



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 07:35 PM EDT

PDB ID : 7JZA
Title : Dihydrodipicolinate synthase S48F mutant with lysine in the allosteric site,
and pyruvate and succinic semi-aldehyde in the catalytic site
Authors : Board, A.J.; Dobson, R.C.J.
Deposited on : 2020-09-01
Resolution : 1.82 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 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

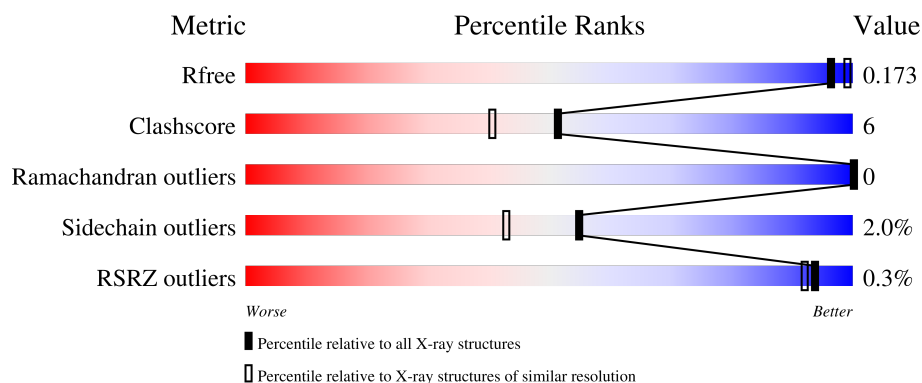
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	A	292	<div> <div></div> <div>87%</div> <div>12%</div> </div>
1	B	292	<div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5165 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	8	0
			2213	1399	386	414	14			
1	B	292	Total	C	N	O	S	0	9	0
			2229	1411	386	417	15			

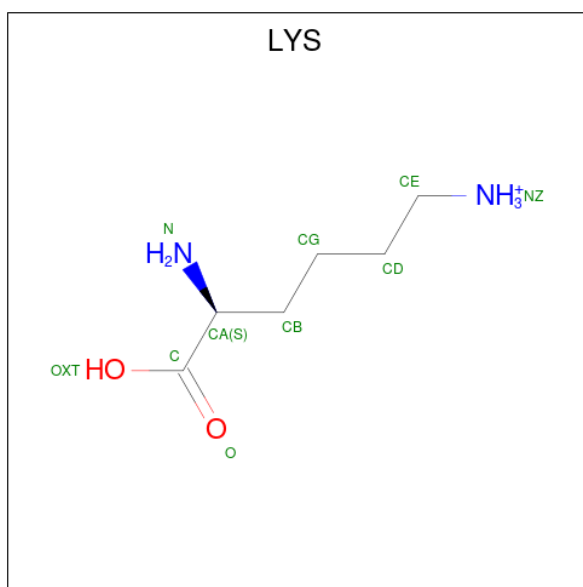
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	PHE	SER	engineered mutation	UNP A0A066Q637
B	48	PHE	SER	engineered mutation	UNP A0A066Q637

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

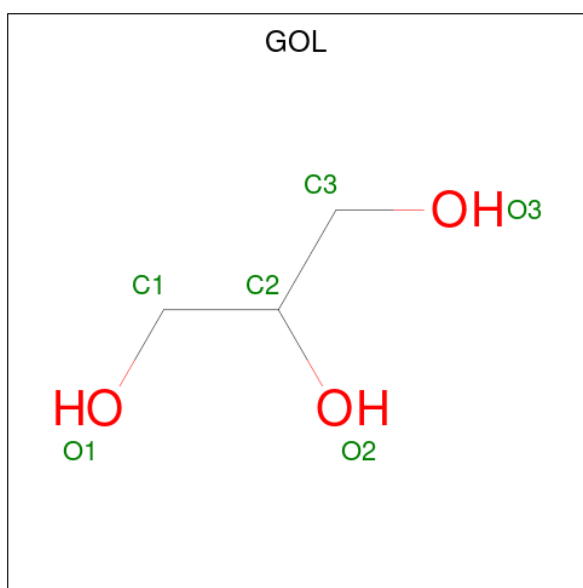
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	2	Total	K	0	0
			2	2		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

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



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

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

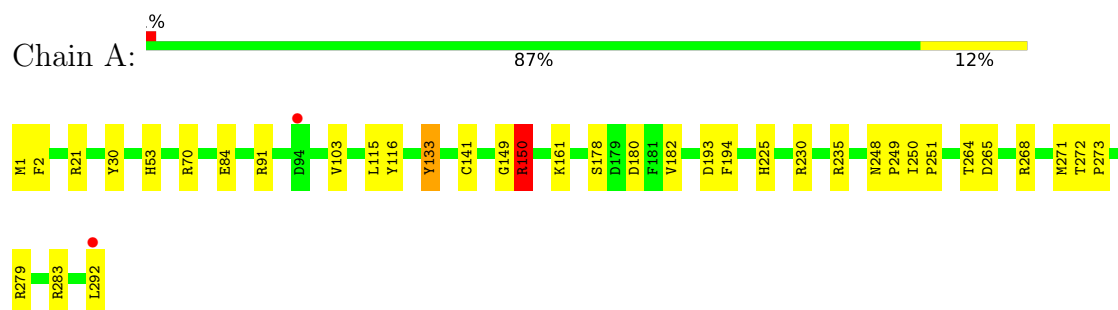
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	330	Total	O	0	0
			330	330		
5	B	352	Total	O	0	0
			352	352		

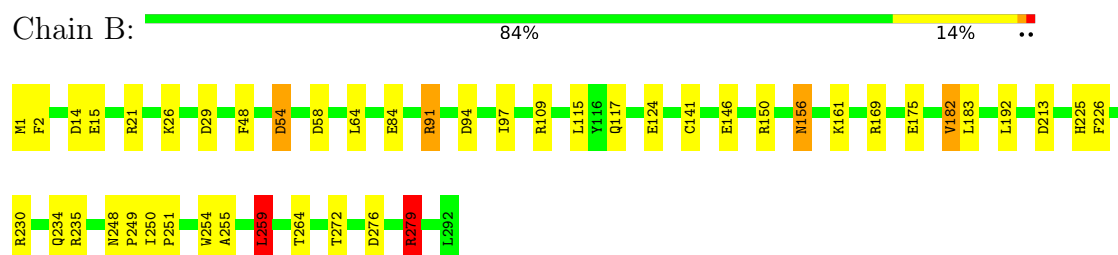
3 Residue-property plots

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-hydroxy-tetrahydronicotinate synthase



- Molecule 1: 4-hydroxy-tetrahydronicotinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.30Å 121.30Å 109.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.36 – 1.82 33.36 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.36-1.82) 100.0 (33.36-1.82)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.15 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.136 , 0.165 0.149 , 0.173	Depositor DCC
R_{free} test set	4166 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5165	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: K, GOL, VPV

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	1.33	5/2249 (0.2%)	1.33	18/3057 (0.6%)
1	B	1.14	3/2270 (0.1%)	1.17	19/3083 (0.6%)
All	All	1.24	8/4519 (0.2%)	1.25	37/6140 (0.6%)

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	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLU	CB-CG	-6.69	1.39	1.52
1	B	84	GLU	CB-CG	-6.68	1.39	1.52
1	A	149	GLY	N-CA	5.92	1.54	1.46
1	B	175	GLU	CB-CG	-5.78	1.41	1.52
1	A	21	ARG	CG-CD	-5.62	1.37	1.51
1	B	84	GLU	CG-CD	5.22	1.59	1.51
1	A	133	TYR	CG-CD2	5.15	1.45	1.39
1	A	30	TYR	CG-CD2	5.01	1.45	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	A	21	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	A	21	ARG	NE-CZ-NH1	9.80	125.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	A	271	MET	CG-SD-CE	-8.85	86.05	100.20
1	A	133	TYR	CB-CG-CD1	8.76	126.25	121.00
1	A	279	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	B	276	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	235	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	B	54[A]	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	B	54[B]	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	91	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	213	ASP	CB-CG-OD2	-7.20	111.83	118.30
1	B	183[A]	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	B	183[B]	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	B	29	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	283[A]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	283[B]	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	235	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	279	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	A	268	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	169	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	70	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	150[A]	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	A	150[B]	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	B	91	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	279	ARG	CG-CD-NE	-5.63	99.98	111.80
1	B	259[A]	LEU	CB-CG-CD1	5.57	120.47	111.00
1	B	259[B]	LEU	CB-CG-CD1	5.57	120.47	111.00
1	B	169	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	193	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	182	VAL	CG1-CB-CG2	-5.38	102.30	110.90
1	B	29	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	133	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	194	PHE	CB-CG-CD1	5.25	124.48	120.80
1	B	150	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	14	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	279	ARG	Sidechain

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	2213	0	2222	20	0
1	B	2229	0	2242	29	1
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	12	2	0
3	B	10	0	12	0	0
4	A	12	0	16	1	0
4	B	6	0	8	1	0
5	A	330	0	0	8	2
5	B	352	0	0	16	3
All	All	5165	0	4512	50	3

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 6.

All (50) 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:B:94:ASP:CB	5:B:633:HOH:O	2.14	0.95
1:B:21[A]:ARG:NH1	5:B:401:HOH:O	1.87	0.95
1:B:146:GLU:CG	5:B:752:HOH:O	2.15	0.93
1:A:53[B]:HIS:HD2	5:A:579:HOH:O	1.49	0.93
1:B:117:GLN:HG3	5:B:664:HOH:O	1.75	0.85
1:B:124:GLU:HG3	5:B:618:HOH:O	1.74	0.84
1:A:53[A]:HIS:HD2	3:A:302:LYS:HE2	1.43	0.84
4:B:303:GOL:O1	5:B:402:HOH:O	1.96	0.82
1:B:156:ASN:HD22	1:B:156:ASN:H	1.27	0.82
1:A:230:ARG:NH1	5:A:402:HOH:O	2.15	0.80
1:B:255:ALA:O	1:B:259[B]:LEU:HD23	1.83	0.77
1:B:234[B]:GLN:NE2	5:B:406:HOH:O	2.19	0.76
1:A:1:MET:CA	5:A:647:HOH:O	2.37	0.72
1:B:1:MET:N	5:B:407:HOH:O	2.22	0.71
1:A:272:THR:OG1	5:A:401:HOH:O	1.86	0.70
1:A:53[A]:HIS:CD2	3:A:302:LYS:HE2	2.29	0.67
1:B:225:HIS:HE1	5:B:671:HOH:O	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230[A]:ARG:NH1	5:B:408:HOH:O	2.23	0.62
1:B:250:ILE:HB	1:B:251:PRO:HD3	1.82	0.61
1:B:58[A]:ASP:OD1	5:B:405:HOH:O	2.16	0.60
1:B:91:ARG:NH1	5:B:404:HOH:O	2.12	0.60
1:A:2:PHE:O	1:A:182[A]:VAL:HG11	2.05	0.57
1:B:225:HIS:HD2	5:B:683:HOH:O	1.87	0.56
1:B:234[B]:GLN:CD	5:B:406:HOH:O	2.43	0.55
1:A:53[B]:HIS:CD2	5:A:579:HOH:O	2.36	0.54
1:B:156:ASN:HD22	1:B:156:ASN:N	2.00	0.54
1:B:248:ASN:ND2	1:B:249:PRO:HA	2.23	0.53
1:A:116:TYR:CE1	1:A:150[A]:ARG:HD2	2.45	0.52
1:B:64:LEU:HD11	1:B:97:ILE:HG23	1.93	0.51
1:A:150[B]:ARG:NH1	5:A:405:HOH:O	2.26	0.50
1:A:250:ILE:HB	1:A:251:PRO:HD3	1.94	0.49
4:A:304:GOL:H2	1:B:109:ARG:HH12	1.78	0.49
1:A:272:THR:HB	1:A:273:PRO:CD	2.43	0.49
1:B:248:ASN:HD22	1:B:249:PRO:HA	1.79	0.47
1:A:248:ASN:HD22	1:A:249:PRO:HA	1.80	0.46
1:A:225:HIS:HD2	5:A:679:HOH:O	1.99	0.46
1:B:234[B]:GLN:CD	5:B:679:HOH:O	2.54	0.45
1:A:248:ASN:ND2	1:A:249:PRO:HA	2.32	0.45
1:B:115:LEU:HD11	1:B:141[B]:CYS:SG	2.57	0.44
1:A:265:ASP:OD2	5:A:403:HOH:O	2.20	0.44
1:B:272:THR:OG1	5:B:403:HOH:O	2.10	0.44
1:B:2:PHE:O	1:B:182:VAL:HG11	2.18	0.43
1:A:103:VAL:HA	1:A:133:TYR:HB3	2.01	0.43
1:A:115:LEU:HD11	1:A:141[A]:CYS:SG	2.58	0.43
1:A:150[A]:ARG:HH11	1:A:150[A]:ARG:HD3	1.61	0.43
1:A:178:SER:OG	1:A:180:ASP:OD1	2.35	0.42
1:B:226:PHE:O	1:B:230[A]:ARG:HG3	2.20	0.42
1:B:192:LEU:CD2	1:B:230[A]:ARG:HG2	2.49	0.41
1:B:192:LEU:HD23	1:B:230[A]:ARG:HG2	2.02	0.41
1:B:254:TRP:CE2	1:B:279:ARG:HG2	2.55	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:597:HOH:O	5:B:454:HOH:O[3_654]	2.07	0.13
5:A:721:HOH:O	5:B:681:HOH:O[3_654]	2.10	0.10
1:B:26:LYS:CD	5:B:496:HOH:O[2_545]	2.10	0.10

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	297/292 (102%)	293 (99%)	4 (1%)	0	100	100
1	B	298/292 (102%)	294 (99%)	4 (1%)	0	100	100
All	All	595/584 (102%)	587 (99%)	8 (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	A	233/237 (98%)	229 (98%)	4 (2%)	60	50
1	B	233/237 (98%)	225 (97%)	8 (3%)	37	22
All	All	466/474 (98%)	454 (97%)	12 (3%)	55	32

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

Mol	Chain	Res	Type
1	A	150[A]	ARG
1	A	150[B]	ARG
1	A	264	THR
1	A	292	LEU
1	B	15	GLU
1	B	48	PHE
1	B	54[A]	ASP
1	B	54[B]	ASP

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Mol	Chain	Res	Type
1	B	156	ASN
1	B	259[A]	LEU
1	B	259[B]	LEU
1	B	264	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	233	ASN
1	A	248	ASN
1	B	90	GLN
1	B	156	ASN
1	B	225	HIS
1	B	233	ASN
1	B	248	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	VPV	A	161	1	13,20,21	1.86	3 (23%)	10,24,26	2.43	5 (50%)
1	VPV	B	161	1	13,20,21	1.96	3 (23%)	10,24,26	1.52	4 (40%)

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
1	VPV	A	161	1	-	2/15/23/25	-
1	VPV	B	161	1	-	4/15/23/25	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	VPV	C5-C1	-5.14	1.45	1.51
1	A	161	VPV	C5-C1	-4.65	1.45	1.51
1	B	161	VPV	O10-C6	3.26	1.53	1.43
1	A	161	VPV	CA-N	-2.79	1.39	1.48
1	B	161	VPV	C2-C1	-2.67	1.48	1.52
1	A	161	VPV	C7-C8	-2.05	1.43	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	VPV	O10-C6-C5	-4.05	98.89	109.65
1	A	161	VPV	C8-C7-C6	-3.34	108.63	115.05
1	A	161	VPV	C7-C6-C5	3.27	124.55	112.78
1	A	161	VPV	C5-C1-NZ	-3.03	116.12	123.33
1	A	161	VPV	C7-C8-C9	-2.84	107.49	113.59
1	B	161	VPV	C7-C8-C9	-2.71	107.77	113.59
1	B	161	VPV	C8-C7-C6	-2.14	110.93	115.05
1	B	161	VPV	C5-C1-NZ	-2.12	118.30	123.33
1	B	161	VPV	O10-C6-C5	-2.11	104.05	109.65

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	161	VPV	C2-C1-C5-C6
1	A	161	VPV	NZ-C1-C5-C6
1	B	161	VPV	C2-C1-C5-C6
1	B	161	VPV	NZ-C1-C5-C6
1	B	161	VPV	C1-C5-C6-O10
1	B	161	VPV	C1-C5-C6-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	A	303	-	5,5,5	1.34	0	5,5,5	1.43	1 (20%)
4	GOL	A	304	-	5,5,5	0.84	0	5,5,5	0.54	0
3	LYS	A	302	-	5,9,9	2.30	1 (20%)	4,10,10	1.11	0
3	LYS	B	302	-	5,9,9	2.07	1 (20%)	4,10,10	0.54	0
4	GOL	B	303	-	5,5,5	0.38	0	5,5,5	0.68	0

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	A	303	-	-	0/4/4/4	-
4	GOL	A	304	-	-	4/4/4/4	-
3	LYS	A	302	-	-	1/5/9/9	-
3	LYS	B	302	-	-	0/5/9/9	-
4	GOL	B	303	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	LYS	CA-N	4.90	1.58	1.47
3	B	302	LYS	CA-N	4.49	1.57	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	303	GOL	O1-C1-C2	2.30	121.21	110.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

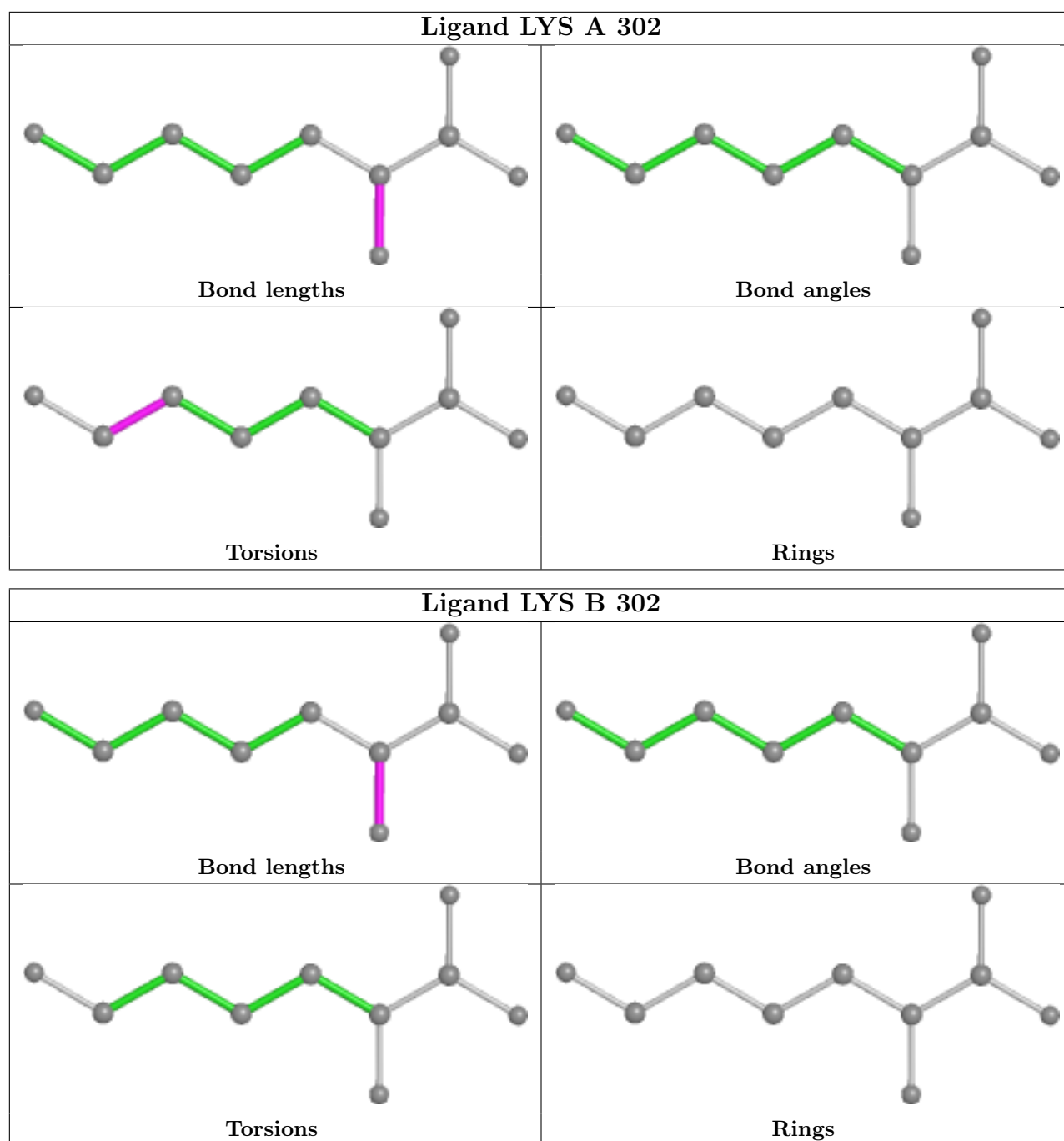
Mol	Chain	Res	Type	Atoms
4	A	304	GOL	O1-C1-C2-C3
4	A	304	GOL	C1-C2-C3-O3
4	B	303	GOL	C1-C2-C3-O3
4	A	304	GOL	O1-C1-C2-O2
4	A	304	GOL	O2-C2-C3-O3
4	B	303	GOL	O2-C2-C3-O3
3	A	302	LYS	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	GOL	1	0
3	A	302	LYS	2	0
4	B	303	GOL	1	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	291/292 (99%)	-0.51	2 (0%) 87 86	10, 17, 30, 56	0
1	B	291/292 (99%)	-0.69	0 100 100	9, 14, 26, 51	0
All	All	582/584 (99%)	-0.60	2 (0%) 94 92	9, 16, 29, 56	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	LEU	2.9
1	A	94	ASP	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	VPV	A	161	21/22	0.97	0.11	10,13,20,27	0
1	VPV	B	161	21/22	0.97	0.09	7,11,18,21	0

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,

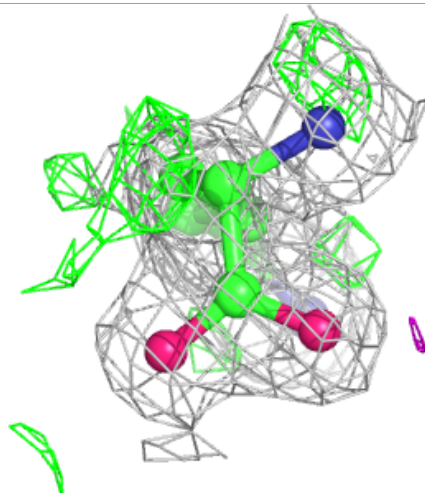
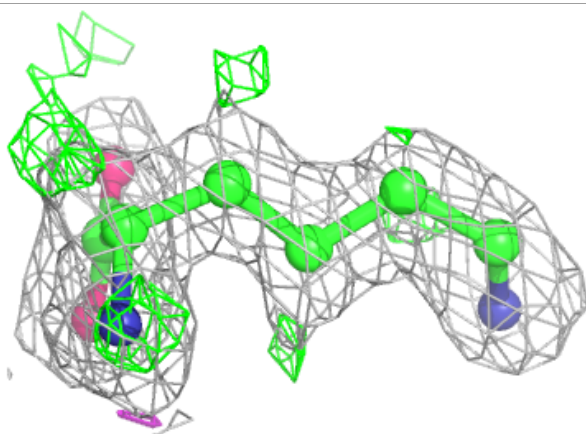
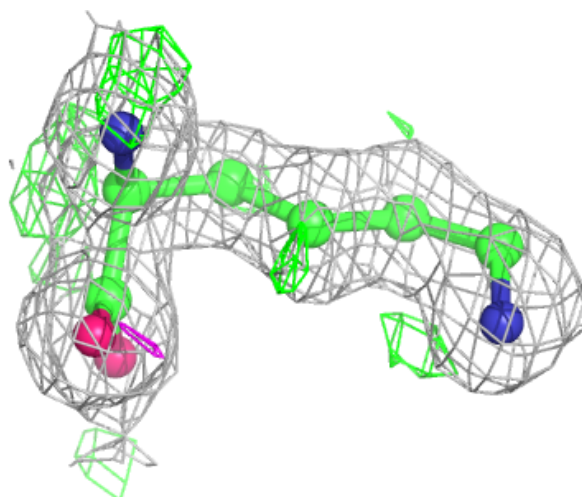
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	304	6/6	0.74	0.21	52,57,59,60	0
4	GOL	A	303	6/6	0.91	0.14	31,50,57,58	0
3	LYS	A	302	10/10	0.92	0.12	11,20,25,26	0
3	LYS	B	302	10/10	0.93	0.10	11,22,28,29	0
4	GOL	B	303	6/6	0.95	0.08	38,45,53,59	0
2	K	A	301	1/1	0.98	0.05	23,23,23,23	0
2	K	B	304	1/1	0.99	0.10	32,32,32,32	0
2	K	B	301	1/1	0.99	0.03	18,18,18,18	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.

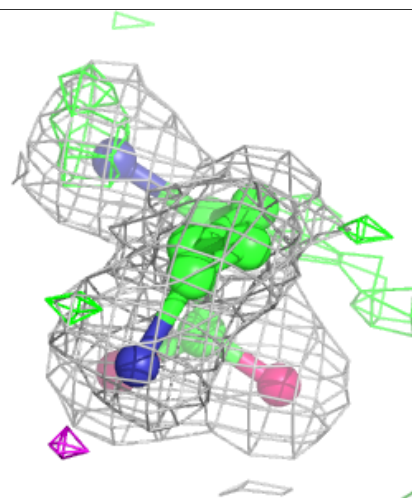
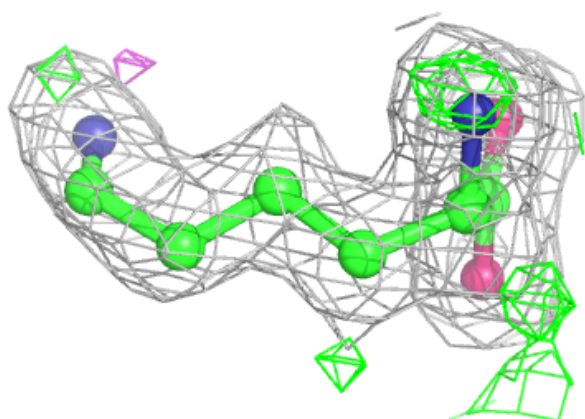
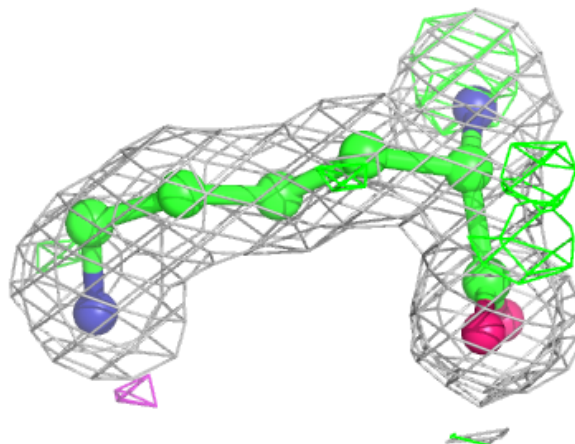
Electron density around LYS A 302:

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 B 302:

$2mF_o-DF_c$ (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.