



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 08:10 PM JST

PDB ID : 8ZK6 / pdb\_00008zk6  
Title : Crystal structure of the Decarboxylase KDC4427 from Enterobacter sp. CGMCC 5087  
Authors : Dong, S.; Liu, L.; Zhang, H.  
Deposited on : 2024-05-15  
Resolution : 1.94 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

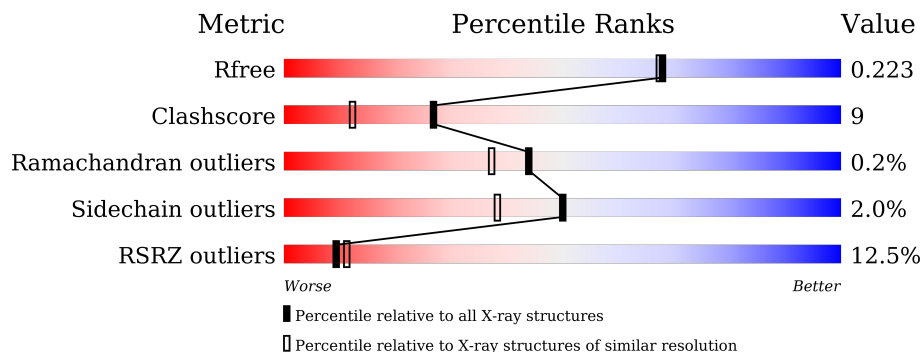
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	
1	B	566	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9196 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
			4129	2618	720	769	22			
1	B	537	Total	C	N	O	S	0	0	0
			4115	2608	718	767	22			

There are 28 discrepancies between the modelled and reference sequences:

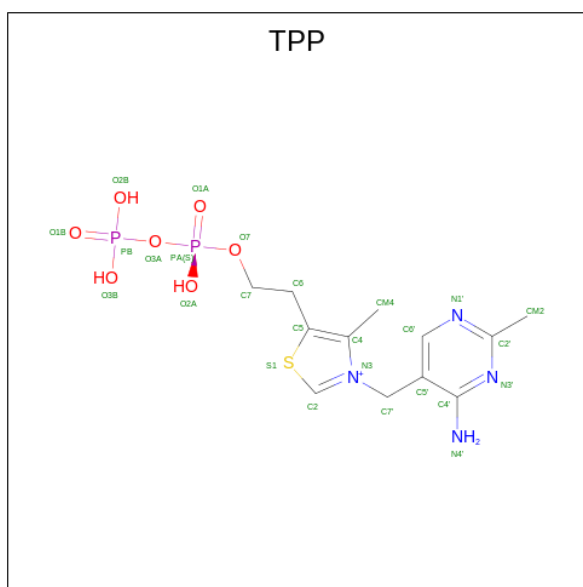
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A2U3EYQ2
A	-12	GLY	-	expression tag	UNP A0A2U3EYQ2
A	-11	SER	-	expression tag	UNP A0A2U3EYQ2
A	-10	SER	-	expression tag	UNP A0A2U3EYQ2
A	-9	HIS	-	expression tag	UNP A0A2U3EYQ2
A	-8	HIS	-	expression tag	UNP A0A2U3EYQ2
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
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
B	-3	SER	-	expression tag	UNP A0A2U3EYQ2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLN	-	expression tag	UNP A0A2U3EYQ2
B	-1	ASP	-	expression tag	UNP A0A2U3EYQ2
B	0	PRO	-	expression tag	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		

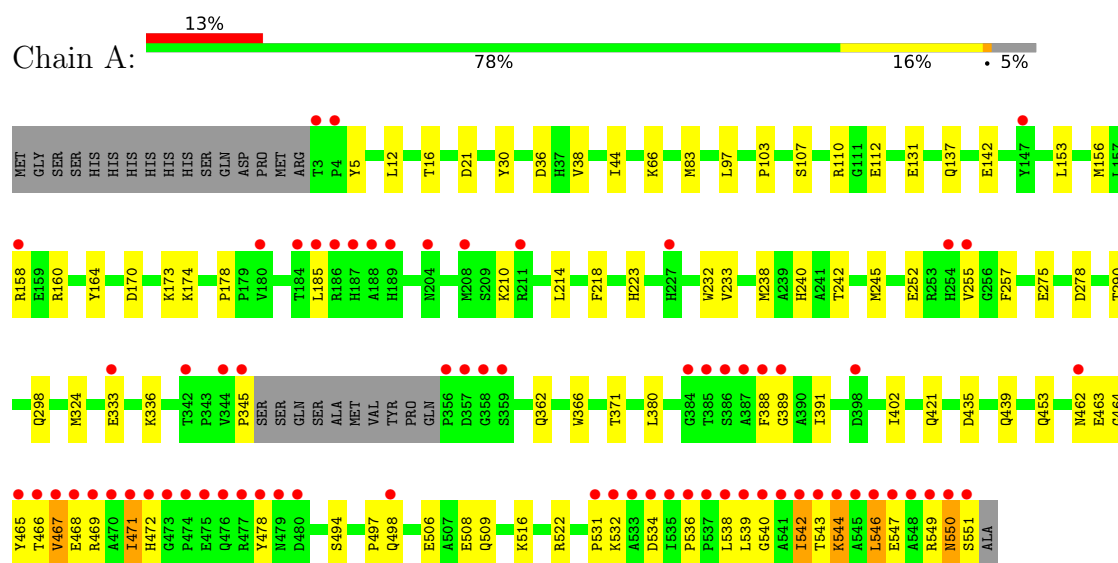
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	418	Total 418	O 418	0	0
4	B	480	Total 480	O 480	0	0

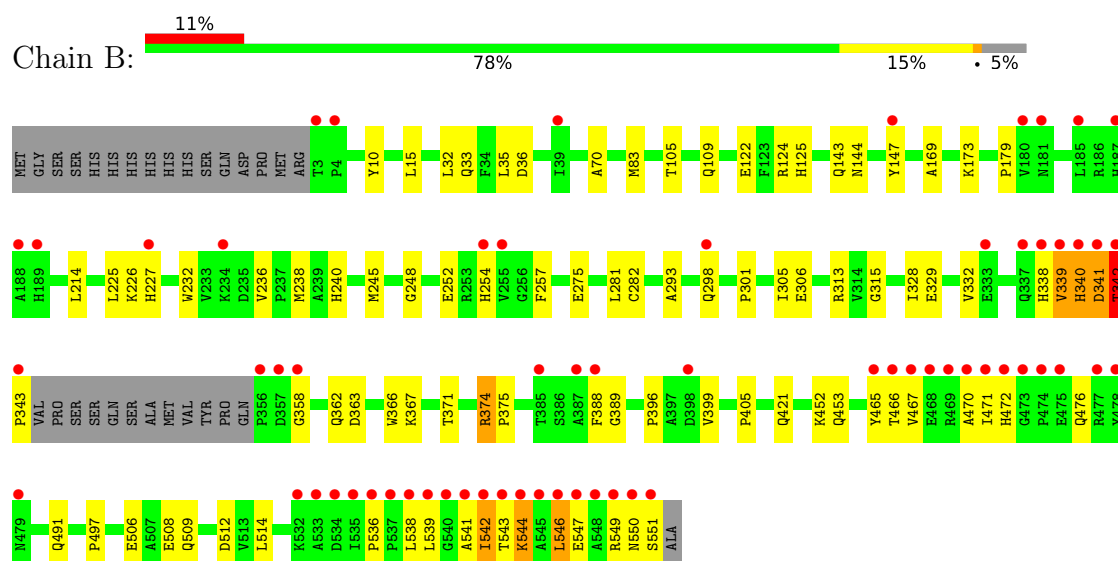
### 3 Residue-property plots [i](#)

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: Indolepyruvate decarboxylase



#### • Molecule 1: Indolepyruvate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.23Å 170.29Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.68 – 1.94 78.68 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.4 (78.68-1.94) 87.6 (78.68-1.94)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.208 , 0.224 0.209 , 0.223	Depositor DCC
$R_{free}$ test set	98109 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/4224	0.58	1/5756 (0.0%)
1	B	0.34	0/4209	0.59	3/5734 (0.1%)
All	All	0.35	0/8433	0.58	4/11490 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	HIS	CA-C-N	6.22	133.42	121.54
1	B	340	HIS	C-N-CA	6.22	133.42	121.54
1	B	342	THR	N-CA-C	5.94	118.10	109.84
1	A	546	LEU	N-CA-C	-5.44	105.94	113.18

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4129	0	4071	82	0
1	B	4115	0	4055	83	0
2	A	26	0	16	4	0
2	B	26	0	16	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	418	0	0	9	2
4	B	480	0	0	18	2
All	All	9196	0	8158	149	2

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 (149) 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:173:LYS:NZ	1:B:550:ASN:HB3	1.40	1.37
1:A:549:ARG:CD	4:B:712:HOH:O	2.11	0.96
1:A:173:LYS:HZ2	1:B:550:ASN:HB3	1.23	0.94
1:A:173:LYS:NZ	1:B:550:ASN:CB	2.31	0.93
1:A:173:LYS:HZ3	1:B:550:ASN:HB3	1.35	0.90
1:A:549:ARG:HD3	4:B:712:HOH:O	1.75	0.81
1:A:549:ARG:HD2	4:B:712:HOH:O	1.78	0.80
1:A:543:THR:OG1	1:A:544:LYS:HD3	1.85	0.77
1:A:160:ARG:NH1	4:A:703:HOH:O	2.19	0.76
1:B:541:ALA:O	1:B:544:LYS:HD3	1.85	0.76
1:A:516:LYS:NZ	4:A:704:HOH:O	2.19	0.74
1:A:462:ASN:ND2	1:A:466:THR:OG1	2.25	0.70
1:A:391:ILE:HG21	1:A:538:LEU:HD22	1.74	0.69
1:B:465:TYR:N	4:B:707:HOH:O	2.24	0.69
1:A:550:ASN:O	1:B:173:LYS:NZ	2.25	0.69
1:A:550:ASN:HB3	1:B:169:ALA:HB3	1.75	0.68
1:A:371:THR:OG1	4:A:701:HOH:O	2.12	0.68
1:A:463:GLU:HB2	1:A:532:LYS:HE2	1.74	0.67
1:B:371:THR:OG1	4:B:702:HOH:O	2.13	0.67
1:B:275:GLU:OE1	4:B:701:HOH:O	2.12	0.66
1:A:467:VAL:HG12	2:A:601:TPP:O3B	1.96	0.66
1:B:371:THR:O	1:B:374:ARG:NH2	2.30	0.65
1:A:173:LYS:HZ2	1:B:550:ASN:CB	2.01	0.65
1:B:476:GLN:NE2	4:B:711:HOH:O	2.28	0.65
1:A:539:LEU:O	1:A:543:THR:HG23	1.96	0.65
1:A:173:LYS:HZ1	1:B:550:ASN:HB3	1.56	0.64
1:B:512:ASP:OD1	4:B:703:HOH:O	2.14	0.64
1:B:465:TYR:C	4:B:707:HOH:O	2.40	0.64
2:B:601:TPP:H2	4:B:1040:HOH:O	1.97	0.64
1:B:214:LEU:HB2	1:B:238:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:PRO:O	4:A:702:HOH:O	2.16	0.61
1:B:549:ARG:HD3	1:B:549:ARG:H	1.64	0.61
1:B:15:LEU:HD11	1:B:70:ALA:HB2	1.82	0.61
1:B:549:ARG:HH11	1:B:549:ARG:HG2	1.65	0.60
1:B:124:ARG:HG2	1:B:124:ARG:HH11	1.67	0.60
1:A:173:LYS:HZ3	1:B:550:ASN:CB	2.06	0.59
1:A:550:ASN:CB	1:B:169:ALA:HB3	2.32	0.59
1:A:498:GLN:HG3	1:A:522:ARG:HG2	1.85	0.59
1:A:170:ASP:HA	1:B:550:ASN:OD1	2.03	0.58
1:B:124:ARG:NH1	4:B:718:HOH:O	2.35	0.58
1:B:143:GLN:HG3	4:B:968:HOH:O	2.05	0.57
1:B:549:ARG:HG2	1:B:549:ARG:NH1	2.19	0.56
1:A:83:MET:SD	1:B:83:MET:SD	3.04	0.56
1:A:107:SER:OG	1:B:549:ARG:NH1	2.38	0.56
1:B:293:ALA:HA	1:B:542:ILE:HD13	1.88	0.56
1:A:255:VAL:HG12	4:A:948:HOH:O	2.05	0.55
1:A:290:THR:HG23	1:A:388:PHE:CZ	2.43	0.54
1:B:491:GLN:HA	1:B:497:PRO:HG3	1.90	0.53
1:A:110:ARG:NH1	1:A:112:GLU:OE2	2.42	0.53
1:B:105:THR:O	1:B:109:GLN:HG3	2.09	0.53
1:A:12:LEU:HD21	1:A:38:VAL:HG22	1.91	0.52
1:B:122:GLU:HB2	4:B:808:HOH:O	2.09	0.52
1:A:362:GLN:OE1	1:A:536:PRO:HG3	2.09	0.52
1:B:342:THR:HB	1:B:343:PRO:CD	2.39	0.52
1:B:363:ASP:OD1	1:B:367:LYS:NZ	2.37	0.52
1:A:508:GLU:H	1:A:508:GLU:CD	2.17	0.52
1:A:421:GLN:HG2	1:A:453:GLN:HB3	1.91	0.52
1:A:233:VAL:HG21	1:A:240:HIS:CG	2.44	0.51
1:B:396:PRO:HD2	1:B:399:VAL:HG21	1.93	0.51
1:B:471:ILE:HG13	1:B:546:LEU:HD12	1.92	0.51
1:B:467:VAL:O	1:B:471:ILE:HD13	2.10	0.51
1:A:131:GLU:OE2	4:A:705:HOH:O	2.19	0.51
1:A:21:ASP:OD2	1:A:66:LYS:NZ	2.43	0.51
1:B:293:ALA:HA	1:B:542:ILE:CD1	2.41	0.50
1:B:374:ARG:HG3	1:B:375:PRO:HD2	1.93	0.50
1:A:5:TYR:CD2	1:A:178:PRO:HG3	2.47	0.50
1:B:254:HIS:ND1	4:B:717:HOH:O	2.34	0.50
1:B:549:ARG:HD3	1:B:549:ARG:N	2.26	0.50
1:B:252:GLU:HB3	1:B:257:PHE:CE1	2.47	0.49
1:A:391:ILE:HD13	1:A:538:LEU:HD22	1.94	0.49
1:B:226:LYS:HE3	1:B:248:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LEU:O	1:B:543:THR:HG23	2.13	0.49
1:A:551:SER:HB2	1:B:33:GLN:OE1	2.12	0.49
1:A:137:GLN:HB3	1:A:164:TYR:HB3	1.95	0.48
1:B:342:THR:CB	1:B:343:PRO:CD	2.91	0.48
1:A:232:TRP:NE1	1:A:238:MET:HE1	2.28	0.48
1:B:245:MET:HG2	1:B:405:PRO:HD2	1.95	0.48
1:A:467:VAL:HG11	2:A:601:TPP:S1	2.53	0.48
1:B:306:GLU:HG2	1:B:313:ARG:HB3	1.96	0.48
1:B:470:ALA:HB1	1:B:543:THR:HG21	1.96	0.48
1:B:362:GLN:OE1	1:B:536:PRO:HG3	2.14	0.47
1:B:144:ASN:HA	1:B:147:TYR:CE1	2.49	0.47
1:B:281:LEU:HD23	1:B:305:ILE:HB	1.96	0.47
1:B:366:TRP:CE2	1:B:389:GLY:HA3	2.50	0.47
1:A:275:GLU:HG2	1:A:298:GLN:O	2.15	0.47
1:B:329:GLU:OE2	4:B:704:HOH:O	2.19	0.47
1:A:218:PHE:HB3	1:A:245:MET:HB3	1.96	0.47
1:A:333:GLU:OE1	4:A:706:HOH:O	2.20	0.47
1:A:290:THR:HG23	1:A:388:PHE:HZ	1.78	0.47
1:A:464:GLY:HA3	1:A:469:ARG:NH2	2.30	0.46
1:B:396:PRO:HG3	4:B:1097:HOH:O	2.16	0.46
1:B:452:LYS:HE3	1:B:452:LYS:HA	1.96	0.46
1:B:122:GLU:HG2	1:B:125:HIS:CE1	2.50	0.46
1:A:214:LEU:O	1:A:240:HIS:HA	2.16	0.46
1:A:97:LEU:HD22	1:A:153:LEU:HD21	1.98	0.46
1:A:223:HIS:CD2	1:A:324:MET:HE1	2.51	0.46
1:A:233:VAL:HG22	4:A:934:HOH:O	2.16	0.46
1:A:36:ASP:OD2	1:B:472:HIS:NE2	2.43	0.46
1:A:366:TRP:CE2	1:A:389:GLY:HA3	2.51	0.46
1:B:275:GLU:HG2	1:B:298:GLN:O	2.15	0.46
1:A:223:HIS:CG	1:A:324:MET:HE1	2.50	0.46
1:A:142:GLU:HG3	1:A:174:LYS:HG2	1.98	0.45
1:A:252:GLU:HB3	1:A:257:PHE:CE2	2.52	0.45
1:A:467:VAL:O	1:A:471:ILE:HG23	2.16	0.45
1:B:358:GLY:HA2	1:B:508:GLU:OE1	2.17	0.45
1:B:508:GLU:H	1:B:508:GLU:CD	2.24	0.45
1:A:472:HIS:NE2	1:B:36:ASP:OD2	2.50	0.45
2:B:601:TPP:HN42	2:B:601:TPP:C2	2.30	0.45
1:A:158:ARG:HB2	1:A:185:LEU:HD11	1.99	0.44
1:A:531:PRO:HB2	1:A:534:ASP:HB2	1.99	0.44
1:A:551:SER:HA	1:B:173:LYS:HE3	1.98	0.44
1:A:232:TRP:HE1	1:A:238:MET:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ASN:HD21	1:A:466:THR:CB	2.29	0.44
1:B:467:VAL:HG11	2:B:601:TPP:S1	2.57	0.44
1:B:338:HIS:O	1:B:339:VAL:C	2.61	0.44
1:B:472:HIS:HB2	1:B:547:GLU:OE1	2.18	0.44
1:B:10:TYR:CE2	1:B:179:PRO:HG3	2.53	0.43
1:B:214:LEU:O	1:B:240:HIS:HA	2.18	0.43
1:A:540:GLY:O	1:A:544:LYS:HG2	2.18	0.43
1:A:16:THR:HG22	1:A:44:ILE:HD11	2.01	0.42
1:B:466:THR:HB	2:B:601:TPP:O1B	2.19	0.42
1:A:380:LEU:HG	1:A:402:ILE:HB	2.02	0.42
1:A:471:ILE:HD12	1:A:472:HIS:HB2	2.01	0.42
2:A:601:TPP:H2	4:B:1033:HOH:O	2.18	0.42
1:A:466:THR:HA	1:A:469:ARG:HB2	2.02	0.42
1:B:124:ARG:HH11	1:B:124:ARG:CG	2.30	0.42
1:A:97:LEU:HB2	1:A:156:MET:HE1	2.02	0.42
1:B:282:CYS:O	1:B:306:GLU:HA	2.20	0.42
1:A:435:ASP:O	1:A:439:GLN:HG3	2.19	0.42
1:A:336:LYS:NZ	4:A:719:HOH:O	2.39	0.41
1:A:494:SER:HB3	1:A:497:PRO:HG3	2.02	0.41
1:B:232:TRP:CG	1:B:332:VAL:HG22	2.55	0.41
1:B:227:HIS:ND1	4:B:709:HOH:O	2.25	0.41
1:A:137:GLN:HA	1:A:164:TYR:O	2.20	0.41
1:B:506:GLU:HB2	1:B:509:GLN:HG3	2.02	0.41
1:A:544:LYS:N	1:A:544:LYS:CD	2.81	0.41
1:B:421:GLN:HG2	1:B:453:GLN:HB3	2.02	0.41
1:A:471:ILE:HD11	1:B:32:LEU:HD12	2.02	0.41
1:A:538:LEU:O	1:A:542:ILE:HG13	2.21	0.41
1:B:236:VAL:CG1	1:B:339:VAL:HB	2.51	0.41
1:A:465:TYR:CD1	2:A:601:TPP:H61	2.56	0.41
1:B:301:PRO:O	1:B:315:GLY:HA2	2.21	0.41
1:A:506:GLU:HB2	1:A:509:GLN:HG3	2.03	0.40
1:B:225:LEU:HD13	1:B:328:ILE:HD12	2.02	0.40
1:B:388:PHE:HB3	1:B:538:LEU:HD23	2.02	0.40
1:A:30:TYR:CZ	1:A:103:PRO:HG3	2.57	0.40
1:A:210:LYS:HB2	1:A:278:ASP:OD2	2.21	0.40
1:B:514:LEU:HD23	1:B:514:LEU:HA	1.93	0.40
1:A:478:TYR:CG	1:B:35:LEU:HD13	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:724:HOH:O	4:B:785:HOH:O[6_555]	2.18	0.02
4:A:820:HOH:O	4:B:738:HOH:O[8_455]	2.18	0.02

## 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%)	519 (97%)	16 (3%)	0	100	100
1	B	533/566 (94%)	521 (98%)	10 (2%)	2 (0%)	30	22
All	All	1068/1132 (94%)	1040 (97%)	26 (2%)	2 (0%)	44	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	VAL
1	B	341	ASP

### 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	432/458 (94%)	423 (98%)	9 (2%)	48	36
1	B	430/458 (94%)	422 (98%)	8 (2%)	52	41
All	All	862/916 (94%)	845 (98%)	17 (2%)	50	38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	THR
1	A	467	VAL
1	A	468	GLU
1	A	471	ILE
1	A	542	ILE
1	A	544	LYS
1	A	546	LEU
1	A	547	GLU
1	A	550	ASN
1	B	340	HIS
1	B	341	ASP
1	B	342	THR
1	B	374	ARG
1	B	542	ILE
1	B	544	LYS
1	B	546	LEU
1	B	551	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	453	GLN
1	A	462	ASN
1	B	189	HIS
1	B	421	GLN
1	B	439	GLN
1	B	498	GLN
1	B	519	HIS

### 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	B	601	3	22,27,27	0.56	0	29,40,40	0.72	1 (3%)
2	TPP	A	601	3	22,27,27	0.65	0	29,40,40	0.77	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	B	601	3	-	6/16/17/17	0/2/2/2
2	TPP	A	601	3	-	4/16/17/17	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	B	601	TPP	C5-C4-N3	2.05	111.67	107.57

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

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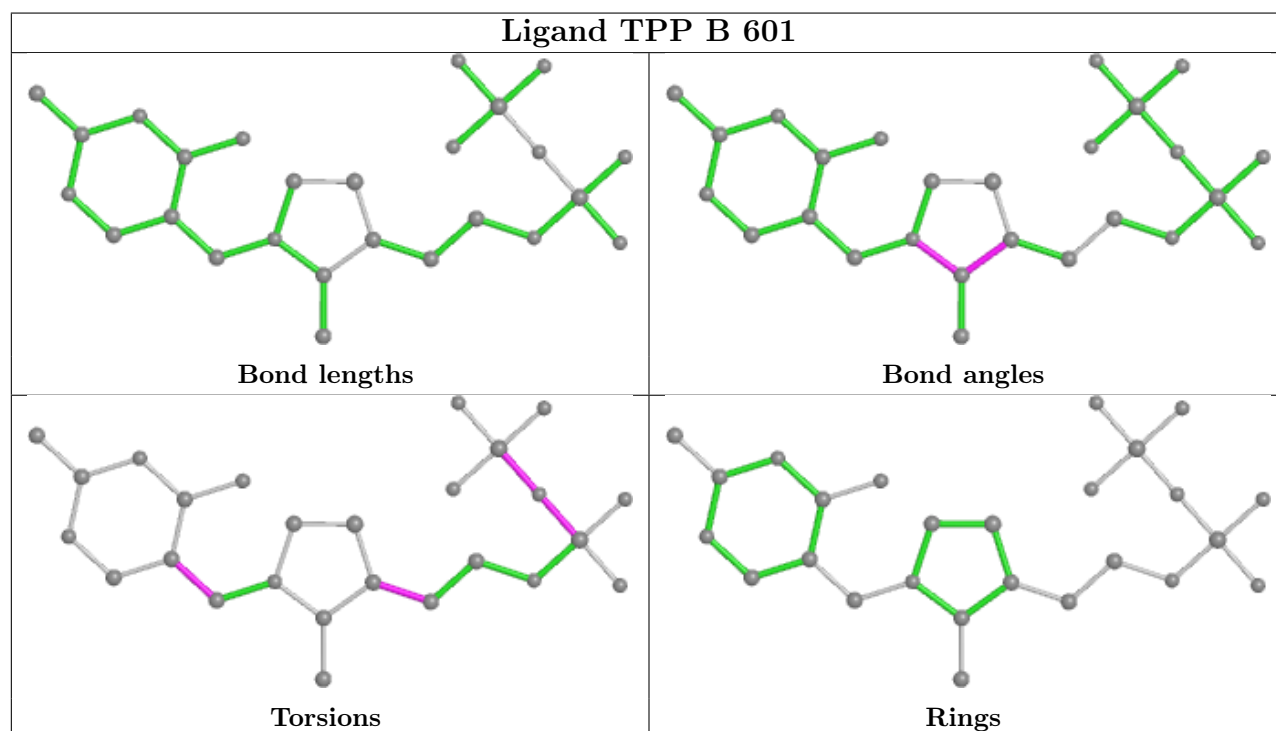
Mol	Chain	Res	Type	Atoms
2	B	601	TPP	C4'-C5'-C7'-N3
2	B	601	TPP	PA-O3A-PB-O2B
2	B	601	TPP	PB-O3A-PA-O2A

There are no ring outliers.

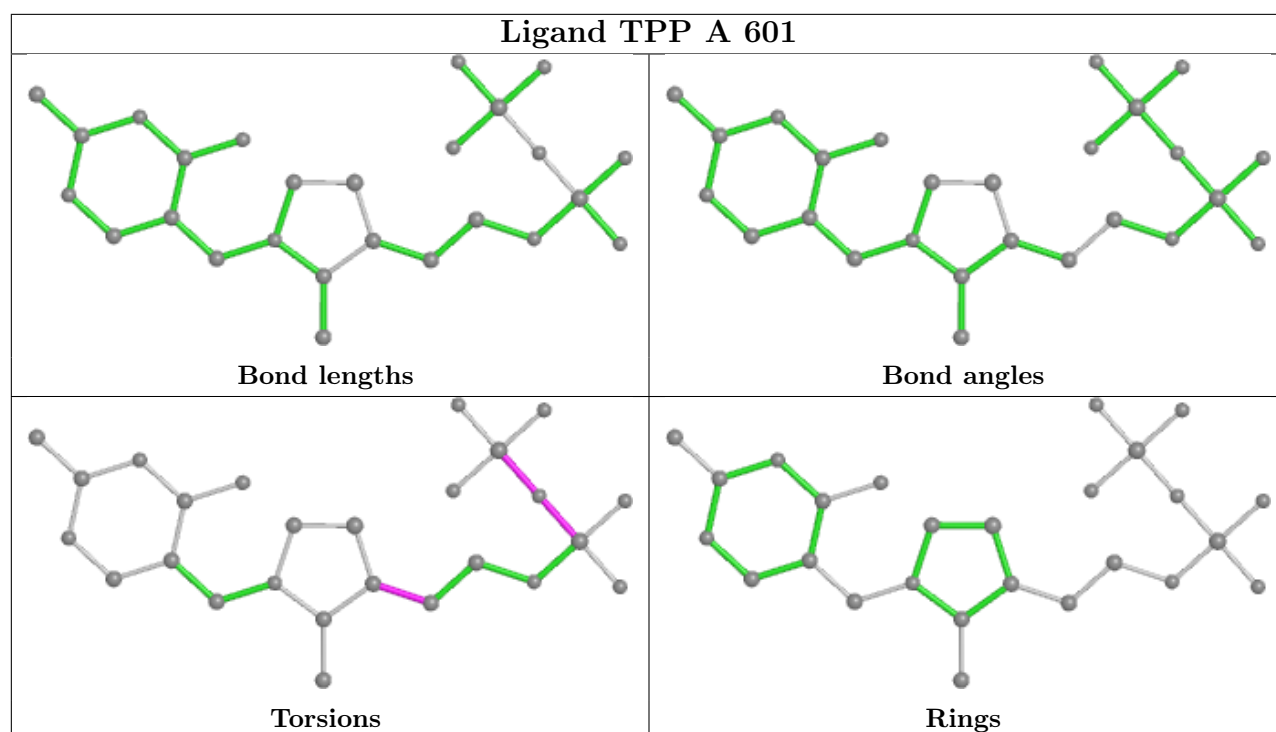
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	TPP	4	0
2	A	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 [i](#)

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	539/566 (95%)	0.95	71 (13%)	8 10	15, 26, 69, 117	0
1	B	537/566 (94%)	0.76	64 (11%)	10 12	15, 25, 60, 102	0
All	All	1076/1132 (95%)	0.86	135 (12%)	9 11	15, 26, 64, 117	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	ILE	10.9
1	A	538	LEU	10.6
1	A	546	LEU	10.4
1	A	539	LEU	10.3
1	A	388	PHE	9.8
1	B	546	LEU	9.3
1	A	467	VAL	9.0
1	A	545	ALA	8.6
1	B	545	ALA	8.4
1	A	535	ILE	8.3
1	B	551	SER	8.3
1	A	474	PRO	8.2
1	A	356	PRO	8.0
1	A	541	ALA	7.8
1	A	471	ILE	7.6
1	B	542	ILE	7.5
1	A	550	ASN	7.5
1	B	539	LEU	7.4
1	B	339	VAL	7.3
1	B	388	PHE	7.2
1	B	550	ASN	7.1
1	A	549	ARG	7.1
1	A	548	ALA	7.0
1	A	551	SER	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	540	GLY	6.9
1	A	536	PRO	6.8
1	B	549	ARG	6.8
1	B	548	ALA	6.6
1	B	538	LEU	6.5
1	B	356	PRO	6.5
1	B	543	THR	6.4
1	B	547	GLU	6.3
1	A	357	ASP	6.2
1	A	543	THR	6.1
1	B	541	ALA	5.9
1	B	471	ILE	5.8
1	A	537	PRO	5.8
1	A	473	GLY	5.6
1	B	536	PRO	5.6
1	B	387	ALA	5.5
1	B	467	VAL	5.5
1	A	547	GLU	5.4
1	A	466	THR	5.4
1	A	385	THR	5.4
1	A	470	ALA	5.4
1	B	544	LYS	5.3
1	B	474	PRO	5.3
1	A	3	THR	5.2
1	B	340	HIS	5.2
1	B	535	ILE	5.2
1	A	344	VAL	5.1
1	A	387	ALA	5.1
1	A	478	TYR	4.8
1	A	533	ALA	4.7
1	A	544	LYS	4.6
1	B	540	GLY	4.5
1	B	357	ASP	4.2
1	B	537	PRO	4.2
1	A	187	HIS	4.2
1	A	534	ASP	4.1
1	B	473	GLY	4.1
1	B	472	HIS	4.1
1	B	187	HIS	4.0
1	B	341	ASP	4.0
1	A	475	GLU	3.9
1	A	472	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	180	VAL	3.9
1	A	184	THR	3.9
1	B	3	THR	3.8
1	B	227	HIS	3.7
1	B	188	ALA	3.7
1	A	345	PRO	3.6
1	A	465	TYR	3.6
1	A	185	LEU	3.5
1	B	475	GLU	3.5
1	B	470	ALA	3.4
1	A	342	THR	3.4
1	A	498	GLN	3.4
1	B	478	TYR	3.3
1	A	469	ARG	3.3
1	B	533	ALA	3.2
1	B	385	THR	3.2
1	A	386	SER	3.2
1	A	186	ARG	3.2
1	A	532	LYS	3.2
1	A	4	PRO	3.1
1	B	343	PRO	3.1
1	A	358	GLY	3.0
1	A	479	ASN	3.0
1	B	342	THR	3.0
1	B	532	LYS	3.0
1	A	227	HIS	3.0
1	A	468	GLU	2.9
1	B	466	THR	2.9
1	B	189	HIS	2.8
1	B	534	ASP	2.8
1	B	469	ARG	2.8
1	A	477	ARG	2.7
1	A	384	GLY	2.7
1	B	398	ASP	2.6
1	A	188	ALA	2.6
1	B	465	TYR	2.6
1	A	398	ASP	2.6
1	B	337	GLN	2.6
1	A	480	ASP	2.6
1	A	211	ARG	2.6
1	A	476	GLN	2.6
1	B	254	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	468	GLU	2.5
1	B	4	PRO	2.4
1	B	39	ILE	2.4
1	B	147	TYR	2.4
1	B	358	GLY	2.4
1	A	389	GLY	2.4
1	A	359	SER	2.4
1	A	531	PRO	2.4
1	A	255	VAL	2.4
1	A	333	GLU	2.3
1	A	204	ASN	2.3
1	B	185	LEU	2.2
1	B	338	HIS	2.2
1	B	479	ASN	2.2
1	B	234	LYS	2.2
1	A	254	HIS	2.2
1	B	255	VAL	2.1
1	B	298	GLN	2.1
1	A	147	TYR	2.1
1	A	462	ASN	2.1
1	A	189	HIS	2.0
1	A	180	VAL	2.0
1	B	333	GLU	2.0
1	A	208	MET	2.0
1	A	158	ARG	2.0
1	B	181	ASN	2.0
1	B	477	ARG	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.

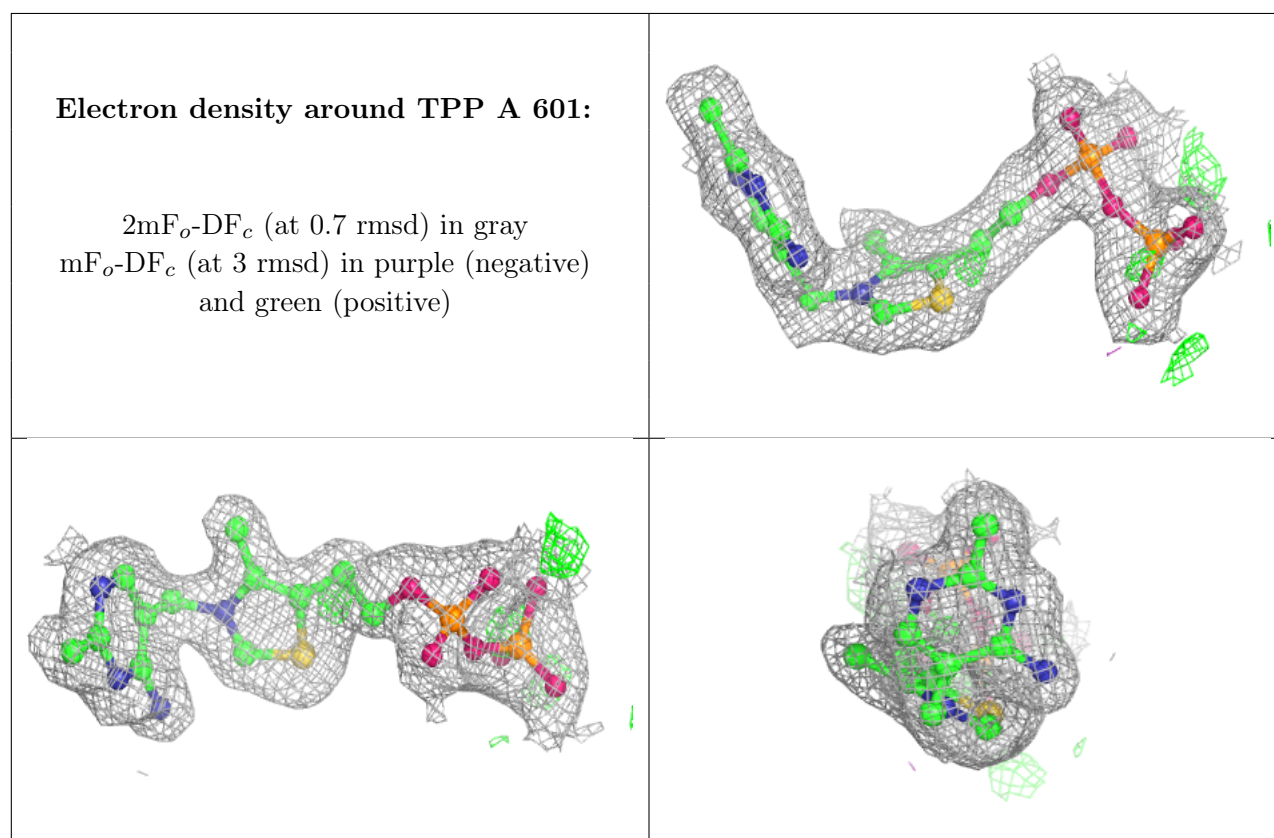
## 6.4 Ligands [i](#)

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.

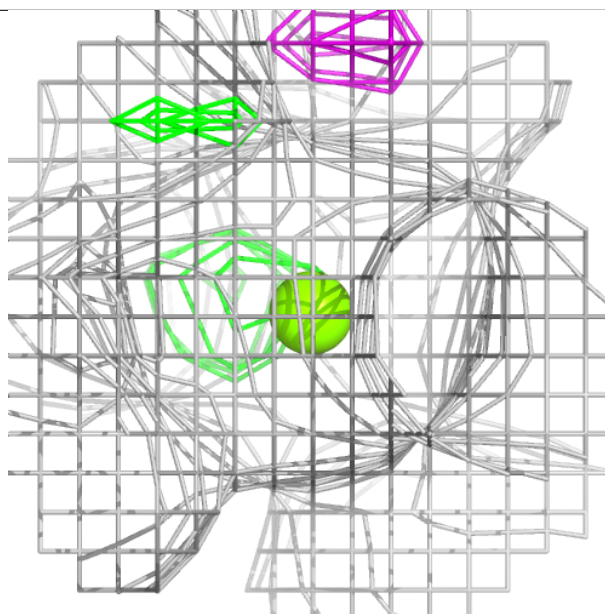
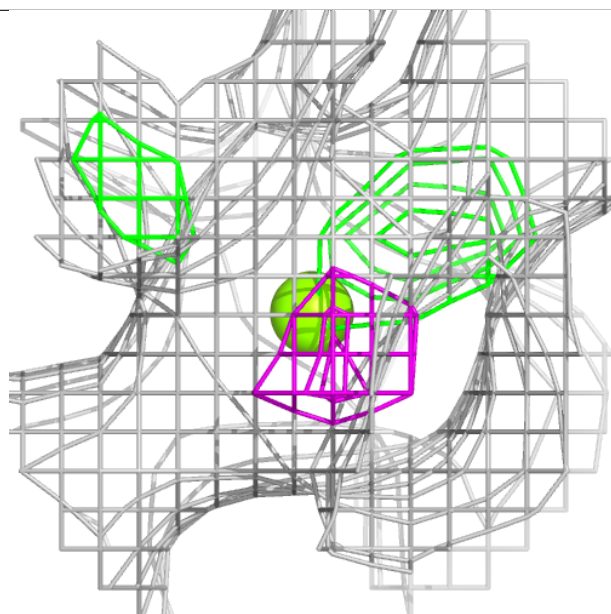
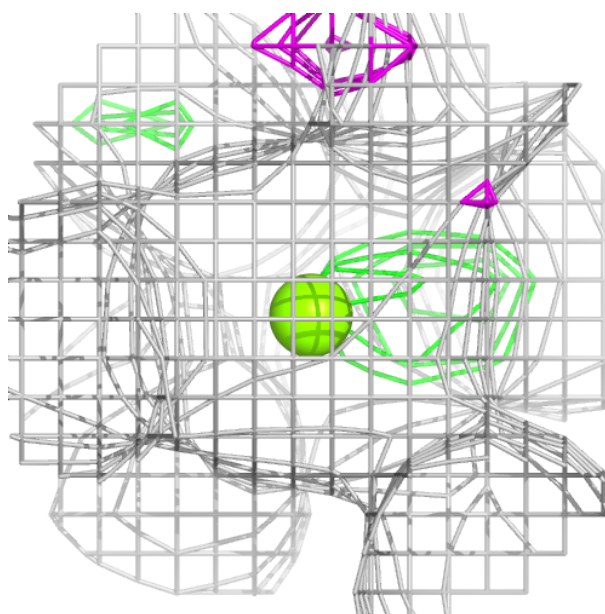
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPP	A	601	26/26	0.95	0.09	14,26,36,39	0
3	MG	B	602	1/1	0.95	0.10	23,23,23,23	0
2	TPP	B	601	26/26	0.96	0.08	17,26,35,37	0
3	MG	A	602	1/1	0.97	0.13	23,23,23,23	0

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.



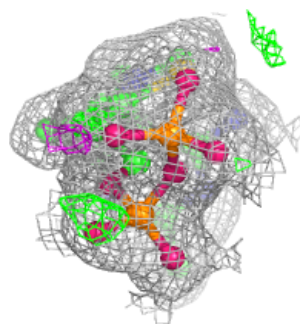
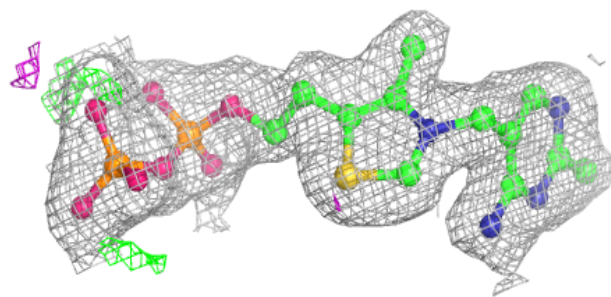
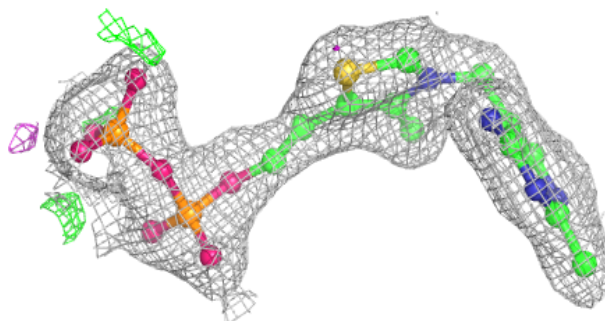
**Electron density around MG B 602:**

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



**Electron density around TPP B 601:**

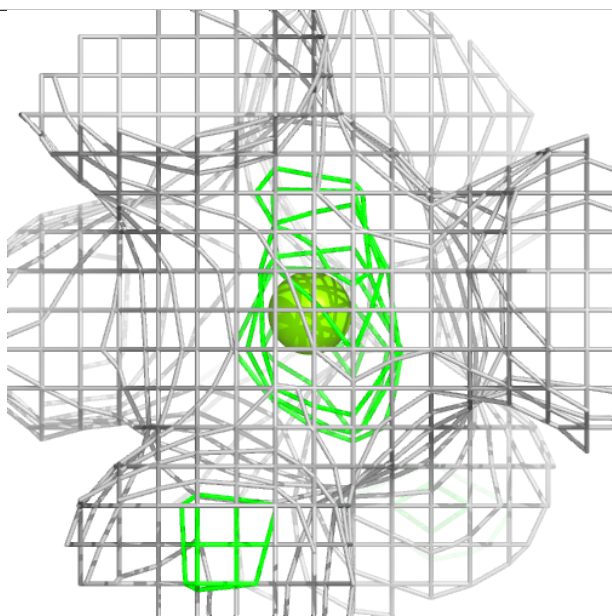
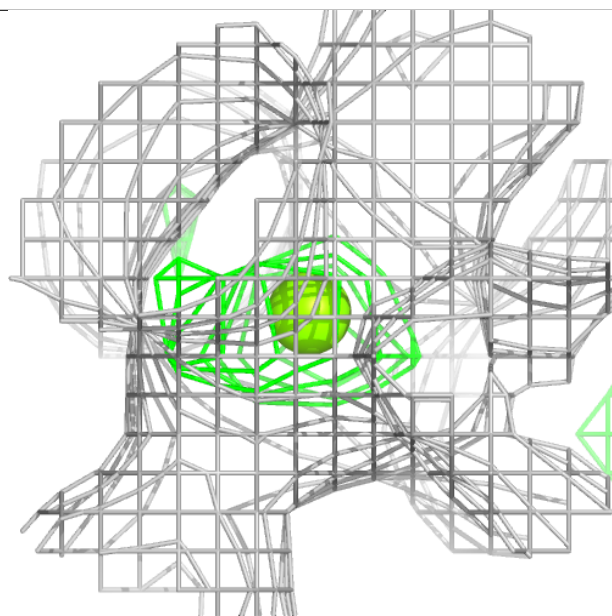
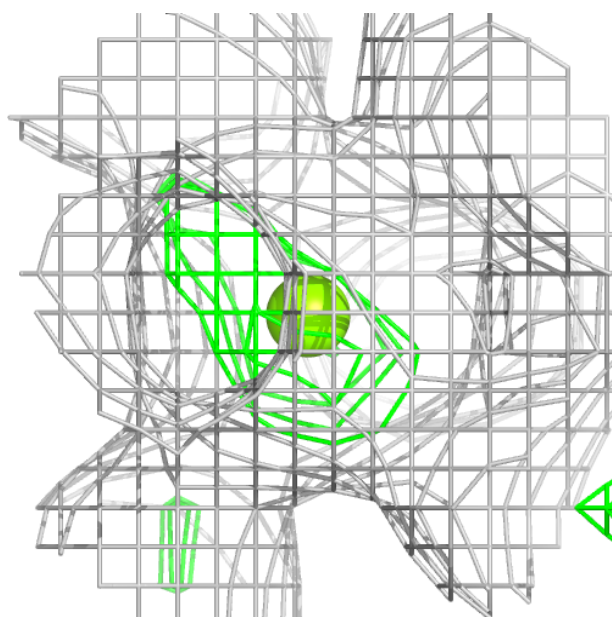
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.