Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 04:29 pm GMT

PDB ID	:	4Z3Z
Title	:	Active site complex BamBC of Benzoyl Coenzyme A reductase in complex with Zinc
Authors	:	Weinert, T.; Kung, J.W.; Weidenweber, S.; Huwiler, S.G.; Boll, M.; Ermler, U.
Deposited on	:	2015-04-01
Resolution	:	2.67 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

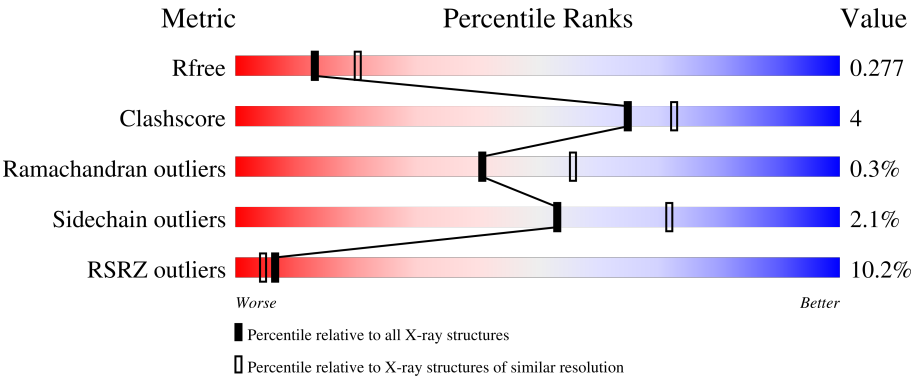
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	35% 88% 12%
1	B	653	3% 89% 10%
1	C	653	6% 88% 11%
1	D	653	4% 87% 12%

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Mol	Chain	Length	Quality of chain
2	E	179	5% 74% 16% 9%
2	F	179	7% 78% 16% 5%
2	G	179	% 78% 16% 6%
2	H	179	% 79% 11% 10%

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
4	SF4	D	702	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 26146 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	0	0	0
			5180	3308	875	963	34			
1	B	652	Total	C	N	O	S	0	0	0
			5180	3308	875	963	34			
1	C	652	Total	C	N	O	S	0	0	0
			5180	3308	875	963	34			
1	D	652	Total	C	N	O	S	0	0	0
			5180	3308	875	963	34			

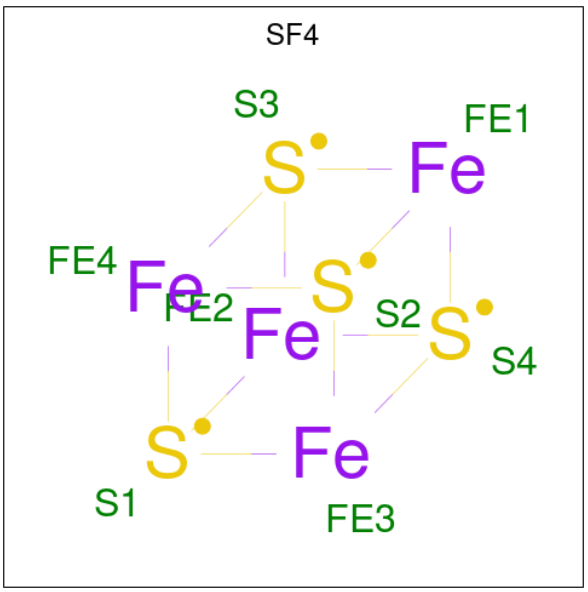
- Molecule 2 is a protein called Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	163	Total	C	N	O	S	0	0	0
			1237	769	218	236	14			
2	F	170	Total	C	N	O	S	0	1	0
			1317	816	226	261	14			
2	G	169	Total	C	N	O	S	0	2	0
			1315	814	228	259	14			
2	H	161	Total	C	N	O	S	0	0	0
			1221	758	213	236	14			

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

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

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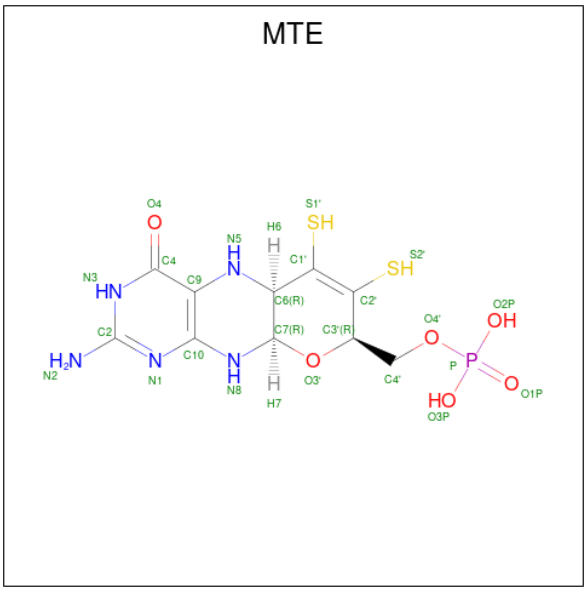
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Fe S 8 4 4	0	0
4	H	1	Total Fe S 8 4 4	0	0
4	H	1	Total Fe S 8 4 4	0	0

- 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 C N O P S 24 10 5 6 1 2	0	0
5	A	1	Total C N O P S 24 10 5 6 1 2	0	0
5	B	1	Total C N O P S 24 10 5 6 1 2	0	0
5	B	1	Total C N O P S 24 10 5 6 1 2	0	0
5	C	1	Total C N O P S 24 10 5 6 1 2	0	0
5	C	1	Total C N O P S 24 10 5 6 1 2	0	0
5	D	1	Total C N O P S 24 10 5 6 1 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).

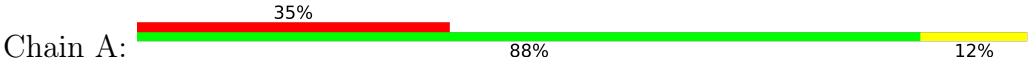
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0
8	B	1	Total Zn 1 1	0	0
8	C	1	Total Zn 1 1	0	0
8	D	1	Total Zn 1 1	0	0

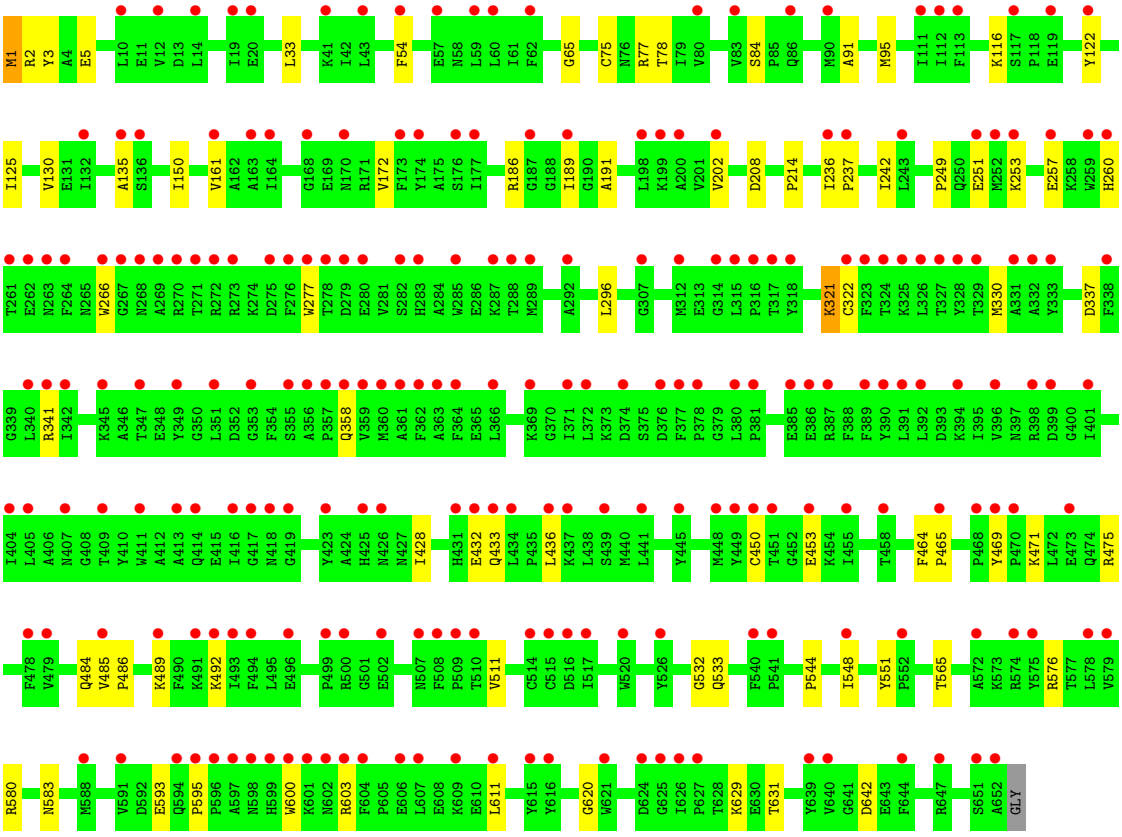
3 Residue-property plots (i)

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

• Molecule 1: Benzoyl-CoA reductase, putative

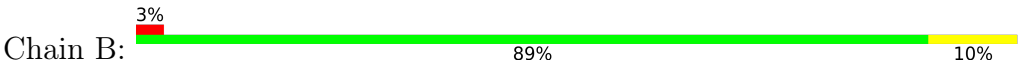
Chain A:

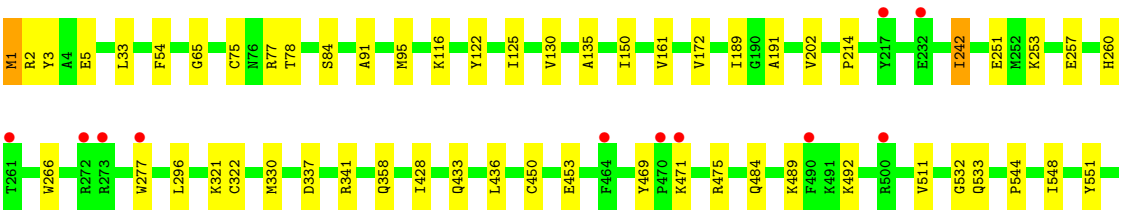


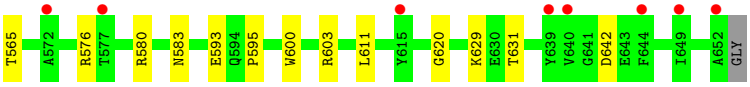


• Molecule 1: Benzoyl-CoA reductase, putative

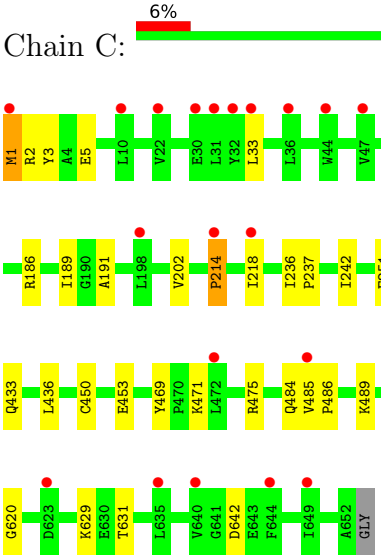
Chain B:



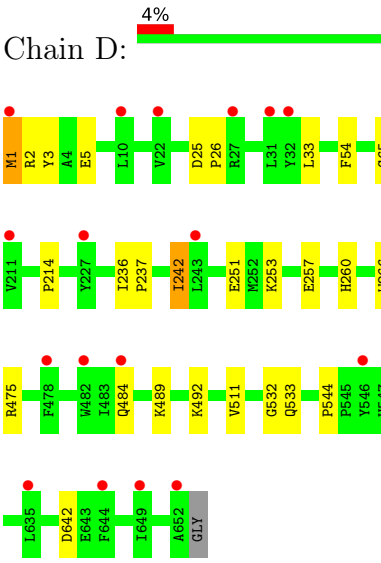




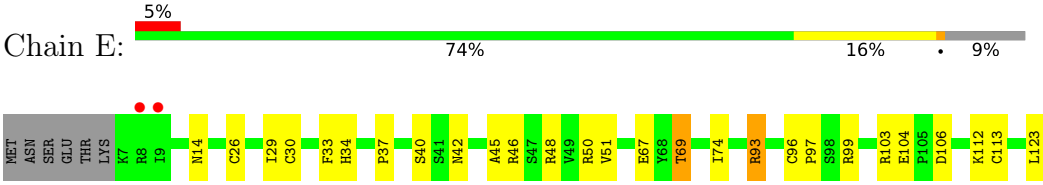
• Molecule 1: Benzoyl-CoA reductase, putative

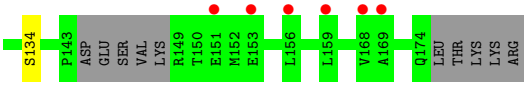


• Molecule 1: Benzoyl-CoA reductase, putative



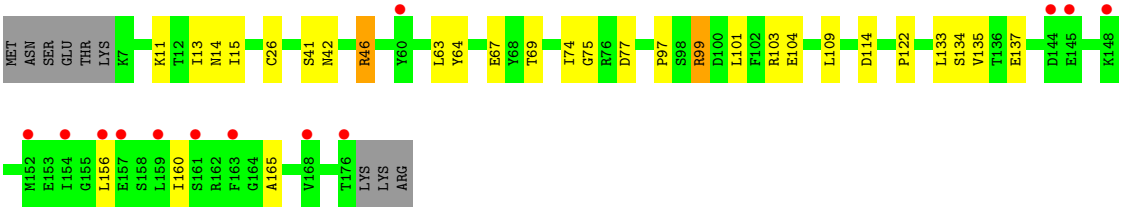
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein





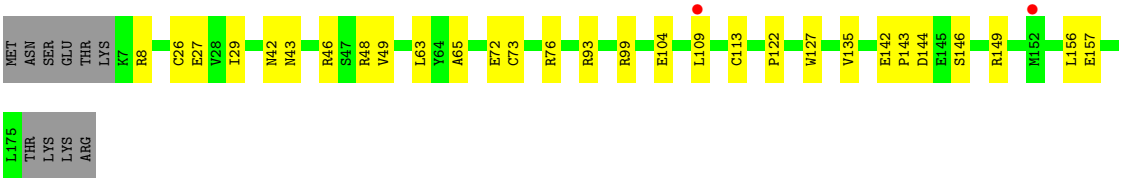
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain F:



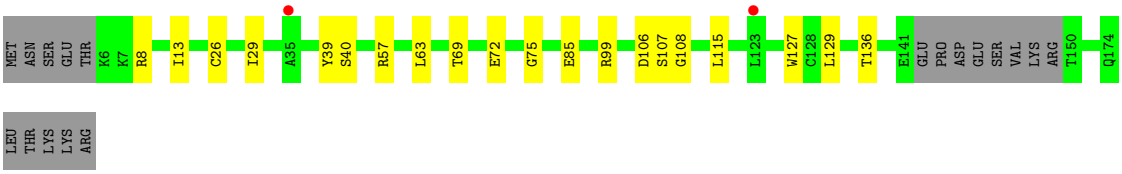
• Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.24Å 117.43Å 143.08Å 90.00° 111.04° 90.00°	Depositor
Resolution (Å)	82.51 – 2.67 82.51 – 2.67	Depositor EDS
% Data completeness (in resolution range)	97.2 (82.51-2.67) 97.4 (82.51-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.232 , 0.274 0.237 , 0.277	Depositor DCC
R_{free} test set	1393 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26146	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.23	0/5306	0.39	0/7172
1	B	0.23	0/5306	0.39	0/7172
1	C	0.23	0/5306	0.39	0/7172
1	D	0.23	0/5306	0.39	0/7172
2	E	0.26	0/1259	0.42	0/1705
2	F	0.27	0/1343	0.44	0/1819
2	G	0.26	0/1344	0.44	0/1819
2	H	0.24	0/1242	0.41	0/1681
All	All	0.24	0/26412	0.40	0/35712

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

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	5110	41	0
1	B	5180	0	5110	33	0
1	C	5180	0	5110	39	0
1	D	5180	0	5110	43	0
2	E	1237	0	1181	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1317	0	1266	16	0
2	G	1315	0	1263	18	0
2	H	1221	0	1158	13	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	2	0
4	E	24	0	0	2	0
4	F	24	0	0	1	0
4	G	24	0	0	2	0
4	H	24	0	0	1	0
5	A	48	0	20	4	0
5	B	48	0	20	1	0
5	C	48	0	20	3	0
5	D	48	0	20	1	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
All	All	26146	0	25388	210	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 4.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:73:CYS:HB2	4:G:1003:SF4:S1	2.03	0.97
3:C:701:UNL:X	5:C:703:MTE:S1'	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:HIS:NE2	4:E:1002:SF4:S1	2.57	0.77
1:D:299:CYS:HB2	4:D:702:SF4:S3	2.29	0.73
1:A:322:CYS:HB3	5:A:704:MTE:S1'	2.30	0.70
2:G:72:GLU:OE1	2:G:76:ARG:NH2	2.21	0.70
1:B:84:SER:HB2	1:B:91:ALA:HB2	1.74	0.69
1:D:84:SER:HB2	1:D:91:ALA:HB2	1.74	0.69
1:A:84:SER:HB2	1:A:91:ALA:HB2	1.74	0.68
1:C:84:SER:HB2	1:C:91:ALA:HB2	1.74	0.68
2:E:93:ARG:NH1	2:F:75:GLY:O	2.31	0.64
2:F:122:PRO:HG2	2:F:135:VAL:HG11	1.79	0.63
1:D:251:GLU:OE1	1:D:260:HIS:HE1	1.80	0.62
2:E:112:LYS:HE2	2:F:74:ILE:HG13	1.81	0.62
1:A:251:GLU:OE1	1:A:260:HIS:HE1	1.80	0.62
1:C:251:GLU:OE1	1:C:260:HIS:HE1	1.80	0.62
1:A:321:LYS:HD3	5:A:703:MTE:H4'2	1.82	0.62
1:A:484:GLN:HG2	1:A:544:PRO:HD2	1.82	0.62
2:G:93:ARG:NH1	2:H:75:GLY:O	2.29	0.62
2:G:72:GLU:OE2	2:H:8:ARG:NH2	2.29	0.62
1:D:484:GLN:HG2	1:D:544:PRO:HD2	1.82	0.61
1:C:484:GLN:HG2	1:C:544:PRO:HD2	1.82	0.61
1:B:251:GLU:OE1	1:B:260:HIS:HE1	1.80	0.61
1:B:484:GLN:HG2	1:B:544:PRO:HD2	1.82	0.61
1:D:629:LYS:NZ	1:D:642:ASP:OD1	2.35	0.60
1:C:629:LYS:NZ	1:C:642:ASP:OD1	2.35	0.60
1:B:629:LYS:NZ	1:B:642:ASP:OD1	2.35	0.60
2:F:11:LYS:HG2	2:F:137:GLU:HG2	1.84	0.60
1:A:629:LYS:NZ	1:A:642:ASP:OD1	2.35	0.59
2:F:99:ARG:HG3	2:F:101:LEU:HB2	1.85	0.59
2:E:106:ASP:OD1	2:E:106:ASP:N	2.35	0.59
1:C:161:VAL:HG22	1:C:202:VAL:HG22	1.85	0.59
1:A:161:VAL:HG22	1:A:202:VAL:HG22	1.85	0.58
1:B:161:VAL:HG22	1:B:202:VAL:HG22	1.85	0.58
1:A:511:VAL:HG13	1:A:611:LEU:HD23	1.85	0.58
1:D:161:VAL:HG22	1:D:202:VAL:HG22	1.85	0.58
2:G:104:GLU:HG3	2:G:109:LEU:HB2	1.86	0.58
1:B:511:VAL:HG13	1:B:611:LEU:HD23	1.85	0.58
1:D:511:VAL:HG13	1:D:611:LEU:HD23	1.85	0.57
1:C:511:VAL:HG13	1:C:611:LEU:HD23	1.85	0.56
1:D:150:ILE:HG21	1:D:202:VAL:HG21	1.88	0.56
1:B:150:ILE:HG21	1:B:202:VAL:HG21	1.88	0.55
1:C:150:ILE:HG21	1:C:202:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:SD	1:B:2:ARG:N	2.79	0.55
1:D:620:GLY:HA3	1:D:631:THR:HG21	1.89	0.54
1:A:150:ILE:HG21	1:A:202:VAL:HG21	1.88	0.54
1:B:620:GLY:HA3	1:B:631:THR:HG21	1.89	0.54
1:C:620:GLY:HA3	1:C:631:THR:HG21	1.89	0.54
1:A:620:GLY:HA3	1:A:631:THR:HG21	1.89	0.54
1:D:358:GLN:NE2	1:D:433:GLN:O	2.40	0.54
1:D:303:PRO:HG3	2:E:129:LEU:HD22	1.89	0.54
1:D:75:CYS:HA	1:D:533:GLN:HA	1.90	0.54
1:A:489:LYS:HA	1:A:492:LYS:HD2	1.90	0.53
1:B:489:LYS:HA	1:B:492:LYS:HD2	1.90	0.53
1:C:75:CYS:HA	1:C:533:GLN:HA	1.90	0.53
1:D:489:LYS:HA	1:D:492:LYS:HD2	1.90	0.53
1:C:358:GLN:NE2	1:C:433:GLN:O	2.40	0.53
2:H:57:ARG:NH1	2:H:85:GLU:O	2.41	0.53
1:D:1:MET:SD	1:D:2:ARG:N	2.79	0.53
1:C:1:MET:SD	1:C:2:ARG:N	2.79	0.53
1:C:489:LYS:HA	1:C:492:LYS:HD2	1.90	0.53
1:B:75:CYS:HA	1:B:533:GLN:HA	1.90	0.52
1:A:75:CYS:HA	1:A:533:GLN:HA	1.90	0.52
2:E:30:CYS:SG	2:E:34:HIS:ND1	2.83	0.52
2:G:149:ARG:NH1	2:G:157:GLU:OE1	2.42	0.52
2:H:106:ASP:OD1	2:H:106:ASP:N	2.37	0.51
1:A:469:TYR:HB2	1:A:475:ARG:HG2	1.92	0.51
2:G:65:ALA:HB3	2:G:113:CYS:H	1.75	0.51
1:A:358:GLN:NE2	1:A:433:GLN:O	2.40	0.51
1:C:469:TYR:HB2	1:C:475:ARG:HG2	1.92	0.51
2:E:67:GLU:OE2	2:E:112:LYS:NZ	2.35	0.51
1:B:469:TYR:HB2	1:B:475:ARG:HG2	1.92	0.50
1:D:94:MET:O	5:D:704:MTE:O2P	2.30	0.50
1:A:1:MET:SD	1:A:2:ARG:N	2.79	0.50
2:E:69:THR:HB	2:F:67[B]:GLU:HG3	1.92	0.50
1:D:469:TYR:HB2	1:D:475:ARG:HG2	1.92	0.50
1:B:358:GLN:NE2	1:B:433:GLN:O	2.40	0.49
1:A:322:CYS:CB	5:A:704:MTE:S1'	2.86	0.49
1:C:303:PRO:HG3	2:H:129:LEU:HD22	1.94	0.49
2:E:46:ARG:NH2	2:E:104:GLU:OE1	2.44	0.49
1:D:125:ILE:HG12	1:D:130:VAL:HG13	1.95	0.49
2:G:29:ILE:HD13	2:G:127:TRP:CZ2	2.47	0.49
1:B:600:TRP:HB2	1:B:603:ARG:HD3	1.95	0.49
1:A:125:ILE:HG12	1:A:130:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:TRP:HB2	1:D:603:ARG:HD3	1.95	0.48
1:C:125:ILE:HG12	1:C:130:VAL:HG13	1.95	0.48
1:C:600:TRP:HB2	1:C:603:ARG:HD3	1.95	0.48
1:A:600:TRP:HB2	1:A:603:ARG:HD3	1.95	0.48
1:C:351:LEU:O	5:C:704:MTE:N2	2.42	0.48
1:B:3:TYR:O	1:B:5:GLU:N	2.47	0.48
1:B:322:CYS:HB3	5:B:704:MTE:S1'	2.54	0.48
1:B:125:ILE:HG12	1:B:130:VAL:HG13	1.95	0.48
2:E:74:ILE:HD12	2:F:114:ASP:HA	1.96	0.48
1:A:548:ILE:HG13	1:A:565:THR:HG23	1.96	0.47
1:A:186:ARG:NH2	1:A:432:GLU:O	2.34	0.47
1:D:186:ARG:NH2	1:D:432:GLU:O	2.34	0.47
2:E:48:ARG:HB3	2:E:113:CYS:HB2	1.97	0.47
1:A:249:PRO:HG2	3:A:701:UNL:X	2.43	0.47
2:G:122:PRO:HB3	4:G:1002:SF4:S2	2.55	0.46
2:G:48:ARG:HB3	2:G:113:CYS:HB2	1.97	0.46
1:C:548:ILE:HG13	1:C:565:THR:HG23	1.97	0.46
1:A:54:PHE:O	1:A:116:LYS:NZ	2.45	0.46
1:B:548:ILE:HG13	1:B:565:THR:HG23	1.96	0.46
1:D:548:ILE:HG13	1:D:565:THR:HG23	1.97	0.46
2:G:8:ARG:NH2	2:H:72:GLU:OE1	2.45	0.46
2:E:29:ILE:HG13	2:E:123:LEU:HB3	1.98	0.46
2:F:122:PRO:HB3	4:F:1002:SF4:S2	2.56	0.46
1:C:322:CYS:HB2	5:C:703:MTE:S2'	2.56	0.46
1:B:337:ASP:O	1:B:341:ARG:HG3	2.16	0.45
1:D:453:GLU:OE1	1:D:583:ASN:ND2	2.50	0.45
1:C:236:ILE:HA	1:C:237:PRO:HD3	1.82	0.45
2:G:65:ALA:O	2:G:93:ARG:NH2	2.50	0.45
1:A:337:ASP:O	1:A:341:ARG:HG3	2.16	0.45
1:B:266:TRP:CE3	1:B:330:MET:HA	2.52	0.45
1:D:266:TRP:CE3	1:D:330:MET:HA	2.52	0.45
2:F:97:PRO:HA	2:F:103:ARG:NH1	2.32	0.45
2:H:115:LEU:HA	4:H:1002:SF4:S1	2.56	0.45
1:A:3:TYR:O	1:A:5:GLU:N	2.47	0.45
1:D:511:VAL:HG13	1:D:611:LEU:HA	1.99	0.45
1:A:453:GLU:OE1	1:A:583:ASN:ND2	2.50	0.45
1:B:453:GLU:OE1	1:B:583:ASN:ND2	2.50	0.45
1:C:218:ILE:HG12	2:H:39:TYR:CE1	2.50	0.45
1:D:54:PHE:O	1:D:116:LYS:NZ	2.46	0.45
1:D:3:TYR:O	1:D:5:GLU:N	2.47	0.45
1:D:337:ASP:O	1:D:341:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ARG:NH2	1:C:432:GLU:O	2.34	0.45
1:C:266:TRP:CE3	1:C:330:MET:HA	2.52	0.45
1:C:511:VAL:HG13	1:C:611:LEU:HA	1.99	0.45
2:F:64:TYR:OH	2:F:133:LEU:HD13	2.17	0.45
1:A:266:TRP:CE3	1:A:330:MET:HA	2.52	0.44
1:A:511:VAL:HG13	1:A:611:LEU:HA	1.99	0.44
1:B:511:VAL:HG13	1:B:611:LEU:HA	1.99	0.44
1:D:253:LYS:HE2	1:D:296:LEU:HD13	1.99	0.44
1:A:253:LYS:HE2	1:A:296:LEU:HD13	1.99	0.44
1:B:253:LYS:HE2	1:B:296:LEU:HD13	1.99	0.44
1:C:3:TYR:O	1:C:5:GLU:N	2.47	0.44
1:C:337:ASP:O	1:C:341:ARG:HG3	2.17	0.44
1:C:453:GLU:OE1	1:C:583:ASN:ND2	2.50	0.44
1:D:65:GLY:HA3	1:D:532:GLY:HA3	2.00	0.44
1:C:253:LYS:HE2	1:C:296:LEU:HD13	1.99	0.44
2:F:104:GLU:HG3	2:F:109:LEU:HB2	2.00	0.44
1:A:65:GLY:HA3	1:A:532:GLY:HA3	2.00	0.44
2:H:29:ILE:HD13	2:H:127:TRP:CZ2	2.53	0.44
1:D:77:ARG:NH1	4:D:702:SF4:S3	2.88	0.43
1:A:580:ARG:NH1	1:A:593:GLU:OE2	2.45	0.43
2:F:14:ASN:HB2	2:F:134:SER:OG	2.18	0.43
2:E:37:PRO:HG2	2:E:40:SER:HB3	2.00	0.43
2:G:43:ASN:HD22	2:G:46:ARG:NH1	2.16	0.43
1:B:54:PHE:O	1:B:116:LYS:NZ	2.45	0.43
1:B:580:ARG:NH1	1:B:593:GLU:OE2	2.45	0.43
1:D:580:ARG:NH1	1:D:593:GLU:OE2	2.45	0.43
1:A:464:PHE:HA	1:A:465:PRO:HD3	1.94	0.43
1:C:65:GLY:HA3	1:C:532:GLY:HA3	2.00	0.43
2:G:156:LEU:HD23	2:G:156:LEU:HA	1.84	0.43
1:B:242:ILE:H	1:B:242:ILE:HG12	1.56	0.43
1:B:257:GLU:HB2	1:B:277:TRP:CH2	2.54	0.42
1:D:78:THR:HB	1:D:95:MET:HG2	2.01	0.42
2:E:34:HIS:CE1	2:E:48:ARG:HD3	2.53	0.42
1:B:65:GLY:HA3	1:B:532:GLY:HA3	2.00	0.42
1:C:214:PRO:HG3	2:H:40:SER:HA	2.00	0.42
1:D:71:PRO:HD3	2:E:42:ASN:ND2	2.33	0.42
1:B:78:THR:HB	1:B:95:MET:HG2	2.01	0.42
2:E:33:PHE:HB2	2:E:123:LEU:HD22	2.01	0.42
1:A:78:THR:HB	1:A:95:MET:HG2	2.01	0.42
1:C:257:GLU:HB2	1:C:277:TRP:CH2	2.54	0.42
1:D:236:ILE:HA	1:D:237:PRO:HD3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLU:HB2	1:D:277:TRP:CH2	2.54	0.42
1:C:485:VAL:HA	1:C:486:PRO:HD3	1.91	0.42
1:A:208:ASP:OD1	2:F:46:ARG:NH1	2.52	0.42
1:A:257:GLU:HB2	1:A:277:TRP:CH2	2.54	0.42
1:D:464:PHE:HA	1:D:465:PRO:HD3	1.93	0.42
1:A:428:ILE:HD11	1:A:595:PRO:HA	2.02	0.42
1:C:78:THR:HB	1:C:95:MET:HG2	2.01	0.42
1:A:172:VAL:O	1:A:191:ALA:HB2	2.20	0.41
1:A:485:VAL:HA	1:A:486:PRO:HD3	1.91	0.41
1:B:172:VAL:O	1:B:191:ALA:HB2	2.20	0.41
1:D:172:VAL:O	1:D:191:ALA:HB2	2.20	0.41
1:D:122:TYR:HD2	1:D:135:ALA:HB2	1.85	0.41
1:C:172:VAL:O	1:C:191:ALA:HB2	2.20	0.41
1:D:450:CYS:SG	1:D:595:PRO:HD3	2.61	0.41
2:E:14:ASN:HB2	2:E:134:SER:O	2.21	0.41
2:E:51:VAL:HG21	4:E:1001:SF4:S2	2.60	0.41
2:F:77:ASP:OD1	2:F:77:ASP:N	2.45	0.41
2:G:142:GLU:HA	2:G:143:PRO:HD3	1.86	0.41
1:A:95:MET:HA	5:A:703:MTE:O3P	2.21	0.41
1:B:122:TYR:HD2	1:B:135:ALA:HB2	1.85	0.41
2:F:13:ILE:O	2:F:15:ILE:HG13	2.20	0.41
1:B:450:CYS:SG	1:B:595:PRO:HD3	2.61	0.41
1:C:450:CYS:SG	1:C:595:PRO:HD3	2.61	0.41
2:E:29:ILE:HD13	2:E:127:TRP:CZ2	2.56	0.41
1:A:122:TYR:HD2	1:A:135:ALA:HB2	1.85	0.41
2:H:63:LEU:HD23	2:H:63:LEU:HA	1.89	0.41
1:B:428:ILE:HD11	1:B:595:PRO:HA	2.03	0.41
2:G:144:ASP:OD1	2:G:146:SER:OG	2.25	0.41
1:C:122:TYR:HD2	1:C:135:ALA:HB2	1.85	0.41
1:D:25:ASP:HA	1:D:26:PRO:HD2	1.92	0.41
1:D:428:ILE:HD11	1:D:595:PRO:HA	2.02	0.41
2:G:76:ARG:O	2:H:13:ILE:N	2.38	0.41
1:D:619:LYS:HA	1:D:619:LYS:HD3	1.93	0.40
2:F:160:ILE:HG23	2:F:165:ALA:HA	2.02	0.40
1:A:236:ILE:HA	1:A:237:PRO:HD3	1.82	0.40
1:C:428:ILE:HD11	1:C:595:PRO:HA	2.02	0.40
2:E:45:ALA:HA	2:E:50:ARG:NH1	2.36	0.40
1:A:450:CYS:SG	1:A:595:PRO:HD3	2.61	0.40
1:C:218:ILE:HG12	2:H:39:TYR:CD1	2.57	0.40
1:D:242:ILE:H	1:D:242:ILE:HG12	1.56	0.40
2:G:27:GLU:HG2	2:G:49:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ARG:NH1	1:C:593:GLU:OE2	2.45	0.40
1:D:441:LEU:HA	1:D:600:TRP:CD1	2.56	0.40
2:E:97:PRO:HA	2:E:103:ARG:NH1	2.37	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%)	614 (94%)	34 (5%)	2 (0%)	41	56
1	B	650/653 (100%)	613 (94%)	35 (5%)	2 (0%)	41	56
1	C	650/653 (100%)	613 (94%)	35 (5%)	2 (0%)	41	56
1	D	650/653 (100%)	613 (94%)	35 (5%)	2 (0%)	41	56
2	E	159/179 (89%)	151 (95%)	8 (5%)	0	100	100
2	F	169/179 (94%)	157 (93%)	11 (6%)	1 (1%)	25	37
2	G	169/179 (94%)	154 (91%)	15 (9%)	0	100	100
2	H	157/179 (88%)	146 (93%)	9 (6%)	2 (1%)	12	18
All	All	3254/3328 (98%)	3061 (94%)	182 (6%)	11 (0%)	41	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	107	SER
1	A	33	LEU
1	B	33	LEU
1	C	33	LEU
1	D	33	LEU
2	F	42	ASN
1	A	214	PRO

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Mol	Chain	Res	Type
1	B	214	PRO
1	C	214	PRO
1	D	214	PRO
2	H	108	GLY

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%)	537 (98%)	9 (2%)	62	78
1	B	546/548 (100%)	537 (98%)	9 (2%)	62	78
1	C	546/548 (100%)	537 (98%)	9 (2%)	62	78
1	D	546/548 (100%)	537 (98%)	9 (2%)	62	78
2	E	134/159 (84%)	129 (96%)	5 (4%)	34	50
2	F	148/159 (93%)	141 (95%)	7 (5%)	26	40
2	G	147/159 (92%)	142 (97%)	5 (3%)	37	53
2	H	132/159 (83%)	128 (97%)	4 (3%)	41	59
All	All	2745/2828 (97%)	2688 (98%)	57 (2%)	53	72

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	77	ARG
1	A	189	ILE
1	A	242	ILE
1	A	321	LYS
1	A	436	LEU
1	A	471	LYS
1	A	551	TYR
1	A	576	ARG
1	B	1	MET
1	B	77	ARG

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Mol	Chain	Res	Type
1	B	189	ILE
1	B	242	ILE
1	B	321	LYS
1	B	436	LEU
1	B	471	LYS
1	B	551	TYR
1	B	576	ARG
1	C	1	MET
1	C	77	ARG
1	C	189	ILE
1	C	242	ILE
1	C	321	LYS
1	C	436	LEU
1	C	471	LYS
1	C	551	TYR
1	C	576	ARG
1	D	1	MET
1	D	77	ARG
1	D	189	ILE
1	D	242	ILE
1	D	321	LYS
1	D	436	LEU
1	D	471	LYS
1	D	551	TYR
1	D	576	ARG
2	E	26	CYS
2	E	69	THR
2	E	93	ARG
2	E	96	CYS
2	E	99	ARG
2	F	26	CYS
2	F	41	SER
2	F	46	ARG
2	F	63	LEU
2	F	69	THR
2	F	99	ARG
2	F	156	LEU
2	G	26	CYS
2	G	42	ASN
2	G	63	LEU
2	G	99	ARG
2	G	135	VAL

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Mol	Chain	Res	Type
2	H	26	CYS
2	H	69	THR
2	H	99	ARG
2	H	136	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	GLN
1	B	463	GLN
1	C	463	GLN
1	D	463	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	F	1001	2	0,12,12	-	-	-		
5	MTE	A	704	6,7,5	21,26,26	2.76	10 (47%)	21,40,40	2.54	6 (28%)
5	MTE	A	703	6,7,5	21,26,26	3.00	10 (47%)	21,40,40	2.25	7 (33%)
4	SF4	H	1001	2	0,12,12	-	-	-		
4	SF4	D	702	1	0,12,12	-	-	-		
4	SF4	F	1003	2	0,12,12	-	-	-		
5	MTE	B	703	6,7	21,26,26	2.77	9 (42%)	21,40,40	1.97	6 (28%)
4	SF4	E	1001	2	0,12,12	-	-	-		
4	SF4	G	1003	2	0,12,12	-	-	-		
5	MTE	B	704	6,7	21,26,26	2.85	9 (42%)	21,40,40	2.47	4 (19%)
4	SF4	G	1002	2	0,12,12	-	-	-		
4	SF4	F	1002	2	0,12,12	-	-	-		
4	SF4	H	1002	2	0,12,12	-	-	-		
5	MTE	C	703	6,7	21,26,26	2.76	9 (42%)	21,40,40	2.21	4 (19%)
4	SF4	A	702	1	0,12,12	-	-	-		
4	SF4	H	1003	2	0,12,12	-	-	-		
5	MTE	D	704	6,7	21,26,26	2.72	9 (42%)	21,40,40	2.30	5 (23%)
4	SF4	E	1003	2	0,12,12	-	-	-		
4	SF4	G	1001	2	0,12,12	-	-	-		
4	SF4	C	702	1	0,12,12	-	-	-		
4	SF4	E	1002	2	0,12,12	-	-	-		
4	SF4	B	702	1	0,12,12	-	-	-		
5	MTE	C	704	6,7	21,26,26	2.82	10 (47%)	21,40,40	2.06	5 (23%)
5	MTE	D	703	6,7	21,26,26	2.68	10 (47%)	21,40,40	2.02	4 (19%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MTE	B	704	6,7	-	3/6/34/34	0/3/3/3
4	SF4	G	1002	2	-	-	0/6/5/5
4	SF4	F	1002	2	-	-	0/6/5/5
4	SF4	H	1002	2	-	-	0/6/5/5
5	MTE	C	703	6,7	-	0/6/34/34	0/3/3/3
4	SF4	A	702	1	-	-	0/6/5/5
4	SF4	H	1003	2	-	-	0/6/5/5
5	MTE	D	704	6,7	-	3/6/34/34	0/3/3/3
4	SF4	E	1003	2	-	-	0/6/5/5
4	SF4	G	1001	2	-	-	0/6/5/5
4	SF4	C	702	1	-	-	0/6/5/5
4	SF4	E	1002	2	-	-	0/6/5/5
4	SF4	B	702	1	-	-	0/6/5/5
5	MTE	C	704	6,7	-	3/6/34/34	0/3/3/3
5	MTE	D	703	6,7	-	2/6/34/34	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	MTE	C9-C10	-6.86	1.28	1.41
5	A	704	MTE	C9-C10	-6.63	1.28	1.41
5	A	703	MTE	C9-C10	-6.43	1.29	1.41
5	D	704	MTE	C9-C10	-6.32	1.29	1.41
5	C	704	MTE	C9-C10	-6.25	1.29	1.41
5	D	703	MTE	C9-C10	-6.23	1.29	1.41
5	B	703	MTE	C9-C10	-6.22	1.29	1.41
5	C	703	MTE	C9-C10	-6.20	1.29	1.41
5	B	704	MTE	C7-C6	-5.99	1.48	1.53
5	D	704	MTE	C9-C4	5.49	1.49	1.41
5	A	704	MTE	C9-C4	5.26	1.48	1.41
5	A	703	MTE	C7-C6	-5.25	1.49	1.53
5	A	703	MTE	C9-C4	5.21	1.48	1.41
5	C	704	MTE	C9-C4	5.18	1.48	1.41
5	B	703	MTE	C2-N2	4.94	1.43	1.33
5	A	703	MTE	C2-N2	4.93	1.43	1.33
5	A	704	MTE	C2-N2	4.89	1.43	1.33
5	C	703	MTE	C7-C6	-4.88	1.49	1.53
5	D	703	MTE	C2-N2	4.81	1.43	1.33
5	C	704	MTE	C2-N2	4.75	1.43	1.33
5	C	704	MTE	C7-C6	-4.73	1.49	1.53
5	B	703	MTE	C9-C4	4.71	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	703	MTE	C7-C6	-4.70	1.49	1.53
5	B	704	MTE	C2-N2	4.69	1.43	1.33
5	C	703	MTE	C2-N2	4.66	1.43	1.33
5	D	704	MTE	C2-N2	4.65	1.43	1.33
5	C	703	MTE	C9-C4	4.64	1.47	1.41
5	D	704	MTE	C7-C6	-4.48	1.50	1.53
5	A	703	MTE	O3'-C7	-4.09	1.37	1.43
5	D	703	MTE	C7-C6	-4.04	1.50	1.53
5	B	704	MTE	C9-C4	4.02	1.47	1.41
5	D	703	MTE	C9-C4	3.88	1.46	1.41
5	A	704	MTE	C7-C6	-3.78	1.50	1.53
5	B	703	MTE	O3'-C7	-3.73	1.38	1.43
5	C	703	MTE	O3'-C7	-3.47	1.38	1.43
5	D	703	MTE	O3'-C7	-3.42	1.38	1.43
5	A	703	MTE	C4-N3	3.38	1.38	1.33
5	C	704	MTE	O3'-C7	-3.36	1.38	1.43
5	A	703	MTE	O3'-C3'	-3.31	1.39	1.43
5	D	703	MTE	C4-N3	3.22	1.38	1.33
5	C	703	MTE	O3'-C3'	-3.17	1.39	1.43
5	C	704	MTE	C4-N3	3.15	1.38	1.33
5	D	704	MTE	C4-N3	3.15	1.38	1.33
5	C	703	MTE	C4-N3	3.12	1.38	1.33
5	A	704	MTE	C4-N3	3.11	1.38	1.33
5	A	704	MTE	O3'-C7	-3.07	1.39	1.43
5	B	704	MTE	O3'-C7	-3.07	1.39	1.43
5	B	704	MTE	C4-N3	3.04	1.38	1.33
5	B	704	MTE	O3'-C3'	-3.02	1.39	1.43
5	D	703	MTE	O3'-C3'	-3.00	1.39	1.43
5	B	703	MTE	C4-N3	2.88	1.38	1.33
5	C	704	MTE	C10-N1	2.86	1.40	1.34
5	C	704	MTE	O3'-C3'	-2.85	1.39	1.43
5	A	703	MTE	C10-N1	2.79	1.39	1.34
5	A	704	MTE	O3'-C3'	-2.75	1.40	1.43
5	A	703	MTE	C2-N3	2.68	1.40	1.35
5	D	704	MTE	C10-N1	2.67	1.39	1.34
5	B	703	MTE	C2-N3	2.64	1.40	1.35
5	A	704	MTE	C10-N1	2.63	1.39	1.34
5	D	704	MTE	O3'-C7	-2.62	1.40	1.43
5	C	703	MTE	C10-N1	2.60	1.39	1.34
5	D	703	MTE	C10-N1	2.59	1.39	1.34
5	B	703	MTE	C10-N1	2.58	1.39	1.34
5	D	703	MTE	C2-N3	2.55	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	704	MTE	C2-N3	2.47	1.39	1.35
5	B	703	MTE	O3'-C3'	-2.44	1.40	1.43
5	C	703	MTE	C2-N3	2.43	1.39	1.35
5	A	704	MTE	C2-N3	2.39	1.39	1.35
5	B	704	MTE	C10-N1	2.36	1.39	1.34
5	A	704	MTE	C9-N5	2.26	1.42	1.38
5	D	704	MTE	O3'-C3'	-2.25	1.40	1.43
5	B	704	MTE	C2-N3	2.22	1.39	1.35
5	D	704	MTE	C2-N3	2.21	1.39	1.35
5	C	704	MTE	C9-N5	2.05	1.42	1.38
5	A	703	MTE	C9-N5	2.05	1.42	1.38
5	D	703	MTE	C9-N5	2.01	1.42	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	703	MTE	C10-C9-C4	7.46	121.19	114.57
5	B	704	MTE	C10-C9-C4	7.44	121.18	114.57
5	C	704	MTE	C10-C9-C4	7.01	120.80	114.57
5	A	703	MTE	C10-C9-C4	7.00	120.79	114.57
5	D	704	MTE	C10-C9-C4	6.97	120.76	114.57
5	A	704	MTE	O3'-C7-C6	6.93	113.59	108.96
5	B	703	MTE	C10-C9-C4	6.92	120.72	114.57
5	D	703	MTE	C10-C9-C4	6.86	120.67	114.57
5	A	704	MTE	C10-C9-C4	5.82	119.74	114.57
5	B	704	MTE	O3'-C7-C6	-4.90	105.69	108.96
5	B	704	MTE	O3'-C7-N8	-4.70	103.73	108.57
5	A	704	MTE	O3'-C7-N8	-4.54	103.90	108.57
5	D	704	MTE	O3'-C7-C6	4.36	111.87	108.96
5	A	703	MTE	O3'-C7-N8	3.80	112.48	108.57
5	C	703	MTE	O3'-C7-C6	-3.56	106.59	108.96
5	C	704	MTE	O3'-C7-N8	-3.16	105.32	108.57
5	D	704	MTE	C2-N1-C10	3.05	121.38	114.54
5	A	704	MTE	C2-N1-C10	2.98	121.22	114.54
5	A	703	MTE	C2-N1-C10	2.97	121.20	114.54
5	B	704	MTE	C2-N1-C10	2.80	120.81	114.54
5	C	703	MTE	C2-N1-C10	2.75	120.71	114.54
5	C	704	MTE	C2-N1-C10	2.73	120.67	114.54
5	D	704	MTE	C9-C10-N8	2.72	120.62	118.13
5	B	703	MTE	C2-N1-C10	2.69	120.58	114.54
5	A	703	MTE	O3'-C7-C6	-2.68	107.18	108.96
5	D	704	MTE	C4-C9-N5	2.62	121.32	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	703	MTE	C9-C10-N8	2.58	120.49	118.13
5	A	704	MTE	C9-C10-N8	2.56	120.47	118.13
5	D	703	MTE	C2-N1-C10	2.53	120.21	114.54
5	D	703	MTE	O3'-C7-C6	-2.39	107.37	108.96
5	A	703	MTE	C9-C10-N8	2.37	120.30	118.13
5	A	703	MTE	C4-C9-N5	2.26	121.01	119.12
5	D	703	MTE	C9-C10-N8	2.19	120.14	118.13
5	C	704	MTE	O3'-C7-C6	2.18	110.42	108.96
5	A	704	MTE	N1-C2-N3	-2.09	122.14	125.42
5	B	703	MTE	C10-N8-C7	-2.08	119.60	123.67
5	C	704	MTE	C9-C10-N8	2.07	120.02	118.13
5	A	703	MTE	N1-C2-N3	-2.03	122.23	125.42
5	B	703	MTE	O3'-C7-C6	-2.03	107.61	108.96
5	B	703	MTE	N1-C2-N3	-2.02	122.25	125.42
5	B	703	MTE	C9-C10-N8	2.00	119.96	118.13

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	703	MTE	O3'-C3'-C4'-O4'
5	A	703	MTE	C4'-O4'-P-O2P
5	A	704	MTE	C4'-O4'-P-O1P
5	A	704	MTE	C4'-O4'-P-O2P
5	A	704	MTE	C4'-O4'-P-O3P
5	B	704	MTE	C4'-O4'-P-O2P
5	B	704	MTE	C4'-O4'-P-O3P
5	C	704	MTE	C4'-O4'-P-O1P
5	C	704	MTE	C4'-O4'-P-O2P
5	C	704	MTE	C4'-O4'-P-O3P
5	D	703	MTE	O3'-C3'-C4'-O4'
5	D	703	MTE	C4'-O4'-P-O2P
5	D	704	MTE	C4'-O4'-P-O1P
5	D	704	MTE	C4'-O4'-P-O2P
5	D	704	MTE	C4'-O4'-P-O3P
5	B	704	MTE	C4'-O4'-P-O1P

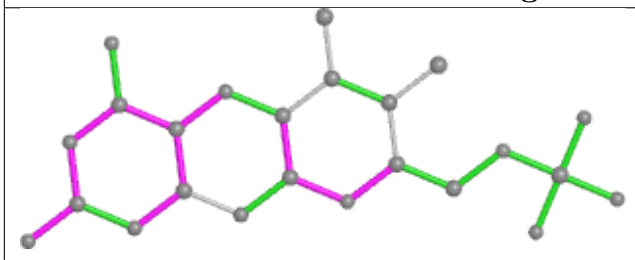
There are no ring outliers.

13 monomers are involved in 17 short contacts:

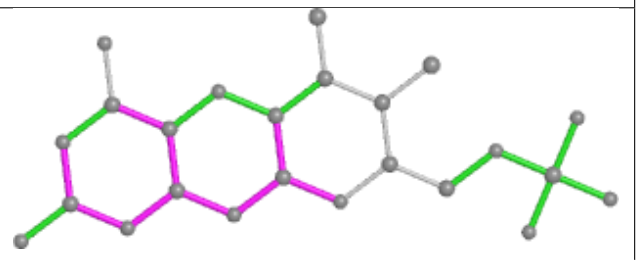
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	MTE	2	0
5	A	703	MTE	2	0
4	D	702	SF4	2	0
4	E	1001	SF4	1	0
4	G	1003	SF4	1	0
5	B	704	MTE	1	0
4	G	1002	SF4	1	0
4	F	1002	SF4	1	0
4	H	1002	SF4	1	0
5	C	703	MTE	2	0
5	D	704	MTE	1	0
4	E	1002	SF4	1	0
5	C	704	MTE	1	0

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

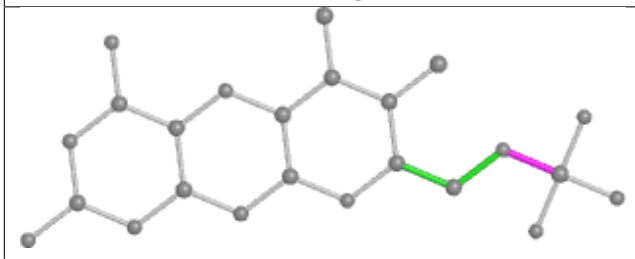
Ligand MTE A 704



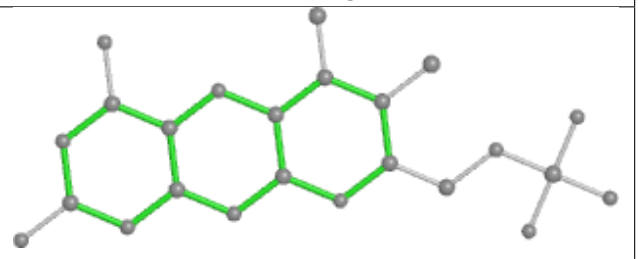
Bond lengths



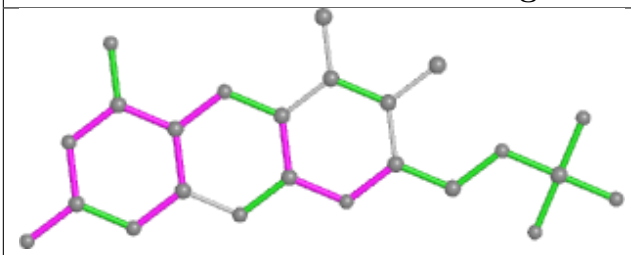
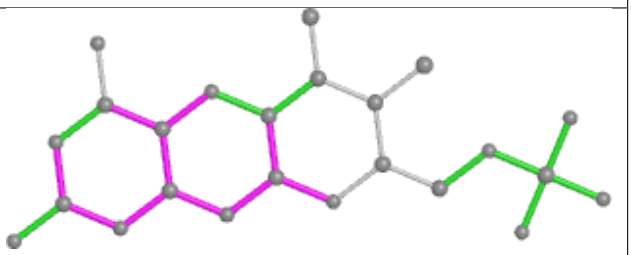
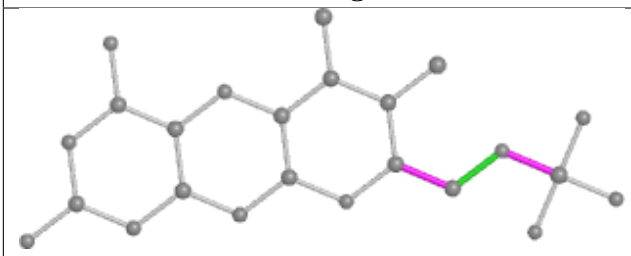
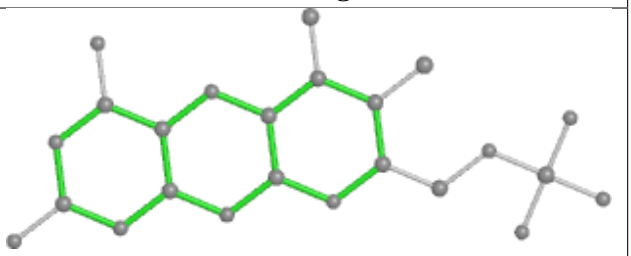
Bond angles

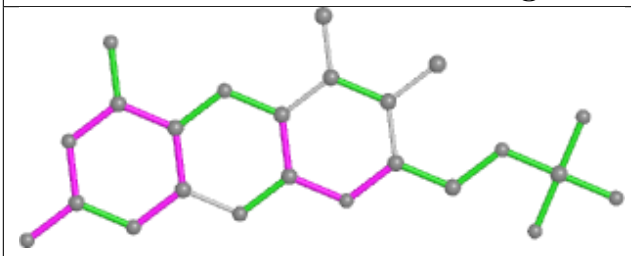
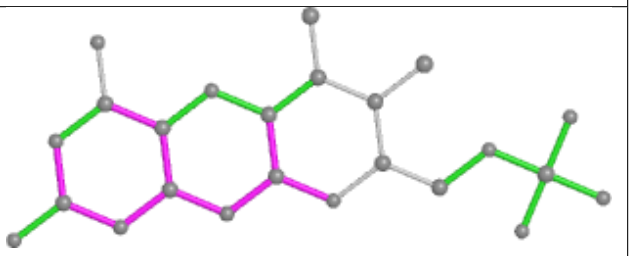
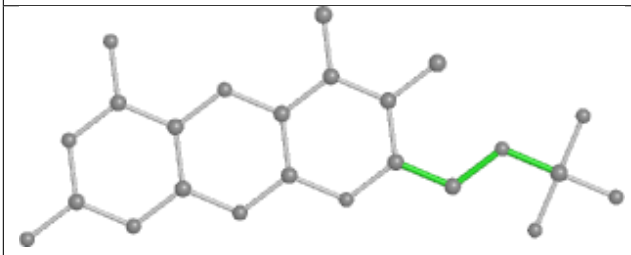
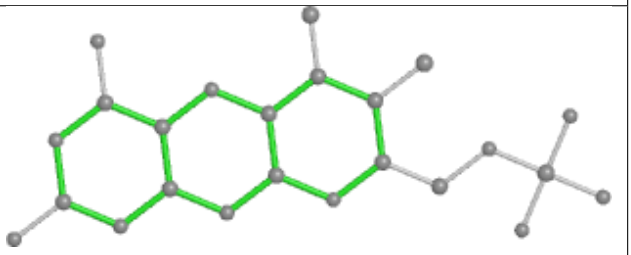


Torsions

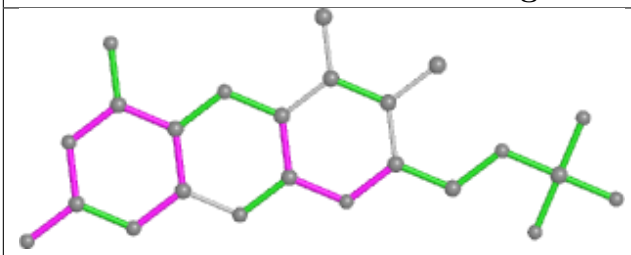


Rings

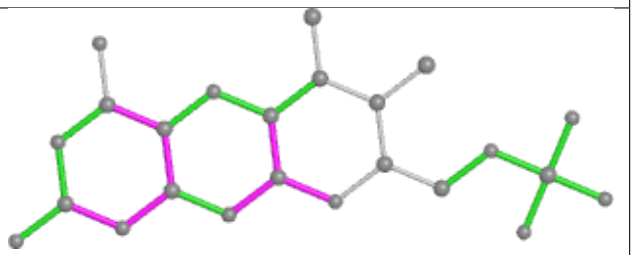
Ligand MTE A 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MTE B 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

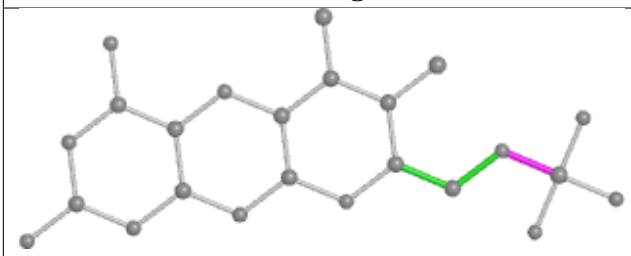
Ligand MTE B 704



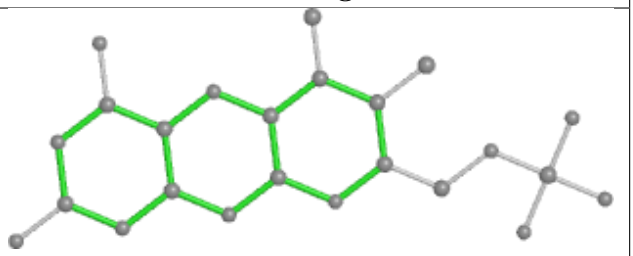
Bond lengths



Bond angles

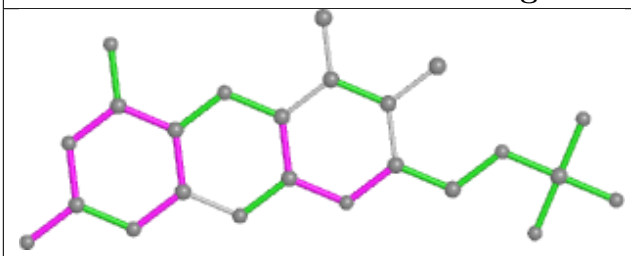


Torsions

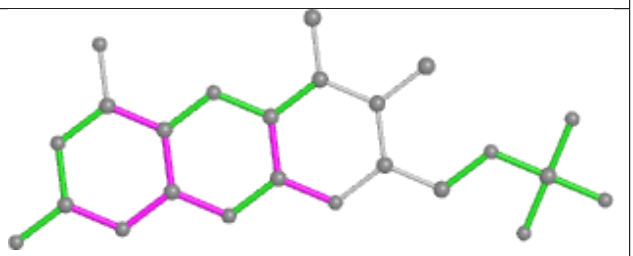


Rings

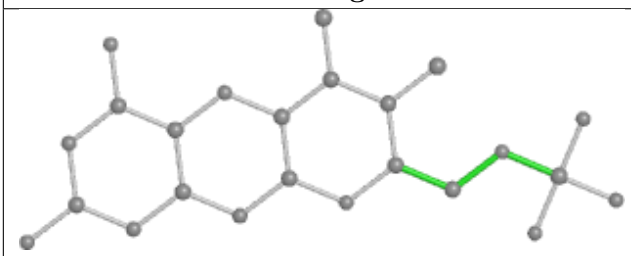
Ligand MTE C 703



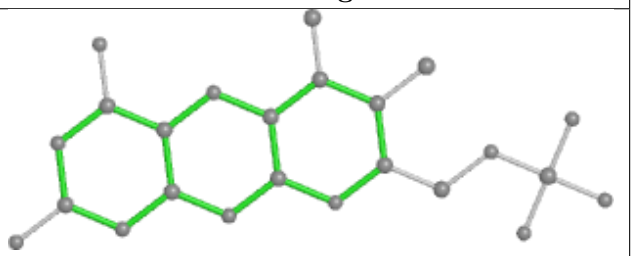
Bond lengths



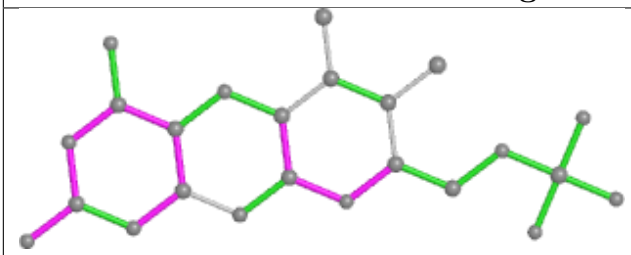
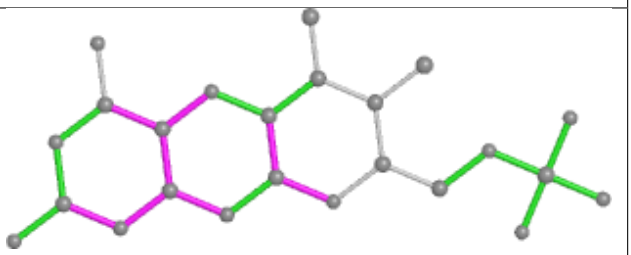
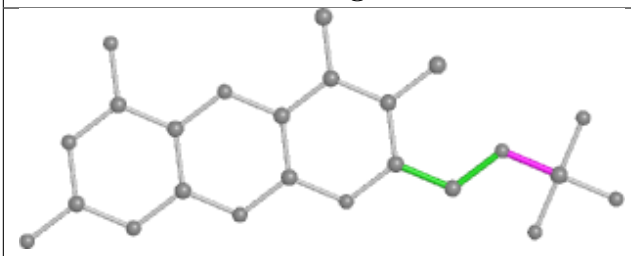
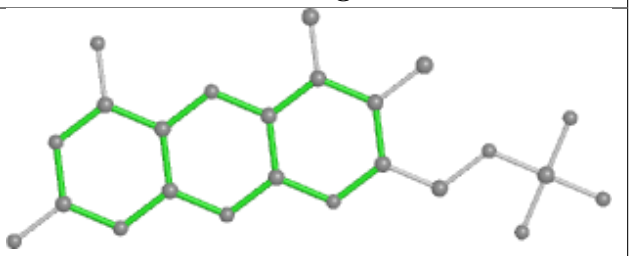
Bond angles

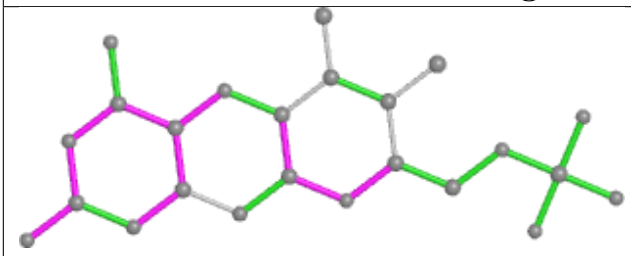
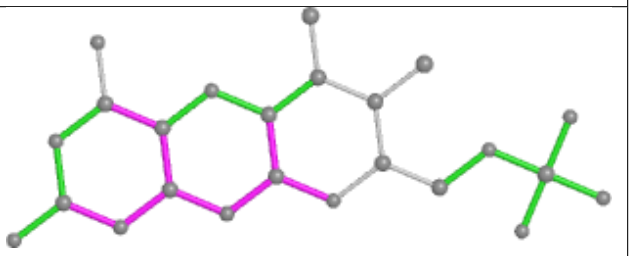
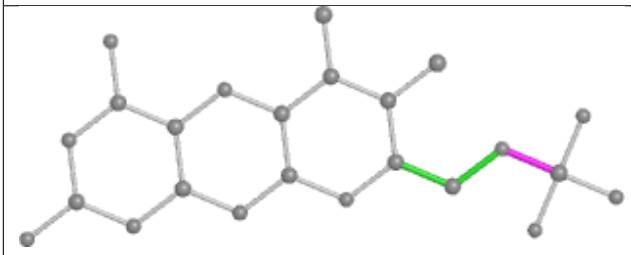
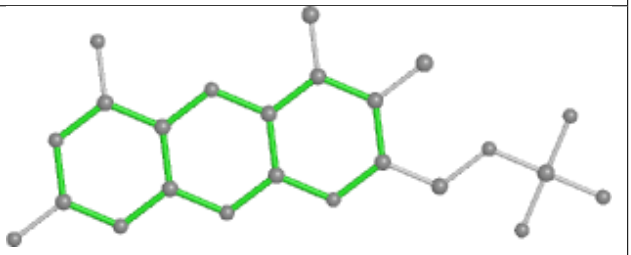


Torsions

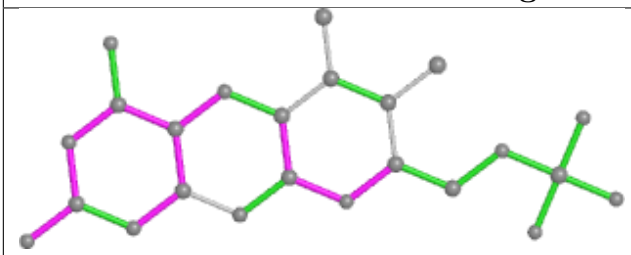


Rings

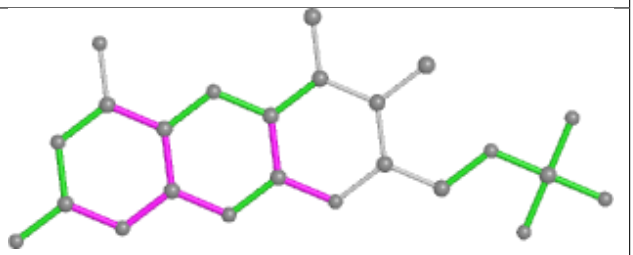
Ligand MTE D 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MTE C 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

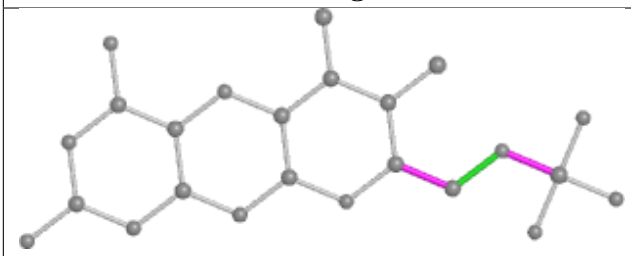
Ligand MTE D 703



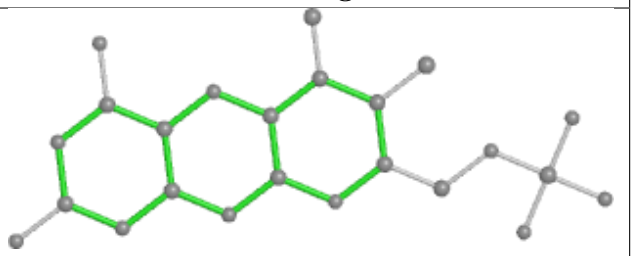
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	652/653 (99%)	1.84	229 (35%) 0 0	60, 173, 256, 390	0
1	B	652/653 (99%)	0.26	19 (2%) 51 48	51, 87, 147, 186	0
1	C	652/653 (99%)	0.34	36 (5%) 25 21	55, 103, 147, 175	0
1	D	652/653 (99%)	0.27	25 (3%) 40 36	45, 93, 145, 185	0
2	E	163/179 (91%)	0.27	9 (5%) 25 21	55, 101, 155, 188	0
2	F	170/179 (94%)	0.39	13 (7%) 13 11	48, 79, 164, 175	0
2	G	169/179 (94%)	0.10	2 (1%) 79 77	56, 92, 167, 178	0
2	H	161/179 (89%)	0.17	2 (1%) 79 77	58, 103, 145, 180	0
All	All	3271/3328 (98%)	0.59	335 (10%) 6 4	45, 103, 209, 390	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	ASP	11.8
1	A	434	LEU	11.0
1	A	357	PRO	10.7
1	A	423	TYR	10.7
1	A	362	PHE	9.7
1	A	611	LEU	9.4
1	A	325	LYS	9.2
1	A	269	ALA	9.1
1	A	625	GLY	9.0
1	A	591	VAL	8.8
1	A	366	LEU	8.4
1	A	272	ARG	8.0
1	A	364	PHE	8.0
1	A	331	ALA	7.9
1	A	606	GLU	7.9
1	A	579	VAL	7.8

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Mol	Chain	Res	Type	RSRZ
1	A	327	THR	7.7
1	A	289	MET	7.7
1	A	261	THR	7.3
1	A	627	PRO	7.2
1	A	377	PHE	7.2
1	A	276	PHE	7.2
1	A	418	ASN	7.1
1	A	361	ALA	7.1
1	A	509	PRO	6.8
1	A	575	TYR	6.8
1	A	405	LEU	6.8
1	A	260	HIS	6.8
1	A	494	PHE	6.7
1	A	355	SER	6.7
1	A	599	HIS	6.7
1	A	264	PHE	6.6
1	A	517	ILE	6.6
1	A	174	TYR	6.5
1	A	374	ASP	6.5
1	A	380	LEU	6.4
2	F	152	MET	6.4
1	A	595	PRO	6.4
1	A	349	TYR	6.3
1	D	557	ALA	6.3
1	A	359	VAL	6.3
1	A	416	ILE	6.3
1	A	329	THR	6.0
1	A	493	ILE	5.9
1	A	315	LEU	5.8
1	A	363	ALA	5.8
1	D	482	TRP	5.8
1	A	526	TYR	5.6
1	A	62	PHE	5.6
1	A	333	TYR	5.5
1	A	426	ASN	5.5
1	A	439	SER	5.5
1	A	479	VAL	5.4
1	A	597	ALA	5.2
1	A	168	GLY	5.2
1	A	262	GLU	5.1
1	A	396	VAL	5.0
1	A	389	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	273	ARG	5.0
1	A	469	TYR	4.9
1	A	243	LEU	4.9
1	A	340	LEU	4.9
1	A	198	LEU	4.8
1	A	135	ALA	4.8
1	A	601	LYS	4.8
1	A	499	PRO	4.7
2	F	168	VAL	4.7
1	A	351	LEU	4.6
1	A	132	ILE	4.6
1	C	1	MET	4.5
2	E	151	GLU	4.5
1	A	450	CYS	4.5
1	B	652	ALA	4.5
1	A	616	TYR	4.4
1	A	200	ALA	4.4
1	A	381	PRO	4.4
1	B	471	LYS	4.4
1	A	288	THR	4.3
1	A	414	GLN	4.3
1	C	640	VAL	4.2
2	F	145	GLU	4.1
1	A	401	ILE	4.1
1	A	111	ILE	4.1
1	A	271	THR	4.1
1	A	328	TYR	4.1
1	A	394	LYS	4.1
1	A	353	GLY	4.1
1	A	600	TRP	4.1
1	A	453	GLU	4.0
1	A	358	GLN	4.0
2	F	156	LEU	4.0
1	A	285	TRP	4.0
2	F	144	ASP	4.0
1	A	392	LEU	4.0
1	A	594	GLN	3.9
1	A	615	TYR	3.9
1	C	562	GLU	3.9
1	A	371	ILE	3.9
1	A	390	TYR	3.8
1	A	385	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	324	THR	3.8
1	A	345	LYS	3.8
1	A	237	PRO	3.8
1	A	338	PHE	3.8
1	C	10	LEU	3.8
1	A	122	TYR	3.7
1	A	449	TYR	3.7
1	A	491	LYS	3.7
1	A	500	ARG	3.7
1	A	508	PHE	3.7
2	E	169	ALA	3.7
1	A	90	MET	3.7
1	A	280	GLU	3.7
1	A	626	ILE	3.7
1	D	31	LEU	3.7
1	A	455	ILE	3.7
1	A	314	GLY	3.7
1	A	425	HIS	3.6
1	A	173	PHE	3.6
1	B	490	PHE	3.6
1	A	376	ASP	3.6
1	A	270	ARG	3.6
1	A	548	ILE	3.5
1	C	108	TYR	3.5
1	A	199	LYS	3.5
1	A	604	PHE	3.4
1	A	432	GLU	3.4
1	A	170	ASN	3.4
1	A	14	LEU	3.4
1	D	568	LEU	3.4
1	A	507	ASN	3.4
1	A	86	GLN	3.4
2	F	176	THR	3.3
1	A	57	GLU	3.3
1	A	202	VAL	3.3
1	A	164	ILE	3.3
1	C	555	ILE	3.3
1	A	251	GLU	3.3
1	A	515	CYS	3.3
2	F	148	LYS	3.3
1	A	113	PHE	3.3
1	A	342	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	263	ASN	3.2
2	F	154	ILE	3.2
1	A	640	VAL	3.2
1	A	441	LEU	3.2
1	A	277	TRP	3.2
1	A	624	ASP	3.2
1	A	448	MET	3.1
1	A	266	TRP	3.1
1	A	253	LYS	3.1
1	A	433	GLN	3.1
1	A	268	ASN	3.1
1	A	609	LYS	3.1
1	A	43	LEU	3.1
1	A	176	SER	3.1
1	A	117	SER	3.0
1	A	20	GLU	3.0
1	A	322	CYS	3.0
1	A	419	GLY	3.0
1	A	283	HIS	3.0
1	A	387	ARG	3.0
1	C	36	LEU	3.0
1	A	332	ALA	3.0
1	A	470	PRO	3.0
1	C	33	LEU	3.0
1	A	267	GLY	3.0
1	A	652	ALA	3.0
1	A	598	ASN	3.0
1	A	259	TRP	3.0
1	A	411	TRP	2.9
1	A	473	GLU	2.9
1	C	154	LEU	2.9
1	D	32	TYR	2.9
1	A	485	VAL	2.9
2	E	156	LEU	2.9
1	A	502	GLU	2.9
1	B	470	PRO	2.9
1	A	19	ILE	2.9
1	A	644	PHE	2.9
1	A	318	TYR	2.9
1	A	588	MET	2.9
2	F	157	GLU	2.9
1	A	413	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.9
1	D	546	TYR	2.8
1	A	431	HIS	2.8
1	A	60	LEU	2.8
1	A	489	LYS	2.8
1	A	404	ILE	2.8
1	A	651	SER	2.8
1	C	362	PHE	2.8
1	A	278	THR	2.8
1	A	436	LEU	2.8
1	A	417	GLY	2.8
1	A	341	ARG	2.8
1	A	292	ALA	2.7
1	A	369	LYS	2.7
1	A	596	PRO	2.7
1	D	579	VAL	2.7
1	B	572	ALA	2.7
1	A	437	LYS	2.7
1	A	312	MET	2.7
2	G	152	MET	2.7
1	A	10	LEU	2.7
1	A	287	LYS	2.7
1	A	282	SER	2.7
1	A	307	GLY	2.7
1	A	399	ASP	2.7
1	A	360	MET	2.7
1	C	615	TYR	2.7
1	D	649	ILE	2.7
1	A	458	THR	2.7
1	D	635	LEU	2.7
1	C	644	PHE	2.7
1	C	31	LEU	2.6
1	C	649	ILE	2.6
1	A	468	PRO	2.6
1	A	326	LEU	2.6
1	C	623	ASP	2.6
1	A	621	TRP	2.6
1	B	232	GLU	2.6
1	A	409	THR	2.6
2	G	109	LEU	2.6
1	A	279	ASP	2.6
1	D	478	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	451	THR	2.6
2	E	8	ARG	2.6
1	A	514	CYS	2.6
1	A	119	GLU	2.6
1	A	398	ARG	2.6
1	C	218	ILE	2.5
1	C	382	GLU	2.5
1	D	10	LEU	2.5
1	A	478	PHE	2.5
1	A	639	TYR	2.5
1	A	41	LYS	2.5
1	A	540	PHE	2.5
2	F	163	PHE	2.5
1	A	347	THR	2.5
1	A	189	ILE	2.5
1	B	277	TRP	2.5
2	E	159	LEU	2.5
1	A	407	ASN	2.5
1	A	236	ILE	2.5
1	D	469	TYR	2.5
2	F	161	SER	2.4
1	A	372	LEU	2.4
1	A	603	ARG	2.4
1	B	639	TYR	2.4
1	C	123	LEU	2.4
1	C	472	LEU	2.4
1	D	548	ILE	2.4
1	C	47	VAL	2.4
1	D	211	VAL	2.4
2	E	9	ILE	2.4
2	E	168	VAL	2.4
2	F	159	LEU	2.4
1	C	22	VAL	2.4
1	C	102	GLU	2.4
1	A	445	TYR	2.4
1	A	356	ALA	2.4
1	A	516	ASP	2.4
1	C	32	TYR	2.3
1	A	492	LYS	2.3
1	A	80	VAL	2.3
1	A	161	VAL	2.3
1	A	510	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	386	GLU	2.3
1	D	615	TYR	2.3
1	A	602	ASN	2.3
1	A	541	PRO	2.3
2	H	35	ALA	2.3
1	A	136	SER	2.3
1	A	163	ALA	2.3
1	B	615	TYR	2.3
2	F	60	TYR	2.3
1	A	574	ARG	2.3
1	B	500	ARG	2.3
1	C	554	PHE	2.3
1	D	22	VAL	2.2
1	C	485	VAL	2.2
1	C	44	TRP	2.2
1	A	317	THR	2.2
1	C	30	GLU	2.2
1	A	378	PRO	2.2
1	A	54	PHE	2.2
1	B	644	PHE	2.2
1	C	113	PHE	2.2
1	D	554	PHE	2.2
1	B	272	ARG	2.2
1	A	465	PRO	2.2
1	B	261	THR	2.2
1	B	217	TYR	2.2
1	A	59	LEU	2.2
1	A	391	LEU	2.2
1	A	252	MET	2.2
1	A	572	ALA	2.2
1	A	112	ILE	2.2
1	C	111	ILE	2.2
1	A	647	ARG	2.2
1	C	377	PHE	2.2
1	D	561	ILE	2.1
1	C	198	LEU	2.1
2	E	129	LEU	2.1
1	A	520	TRP	2.1
1	B	464	PHE	2.1
1	D	484	GLN	2.1
1	A	187	GLY	2.1
1	A	552	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	27	ARG	2.1
1	C	420	ALA	2.1
1	B	577	THR	2.1
1	A	83	VAL	2.1
1	A	607	LEU	2.1
1	C	575	TYR	2.1
1	B	649	ILE	2.1
1	C	60	LEU	2.1
1	B	273	ARG	2.1
2	E	153	GLU	2.1
1	A	12	VAL	2.1
1	A	177	ILE	2.1
1	A	316	PRO	2.1
1	A	257	GLU	2.1
1	A	496	GLU	2.1
1	B	640	VAL	2.0
1	C	214	PRO	2.0
1	D	227	TYR	2.0
1	D	652	ALA	2.0
1	C	635	LEU	2.0
2	H	123	LEU	2.0
1	D	644	PHE	2.0
1	A	578	LEU	2.0
1	D	243	LEU	2.0
1	A	323	PHE	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^{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.

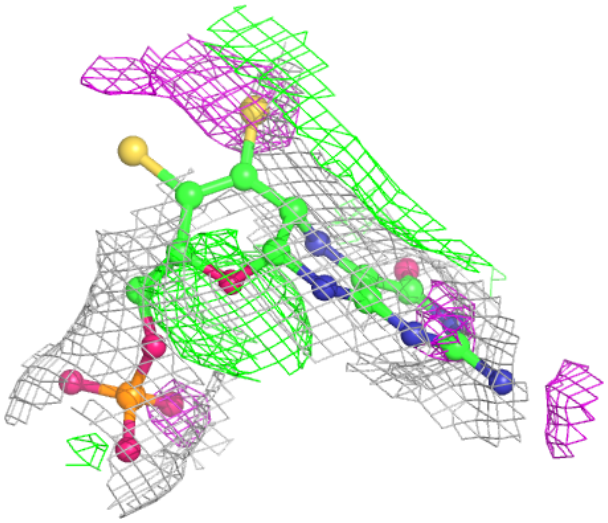
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	ZN	A	707	1/1	0.73	0.16	67,67,67,67	1
7	MG	A	706	1/1	0.75	0.10	100,100,100,100	0
3	UNL	A	701	1/-	0.91	0.42	55,55,55,55	0
5	MTE	A	703	24/24	0.93	0.19	39,93,108,267	0
5	MTE	A	704	24/24	0.94	0.15	78,82,110,178	0
4	SF4	A	702	8/8	0.95	0.13	65,92,124,143	0
7	MG	B	706	1/1	0.95	0.22	64,64,64,64	0
6	W	A	705	1/1	0.95	0.14	111,111,111,111	0
5	MTE	B	703	24/24	0.96	0.17	31,53,61,142	0
5	MTE	B	704	24/24	0.96	0.19	55,66,73,117	0
5	MTE	C	703	24/24	0.96	0.15	46,69,86,87	0
5	MTE	D	703	24/24	0.96	0.18	38,60,70,94	0
8	ZN	C	707	1/1	0.96	0.11	76,76,76,76	1
3	UNL	C	701	1/-	0.97	0.39	83,83,83,83	0
7	MG	C	706	1/1	0.97	0.18	47,47,47,47	0
8	ZN	D	707	1/1	0.97	0.07	89,89,89,89	1
5	MTE	C	704	24/24	0.98	0.16	39,60,94,112	0
4	SF4	H	1003	8/8	0.98	0.16	60,75,90,104	0
7	MG	D	706	1/1	0.98	0.13	43,43,43,43	0
5	MTE	D	704	24/24	0.98	0.16	38,55,75,82	0
3	UNL	B	701	1/-	0.98	0.37	60,60,60,60	0
4	SF4	F	1002	8/8	0.98	0.20	41,45,61,70	0
4	SF4	E	1001	8/8	0.99	0.19	56,71,77,117	0
4	SF4	E	1002	8/8	0.99	0.17	56,76,99,147	0
4	SF4	E	1003	8/8	0.99	0.18	60,66,75,77	0
4	SF4	F	1001	8/8	0.99	0.15	44,49,50,59	0
3	UNL	D	701	1/-	0.99	0.27	87,87,87,87	0
4	SF4	F	1003	8/8	0.99	0.17	54,69,73,85	0
4	SF4	G	1001	8/8	0.99	0.19	52,55,56,59	0
6	W	C	705	1/1	0.99	0.27	78,78,78,78	0
6	W	D	705	1/1	0.99	0.21	67,67,67,67	0
4	SF4	G	1002	8/8	0.99	0.18	47,54,65,73	0
4	SF4	G	1003	8/8	0.99	0.19	78,80,89,152	0
4	SF4	H	1001	8/8	0.99	0.20	55,69,76,82	0
4	SF4	H	1002	8/8	0.99	0.17	64,90,98,99	0
4	SF4	B	702	8/8	0.99	0.16	44,56,66,73	0
8	ZN	B	707	1/1	0.99	0.09	40,40,40,40	1
4	SF4	C	702	8/8	0.99	0.15	56,64,74,83	0
4	SF4	D	702	8/8	0.99	0.15	59,66,75,83	0
6	W	B	705	1/1	1.00	0.26	80,80,80,80	0

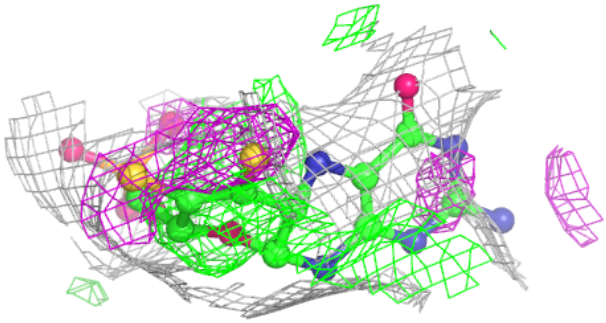
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

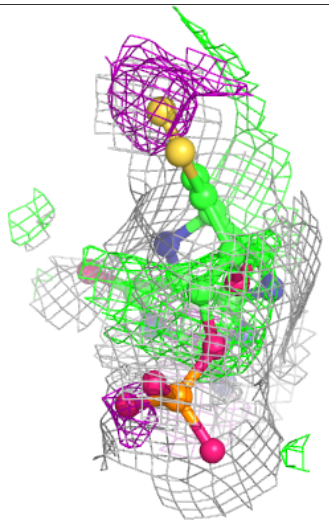
orientation to approximate a three-dimensional view.

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)

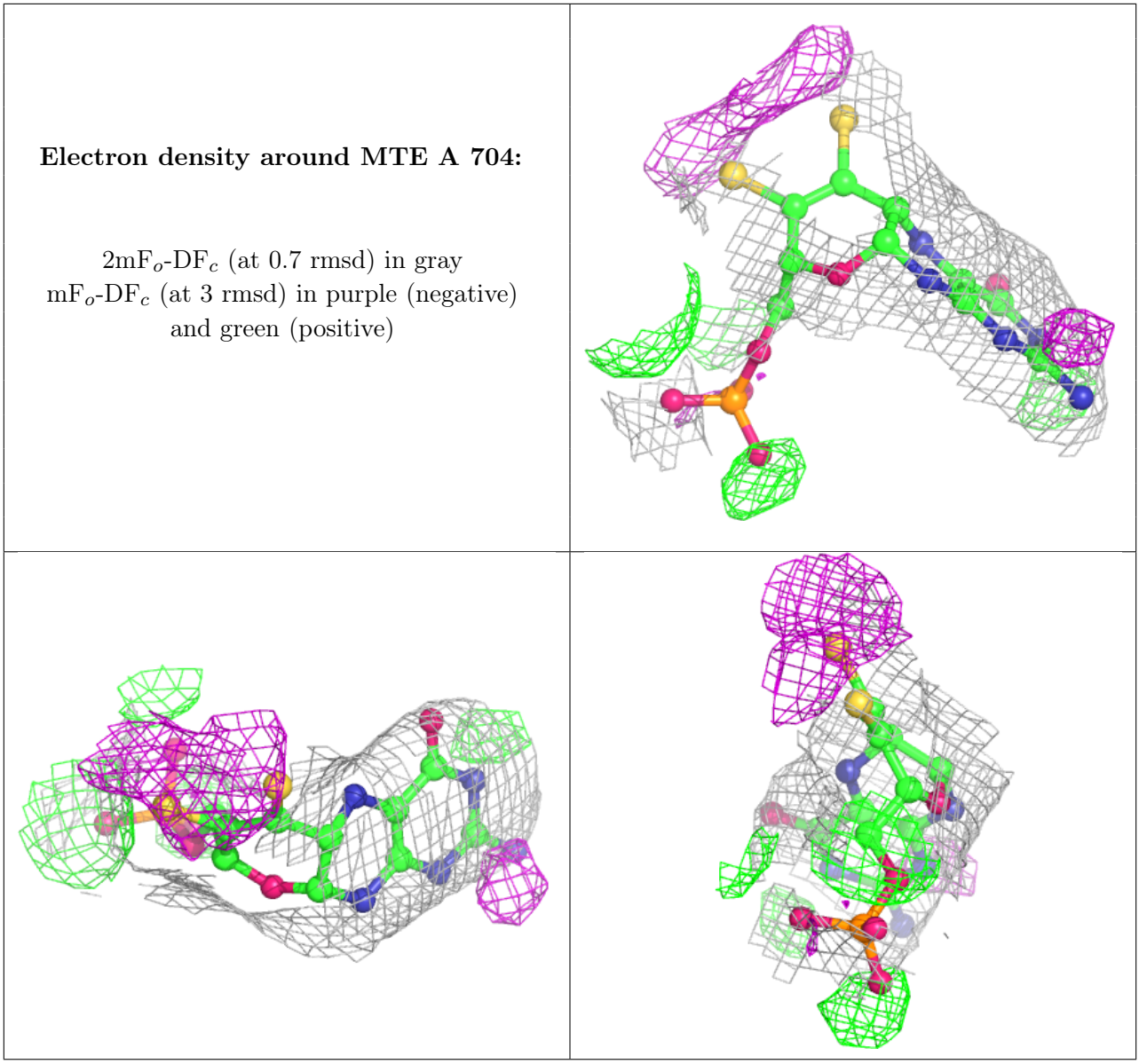






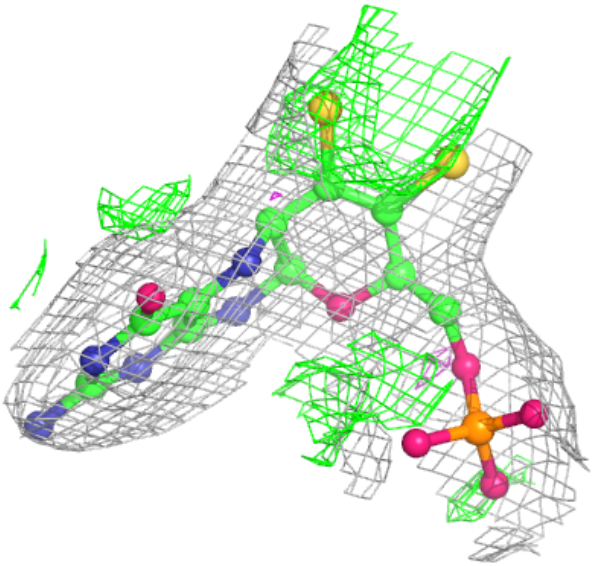
Electron density around MTE A 704:

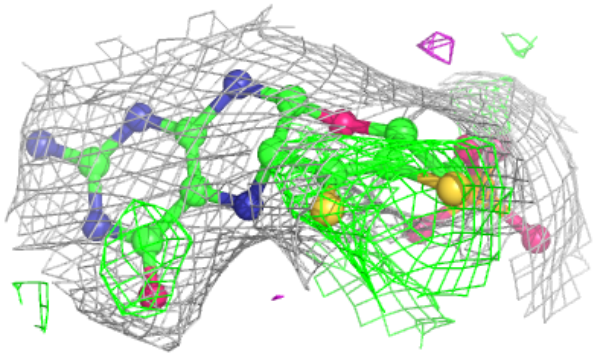
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

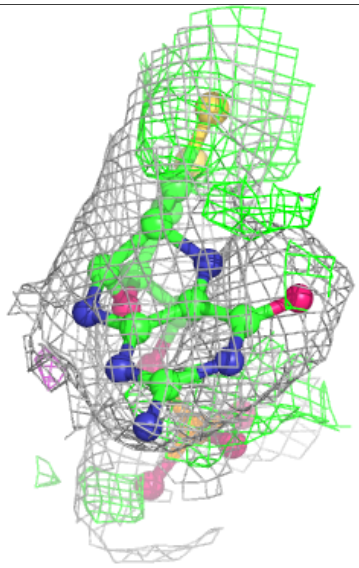


Electron density around MTE B 703:

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

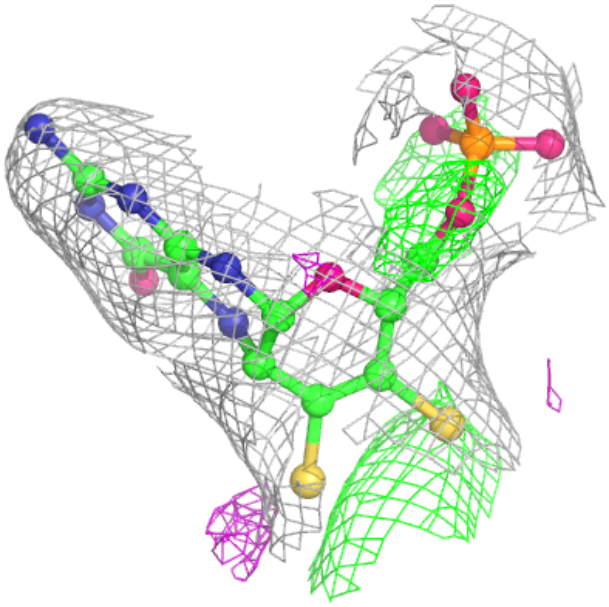


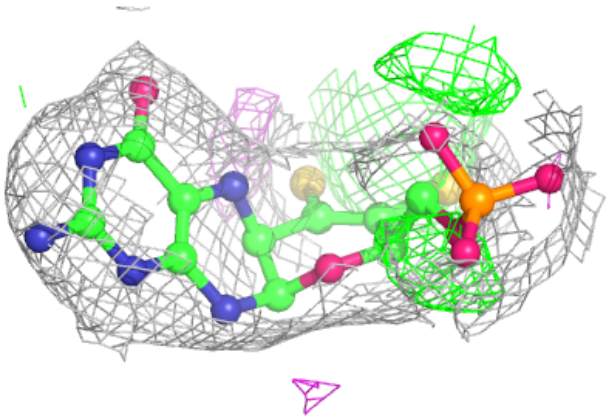


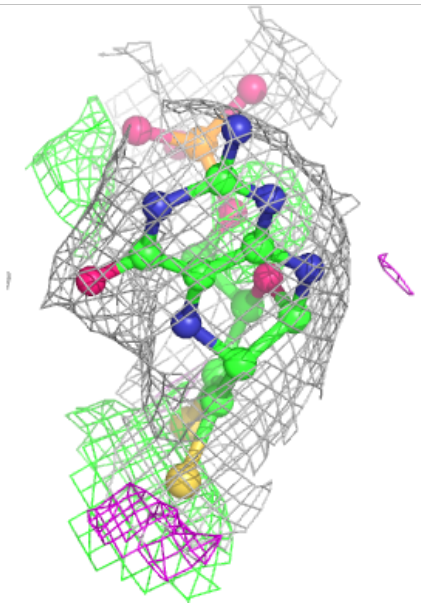


Electron density around MTE B 704:

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

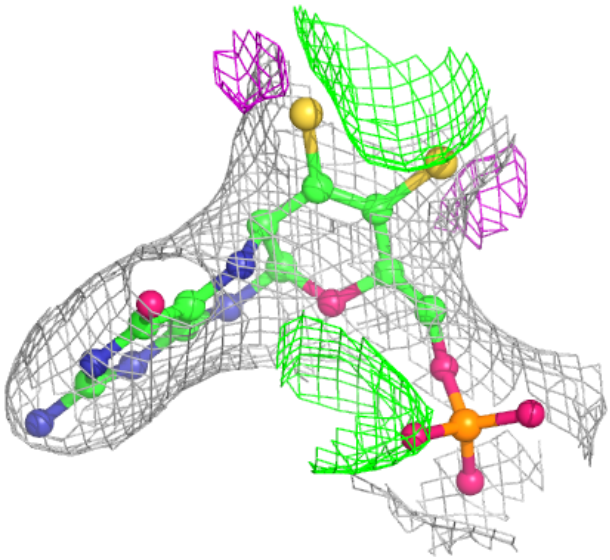


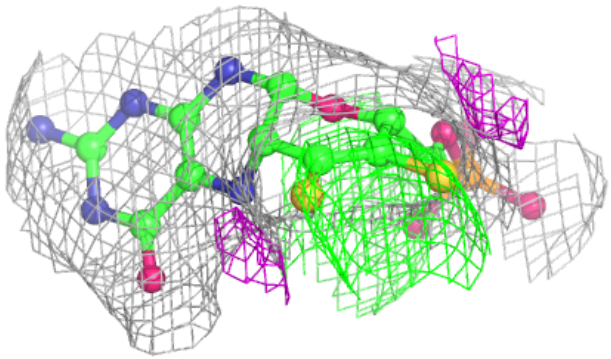


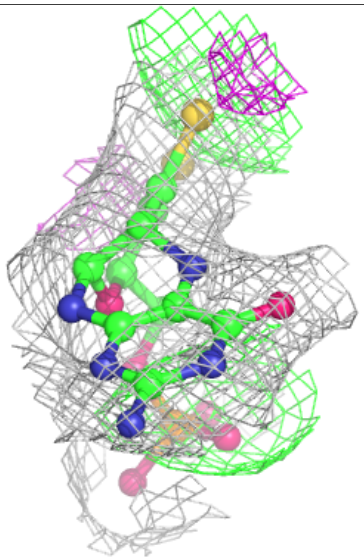


Electron density around MTE C 703:

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

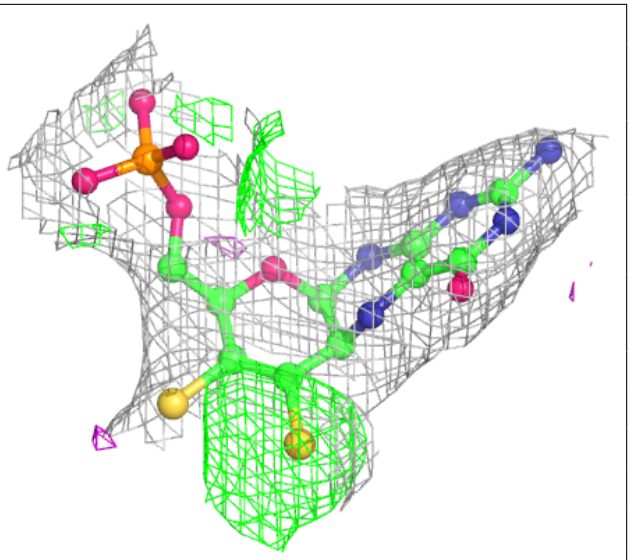


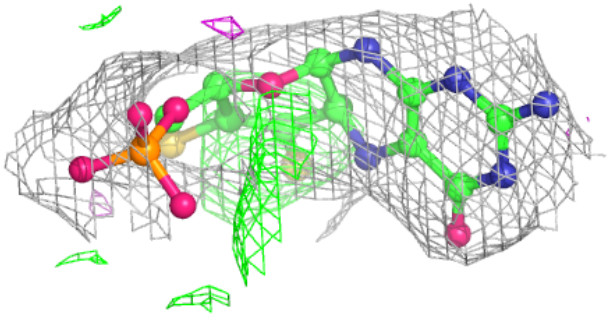


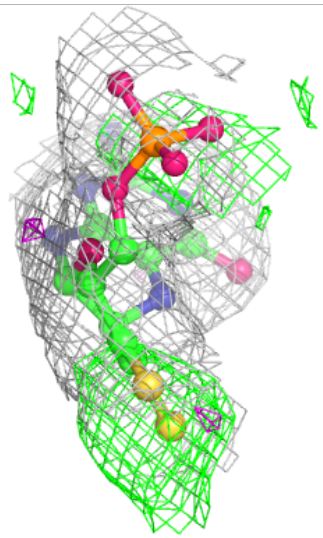


Electron density around MTE D 703:

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

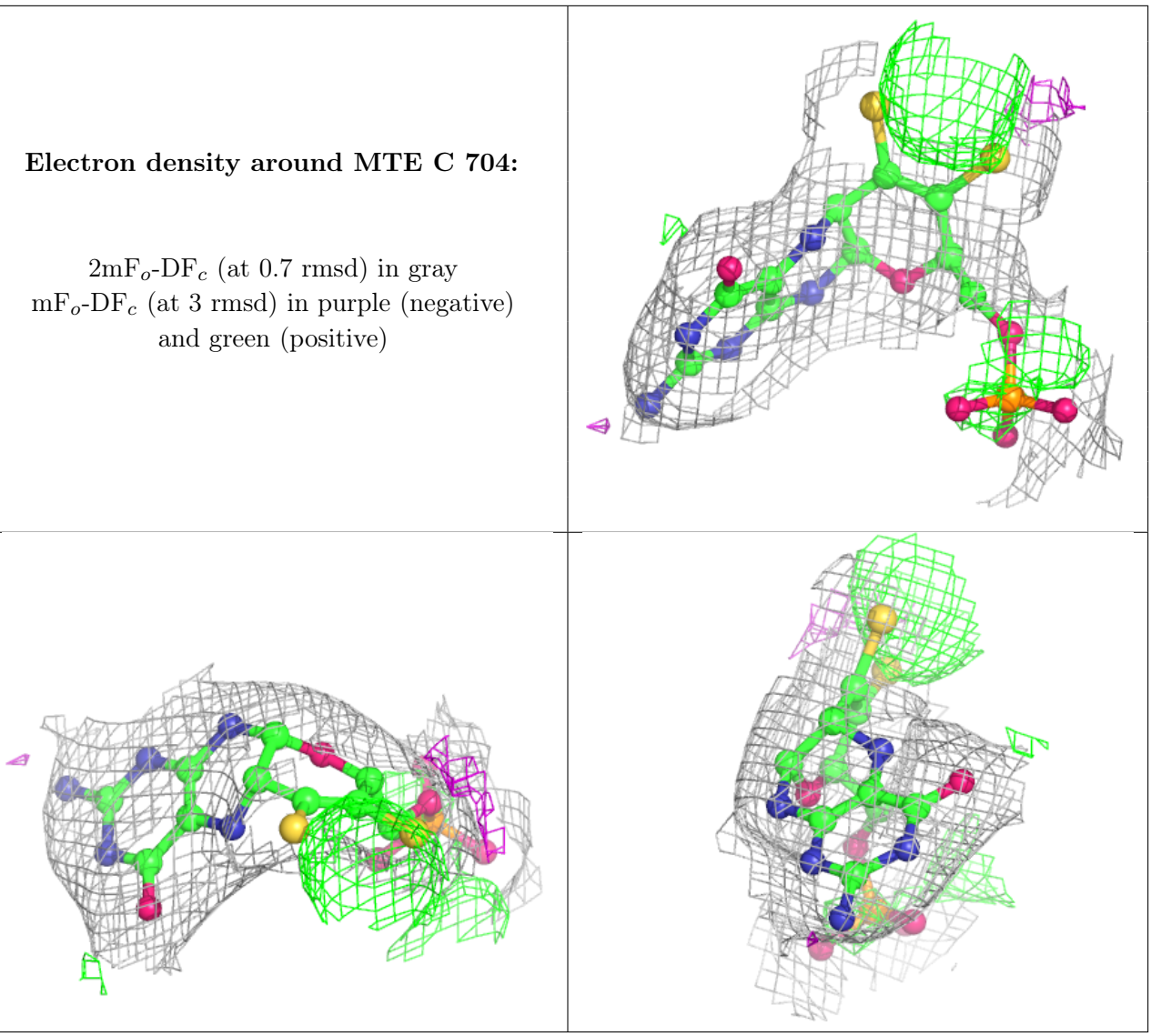






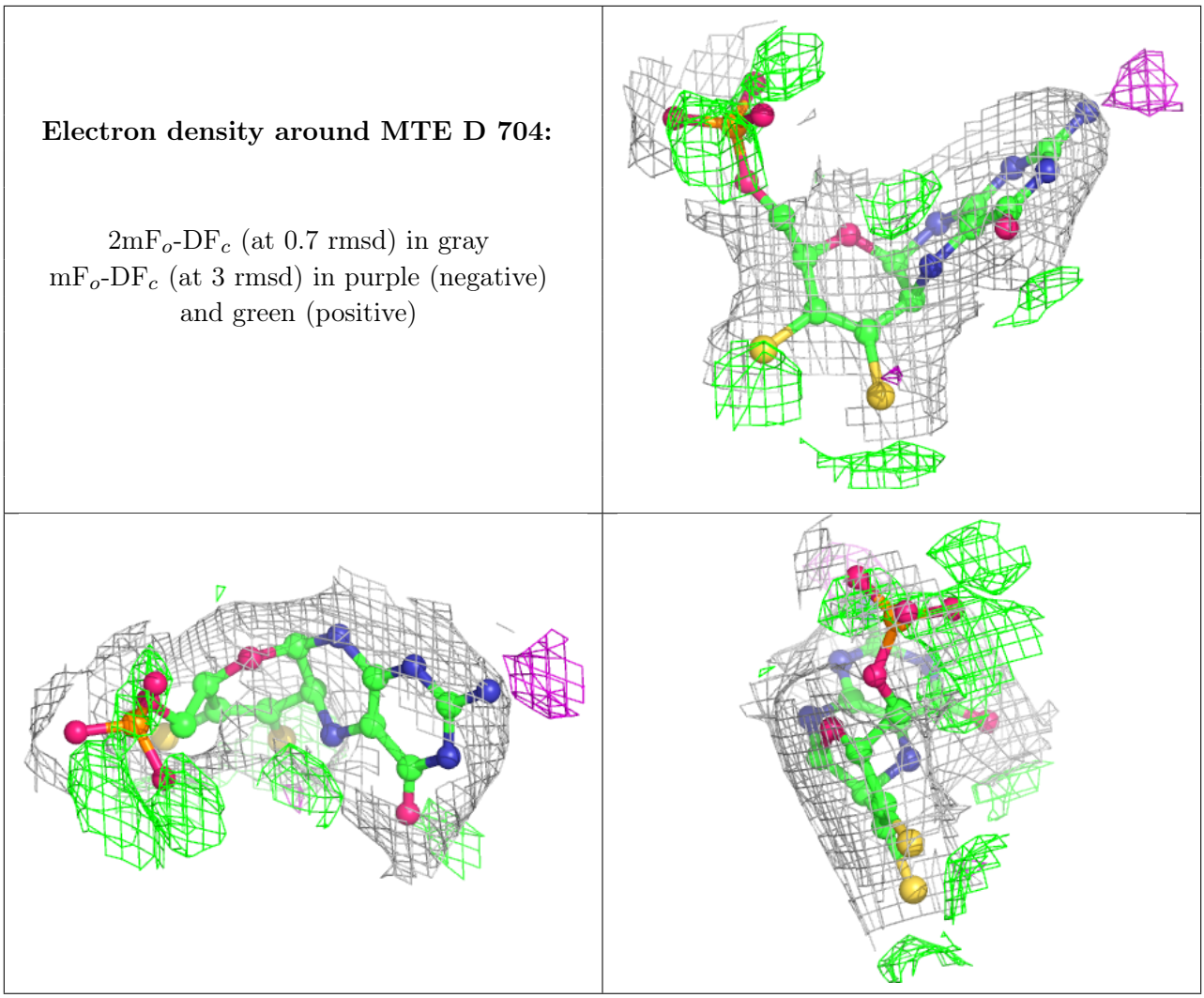
Electron density around MTE C 704:

$2mF_o$-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)



6.5 Other polymers

There are no such residues in this entry.