



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 08:10 PM JST

PDB ID : 8ZK9 / pdb\_00008zk9  
Title : Crystal structure of the Decarboxylase KDC4427 mutant E468L in complex with phenylpyruvic acid  
Authors : Dong, S.; Liu, L.; Zhang, H.  
Deposited on : 2024-05-15  
Resolution : 2.03 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](mailto: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>.

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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

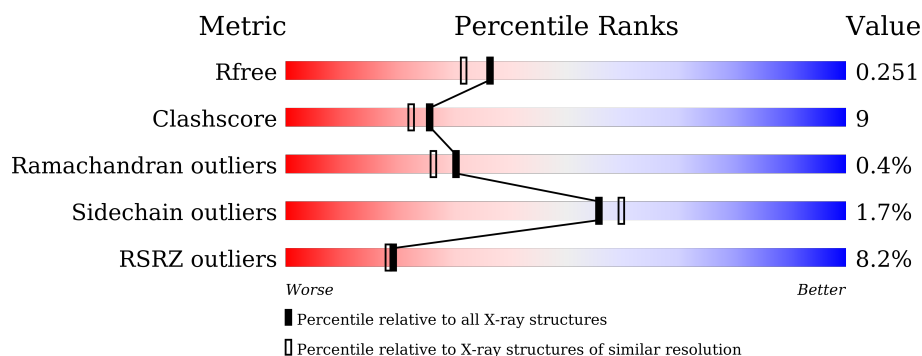
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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  $\geq 3$ , 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	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div> </div>
1	B	566	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TPP	A	601	-	-	X	-
2	TPP	B	601	-	-	X	-
4	PPY	A	603	-	-	X	-
4	PPY	B	603	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8696 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	536	Total	C	N	O	S	0	0	0
			4108	2609	715	762	22			
1	B	536	Total	C	N	O	S	0	0	0
			4108	2606	718	762	22			

There are 30 discrepancies between the modelled and reference sequences:

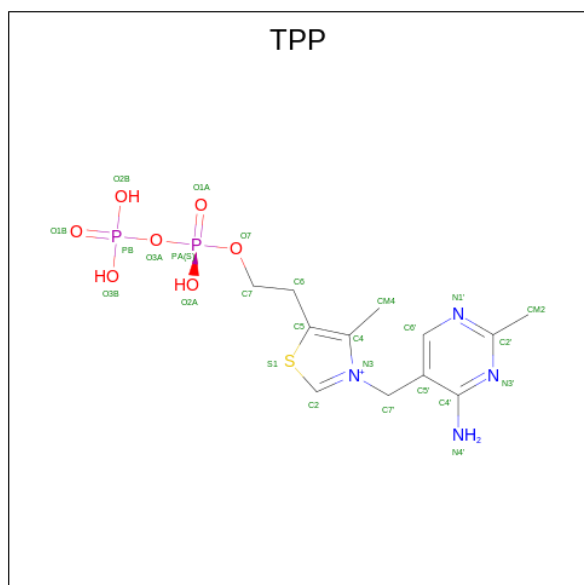
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A2U3EYQ2
A	-12	GLY	-	expression tag	UNP A0A2U3EYQ2
A	-11	SER	-	expression tag	UNP A0A2U3EYQ2
A	-10	SER	-	expression tag	UNP A0A2U3EYQ2
A	-9	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-8	HIS	-	expression tag	UNP A0A2U3EYQ2
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

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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).

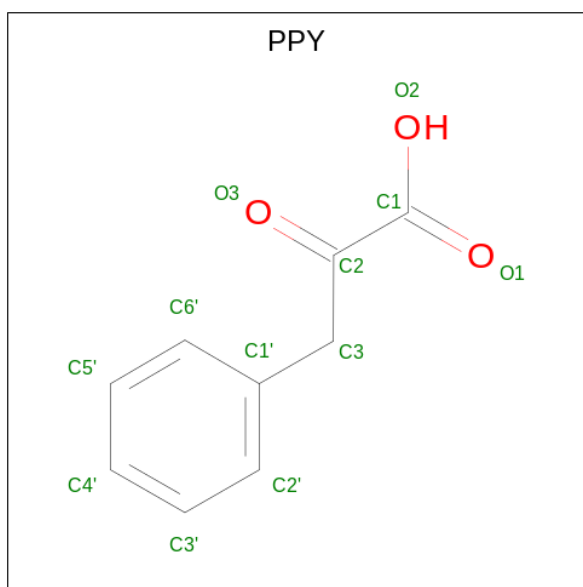


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- 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 3-PHENYLPYRUVIC ACID (CCD ID: PPY) (formula:  $C_9H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	9	3		
4	B	1	Total	C	O	0	0
			12	9	3		

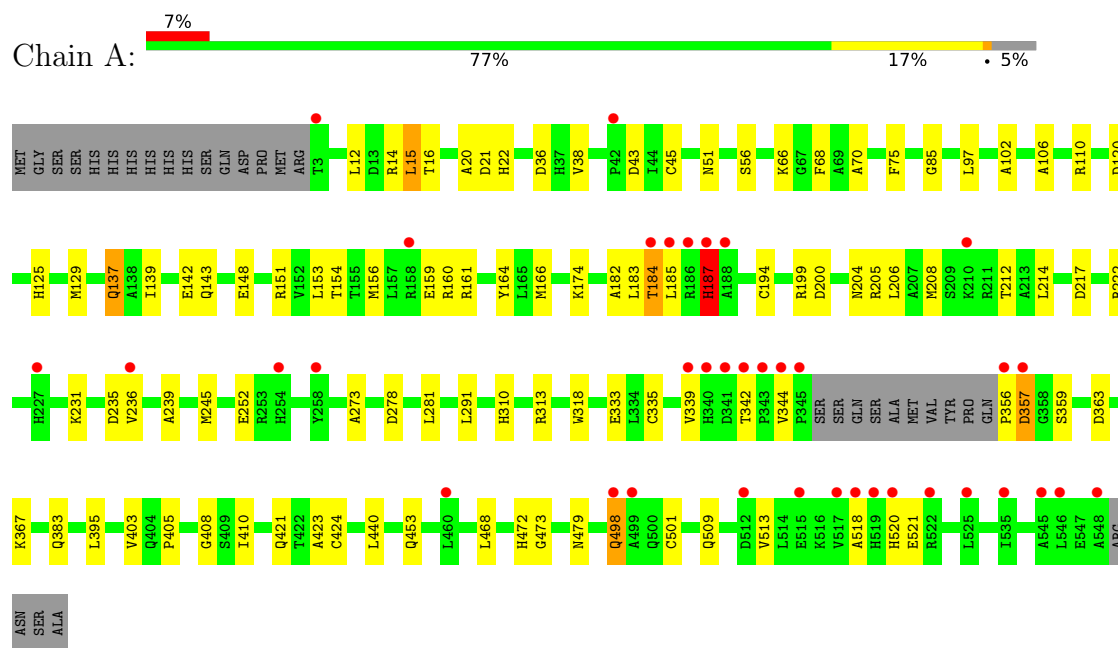
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total	O	0	0
			213	213		
5	B	189	Total	O	0	0
			189	189		

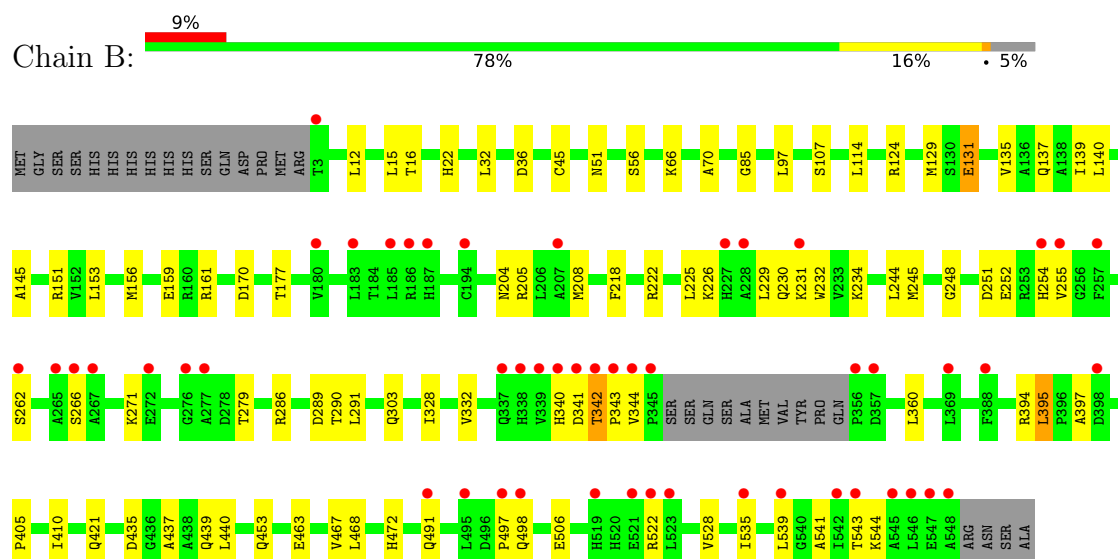
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	115.92Å 136.52Å 77.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.27 – 2.03 64.27 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.8 (64.27-2.03) 98.3 (64.27-2.03)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.220 , 0.254 0.219 , 0.251	Depositor DCC
$R_{free}$ test set	3948 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	1.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PPY, MG, TPP

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	0.42	1/4204 (0.0%)	0.47	2/5730 (0.0%)
1	B	0.46	1/4202 (0.0%)	0.51	4/5724 (0.1%)
All	All	0.44	2/8406 (0.0%)	0.49	6/11454 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	GLU	C-O	-6.38	1.18	1.24
1	A	200	ASP	CA-C	-5.02	1.46	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	HIS	N-CA-C	8.42	121.19	110.24
1	B	342	THR	CA-C-N	6.73	128.25	119.84
1	B	342	THR	C-N-CA	6.73	128.25	119.84
1	B	234	LYS	N-CA-C	-5.61	104.56	111.40
1	B	395	LEU	N-CA-C	5.12	116.33	109.83
1	A	501	CYS	N-CA-C	5.11	117.57	109.50

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	4108	0	4057	67	0
1	B	4108	0	4049	65	0
2	A	26	0	16	15	0
2	B	26	0	16	20	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	7	12	0
4	B	12	0	7	13	0
5	A	213	0	0	4	0
5	B	189	0	0	8	0
All	All	8696	0	8152	155	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 (155) 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)
4:A:603:PPY:C2	2:B:601:TPP:H2	1.34	1.53
2:A:601:TPP:H2	4:B:603:PPY:C2	1.31	1.52
4:A:603:PPY:C2	2:B:601:TPP:C2	2.10	1.28
2:A:601:TPP:C2	4:B:603:PPY:C2	2.14	1.26
4:A:603:PPY:O3	2:B:601:TPP:H2	1.38	1.24
2:A:601:TPP:H2	4:B:603:PPY:O3	1.46	1.15
4:A:603:PPY:C3	2:B:601:TPP:C2	2.24	1.14
2:A:601:TPP:C2	4:B:603:PPY:C3	2.29	1.09
2:A:601:TPP:H2	4:B:603:PPY:C3	1.83	1.07
4:A:603:PPY:H31	2:B:601:TPP:S1	1.94	1.06
4:A:603:PPY:C3	2:B:601:TPP:H2	1.89	1.01
4:A:603:PPY:C3	2:B:601:TPP:S1	2.51	0.98
2:A:601:TPP:S1	4:B:603:PPY:H31	2.05	0.95
1:A:187:HIS:H	1:A:187:HIS:CD2	1.93	0.87
2:A:601:TPP:S1	4:B:603:PPY:C3	2.63	0.87
1:B:266:SER:HB2	1:B:271:LYS:HG3	1.61	0.82
4:A:603:PPY:H31	2:B:601:TPP:C2	2.04	0.82
2:A:601:TPP:C2	4:B:603:PPY:H31	2.09	0.79
1:A:15:LEU:HD21	1:A:70:ALA:HB2	1.67	0.76
1:A:137:GLN:HB3	1:A:164:TYR:HB3	1.70	0.74
4:A:603:PPY:H32	2:B:601:TPP:S1	2.31	0.70
1:A:154:THR:CG2	1:A:185:LEU:HG	2.20	0.70
2:B:601:TPP:H2	2:B:601:TPP:HN42	1.56	0.70
1:B:177:THR:HG23	5:B:859:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LYS:HE3	1:B:248:GLY:O	1.92	0.68
1:A:521:GLU:OE1	1:A:521:GLU:N	2.20	0.67
1:A:245:MET:HG3	1:A:291:LEU:HD11	1.77	0.67
2:B:601:TPP:C2	2:B:601:TPP:HN42	2.07	0.66
1:A:154:THR:HG21	1:A:185:LEU:HG	1.77	0.66
1:A:194:CYS:SG	5:A:885:HOH:O	2.55	0.64
1:B:225:LEU:HD23	1:B:328:ILE:CD1	2.27	0.64
1:B:205:ARG:NH1	1:B:279:THR:OG1	2.29	0.64
1:B:245:MET:HE3	1:B:291:LEU:HD11	1.80	0.62
1:B:245:MET:HG3	1:B:405:PRO:HD2	1.81	0.62
1:A:21:ASP:OD2	1:A:66:LYS:NZ	2.32	0.62
1:B:328:ILE:O	1:B:332:VAL:HG23	2.00	0.62
1:A:245:MET:HG2	1:A:405:PRO:HD2	1.83	0.60
2:A:601:TPP:S1	4:B:603:PPY:H32	2.42	0.59
4:A:603:PPY:O3	2:B:601:TPP:N4'	2.34	0.59
4:A:603:PPY:H32	2:B:601:TPP:C2	2.28	0.58
1:B:225:LEU:HD23	1:B:328:ILE:HD12	1.85	0.57
1:A:143:GLN:HG3	5:A:882:HOH:O	2.05	0.57
1:B:467:VAL:CG1	2:B:601:TPP:H62	2.35	0.57
1:B:491:GLN:HA	1:B:497:PRO:HG3	1.87	0.57
1:B:15:LEU:HD11	1:B:70:ALA:HB2	1.87	0.56
1:A:106:ALA:O	1:A:110:ARG:HG3	2.05	0.56
1:A:182:ALA:O	1:A:184:THR:HG22	2.06	0.56
1:A:383:GLN:HG3	1:A:408:GLY:HA2	1.86	0.56
2:A:601:TPP:C2	4:B:603:PPY:H32	2.34	0.56
1:A:159:GLU:OE2	1:A:310:HIS:NE2	2.38	0.56
1:A:214:LEU:HD12	1:A:281:LEU:HB2	1.88	0.56
1:B:12:LEU:O	1:B:16:THR:HG23	2.06	0.56
1:B:506:GLU:HB3	5:B:820:HOH:O	2.06	0.55
1:A:156:MET:HG2	1:A:161:ARG:O	2.07	0.55
1:A:139:ILE:HG12	1:A:166:MET:HE3	1.89	0.55
1:B:244:LEU:HB3	1:B:291:LEU:HD22	1.88	0.54
2:A:601:TPP:H2	4:B:603:PPY:H31	1.77	0.54
1:B:135:VAL:HG21	1:B:159:GLU:HG3	1.90	0.53
1:A:498:GLN:H	1:A:498:GLN:CD	2.18	0.51
1:B:97:LEU:HD22	1:B:153:LEU:HD21	1.91	0.51
1:A:154:THR:HG23	1:A:185:LEU:HG	1.93	0.51
1:B:232:TRP:O	1:B:232:TRP:HD1	1.93	0.51
1:B:467:VAL:HG12	2:B:601:TPP:H62	1.93	0.51
1:A:509:GLN:O	1:A:513:VAL:HG23	2.11	0.50
1:A:199:ARG:NH1	1:A:333:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HB2	1:A:318:TRP:CD2	2.47	0.49
1:A:97:LEU:HD22	1:A:153:LEU:HD21	1.94	0.49
1:A:468:LEU:HD22	1:B:32:LEU:HD11	1.93	0.49
1:B:66:LYS:NZ	5:B:710:HOH:O	2.30	0.49
1:B:226:LYS:CE	1:B:248:GLY:O	2.61	0.49
1:B:124:ARG:HE	1:B:139:ILE:HD13	1.78	0.49
1:A:217:ASP:OD2	1:A:245:MET:HB2	2.12	0.49
1:B:159:GLU:O	5:B:701:HOH:O	2.20	0.49
1:A:120:ASP:OD2	1:A:125:HIS:HE1	1.95	0.49
1:A:421:GLN:HG2	1:A:453:GLN:HB3	1.95	0.49
1:B:140:LEU:HD22	1:B:145:ALA:HA	1.95	0.49
1:B:22:HIS:CD2	1:B:45:CYS:HB3	2.48	0.48
1:A:142:GLU:CD	1:A:174:LYS:HE2	2.37	0.48
1:A:204:ASN:O	1:A:208:MET:HG2	2.12	0.48
1:B:468:LEU:HD11	2:B:601:TPP:CM4	2.43	0.48
1:A:239:ALA:HB1	1:A:273:ALA:HB1	1.96	0.48
4:A:603:PPY:C1	2:B:601:TPP:H7'2	2.44	0.48
1:A:222:ARG:HD3	5:A:879:HOH:O	2.13	0.48
1:A:16:THR:HG21	1:A:43:ASP:HB2	1.96	0.48
2:A:601:TPP:C2	2:A:601:TPP:HN42	2.27	0.47
1:A:356:PRO:O	1:A:357:ASP:HB3	2.14	0.47
1:A:403:VAL:HG13	1:A:405:PRO:HD3	1.96	0.47
1:A:212:THR:HB	1:A:339:VAL:HG21	1.97	0.47
1:A:231:LYS:NZ	1:A:235:ASP:OD2	2.48	0.47
1:B:226:LYS:HE2	1:B:230:GLN:NE2	2.30	0.47
1:A:424:CYS:SG	5:A:892:HOH:O	2.61	0.46
1:A:472:HIS:NE2	1:B:36:ASP:OD2	2.27	0.46
1:B:435:ASP:N	1:B:435:ASP:OD1	2.48	0.46
1:B:56:SER:OG	1:B:85:GLY:HA3	2.15	0.46
1:A:252:GLU:HG3	1:A:395:LEU:HB2	1.98	0.46
2:B:601:TPP:C2	2:B:601:TPP:N4'	2.77	0.46
1:A:363:ASP:OD1	1:A:367:LYS:HE2	2.15	0.46
1:B:245:MET:HG3	1:B:405:PRO:CD	2.46	0.46
1:B:535:ILE:CG1	1:B:539:LEU:HD22	2.46	0.46
1:A:159:GLU:CD	1:A:310:HIS:HE2	2.24	0.46
1:A:236:VAL:HG11	1:A:335:CYS:HB3	1.98	0.46
1:A:335:CYS:O	1:A:339:VAL:HG12	2.15	0.46
1:A:187:HIS:CD2	1:A:187:HIS:N	2.72	0.46
1:B:360:LEU:HD13	1:B:528:VAL:HG13	1.96	0.46
1:B:410:ILE:HD12	1:B:437:ALA:HA	1.98	0.46
1:B:232:TRP:CD1	1:B:232:TRP:C	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HD2	1:B:208:MET:HE3	1.97	0.45
1:B:463:GLU:OE2	5:B:702:HOH:O	2.21	0.45
1:B:498:GLN:HB3	1:B:522:ARG:HD2	1.99	0.45
1:A:15:LEU:HD22	1:A:20:ALA:HB3	1.98	0.45
1:A:498:GLN:H	1:A:498:GLN:NE2	2.14	0.45
1:A:75:PHE:HB2	1:A:102:ALA:HA	1.99	0.45
1:A:440:LEU:HG	1:B:51:ASN:HB3	1.98	0.44
1:A:520:HIS:CD2	1:A:520:HIS:O	2.70	0.44
1:B:204:ASN:O	1:B:208:MET:HE2	2.17	0.44
1:B:421:GLN:HG2	1:B:453:GLN:HB3	2.00	0.44
1:B:539:LEU:HD23	1:B:543:THR:HG23	2.00	0.44
1:B:498:GLN:O	1:B:522:ARG:HD3	2.16	0.44
1:A:473:GLY:O	1:A:479:ASN:ND2	2.50	0.44
1:B:252:GLU:HG3	1:B:395:LEU:HB2	1.99	0.44
1:B:435:ASP:O	1:B:439:GLN:HG3	2.18	0.44
1:A:160:ARG:HD2	1:A:222:ARG:O	2.17	0.43
2:A:601:TPP:H7'2	4:B:603:PPY:C1	2.48	0.43
1:B:232:TRP:O	1:B:232:TRP:CD1	2.70	0.43
1:B:251:ASP:N	5:B:714:HOH:O	2.32	0.43
1:A:12:LEU:HD21	1:A:38:VAL:HG22	2.00	0.43
1:A:148:GLU:OE2	1:A:151:ARG:NE	2.47	0.43
1:B:170:ASP:O	5:B:703:HOH:O	2.22	0.43
1:B:218:PHE:O	1:B:222:ARG:HG2	2.18	0.43
1:B:440:LEU:CD2	2:B:601:TPP:HM23	2.49	0.43
1:A:51:ASN:HB3	1:B:440:LEU:HG	2.00	0.43
1:A:231:LYS:NZ	1:A:235:ASP:OD1	2.49	0.43
1:B:107:SER:HB3	1:B:114:LEU:HD11	2.00	0.43
1:B:289:ASP:OD1	1:B:290:THR:N	2.52	0.43
1:B:151:ARG:NH1	5:B:721:HOH:O	2.39	0.42
1:A:206:LEU:HD21	1:A:281:LEU:HD21	2.00	0.42
1:B:131:GLU:HA	1:B:137:GLN:NE2	2.34	0.42
1:B:254:HIS:CD2	1:B:255:VAL:O	2.73	0.42
1:A:36:ASP:OD2	1:B:472:HIS:NE2	2.38	0.42
1:A:245:MET:HG2	1:A:405:PRO:CD	2.49	0.41
1:A:15:LEU:HD23	1:A:68:PHE:HE2	1.85	0.41
1:A:56:SER:OG	1:A:85:GLY:HA3	2.20	0.41
1:A:205:ARG:NH2	1:A:278:ASP:O	2.53	0.41
1:A:22:HIS:CD2	1:A:45:CYS:HB3	2.56	0.41
1:A:14:ARG:HD2	1:A:183:LEU:HB2	2.03	0.41
2:A:601:TPP:C2	4:B:603:PPY:C1	2.93	0.41
1:B:279:THR:HA	1:B:303:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:ALA:HA	1:B:544:LYS:HG2	2.02	0.41
1:A:129:MET:HG2	1:B:129:MET:O	2.21	0.41
1:B:156:MET:HG2	1:B:161:ARG:O	2.21	0.41
1:B:286:ARG:HD3	1:B:286:ARG:HA	1.87	0.41
1:B:251:ASP:OD2	1:B:397:ALA:HB2	2.21	0.41
1:A:410:ILE:HG12	2:A:601:TPP:C4'	2.51	0.40
1:A:66:LYS:HG3	1:A:423:ALA:HB1	2.04	0.40
1:B:467:VAL:HG12	2:B:601:TPP:O2B	2.21	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	532/566 (94%)	519 (98%)	11 (2%)	2 (0%)	30	26
1	B	532/566 (94%)	522 (98%)	8 (2%)	2 (0%)	30	26
All	All	1064/1132 (94%)	1041 (98%)	19 (2%)	4 (0%)	30	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	ASP
1	B	343	PRO
1	B	344	VAL
1	A	518	ALA

### 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	430/458 (94%)	422 (98%)	8 (2%)	52	55
1	B	428/458 (93%)	421 (98%)	7 (2%)	58	62
All	All	858/916 (94%)	843 (98%)	15 (2%)	56	60

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

Mol	Chain	Res	Type
1	A	15	LEU
1	A	137	GLN
1	A	184	THR
1	A	187	HIS
1	A	342	THR
1	A	344	VAL
1	A	359	SER
1	A	498	GLN
1	B	229	LEU
1	B	231	LYS
1	B	262	SER
1	B	340	HIS
1	B	341	ASP
1	B	342	THR
1	B	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	137	GLN
1	A	187	HIS
1	A	204	ASN
1	A	223	HIS
1	A	254	HIS
1	A	298	GLN
1	A	498	GLN
1	A	500	GLN
1	B	33	GLN
1	B	137	GLN
1	B	181	ASN

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Mol	Chain	Res	Type
1	B	223	HIS
1	B	254	HIS
1	B	340	HIS
1	B	520	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PPY	A	603	-	12,12,12	1.66	1 (8%)	15,15,15	1.20	1 (6%)
2	TPP	B	601	3	22,27,27	1.50	2 (9%)	29,40,40	2.12	7 (24%)
4	PPY	B	603	-	12,12,12	1.66	1 (8%)	15,15,15	1.22	2 (13%)
2	TPP	A	601	3	22,27,27	2.39	8 (36%)	29,40,40	1.83	6 (20%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PPY	A	603	-	-	0/8/8/8	0/1/1/1
2	TPP	B	601	3	-	4/16/17/17	0/2/2/2
4	PPY	B	603	-	-	0/8/8/8	0/1/1/1
2	TPP	A	601	3	-	3/16/17/17	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TPP	C4-N3	-7.73	1.33	1.39
2	B	601	TPP	C4-N3	-5.36	1.35	1.39
4	A	603	PPY	C2-C1	-5.29	1.46	1.53
4	B	603	PPY	C2-C1	-5.28	1.46	1.53
2	A	601	TPP	C6-C5	-4.22	1.49	1.50
2	B	601	TPP	C5'-C4'	3.28	1.48	1.42
2	A	601	TPP	PB-O2B	-3.07	1.43	1.54
2	A	601	TPP	PB-O3B	-2.99	1.43	1.54
2	A	601	TPP	C5'-C4'	2.45	1.47	1.42
2	A	601	TPP	C4'-N3'	-2.19	1.31	1.35
2	A	601	TPP	C7'-N3	-2.18	1.44	1.48
2	A	601	TPP	PA-O2A	-2.04	1.45	1.55

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TPP	C6-C5-C4	6.96	133.02	127.43
2	A	601	TPP	C6-C5-C4	4.77	131.26	127.43
2	A	601	TPP	N4'-C4'-N3'	4.27	123.06	117.03
2	B	601	TPP	PA-O3A-PB	-3.58	120.55	132.83
2	B	601	TPP	C6'-N1'-C2'	3.58	122.05	115.96
4	A	603	PPY	C1'-C3-C2	-3.21	109.47	113.64
2	A	601	TPP	C5'-C4'-N4'	-3.20	117.64	122.19
4	B	603	PPY	C1'-C3-C2	-3.18	109.51	113.64
2	A	601	TPP	C6'-N1'-C2'	3.05	121.15	115.96
2	B	601	TPP	N4'-C4'-N3'	2.65	120.77	117.03
2	B	601	TPP	C5'-C6'-N1'	-2.63	119.43	123.82
2	B	601	TPP	C5'-C7'-N3	-2.30	109.45	113.28
2	B	601	TPP	N1'-C2'-N3'	-2.26	121.66	125.54
2	A	601	TPP	CM2-C2'-N3'	2.06	120.37	117.15
4	B	603	PPY	O1-C1-C2	-2.05	118.98	121.72
2	A	601	TPP	O3B-PB-O1B	2.01	118.53	110.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

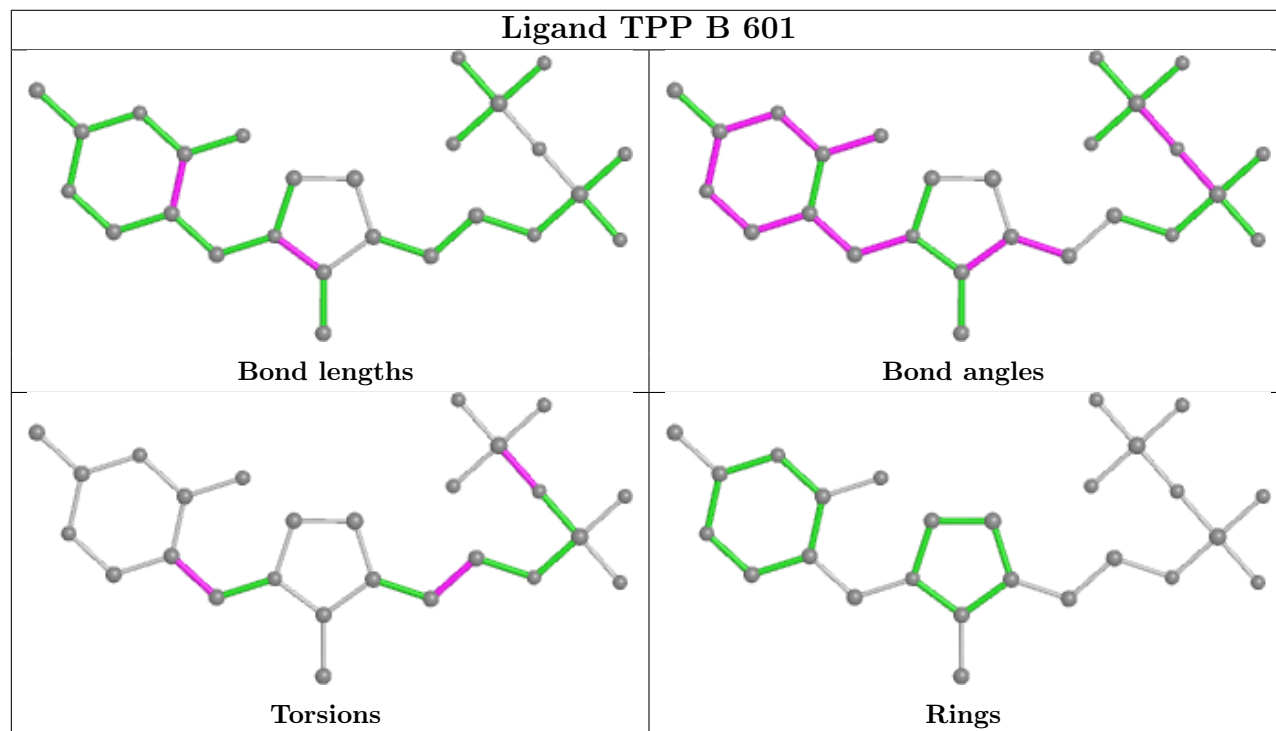
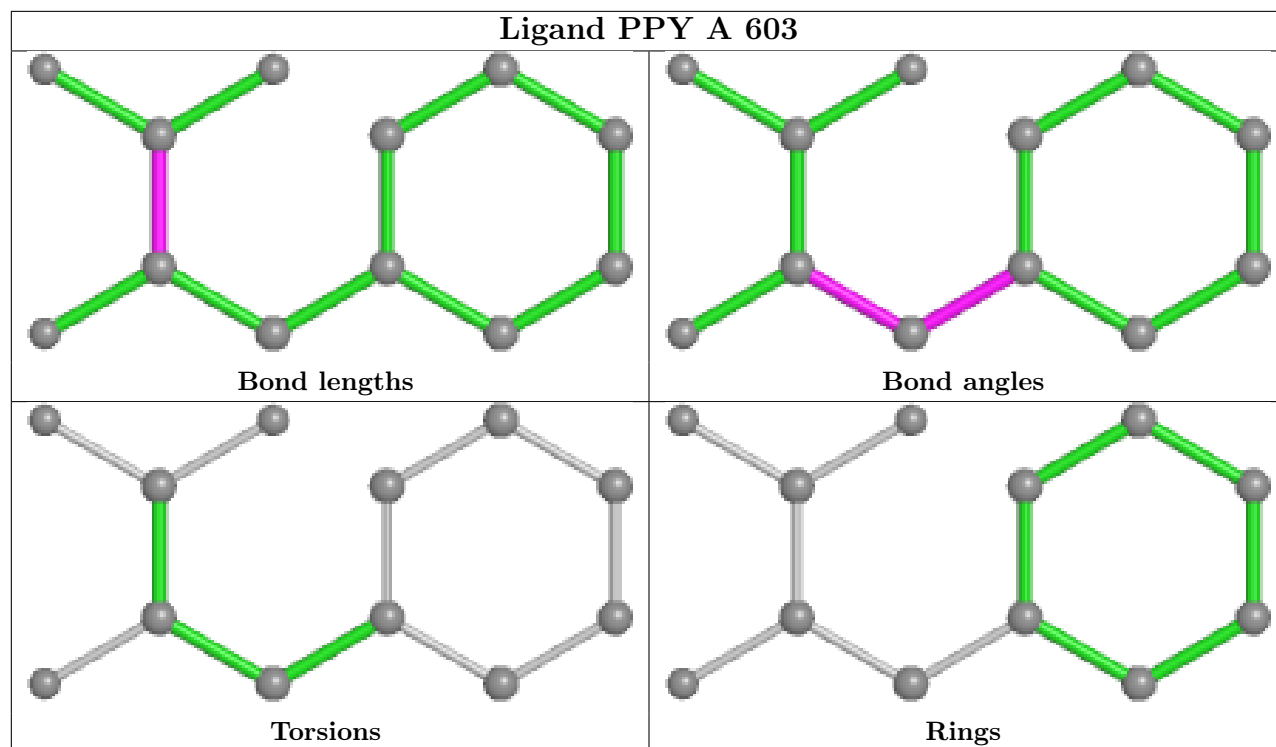
Mol	Chain	Res	Type	Atoms
2	B	601	TPP	PA-O3A-PB-O3B
2	A	601	TPP	PA-O3A-PB-O2B
2	A	601	TPP	C4'-C5'-C7'-N3
2	B	601	TPP	C4'-C5'-C7'-N3
2	B	601	TPP	PA-O3A-PB-O1B
2	B	601	TPP	C5-C6-C7-O7
2	A	601	TPP	PA-O3A-PB-O3B

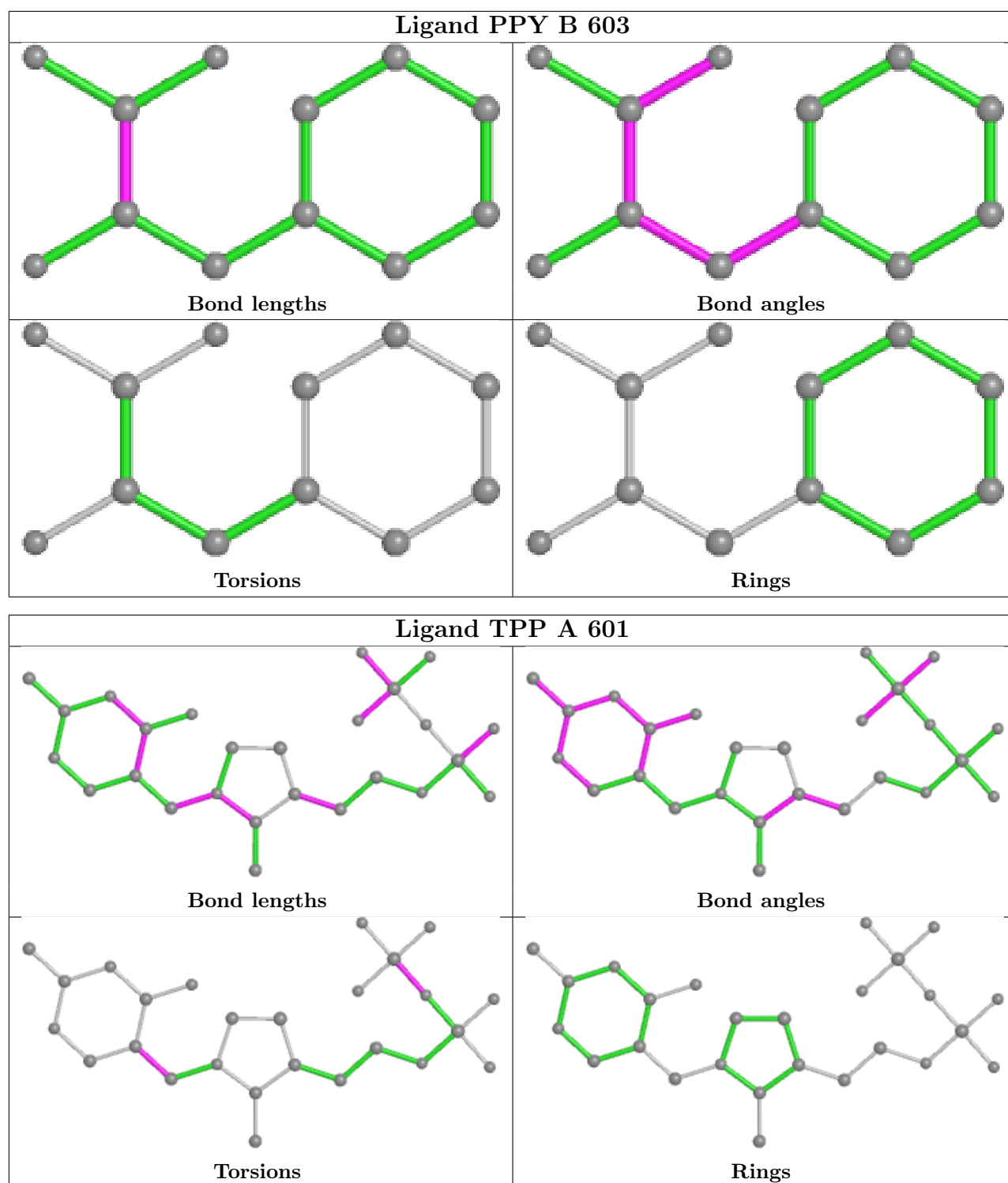
There are no ring outliers.

4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	PPY	12	0
2	B	601	TPP	20	0
4	B	603	PPY	13	0
2	A	601	TPP	15	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	536/566 (94%)	0.78	37 (6%)	24 23	26, 37, 62, 95	0
1	B	536/566 (94%)	0.85	51 (9%)	15 14	26, 39, 67, 109	0
All	All	1072/1132 (94%)	0.82	88 (8%)	19 18	26, 38, 65, 109	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	VAL	7.0
1	B	548	ALA	6.4
1	A	356	PRO	6.4
1	B	343	PRO	6.2
1	A	344	VAL	6.2
1	A	345	PRO	5.4
1	A	185	LEU	5.3
1	A	548	ALA	4.9
1	B	356	PRO	4.7
1	A	498	GLN	4.6
1	B	345	PRO	4.4
1	A	341	ASP	4.4
1	B	545	ALA	4.2
1	A	187	HIS	4.2
1	A	343	PRO	4.0
1	B	266	SER	3.8
1	B	546	LEU	3.7
1	A	357	ASP	3.6
1	A	342	THR	3.5
1	B	3	THR	3.5
1	B	342	THR	3.3
1	A	340	HIS	3.3
1	B	185	LEU	3.3
1	B	227	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	535	ILE	3.3
1	A	512	ASP	3.3
1	B	543	THR	3.3
1	B	257	PHE	3.2
1	B	542	ILE	3.2
1	A	3	THR	3.1
1	B	338	HIS	3.1
1	B	497	PRO	3.1
1	B	498	GLN	3.0
1	B	262	SER	3.0
1	B	254	HIS	3.0
1	A	519	HIS	3.0
1	B	341	ASP	2.9
1	A	186	ARG	2.9
1	B	369	LEU	2.8
1	B	339	VAL	2.7
1	B	228	ALA	2.6
1	A	545	ALA	2.5
1	B	522	ARG	2.5
1	B	521	GLU	2.5
1	A	546	LEU	2.5
1	B	276	GLY	2.5
1	B	267	ALA	2.5
1	B	337	GLN	2.5
1	A	254	HIS	2.5
1	A	520	HIS	2.5
1	B	340	HIS	2.5
1	B	277	ALA	2.5
1	B	357	ASP	2.4
1	B	207	ALA	2.4
1	A	184	THR	2.4
1	B	547	GLU	2.4
1	A	339	VAL	2.4
1	A	517	VAL	2.4
1	A	158	ARG	2.4
1	A	188	ALA	2.3
1	B	398	ASP	2.3
1	A	460	LEU	2.3
1	B	495	LEU	2.3
1	B	539	LEU	2.3
1	B	388	PHE	2.3
1	A	42	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	255	VAL	2.3
1	B	491	GLN	2.3
1	A	525	LEU	2.2
1	B	265	ALA	2.2
1	A	210	LYS	2.2
1	B	187	HIS	2.2
1	B	519	HIS	2.2
1	A	499	ALA	2.2
1	B	186	ARG	2.2
1	A	227	HIS	2.2
1	A	518	ALA	2.1
1	A	522	ARG	2.1
1	B	183	LEU	2.1
1	B	272	GLU	2.1
1	A	535	ILE	2.1
1	A	515	GLU	2.1
1	B	194	CYS	2.1
1	B	231	LYS	2.1
1	B	523	LEU	2.1
1	B	180	VAL	2.0
1	A	258	TYR	2.0
1	A	236	VAL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PPY	A	603	12/12	0.55	0.22	46,52,56,57	0

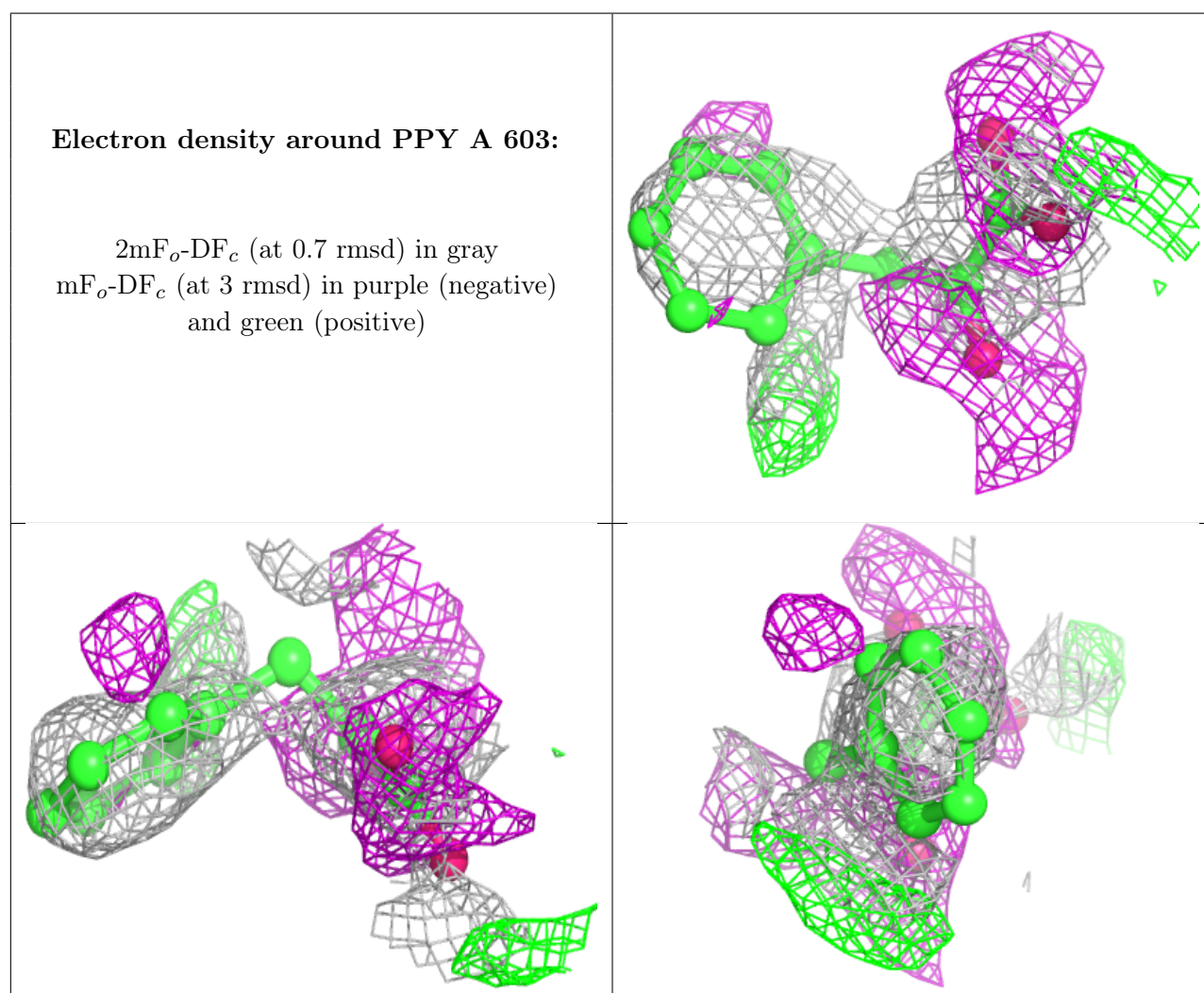
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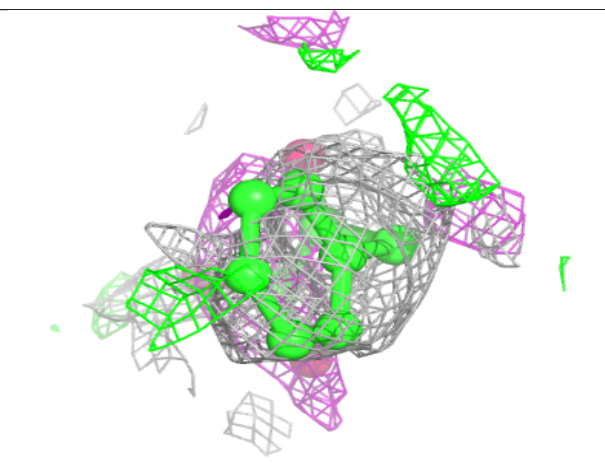
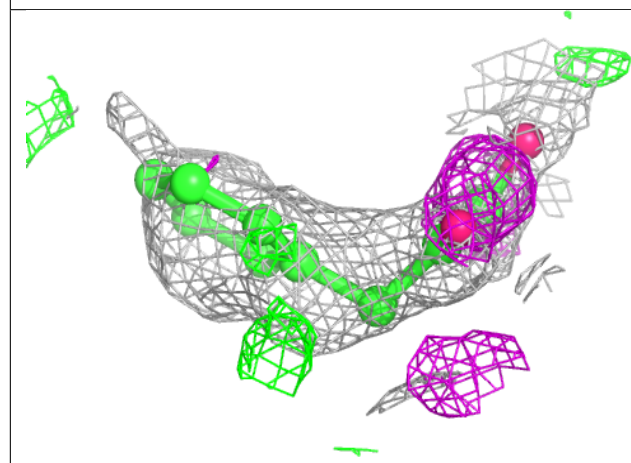
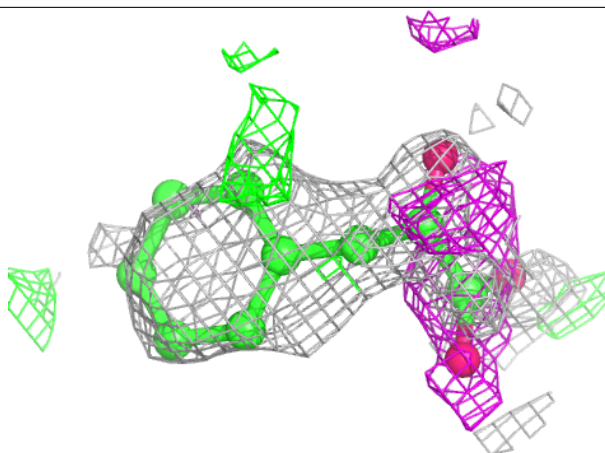
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PPY	B	603	12/12	0.62	0.23	48,55,60,61	0
2	TPP	B	601	26/26	0.87	0.15	20,31,43,58	0
2	TPP	A	601	26/26	0.95	0.08	17,28,43,55	0
3	MG	A	602	1/1	0.98	0.04	24,24,24,24	0
3	MG	B	602	1/1	0.98	0.03	26,26,26,26	0

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.

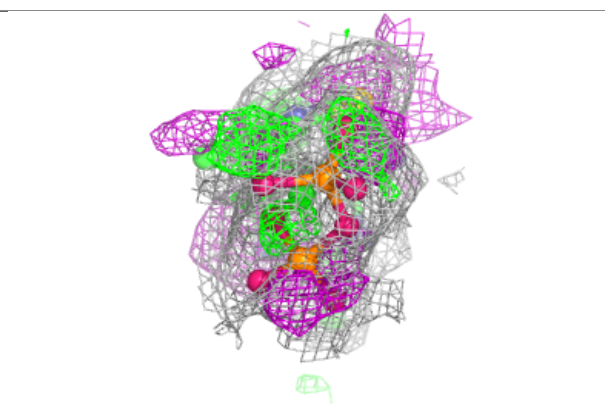
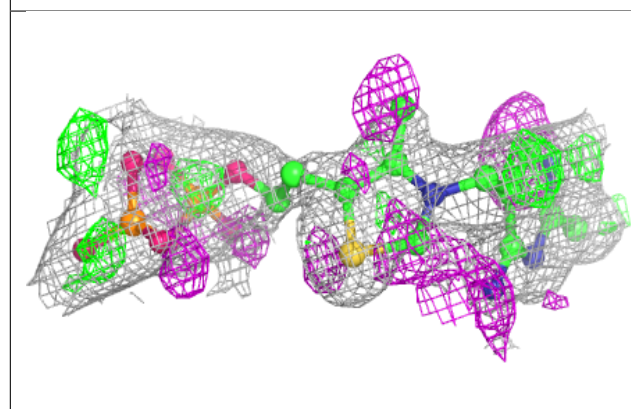
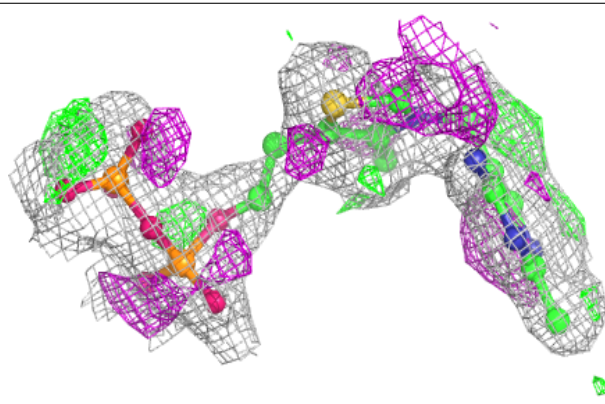


**Electron density around PPY B 603:**

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

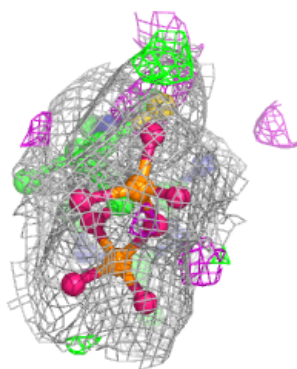
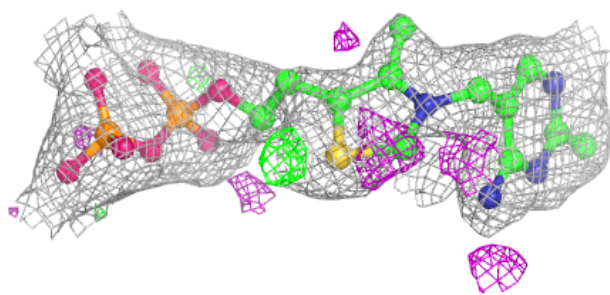
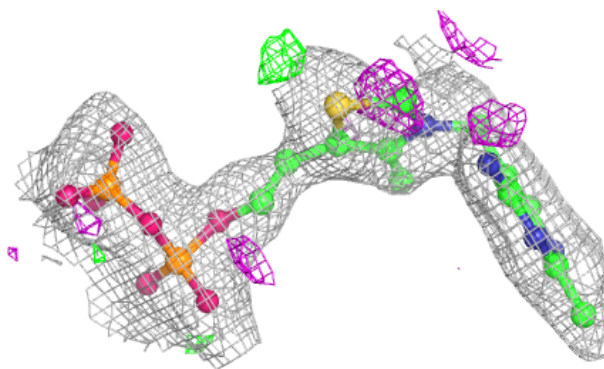
**Electron density around TPP B 601:**

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



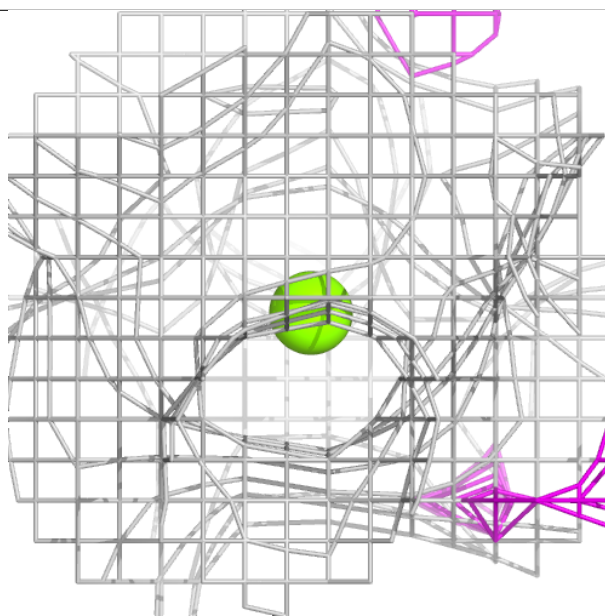
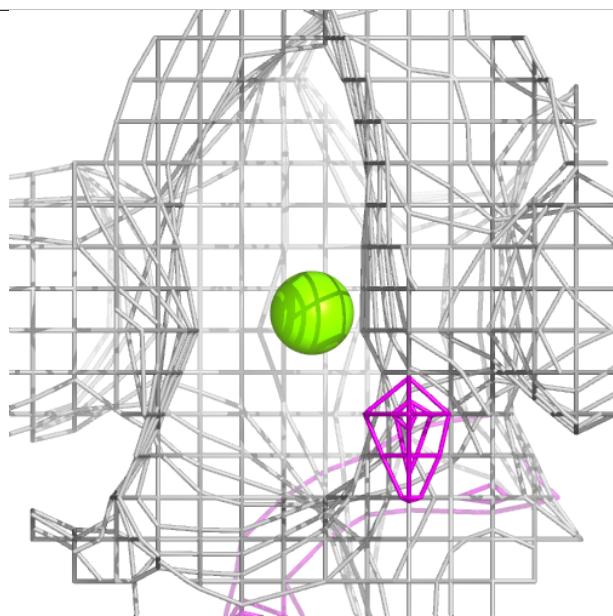
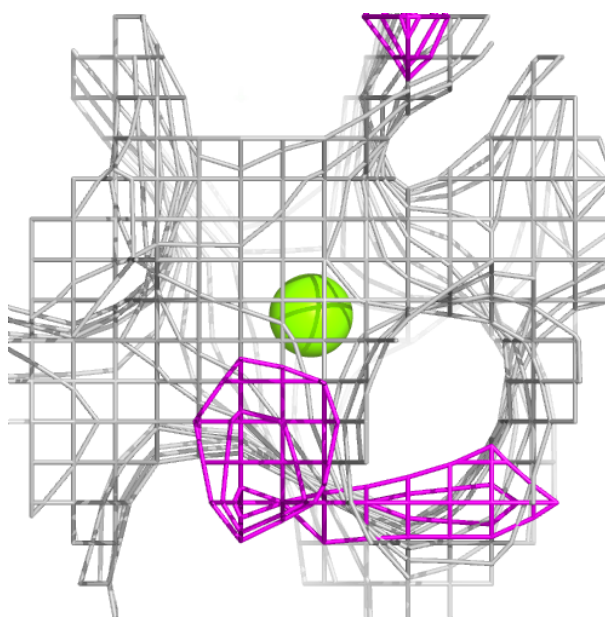
**Electron density around TPP A 601:**

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



**Electron density around MG A 602:**

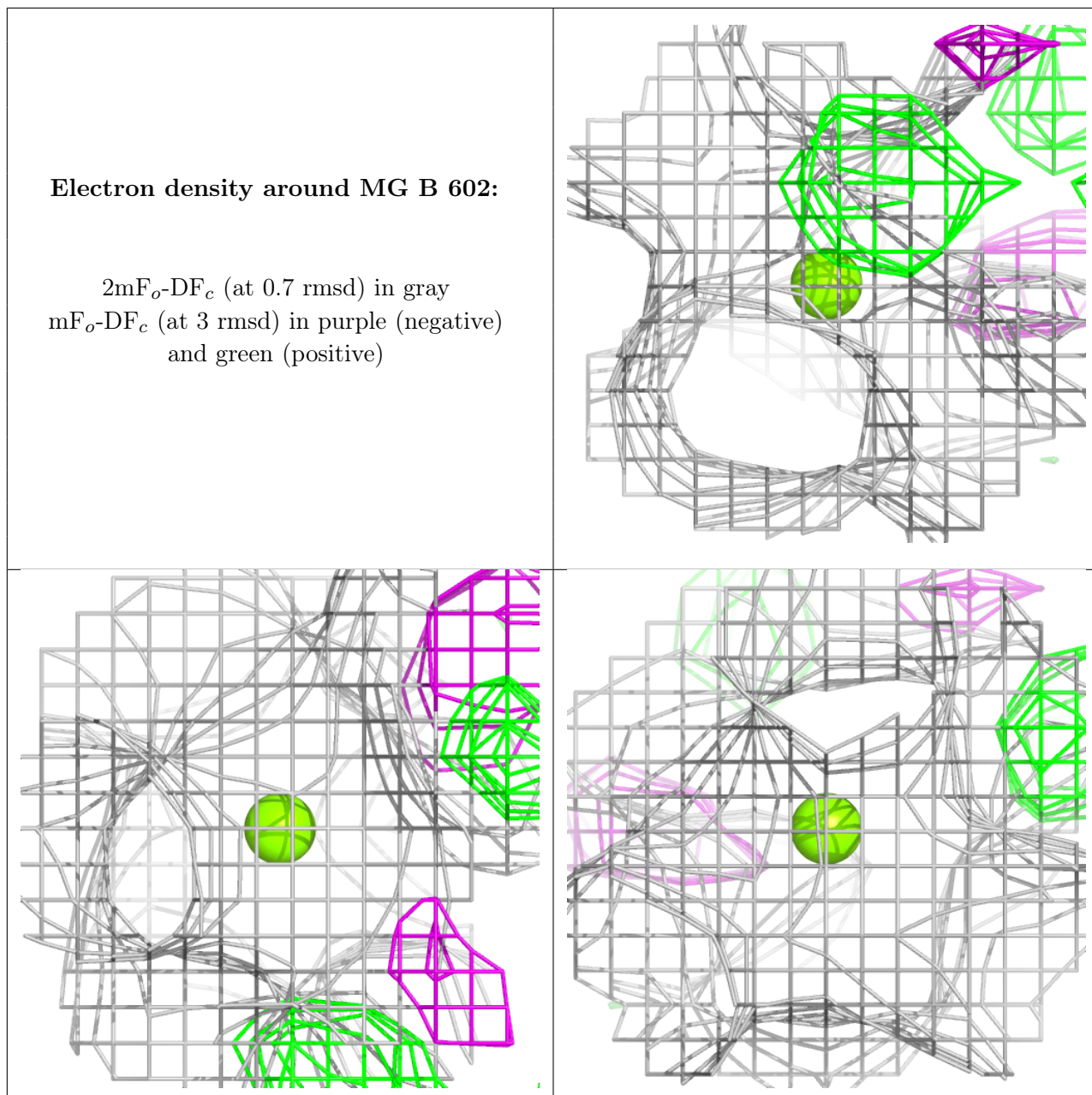
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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 ⓘ

There are no such residues in this entry.