



# Full wwPDB X-ray Structure Validation 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)

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](mailto: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>.

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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

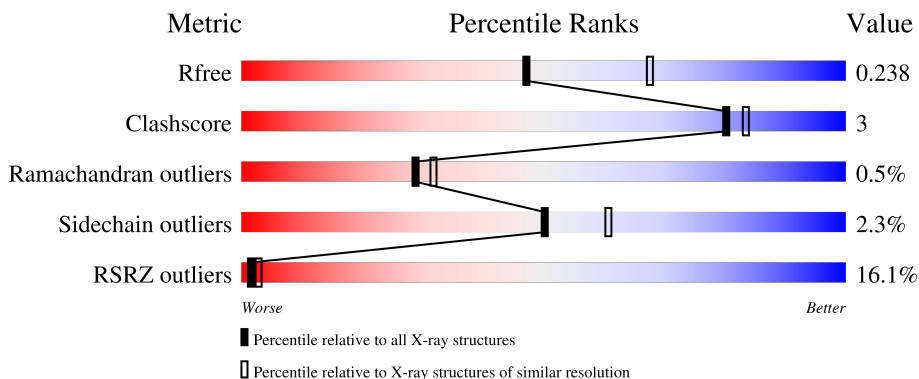
# 1 Overall quality at a glance

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  $\geq 3$ , 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	
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 [i](#)

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
			Total	C	N	O	S			
1	A	652	5180	3308	875	963	34	0	0	0
1	B	652	5180	3308	875	963	34	0	0	0
1	C	652	5185	3311	875	965	34	0	0	0
1	D	652	5180	3308	875	963	34	0	0	0

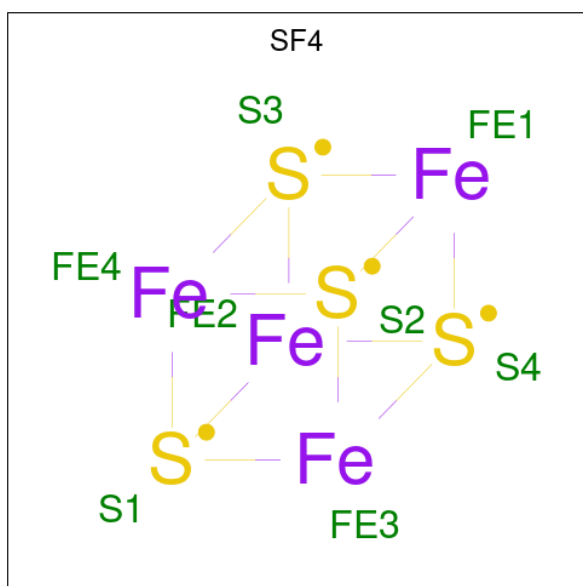
- Molecule 2 is a protein called Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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 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<sub>4</sub>S<sub>4</sub>).



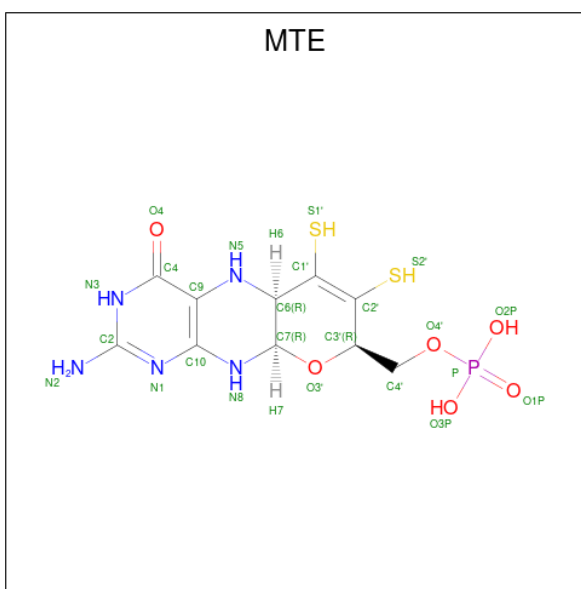
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4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

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

- 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<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>PS<sub>2</sub>).



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

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

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

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

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

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

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

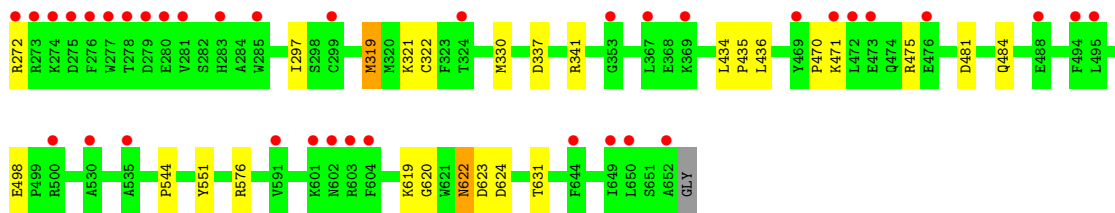
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		
8	B	1	Total	Zn	0	0
			1	1		
8	C	1	Total	Zn	0	0
			1	1		
8	D	1	Total	Zn	0	0
			1	1		

- Molecule 9 is water.

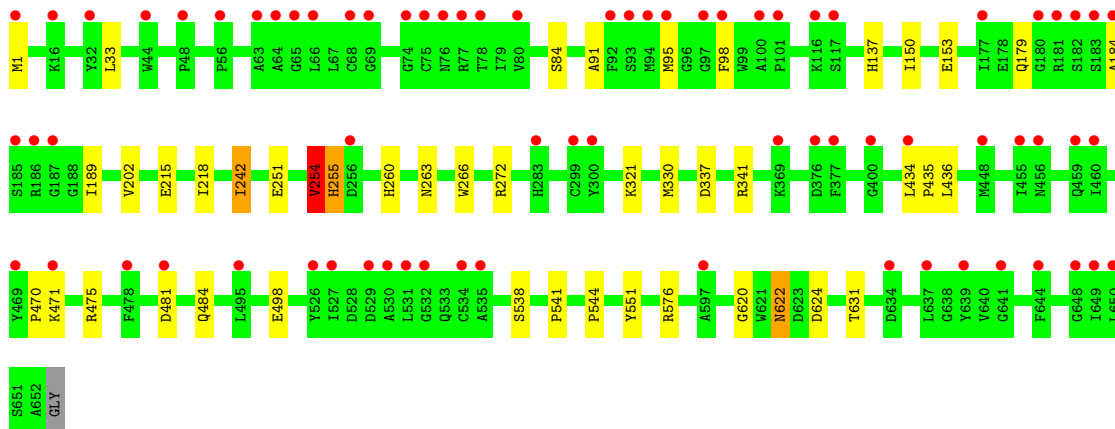
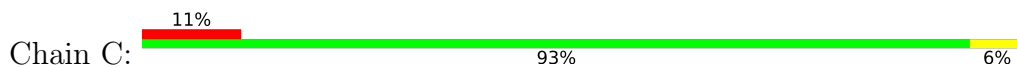
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	11	Total O 11 11	0	0
9	B	37	Total O 37 37	0	0
9	C	22	Total O 22 22	0	0
9	D	24	Total O 24 24	0	0
9	E	9	Total O 9 9	0	0
9	F	12	Total O 12 12	0	0
9	G	10	Total O 10 10	0	0
9	H	14	Total O 14 14	0	0



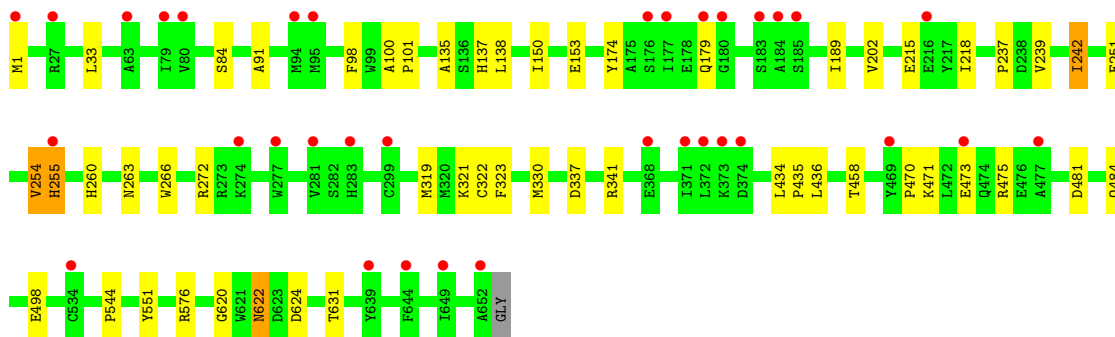
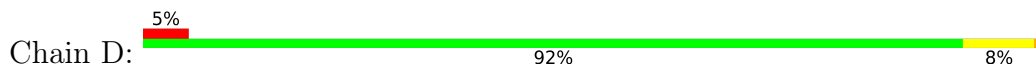




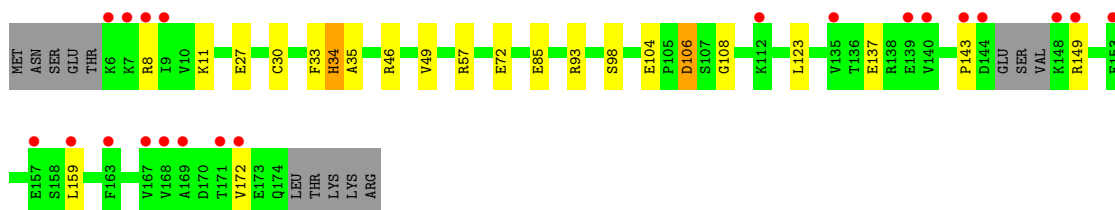
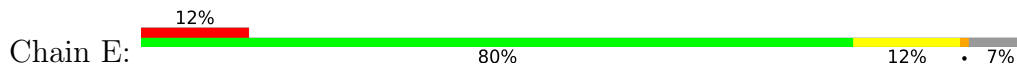
- Molecule 1: Benzoyl-CoA reductase, putative



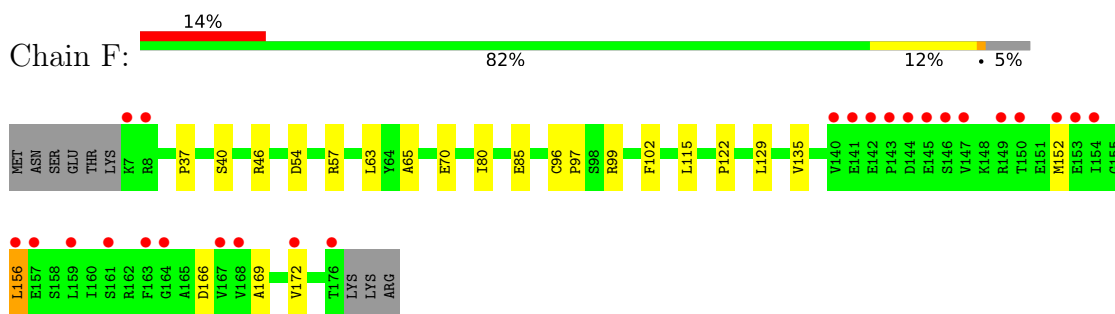
- Molecule 1: Benzoyl-CoA reductase, putative



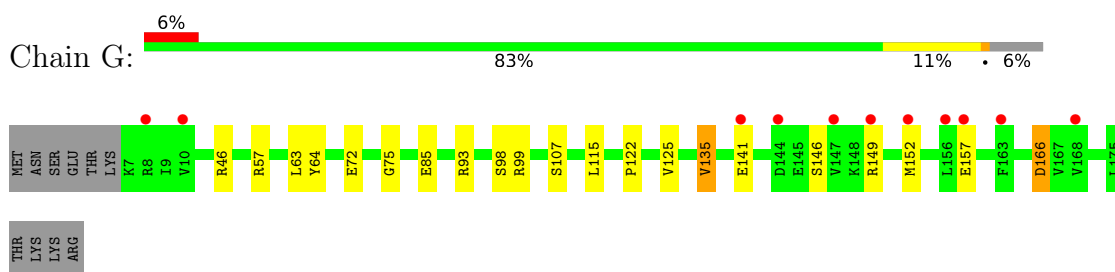
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein



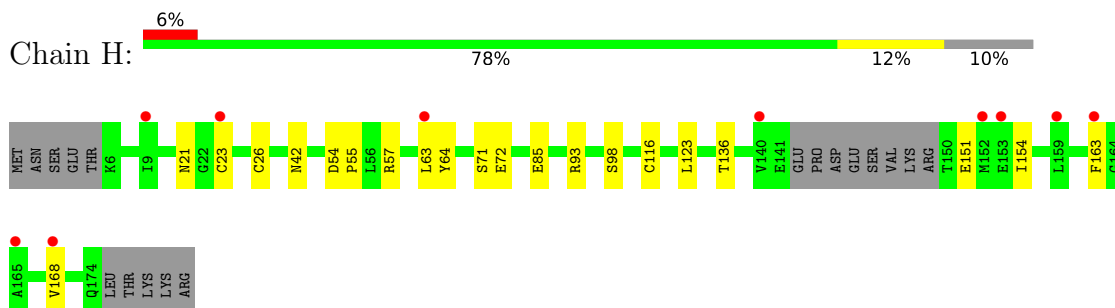
- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein



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



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.34Å)	Xtrriage
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 <sup>2</sup> )	61.0	Xtrriage
Anisotropy	0.190	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	26313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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.

All (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
2:G:122:PRO:HG2	2:G:135:VAL:HG11	1.76	0.67
1:D:322:CYS:SG	5:D:704:MTE:S1'	2.93	0.66
1:D:434:LEU:HD22	1:D:435:PRO:HD2	1.79	0.64
1:B:434:LEU:HD22	1:B:435:PRO:HD2	1.79	0.64
1:A:185:SER:HB2	5:A:704:MTE:H4'1	1.81	0.63
2:F:80:ILE:HG12	2:F:85:GLU:HG2	1.81	0.62
1:A:434:LEU:HD22	1:A:435:PRO:HD2	1.80	0.62
1:B:254:VAL:O	1:B:255:HIS:ND1	2.33	0.61
2:E:159:LEU:HD13	2:F:156:LEU:HD22	1.81	0.61
1:C:254:VAL:O	1:C:255:HIS:ND1	2.34	0.60
1:D:254:VAL:O	1:D:255:HIS:ND1	2.34	0.60
1:C:434:LEU:HD22	1:C:435:PRO:HD2	1.84	0.60
1:A:254:VAL:O	1:A:255:HIS:ND1	2.35	0.59
2:H:57:ARG:NH1	2:H:85:GLU:O	2.36	0.59
2:E:172:VAL:HG21	2:F:172:VAL:HG21	1.86	0.57
2:G:149:ARG:NH1	2:G:157:GLU:OE1	2.38	0.56
2:F:37:PRO:HG2	2:F:40:SER:HB3	1.87	0.56
2:G:107:SER:HA	2:H:151:GLU:HB3	1.86	0.55
1:A:98:PHE:H	1:A:179:GLN:HE22	1.55	0.54
2:G:57:ARG:NH1	2:G:85:GLU:O	2.40	0.54
1:A:222:ASN:ND2	9:A:801:HOH:O	2.35	0.53
3:D:701:UNL:X	5:D:703:MTE:S1'	2.95	0.53
1:A:622:ASN:HD22	1:A:624:ASP:H	1.55	0.52
1:D:137:HIS:NE2	1:D:153:GLU:OE2	2.43	0.52
1:B:137:HIS:NE2	1:B:153:GLU:OE2	2.43	0.51
1:B:98:PHE:H	1:B:179:GLN:HE22	1.58	0.51
1:A:337:ASP:O	1:A:341:ARG:HG3	2.11	0.51
2:G:146:SER:HB3	2:H:71:SER:HB2	1.92	0.51
2:G:64:TYR:O	2:G:93:ARG:HD2	2.11	0.50
1:B:337:ASP:O	1:B:341:ARG:HG3	2.12	0.50
2:E:46:ARG:NH2	2:E:104:GLU:OE1	2.44	0.50
1:D:84:SER:HB2	1:D:91:ALA:HB2	1.93	0.50
1:B:84:SER:HB2	1:B:91:ALA:HB2	1.93	0.50
1:D:98:PHE:H	1:D:179:GLN:HE22	1.59	0.50
1:C:622:ASN:HD22	1:C:624:ASP:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:SER:HB2	1:C:91:ALA:HB2	1.92	0.50
1:A:137:HIS:NE2	1:A:153:GLU:OE2	2.44	0.49
1:B:622:ASN:HD22	1:B:624:ASP:H	1.60	0.49
1:D:337:ASP:O	1:D:341:ARG:HG3	2.11	0.49
1:D:622:ASN:HD22	1:D:624:ASP:H	1.60	0.49
1:C:98:PHE:H	1:C:179:GLN:HE22	1.59	0.49
2:F:115:LEU:HA	4:F:1002:SF4:S2	2.53	0.49
1:C:337:ASP:O	1:C:341:ARG:HG3	2.13	0.49
2:G:46:ARG:HD3	9:G:1108:HOH:O	2.13	0.48
1:A:84:SER:HB2	1:A:91:ALA:HB2	1.94	0.48
1:C:137:HIS:NE2	1:C:153:GLU:OE2	2.46	0.48
1:D:263:ASN:OD1	1:D:272:ARG:NH2	2.47	0.47
2:H:64:TYR:O	2:H:93:ARG:HD2	2.13	0.47
1:D:484:GLN:HG2	1:D:544:PRO:HD2	1.96	0.47
2:F:152:MET:HG2	2:F:156:LEU:HD23	1.95	0.47
2:E:11:LYS:HG2	2:E:137:GLU:HG2	1.98	0.46
2:F:122:PRO:HB3	4:F:1002:SF4:S2	2.55	0.46
1:A:484:GLN:HG2	1:A:544:PRO:HD2	1.97	0.46
1:C:263:ASN:OD1	1:C:272:ARG:NH2	2.49	0.46
1:C:254:VAL:HB	1:C:255:HIS:H	1.34	0.46
2:G:75:GLY:O	2:H:93:ARG:NH1	2.47	0.46
1:A:529:ASP:OD1	5:A:703:MTE:N2	2.49	0.46
1:D:242:ILE:H	1:D:242:ILE:HD13	1.81	0.45
2:E:33:PHE:C	2:E:35:ALA:H	2.20	0.45
2:F:166:ASP:OD1	2:F:166:ASP:N	2.47	0.45
1:B:263:ASN:OD1	1:B:272:ARG:NH2	2.49	0.45
1:D:251:GLU:OE1	1:D:260:HIS:HE1	1.92	0.45
1:B:242:ILE:HD13	1:B:242:ILE:H	1.82	0.45
1:B:619:LYS:HD3	1:B:619:LYS:HA	1.83	0.45
2:H:116:CYS:SG	2:H:123:LEU:HD12	2.56	0.45
2:H:154:ILE:H	2:H:154:ILE:HD12	1.81	0.45
1:C:251:GLU:OE1	1:C:260:HIS:HE1	1.93	0.45
1:C:484:GLN:HG2	1:C:544:PRO:HD2	1.99	0.45
2:E:172:VAL:HG11	2:F:169:ALA:HA	1.98	0.45
2:G:152:MET:HB2	2:H:163:PHE:CE1	2.52	0.45
1:A:180:GLY:N	9:A:802:HOH:O	2.49	0.44
1:C:620:GLY:HA3	1:C:631:THR:HG21	1.99	0.44
2:F:96:CYS:SG	2:F:97:PRO:HD2	2.57	0.44
1:D:322:CYS:SG	1:D:323:PHE:N	2.90	0.44
2:G:141:GLU:H	2:G:141:GLU:HG2	1.55	0.44
2:G:115:LEU:HA	4:G:1002:SF4:S2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:OD1	1:A:272:ARG:NH2	2.51	0.44
2:G:122:PRO:HB3	4:G:1002:SF4:S2	2.58	0.44
1:D:100:ALA:HB3	1:D:101:PRO:HD3	2.00	0.44
1:B:266:TRP:CE3	1:B:330:MET:HA	2.53	0.43
1:B:484:GLN:HG2	1:B:544:PRO:HD2	2.00	0.43
1:C:242:ILE:H	1:C:242:ILE:HD13	1.83	0.43
1:C:266:TRP:CE3	1:C:330:MET:HA	2.54	0.43
2:G:125:VAL:HG21	2:G:135:VAL:HG12	2.00	0.43
1:B:189:ILE:H	1:B:189:ILE:HD13	1.83	0.43
1:D:135:ALA:HB1	1:D:138:LEU:HD12	1.99	0.43
1:A:242:ILE:H	1:A:242:ILE:HD13	1.84	0.43
1:D:473:GLU:OE2	1:D:473:GLU:N	2.52	0.43
1:A:620:GLY:HA3	1:A:631:THR:HG21	2.00	0.43
1:C:481:ASP:OD1	1:C:481:ASP:N	2.51	0.43
1:A:218:ILE:HD12	1:A:218:ILE:HA	1.87	0.43
1:A:189:ILE:H	1:A:189:ILE:HD13	1.84	0.43
1:A:266:TRP:CE3	1:A:330:MET:HA	2.53	0.43
1:D:266:TRP:CE3	1:D:330:MET:HA	2.54	0.43
2:F:65:ALA:HB2	2:F:102:PHE:CD1	2.53	0.43
1:A:135:ALA:HB1	1:A:138:LEU:HD12	2.01	0.42
1:A:150:ILE:HG21	1:A:202:VAL:HG21	2.02	0.42
1:A:322:CYS:SG	3:A:701:UNL:X	3.08	0.42
1:C:150:ILE:HG21	1:C:202:VAL:HG21	2.02	0.42
1:C:475:ARG:NH2	1:C:498:GLU:HG2	2.35	0.42
1:D:620:GLY:HA3	1:D:631:THR:HG21	2.01	0.42
2:E:72:GLU:HG2	2:E:98:SER:HB3	2.02	0.42
2:E:27:GLU:HG2	2:E:49:VAL:O	2.20	0.42
1:A:481:ASP:OD1	1:A:481:ASP:N	2.52	0.42
1:A:303:PRO:HG3	2:F:129:LEU:HD22	2.02	0.42
1:B:297:ILE:HD11	1:B:319:MET:HG2	2.02	0.41
1:B:481:ASP:OD1	1:B:481:ASP:N	2.52	0.41
1:D:481:ASP:OD1	1:D:481:ASP:N	2.53	0.41
2:E:104:GLU:HB2	2:E:108:GLY:H	1.85	0.41
2:G:152:MET:HE2	2:H:168:VAL:HA	2.03	0.41
1:A:77:ARG:NH1	4:A:702:SF4:S3	2.93	0.41
2:H:21:ASN:OD1	2:H:23:CYS:HB3	2.20	0.41
2:H:72:GLU:HG2	2:H:98:SER:HB3	2.03	0.41
1:B:475:ARG:NH2	1:B:498:GLU:HG2	2.35	0.41
1:D:458:THR:HB	3:D:701:UNL:X	2.50	0.41
1:A:475:ARG:NH2	1:A:498:GLU:HG2	2.36	0.41
2:E:8:ARG:HE	2:E:143:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:ASP:OD1	2:E:106:ASP:N	2.34	0.41
1:B:620:GLY:HA3	1:B:631:THR:HG21	2.02	0.41
2:F:54:ASP:OD2	2:F:57:ARG:NE	2.53	0.41
1:B:150:ILE:HG21	1:B:202:VAL:HG21	2.03	0.41
1:C:218:ILE:HD12	1:C:218:ILE:HA	1.91	0.41
1:D:218:ILE:HD12	1:D:218:ILE:HA	1.92	0.41
1:D:475:ARG:NH2	1:D:498:GLU:HG2	2.36	0.41
1:A:78:THR:OG1	1:A:100:ALA:HB2	2.21	0.41
1:B:623:ASP:OD1	1:B:623:ASP:N	2.52	0.41
2:E:57:ARG:NH1	2:E:85:GLU:O	2.50	0.41
2:H:54:ASP:HA	2:H:55:PRO:HD3	1.90	0.41
1:C:95:MET:HE3	1:C:184:ALA:H	1.85	0.41
1:A:622:ASN:ND2	1:A:624:ASP:H	2.19	0.40
1:C:538:SER:O	1:C:541:PRO:HD2	2.21	0.40
1:D:150:ILE:HG21	1:D:202:VAL:HG21	2.02	0.40
1:B:322:CYS:SG	3:B:701:UNL:X	3.10	0.40
1:D:237:PRO:O	1:D:239:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	VAL
1	B	254	VAL
1	C	254	VAL
1	D	254	VAL
1	A	255	HIS
1	B	33	LEU
1	B	255	HIS
1	C	255	HIS
1	D	255	HIS
2	E	34	HIS
1	A	33	LEU
1	C	33	LEU
1	D	33	LEU
1	C	470	PRO
1	D	470	PRO
1	A	470	PRO
1	B	470	PRO

### 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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	189	ILE
1	A	215	GLU
1	A	242	ILE
1	A	319	MET
1	A	321	LYS
1	A	436	LEU
1	A	471	LYS
1	A	551	TYR
1	A	576	ARG
1	A	622	ASN
1	B	1	MET
1	B	189	ILE
1	B	215	GLU
1	B	242	ILE
1	B	319	MET
1	B	321	LYS
1	B	436	LEU
1	B	471	LYS
1	B	551	TYR
1	B	576	ARG
1	B	622	ASN
1	C	1	MET
1	C	189	ILE
1	C	215	GLU
1	C	242	ILE
1	C	254	VAL
1	C	321	LYS
1	C	436	LEU
1	C	471	LYS
1	C	551	TYR
1	C	576	ARG
1	C	622	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	1	MET
1	D	174	TYR
1	D	189	ILE
1	D	215	GLU
1	D	242	ILE
1	D	319	MET
1	D	321	LYS
1	D	436	LEU
1	D	471	LYS
1	D	551	TYR
1	D	576	ARG
1	D	622	ASN
2	E	93	ARG
2	E	106	ASP
2	E	123	LEU
2	E	149	ARG
2	F	46	ARG
2	F	63	LEU
2	F	70	GLU
2	F	99	ARG
2	F	135	VAL
2	F	156	LEU
2	G	63	LEU
2	G	99	ARG
2	G	135	VAL
2	G	166	ASP
2	H	26	CYS
2	H	42	ASN
2	H	63	LEU
2	H	136	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	179	GLN
1	A	463	GLN
1	A	622	ASN
1	B	179	GLN
1	B	463	GLN
1	B	622	ASN
1	C	179	GLN
1	C	463	GLN

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Mol	Chain	Res	Type
1	C	622	ASN
1	D	179	GLN
1	D	463	GLN
1	D	622	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	702	1	-	-	0/6/5/5
4	SF4	G	1001	2	-	-	0/6/5/5
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

All (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
5	C	703	MTE	C9-C10	-6.00	1.30	1.41
5	D	704	MTE	C9-C10	-5.84	1.30	1.41
5	B	704	MTE	C7-C6	-5.78	1.49	1.53
5	D	703	MTE	C9-C10	-5.76	1.30	1.41
5	C	704	MTE	C7-C6	-5.72	1.49	1.53
5	A	703	MTE	C9-C4	5.36	1.48	1.41
5	C	704	MTE	C9-C4	5.28	1.48	1.41
5	D	704	MTE	C9-C4	5.20	1.48	1.41
5	B	703	MTE	C7-C6	-5.10	1.49	1.53
5	B	703	MTE	C9-C4	5.03	1.48	1.41
5	B	703	MTE	C2-N2	4.94	1.43	1.33
5	A	704	MTE	C9-C4	4.92	1.48	1.41
5	D	704	MTE	C7-C6	-4.87	1.49	1.53
5	A	703	MTE	C2-N2	4.85	1.43	1.33
5	D	703	MTE	C2-N2	4.83	1.43	1.33
5	A	704	MTE	C2-N2	4.83	1.43	1.33
5	D	704	MTE	C2-N2	4.70	1.43	1.33
5	B	704	MTE	C2-N2	4.66	1.43	1.33
5	C	703	MTE	C2-N2	4.62	1.43	1.33
5	B	704	MTE	C9-C4	4.56	1.47	1.41
5	D	703	MTE	C9-C4	4.47	1.47	1.41
5	C	703	MTE	C9-C4	4.43	1.47	1.41
5	C	704	MTE	C2-N2	4.35	1.42	1.33
5	A	703	MTE	C7-C6	-4.25	1.50	1.53
5	C	703	MTE	C7-C6	-3.79	1.50	1.53
5	D	703	MTE	C4-N3	3.54	1.39	1.33
5	A	703	MTE	O3'-C7	-3.40	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	704	MTE	C4-N3	3.38	1.38	1.33
5	C	703	MTE	C4-N3	3.37	1.38	1.33
5	B	703	MTE	O3'-C3'	-3.34	1.39	1.43
5	A	704	MTE	C4-N3	3.32	1.38	1.33
5	B	704	MTE	O3'-C7	-3.32	1.39	1.43
5	B	703	MTE	C4-N3	3.30	1.38	1.33
5	D	703	MTE	O3'-C3'	-3.23	1.39	1.43
5	A	703	MTE	C4-N3	3.20	1.38	1.33
5	D	704	MTE	C4-N3	3.19	1.38	1.33
5	C	703	MTE	O3'-C3'	-3.18	1.39	1.43
5	C	704	MTE	O3'-C3'	-3.15	1.39	1.43
5	D	703	MTE	O3'-C7	-3.13	1.39	1.43
5	D	703	MTE	C2-N3	3.04	1.40	1.35
5	B	704	MTE	O3'-C3'	-2.99	1.39	1.43
5	B	703	MTE	O3'-C7	-2.96	1.39	1.43
5	C	704	MTE	O3'-C7	-2.93	1.39	1.43
5	B	704	MTE	C4-N3	2.91	1.38	1.33
5	A	703	MTE	O3'-C3'	-2.88	1.39	1.43
5	A	703	MTE	C10-N1	2.75	1.39	1.34
5	C	703	MTE	C10-N1	2.74	1.39	1.34
5	A	704	MTE	C10-N1	2.73	1.39	1.34
5	C	703	MTE	O3'-C7	-2.70	1.39	1.43
5	D	703	MTE	C10-N1	2.69	1.39	1.34
5	D	704	MTE	C10-N1	2.66	1.39	1.34
5	A	704	MTE	O3'-C3'	-2.63	1.40	1.43
5	D	704	MTE	C2-N3	2.62	1.40	1.35
5	A	704	MTE	C7-C6	-2.62	1.51	1.53
5	A	704	MTE	C2-N3	2.60	1.40	1.35
5	A	703	MTE	C9-N5	2.57	1.43	1.38
5	C	704	MTE	C10-N1	2.56	1.39	1.34
5	B	704	MTE	C2-N3	2.54	1.39	1.35
5	A	704	MTE	O3'-C7	-2.51	1.40	1.43
5	B	704	MTE	C10-N1	2.51	1.39	1.34
5	B	703	MTE	C10-N1	2.51	1.39	1.34
5	D	703	MTE	C9-N5	2.45	1.43	1.38
5	A	703	MTE	C2-N3	2.44	1.39	1.35
5	C	703	MTE	C9-N5	2.44	1.43	1.38
5	B	703	MTE	C2-N3	2.43	1.39	1.35
5	C	704	MTE	C2-N3	2.43	1.39	1.35
5	A	703	MTE	C1'-C2'	2.42	1.51	1.35
5	D	704	MTE	C9-N5	2.39	1.42	1.38
5	D	704	MTE	O3'-C7	-2.27	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	703	MTE	C2-N3	2.27	1.39	1.35
5	D	703	MTE	C7-C6	-2.25	1.51	1.53
5	C	704	MTE	C9-N5	2.09	1.42	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	B	703	MTE	C10-C9-C4	6.57	120.41	114.57
5	C	704	MTE	C10-C9-C4	6.52	120.36	114.57
5	C	703	MTE	C10-C9-C4	6.31	120.18	114.57
5	A	704	MTE	O3'-C7-N8	6.31	115.05	108.57
5	B	704	MTE	O3'-C7-C6	-6.27	104.78	108.96
5	A	703	MTE	C10-C9-C4	5.76	119.69	114.57
5	D	703	MTE	C10-C9-C4	5.38	119.35	114.57
5	B	704	MTE	O3'-C7-N8	-5.33	103.09	108.57
5	A	703	MTE	O3'-C7-N8	4.98	113.68	108.57
5	D	704	MTE	O3'-C7-N8	-4.37	104.08	108.57
5	D	703	MTE	C9-C10-N8	4.09	121.88	118.13
5	C	703	MTE	O3'-C7-C6	-3.99	106.30	108.96
5	C	704	MTE	C9-C10-N8	3.19	121.05	118.13
5	B	703	MTE	C9-C10-N8	3.09	120.95	118.13
5	B	704	MTE	C9-C10-N8	3.05	120.92	118.13
5	B	703	MTE	C2-N1-C10	3.00	121.27	114.54
5	A	704	MTE	C2-N1-C10	2.99	121.25	114.54
5	D	704	MTE	P-O4'-C4'	2.86	126.17	118.30
5	C	703	MTE	C2-N1-C10	2.78	120.77	114.54
5	A	704	MTE	C9-C10-N8	2.78	120.67	118.13
5	D	703	MTE	C2-N1-C10	2.77	120.75	114.54
5	C	704	MTE	C2-N1-C10	2.76	120.72	114.54
5	D	704	MTE	C2-N1-C10	2.74	120.68	114.54
5	C	704	MTE	C4-C9-N5	2.73	121.41	119.12
5	A	703	MTE	C2-N1-C10	2.72	120.63	114.54
5	B	704	MTE	C2-N1-C10	2.71	120.62	114.54
5	C	703	MTE	C9-C10-N8	2.71	120.61	118.13
5	A	703	MTE	C4-C9-N5	2.65	121.35	119.12
5	D	703	MTE	N1-C2-N3	-2.54	121.44	125.42
5	A	703	MTE	C9-C10-N8	2.50	120.42	118.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	703	MTE	C10-N8-C7	-2.46	118.86	123.67
5	B	703	MTE	C10-N8-C7	-2.34	119.08	123.67
5	B	703	MTE	O3'-C7-C6	-2.33	107.41	108.96
5	D	703	MTE	N2-C2-N3	2.29	120.81	117.25
5	B	703	MTE	N1-C2-N3	-2.20	121.97	125.42
5	D	704	MTE	C10-N8-C7	-2.16	119.44	123.67
5	D	704	MTE	C9-C10-N8	2.14	120.09	118.13
5	D	703	MTE	C10-N8-C7	-2.12	119.51	123.67
5	A	704	MTE	O3P-P-O4'	2.08	112.28	106.73
5	B	704	MTE	C10-N8-C7	-2.03	119.69	123.67
5	A	703	MTE	N1-C2-N3	-2.00	122.28	125.42

There are no chirality outliers.

All (12) torsion outliers are listed below:

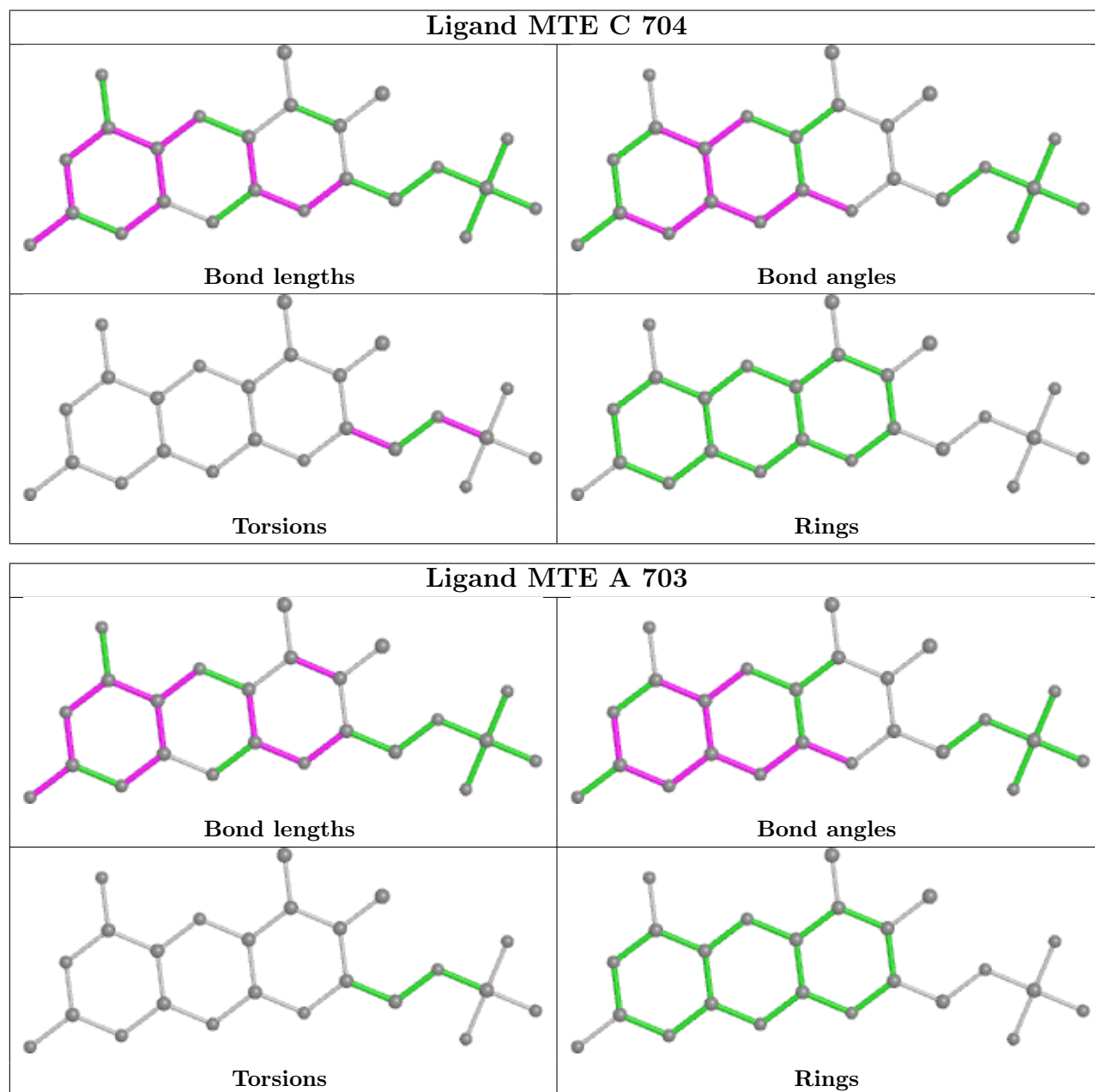
Mol	Chain	Res	Type	Atoms
5	A	704	MTE	C2'-C3'-C4'-O4'
5	A	704	MTE	O3'-C3'-C4'-O4'
5	B	704	MTE	C4'-O4'-P-O1P
5	B	704	MTE	C4'-O4'-P-O2P
5	B	704	MTE	C4'-O4'-P-O3P
5	C	704	MTE	C4'-O4'-P-O2P
5	C	704	MTE	C4'-O4'-P-O3P
5	C	704	MTE	C4'-O4'-P-O1P
5	B	704	MTE	C2'-C3'-C4'-O4'
5	C	704	MTE	C2'-C3'-C4'-O4'
5	B	704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

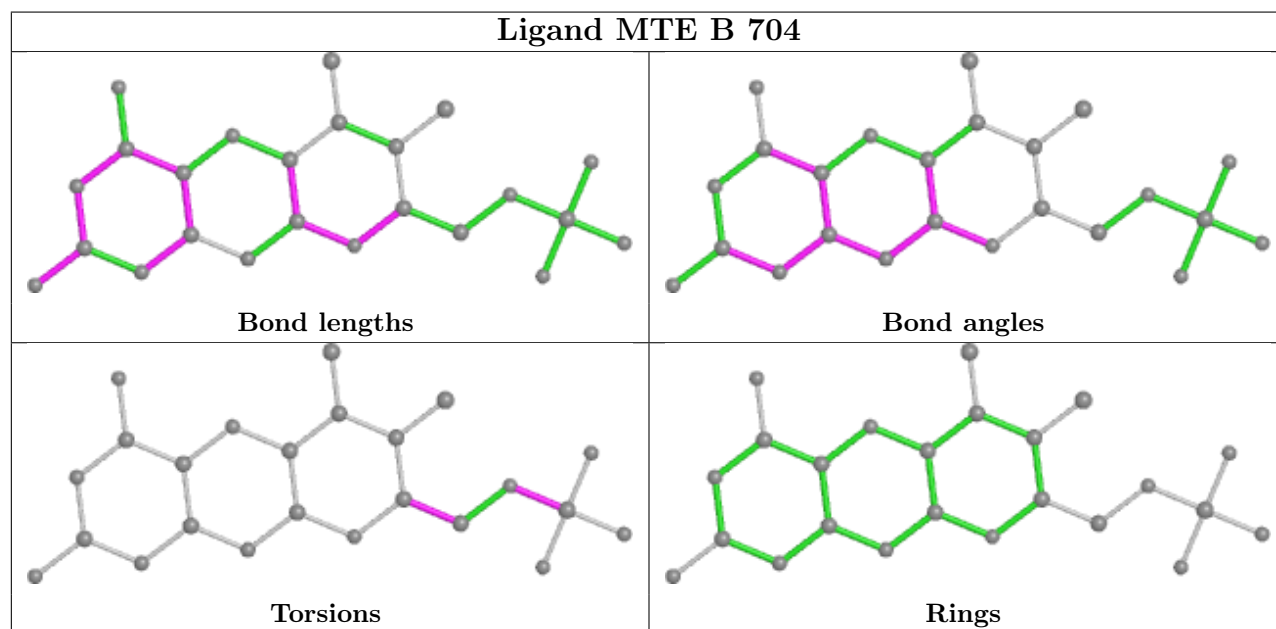
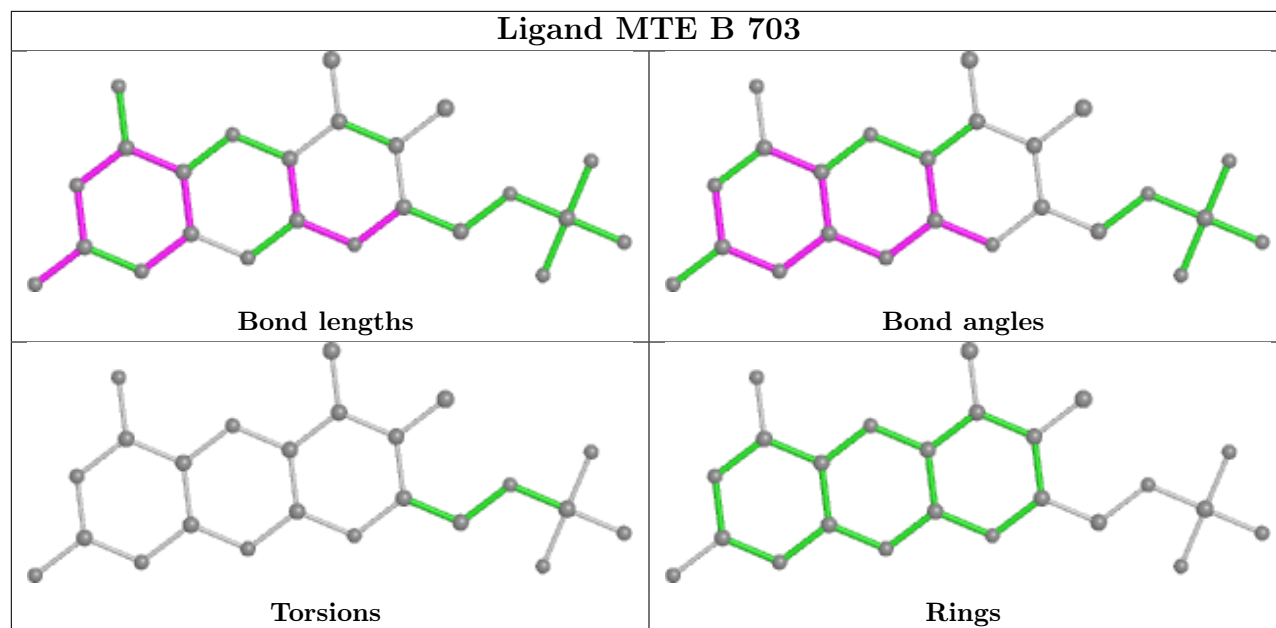
There are no ring outliers.

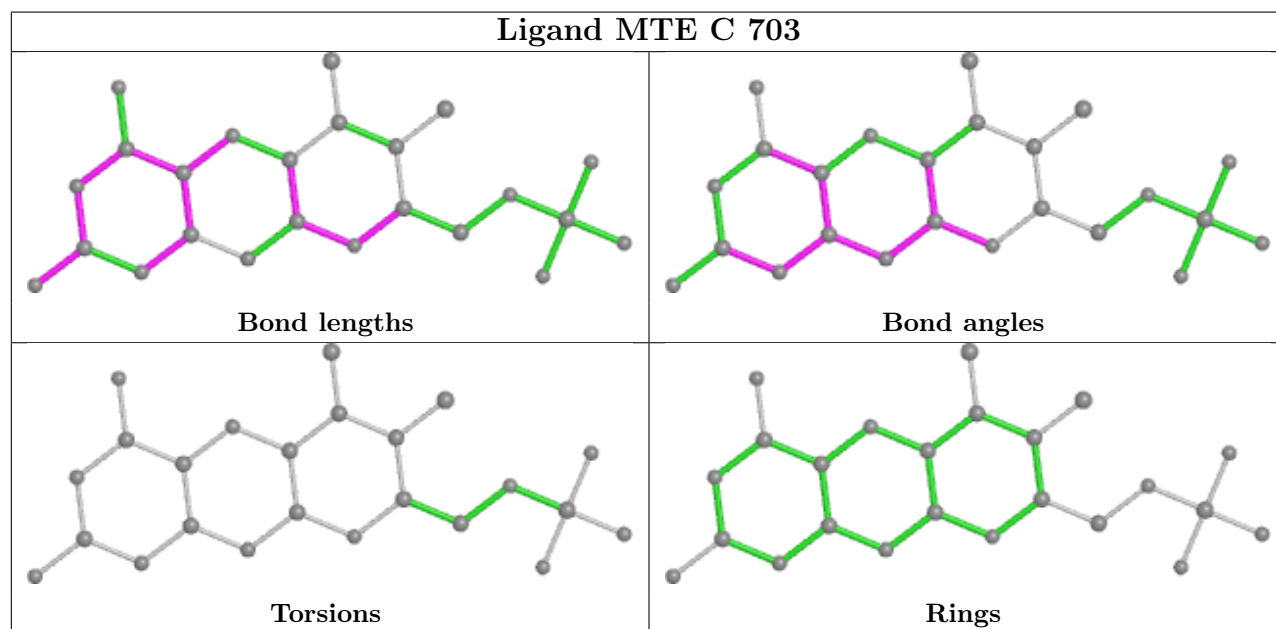
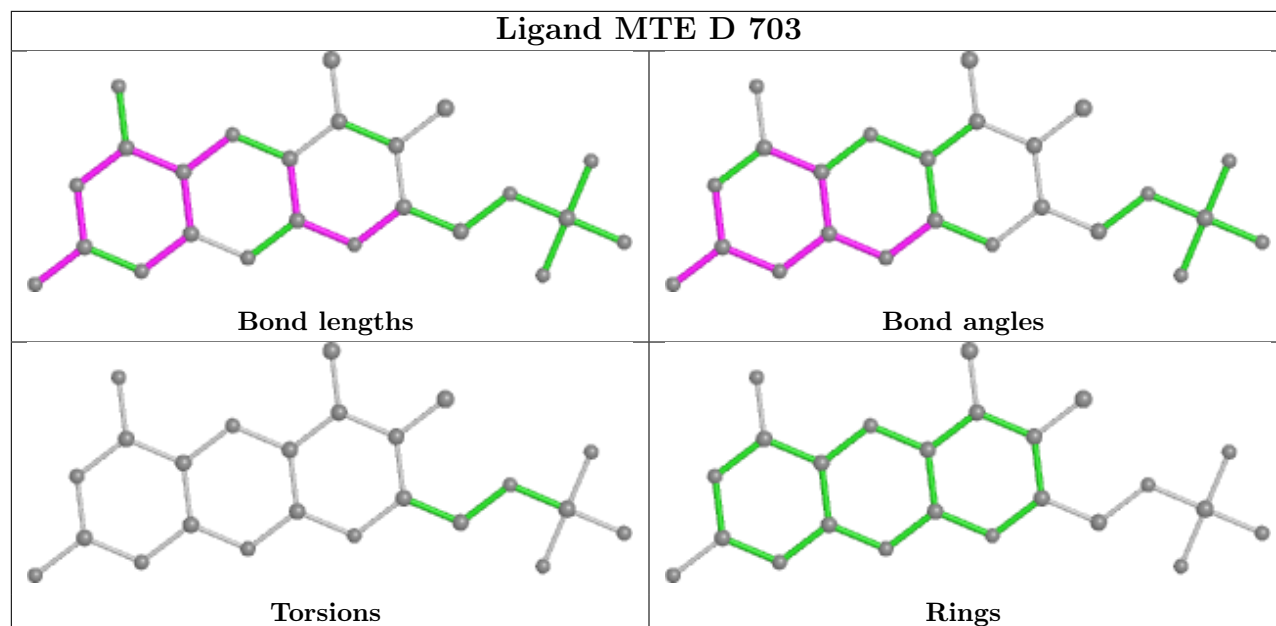
8 monomers are involved in 11 short contacts:

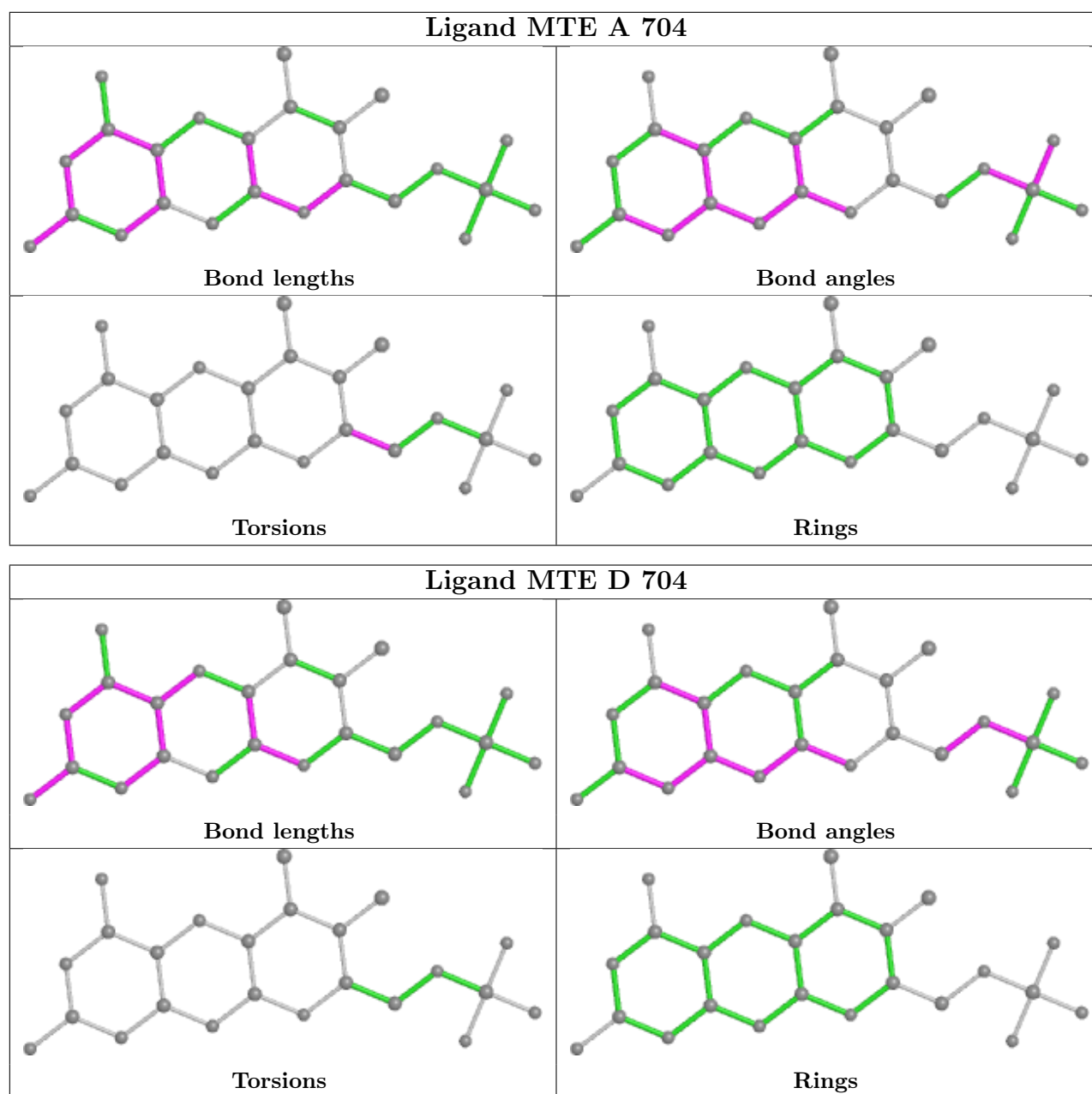
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	703	MTE	2	0
4	A	702	SF4	1	0
4	E	1002	SF4	1	0
5	D	703	MTE	1	0
5	A	704	MTE	1	0
5	D	704	MTE	1	0
4	G	1002	SF4	2	0
4	F	1002	SF4	2	0

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 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	A	401	ILE	9.5
1	A	277	TRP	9.1
1	A	285	TRP	9.0
1	A	359	VAL	8.9
1	A	416	ILE	8.8
1	A	377	PHE	8.7
1	A	625	GLY	8.6
1	A	607	LEU	8.4
1	A	421	GLU	8.2
1	A	281	VAL	7.9
1	A	440	MET	7.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	652	ALA	7.8
1	A	271	THR	7.6
2	E	144	ASP	7.3
1	A	471	LYS	7.1
1	A	372	LEU	6.9
1	A	267	GLY	6.7
1	A	500	ARG	6.6
1	A	394	LYS	6.5
1	A	396	VAL	6.4
1	C	68	CYS	6.4
1	A	503	LYS	6.4
1	A	260	HIS	6.3
1	A	263	ASN	6.3
1	A	390	TYR	6.3
1	A	370	GLY	6.3
1	A	135	ALA	6.2
1	A	499	PRO	6.1
1	A	289	MET	6.0
1	A	276	PHE	6.0
1	A	332	ALA	6.0
1	A	603	ARG	5.9
1	A	645	ILE	5.9
1	A	383	GLY	5.8
1	A	261	THR	5.8
1	A	173	PHE	5.8
1	A	283	HIS	5.8
1	A	392	LEU	5.7
1	A	494	PHE	5.7
1	A	473	GLU	5.6
1	A	506	PRO	5.5
1	A	495	LEU	5.5
1	A	236	ILE	5.3
1	A	329	THR	5.3
1	A	374	ASP	5.3
1	C	644	PHE	5.2
1	A	94	MET	5.1
1	A	241	PRO	5.1
1	A	378	PRO	5.1
1	A	369	LYS	5.1
1	A	419	GLY	5.1
1	A	371	ILE	5.1
1	A	272	ARG	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	391	LEU	5.0
1	A	299	CYS	5.0
1	A	474	GLN	5.0
1	A	360	MET	5.0
1	A	362	PHE	5.0
1	B	652	ALA	5.0
1	A	238	ASP	5.0
1	A	615	TYR	5.0
1	A	387	ARG	5.0
1	A	264	PHE	5.0
1	A	280	GLU	4.9
1	A	184	ALA	4.9
1	A	650	LEU	4.9
1	A	450	CYS	4.9
1	A	379	GLY	4.8
1	A	185	SER	4.8
2	H	163	PHE	4.8
1	A	651	SER	4.7
1	A	166	LYS	4.7
1	A	258	LYS	4.7
2	F	168	VAL	4.6
1	A	508	PHE	4.6
1	A	641	GLY	4.6
1	A	472	LEU	4.6
1	A	454	LYS	4.5
1	A	259	TRP	4.5
1	A	187	GLY	4.5
1	A	275	ASP	4.5
1	A	496	GLU	4.5
1	A	414	GLN	4.5
1	A	402	GLY	4.5
2	E	148	LYS	4.5
1	A	367	LEU	4.5
1	A	600	TRP	4.5
1	C	530	ALA	4.5
1	B	277	TRP	4.5
1	A	182	SER	4.4
2	G	168	VAL	4.4
1	A	455	ILE	4.4
1	B	473	GLU	4.4
1	A	249	PRO	4.4
1	A	357	PRO	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	143	PRO	4.4
2	F	7	LYS	4.4
2	F	145	GLU	4.4
1	C	377	PHE	4.3
1	A	604	PHE	4.3
2	G	149	ARG	4.3
2	E	159	LEU	4.3
1	A	611	LEU	4.3
1	A	491	LYS	4.3
1	A	373	LYS	4.3
1	A	475	ARG	4.2
1	A	183	SER	4.2
1	A	389	PHE	4.2
2	F	144	ASP	4.2
1	A	381	PRO	4.2
2	G	152	MET	4.1
1	A	331	ALA	4.1
1	A	95	MET	4.1
1	A	509	PRO	4.1
1	A	411	TRP	4.1
1	B	280	GLU	4.1
1	A	132	ILE	4.1
1	D	1	MET	4.1
1	C	75	CYS	4.1
2	H	140	VAL	4.1
1	A	526	TYR	4.1
1	A	57	GLU	4.1
1	D	277	TRP	4.0
1	A	376	ASP	4.0
1	C	1	MET	4.0
1	A	412	ALA	4.0
1	A	591	VAL	4.0
1	A	457	ILE	4.0
1	B	94	MET	4.0
1	B	472	LEU	4.0
1	A	59	LEU	4.0
2	H	159	LEU	4.0
1	A	445	TYR	3.9
1	A	363	ALA	3.9
1	A	418	ASN	3.9
1	A	502	GLU	3.9
1	A	644	PHE	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	168	GLY	3.9
2	F	147	VAL	3.9
1	A	439	SER	3.9
1	A	327	THR	3.9
1	A	54	PHE	3.9
1	A	375	SER	3.8
1	A	162	ALA	3.8
1	A	382	GLU	3.8
1	A	93	SER	3.8
1	A	597	ALA	3.8
1	A	380	LEU	3.8
1	A	78	THR	3.7
1	A	446	TYR	3.7
1	A	313	GLU	3.7
1	C	534	CYS	3.7
1	A	174	TYR	3.7
1	A	90	MET	3.7
1	A	460	ILE	3.7
1	A	441	LEU	3.7
1	A	447	LEU	3.7
1	B	274	LYS	3.7
1	A	268	ASN	3.7
1	A	262	GLU	3.7
1	A	385	GLU	3.7
1	A	237	PRO	3.7
1	B	650	LEU	3.6
1	A	602	ASN	3.6
1	A	52	GLU	3.6
1	A	609	LYS	3.6
1	B	275	ASP	3.6
1	A	589	ARG	3.6
1	B	602	ASN	3.6
1	B	500	ARG	3.6
1	D	469	TYR	3.6
1	A	278	THR	3.6
1	B	79	ILE	3.6
1	A	435	PRO	3.6
2	F	154	ILE	3.5
2	F	156	LEU	3.5
1	A	269	ALA	3.5
1	A	458	THR	3.5
1	A	186	ARG	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	92	PHE	3.5
1	A	448	MET	3.5
1	A	340	LEU	3.5
1	A	640	VAL	3.5
2	G	163	PHE	3.5
1	A	273	ARG	3.5
2	F	159	LEU	3.5
1	A	633	ASP	3.5
1	A	464	PHE	3.4
1	A	342	ILE	3.4
1	B	278	THR	3.4
1	A	621	TRP	3.4
1	A	120	LEU	3.4
2	E	168	VAL	3.4
1	A	355	SER	3.4
1	D	184	ALA	3.4
1	D	652	ALA	3.4
1	A	520	TRP	3.4
1	A	449	TYR	3.4
1	A	279	ASP	3.4
1	A	356	ALA	3.4
1	A	456	ASN	3.4
1	B	471	LYS	3.4
1	C	471	LYS	3.4
1	A	599	HIS	3.3
2	E	172	VAL	3.3
1	C	94	MET	3.3
1	C	535	ALA	3.3
1	A	336	LEU	3.3
1	C	32	TYR	3.3
2	H	168	VAL	3.3
1	A	312	MET	3.3
1	A	314	GLY	3.3
1	B	494	PHE	3.3
1	A	393	ASP	3.3
1	A	530	ALA	3.3
1	B	283	HIS	3.3
1	B	369	LYS	3.2
2	F	152	MET	3.2
1	C	649	ILE	3.2
1	A	76	ASN	3.2
1	C	44	TRP	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	62	PHE	3.2
1	A	505	MET	3.2
1	A	535	ALA	3.2
1	A	79	ILE	3.2
2	E	171	THR	3.2
1	A	287	LYS	3.2
2	E	139	GLU	3.2
1	A	270	ARG	3.2
1	D	177	ILE	3.1
1	A	469	TYR	3.1
1	A	75	CYS	3.1
1	A	189	ILE	3.1
1	A	479	VAL	3.1
1	A	529	ASP	3.1
1	D	283	HIS	3.1
1	C	300	TYR	3.1
1	C	650	LEU	3.1
1	A	630	GLU	3.1
1	A	80	VAL	3.1
1	B	183	SER	3.1
1	B	272	ARG	3.1
1	A	136	SER	3.1
1	B	182	SER	3.1
1	A	608	GLU	3.0
1	A	430	LYS	3.0
1	C	76	ASN	3.0
1	C	183	SER	3.0
1	A	254	VAL	3.0
2	E	140	VAL	3.0
1	C	526	TYR	3.0
1	A	65	GLY	3.0
1	A	631	THR	3.0
2	F	143	PRO	3.0
1	A	511	VAL	3.0
1	A	351	LEU	3.0
1	A	406	ALA	3.0
1	B	63	ALA	3.0
1	A	646	LYS	3.0
1	B	80	VAL	3.0
2	F	140	VAL	3.0
1	A	507	ASN	3.0
1	A	629	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	99	TRP	3.0
1	C	181	ARG	3.0
1	A	481	ASP	2.9
1	C	93	SER	2.9
1	A	649	ILE	2.9
1	C	77	ARG	2.9
1	A	92	PHE	2.9
1	A	239	VAL	2.9
1	A	282	SER	2.9
1	B	93	SER	2.9
1	C	97	GLY	2.9
1	B	649	ILE	2.9
1	C	400	GLY	2.9
1	B	95	MET	2.9
1	B	240	MET	2.9
1	D	216	GLU	2.9
1	C	455	ILE	2.9
1	A	91	ALA	2.9
1	A	328	TYR	2.8
1	A	19	ILE	2.8
1	A	315	LEU	2.8
1	A	77	ARG	2.8
2	E	6	LYS	2.8
1	A	424	ALA	2.8
1	B	603	ARG	2.8
2	G	144	ASP	2.8
1	A	274	LYS	2.8
1	A	459	GLN	2.8
1	A	434	LEU	2.8
1	B	180	GLY	2.8
1	A	577	THR	2.8
1	B	476	GLU	2.8
1	C	460	ILE	2.8
1	A	63	ALA	2.8
1	A	134	ASP	2.8
1	C	187	GLY	2.8
1	A	286	GLU	2.8
1	A	478	PHE	2.7
1	A	618	LEU	2.7
2	F	176	THR	2.7
1	B	273	ARG	2.7
1	A	410	TYR	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	64	ALA	2.7
1	C	74	GLY	2.7
1	A	388	PHE	2.7
2	E	149	ARG	2.7
2	F	149	ARG	2.7
1	C	634	ASP	2.7
1	A	595	PRO	2.7
1	A	596	PRO	2.7
1	A	119	GLU	2.7
1	A	498	GLU	2.7
1	D	183	SER	2.7
1	A	338	PHE	2.7
1	D	281	VAL	2.7
2	G	8	ARG	2.7
1	A	345	LYS	2.7
2	F	142	GLU	2.7
1	C	184	ALA	2.7
1	A	323	PHE	2.7
1	C	78	THR	2.7
2	F	161	SER	2.7
1	A	201	VAL	2.7
1	B	604	PHE	2.7
1	A	422	ASP	2.6
1	B	184	ALA	2.6
1	A	531	LEU	2.6
1	C	531	LEU	2.6
1	D	644	PHE	2.6
1	D	274	LYS	2.6
1	A	68	CYS	2.6
1	A	177	ILE	2.6
1	C	283	HIS	2.6
1	D	63	ALA	2.6
1	B	35	GLY	2.6
1	B	78	THR	2.6
1	A	318	TYR	2.6
2	G	156	LEU	2.6
1	D	94	MET	2.6
1	D	368	GLU	2.6
1	D	649	ILE	2.6
1	A	620	GLY	2.6
1	A	594	GLN	2.6
1	A	307	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	530	ALA	2.6
2	E	9	ILE	2.6
1	B	259	TRP	2.6
1	A	537	LEU	2.6
2	F	172	VAL	2.6
1	B	96	GLY	2.6
1	B	535	ALA	2.6
1	A	490	PHE	2.5
1	C	95	MET	2.5
2	E	163	PHE	2.5
1	A	349	TYR	2.5
1	D	179	GLN	2.5
1	A	35	GLY	2.5
1	C	80	VAL	2.5
2	E	7	LYS	2.5
1	D	534	CYS	2.5
1	A	243	LEU	2.5
1	A	622	ASN	2.5
2	E	167	VAL	2.5
1	C	100	ALA	2.5
1	A	480	GLU	2.5
1	A	606	GLU	2.5
1	A	316	PRO	2.5
1	A	44	TRP	2.5
1	B	644	PHE	2.5
2	E	157	GLU	2.5
1	A	613	ASP	2.5
1	B	276	PHE	2.5
1	B	285	TRP	2.5
1	A	425	HIS	2.5
1	C	69	GLY	2.5
1	C	66	LEU	2.5
1	B	92	PHE	2.4
1	C	478	PHE	2.4
1	C	597	ALA	2.4
1	A	350	GLY	2.4
1	A	395	ILE	2.4
1	A	117	SER	2.4
1	A	635	LEU	2.4
1	C	101	PRO	2.4
1	A	153	GLU	2.4
1	B	255	HIS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	150	THR	2.4
2	F	157	GLU	2.4
1	A	444	ILE	2.4
1	D	79	ILE	2.4
1	A	466	GLN	2.4
1	A	443	PRO	2.4
1	A	451	THR	2.4
1	B	601	LYS	2.4
1	A	333	TYR	2.4
1	D	639	TYR	2.4
1	B	495	LEU	2.4
1	C	180	GLY	2.4
1	C	529	ASP	2.4
1	A	53	PRO	2.4
1	D	473	GLU	2.4
1	C	637	LEU	2.4
1	D	255	HIS	2.4
2	H	152	MET	2.4
1	A	98	PHE	2.4
1	D	374	ASP	2.3
1	A	178	GLU	2.3
1	A	540	PHE	2.3
1	B	281	VAL	2.3
1	A	534	CYS	2.3
1	A	462	GLY	2.3
1	C	641	GLY	2.3
2	G	141	GLU	2.3
2	H	9	ILE	2.3
1	A	467	ALA	2.3
1	B	367	LEU	2.3
1	D	27	ARG	2.3
1	B	591	VAL	2.3
1	C	481	ASP	2.3
1	B	353	GLY	2.3
1	D	180	GLY	2.3
1	A	310	ILE	2.3
1	C	299	CYS	2.3
1	A	66	LEU	2.3
1	A	581	ALA	2.3
1	B	175	ALA	2.3
1	D	176	SER	2.3
1	D	185	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	112	LYS	2.3
1	A	13	ASP	2.3
1	A	64	ALA	2.3
1	D	372	LEU	2.3
1	C	369	LYS	2.3
1	A	297	ILE	2.3
1	C	527	ILE	2.3
1	B	179	GLN	2.3
1	C	469	TYR	2.3
1	D	299	CYS	2.3
1	A	525	HIS	2.3
1	A	516	ASP	2.3
1	C	456	ASN	2.3
1	A	493	ILE	2.3
1	A	34	GLY	2.2
2	F	167	VAL	2.2
1	A	311	SER	2.2
1	A	400	GLY	2.2
1	B	324	THR	2.2
2	H	63	LEU	2.2
1	A	642	ASP	2.2
1	D	80	VAL	2.2
1	C	116	LYS	2.2
1	A	404	ILE	2.2
1	C	117	SER	2.2
1	C	182	SER	2.2
2	F	163	PHE	2.2
1	B	488	GLU	2.2
1	A	113	PHE	2.2
1	B	279	ASP	2.2
1	C	98	PHE	2.2
1	A	426	ASN	2.2
2	E	153	GLU	2.2
1	C	63	ALA	2.2
2	E	169	ALA	2.2
1	A	497	TRP	2.2
1	D	371	ILE	2.2
1	A	138	LEU	2.2
2	F	8	ARG	2.2
1	A	50	GLU	2.2
1	A	624	ASP	2.2
2	F	141	GLU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	157	GLU	2.2
2	E	135	VAL	2.2
1	A	100	ALA	2.2
1	C	532	GLY	2.2
1	D	373	LYS	2.1
1	C	177	ILE	2.1
1	A	36	LEU	2.1
1	C	48	PRO	2.1
2	E	8	ARG	2.1
1	C	639	TYR	2.1
2	H	153	GLU	2.1
1	A	361	ALA	2.1
1	A	572	ALA	2.1
1	C	185	SER	2.1
1	C	434	LEU	2.1
1	C	495	LEU	2.1
1	D	95	MET	2.1
1	B	260	HIS	2.1
1	A	170	ASN	2.1
1	A	215	GLU	2.1
1	A	436	LEU	2.1
1	B	97	GLY	2.1
2	F	146	SER	2.1
1	B	299	CYS	2.1
1	C	459	GLN	2.1
1	A	96	GLY	2.1
1	A	532	GLY	2.1
1	C	186	ARG	2.1
2	F	153	GLU	2.1
2	H	23	CYS	2.1
2	G	147	VAL	2.1
1	C	648	GLY	2.1
2	F	164	GLY	2.1
2	G	10	VAL	2.1
1	A	627	PRO	2.1
1	A	431	HIS	2.0
1	D	477	ALA	2.0
1	C	56	PRO	2.0
1	A	306	CYS	2.0
1	C	256	ASP	2.0
1	C	448	MET	2.0
1	B	188	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	81	SER	2.0
2	H	165	ALA	2.0
1	C	16	LYS	2.0
1	B	469	TYR	2.0
1	A	14	LEU	2.0
1	A	240	MET	2.0
1	C	65	GLY	2.0
1	C	376	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	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

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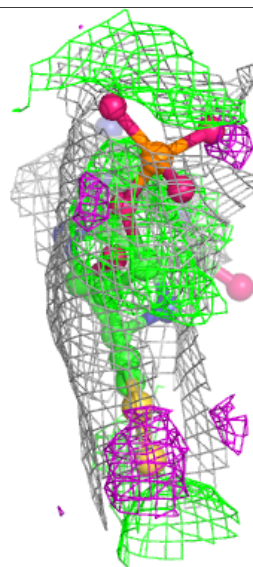
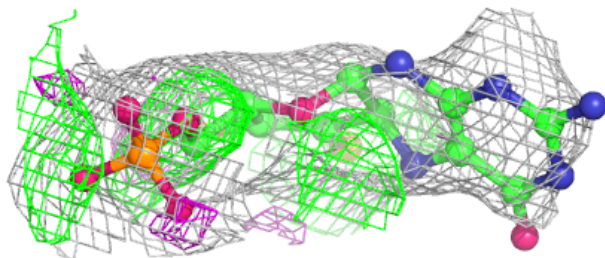
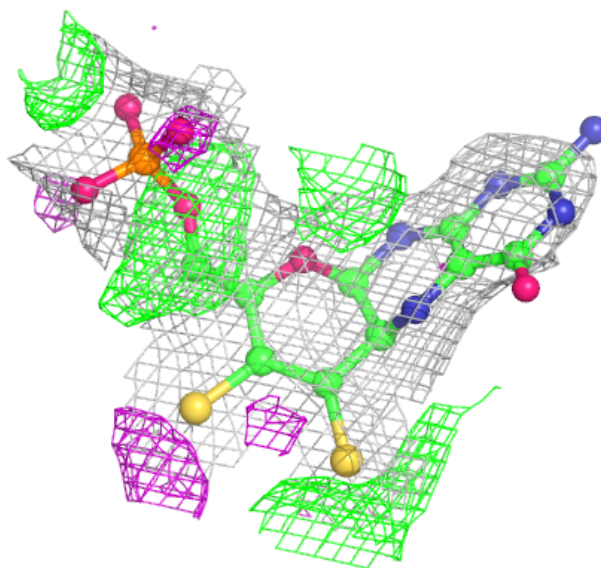
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MTE	B	703	24/24	0.96	0.23	41,54,59,65	0
7	MG	B	706	1/1	0.96	0.41	59,59,59,59	0
5	MTE	D	703	24/24	0.96	0.22	34,54,66,66	0
4	SF4	A	702	8/8	0.97	0.15	85,98,123,150	0
3	UNL	A	701	1/-	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
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.

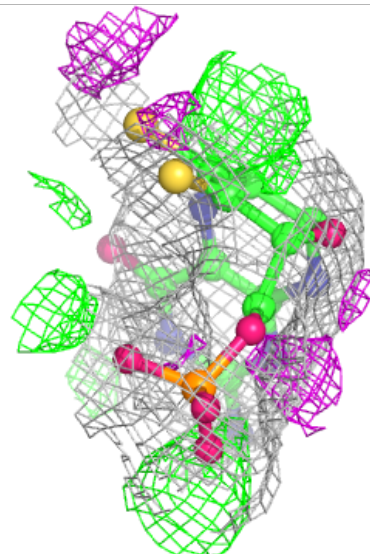
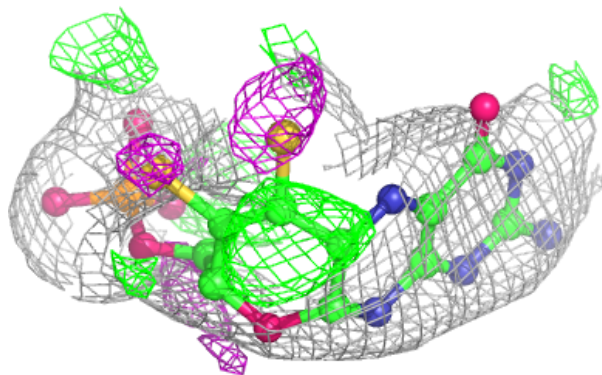
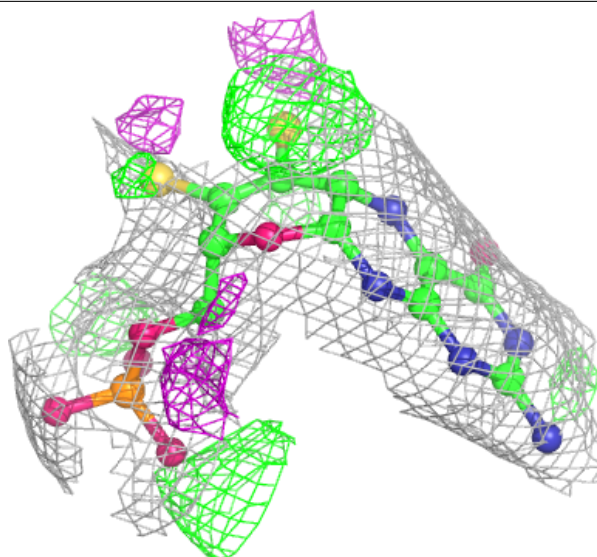
**Electron density around MTE A 703:**

$2mF_o-DF_c$  (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:**

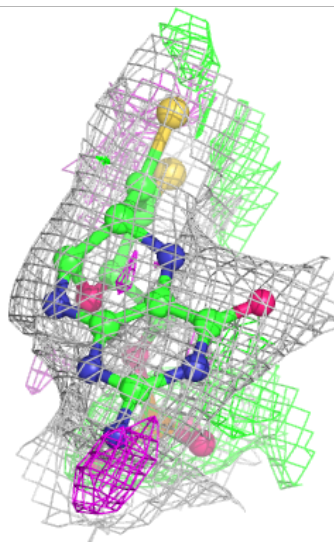
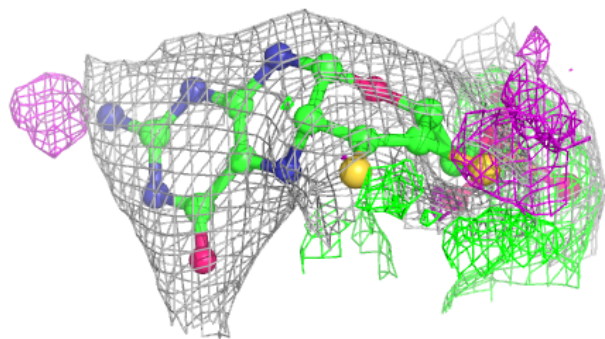
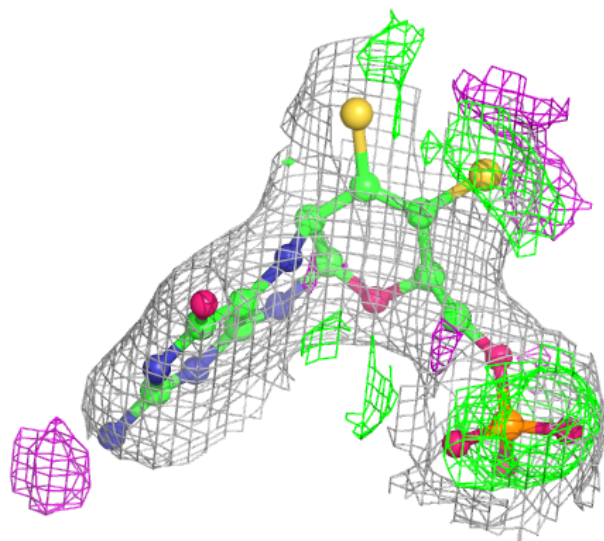
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





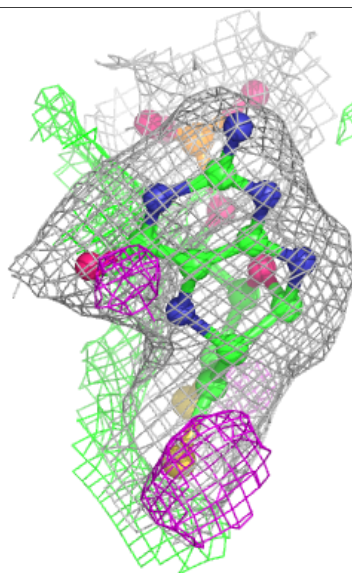
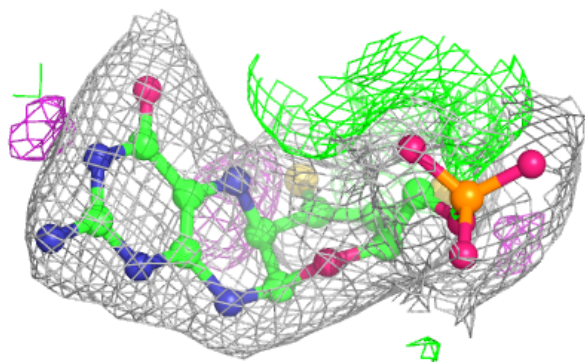
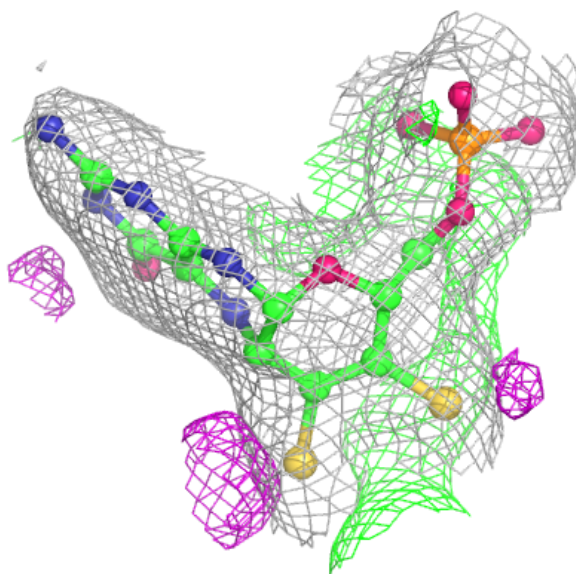
**Electron density around MTE C 704:**

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



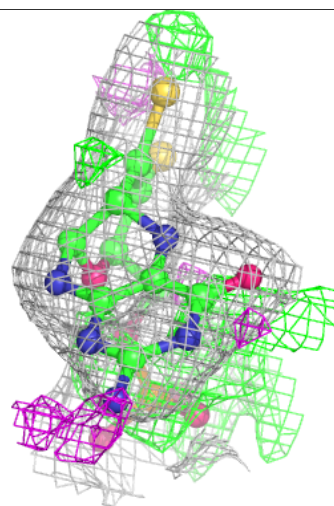
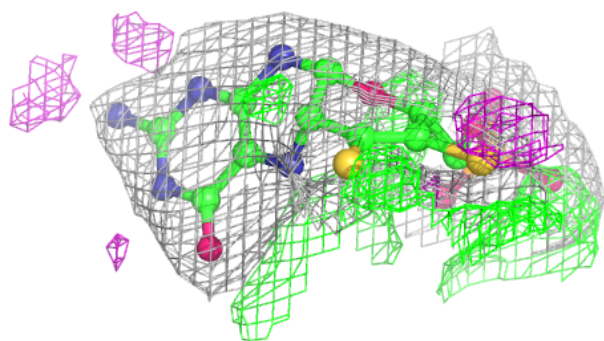
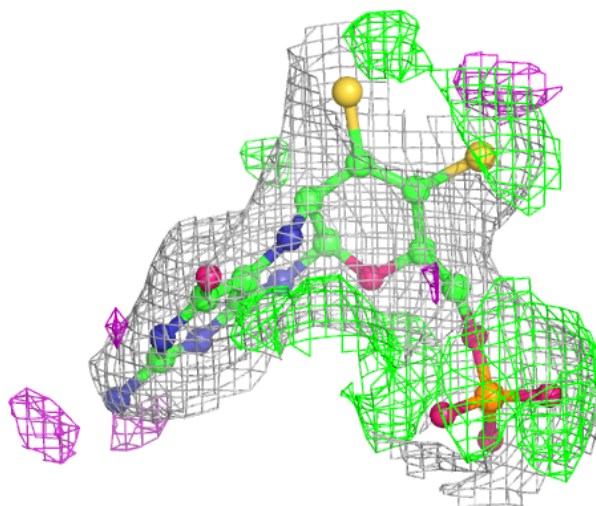
**Electron density around MTE B 704:**

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



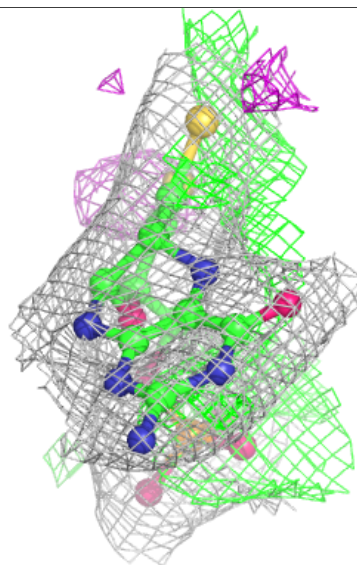
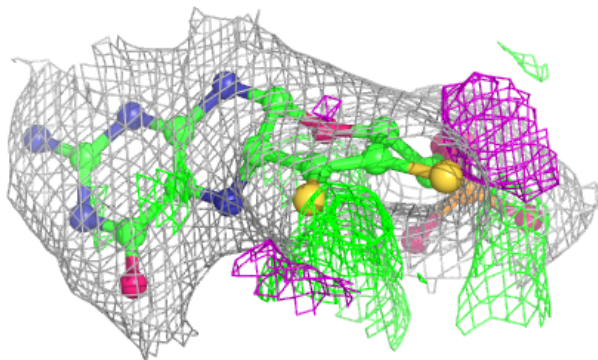
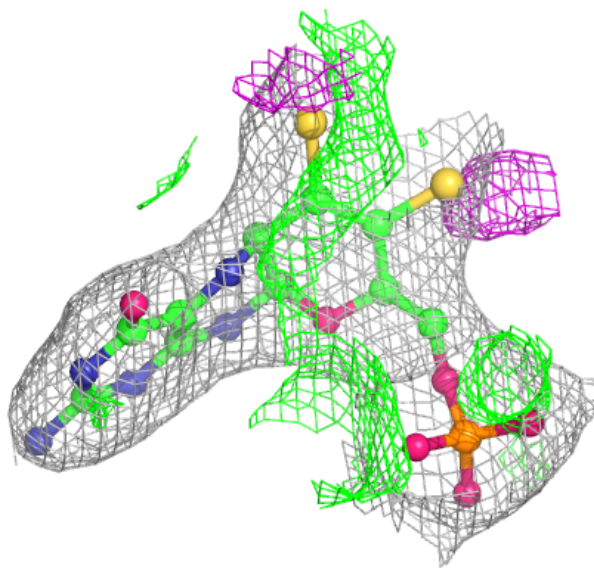
**Electron density around MTE D 704:**

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



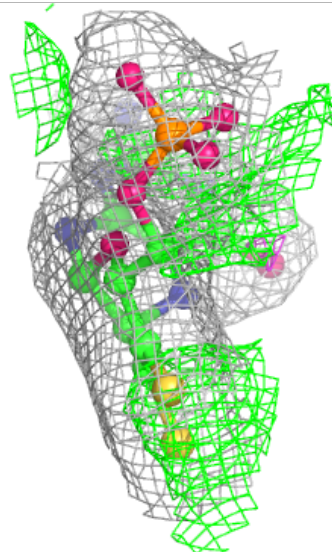
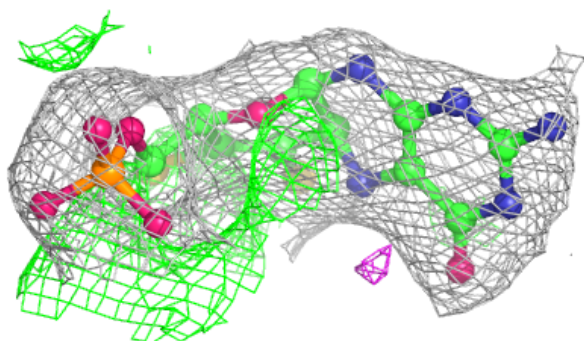
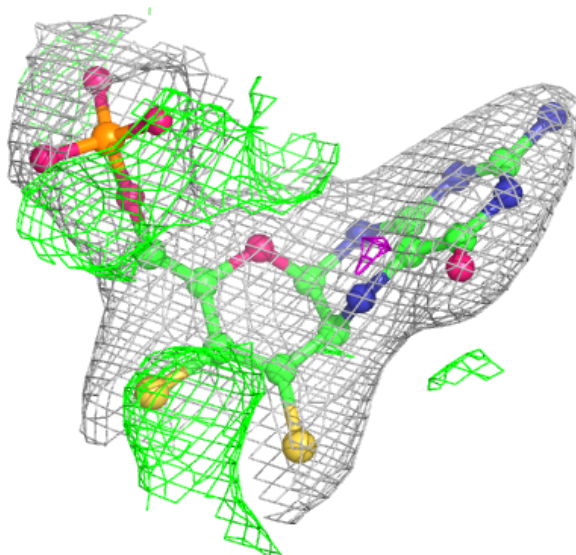
**Electron density around MTE C 703:**

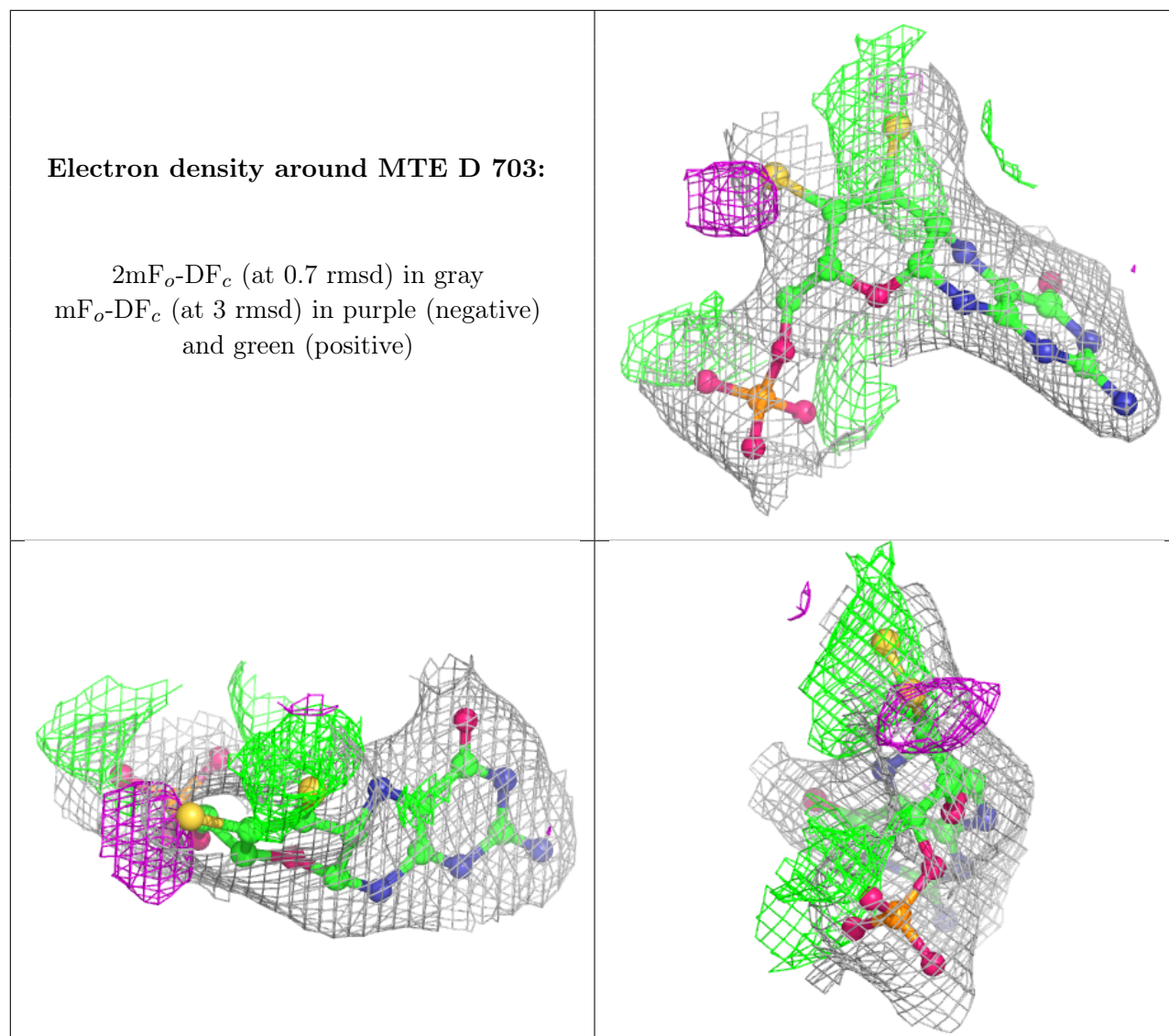
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.