



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2026 – 02:10 PM EDT

PDB ID : 36AD / pdb_000036ad
Title : Fumarate hydratase (human mitochondrial)
Authors : Weaver, T.M.; May, J.F.; Bhattacharyya, B.; Strauss, L.A.
Deposited on : 2026-05-27
Resolution : 2.11 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

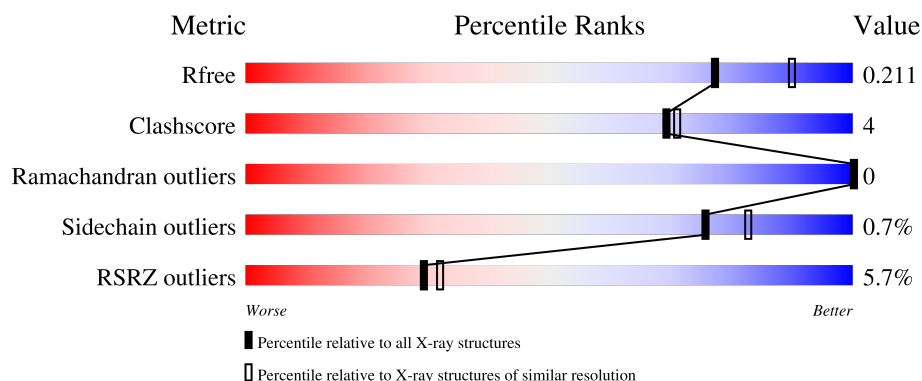
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	510	<div> <div>4%</div> <div>80%</div> <div>9%</div> <div>11%</div> </div>
1	B	510	<div> <div>6%</div> <div>83%</div> <div>7%</div> <div>9%</div> </div>
1	C	510	<div> <div>5%</div> <div>74%</div> <div>8%</div> <div>17%</div> </div>
1	D	510	<div> <div>5%</div> <div>82%</div> <div>8%</div> <div>10%</div> </div>

2 Entry composition [i](#)

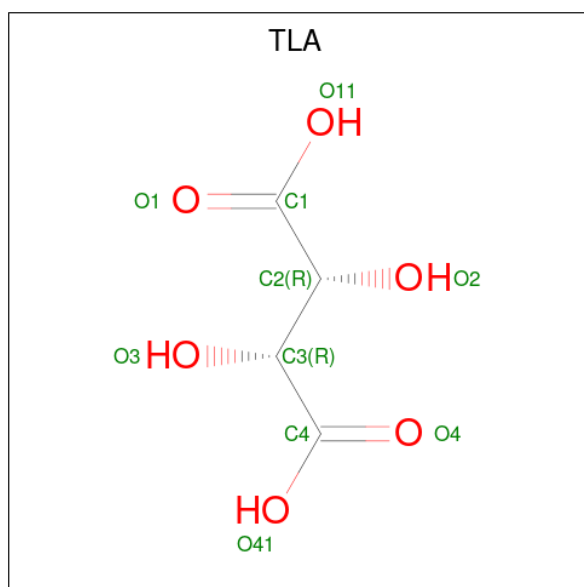
There are 3 unique types of molecules in this entry. The entry contains 27183 atoms, of which 13073 are hydrogens and 0 are deuteriums.

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 Fumarate hydratase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	H	N	O	S	0	3	0
			6801	2180	3348	598	654	21			
1	B	462	Total	C	H	N	O	S	0	2	0
			6843	2201	3355	604	661	22			
1	C	421	Total	C	H	N	O	S	0	4	0
			6189	2011	3000	553	602	23			
1	D	458	Total	C	H	N	O	S	0	6	0
			6855	2202	3370	604	657	22			

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆) (labeled as "Ligand of Interest" by depositor).



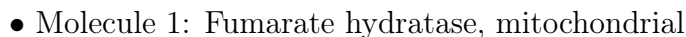
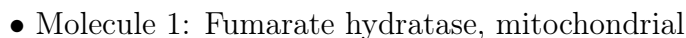
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	4	6		

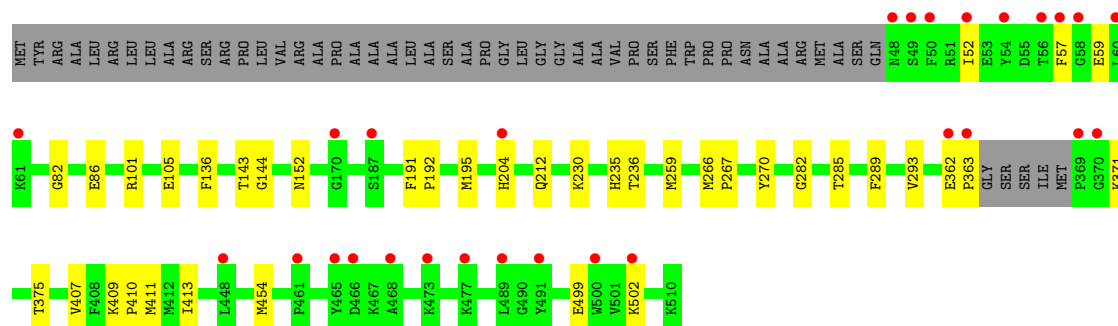
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total 142	O 142	0	0
3	B	127	Total 127	O 127	0	0
3	C	110	Total 110	O 110	0	0
3	D	106	Total 106	O 106	0	0

i

- Molecule 1: Fumarate hydratase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.49Å 189.49Å 115.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.98 – 2.11 66.98 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.98-2.11) 99.9 (66.98-2.11)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.179 , 0.211 0.179 , 0.211	Depositor DCC
R_{free} test set	6914 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27183	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: TLA

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	0.10	0/3528	0.27	0/4775
1	B	0.09	0/3562	0.27	0/4822
1	C	0.10	0/3259	0.28	0/4410
1	D	0.09	0/3571	0.27	0/4833
All	All	0.10	0/13920	0.27	0/18840

There are no bond length outliers.

There are no bond angle outliers.

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	3453	3348	3486	34	0
1	B	3488	3355	3520	22	0
1	C	3189	3000	3220	29	0
1	D	3485	3370	3524	25	0
2	C	10	0	4	0	0
3	A	142	0	0	0	0
3	B	127	0	0	0	0
3	C	110	0	0	0	0
3	D	106	0	0	0	0
All	All	14110	13073	13754	96	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 4.

All (96) 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:C:147[A]:THR:HG22	1:C:187:SER:HB2	1.42	0.96
1:C:147[A]:THR:HG22	1:C:187:SER:CB	2.18	0.74
1:C:145:SER:OG	1:C:147[A]:THR:HG23	1.89	0.73
1:B:470:LYS:HD3	1:B:491:TYR:OH	1.89	0.71
1:A:54:TYR:CE1	1:A:59:GLU:HB2	2.27	0.70
1:A:143[B]:THR:HG21	1:A:147[B]:THR:HG22	1.72	0.69
1:B:238:ASP:O	1:D:371:LYS:HE2	1.95	0.66
1:A:362:GLU:HB3	1:A:363:PRO:HD2	1.78	0.65
1:A:375:THR:HG22	1:D:143[A]:THR:HG22	1.79	0.65
1:D:499:GLU:O	1:D:502:LYS:HE3	1.97	0.65
1:B:101:ARG:NH1	1:B:105:GLU:OE1	2.29	0.64
1:D:362:GLU:HB3	1:D:363:PRO:HD2	1.80	0.64
1:C:368:MET:HA	1:C:368:MET:HE3	1.80	0.64
1:C:77:MET:O	1:C:80:LYS:HE3	1.99	0.62
1:C:101:ARG:NH1	1:C:105:GLU:OE1	2.35	0.59
1:D:101:ARG:NH1	1:D:105:GLU:OE1	2.29	0.58
1:D:289:PHE:CZ	1:D:293[B]:VAL:HG21	2.38	0.58
1:A:50:PHE:CE2	1:A:61:LYS:HE3	2.39	0.57
1:A:469:ALA:HA	1:C:367:ILE:HD12	1.87	0.57
1:A:101:ARG:NH1	1:A:105:GLU:OE1	2.33	0.57
1:C:118[B]:ASN:OD1	1:C:122:LYS:NZ	2.39	0.56
1:A:143[B]:THR:HG21	1:A:147[B]:THR:CG2	2.36	0.56
1:A:493:THR:HG23	1:A:496:GLN:H	1.71	0.56
1:B:484:GLU:O	1:B:488:GLU:HG3	2.07	0.55
1:C:365:SER:O	1:C:366:SER:HB3	2.06	0.55
1:B:393:ALA:HB1	1:B:411:MET:HE1	1.89	0.55
1:B:493:THR:HG23	1:B:496:GLN:H	1.72	0.53
1:C:368:MET:HE3	1:C:368:MET:CA	2.38	0.53
1:A:466:ASP:O	1:A:470:LYS:HG3	2.09	0.53
1:A:375:THR:CG2	1:D:143[A]:THR:HG22	2.38	0.53
1:B:282:GLY:O	1:B:285:THR:HG22	2.09	0.52
1:B:143[B]:THR:HG22	1:C:375:THR:HG22	1.92	0.52
1:B:365:SER:HB3	1:B:368:MET:HB2	1.91	0.52
1:A:77:MET:O	1:A:80:LYS:HE3	2.11	0.50
1:C:282:GLY:O	1:C:285:THR:HG22	2.12	0.50
1:A:143[A]:THR:HG22	1:D:375:THR:CG2	2.42	0.49
1:C:456:VAL:O	1:C:457:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:PHE:HA	1:D:152:ASN:HD21	1.78	0.48
1:B:368:MET:HE3	1:B:368:MET:HA	1.96	0.48
1:D:52:ILE:HG23	1:D:59:GLU:HG3	1.94	0.48
1:A:143[A]:THR:HG22	1:D:375:THR:HG22	1.95	0.48
1:A:397:GLY:HA3	1:A:411:MET:HE1	1.96	0.48
1:C:144:GLY:HA3	1:C:407:VAL:O	2.14	0.48
1:C:367:ILE:O	1:C:367:ILE:HG13	2.12	0.47
1:D:282:GLY:O	1:D:285:THR:HG22	2.15	0.47
1:B:136:PHE:HA	1:B:152:ASN:HD21	1.79	0.47
1:D:144:GLY:HA3	1:D:407:VAL:O	2.14	0.47
1:D:235:HIS:O	1:D:236:THR:OG1	2.28	0.47
1:B:385:ALA:HB3	1:C:411[B]:MET:HE3	1.96	0.47
1:B:144:GLY:HA3	1:B:407:VAL:O	2.15	0.46
1:D:266:MET:N	1:D:267:PRO:CD	2.78	0.46
1:A:350:ARG:CZ	1:C:453:LEU:HD21	2.45	0.46
1:A:350:ARG:NH2	1:C:453:LEU:HD21	2.30	0.46
1:A:486:ALA:HB1	1:A:492:LEU:HD11	1.97	0.46
1:A:50:PHE:HE2	1:A:52:ILE:HD11	1.82	0.46
1:C:138:LEU:HD13	1:C:148:GLN:HB3	1.97	0.46
1:D:204[A]:HIS:NE2	1:D:270:TYR:OH	2.42	0.45
1:C:266:MET:N	1:C:267:PRO:CD	2.80	0.45
1:D:82:GLY:HA3	1:D:86:GLU:HG3	1.99	0.45
1:B:289:PHE:O	1:B:293:VAL:HG23	2.16	0.45
1:A:144:GLY:HA3	1:A:407:VAL:O	2.18	0.44
1:B:82:GLY:HA3	1:B:86:GLU:HG3	1.99	0.44
1:A:82:GLY:HA3	1:A:86:GLU:HG3	1.99	0.44
1:B:138:LEU:HD13	1:B:148:GLN:HB3	2.00	0.44
1:B:266:MET:N	1:B:267:PRO:CD	2.80	0.44
1:D:212:GLN:OE1	1:D:259:MET:HE1	2.18	0.44
1:A:266:MET:N	1:A:267:PRO:CD	2.81	0.44
1:C:136:PHE:HA	1:C:152:ASN:HD21	1.83	0.44
1:A:371:LYS:HG3	1:C:237:GLN:HB3	2.00	0.43
1:A:385:ALA:HB3	1:D:411[B]:MET:HE3	1.99	0.43
1:A:136:PHE:HA	1:A:152:ASN:HD21	1.82	0.43
1:B:77:MET:O	1:B:80:LYS:HE3	2.19	0.43
1:B:195:MET:HB2	1:B:413:ILE:HD13	2.00	0.43
1:C:82:GLY:HA3	1:C:86:GLU:HG3	2.01	0.43
1:C:409:LYS:HB2	1:C:410:PRO:HD3	2.00	0.43
1:A:204:HIS:HE2	1:A:270:TYR:HH	1.64	0.43
1:A:282:GLY:O	1:A:285:THR:HG22	2.18	0.43
1:A:360:GLU:HG2	1:D:57:PHE:HZ	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:C	1:A:492:LEU:HD12	2.44	0.42
1:B:409:LYS:HB2	1:B:410:PRO:HD3	2.00	0.42
1:D:195:MET:HB2	1:D:413:ILE:HD13	2.00	0.42
1:A:411:MET:HE3	1:A:411:MET:HB3	1.96	0.42
1:A:489:LEU:HD13	1:A:491:TYR:HE2	1.84	0.42
1:D:409:LYS:HB2	1:D:410:PRO:HD3	2.02	0.41
1:C:367:ILE:C	1:C:369:PRO:HD3	2.45	0.41
1:A:204:HIS:NE2	1:A:270:TYR:OH	2.44	0.41
1:C:204:HIS:HE2	1:C:270:TYR:HH	1.58	0.41
1:C:368:MET:HA	1:C:368:MET:CE	2.47	0.41
1:A:409:LYS:HB2	1:A:410:PRO:HD3	2.03	0.41
1:B:266:MET:O	1:B:267:PRO:C	2.64	0.41
1:C:195:MET:HB2	1:C:413:ILE:HD13	2.02	0.41
1:D:191:PHE:N	1:D:192:PRO:HD2	2.36	0.40
1:D:192:PRO:HA	1:D:195:MET:HG2	2.04	0.40
1:A:192:PRO:HA	1:A:195:MET:HG2	2.04	0.40
1:B:368:MET:HE1	1:D:454:MET:SD	2.61	0.40
1:C:362:GLU:HB3	1:C:363:PRO:HD2	2.03	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	455/510 (89%)	446 (98%)	9 (2%)	0	100	100
1	B	462/510 (91%)	453 (98%)	9 (2%)	0	100	100
1	C	421/510 (82%)	410 (97%)	11 (3%)	0	100	100
1	D	460/510 (90%)	453 (98%)	7 (2%)	0	100	100
All	All	1798/2040 (88%)	1762 (98%)	36 (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	369/403 (92%)	366 (99%)	3 (1%)	73	80
1	B	373/403 (93%)	371 (100%)	2 (0%)	81	87
1	C	344/403 (85%)	340 (99%)	4 (1%)	63	71
1	D	374/403 (93%)	373 (100%)	1 (0%)	86	91
All	All	1460/1612 (91%)	1450 (99%)	10 (1%)	76	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	LYS
1	A	371	LYS
1	A	407	VAL
1	B	187	SER
1	B	230	LYS
1	C	187	SER
1	C	230	LYS
1	C	307	THR
1	C	443	GLU
1	D	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	386	GLN
1	B	152	ASN
1	B	329	ASN
1	B	386	GLN
1	B	415	ASN
1	B	446	ASN
1	C	64	ASN
1	C	152	ASN

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Mol	Chain	Res	Type
1	C	237	GLN
1	C	284	ASN
1	C	361	ASN
1	C	386	GLN
1	C	402	HIS
1	C	415	ASN
1	D	152	ASN
1	D	402	HIS
1	D	415	ASN

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](#)

1 ligand is modelled in this entry.

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	TLA	C	601	-	9,9,9	1.04	0	12,12,12	1.26	2 (16%)

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	TLA	C	601	-	-	4/12/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	TLA	O41-C4-C3	2.39	119.96	113.31
2	C	601	TLA	O11-C1-C2	2.36	119.88	113.31

There are no chirality outliers.

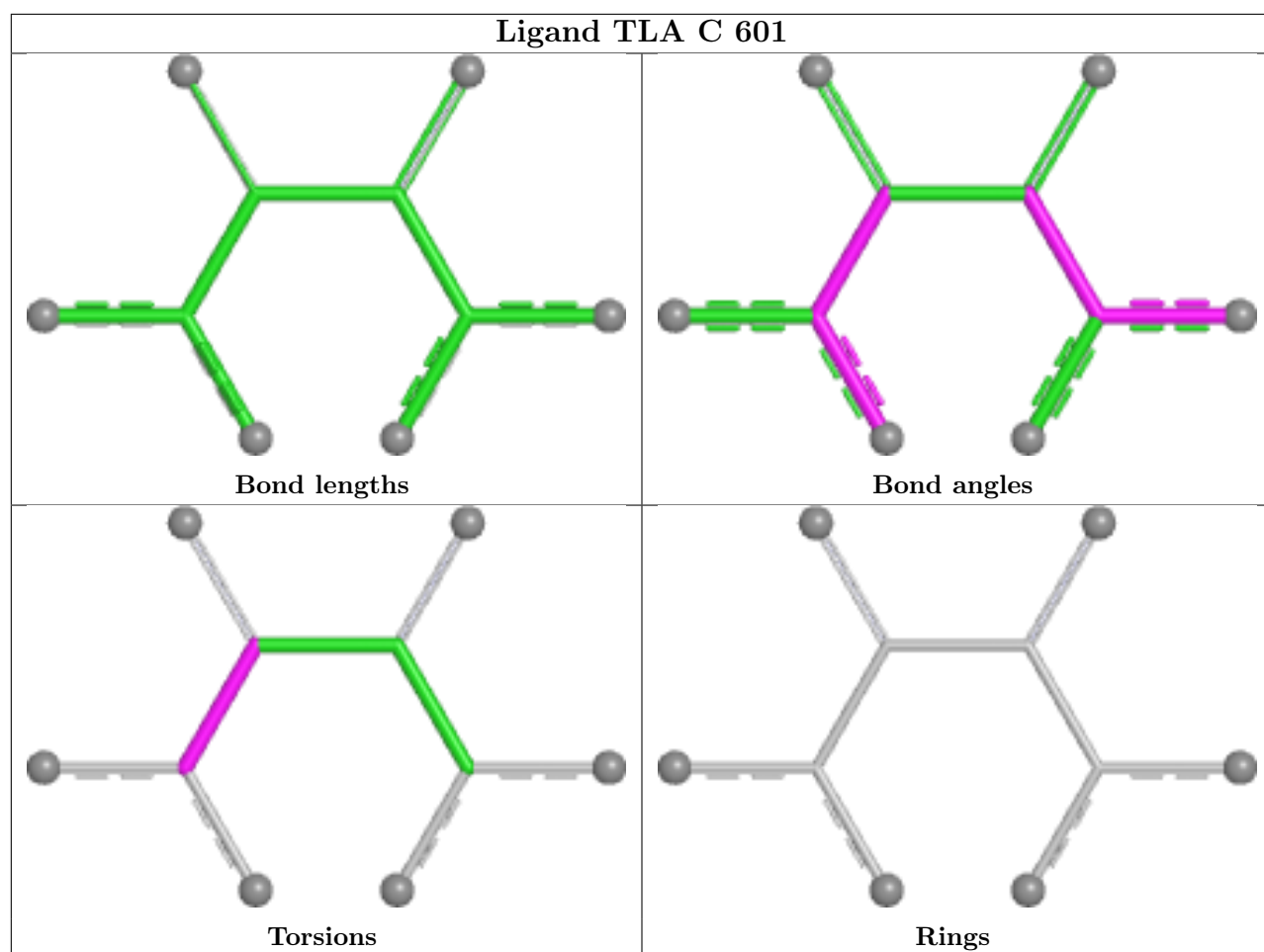
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	TLA	O3-C3-C4-O4
2	C	601	TLA	O3-C3-C4-O41
2	C	601	TLA	C2-C3-C4-O4
2	C	601	TLA	C2-C3-C4-O41

There are no ring outliers.

No monomer is involved in short contacts.

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	456/510 (89%)	0.01	22 (4%)	35	38	32, 52, 98, 110	5 (1%)
1	B	462/510 (90%)	0.14	29 (6%)	26	28	32, 57, 110, 126	4 (0%)
1	C	421/510 (82%)	0.10	24 (5%)	29	32	24, 57, 89, 117	6 (1%)
1	D	458/510 (89%)	0.10	28 (6%)	27	29	22, 55, 108, 122	8 (1%)
All	All	1797/2040 (88%)	0.09	103 (5%)	29	32	22, 55, 102, 126	23 (1%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	369	PRO	7.4
1	D	363	PRO	7.1
1	C	457	THR	7.0
1	A	363	PRO	7.0
1	C	500	TRP	6.7
1	A	370	GLY	6.0
1	A	56	THR	5.8
1	D	56	THR	5.6
1	C	501	VAL	5.5
1	C	456	VAL	5.1
1	A	372	VAL	5.1
1	C	448	LEU	4.8
1	C	363	PRO	4.8
1	C	367	ILE	4.7
1	A	371	LYS	4.4
1	C	365	SER	4.3
1	A	57	PHE	4.1
1	B	56	THR	3.9
1	C	455	LEU	3.7
1	C	366	SER	3.6
1	C	499	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	364	GLY	3.4
1	D	465	TYR	3.4
1	C	56	THR	3.3
1	D	49	SER	3.2
1	D	54	TYR	3.2
1	B	50	PHE	3.2
1	B	367	ILE	3.2
1	B	472	ALA	3.1
1	B	489	LEU	3.1
1	B	465	TYR	3.1
1	D	50	PHE	3.1
1	A	55	ASP	3.1
1	C	453	LEU	3.1
1	D	466	ASP	3.1
1	B	49	SER	3.1
1	B	364	GLY	3.0
1	B	371	LYS	3.0
1	C	450	ASN	3.0
1	D	362	GLU	2.9
1	A	465	TYR	2.9
1	D	204[A]	HIS	2.9
1	A	50	PHE	2.8
1	B	363	PRO	2.8
1	B	477	LYS	2.8
1	D	60	LEU	2.8
1	B	482	LEU	2.8
1	D	58	GLY	2.7
1	D	491	TYR	2.7
1	A	52	ILE	2.7
1	B	468	ALA	2.7
1	C	454	MET	2.7
1	A	54	TYR	2.6
1	C	446	ASN	2.6
1	B	369	PRO	2.6
1	D	461	PRO	2.6
1	C	50	PHE	2.5
1	A	463	ILE	2.5
1	D	477	LYS	2.5
1	B	455	LEU	2.5
1	D	57	PHE	2.5
1	A	49	SER	2.5
1	B	492	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	61	LYS	2.4
1	A	470	LYS	2.4
1	C	371	LYS	2.4
1	B	370	GLY	2.4
1	A	497	PHE	2.4
1	B	462	HIS	2.4
1	A	487	ILE	2.3
1	D	473	LYS	2.3
1	C	49	SER	2.3
1	D	187	SER	2.3
1	D	370	GLY	2.3
1	C	452	SER	2.3
1	A	60	LEU	2.3
1	B	500	TRP	2.3
1	A	491	TYR	2.2
1	C	368	MET	2.2
1	B	362	GLU	2.2
1	C	115	LYS	2.2
1	B	491	TYR	2.2
1	D	500	TRP	2.2
1	A	362	GLU	2.1
1	B	52	ILE	2.1
1	B	469	ALA	2.1
1	D	489	LEU	2.1
1	B	474	THR	2.1
1	A	477	LYS	2.1
1	B	504	LYS	2.1
1	D	502	LYS	2.1
1	A	488	GLU	2.1
1	B	471	ILE	2.1
1	D	448	LEU	2.1
1	C	369	PRO	2.1
1	D	170	GLY	2.1
1	D	52	ILE	2.1
1	A	84	VAL	2.1
1	B	497	PHE	2.1
1	D	48	ASN	2.0
1	B	372	VAL	2.0
1	B	187	SER	2.0
1	D	468	ALA	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](#)

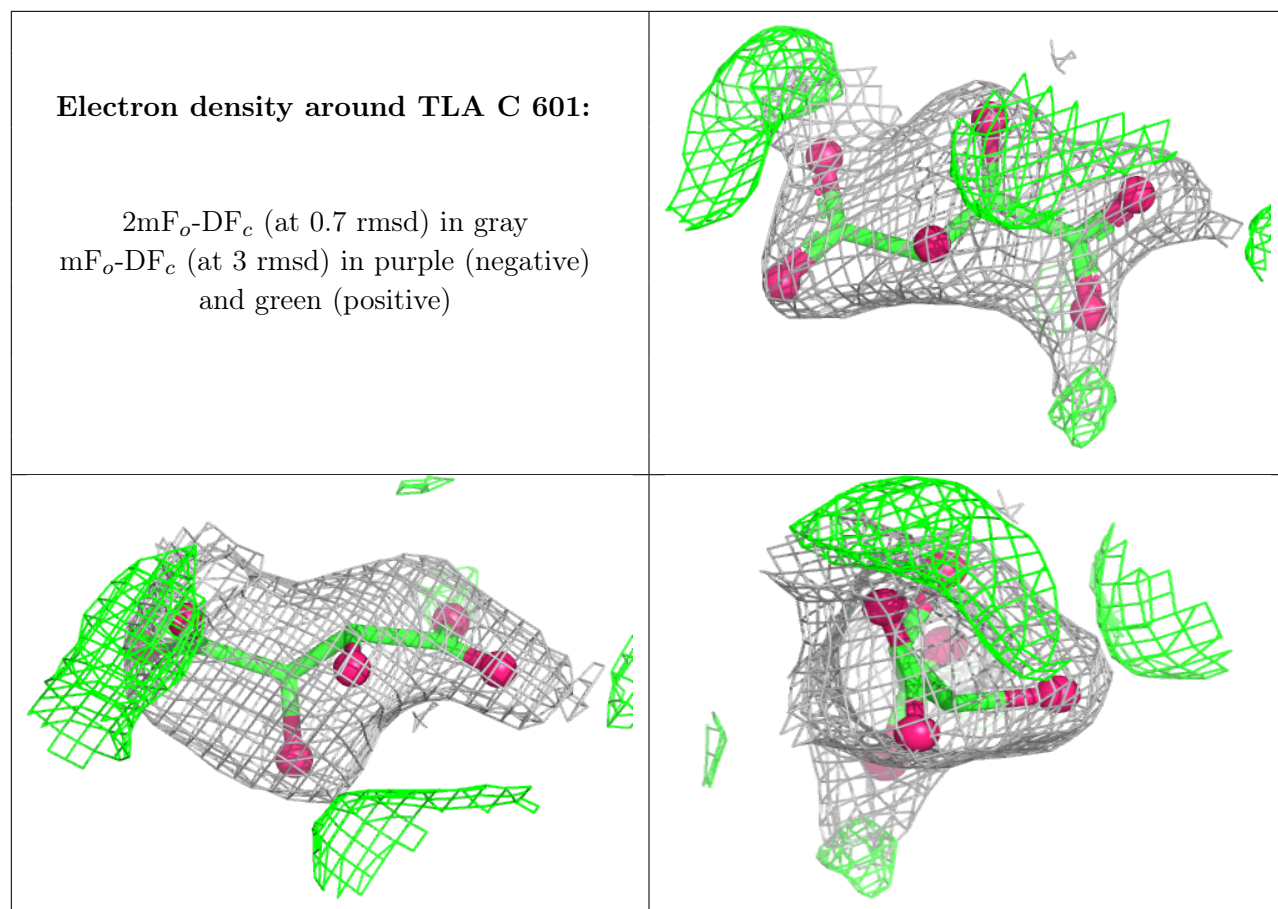
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
2	TLA	C	601	10/10	0.79	0.18	76,88,93,93	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.