



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2026 – 07:17 am BST

PDB ID : 6F2M / pdb_00006f2m
Title : Structure of the bacteriophage T5 distal tail protein pb9 co-crystallized with 10mM Tb-Xo4
Authors : Engilberge, S.; Riobe, F.; Di Pietro, S.; Breyton, C.; Girard, E.; Dumont, E.; Maury, O.
Deposited on : 2017-11-24
Resolution : 1.80 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

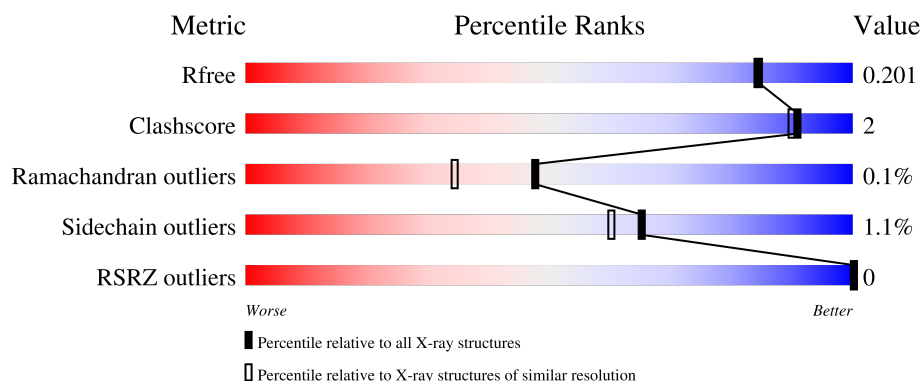
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	
1	C	217	
1	D	217	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12215 atoms, of which 5695 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 Distal tail protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	185	Total	C	H	N	O	S	0	1	0
			2883	936	1421	238	286	2			
1	B	172	Total	C	H	N	O	S	0	0	0
			2712	883	1343	221	263	2			
1	C	185	Total	C	H	N	O	S	0	0	0
			2877	934	1418	238	285	2			
1	D	185	Total	C	H	N	O	S	0	2	0
			2895	940	1426	239	288	2			

There are 52 discrepancies between the modelled and reference sequences:

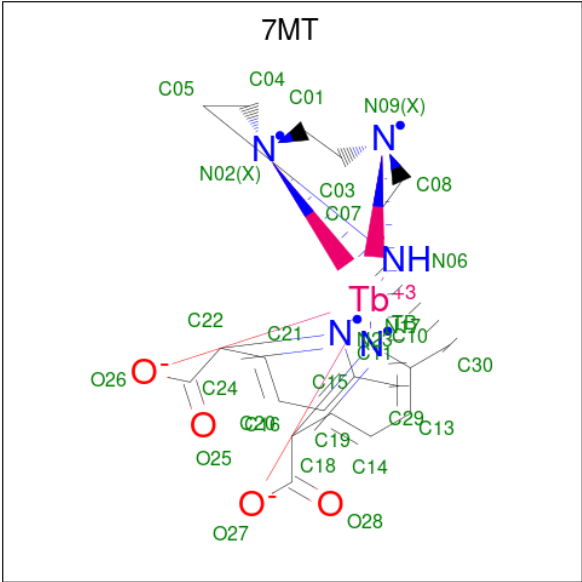
Chain	Residue	Modelled	Actual	Comment	Reference
A	205	GLU	-	expression tag	UNP Q6QGE8
A	206	ASN	-	expression tag	UNP Q6QGE8
A	207	LEU	-	expression tag	UNP Q6QGE8
A	208	TYR	-	expression tag	UNP Q6QGE8
A	209	PHE	-	expression tag	UNP Q6QGE8
A	210	GLN	-	expression tag	UNP Q6QGE8
A	211	GLY	-	expression tag	UNP Q6QGE8
A	212	HIS	-	expression tag	UNP Q6QGE8
A	213	HIS	-	expression tag	UNP Q6QGE8
A	214	HIS	-	expression tag	UNP Q6QGE8
A	215	HIS	-	expression tag	UNP Q6QGE8
A	216	HIS	-	expression tag	UNP Q6QGE8
A	217	HIS	-	expression tag	UNP Q6QGE8
B	205	GLU	-	expression tag	UNP Q6QGE8
B	206	ASN	-	expression tag	UNP Q6QGE8
B	207	LEU	-	expression tag	UNP Q6QGE8
B	208	TYR	-	expression tag	UNP Q6QGE8
B	209	PHE	-	expression tag	UNP Q6QGE8
B	210	GLN	-	expression tag	UNP Q6QGE8
B	211	GLY	-	expression tag	UNP Q6QGE8
B	212	HIS	-	expression tag	UNP Q6QGE8

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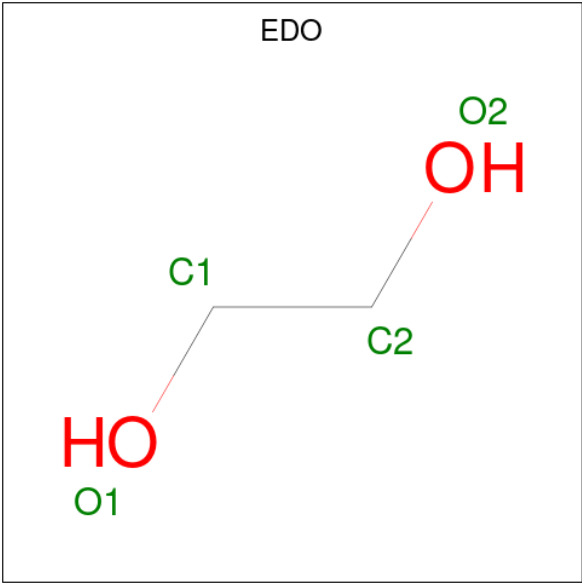
Chain	Residue	Modelled	Actual	Comment	Reference
B	213	HIS	-	expression tag	UNP Q6QGE8
B	214	HIS	-	expression tag	UNP Q6QGE8
B	215	HIS	-	expression tag	UNP Q6QGE8
B	216	HIS	-	expression tag	UNP Q6QGE8
B	217	HIS	-	expression tag	UNP Q6QGE8
C	205	GLU	-	expression tag	UNP Q6QGE8
C	206	ASN	-	expression tag	UNP Q6QGE8
C	207	LEU	-	expression tag	UNP Q6QGE8
C	208	TYR	-	expression tag	UNP Q6QGE8
C	209	PHE	-	expression tag	UNP Q6QGE8
C	210	GLN	-	expression tag	UNP Q6QGE8
C	211	GLY	-	expression tag	UNP Q6QGE8
C	212	HIS	-	expression tag	UNP Q6QGE8
C	213	HIS	-	expression tag	UNP Q6QGE8
C	214	HIS	-	expression tag	UNP Q6QGE8
C	215	HIS	-	expression tag	UNP Q6QGE8
C	216	HIS	-	expression tag	UNP Q6QGE8
C	217	HIS	-	expression tag	UNP Q6QGE8
D	205	GLU	-	expression tag	UNP Q6QGE8
D	206	ASN	-	expression tag	UNP Q6QGE8
D	207	LEU	-	expression tag	UNP Q6QGE8
D	208	TYR	-	expression tag	UNP Q6QGE8
D	209	PHE	-	expression tag	UNP Q6QGE8
D	210	GLN	-	expression tag	UNP Q6QGE8
D	211	GLY	-	expression tag	UNP Q6QGE8
D	212	HIS	-	expression tag	UNP Q6QGE8
D	213	HIS	-	expression tag	UNP Q6QGE8
D	214	HIS	-	expression tag	UNP Q6QGE8
D	215	HIS	-	expression tag	UNP Q6QGE8
D	216	HIS	-	expression tag	UNP Q6QGE8
D	217	HIS	-	expression tag	UNP Q6QGE8

- Molecule 2 is Tb-Xo4 (CCD ID: 7MT) (formula: C₂₀H₂₃N₅O₄Tb).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	Tb	0	0
			53	20	23	5	4	1		
2	C	1	Total	C	H	N	O	Tb	0	0
			53	20	23	5	4	1		
2	D	1	Total	C	H	N	O	Tb	0	0
			53	20	23	5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is TERBIUM(III) ION (CCD ID: TB) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Tb	0	0
			1	1		
6	D	1	Total	Tb	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	171	Total	O	0	0
			171	171		
7	B	154	Total	O	0	0
			154	154		
7	C	161	Total	O	0	0
			161	161		
7	D	169	Total	O	0	0
			169	169		

- Molecule 1: Distal tail protein



- [illegible]

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|----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | E18 | S19 | V20 | D26 | PRO | NET | ILE | ARG | ASP | GLU | LEU | PRO | ASN | GLY | LYS | VAL | LYS | GLU | VAL | LYS | ILE | SER | A45 | D77 | L83 | T99 | N12 | T175 | S203 | LEU | GLU | ASN | LEU | TYR | PHE | GLN | GLY | HIS | HIS | HIS | HIS |
|----|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|--|----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| HIS | | H1 | D26 | PRO | MET | TLE | ARG | ASP | GLU | LEU | PRO | ASN | GLY | LYS | VAL | LYS | GLU | VAL | LYS | TLE | SER | A46 | T75 | G76 | D77 | V81 | E87 | A88 | F89 | I109 | T139 | L177 | M178 | N179 | G180 | S194 | L200 | S203 | LEU | GLU | ASN | LEU | TYR | PHE | GLN | GLY | HIS | HIS | HIS | HIS |
|-----|--|----|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.40Å 95.24Å 71.58Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	48.16 – 1.80 48.16 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.16-1.80) 95.9 (48.16-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.79Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.178 , 0.203 0.181 , 0.201	Depositor DCC
R_{free} test set	4210 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.188 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12215	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, 7MT, TB, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	0/1501	0.97	1/2040 (0.0%)
1	B	0.78	0/1403	0.95	2/1906 (0.1%)
1	C	0.76	0/1495	0.97	2/2032 (0.1%)
1	D	0.79	0/1511	1.00	2/2054 (0.1%)
All	All	0.77	0/5910	0.97	7/8032 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	THR	N-CA-C	-6.50	101.77	110.55
1	B	77	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	77	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	77	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	21	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	77	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	175	THR	N-CA-C	5.08	116.70	109.14

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	1462	1421	1427	6	0
1	B	1369	1343	1347	6	0
1	C	1459	1418	1422	3	0
1	D	1469	1426	1432	5	0
2	A	30	23	0	0	0
2	C	30	23	0	0	0
2	D	30	23	0	0	0
3	A	8	12	12	1	0
3	C	4	6	6	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	171	0	0	1	0
7	B	154	0	0	0	0
7	C	161	0	0	0	0
7	D	169	0	0	0	0
All	All	6520	5695	5646	19	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 2.

All (19) 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:B:113:THR:O	1:B:116:THR:HG22	1.89	0.72
1:A:75:THR:O	1:A:77:ASP:N	2.31	0.59
1:A:95:THR:HG21	7:A:403:HOH:O	2.03	0.59
1:B:81:VAL:HG21	1:B:200:LEU:HD13	1.91	0.52
1:D:87:GLU:HG3	1:D:89:PHE:CE2	2.46	0.50
1:B:87:GLU:HG3	1:B:89:PHE:CE2	2.48	0.49
1:D:81:VAL:HG21	1:D:200:LEU:HD13	1.95	0.49
1:A:75:THR:O	1:A:75:THR:OG1	2.28	0.47
1:A:18:GLU:OE1	1:A:18:GLU:HA	2.16	0.46
1:A:126:LEU:HD12	3:A:303:EDO:H11	1.96	0.46
1:B:139:THR:HG22	1:D:139:THR:HG22	1.98	0.45
1:C:20:VAL:HG11	1:C:83:LEU:HD22	1.99	0.44
1:D:87:GLU:CG	1:D:89:PHE:CE2	3.02	0.42
1:A:179:ASN:ND2	1:A:199:SER:H	2.17	0.42
1:B:87:GLU:CG	1:B:89:PHE:CE2	3.03	0.41
1:C:18:GLU:OE1	1:C:18:GLU:HA	2.19	0.41
1:B:126:LEU:HD23	1:B:137:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:THR:OG1	1:C:112:ASN:HB3	2.21	0.41
1:D:177:LEU:C	1:D:178:MET:HE2	2.45	0.41

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	182/217 (84%)	180 (99%)	2 (1%)	0	100	100
1	B	166/217 (76%)	162 (98%)	4 (2%)	0	100	100
1	C	181/217 (83%)	180 (99%)	1 (1%)	0	100	100
1	D	183/217 (84%)	181 (99%)	1 (0%)	1 (0%)	24	14
All	All	712/868 (82%)	703 (99%)	8 (1%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	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	164/193 (85%)	160 (98%)	4 (2%)	43	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	153/193 (79%)	152 (99%)	1 (1%)	76	73
1	C	163/193 (84%)	163 (100%)	0	100	100
1	D	165/193 (86%)	163 (99%)	2 (1%)	63	57
All	All	645/772 (84%)	638 (99%)	7 (1%)	65	60

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	95	THR
1	A	96	LYS
1	A	179	ASN
1	B	109	ILE
1	D	109	ILE
1	D	194	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	169	ASN
1	A	179	ASN
1	B	25	ASN
1	B	51	ASN
1	C	169	ASN
1	D	46	GLN
1	D	114	ASN
1	D	169	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
2	7MT	C	301	1	31,38,38	2.94	8 (25%)	29,76,76	1.95	7 (24%)
2	7MT	D	302	1	31,38,38	2.06	8 (25%)	29,76,76	1.65	8 (27%)
2	7MT	A	301	1	31,38,38	1.89	7 (22%)	29,76,76	1.99	7 (24%)
3	EDO	C	302	-	3,3,3	0.46	0	2,2,2	0.89	0
3	EDO	A	303	-	3,3,3	0.52	0	2,2,2	0.25	0
3	EDO	A	302	-	3,3,3	0.50	0	2,2,2	0.09	0

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
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	C	302	-	-	0/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	7MT	TB-N17	-12.50	2.31	2.50
2	D	302	7MT	TB-N17	7.13	2.60	2.50
2	C	301	7MT	TB-N23	6.40	2.59	2.50
2	A	301	7MT	TB-N17	-6.33	2.40	2.50
2	C	301	7MT	C30-C10	3.56	1.55	1.49
2	A	301	7MT	C30-C10	3.50	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	7MT	C29-C11	3.48	1.55	1.49
2	A	301	7MT	C29-C11	3.37	1.55	1.49
2	C	301	7MT	C29-C11	3.36	1.55	1.49
2	D	302	7MT	C30-C10	3.24	1.55	1.49
2	A	301	7MT	C04-N02	-2.99	1.45	1.49
2	C	301	7MT	C04-N02	-2.98	1.45	1.49
2	D	302	7MT	O26-C24	-2.80	1.22	1.28
2	D	302	7MT	TB-N23	2.69	2.54	2.50
2	D	302	7MT	O28-C18	2.52	1.26	1.21
2	D	302	7MT	O25-C24	2.49	1.26	1.21
2	A	301	7MT	O28-C18	2.33	1.26	1.21
2	C	301	7MT	O28-C18	2.29	1.26	1.21
2	C	301	7MT	O25-C24	2.22	1.26	1.21
2	A	301	7MT	O25-C24	2.20	1.26	1.21
2	D	302	7MT	C16-N17	-2.17	1.34	1.38
2	C	301	7MT	C16-C18	2.06	1.53	1.49
2	A	301	7MT	C16-C18	2.04	1.53	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	7MT	C05-C04-N02	-4.65	109.19	112.86
2	C	301	7MT	C05-C04-N02	-4.57	109.25	112.86
2	A	301	7MT	C07-C08-N09	-4.45	109.35	112.86
2	C	301	7MT	C03-C01-N02	-4.14	109.59	112.86
2	A	301	7MT	C03-C01-N02	-4.08	109.64	112.86
2	C	301	7MT	C01-C03-N09	-4.07	109.65	112.86
2	C	301	7MT	C07-C08-N09	-4.04	109.67	112.86
2	A	301	7MT	C01-C03-N09	-4.02	109.68	112.86
2	D	302	7MT	C29-C11-N23	-3.61	114.93	118.77
2	D	302	7MT	O26-C24-O25	-3.34	119.29	125.24
2	D	302	7MT	O27-C18-O28	-3.14	119.64	125.24
2	A	301	7MT	O27-C18-O28	-2.94	119.99	125.24
2	A	301	7MT	O26-C24-O25	-2.93	120.02	125.24
2	C	301	7MT	O26-C24-O25	-2.93	120.02	125.24
2	C	301	7MT	O27-C18-O28	-2.91	120.04	125.24
2	D	302	7MT	C08-N09-C03	2.91	114.28	109.86
2	D	302	7MT	C13-C10-N17	-2.67	119.87	124.20
2	D	302	7MT	C30-C10-N17	-2.66	115.94	118.77
2	D	302	7MT	C19-C11-N23	-2.43	120.26	124.20
2	A	301	7MT	C13-C10-N17	-2.30	120.46	124.20
2	C	301	7MT	C13-C10-N17	-2.27	120.52	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	7MT	C01-C03-N09	2.09	114.51	112.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2

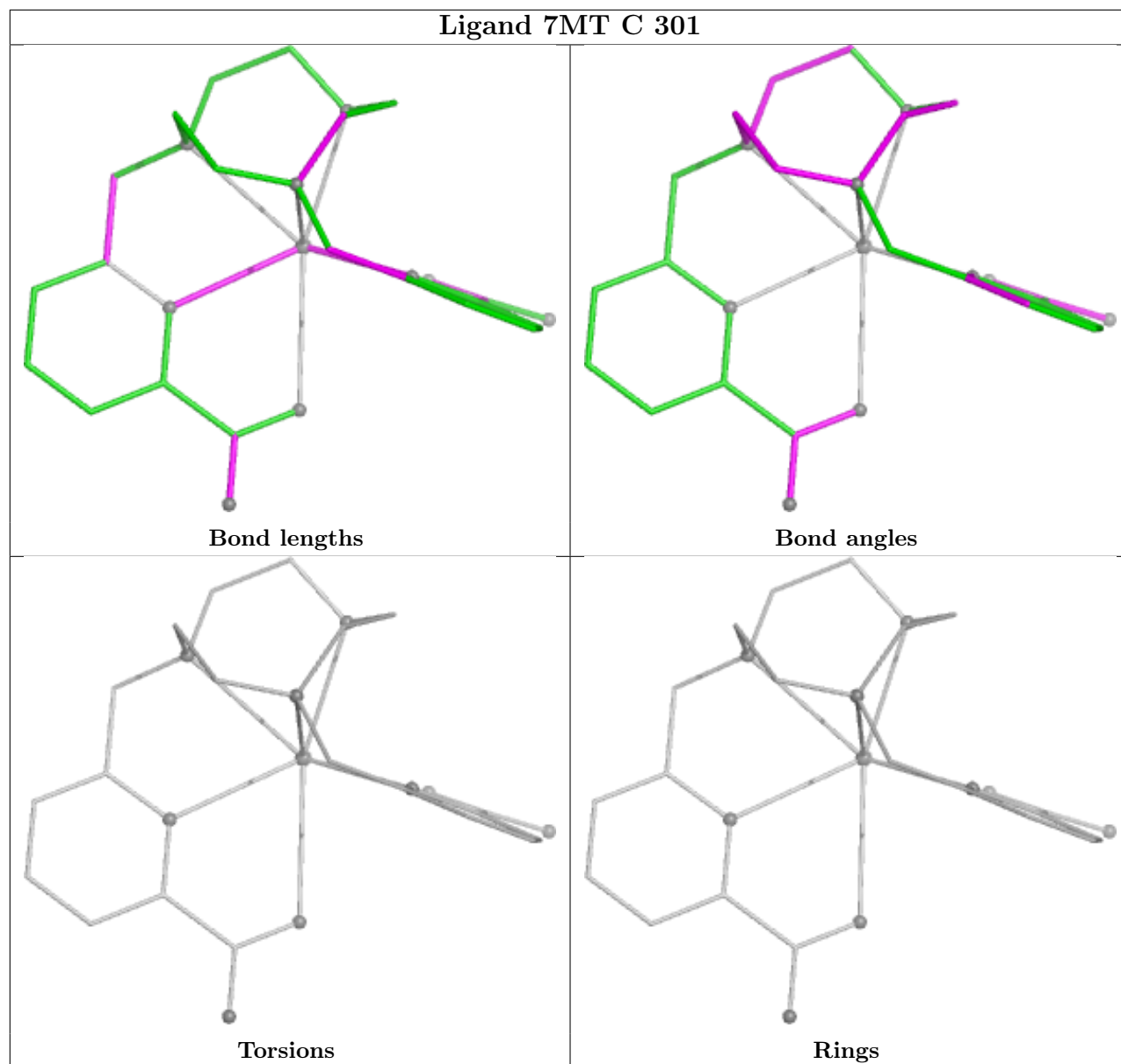
There are no ring outliers.

1 monomer is involved in 1 short contact:

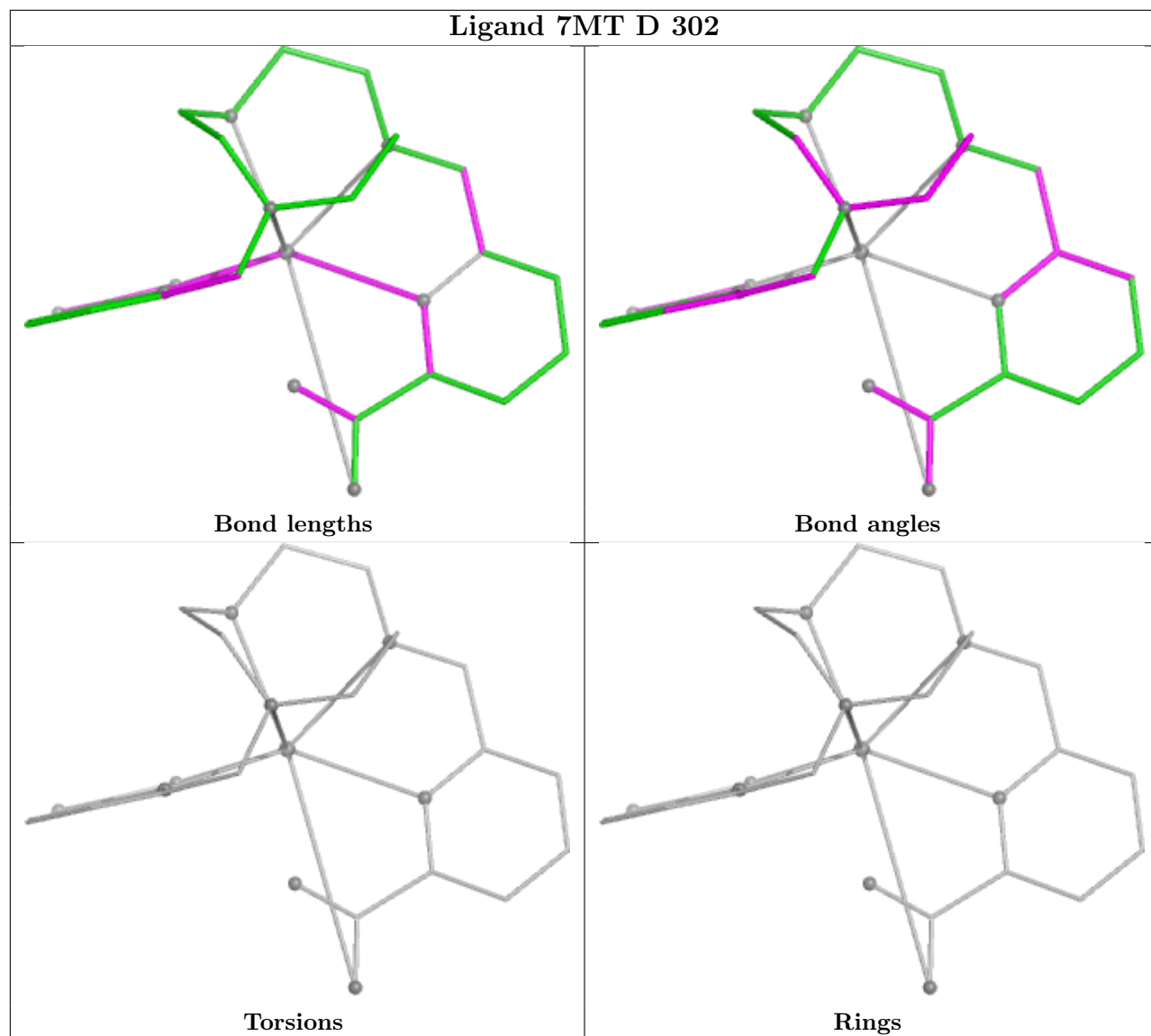
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	EDO	1	0

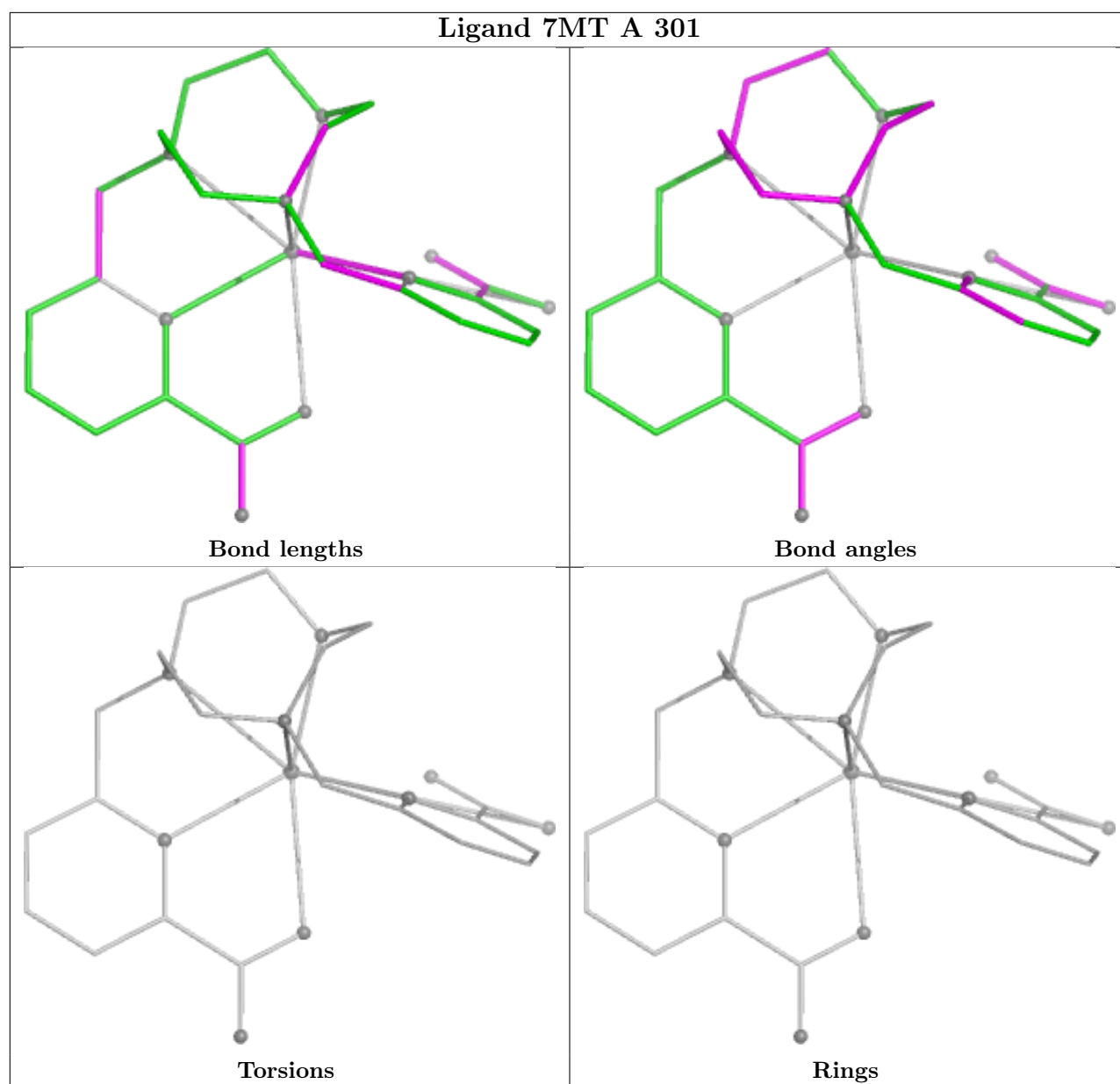
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 7MT C 301



Ligand 7MT D 302





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	185/217 (85%)	-1.30	0 100 100	21, 32, 53, 75	2 (1%)
1	B	172/217 (79%)	-1.26	0 100 100	21, 32, 59, 79	0
1	C	185/217 (85%)	-1.27	0 100 100	26, 32, 56, 83	0
1	D	185/217 (85%)	-1.24	0 100 100	16, 30, 77, 96	3 (1%)
All	All	727/868 (83%)	-1.27	0 100 100	16, 32, 60, 96	5 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	302	4/4	0.97	0.09	49,50,53,53	10
3	EDO	A	303	4/4	0.98	0.08	32,40,46,46	0
3	EDO	C	302	4/4	0.99	0.06	49,50,51,51	10
4	CL	A	304	1/1	0.99	0.07	71,71,71,71	0

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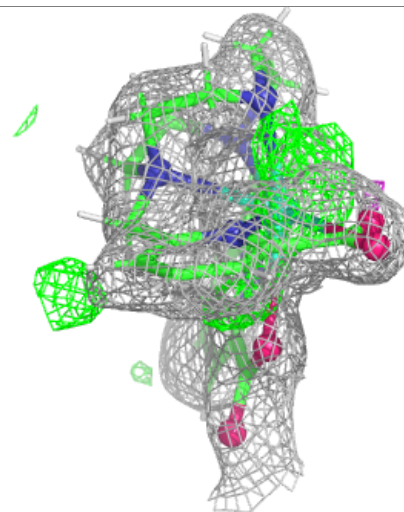
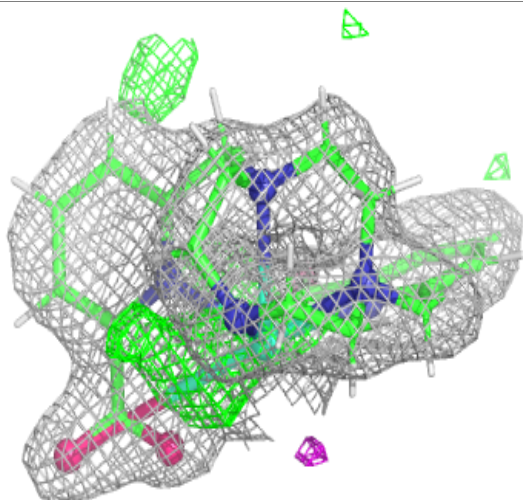
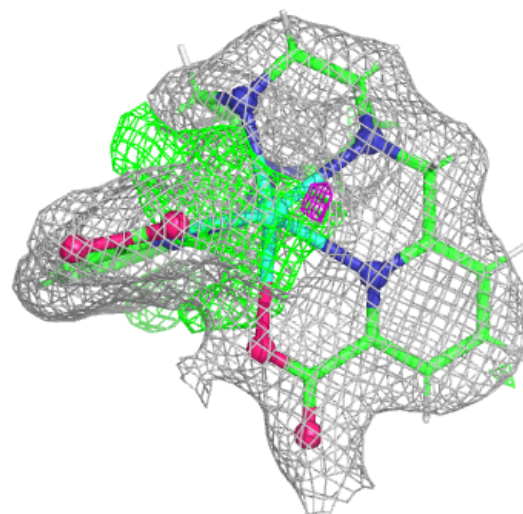
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	7MT	C	301	30/30	1.00	0.03	28,33,36,39	53
2	7MT	D	302	30/30	1.00	0.03	22,33,36,45	53
2	7MT	A	301	30/30	1.00	0.04	28,32,36,39	53
5	NA	A	305	1/1	1.00	0.08	39,39,39,39	0
6	TB	B	301	1/1	1.00	0.07	37,37,37,37	1
6	TB	D	301	1/1	1.00	0.14	42,42,42,42	1

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.

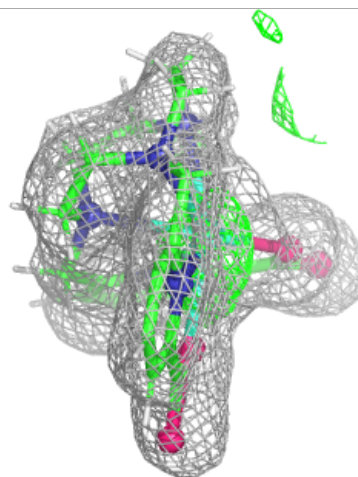
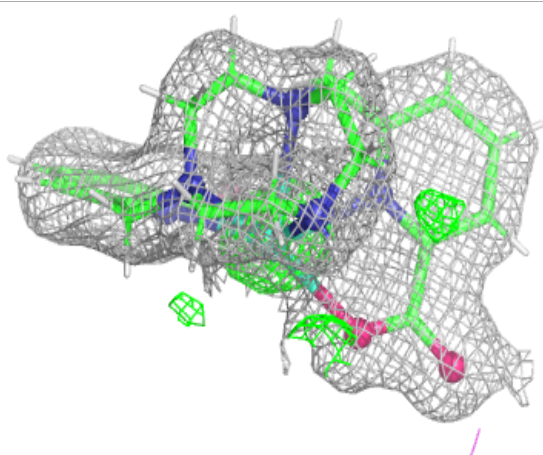
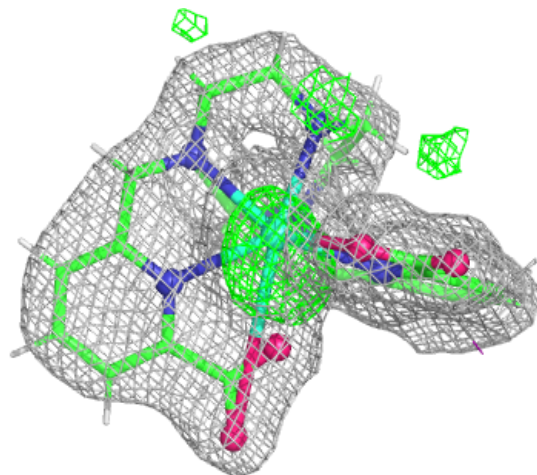
Electron density around 7MT C 301:

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



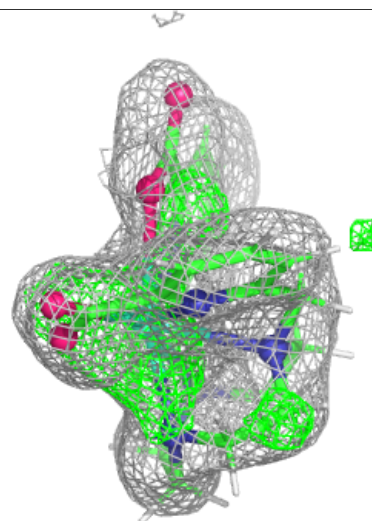
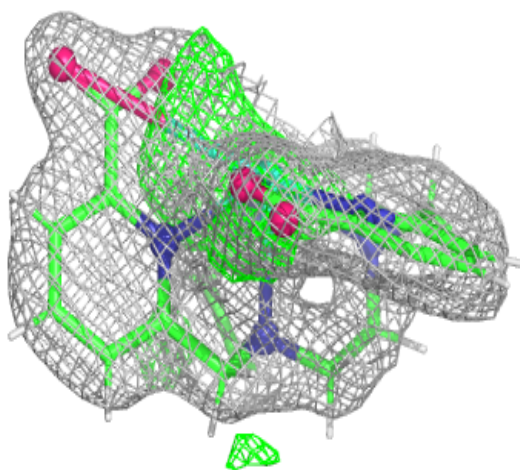
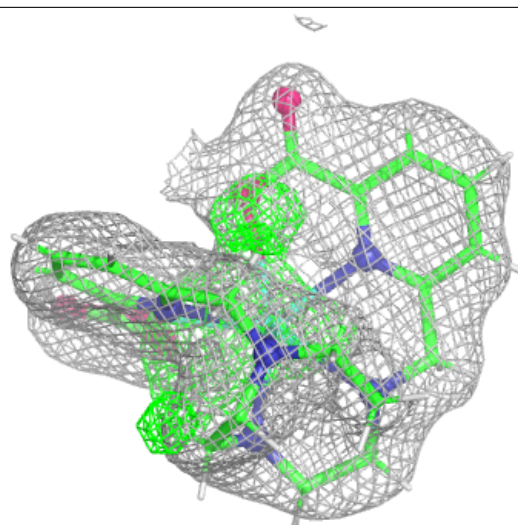
Electron density around 7MT D 302:

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



Electron density around 7MT A 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.