



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2025 – 08:19 PM JST

PDB ID : 9JHU / pdb_00009jhu
Title : Complex structure of AtHPPD with inhibitor CLJ788
Authors : Ying, R.-N.; Lin, H.-Y.; Yang, G.-F.
Deposited on : 2024-09-10
Resolution : 2.00 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

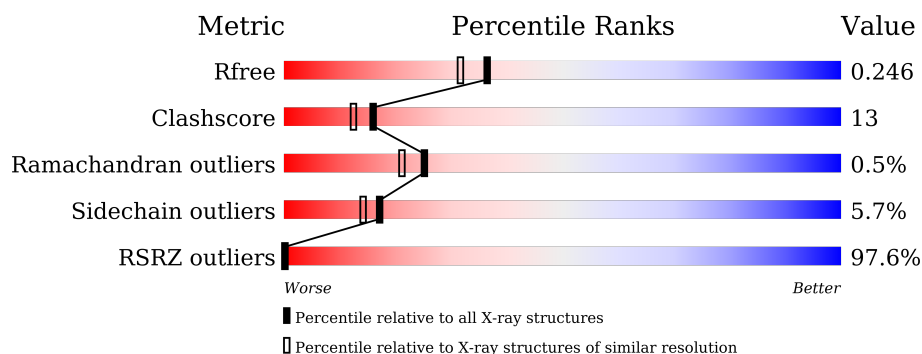
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	402	<div> <div>93%</div> <div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div> </div>

2 Entry composition [i](#)

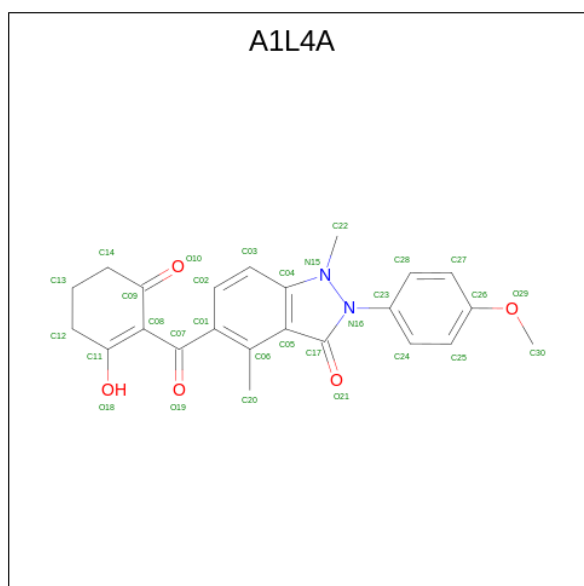
There are 4 unique types of molecules in this entry. The entry contains 2936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	381	2870	1824	490	543	13	0	1	0

- Molecule 2 is 2-(4-methoxyphenyl)-1,4-dimethyl-5-(2-oxidanyl-6-oxidanylidene-cyclohexen-1-yl)carbonyl-indazol-3-one (CCD ID: A1L4A) (formula: C₂₃H₂₂N₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	23	2	5	0	0

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		

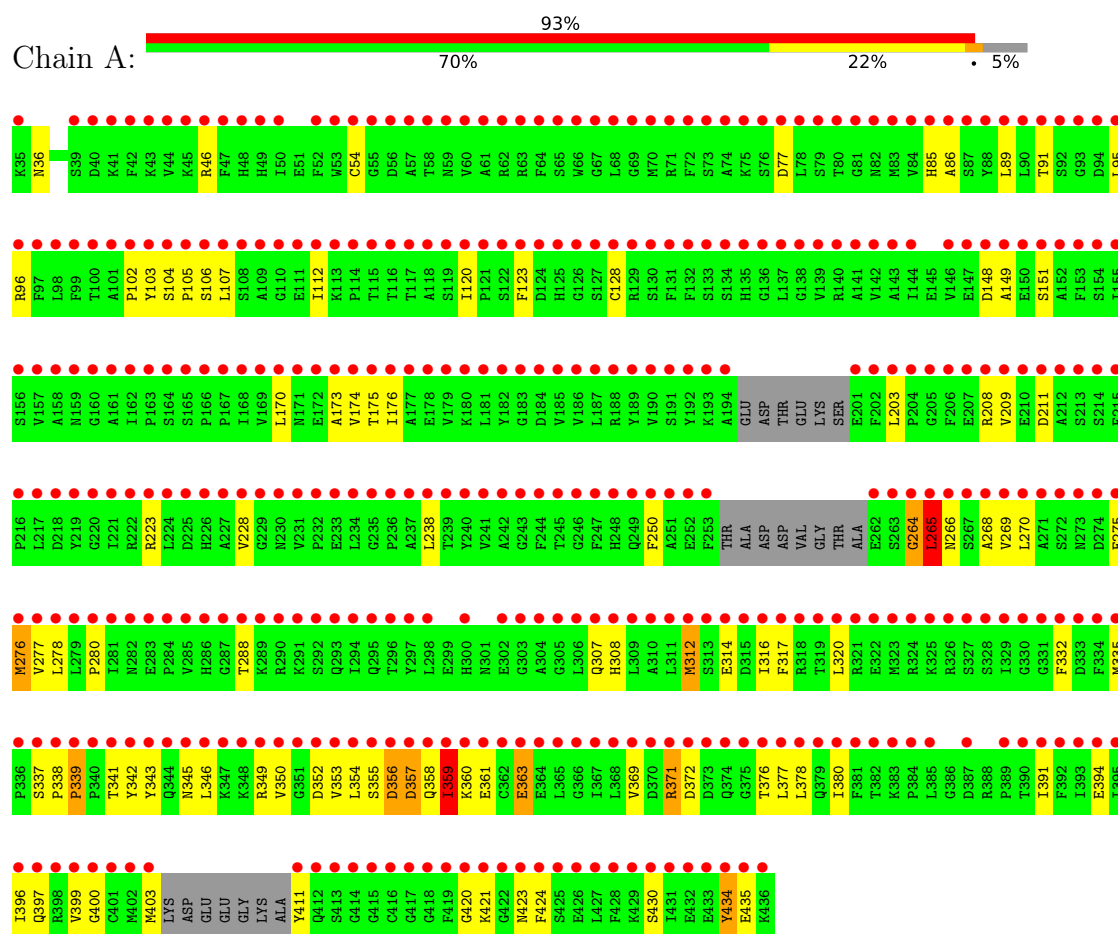
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		

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: 4-hydroxyphenylpyruvate dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.54Å 84.45Å 63.84Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	39.31 – 2.00 39.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.31-2.00) 97.2 (39.31-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.218 , 0.244 0.223 , 0.246	Depositor DCC
R_{free} test set	1338 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	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	0.96	EDS
Total number of atoms	2936	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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: A1L4A, CO

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	1.04	17/2942 (0.6%)	0.94	14/3990 (0.4%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	VAL	C-O	-7.71	1.16	1.24
1	A	278	LEU	C-O	-6.74	1.16	1.24
1	A	312	MET	C-O	-6.21	1.16	1.23
1	A	36	ASN	C-O	-6.16	1.19	1.24
1	A	277	VAL	C-O	-6.11	1.17	1.24
1	A	332	PHE	C-O	-6.06	1.16	1.23
1	A	173	ALA	CA-C	-5.82	1.45	1.52
1	A	104	SER	C-O	-5.80	1.16	1.24
1	A	106	SER	C-O	-5.77	1.17	1.24
1	A	359	ILE	C-O	-5.73	1.17	1.24
1	A	36	ASN	N-CA	-5.47	1.41	1.46
1	A	36	ASN	CA-C	-5.38	1.46	1.52
1	A	107	LEU	C-O	-5.27	1.17	1.24
1	A	105	PRO	C-O	-5.27	1.18	1.24
1	A	359	ILE	CA-C	-5.24	1.46	1.52
1	A	173	ALA	C-O	-5.22	1.17	1.24
1	A	339	PRO	C-O	-5.08	1.20	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	GLN	N-CA-C	-8.62	101.08	111.69
1	A	338	PRO	CA-C-N	7.89	125.42	119.66
1	A	338	PRO	C-N-CA	7.89	125.42	119.66
1	A	264	GLY	N-CA-C	7.79	131.65	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	SER	CA-C-N	7.52	128.13	120.38
1	A	337	SER	C-N-CA	7.52	128.13	120.38
1	A	359	ILE	CB-CA-C	-7.43	102.28	111.87
1	A	266	ASN	N-CA-C	-6.89	96.13	110.80
1	A	36	ASN	CA-C-N	6.52	126.15	119.56
1	A	36	ASN	C-N-CA	6.52	126.15	119.56
1	A	265	LEU	N-CA-C	6.41	120.30	110.36
1	A	339	PRO	N-CA-C	6.04	116.27	110.47
1	A	357	ASP	N-CA-C	-5.74	98.58	110.80
1	A	435	GLU	N-CA-C	-5.45	104.98	111.69

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	2870	0	2722	73	0
2	A	30	0	0	0	0
3	A	1	0	0	0	0
4	A	35	0	0	3	0
All	All	2936	0	2722	73	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 13.

All (73) 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:276:MET:HA	1:A:276:MET:HE2	1.25	1.12
1:A:346:LEU:HD23	1:A:349:ARG:NH1	1.65	1.11
1:A:346:LEU:HD23	1:A:349:ARG:HH12	1.32	0.94
1:A:376:THR:CG2	1:A:399:VAL:HG13	2.04	0.87
1:A:276:MET:HA	1:A:276:MET:CE	2.05	0.86
1:A:317:PHE:CD1	1:A:361:GLU:OE2	2.31	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:HA	1:A:359:ILE:HB	1.61	0.81
1:A:346:LEU:CD2	1:A:349:ARG:HH12	1.97	0.76
1:A:345:ASN:O	1:A:349:ARG:HD3	1.87	0.74
1:A:265:LEU:N	1:A:265:LEU:HD12	2.03	0.74
1:A:46:ARG:NH2	1:A:276:MET:HG3	2.03	0.73
1:A:376:THR:HG23	1:A:399:VAL:CG1	2.19	0.72
1:A:341:THR:HG21	1:A:430:SER:O	1.91	0.70
1:A:314:GLU:O	1:A:397:GLN:NE2	2.21	0.70
1:A:376:THR:HG23	1:A:399:VAL:HG13	1.76	0.67
1:A:46:ARG:CZ	1:A:276:MET:HG3	2.25	0.66
1:A:376:THR:CG2	1:A:399:VAL:CG1	2.76	0.64
1:A:149:ALA:HB3	1:A:175:THR:OG1	1.97	0.64
1:A:376:THR:HG22	1:A:399:VAL:O	1.98	0.62
1:A:238:LEU:HD11	1:A:268:ALA:CB	2.30	0.61
1:A:350:VAL:HG12	1:A:350:VAL:O	2.00	0.61
1:A:265:LEU:HD12	1:A:265:LEU:H	1.67	0.59
1:A:353:VAL:HG12	1:A:354:LEU:HD12	1.84	0.59
1:A:369:VAL:HG22	1:A:378:LEU:HD23	1.84	0.59
1:A:341:THR:HG22	1:A:434:TYR:HB2	1.84	0.58
1:A:316:ILE:HG12	1:A:316:ILE:O	2.03	0.58
1:A:339:PRO:HB2	1:A:341:THR:HG22	1.84	0.58
1:A:238:LEU:HD11	1:A:268:ALA:HB3	1.84	0.58
1:A:276:MET:HE2	1:A:276:MET:CA	2.17	0.56
1:A:376:THR:HG23	1:A:399:VAL:HG12	1.87	0.56
1:A:400:GLY:N	4:A:602:HOH:O	2.31	0.55
1:A:341:THR:CG2	1:A:434:TYR:HB2	2.38	0.54
1:A:228:VAL:HG21	1:A:308:HIS:CE1	2.42	0.54
1:A:342:TYR:HA	1:A:430:SER:OG	2.07	0.54
1:A:346:LEU:CD2	1:A:349:ARG:NH1	2.52	0.53
1:A:265:LEU:N	1:A:265:LEU:CD1	2.72	0.53
1:A:317:PHE:HD1	1:A:361:GLU:OE2	1.89	0.52
1:A:343:TYR:CG	1:A:363:GLU:HG3	2.45	0.51
1:A:434:TYR:C	1:A:434:TYR:CD2	2.87	0.51
1:A:403:MET:HB2	1:A:411:TYR:CE2	2.46	0.50
1:A:399:VAL:HG23	4:A:602:HOH:O	2.13	0.49
1:A:320:LEU:HD11	1:A:380:ILE:HG21	1.93	0.49
1:A:276:MET:CE	1:A:276:MET:CA	2.86	0.48
1:A:352:ASP:OD1	1:A:353:VAL:HG23	2.13	0.48
1:A:102:PRO:HD3	1:A:128:CYS:SG	2.54	0.47
1:A:420:GLY:O	1:A:423:ASN:HB2	2.14	0.46
1:A:265:LEU:H	1:A:265:LEU:CD1	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLN:O	1:A:391:ILE:HA	2.16	0.46
1:A:228:VAL:HG22	1:A:280:PRO:HB2	1.97	0.45
1:A:91:THR:HA	1:A:95:LEU:O	2.17	0.44
1:A:250:PHE:CE2	1:A:275:GLU:OE2	2.71	0.44
1:A:434:TYR:O	1:A:434:TYR:CG	2.70	0.43
1:A:148:ASP:HB3	1:A:151:SER:HB3	2.00	0.43
1:A:85:HIS:HE1	1:A:120:ILE:H	1.65	0.43
1:A:223:ARG:HE	1:A:312:MET:CE	2.32	0.43
1:A:399:VAL:HA	4:A:602:HOH:O	2.18	0.43
1:A:89:LEU:HD11	1:A:96:ARG:HB3	2.01	0.43
1:A:170:LEU:HD12	1:A:176:ILE:HD12	2.01	0.43
1:A:238:LEU:HD22	1:A:270:LEU:HD21	2.01	0.42
1:A:176:ILE:HD11	1:A:203:LEU:HD22	2.01	0.42
1:A:421:LYS:O	1:A:424:PHE:HD1	2.02	0.42
1:A:394:GLU:HG2	1:A:396:ILE:HG23	2.01	0.42
1:A:102:PRO:HB3	1:A:123:PHE:HZ	1.84	0.42
1:A:77:ASP:HB2	1:A:103:TYR:OH	2.20	0.42
1:A:342:TYR:O	1:A:346:LEU:HG	2.20	0.42
1:A:250:PHE:HB3	1:A:269:VAL:HB	2.02	0.41
1:A:352:ASP:OD1	1:A:371:ARG:NH2	2.54	0.41
1:A:341:THR:CG2	1:A:434:TYR:CB	2.99	0.41
1:A:86:ALA:HB2	1:A:103:TYR:CZ	2.56	0.40
1:A:376:THR:HG21	1:A:399:VAL:HG13	1.93	0.40
1:A:353:VAL:HG23	1:A:371:ARG:HH22	1.87	0.40
1:A:353:VAL:HG11	1:A:376:THR:HG21	2.03	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	374/402 (93%)	357 (96%)	15 (4%)	2 (0%)	25	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	GLY
1	A	357	ASP

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	299/338 (88%)	282 (94%)	17 (6%)	17	14

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	208	ARG
1	A	209	VAL
1	A	211	ASP
1	A	265	LEU
1	A	276	MET
1	A	288	THR
1	A	335	MET
1	A	355	SER
1	A	356	ASP
1	A	359	ILE
1	A	360	LYS
1	A	363	GLU
1	A	371	ARG
1	A	372	ASP
1	A	377	LEU
1	A	434	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
2	A1L4A	A	501	3	33,33,33	5.15	19 (57%)	44,49,49	1.89	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1L4A	A	501	3	-	5/14/28/28	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1L4A	C03-C04	9.66	1.55	1.39
2	A	501	A1L4A	C05-C06	9.52	1.54	1.40
2	A	501	A1L4A	C01-C06	8.98	1.52	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1L4A	C25-C24	8.35	1.53	1.38
2	A	501	A1L4A	C25-C26	7.65	1.54	1.38
2	A	501	A1L4A	C03-C02	7.36	1.52	1.38
2	A	501	A1L4A	C24-C23	7.32	1.53	1.39
2	A	501	A1L4A	C02-C01	7.22	1.51	1.39
2	A	501	A1L4A	C28-C23	7.13	1.53	1.39
2	A	501	A1L4A	C27-C28	7.10	1.51	1.38
2	A	501	A1L4A	C27-C26	6.78	1.52	1.38
2	A	501	A1L4A	N16-N15	6.57	1.49	1.40
2	A	501	A1L4A	C17-N16	6.39	1.48	1.40
2	A	501	A1L4A	C08-C09	4.40	1.56	1.46
2	A	501	A1L4A	C05-C04	3.96	1.48	1.41
2	A	501	A1L4A	C08-C11	3.31	1.49	1.39
2	A	501	A1L4A	O18-C11	3.10	1.40	1.32
2	A	501	A1L4A	C04-N15	2.84	1.47	1.37
2	A	501	A1L4A	C14-C09	2.62	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1L4A	C24-C23-N16	5.20	128.63	119.57
2	A	501	A1L4A	C28-C23-N16	-5.06	110.75	119.57
2	A	501	A1L4A	C01-C07-C08	4.31	128.24	120.77
2	A	501	A1L4A	C22-N15-N16	3.93	128.63	118.08
2	A	501	A1L4A	C09-C08-C11	-3.64	115.25	119.27
2	A	501	A1L4A	O19-C07-C01	-3.08	112.26	120.29
2	A	501	A1L4A	C23-N16-N15	2.63	125.92	120.71
2	A	501	A1L4A	C14-C09-C08	2.07	120.84	116.95
2	A	501	A1L4A	C25-C24-C23	-2.07	117.60	120.32

There are no chirality outliers.

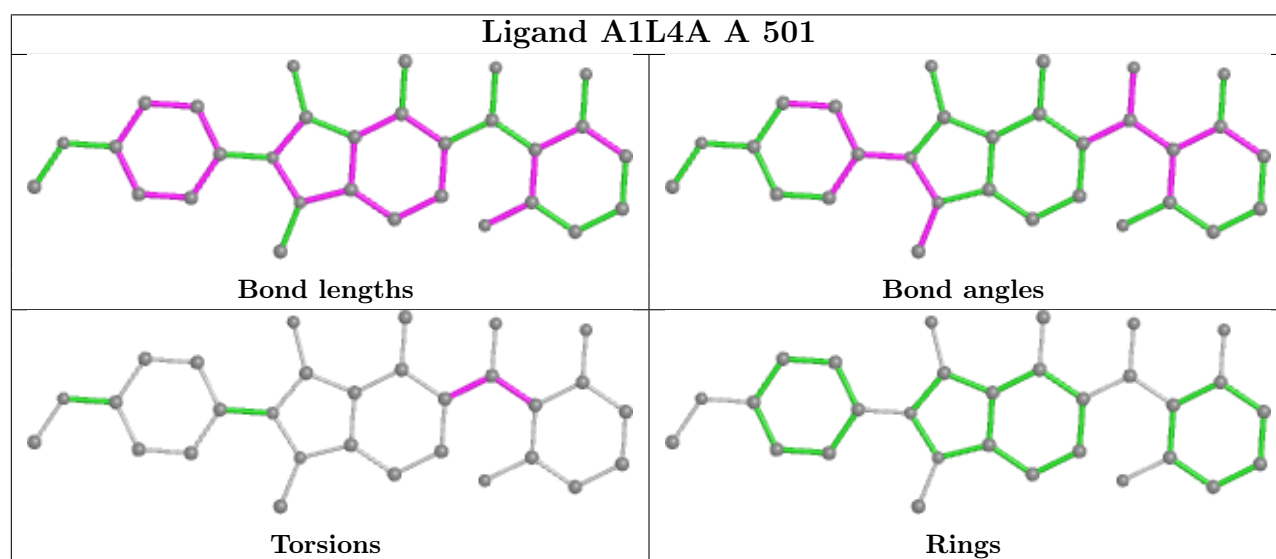
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1L4A	C01-C07-C08-C09
2	A	501	A1L4A	C01-C07-C08-C11
2	A	501	A1L4A	O19-C07-C08-C09
2	A	501	A1L4A	O19-C07-C08-C11
2	A	501	A1L4A	C06-C01-C07-O19

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 ⓘ

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	381/402 (94%)	4.55	372 (97%) 0 0	37, 53, 94, 108	1 (0%)

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	TYR	11.7
1	A	217	LEU	9.6
1	A	215	PHE	9.5
1	A	436	LYS	9.3
1	A	339	PRO	9.3
1	A	366	GLY	9.2
1	A	365	LEU	9.1
1	A	342	TYR	9.0
1	A	354	LEU	9.0
1	A	338	PRO	8.8
1	A	329	ILE	8.6
1	A	320	LEU	8.5
1	A	424	PHE	8.5
1	A	428	PHE	8.5
1	A	328	SER	8.5
1	A	212	ALA	8.4
1	A	253	PHE	8.4
1	A	211	ASP	8.4
1	A	216	PRO	8.0
1	A	214	SER	8.0
1	A	346	LEU	7.9
1	A	419	PHE	7.9
1	A	213	SER	7.8
1	A	286	HIS	7.8
1	A	367	ILE	7.6
1	A	357	ASP	7.6
1	A	340	PRO	7.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	369	VAL	7.6
1	A	66	TRP	7.6
1	A	368	LEU	7.5
1	A	393	ILE	7.5
1	A	234	LEU	7.5
1	A	327	SER	7.4
1	A	116	THR	7.4
1	A	420	GLY	7.3
1	A	238	LEU	7.2
1	A	433	GLU	7.2
1	A	427	LEU	7.2
1	A	341	THR	7.1
1	A	411	TYR	7.1
1	A	429	LYS	7.0
1	A	303	GLY	7.0
1	A	73	SER	6.9
1	A	279	LEU	6.9
1	A	304	ALA	6.9
1	A	84	VAL	6.8
1	A	422	GLY	6.8
1	A	219	TYR	6.7
1	A	269	VAL	6.7
1	A	360	LYS	6.7
1	A	381	PHE	6.7
1	A	115	THR	6.7
1	A	361	GLU	6.7
1	A	337	SER	6.7
1	A	112	ILE	6.5
1	A	426	GLU	6.5
1	A	72	PHE	6.5
1	A	345	ASN	6.4
1	A	65	SER	6.3
1	A	353	VAL	6.2
1	A	290	ARG	6.2
1	A	181	LEU	6.2
1	A	350	VAL	6.2
1	A	268	ALA	6.2
1	A	128	CYS	6.1
1	A	425	SER	6.1
1	A	298	LEU	6.0
1	A	343	TYR	6.0
1	A	287	GLY	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	330	GLY	6.0
1	A	375	GLY	6.0
1	A	205	GLY	5.9
1	A	78	LEU	5.9
1	A	44	VAL	5.9
1	A	42	PHE	5.8
1	A	317	PHE	5.8
1	A	359	ILE	5.8
1	A	94	ASP	5.8
1	A	210	GLU	5.8
1	A	378	LEU	5.8
1	A	423	ASN	5.8
1	A	395	ILE	5.8
1	A	401	CYS	5.8
1	A	377	LEU	5.7
1	A	380	ILE	5.7
1	A	336	PRO	5.7
1	A	157	VAL	5.7
1	A	147	GLU	5.7
1	A	431	ILE	5.7
1	A	278	LEU	5.6
1	A	324	ARG	5.6
1	A	203	LEU	5.6
1	A	285	VAL	5.6
1	A	352	ASP	5.6
1	A	103	TYR	5.6
1	A	120	ILE	5.6
1	A	362	CYS	5.5
1	A	225	ASP	5.5
1	A	202	PHE	5.5
1	A	289	LYS	5.5
1	A	187	LEU	5.5
1	A	241	VAL	5.4
1	A	113[A]	LYS	5.4
1	A	364	GLU	5.4
1	A	243	GLY	5.4
1	A	316	ILE	5.4
1	A	123	PHE	5.4
1	A	150	GLU	5.4
1	A	244	PHE	5.4
1	A	421	LYS	5.3
1	A	68	LEU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	239	THR	5.3
1	A	370	ASP	5.3
1	A	132	PHE	5.3
1	A	209	VAL	5.2
1	A	277	VAL	5.2
1	A	412	GLN	5.2
1	A	262	GLU	5.2
1	A	179	VAL	5.2
1	A	91	THR	5.2
1	A	50	ILE	5.2
1	A	358	GLN	5.2
1	A	206	PHE	5.1
1	A	351	GLY	5.1
1	A	70	MET	5.1
1	A	114	PRO	5.1
1	A	47	PHE	5.1
1	A	323	MET	5.1
1	A	311	LEU	5.1
1	A	158	ALA	5.1
1	A	435	GLU	5.1
1	A	153	PHE	5.0
1	A	263	SER	5.0
1	A	169	VAL	5.0
1	A	71	ARG	5.0
1	A	242	ALA	5.0
1	A	309	LEU	4.9
1	A	349	ARG	4.9
1	A	416	CYS	4.9
1	A	162	ILE	4.9
1	A	67	GLY	4.9
1	A	237	ALA	4.9
1	A	335	MET	4.9
1	A	185	VAL	4.9
1	A	399	VAL	4.9
1	A	305	GLY	4.9
1	A	432	GLU	4.8
1	A	265	LEU	4.8
1	A	296	THR	4.8
1	A	218	ASP	4.8
1	A	270	LEU	4.8
1	A	266	ASN	4.8
1	A	201	GLU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	231	VAL	4.7
1	A	295	GLN	4.7
1	A	152	ALA	4.7
1	A	382	THR	4.7
1	A	325	LYS	4.7
1	A	118	ALA	4.7
1	A	267	SER	4.7
1	A	81	GLY	4.7
1	A	223	ARG	4.7
1	A	117	THR	4.7
1	A	224	LEU	4.7
1	A	280	PRO	4.7
1	A	402	MET	4.6
1	A	110	GLY	4.6
1	A	119	SER	4.6
1	A	376	THR	4.6
1	A	131	PHE	4.6
1	A	403	MET	4.6
1	A	92	SER	4.5
1	A	326	ARG	4.5
1	A	334	PHE	4.5
1	A	194	ALA	4.4
1	A	176	ILE	4.4
1	A	396	ILE	4.4
1	A	86	ALA	4.4
1	A	142	VAL	4.4
1	A	168	ILE	4.4
1	A	121	PRO	4.4
1	A	204	PRO	4.4
1	A	149	ALA	4.4
1	A	430	SER	4.4
1	A	170	LEU	4.4
1	A	400	GLY	4.3
1	A	40	ASP	4.3
1	A	373	ASP	4.3
1	A	392	PHE	4.3
1	A	319	THR	4.3
1	A	232	PRO	4.3
1	A	228	VAL	4.3
1	A	371	ARG	4.2
1	A	101	ALA	4.2
1	A	221	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	189	TYR	4.2
1	A	288	THR	4.2
1	A	208	ARG	4.2
1	A	245	THR	4.2
1	A	348	LYS	4.2
1	A	374	GLN	4.2
1	A	247	PHE	4.2
1	A	107	LEU	4.1
1	A	54	CYS	4.1
1	A	90	LEU	4.1
1	A	331	GLY	4.1
1	A	355	SER	4.0
1	A	356	ASP	4.0
1	A	175	THR	4.0
1	A	385	LEU	4.0
1	A	171	ASN	4.0
1	A	62	ARG	4.0
1	A	291	LYS	4.0
1	A	190	VAL	4.0
1	A	294	ILE	4.0
1	A	347	LYS	4.0
1	A	100	THR	4.0
1	A	281	ILE	4.0
1	A	192	TYR	3.9
1	A	284	PRO	3.9
1	A	391	ILE	3.9
1	A	387	ASP	3.9
1	A	251	ALA	3.8
1	A	58	THR	3.8
1	A	83	MET	3.8
1	A	344	GLN	3.8
1	A	154	SER	3.8
1	A	372	ASP	3.8
1	A	363	GLU	3.8
1	A	161	ALA	3.8
1	A	312	MET	3.8
1	A	88	TYR	3.8
1	A	52	PHE	3.8
1	A	126	GLY	3.8
1	A	141	ALA	3.8
1	A	93	GLY	3.7
1	A	235	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	148	ASP	3.7
1	A	146	VAL	3.7
1	A	186	VAL	3.7
1	A	322	GLU	3.7
1	A	174	VAL	3.7
1	A	143	ALA	3.7
1	A	87	SER	3.7
1	A	80	THR	3.6
1	A	321	ARG	3.6
1	A	264	GLY	3.6
1	A	248	HIS	3.6
1	A	230	ASN	3.6
1	A	173	ALA	3.5
1	A	207	GLU	3.5
1	A	313	SER	3.5
1	A	137	LEU	3.5
1	A	109	ALA	3.5
1	A	315	ASP	3.5
1	A	379	GLN	3.5
1	A	99	PHE	3.5
1	A	250	PHE	3.5
1	A	124	ASP	3.4
1	A	172	GLU	3.4
1	A	252	GLU	3.4
1	A	130	SER	3.4
1	A	293	GLN	3.4
1	A	57	ALA	3.4
1	A	415	GLY	3.4
1	A	159	ASN	3.4
1	A	292	SER	3.4
1	A	144	ILE	3.4
1	A	63	ARG	3.4
1	A	220	GLY	3.4
1	A	138	GLY	3.3
1	A	177	ALA	3.3
1	A	249	GLN	3.3
1	A	222	ARG	3.3
1	A	95	LEU	3.3
1	A	333	ASP	3.3
1	A	418	GLY	3.3
1	A	60	VAL	3.3
1	A	383	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	332	PHE	3.3
1	A	82	ASN	3.2
1	A	156	SER	3.2
1	A	236	PRO	3.2
1	A	59	ASN	3.2
1	A	155	ILE	3.2
1	A	140	ARG	3.2
1	A	163	PRO	3.2
1	A	166	PRO	3.2
1	A	53	TRP	3.2
1	A	394	GLU	3.2
1	A	134	SER	3.2
1	A	160	GLY	3.1
1	A	104	SER	3.1
1	A	122	SER	3.1
1	A	102	PRO	3.1
1	A	275	GLU	3.1
1	A	193	LYS	3.1
1	A	56	ASP	3.1
1	A	229	GLY	3.1
1	A	240	TYR	3.0
1	A	85	HIS	3.0
1	A	246	GLY	3.0
1	A	125	HIS	3.0
1	A	397	GLN	3.0
1	A	167	PRO	2.9
1	A	106	SER	2.9
1	A	46	ARG	2.9
1	A	129	ARG	2.9
1	A	43	LYS	2.9
1	A	182	TYR	2.9
1	A	389	PRO	2.9
1	A	127	SER	2.9
1	A	318	ARG	2.9
1	A	35	LYS	2.9
1	A	45	LYS	2.9
1	A	98	LEU	2.9
1	A	297	TYR	2.9
1	A	283	GLU	2.8
1	A	417	GLY	2.8
1	A	180	LYS	2.8
1	A	272	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	390	THR	2.8
1	A	307	GLN	2.8
1	A	188	ARG	2.8
1	A	41	LYS	2.8
1	A	111	GLU	2.7
1	A	151	SER	2.7
1	A	398	ARG	2.7
1	A	310	ALA	2.7
1	A	133	SER	2.7
1	A	75	LYS	2.7
1	A	164	SER	2.7
1	A	178	GLU	2.7
1	A	64	PHE	2.6
1	A	184	ASP	2.6
1	A	306	LEU	2.6
1	A	97	PHE	2.6
1	A	49	HIS	2.6
1	A	135	HIS	2.6
1	A	308	HIS	2.6
1	A	273	ASN	2.6
1	A	274	ASP	2.6
1	A	300	HIS	2.5
1	A	105	PRO	2.5
1	A	136	GLY	2.5
1	A	48	HIS	2.5
1	A	233	GLU	2.5
1	A	414	GLY	2.5
1	A	74	ALA	2.5
1	A	227	ALA	2.5
1	A	413	SER	2.4
1	A	77	ASP	2.4
1	A	384	PRO	2.4
1	A	55	GLY	2.4
1	A	89	LEU	2.4
1	A	226	HIS	2.4
1	A	165	SER	2.4
1	A	139	VAL	2.4
1	A	39	SER	2.3
1	A	271	ALA	2.3
1	A	314	GLU	2.3
1	A	276	MET	2.3
1	A	79	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	191	SER	2.3
1	A	61	ALA	2.2
1	A	282	ASN	2.2
1	A	69	GLY	2.1
1	A	96	ARG	2.1
1	A	76	SER	2.1
1	A	183	GLY	2.1
1	A	108	SER	2.0
1	A	302	GLU	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](#)

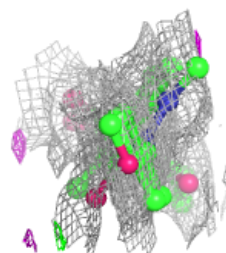
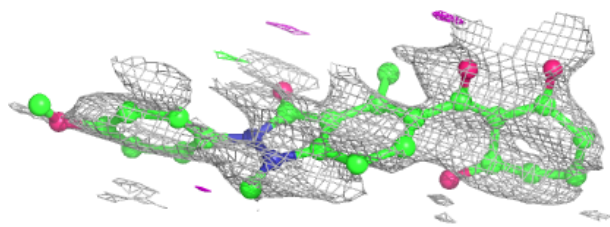
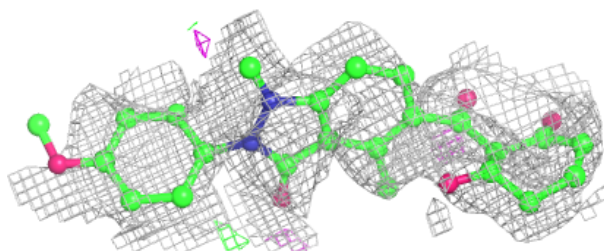
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1L4A	A	501	30/30	0.60	0.30	55,73,82,82	0
3	CO	A	502	1/1	0.95	0.06	50,50,50,50	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.

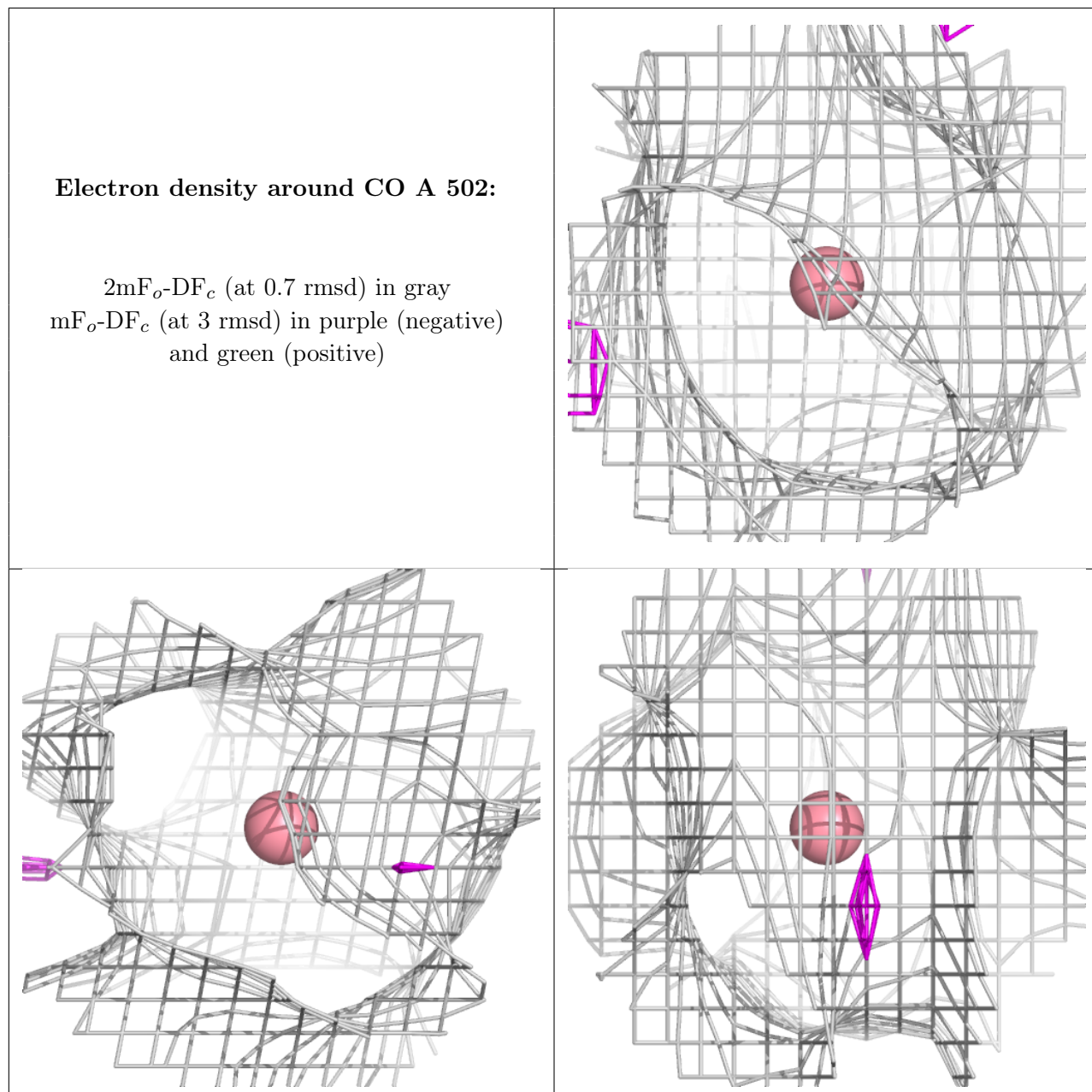
Electron density around A1L4A A 501:

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



Electron density around CO A 502:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.