



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 PM UTC

PDB ID : 1TG5 / pdb_00001tg5
Title : Crystal structures of plant 4-hydroxyphenylpyruvate dioxygenases complexed with DAS645
Authors : Yang, C.; Pflugrath, J.W.; Camper, D.L.; Foster, M.L.; Pernich, D.J.; Walsh, T.A.
Deposited on : 2004-05-28
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

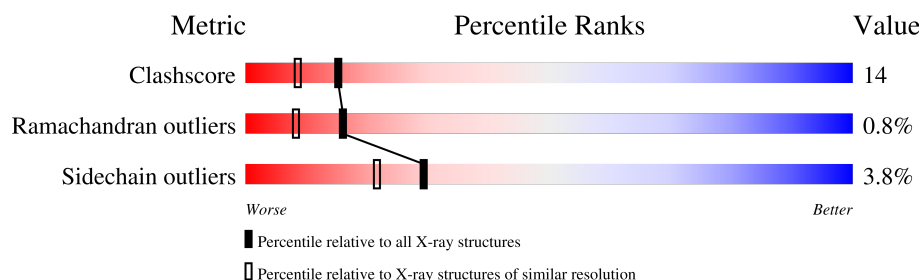
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	424	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	645	A	501[A]	-	X	-	-
3	645	A	501[B]	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3173 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 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	1	0
			2873	1828	489	544	12			

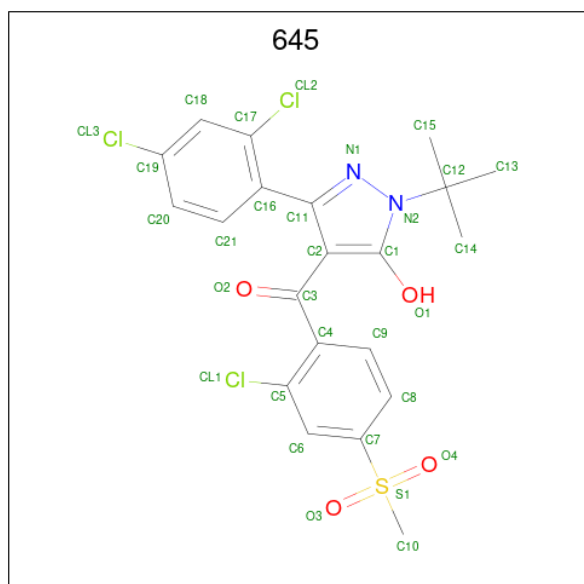
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P93836

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is [1-TERT-BUTYL-3-(2,4-DICHLOROPHENYL)-5-HYDROXY-1H-PYRAZO L-4-YL][2-CHLORO-4-(METHYLSULFONYL)PHENYL]METHANONE (CCD ID: 645) (formula: C₂₁H₁₉Cl₃N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	1
			39	27	5	2	4	1		

- Molecule 4 is water.

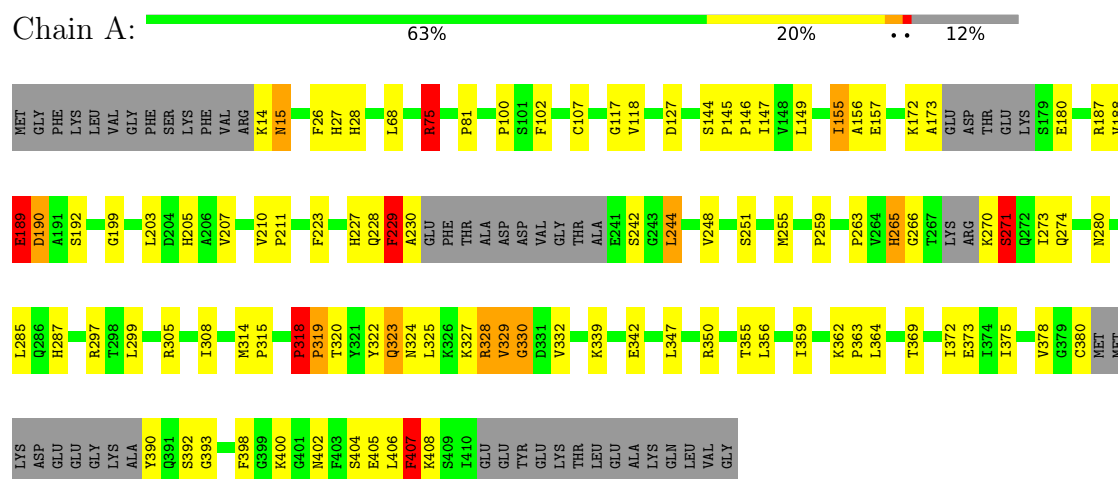
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	260	Total	O	0	0
			260	260		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.46Å 83.87Å 63.30Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.188 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3173	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, 645

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	0.42	0/2943	1.24	20/3975 (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	A	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	PRO	N-CA-C	10.67	120.72	110.47
1	A	205	HIS	CA-CB-CG	9.41	123.21	113.80
1	A	323	GLN	CB-CG-CD	9.01	127.92	112.60
1	A	407	PHE	CA-CB-CG	-8.73	105.07	113.80
1	A	265	HIS	N-CA-C	7.71	119.73	108.86
1	A	318	PRO	CB-CA-C	-7.36	104.47	111.39
1	A	265	HIS	CA-C-O	7.03	129.20	121.40
1	A	287	HIS	CA-CB-CG	6.95	120.75	113.80
1	A	223	PHE	CA-CB-CG	6.62	120.42	113.80
1	A	318	PRO	O-C-N	6.44	124.27	121.31
1	A	229	PHE	N-CA-C	-6.32	105.05	112.89
1	A	318	PRO	CA-C-O	6.24	125.39	120.90
1	A	271	SER	N-CA-CB	6.21	119.09	109.97
1	A	188	VAL	CA-C-O	-6.14	115.19	121.70
1	A	75	ARG	CD-NE-CZ	5.91	132.68	124.40
1	A	190	ASP	CA-CB-CG	5.80	118.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	PRO	N-CA-CB	5.30	106.16	103.19
1	A	265	HIS	CB-CG-ND1	-5.28	114.78	122.70
1	A	322	TYR	CA-CB-CG	-5.11	104.69	113.90
1	A	328	ARG	CA-C-O	-5.02	113.73	119.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	GLU	Peptide
1	A	318	PRO	Peptide

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	2873	0	2810	77	0
2	A	1	0	0	0	0
3	A	39	0	6	2	0
4	A	260	0	0	6	0
All	All	3173	0	2816	78	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 14.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:HIS:HE1	1:A:274:GLN:HB2	1.22	1.01
1:A:190:ASP:HB3	1:A:192:SER:H	1.32	0.95
1:A:265:HIS:CE1	1:A:274:GLN:HB2	2.10	0.87
1:A:265:HIS:CD2	1:A:271:SER:H	2.02	0.78
1:A:155:ILE:HD13	4:A:1172:HOH:O	1.87	0.74
1:A:100:PRO:HG3	1:A:149:LEU:HD21	1.71	0.73
1:A:255:MET:HA	1:A:255:MET:HE2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:HIS:NE2	1:A:271:SER:N	2.35	0.72
1:A:325:LEU:HD23	1:A:328:ARG:HE	1.56	0.71
1:A:265:HIS:NE2	1:A:271:SER:HB3	2.06	0.69
1:A:328:ARG:NH1	1:A:405:GLU:HG3	2.08	0.69
1:A:228:GLN:HG2	1:A:230:ALA:HB2	1.80	0.64
1:A:242:SER:HB2	1:A:244:LEU:CD2	2.28	0.63
1:A:380:CYS:HB3	1:A:392:SER:H	1.62	0.63
1:A:189:GLU:O	1:A:189:GLU:HG3	1.99	0.62
1:A:328:ARG:HH12	1:A:405:GLU:HG3	1.65	0.61
1:A:324:ASN:HB3	1:A:327:LYS:HE3	1.83	0.60
1:A:149:LEU:HD13	4:A:1100:HOH:O	2.04	0.57
1:A:68:LEU:HD11	1:A:75:ARG:HB3	1.87	0.56
1:A:325:LEU:HD22	1:A:329:VAL:HG22	1.88	0.56
1:A:404:SER:O	1:A:408:LYS:HB2	2.06	0.56
1:A:207:VAL:HG22	1:A:259:PRO:HG2	1.89	0.55
1:A:230:ALA:HA	1:A:248:VAL:H	1.72	0.55
1:A:400:LYS:HA	3:A:501[A]:645:CL2	2.45	0.53
1:A:270:LYS:HE3	1:A:274:GLN:HG3	1.89	0.53
1:A:229:PHE:O	1:A:230:ALA:C	2.54	0.51
1:A:255:MET:HA	1:A:255:MET:CE	2.41	0.50
1:A:305:ARG:HA	1:A:308:ILE:HG12	1.93	0.50
1:A:265:HIS:NE2	1:A:270:LYS:HG2	2.26	0.50
1:A:210:VAL:HB	1:A:211:PRO:HD2	1.95	0.49
1:A:118:VAL:HG11	1:A:285:LEU:HD13	1.94	0.49
1:A:255:MET:HE3	1:A:393:GLY:HA3	1.93	0.49
1:A:228:GLN:CG	1:A:230:ALA:HB2	2.43	0.49
1:A:329:VAL:O	1:A:330:GLY:C	2.56	0.48
1:A:199:GLY:HA3	1:A:297:ARG:HH12	1.78	0.48
1:A:263:PRO:HB3	1:A:273:ILE:HB	1.96	0.48
1:A:314:MET:HE3	1:A:315:PRO:HD2	1.96	0.47
1:A:325:LEU:HD22	1:A:329:VAL:CG2	2.44	0.47
1:A:265:HIS:CE1	1:A:274:GLN:CB	2.89	0.47
1:A:299:LEU:HD11	1:A:359:ILE:HG21	1.95	0.47
1:A:228:GLN:HE21	1:A:230:ALA:HB2	1.79	0.47
1:A:373:GLU:HG2	1:A:375:ILE:HG23	1.97	0.46
1:A:364:LEU:HD11	1:A:372:ILE:HG13	1.97	0.46
1:A:14:LYS:HG2	1:A:15:ASN:N	2.31	0.46
1:A:318:PRO:O	1:A:319:PRO:C	2.58	0.46
1:A:155:ILE:HG12	1:A:156:ALA:N	2.30	0.45
1:A:332:VAL:HG21	1:A:355:THR:OG1	2.15	0.45
1:A:187:ARG:HG2	4:A:1147:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:MET:HE3	1:A:393:GLY:CA	2.46	0.45
1:A:299:LEU:HD11	1:A:359:ILE:HD13	1.99	0.45
1:A:145:PRO:O	1:A:147:ILE:HD12	2.17	0.45
1:A:172:LYS:O	1:A:173:ALA:HB3	2.17	0.45
1:A:242:SER:HB2	1:A:244:LEU:HD23	1.99	0.45
1:A:27:HIS:O	1:A:28:HIS:HB3	2.17	0.44
1:A:320:THR:O	1:A:323:GLN:HB2	2.17	0.44
1:A:390:TYR:C	1:A:390:TYR:CD1	2.96	0.44
1:A:280:ASN:HD22	1:A:369:THR:HG21	1.81	0.44
1:A:305:ARG:HA	1:A:308:ILE:CG1	2.48	0.44
1:A:81:PRO:HD3	1:A:107:CYS:SG	2.58	0.44
1:A:227:HIS:HE1	1:A:251:SER:O	2.01	0.43
1:A:347:LEU:HD23	1:A:406:LEU:HD22	2.00	0.43
1:A:146:PRO:HA	1:A:155:ILE:O	2.19	0.43
1:A:81:PRO:HB3	1:A:102:PHE:HZ	1.83	0.42
1:A:127:ASP:HB3	4:A:1255:HOH:O	2.19	0.42
1:A:144:SER:HB3	1:A:157:GLU:HB2	2.01	0.42
1:A:406:LEU:O	1:A:407:PHE:C	2.62	0.42
1:A:265:HIS:NE2	1:A:270:LYS:CG	2.83	0.41
1:A:402:ASN:O	1:A:406:LEU:HG	2.20	0.41
1:A:117:GLY:HA3	4:A:1109:HOH:O	2.19	0.41
1:A:339:LYS:O	1:A:342:GLU:HB3	2.21	0.41
1:A:404:SER:HB3	4:A:1160:HOH:O	2.20	0.41
1:A:265:HIS:HB3	1:A:266:GLY:H	1.62	0.41
1:A:229:PHE:O	1:A:229:PHE:HD2	2.04	0.41
1:A:362:LYS:HB3	1:A:363:PRO:HD2	2.02	0.41
1:A:26:PHE:CG	1:A:203:LEU:HD23	2.56	0.40

There are no symmetry-related clashes.

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	362/424 (85%)	339 (94%)	20 (6%)	3 (1%)	16 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	GLY
1	A	407	PHE
1	A	319	PRO

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	313/356 (88%)	301 (96%)	12 (4%)	29 21

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	75	ARG
1	A	155	ILE
1	A	180	GLU
1	A	189	GLU
1	A	229	PHE
1	A	244	LEU
1	A	271	SER
1	A	329	VAL
1	A	350	ARG
1	A	356	LEU
1	A	378	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS

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Mol	Chain	Res	Type
1	A	228	GLN
1	A	280	ASN
1	A	324	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	645	A	501[A]	-	32,33,33	7.89	24 (75%)	46,52,52	5.90	33 (71%)
3	645	A	501[B]	-	32,33,33	7.79	24 (75%)	46,52,52	5.96	33 (71%)

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
3	645	A	501[A]	-	-	9/24/24/24	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	645	A	501[B]	-	-	7/24/24/24	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501[A]	645	C19-CL3	-20.73	1.26	1.74
3	A	501[B]	645	C19-CL3	-19.94	1.27	1.74
3	A	501[A]	645	O2-C3	17.21	1.59	1.23
3	A	501[B]	645	O2-C3	17.21	1.59	1.23
3	A	501[A]	645	C4-C3	-13.63	1.22	1.49
3	A	501[B]	645	C4-C3	-13.63	1.22	1.49
3	A	501[A]	645	C7-S1	-13.53	1.63	1.77
3	A	501[B]	645	C7-S1	-13.53	1.63	1.77
3	A	501[A]	645	C17-CL2	-10.41	1.49	1.73
3	A	501[A]	645	C5-CL1	-10.37	1.49	1.73
3	A	501[B]	645	C5-CL1	-10.37	1.49	1.73
3	A	501[A]	645	C21-C16	-10.10	1.24	1.39
3	A	501[B]	645	C17-CL2	-9.94	1.50	1.73
3	A	501[A]	645	C16-C17	9.58	1.53	1.39
3	A	501[B]	645	C16-C17	9.57	1.53	1.39
3	A	501[B]	645	C21-C16	-9.46	1.25	1.39
3	A	501[A]	645	C2-C1	-9.22	1.22	1.40
3	A	501[B]	645	C2-C1	-9.22	1.22	1.40
3	A	501[B]	645	C18-C17	8.87	1.53	1.38
3	A	501[A]	645	C18-C17	8.67	1.52	1.38
3	A	501[A]	645	C4-C5	7.70	1.50	1.39
3	A	501[B]	645	C4-C5	7.70	1.50	1.39
3	A	501[A]	645	C10-S1	-6.83	1.51	1.75
3	A	501[B]	645	C10-S1	-6.83	1.51	1.75
3	A	501[A]	645	C16-C11	-6.29	1.37	1.48
3	A	501[B]	645	C16-C11	-6.16	1.37	1.48
3	A	501[B]	645	C20-C19	6.09	1.49	1.38
3	A	501[A]	645	C20-C19	6.08	1.49	1.38
3	A	501[A]	645	C12-N2	-4.87	1.43	1.50
3	A	501[B]	645	C12-N2	-4.87	1.43	1.50
3	A	501[A]	645	C11-N1	4.47	1.40	1.33
3	A	501[B]	645	C11-N1	4.47	1.40	1.33
3	A	501[A]	645	C6-C7	4.18	1.46	1.39
3	A	501[B]	645	C6-C7	4.18	1.46	1.39
3	A	501[A]	645	O3-S1	-3.93	1.34	1.44
3	A	501[B]	645	O3-S1	-3.93	1.34	1.44
3	A	501[A]	645	C13-C12	3.68	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501[B]	645	C13-C12	3.68	1.60	1.52
3	A	501[A]	645	C9-C4	3.48	1.45	1.39
3	A	501[B]	645	C9-C4	3.48	1.45	1.39
3	A	501[B]	645	C21-C20	-3.48	1.33	1.38
3	A	501[A]	645	C2-C11	3.45	1.50	1.43
3	A	501[B]	645	C2-C11	3.45	1.50	1.43
3	A	501[A]	645	C21-C20	-3.28	1.33	1.38
3	A	501[A]	645	C2-C3	-2.49	1.41	1.48
3	A	501[B]	645	C2-C3	-2.49	1.41	1.48
3	A	501[A]	645	O1-C1	-2.23	1.24	1.31
3	A	501[B]	645	O1-C1	-2.23	1.24	1.31

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[A]	645	O4-S1-O3	-18.40	86.79	117.99
3	A	501[B]	645	O4-S1-O3	-18.40	86.79	117.99
3	A	501[B]	645	C18-C17-C16	-16.26	108.29	121.59
3	A	501[A]	645	O3-S1-C10	14.43	129.65	108.47
3	A	501[B]	645	O3-S1-C10	14.43	129.65	108.47
3	A	501[A]	645	C18-C17-C16	-13.73	110.36	121.59
3	A	501[A]	645	C17-C16-C11	-9.65	111.07	122.68
3	A	501[A]	645	C14-C12-N2	8.60	122.26	108.64
3	A	501[B]	645	C14-C12-N2	8.60	122.26	108.64
3	A	501[A]	645	C6-C7-S1	8.04	125.48	119.02
3	A	501[B]	645	C6-C7-S1	8.04	125.48	119.02
3	A	501[B]	645	C16-C11-N1	-7.91	106.95	119.73
3	A	501[B]	645	C17-C18-C19	7.78	127.51	118.72
3	A	501[A]	645	C5-C6-C7	7.78	123.95	118.80
3	A	501[B]	645	C5-C6-C7	7.78	123.95	118.80
3	A	501[A]	645	O2-C3-C2	-7.10	107.09	119.89
3	A	501[B]	645	O2-C3-C2	-7.10	107.09	119.89
3	A	501[A]	645	C20-C21-C16	7.07	132.50	120.86
3	A	501[A]	645	O3-S1-C7	6.73	113.46	108.23
3	A	501[B]	645	O3-S1-C7	6.73	113.46	108.23
3	A	501[A]	645	C16-C11-N1	-6.64	109.01	119.73
3	A	501[A]	645	C13-C12-N2	-6.56	98.26	108.64
3	A	501[B]	645	C13-C12-N2	-6.56	98.26	108.64
3	A	501[B]	645	C20-C21-C16	6.45	131.49	120.86
3	A	501[A]	645	C18-C17-CL2	6.30	128.76	118.45
3	A	501[B]	645	C17-C16-C11	-5.51	116.05	122.68
3	A	501[A]	645	C5-C4-C3	-5.50	115.70	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[B]	645	C5-C4-C3	-5.50	115.70	123.06
3	A	501[B]	645	C20-C19-C18	-5.35	114.53	121.53
3	A	501[A]	645	C17-C18-C19	5.15	124.53	118.72
3	A	501[A]	645	C3-C2-C1	4.96	137.48	119.83
3	A	501[B]	645	C3-C2-C1	4.96	137.48	119.83
3	A	501[A]	645	C21-C16-C11	4.84	128.99	119.72
3	A	501[A]	645	O4-S1-C7	4.67	111.86	108.23
3	A	501[B]	645	O4-S1-C7	4.67	111.86	108.23
3	A	501[A]	645	C20-C19-CL3	4.60	126.15	119.36
3	A	501[B]	645	C20-C19-CL3	4.36	125.80	119.36
3	A	501[A]	645	C9-C4-C3	4.26	129.04	119.37
3	A	501[B]	645	C9-C4-C3	4.26	129.04	119.37
3	A	501[B]	645	C16-C17-CL2	4.18	127.19	121.01
3	A	501[A]	645	C20-C19-C18	-3.91	116.42	121.53
3	A	501[A]	645	C2-C1-N2	3.86	112.41	107.77
3	A	501[B]	645	C2-C1-N2	3.86	112.41	107.77
3	A	501[B]	645	C18-C17-CL2	3.71	124.52	118.45
3	A	501[A]	645	C6-C5-C4	-3.64	118.61	121.59
3	A	501[B]	645	C6-C5-C4	-3.64	118.61	121.59
3	A	501[A]	645	C14-C12-C13	-3.29	102.15	109.48
3	A	501[B]	645	C14-C12-C13	-3.29	102.15	109.48
3	A	501[A]	645	C8-C7-C6	-3.21	116.71	120.68
3	A	501[B]	645	C8-C7-C6	-3.21	116.71	120.68
3	A	501[A]	645	C2-C11-N1	-3.20	108.41	111.62
3	A	501[B]	645	C2-C11-N1	-3.20	108.41	111.62
3	A	501[A]	645	O2-C3-C4	3.04	128.18	120.41
3	A	501[B]	645	O2-C3-C4	3.04	128.18	120.41
3	A	501[A]	645	C21-C20-C19	-2.99	116.23	119.24
3	A	501[B]	645	C21-C16-C17	2.59	120.82	117.79
3	A	501[A]	645	C8-C7-S1	-2.54	117.33	119.58
3	A	501[B]	645	C8-C7-S1	-2.54	117.33	119.58
3	A	501[A]	645	C9-C4-C5	-2.19	115.23	117.79
3	A	501[B]	645	C9-C4-C5	-2.19	115.23	117.79
3	A	501[A]	645	C15-C12-N2	2.17	112.08	108.64
3	A	501[B]	645	C15-C12-N2	2.17	112.08	108.64
3	A	501[A]	645	C12-N2-N1	2.12	121.53	117.83
3	A	501[B]	645	C12-N2-N1	2.12	121.53	117.83
3	A	501[A]	645	C9-C8-C7	2.05	121.43	119.44
3	A	501[B]	645	C9-C8-C7	2.05	121.43	119.44

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501[A]	645	C14-C12-N2-C1
3	A	501[B]	645	C14-C12-N2-C1
3	A	501[A]	645	C6-C7-S1-O3
3	A	501[B]	645	C6-C7-S1-O3
3	A	501[A]	645	C8-C7-S1-O3
3	A	501[B]	645	C8-C7-S1-O3
3	A	501[A]	645	C13-C12-N2-C1
3	A	501[B]	645	C13-C12-N2-C1
3	A	501[A]	645	C14-C12-N2-N1
3	A	501[B]	645	C14-C12-N2-N1
3	A	501[A]	645	C13-C12-N2-N1
3	A	501[B]	645	C13-C12-N2-N1
3	A	501[A]	645	O2-C3-C4-C9
3	A	501[B]	645	O2-C3-C4-C9
3	A	501[A]	645	C2-C11-C16-C17
3	A	501[A]	645	C2-C11-C16-C21

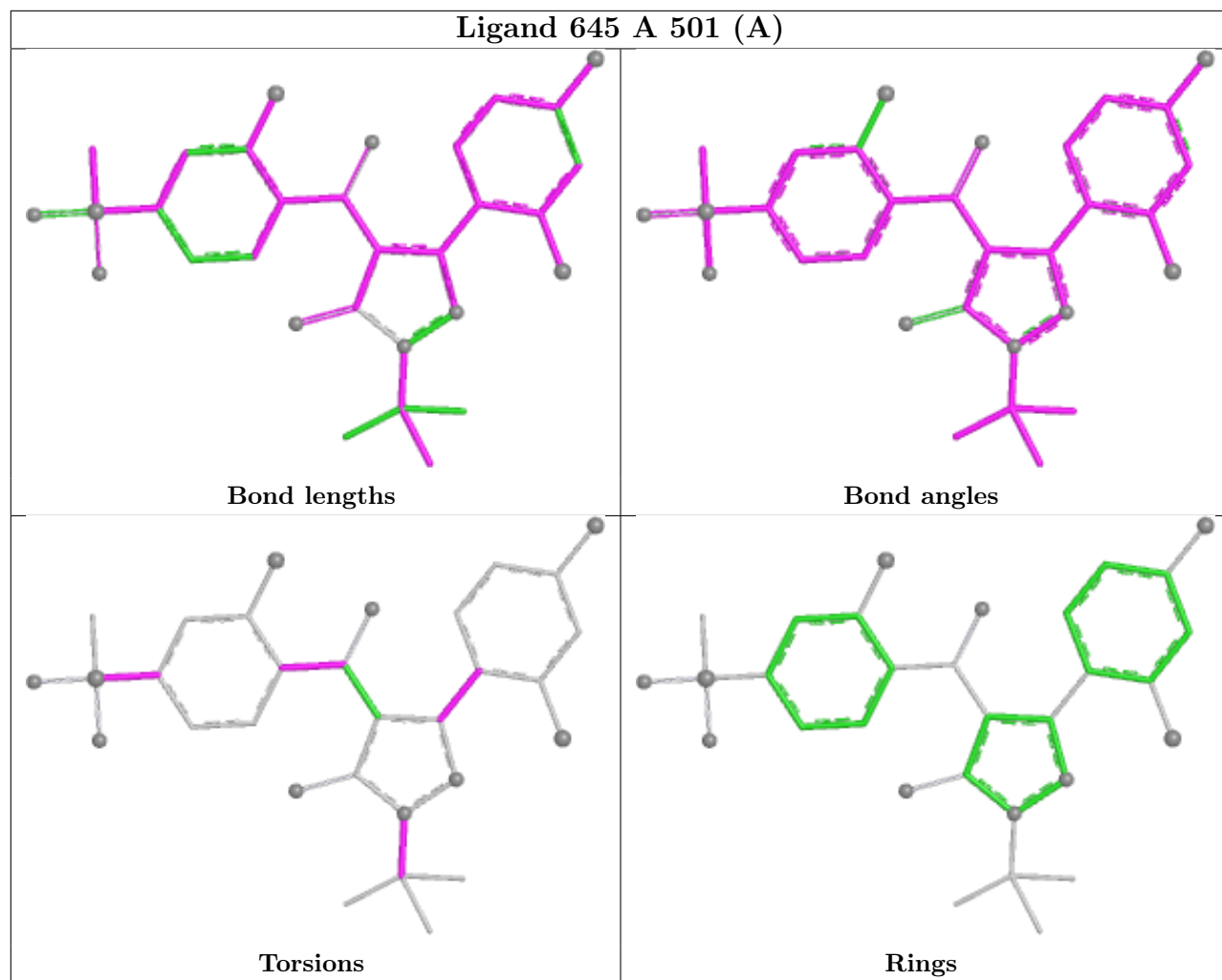
There are no ring outliers.

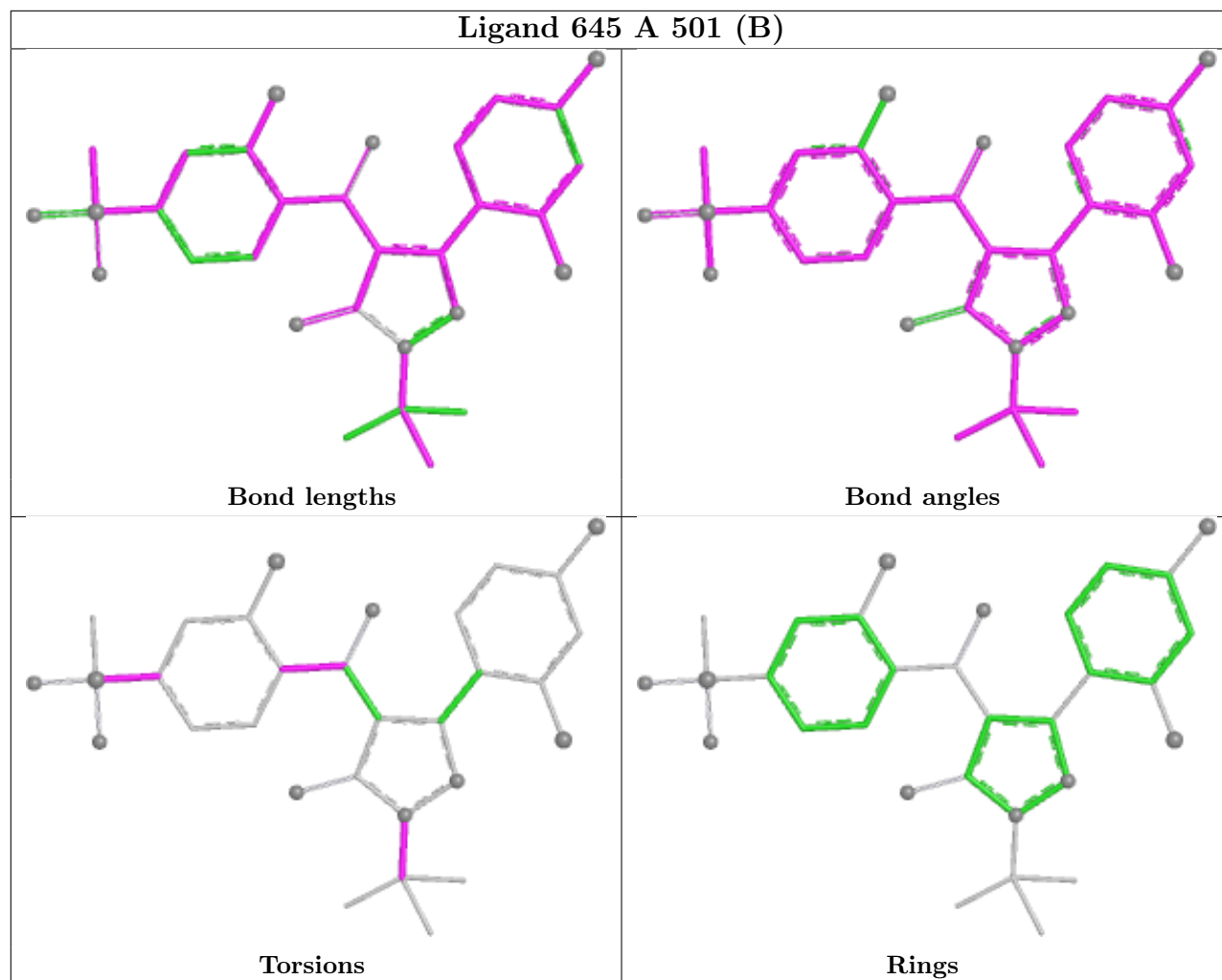
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501[A]	645	2	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.

Ligand 645 A 501 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.