



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2021 – 10:26 AM EDT

PDB ID : 6VVH
Title : Arabidopsis thaliana dihydrodipicolinate synthase isoform 1 (DHDPS1) in complex with lysine
Authors : Lee, M.; Hall, C.J.
Deposited on : 2020-02-18
Resolution : 1.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

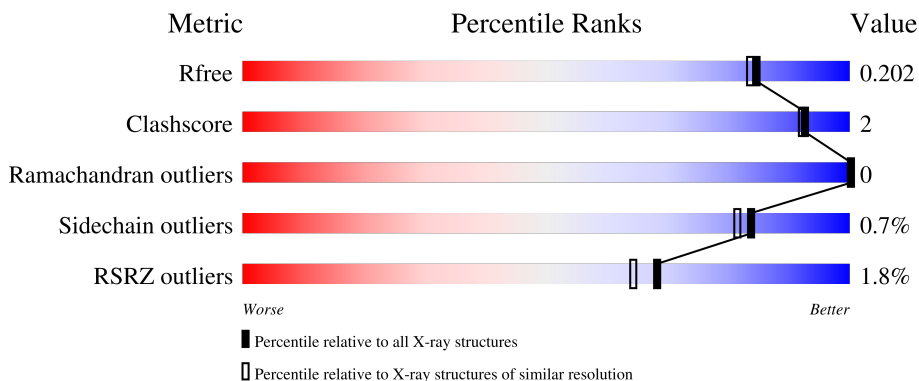
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	AAA	321	<div> <div>0%</div> <div>93%</div> <div>5%</div> <div>2%</div> </div>
1	BBB	321	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>2%</div> </div>
1	CCC	321	<div> <div>2%</div> <div>95%</div> <div>2%</div> <div>2%</div> </div>
1	DDD	321	<div> <div>2%</div> <div>95%</div> <div>2%</div> <div>2%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11023 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-hydroxy-tetrahydrodipicolinate synthase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	308	Total	C	N	O	S	0	12	0
			2474	1565	445	449	15			
1	BBB	313	Total	C	N	O	S	0	16	0
			2525	1598	447	465	15			
1	CCC	312	Total	C	N	O	S	0	10	0
			2474	1562	434	463	15			
1	DDD	312	Total	C	N	O	S	0	7	0
			2463	1554	435	458	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	45	GLY	-	expression tag	UNP Q9LZX6
AAA	46	PRO	-	expression tag	UNP Q9LZX6
AAA	47	GLY	-	expression tag	UNP Q9LZX6
AAA	48	SER	-	expression tag	UNP Q9LZX6
BBB	45	GLY	-	expression tag	UNP Q9LZX6
BBB	46	PRO	-	expression tag	UNP Q9LZX6
BBB	47	GLY	-	expression tag	UNP Q9LZX6
BBB	48	SER	-	expression tag	UNP Q9LZX6
CCC	45	GLY	-	expression tag	UNP Q9LZX6
CCC	46	PRO	-	expression tag	UNP Q9LZX6
CCC	47	GLY	-	expression tag	UNP Q9LZX6
CCC	48	SER	-	expression tag	UNP Q9LZX6
DDD	45	GLY	-	expression tag	UNP Q9LZX6
DDD	46	PRO	-	expression tag	UNP Q9LZX6
DDD	47	GLY	-	expression tag	UNP Q9LZX6
DDD	48	SER	-	expression tag	UNP Q9LZX6

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			10	6	2	2		
2	BBB	1	Total	C	N	O	0	0
			10	6	2	2		
2	CCC	1	Total	C	N	O	0	0
			10	6	2	2		
2	DDD	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

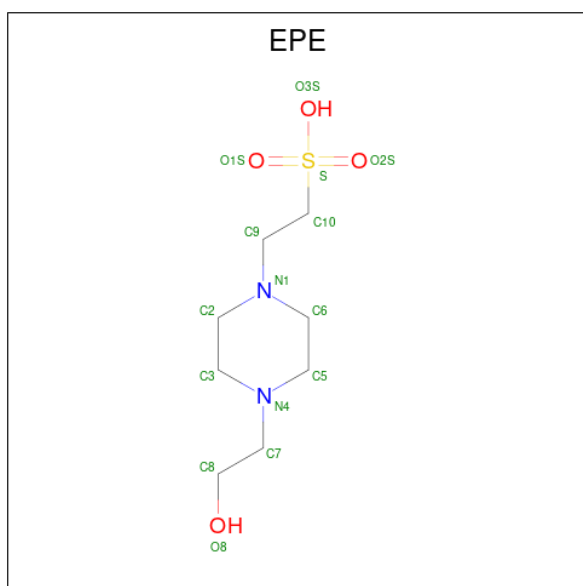
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Na	0	0
			1	1		
3	BBB	1	Total	Na	0	0
			1	1		
3	CCC	1	Total	Na	0	0
			1	1		
3	DDD	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	C	O	0	0
			6	3	3		
4	DDD	1	Total	C	O	0	0
			6	3	3		
4	DDD	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	DDD	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

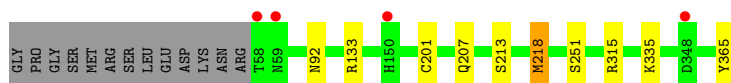
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	217	Total	O	0	0
			217	217		
6	BBB	272	Total	O	0	0
			272	272		
6	CCC	262	Total	O	0	0
			262	262		
6	DDD	259	Total	O	0	0
			259	259		

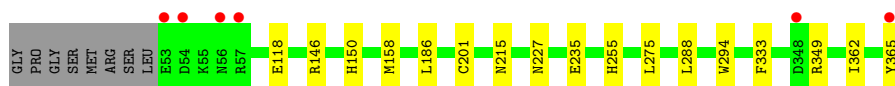
3 Residue-property plots [i](#)

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-hydroxy-tetrahydronicotinate synthase 1, chloroplastic



- Molecule 1: 4-hydroxy-tetrahydronicotinate synthase 1, chloroplastic



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- Molecule 1: 4-hydroxy-tetrahydronicotinate synthase 1, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.04Å 97.63Å 176.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.93 – 1.79 45.89 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.93-1.79) 99.4 (45.89-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.166 , 0.196 0.175 , 0.202	Depositor DCC
R_{free} test set	7721 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11023	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: NA, EPE, GOL

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	AAA	0.64	0/2563	0.74	0/3472
1	BBB	0.65	1/2625 (0.0%)	0.72	0/3557
1	CCC	0.66	0/2556	0.76	0/3467
1	DDD	0.67	0/2536	0.76	0/3437
All	All	0.66	1/10280 (0.0%)	0.74	0/13933

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	118	GLU	CD-OE2	-5.03	1.20	1.25

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	AAA	2474	0	2490	7	0
1	BBB	2525	0	2536	16	0
1	CCC	2474	0	2452	6	0
1	DDD	2463	0	2446	5	0
2	AAA	10	0	12	0	0
2	BBB	10	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	10	0	12	0	0
2	DDD	10	0	12	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	BBB	6	0	8	0	0
4	DDD	12	0	16	0	0
5	DDD	15	0	18	0	0
6	AAA	217	0	0	3	0
6	BBB	272	0	0	3	0
6	CCC	262	0	0	3	0
6	DDD	259	0	0	2	0
All	All	11023	0	10014	30	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 2.

The worst 5 of 30 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:BBB:349[B]:ARG:HH11	1:BBB:349[B]:ARG:HG3	1.14	1.10
1:BBB:349[B]:ARG:HH11	1:BBB:349[B]:ARG:CG	1.87	0.88
1:AAA:315[B]:ARG:NH1	6:AAA:501:HOH:O	2.19	0.74
1:BBB:349[B]:ARG:HG3	1:BBB:349[B]:ARG:NH1	1.96	0.73
1:BBB:275[B]:LEU:HD11	1:BBB:288:LEU:HD12	1.77	0.67

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	AAA	318/321 (99%)	314 (99%)	4 (1%)	0	100	100
1	BBB	327/321 (102%)	323 (99%)	4 (1%)	0	100	100
1	CCC	320/321 (100%)	316 (99%)	4 (1%)	0	100	100
1	DDD	317/321 (99%)	313 (99%)	4 (1%)	0	100	100
All	All	1282/1284 (100%)	1266 (99%)	16 (1%)	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	AAA	272/272 (100%)	267 (98%)	5 (2%)	59	48
1	BBB	279/272 (103%)	278 (100%)	1 (0%)	91	89
1	CCC	272/272 (100%)	271 (100%)	1 (0%)	91	89
1	DDD	270/272 (99%)	269 (100%)	1 (0%)	91	89
All	All	1093/1088 (100%)	1085 (99%)	8 (1%)	84	81

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	201	CYS
1	CCC	201	CYS
1	AAA	251	SER
1	AAA	218[B]	MET
1	BBB	201	CYS

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

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	DDD	402	-	5,5,5	0.08	0	5,5,5	0.21	0
2	LYS	BBB	402	-	5,9,9	0.42	0	4,10,10	0.78	0
2	LYS	DDD	404	-	5,9,9	0.58	0	4,10,10	0.71	0
2	LYS	AAA	401	-	5,9,9	0.61	0	4,10,10	0.96	0
4	GOL	DDD	403	-	5,5,5	0.23	0	5,5,5	0.33	0
4	GOL	BBB	401	-	5,5,5	0.16	0	5,5,5	0.24	0
2	LYS	CCC	401	-	5,9,9	0.37	0	4,10,10	0.62	0
5	EPE	DDD	401	-	15,15,15	2.13	1 (6%)	18,20,20	1.55	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	DDD	402	-	-	0/4/4/4	-
2	LYS	BBB	402	-	-	0/5/9/9	-
2	LYS	DDD	404	-	-	0/5/9/9	-
2	LYS	AAA	401	-	-	0/5/9/9	-
4	GOL	DDD	403	-	-	0/4/4/4	-
4	GOL	BBB	401	-	-	0/4/4/4	-
2	LYS	CCC	401	-	-	0/5/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	DDD	401	-	-	6/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	DDD	401	EPE	C10-S	-8.06	1.66	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	DDD	401	EPE	O2S-S-C10	4.93	112.85	106.92

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

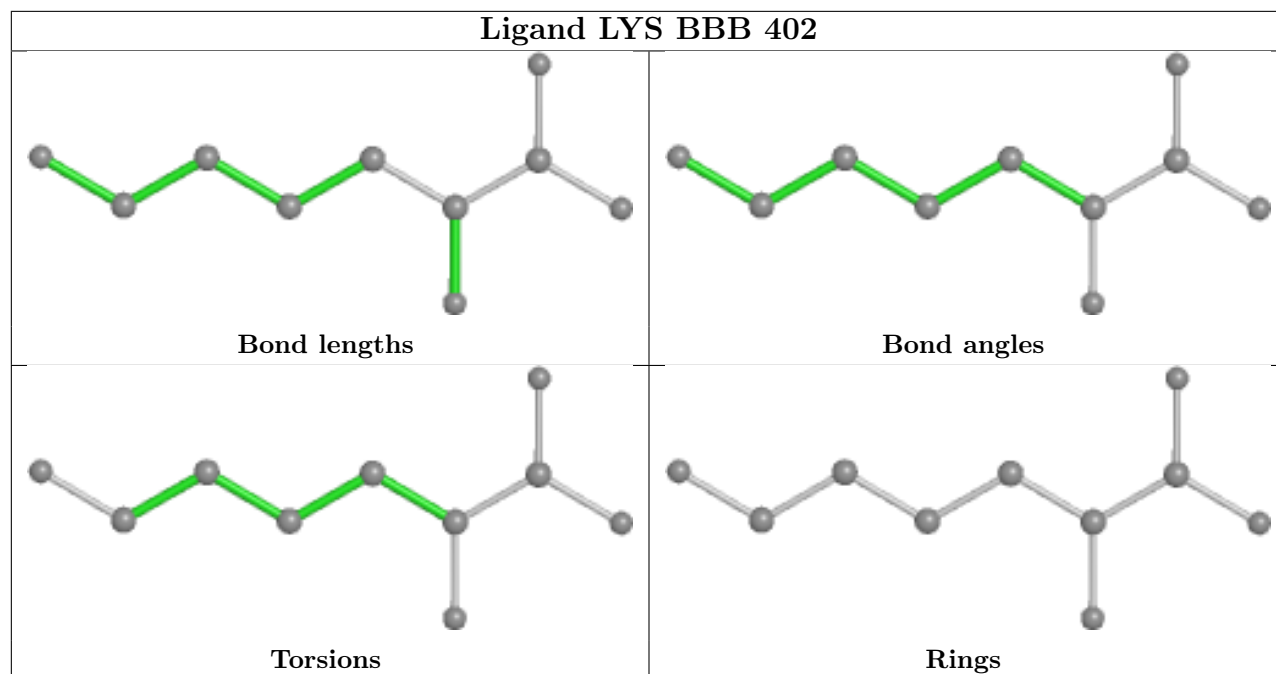
Mol	Chain	Res	Type	Atoms
5	DDD	401	EPE	C8-C7-N4-C3
5	DDD	401	EPE	C9-C10-S-O2S
5	DDD	401	EPE	N4-C7-C8-O8
5	DDD	401	EPE	C10-C9-N1-C2
5	DDD	401	EPE	C10-C9-N1-C6

There are no ring outliers.

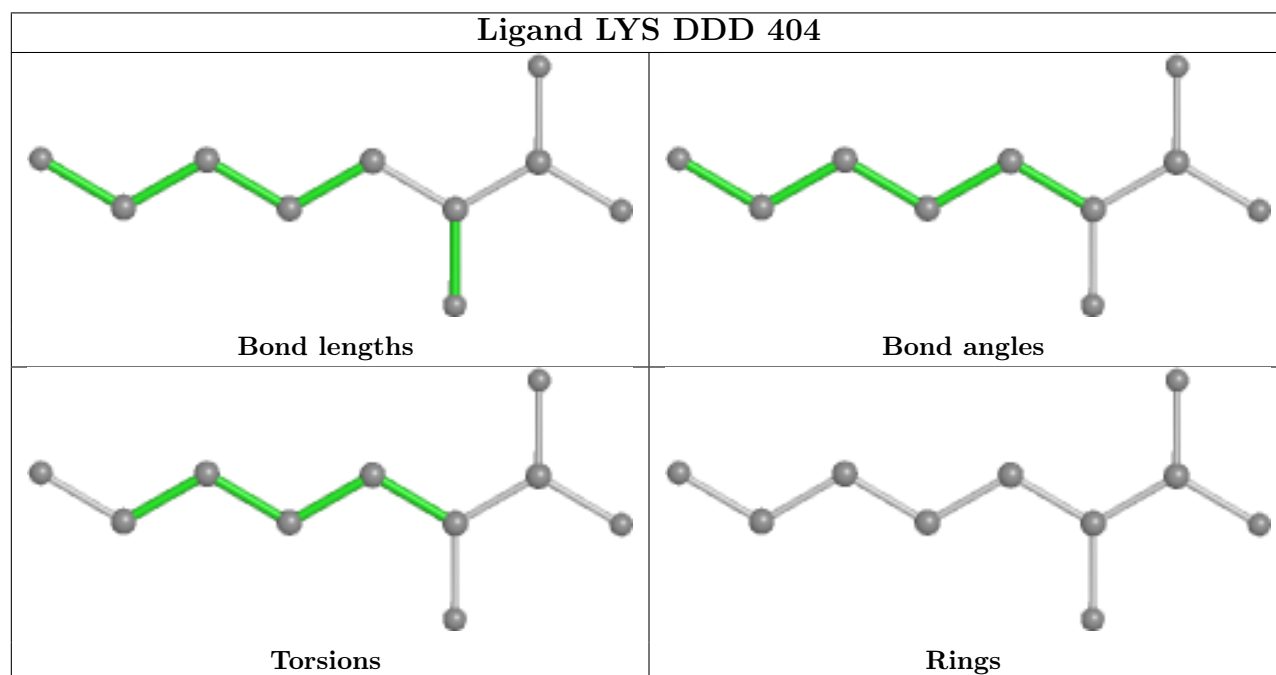
No monomer is involved in short contacts.

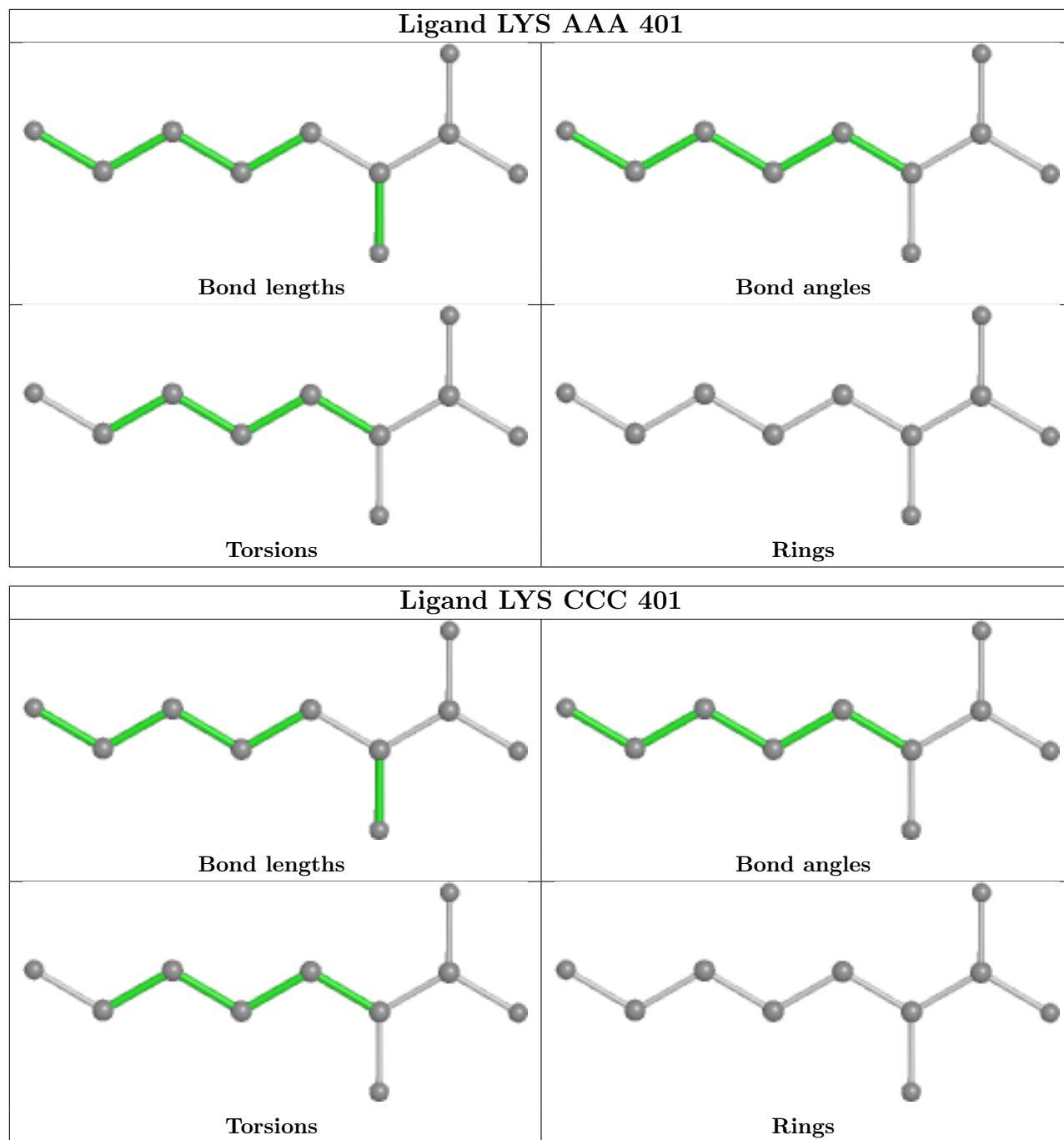
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand LYS BBB 402



Ligand LYS DDD 404





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	AAA	308/321 (95%)	-0.04	4 (1%) 77 74	19, 28, 43, 76	0
1	BBB	313/321 (97%)	-0.27	6 (1%) 66 63	18, 24, 37, 74	0
1	CCC	312/321 (97%)	-0.02	5 (1%) 72 68	18, 27, 41, 90	0
1	DDD	312/321 (97%)	-0.24	7 (2%) 62 57	18, 25, 41, 64	0
All	All	1245/1284 (96%)	-0.15	22 (1%) 68 64	18, 26, 41, 90	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	365	TYR	5.6
1	DDD	55	LYS	3.8
1	AAA	58	THR	3.8
1	BBB	365	TYR	3.5
1	CCC	54	ASP	3.4

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 monosaccharides in this entry.

6.4 Ligands [i](#)

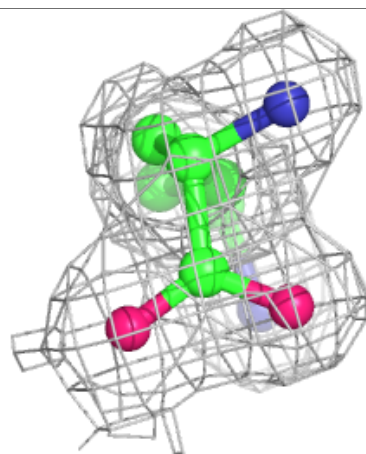
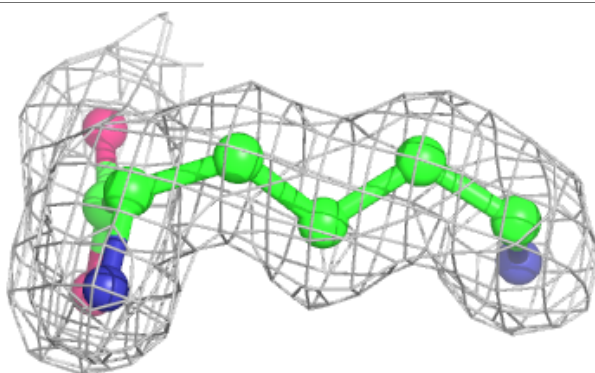
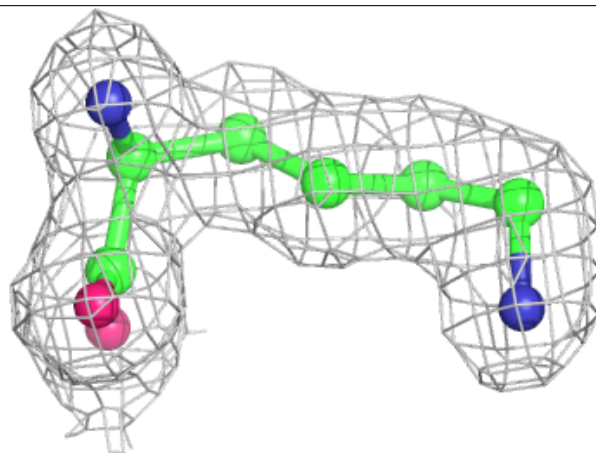
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EPE	DDD	401	15/15	0.83	0.39	33,38,40,41	15
4	GOL	DDD	403	6/6	0.90	0.10	27,32,33,34	0
2	LYS	AAA	401	10/10	0.94	0.15	19,21,23,23	0
2	LYS	CCC	401	10/10	0.95	0.12	19,20,21,22	0
4	GOL	BBB	401	6/6	0.95	0.12	26,27,29,31	0
2	LYS	DDD	404	10/10	0.96	0.14	20,21,24,24	0
2	LYS	BBB	402	10/10	0.96	0.12	20,21,22,23	0
4	GOL	DDD	402	6/6	0.98	0.12	24,26,27,28	0
3	NA	AAA	402	1/1	0.99	0.12	27,27,27,27	0
3	NA	BBB	403	1/1	0.99	0.17	22,22,22,22	0
3	NA	CCC	402	1/1	0.99	0.14	24,24,24,24	0
3	NA	DDD	405	1/1	0.99	0.17	25,25,25,25	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.

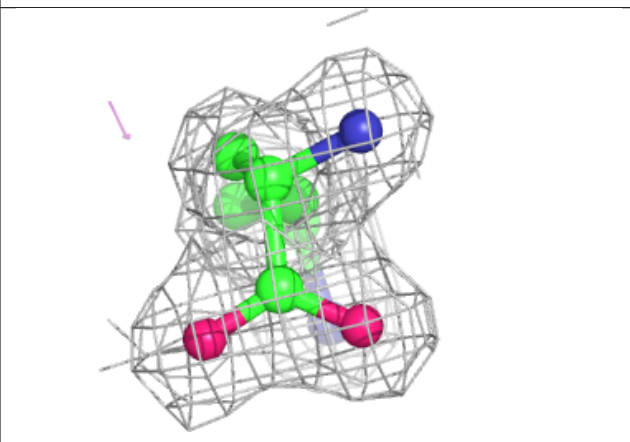
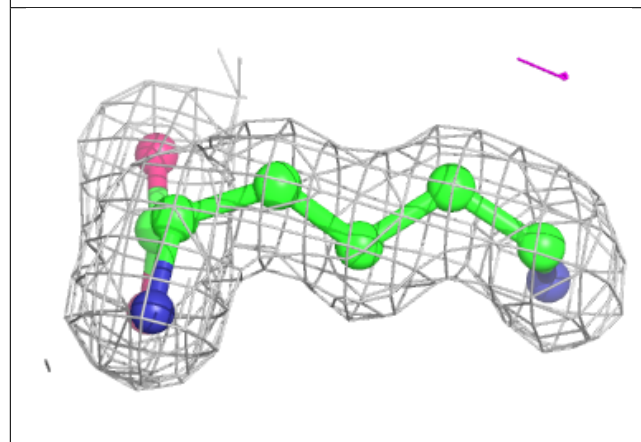
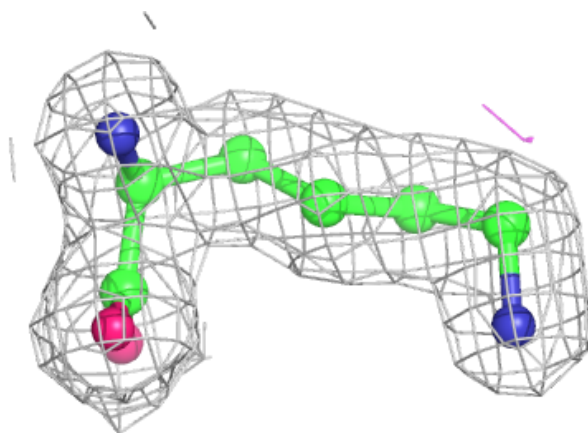
Electron density around LYS AAA 401:

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

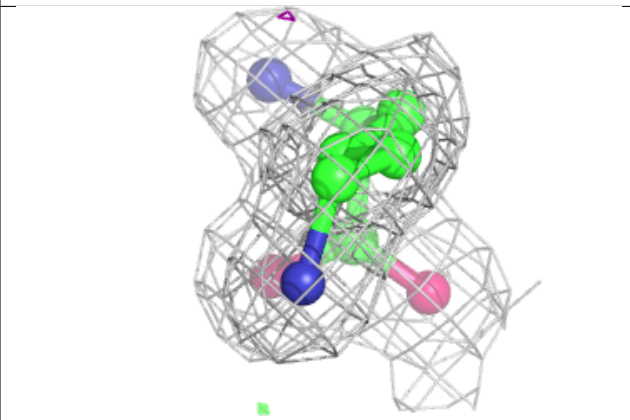
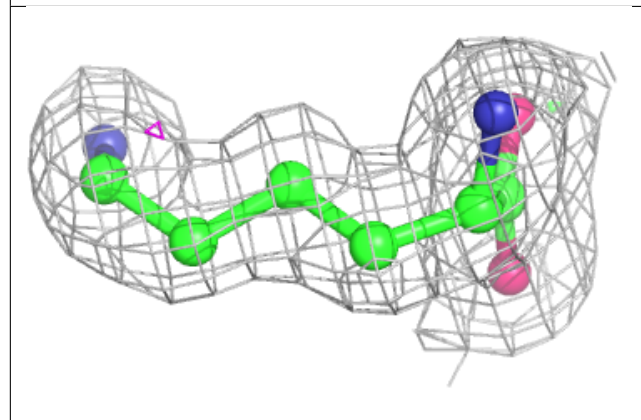
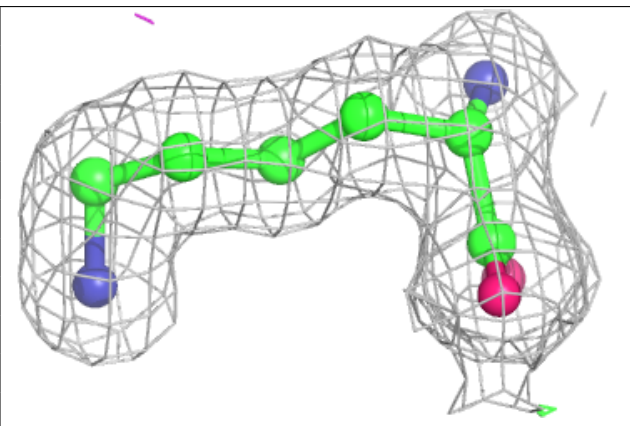


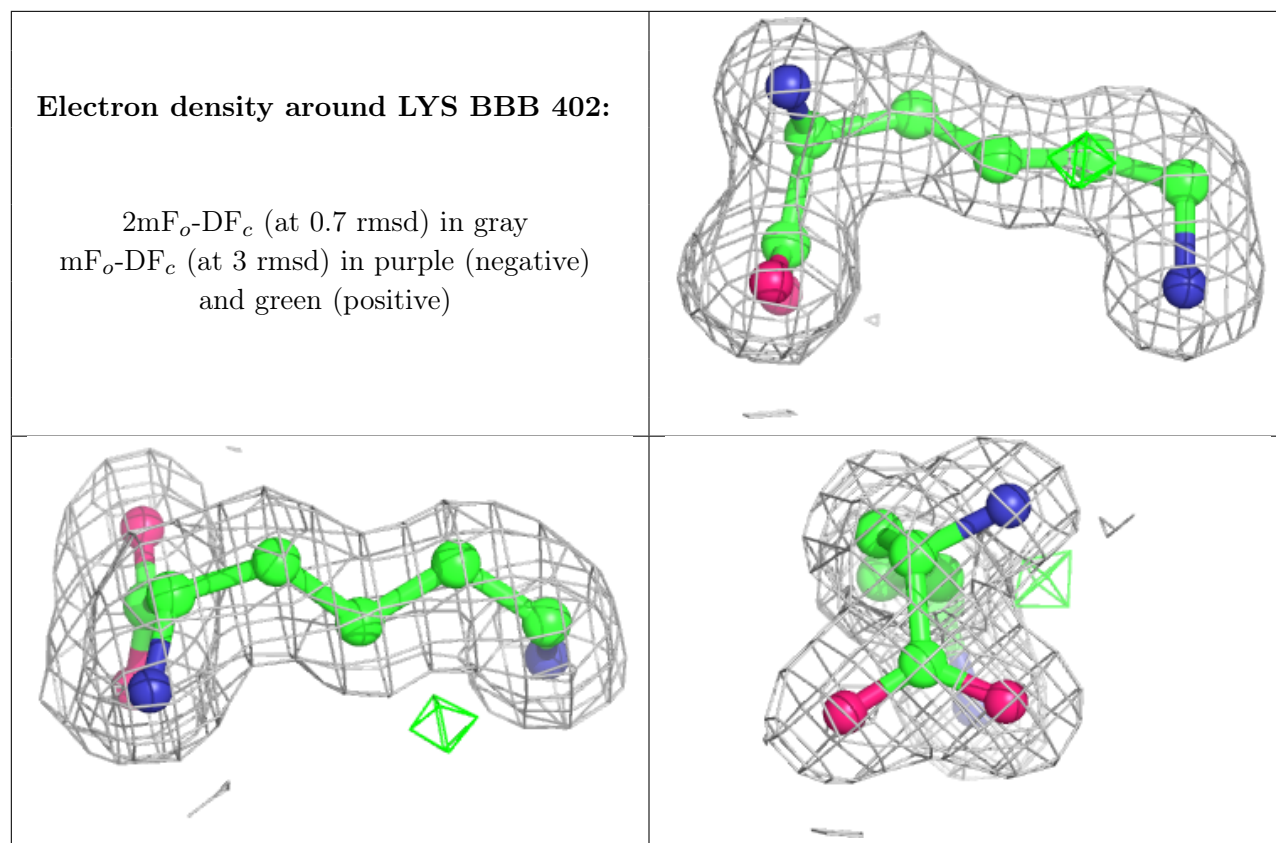
Electron density around LYS CCC 401:

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

**Electron density around LYS DDD 404:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.