



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 08:09 PM JST

PDB ID : 8ZK7 / pdb_00008zk7
Title : Crystal structure of the Decarboxylase KDC4427 mutant E468L from Enterobacter sp. CGMCC 5087
Authors : Dong, S.; Liu, L.; Zhang, H.
Deposited on : 2024-05-15
Resolution : 2.32 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

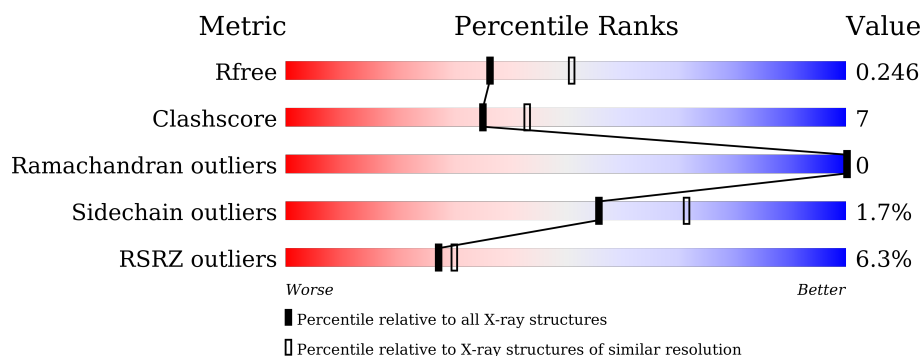
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	566	 6% 80% 14% • 5%
1	B	566	 6% 78% 16% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8662 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 Indolepyruvate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4139	2625	725	767	22			
1	B	539	Total	C	N	O	S	0	0	0
			4139	2625	725	767	22			

There are 30 discrepancies between the modelled and reference sequences:

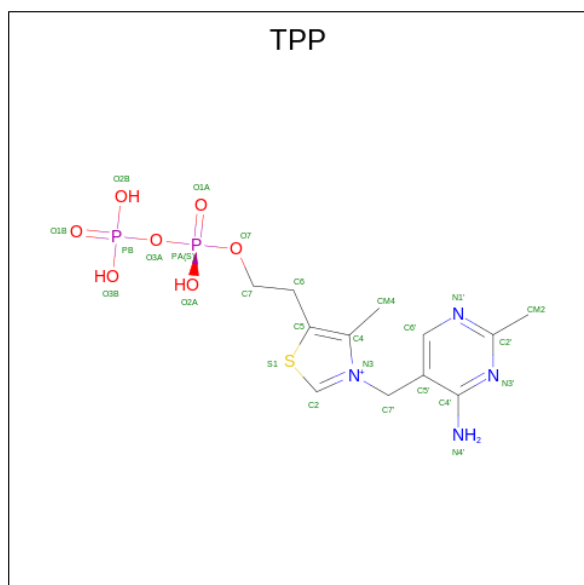
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A2U3EYQ2
A	-12	GLY	-	expression tag	UNP A0A2U3EYQ2
A	-11	SER	-	expression tag	UNP A0A2U3EYQ2
A	-10	SER	-	expression tag	UNP A0A2U3EYQ2
A	-9	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-8	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-7	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-6	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-5	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-4	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-3	SER	-	expression tag	UNP A0A2U3EYQ2
A	-2	GLN	-	expression tag	UNP A0A2U3EYQ2
A	-1	ASP	-	expression tag	UNP A0A2U3EYQ2
A	0	PRO	-	expression tag	UNP A0A2U3EYQ2
A	468	LEU	GLU	engineered mutation	UNP A0A2U3EYQ2
B	-13	MET	-	initiating methionine	UNP A0A2U3EYQ2
B	-12	GLY	-	expression tag	UNP A0A2U3EYQ2
B	-11	SER	-	expression tag	UNP A0A2U3EYQ2
B	-10	SER	-	expression tag	UNP A0A2U3EYQ2
B	-9	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-8	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-7	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-6	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-5	HIS	-	expression tag	UNP A0A2U3EYQ2
B	-4	HIS	-	expression tag	UNP A0A2U3EYQ2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	expression tag	UNP A0A2U3EYQ2
B	-2	GLN	-	expression tag	UNP A0A2U3EYQ2
B	-1	ASP	-	expression tag	UNP A0A2U3EYQ2
B	0	PRO	-	expression tag	UNP A0A2U3EYQ2
B	468	LEU	GLU	engineered mutation	UNP A0A2U3EYQ2

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

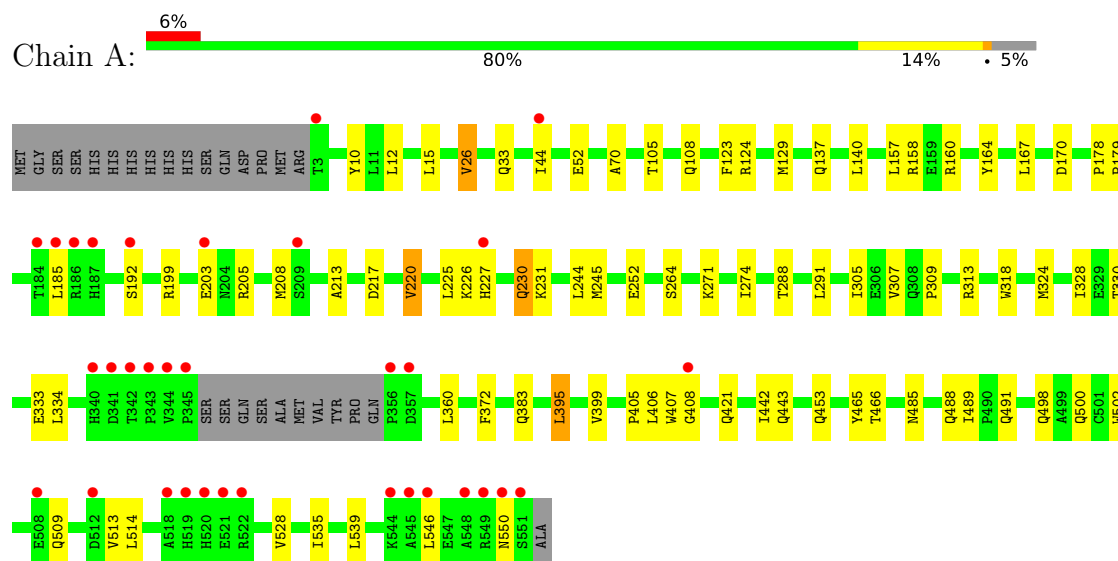
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total 173	O 173	0	0
4	B	157	Total 157	O 157	0	0

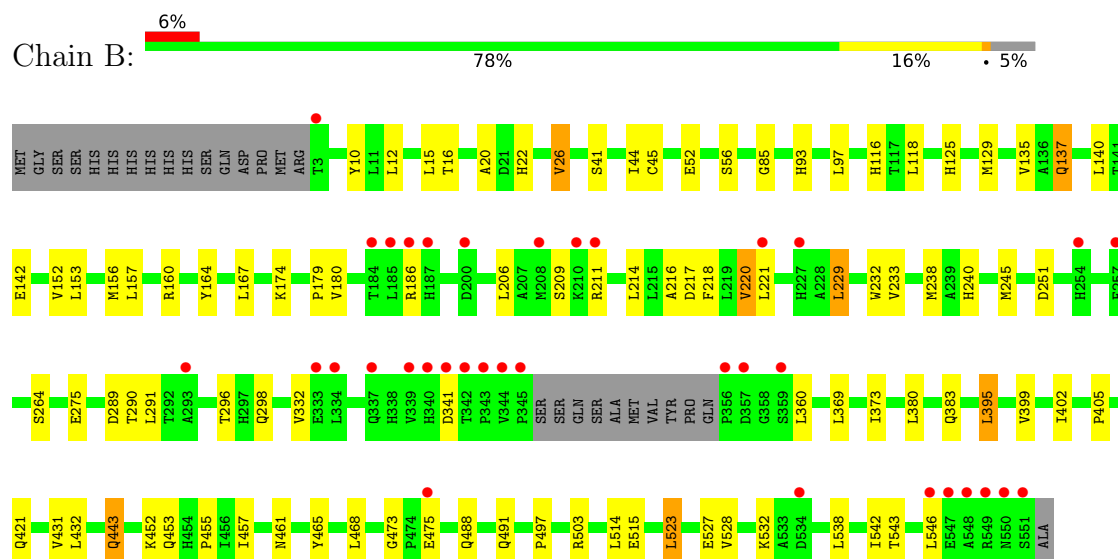
3 Residue-property plots

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 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: Indolepyruvate decarboxylase



• Molecule 1: Indolepyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.60Å 137.05Å 77.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.53 – 2.32 68.53 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (68.53-2.32) 99.6 (68.53-2.32)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.203 , 0.247 0.204 , 0.246	Depositor DCC
R_{free} test set	2733 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	1.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8662	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: TPP, 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	0.45	1/4235 (0.0%)	0.54	1/5770 (0.0%)
1	B	0.48	3/4235 (0.1%)	0.52	1/5770 (0.0%)
All	All	0.47	4/8470 (0.0%)	0.53	2/11540 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	VAL	C-O	-7.77	1.16	1.24
1	B	137	GLN	C-O	-5.76	1.16	1.23
1	A	442	ILE	C-O	-5.48	1.17	1.24
1	B	251	ASP	C-O	-5.31	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	ASP	N-CA-C	-5.95	100.14	109.25
1	A	395	LEU	N-CA-C	5.23	116.41	109.93

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	4139	0	4092	58	0
1	B	4139	0	4092	63	0
2	A	26	0	16	3	0
2	B	26	0	16	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	173	0	0	5	0
4	B	157	0	0	7	0
All	All	8662	0	8216	121	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 7.

All (121) 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:A:137:GLN:HG2	1:A:164:TYR:HB3	1.39	1.00
1:B:455:PRO:HD2	1:B:523:LEU:HD22	1.59	0.85
1:A:443:GLN:HE22	1:B:443:GLN:HE22	1.28	0.80
1:B:218:PHE:HA	1:B:221:LEU:HD12	1.66	0.78
1:A:12:LEU:HD22	1:A:44:ILE:HG21	1.69	0.75
1:B:503:ARG:NH2	4:B:705:HOH:O	2.24	0.70
1:B:383:GLN:NE2	4:B:706:HOH:O	2.24	0.69
1:B:542:ILE:O	1:B:546:LEU:HG	1.92	0.68
1:B:137:GLN:HG3	1:B:164:TYR:HB3	1.74	0.68
1:A:192:SER:N	4:A:702:HOH:O	2.22	0.67
1:A:395:LEU:HD22	1:A:399:VAL:HG11	1.76	0.66
1:A:535:ILE:HD12	1:A:539:LEU:HD23	1.79	0.65
1:A:407:TRP:O	1:B:116:HIS:HD2	1.79	0.65
1:B:369:LEU:HD11	1:B:432:LEU:HD21	1.79	0.64
2:A:601:TPP:HN42	2:A:601:TPP:C2	2.11	0.62
1:A:205:ARG:HG2	1:A:305:ILE:HD11	1.83	0.61
1:A:124:ARG:NH2	4:A:712:HOH:O	2.35	0.60
1:B:488:GLN:O	1:B:491:GLN:HG3	2.00	0.59
1:A:485:ASN:ND2	1:A:488:GLN:HG3	2.18	0.58
1:B:395:LEU:HG	1:B:399:VAL:HG11	1.86	0.58
1:A:245:MET:HG2	1:A:405:PRO:HD2	1.86	0.57
1:A:226:LYS:O	1:A:230:GLN:HG2	2.05	0.57
1:B:118:LEU:HD12	1:B:125:HIS:CD2	2.39	0.57
1:B:421:GLN:HG2	1:B:453:GLN:HB3	1.86	0.57
1:B:232:TRP:O	1:B:232:TRP:HD1	1.88	0.56
1:B:532:LYS:NZ	4:B:718:HOH:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:HG12	1:A:324:MET:HG3	1.88	0.56
1:B:12:LEU:O	1:B:16:THR:HG23	2.06	0.55
1:B:380:LEU:HG	1:B:402:ILE:HB	1.89	0.54
1:B:455:PRO:CD	1:B:523:LEU:HD22	2.33	0.54
1:B:97:LEU:HD22	1:B:153:LEU:HD21	1.89	0.54
1:A:158:ARG:HD2	4:A:792:HOH:O	2.07	0.54
1:B:245:MET:HG3	1:B:405:PRO:HG2	1.90	0.54
1:A:309:PRO:HA	1:A:324:MET:HE2	1.91	0.53
1:B:56:SER:OG	1:B:85:GLY:HA3	2.09	0.53
1:B:452:LYS:NZ	4:B:721:HOH:O	2.42	0.53
1:B:142:GLU:HG3	1:B:174:LYS:HG3	1.90	0.53
1:A:15:LEU:HD11	1:A:70:ALA:HB2	1.91	0.52
1:B:473:GLY:HA2	1:B:475:GLU:OE2	2.08	0.52
1:A:466:THR:HG22	1:A:535:ILE:HD11	1.91	0.52
1:A:421:GLN:HG2	1:A:453:GLN:HB3	1.91	0.52
1:B:245:MET:HE3	1:B:291:LEU:HD11	1.91	0.51
1:A:26:VAL:HG13	1:A:52:GLU:HG3	1.92	0.51
1:A:244:LEU:HB3	1:A:291:LEU:HD22	1.92	0.51
2:B:601:TPP:HN42	2:B:601:TPP:C2	2.23	0.51
1:A:217:ASP:O	1:A:220:VAL:HG13	2.11	0.51
1:A:307:VAL:CG1	1:A:324:MET:HG3	2.42	0.50
1:A:199:ARG:NH2	1:A:333:GLU:OE1	2.44	0.50
1:A:199:ARG:O	1:A:203:GLU:HG3	2.12	0.50
1:A:217:ASP:OD2	1:A:245:MET:HB2	2.12	0.50
1:B:140:LEU:HD12	1:B:167:LEU:HD13	1.93	0.49
1:A:360:LEU:HD13	1:A:528:VAL:HG13	1.94	0.49
1:B:218:PHE:HB3	1:B:245:MET:HB3	1.95	0.49
1:A:500:GLN:HG2	1:A:502:TRP:CZ2	2.47	0.49
1:A:10:TYR:CE2	1:A:179:PRO:HG3	2.48	0.49
1:B:232:TRP:CD1	1:B:232:TRP:C	2.91	0.48
1:A:157:LEU:HD13	1:A:185:LEU:HG	1.96	0.48
1:B:157:LEU:O	1:B:160:ARG:HD3	2.14	0.47
1:A:330:THR:O	1:A:334:LEU:HG	2.13	0.47
1:A:500:GLN:HG2	1:A:502:TRP:CH2	2.49	0.47
1:A:264:SER:HA	1:A:271:LYS:HE2	1.97	0.47
1:A:383:GLN:HG3	1:A:408:GLY:HA2	1.96	0.47
1:A:491:GLN:H	1:A:491:GLN:CD	2.23	0.47
1:B:360:LEU:HD13	1:B:528:VAL:HG13	1.97	0.47
1:A:245:MET:HG2	1:A:405:PRO:CD	2.45	0.46
1:B:217:ASP:O	1:B:220:VAL:HG13	2.16	0.46
1:B:216:ALA:HB2	1:B:229:LEU:HD22	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:HA	1:A:208:MET:HE2	1.98	0.46
1:B:26:VAL:HG13	1:B:52:GLU:HG3	1.98	0.46
1:B:543:THR:HA	1:B:546:LEU:HD12	1.98	0.46
1:A:509:GLN:O	1:A:513:VAL:HG23	2.15	0.45
1:A:539:LEU:HD12	1:A:539:LEU:O	2.16	0.45
1:A:105:THR:OG1	1:A:170:ASP:OD2	2.26	0.45
2:A:601:TPP:HN42	2:A:601:TPP:H2	1.80	0.45
1:A:288:THR:HG21	1:A:406:LEU:HD13	1.98	0.45
1:A:498:GLN:HB2	4:A:766:HOH:O	2.15	0.45
1:A:313:ARG:HB2	1:A:318:TRP:CD2	2.51	0.45
1:B:15:LEU:CD2	1:B:20:ALA:HB3	2.47	0.45
1:B:41:SER:OG	1:B:44:ILE:HG22	2.16	0.45
1:B:465:TYR:CD1	2:B:601:TPP:H61	2.51	0.45
1:B:214:LEU:HD21	1:B:229:LEU:HD23	1.98	0.45
1:A:225:LEU:HD13	1:A:328:ILE:HD12	1.99	0.44
1:B:186:ARG:HA	4:B:785:HOH:O	2.17	0.44
1:B:275:GLU:HG2	1:B:298:GLN:O	2.17	0.44
1:A:535:ILE:HG23	1:A:539:LEU:HB3	2.00	0.44
1:B:491:GLN:HA	1:B:497:PRO:HG3	1.99	0.44
1:A:140:LEU:HD12	1:A:167:LEU:HD13	1.98	0.43
1:A:465:TYR:CD1	2:A:601:TPP:H61	2.53	0.43
1:B:211:ARG:HG3	1:B:341:ASP:HB2	2.00	0.43
1:B:93:HIS:HD2	4:B:710:HOH:O	2.01	0.43
1:B:232:TRP:CG	1:B:332:VAL:HG22	2.53	0.43
1:B:232:TRP:HE1	1:B:238:MET:CE	2.32	0.43
1:A:129:MET:HG2	1:B:129:MET:O	2.19	0.43
1:B:468:LEU:HD11	2:B:601:TPP:HM42	1.99	0.43
1:A:178:PRO:HA	1:A:179:PRO:HD3	1.91	0.43
1:B:22:HIS:CD2	1:B:45:CYS:HB3	2.54	0.42
1:B:373:ILE:O	4:B:702:HOH:O	2.21	0.42
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.80	0.42
1:A:227:HIS:HB3	4:A:750:HOH:O	2.19	0.42
1:A:231:LYS:HE2	1:A:231:LYS:HB3	1.83	0.42
1:B:214:LEU:O	1:B:240:HIS:HA	2.20	0.42
1:B:461:ASN:ND2	1:B:527:GLU:OE2	2.50	0.42
1:A:160:ARG:HA	1:A:160:ARG:HD3	1.75	0.42
1:A:491:GLN:CD	1:A:491:GLN:N	2.78	0.42
1:A:129:MET:O	1:B:129:MET:HG2	2.20	0.42
1:A:213:ALA:HB1	1:A:274:ILE:HD13	2.01	0.42
1:B:206:LEU:O	1:B:209:SER:OG	2.37	0.42
1:A:108:GLN:HA	1:A:123:PHE:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:HD22	1:A:550:ASN:OD1	2.21	0.41
1:B:289:ASP:OD1	1:B:290:THR:N	2.52	0.41
1:B:514:LEU:HD23	1:B:514:LEU:HA	1.92	0.41
1:A:372:PHE:CD1	1:A:514:LEU:HB3	2.56	0.41
1:B:264:SER:HB3	1:B:296:THR:HB	2.02	0.41
1:B:431:VAL:HB	1:B:457:ILE:HA	2.03	0.41
2:B:601:TPP:HN42	2:B:601:TPP:H2	1.85	0.41
1:B:10:TYR:CE2	1:B:179:PRO:HG3	2.56	0.41
1:B:152:VAL:O	1:B:156:MET:HG3	2.21	0.41
1:A:252:GLU:HG3	1:A:395:LEU:HB2	2.02	0.40
1:B:232:TRP:HE1	1:B:238:MET:HE1	1.85	0.40
1:B:160:ARG:HA	1:B:160:ARG:HD2	1.78	0.40
1:B:232:TRP:NE1	1:B:238:MET:CE	2.85	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	535/566 (94%)	525 (98%)	10 (2%)	0	100	100
1	B	535/566 (94%)	523 (98%)	12 (2%)	0	100	100
All	All	1070/1132 (94%)	1048 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	434/458 (95%)	429 (99%)	5 (1%)	67	80
1	B	434/458 (95%)	424 (98%)	10 (2%)	45	62
All	All	868/916 (95%)	853 (98%)	15 (2%)	56	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	33	GLN
1	A	220	VAL
1	A	230	GLN
1	A	489	ILE
1	B	26	VAL
1	B	180	VAL
1	B	220	VAL
1	B	229	LEU
1	B	233	VAL
1	B	395	LEU
1	B	443	GLN
1	B	515	GLU
1	B	523	LEU
1	B	538	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	254	HIS
1	A	298	GLN
1	A	338	HIS
1	A	383	GLN
1	A	421	GLN
1	A	443	GLN
1	B	93	HIS
1	B	116	HIS
1	B	137	GLN
1	B	337	GLN
1	B	338	HIS
1	B	421	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TPP	A	601	3	22,27,27	0.49	0	29,40,40	0.73	1 (3%)
2	TPP	B	601	3	22,27,27	0.49	0	29,40,40	0.75	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
2	TPP	A	601	3	-	5/16/17/17	0/2/2/2
2	TPP	B	601	3	-	6/16/17/17	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	TPP	C5-C4-N3	2.06	111.68	107.57

There are no chirality outliers.

All (11) torsion outliers are listed below:

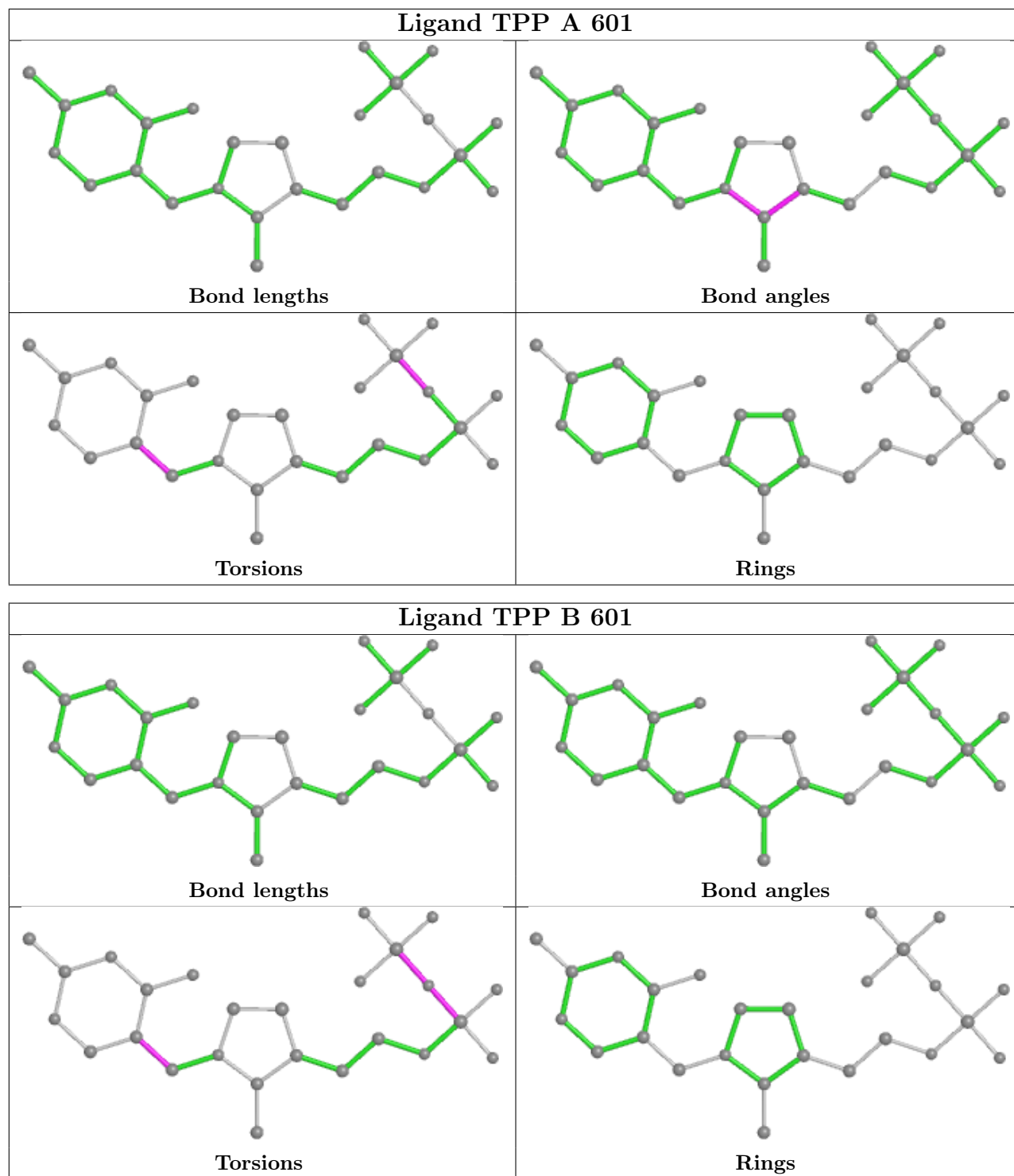
Mol	Chain	Res	Type	Atoms
2	A	601	TPP	C4'-C5'-C7'-N3
2	B	601	TPP	C4'-C5'-C7'-N3
2	B	601	TPP	PA-O3A-PB-O1B
2	A	601	TPP	PA-O3A-PB-O3B
2	B	601	TPP	PB-O3A-PA-O1A
2	A	601	TPP	PA-O3A-PB-O1B
2	B	601	TPP	PB-O3A-PA-O2A
2	A	601	TPP	PA-O3A-PB-O2B
2	B	601	TPP	PA-O3A-PB-O2B
2	B	601	TPP	PA-O3A-PB-O3B
2	A	601	TPP	C6'-C5'-C7'-N3

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TPP	3	0
2	B	601	TPP	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.



5.7 Other polymers [\(i\)](#)

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	539/566 (95%)	0.40	33 (6%) 28 31	23, 36, 61, 112	0
1	B	539/566 (95%)	0.50	35 (6%) 26 29	22, 38, 70, 126	0
All	All	1078/1132 (95%)	0.45	68 (6%) 27 30	22, 37, 69, 126	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	VAL	8.3
1	B	185	LEU	8.0
1	B	344	VAL	7.7
1	B	345	PRO	7.0
1	A	345	PRO	6.8
1	B	548	ALA	6.0
1	B	356	PRO	5.9
1	B	546	LEU	5.6
1	A	356	PRO	5.3
1	A	185	LEU	4.9
1	B	357	ASP	4.9
1	A	357	ASP	4.8
1	A	548	ALA	4.7
1	B	340	HIS	4.4
1	B	187	HIS	4.4
1	B	551	SER	4.2
1	B	550	ASN	4.2
1	B	549	ARG	4.2
1	B	343	PRO	4.1
1	A	342	THR	3.9
1	A	187	HIS	3.8
1	B	3	THR	3.7
1	B	342	THR	3.6
1	B	341	ASP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	343	PRO	3.5
1	A	549	ARG	3.5
1	A	550	ASN	3.4
1	A	341	ASP	3.4
1	A	512	ASP	3.4
1	A	3	THR	3.3
1	A	186	ARG	3.3
1	A	340	HIS	3.2
1	A	203	GLU	3.2
1	B	184	THR	3.2
1	A	551	SER	3.2
1	A	519	HIS	3.1
1	B	208	MET	3.0
1	A	508	GLU	3.0
1	A	546	LEU	3.0
1	A	521	GLU	2.9
1	B	547	GLU	2.9
1	B	254	HIS	2.7
1	A	184	THR	2.7
1	A	522	ARG	2.7
1	B	186	ARG	2.7
1	B	210	LYS	2.7
1	A	44	ILE	2.7
1	A	545	ALA	2.7
1	A	518	ALA	2.6
1	A	209	SER	2.6
1	B	211	ARG	2.6
1	B	339	VAL	2.5
1	B	359	SER	2.3
1	B	293	ALA	2.3
1	B	200	ASP	2.3
1	B	227	HIS	2.3
1	A	408	GLY	2.2
1	B	475	GLU	2.2
1	B	337	GLN	2.2
1	A	227	HIS	2.1
1	A	192	SER	2.1
1	B	333	GLU	2.1
1	B	534	ASP	2.1
1	A	520	HIS	2.0
1	B	334	LEU	2.0
1	B	257	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	544	LYS	2.0
1	B	221	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

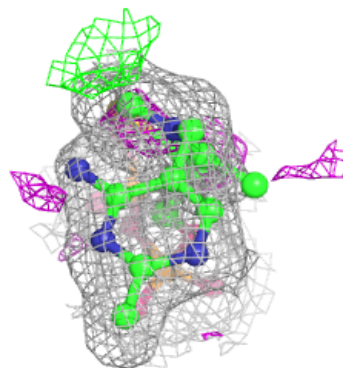
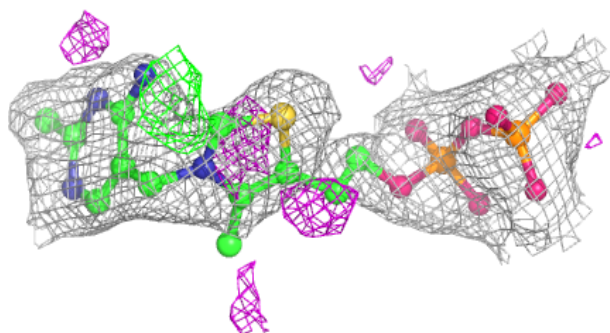
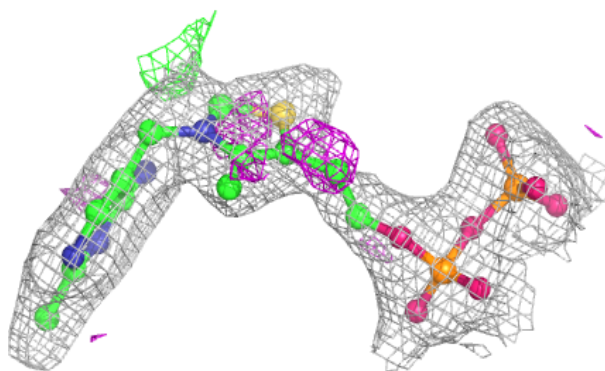
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TPP	A	601	26/26	0.95	0.10	15,29,41,48	0
2	TPP	B	601	26/26	0.96	0.09	23,30,40,54	0
3	MG	A	602	1/1	0.99	0.03	26,26,26,26	0
3	MG	B	602	1/1	1.00	0.05	26,26,26,26	0

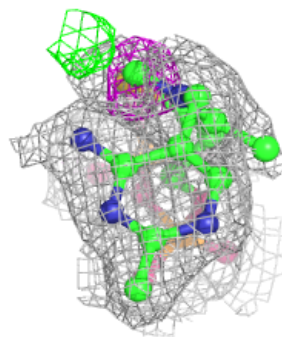
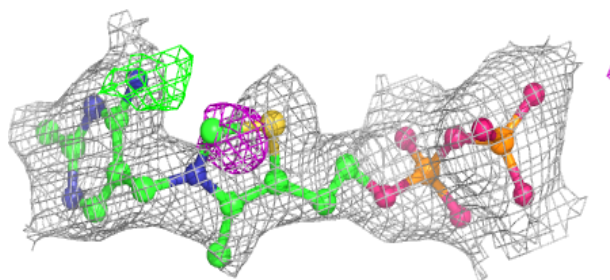
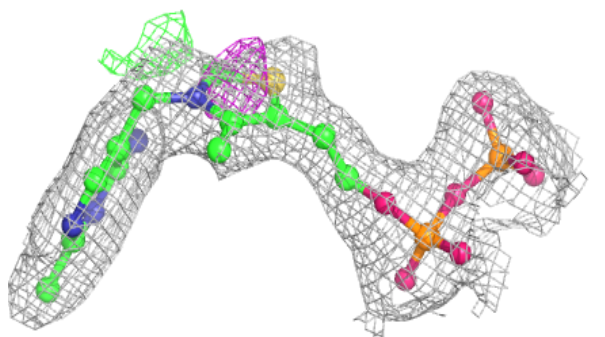
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 601:

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

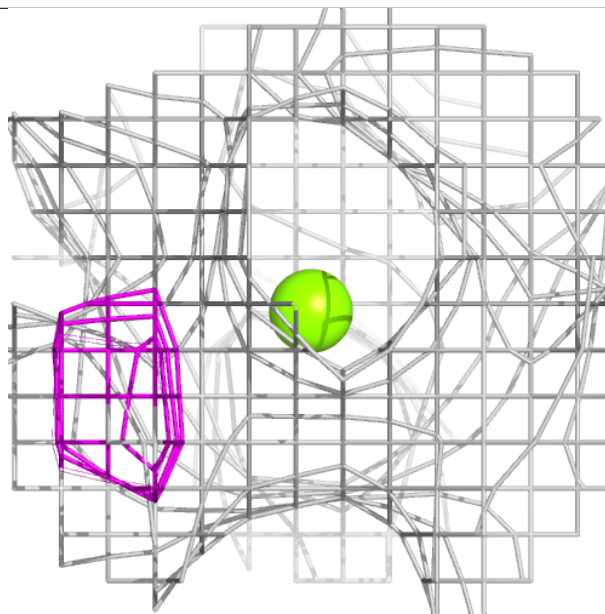
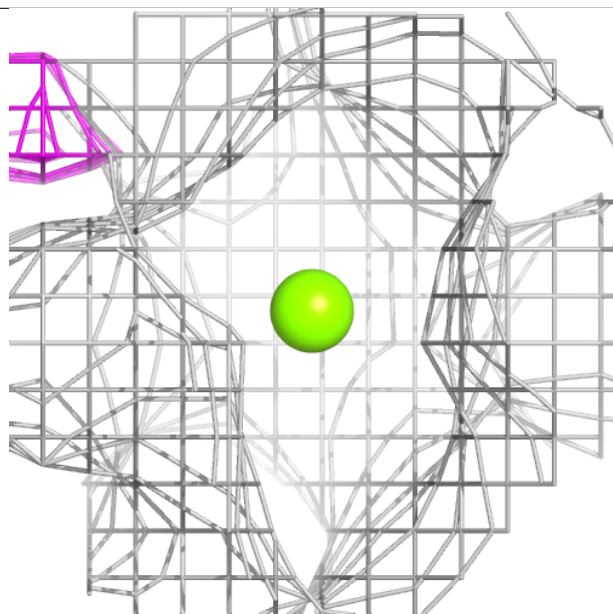
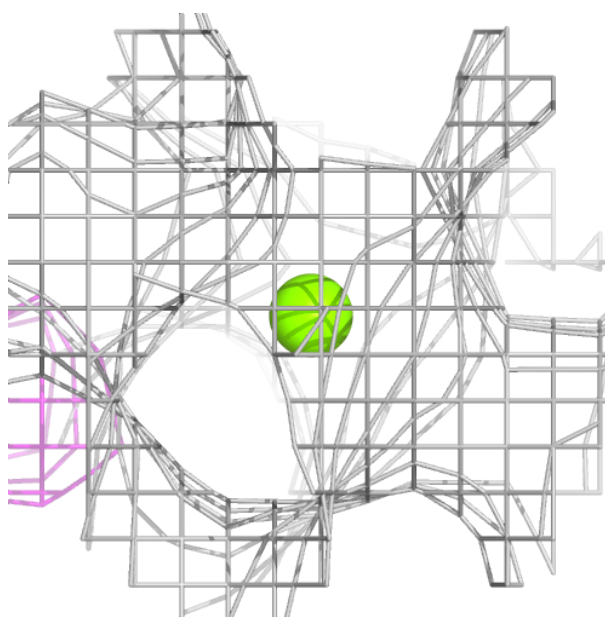
**Electron density around TPP B 601:**

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



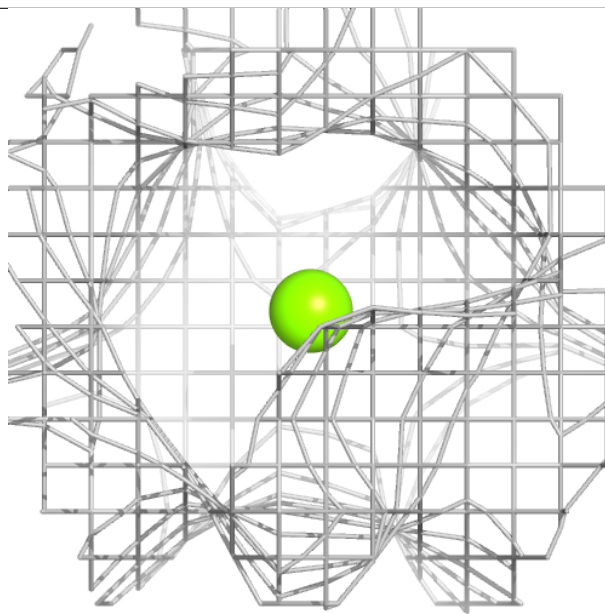
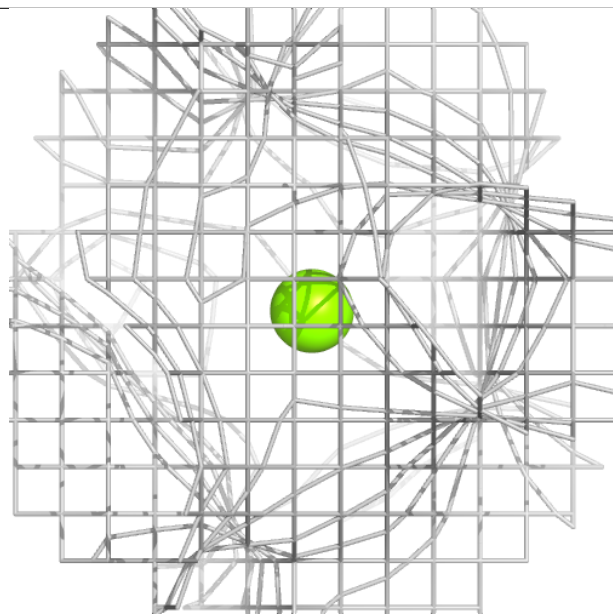
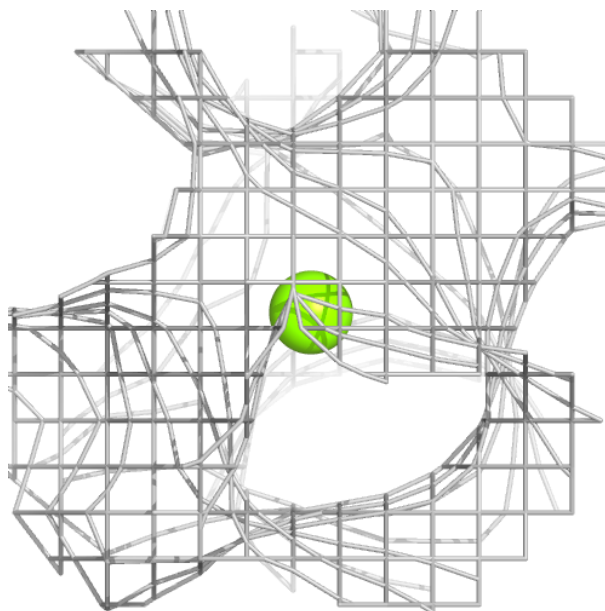
Electron density around MG A 602:

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



Electron density around MG B 602:

$2mF_o-DF_c$ (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.