

wwPDB X-ray Structure Validation Summary Report (i)

Dec 9, 2021 – 12:06 AM EST

PDB ID : 7SZP

Title : Crystal Structure of Histidinol-phosphate aminotransferase from Klebsiella

pneumoniae subsp. pneumoniae (strain HS11286)

Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)

Deposited on : 2021-11-29

Resolution : 1.80 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 (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: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.24

buster-report : 1.1.7 (2018)

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

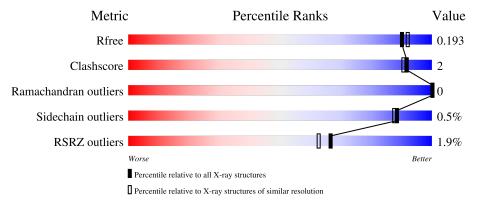
Validation Pipeline (wwPDB-VP) : 2.24

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 1.80 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
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 <=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	361	94%	
1	В	361	94%	
1	С	361	91%	6% •
1	D	361	91%	7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	D	401	-	-	X	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12541 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 Histidinol-phosphate aminotransferase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Λ	353	Total	С	N	О	S	0	8	0
1	A	ააა	2742	1737	469	523	13	0	8	
1	В	350	Total	С	N	О	S	0	6	0
1	Б		2708	1716	460	519	13	U	U	0
1	С	347	Total	С	N	О	S	0	3	0
1		347	2667	1691	454	509	13	0) 	0
1	D	D 351	Total	С	N	О	S	0	9	0
1	D		2730	1731	466	520	13			U

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP W9BAC7
A	-6	ALA	-	expression tag	UNP W9BAC7
A	-5	HIS	-	expression tag	UNP W9BAC7
A	-4	HIS	-	expression tag	UNP W9BAC7
A	-3	HIS	-	expression tag	UNP W9BAC7
A	-2	HIS	-	expression tag	UNP W9BAC7
A	-1	HIS	-	expression tag	UNP W9BAC7
A	0	HIS	-	expression tag	UNP W9BAC7
В	-7	MET	-	initiating methionine	UNP W9BAC7
В	-6	ALA	_	expression tag	UNP W9BAC7
В	-5	HIS	-	expression tag	UNP W9BAC7
В	-4	HIS	_	expression tag	UNP W9BAC7
В	-3	HIS	-	expression tag	UNP W9BAC7
В	-2	HIS	_	expression tag	UNP W9BAC7
В	-1	HIS	-	expression tag	UNP W9BAC7
В	0	HIS	-	expression tag	UNP W9BAC7
С	-7	MET	-	initiating methionine	UNP W9BAC7
С	-6	ALA	-	expression tag	UNP W9BAC7
С	-5	HIS	-	expression tag	UNP W9BAC7
С	-4	HIS	-	expression tag	UNP W9BAC7
С	-3	HIS	-	expression tag	UNP W9BAC7

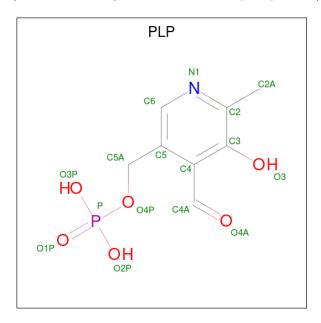
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Chain	Residue	Modelled	Actual	Comment	Reference
С	-2	HIS	-	expression tag	UNP W9BAC7
С	-1	HIS	-	expression tag	UNP W9BAC7
С	0	HIS	-	expression tag	UNP W9BAC7
D	-7	MET	-	initiating methionine	UNP W9BAC7
D	-6	ALA	-	expression tag	UNP W9BAC7
D	-5	HIS	-	expression tag	UNP W9BAC7
D	-4	HIS	-	expression tag	UNP W9BAC7
D	-3	HIS	-	expression tag	UNP W9BAC7
D	-2	HIS	-	expression tag	UNP W9BAC7
D	-1	HIS	-	expression tag	UNP W9BAC7
D	0	HIS	-	expression tag	UNP W9BAC7

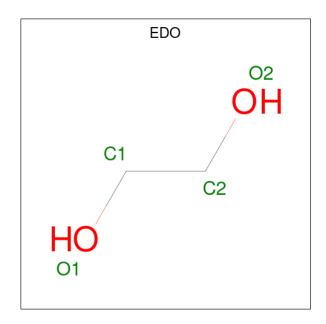
 \bullet Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P)$ (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	Δ	1	Total	С	N	О	Р	0	0
2		1	16	8	1	6	1		U
2	R	1	Total	С	N	Ο	Р	0	0
2	Ъ	1	16	8	1	6	1		0
2	С	1	Total	С	N	О	Р	0	0
2		1	16	8	1	6	1	0	U
2	D	D 1	Total	С	N	О	Р	0	0
	D		16	8	1	6	1		0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

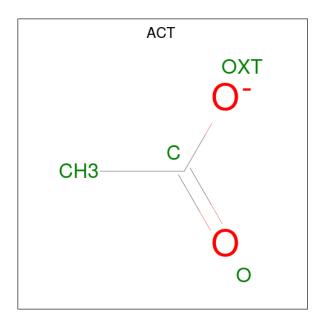




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	В	1	Total C O 4 2 2	0	0
3	В	1	Total C O 4 2 2	0	0
3	С	1	Total C O 4 2 2	0	0
3	С	1	Total C O 4 2 2	0	0
3	С	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

 \bullet Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	В	1	Total C O 4 2 2	0	0
4	В	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Cl 1 1	0	0

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	1	Total Ca 1 1	0	0

• Molecule 7 is water.

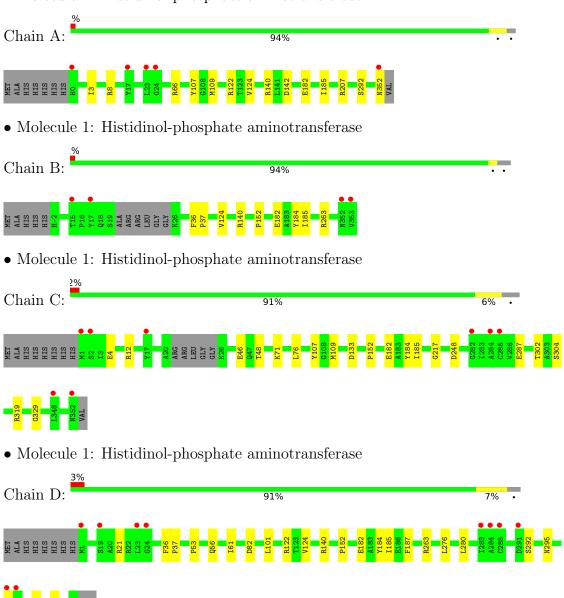
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	433	Total O 447 447	0	14
7	В	415	Total O 424 424	0	9
7	С	355	Total O 364 364	0	10
7	D	314	Total O 321 321	0	7



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: Histidinol-phosphate aminotransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	106.40Å 111.61Å 119.32Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.55 - 1.80	Depositor
Resolution (A)	47.16 - 1.80	EDS
% Data completeness	98.3 (44.55-1.80)	Depositor
(in resolution range)	98.3 (47.16-1.80)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.14 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.20rc3-4406	Depositor
D.D.	0.151 , 0.193	Depositor
R, R_{free}	0.151 , 0.193	DCC
R_{free} test set	2038 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 50.0	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12541	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.81% 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, EDO, ACT, CL, CA

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	0/2817	0.62	0/3842	
1	В	0.43	0/2777	0.64	0/3790	
1	С	0.39	0/2725	0.61	$1/3721 \ (0.0\%)$	
1	D	0.38	0/2807	0.60	0/3830	
All	All	0.41	0/11126	0.62	1/15183 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	С	248	ASP	CB-CG-OD1	5.27	123.05	118.30

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	A	2742	0	2754	8	0
1	В	2708	0	2704	5	0
1	С	2667	0	2663	11	0
1	D	2730	0	2742	12	0
2	A	16	0	7	0	0
2	В	16	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	16	0	7	0	0
2	D	16	0	8	1	0
3	A	12	0	18	1	0
3	В	8	0	12	0	0
3	С	12	0	18	0	0
3	D	8	0	12	1	0
4	A	8	0	6	0	0
4	В	8	0	6	0	0
4	С	8	0	6	1	0
4	D	8	0	6	2	0
5	В	1	0	0	0	0
6	С	1	0	0	0	0
7	A	447	0	0	3	0
7	В	424	0	0	1	0
7	С	364	0	0	2	0
7	D	321	0	0	0	0
All	All	12541	0	10976	36	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 36 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:C:319:ARG:HH21	4:C:405:ACT:H3	1.39	0.84	
1:A:8:ARG:NH1	7:A:501:HOH:O	2.12	0.77	
4:D:401:ACT:H2	2:D:402:PLP:H5A1	1.78	0.66	
1:D:82:ASP:OD2	4:D:401:ACT:H1	2.05	0.57	
1:C:71:LYS:NZ	7:C:510:HOH:O	2.43	0.52	

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 ba	ackbone	conformation	was
analysed, and the total number	r of residue	es.					

Mol	Chain	Analysed	Favoured Allowed		Outliers	Percentiles		
1	A	359/361 (99%)	356 (99%)	3 (1%)	0	100	100	
1	В	352/361 (98%)	348 (99%)	4 (1%)	0	100	100	
1	\mathbf{C}	346/361 (96%)	341 (99%)	5 (1%)	0	100	100	
1	D	358/361 (99%)	354 (99%)	4 (1%)	0	100	100	
All	All	1415/1444 (98%)	1399 (99%)	16 (1%)	0	100	100	

There are no Ramachandran outliers to report.

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	Percentiles		
1	A	294/299 (98%)	292 (99%)	2 (1%)	84	81	
1	В	292/299~(98%)	292 (100%)	0	100	100	
1	С	284/299 (95%)	283 (100%)	1 (0%)	91	89	
1	D	292/299~(98%)	289 (99%)	3 (1%)	76	71	
All	All	$1162/1196 \ (97\%)$	1156 (100%)	6 (0%)	88	87	

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	21	ARG
1	D	292	SER
1	D	328	SER
1	A	292	SER
1	A	3	ILE

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



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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).

Mal	Т	Clasia.	Das	Link	В	ond leng	$_{ m gths}$	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	С	406	-	1,3,3	5.04	1 (100%)	0,3,3	_	-
4	ACT	A	406	-	1,3,3	5.64	1 (100%)	0,3,3	-	-
4	ACT	D	401	-	1,3,3	7.86	1 (100%)	0,3,3	-	-
3	EDO	В	404	-	3,3,3	0.56	0	2,2,2	0.18	0
4	ACT	С	405	-	1,3,3	5.96	1 (100%)	0,3,3	_	-
4	ACT	D	405	-	1,3,3	6.61	1 (100%)	0,3,3	-	-
2	PLP	С	401	-	16,16,16	0.61	0	20,23,23	0.85	1 (5%)
3	EDO	В	403	-	3,3,3	0.52	0	2,2,2	0.45	0
4	ACT	В	401	-	1,3,3	7.85	1 (100%)	0,3,3	-	-
3	EDO	С	404	-	3,3,3	0.64	0	2,2,2	0.20	0
3	EDO	D	404	-	3,3,3	0.51	0	2,2,2	0.29	0
3	EDO	A	404	-	3,3,3	0.72	0	2,2,2	0.16	0
2	PLP	В	402	-	16,16,16	0.62	0	20,23,23	0.86	0
3	EDO	A	402	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	С	403	-	3,3,3	0.52	0	2,2,2	0.29	0
3	EDO	A	403	-	3,3,3	0.47	0	2,2,2	0.26	0



Mol	Iol Type Chain Res		Dec	Link	Bond lengths			Bond angles			
MIOI	Туре	Chain	rtes	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	С	402	-	3,3,3	0.49	0	2,2,2	0.26	0	
2	PLP	A	401	-	16,16,16	0.47	0	20,23,23	0.82	1 (5%)	
3	EDO	D	403	-	3,3,3	0.48	0	2,2,2	0.26	0	
4	ACT	В	405	-	1,3,3	6.11	1 (100%)	0,3,3	_	-	
2	PLP	D	402	-	16,16,16	0.34	0	20,23,23	0.73	0	
4	ACT	A	405	-	1,3,3	6.48	1 (100%)	0,3,3	-	-	

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
3	EDO	С	402	-	-	0/1/1/1	-
2	PLP	A	401	-	-	5/8/8/8	0/1/1/1
3	EDO	D	403	-	-	0/1/1/1	-
3	EDO	С	404	_	-	0/1/1/1	-
3	EDO	D	404	-	-	0/1/1/1	-
2	PLP	D	402	_	-	4/8/8/8	0/1/1/1
3	EDO	A	404	-	-	0/1/1/1	-
2	PLP	В	402	-	-	2/8/8/8	0/1/1/1
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	С	403	-	-	0/1/1/1	-
2	PLP	С	401	-	-	4/8/8/8	0/1/1/1
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	В	403	-	-	1/1/1/1	-
3	EDO	В	404	-	-	0/1/1/1	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
4	D	401	ACT	СН3-С	7.86	1.58	1.48
4	В	401	ACT	СН3-С	7.85	1.58	1.48
4	D	405	ACT	СН3-С	6.61	1.57	1.48
4	A	405	ACT	СН3-С	6.48	1.57	1.48
4	В	405	ACT	СН3-С	6.11	1.56	1.48

All (2) bond angle outliers are listed below:



Mo	l Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$\operatorname{Ideal}({}^{o})$
2	С	401	PLP	O3P-P-O4P	-2.12	101.10	106.73
2	A	401	PLP	O3P-P-O4P	-2.12	101.10	106.73

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLP	C5A-O4P-P-O1P
2	A	401	PLP	C5A-O4P-P-O2P
2	A	401	PLP	C5A-O4P-P-O3P
2	В	402	PLP	C5A-O4P-P-O2P
2	В	402	PLP	C5A-O4P-P-O3P

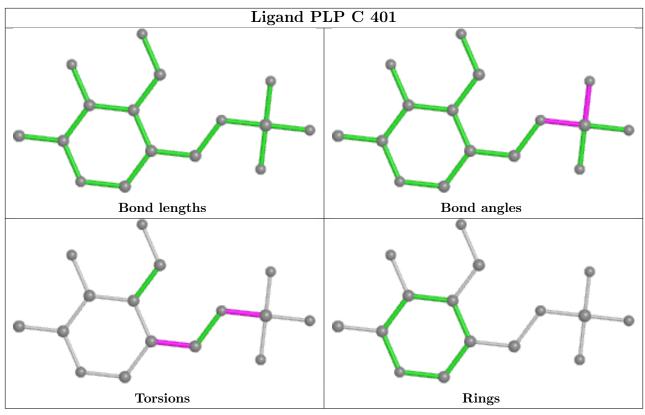
There are no ring outliers.

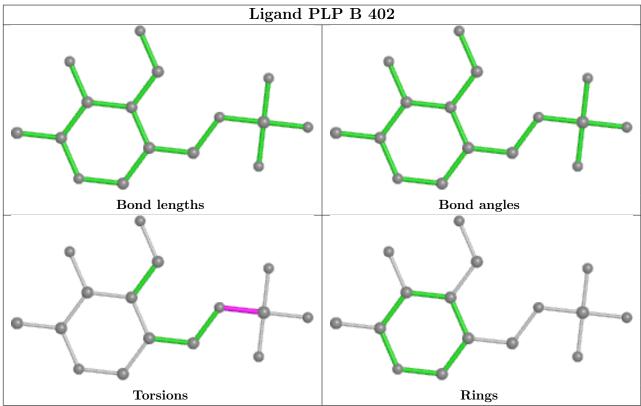
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	ACT	2	0
4	С	405	ACT	1	0
3	A	402	EDO	1	0
3	D	403	EDO	1	0
2	D	402	PLP	1	0

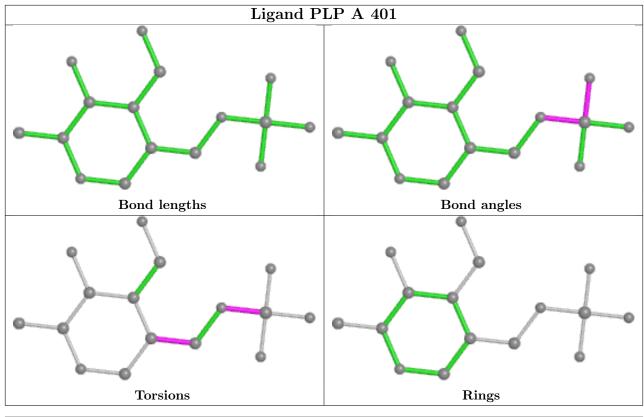
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

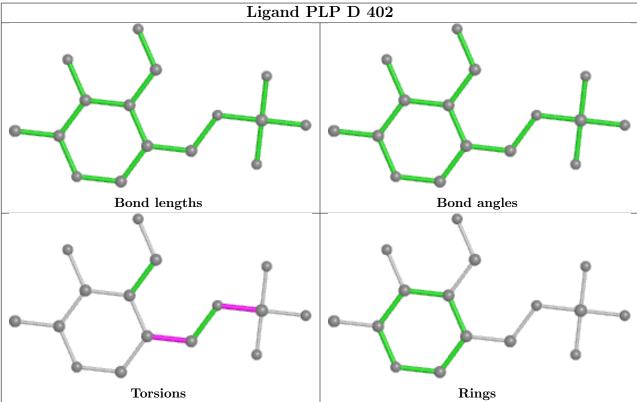












5.7 Other polymers (i)

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>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	353/361 (97%)	-0.28	5 (1%) 75 72	13, 20, 36, 73	0
1	В	350/361 (96%)	-0.31	4 (1%) 80 78	12, 20, 35, 70	0
1	С	347/361 (96%)	-0.23	8 (2%) 60 56	16, 25, 53, 84	0
1	D	351/361 (97%)	-0.18	10 (2%) 53 47	17, 27, 50, 76	0
All	All	1401/1444 (97%)	-0.25	27 (1%) 66 63	12, 22, 48, 84	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	LEU	7.7
1	A	352	ASN	4.4
1	A	23	LEU	4.0
1	С	1	MET	3.7
1	С	17	TYR	3.3

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)

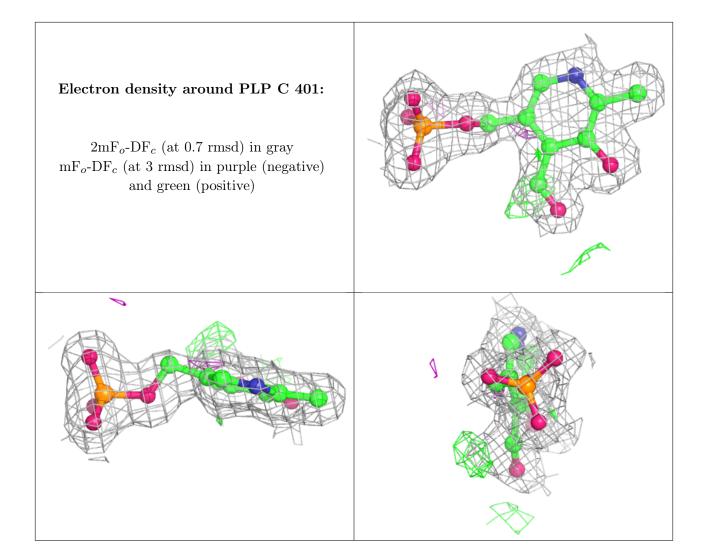
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



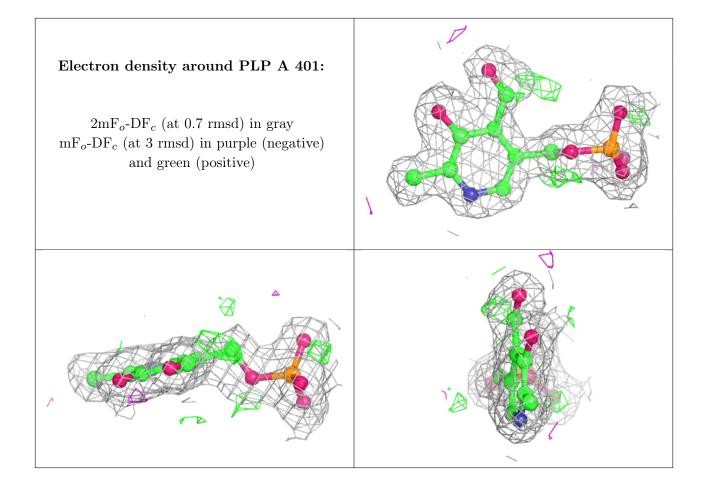
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
4	ACT	С	406	4/4	0.75	0.18	32,46,46,49	0
4	ACT	D	401	4/4	0.75	0.17	29,39,46,48	0
4	ACT	В	401	4/4	0.82	0.16	40,40,48,48	0
3	EDO	С	402	4/4	0.83	0.16	28,29,29,30	0
3	EDO	В	403	4/4	0.83	0.22	27,30,33,34	0
4	ACT	A	406	4/4	0.85	0.16	31,38,41,43	0
3	EDO	A	402	4/4	0.86	0.12	29,29,30,31	0
3	EDO	D	403	4/4	0.89	0.17	32,34,39,40	0
3	EDO	С	404	4/4	0.91	0.12	26,27,27,27	0
3	EDO	В	404	4/4	0.91	0.18	19,32,32,34	0
3	EDO	A	403	4/4	0.93	0.14	20,28,33,37	0
3	EDO	D	404	4/4	0.93	0.11	25,34,35,37	0
4	ACT	D	405	4/4	0.93	0.10	33,34,36,37	0
4	ACT	В	405	4/4	0.94	0.13	25,33,37,43	0
3	EDO	A	404	4/4	0.94	0.17	20,21,22,24	0
4	ACT	A	405	4/4	0.95	0.11	33,35,35,35	0
4	ACT	С	405	4/4	0.96	0.13	25,34,35,39	0
3	EDO	С	403	4/4	0.96	0.11	20,26,33,36	0
2	PLP	С	401	16/16	0.97	0.09	18,20,33,38	0
6	CA	С	407	1/1	0.97	0.09	32,32,32,32	0
2	PLP	A	401	16/16	0.98	0.11	14,19,31,32	0
2	PLP	D	402	16/16	0.98	0.10	18,21,32,37	0
2	PLP	В	402	16/16	0.98	0.09	15,18,31,36	0
5	CL	В	406	1/1	0.99	0.07	19,19,19,19	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.

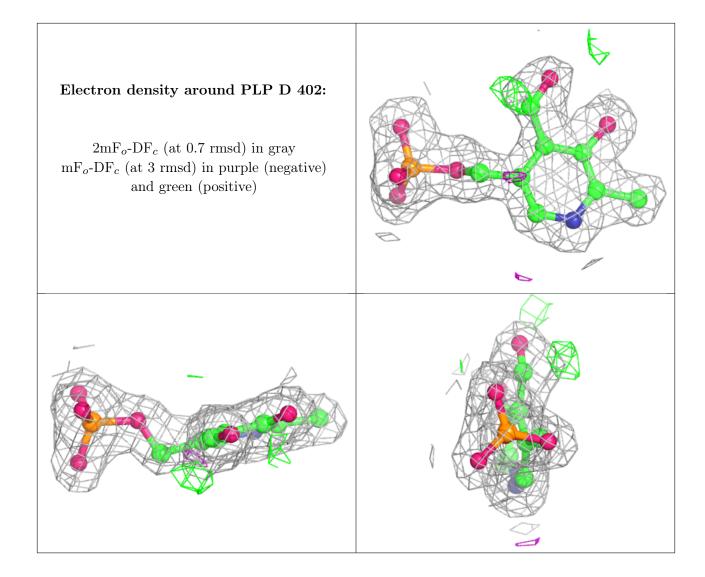




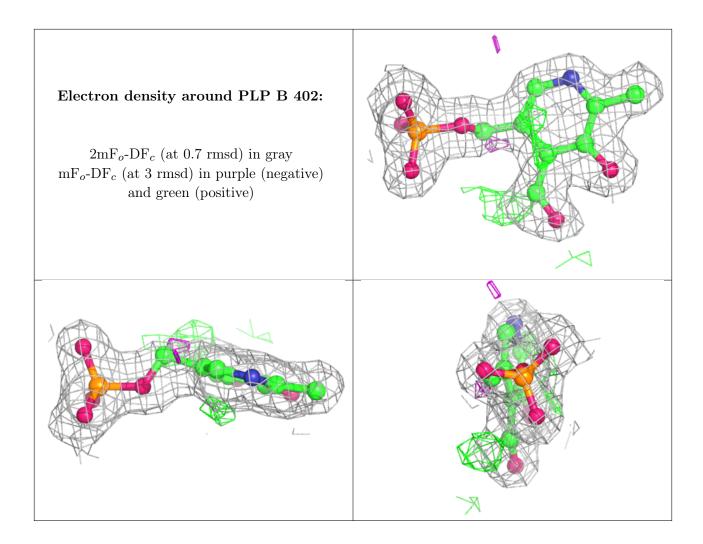












6.5 Other polymers (i)

There are no such residues in this entry.

