



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:04 PM UTC

PDB ID : 1QGD / pdb_00001qgd
Title : TRANSKETOLASE FROM ESCHERICHIA COLI
Authors : Isupov, M.N.; Littlechild, J.A.
Deposited on : 1999-04-23
Resolution : 1.90 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

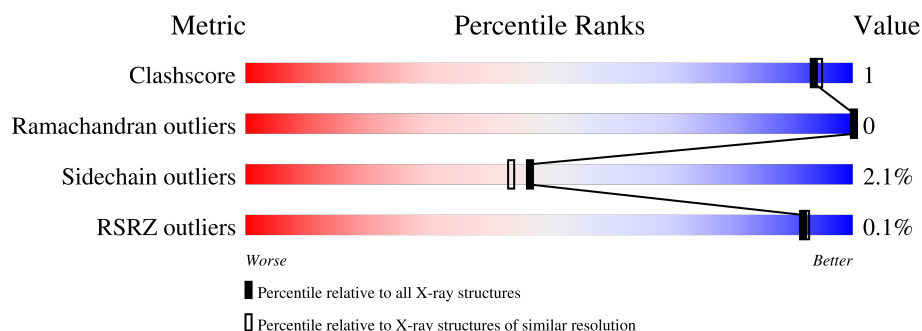
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	662	 93% 7%
1	B	662	 92% 6% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11273 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 PROTEIN (TRANSKETOLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	4	0
			5072	3206	874	966	26			
1	B	662	Total	C	N	O	S	0	5	0
			5072	3206	874	966	26			

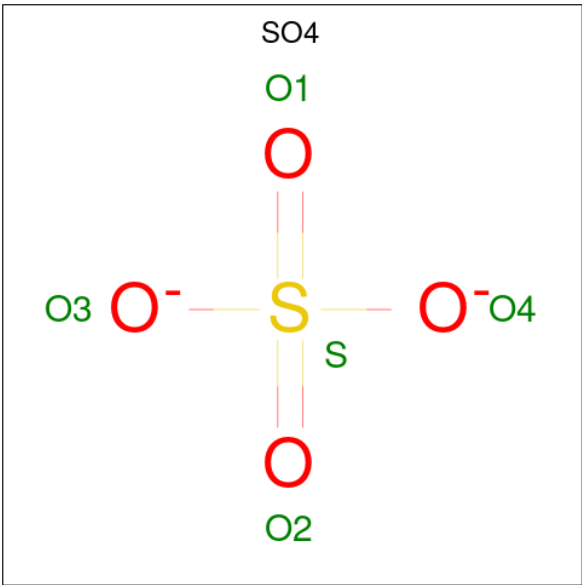
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	LYS	TYR	SEE REMARK 999	UNP P27302
B	105	LYS	TYR	SEE REMARK 999	UNP P27302
A	486	PRO	SER	SEE REMARK 999	UNP P27302
B	486	PRO	SER	SEE REMARK 999	UNP P27302

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

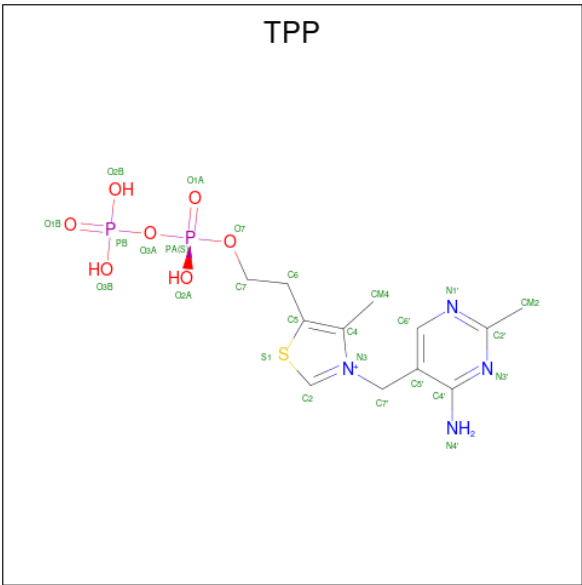
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

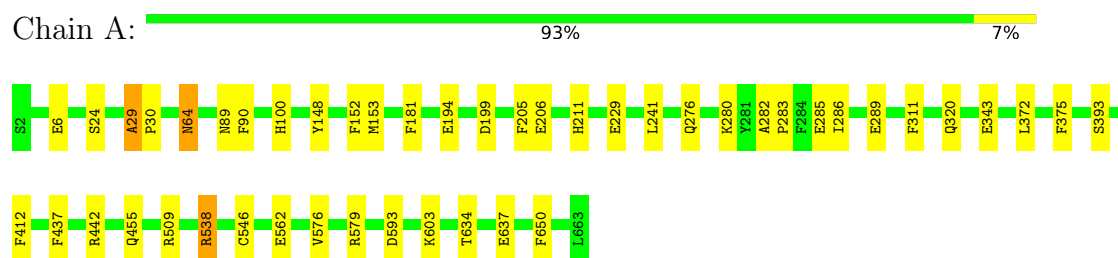
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	542	Total 542	O 542	0	0
5	B	523	Total 523	O 523	0	0

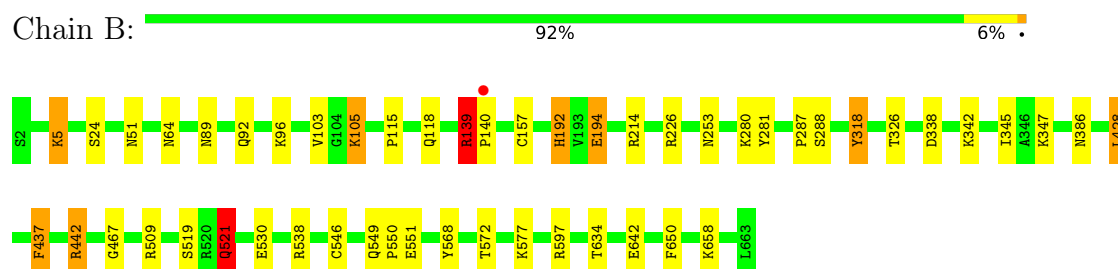
3 Residue-property plots

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: PROTEIN (TRANSKETOLASE)



• Molecule 1: PROTEIN (TRANSKETOLASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.85Å 126.00Å 151.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.5 (10.00-1.90) 96.7 (10.00-1.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.132 , 0.176 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11273	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, CA, 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	0.91	0/5189	1.54	33/7030 (0.5%)
1	B	0.90	1/5189 (0.0%)	1.54	32/7030 (0.5%)
All	All	0.91	1/10378 (0.0%)	1.54	65/14060 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	TYR	CA-CB	5.16	1.59	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	CG-CD-NE	12.90	140.37	112.00
1	A	538	ARG	CD-NE-CZ	10.92	139.69	124.40
1	B	139	ARG	O-C-N	-8.95	114.11	121.80
1	B	192	HIS	CA-CB-CG	-8.29	105.51	113.80
1	A	593	ASP	CA-CB-CG	7.93	120.53	112.60
1	B	442	ARG	NE-CZ-NH2	7.83	126.24	119.20
1	A	412	PHE	CA-CB-CG	7.45	121.25	113.80
1	B	214	ARG	NE-CZ-NH2	7.34	125.81	119.20
1	A	579	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	B	115	PRO	N-CA-CB	7.11	106.90	102.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	PHE	CA-CB-CG	6.89	120.69	113.80
1	B	509	ARG	CG-CD-NE	-6.52	97.65	112.00
1	B	597	ARG	CD-NE-CZ	6.50	133.50	124.40
1	A	509	ARG	CD-NE-CZ	6.39	133.34	124.40
1	B	139	ARG	CD-NE-CZ	-6.38	115.47	124.40
1	A	437	PHE	CA-CB-CG	-6.35	107.45	113.80
1	A	64	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	153	MET	CA-CB-CG	6.29	126.68	114.10
1	B	386	ASN	CA-CB-CG	6.19	118.79	112.60
1	B	650	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	311	PHE	CA-CB-CG	-6.11	107.69	113.80
1	B	521	GLN	OE1-CD-NE2	-6.08	116.53	122.60
1	B	89	ASN	CA-CB-CG	-6.05	106.55	112.60
1	A	206	GLU	CA-CB-CG	-6.01	102.08	114.10
1	A	89	ASN	CA-CB-CG	-5.90	106.70	112.60
1	A	286	ILE	CA-C-O	-5.89	115.86	119.51
1	B	253	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	650	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	211	HIS	O-C-N	-5.81	116.60	123.22
1	B	509	ARG	CD-NE-CZ	5.79	132.50	124.40
1	A	509	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	B	140	PRO	CA-C-O	-5.68	115.30	121.27
1	A	148	TYR	CA-CB-CG	-5.66	103.72	113.90
1	B	24	SER	CA-C-N	-5.62	114.58	122.85
1	B	24	SER	C-N-CA	-5.62	114.58	122.85
1	B	157	CYS	N-CA-CB	-5.60	101.89	110.12
1	A	100	HIS	CA-CB-CG	-5.51	108.29	113.80
1	B	51	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	24	SER	CA-C-O	-5.48	114.86	120.89
1	A	576	VAL	CA-C-O	-5.46	114.62	121.11
1	A	285	GLU	CB-CG-CD	5.38	121.75	112.60
1	B	467	GLY	N-CA-C	5.30	119.96	110.95
1	B	103	VAL	CA-C-O	5.25	127.00	121.59
1	B	442	ARG	N-CA-C	5.24	117.40	111.11
1	A	229	GLU	CA-CB-CG	-5.23	103.64	114.10
1	B	345	ILE	CA-C-O	5.23	126.39	120.95
1	A	343	GLU	CA-CB-CG	5.21	124.52	114.10
1	B	519	SER	O-C-N	5.19	128.76	122.94
1	B	118	GLN	CA-C-N	-5.17	114.31	120.00
1	B	118	GLN	C-N-CA	-5.17	114.31	120.00
1	B	538	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	A	372	LEU	CA-C-N	5.14	124.80	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	LEU	C-N-CA	5.14	124.80	119.56
1	A	194	GLU	CB-CG-CD	-5.11	103.91	112.60
1	A	393	SER	CB-CA-C	-5.11	101.72	109.89
1	B	92	GLN	CA-C-O	5.09	127.87	121.66
1	A	152	PHE	CA-C-N	-5.09	113.97	122.21
1	A	152	PHE	C-N-CA	-5.09	113.97	122.21
1	B	437	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	326	THR	N-CA-CB	-5.05	102.69	110.12
1	A	205	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	29	ALA	CA-C-O	5.04	123.23	118.34
1	A	455	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	139	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	199	ASP	CB-CA-C	-5.00	100.66	109.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	437	PHE	Mainchain

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	5072	0	4938	8	0
1	B	5072	0	4932	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	26	0	16	0	0
4	B	26	0	16	1	0
5	A	542	0	0	5	0
5	B	523	0	0	5	0
All	All	11273	0	9902	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 1.

All (29) 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:521:GLN:H	1:B:521:GLN:HE21	1.23	0.87
1:B:551:GLU:HG3	1:B:577:LYS:HB2	1.76	0.66
1:B:338:ASP:O	1:B:342:LYS:HG3	2.00	0.62
1:A:634:THR:HB	5:A:962:HOH:O	2.00	0.61
1:B:5:LYS:H	1:B:5:LYS:HD2	1.67	0.60
1:B:521:GLN:H	1:B:521:GLN:NE2	1.96	0.59
1:B:139:ARG:HG3	1:B:318:TYR:CE2	2.43	0.54
1:B:521:GLN:HE21	1:B:521:GLN:N	2.02	0.52
1:A:538:ARG:NH2	5:A:864:HOH:O	2.46	0.48
1:A:546:CYS:HB3	5:A:875:HOH:O	2.14	0.48
1:B:568:TYR:O	1:B:572:THR:HG23	2.13	0.48
5:A:1085:HOH:O	4:B:670:TPP:H2	2.14	0.47
1:B:546:CYS:HB3	5:B:925:HOH:O	2.14	0.46
1:B:549:GLN:HG2	1:B:550:PRO:HD2	1.96	0.46
1:A:181:PHE:CE2	1:A:241:LEU:HD12	2.52	0.45
1:B:5:LYS:NZ	5:B:1181:HOH:O	2.50	0.45
1:B:226:ARG:HG3	5:B:990:HOH:O	2.17	0.45
1:B:192:HIS:HB3	1:B:194:GLU:OE2	2.18	0.44
1:B:139:ARG:HH11	1:B:139:ARG:HD3	1.38	0.44
1:B:442:ARG:NH1	5:B:736:HOH:O	2.39	0.43
1:B:428:LEU:C	1:B:428:LEU:HD12	2.43	0.43
1:B:281:TYR:CZ	1:B:287:PRO:HG3	2.54	0.42
1:B:634:THR:HB	5:B:957:HOH:O	2.19	0.42
1:A:562:GLU:HG3	5:A:1007:HOH:O	2.20	0.41
1:A:282:ALA:HB1	1:A:283:PRO:HD2	2.03	0.41
1:B:549:GLN:CG	1:B:550:PRO:HD2	2.50	0.41
1:A:442:ARG:HG3	1:A:442:ARG:HH11	1.84	0.41
1:A:29:ALA:N	1:A:30:PRO:CD	2.84	0.40
1:B:96:LYS:HA	1:B:105:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

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	514/662 (78%)	505 (98%)	9 (2%)	0	100	100
1	B	660/662 (100%)	649 (98%)	11 (2%)	0	100	100
All	All	1174/1324 (89%)	1154 (98%)	20 (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	515/515 (100%)	506 (98%)	9 (2%)	53	52
1	B	515/515 (100%)	502 (98%)	13 (2%)	42	37
All	All	1030/1030 (100%)	1008 (98%)	22 (2%)	47	44

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	64	ASN
1	A	276	GLN
1	A	280	LYS
1	A	289	GLU
1	A	320	GLN
1	A	375	PHE
1	A	603	LYS
1	A	637	GLU
1	B	5	LYS
1	B	64	ASN
1	B	105	LYS
1	B	139	ARG
1	B	194	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	LYS
1	B	288	SER
1	B	347	LYS
1	B	428	LEU
1	B	521	GLN
1	B	530	GLU
1	B	642	GLU
1	B	658	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	A	455	GLN
1	A	510	GLN
1	B	510	GLN
1	B	521	GLN
1	B	522	ASN

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 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	TPP	A	670	2	26,27,27	1.28	2 (7%)	38,40,40	1.78	12 (31%)
3	SO4	B	680	-	4,4,4	0.64	0	6,6,6	0.15	0
3	SO4	A	680	-	4,4,4	0.66	0	6,6,6	0.36	0
4	TPP	B	670	2	26,27,27	1.01	1 (3%)	38,40,40	1.73	9 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TPP	A	670	2	-	3/17/17/17	0/2/2/2
4	TPP	B	670	2	-	4/17/17/17	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	670	TPP	C4'-N3'	3.45	1.39	1.35
4	B	670	TPP	C6'-N1'	2.46	1.39	1.34
4	A	670	TPP	PA-O3A	-2.16	1.57	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	670	TPP	C2-S1-C5	-4.72	88.09	91.22
4	B	670	TPP	C5'-C4'-N4'	3.88	127.36	122.14
4	A	670	TPP	C6-C5-C4	-3.55	119.27	128.17
4	A	670	TPP	CM4-C4-N3	3.34	128.29	120.57
4	B	670	TPP	C6-C5-C4	-3.32	119.84	128.17
4	A	670	TPP	C6-C5-S1	3.21	128.41	120.90
4	A	670	TPP	C2-S1-C5	-3.20	89.10	91.22
4	A	670	TPP	C5'-C7'-N3	-2.99	106.52	112.97
4	A	670	TPP	O3B-PB-O2B	2.81	118.34	107.80
4	B	670	TPP	C5'-C7'-N3	-2.59	107.38	112.97
4	B	670	TPP	C4-C5-S1	2.55	114.54	110.56
4	B	670	TPP	N4'-C4'-N3'	-2.53	113.62	117.03
4	A	670	TPP	CM4-C4-C5	-2.46	121.45	127.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	670	TPP	CM2-C2'-N1'	2.44	119.80	117.20
4	B	670	TPP	CM2-C2'-N1'	2.39	119.74	117.20
4	A	670	TPP	N1'-C2'-N3'	-2.33	121.66	125.53
4	A	670	TPP	N4'-C4'-N3'	-2.32	113.89	117.03
4	A	670	TPP	O7-PA-O1A	-2.22	100.14	108.94
4	B	670	TPP	O7-PA-O1A	-2.22	100.14	108.94
4	A	670	TPP	C6'-N1'-C2'	2.12	119.56	116.07
4	B	670	TPP	C6-C5-S1	2.01	125.61	120.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

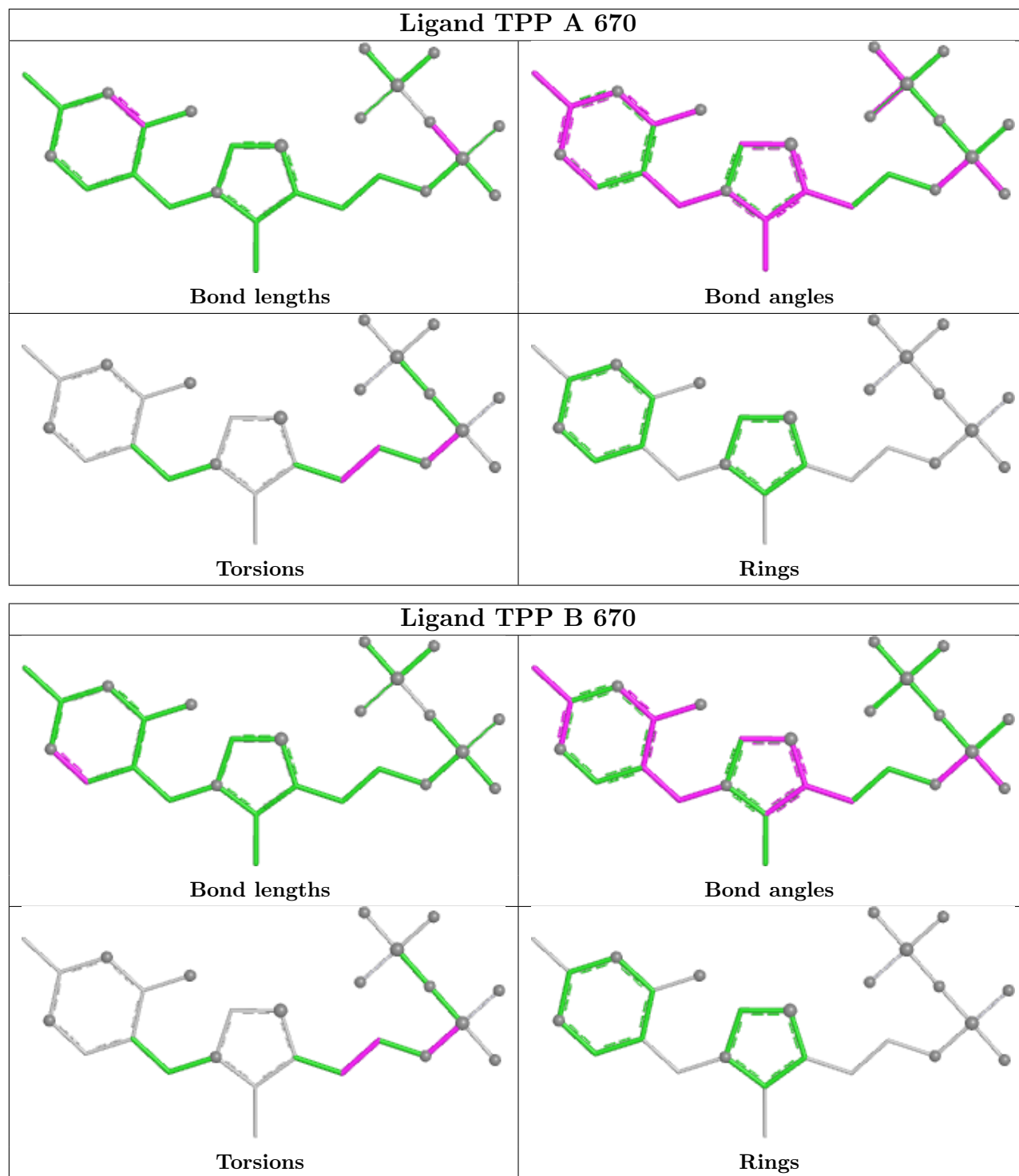
Mol	Chain	Res	Type	Atoms
4	A	670	TPP	C5-C6-C7-O7
4	A	670	TPP	C7-O7-PA-O2A
4	B	670	TPP	C5-C6-C7-O7
4	B	670	TPP	C7-O7-PA-O2A
4	B	670	TPP	C7-O7-PA-O3A
4	A	670	TPP	C7-O7-PA-O3A
4	B	670	TPP	C7-O7-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	670	TPP	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	662/662 (100%)	-1.01	0 100 100	6, 14, 32, 59	1 (0%)
1	B	662/662 (100%)	-0.99	1 (0%) 91 92	6, 14, 34, 53	1 (0%)
All	All	1324/1324 (100%)	-1.00	1 (0%) 92 92	6, 14, 33, 59	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	PRO	2.8

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	680	5/5	0.94	0.09	47,49,53,53	0
3	SO4	B	680	5/5	0.96	0.07	44,47,49,50	0
4	TPP	B	670	26/26	0.97	0.05	9,16,30,37	0
4	TPP	A	670	26/26	0.98	0.05	10,16,30,31	0

Continued on next page...

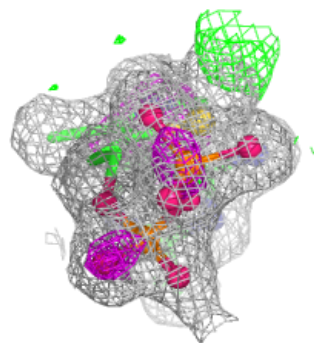
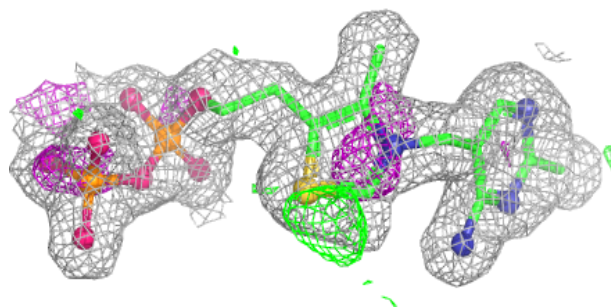
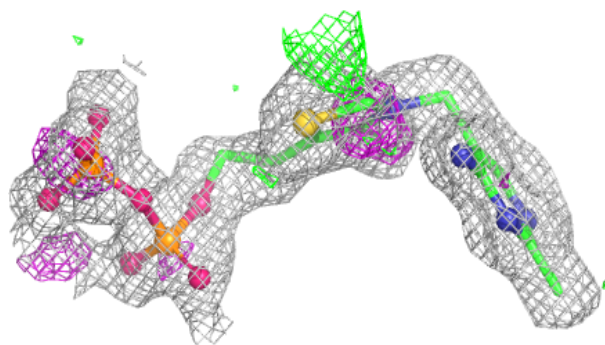
Continued from previous page...

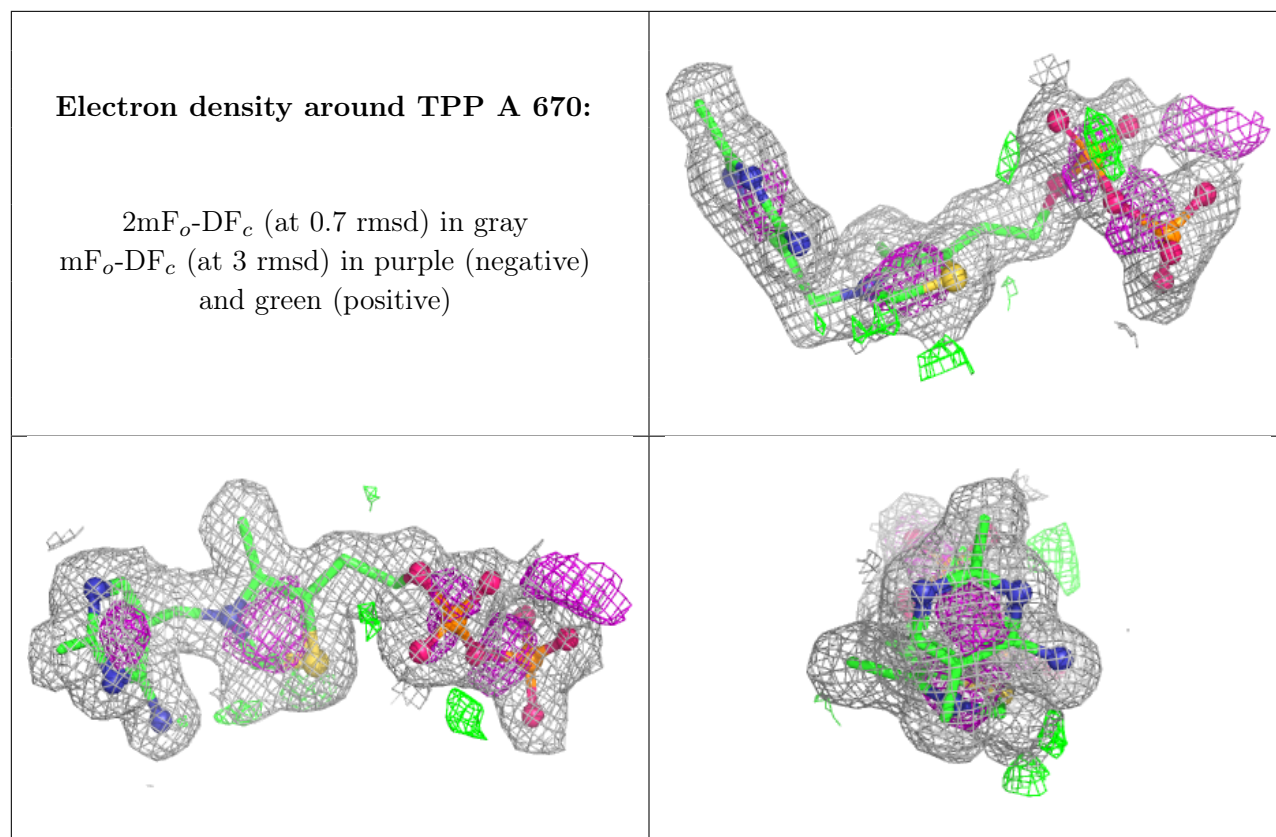
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	675	1/1	0.99	0.06	12,12,12,12	0
2	CA	B	675	1/1	1.00	0.06	14,14,14,14	0

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 B 670:

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.