



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:56 PM UTC

PDB ID : 4Z3X / pdb_00004z3x
Title : Active site complex BamBC of Benzoyl Coenzyme A reductase in complex with 1-Monoenoyl-CoA
Authors : Weinert, T.; Kung, J.W.; Weidenweber, S.; Huwiler, S.G.; Boll, M.; Ermler, U.
Deposited on : 2015-04-01
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

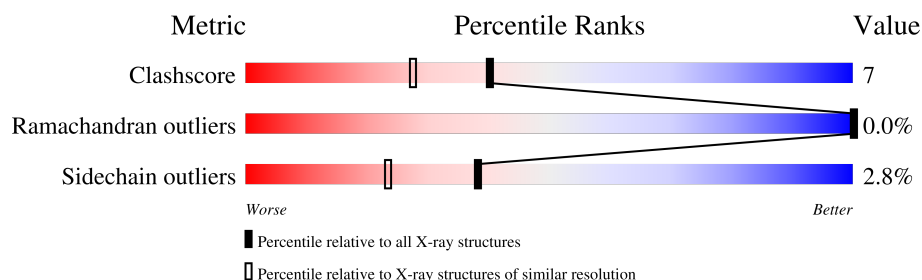
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	653	87% 13% .
1	B	653	88% 12%
1	C	653	82% 16% .
1	D	653	80% 19% .
2	E	179	72% 18% . . 7%
2	F	179	80% 14% . 5%
2	G	179	75% 17% . . 6%
2	H	179	74% 15% . 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
3	SF4	H	1003	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27713 atoms, of which 60 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

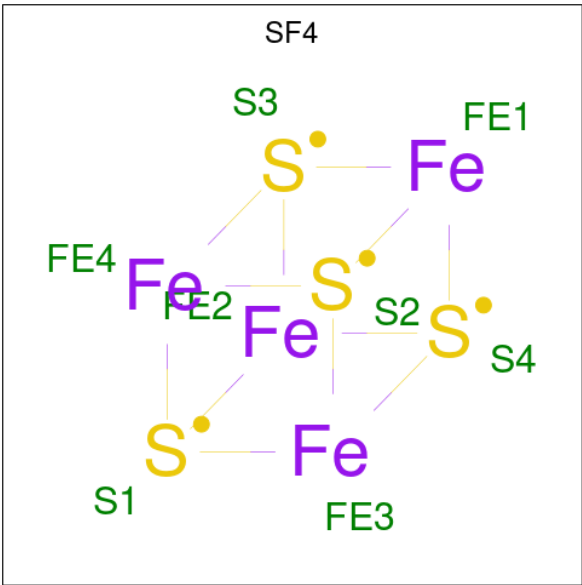
- Molecule 1 is a protein called Benzoyl-CoA reductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	653	Total	C	N	O	S	0	1	0
			5187	3312	875	966	34			
1	B	653	Total	C	N	O	S	0	0	0
			5185	3311	876	964	34			
1	C	653	Total	C	N	O	S	0	0	0
			5181	3309	876	962	34			
1	D	652	Total	C	N	O	S	0	0	0
			5181	3309	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	166	Total	C	N	O	S	0	0	0
			1260	784	223	239	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 IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



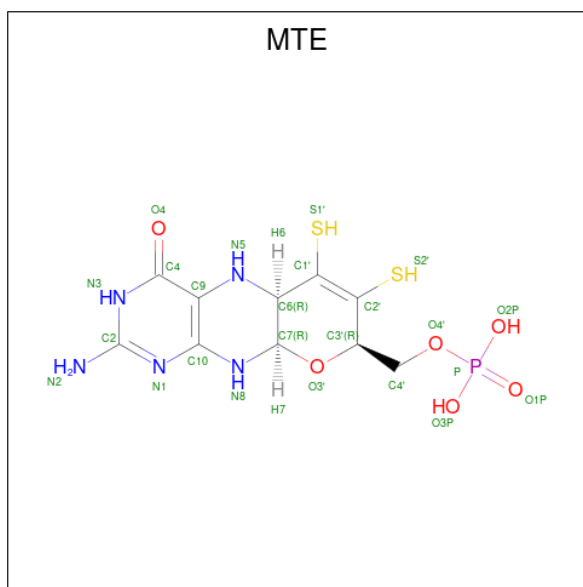
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3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

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

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



- Molecule 5 is TUNGSTEN ION (CCD ID: W) (formula: W).

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

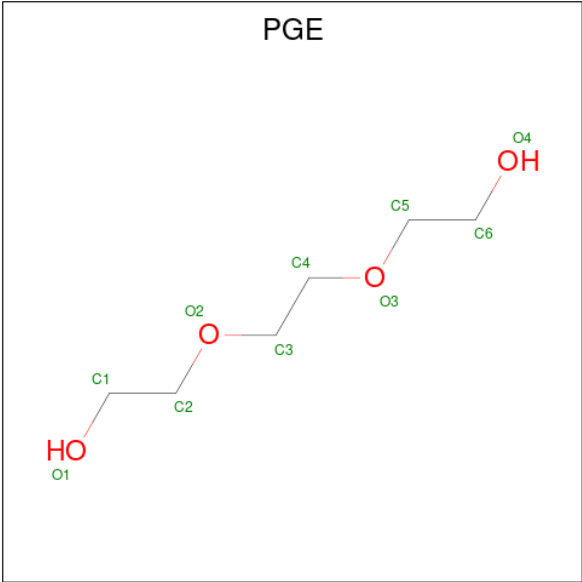
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

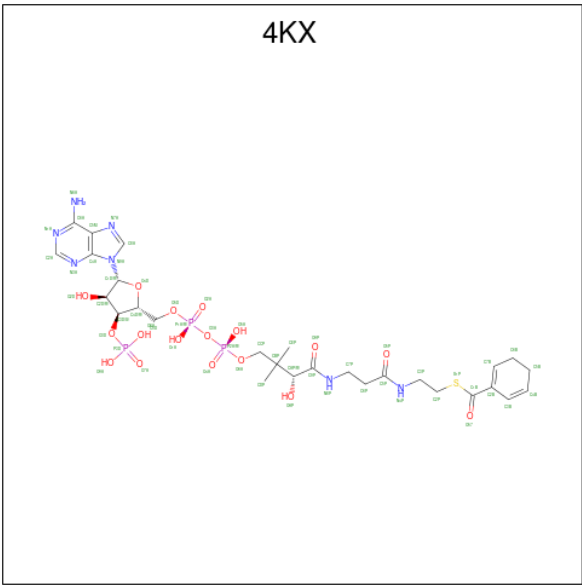
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total X 1 1	0	0
7	B	1	Total X 1 1	0	0
7	C	1	Total X 1 1	0	0
7	D	1	Total X 1 1	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 9 is 1,5 Dienoyl-CoA (CCD ID: 4KX) (formula: C₂₈H₄₂N₇O₁₇P₃S).



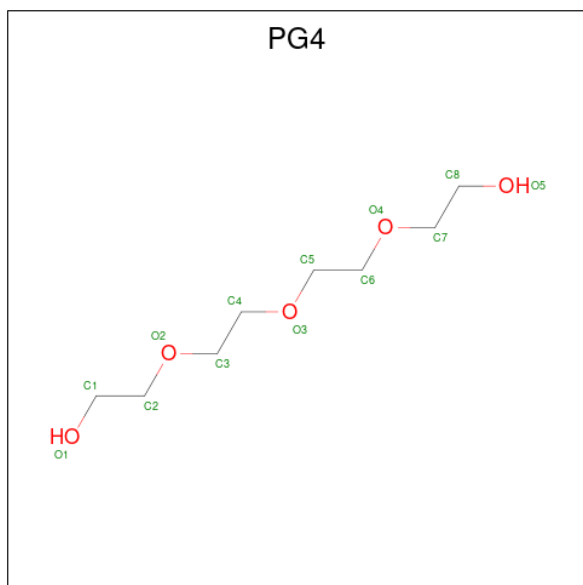
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	A	1	Total	C	N	O	P	S	0	0
			56	28	7	17	3	1		

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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 11 is water.

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

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

3 Residue-property plots

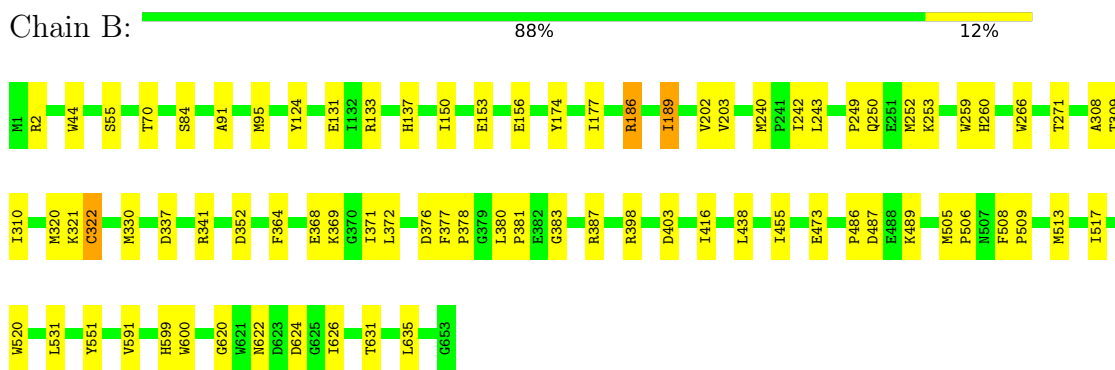
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

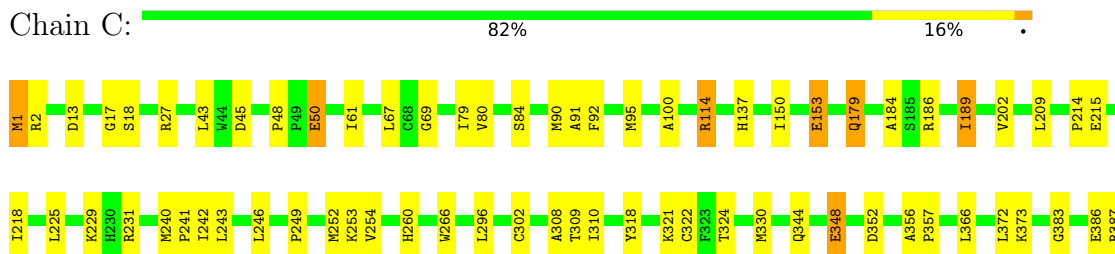
- Molecule 1: Benzoyl-CoA reductase, putative

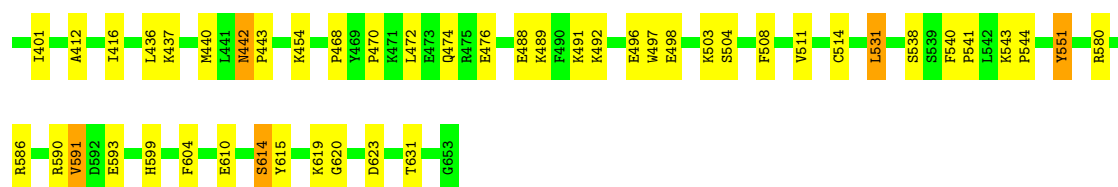


- Molecule 1: Benzoyl-CoA reductase, putative

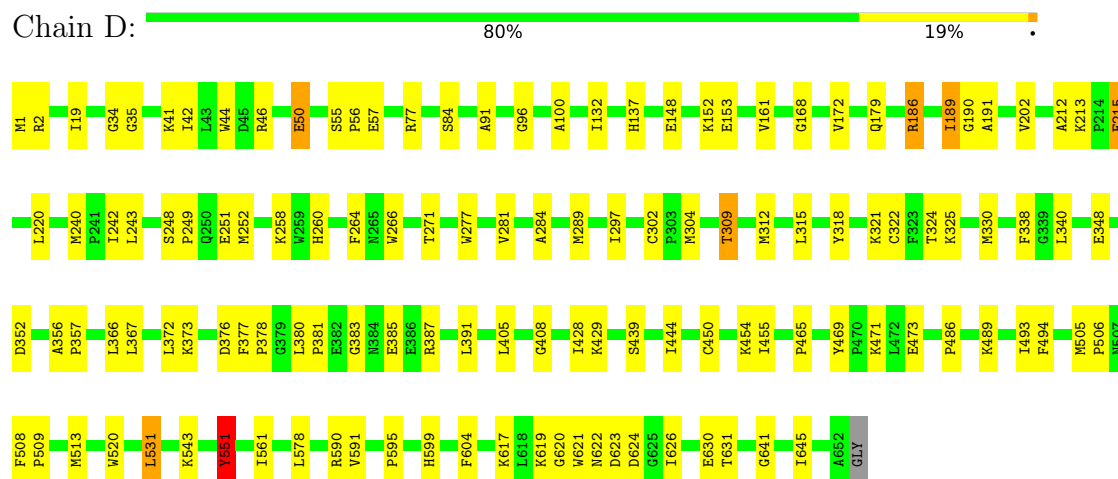


- Molecule 1: Benzoyl-CoA reductase, putative

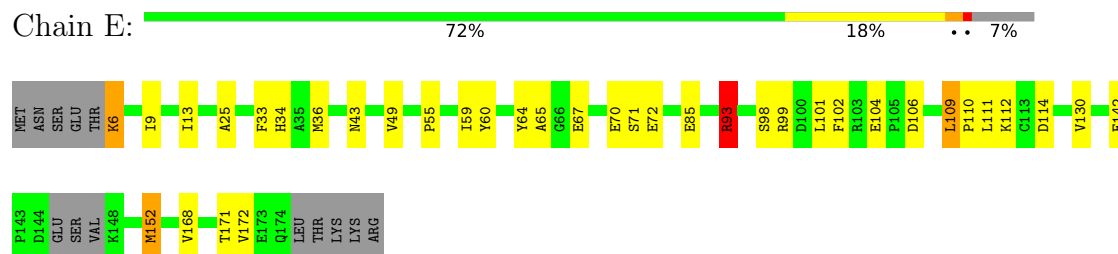




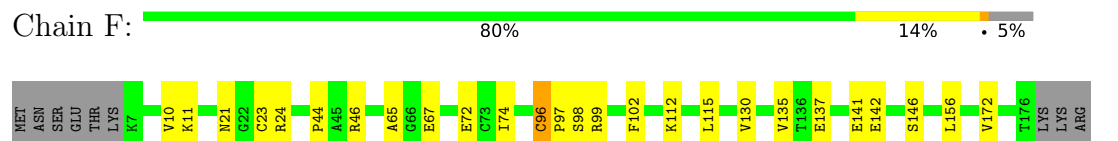
- Molecule 1: Benzoyl-CoA reductase, putative

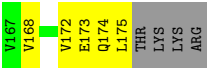


- Molecule 2: Iron-sulfur cluster-binding oxidoreductase, putative benzoyl-CoA reductase electron transfer protein



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4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

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

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MTE, W, PGE, 4KX, PG4, UNL, SF4, 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	0.92	2/5316 (0.0%)	0.95	7/7187 (0.1%)
1	B	0.79	1/5311 (0.0%)	0.93	7/7179 (0.1%)
1	C	1.02	3/5307 (0.1%)	1.10	12/7174 (0.2%)
1	D	1.11	7/5307 (0.1%)	1.14	23/7174 (0.3%)
2	E	1.15	4/1282 (0.3%)	1.22	10/1734 (0.6%)
2	F	1.08	0/1343	1.18	3/1819 (0.2%)
2	G	1.07	3/1344 (0.2%)	1.12	4/1819 (0.2%)
2	H	1.04	2/1242 (0.2%)	1.11	4/1681 (0.2%)
All	All	0.99	22/26452 (0.1%)	1.06	70/35767 (0.2%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	25	ALA	CA-CB	7.34	1.65	1.53
2	E	93	ARG	CD-NE	-7.21	1.36	1.46
1	D	309	THR	CA-CB	6.68	1.64	1.53
1	D	284	ALA	CA-CB	-6.27	1.43	1.53
1	A	203	VAL	CA-C	6.07	1.60	1.52
1	C	179	GLN	CA-CB	6.02	1.60	1.52
2	E	49	VAL	CA-CB	5.67	1.61	1.54
2	G	61	VAL	CA-C	5.59	1.58	1.52
1	D	168	GLY	C-O	5.57	1.30	1.23
1	D	297	ILE	C-O	5.56	1.29	1.23
1	C	100	ALA	C-O	-5.45	1.19	1.24
2	G	99	ARG	CA-C	5.43	1.59	1.52
1	C	67	LEU	CA-C	5.35	1.60	1.52
1	D	212	ALA	CA-CB	5.34	1.61	1.53
2	H	62	PRO	CA-C	5.26	1.58	1.52
1	D	100	ALA	CA-CB	5.23	1.61	1.53
2	H	18	ASP	C-O	-5.23	1.17	1.24
1	B	203	VAL	CA-C	5.20	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	130	VAL	CA-C	5.18	1.58	1.52
1	D	324	THR	CA-CB	5.13	1.62	1.53
2	G	49	VAL	C-O	5.10	1.29	1.24
1	A	455	ILE	CA-CB	5.09	1.61	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	454	LYS	N-CA-C	-8.81	101.96	112.89
1	D	469	TYR	CA-C-N	8.47	128.45	119.05
1	D	469	TYR	C-N-CA	8.47	128.45	119.05
1	C	442	ASN	CA-C-N	8.04	127.97	119.05
1	C	442	ASN	C-N-CA	8.04	127.97	119.05
1	D	543	LYS	CA-C-N	7.87	125.33	119.66
1	D	543	LYS	C-N-CA	7.87	125.33	119.66
2	G	121	GLU	N-CA-C	7.75	115.20	108.22
1	D	186	ARG	NE-CZ-NH1	7.60	129.10	121.50
2	F	46	ARG	CG-CD-NE	-7.54	95.42	112.00
2	E	93	ARG	NE-CZ-NH1	-7.19	114.31	121.50
1	A	44	TRP	CA-C-N	-7.14	110.75	122.54
1	A	44	TRP	C-N-CA	-7.14	110.75	122.54
1	B	44	TRP	CA-C-N	-7.10	110.83	122.54
1	B	44	TRP	C-N-CA	-7.10	110.83	122.54
2	H	109	LEU	CA-C-N	7.08	127.07	119.78
2	H	109	LEU	C-N-CA	7.08	127.07	119.78
2	E	142	GLU	CA-C-N	6.84	127.77	120.11
2	E	142	GLU	C-N-CA	6.84	127.77	120.11
1	D	186	ARG	NE-CZ-NH2	-6.69	113.18	119.20
1	C	302	CYS	CA-C-N	6.54	127.11	120.04
1	C	302	CYS	C-N-CA	6.54	127.11	120.04
1	C	604	PHE	CA-C-N	6.53	126.77	119.32
1	C	604	PHE	C-N-CA	6.53	126.77	119.32
2	G	47	SER	N-CA-C	6.52	119.69	110.23
2	F	96	CYS	CA-C-N	6.49	126.62	119.87
2	F	96	CYS	C-N-CA	6.49	126.62	119.87
2	E	93	ARG	NE-CZ-NH2	6.46	125.01	119.20
1	D	551	TYR	CA-C-N	-6.37	111.98	119.05
1	D	551	TYR	C-N-CA	-6.37	111.98	119.05
2	G	46	ARG	CG-CD-NE	-6.28	98.19	112.00
1	D	302	CYS	CA-C-N	-6.13	113.48	120.89
1	D	302	CYS	C-N-CA	-6.13	113.48	120.89
1	D	44	TRP	CA-C-N	-6.02	113.21	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	TRP	C-N-CA	-6.02	113.21	122.60
1	C	543	LYS	CA-C-N	5.98	126.54	120.38
1	C	543	LYS	C-N-CA	5.98	126.54	120.38
1	C	67	LEU	N-CA-C	5.97	119.53	112.72
2	H	19	LYS	N-CA-C	-5.65	106.37	113.72
1	D	309	THR	N-CA-C	-5.63	102.15	110.48
2	H	23	CYS	N-CA-C	5.61	118.33	111.82
1	D	271	THR	N-CA-C	5.59	117.51	108.34
1	A	186	ARG	NE-CZ-NH2	-5.56	114.20	119.20
2	E	109	LEU	CA-C-N	5.51	125.27	119.76
2	E	109	LEU	C-N-CA	5.51	125.27	119.76
1	B	70	THR	CA-C-N	-5.45	115.27	120.83
1	B	70	THR	C-N-CA	-5.45	115.27	120.83
2	E	59	ILE	N-CA-C	5.41	115.89	107.99
1	D	630	GLU	N-CA-C	5.41	117.60	111.11
2	E	93	ARG	CB-CG-CD	-5.37	98.95	111.30
1	D	100	ALA	CA-C-N	-5.32	113.14	119.05
1	D	100	ALA	C-N-CA	-5.32	113.14	119.05
2	E	43	ASN	CA-C-N	-5.32	114.14	119.56
2	E	43	ASN	C-N-CA	-5.32	114.14	119.56
1	B	322	CYS	CB-CA-C	-5.31	109.47	115.79
1	D	220	LEU	N-CA-C	-5.31	105.66	111.82
1	B	271	THR	N-CA-C	5.30	117.04	108.41
1	A	70	THR	CA-C-N	-5.29	115.43	120.83
1	A	70	THR	C-N-CA	-5.29	115.43	120.83
1	A	271	THR	N-CA-C	5.28	117.02	108.41
1	A	322	CYS	CB-CA-C	-5.22	109.58	115.79
1	D	604	PHE	CA-C-N	5.15	125.19	119.32
1	D	604	PHE	C-N-CA	5.15	125.19	119.32
1	C	214	PRO	CA-C-N	5.14	127.94	120.79
1	C	214	PRO	C-N-CA	5.14	127.94	120.79
2	G	93	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	D	444	ILE	N-CA-C	-5.13	105.70	110.53
1	C	153	GLU	CB-CA-C	-5.08	102.05	110.68
1	B	186	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	D	408	GLY	CA-C-O	-5.03	118.22	122.29

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	5187	0	5113	56	0
1	B	5185	0	5118	52	0
1	C	5181	0	5114	88	0
1	D	5181	0	5115	68	0
2	E	1260	0	1209	20	0
2	F	1317	0	1266	16	0
2	G	1315	0	1263	30	0
2	H	1221	0	1158	23	0
3	A	8	0	0	1	0
3	B	8	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
3	E	24	0	0	0	0
3	F	24	0	0	1	0
3	G	24	0	0	0	0
3	H	24	0	0	3	0
4	A	48	0	20	2	0
4	B	48	0	20	5	0
4	C	48	0	20	1	0
4	D	48	0	20	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	20	28	28	2	0
8	D	10	14	14	1	0
9	A	56	0	38	4	0
9	B	56	0	38	4	0
9	C	112	0	76	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	56	0	38	4	0
10	D	13	18	18	1	0
11	A	261	0	0	3	1
11	B	118	0	0	2	0
11	C	226	0	0	6	0
11	D	230	0	0	3	0
11	E	90	0	0	2	0
11	F	90	0	0	0	0
11	G	71	0	0	0	0
11	H	65	0	0	4	0
All	All	27653	60	25686	344	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (344) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:SD	1:C:2:ARG:N	2.35	1.00
2:G:152:MET:HE3	2:G:156:LEU:HD11	1.42	0.99
2:H:152:MET:HE3	2:H:156:LEU:HD11	1.52	0.89
1:D:84:SER:HB2	1:D:91:ALA:HB2	1.57	0.86
1:D:137:HIS:NE2	1:D:153:GLU:OE2	2.10	0.84
2:G:152:MET:HE3	2:G:156:LEU:CD1	2.07	0.84
2:G:64:TYR:O	2:G:93:ARG:HD2	1.78	0.84
1:A:137:HIS:NE2	1:A:153:GLU:OE2	2.12	0.82
1:B:137:HIS:NE2	1:B:153:GLU:OE2	2.12	0.81
1:D:186:ARG:HD2	1:D:352:ASP:OD2	1.83	0.79
1:C:252:MET:CE	1:C:308:ALA:HB3	2.13	0.78
2:G:163:PHE:CE2	2:H:152:MET:HB3	2.19	0.78
1:A:372:LEU:HD11	1:A:416:ILE:HD13	1.67	0.76
1:B:372:LEU:HD11	1:B:416:ILE:HD13	1.67	0.76
1:B:150:ILE:HG21	1:B:202:VAL:HG21	1.67	0.76
1:A:150:ILE:HG21	1:A:202:VAL:HG21	1.67	0.76
1:B:242:ILE:HG13	1:B:243:LEU:HG	1.68	0.76
1:A:242:ILE:HG13	1:A:243:LEU:HG	1.68	0.75
1:A:380:LEU:HD12	1:A:381:PRO:HD2	1.67	0.75
1:A:249:PRO:HG2	9:A:709:4KX:H4B	1.70	0.74
1:B:380:LEU:HD12	1:B:381:PRO:HD2	1.67	0.74
1:C:137:HIS:NE2	1:C:153:GLU:OE2	2.19	0.74
1:A:624:ASP:OD2	11:A:801:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:MET:HE1	1:C:310:ILE:HD11	1.70	0.73
1:C:620:GLY:HA3	1:C:631:THR:HG21	1.71	0.72
1:C:249:PRO:HG2	9:C:707[A]:4KX:H4B	1.69	0.72
1:D:240:MET:HE2	1:D:242:ILE:HG12	1.71	0.71
2:G:152:MET:CE	2:H:168:VAL:HA	2.21	0.71
1:D:242:ILE:HG13	1:D:243:LEU:HG	1.73	0.71
2:G:152:MET:CE	2:G:156:LEU:HD11	2.18	0.70
1:D:383:GLY:O	1:D:387:ARG:HG3	1.93	0.69
1:C:249:PRO:HG2	9:C:707[B]:4KX:H4B	1.74	0.69
1:B:252:MET:CE	1:B:308:ALA:HB3	2.23	0.69
1:C:249:PRO:CG	9:C:707[A]:4KX:H4B	2.22	0.69
1:A:252:MET:CE	1:A:308:ALA:HB3	2.24	0.68
2:H:152:MET:HE3	2:H:156:LEU:CD1	2.23	0.68
1:C:252:MET:CE	1:C:310:ILE:HD11	2.24	0.68
1:B:84:SER:HB2	1:B:91:ALA:HB2	1.75	0.68
2:G:67[B]:GLU:CD	2:G:67[B]:GLU:H	2.00	0.68
1:C:366:LEU:HB3	1:C:372:LEU:HD13	1.75	0.68
1:B:260:HIS:NE2	9:B:707:4KX:H5B	2.08	0.68
1:A:84:SER:HB2	1:A:91:ALA:HB2	1.75	0.68
1:C:252:MET:HE3	1:C:308:ALA:HB3	1.77	0.67
1:C:252:MET:HE2	1:C:308:ALA:HB3	1.76	0.66
1:C:249:PRO:CG	9:C:707[B]:4KX:H4B	2.25	0.66
1:D:471:LYS:HB3	1:D:473:GLU:OE1	1.96	0.65
2:G:152:MET:HE1	2:H:168:VAL:HG22	1.78	0.65
1:A:131:GLU:OE2	1:A:133:ARG:NE	2.22	0.64
1:A:252:MET:HE3	1:A:308:ALA:HB3	1.80	0.63
1:A:240:MET:HE2	1:A:242:ILE:HG12	1.80	0.63
1:A:372:LEU:HD23	1:A:377:PHE:CE1	2.34	0.63
1:B:240:MET:HE2	1:B:242:ILE:HG12	1.81	0.63
1:B:252:MET:HE3	1:B:308:ALA:HB3	1.79	0.63
1:B:383:GLY:O	1:B:387:ARG:HG3	1.99	0.63
1:A:383:GLY:O	1:A:387:ARG:HG3	1.99	0.63
2:G:63:LEU:HD11	2:G:92:CYS:O	1.99	0.62
1:B:322:CYS:HB3	4:B:703:MTE:S1'	2.38	0.62
1:B:372:LEU:HD23	1:B:377:PHE:CE1	2.34	0.62
2:E:64:TYR:O	2:E:93:ARG:CD	2.48	0.62
1:A:186:ARG:HD2	1:A:352:ASP:OD2	2.00	0.61
1:B:189:ILE:HD13	1:B:189:ILE:H	1.65	0.61
1:D:249:PRO:CG	9:D:709:4KX:H4B	2.31	0.61
1:D:338:PHE:CD1	1:D:385:GLU:HG3	2.35	0.61
2:G:72:GLU:HG2	2:G:98:SER:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HD13	1:A:189:ILE:H	1.65	0.60
1:C:242:ILE:HG13	1:C:243:LEU:HG	1.82	0.60
1:B:186:ARG:HD2	1:B:352:ASP:OD2	2.01	0.60
1:B:131:GLU:OE2	1:B:133:ARG:NE	2.23	0.60
1:D:266:TRP:CE3	1:D:330:MET:HA	2.36	0.60
1:C:620:GLY:CA	1:C:631:THR:HG21	2.30	0.60
2:E:172:VAL:HG21	2:F:172:VAL:HG21	1.84	0.60
2:G:103[A]:ARG:HD2	2:G:108:GLY:O	2.02	0.60
1:C:580:ARG:HH22	1:C:593:GLU:CD	2.10	0.59
2:G:29:ILE:HD13	2:G:127:TRP:CZ2	2.37	0.59
2:H:14:ASN:ND2	11:H:1102:HOH:O	2.19	0.59
1:C:260:HIS:NE2	9:C:707[B]:4KX:H5B	2.18	0.59
1:C:84:SER:HB2	1:C:91:ALA:HB2	1.84	0.58
1:D:186:ARG:HD3	1:D:352:ASP:OD1	2.03	0.58
1:D:591:VAL:HG21	11:D:1029:HOH:O	2.02	0.58
2:E:64:TYR:O	2:E:93:ARG:HD3	2.04	0.58
2:G:173:GLU:O	2:G:175:LEU:N	2.29	0.58
1:D:240:MET:H	10:D:708:PG4:H72	1.68	0.58
1:D:376:ASP:C	1:D:378:PRO:HD3	2.29	0.57
2:F:72:GLU:CG	2:F:98:SER:HB3	2.34	0.57
1:B:337:ASP:O	1:B:341:ARG:HG3	2.04	0.57
1:C:43:LEU:HD12	1:C:90:MET:HE3	1.85	0.57
1:A:158:ARG:NH1	11:A:808:HOH:O	2.37	0.57
1:C:489:LYS:HA	1:C:492:LYS:CD	2.35	0.57
2:G:146:SER:HB3	2:H:71:SER:HB2	1.87	0.57
1:B:252:MET:HE1	1:B:310:ILE:HD11	1.87	0.57
1:C:489:LYS:HA	1:C:492:LYS:HD3	1.87	0.57
2:G:152:MET:HE2	2:H:168:VAL:HA	1.86	0.57
2:G:163:PHE:CD2	2:H:152:MET:HB3	2.39	0.56
1:D:366:LEU:HB3	1:D:372:LEU:HD13	1.87	0.56
1:B:249:PRO:HG2	9:B:707:4KX:H4B	1.88	0.56
1:C:615:TYR:CZ	1:C:619:LYS:HE3	2.40	0.56
1:C:591:VAL:HG22	11:C:858:HOH:O	2.06	0.56
1:D:380:LEU:HD12	1:D:381:PRO:HD2	1.88	0.56
1:A:252:MET:HE1	1:A:310:ILE:HD11	1.88	0.56
1:A:337:ASP:O	1:A:341:ARG:HG3	2.05	0.56
2:G:152:MET:HE1	2:H:168:VAL:HA	1.87	0.56
1:D:620:GLY:HA3	1:D:631:THR:HG21	1.88	0.56
2:E:65:ALA:HB2	2:E:102:PHE:CD1	2.41	0.56
1:D:428:ILE:HG22	1:D:429:LYS:HG3	1.88	0.55
1:C:538:SER:O	1:C:544:PRO:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:ASN:HB3	1:D:624:ASP:H	1.72	0.55
1:D:1:MET:HG3	1:D:2:ARG:O	2.07	0.55
2:H:131:GLY:HA2	11:H:1143:HOH:O	2.06	0.55
9:C:707[B]:4KX:H5DA	9:C:707[B]:4KX:H8A	1.88	0.54
2:G:173:GLU:C	2:G:175:LEU:H	2.12	0.54
1:B:372:LEU:CD1	1:B:416:ILE:HD13	2.35	0.54
1:B:259:TRP:HE1	9:B:707:4KX:HDPB	1.72	0.54
1:B:473:GLU:CD	1:B:473:GLU:H	2.16	0.54
1:A:372:LEU:CD1	1:A:416:ILE:HD13	2.35	0.54
1:D:591:VAL:HG23	11:D:848:HOH:O	2.08	0.54
1:D:249:PRO:HG2	9:D:709:4KX:H4B	1.89	0.54
2:G:27:GLU:HG2	2:G:49:VAL:O	2.07	0.54
2:H:7:LYS:O	11:H:1101:HOH:O	2.18	0.54
1:A:473:GLU:CD	1:A:473:GLU:H	2.16	0.54
1:C:189:ILE:HD13	1:C:189:ILE:H	1.72	0.53
2:E:71:SER:HB2	2:F:146:SER:HB3	1.91	0.53
1:C:260:HIS:NE2	9:C:707[A]:4KX:H5B	2.23	0.53
1:C:620:GLY:O	1:C:631:THR:HG21	2.09	0.53
1:A:252:MET:HE2	1:A:308:ALA:HB3	1.91	0.53
1:B:186:ARG:HD3	1:B:352:ASP:OD1	2.09	0.53
1:D:56:PRO:HD2	1:D:57:GLU:OE1	2.09	0.53
1:C:95:MET:HE3	1:C:184:ALA:H	1.73	0.52
2:G:29:ILE:HD13	2:G:127:TRP:CE2	2.44	0.52
1:D:148:GLU:O	1:D:152:LYS:HG3	2.10	0.52
2:E:70:GLU:HG2	11:E:1148:HOH:O	2.10	0.52
1:A:186:ARG:HD3	1:A:352:ASP:OD1	2.09	0.52
1:B:124:TYR:OH	1:B:156:GLU:OE2	2.23	0.51
1:C:472:LEU:O	1:C:476:GLU:HG3	2.09	0.51
2:E:64:TYR:O	2:E:93:ARG:HD2	2.09	0.51
2:H:85:GLU:HB3	11:H:1105:HOH:O	2.08	0.51
1:C:322:CYS:HB3	4:C:703:MTE:S1'	2.51	0.51
1:C:383:GLY:O	1:C:387:ARG:HG3	2.11	0.51
1:B:252:MET:HE2	1:B:308:ALA:HB3	1.91	0.51
1:C:511:VAL:HG21	1:C:610:GLU:HG2	1.92	0.51
1:C:13:ASP:HB3	1:C:18:SER:OG	2.10	0.51
1:A:124:TYR:OH	1:A:156:GLU:OE2	2.23	0.51
1:D:186:ARG:HD2	1:D:352:ASP:CG	2.35	0.51
2:E:67:GLU:OE2	2:E:112:LYS:NZ	2.40	0.51
2:F:23:CYS:O	2:F:24:ARG:HB2	2.11	0.51
1:A:240:MET:HG2	8:A:708:PGE:O1	2.11	0.51
1:B:620:GLY:HA3	1:B:631:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:MET:CE	1:B:310:ILE:HD11	2.42	0.50
1:C:240:MET:HE2	1:C:242:ILE:HG23	1.93	0.50
9:A:709:4KX:O2A	11:A:802:HOH:O	2.20	0.50
1:C:412:ALA:O	1:C:416:ILE:HG13	2.12	0.50
1:A:398:ARG:HB3	1:A:403:ASP:OD1	2.11	0.50
1:C:186:ARG:NH2	11:C:805:HOH:O	2.42	0.50
1:D:322:CYS:HB2	4:D:703:MTE:S2'	2.52	0.50
1:C:356:ALA:HB3	1:C:357:PRO:HD3	1.92	0.50
1:A:252:MET:CE	1:A:310:ILE:HD11	2.42	0.50
2:F:115:LEU:HA	3:F:1002:SF4:S2	2.52	0.50
1:B:369:LYS:HG3	1:B:369:LYS:O	2.12	0.50
1:A:249:PRO:CG	9:A:709:4KX:H4B	2.41	0.49
1:B:249:PRO:CG	9:B:707:4KX:H4B	2.43	0.49
2:E:168:VAL:O	2:E:172:VAL:HG23	2.12	0.49
1:C:186:ARG:HD3	1:C:352:ASP:OD1	2.11	0.49
2:F:72:GLU:HG2	2:F:98:SER:HB3	1.95	0.49
1:C:366:LEU:CB	1:C:372:LEU:HD13	2.41	0.49
1:B:398:ARG:HB3	1:B:403:ASP:OD1	2.12	0.49
1:D:215:GLU:CD	1:D:215:GLU:H	2.21	0.49
1:D:493:ILE:HD13	1:D:513:MET:HB3	1.93	0.49
9:A:709:4KX:O9P	9:A:709:4KX:HCPA	2.13	0.49
2:H:153:GLU:O	2:H:157:GLU:HG3	2.13	0.49
1:C:443:PRO:HB2	1:C:514:CYS:SG	2.53	0.49
1:A:369:LYS:O	1:A:369:LYS:HG3	2.12	0.49
1:D:590:ARG:HD2	1:D:623:ASP:O	2.12	0.49
2:G:168:VAL:O	2:G:172:VAL:HG23	2.13	0.49
1:A:438:LEU:O	1:A:600:TRP:HA	2.13	0.48
1:B:250:GLN:OE1	1:B:253:LYS:HE3	2.12	0.48
1:B:322:CYS:CB	4:B:703:MTE:S1'	2.98	0.48
1:A:620:GLY:HA3	1:A:631:THR:HG21	1.93	0.48
1:A:250:GLN:OE1	1:A:253:LYS:HE3	2.13	0.48
1:C:386:GLU:H	1:C:386:GLU:CD	2.21	0.48
2:G:67[B]:GLU:HG2	3:H:1003:SF4:S4	2.53	0.48
1:C:436:LEU:O	1:C:437:LYS:HD3	2.14	0.48
1:A:95:MET:HE1	1:A:177:ILE:HG22	1.96	0.47
1:B:438:LEU:O	1:B:600:TRP:HA	2.13	0.47
1:C:503:LYS:C	1:C:508:PHE:HB3	2.40	0.47
1:C:610:GLU:O	1:C:614:SER:OG	2.31	0.47
2:E:33:PHE:HD2	2:E:34:HIS:CE1	2.33	0.47
1:A:322:CYS:CB	4:A:702:MTE:S2'	3.02	0.47
2:H:67:GLU:OE1	2:H:112:LYS:NZ	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:GLU:O	1:C:491:LYS:HB2	2.14	0.47
1:D:322:CYS:CB	4:D:703:MTE:S2'	3.02	0.47
1:D:617:LYS:HD3	11:D:1002:HOH:O	2.14	0.47
2:G:107:SER:HA	2:H:151:GLU:HB3	1.96	0.47
1:C:186:ARG:HD3	1:C:352:ASP:CG	2.40	0.47
1:D:172:VAL:O	1:D:191:ALA:HB2	2.15	0.47
1:D:312:MET:HB2	1:D:315:LEU:HD12	1.97	0.47
2:E:71:SER:CB	2:F:146:SER:HB3	2.45	0.47
1:B:95:MET:HE1	1:B:177:ILE:HG22	1.96	0.47
1:D:465:PRO:HG2	1:D:494:PHE:CE1	2.49	0.47
1:B:622:ASN:HB2	1:B:626:ILE:H	1.80	0.46
2:H:150:THR:OG1	2:H:151:GLU:N	2.47	0.46
1:C:79:ILE:N	1:C:79:ILE:HD12	2.30	0.46
1:A:622:ASN:HB2	1:A:626:ILE:H	1.81	0.46
1:D:348:GLU:OE2	1:D:348:GLU:HA	2.15	0.46
1:D:304:MET:HE3	1:D:304:MET:HA	1.98	0.46
1:D:531:LEU:HD23	1:D:551:TYR:CE1	2.50	0.46
1:C:95:MET:HE3	1:C:184:ALA:N	2.31	0.46
1:D:161:VAL:HG22	1:D:202:VAL:HG13	1.98	0.46
1:A:322:CYS:HB2	4:A:702:MTE:S2'	2.55	0.46
1:C:242:ILE:HG22	1:C:254:VAL:HB	1.98	0.46
2:E:152:MET:HE2	2:E:152:MET:HB3	1.81	0.46
1:B:622:ASN:HB3	1:B:624:ASP:H	1.80	0.45
1:C:150:ILE:HG21	1:C:202:VAL:HG21	1.96	0.45
2:H:64:TYR:O	2:H:93:ARG:HD2	2.16	0.45
1:D:19:ILE:HD11	1:D:132:ILE:HG13	1.98	0.45
1:D:50:GLU:H	1:D:50:GLU:CD	2.22	0.45
1:A:299:CYS:HB2	3:A:701:SF4:S3	2.57	0.45
2:F:96:CYS:SG	2:F:97:PRO:HD2	2.56	0.45
1:C:92:PHE:O	1:C:454:LYS:HE2	2.17	0.45
1:C:372:LEU:HD11	1:C:416:ILE:HG21	1.99	0.45
2:E:85:GLU:HB3	11:E:1128:HOH:O	2.15	0.45
2:G:74:ILE:HD12	2:H:114:ASP:HA	1.98	0.45
1:A:622:ASN:HB3	1:A:624:ASP:H	1.81	0.45
1:C:241:PRO:HB2	1:C:254:VAL:HG21	1.99	0.45
1:D:372:LEU:C	1:D:373:LYS:HD2	2.41	0.45
1:D:391:LEU:HD11	1:D:405:LEU:HD12	1.98	0.45
2:G:173:GLU:C	2:G:175:LEU:N	2.75	0.45
1:B:486:PRO:HD3	1:B:520:TRP:CE2	2.52	0.45
1:C:318:TYR:CE1	1:C:344:GLN:HB2	2.52	0.45
1:D:505:MET:HB3	1:D:506:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLY:C	1:C:209:LEU:HD23	2.42	0.44
1:C:383:GLY:HA3	1:C:386:GLU:OE1	2.16	0.44
1:A:54:PHE:O	1:A:116:LYS:NZ	2.41	0.44
1:C:13:ASP:O	1:C:17:GLY:N	2.47	0.44
1:A:486:PRO:HD3	1:A:520:TRP:CE2	2.52	0.44
1:C:218:ILE:HD12	1:C:218:ILE:HA	1.75	0.44
1:A:376:ASP:C	1:A:378:PRO:HD3	2.43	0.44
1:C:324:THR:HG23	11:C:848:HOH:O	2.18	0.44
1:B:508:PHE:HA	1:B:509:PRO:C	2.43	0.44
1:C:240:MET:SD	1:C:242:ILE:HG12	2.58	0.44
1:D:213:LYS:NZ	8:D:707:PGE:H52	2.33	0.44
1:C:470:PRO:HD2	1:C:474:GLN:OE1	2.18	0.44
1:C:590:ARG:NH1	1:C:623:ASP:O	2.45	0.44
1:D:248:SER:O	1:D:249:PRO:C	2.61	0.44
2:F:141:GLU:HG3	2:F:142:GLU:OE2	2.18	0.44
1:A:508:PHE:HA	1:A:509:PRO:C	2.43	0.43
2:E:114:ASP:HA	2:F:74:ILE:HD13	1.98	0.43
1:B:376:ASP:C	1:B:378:PRO:HD3	2.43	0.43
1:D:251:GLU:HB3	1:D:325:LYS:HD3	2.00	0.43
1:A:189:ILE:HD13	1:A:189:ILE:N	2.31	0.43
1:C:348:GLU:OE2	1:C:348:GLU:HA	2.17	0.43
1:C:540:PHE:HB3	1:C:541:PRO:HD3	2.00	0.43
1:D:356:ALA:HB3	1:D:357:PRO:HD3	2.00	0.43
1:B:372:LEU:HD23	1:B:377:PHE:CZ	2.54	0.43
2:E:6:LYS:O	2:E:6:LYS:HD3	2.17	0.43
1:B:189:ILE:H	1:B:189:ILE:CD1	2.31	0.43
1:C:372:LEU:HD11	1:C:416:ILE:HD13	1.99	0.43
1:D:77:ARG:CZ	1:D:96:GLY:HA3	2.48	0.43
1:B:505:MET:HB3	1:B:506:PRO:HA	2.01	0.43
2:E:72:GLU:HG2	2:E:98:SER:HB3	2.00	0.43
2:F:65:ALA:HB2	2:F:102:PHE:CD1	2.54	0.43
2:H:66:GLY:O	2:H:112:LYS:HG3	2.19	0.43
1:B:487:ASP:OD1	1:B:489:LYS:HG2	2.18	0.43
1:C:468:PRO:HB3	1:C:497:TRP:CG	2.53	0.43
1:D:367:LEU:HD22	1:D:377:PHE:CE1	2.54	0.43
2:E:36:MET:HB2	2:E:36:MET:HE3	1.49	0.43
1:A:372:LEU:HD23	1:A:377:PHE:CZ	2.54	0.42
1:A:505:MET:HB3	1:A:506:PRO:HA	2.01	0.42
1:D:186:ARG:CD	1:D:352:ASP:CG	2.91	0.42
1:D:189:ILE:HD13	1:D:189:ILE:H	1.83	0.42
1:C:27:ARG:HG3	1:C:27:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:ASN:HB2	1:D:626:ILE:H	1.84	0.42
1:A:487:ASP:OD1	1:A:489:LYS:HG2	2.19	0.42
1:C:225:LEU:O	1:C:229:LYS:HG3	2.19	0.42
1:C:260:HIS:CE1	9:C:707[B]:4KX:H5B	2.53	0.42
2:G:156:LEU:CD2	2:H:159:LEU:HD13	2.49	0.42
1:B:266:TRP:CE3	1:B:330:MET:HA	2.54	0.42
1:B:322:CYS:HB2	4:B:702:MTE:S2'	2.59	0.42
1:C:266:TRP:CE3	1:C:330:MET:HA	2.54	0.42
1:D:41:LYS:HA	1:D:578:LEU:HD21	2.02	0.42
2:H:64:TYR:O	2:H:93:ARG:CD	2.67	0.42
1:B:635:LEU:HG	11:B:872:HOH:O	2.18	0.42
1:D:318:TYR:OH	1:D:340:LEU:O	2.32	0.42
1:C:186:ARG:CD	1:C:352:ASP:OD2	2.68	0.42
1:B:322:CYS:CB	4:B:702:MTE:S2'	3.08	0.42
1:C:373:LYS:HB3	1:C:373:LYS:HE2	1.83	0.42
2:G:67[B]:GLU:CG	3:H:1003:SF4:S4	3.08	0.42
2:G:166:ASP:OD1	2:G:166:ASP:N	2.45	0.42
1:A:369:LYS:CG	1:A:371:ILE:HG13	2.50	0.42
1:C:531:LEU:HD23	1:C:551:TYR:CE1	2.54	0.42
1:D:258:LYS:HB2	1:D:277:TRP:CD1	2.54	0.42
1:A:266:TRP:CE3	1:A:330:MET:HA	2.54	0.42
1:C:114:ARG:HD3	11:C:1005:HOH:O	2.19	0.41
1:C:231:ARG:HG2	1:C:246:LEU:HG	2.01	0.41
1:B:369:LYS:CG	1:B:371:ILE:HG13	2.50	0.41
1:C:511:VAL:HG11	1:C:614:SER:OG	2.20	0.41
1:A:364:PHE:O	1:A:368:GLU:HB2	2.21	0.41
1:D:450:CYS:SG	1:D:595:PRO:HD3	2.60	0.41
1:B:189:ILE:HD13	1:B:189:ILE:N	2.32	0.41
1:C:503:LYS:O	1:C:508:PHE:HB3	2.20	0.41
9:D:709:4KX:O9P	9:D:709:4KX:HCPA	2.20	0.41
1:A:481:ASP:OD1	1:A:481:ASP:N	2.53	0.41
1:C:260:HIS:CE1	9:C:707[A]:4KX:H5B	2.55	0.41
1:C:442:ASN:HA	1:C:443:PRO:HD2	1.76	0.41
2:F:11:LYS:HG2	2:F:137:GLU:HG2	2.01	0.41
2:G:123:LEU:HD23	2:G:123:LEU:HA	1.78	0.41
1:A:172:VAL:O	1:A:191:ALA:HB2	2.21	0.41
1:D:260:HIS:NE2	9:D:709:4KX:H5B	2.36	0.41
2:F:21:ASN:ND2	2:F:130:VAL:HG11	2.36	0.41
1:A:189:ILE:H	1:A:189:ILE:CD1	2.31	0.41
1:B:252:MET:SD	1:B:320:MET:HG2	2.61	0.41
1:B:513:MET:O	1:B:517:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:MET:HE3	1:D:289:MET:HE1	2.02	0.41
1:D:264:PHE:HB2	1:D:330:MET:HE1	2.03	0.41
1:A:466:GLN:HB2	8:A:708:PGE:H3	2.03	0.41
4:B:703:MTE:H6	11:B:859:HOH:O	2.21	0.41
1:C:61:ILE:O	1:C:80:VAL:HA	2.21	0.41
1:C:440:MET:HE2	1:C:440:MET:HB2	1.91	0.41
1:C:488:GLU:O	1:C:492:LYS:HD2	2.21	0.41
1:C:496:GLU:OE2	1:C:503:LYS:NZ	2.40	0.41
1:C:498:GLU:O	1:C:504:SER:HA	2.21	0.41
1:D:266:TRP:CZ3	1:D:330:MET:HA	2.56	0.41
1:D:641:GLY:O	1:D:645:ILE:HG13	2.21	0.41
2:E:55:PRO:HA	2:E:60:TYR:OH	2.20	0.41
2:E:104:GLU:CD	2:E:111:LEU:HD21	2.46	0.41
2:F:142:GLU:CD	2:F:142:GLU:H	2.29	0.41
1:B:364:PHE:O	1:B:368:GLU:HB2	2.20	0.41
1:D:486:PRO:HD3	1:D:520:TRP:CE2	2.56	0.41
1:C:253:LYS:HG2	1:C:296:LEU:HD13	2.02	0.40
1:C:619:LYS:NZ	11:C:819:HOH:O	2.52	0.40
1:A:252:MET:SD	1:A:320:MET:HG2	2.61	0.40
2:E:109:LEU:HB3	2:E:110:PRO:HD2	2.04	0.40
2:F:67[A]:GLU:OE1	2:F:112:LYS:NZ	2.42	0.40
1:A:489:LYS:O	1:A:493:ILE:HG13	2.22	0.40
1:C:48:PRO:HB2	1:C:50:GLU:OE1	2.22	0.40
1:C:586:ARG:NH2	11:C:812:HOH:O	2.48	0.40
1:D:34:GLY:O	1:D:35:GLY:C	2.64	0.40
1:D:619:LYS:HB3	1:D:621:TRP:CE2	2.56	0.40
2:H:115:LEU:HA	3:H:1002:SF4:S1	2.61	0.40
1:D:189:ILE:HG12	1:D:190:GLY:N	2.36	0.40
1:A:580:ARG:NH2	1:A:593:GLU:OE1	2.45	0.40
1:D:42:ILE:HG23	1:D:46:ARG:HD3	2.03	0.40
1:D:489:LYS:O	1:D:493:ILE:HG13	2.21	0.40
1:D:508:PHE:HA	1:D:509:PRO:C	2.47	0.40
2:G:103[B]:ARG:HD2	2:G:108:GLY:O	2.21	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	652/653 (100%)	628 (96%)	24 (4%)	0	100	100
1	B	651/653 (100%)	627 (96%)	24 (4%)	0	100	100
1	C	651/653 (100%)	629 (97%)	22 (3%)	0	100	100
1	D	650/653 (100%)	623 (96%)	27 (4%)	0	100	100
2	E	162/179 (90%)	157 (97%)	5 (3%)	0	100	100
2	F	169/179 (94%)	167 (99%)	2 (1%)	0	100	100
2	G	169/179 (94%)	166 (98%)	2 (1%)	1 (1%)	21	10
2	H	157/179 (88%)	155 (99%)	2 (1%)	0	100	100
All	All	3261/3328 (98%)	3152 (97%)	108 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	174	GLN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	547/548 (100%)	536 (98%)	11 (2%)	48	36
1	B	547/548 (100%)	536 (98%)	11 (2%)	48	36
1	C	546/548 (100%)	530 (97%)	16 (3%)	37	22
1	D	547/548 (100%)	533 (97%)	14 (3%)	40	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	136/159 (86%)	127 (93%)	9 (7%)	15	4
2	F	148/159 (93%)	143 (97%)	5 (3%)	32	17
2	G	147/159 (92%)	141 (96%)	6 (4%)	27	12
2	H	132/159 (83%)	128 (97%)	4 (3%)	36	21
All	All	2750/2828 (97%)	2674 (97%)	76 (3%)	38	23

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	55	SER
1	A	174	TYR
1	A	189	ILE
1	A	309	THR
1	A	321	LYS
1	A	455	ILE
1	A	531	LEU
1	A	551	TYR
1	A	591	VAL
1	A	599	HIS
1	B	2	ARG
1	B	55	SER
1	B	174	TYR
1	B	189	ILE
1	B	309	THR
1	B	321	LYS
1	B	455	ILE
1	B	531	LEU
1	B	551	TYR
1	B	591	VAL
1	B	599	HIS
1	C	1	MET
1	C	45	ASP
1	C	50	GLU
1	C	114	ARG
1	C	179	GLN
1	C	189	ILE
1	C	215	GLU
1	C	309	THR
1	C	321	LYS
1	C	348	GLU

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Mol	Chain	Res	Type
1	C	401	ILE
1	C	531	LEU
1	C	551	TYR
1	C	591	VAL
1	C	599	HIS
1	C	614	SER
1	D	50	GLU
1	D	55	SER
1	D	179	GLN
1	D	189	ILE
1	D	215	GLU
1	D	281	VAL
1	D	309	THR
1	D	321	LYS
1	D	439	SER
1	D	455	ILE
1	D	531	LEU
1	D	551	TYR
1	D	561	ILE
1	D	599	HIS
2	E	6	LYS
2	E	9	ILE
2	E	13	ILE
2	E	93	ARG
2	E	99	ARG
2	E	101	LEU
2	E	106	ASP
2	E	152	MET
2	E	171	THR
2	F	10	VAL
2	F	44	PRO
2	F	99	ARG
2	F	135	VAL
2	F	156	LEU
2	G	63	LEU
2	G	93	ARG
2	G	99	ARG
2	G	101	LEU
2	G	135	VAL
2	G	160	ILE
2	H	36	MET
2	H	63	LEU

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Mol	Chain	Res	Type
2	H	93	ARG
2	H	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	602	ASN
1	B	427	ASN
1	B	602	ASN
1	C	427	ASN
1	C	456	ASN
1	D	433	GLN
2	E	42	ASN
2	F	42	ASN
2	G	14	ASN
2	G	42	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 8 are monoatomic and 4 are unknown - leaving 33 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTE	C	702	5,6	21,26,26	2.18	4 (19%)	19,40,40	2.94	9 (47%)
4	MTE	C	703	5,6	21,26,26	2.81	6 (28%)	19,40,40	2.18	5 (26%)
3	SF4	F	1001	2	0,12,12	-	-	-	-	-
8	PGE	A	707	-	9,9,9	0.56	0	8,8,8	0.61	0
9	4KX	C	707[A]	-	53,59,59	1.20	2 (3%)	77,87,87	1.08	5 (6%)
3	SF4	D	702	1	0,12,12	-	-	-	-	-
4	MTE	D	703	5,6	21,26,26	2.35	7 (33%)	19,40,40	2.03	6 (31%)
10	PG4	D	708	-	12,12,12	0.66	0	11,11,11	0.57	0
3	SF4	G	1002	2	0,12,12	-	-	-	-	-
3	SF4	G	1003	2	0,12,12	-	-	-	-	-
3	SF4	H	1002	2	0,12,12	-	-	-	-	-
9	4KX	A	709	-	53,59,59	1.24	2 (3%)	77,87,87	1.10	6 (7%)
4	MTE	A	702	5,6	21,26,26	2.47	9 (42%)	19,40,40	2.09	3 (15%)
3	SF4	F	1003	2	0,12,12	-	-	-	-	-
3	SF4	B	701	1	0,12,12	-	-	-	-	-
3	SF4	E	1002	2	0,12,12	-	-	-	-	-
9	4KX	D	709	-	53,59,59	1.24	2 (3%)	77,87,87	1.07	7 (9%)
3	SF4	E	1003	2	0,12,12	-	-	-	-	-
3	SF4	A	701	1	0,12,12	-	-	-	-	-
3	SF4	C	701	1	0,12,12	-	-	-	-	-
3	SF4	H	1001	2	0,12,12	-	-	-	-	-
4	MTE	B	703	5,6	21,26,26	2.53	7 (33%)	19,40,40	2.74	8 (42%)
8	PGE	D	707	-	9,9,9	0.45	0	8,8,8	0.52	0
3	SF4	F	1002	2	0,12,12	-	-	-	-	-
9	4KX	C	707[B]	-	53,59,59	1.25	2 (3%)	77,87,87	1.11	5 (6%)
4	MTE	A	703	5,6	21,26,26	2.95	6 (28%)	19,40,40	3.44	8 (42%)
8	PGE	A	708	-	9,9,9	0.82	0	8,8,8	0.82	0
4	MTE	D	704	5,6	21,26,26	3.34	6 (28%)	19,40,40	3.08	10 (52%)
3	SF4	E	1001	2	0,12,12	-	-	-	-	-
4	MTE	B	702	5,6	21,26,26	2.84	8 (38%)	19,40,40	2.19	7 (36%)
3	SF4	H	1003	2	0,12,12	-	-	-	-	-
9	4KX	B	707	-	53,59,59	1.24	3 (5%)	77,87,87	1.18	6 (7%)
3	SF4	G	1001	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	MTE	C	702	5,6	-	0/6/34/34	0/3/3/3
4	MTE	C	703	5,6	-	0/6/34/34	0/3/3/3
3	SF4	F	1001	2	-	-	0/6/5/5
8	PGE	A	707	-	-	3/7/7/7	-
9	4KX	C	707[A]	-	-	3/53/79/79	0/4/4/4
3	SF4	D	702	1	-	-	0/6/5/5
4	MTE	D	703	5,6	-	0/6/34/34	0/3/3/3
10	PG4	D	708	-	-	6/10/10/10	-
3	SF4	G	1002	2	-	-	0/6/5/5
3	SF4	G	1003	2	-	-	0/6/5/5
3	SF4	H	1002	2	-	-	0/6/5/5
9	4KX	A	709	-	-	1/53/79/79	0/4/4/4
4	MTE	A	702	5,6	-	1/6/34/34	0/3/3/3
3	SF4	F	1003	2	-	-	0/6/5/5
3	SF4	B	701	1	-	-	0/6/5/5
3	SF4	E	1002	2	-	-	0/6/5/5
9	4KX	D	709	-	-	3/53/79/79	0/4/4/4
3	SF4	E	1003	2	-	-	0/6/5/5
3	SF4	A	701	1	-	-	0/6/5/5
3	SF4	C	701	1	-	-	0/6/5/5
3	SF4	H	1001	2	-	-	0/6/5/5
4	MTE	B	703	5,6	-	2/6/34/34	0/3/3/3
8	PGE	D	707	-	-	2/7/7/7	-
3	SF4	F	1002	2	-	-	0/6/5/5
9	4KX	C	707[B]	-	-	21/53/79/79	0/4/4/4
4	MTE	A	703	5,6	-	0/6/34/34	0/3/3/3
8	PGE	A	708	-	-	5/7/7/7	-
4	MTE	D	704	5,6	-	0/6/34/34	0/3/3/3
3	SF4	E	1001	2	-	-	0/6/5/5
3	SF4	G	1001	2	-	-	0/6/5/5
4	MTE	B	702	5,6	-	0/6/34/34	0/3/3/3
3	SF4	H	1003	2	-	-	0/6/5/5
9	4KX	B	707	-	-	4/53/79/79	0/4/4/4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	704	MTE	C10-N8	13.15	1.49	1.35
4	C	703	MTE	C10-N8	9.84	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	MTE	C10-N8	8.93	1.44	1.35
4	B	702	MTE	C10-N8	8.82	1.44	1.35
9	C	707[A]	4KX	C3B-C4B	7.62	1.52	1.33
9	C	707[B]	4KX	C3B-C4B	7.62	1.52	1.33
9	B	707	4KX	C3B-C4B	7.48	1.52	1.33
9	A	709	4KX	C3B-C4B	7.40	1.52	1.33
9	D	709	4KX	C3B-C4B	7.09	1.51	1.33
4	D	703	MTE	C10-N8	6.88	1.42	1.35
4	B	703	MTE	C10-N8	6.50	1.42	1.35
4	C	702	MTE	C9-C10	-5.88	1.28	1.38
4	B	703	MTE	C9-C10	-5.52	1.29	1.38
4	C	702	MTE	C10-N8	5.42	1.41	1.35
4	C	703	MTE	C2-N2	5.05	1.46	1.34
4	A	702	MTE	C6-N5	5.01	1.52	1.46
4	A	702	MTE	C10-N8	4.85	1.40	1.35
4	A	703	MTE	C6-N5	4.83	1.51	1.46
4	B	702	MTE	C9-C10	-4.45	1.31	1.38
4	A	703	MTE	C7-C6	-4.26	1.50	1.53
4	A	703	MTE	C9-C10	-4.25	1.31	1.38
9	D	709	4KX	C3B-C2B	4.23	1.52	1.43
4	B	702	MTE	C2-N2	4.15	1.43	1.34
4	B	703	MTE	C6-N5	-4.12	1.41	1.46
4	A	703	MTE	C2-N2	4.11	1.43	1.34
4	D	704	MTE	C9-C10	-3.98	1.31	1.38
9	C	707[B]	4KX	C3B-C2B	3.87	1.51	1.43
4	A	702	MTE	C2-N2	3.85	1.43	1.34
9	A	709	4KX	C3B-C2B	3.85	1.51	1.43
9	C	707[A]	4KX	C3B-C2B	3.84	1.51	1.43
4	D	704	MTE	C6-N5	3.82	1.50	1.46
4	D	703	MTE	C2-N2	3.75	1.43	1.34
4	A	702	MTE	P-O3P	-3.72	1.41	1.54
9	B	707	4KX	C3B-C2B	3.61	1.50	1.43
4	B	703	MTE	C2-N2	3.50	1.42	1.34
4	B	702	MTE	O3'-C7	-3.43	1.38	1.43
4	D	703	MTE	C9-C10	-3.33	1.33	1.38
4	D	703	MTE	C9-N5	3.33	1.45	1.37
4	A	702	MTE	O3'-C7	-3.28	1.38	1.43
4	B	703	MTE	C10-N1	3.09	1.40	1.36
4	C	703	MTE	C9-C10	-2.98	1.33	1.38
4	A	703	MTE	C9-C4	2.97	1.50	1.41
4	B	702	MTE	C9-C4	2.96	1.50	1.41
4	A	702	MTE	P-O1P	2.92	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	703	MTE	C10-N1	2.92	1.40	1.36
4	A	702	MTE	C9-N5	2.85	1.44	1.37
4	C	702	MTE	C2-N2	2.79	1.40	1.34
4	A	702	MTE	O4-C4	2.76	1.28	1.23
4	B	702	MTE	C9-N5	2.72	1.44	1.37
4	D	704	MTE	C2-N2	2.65	1.40	1.34
4	C	703	MTE	C9-N5	2.52	1.43	1.37
4	A	702	MTE	C10-N1	2.50	1.40	1.36
4	D	704	MTE	C9-C4	2.49	1.49	1.41
4	B	702	MTE	C7-C6	-2.37	1.51	1.53
9	B	707	4KX	P3D-O3D	2.33	1.63	1.59
4	B	703	MTE	C7-C6	-2.32	1.51	1.53
4	D	703	MTE	C9-C4	2.27	1.48	1.41
4	D	704	MTE	C2-N1	2.19	1.38	1.33
4	C	703	MTE	C9-C4	2.18	1.48	1.41
4	B	703	MTE	O3'-C3'	-2.16	1.39	1.43
4	D	703	MTE	O3'-C7	-2.10	1.40	1.43
4	B	702	MTE	P-O1P	2.10	1.57	1.50
4	C	702	MTE	C9-C4	2.04	1.48	1.41
4	D	703	MTE	C7-N8	2.01	1.48	1.45

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	704	MTE	O3'-C7-N8	-8.97	100.46	108.61
4	A	703	MTE	O3'-C7-N8	-7.97	101.37	108.61
4	A	703	MTE	C2-N1-C10	7.01	125.74	113.36
4	B	703	MTE	O3'-C7-N8	-6.97	102.28	108.61
4	A	702	MTE	C7-C6-N5	6.49	114.24	107.87
4	C	702	MTE	O3'-C7-C6	6.47	113.28	108.96
4	C	703	MTE	O3'-C7-N8	-6.23	102.95	108.61
4	C	702	MTE	C2-N3-C4	-6.09	114.07	125.11
4	A	703	MTE	C2-N3-C4	-5.92	114.36	125.11
9	C	707[B]	4KX	C5B-C4B-C3B	-5.92	111.30	122.95
9	C	707[A]	4KX	C5B-C4B-C3B	-5.88	111.39	122.95
9	B	707	4KX	C5B-C4B-C3B	-5.62	111.89	122.95
4	A	703	MTE	O3'-C7-C6	-5.19	105.50	108.96
4	B	703	MTE	O4-C4-C9	-4.99	115.24	127.26
4	B	703	MTE	C2-N3-C4	-4.94	116.15	125.11
4	D	704	MTE	C2-N3-C4	-4.88	116.26	125.11
4	B	702	MTE	C2-N1-C10	4.88	121.97	113.36
4	D	703	MTE	C2-N3-C4	-4.87	116.28	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	709	4KX	C5B-C4B-C3B	-4.70	113.70	122.95
9	B	707	4KX	C2P-S1P-C1B	4.68	105.36	99.85
4	B	702	MTE	C2-N3-C4	-4.61	116.75	125.11
4	C	702	MTE	O3'-C7-N8	-4.60	104.43	108.61
4	A	702	MTE	O3'-C7-N8	-4.54	104.48	108.61
9	A	709	4KX	C4B-C3B-C2B	-4.44	111.31	121.50
9	D	709	4KX	C5B-C4B-C3B	-4.39	114.31	122.95
9	C	707[B]	4KX	C4B-C3B-C2B	-4.23	111.78	121.50
9	C	707[A]	4KX	C4B-C3B-C2B	-4.21	111.83	121.50
4	D	704	MTE	O3'-C7-C6	4.18	111.75	108.96
9	B	707	4KX	C4B-C3B-C2B	-4.14	111.99	121.50
4	C	702	MTE	O3P-P-O4'	3.99	117.08	106.67
4	C	703	MTE	C2-N1-C10	3.82	120.11	113.36
4	D	704	MTE	C2-N1-C10	3.81	120.08	113.36
4	A	703	MTE	C9-C4-N3	3.75	122.42	112.13
4	C	702	MTE	O4-C4-C9	-3.62	118.54	127.26
4	D	703	MTE	C2-N1-C10	3.29	119.16	113.36
9	D	709	4KX	C4B-C3B-C2B	-3.24	114.07	121.50
4	C	702	MTE	C9-C4-N3	3.22	120.96	112.13
4	B	703	MTE	O4'-C4'-C3'	3.09	116.22	108.58
4	C	703	MTE	O4'-P-O1P	2.97	114.48	106.44
9	A	709	4KX	O5A-P2A-O6A	2.92	120.80	107.57
9	B	707	4KX	P3D-O3D-C3D	2.89	131.16	123.43
4	D	704	MTE	O2P-P-O1P	-2.89	99.58	110.83
4	D	703	MTE	C9-C4-N3	2.88	120.04	112.13
4	B	702	MTE	C9-C4-N3	2.85	119.96	112.13
4	D	703	MTE	C7-C6-N5	2.84	110.66	107.87
4	D	704	MTE	O2P-P-O4'	2.79	113.95	106.67
9	D	709	4KX	C2P-S1P-C1B	2.78	103.12	99.85
4	A	703	MTE	C4-C9-N5	2.77	123.83	116.27
4	B	702	MTE	O2P-P-O4'	2.72	113.75	106.67
4	B	703	MTE	O4-C4-N3	2.71	125.20	120.11
4	B	703	MTE	C9-C4-N3	2.71	119.56	112.13
4	D	703	MTE	O3'-C7-N8	-2.70	106.16	108.61
4	D	704	MTE	C9-C4-N3	2.64	119.38	112.13
4	D	704	MTE	O4-C4-N3	-2.56	115.30	120.11
4	C	703	MTE	C2-N3-C4	-2.52	120.54	125.11
4	C	702	MTE	C2-N1-C10	2.50	117.77	113.36
9	D	709	4KX	O1A-P1A-O3A	-2.48	100.56	107.27
9	C	707[B]	4KX	C2P-S1P-C1B	2.46	102.75	99.85
9	C	707[A]	4KX	C5B-C6B-C7B	-2.46	112.52	118.93
4	D	703	MTE	O4-C4-C9	-2.45	121.35	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	707[B]	4KX	C5B-C6B-C7B	-2.45	112.53	118.93
4	A	703	MTE	O4-C4-N3	-2.43	115.54	120.11
9	B	707	4KX	C5B-C6B-C7B	-2.43	112.59	118.93
4	A	702	MTE	C2-N3-C4	-2.40	120.75	125.11
4	D	704	MTE	C4-C9-N5	2.38	122.75	116.27
9	C	707[A]	4KX	C2P-S1P-C1B	2.34	102.61	99.85
4	B	702	MTE	O4-C4-C9	-2.34	121.62	127.26
4	B	703	MTE	C2-N1-C10	2.34	117.48	113.36
4	B	703	MTE	O4'-P-O1P	2.33	112.73	106.44
9	A	709	4KX	C5B-C6B-C7B	-2.32	112.87	118.93
9	C	707[A]	4KX	O57-C1B-C2B	-2.32	118.65	123.35
4	C	702	MTE	O3P-P-O1P	-2.27	101.98	110.83
9	C	707[B]	4KX	O57-C1B-C2B	-2.27	118.75	123.35
9	D	709	4KX	C5B-C6B-C7B	-2.24	113.08	118.93
4	B	702	MTE	O4'-P-O1P	2.19	112.36	106.44
4	A	703	MTE	O4-C4-C9	-2.18	122.00	127.26
9	A	709	4KX	C7B-C2B-C1B	2.17	123.87	119.37
9	A	709	4KX	P3D-O3D-C3D	2.16	129.21	123.43
9	D	709	4KX	O5D-P1A-O2A	2.16	117.49	108.94
4	B	702	MTE	C7-C6-N5	2.14	109.97	107.87
4	C	703	MTE	O4-C4-C9	-2.13	122.12	127.26
9	B	707	4KX	C7B-C2B-C1B	2.12	123.76	119.37
4	D	704	MTE	O3P-P-O2P	2.10	115.66	107.80
4	C	702	MTE	N2-C2-N1	-2.09	115.59	119.67
9	D	709	4KX	C7B-C2B-C1B	2.02	123.55	119.37

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	MTE	C4'-O4'-P-O2P
4	B	703	MTE	C4'-O4'-P-O3P
9	B	707	4KX	N8P-C9P-CAP-OAP
9	C	707[B]	4KX	C5D-O5D-P1A-O1A
9	C	707[B]	4KX	C5D-O5D-P1A-O3A
9	C	707[B]	4KX	CCP-O6A-P2A-O3A
9	C	707[B]	4KX	CCP-O6A-P2A-O4A
9	C	707[B]	4KX	CCP-O6A-P2A-O5A
9	C	707[B]	4KX	CBP-CCP-O6A-P2A
9	C	707[B]	4KX	N8P-C9P-CAP-CBP
9	C	707[B]	4KX	O9P-C9P-CAP-CBP
9	C	707[B]	4KX	CAP-CBP-CCP-O6A

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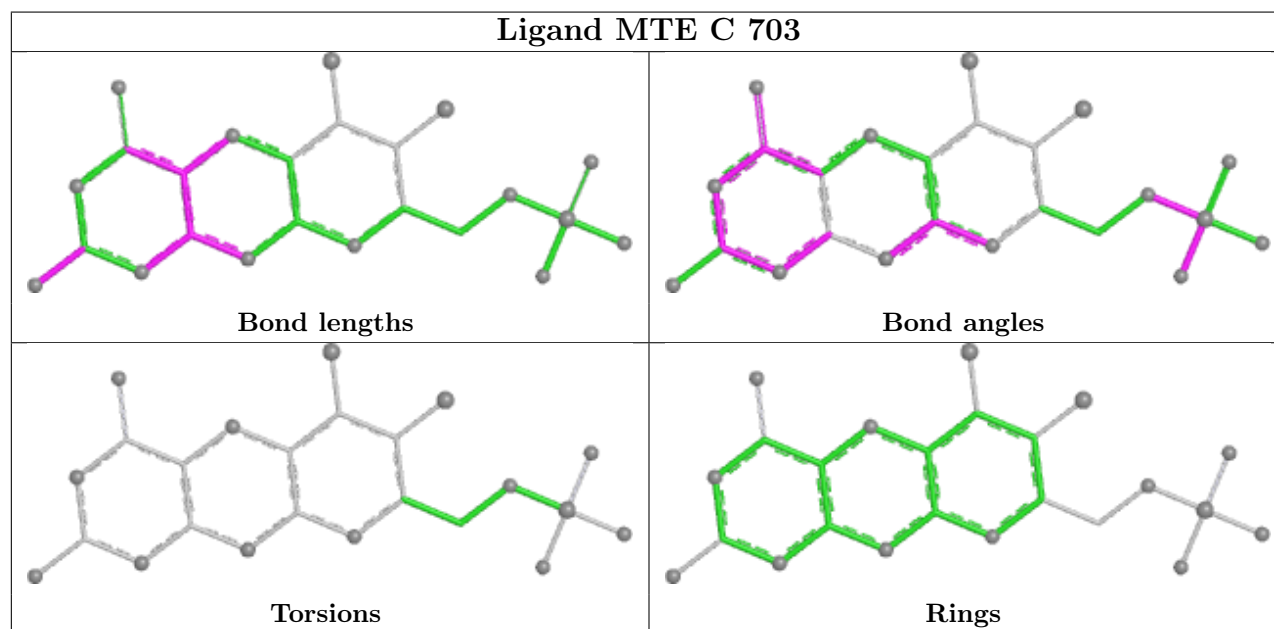
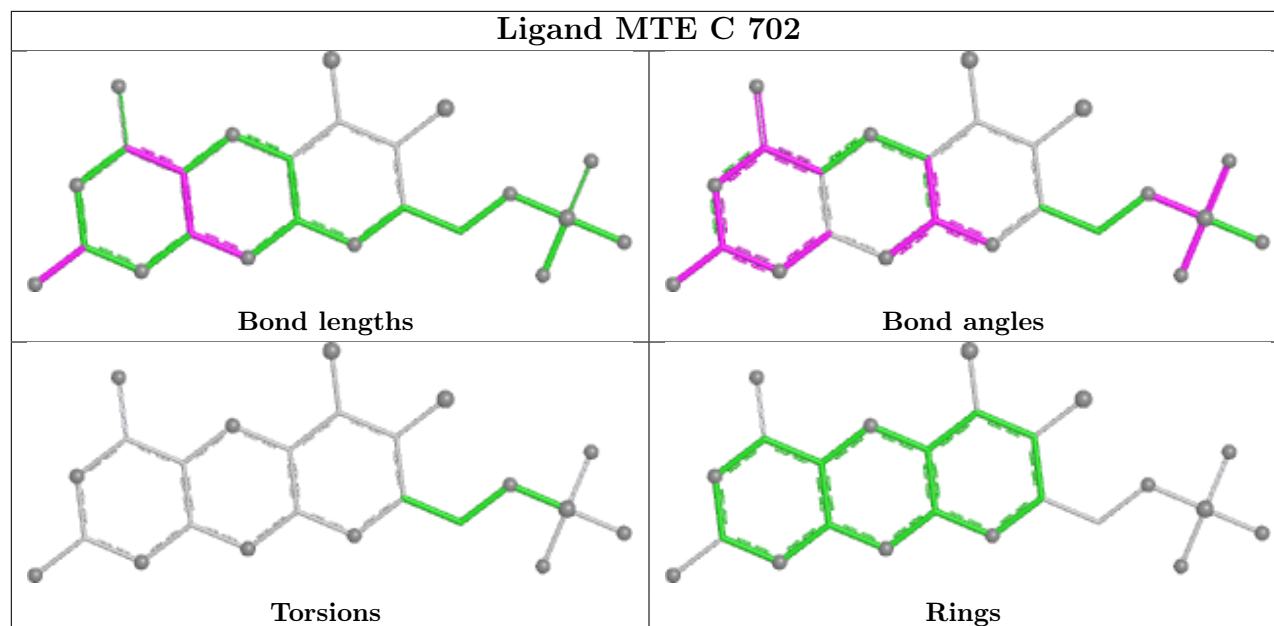
Mol	Chain	Res	Type	Atoms
9	C	707[B]	4KX	CDP-CBP-CCP-O6A
9	C	707[B]	4KX	CEP-CBP-CCP-O6A
9	C	707[B]	4KX	O5P-C5P-C6P-C7P
9	C	707[B]	4KX	N4P-C5P-C6P-C7P
8	A	707	PGE	O2-C3-C4-O3
8	A	708	PGE	O3-C5-C6-O4
10	D	708	PG4	O1-C1-C2-O2
8	D	707	PGE	O1-C1-C2-O2
8	A	708	PGE	O1-C1-C2-O2
10	D	708	PG4	O2-C3-C4-O3
10	D	708	PG4	C4-C3-O2-C2
9	B	707	4KX	O9P-C9P-CAP-OAP
9	C	707[B]	4KX	C2D-C3D-O3D-P3D
8	A	707	PGE	O1-C1-C2-O2
9	C	707[B]	4KX	N8P-C9P-CAP-OAP
9	B	707	4KX	N4P-C5P-C6P-C7P
9	C	707[B]	4KX	C4D-C3D-O3D-P3D
8	A	708	PGE	C6-C5-O3-C4
8	A	708	PGE	C3-C4-O3-C5
8	D	707	PGE	C6-C5-O3-C4
8	A	708	PGE	C1-C2-O2-C3
9	B	707	4KX	O5P-C5P-C6P-C7P
10	D	708	PG4	C6-C5-O3-C4
9	C	707[B]	4KX	C5D-O5D-P1A-O2A
9	D	709	4KX	O5P-C5P-C6P-C7P
4	A	702	MTE	C4'-O4'-P-O1P
9	D	709	4KX	N4P-C5P-C6P-C7P
9	C	707[B]	4KX	C3D-O3D-P3D-O8A
9	D	709	4KX	C3D-O3D-P3D-O9A
10	D	708	PG4	C5-C6-O4-C7
8	A	707	PGE	C6-C5-O3-C4
9	C	707[B]	4KX	P2A-O3A-P1A-O1A
9	C	707[A]	4KX	C3D-O3D-P3D-O8A
9	C	707[A]	4KX	O5P-C5P-C6P-C7P
9	A	709	4KX	N4P-C5P-C6P-C7P
9	C	707[A]	4KX	N4P-C5P-C6P-C7P
9	C	707[B]	4KX	C4D-C5D-O5D-P1A
10	D	708	PG4	C8-C7-O4-C6
9	C	707[B]	4KX	C2P-C3P-N4P-C5P

There are no ring outliers.

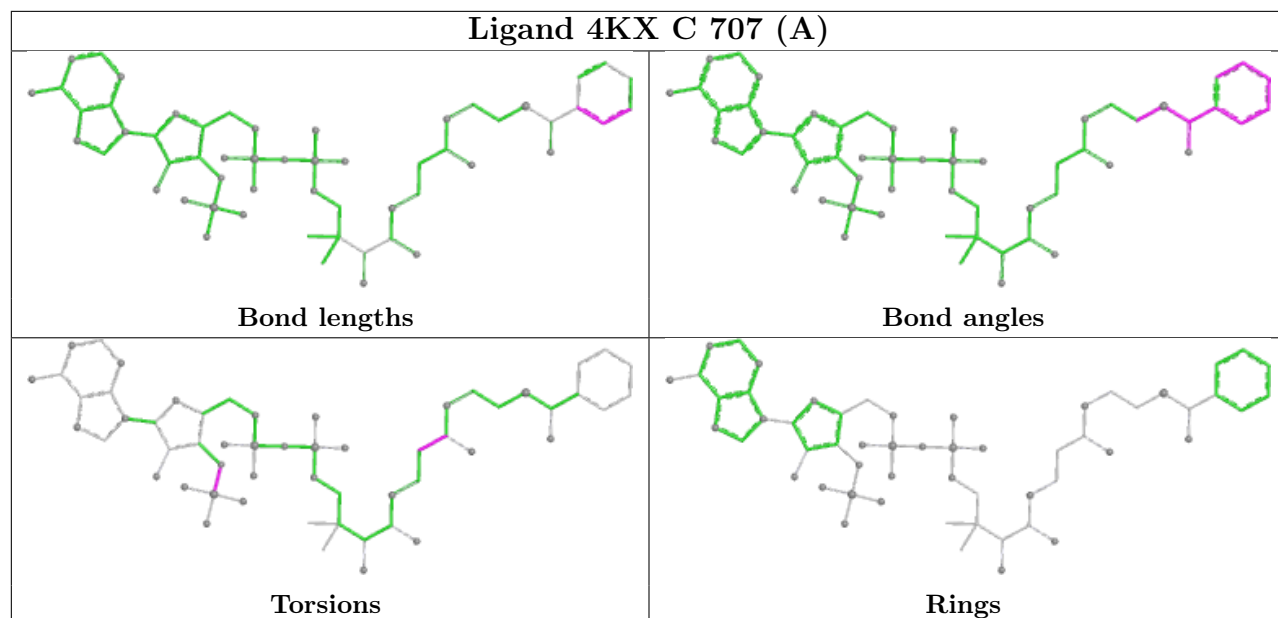
17 monomers are involved in 40 short contacts:

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

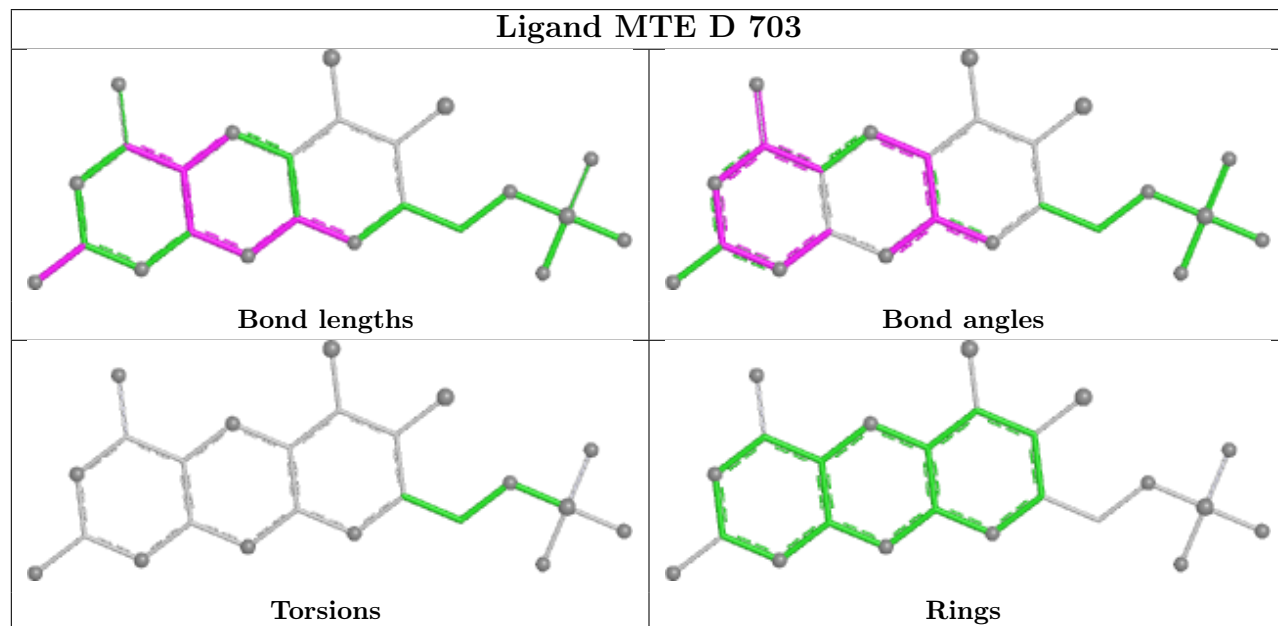
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



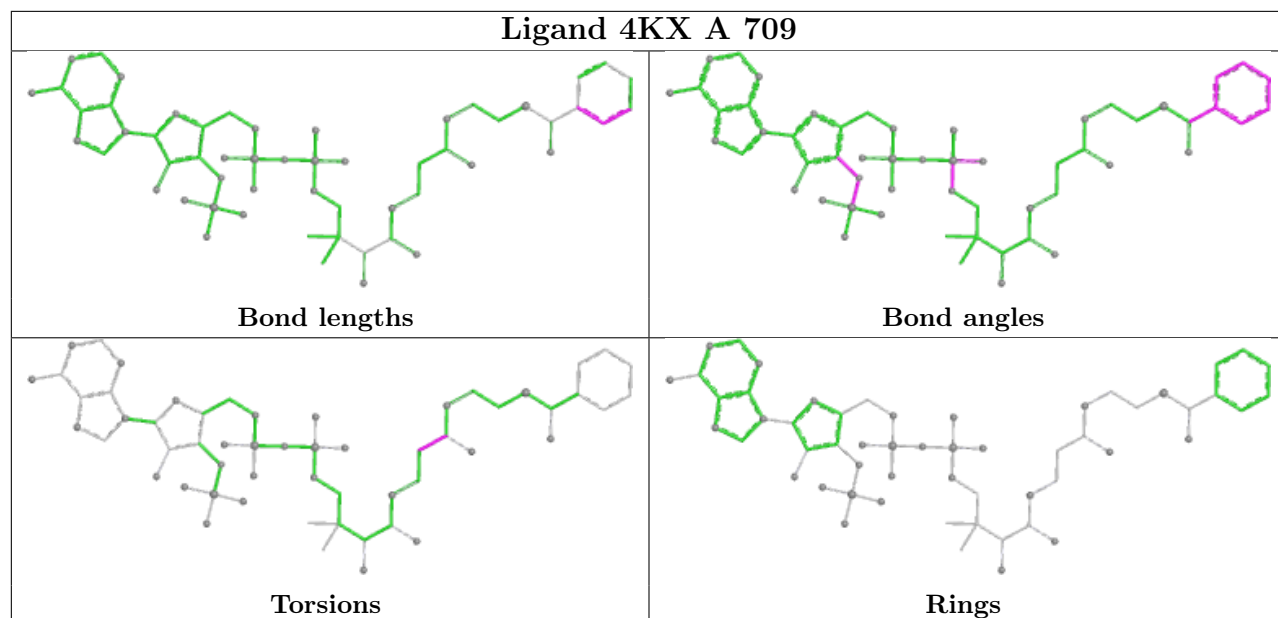
Ligand 4KX C 707 (A)



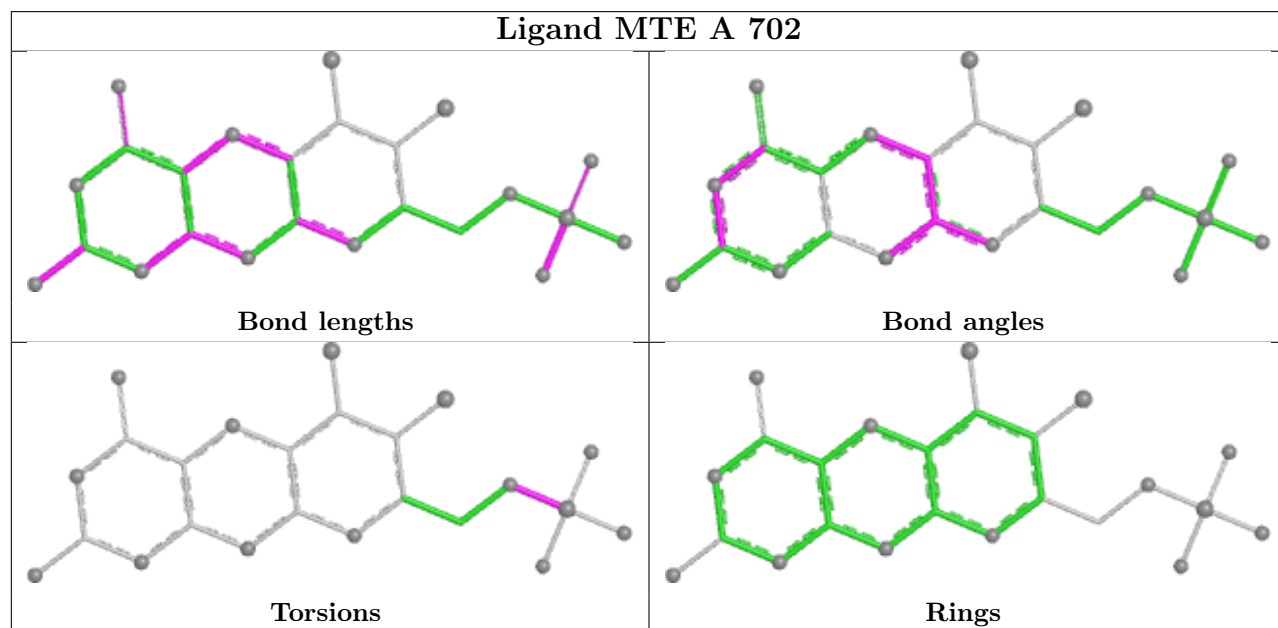
Ligand MTE D 703



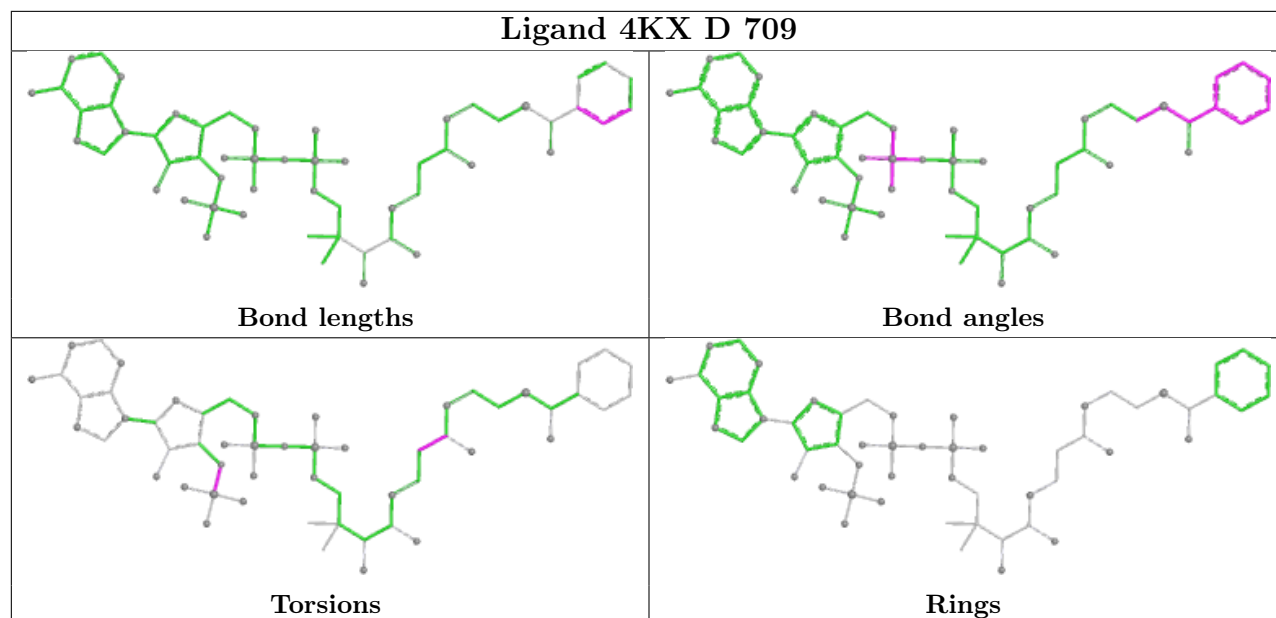
Ligand 4KX A 709



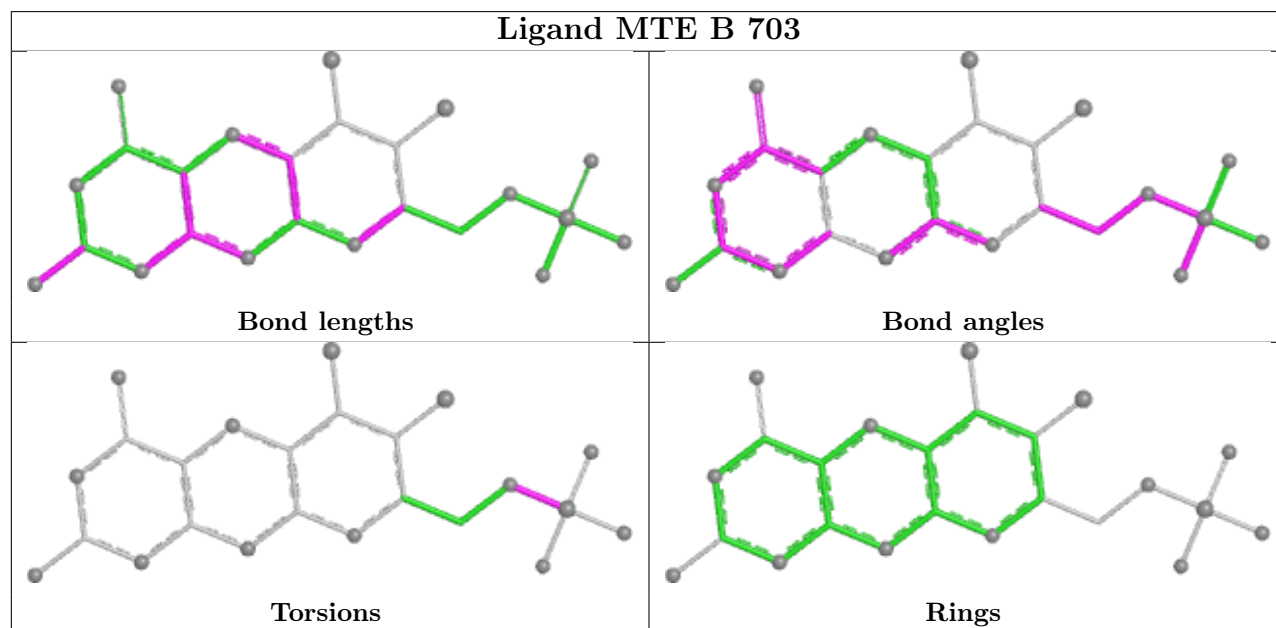
Ligand MTE A 702



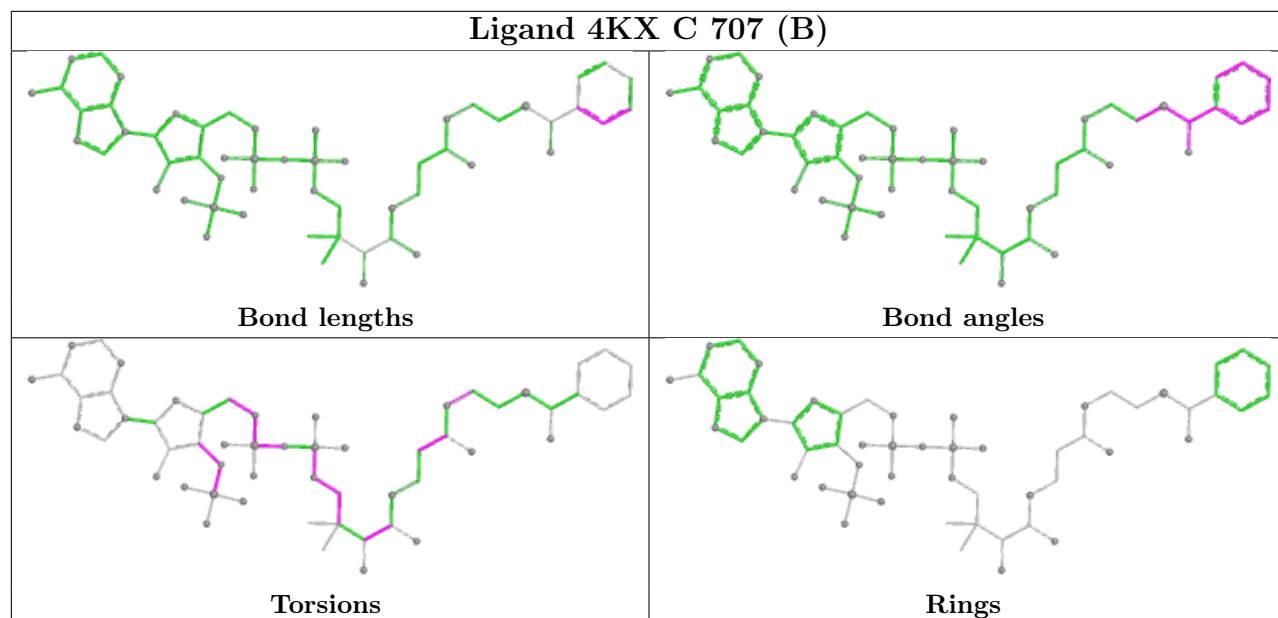
Ligand 4KX D 709



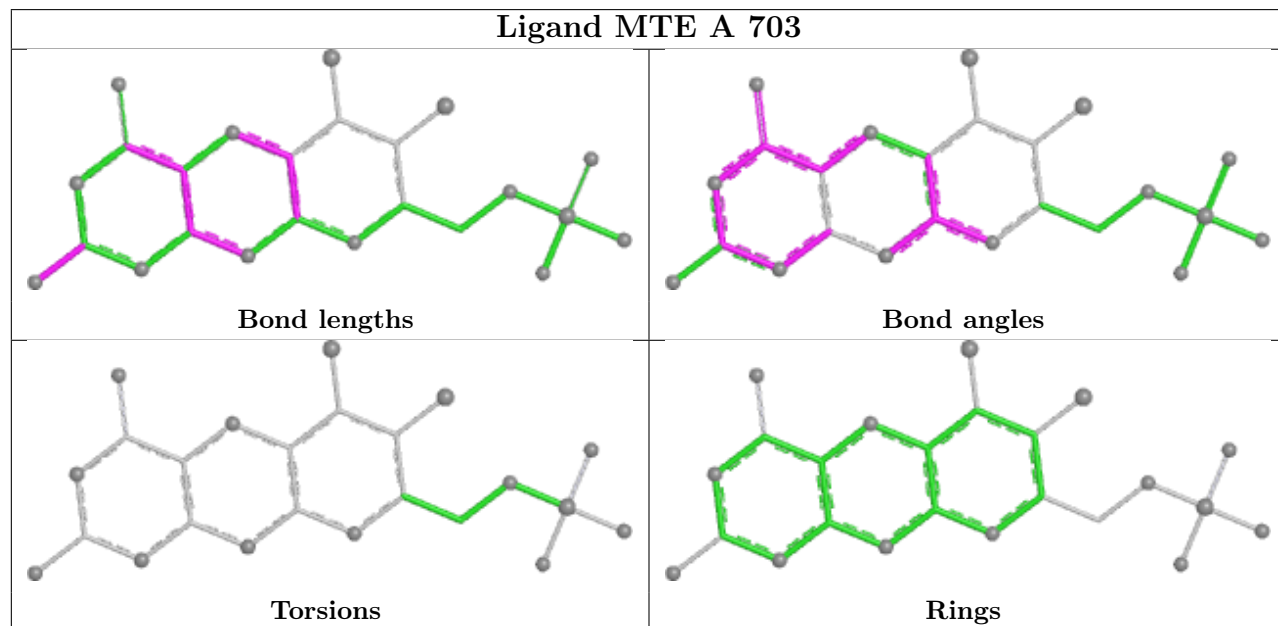
Ligand MTE B 703

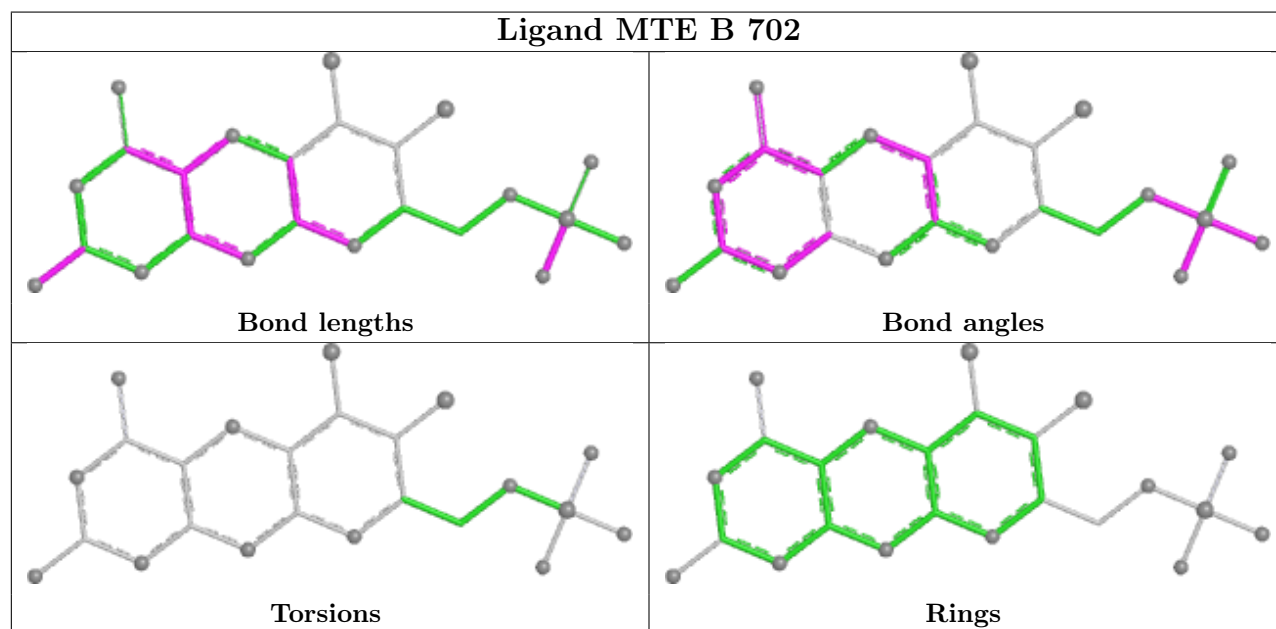
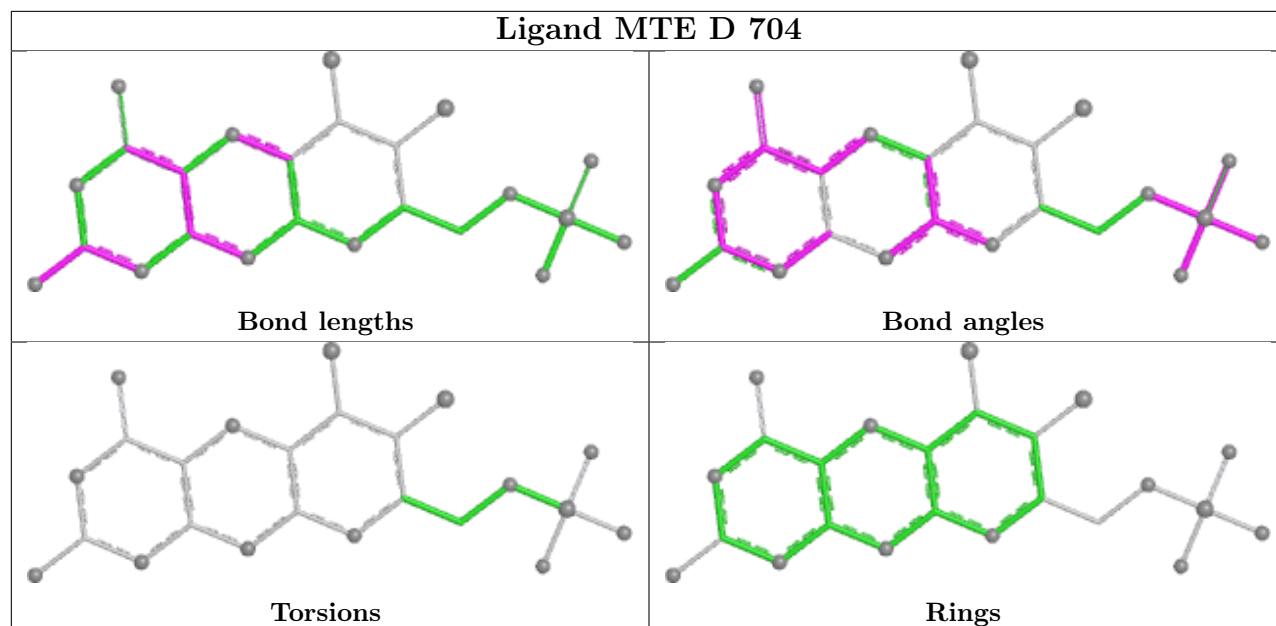


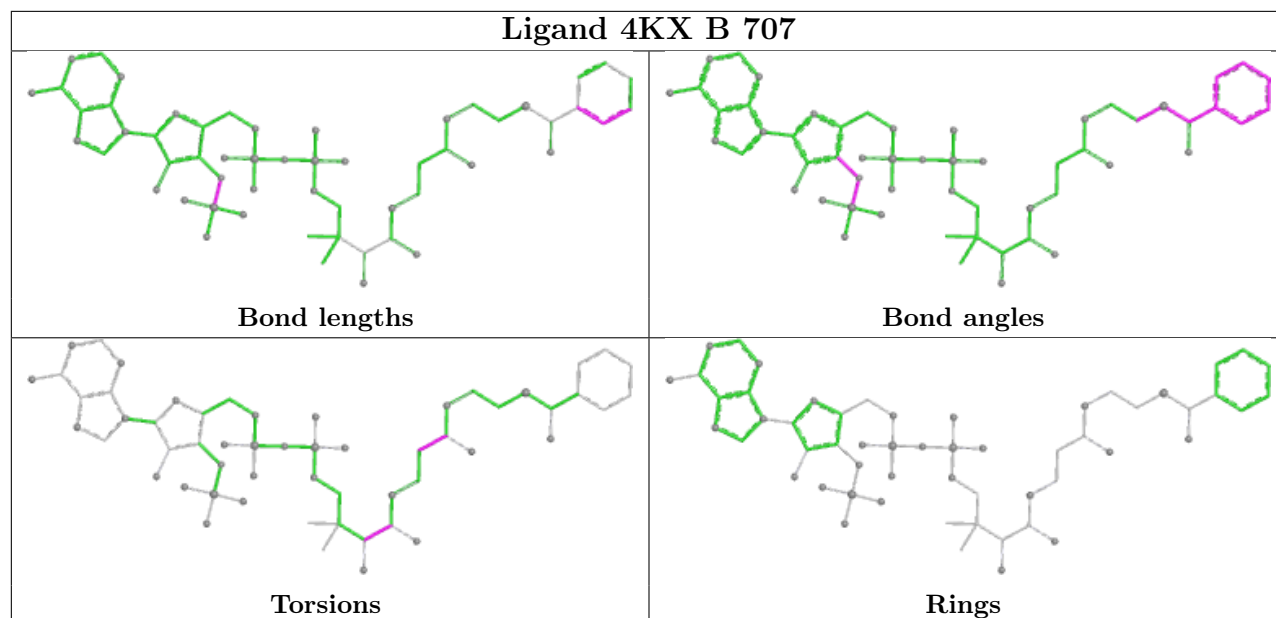
Ligand 4KX C 707 (B)



Ligand MTE A 703







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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

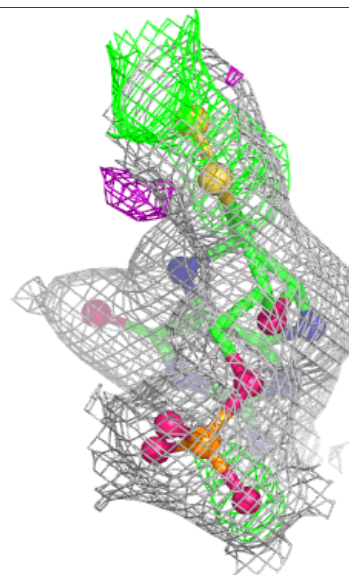
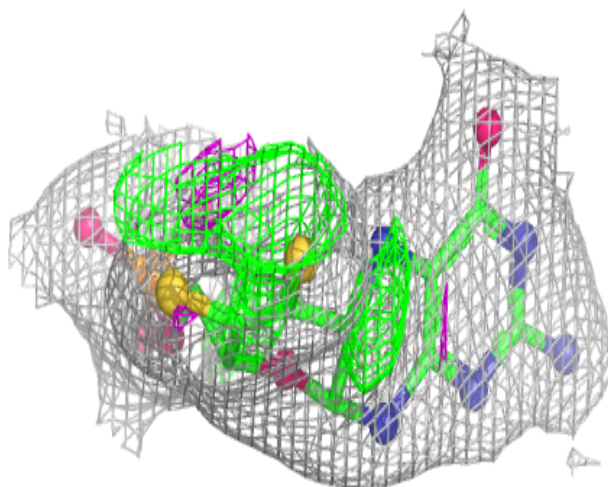
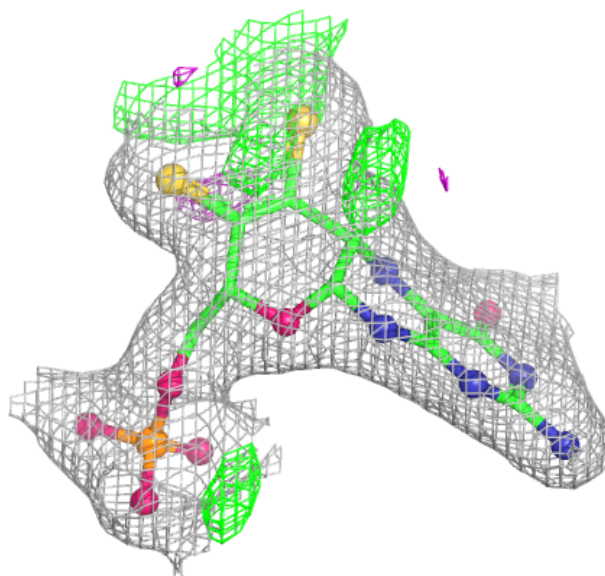
6.4 Ligands

EDS failed to run properly - this section is therefore empty.

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.

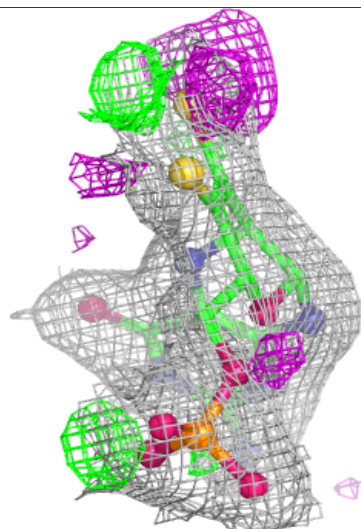
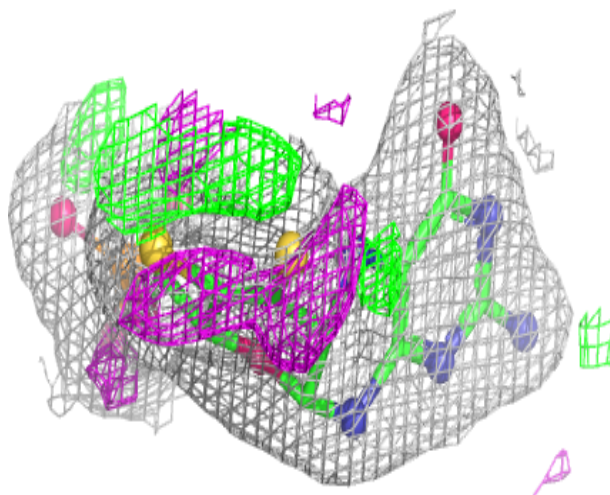
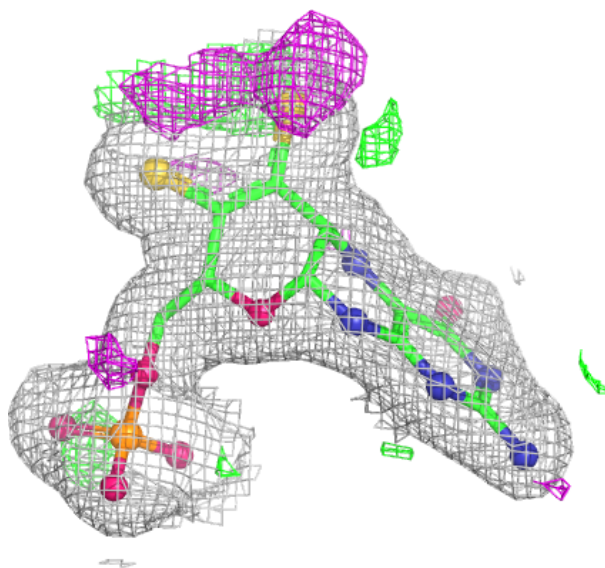
Electron density around MTE A 702:

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



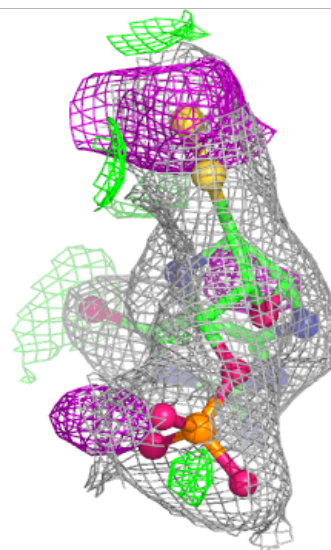
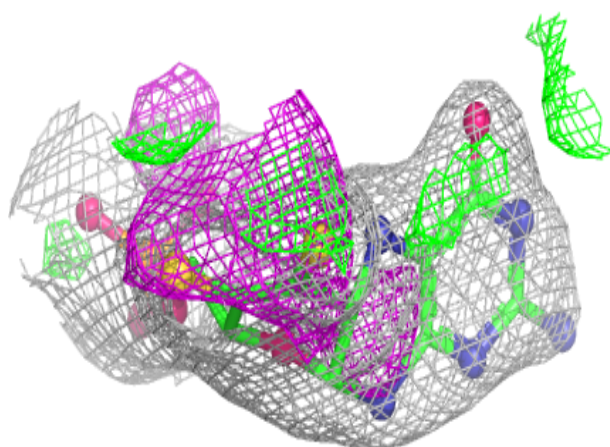
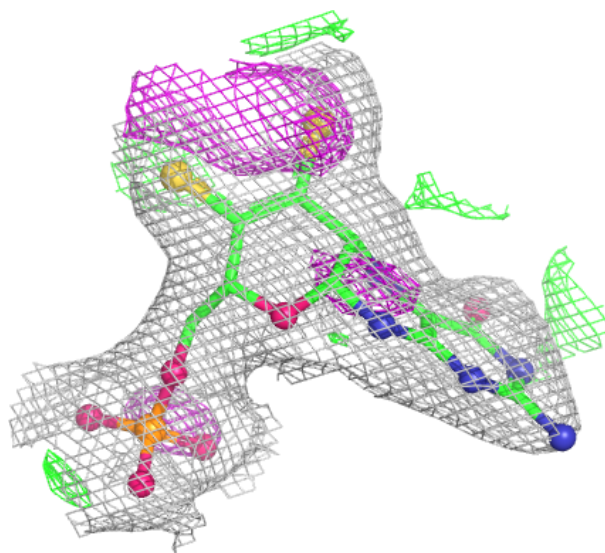
Electron density around MTE A 703:

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



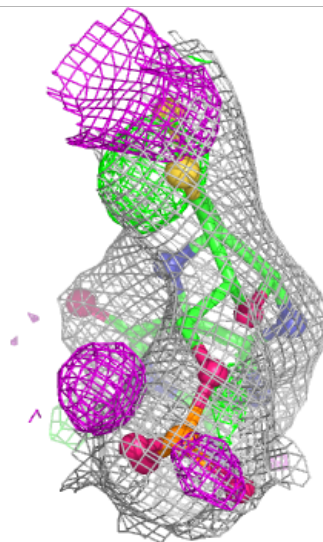
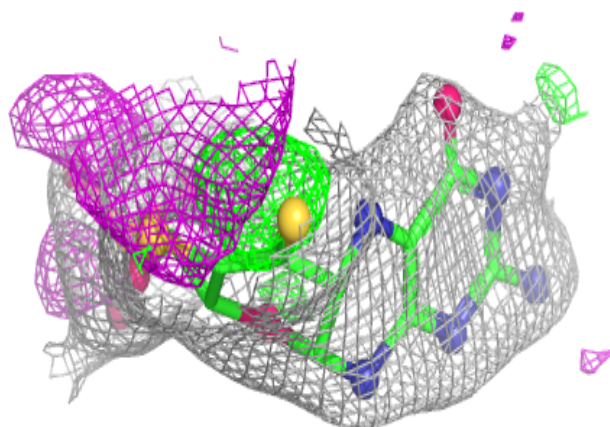
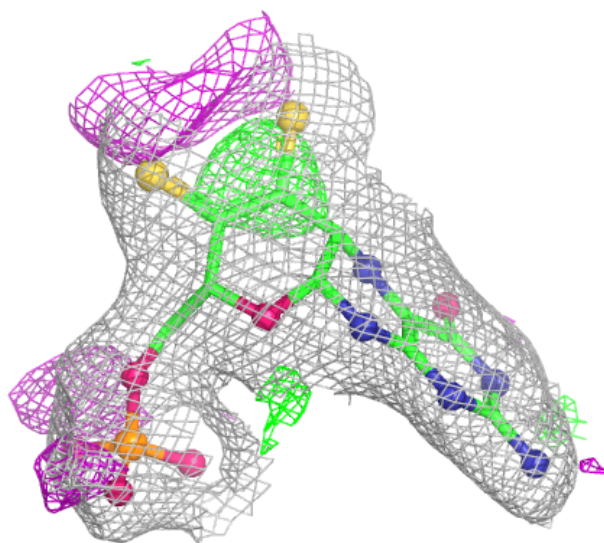
Electron density around MTE B 702:

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



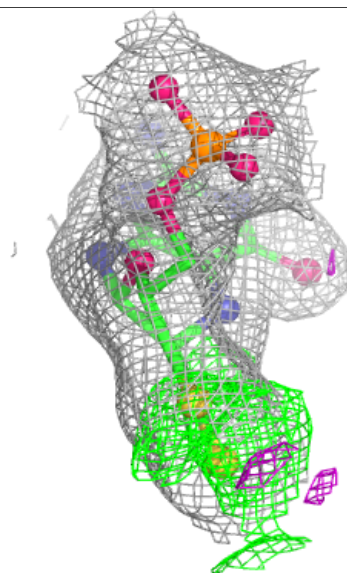
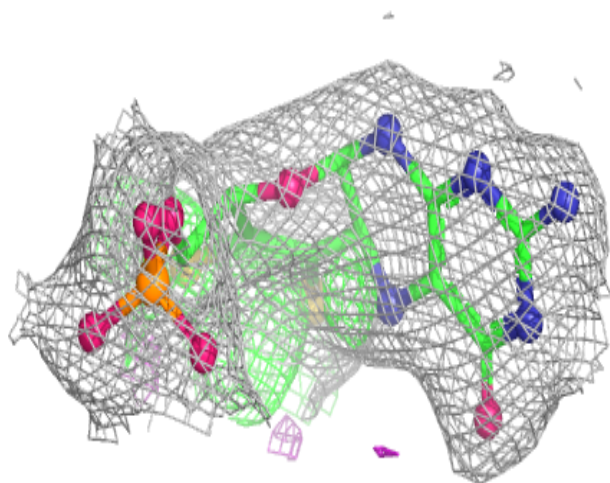
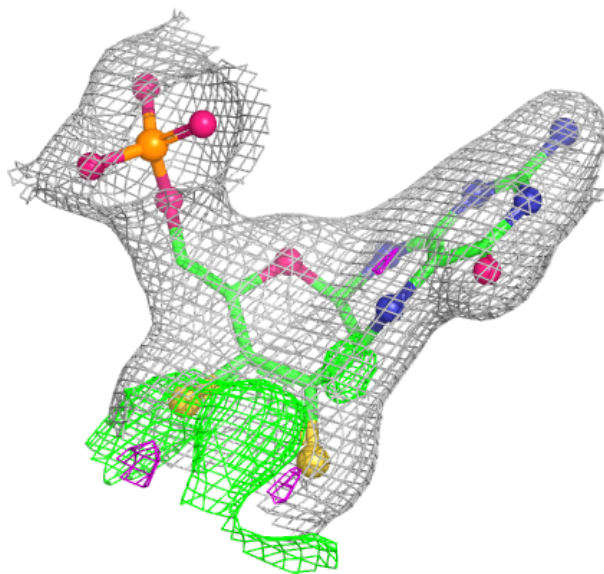
Electron density around MTE B 703:

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



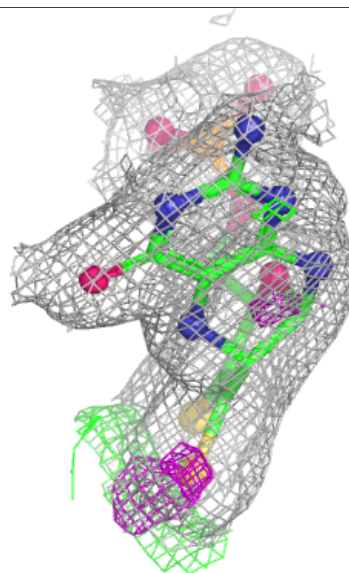
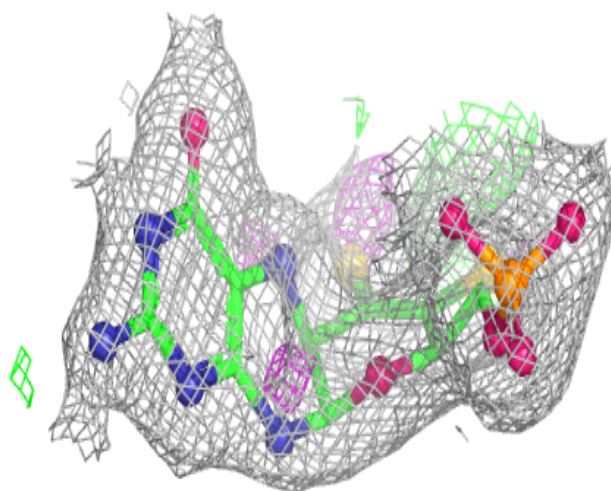
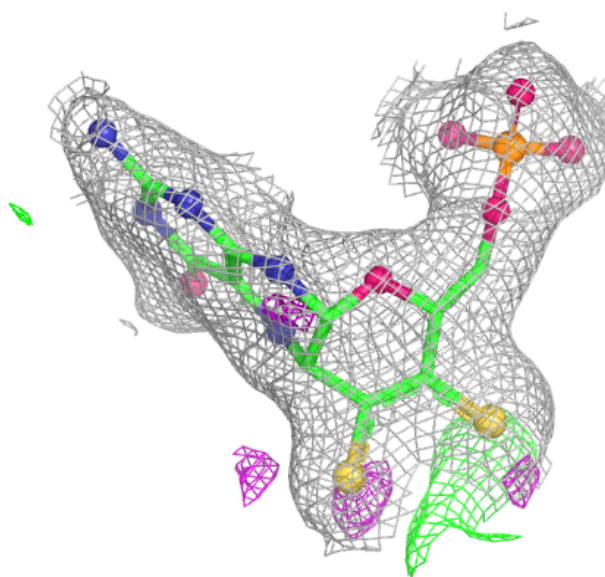
Electron density around MTE C 702:

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



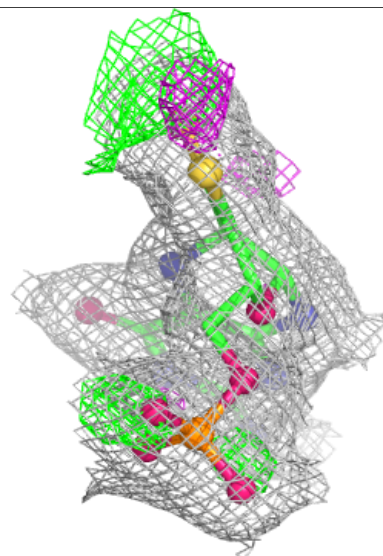
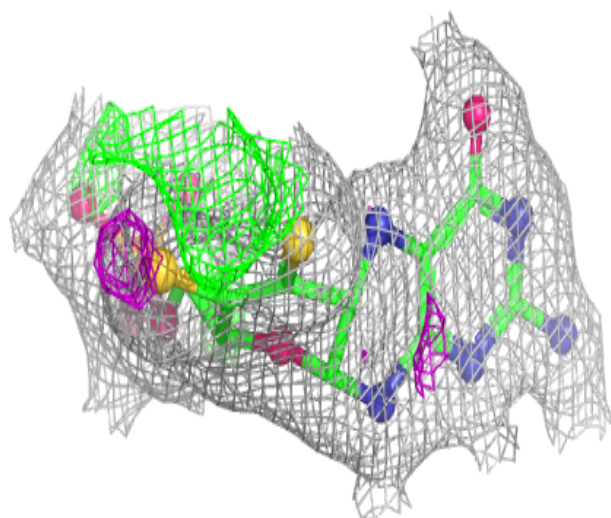
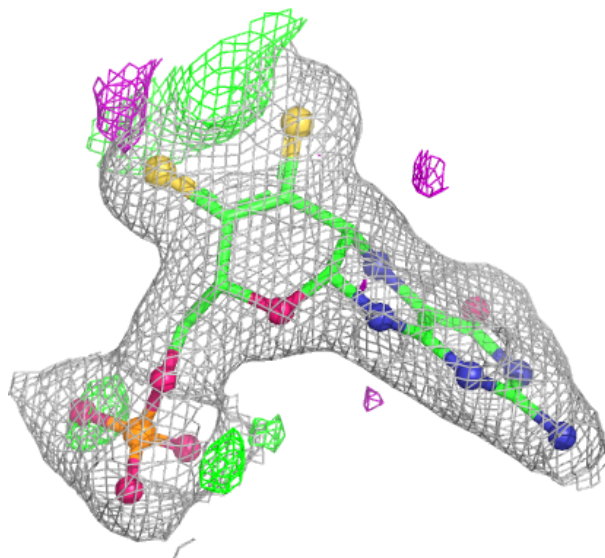
Electron density around MTE C 703:

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



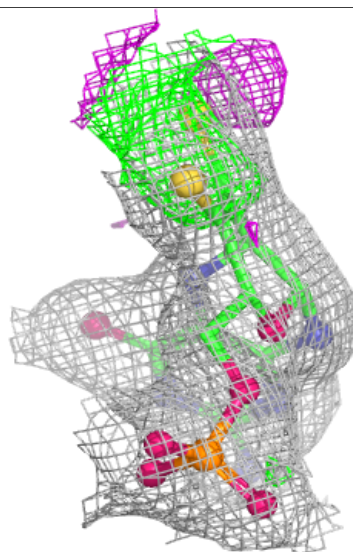
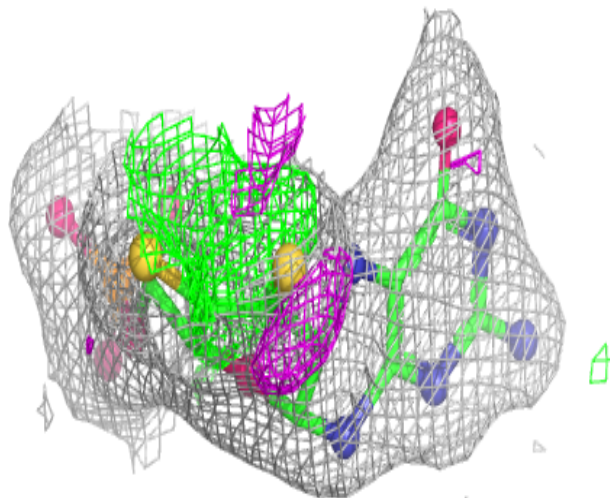
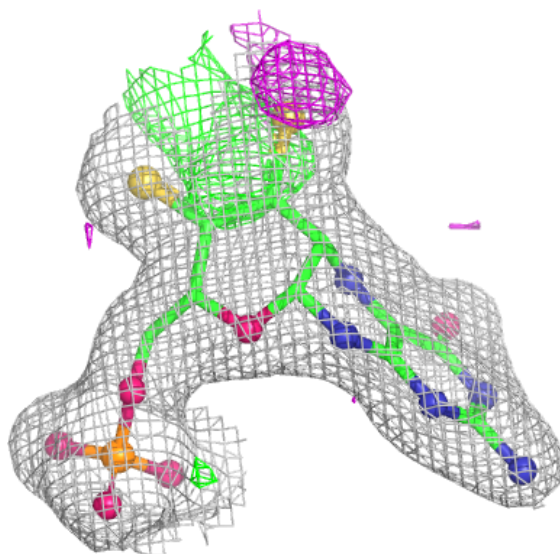
Electron density around MTE D 703:

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



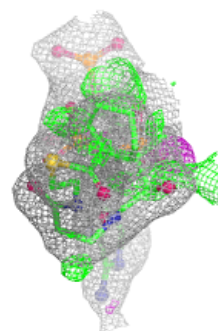
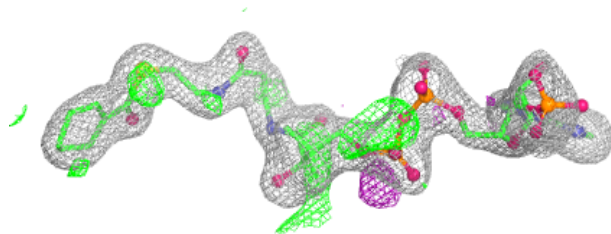
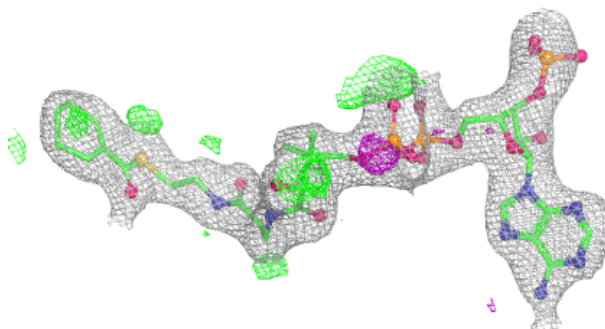
Electron density around MTE D 704:

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

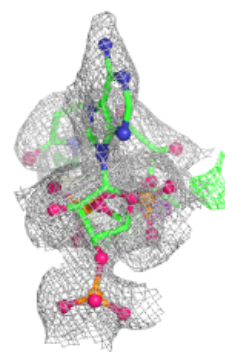
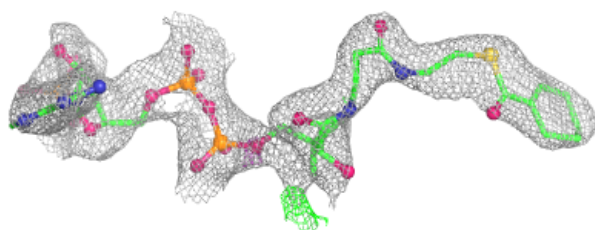
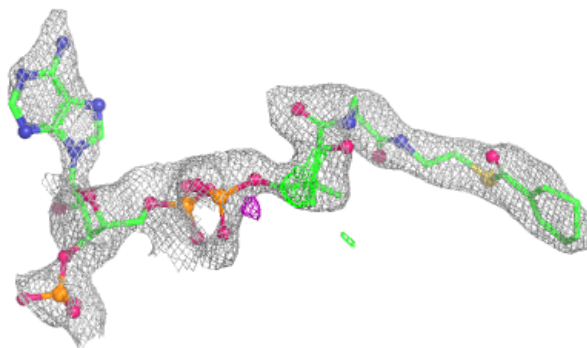


Electron density around 4KX A 709:

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

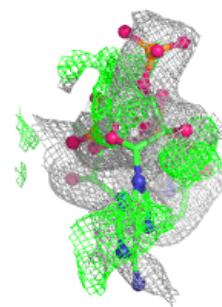
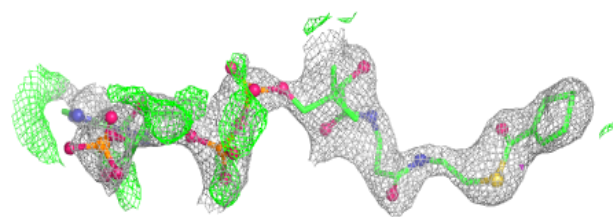
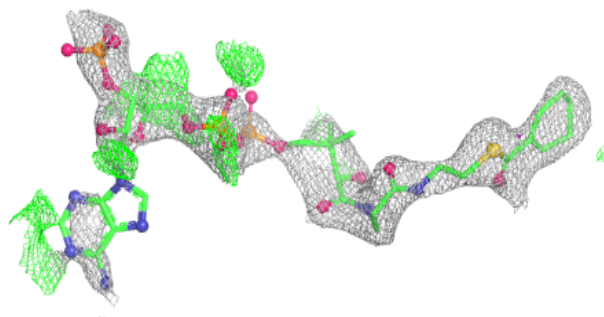
**Electron density around 4KX B 707:**

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

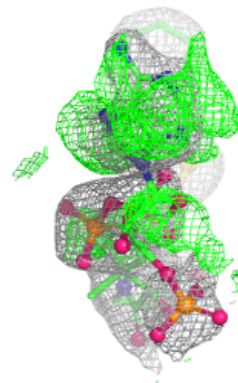
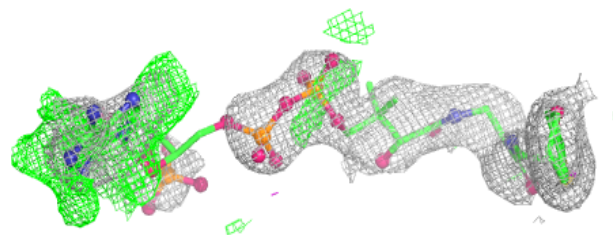
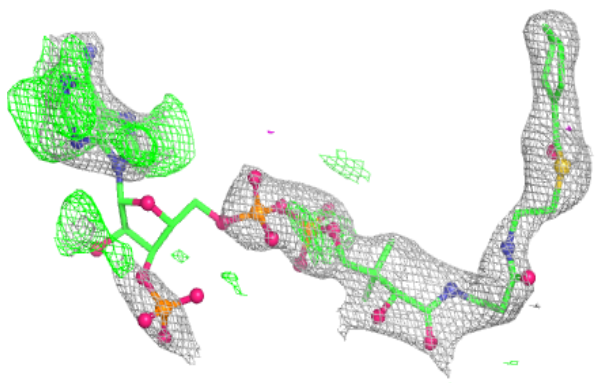


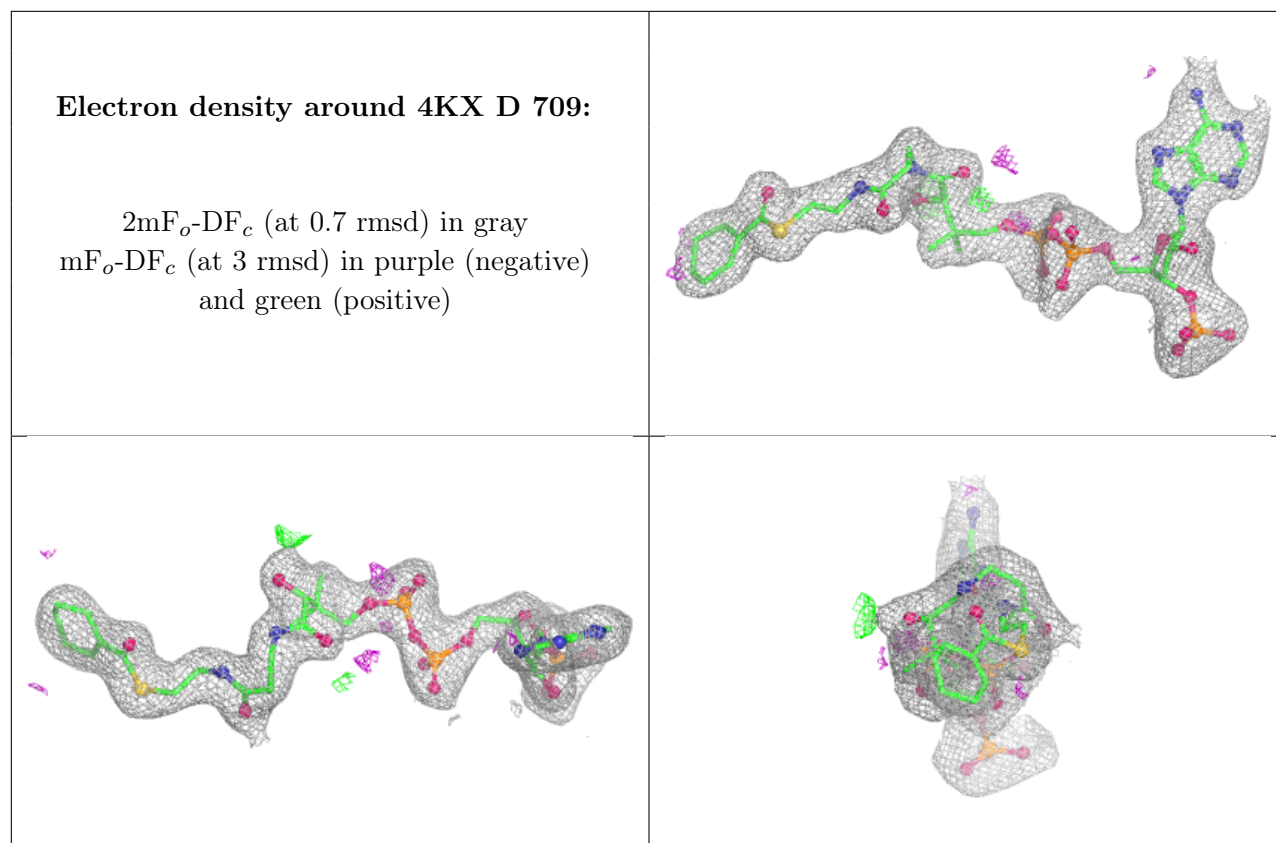
Electron density around 4KX C 707 (A):

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

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

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





6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.