

Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2022 – 04:53 pm GMT

PDB ID : 7BA4

Title: Structure of Cystathionine gamma-lyase from Pseudomonas aeruginosa

Authors: Fernandez-Rodriguez, C.; Oyenarte, I.; Gonzalez-Recio, I.; Majtan, T.;

Astegno, A.; Martinez-Cruz, L.A.

Deposited on : 2020-12-15

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.26

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

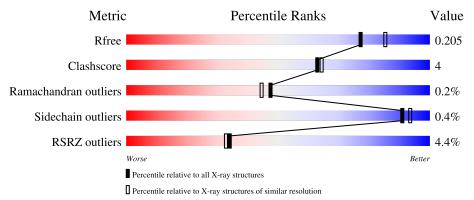
Validation Pipeline (wwPDB-VP) : 2.26

1 Overall quality at a glance (i)

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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	400	84%	10%	6%
1	В	400	5% 84%	8%	8%
1	С	400	81%	11%	8%
1	D	400	82%	8%	10%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12573 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 Cystathionine gamma-lyase.

Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	Trace	
1	Λ	377	Total	С	N	О	S	0	4	0
1	A	311	2915	1835	539	531	10	U	4	
1	В	370	Total	С	N	О	S	0	2	0
1	Б	370	2838	1788	519	522	9	U	2	
1	С	366	Total	С	N	О	S	0	2	0
1		300	2815	1776	516	514	9	U	2	
1	D	358	Total	С	N	О	S	0	3	0
1	ש	330	2768	1746	508	505	9	U	3	

There are 24 discrepancies between the modelled and reference sequences:

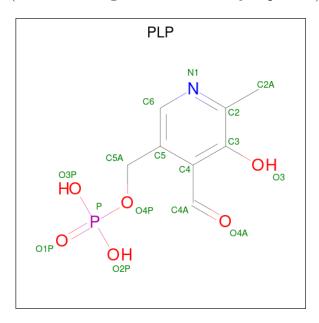
Chain	Residue	Modelled	Actual	Comment	Reference
			rectaar		
A	395	HIS	-	expression tag	UNP A0A509J8D5
A	396	HIS	-	expression tag	UNP A0A509J8D5
A	397	HIS	-	expression tag	UNP A0A509J8D5
A	398	HIS	-	expression tag	UNP A0A509J8D5
A	399	HIS	-	expression tag	UNP A0A509J8D5
A	400	HIS	-	expression tag	UNP A0A509J8D5
В	395	HIS	-	expression tag	UNP A0A509J8D5
В	396	HIS	-	expression tag	UNP A0A509J8D5
В	397	HIS	-	expression tag	UNP A0A509J8D5
В	398	HIS	-	expression tag	UNP A0A509J8D5
В	399	HIS	-	expression tag	UNP A0A509J8D5
В	400	HIS	-	expression tag	UNP A0A509J8D5
С	395	HIS	-	expression tag	UNP A0A509J8D5
С	396	HIS	-	expression tag	UNP A0A509J8D5
С	397	HIS	-	expression tag	UNP A0A509J8D5
С	398	HIS	-	expression tag	UNP A0A509J8D5
С	399	HIS	-	expression tag	UNP A0A509J8D5
С	400	HIS	-	expression tag	UNP A0A509J8D5
D	395	HIS	-	expression tag	UNP A0A509J8D5
D	396	HIS	-	expression tag	UNP A0A509J8D5
D	397	HIS	-	expression tag	UNP A0A509J8D5



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	398	HIS	-	expression tag	UNP A0A509J8D5
D	399	HIS	-	expression tag	UNP A0A509J8D5
D	400	HIS	-	expression tag	UNP A0A509J8D5

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Λ	1	Total C N O P	0	0
2	А	1	15 8 1 5 1	0	U
2	В	1	Total C N O P	0	0
2	Б	1	15 8 1 5 1	0	U
2	C	1	Total C N O P	0	0
2	C	1	15 8 1 5 1	0	U
2	D	1	Total C N O P	0	0
2	D	1	15 8 1 5 1		U

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	259	Total O 259 259	0	0
3	В	334	Total O 334 334	0	0
3	С	264	Total O 264 264	0	0



Continued from previous page...

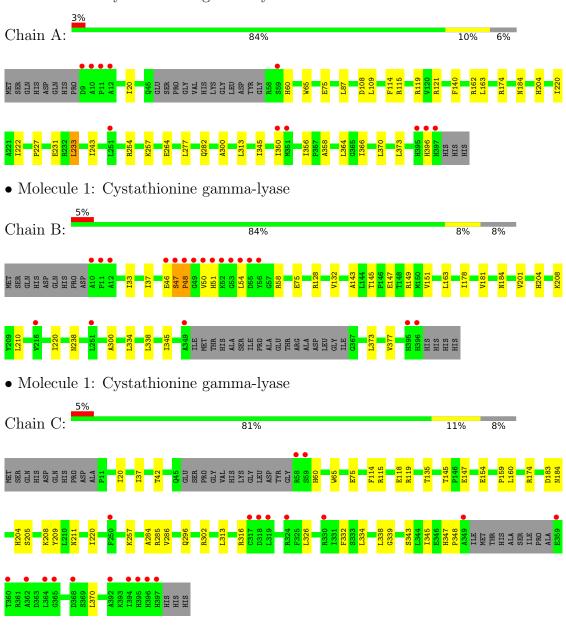
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	320	Total O 320 320	0	0



3 Residue-property plots (i)

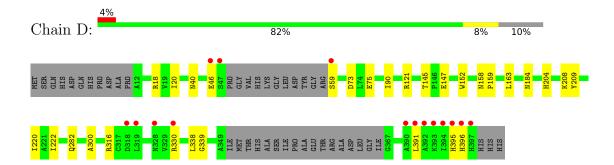
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cystathionine gamma-lyase



• Molecule 1: Cystathionine gamma-lyase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	79.30Å 79.30Å 446.67Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.45 - 2.00	Depositor
Resolution (A)	54.45 - 2.00	EDS
% Data completeness	99.7 (54.45-2.00)	Depositor
(in resolution range)	99.7 (54.45-2.00)	EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.52 (at 2.00 Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D.D.	0.160 , 0.205	Depositor
R, R_{free}	0.160 , 0.205	DCC
R_{free} test set	5679 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.44, < L^2> = 0.26$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12573	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: 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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.44	0/2986	0.60	0/4054	
1	В	0.47	0/2901	0.62	0/3939	
1	С	0.47	0/2874	0.61	0/3901	
1	D	0.46	0/2832	0.61	0/3843	
All	All	0.46	0/11593	0.61	0/15737	

There are no bond length outliers.

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	2915	0	2900	30	0
1	В	2838	0	2806	25	0
1	С	2815	0	2780	29	0
1	D	2768	0	2742	21	0
2	A	15	0	7	0	0
2	В	15	0	7	0	0
2	С	15	0	6	1	0
2	D	15	0	6	0	0
3	A	259	0	0	4	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	334	0	0	1	0
3	С	264	0	0	1	0
3	D	320	0	0	2	0
All	All	12573	0	11254	98	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 4.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		${\rm distance} (\mathring{\rm A})$	overlap (Å)
1:C:154:GLU:HG2	1:C:183:ASP:HB3	1.69	0.75
1:D:59:SER:N	3:D:601:HOH:O	2.22	0.71
1:A:119:ARG:HG2	1:A:356:ILE:HD11	1.73	0.70
1:D:282:GLN:HG3	1:D:396:HIS:CE1	2.28	0.69
1:C:285:ARG:HD2	1:C:286:VAL:H	1.58	0.67
1:A:162:ARG:HH21	1:A:364:LEU:HG	1.60	0.66
1:A:184:ASN:HB3	1:A:204[B]:HIS:CE1	2.33	0.64
1:C:285:ARG:HD2	1:C:286:VAL:N	2.13	0.64
1:B:75:GLU:OE1	1:B:204[B]:HIS:NE2	2.32	0.62
1:C:302:ARG:NH2	3:C:606:HOH:O	2.33	0.61
1:B:46:GLU:HB2	1:B:50:VAL:HG12	1.86	0.58
1:C:75:GLU:OE2	1:C:204[A]:HIS:NE2	2.35	0.58
1:B:184:ASN:HB3	1:B:204[B]:HIS:CE1	2.38	0.57
1:A:227:PRO:O	1:A:231:GLU:HG2	2.06	0.56
1:D:184:ASN:HB3	1:D:204[A]:HIS:CE1	2.42	0.55
1:A:356:ILE:HD12	1:A:358:ALA:HB3	1.89	0.54
1:B:151:VAL:HG23	1:B:178:ILE:HG21	1.90	0.54
1:B:47:SER:OG	1:B:48:PRO:HD3	2.07	0.54
1:A:204[A]:HIS:HB2	1:A:220:ILE:HG22	1.90	0.54
1:C:326:LEU:HD11	1:C:347:HIS:HB2	1.89	0.53
3:A:802:HOH:O	1:D:40:ASN:HB2	2.09	0.53
1:A:204[B]:HIS:HB2	1:A:220:ILE:HG22	1.90	0.53
1:C:145:THR:OG1	1:C:147:GLU:HG2	2.09	0.52
1:A:345:ILE:HG13	1:A:373:LEU:HD23	1.91	0.52
1:D:75:GLU:OE2	1:D:204[A]:HIS:NE2	2.34	0.51
1:C:114:PHE:CE1	1:C:118:GLU:HG3	2.46	0.50
1:C:174:ARG:HH21	1:C:174:ARG:HG2	1.76	0.50
1:A:60:HIS:HB2	1:A:65:TRP:CZ2	2.46	0.50
1:C:209:TYR:CE1	1:C:339:GLY:HA2	2.46	0.50
1:B:208:LYS:HD2	1:B:338:LEU:HG	1.93	0.49
		Continu	ed on nert page



 $Continued\ from\ previous\ page...$

Continuea from previ		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:D:90:ILE:HG23	1:D:152:TRP:CH2	2.47	0.49
1:A:366:ILE:HG23	1:A:370:LEU:HD23	1.94	0.49
1:A:87:LEU:HD12	1:B:58:ARG:CZ	2.43	0.49
1:A:254:ARG:NH2	1:C:211:ASN:OD1	2.45	0.49
1:C:135:THR:HG22	1:C:296:GLN:HE22	1.77	0.48
1:B:181:VAL:HG22	1:B:201:VAL:HB	1.96	0.48
1:C:60:HIS:HA	1:C:65[B]:TRP:CZ2	2.48	0.48
1:C:184:ASN:HB3	1:C:204[A]:HIS:CE1	2.49	0.48
1:C:184:ASN:HB3	1:C:204[B]:HIS:CE1	2.49	0.48
1:A:109:LEU:HD21	1:A:114:PHE:HD1	1.79	0.47
1:D:204[A]:HIS:HB2	1:D:220:ILE:HG22	1.96	0.47
1:D:18:ARG:HD2	1:D:73:ASP:OD2	2.14	0.47
1:B:163:LEU:HD11	1:B:300:ALA:HB2	1.97	0.47
1:C:20:ILE:HA	1:C:257:LYS:HD3	1.96	0.47
1:A:184:ASN:HB3	1:A:204[A]:HIS:CE1	2.51	0.46
1:B:54:LEU:HD22	1:B:238:ASN:HB2	1.97	0.46
1:C:159:PRO:HD2	1:C:160:LEU:HD22	1.98	0.46
1:D:282:GLN:HA	1:D:396:HIS:NE2	2.31	0.46
1:A:115:ARG:HH11	1:B:54:LEU:HD23	1.81	0.46
1:A:163:LEU:HD11	1:A:300:ALA:HB2	1.98	0.46
1:A:282:GLN:HA	1:A:396:HIS:CE1	2.51	0.45
1:B:204[A]:HIS:HB2	1:B:220:ILE:HG22	1.97	0.45
1:C:284:ALA:HB2	1:C:316:ARG:HG2	1.99	0.45
1:D:163:LEU:HD11	1:D:300:ALA:HB2	1.98	0.45
1:D:145:THR:OG1	1:D:147:GLU:HG2	2.17	0.45
1:B:345:ILE:HG13	1:B:373:LEU:HD23	1.98	0.45
1:B:33:ILE:HD12	1:C:42:THR:HG23	2.00	0.44
1:B:145:THR:OG1	1:B:147:GLU:HG2	2.18	0.44
1:B:184:ASN:HB3	1:B:204[A]:HIS:CE1	2.51	0.44
1:C:348:PRO:HG2	1:C:370:LEU:HD23	1.99	0.44
1:A:350:ILE:HD12	3:A:827:HOH:O	2.17	0.44
1:D:184:ASN:HB3	1:D:204[B]:HIS:CE1	2.53	0.44
1:A:243:ILE:HD12	1:A:243:ILE:O	2.18	0.43
1:C:115:ARG:HG3	1:C:119:ARG:HD3	2.00	0.43
1:A:174:ARG:HG3	3:A:669:HOH:O	2.18	0.43
1:A:264:GLU:OE1	3:A:601:HOH:O	2.21	0.43
1:D:209:TYR:CE1	1:D:339:GLY:HA2	2.53	0.43
1:A:75:GLU:HG3	1:A:222:ILE:HD13	2.01	0.43
1:D:316:ARG:NH2	3:D:609:HOH:O	2.43	0.43
1:B:37:ILE:HB	1:C:37:ILE:HB	2.00	0.43
1:B:204[B]:HIS:HB2	1:B:220:ILE:HG22	1.99	0.43



Continued from previous page...

A	A. 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:A:75:GLU:OE1	1:A:204[B]:HIS:NE2	2.42	0.43
1:A:20:ILE:HA	1:A:257:LYS:HD3	2.00	0.42
1:C:208:LYS:HD2	1:C:338:LEU:HG	2.00	0.42
1:A:277:LEU:HD13	1:A:313:LEU:HD23	2.02	0.42
1:C:332:PHE:CD2	1:C:343:SER:HB3	2.54	0.42
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.80	0.42
1:D:282:GLN:HG2	1:D:391:LEU:O	2.20	0.42
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.91	0.42
1:A:313:LEU:HD12	1:A:313:LEU:O	2.20	0.41
1:D:121:ARG:HD3	1:D:121:ARG:HA	1.91	0.41
1:D:158:ASN:HA	1:D:159:PRO:HA	1.82	0.41
1:C:204[B]:HIS:HB2	1:C:220:ILE:HG22	2.02	0.41
1:B:334:LEU:HD23	1:B:345:ILE:HG23	2.03	0.41
1:C:334:LEU:HD12	1:C:345:ILE:O	2.20	0.41
1:B:377:VAL:HG23	1:D:20:ILE:HD11	2.02	0.41
1:C:334:LEU:HD23	1:D:46:GLU:HA	2.03	0.41
1:B:132:VAL:HG11	1:B:143:ALA:CB	2.51	0.41
1:A:282:GLN:HG3	1:A:396:HIS:NE2	2.36	0.41
1:C:205:SER:HB2	2:C:501:PLP:O4P	2.21	0.41
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.96	0.40
1:C:332:PHE:CE2	1:C:343:SER:HB3	2.57	0.40
1:A:108:ASP:OD1	1:A:108:ASP:N	2.52	0.40
1:B:128:ARG:HD2	1:B:128:ARG:HA	1.83	0.40
1:B:149:ARG:HD3	3:B:833:HOH:O	2.20	0.40
1:D:75:GLU:HG3	1:D:222:ILE:HD13	2.03	0.40
1:B:132:VAL:HG11	1:B:143:ALA:HB2	2.03	0.40
1:D:208:LYS:HD2	1:D:338:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	377/400~(94%)	371 (98%)	6 (2%)	0	100	100
1	В	368/400~(92%)	361 (98%)	4 (1%)	3 (1%)	19	13
1	C	362/400~(90%)	355 (98%)	7 (2%)	0	100	100
1	D	355/400~(89%)	347 (98%)	8 (2%)	0	100	100
All	All	$1462/1600 \; (91\%)$	1434 (98%)	25 (2%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	48	PRO
1	В	51	HIS
1	В	47	SER

5.3.2 Protein sidechains (i)

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	Perce	ntiles
1	A	303/320 (95%)	301 (99%)	2 (1%)	84	88
1	В	293/320 (92%)	293 (100%)	0	100	100
1	С	289/320 (90%)	288 (100%)	1 (0%)	92	95
1	D	287/320 (90%)	285 (99%)	2 (1%)	84	88
All	All	1172/1280 (92%)	1167 (100%)	5 (0%)	91	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	PHE
1	A	233	LEU
1	С	313	LEU
1	D	330	ARG
1	D	395	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	В	45	GLN
1	С	395	HIS
1	D	138	GLN
1	D	397	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	Mol Type Chain Res		Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	В	501	1	15,15,16	1.05	2 (13%)	20,22,23	1.09	2 (10%)
2	PLP	С	501	1	15,15,16	1.02	1 (6%)	20,22,23	1.11	1 (5%)
2	PLP	D	501	1	15,15,16	1.02	1 (6%)	20,22,23	1.29	2 (10%)
2	PLP	A	501	1	15,15,16	1.06	2 (13%)	20,22,23	1.54	3 (15%)

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	В	501	1	-	0/6/6/8	0/1/1/1
2	PLP	С	501	1	=	0/6/6/8	0/1/1/1
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1
2	PLP	A	501	1	=	0/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
2	С	501	PLP	C2-N1	2.57	1.38	1.33
2	В	501	PLP	C6-N1	2.44	1.39	1.34
2	В	501	PLP	C2-N1	2.37	1.38	1.33
2	A	501	PLP	C2-N1	2.35	1.38	1.33
2	A	501	PLP	C6-N1	2.28	1.39	1.34
2	D	501	PLP	C2-N1	2.09	1.37	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	A	501	PLP	O4P-C5A-C5	3.86	116.72	109.35
2	В	501	PLP	C6-C5-C4	2.96	120.49	118.16
2	D	501	PLP	O4P-C5A-C5	2.71	114.52	109.35
2	D	501	PLP	O2P-P-O4P	2.62	113.71	106.73
2	A	501	PLP	C4A-C4-C5	2.37	123.37	120.94
2	A	501	PLP	C4A-C4-C3	-2.17	116.82	120.50
2	С	501	PLP	O4P-C5A-C5	2.11	113.38	109.35
2	В	501	PLP	C5-C6-N1	-2.01	120.46	123.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

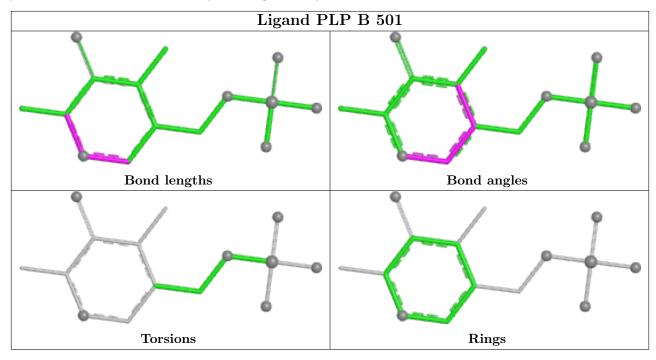
1 monomer is involved in 1 short contact:

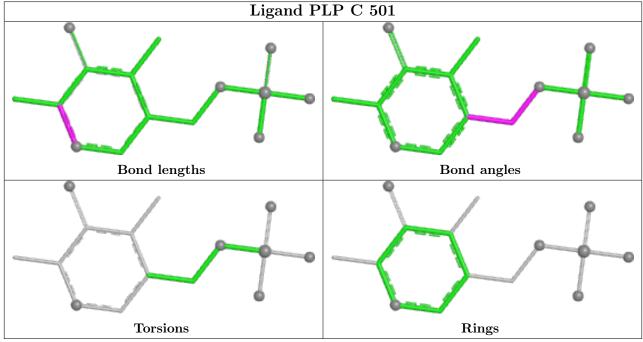
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	501	PLP	1	0

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 then 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

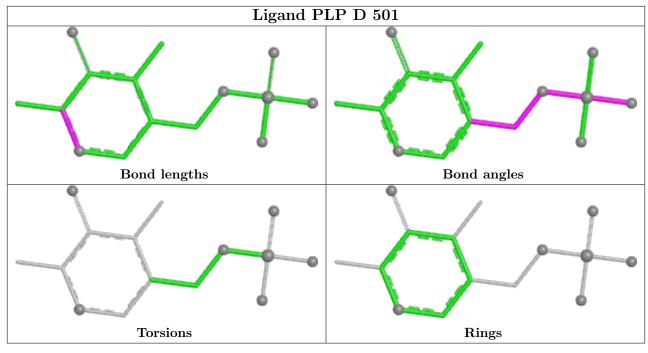


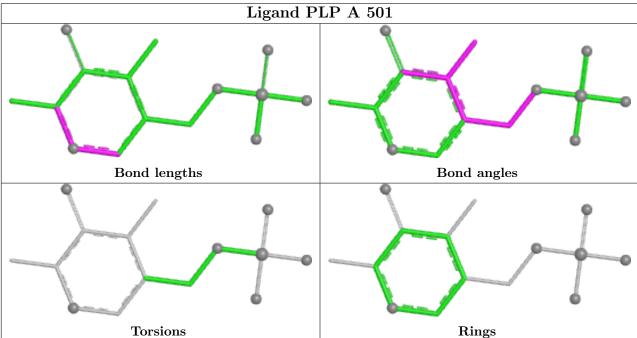
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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, 95^{th} 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>	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	377/400 (94%)	-0.22	11 (2%) 51 50	24, 35, 67, 145	0
1	В	370/400 (92%)	-0.12	19 (5%) 28 27	24, 34, 76, 155	0
1	С	366/400 (91%)	-0.08	20 (5%) 25 24	24, 34, 70, 141	1 (0%)
1	D	358/400 (89%)	-0.10	15 (4%) 36 35	22, 34, 63, 144	1 (0%)
All	All	1471/1600 (91%)	-0.13	65 (4%) 34 33	22, 34, 69, 155	2 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	54	LEU	10.4
1	D	396	HIS	8.4
1	В	51	HIS	8.2
1	В	50	VAL	7.7
1	В	53	GLY	7.7
1	С	360	THR	7.2
1	В	49	GLY	7.2
1	С	397	HIS	7.1
1	A	9	ASP	6.7
1	С	359	GLU	6.3
1	В	52	LYS	5.6
1	В	48	PRO	5.5
1	В	47	SER	5.5
1	A	10	ALA	5.3
1	D	395	HIS	5.1
1	С	396	HIS	4.8
1	D	397	HIS	4.7
1	D	46	GLU	4.5
1	В	56	TYR	4.5
1	D	394	ILE	4.2
1	В	10	ALA	4.2



Continued from previous page...

Mol	nued fron Chain	Res	Type	RSRZ
1	A	395	HIS	4.2
1	В	396	HIS	4.2
1	A	397	HIS	4.1
1	С	364	LEU	4.0
1	A	396	HIS	4.0
1	В	395	HIS	3.8
1	В	11	PRO	3.4
1	С	365	GLY	3.3
1	C C	368	ASP	3.3
1	С	349	ALA	3.2
1	A	350	ILE	3.2
1	С	319	LEU	3.1
1	D	391	LEU	3.0
1	D	47	SER	2.9
1	В	55	ASP	2.9
1	A	12	ALA	2.9
1	A	59	SER	2.9
1	D	59	SER	2.9
1	С	395	HIS	2.9
1	D	330	ARG	2.8
1	A	251	LEU	2.7
1	С	59	SER	2.6
1	С	362	ALA	2.5
1	В	12	ALA	2.5
1	С	394	ILE	2.4
1	В	251	LEU	2.3
1	С	317	CYS	2.3
1	D	319	LEU	2.3
1	В	216	VAL	2.3
1	С	250	PHE	2.3
1	D	318	ASP	2.2
1	В	46	GLU	2.2
1	A	351	MET	2.2
1	A	11	PRO	2.2
1	D	392	ALA	2.2
1	D	328	ASN	2.2
1	С	324	ARG	2.1
1	D	390	ALA	2.1
1	С	318	ASP	2.1
1	В	349	ALA	2.1
1	С	392	ALA	2.1
1	С	330	ARG	2.1



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	С	58	ARG	2.1
1	D	393	LYS	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 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, 95^{th} 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.

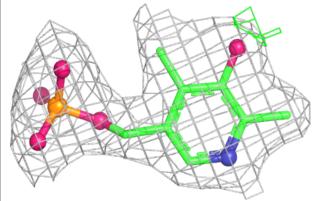
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	PLP	A	501	15/16	0.98	0.09	27,30,35,35	0
2	PLP	В	501	15/16	0.98	0.10	28,33,37,39	0
2	PLP	D	501	15/16	0.98	0.09	24,30,35,38	0
2	PLP	С	501	15/16	0.99	0.10	23,32,36,36	0

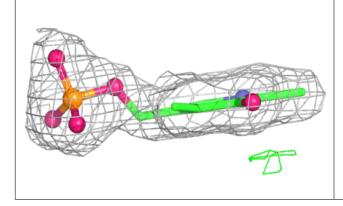
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

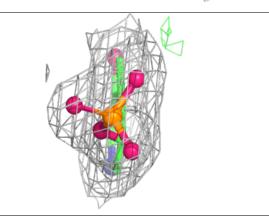


Electron density around PLP A 501:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

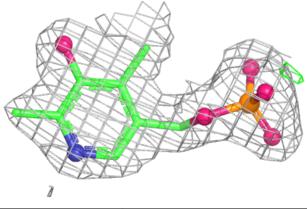


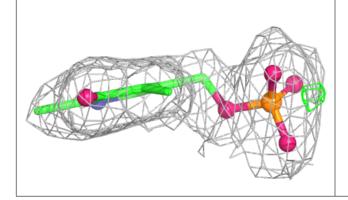


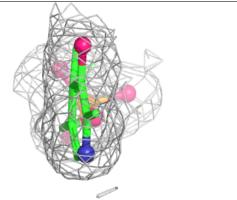


Electron density around PLP B 501:

 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



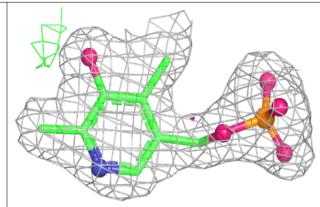


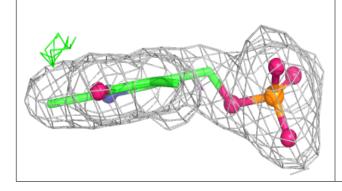


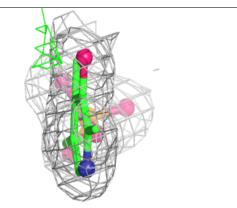


Electron density around PLP D 501:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

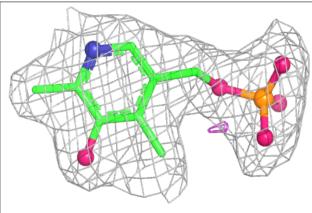


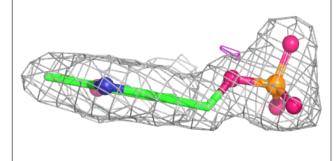


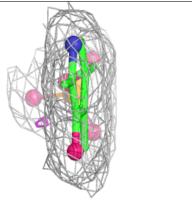


Electron density around PLP C 501:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

