



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:54 AM UTC

PDB ID : 1E2K / pdb_00001e2k
Title : Kinetics and crystal structure of the wild-type and the engineered Y101F mutant of Herpes simplex virus type 1 thymidine kinase interacting with (North)-methanocarpa-thymidine
Authors : Vogt, J.; Scapozza, L.; Schulz, G.E.
Deposited on : 2000-05-23
Resolution : 1.70 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	:	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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

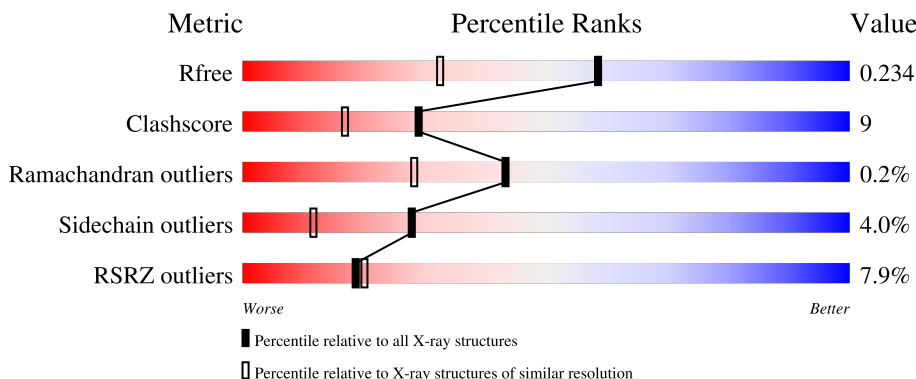
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	331	
1	B	331	

2 Entry composition [i](#)

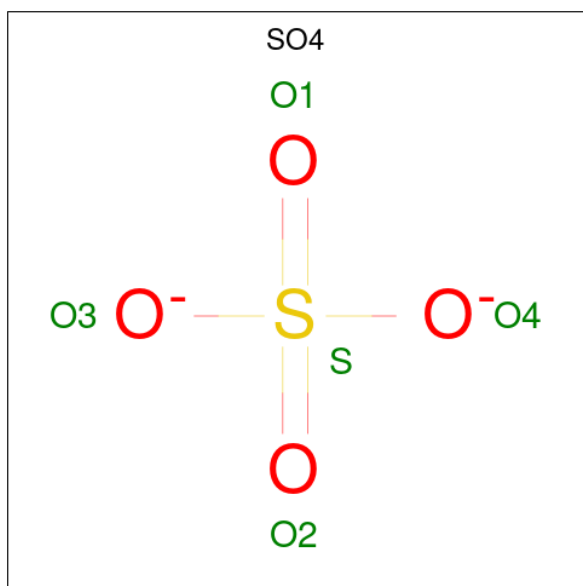
There are 4 unique types of molecules in this entry. The entry contains 5169 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDINE KINASE.

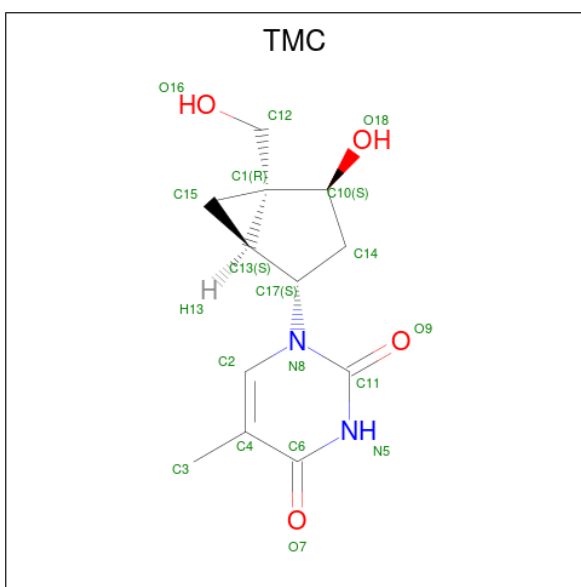
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2350	1498	410	426	16			
1	B	316	Total	C	N	O	S	0	0	0
			2409	1534	421	438	16			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1-[4-HYDROXY-5-(HYDROXYMETHYL)BICYCLO[3.1.0]HEX-2-YL]-5-METHYLPYRIMIDINE-2,4(1H,3H)-DIONE (CCD ID: TMC) (formula: C₁₂H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	12	2	4		
3	B	1	Total	C	N	O	0	0
			18	12	2	4		

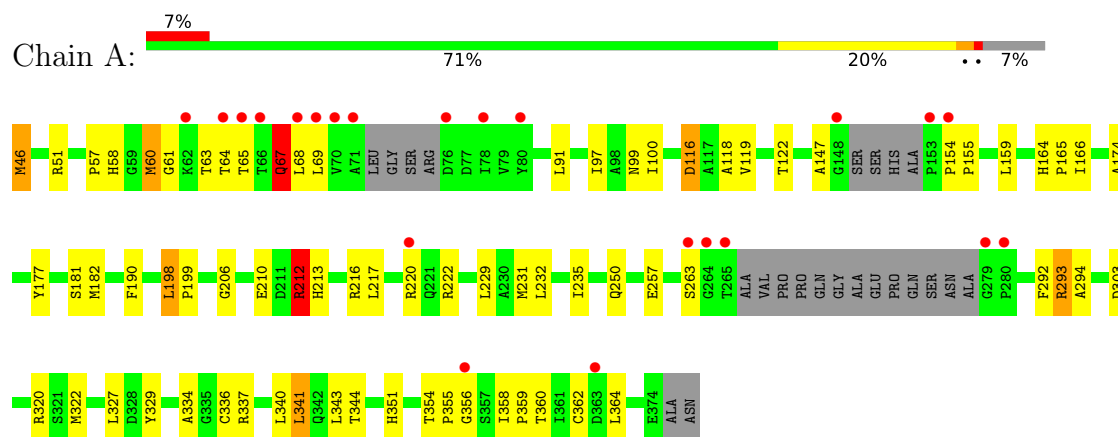
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total	O	0	0
			180	180		
4	B	184	Total	O	0	0
			184	184		

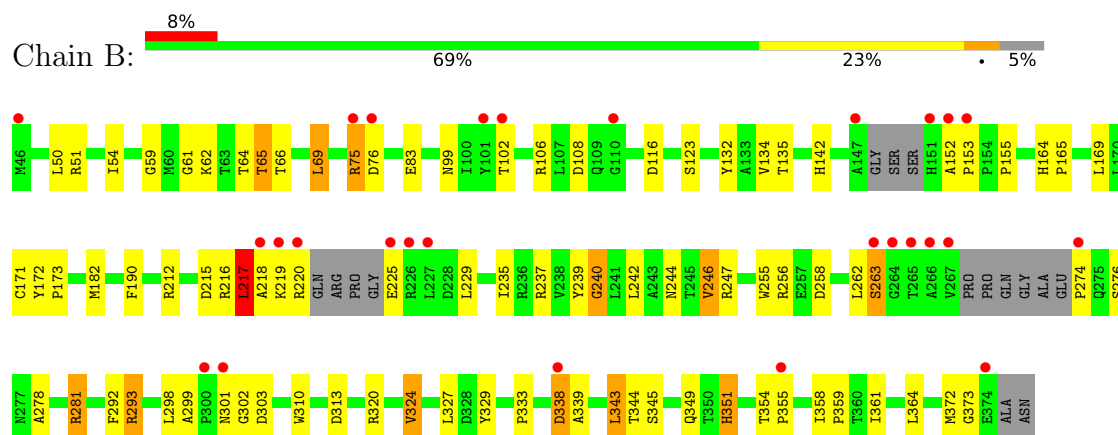
3 Residue-property plots

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

• Molecule 1: THYMIDINE KINASE



• Molecule 1: THYMIDINE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.00Å 117.70Å 108.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-1.70) 99.4 (20.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.252 0.197 , 0.234	Depositor DCC
R_{free} test set	3989 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5169	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: SO4, TMC

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	1.13	1/2404 (0.0%)	1.74	37/3279 (1.1%)
1	B	1.09	2/2464 (0.1%)	1.79	37/3363 (1.1%)
All	All	1.11	3/4868 (0.1%)	1.77	74/6642 (1.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	ARG	N-CA	5.13	1.52	1.46
1	B	240	GLY	CA-C	5.06	1.57	1.52
1	A	174	ALA	N-CA	5.03	1.52	1.46

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	ASP	CA-CB-CG	20.84	133.44	112.60
1	B	281	ARG	CD-NE-CZ	12.42	141.79	124.40
1	A	212	ARG	CG-CD-NE	11.45	137.19	112.00
1	A	212	ARG	CD-NE-CZ	8.57	136.41	124.40
1	B	212	ARG	CD-NE-CZ	8.41	136.17	124.40
1	A	303	ASP	CA-CB-CG	8.10	120.70	112.60
1	A	340	LEU	CA-C-O	8.10	129.33	120.82
1	B	64	THR	CA-C-O	8.02	129.24	120.82
1	A	320	ARG	NE-CZ-NH2	-7.64	112.33	119.20
1	A	99	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	A	292	PHE	CA-CB-CG	-7.52	106.28	113.80
1	A	116	ASP	CA-CB-CG	7.44	120.04	112.60
1	A	58	HIS	CA-CB-CG	7.41	121.21	113.80
1	B	242	LEU	CA-C-O	-7.39	112.71	120.55
1	A	51	ARG	CD-NE-CZ	7.25	134.55	124.40
1	B	237	ARG	CD-NE-CZ	7.11	134.35	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ARG	CD-NE-CZ	7.09	134.33	124.40
1	B	293	ARG	CA-C-N	7.03	130.47	120.49
1	B	293	ARG	C-N-CA	7.03	130.47	120.49
1	B	171	CYS	N-CA-C	6.90	118.60	111.14
1	A	293	ARG	N-CA-C	-6.78	105.34	112.93
1	A	351	HIS	CA-CB-CG	-6.69	107.11	113.80
1	B	292	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	320	ARG	NE-CZ-NH1	6.48	127.98	121.50
1	A	210	GLU	N-CA-C	6.36	117.88	111.07
1	B	324	VAL	N-CA-C	6.36	117.08	108.17
1	B	313	ASP	CA-C-O	6.34	127.27	120.55
1	B	239	TYR	O-C-N	6.30	130.03	122.27
1	A	340	LEU	O-C-N	-6.17	115.72	122.07
1	A	320	ARG	CD-NE-CZ	-6.13	115.82	124.40
1	B	302	GLY	N-CA-C	6.06	122.29	115.08
1	A	235	ILE	CA-C-O	6.05	127.01	120.47
1	B	132	TYR	CB-CG-CD1	6.04	129.86	120.80
1	A	250	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	A	231	MET	O-C-N	-5.99	114.91	122.27
1	B	255	TRP	O-C-N	5.93	129.16	122.22
1	B	246	VAL	O-C-N	5.91	127.60	121.87
1	B	338	ASP	CB-CA-C	-5.85	101.95	110.96
1	B	108	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	351	HIS	N-CA-C	-5.81	103.03	110.53
1	A	250	GLN	CG-CD-NE2	-5.80	107.69	116.40
1	A	212	ARG	CA-CB-CG	5.68	125.45	114.10
1	B	244	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	B	303	ASP	N-CA-CB	5.46	118.72	110.42
1	B	372	MET	N-CA-C	5.45	120.80	113.72
1	B	132	TYR	CB-CG-CD2	-5.43	112.65	120.80
1	B	373	GLY	N-CA-C	-5.41	104.80	112.37
1	A	177	TYR	N-CA-C	-5.38	105.41	111.28
1	B	256	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	A	60	MET	N-CA-CB	-5.34	102.68	110.53
1	B	99	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	147	ALA	N-CA-C	-5.33	106.79	113.72
1	B	281	ARG	CB-CG-CD	-5.28	99.15	111.30
1	A	190	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	320	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	B	343	LEU	CA-C-O	5.26	126.04	120.10
1	B	83	GLU	N-CA-C	-5.25	103.17	109.83
1	B	134	VAL	CA-C-O	-5.24	115.29	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ALA	O-C-N	-5.23	116.64	121.30
1	B	218	ALA	CA-C-N	5.23	133.40	122.58
1	B	218	ALA	C-N-CA	5.23	133.40	122.58
1	B	83	GLU	CA-CB-CG	5.21	124.52	114.10
1	A	91	LEU	N-CA-C	5.21	116.64	111.07
1	A	67	GLN	CA-C-N	5.18	127.23	120.28
1	A	67	GLN	C-N-CA	5.18	127.23	120.28
1	A	320	ARG	N-CA-C	5.12	117.53	111.33
1	A	206	GLY	CA-C-O	5.06	129.38	120.57
1	A	356	GLY	CA-C-N	-5.04	113.89	120.44
1	A	356	GLY	C-N-CA	-5.04	113.89	120.44
1	B	217	LEU	O-C-N	-5.04	116.78	122.12
1	A	100	ILE	O-C-N	5.02	126.83	121.91
1	A	257	GLU	CA-CB-CG	5.02	124.14	114.10
1	A	343	LEU	O-C-N	-5.01	115.88	122.39
1	B	240	GLY	N-CA-C	-5.00	106.70	112.50

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	2350	0	2363	39	0
1	B	2409	0	2424	47	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	18	0	16	1	0
3	B	18	0	16	0	0
4	A	180	0	0	1	0
4	B	184	0	0	8	0
All	All	5169	0	4819	84	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 9.

All (84) 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:354:THR:HB	1:B:355:PRO:HD2	1.47	0.96
1:A:212:ARG:NH2	1:A:216:ARG:HH21	1.70	0.87
1:B:65:THR:HG22	4:B:2167:HOH:O	1.81	0.80
1:B:216:ARG:O	1:B:219:LYS:HG3	1.83	0.79
1:B:61:GLY:O	1:B:65:THR:HG23	1.83	0.79
1:A:341:LEU:O	1:A:344:THR:HG22	1.86	0.75
1:B:220:ARG:HE	1:B:225:GLU:HB2	1.57	0.70
1:A:198:LEU:HB3	1:A:199:PRO:HD2	1.75	0.67
1:B:62:LYS:O	1:B:66:THR:HG23	1.95	0.67
1:B:75:ARG:HD2	1:B:75:ARG:H	1.59	0.66
1:B:54:ILE:HG13	1:B:66:THR:HG22	1.76	0.65
1:B:66:THR:HG21	4:B:2016:HOH:O	1.94	0.65
1:B:246:VAL:HG21	1:B:324:VAL:HG21	1.81	0.62
1:B:274:PRO:N	4:B:2129:HOH:O	2.33	0.61
1:A:64:THR:O	1:A:68:LEU:HD23	2.02	0.60
1:A:61:GLY:HA2	1:A:220:ARG:NH1	2.16	0.60
1:A:65:THR:HG21	1:A:336:CYS:HB2	1.84	0.60
1:B:262:LEU:O	1:B:263:SER:C	2.45	0.60
1:A:198:LEU:HB3	1:A:199:PRO:CD	2.35	0.57
1:A:327:LEU:HD23	1:A:329:TYR:CZ	2.40	0.57
1:A:334:ALA:HB1	1:A:337:ARG:NH2	2.19	0.56
1:A:65:THR:HG21	1:A:336:CYS:CB	2.36	0.56
1:B:102:THR:O	1:B:106:ARG:HG3	2.06	0.56
1:B:339:ALA:O	1:B:343:LEU:HD23	2.06	0.56
1:A:97:ILE:HD13	3:A:500:TMC:H152	1.89	0.55
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.42	0.54
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.90	0.54
1:B:293:ARG:HD3	4:B:2145:HOH:O	2.07	0.54
1:A:65:THR:CG2	1:A:336:CYS:HB2	2.38	0.53
1:B:217:LEU:O	1:B:219:LYS:N	2.39	0.53
1:B:69:LEU:C	1:B:69:LEU:HD13	2.34	0.52
1:B:358:ILE:HB	1:B:359:PRO:HD3	1.90	0.52
1:A:46:MET:HE2	1:A:46:MET:HA	1.92	0.52
1:A:166:ILE:HD13	1:A:322:MET:HE1	1.91	0.52
1:A:213:HIS:CE1	1:A:232:LEU:HD11	2.44	0.52
1:B:354:THR:HB	1:B:355:PRO:CD	2.29	0.51
1:B:50:LEU:HD21	1:B:344:THR:HG23	1.93	0.50
1:B:54:ILE:HG13	1:B:66:THR:CG2	2.41	0.50
1:B:69:LEU:HD13	1:B:69:LEU:O	2.12	0.49
1:A:122:THR:HB	1:B:123:SER:OG	2.12	0.49
1:A:60:MET:HG2	1:A:329:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:HD2	1:B:75:ARG:N	2.27	0.48
1:A:164:HIS:ND1	1:A:166:ILE:HG12	2.28	0.48
1:A:57:PRO:HD2	1:A:60:MET:HE1	1.94	0.48
1:A:63:THR:HG22	1:A:67:GLN:HE22	1.79	0.48
1:A:364:LEU:HD22	1:B:310:TRP:CZ2	2.49	0.48
1:A:63:THR:HG22	1:A:67:GLN:NE2	2.28	0.48
1:B:258:ASP:OD2	1:B:281:ARG:NH2	2.47	0.48
1:B:276:SER:HB2	1:B:324:VAL:HB	1.96	0.48
1:B:345:SER:HB2	4:B:2173:HOH:O	2.12	0.48
1:B:152:ALA:HB1	1:B:153:PRO:HD2	1.94	0.47
1:B:351:HIS:HB3	4:B:2001:HOH:O	2.13	0.47
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.49	0.47
1:A:263:SER:HB2	4:A:2132:HOH:O	2.14	0.47
1:B:169:LEU:O	1:B:190:PHE:HB3	2.15	0.46
1:B:155:PRO:HD3	1:B:349:GLN:NE2	2.31	0.46
1:A:46:MET:HA	1:A:46:MET:CE	2.46	0.46
1:A:217:LEU:HD22	1:A:232:LEU:HD22	1.98	0.46
1:B:59:GLY:HA3	1:B:217:LEU:HD11	1.98	0.45
1:B:333:PRO:HA	4:B:2167:HOH:O	2.16	0.45
1:A:263:SER:HG	1:A:293:ARG:HE	1.61	0.45
1:B:235:ILE:HD12	1:B:235:ILE:HA	1.92	0.43
1:B:278:ALA:HB3	4:B:2131:HOH:O	2.17	0.43
1:A:212:ARG:HH22	1:A:216:ARG:HH21	1.57	0.43
1:B:182:MET:HE2	1:B:182:MET:HB3	1.88	0.43
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.75	0.43
1:B:172:TYR:N	1:B:173:PRO:CD	2.82	0.43
1:B:59:GLY:HA3	1:B:217:LEU:CD1	2.49	0.43
1:A:364:LEU:C	1:A:364:LEU:HD13	2.44	0.43
1:B:327:LEU:HD23	1:B:329:TYR:CZ	2.53	0.42
1:A:182:MET:HE3	1:A:182:MET:HB2	1.87	0.42
1:A:118:ALA:HA	1:A:181:SER:O	2.20	0.42
1:A:116:ASP:O	1:A:119:VAL:HG22	2.20	0.42
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.85	0.41
1:B:240:GLY:HA2	1:B:274:PRO:HG2	2.03	0.41
1:B:338:ASP:O	1:B:339:ALA:C	2.62	0.41
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.92	0.41
1:B:152:ALA:HB1	1:B:153:PRO:CD	2.50	0.41
1:B:299:ALA:HB3	1:B:301:ASN:OD1	2.21	0.41
1:A:212:ARG:NH2	1:A:216:ARG:NH2	2.53	0.41
1:B:135:THR:HG23	1:B:364:LEU:HD11	2.03	0.41
1:A:354:THR:HB	1:A:355:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:HB3	1:B:361:ILE:HD11	2.03	0.40
1:A:164:HIS:CD2	1:A:165:PRO:HD2	2.57	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	300/331 (91%)	292 (97%)	8 (3%)	0	100	100
1	B	308/331 (93%)	300 (97%)	7 (2%)	1 (0%)	36	22
All	All	608/662 (92%)	592 (97%)	15 (2%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	SER

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	247/264 (94%)	237 (96%)	10 (4%)	28	12
1	B	254/264 (96%)	244 (96%)	10 (4%)	28	12
All	All	501/528 (95%)	481 (96%)	20 (4%)	28	12

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	67	GLN
1	A	69	LEU
1	A	159	LEU
1	A	198	LEU
1	A	212	ARG
1	A	229	LEU
1	A	341	LEU
1	A	360	THR
1	A	362	CYS
1	B	51	ARG
1	B	65	THR
1	B	69	LEU
1	B	75	ARG
1	B	76	ASP
1	B	116	ASP
1	B	215	ASP
1	B	217	LEU
1	B	229	LEU
1	B	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	B	202	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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	SO4	B	400	-	4,4,4	0.81	0	6,6,6	0.54	0
3	TMC	B	500	-	19,20,20	1.14	1 (5%)	23,32,32	2.40	6 (26%)
3	TMC	A	500	-	19,20,20	1.48	3 (15%)	23,32,32	3.36	14 (60%)
2	SO4	A	400	-	4,4,4	0.79	0	6,6,6	0.36	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	TMC	A	500	-	-	3/7/29/29	0/3/3/3
3	TMC	B	500	-	-	1/7/29/29	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	TMC	C14-C17	3.26	1.59	1.53
3	A	500	TMC	C11-N5	2.87	1.43	1.38
3	A	500	TMC	O7-C6	2.75	1.28	1.23
3	A	500	TMC	C6-C4	-2.39	1.40	1.44

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	TMC	C14-C17-N8	-8.53	102.20	113.42
3	A	500	TMC	C4-C6-N5	6.84	121.27	115.32
3	A	500	TMC	C2-N8-C11	6.13	127.41	121.30
3	A	500	TMC	C14-C17-N8	-5.84	105.74	113.42
3	A	500	TMC	C3-C4-C6	5.07	124.19	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	TMC	O9-C11-N8	4.77	129.01	122.80
3	A	500	TMC	C1-C13-C17	-3.84	105.39	108.39
3	B	500	TMC	C1-C13-C17	-3.84	105.40	108.39
3	A	500	TMC	C2-C4-C6	-3.56	115.09	118.02
3	A	500	TMC	N5-C11-N8	-3.51	110.32	114.89
3	B	500	TMC	O7-C6-C4	-3.44	120.98	124.92
3	B	500	TMC	O9-C11-N8	3.18	126.93	122.80
3	A	500	TMC	O18-C10-C14	2.99	118.44	111.33
3	A	500	TMC	O7-C6-N5	-2.83	114.79	120.11
3	A	500	TMC	C17-N8-C11	-2.82	114.03	117.41
3	A	500	TMC	C1-C15-C13	2.64	61.43	59.98
3	B	500	TMC	O16-C12-C1	-2.63	105.94	112.39
3	B	500	TMC	O7-C6-N5	2.46	124.74	120.11
3	A	500	TMC	C10-C14-C17	2.26	107.69	104.28
3	A	500	TMC	C6-N5-C11	-2.17	124.49	127.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	TMC	C10-C1-C12-O16
3	A	500	TMC	C15-C1-C12-O16
3	B	500	TMC	C10-C1-C12-O16
3	A	500	TMC	C13-C1-C12-O16

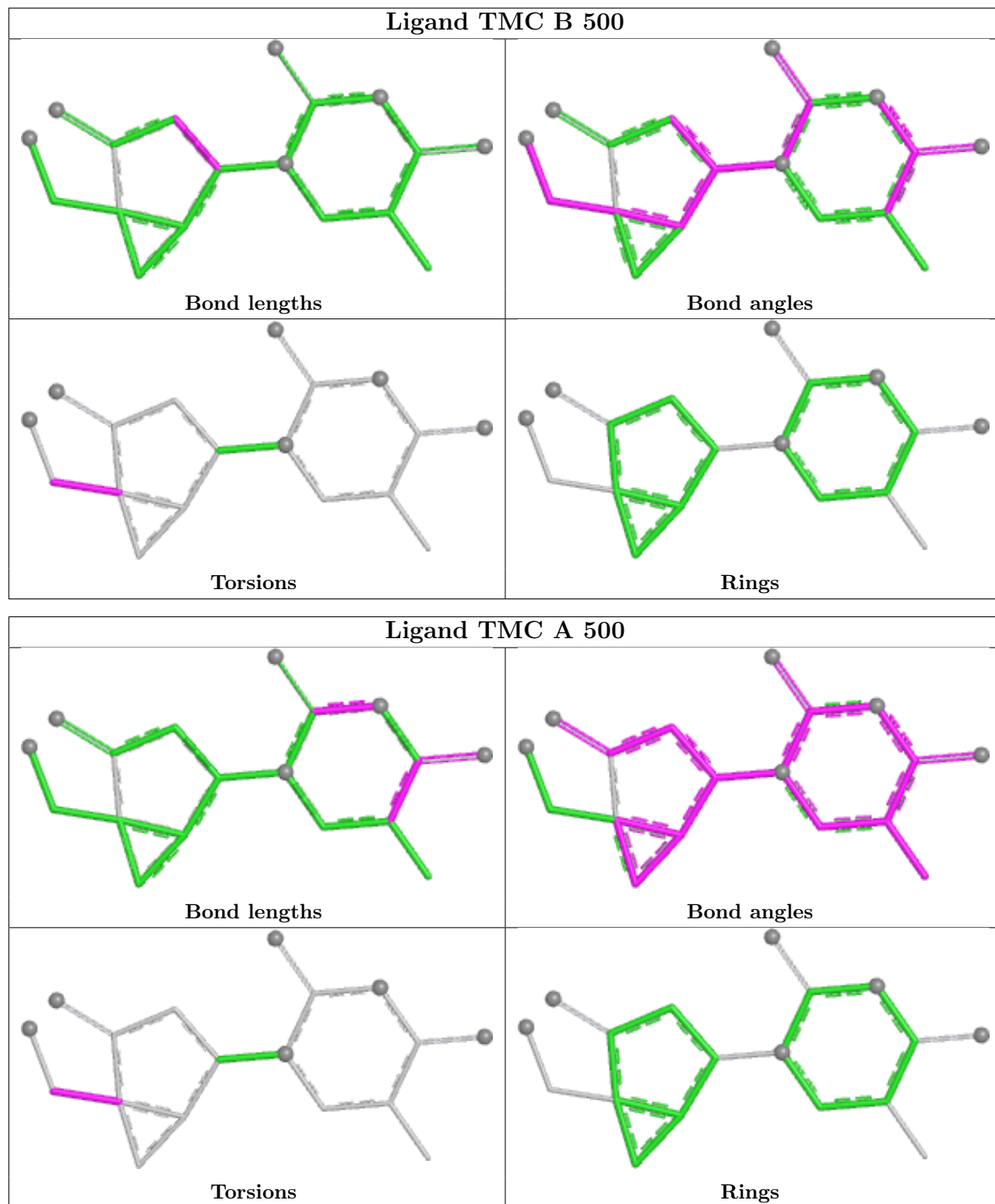
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	TMC	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.



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, 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	308/331 (93%)	0.37	22 (7%) 22 24	18, 27, 61, 112	0
1	B	316/331 (95%)	0.43	27 (8%) 16 17	17, 27, 65, 115	0
All	All	624/662 (94%)	0.40	49 (7%) 18 20	17, 27, 64, 115	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	VAL	7.3
1	A	264	GLY	5.8
1	B	338	ASP	5.5
1	B	266	ALA	5.4
1	A	148	GLY	5.3
1	A	70	VAL	5.3
1	B	265	THR	5.0
1	A	69	LEU	4.8
1	B	218	ALA	4.7
1	A	153	PRO	4.6
1	A	68	LEU	4.4
1	B	152	ALA	4.4
1	A	265	THR	4.3
1	A	71	ALA	4.2
1	B	300	PRO	4.2
1	A	279	GLY	4.2
1	B	153	PRO	4.1
1	B	227	LEU	4.1
1	B	219	LYS	4.1
1	B	264	GLY	3.8
1	A	76	ASP	3.7
1	A	263	SER	3.6
1	A	65	THR	3.5
1	B	220	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	301	ASN	3.4
1	B	46	MET	3.4
1	B	263	SER	3.1
1	B	225	GLU	3.1
1	B	151	HIS	3.0
1	A	66	THR	2.8
1	B	374	GLU	2.8
1	B	147	ALA	2.7
1	B	226	ARG	2.7
1	A	64	THR	2.7
1	B	101	TYR	2.7
1	B	102	THR	2.7
1	A	62	LYS	2.6
1	A	220	ARG	2.6
1	A	363	ASP	2.4
1	B	274	PRO	2.3
1	B	75	ARG	2.3
1	B	110	GLY	2.3
1	A	280	PRO	2.3
1	A	80	TYR	2.2
1	A	154	PRO	2.2
1	A	78	ILE	2.2
1	B	76	ASP	2.1
1	B	355	PRO	2.1
1	A	356	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

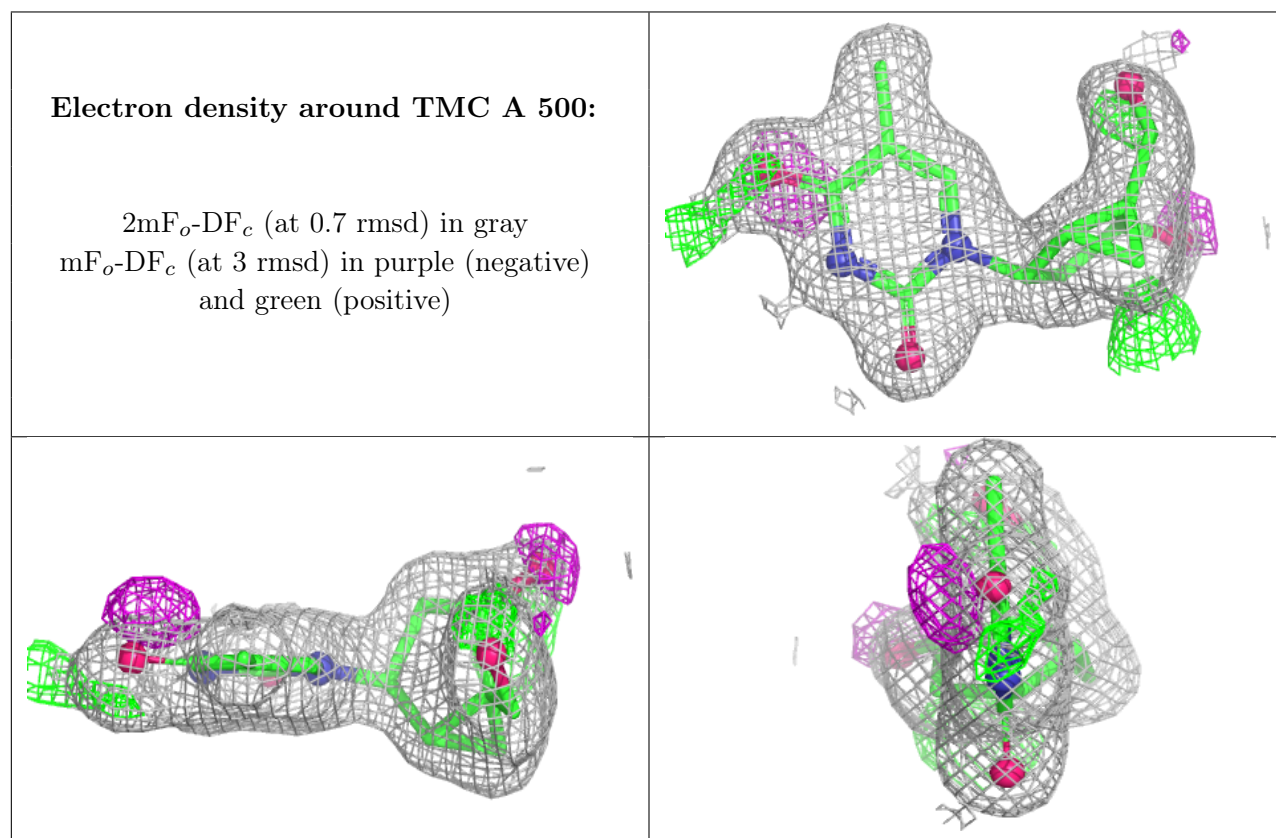
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

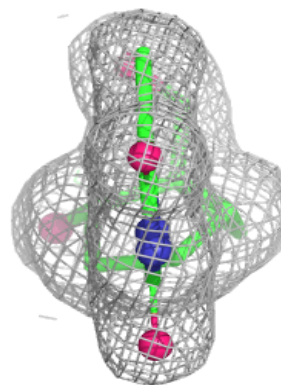
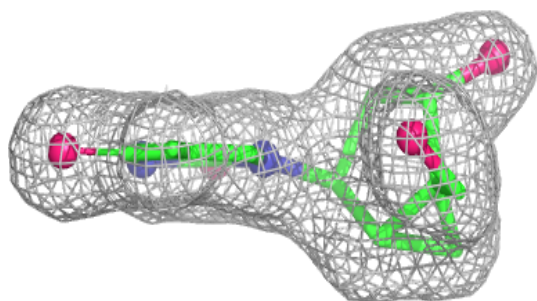
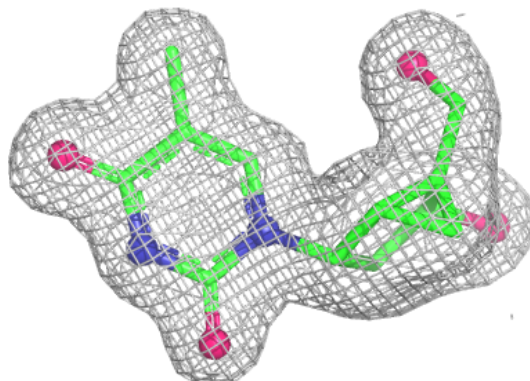
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TMC	A	500	18/18	0.91	0.10	20,23,38,51	0
3	TMC	B	500	18/18	0.94	0.07	18,26,31,34	0
2	SO4	A	400	5/5	0.95	0.10	32,33,38,42	0
2	SO4	B	400	5/5	0.98	0.06	27,27,32,33	0

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 TMC B 500:

$2mF_o-DF_c$ (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.