



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:30 AM UTC

PDB ID : 9LLS / pdb_00009lls
Title : Crystal structure of Ornithine decarboxylase H346A mutant
Authors : Kim, D.S.; Park, J.H.; Adiko, N.N.; Seo, H.T.
Deposited on : 2025-01-17
Resolution : 2.69 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

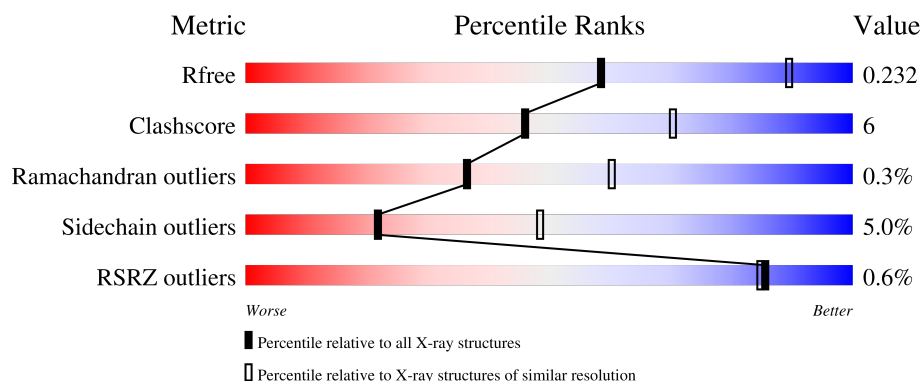
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	694	84% 14% .
1	B	694	82% 15% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10709 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.

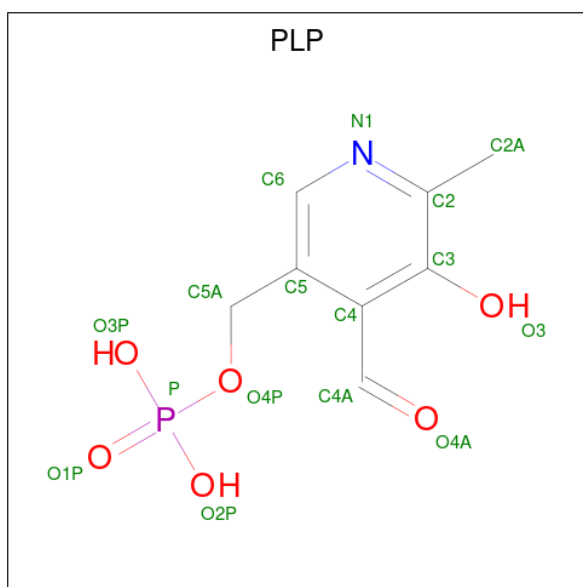
- Molecule 1 is a protein called Ornithine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	694	Total	C	N	O	S	0	0	0
			5339	3419	914	998	8			
1	B	692	Total	C	N	O	S	0	0	0
			5327	3412	912	995	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ASP	ASN	conflict	UNP A0AAN4BJQ6
A	66	TYR	HIS	conflict	UNP A0AAN4BJQ6
A	102	GLU	GLY	conflict	UNP A0AAN4BJQ6
A	346	ALA	HIS	engineered mutation	UNP A0AAN4BJQ6
A	455	VAL	ALA	conflict	UNP A0AAN4BJQ6
A	620	ASP	GLU	conflict	UNP A0AAN4BJQ6
A	654	GLU	PRO	conflict	UNP A0AAN4BJQ6
A	684	ALA	LYS	conflict	UNP A0AAN4BJQ6
A	695	ALA	ASP	conflict	UNP A0AAN4BJQ6
B	17	ASP	ASN	conflict	UNP A0AAN4BJQ6
B	66	TYR	HIS	conflict	UNP A0AAN4BJQ6
B	102	GLU	GLY	conflict	UNP A0AAN4BJQ6
B	346	ALA	HIS	engineered mutation	UNP A0AAN4BJQ6
B	455	VAL	ALA	conflict	UNP A0AAN4BJQ6
B	620	ASP	GLU	conflict	UNP A0AAN4BJQ6
B	654	GLU	PRO	conflict	UNP A0AAN4BJQ6
B	684	ALA	LYS	conflict	UNP A0AAN4BJQ6
B	695	ALA	ASP	conflict	UNP A0AAN4BJQ6

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	15	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	15	0
			15	8	1	5	1		

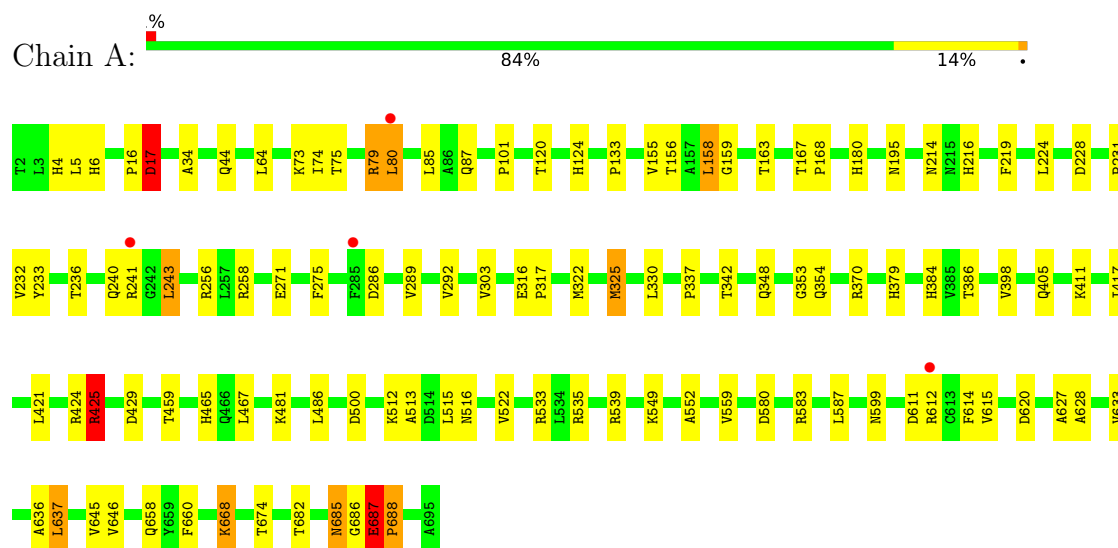
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	8	Total	O	0	0
			8	8		

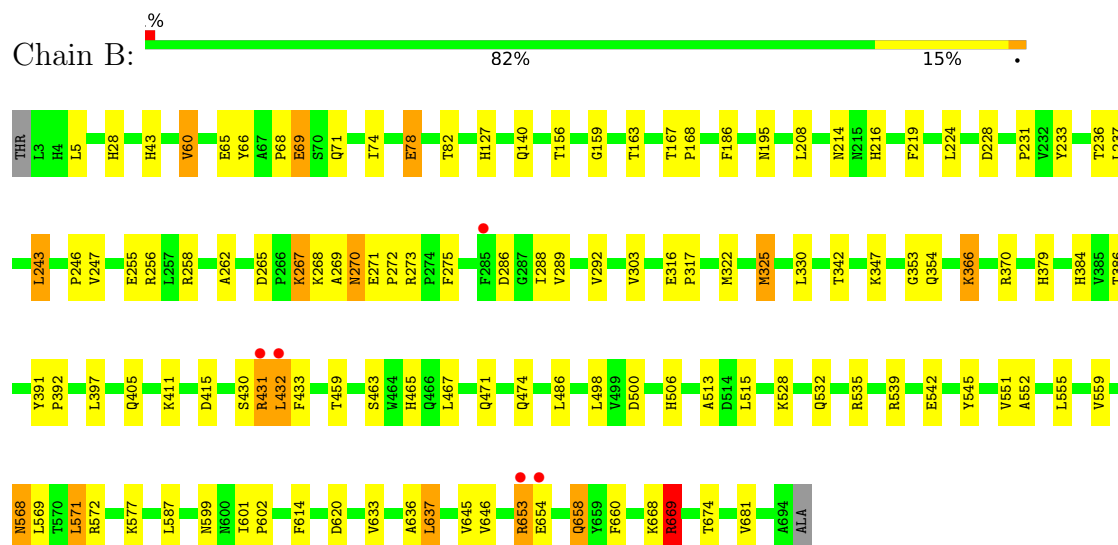
3 Residue-property plots

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: Ornithine decarboxylase



• Molecule 1: Ornithine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.36Å 72.38Å 78.05Å 114.65° 107.28° 100.49°	Depositor
Resolution (Å)	29.34 – 2.69 29.34 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.34-2.69) 97.8 (29.34-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.41 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.171 , 0.231 0.182 , 0.232	Depositor DCC
R_{free} test set	1721 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10709	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	7/5477 (0.1%)	1.03	4/7489 (0.1%)
1	B	0.68	7/5465 (0.1%)	1.03	4/7472 (0.1%)
All	All	0.67	14/10942 (0.1%)	1.03	8/14961 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	HIS	CE1-NE2	6.71	1.39	1.32
1	A	180	HIS	CE1-NE2	6.53	1.39	1.32
1	A	384	HIS	CE1-NE2	6.40	1.39	1.32
1	B	379	HIS	CE1-NE2	6.25	1.38	1.32
1	A	216	HIS	CE1-NE2	6.18	1.38	1.32
1	B	127	HIS	CE1-NE2	6.14	1.38	1.32
1	B	384	HIS	CE1-NE2	6.04	1.38	1.32
1	A	4	HIS	CE1-NE2	5.94	1.38	1.32
1	B	28	HIS	CE1-NE2	5.60	1.38	1.32
1	B	506	HIS	CE1-NE2	5.49	1.38	1.32
1	B	43	HIS	CE1-NE2	5.47	1.38	1.32
1	A	124	HIS	CE1-NE2	5.46	1.38	1.32
1	A	379	HIS	CE1-NE2	5.21	1.37	1.32
1	A	6	HIS	CE1-NE2	5.16	1.37	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PRO	N-CA-C	6.50	124.50	111.69
1	B	231	PRO	N-CA-C	6.40	124.29	111.69
1	A	688	PRO	N-CA-C	5.97	120.28	110.55
1	A	620	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	620	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	568	ASN	CA-CB-CG	5.50	118.10	112.60
1	B	415	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	232	VAL	N-CA-C	-5.33	100.07	107.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	ARG	Sidechain
1	A	425	ARG	Sidechain
1	A	79	ARG	Sidechain
1	B	273	ARG	Sidechain
1	B	370	ARG	Sidechain
1	B	669	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	5339	0	5275	60	0
1	B	5327	0	5263	68	0
2	A	15	0	7	0	0
2	B	15	0	6	0	0
3	A	5	0	0	0	0
3	B	8	0	0	0	0
All	All	10709	0	10551	123	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 6.

All (123) 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:237:LEU:HD12	1:B:246:PRO:HG2	1.50	0.94
1:B:208:LEU:HG	1:B:268:LYS:HD2	1.64	0.79
1:B:535:ARG:HG3	1:B:539:ARG:HE	1.48	0.78
1:B:551:VAL:HG22	1:B:571:LEU:HD23	1.64	0.78
1:A:64:LEU:HD22	1:A:74:ILE:HG21	1.70	0.71
1:A:535:ARG:HG3	1:A:539:ARG:HE	1.53	0.70
1:B:535:ARG:NH2	1:B:539:ARG:HG3	2.10	0.67
1:B:471:GLN:H	1:B:474:GLN:HE21	1.44	0.66
1:B:535:ARG:HH22	1:B:539:ARG:HG3	1.62	0.65
1:A:337:PRO:HA	1:A:370:ARG:HH12	1.59	0.65
1:B:68:PRO:O	1:B:69:GLU:O	2.15	0.64
1:A:243:LEU:HD13	1:A:286:ASP:HB3	1.79	0.63
1:A:515:LEU:HD11	1:A:587:LEU:HD23	1.80	0.63
1:A:120:THR:HG21	1:B:347:LYS:CD	2.30	0.62
1:A:535:ARG:NH2	1:A:539:ARG:HG3	2.15	0.60
1:A:120:THR:HG21	1:B:347:LYS:HD3	1.82	0.60
1:B:515:LEU:HD11	1:B:587:LEU:HD23	1.82	0.60
1:A:682:THR:HA	1:A:687:GLU:O	2.01	0.59
1:B:552:ALA:HA	1:B:559:VAL:HG21	1.85	0.59
1:A:580:ASP:OD1	1:A:583:ARG:NH1	2.35	0.58
1:A:258:ARG:NH1	1:A:271:GLU:O	2.33	0.58
1:B:601:ILE:HG23	1:B:653:ARG:CZ	2.33	0.57
1:B:465:HIS:HD2	1:B:467:LEU:H	1.52	0.57
1:A:535:ARG:HH22	1:A:539:ARG:HG3	1.70	0.57
1:A:233:TYR:H	1:A:599:ASN:HD21	1.53	0.57
1:B:431:ARG:HG2	1:B:542:GLU:OE1	2.05	0.57
1:B:258:ARG:NH1	1:B:271:GLU:O	2.37	0.57
1:B:243:LEU:HD13	1:B:286:ASP:HB3	1.87	0.56
1:A:133:PRO:HB3	1:B:5:LEU:HD11	1.88	0.56
1:A:465:HIS:HD2	1:A:467:LEU:H	1.54	0.55
1:B:471:GLN:H	1:B:474:GLN:NE2	2.04	0.55
1:A:552:ALA:HA	1:A:559:VAL:HG21	1.89	0.55
1:B:322:MET:HA	1:B:325:MET:HE3	1.89	0.54
1:B:140:GLN:HA	1:B:140:GLN:HE21	1.73	0.54
1:B:233:TYR:H	1:B:599:ASN:HD21	1.56	0.53
1:A:322:MET:HA	1:A:325:MET:HE3	1.91	0.53
1:B:545:TYR:CZ	1:B:572:ARG:HG3	2.44	0.53
1:B:465:HIS:CD2	1:B:467:LEU:HB2	2.44	0.52
1:B:430:SER:HA	1:B:431:ARG:HH21	1.73	0.52
1:A:337:PRO:HA	1:A:370:ARG:NH1	2.24	0.52
1:A:386:THR:HG21	1:B:354:GLN:HG2	1.91	0.52
1:A:645:VAL:HG23	1:A:646:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:LYS:HA	1:B:271:GLU:CD	2.35	0.52
1:A:101:PRO:HG2	1:A:398:VAL:HG12	1.90	0.52
1:B:316:GLU:N	1:B:317:PRO:CD	2.73	0.51
1:B:577:LYS:HD3	1:B:669:ARG:HH12	1.75	0.51
1:A:348:GLN:HE22	1:A:481:LYS:NZ	2.08	0.51
1:A:75:THR:HG21	1:A:87:GLN:NE2	2.26	0.51
1:B:459:THR:O	1:B:465:HIS:HE1	1.93	0.50
1:B:602:PRO:HD2	1:B:653:ARG:HH12	1.76	0.50
1:A:316:GLU:N	1:A:317:PRO:CD	2.75	0.50
1:A:44:GLN:OE1	1:A:44:GLN:N	2.41	0.49
1:B:498:LEU:HD21	1:B:571:LEU:HD22	1.94	0.49
1:B:465:HIS:HD2	1:B:467:LEU:HB2	1.77	0.49
1:A:685:ASN:HD22	1:A:686:GLY:H	1.60	0.48
1:A:167:THR:N	1:A:168:PRO:CD	2.77	0.48
1:A:465:HIS:CD2	1:A:467:LEU:HB2	2.48	0.48
1:A:658:GLN:O	1:A:658:GLN:NE2	2.47	0.48
1:A:459:THR:O	1:A:465:HIS:HE1	1.97	0.48
1:A:417:ILE:HD13	1:A:522:VAL:HG11	1.96	0.47
1:B:167:THR:N	1:B:168:PRO:CD	2.77	0.47
1:B:645:VAL:HG23	1:B:646:VAL:HG23	1.96	0.47
1:A:195:ASN:HD22	1:A:342:THR:HG21	1.78	0.47
1:A:465:HIS:HD2	1:A:467:LEU:HB2	1.79	0.47
1:B:262:ALA:HA	1:B:265:ASP:O	2.16	0.46
1:B:292:VAL:HG23	1:B:330:LEU:HD21	1.97	0.46
1:A:465:HIS:CD2	1:A:467:LEU:H	2.34	0.46
1:B:258:ARG:NH2	1:B:272:PRO:O	2.47	0.46
1:B:78:GLU:H	1:B:78:GLU:HG2	1.47	0.46
1:A:275:PHE:HB2	1:A:303:VAL:HG12	1.98	0.46
1:B:246:PRO:HD3	1:B:288:ILE:HG21	1.97	0.46
1:B:432:LEU:HD12	1:B:542:GLU:HA	1.98	0.46
1:B:186:PHE:HB3	1:B:397:LEU:HD13	1.98	0.46
1:A:348:GLN:HE22	1:A:481:LYS:HZ2	1.65	0.45
1:B:267:LYS:C	1:B:269:ALA:N	2.73	0.45
1:B:366:LYS:HB2	1:B:366:LYS:HE3	1.61	0.45
1:A:614:PHE:HB2	1:A:633:VAL:HB	1.99	0.45
1:B:637:LEU:C	1:B:637:LEU:HD12	2.42	0.45
1:B:636:ALA:HB1	1:B:660:PHE:CZ	2.51	0.45
1:A:224:LEU:O	1:A:228:ASP:HA	2.17	0.44
1:A:636:ALA:HB1	1:A:660:PHE:CZ	2.52	0.44
1:B:353:GLY:O	1:B:354:GLN:HB2	2.17	0.44
1:B:275:PHE:HB2	1:B:303:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ASP:HB2	1:A:513:ALA:HB2	1.99	0.44
1:B:658:GLN:O	1:B:658:GLN:NE2	2.50	0.44
1:B:267:LYS:O	1:B:268:LYS:C	2.60	0.43
1:B:500:ASP:HB2	1:B:513:ALA:HB2	1.99	0.43
1:B:214:ASN:CG	1:B:236:THR:HG21	2.44	0.43
1:A:16:PRO:O	1:A:17:ASP:HB3	2.18	0.43
1:A:214:ASN:CG	1:A:236:THR:HG21	2.43	0.43
1:A:241:ARG:HH22	1:A:486:LEU:H	1.66	0.43
1:B:224:LEU:O	1:B:228:ASP:HA	2.18	0.43
1:B:614:PHE:HB2	1:B:633:VAL:HB	2.00	0.43
1:A:292:VAL:HG23	1:A:330:LEU:HD21	2.00	0.43
1:B:65:GLU:O	1:B:66:TYR:HB3	2.18	0.43
1:B:195:ASN:HD22	1:B:342:THR:HG21	1.84	0.43
1:B:270:ASN:OD1	1:B:270:ASN:N	2.51	0.42
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.69	0.42
1:A:637:LEU:HD12	1:A:637:LEU:C	2.45	0.42
1:A:687:GLU:OE2	1:A:687:GLU:HA	2.16	0.42
1:B:60:VAL:HG12	1:B:74:ILE:HG23	2.02	0.42
1:A:417:ILE:O	1:A:421:LEU:HG	2.19	0.42
1:B:60:VAL:CG1	1:B:74:ILE:HG23	2.50	0.42
1:B:269:ALA:C	1:B:271:GLU:H	2.27	0.42
1:A:421:LEU:O	1:A:425:ARG:HD3	2.20	0.42
1:B:465:HIS:CD2	1:B:467:LEU:H	2.35	0.42
1:A:611:ASP:O	1:A:615:VAL:HG23	2.20	0.42
1:A:687:GLU:CB	1:A:688:PRO:HD3	2.50	0.42
1:B:528:LYS:O	1:B:532:GLN:HG3	2.21	0.41
1:A:155:VAL:CG1	1:A:158:LEU:HD22	2.49	0.41
1:B:432:LEU:HB2	1:B:542:GLU:HG2	2.01	0.41
1:A:156:THR:O	1:A:159:GLY:N	2.52	0.41
1:A:241:ARG:NH2	1:A:516:ASN:O	2.53	0.41
1:A:80:LEU:HD22	1:A:85:LEU:HG	2.02	0.41
1:A:353:GLY:O	1:A:354:GLN:HB2	2.21	0.41
1:A:627:ALA:O	1:A:628:ALA:C	2.62	0.41
1:B:156:THR:O	1:B:159:GLY:N	2.52	0.41
1:B:391:TYR:N	1:B:392:PRO:CD	2.84	0.41
1:B:433:PHE:CE1	1:B:486:LEU:HD21	2.55	0.40
1:A:668:LYS:HE2	1:A:668:LYS:HB3	1.50	0.40
1:B:555:LEU:HD12	1:B:571:LEU:HD21	2.04	0.40
1:A:5:LEU:HB2	1:A:34:ALA:HB2	2.04	0.40
1:A:354:GLN:HG2	1:B:386:THR:HG21	2.04	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	692/694 (100%)	674 (97%)	16 (2%)	2 (0%)	36	60
1	B	690/694 (99%)	669 (97%)	19 (3%)	2 (0%)	36	60
All	All	1382/1388 (100%)	1343 (97%)	35 (2%)	4 (0%)	36	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	B	69	GLU
1	A	687	GLU
1	B	432	LEU

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	554/554 (100%)	529 (96%)	25 (4%)	24	52
1	B	553/554 (100%)	523 (95%)	30 (5%)	20	45
All	All	1107/1108 (100%)	1052 (95%)	55 (5%)	22	48

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	73	LYS

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Mol	Chain	Res	Type
1	A	79	ARG
1	A	80	LEU
1	A	158	LEU
1	A	163	THR
1	A	219	PHE
1	A	240	GLN
1	A	243	LEU
1	A	256	ARG
1	A	289	VAL
1	A	325	MET
1	A	405	GLN
1	A	411	LYS
1	A	425	ARG
1	A	429	ASP
1	A	512	LYS
1	A	533	ARG
1	A	549	LYS
1	A	612	ARG
1	A	637	LEU
1	A	668	LYS
1	A	674	THR
1	A	685	ASN
1	A	687	GLU
1	B	60	VAL
1	B	71	GLN
1	B	78	GLU
1	B	82	THR
1	B	163	THR
1	B	219	PHE
1	B	243	LEU
1	B	247	VAL
1	B	255	GLU
1	B	256	ARG
1	B	267	LYS
1	B	270	ASN
1	B	289	VAL
1	B	325	MET
1	B	366	LYS
1	B	405	GLN
1	B	411	LYS
1	B	431	ARG
1	B	463	SER

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Mol	Chain	Res	Type
1	B	568	ASN
1	B	569	LEU
1	B	571	LEU
1	B	637	LEU
1	B	653	ARG
1	B	654	GLU
1	B	658	GLN
1	B	668	LYS
1	B	669	ARG
1	B	674	THR
1	B	681	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	28	HIS
1	A	48	GLN
1	A	87	GLN
1	A	124	HIS
1	A	139	HIS
1	A	189	ASN
1	A	195	ASN
1	A	196	ASN
1	A	215	ASN
1	A	221	ASN
1	A	348	GLN
1	A	357	GLN
1	A	368	GLN
1	A	405	GLN
1	A	465	HIS
1	A	532	GLN
1	A	584	GLN
1	A	590	GLN
1	A	599	ASN
1	A	658	GLN
1	A	685	ASN
1	B	6	HIS
1	B	28	HIS
1	B	124	HIS
1	B	140	GLN
1	B	189	ASN

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Mol	Chain	Res	Type
1	B	195	ASN
1	B	196	ASN
1	B	215	ASN
1	B	221	ASN
1	B	368	GLN
1	B	405	GLN
1	B	465	HIS
1	B	474	GLN
1	B	532	GLN
1	B	584	GLN
1	B	599	ASN
1	B	618	GLN
1	B	658	GLN

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](#)

2 ligands 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	$\# Z > 2$
2	PLP	B	701	-	15,15,16	0.81	1 (6%)	21,22,23	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	A	701	-	15,15,16	0.75	1 (6%)	21,22,23	0.69	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
2	PLP	B	701	-	-	5/6/6/8	0/1/1/1
2	PLP	A	701	-	-	3/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	PLP	C4A-C4	-2.48	1.46	1.51
2	A	701	PLP	C4A-C4	-2.36	1.46	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

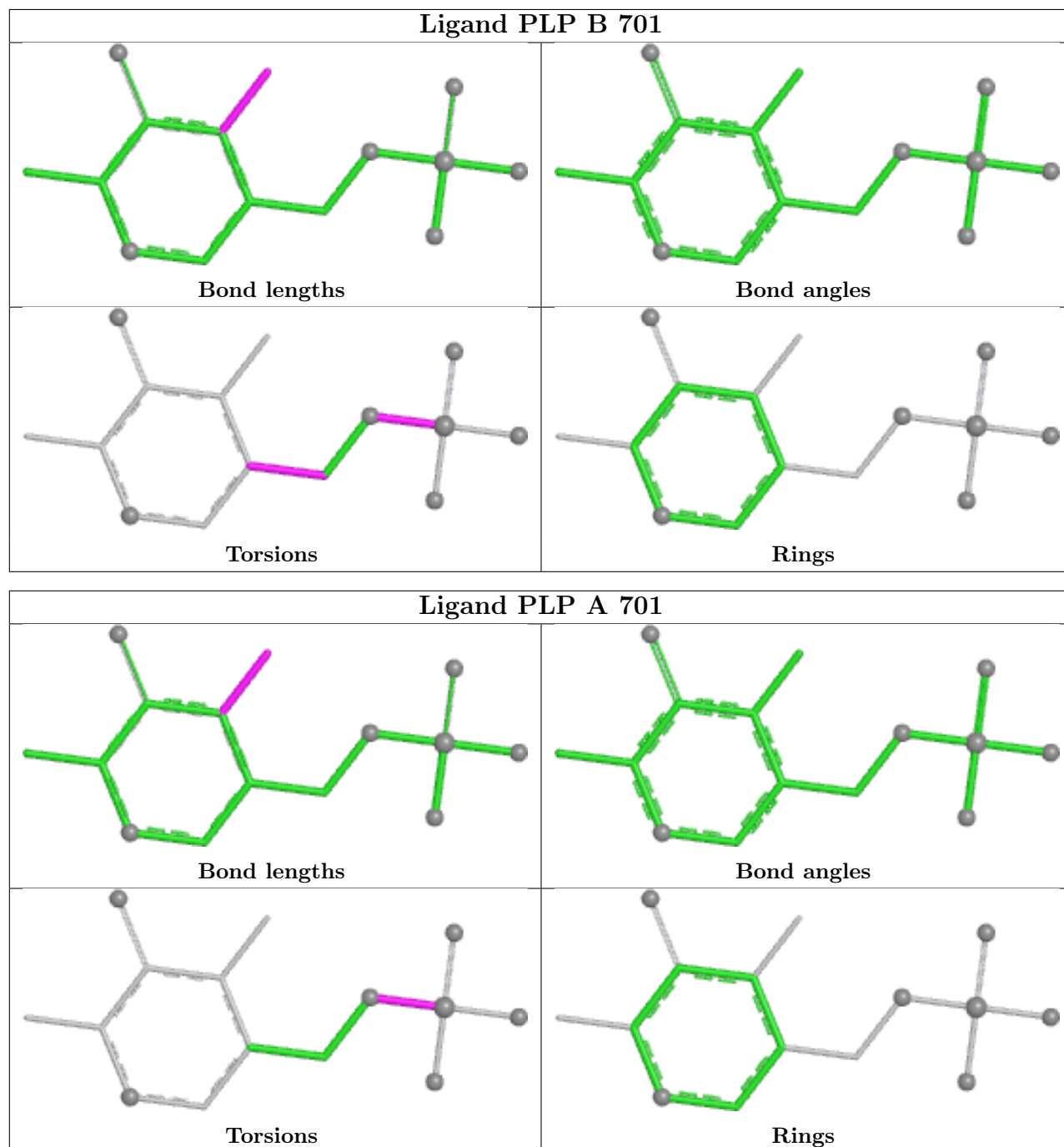
Mol	Chain	Res	Type	Atoms
2	A	701	PLP	C5A-O4P-P-O1P
2	A	701	PLP	C5A-O4P-P-O2P
2	A	701	PLP	C5A-O4P-P-O3P
2	B	701	PLP	C4-C5-C5A-O4P
2	B	701	PLP	C5A-O4P-P-O2P
2	B	701	PLP	C5A-O4P-P-O1P
2	B	701	PLP	C6-C5-C5A-O4P
2	B	701	PLP	C5A-O4P-P-O3P

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 ⓘ

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	694/694 (100%)	-0.32	4 (0%)	85 85	18, 41, 67, 108	0
1	B	692/694 (99%)	-0.33	5 (0%)	84 83	22, 39, 68, 101	0
All	All	1386/1388 (99%)	-0.33	9 (0%)	85 85	18, 40, 68, 108	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	431	ARG	3.2
1	A	241	ARG	2.7
1	B	653	ARG	2.6
1	B	285	PHE	2.5
1	A	285	PHE	2.3
1	B	432	LEU	2.2
1	B	654	GLU	2.1
1	A	612	ARG	2.1
1	A	80	LEU	2.1

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,

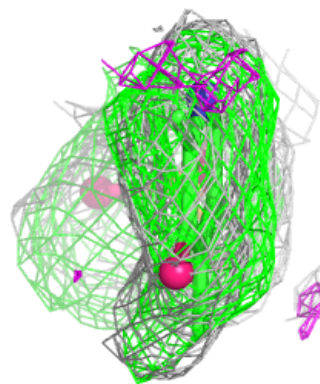
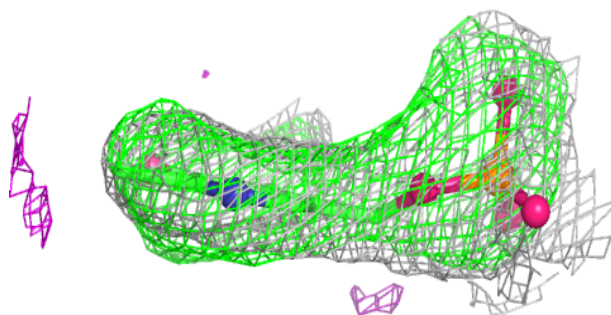
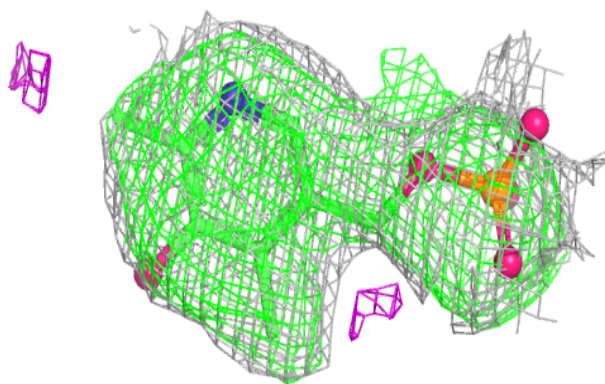
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	A	701	15/16	-	-	16,16,16,16	15
2	PLP	B	701	15/16	-	-	21,21,21,21	15

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.

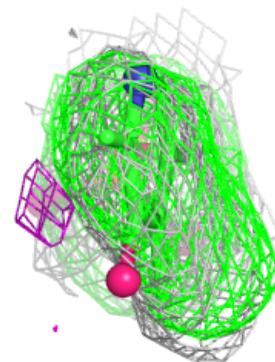
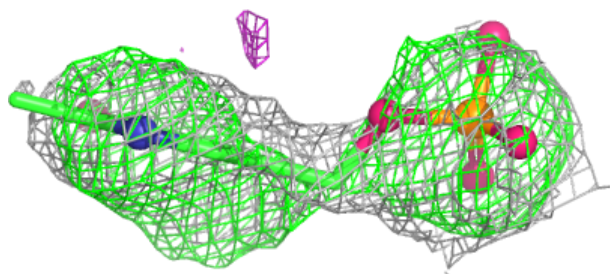
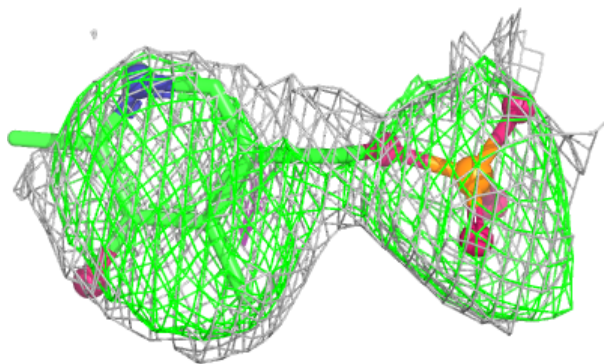
Electron density around PLP A 701:

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 PLP B 701:

$2mF_o-DF_c$ (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.