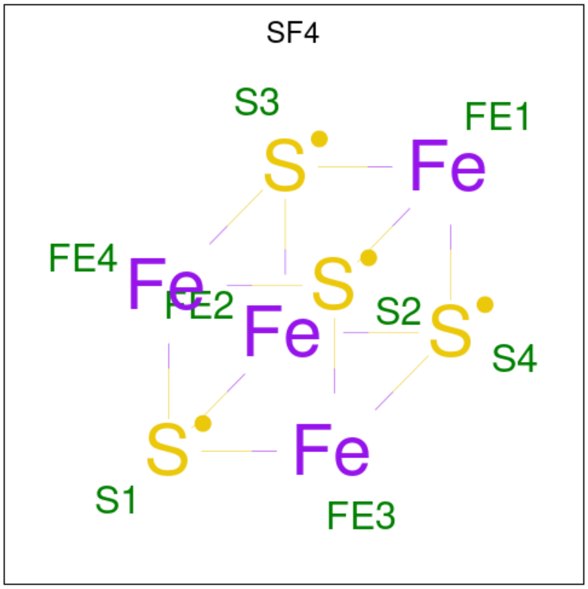
- Molecule 2 is a protein called Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein.

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

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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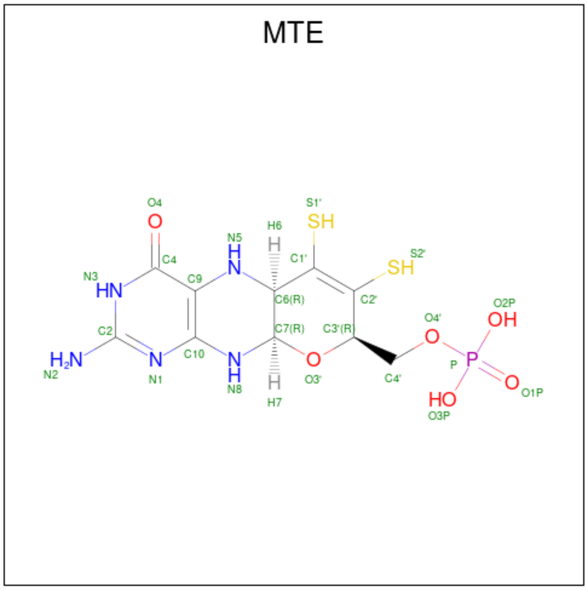
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total 8	Fe 4	S 4	0	0
4	H	1	Total 8	Fe 4	S 4	0	0
4	H	1	Total 8	Fe 4	S 4	0	0

- Molecule 5 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: $C_{10}H_{14}N_5O_6PS_2$).



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

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

- Molecule 6 is TUNGSTEN ION (three-letter code: W) (formula: W).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0
8	B	1	Total Zn 1 1	0	0
8	C	1	Total Zn 1 1	0	0
8	D	1	Total Zn 1 1	0	0

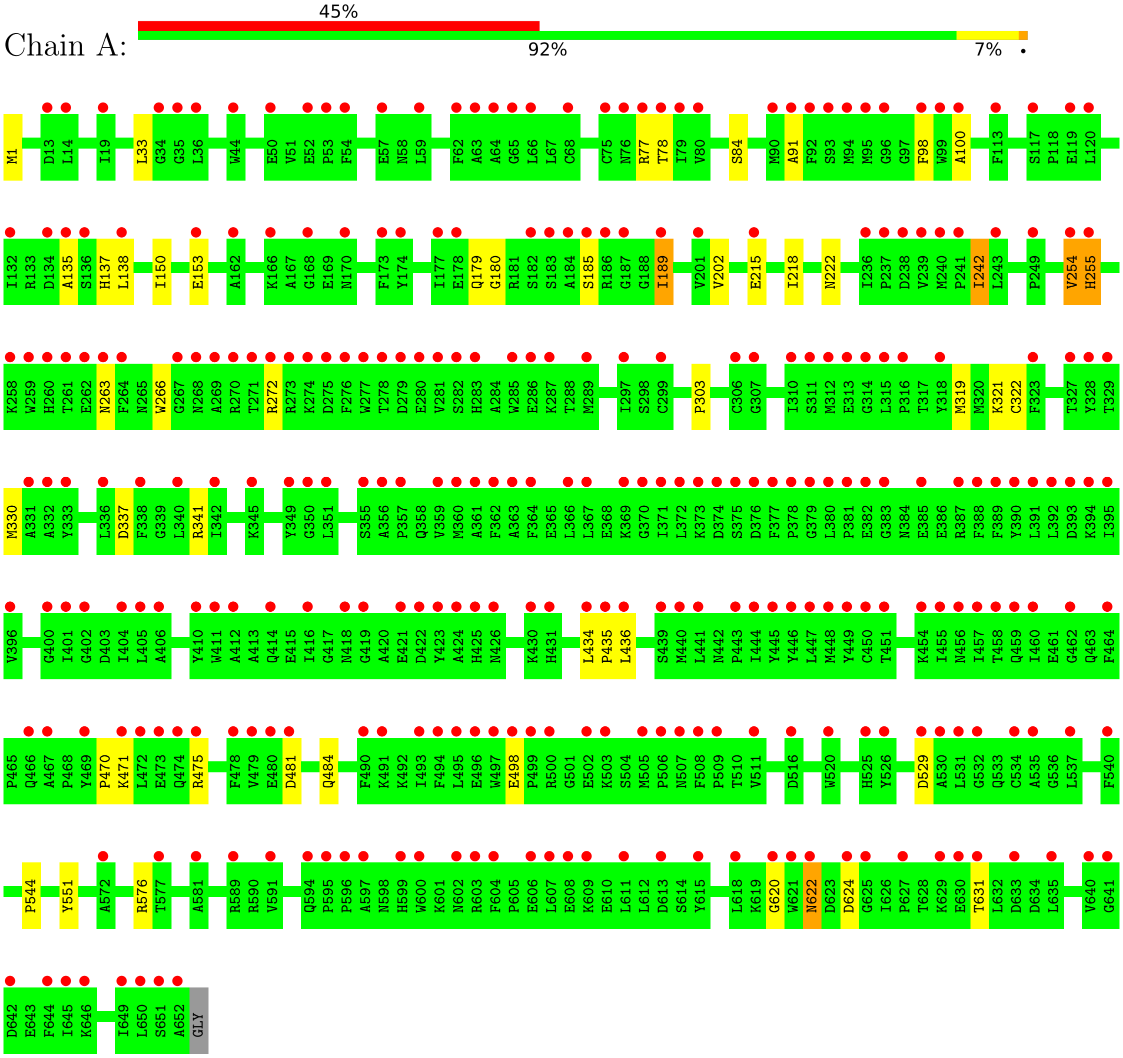
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	11	Total O 11 11	0	0
9	B	37	Total O 37 37	0	0
9	C	22	Total O 22 22	0	0
9	D	24	Total O 24 24	0	0
9	E	9	Total O 9 9	0	0
9	F	12	Total O 12 12	0	0
9	G	10	Total O 10 10	0	0
9	H	14	Total O 14 14	0	0

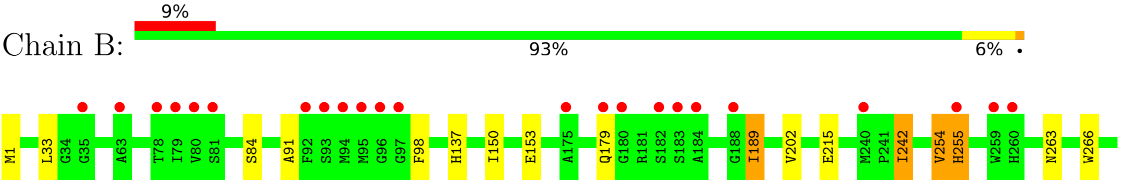
3 Residue-property plots ⓘ

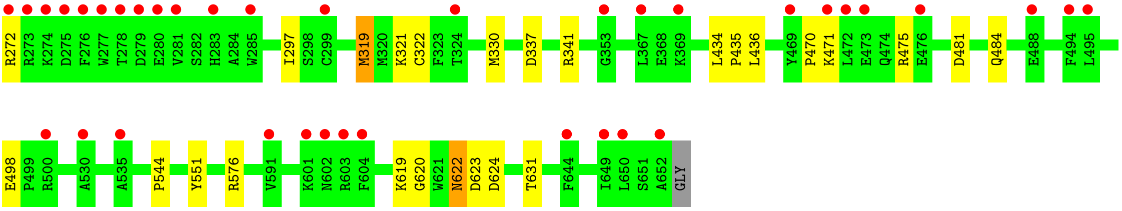
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Benzoyl-CoA reductase, putative



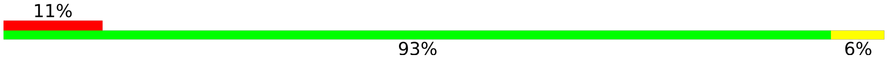
- Molecule 1: Benzoyl-CoA reductase, putative

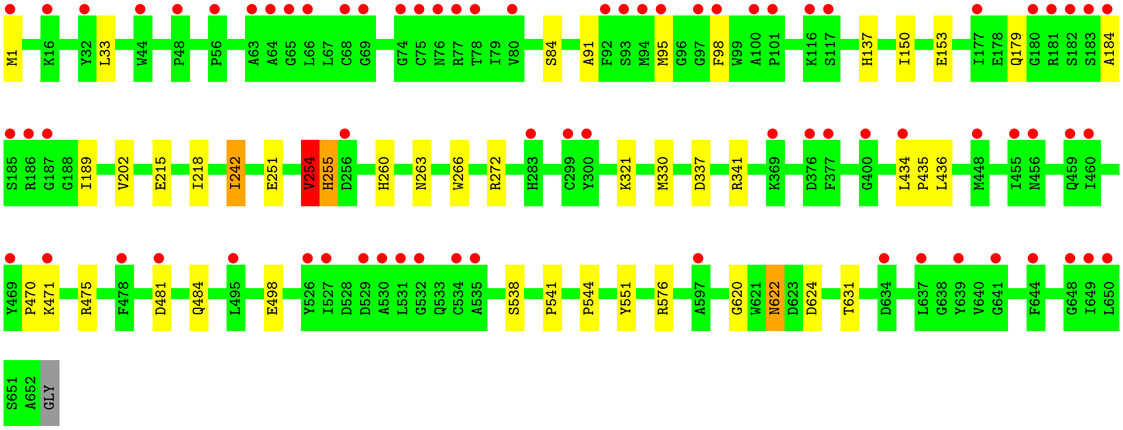




- Molecule 1: Benzoyl-CoA reductase, putative

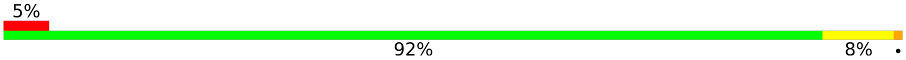
Chain C:

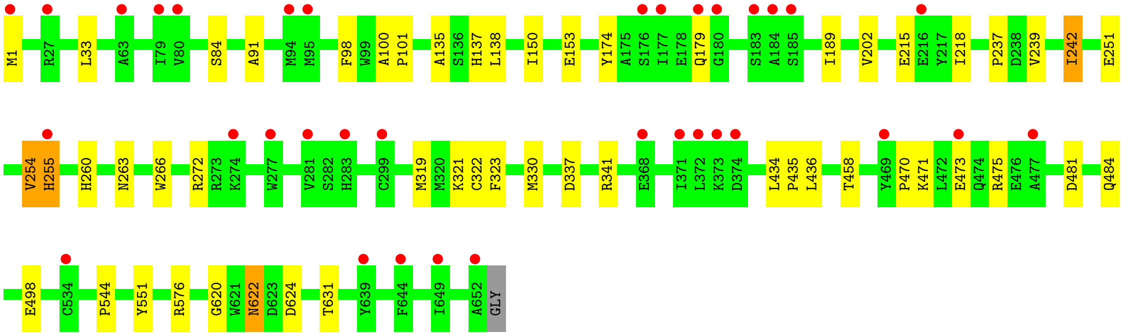




- Molecule 1: Benzoyl-CoA reductase, putative

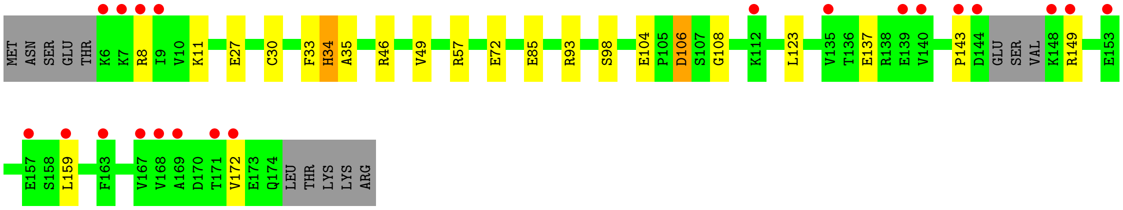
Chain D:



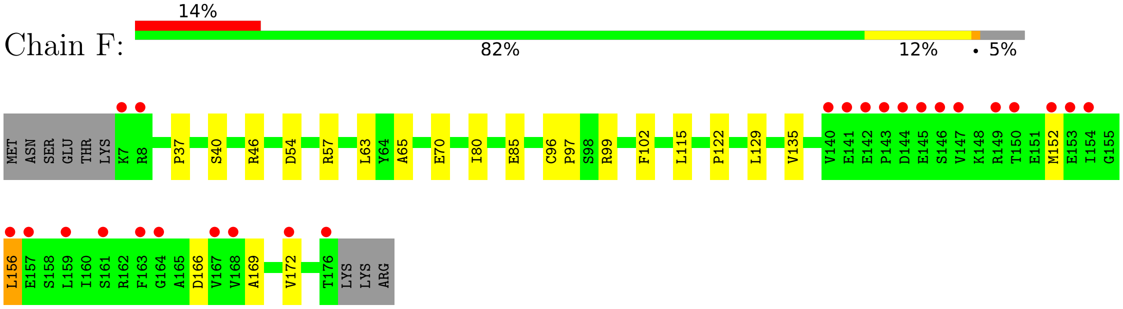


- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

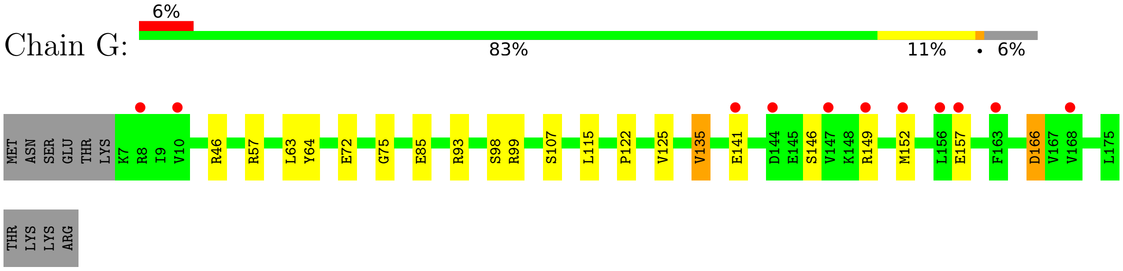
Chain E:



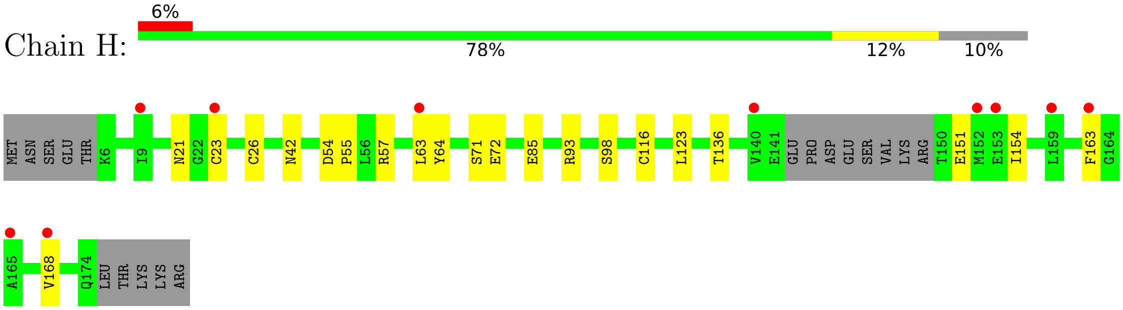
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein



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



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



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	125.19Å 116.82Å 143.60Å 90.00° 110.39° 90.00°	Depositor
Resolution (Å)	49.50 – 2.35 49.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.50-2.35) 98.5 (49.50-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.238 0.214 , 0.238	Depositor DCC
R_{free} test set	1594 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26313	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.26	0/5306	0.41	0/7172
1	B	0.30	0/5306	0.43	0/7172
1	C	0.30	0/5311	0.43	0/7179
1	D	0.32	0/5306	0.43	0/7172
2	E	0.37	0/1282	0.50	0/1734
2	F	0.37	0/1343	0.51	0/1819
2	G	0.36	0/1344	0.51	0/1819
2	H	0.34	0/1242	0.50	0/1681
All	All	0.31	0/26440	0.44	0/35748

There are no bond length outliers.

There are no bond angle outliers.

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	5180	0	5111	27	0
1	B	5180	0	5111	20	0
1	C	5185	0	5120	20	0
1	D	5180	0	5111	24	0
2	E	1260	0	1209	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1317	0	1266	13	0
2	G	1315	0	1263	16	0
2	H	1221	0	1158	12	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	2	0
4	A	8	0	0	1	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	0	0
4	E	24	0	0	1	0
4	F	24	0	0	2	0
4	G	24	0	0	2	0
4	H	24	0	0	0	0
5	A	48	0	22	3	0
5	B	48	0	23	0	0
5	C	48	0	20	0	0
5	D	48	0	20	2	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	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	11	0	0	2	0
9	B	37	0	0	0	0
9	C	22	0	0	0	0
9	D	24	0	0	0	0
9	E	9	0	0	0	0
9	F	12	0	0	0	0
9	G	10	0	0	1	0
9	H	14	0	0	0	0
All	All	26313	0	25434	139	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 3.

The worst 5 of 139 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)
3:A:701:UNL:X	5:A:703:MTE:S1'	2.61	0.88
2:G:166:ASP:OD1	2:G:166:ASP:N	2.24	0.71
2:G:72:GLU:HG2	2:G:98:SER:HB3	1.71	0.71
2:E:30:CYS:SG	2:E:34:HIS:ND1	2.65	0.68
2:E:34:HIS:NE2	4:E:1002:SF4:S1	2.67	0.67

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	650/653 (100%)	620 (95%)	26 (4%)	4 (1%)	25	27
1	B	650/653 (100%)	621 (96%)	25 (4%)	4 (1%)	25	27
1	C	650/653 (100%)	619 (95%)	27 (4%)	4 (1%)	25	27
1	D	650/653 (100%)	618 (95%)	28 (4%)	4 (1%)	25	27
2	E	162/179 (90%)	157 (97%)	4 (2%)	1 (1%)	25	27
2	F	169/179 (94%)	162 (96%)	7 (4%)	0	100	100
2	G	169/179 (94%)	163 (96%)	6 (4%)	0	100	100
2	H	157/179 (88%)	151 (96%)	6 (4%)	0	100	100
All	All	3257/3328 (98%)	3111 (96%)	129 (4%)	17 (0%)	29	32

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	VAL
1	B	254	VAL
1	C	254	VAL

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Mol	Chain	Res	Type
1	D	254	VAL
1	A	255	HIS

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	546/548 (100%)	535 (98%)	11 (2%)	55	66
1	B	546/548 (100%)	535 (98%)	11 (2%)	55	66
1	C	548/548 (100%)	537 (98%)	11 (2%)	55	66
1	D	546/548 (100%)	534 (98%)	12 (2%)	52	63
2	E	136/159 (86%)	132 (97%)	4 (3%)	42	52
2	F	148/159 (93%)	142 (96%)	6 (4%)	30	37
2	G	147/159 (92%)	143 (97%)	4 (3%)	44	55
2	H	132/159 (83%)	128 (97%)	4 (3%)	41	50
All	All	2749/2828 (97%)	2686 (98%)	63 (2%)	50	61

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	436	LEU
2	G	63	LEU
1	D	189	ILE
2	F	156	LEU
2	H	26	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	463	GLN
1	C	622	ASN
1	D	622	ASN

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Mol	Chain	Res	Type
1	D	179	GLN
1	B	179	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 4 are unknown and 12 are monoatomic - leaving 24 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	SF4	G	1003	2	0,12,12	-	-	-		
5	MTE	C	704	6,7	21,26,26	2.87	10 (47%)	21,40,40	2.54	5 (23%)
4	SF4	F	1001	2	0,12,12	-	-	-		
4	SF4	E	1003	2	0,12,12	-	-	-		
4	SF4	H	1002	2	0,12,12	-	-	-		
4	SF4	H	1003	2	0,12,12	-	-	-		
4	SF4	H	1001	2	0,12,12	-	-	-		
5	MTE	A	703	6,5,7	21,26,26	2.86	11 (52%)	21,40,40	2.17	6 (28%)
4	SF4	A	702	1	0,12,12	-	-	-		
5	MTE	B	703	6,7	21,26,26	2.84	9 (42%)	21,40,40	2.11	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	SF4	E	1002	2	0,12,12	-	-	-		
5	MTE	B	704	6,7	21,26,26	2.80	9 (42%)	21,40,40	2.72	6 (28%)
4	SF4	D	702	1	0,12,12	-	-	-		
4	SF4	F	1003	2	0,12,12	-	-	-		
4	SF4	E	1001	2	0,12,12	-	-	-		
5	MTE	D	703	6,7	21,26,26	2.63	10 (47%)	21,40,40	2.01	6 (28%)
5	MTE	C	703	6,7	21,26,26	2.65	10 (47%)	21,40,40	2.09	5 (23%)
5	MTE	A	704	6,5,7	21,26,26	2.70	9 (42%)	21,40,40	3.05	6 (28%)
4	SF4	B	702	1	0,12,12	-	-	-		
4	SF4	G	1001	2	0,12,12	-	-	-		
5	MTE	D	704	6,7	21,26,26	2.71	9 (42%)	21,40,40	2.28	6 (28%)
4	SF4	C	702	1	0,12,12	-	-	-		
4	SF4	G	1002	2	0,12,12	-	-	-		
4	SF4	F	1002	2	0,12,12	-	-	-		

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	SF4	G	1003	2	-	-	0/6/5/5
5	MTE	C	704	6,7	-	5/6/34/34	0/3/3/3
4	SF4	F	1001	2	-	-	0/6/5/5
4	SF4	E	1003	2	-	-	0/6/5/5
4	SF4	H	1002	2	-	-	0/6/5/5
4	SF4	H	1003	2	-	-	0/6/5/5
5	MTE	A	703	6,5,7	-	0/6/34/34	0/3/3/3
4	SF4	H	1001	2	-	-	0/6/5/5
4	SF4	A	702	1	-	-	0/6/5/5
5	MTE	B	703	6,7	-	0/6/34/34	0/3/3/3
4	SF4	E	1002	2	-	-	0/6/5/5
5	MTE	B	704	6,7	-	5/6/34/34	0/3/3/3
4	SF4	D	702	1	-	-	0/6/5/5
4	SF4	F	1003	2	-	-	0/6/5/5
4	SF4	E	1001	2	-	-	0/6/5/5
5	MTE	D	703	6,7	-	0/6/34/34	0/3/3/3
5	MTE	C	703	6,7	-	0/6/34/34	0/3/3/3
5	MTE	A	704	6,5,7	-	2/6/34/34	0/3/3/3
4	SF4	B	702	1	-	-	0/6/5/5
4	SF4	G	1001	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MTE	D	704	6,7	-	0/6/34/34	0/3/3/3
4	SF4	C	702	1	-	-	0/6/5/5
4	SF4	G	1002	2	-	-	0/6/5/5
4	SF4	F	1002	2	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	MTE	C9-C10	-6.82	1.28	1.41
5	B	703	MTE	C9-C10	-6.36	1.29	1.41
5	C	704	MTE	C9-C10	-6.17	1.29	1.41
5	B	704	MTE	C9-C10	-6.14	1.29	1.41
5	A	703	MTE	C9-C10	-6.03	1.30	1.41

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704	MTE	O3'-C7-C6	8.47	114.61	108.96
5	B	704	MTE	C10-C9-C4	7.28	121.03	114.57
5	D	704	MTE	C10-C9-C4	6.96	120.75	114.57
5	A	704	MTE	C10-C9-C4	6.88	120.68	114.57
5	C	704	MTE	O3'-C7-N8	-6.78	101.60	108.57

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	704	MTE	C2'-C3'-C4'-O4'
5	A	704	MTE	O3'-C3'-C4'-O4'
5	B	704	MTE	C4'-O4'-P-O1P
5	B	704	MTE	C4'-O4'-P-O2P
5	B	704	MTE	C4'-O4'-P-O3P

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	MTE	2	0
4	A	702	SF4	1	0
4	E	1002	SF4	1	0
5	D	703	MTE	1	0

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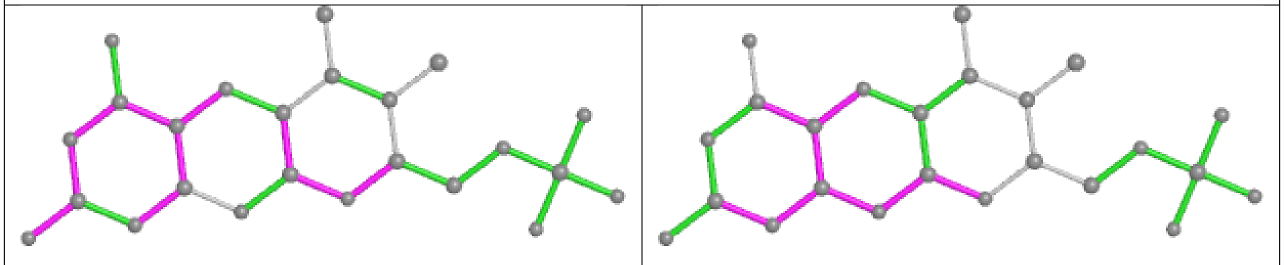
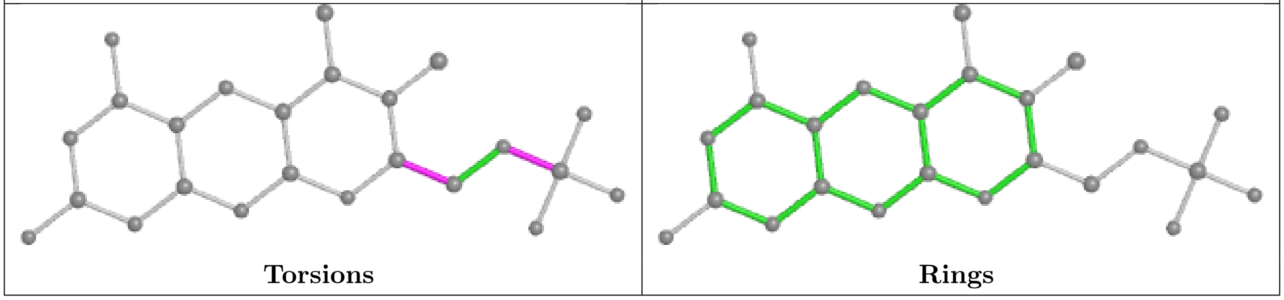
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	MTE	1	0
5	D	704	MTE	1	0
4	G	1002	SF4	2	0
4	F	1002	SF4	2	0

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

Ligand MTE C 704

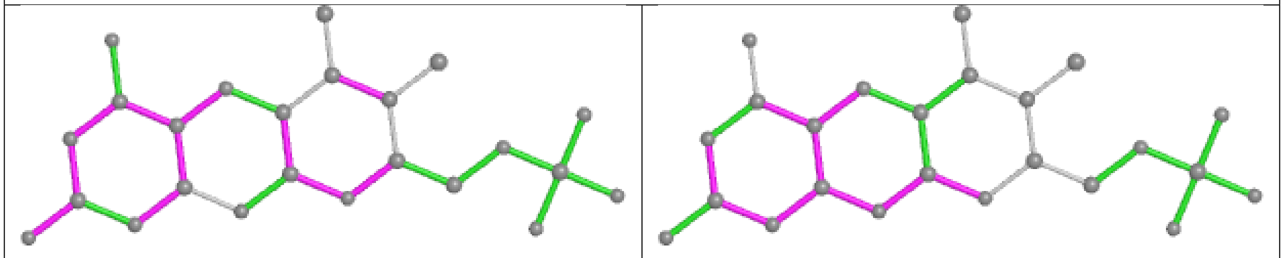


Bond lengths **Bond angles**

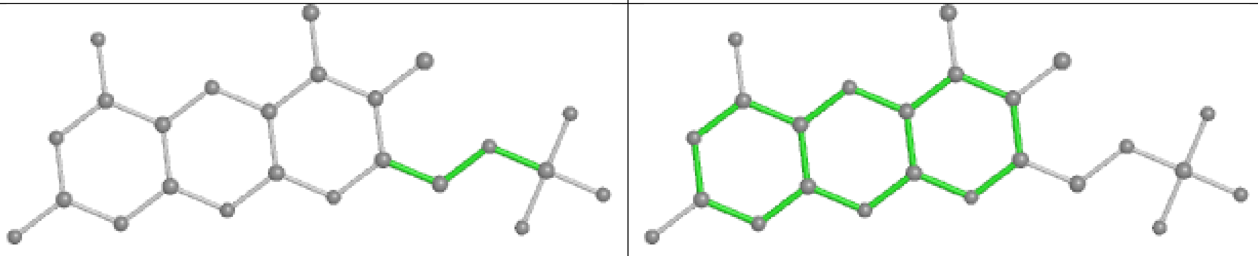


Torsions **Rings**

Ligand MTE A 703

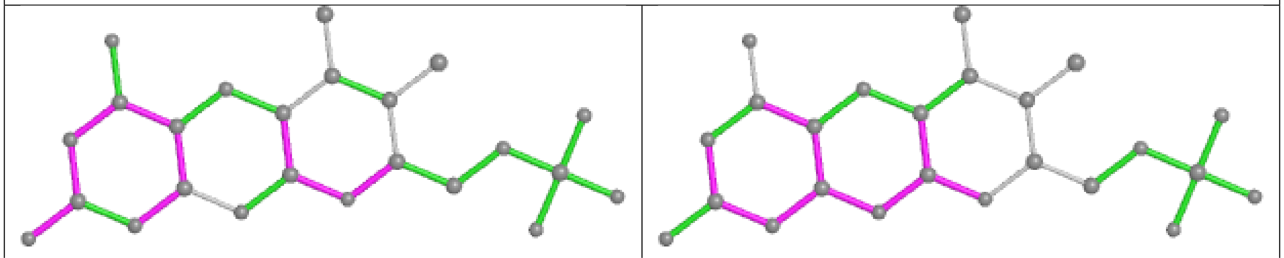


Bond lengths Bond angles

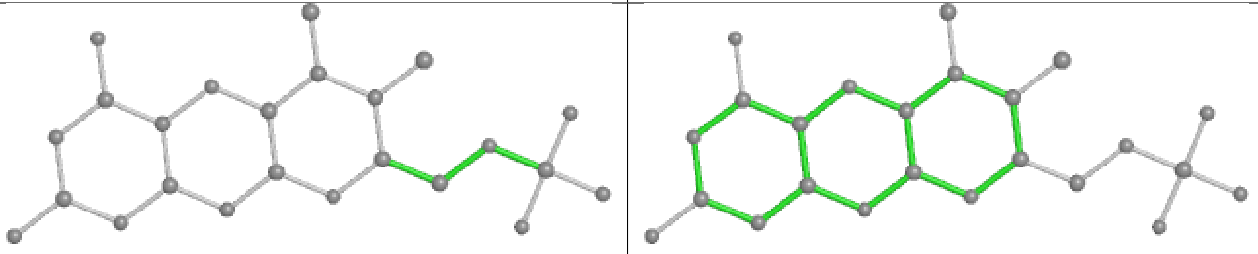


Torsions Rings

Ligand MTE B 703

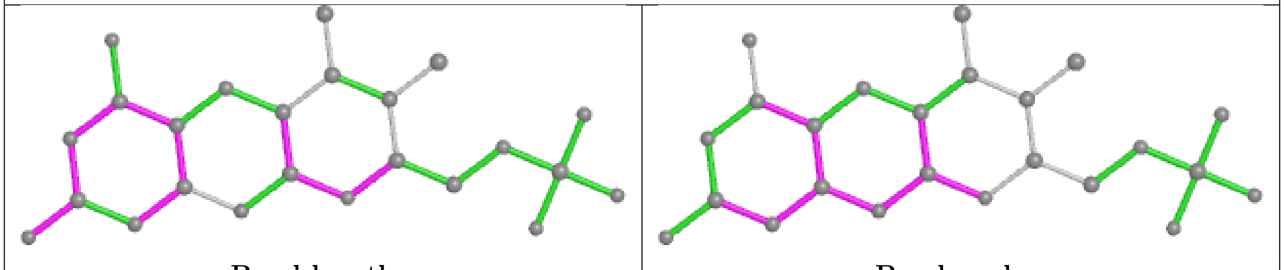


Bond lengths Bond angles



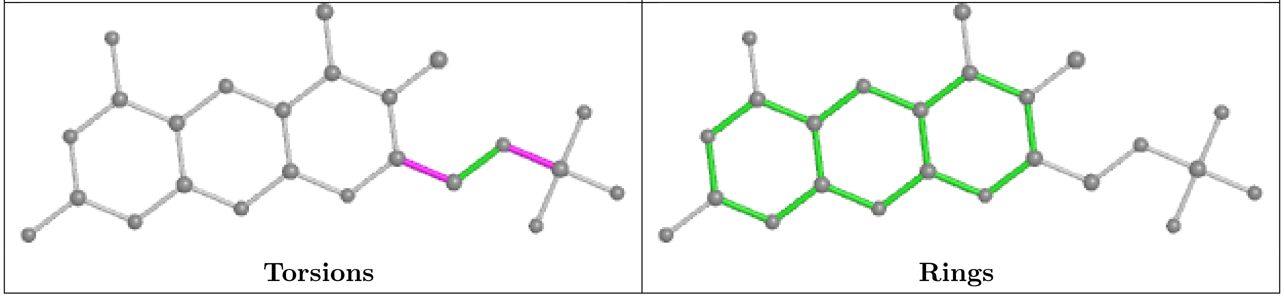
Torsions Rings

Ligand MTE B 704



Bond lengths

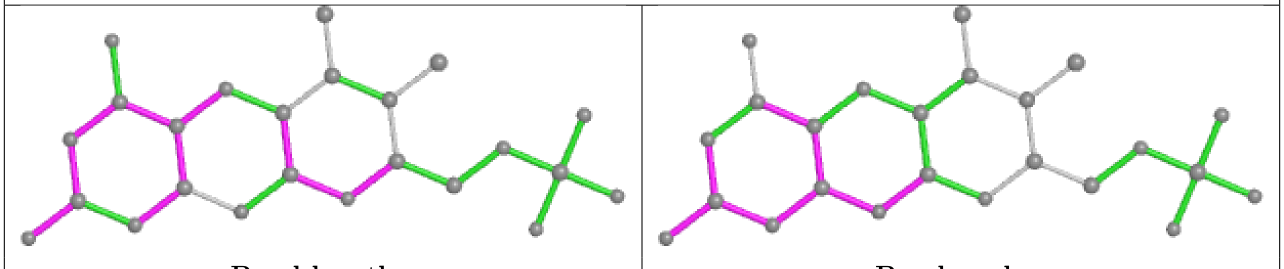
Bond angles



Torsions

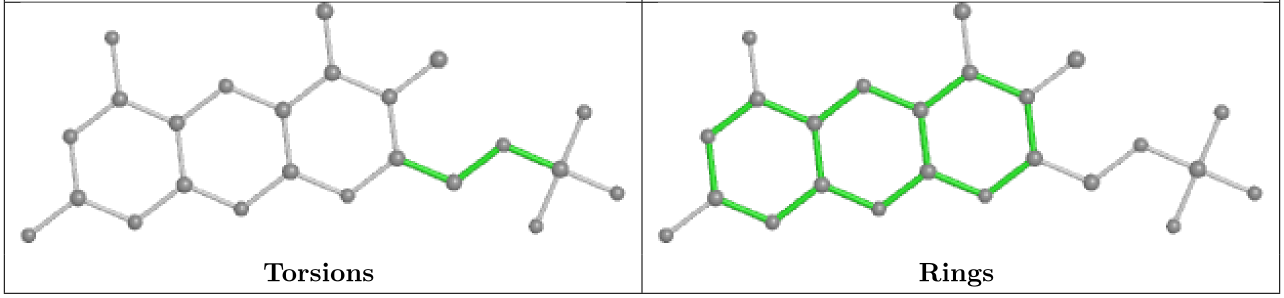
Rings

Ligand MTE D 703



Bond lengths

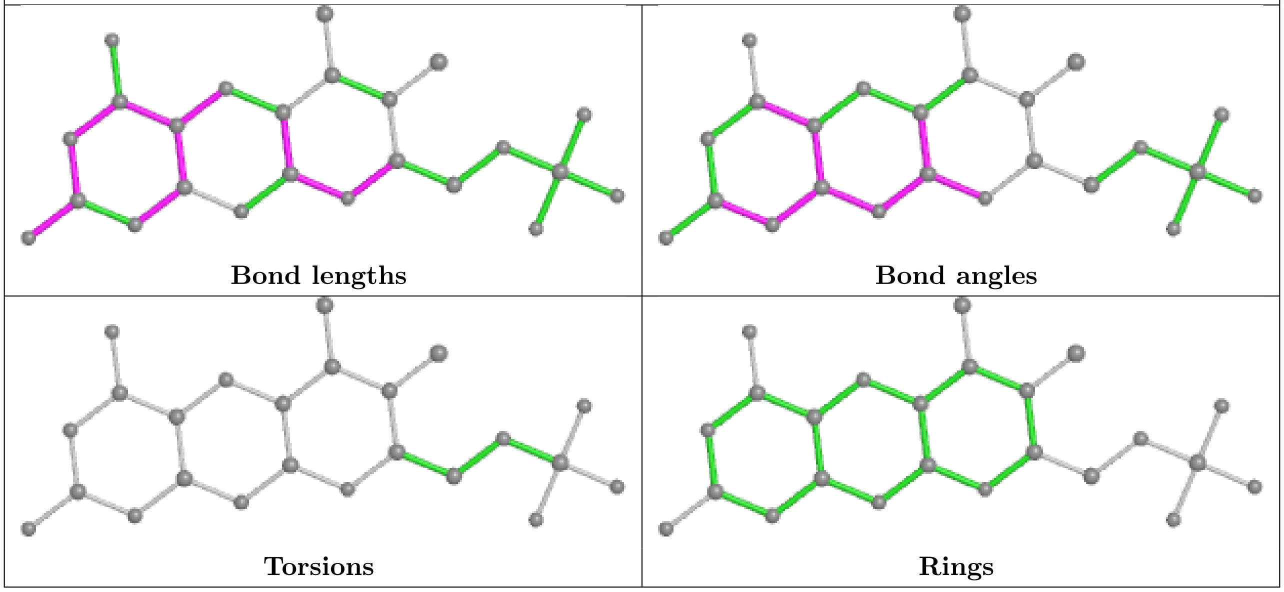
Bond angles



Torsions

Rings

Ligand MTE C 703



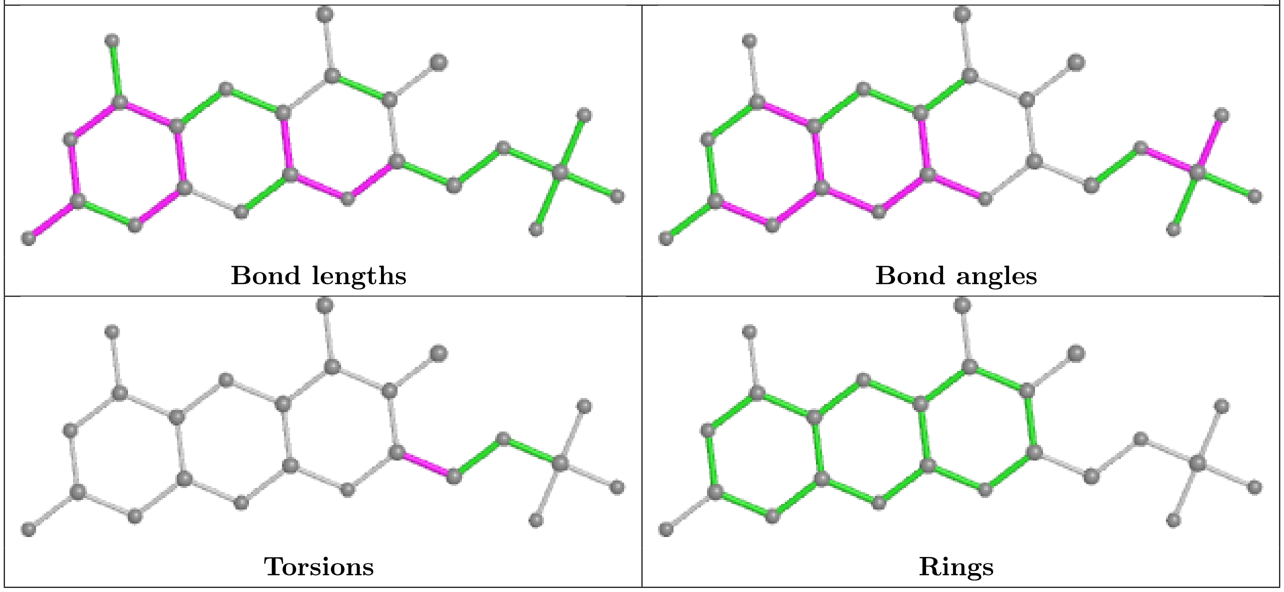
Bond lengths

Bond angles

Torsions

Rings

Ligand MTE A 704



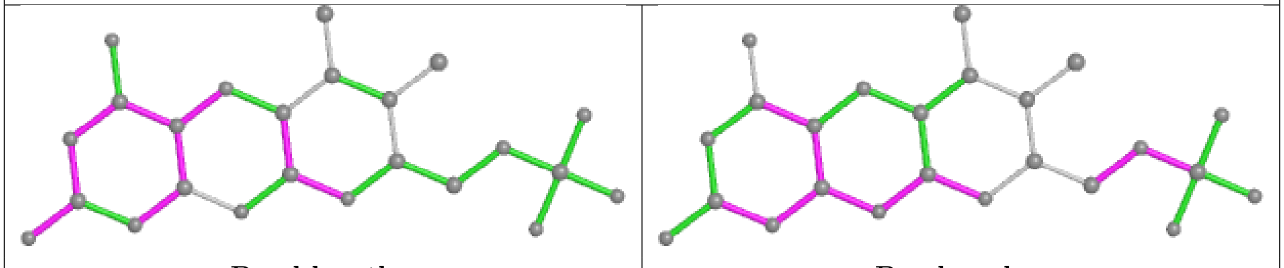
Bond lengths

Bond angles

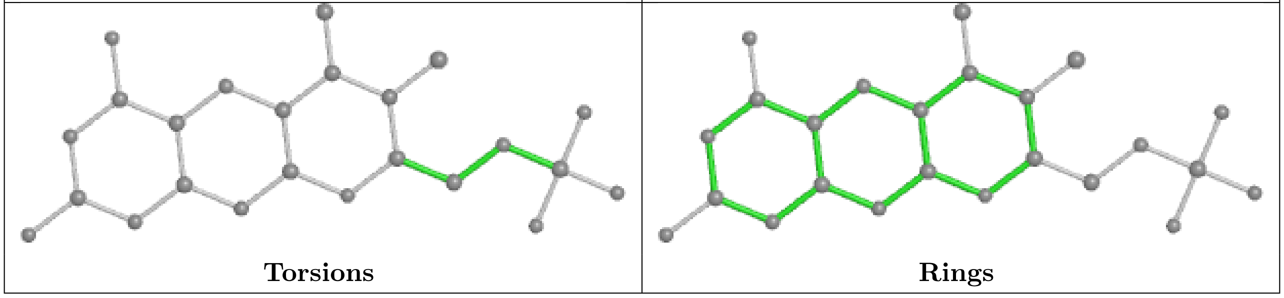
Torsions

Rings

Ligand MTE D 704



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (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	652/653 (99%)	2.25	294 (45%)	0	0	65, 151, 230, 286	0
1	B	652/653 (99%)	0.62	60 (9%)	9	14	53, 82, 134, 173	0
1	C	652/653 (99%)	0.75	73 (11%)	5	8	54, 89, 124, 145	0
1	D	652/653 (99%)	0.48	34 (5%)	27	39	54, 82, 118, 144	0
2	E	166/179 (92%)	0.69	21 (12%)	3	6	62, 85, 124, 219	0
2	F	170/179 (94%)	0.58	25 (14%)	2	3	55, 78, 121, 147	0
2	G	169/179 (94%)	0.39	11 (6%)	18	27	54, 72, 153, 188	0
2	H	161/179 (89%)	0.57	10 (6%)	20	29	57, 79, 140, 151	0
All	All	3274/3328 (98%)	0.93	528 (16%)	1	3	53, 89, 184, 286	0

The worst 5 of 528 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	TYR	13.4
1	A	366	LEU	11.7
1	A	255	HIS	11.1
1	A	405	LEU	10.8
1	A	364	PHE	10.2

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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	A	706	1/1	0.54	0.16	86,86,86,86	0
5	MTE	A	703	24/24	0.86	0.24	89,101,106,269	0
7	MG	D	706	1/1	0.86	0.31	47,47,47,47	0
8	ZN	A	707	1/1	0.86	0.07	65,65,65,65	1
6	W	A	705	1/1	0.88	0.18	131,131,131,131	0
3	UNL	C	701	1/-	0.90	0.51	67,67,67,67	0
5	MTE	A	704	24/24	0.91	0.26	81,101,118,296	0
5	MTE	C	704	24/24	0.93	0.24	45,61,112,116	0
7	MG	C	706	1/1	0.93	0.34	49,49,49,49	0
8	ZN	C	707	1/1	0.93	0.06	58,58,58,58	1
8	ZN	B	707	1/1	0.94	0.10	57,57,57,57	1
5	MTE	B	704	24/24	0.95	0.25	56,63,67,69	0
8	ZN	D	707	1/1	0.95	0.07	60,60,60,60	1
5	MTE	D	704	24/24	0.96	0.18	44,53,63,97	0
5	MTE	C	703	24/24	0.96	0.27	45,58,60,67	0
5	MTE	B	703	24/24	0.96	0.23	41,54,59,65	0
7	MG	B	706	1/1	0.96	0.41	59,59,59,59	0
5	MTE	D	703	24/24	0.96	0.22	34,54,66,66	0
4	SF4	A	702	8/8	0.97	0.15	85,98,123,150	0
3	UNL	A	701	1/-	0.97	0.43	56,56,56,56	0
4	SF4	C	702	8/8	0.98	0.12	52,59,65,72	0
4	SF4	D	702	8/8	0.98	0.12	53,57,66,71	0
4	SF4	E	1001	8/8	0.98	0.13	56,60,65,66	0
4	SF4	E	1002	8/8	0.98	0.12	61,65,70,80	0
4	SF4	F	1002	8/8	0.98	0.12	46,49,51,51	0
4	SF4	G	1003	8/8	0.98	0.10	56,62,64,73	0
4	SF4	H	1002	8/8	0.98	0.13	64,66,76,82	0
4	SF4	B	702	8/8	0.98	0.13	43,54,60,68	0
4	SF4	H	1003	8/8	0.99	0.11	59,61,66,67	0
6	W	B	705	1/1	0.99	0.21	77,77,77,77	0
6	W	C	705	1/1	0.99	0.17	68,68,68,68	0
6	W	D	705	1/1	0.99	0.17	71,71,71,71	0
4	SF4	F	1001	8/8	0.99	0.12	49,53,54,60	0
3	UNL	B	701	1/-	0.99	0.52	62,62,62,62	0
4	SF4	F	1003	8/8	0.99	0.09	50,59,62,70	0
4	SF4	G	1001	8/8	0.99	0.12	50,53,55,65	0
4	SF4	G	1002	8/8	0.99	0.09	53,57,59,59	0

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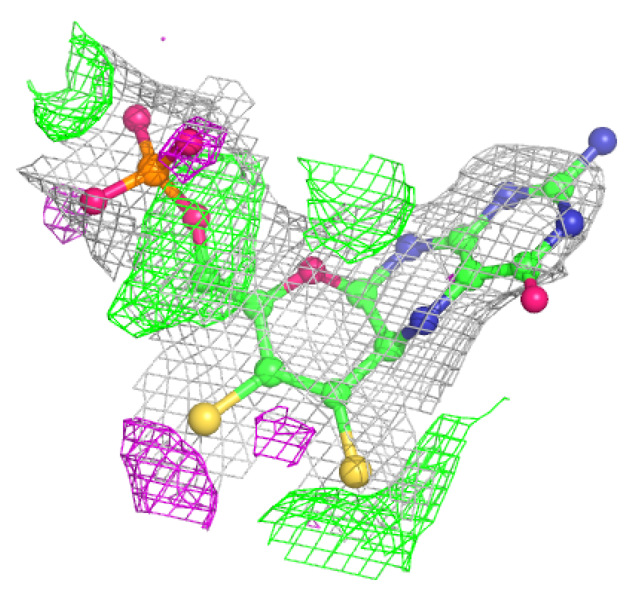
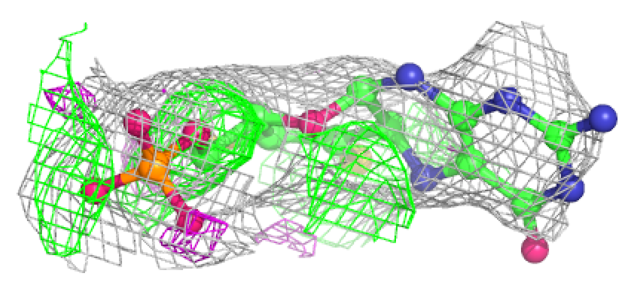
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UNL	D	701	1/-	0.99	0.33	94,94,94,94	0
4	SF4	H	1001	8/8	0.99	0.15	53,57,63,67	0
4	SF4	E	1003	8/8	0.99	0.09	54,57,62,63	0

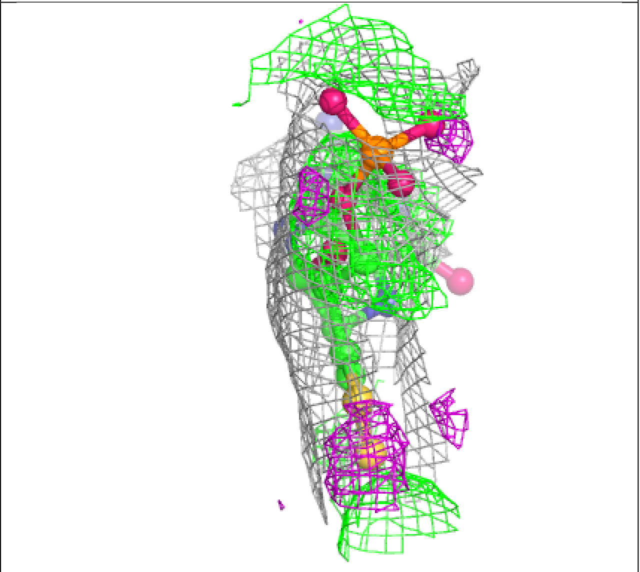
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

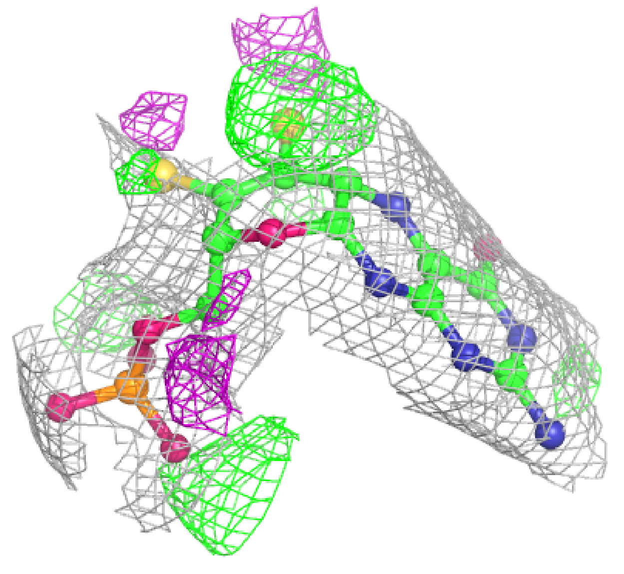


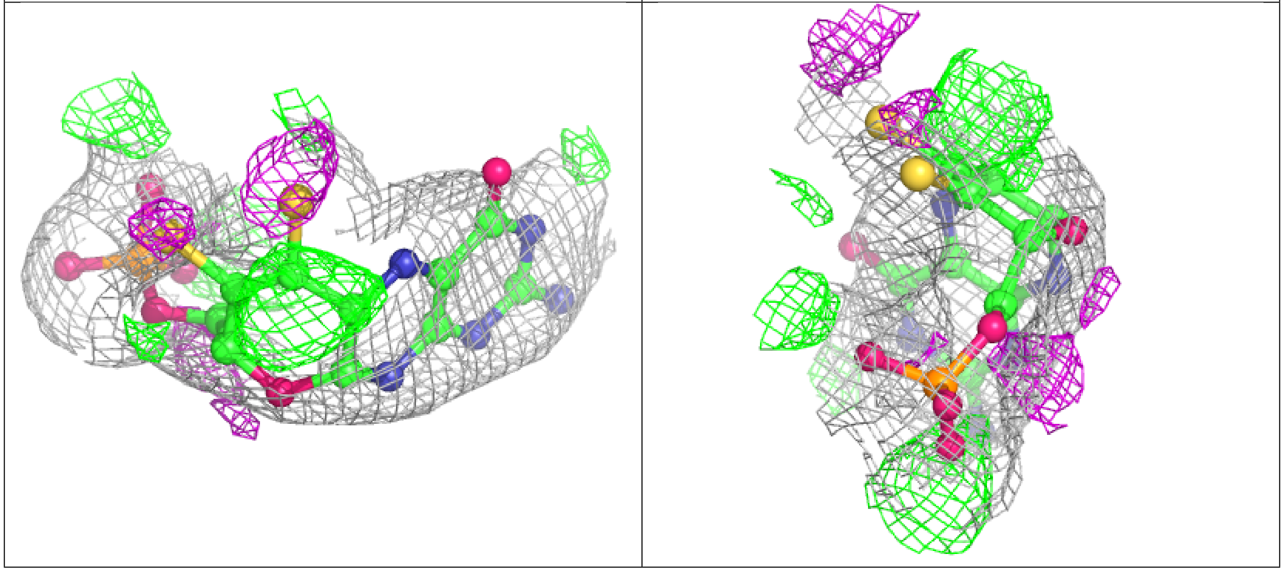




Electron density around MTE A 704:

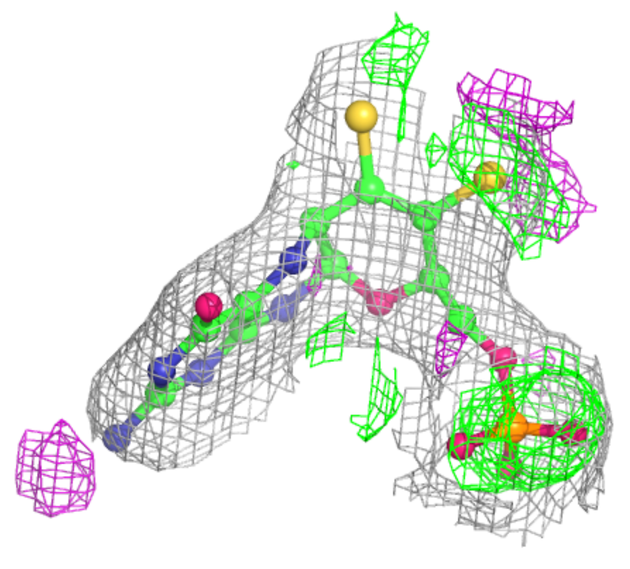
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

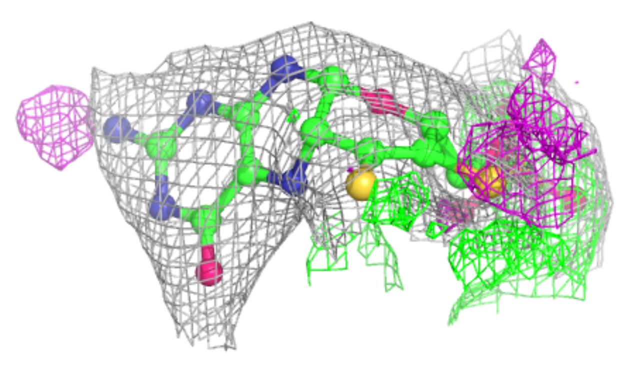


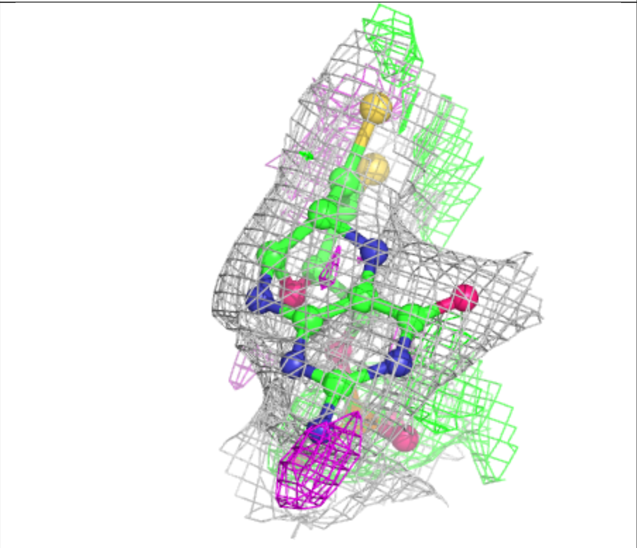


Electron density around MTE C 704:

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

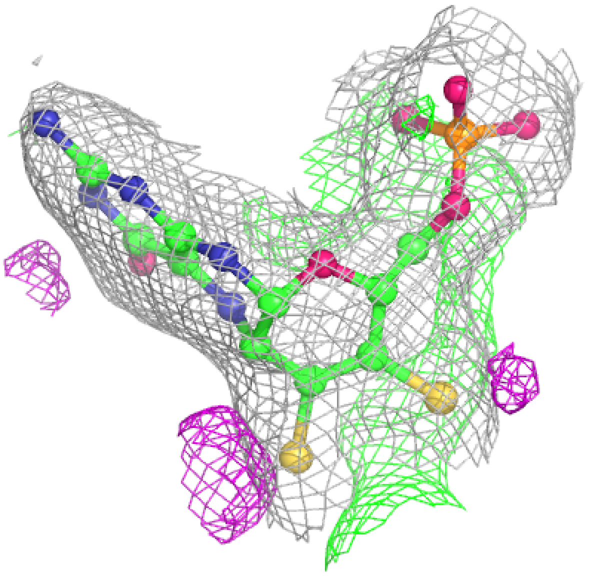


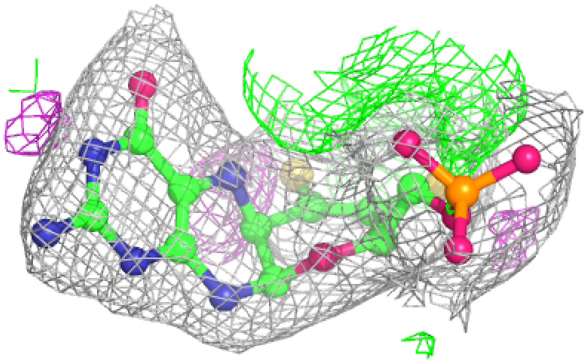


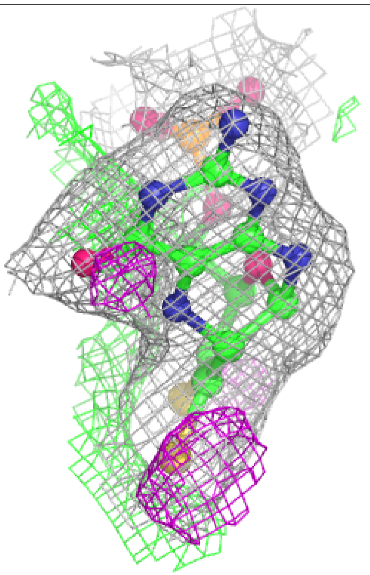


Electron density around MTE B 704:

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

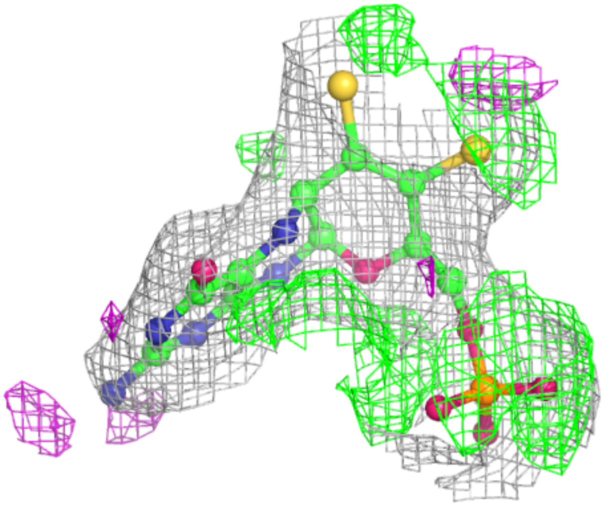


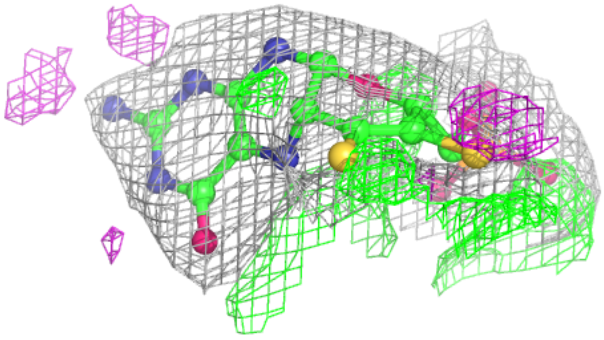


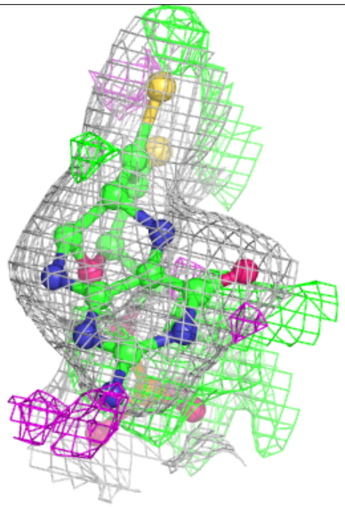


Electron density around MTE D 704:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

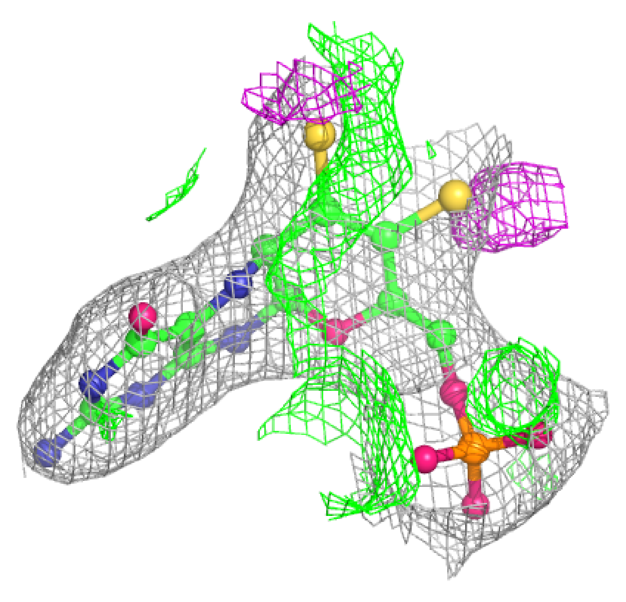


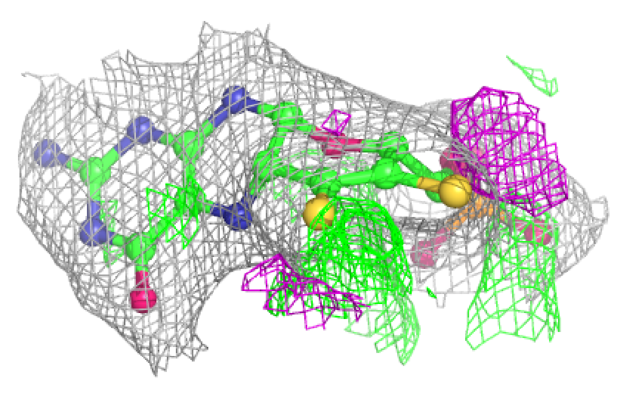


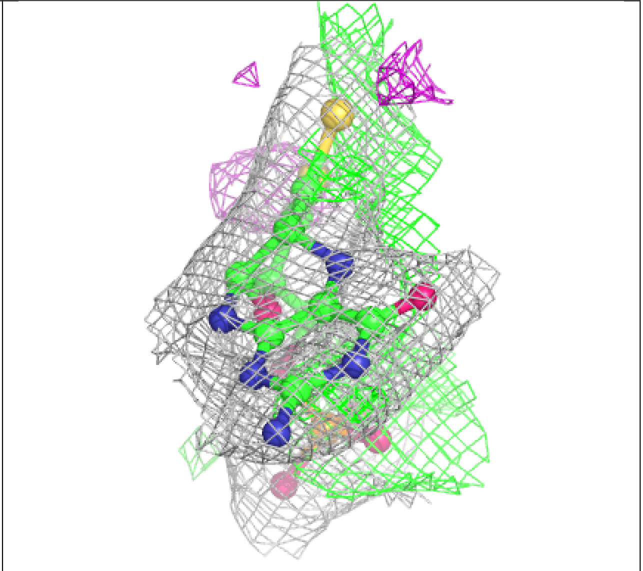


Electron density around MTE C 703:

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

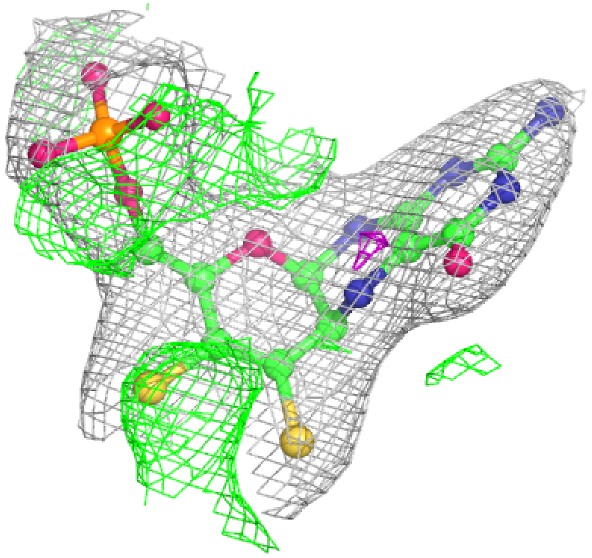


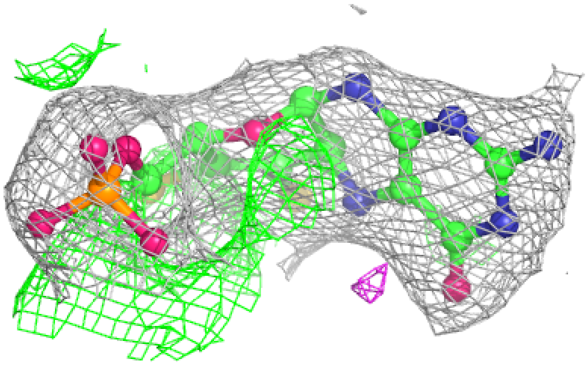


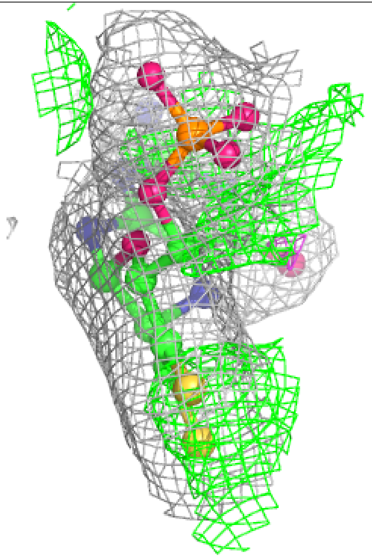


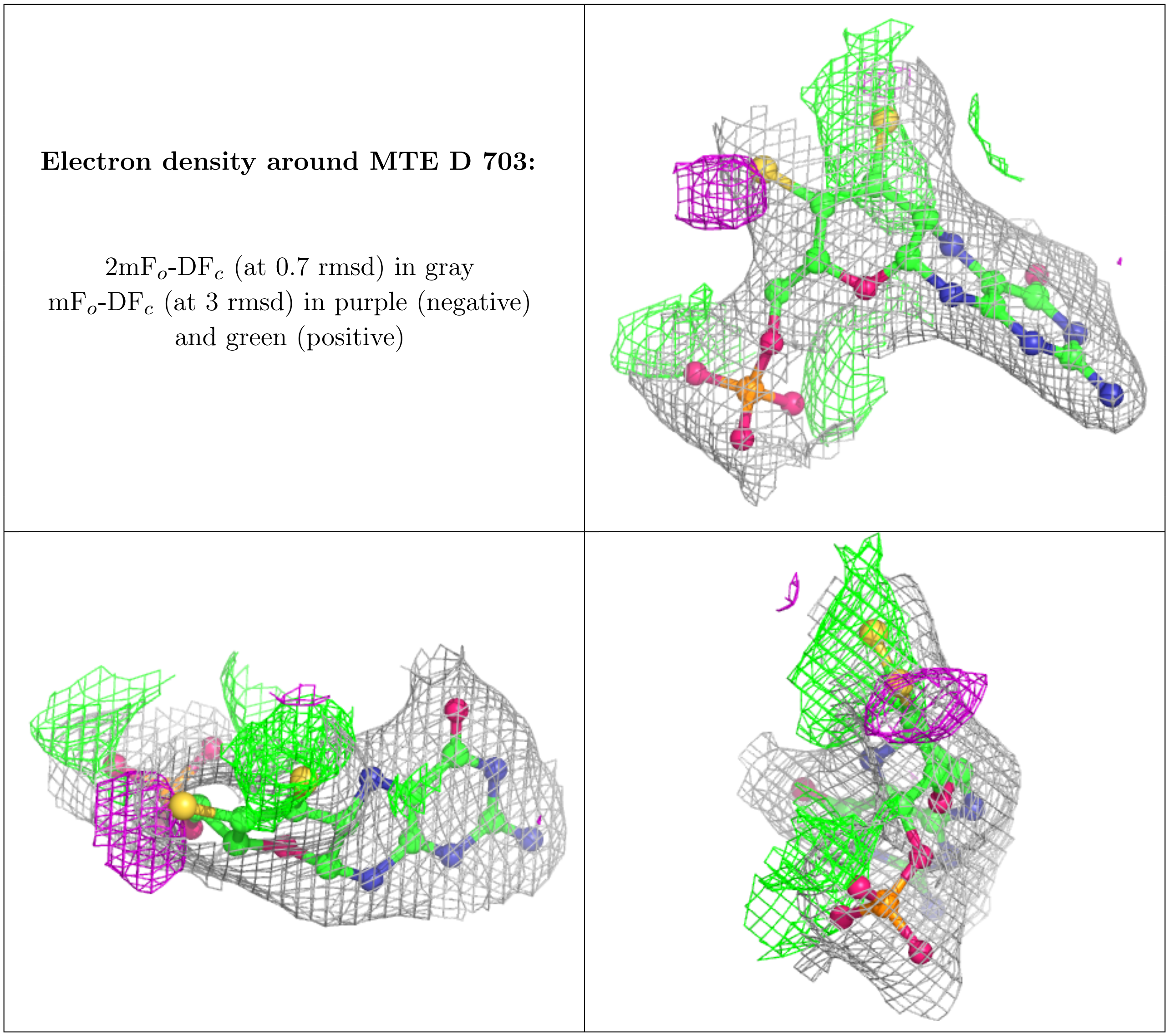
Electron density around MTE B 703:

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 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 ⓘ

There are no such residues in this entry.