Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 10:42 pm GMT

PDB ID	:	4COK
Title	:	Functional and Structural Characterization of Pyruvate decarboxylase from Gluconoacetobacter diazotrophicus
Authors	:	vanZyl, L.J.; Schubert, W.-D.; Tuffin, M.; Cowan, D.A.
Deposited on	:	2014-01-29
Resolution	:	1.69 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

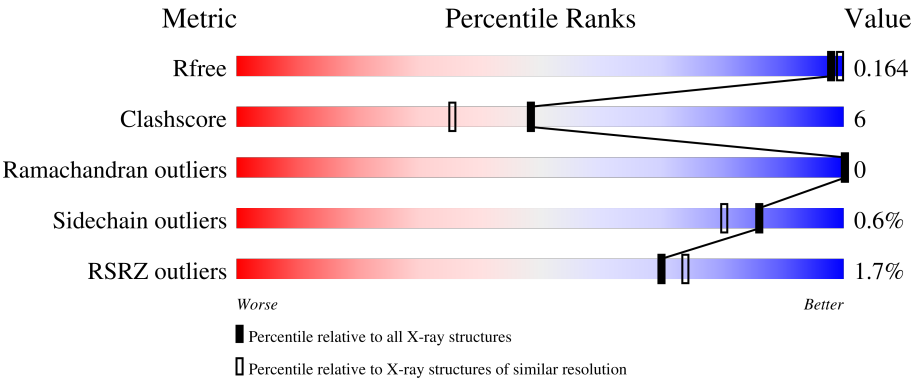
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

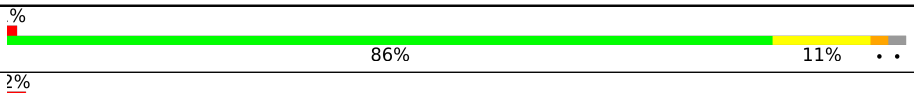
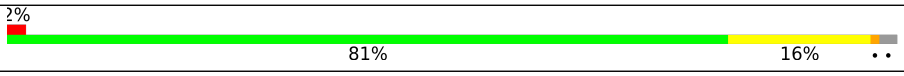
The reported resolution of this entry is 1.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	558	
1	B	558	

2 Entry composition

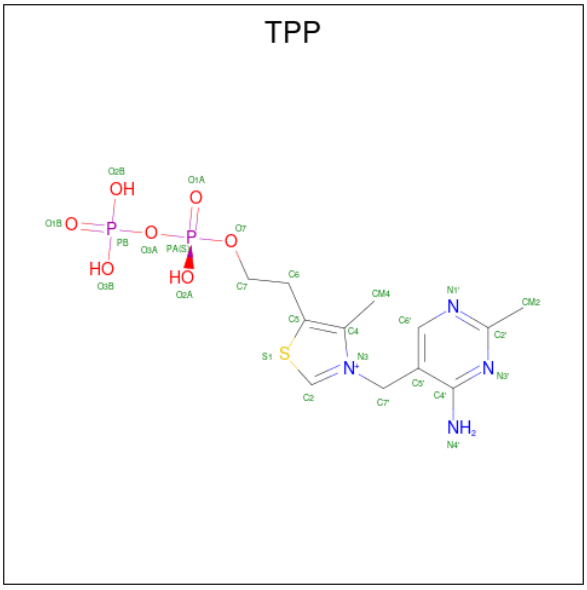
There are 5 unique types of molecules in this entry. The entry contains 9847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	35	1
			4304	2713	770	794	27			
1	B	549	Total	C	N	O	S	0	36	0
			4312	2724	773	788	27			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

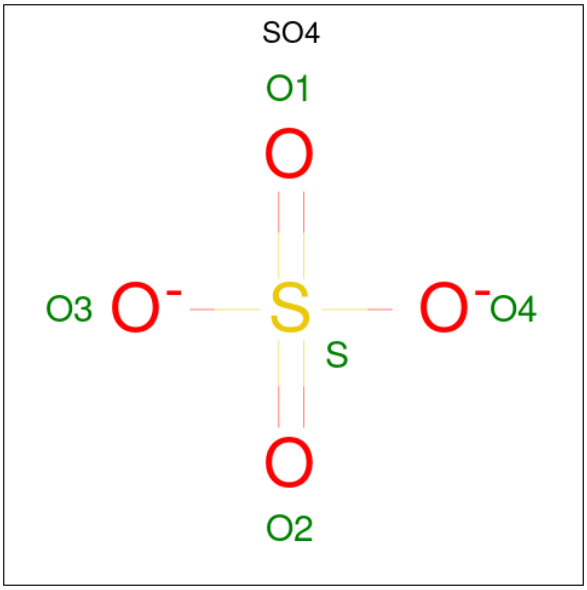


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

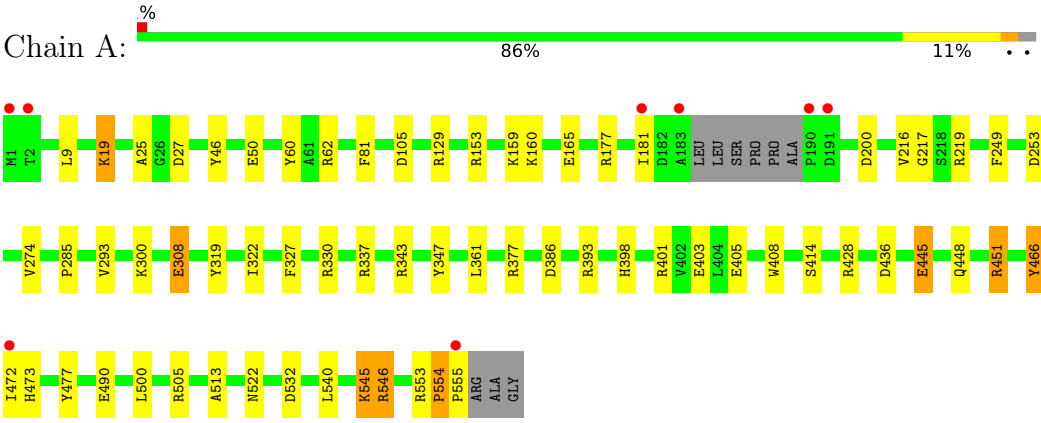
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	632	Total O 632 632	0	0
5	B	535	Total O 535 535	0	0

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.

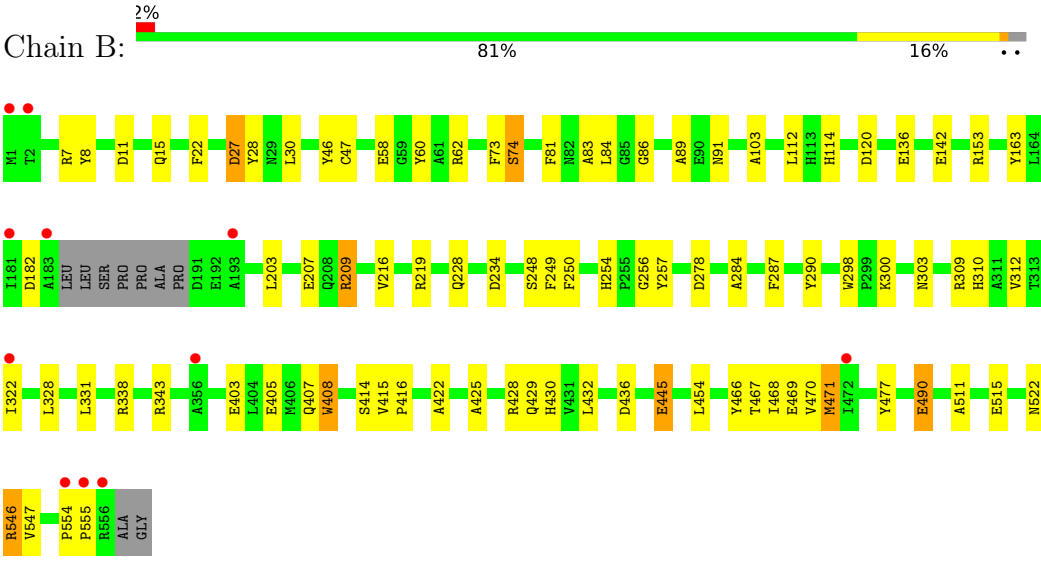
• Molecule 1: PYRUVATE DECARBOXYLASE

Chain A:



• Molecule 1: PYRUVATE DECARBOXYLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.07Å 140.96Å 91.06Å 90.00° 125.78° 90.00°	Depositor
Resolution (Å)	84.06 – 1.69 45.03 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (84.06-1.69) 99.4 (45.03-1.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.132 , 0.163 0.132 , 0.164	Depositor DCC
R_{free} test set	7314 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9847	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPP, MG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.54	23/4483 (0.5%)	1.33	36/6091 (0.6%)
1	B	1.55	36/4506 (0.8%)	1.31	30/6124 (0.5%)
All	All	1.54	59/8989 (0.7%)	1.32	66/12215 (0.5%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	GLU	CD-OE2	13.40	1.40	1.25
1	A	490	GLU	CG-CD	10.97	1.68	1.51
1	B	74	SER	CB-OG	-9.52	1.29	1.42
1	B	515	GLU	CG-CD	9.20	1.65	1.51
1	B	142	GLU	CG-CD	8.53	1.64	1.51
1	A	165	GLU	CG-CD	8.06	1.64	1.51
1	B	81	PHE	CD1-CE1	7.25	1.53	1.39
1	B	83	ALA	CA-CB	7.12	1.67	1.52
1	B	515	GLU	CD-OE2	7.11	1.33	1.25
1	B	298	TRP	CE3-CZ3	7.01	1.50	1.38
1	A	81	PHE	CD1-CE1	6.94	1.53	1.39
1	A	490	GLU	CB-CG	6.93	1.65	1.52
1	A	408	TRP	CZ3-CH2	6.90	1.51	1.40
1	A	445	GLU	CB-CG	6.82	1.65	1.52
1	B	8	TYR	CE1-CZ	6.78	1.47	1.38
1	B	490[A]	GLU	CG-CD	6.71	1.62	1.51
1	B	490[B]	GLU	CG-CD	6.71	1.62	1.51
1	A	466	TYR	CD1-CE1	6.54	1.49	1.39
1	B	511	ALA	CA-CB	6.44	1.66	1.52
1	A	490	GLU	CD-OE1	6.41	1.32	1.25
1	B	216	VAL	CB-CG2	6.27	1.66	1.52
1	A	513	ALA	CA-CB	6.25	1.65	1.52
1	A	327	PHE	CE1-CZ	6.21	1.49	1.37
1	B	257	TYR	CE2-CZ	6.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	VAL	CB-CG2	6.03	1.65	1.52
1	B	73	PHE	CD2-CE2	5.99	1.51	1.39
1	A	405	GLU	CD-OE1	-5.99	1.19	1.25
1	B	249	PHE	CE1-CZ	5.94	1.48	1.37
1	B	343	ARG	CB-CG	-5.84	1.36	1.52
1	A	327	PHE	CE2-CZ	5.74	1.48	1.37
1	B	60	TYR	CG-CD1	5.67	1.46	1.39
1	A	249	PHE	CE1-CZ	5.64	1.48	1.37
1	B	287	PHE	CD1-CE1	5.61	1.50	1.39
1	A	467	THR	C-O	5.54	1.33	1.23
1	B	248	SER	CB-OG	5.52	1.49	1.42
1	A	414	SER	CA-CB	5.52	1.61	1.52
1	A	472	ILE	CB-CG2	5.51	1.70	1.52
1	B	445	GLU	CG-CD	5.46	1.60	1.51
1	B	103	ALA	CA-CB	5.41	1.63	1.52
1	B	81	PHE	CE1-CZ	5.37	1.47	1.37
1	A	403	GLU	CD-OE2	5.36	1.31	1.25
1	A	19[A]	LYS	CE-NZ	5.34	1.62	1.49
1	A	19[B]	LYS	CE-NZ	5.34	1.62	1.49
1	B	429[A]	GLN	CG-CD	-5.31	1.38	1.51
1	B	429[B]	GLN	CG-CD	-5.31	1.38	1.51
1	B	405	GLU	CG-CD	5.25	1.59	1.51
1	B	28	TYR	CD2-CE2	5.24	1.47	1.39
1	B	136	GLU	CB-CG	5.21	1.62	1.52
1	A	274	VAL	CB-CG1	5.19	1.63	1.52
1	B	403	GLU	CD-OE2	5.18	1.31	1.25
1	B	490[A]	GLU	CB-CG	5.16	1.61	1.52
1	B	490[B]	GLU	CB-CG	5.16	1.61	1.52
1	B	165	GLU	CG-CD	5.08	1.59	1.51
1	B	249	PHE	CE2-CZ	5.07	1.47	1.37
1	B	408	TRP	CE3-CZ3	5.07	1.47	1.38
1	A	293	VAL	CB-CG1	5.04	1.63	1.52
1	B	314	VAL	CB-CG2	5.04	1.63	1.52
1	B	28	TYR	CE2-CZ	-5.04	1.32	1.38
1	B	22	PHE	CE2-CZ	5.02	1.46	1.37

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	A	62	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	554	PRO	N-CA-CB	8.26	113.22	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	554	PRO	N-CA-CB	8.19	113.12	103.30
1	B	177	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	B	209	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	436	ASP	CB-CG-OD1	7.89	125.40	118.30
1	A	471	MET	CG-SD-CE	7.70	112.52	100.20
1	B	471	MET	CG-SD-CE	7.63	112.41	100.20
1	A	27	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	163	TYR	CZ-CE2-CD2	-7.16	113.36	119.80
1	A	377	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	163	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	A	200	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	B	428	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	428	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	451	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	347	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	B	81	PHE	CB-CG-CD2	-6.45	116.28	120.80
1	B	7	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	454	LEU	CB-CG-CD1	-6.32	100.25	111.00
1	A	553	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	532	ASP	CB-CG-OD1	6.22	123.89	118.30
1	A	343	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	62	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	105	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	386	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	330	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	386	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	27	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	300	LYS	CD-CE-NZ	-5.75	98.47	111.70
1	A	500	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	B	546[A]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	546[B]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	331	LEU	CB-CG-CD1	5.64	120.59	111.00
1	A	393	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	377	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	120	ASP	N-CA-CB	-5.59	100.54	110.60
1	A	177	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	8	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	327	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	A	200	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	436	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	258	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	300	LYS	CB-CG-CD	-5.45	97.42	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	84	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	A	361	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	B	300	LYS	CB-CG-CD	-5.41	97.53	111.60
1	B	60	TYR	CG-CD2-CE2	-5.39	116.99	121.30
1	A	445	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	B	250	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	B	27	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	250	PHE	CD1-CE1-CZ	-5.33	113.70	120.10
1	B	81	PHE	CD1-CE1-CZ	-5.27	113.77	120.10
1	A	9	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	B	112	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	A	473	HIS	N-CA-CB	-5.23	101.19	110.60
1	B	22	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	B	74	SER	CB-CA-C	5.20	119.98	110.10
1	A	308	GLU	CA-CB-CG	-5.16	102.04	113.40
1	A	401	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	60	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	60	TYR	CZ-CE2-CD2	-5.10	115.21	119.80
1	B	338	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	278	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	47	CYS	CA-CB-SG	-5.04	104.92	114.00

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	4304	0	4305	38	0
1	B	4312	0	4347	65	0
2	A	26	0	16	6	0
2	B	26	0	16	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
5	A	632	0	0	19	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	535	0	0	19	2
All	All	9847	0	8684	105	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 6.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207[A]:GLU:OE1	5:B:2220:HOH:O	1.54	1.19
1:B:547[A]:VAL:HG13	5:B:2314:HOH:O	1.59	1.03
1:A:153[B]:ARG:HD2	5:A:2223:HOH:O	0.86	1.01
1:B:522[A]:ASN:OD1	5:B:2508:HOH:O	1.90	0.89
1:A:219[B]:ARG:NH1	5:A:2288:HOH:O	1.99	0.87
1:B:254:HIS:HD2	1:B:256:GLY:H	1.20	0.86
1:B:209:ARG:HH21	1:B:303:ASN:HD22	1.22	0.85
1:B:219[A]:ARG:NH1	5:B:2236:HOH:O	2.10	0.84
1:A:522[A]:ASN:OD1	5:A:2601:HOH:O	1.95	0.83
1:B:254:HIS:CD2	1:B:256:GLY:H	2.02	0.77
1:B:219[C]:ARG:NH2	5:B:2240:HOH:O	2.05	0.77
1:A:308:GLU:OE1	5:A:2391:HOH:O	2.05	0.74
5:A:2147:HOH:O	2:B:600:TPP:H2	1.87	0.74
1:A:264:GLU:OE2	1:A:546[A]:ARG:HD3	1.87	0.74
2:A:600:TPP:H2	5:A:2367:HOH:O	1.86	0.73
1:B:11:ASP:O	1:B:15[B]:GLN:HG3	1.88	0.73
1:B:490[B]:GLU:OE1	5:B:2477:HOH:O	2.08	0.71
1:A:468:ILE:HG13	1:A:540[A]:LEU:HD11	1.72	0.71
5:A:2034:HOH:O	1:B:469[A]:GLU:OE2	2.10	0.70
1:B:319:TYR:HB3	1:B:322[B]:ILE:HD11	1.74	0.69
1:A:448:GLN:HE22	1:A:451:ARG:HH11	1.39	0.69
5:A:2245:HOH:O	1:B:555:PRO:CD	2.40	0.68
5:A:2245:HOH:O	1:B:555:PRO:HD3	1.94	0.68
1:B:203:LEU:O	1:B:207[A]:GLU:HG3	1.92	0.68
1:B:546[A]:ARG:HD3	5:B:2525:HOH:O	1.94	0.68
1:B:471:MET:HG3	1:B:540[B]:LEU:CD2	2.25	0.66
1:A:129[A]:ARG:NH2	5:A:2183:HOH:O	2.25	0.66
1:B:471:MET:HG3	1:B:540[B]:LEU:HD22	1.78	0.65
1:B:468:ILE:HG13	1:B:540[A]:LEU:HD11	1.79	0.65
1:B:312:VAL:HG23	1:B:322[A]:ILE:HD11	1.78	0.64
1:B:209:ARG:HH21	1:B:303:ASN:ND2	1.96	0.61
1:A:159[B]:LYS:HE2	5:A:2226:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ALA:O	1:B:430:HIS:HE1	1.85	0.59
1:B:430:HIS:CD2	5:B:2428:HOH:O	2.55	0.59
1:A:471:MET:HG3	1:A:540[B]:LEU:CD2	2.32	0.58
1:A:153[B]:ARG:NH2	1:A:181:ILE:O	2.36	0.58
1:A:159[B]:LYS:CE	5:A:2226:HOH:O	2.52	0.58
1:A:253:ASP:OD1	1:A:398:HIS:HD2	1.87	0.57
1:A:540[B]:LEU:HD23	1:A:540[B]:LEU:C	2.25	0.57
5:A:2245:HOH:O	1:B:555:PRO:HD2	2.04	0.57
1:A:19[B]:LYS:HD2	5:A:2025:HOH:O	2.04	0.56
1:B:182:ASP:O	5:B:2188:HOH:O	2.17	0.56
1:B:207[A]:GLU:CD	5:B:2220:HOH:O	2.16	0.56
1:B:322[A]:ILE:O	1:B:322[A]:ILE:HG13	2.04	0.56
1:B:466:TYR:CD1	2:B:600:TPP:H61	2.42	0.55
1:B:91:ASN:HD21	1:B:219[B]:ARG:HH11	1.54	0.54
1:A:160:LYS:NZ	5:A:2105:HOH:O	2.39	0.54
1:A:555:PRO:HB3	5:B:2199:HOH:O	2.08	0.53
1:A:477:TYR:HB3	1:B:46:TYR:CE1	2.44	0.53
1:B:254:HIS:HD2	1:B:256:GLY:N	2.00	0.53
1:B:546[B]:ARG:NH1	5:B:2526:HOH:O	2.34	0.52
1:A:467:THR:O	1:A:471:MET:HG2	2.10	0.52
1:B:219[A]:ARG:HB2	1:B:284:ALA:HB1	1.90	0.52
1:B:219[A]:ARG:CZ	5:B:2236:HOH:O	2.53	0.51
1:B:546[B]:ARG:NH2	5:B:2526:HOH:O	2.32	0.50
1:A:468:ILE:HG21	2:A:600:TPP:S1	2.52	0.50
1:A:545[A]:LYS:HG3	1:A:546[A]:ARG:CZ	2.41	0.50
1:B:430:HIS:HD2	5:B:2428:HOH:O	1.94	0.50
2:B:600:TPP:HN42	2:B:600:TPP:C2	2.24	0.50
1:B:468:ILE:HG21	2:B:600:TPP:S1	2.52	0.49
1:A:555:PRO:HA	5:B:2199:HOH:O	2.12	0.49
1:A:46:TYR:CE1	1:B:477:TYR:HB3	2.48	0.48
1:A:471:MET:HG3	1:A:540[B]:LEU:HD22	1.94	0.48
1:A:505[A]:ARG:HH11	1:A:505[A]:ARG:HG3	1.79	0.48
1:B:319:TYR:HB3	1:B:322[B]:ILE:CD1	2.44	0.47
1:B:545[B]:LYS:HG3	5:B:2458:HOH:O	2.14	0.47
1:B:468:ILE:HG13	1:B:540[A]:LEU:CD1	2.45	0.47
1:B:15[B]:GLN:HG3	5:B:2009:HOH:O	2.14	0.47
1:B:415:VAL:HB	1:B:416:PRO:HD3	1.97	0.47
1:B:290:TYR:CE1	1:B:547[A]:VAL:HG11	2.49	0.46
1:A:466:TYR:CD1	2:A:600:TPP:H61	2.51	0.46
1:A:471:MET:HB2	1:A:540[B]:LEU:HD21	1.96	0.46
1:B:27:ASP:HA	1:B:30:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153[B]:ARG:HD3	5:A:2222:HOH:O	2.15	0.46
1:B:415:VAL:HB	1:B:416:PRO:CD	2.46	0.46
1:B:467:THR:O	1:B:471:MET:HG2	2.14	0.46
1:B:309[B]:ARG:HG2	1:B:310:HIS:CD2	2.51	0.45
1:A:217:GLY:HA3	1:A:285:PRO:HA	1.99	0.44
1:B:89:ALA:HB1	1:B:407:GLN:HG3	1.99	0.44
1:B:234:ASP:OD1	1:B:254:HIS:HE1	2.00	0.44
1:B:74:SER:HB3	1:B:114:HIS:O	2.19	0.43
1:A:554:PRO:O	5:A:2627:HOH:O	2.21	0.43
1:B:468:ILE:CG2	2:B:600:TPP:S1	3.07	0.43
1:B:471:MET:CG	1:B:540[B]:LEU:CD2	2.96	0.43
1:A:319:TYR:HB3	1:A:322[B]:ILE:CD1	2.49	0.43
1:A:25:ALA:HB2	1:B:477:TYR:HB2	2.01	0.42
1:B:228:GLN:HB3	1:B:328:LEU:HB2	2.01	0.42
1:A:337[B]:ARG:NH2	5:A:2310:HOH:O	2.28	0.42
1:A:468:ILE:CG2	2:A:600:TPP:S1	3.06	0.42
1:B:153:ARG:HH11	1:B:182:ASP:HA	1.84	0.42
1:A:50:GLU:OE2	2:B:600:TPP:N1'	2.53	0.42
2:B:600:TPP:H2	2:B:600:TPP:HN42	1.84	0.42
1:A:159[B]:LYS:NZ	5:A:2226:HOH:O	2.53	0.41
1:B:91:ASN:HD21	1:B:219[B]:ARG:NH1	2.17	0.41
1:B:466:TYR:HB3	2:B:600:TPP:H62	2.03	0.41
1:A:505[A]:ARG:HG3	1:A:505[A]:ARG:NH1	2.36	0.41
2:A:600:TPP:HN42	2:A:600:TPP:C2	2.33	0.41
1:B:86:GLY:HA2	1:B:408:TRP:CG	2.56	0.41
1:B:422:ALA:HA	1:B:430:HIS:CE1	2.56	0.41
1:B:468:ILE:HA	1:B:540[A]:LEU:HD21	2.03	0.41
1:B:547[A]:VAL:CG1	5:B:2314:HOH:O	2.38	0.41
1:A:466:TYR:HB3	2:A:600:TPP:H62	2.03	0.40
1:B:414:SER:HB2	1:B:432:LEU:HD11	2.03	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)
5:A:2134:HOH:O	5:B:2106:HOH:O[2_554]	2.07	0.13
5:A:2125:HOH:O	5:B:2106:HOH:O[2_554]	2.17	0.03

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	580/558 (104%)	566 (98%)	14 (2%)	0	100	100
1	B	582/558 (104%)	571 (98%)	11 (2%)	0	100	100
All	All	1162/1116 (104%)	1137 (98%)	25 (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	437/410 (107%)	432 (99%)	5 (1%)	73	63
1	B	439/410 (107%)	437 (100%)	2 (0%)	88	83
All	All	876/820 (107%)	869 (99%)	7 (1%)	86	74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	GLU
1	A	545[A]	LYS
1	A	545[B]	LYS
1	A	546[A]	ARG
1	A	546[B]	ARG
1	B	58	GLU
1	B	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	44	GLN
1	A	208	GLN
1	A	334	HIS
1	A	398	HIS
1	A	448	GLN
1	A	464	HIS
1	B	44	GLN
1	B	91	ASN
1	B	254	HIS
1	B	303	ASN
1	B	430	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 monosaccharides 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	SO4	A	1557	-	4,4,4	0.63	0	6,6,6	1.07	1 (16%)
4	SO4	A	1556	-	4,4,4	0.30	0	6,6,6	0.91	0
2	TPP	B	600	3	22,27,27	2.89	7 (31%)	29,40,40	1.62	8 (27%)
2	TPP	A	600	3	22,27,27	2.93	9 (40%)	29,40,40	1.88	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
2	TPP	B	600	3	-	4/16/17/17	0/2/2/2
2	TPP	A	600	3	-	2/16/17/17	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	TPP	C4-N3	-9.00	1.31	1.39
2	A	600	TPP	PB-O1B	8.02	1.76	1.50
2	A	600	TPP	C4-N3	-6.72	1.33	1.39
2	B	600	TPP	PB-O2B	-5.79	1.32	1.54
2	B	600	TPP	CM4-C4	4.28	1.58	1.49
2	A	600	TPP	C2-N3	3.96	1.44	1.36
2	A	600	TPP	C6-C5	-3.57	1.49	1.50
2	A	600	TPP	C2'-N1'	3.47	1.39	1.34
2	B	600	TPP	C6-C5	-3.43	1.49	1.50
2	A	600	TPP	PB-O3B	-3.22	1.42	1.54
2	B	600	TPP	C7'-C5'	3.22	1.57	1.51
2	B	600	TPP	C4'-N4'	3.05	1.41	1.34
2	A	600	TPP	CM4-C4	2.83	1.55	1.49
2	B	600	TPP	C7'-N3	2.49	1.53	1.48
2	A	600	TPP	C7'-C5'	2.29	1.56	1.51
2	A	600	TPP	O7-C7	2.02	1.53	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	TPP	C5-C4-N3	4.42	116.42	107.57
2	A	600	TPP	C7'-N3-C2	-3.79	118.50	125.35
2	A	600	TPP	O3B-PB-O1B	3.66	125.02	110.68
2	A	600	TPP	CM4-C4-C5	-3.53	119.88	127.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	TPP	CM2-C2'-N1'	2.92	120.35	117.14
2	B	600	TPP	C7'-N3-C2	-2.73	120.42	125.35
2	B	600	TPP	N1'-C2'-N3'	-2.73	120.84	125.54
2	B	600	TPP	C2'-N3'-C4'	2.67	122.24	118.08
2	A	600	TPP	O3A-PB-O1B	-2.67	96.40	111.19
2	B	600	TPP	N4'-C4'-N3'	2.51	120.58	117.03
4	A	1557	SO4	O4-S-O3	2.23	118.58	109.06
2	B	600	TPP	CM2-C2'-N3'	2.20	120.58	117.15
2	B	600	TPP	C5-C4-N3	2.19	111.96	107.57
2	B	600	TPP	CM4-C4-C5	-2.16	122.87	127.60
2	B	600	TPP	C5'-C6'-N1'	-2.07	120.38	123.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	TPP	C4-C5-C6-C7
2	A	600	TPP	PA-O3A-PB-O2B
2	B	600	TPP	C4-C5-C6-C7
2	B	600	TPP	PA-O3A-PB-O2B
2	B	600	TPP	PA-O3A-PB-O3B
2	B	600	TPP	PA-O3A-PB-O1B

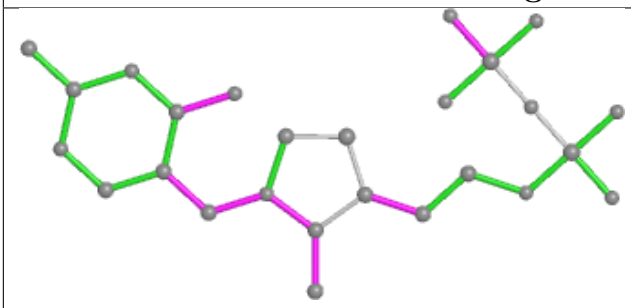
There are no ring outliers.

2 monomers are involved in 14 short contacts:

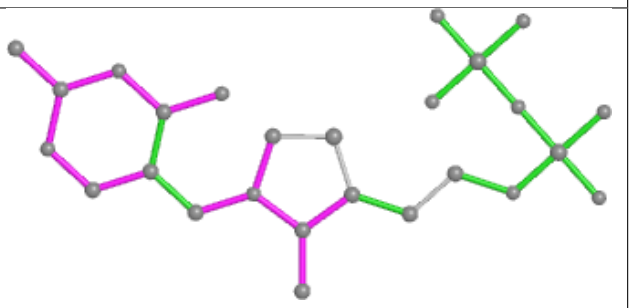
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	TPP	8	0
2	A	600	TPP	6	0

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 then 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.

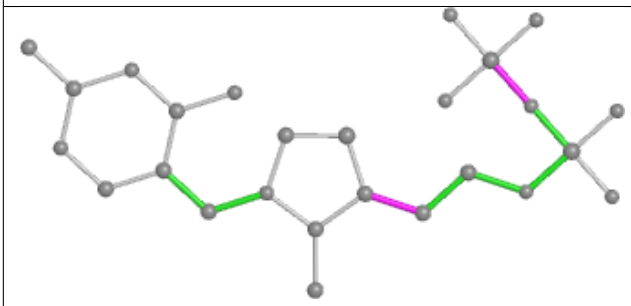
Ligand TPP B 600



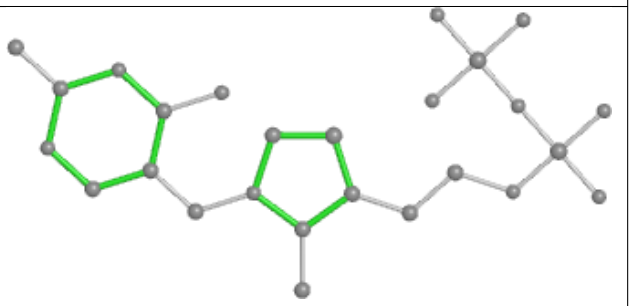
Bond lengths



Bond angles

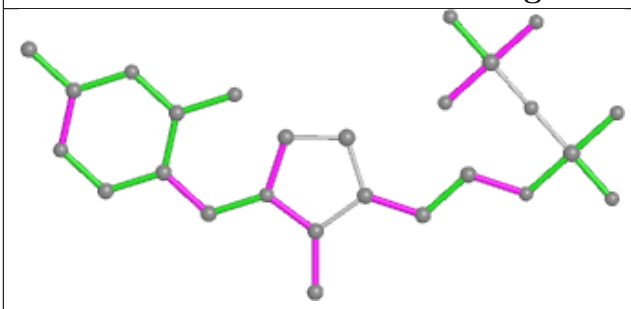


Torsions

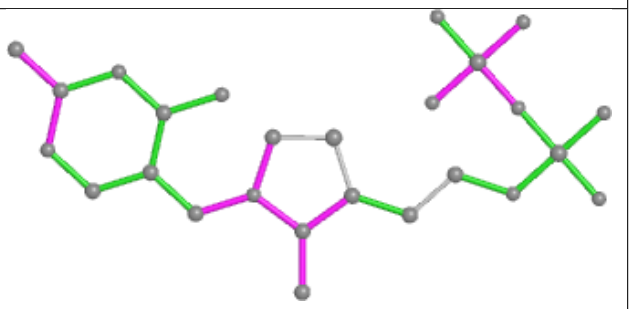


Rings

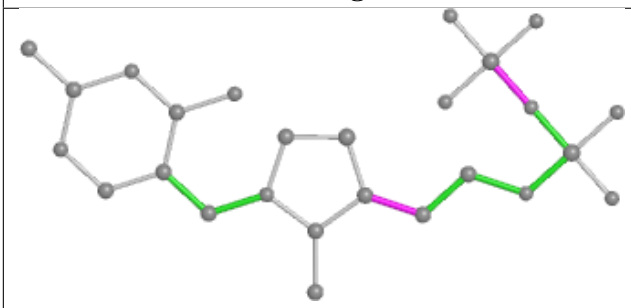
Ligand TPP A 600



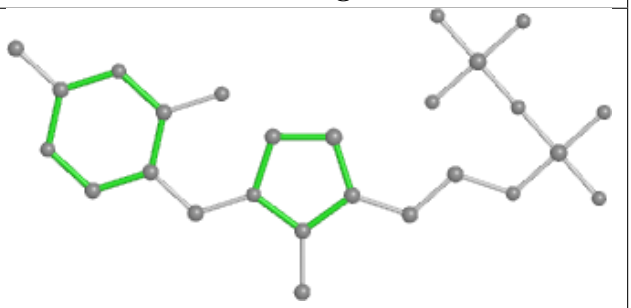
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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^{th} 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	549/558 (98%)	-0.62	8 (1%)	73 77	7, 11, 22, 52	0
1	B	549/558 (98%)	-0.49	11 (2%)	65 69	7, 12, 24, 52	0
All	All	1098/1116 (98%)	-0.56	19 (1%)	70 74	7, 12, 23, 52	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.5
1	B	1	MET	5.5
1	B	555	PRO	5.2
1	A	190	PRO	4.6
1	A	183	ALA	4.1
1	B	183	ALA	3.8
1	A	555	PRO	3.7
1	A	2	THR	3.6
1	B	2	THR	3.0
1	B	556	ARG	3.0
1	B	181	ILE	2.8
1	B	356	ALA	2.6
1	B	322[A]	ILE	2.6
1	B	554	PRO	2.6
1	B	472	ILE	2.5
1	B	193	ALA	2.4
1	A	181	ILE	2.3
1	A	472	ILE	2.2
1	A	191	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

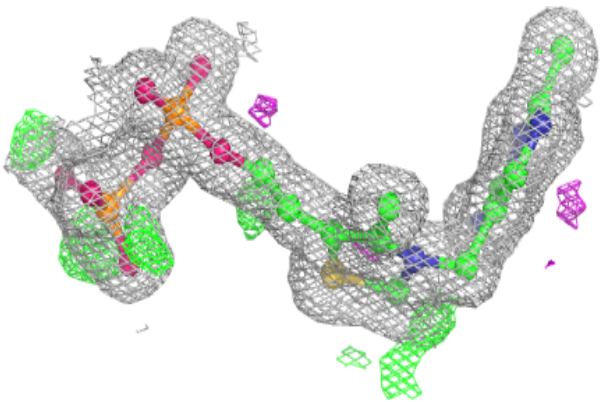
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

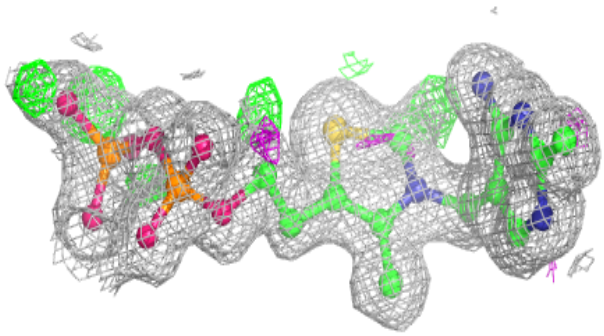
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1557	5/5	0.39	0.24	49,62,66,71	0
4	SO4	A	1556	5/5	0.92	0.24	74,74,75,75	0
2	TPP	A	600	26/26	0.98	0.06	6,11,20,25	0
2	TPP	B	600	26/26	0.98	0.09	8,12,23,26	0
3	MG	A	601	1/1	1.00	0.02	8,8,8,8	0
3	MG	B	601	1/1	1.00	0.04	11,11,11,11	0

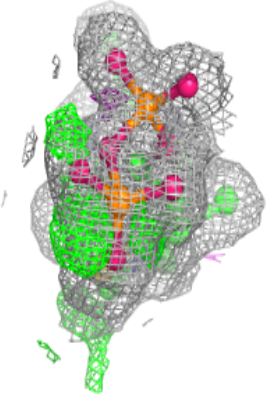
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 600:

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

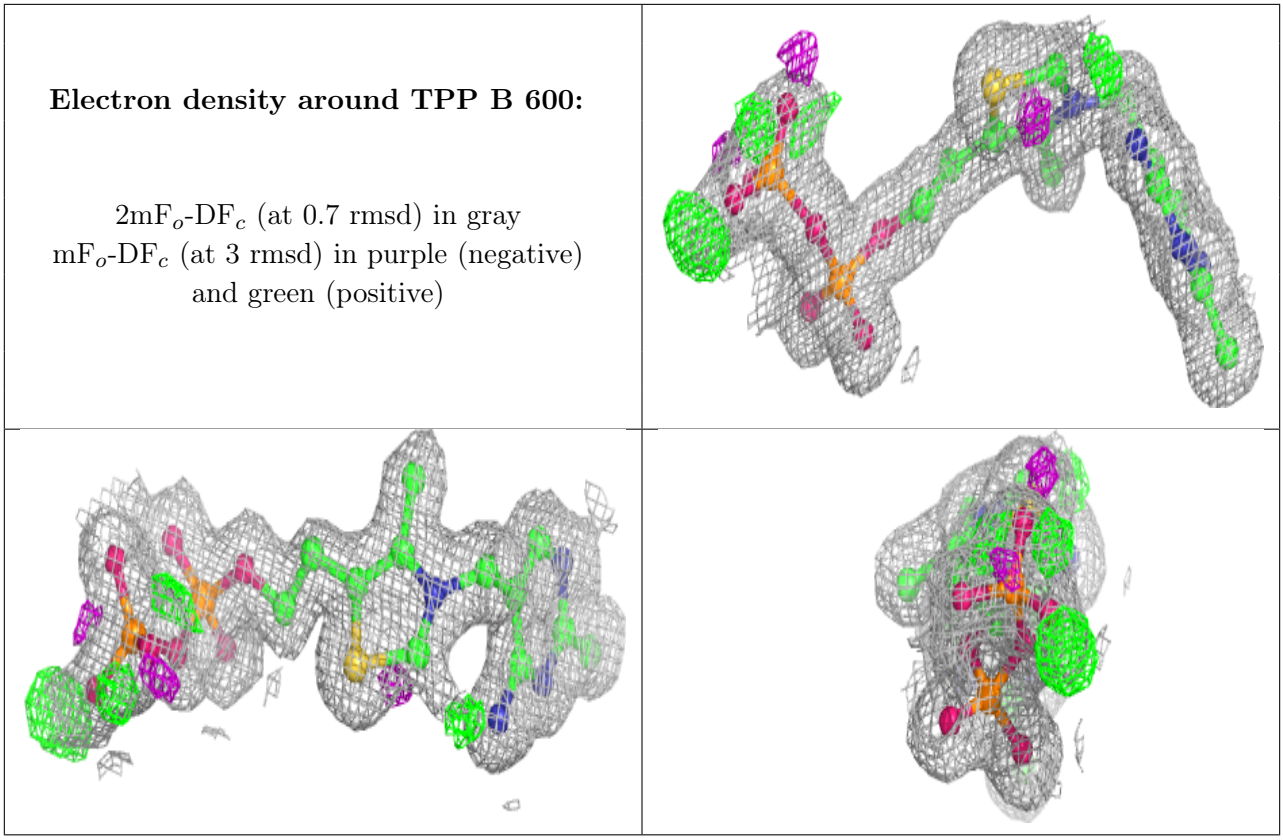






Electron density around TPP B 600:

$2mF_o$-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.