



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:36 AM UTC

PDB ID : 4COK / pdb_00004cok
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

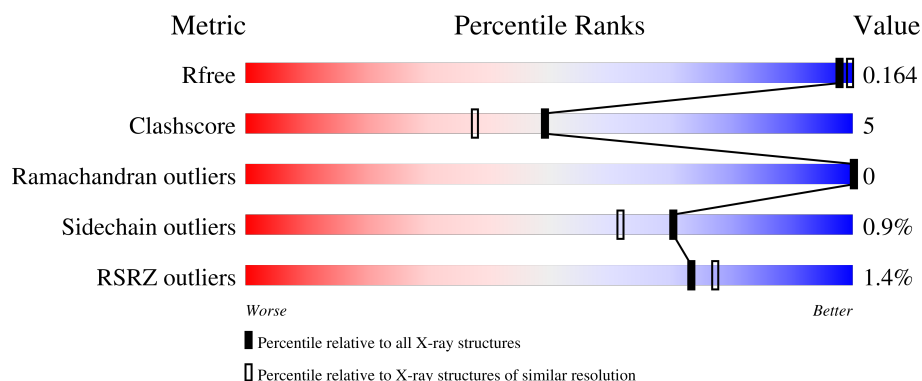
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

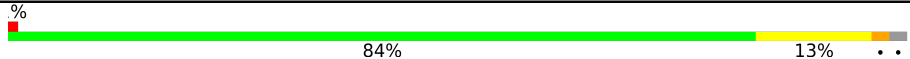
The reported resolution of this entry is 1.69 Å.

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. 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	558	
1	B	558	

2 Entry composition [i](#)

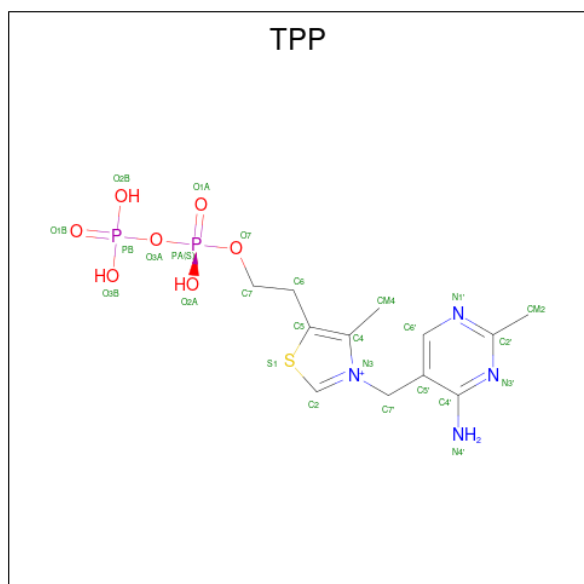
There are 5 unique types of molecules in this entry. The entry contains 9847 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

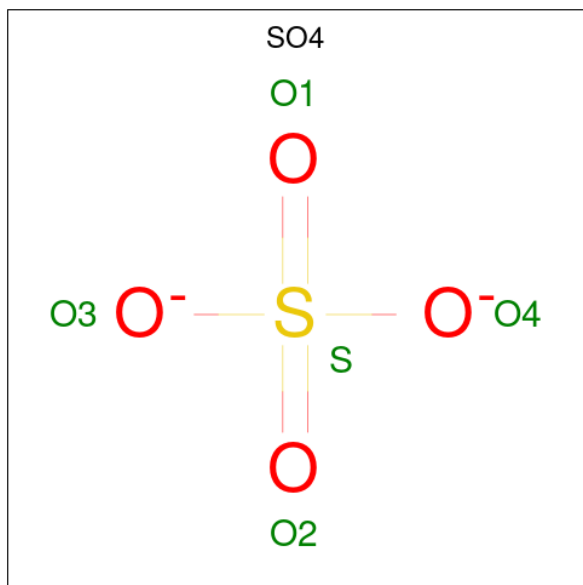


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	
2	B	1	Total	C	N	O	P	S	0
			26	12	4	7	2	1	

- Molecule 3 is MAGNESIUM ION (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

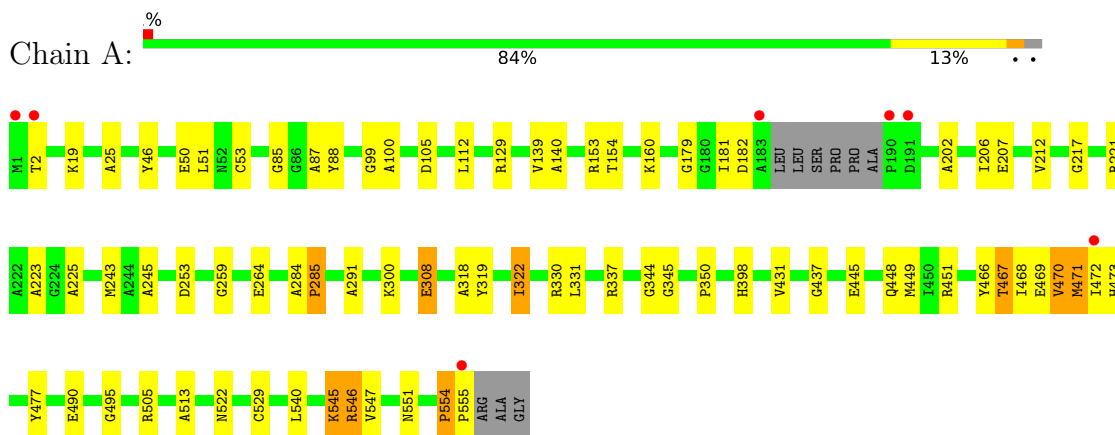
- Molecule 5 is water.

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

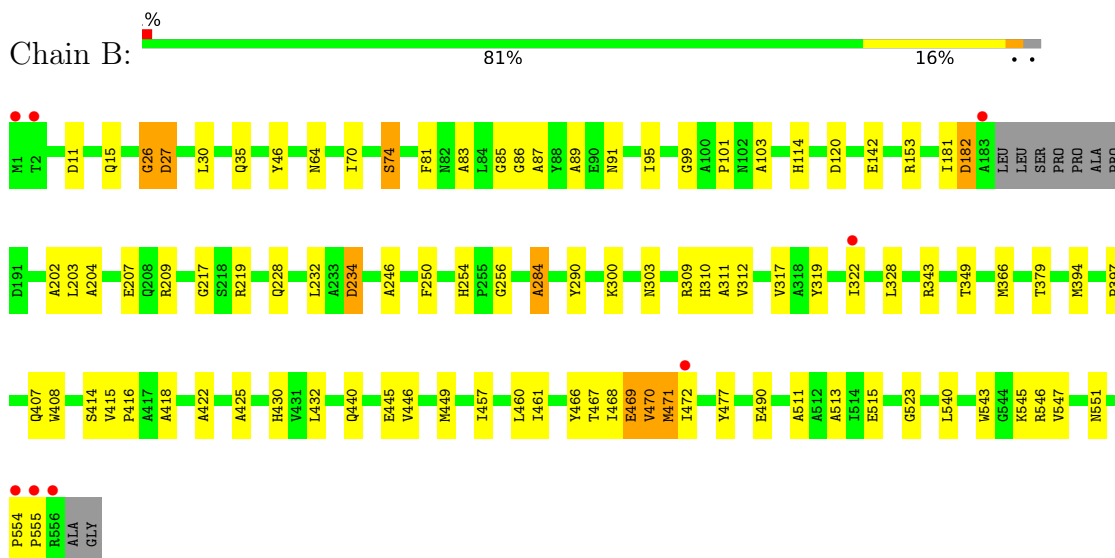
3 Residue-property plots

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



• Molecule 1: PYRUVATE DECARBOXYLASE



4 Data and refinement statistics

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 84.06 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (84.06-1.69) 99.4 (84.06-1.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TPP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.76	54/4483 (1.2%)	1.47	24/6091 (0.4%)
1	B	1.77	42/4506 (0.9%)	1.48	23/6124 (0.4%)
All	All	1.77	96/8989 (1.1%)	1.47	47/12215 (0.4%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	ALA	CA-CB	12.80	1.61	1.52
1	A	472	ILE	CA-CB	9.10	1.65	1.54
1	B	83	ALA	CA-CB	8.50	1.67	1.53
1	A	471	MET	SD-CE	8.38	2.00	1.79
1	A	467	THR	C-O	8.21	1.33	1.24
1	B	511	ALA	CA-CB	8.13	1.66	1.53
1	A	490	GLU	CD-OE2	7.91	1.40	1.25
1	B	234	ASP	N-CA	7.80	1.55	1.46
1	A	513	ALA	CA-CB	7.73	1.65	1.53
1	B	217	GLY	N-CA	7.70	1.52	1.44
1	B	470	VAL	CA-C	7.55	1.62	1.52
1	A	179	GLY	N-CA	7.52	1.52	1.45
1	A	284	ALA	C-O	7.23	1.27	1.23
1	A	490	GLU	N-CA	7.21	1.55	1.46
1	A	284	ALA	CA-CB	7.06	1.57	1.52
1	B	472	ILE	CA-CB	6.91	1.62	1.54
1	B	471	MET	SD-CE	6.85	1.96	1.79
1	B	471	MET	N-CA	6.81	1.54	1.46
1	A	100	ALA	CA-CB	6.68	1.62	1.53
1	A	322[A]	ILE	C-O	6.61	1.31	1.24
1	A	322[B]	ILE	C-O	6.61	1.31	1.24
1	A	490	GLU	CG-CD	6.54	1.68	1.52
1	B	470	VAL	N-CA	-6.53	1.38	1.46
1	B	120	ASP	N-CA	6.48	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	THR	CA-CB	-6.46	1.44	1.53
1	B	103	ALA	CA-CB	6.40	1.63	1.53
1	B	397	PRO	C-O	6.36	1.31	1.23
1	B	70	ILE	CG1-CD1	-6.25	1.27	1.51
1	A	318	ALA	C-O	6.17	1.31	1.24
1	B	74	SER	CB-OG	-6.13	1.29	1.42
1	A	330	ARG	N-CA	6.10	1.53	1.46
1	B	418	ALA	N-CA	5.99	1.53	1.46
1	A	449	MET	CA-CB	5.97	1.62	1.53
1	A	53	CYS	N-CA	5.93	1.53	1.46
1	A	206	ILE	C-O	5.89	1.30	1.24
1	B	27	ASP	C-O	5.88	1.31	1.24
1	A	285	PRO	C-O	5.85	1.30	1.23
1	A	85	GLY	CA-C	5.82	1.58	1.52
1	B	246	ALA	CA-CB	5.79	1.61	1.53
1	A	243	MET	N-CA	5.77	1.53	1.45
1	B	513	ALA	CA-CB	5.77	1.62	1.53
1	A	2	THR	N-CA	5.74	1.53	1.46
1	A	472	ILE	CA-C	5.71	1.58	1.52
1	A	51	LEU	N-CA	5.71	1.53	1.46
1	A	551	ASN	CA-CB	5.70	1.62	1.53
1	A	88	TYR	CA-C	5.67	1.59	1.52
1	A	140	ALA	N-CA	5.51	1.53	1.46
1	B	515	GLU	CG-CD	5.48	1.65	1.52
1	A	331	LEU	CA-CB	5.46	1.61	1.53
1	B	202	ALA	N-CA	5.46	1.53	1.46
1	B	64	ASN	CA-C	-5.45	1.45	1.52
1	A	87	ALA	N-CA	5.45	1.53	1.46
1	B	87	ALA	N-CA	5.45	1.52	1.46
1	A	225	ALA	N-CA	5.44	1.52	1.46
1	B	446	VAL	N-CA	5.42	1.53	1.46
1	B	349	THR	C-O	5.41	1.29	1.24
1	A	154	THR	N-CA	5.41	1.52	1.46
1	A	259	GLY	N-CA	5.41	1.53	1.45
1	B	457	ILE	CA-CB	5.38	1.60	1.54
1	A	245	ALA	N-CA	5.35	1.53	1.46
1	A	345	GLY	N-CA	5.33	1.49	1.44
1	B	449	MET	N-CA	5.31	1.52	1.46
1	B	366	MET	CA-CB	5.29	1.61	1.53
1	B	317	VAL	C-O	-5.28	1.18	1.24
1	B	461	ILE	CA-CB	5.28	1.59	1.53
1	A	206	ILE	CA-CB	-5.27	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	ALA	CA-CB	5.27	1.62	1.53
1	A	112	LEU	N-CA	5.26	1.52	1.45
1	A	472	ILE	CB-CG2	5.26	1.70	1.52
1	A	495	GLY	N-CA	5.23	1.53	1.45
1	B	343	ARG	CB-CG	-5.22	1.36	1.52
1	A	221	ARG	CD-NE	5.21	1.53	1.46
1	A	291	ALA	CA-CB	5.20	1.61	1.53
1	B	311	ALA	N-CA	5.19	1.52	1.46
1	A	212	VAL	N-CA	5.18	1.52	1.46
1	A	437	GLY	N-CA	5.17	1.52	1.45
1	A	473	HIS	N-CA	5.17	1.52	1.46
1	B	551	ASN	CA-CB	5.15	1.61	1.53
1	A	547[A]	VAL	N-CA	-5.13	1.40	1.46
1	A	547[B]	VAL	N-CA	-5.13	1.40	1.46
1	A	554	PRO	CA-C	-5.12	1.47	1.52
1	A	470	VAL	CA-C	5.11	1.59	1.52
1	B	250	PHE	CA-C	5.11	1.57	1.52
1	B	551	ASN	CG-ND2	5.09	1.44	1.33
1	A	207[A]	GLU	C-O	5.09	1.30	1.24
1	A	207[B]	GLU	C-O	5.09	1.30	1.24
1	B	142	GLU	CG-CD	5.08	1.64	1.52
1	A	431	VAL	C-O	-5.07	1.18	1.24
1	B	523	GLY	N-CA	5.04	1.51	1.44
1	B	394[A]	MET	C-O	-5.04	1.17	1.23
1	B	394[B]	MET	C-O	-5.04	1.17	1.23
1	B	81	PHE	CD1-CE1	5.03	1.53	1.38
1	A	318	ALA	CA-CB	5.03	1.60	1.53
1	A	529	CYS	N-CA	5.03	1.52	1.46
1	A	202	ALA	CA-C	5.01	1.59	1.52
1	B	85	GLY	CA-C	5.00	1.57	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	ILE	N-CA-C	-12.94	100.68	111.81
1	B	472	ILE	N-CA-C	-11.70	101.75	111.81
1	B	554	PRO	N-CA-CB	10.45	113.22	103.08
1	A	554	PRO	N-CA-CB	10.35	113.12	103.08
1	A	471	MET	N-CA-C	7.40	122.33	113.16
1	A	470	VAL	N-CA-C	-7.00	102.64	110.62
1	A	51	LEU	N-CA-C	-6.66	103.94	111.07
1	A	2	THR	N-CA-CB	6.65	119.75	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ALA	N-CA-C	-6.55	103.63	111.69
1	A	88	TYR	N-CA-C	-6.38	104.25	111.14
1	A	99	GLY	N-CA-C	-6.32	104.45	112.54
1	A	344	GLY	CA-C-N	-6.13	116.07	122.69
1	A	344	GLY	C-N-CA	-6.13	116.07	122.69
1	A	350	PRO	CB-CA-C	-6.05	103.16	111.21
1	A	300	LYS	CB-CG-CD	-6.03	97.42	111.30
1	A	308	GLU	CA-CB-CG	-6.03	102.04	114.10
1	B	471	MET	N-CA-C	5.99	120.21	113.02
1	B	300	LYS	CB-CG-CD	-5.99	97.53	111.30
1	B	470	VAL	N-CA-C	-5.86	103.08	111.17
1	B	120	ASP	N-CA-CB	-5.74	100.54	110.17
1	A	547[A]	VAL	CA-C-O	5.73	126.65	120.47
1	A	547[B]	VAL	CA-C-O	5.73	126.65	120.47
1	B	543	TRP	CA-C-N	5.66	126.27	119.98
1	B	543	TRP	C-N-CA	5.66	126.27	119.98
1	B	35	GLN	N-CA-C	-5.63	105.22	111.36
1	A	139	VAL	N-CA-C	-5.52	107.74	113.10
1	A	473	HIS	N-CA-CB	-5.50	101.19	110.49
1	B	101	PRO	CB-CA-C	-5.46	104.24	111.23
1	A	437	GLY	N-CA-C	-5.43	106.22	112.73
1	B	99	GLY	N-CA-C	-5.31	105.74	112.54
1	A	179	GLY	O-C-N	-5.29	119.87	123.95
1	A	471	MET	CG-SD-CE	5.28	112.52	100.90
1	B	120	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	471	MET	CG-SD-CE	5.23	112.41	100.90
1	B	232	LEU	N-CA-C	-5.22	105.67	111.36
1	B	95	ILE	N-CA-C	-5.21	100.24	107.80
1	B	85	GLY	N-CA-C	-5.15	106.55	112.73
1	B	182	ASP	N-CA-C	-5.15	107.17	113.50
1	A	105	ASP	CA-C-N	-5.14	113.58	120.87
1	A	105	ASP	C-N-CA	-5.14	113.58	120.87
1	A	449	MET	N-CA-C	-5.13	105.58	111.07
1	B	26	GLY	CA-C-N	-5.10	112.93	120.28
1	B	26	GLY	C-N-CA	-5.10	112.93	120.28
1	B	440	GLN	CA-CB-CG	-5.08	103.94	114.10
1	A	182	ASP	N-CA-C	-5.08	107.22	113.41
1	B	551	ASN	CB-CA-C	-5.08	102.05	110.68
1	B	27	ASP	N-CA-C	5.05	117.51	111.71

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	4304	0	4305	34	0
1	B	4312	0	4347	58	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	14	2
5	B	535	0	0	11	2
All	All	9847	0	8684	94	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 5.

All (94) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:540[B]:LEU:HD23	1:A:540[B]:LEU:C	2.25	0.62
1:B:209:ARG:HH21	1:B:303:ASN:ND2	1.96	0.61
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:253:ASP:OD1	1:A:398:HIS:HD2	1.87	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:469[B]:GLU:O	1:A:470:VAL:C	2.63	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:26:GLY:O	1:B:27:ASP:C	2.63	0.40
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

5.3.1 Protein backbone

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

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%)	65	54
1	B	439/410 (107%)	434 (99%)	5 (1%)	65	54
All	All	876/820 (107%)	866 (99%)	10 (1%)	70	54

All (10) 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	181	ILE
1	B	445	GLU
1	B	460	LEU

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Mol	Chain	Res	Type
1	B	469[A]	GLU
1	B	469[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	334	HIS
1	A	363	ASN
1	A	390	ASN
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	363	ASN
1	B	390	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 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	SO4	A	1556	-	4,4,4	0.40	0	6,6,6	0.75	0
2	TPP	B	600	3	26,27,27	2.38	10 (38%)	38,40,40	1.68	10 (26%)
4	SO4	A	1557	-	4,4,4	0.68	0	6,6,6	0.94	0
2	TPP	A	600	3	26,27,27	2.74	10 (38%)	38,40,40	1.84	10 (26%)

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	-	3/17/17/17	0/2/2/2
2	TPP	A	600	3	-	1/17/17/17	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	TPP	PB-O1B	8.34	1.76	1.50
2	B	600	TPP	PB-O2B	-5.99	1.32	1.54
2	A	600	TPP	C2-N3	4.90	1.44	1.32
2	A	600	TPP	C2-S1	4.78	1.83	1.69
2	B	600	TPP	CM4-C4	4.35	1.58	1.49
2	B	600	TPP	C4-N3	-3.89	1.31	1.39
2	B	600	TPP	C5-C4	3.85	1.43	1.35
2	B	600	TPP	C7'-C5'	3.68	1.57	1.51
2	A	600	TPP	C2'-N1'	3.67	1.39	1.34
2	B	600	TPP	C2-S1	3.41	1.79	1.69
2	A	600	TPP	PB-O3B	-3.33	1.42	1.54
2	A	600	TPP	C5-C4	3.17	1.41	1.35
2	B	600	TPP	C4'-N4'	2.96	1.41	1.34
2	A	600	TPP	C4-N3	-2.92	1.33	1.39
2	A	600	TPP	CM4-C4	2.90	1.55	1.49
2	A	600	TPP	C7'-C5'	2.65	1.56	1.51
2	B	600	TPP	C2-N3	2.42	1.38	1.32
2	B	600	TPP	C7'-N3	2.16	1.53	1.48
2	A	600	TPP	O7-C7	2.10	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	TPP	C5-S1	2.01	1.78	1.72

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	TPP	S1-C2-N3	-4.50	106.60	112.30
2	B	600	TPP	C2-S1-C5	-4.19	88.44	91.22
2	A	600	TPP	O3B-PB-O1B	3.64	125.02	110.83
2	A	600	TPP	O2A-PA-O3A	3.50	116.74	107.27
2	A	600	TPP	CM4-C4-C5	-3.07	119.88	127.75
2	A	600	TPP	O3A-PA-O1A	-2.97	101.78	110.70
2	A	600	TPP	CM2-C2'-N1'	2.95	120.35	117.20
2	B	600	TPP	N1'-C2'-N3'	-2.82	120.84	125.53
2	A	600	TPP	O3A-PB-O1B	-2.78	96.40	111.04
2	B	600	TPP	C2'-N3'-C4'	2.69	122.24	118.10
2	B	600	TPP	O2A-PA-O3A	2.63	114.39	107.27
2	B	600	TPP	N4'-C4'-N3'	2.63	120.58	117.03
2	A	600	TPP	C5-C4-N3	2.61	116.42	111.67
2	B	600	TPP	O3A-PA-O1A	-2.58	102.94	110.70
2	A	600	TPP	O7-C7-C6	-2.53	98.46	108.63
2	A	600	TPP	C7'-N3-C2	-2.39	118.50	123.48
2	B	600	TPP	C6'-C5'-C4'	2.35	118.44	115.55
2	B	600	TPP	CM2-C2'-N3'	2.31	120.58	117.13
2	B	600	TPP	C5'-C6'-N1'	-2.12	120.38	123.83
2	B	600	TPP	C2-N3-C4	2.08	116.87	114.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

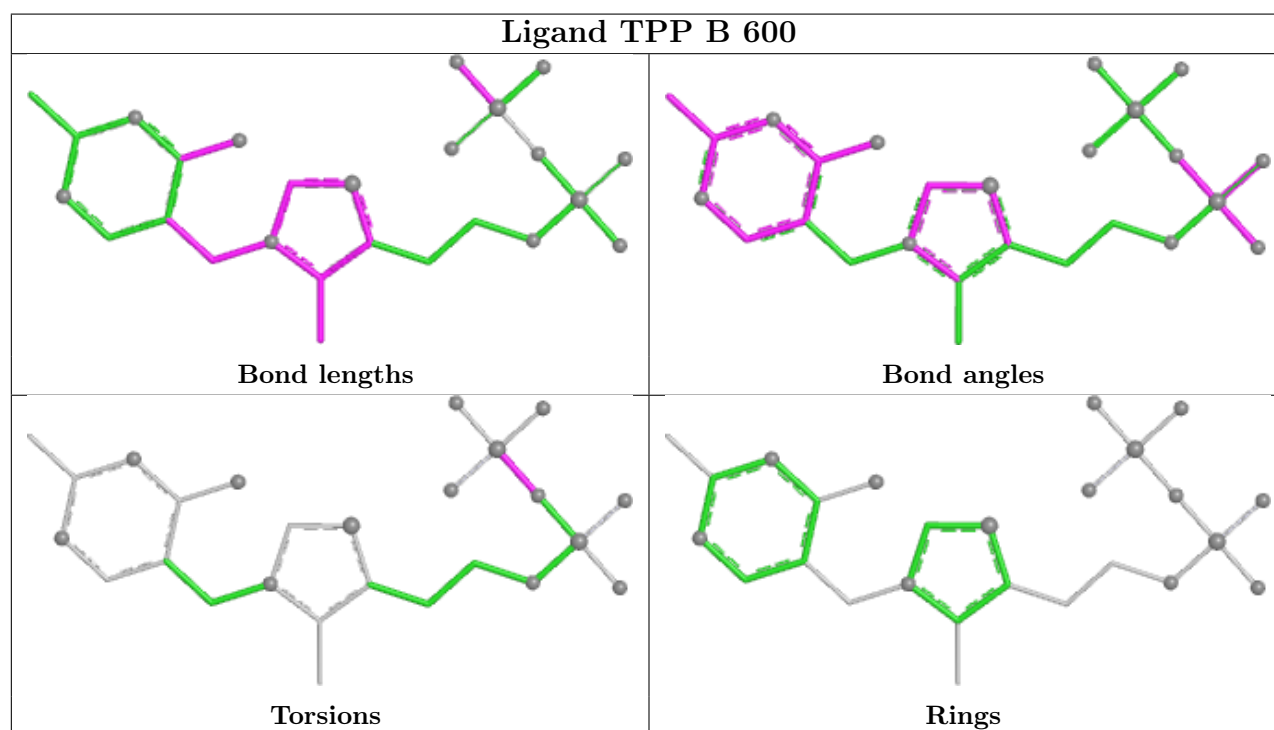
Mol	Chain	Res	Type	Atoms
2	A	600	TPP	PA-O3A-PB-O2B
2	B	600	TPP	PA-O3A-PB-O2B
2	B	600	TPP	PA-O3A-PB-O3B
2	B	600	TPP	PA-O3A-PB-O1B

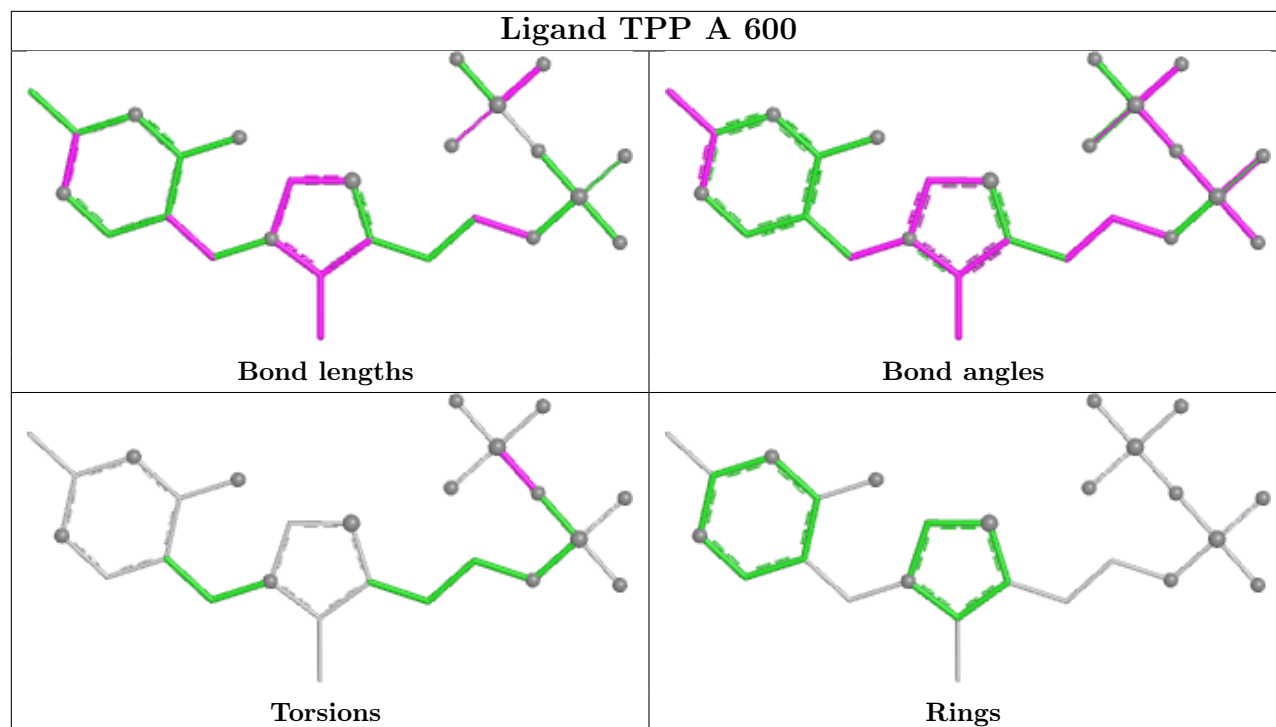
There are no ring outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	549/558 (98%)	-0.83	7 (1%) 75 79	5, 11, 22, 52	35 (6%)
1	B	549/558 (98%)	-0.75	8 (1%) 72 76	5, 12, 24, 52	36 (6%)
All	All	1098/1116 (98%)	-0.79	15 (1%) 73 77	5, 11, 23, 52	71 (6%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	555	PRO	4.7
1	A	183	ALA	4.5
1	B	183	ALA	4.0
1	B	1	MET	3.5
1	A	555	PRO	3.4
1	B	472	ILE	3.1
1	B	2	THR	3.1
1	A	191	ASP	2.7
1	A	472	ILE	2.6
1	A	190	PRO	2.6
1	B	554	PRO	2.5
1	B	322[A]	ILE	2.4
1	A	2	THR	2.2
1	A	1	MET	2.2
1	B	556	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

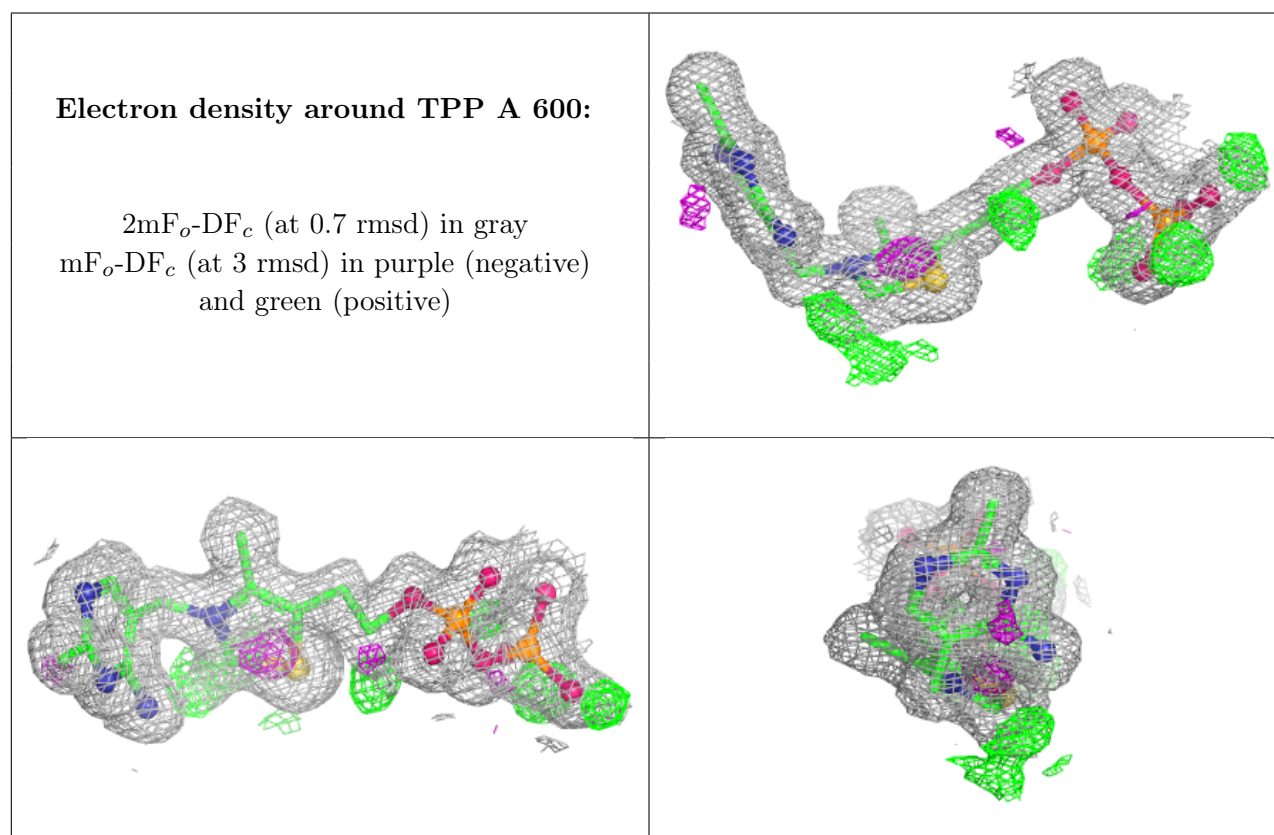
There are no oligosaccharides in this entry.

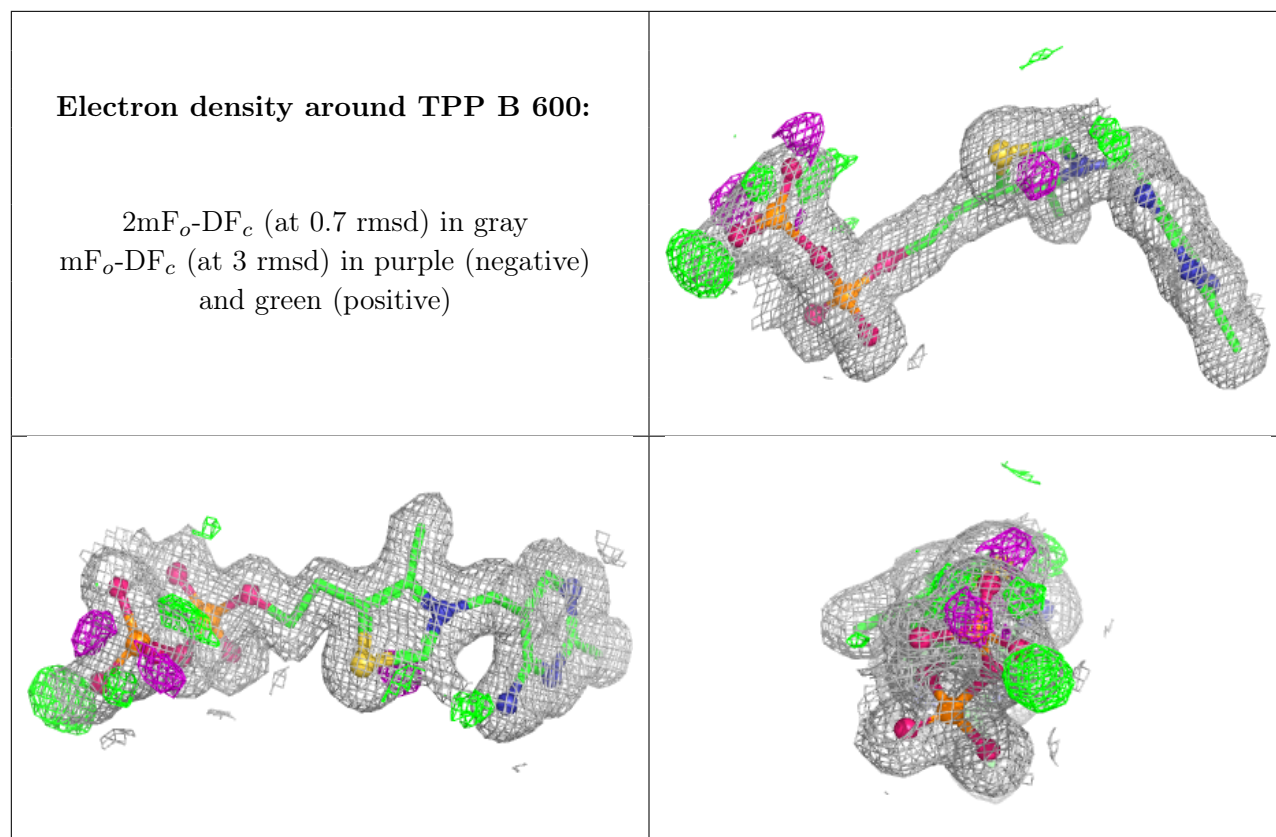
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1557	5/5	0.63	0.18	49,62,66,71	0
4	SO4	A	1556	5/5	0.85	0.17	74,74,75,75	0
2	TPP	A	600	26/26	0.98	0.05	6,11,20,25	0
2	TPP	B	600	26/26	0.98	0.05	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	0.05	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.