



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:49 AM UTC

PDB ID : 9JHU / pdb_00009jhu
Title : Complex structure of AtHPPD with inhibitor CLJ788
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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 Phenix2.0
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

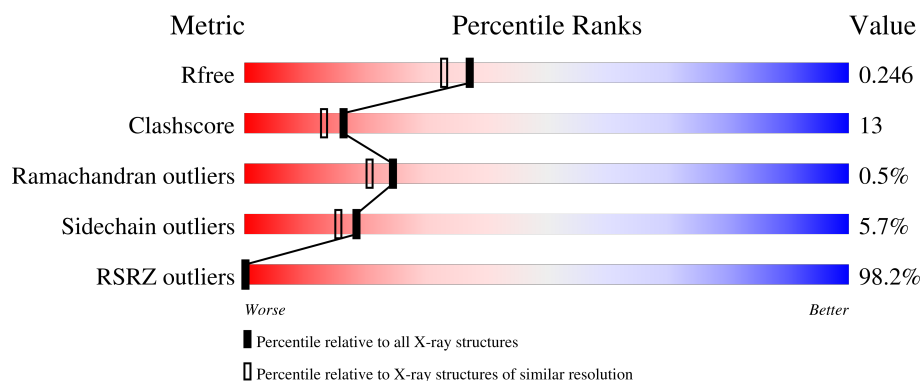
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	93% 70% 22% • 5%

2 Entry composition [i](#)

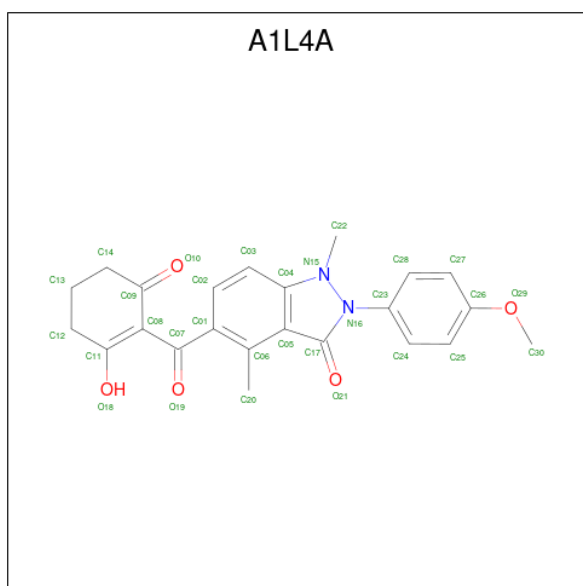
There are 4 unique types of molecules in this entry. The entry contains 2936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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
2	A	1	Total	C	N	O	0	0
			30	23	2	5		

- 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		

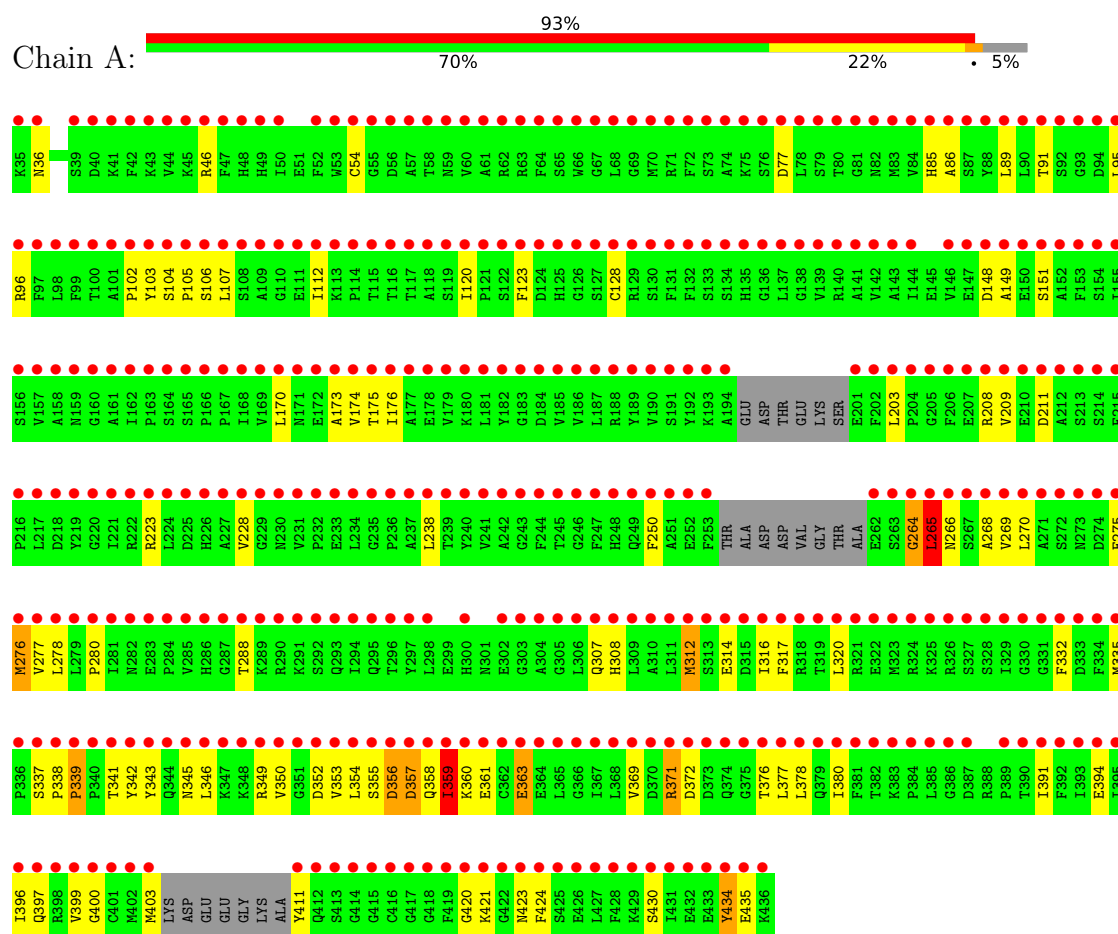
- Molecule 4 is water.

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

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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

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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

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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 ⓘ

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	374/402 (93%)	357 (96%)	15 (4%)	2 (0%)	24	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%)	18	15

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	5.55	20 (60%)	41,49,49	2.84	12 (29%)

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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1L4A	C03-C04	10.37	1.55	1.39
2	A	501	A1L4A	C01-C06	9.66	1.52	1.40
2	A	501	A1L4A	C05-C06	9.57	1.54	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1L4A	C25-C24	9.36	1.53	1.38
2	A	501	A1L4A	C17-N16	8.75	1.48	1.39
2	A	501	A1L4A	C03-C02	8.25	1.52	1.38
2	A	501	A1L4A	C25-C26	8.14	1.54	1.38
2	A	501	A1L4A	C27-C28	7.95	1.51	1.38
2	A	501	A1L4A	C24-C23	7.66	1.53	1.39
2	A	501	A1L4A	C02-C01	7.55	1.51	1.39
2	A	501	A1L4A	C28-C23	7.46	1.53	1.39
2	A	501	A1L4A	C27-C26	7.21	1.52	1.38
2	A	501	A1L4A	N16-N15	6.79	1.49	1.40
2	A	501	A1L4A	C08-C09	4.36	1.56	1.45
2	A	501	A1L4A	C05-C04	4.16	1.48	1.41
2	A	501	A1L4A	C08-C11	3.36	1.49	1.39
2	A	501	A1L4A	C04-N15	3.09	1.47	1.37
2	A	501	A1L4A	O18-C11	2.93	1.40	1.32
2	A	501	A1L4A	C14-C09	2.56	1.54	1.50
2	A	501	A1L4A	O19-C07	-2.02	1.19	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1L4A	C12-C11-C08	-12.71	109.25	122.90
2	A	501	A1L4A	C24-C23-N16	5.38	128.63	119.58
2	A	501	A1L4A	C28-C23-N16	-5.25	110.75	119.58
2	A	501	A1L4A	C22-N15-N16	4.01	128.63	118.00
2	A	501	A1L4A	C01-C07-C08	3.91	128.24	120.83
2	A	501	A1L4A	C09-C08-C11	-3.49	115.25	119.13
2	A	501	A1L4A	O19-C07-C01	-3.19	112.26	120.41
2	A	501	A1L4A	O21-C17-N16	2.91	126.21	124.11
2	A	501	A1L4A	C23-N16-N15	2.72	125.92	120.69
2	A	501	A1L4A	C25-C24-C23	-2.13	117.60	120.30
2	A	501	A1L4A	C06-C01-C07	-2.12	119.70	121.92
2	A	501	A1L4A	C14-C09-C08	2.11	120.84	116.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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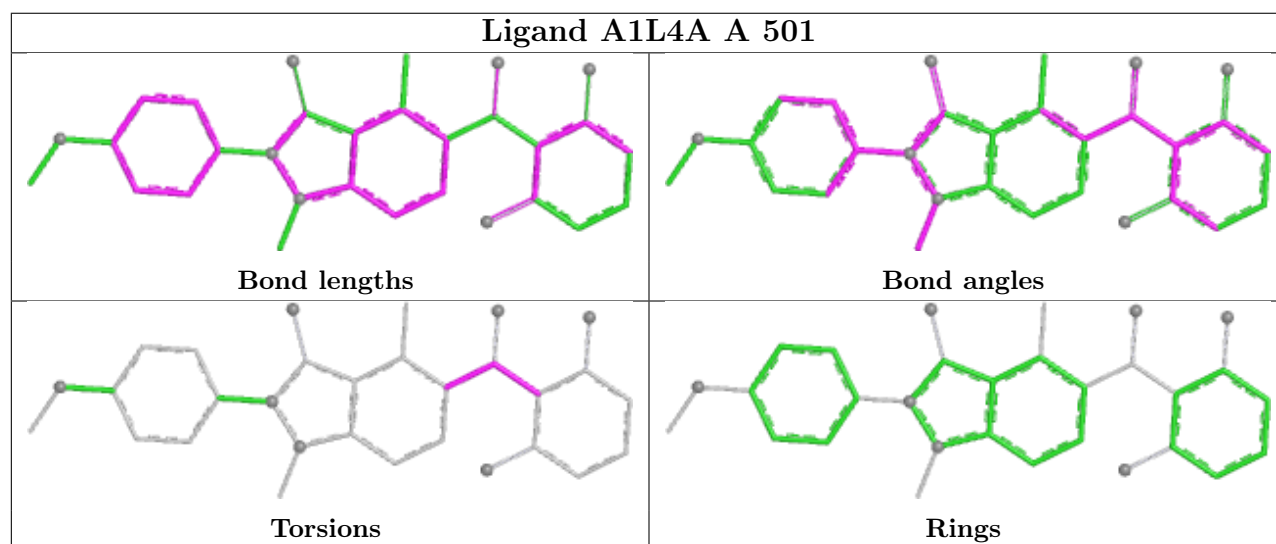
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Mol	Chain	Res	Type	Atoms
2	A	501	A1L4A	C06-C01-C07-O19

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 [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

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%)	4.73	374 (98%) 0 0	37, 53, 94, 108	1 (0%)

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	TYR	12.0
1	A	217	LEU	10.0
1	A	215	PHE	9.8
1	A	339	PRO	9.6
1	A	366	GLY	9.5
1	A	365	LEU	9.4
1	A	436	LYS	9.4
1	A	342	TYR	9.4
1	A	354	LEU	9.3
1	A	338	PRO	9.1
1	A	320	LEU	8.9
1	A	329	ILE	8.9
1	A	424	PHE	8.8
1	A	212	ALA	8.8
1	A	428	PHE	8.8
1	A	328	SER	8.7
1	A	253	PHE	8.7
1	A	211	ASP	8.5
1	A	216	PRO	8.3
1	A	346	LEU	8.2
1	A	214	SER	8.2
1	A	419	PHE	8.2
1	A	213	SER	8.0
1	A	66	TRP	8.0
1	A	286	HIS	8.0
1	A	367	ILE	7.9
1	A	369	VAL	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	340	PRO	7.9
1	A	368	LEU	7.8
1	A	234	LEU	7.8
1	A	393	ILE	7.8
1	A	357	ASP	7.8
1	A	420	GLY	7.6
1	A	116	THR	7.6
1	A	327	SER	7.6
1	A	238	LEU	7.5
1	A	427	LEU	7.4
1	A	411	TYR	7.4
1	A	341	THR	7.4
1	A	303	GLY	7.3
1	A	433	GLU	7.3
1	A	304	ALA	7.2
1	A	279	LEU	7.2
1	A	422	GLY	7.1
1	A	84	VAL	7.1
1	A	429	LYS	7.1
1	A	73	SER	7.1
1	A	269	VAL	7.0
1	A	219	TYR	7.0
1	A	381	PHE	6.9
1	A	115	THR	6.9
1	A	337	SER	6.9
1	A	112	ILE	6.8
1	A	72	PHE	6.8
1	A	360	LYS	6.8
1	A	361	GLU	6.7
1	A	426	GLU	6.6
1	A	345	ASN	6.5
1	A	353	VAL	6.5
1	A	65	SER	6.5
1	A	268	ALA	6.5
1	A	181	LEU	6.5
1	A	350	VAL	6.5
1	A	290	ARG	6.3
1	A	298	LEU	6.3
1	A	128	CYS	6.3
1	A	425	SER	6.3
1	A	343	TYR	6.3
1	A	287	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	330	GLY	6.3
1	A	375	GLY	6.3
1	A	205	GLY	6.2
1	A	78	LEU	6.1
1	A	44	VAL	6.1
1	A	42	PHE	6.1
1	A	317	PHE	6.1
1	A	359	ILE	6.0
1	A	378	LEU	6.0
1	A	377	LEU	6.0
1	A	395	ILE	6.0
1	A	94	ASP	6.0
1	A	380	ILE	6.0
1	A	401	CYS	5.9
1	A	157	VAL	5.9
1	A	423	ASN	5.9
1	A	336	PRO	5.9
1	A	278	LEU	5.9
1	A	431	ILE	5.9
1	A	285	VAL	5.9
1	A	203	LEU	5.9
1	A	210	GLU	5.8
1	A	103	TYR	5.8
1	A	120	ILE	5.8
1	A	352	ASP	5.7
1	A	147	GLU	5.7
1	A	202	PHE	5.7
1	A	324	ARG	5.7
1	A	362	CYS	5.7
1	A	187	LEU	5.7
1	A	243	GLY	5.7
1	A	241	VAL	5.7
1	A	225	ASP	5.7
1	A	316	ILE	5.6
1	A	123	PHE	5.6
1	A	244	PHE	5.6
1	A	68	LEU	5.5
1	A	289	LYS	5.5
1	A	239	THR	5.5
1	A	113[A]	LYS	5.5
1	A	132	PHE	5.5
1	A	364	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	209	VAL	5.5
1	A	277	VAL	5.5
1	A	150	GLU	5.4
1	A	370	ASP	5.4
1	A	179	VAL	5.4
1	A	421	LYS	5.4
1	A	351	GLY	5.4
1	A	50	ILE	5.4
1	A	206	PHE	5.4
1	A	158	ALA	5.4
1	A	91	THR	5.3
1	A	412	GLN	5.3
1	A	114	PRO	5.3
1	A	47	PHE	5.3
1	A	311	LEU	5.3
1	A	70	MET	5.3
1	A	262	GLU	5.3
1	A	358	GLN	5.3
1	A	323	MET	5.3
1	A	153	PHE	5.3
1	A	169	VAL	5.2
1	A	242	ALA	5.2
1	A	263	SER	5.2
1	A	309	LEU	5.2
1	A	162	ILE	5.1
1	A	435	GLU	5.1
1	A	237	ALA	5.1
1	A	67	GLY	5.1
1	A	416	CYS	5.1
1	A	71	ARG	5.1
1	A	305	GLY	5.1
1	A	185	VAL	5.1
1	A	399	VAL	5.1
1	A	265	LEU	5.1
1	A	270	LEU	5.0
1	A	349	ARG	5.0
1	A	335	MET	5.0
1	A	296	THR	5.0
1	A	152	ALA	5.0
1	A	218	ASP	5.0
1	A	231	VAL	5.0
1	A	118	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	4.9
1	A	266	ASN	4.9
1	A	432	GLU	4.9
1	A	382	THR	4.9
1	A	224	LEU	4.9
1	A	110	GLY	4.9
1	A	280	PRO	4.9
1	A	267	SER	4.8
1	A	295	GLN	4.8
1	A	117	THR	4.8
1	A	201	GLU	4.8
1	A	131	PHE	4.8
1	A	402	MET	4.8
1	A	376	THR	4.8
1	A	325	LYS	4.8
1	A	119	SER	4.8
1	A	223	ARG	4.8
1	A	403	MET	4.7
1	A	92	SER	4.7
1	A	334	PHE	4.7
1	A	194	ALA	4.7
1	A	86	ALA	4.7
1	A	149	ALA	4.6
1	A	142	VAL	4.6
1	A	176	ILE	4.6
1	A	396	ILE	4.6
1	A	326	ARG	4.6
1	A	168	ILE	4.6
1	A	121	PRO	4.6
1	A	204	PRO	4.6
1	A	400	GLY	4.6
1	A	170	LEU	4.6
1	A	392	PHE	4.5
1	A	430	SER	4.5
1	A	319	THR	4.5
1	A	232	PRO	4.5
1	A	101	ALA	4.5
1	A	40	ASP	4.5
1	A	373	ASP	4.5
1	A	228	VAL	4.5
1	A	189	TYR	4.4
1	A	221	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	288	THR	4.4
1	A	247	PHE	4.3
1	A	107	LEU	4.3
1	A	371	ARG	4.3
1	A	245	THR	4.3
1	A	90	LEU	4.3
1	A	331	GLY	4.3
1	A	54	CYS	4.3
1	A	374	GLN	4.3
1	A	208	ARG	4.3
1	A	385	LEU	4.2
1	A	348	LYS	4.2
1	A	175	THR	4.2
1	A	190	VAL	4.2
1	A	355	SER	4.2
1	A	294	ILE	4.2
1	A	356	ASP	4.2
1	A	171	ASN	4.2
1	A	281	ILE	4.1
1	A	192	TYR	4.1
1	A	100	THR	4.1
1	A	62	ARG	4.1
1	A	291	LYS	4.1
1	A	391	ILE	4.1
1	A	251	ALA	4.1
1	A	284	PRO	4.1
1	A	347	LYS	4.1
1	A	161	ALA	4.0
1	A	58	THR	4.0
1	A	387	ASP	4.0
1	A	141	ALA	4.0
1	A	83	MET	4.0
1	A	154	SER	4.0
1	A	88	TYR	4.0
1	A	126	GLY	4.0
1	A	52	PHE	4.0
1	A	93	GLY	3.9
1	A	235	GLY	3.9
1	A	344	GLN	3.9
1	A	372	ASP	3.9
1	A	312	MET	3.9
1	A	146	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	186	VAL	3.9
1	A	143	ALA	3.9
1	A	174	VAL	3.9
1	A	363	GLU	3.9
1	A	148	ASP	3.9
1	A	264	GLY	3.8
1	A	87	SER	3.8
1	A	80	THR	3.8
1	A	173	ALA	3.8
1	A	322	GLU	3.8
1	A	248	HIS	3.7
1	A	109	ALA	3.7
1	A	321	ARG	3.7
1	A	230	ASN	3.7
1	A	137	LEU	3.7
1	A	313	SER	3.7
1	A	99	PHE	3.7
1	A	250	PHE	3.7
1	A	315	ASP	3.6
1	A	379	GLN	3.6
1	A	207	GLU	3.6
1	A	57	ALA	3.6
1	A	415	GLY	3.6
1	A	220	GLY	3.6
1	A	144	ILE	3.6
1	A	130	SER	3.6
1	A	124	ASP	3.6
1	A	177	ALA	3.5
1	A	138	GLY	3.5
1	A	292	SER	3.5
1	A	159	ASN	3.5
1	A	293	GLN	3.5
1	A	172	GLU	3.5
1	A	252	GLU	3.5
1	A	95	LEU	3.5
1	A	418	GLY	3.5
1	A	63	ARG	3.5
1	A	60	VAL	3.5
1	A	249	GLN	3.4
1	A	332	PHE	3.4
1	A	333	ASP	3.4
1	A	222	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	53	TRP	3.4
1	A	236	PRO	3.4
1	A	155	ILE	3.4
1	A	156	SER	3.4
1	A	82	ASN	3.4
1	A	163	PRO	3.4
1	A	166	PRO	3.4
1	A	383	LYS	3.3
1	A	160	GLY	3.3
1	A	59	ASN	3.3
1	A	134	SER	3.3
1	A	102	PRO	3.3
1	A	140	ARG	3.3
1	A	104	SER	3.3
1	A	122	SER	3.3
1	A	229	GLY	3.3
1	A	394	GLU	3.2
1	A	56	ASP	3.2
1	A	240	TYR	3.2
1	A	275	GLU	3.2
1	A	193	LYS	3.2
1	A	246	GLY	3.2
1	A	85	HIS	3.2
1	A	167	PRO	3.1
1	A	125	HIS	3.1
1	A	182	TYR	3.1
1	A	397	GLN	3.1
1	A	106	SER	3.1
1	A	389	PRO	3.1
1	A	98	LEU	3.0
1	A	297	TYR	3.0
1	A	127	SER	3.0
1	A	417	GLY	3.0
1	A	46	ARG	3.0
1	A	129	ARG	3.0
1	A	43	LYS	3.0
1	A	318	ARG	3.0
1	A	35	LYS	3.0
1	A	45	LYS	3.0
1	A	272	SER	2.9
1	A	390	THR	2.9
1	A	283	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	2.9
1	A	310	ALA	2.9
1	A	307	GLN	2.9
1	A	188	ARG	2.9
1	A	151	SER	2.9
1	A	41	LYS	2.8
1	A	133	SER	2.8
1	A	398	ARG	2.8
1	A	111	GLU	2.8
1	A	64	PHE	2.8
1	A	164	SER	2.8
1	A	306	LEU	2.8
1	A	97	PHE	2.8
1	A	75	LYS	2.8
1	A	184	ASP	2.8
1	A	49	HIS	2.7
1	A	135	HIS	2.7
1	A	178	GLU	2.7
1	A	308	HIS	2.7
1	A	136	GLY	2.7
1	A	105	PRO	2.7
1	A	273	ASN	2.7
1	A	300	HIS	2.7
1	A	74	ALA	2.7
1	A	227	ALA	2.7
1	A	414	GLY	2.7
1	A	274	ASP	2.7
1	A	48	HIS	2.7
1	A	233	GLU	2.6
1	A	55	GLY	2.6
1	A	384	PRO	2.5
1	A	89	LEU	2.5
1	A	413	SER	2.5
1	A	139	VAL	2.5
1	A	77	ASP	2.5
1	A	165	SER	2.5
1	A	226	HIS	2.5
1	A	271	ALA	2.5
1	A	39	SER	2.5
1	A	61	ALA	2.4
1	A	79	SER	2.4
1	A	191	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	276	MET	2.4
1	A	314	GLU	2.4
1	A	282	ASN	2.3
1	A	69	GLY	2.3
1	A	183	GLY	2.2
1	A	96	ARG	2.2
1	A	76	SER	2.2
1	A	108	SER	2.2
1	A	386	GLY	2.2
1	A	302	GLU	2.1
1	A	36	ASN	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](#)

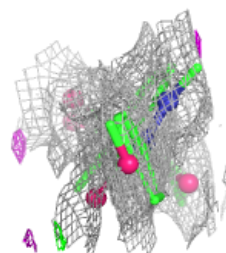
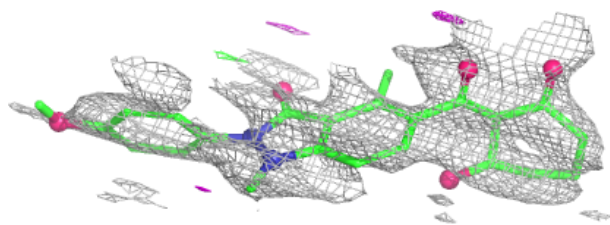
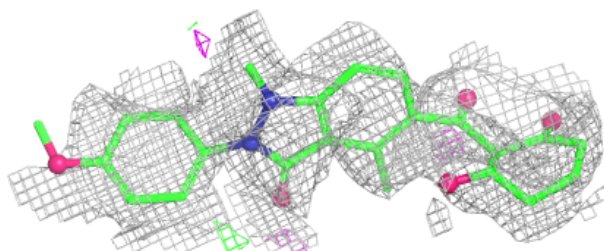
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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.

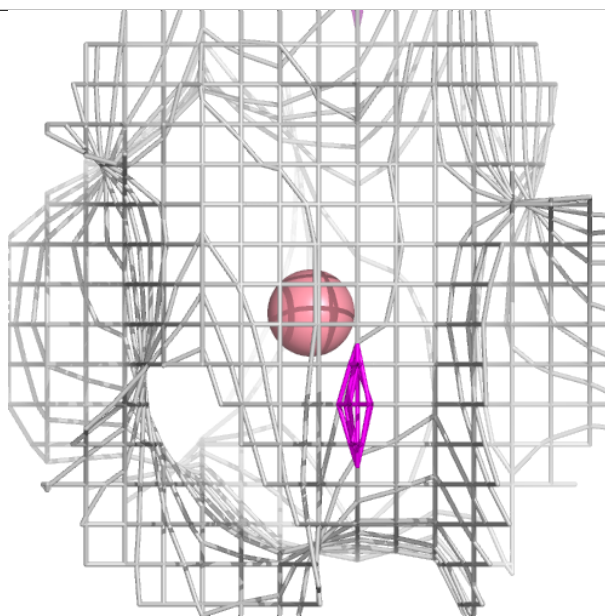
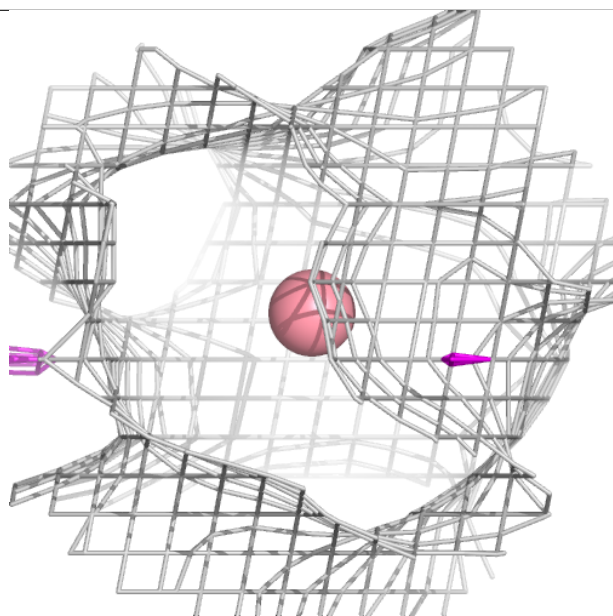
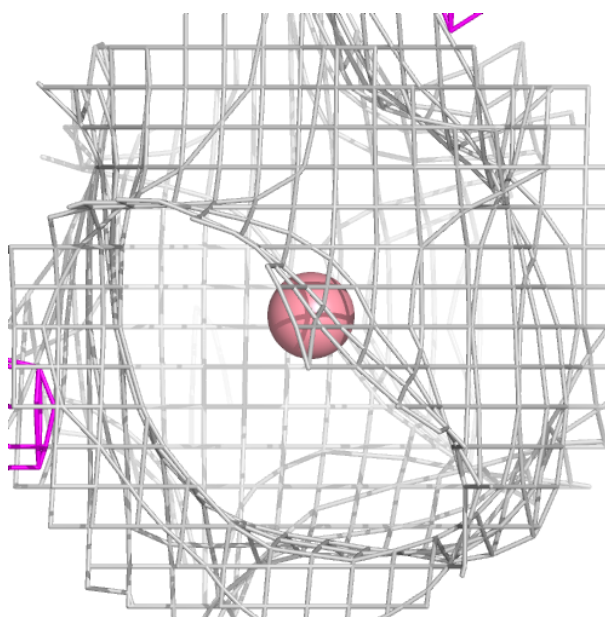
Electron density around A1L4A A 501:

$2mF_o-DF_c$ (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.