



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 06:12 PM EST

PDB ID : 2Q27
Title : Crystal structure of oxalyl-coA decarboxylase from Escherichia coli
Authors : Werther, T.; Zimmer, A.; Wille, G.; Hubner, G.; Weiss, M.S.; Konig, S.
Deposited on : 2007-05-26
Resolution : 2.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

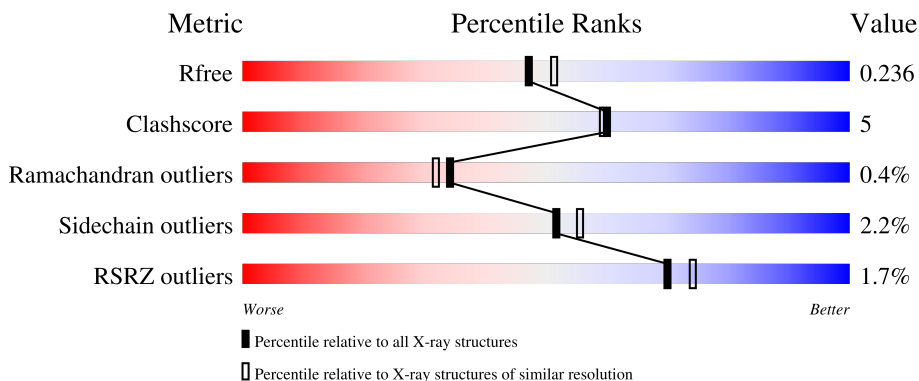
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	564	 2% 87% 9% ..
1	B	564	 % 83% 13% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8798 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 oxalyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	4122	2594	719	787	22	0	0	0
1	B	545	4112	2589	717	784	22	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

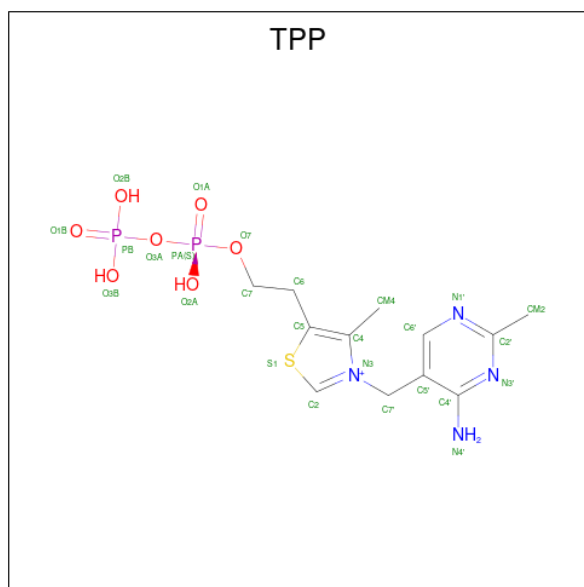
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



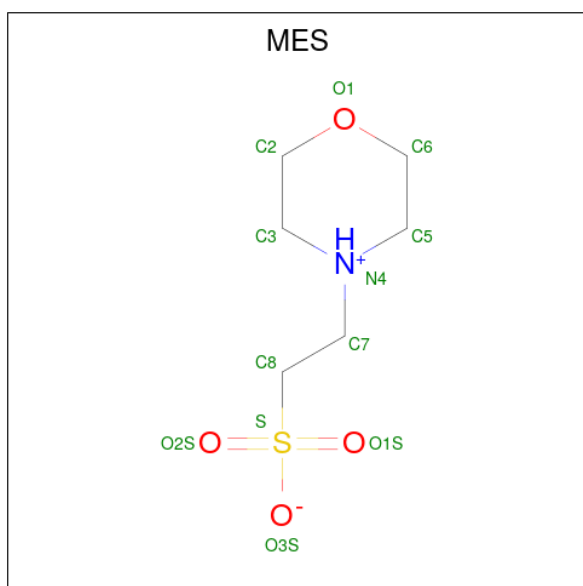
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 26 12 4 7 2 1	0	0
4	B	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	12	6	1	4	1	0	0

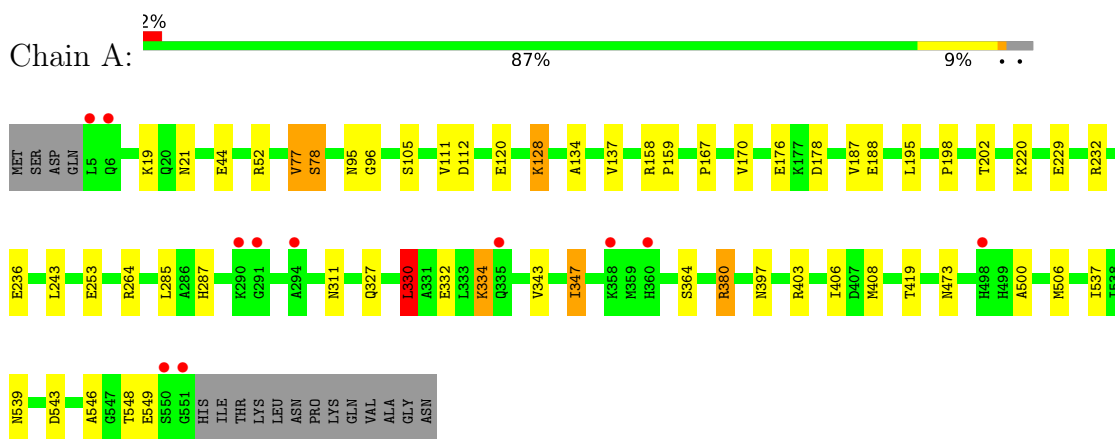
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	247	Total 247	O 247	0	0
7	B	186	Total 186	O 186	0	0

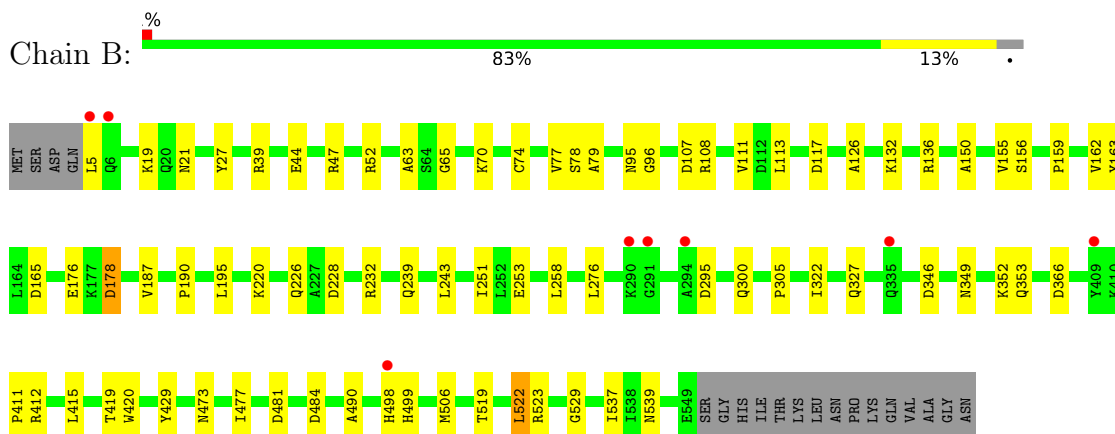
3 Residue-property plots [i](#)

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

- Molecule 1: oxalyl-CoA decarboxylase



- Molecule 1: oxalyl-CoA decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.11Å 145.44Å 147.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.31 – 2.12 18.31 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.2 (18.31-2.12) 97.2 (18.31-2.12)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.13Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.237 0.193 , 0.236	Depositor DCC
R_{free} test set	3939 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8798	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: EDO, MES, MG, TPP, SO4

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	1.11	5/4197 (0.1%)	0.95	4/5704 (0.1%)
1	B	0.99	2/4187 (0.0%)	0.91	9/5691 (0.2%)
All	All	1.05	7/8384 (0.1%)	0.93	13/11395 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	CG-CD	7.15	1.62	1.51
1	A	327	GLN	CG-CD	5.83	1.64	1.51
1	A	500	ALA	CA-CB	5.73	1.64	1.52
1	B	111	VAL	CB-CG2	5.69	1.64	1.52
1	A	236	GLU	CB-CG	5.67	1.62	1.52
1	B	126	ALA	CA-CB	5.64	1.64	1.52
1	A	77	VAL	CB-CG1	5.48	1.64	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	LEU	CB-CG-CD1	-6.57	99.83	111.00
1	B	39	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	52	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	B	107	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	346	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	330	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	403	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	112	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	52	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	B	117	ASP	CB-CG-OD1	5.47	123.23	118.30
1	B	47	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	113	LEU	CA-CB-CG	5.07	126.95	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ASP	CB-CG-OD2	-5.07	113.74	118.30

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	4122	0	4131	36	0
1	B	4112	0	4123	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	0	2	0
3	B	20	0	0	0	0
4	A	26	0	16	0	0
4	B	26	0	16	2	0
5	A	4	0	6	0	0
5	B	4	0	6	3	0
6	A	12	0	12	1	0
6	B	12	0	12	0	0
7	A	247	0	0	4	0
7	B	186	0	0	3	0
All	All	8798	0	8322	76	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 5.

All (76) 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:498:HIS:CD2	1:B:499:HIS:HD2	1.74	1.03
1:B:322:ILE:HD12	5:B:5001:EDO:H11	1.47	0.96
1:B:498:HIS:CD2	1:B:499:HIS:CD2	2.57	0.92
1:A:95:ASN:HD22	1:A:220:LYS:HE2	1.36	0.90
1:B:21:ASN:HD21	1:B:187:VAL:H	1.24	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASN:HD22	1:A:539:ASN:HD21	1.24	0.84
1:B:473:ASN:HD22	1:B:539:ASN:HD21	1.26	0.82
1:B:498:HIS:NE2	1:B:499:HIS:HD2	1.82	0.77
1:A:549:GLU:OE2	6:A:6001:MES:H72	1.87	0.75
1:A:21:ASN:HD21	1:A:187:VAL:H	1.37	0.72
1:A:95:ASN:HD21	1:A:419:THR:H	1.39	0.70
1:B:95:ASN:HD22	1:B:220:LYS:HE3	1.58	0.69
5:B:5001:EDO:H21	7:B:6139:HOH:O	1.95	0.66
1:B:95:ASN:HD21	1:B:419:THR:H	1.42	0.65
1:B:322:ILE:CD1	5:B:5001:EDO:H11	2.24	0.65
1:B:506:MET:HG2	1:B:537:ILE:HD12	1.77	0.65
1:B:498:HIS:NE2	1:B:499:HIS:CD2	2.64	0.63
1:B:96:GLY:HA2	1:B:159:PRO:O	1.99	0.61
1:A:287:HIS:ND1	1:A:311:ASN:ND2	2.51	0.59
1:B:353:GLN:HG2	7:B:6102:HOH:O	2.01	0.59
1:A:158:ARG:HD2	3:A:2009:SO4:O4	2.06	0.55
1:B:21:ASN:ND2	1:B:187:VAL:H	1.99	0.55
1:B:251:ILE:HA	1:B:411:PRO:HB3	1.91	0.53
1:B:232:ARG:NH2	1:B:253:GLU:OE1	2.30	0.52
1:A:543:ASP:HB3	1:A:546:ALA:HB2	1.92	0.52
1:A:95:ASN:ND2	1:A:419:THR:H	2.07	0.52
1:A:397:ASN:HD21	1:A:548:THR:H	1.57	0.52
1:B:176:GLU:OE1	1:B:178:ASP:HB2	2.10	0.52
1:A:128:LYS:HZ3	1:A:134:ALA:HB3	1.74	0.51
1:A:380:ARG:HG2	7:A:6038:HOH:O	2.11	0.49
1:A:364:SER:HB2	7:A:6169:HOH:O	2.11	0.49
1:B:226:GLN:HG2	1:B:412:ARG:CZ	2.43	0.49
1:B:484:ASP:HB2	1:B:490:ALA:O	2.13	0.49
1:A:343:VAL:O	1:A:347:ILE:HG23	2.13	0.47
1:A:232:ARG:NH2	1:A:253:GLU:OE1	2.37	0.47
1:A:96:GLY:HA2	1:A:159:PRO:O	2.15	0.47
1:A:176:GLU:OE2	1:A:178:ASP:HB2	2.15	0.47
1:B:132:LYS:NZ	1:B:156:SER:O	2.48	0.47
1:A:21:ASN:ND2	1:A:187:VAL:H	2.06	0.47
1:B:65:GLY:HA2	1:B:70:LYS:O	2.15	0.46
1:A:78:SER:HB3	1:A:105:SER:HA	1.98	0.46
4:B:4001:TPP:C6'	4:B:4001:TPP:HM42	2.46	0.45
1:A:111:VAL:HG13	1:A:120:GLU:HG3	1.99	0.44
1:B:498:HIS:HD2	1:B:499:HIS:CD2	2.26	0.44
1:A:137:VAL:O	1:A:167:PRO:HD2	2.17	0.44
1:A:198:PRO:O	1:A:202:THR:HG23	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASN:HD22	1:A:220:LYS:CE	2.18	0.44
1:A:220:LYS:HE3	7:A:6127:HOH:O	2.17	0.44
1:A:506:MET:HG2	1:A:537:ILE:HD12	2.00	0.43
1:A:19:LYS:HD2	1:A:44:GLU:HB3	2.01	0.43
1:B:163:TYR:CE2	1:B:165:ASP:HB2	2.53	0.43
1:B:108:ARG:HD2	1:B:136:ARG:HD2	2.01	0.43
1:B:150:ALA:HA	1:B:162:VAL:HG11	2.00	0.43
1:A:330:LEU:O	1:A:334:LYS:HD3	2.19	0.43
1:B:95:ASN:HD22	1:B:220:LYS:CE	2.29	0.43
1:A:195:LEU:HB2	1:B:195:LEU:HB2	2.01	0.43
1:A:220:LYS:NZ	3:A:2008:SO4:O1	2.52	0.42
1:B:63:ALA:HB2	1:B:429:TYR:CD1	2.54	0.42
1:A:406:ILE:HG22	1:A:408:MET:CE	2.49	0.42
1:B:95:ASN:ND2	1:B:419:THR:H	2.12	0.42
1:B:27:TYR:O	1:B:74:CYS:HA	2.20	0.42
1:B:239:GLN:HA	1:B:258:LEU:HD11	2.02	0.41
1:B:327:GLN:HB2	7:B:6128:HOH:O	2.18	0.41
1:B:349:ASN:HD21	1:B:352:LYS:NZ	2.19	0.41
1:B:519:THR:OG1	1:B:523:ARG:NH2	2.53	0.41
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.85	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.90	0.41
1:B:19:LYS:HD2	1:B:44:GLU:HB3	2.02	0.41
1:A:158:ARG:HG2	1:A:158:ARG:NH1	2.36	0.41
1:A:167:PRO:O	1:A:170:VAL:HG12	2.21	0.41
1:B:522:LEU:HD12	1:B:522:LEU:O	2.20	0.40
1:A:158:ARG:NH1	7:A:6070:HOH:O	2.54	0.40
1:B:276:LEU:HB2	1:B:300:GLN:HG3	2.03	0.40
1:B:477:ILE:HG23	4:B:4001:TPP:H71	2.04	0.40
1:A:202:THR:HG22	1:A:332:GLU:OE1	2.22	0.40
1:B:155:VAL:HG21	1:B:190:PRO:HB2	2.03	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	545/564 (97%)	523 (96%)	21 (4%)	1 (0%)	47	48
1	B	543/564 (96%)	517 (95%)	23 (4%)	3 (1%)	25	20
All	All	1088/1128 (96%)	1040 (96%)	44 (4%)	4 (0%)	34	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	VAL
1	B	79	ALA
1	B	77	VAL
1	B	529	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	435/450 (97%)	426 (98%)	9 (2%)	53	57
1	B	434/450 (96%)	424 (98%)	10 (2%)	50	53
All	All	869/900 (97%)	850 (98%)	19 (2%)	52	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	SER
1	A	128	LYS
1	A	188	GLU
1	A	243	LEU
1	A	264	ARG
1	A	330	LEU
1	A	334	LYS
1	A	347	ILE
1	A	380	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	5	LEU
1	B	78	SER
1	B	178	ASP
1	B	228	ASP
1	B	295	ASP
1	B	305	PRO
1	B	366	ASP
1	B	415	LEU
1	B	420	TRP
1	B	522	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	21	ASN
1	A	55	GLN
1	A	95	ASN
1	A	226	GLN
1	A	306	GLN
1	A	311	ASN
1	A	349	ASN
1	A	387	GLN
1	A	397	ASN
1	A	539	ASN
1	B	20	GLN
1	B	21	ASN
1	B	95	ASN
1	B	226	GLN
1	B	239	GLN
1	B	300	GLN
1	B	306	GLN
1	B	311	ASN
1	B	349	ASN
1	B	387	GLN
1	B	397	ASN
1	B	498	HIS
1	B	499	HIS
1	B	539	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
3	SO4	B	2005	-	4,4,4	0.18	0	6,6,6	0.50	0
5	EDO	B	5001	-	3,3,3	0.83	0	2,2,2	0.90	0
3	SO4	B	2007	-	4,4,4	0.31	0	6,6,6	0.51	0
6	MES	B	6002	-	12,12,12	1.89	1 (8%)	14,16,16	2.42	5 (35%)
4	TPP	B	4001	2	22,27,27	2.02	6 (27%)	29,40,40	2.00	12 (41%)
3	SO4	A	2008	-	4,4,4	0.60	0	6,6,6	0.83	0
5	EDO	A	5002	-	3,3,3	0.89	0	2,2,2	0.47	0
3	SO4	A	2001	-	4,4,4	0.28	0	6,6,6	0.77	0
3	SO4	A	2003	-	4,4,4	0.27	0	6,6,6	0.80	0
4	TPP	A	3001	2	22,27,27	2.56	6 (27%)	29,40,40	1.92	9 (31%)
3	SO4	B	2004	-	4,4,4	0.24	0	6,6,6	0.45	0
3	SO4	A	2009	-	4,4,4	0.16	0	6,6,6	0.44	0
3	SO4	A	2006	-	4,4,4	0.82	0	6,6,6	0.69	0
3	SO4	B	2002	-	4,4,4	0.30	0	6,6,6	0.24	0
6	MES	A	6001	-	12,12,12	1.80	1 (8%)	14,16,16	3.16	7 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	5001	-	-	1/1/1/1	-
6	MES	B	6002	-	-	1/6/14/14	0/1/1/1
4	TPP	B	4001	2	-	4/16/17/17	0/2/2/2
5	EDO	A	5002	-	-	0/1/1/1	-
4	TPP	A	3001	2	-	4/16/17/17	0/2/2/2
6	MES	A	6001	-	-	5/6/14/14	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	TPP	C6-C5	8.69	1.54	1.50
4	B	4001	TPP	C6-C5	6.72	1.53	1.50
6	B	6002	MES	C8-S	-6.00	1.69	1.77
6	A	6001	MES	C8-S	-5.54	1.69	1.77
4	A	3001	TPP	C4-N3	-4.16	1.36	1.39
4	A	3001	TPP	C2-N3	3.77	1.43	1.36
4	A	3001	TPP	C6'-N1'	3.09	1.40	1.34
4	A	3001	TPP	C2'-N3'	2.96	1.39	1.34
4	B	4001	TPP	C2'-N3'	2.84	1.39	1.34
4	B	4001	TPP	C4'-N3'	2.56	1.38	1.35
4	B	4001	TPP	C6'-N1'	2.48	1.39	1.34
4	B	4001	TPP	C2'-N1'	2.21	1.37	1.34
4	B	4001	TPP	C2-N3	2.16	1.40	1.36
4	A	3001	TPP	C4'-N3'	2.07	1.38	1.35

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6001	MES	O1S-S-C8	8.03	116.58	106.92
6	B	6002	MES	C5-N4-C3	5.22	120.57	108.83
6	A	6001	MES	C5-N4-C3	5.20	120.53	108.83
4	A	3001	TPP	N1'-C2'-N3'	-4.95	117.02	125.54
6	A	6001	MES	C7-N4-C5	4.24	122.07	111.23
4	B	4001	TPP	C5'-C7'-N3	-4.04	106.56	113.28
4	B	4001	TPP	C6'-N1'-C2'	3.94	122.67	115.96
4	B	4001	TPP	N1'-C2'-N3'	-3.61	119.33	125.54
4	A	3001	TPP	CM2-C2'-N3'	3.52	122.64	117.15
6	B	6002	MES	O1S-S-C8	3.41	111.02	106.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	6002	MES	C7-N4-C3	3.38	119.89	111.23
6	B	6002	MES	C7-N4-C5	3.25	119.54	111.23
4	B	4001	TPP	C5'-C6'-N1'	-3.12	118.63	123.82
4	A	3001	TPP	C6'-N1'-C2'	3.05	121.15	115.96
4	A	3001	TPP	C2'-N3'-C4'	2.97	122.72	118.08
4	A	3001	TPP	CM2-C2'-N1'	2.88	120.31	117.14
4	B	4001	TPP	CM2-C2'-N1'	2.83	120.25	117.14
4	B	4001	TPP	CM4-C4-N3	2.77	126.06	122.53
6	B	6002	MES	O2S-S-C8	2.70	110.17	106.92
4	A	3001	TPP	C5-C4-N3	2.52	112.61	107.57
4	A	3001	TPP	N4'-C4'-N3'	2.49	120.56	117.03
4	B	4001	TPP	CM4-C4-C5	-2.48	122.19	127.60
6	A	6001	MES	C7-N4-C3	2.41	117.40	111.23
4	B	4001	TPP	C6-C5-C4	2.26	129.25	127.43
4	A	3001	TPP	PA-O3A-PB	-2.26	125.08	132.83
6	A	6001	MES	O1-C6-C5	2.21	116.67	111.80
6	A	6001	MES	C6-O1-C2	2.21	117.26	109.89
4	B	4001	TPP	O7-PA-O1A	2.17	117.56	109.07
4	B	4001	TPP	PA-O3A-PB	-2.13	125.51	132.83
4	A	3001	TPP	C5'-C4'-N4'	-2.11	119.20	122.19
4	B	4001	TPP	C5-C4-N3	2.09	111.75	107.57
6	A	6001	MES	O3S-S-O2S	-2.09	106.18	111.27
4	B	4001	TPP	CM2-C2'-N3'	2.08	120.39	117.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3001	TPP	C4-C5-C6-C7
4	A	3001	TPP	PA-O3A-PB-O3B
4	B	4001	TPP	C4-C5-C6-C7
6	A	6001	MES	C8-C7-N4-C5
6	A	6001	MES	C7-C8-S-O2S
6	A	6001	MES	C7-C8-S-O3S
4	B	4001	TPP	PB-O3A-PA-O7
6	A	6001	MES	C7-C8-S-O1S
4	B	4001	TPP	C5'-C7'-N3-C2
6	A	6001	MES	C8-C7-N4-C3
6	B	6002	MES	C8-C7-N4-C5
5	B	5001	EDO	O1-C1-C2-O2
4	A	3001	TPP	PA-O3A-PB-O2B
4	A	3001	TPP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

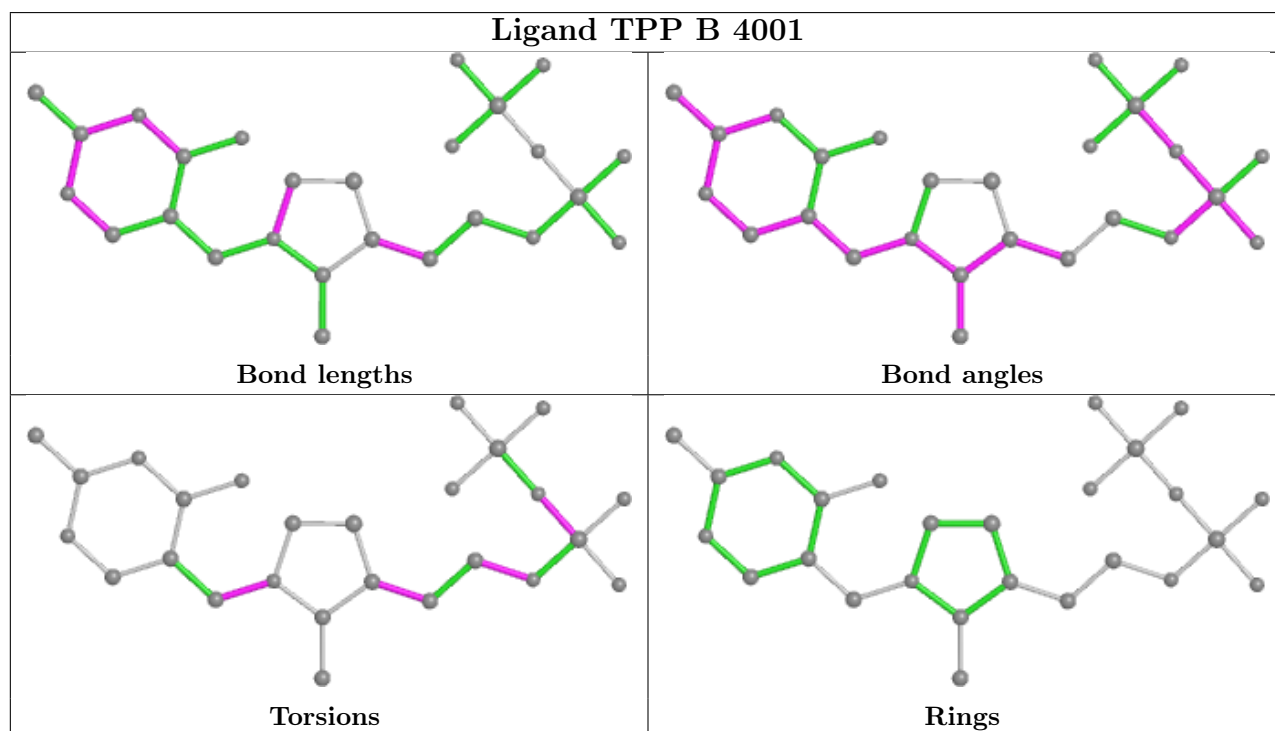
Mol	Chain	Res	Type	Atoms
4	B	4001	TPP	C6-C7-O7-PA

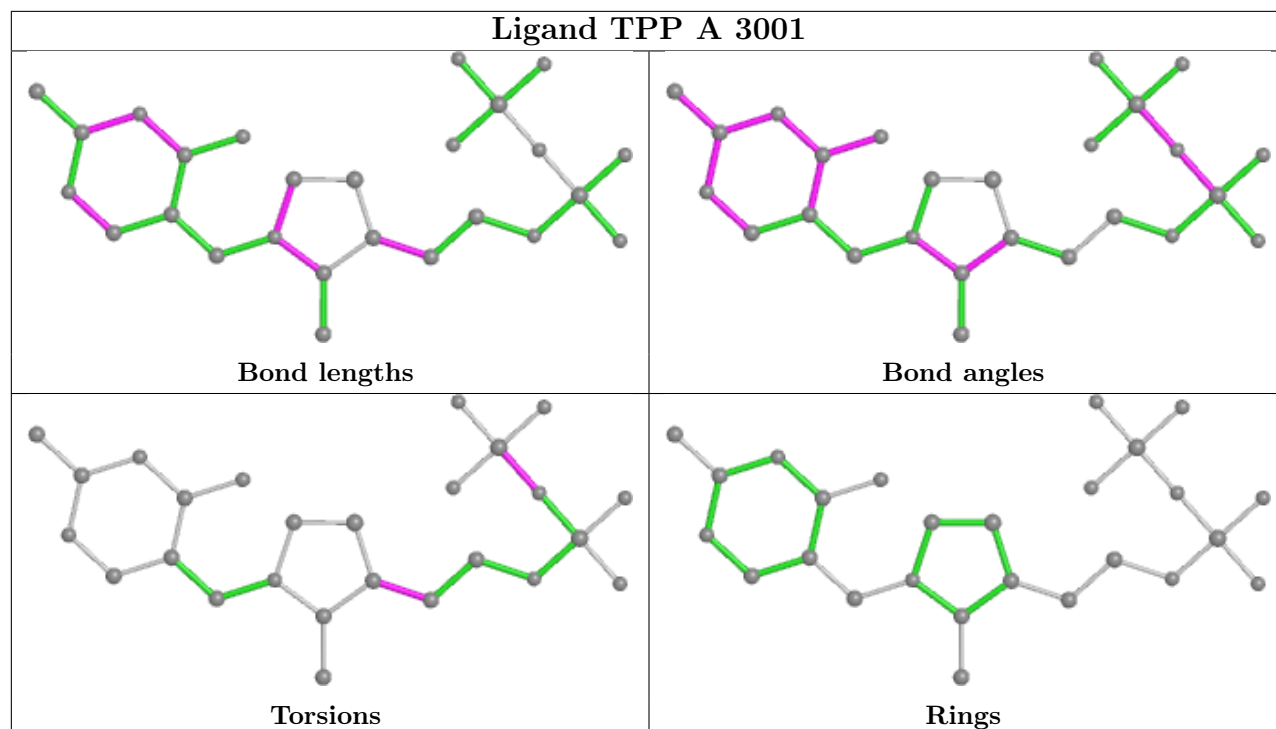
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5001	EDO	3	0
4	B	4001	TPP	2	0
3	A	2008	SO4	1	0
3	A	2009	SO4	1	0
6	A	6001	MES	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 [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	547/564 (96%)	-0.38	11 (2%) 65 69	21, 31, 49, 68	0
1	B	545/564 (96%)	-0.20	8 (1%) 73 77	26, 39, 55, 74	0
All	All	1092/1128 (96%)	-0.29	19 (1%) 70 74	21, 35, 52, 74	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	4.9
1	B	294	ALA	4.5
1	A	5	LEU	4.3
1	A	294	ALA	3.7
1	A	551	GLY	3.6
1	A	335	GLN	3.1
1	B	290	LYS	2.9
1	B	335	GLN	2.8
1	A	290	LYS	2.8
1	B	6	GLN	2.7
1	A	291	GLY	2.6
1	A	550	SER	2.5
1	B	498	HIS	2.4
1	A	6	GLN	2.4
1	B	291	GLY	2.3
1	A	358	LYS	2.2
1	A	498	HIS	2.1
1	A	360	HIS	2.1
1	B	409	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

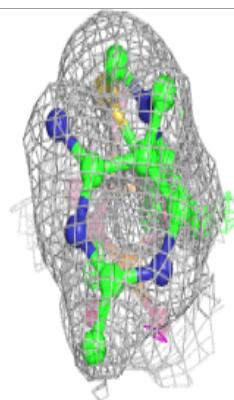
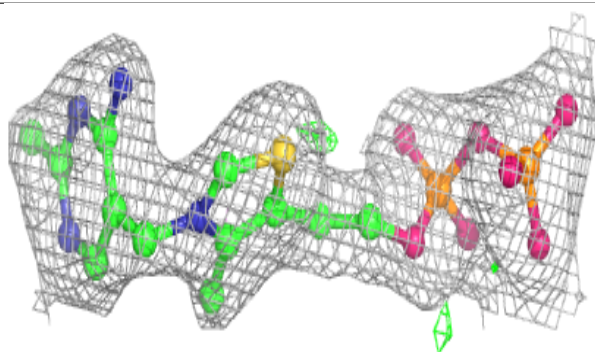
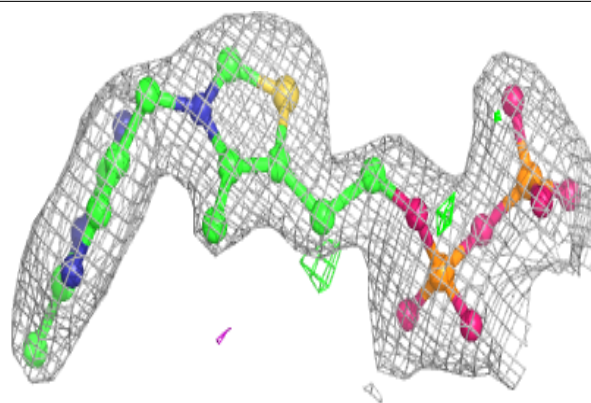
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	2006	5/5	0.66	0.25	90,91,93,94	0
5	EDO	A	5002	4/4	0.80	0.15	49,55,56,61	0
5	EDO	B	5001	4/4	0.81	0.20	43,50,50,55	0
3	SO4	A	2009	5/5	0.82	0.27	121,122,122,124	0
3	SO4	B	2005	5/5	0.82	0.19	90,91,93,93	0
3	SO4	B	2004	5/5	0.84	0.26	84,87,88,90	0
6	MES	B	6002	12/12	0.89	0.24	87,90,92,93	0
3	SO4	A	2003	5/5	0.91	0.23	68,69,72,74	0
6	MES	A	6001	12/12	0.92	0.26	57,59,62,63	0
3	SO4	A	2008	5/5	0.94	0.11	42,45,46,47	0
3	SO4	B	2007	5/5	0.96	0.07	45,47,49,49	0
2	MG	A	1001	1/1	0.98	0.08	27,27,27,27	0
3	SO4	A	2001	5/5	0.98	0.12	47,48,49,50	0
3	SO4	B	2002	5/5	0.98	0.23	57,58,60,61	0
4	TPP	B	4001	26/26	0.98	0.09	30,34,37,38	0
4	TPP	A	3001	26/26	0.99	0.10	22,26,28,30	0
2	MG	B	1002	1/1	0.99	0.03	39,39,39,39	0

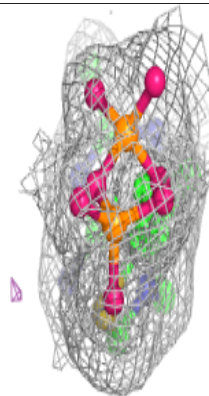
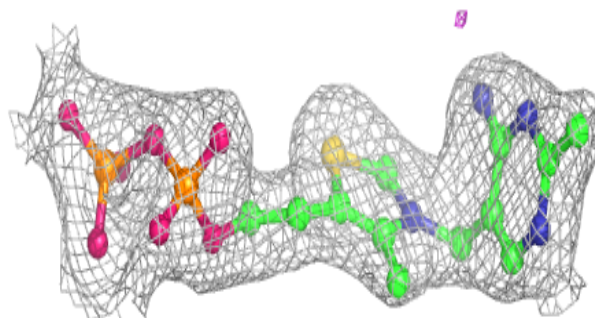
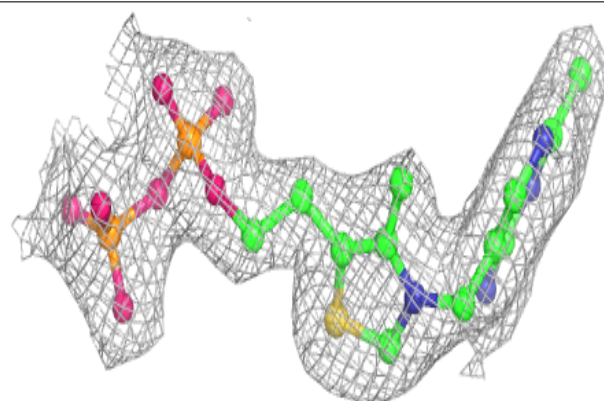
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP B 4001:

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

**Electron density around TPP A 3001:**

$2mF_o-DF_c$ (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.