

# wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2022 – 06:06 pm BST

PDB ID : 7ZGS

Title: Crystal Structure of truncated aspartate transcarbamoylase from Plasmodium

falciparum with bound inhibitor 2-phenylethan-1-amine

Authors : Wang, C.; Zhang, B.

Deposited on : 2022-04-04

Resolution : 2.35 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.30

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)

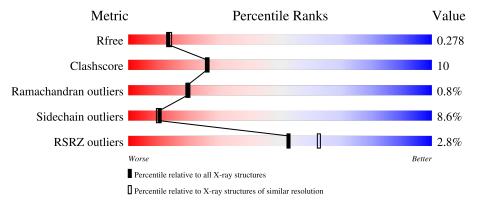
Validation Pipeline (wwPDB-VP) : 2.30

## 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 2.35 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	349	68%	21%	• 7%
1	В	349	75%	19%	5% •
1	С	349	67%	23%	• 5%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16400 atoms, of which 8183 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	Λ	324	Total	С	Н	N	О	S	83	0	0
1	A	324	5248	1674	2632	428	506	8	0.0	0	U
1	В	346	Total	С	Н	N	О	S	88	0	0
1	Б	340	5629	1801	2814	462	544	8	00	0	U
1	С	332	Total	С	Н	N	О	S	85	0	0
1		332	5384	1720	2698	441	517	8	00		0

There are 30 discrepancies between the modelled and reference sequences:

A         376         SER         -         expression tag         UNP A0A5R           A         377         ALA         -         expression tag         UNP A0A5R           A         378         TRP         -         expression tag         UNP A0A5R           A         379         SER         -         expression tag         UNP A0A5R           A         380         HIS         -         expression tag         UNP A0A5R           A         381         PRO         -         expression tag         UNP A0A5R           A         382         GLN         -         expression tag         UNP A0A5R           A         383         PHE         -         expression tag         UNP A0A5R           A         384         GLU         -         expression tag         UNP A0A5R           B         376         SER         -         expression tag         UNP A0A5R           B         377         ALA         -         expression tag         UNP A0A5R	nce
A         378         TRP         -         expression tag         UNP A0A5E           A         379         SER         -         expression tag         UNP A0A5E           A         380         HIS         -         expression tag         UNP A0A5E           A         381         PRO         -         expression tag         UNP A0A5E           A         382         GLN         -         expression tag         UNP A0A5E           A         383         PHE         -         expression tag         UNP A0A5E           A         384         GLU         -         expression tag         UNP A0A5E           A         385         LYS         -         expression tag         UNP A0A5E           B         376         SER         -         expression tag         UNP A0A5E           B         377         ALA         -         expression tag         UNP A0A5E	K1K910
A         379         SER         -         expression tag         UNP A0A5E           A         380         HIS         -         expression tag         UNP A0A5E           A         381         PRO         -         expression tag         UNP A0A5E           A         382         GLN         -         expression tag         UNP A0A5E           A         383         PHE         -         expression tag         UNP A0A5E           A         384         GLU         -         expression tag         UNP A0A5E           A         385         LYS         -         expression tag         UNP A0A5E           B         376         SER         -         expression tag         UNP A0A5E           B         377         ALA         -         expression tag         UNP A0A5E	K1K910
A         380         HIS         -         expression tag         UNP A0A5E           A         381         PRO         -         expression tag         UNP A0A5E           A         382         GLN         -         expression tag         UNP A0A5E           A         383         PHE         -         expression tag         UNP A0A5E           A         384         GLU         -         expression tag         UNP A0A5E           A         385         LYS         -         expression tag         UNP A0A5E           B         376         SER         -         expression tag         UNP A0A5E           B         377         ALA         -         expression tag         UNP A0A5E	K1K910
A         381         PRO         -         expression tag         UNP A0A5E           A         382         GLN         -         expression tag         UNP A0A5E           A         383         PHE         -         expression tag         UNP A0A5E           A         384         GLU         -         expression tag         UNP A0A5E           A         385         LYS         -         expression tag         UNP A0A5E           B         376         SER         -         expression tag         UNP A0A5E           B         377         ALA         -         expression tag         UNP A0A5E	K1K910
A         382         GLN         -         expression tag         UNP A0A5E           A         383         PHE         -         expression tag         UNP A0A5E           A         384         GLU         -         expression tag         UNP A0A5E           A         385         LYS         -         expression tag         UNP A0A5E           B         376         SER         -         expression tag         UNP A0A5E           B         377         ALA         -         expression tag         UNP A0A5E	K1K910
A         383         PHE         -         expression tag         UNP A0A5E           A         384         GLU         -         expression tag         UNP A0A5E           A         385         LYS         -         expression tag         UNP A0A5E           B         376         SER         -         expression tag         UNP A0A5E           B         377         ALA         -         expression tag         UNP A0A5E	K1K910
A         384         GLU         -         expression tag         UNP A0A5E           A         385         LYS         -         expression tag         UNP A0A5E           B         376         SER         -         expression tag         UNP A0A5E           B         377         ALA         -         expression tag         UNP A0A5E	K1K910
A 385 LYS - expression tag UNP A0A5E B 376 SER - expression tag UNP A0A5E B 377 ALA - expression tag UNP A0A5E	K1K910
B 376 SER - expression tag UNP A0A5E B 377 ALA - expression tag UNP A0A5E	K1K910
B 377 ALA - expression tag UNP A0A5H	K1K910
1 0	K1K910
D 970 IDD LIND AGARI	K1K910
B 378 TRP - expression tag UNP A0A5H	K1K910
B 379 SER - expression tag UNP A0A5H	K1K910
B 380 HIS - expression tag UNP A0A5H	K1K910
B 381 PRO - expression tag UNP A0A5H	K1K910
B 382 GLN - expression tag UNP A0A5H	K1K910
B 383 PHE - expression tag UNP A0A5H	K1K910
B 384 GLU - expression tag UNP A0A5H	K1K910
B 385 LYS - expression tag UNP A0A5H	K1K910
C 376 SER - expression tag UNP A0A5H	K1K910
C 377 ALA - expression tag UNP A0A5H	K1K910
C 378 TRP - expression tag UNP A0A5H	K1K910

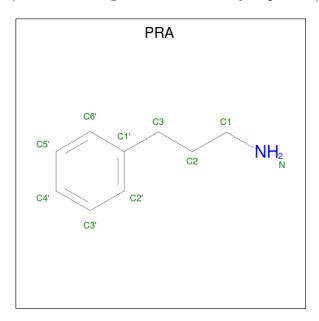
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Chain	Residue	Modelled	Actual	Comment	Reference
С	379	SER	-	expression tag	UNP A0A5K1K910
С	380	HIS	-	expression tag	UNP A0A5K1K910
С	381	PRO	-	expression tag	UNP A0A5K1K910
С	382	GLN	-	expression tag	UNP A0A5K1K910
С	383	PHE	-	expression tag	UNP A0A5K1K910
С	384	GLU	-	expression tag	UNP A0A5K1K910
С	385	LYS	-	expression tag	UNP A0A5K1K910

• Molecule 2 is 3-PHENYLPROPYLAMINE (three-letter code: PRA) (formula:  $C_9H_{13}N$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 23			N 1	0	0
2	В	1	Total 23				0	0
2	С	1	Total 23	C 9	H 13	N 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total O S 5 4 1	0	0
4	С	1	Total O S 5 4 1	0	0

## • Molecule 5 is water.

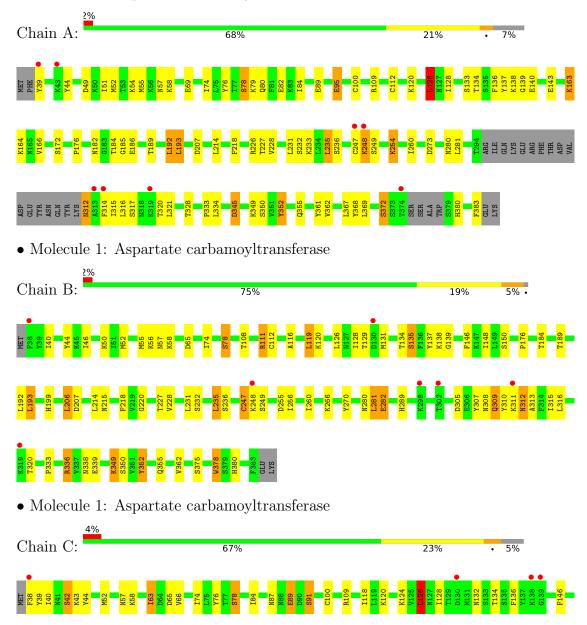
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	В	19	Total O 19 19	0	0
5	С	22	Total O 22 22	0	0



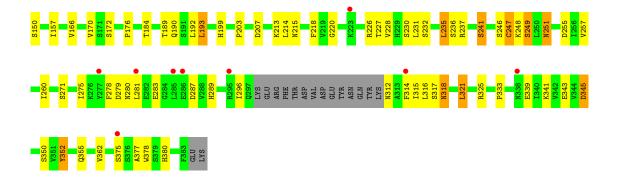
# 3 Residue-property plots (i)

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: Aspartate carbamoyltransferase









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	86.85Å 104.37Å 87.05Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $117.53^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	45.13 - 2.35	Depositor
rtesolution (A)	45.09 - 2.35	EDS
% Data completeness	98.3 (45.13-2.35)	Depositor
(in resolution range)	$95.0 \ (45.09 - 2.35)$	EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.71  (at  2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
$R, R_{free}$	0.217 , $0.272$	Depositor
it, it free	0.218 , $0.278$	DCC
$R_{free}$ test set	2651 reflections $(4.83\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.41, < L^2> = 0.23$	Xtriage
	0.064  for -h-l,k,h	
	0.064  for  l,k,-h-l	
Estimated twinning fraction	0.077  for h,-k,-h-l	Xtriage
	0.069  for -h-l,-k,l	
	0.216  for  l,-k,h	
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16400	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: SO4, PRA, NA

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		Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.78	$2/2664 \ (0.1\%)$	0.98	3/3598 (0.1%)	
1	В	0.78	0/2871	0.98	3/3880 (0.1%)	
1	С	0.77	$1/2738 \ (0.0\%)$	0.99	3/3700 (0.1%)	
All	All	0.78	3/8273 (0.0%)	0.98	9/11178 (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.

$\mathbf{Mol}$	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	С	91	SER	CB-OG	-5.78	1.34	1.42
1	A	143	GLU	CD-OE2	5.71	1.31	1.25
1	A	186	GLU	CD-OE2	5.04	1.31	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	345	ASP	CB-CA-C	9.47	129.34	110.40
1	В	349	LYS	CB-CA-C	9.45	129.31	110.40
1	С	345	ASP	CB-CA-C	7.82	126.03	110.40
1	С	91	SER	N-CA-CB	-6.87	100.19	110.50
1	В	111	ARG	NE-CZ-NH1	-6.29	117.15	120.30

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	375	SER	Peptide

#### 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	2616	2632	2623	54	2
1	В	2815	2814	2807	53	2
1	С	2686	2698	2690	67	0
2	A	10	13	14	4	0
2	В	10	13	14	2	0
2	С	10	13	14	1	0
3	A	1	0	0	0	0
4	С	10	0	0	0	0
5	A	18	0	0	1	0
5	В	19	0	0	0	0
5	С	22	0	0	2	0
All	All	8217	8183	8162	171	2

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 10.

The worst 5 of 171 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:C:109:ARG:HD2	5:C:512:HOH:O	1.66	0.93	
1:B:215:ASN:H	1:B:289:HIS:HD2	1.15	0.92	
1:C:215:ASN:H	1:C:289:HIS:HD2	1.15	0.91	
1:A:136:PHE:O	2:A:401:PRA:N	2.05	0.90	
1:A:281:LEU:HD23	1:A:320:THR:HG21	1.54	0.89	

All (2) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:254:LYS:NZ	1:B:270:TYR:O[1_554]	1.91	0.29
1:A:254:LYS:HZ1	1:B:270:TYR:O[1_554]	1.51	0.09

### 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	Percentiles
1	A	318/349 (91%)	302 (95%)	14 (4%)	2 (1%)	25 26
1	В	344/349 (99%)	321 (93%)	19 (6%)	4 (1%)	13 11
1	С	328/349 (94%)	305 (93%)	21 (6%)	2 (1%)	25 26
All	All	990/1047 (95%)	928 (94%)	54 (6%)	8 (1%)	19 20

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	LYS
1	A	248	LYS
1	В	138	LYS
1	В	248	LYS
1	С	247	CYS

#### 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	304/328 (93%)	274 (90%)	30 (10%)	8 6	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	В	325/328~(99%)	303 (93%)	22 (7%)	16	17	
1	С	311/328 (95%)	282 (91%)	29 (9%)	9	8	
All	All	940/984 (96%)	859 (91%)	81 (9%)	10	10	

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	87	ASN
1	С	255	ASP
1	С	126	LEU
1	С	214	LEU
1	С	317	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	243	ASN
1	С	323	ASN
1	С	289	HIS
1	В	258	ASN
1	С	199	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)

Of 6 ligands modelled in this entry, 1 is 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				
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PRA	A	401	-	10,10,10	0.17	0	11,11,11	0.26	0
2	PRA	С	401	-	10,10,10	0.33	0	11,11,11	0.25	0
4	SO4	С	403	-	4,4,4	0.36	0	6,6,6	0.25	0
2	PRA	В	401	-	10,10,10	0.22	0	11,11,11	0.29	0
4	SO4	С	402	-	4,4,4	0.32	0	6,6,6	0.28	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	PRA	С	401	-	-	1/4/4/4	0/1/1/1
2	PRA	A	401	-	-	3/4/4/4	0/1/1/1
2	PRA	В	401	-	-	2/4/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PRA	C1-C2-C3-C1'
2	С	401	PRA	C1-C2-C3-C1'
2	В	401	PRA	C1-C2-C3-C1'
2	A	401	PRA	C2'-C1'-C3-C2
2	В	401	PRA	N-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

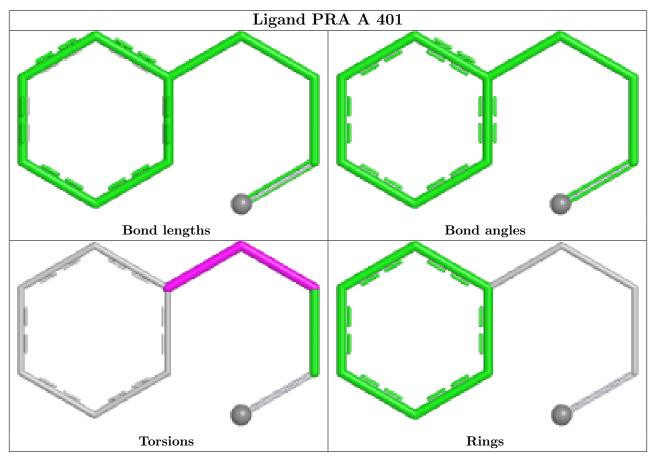
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PRA	4	0

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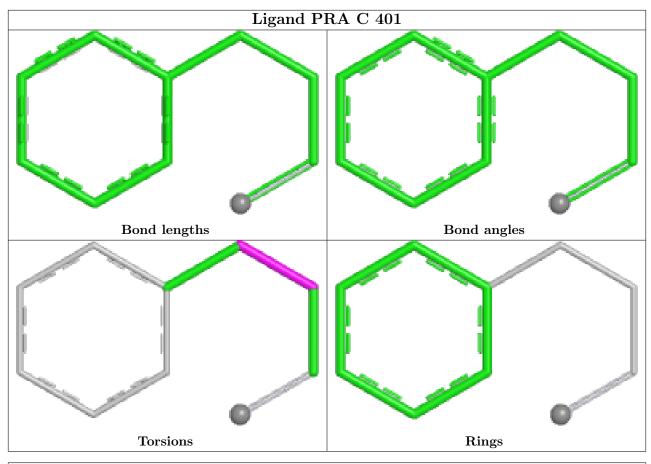
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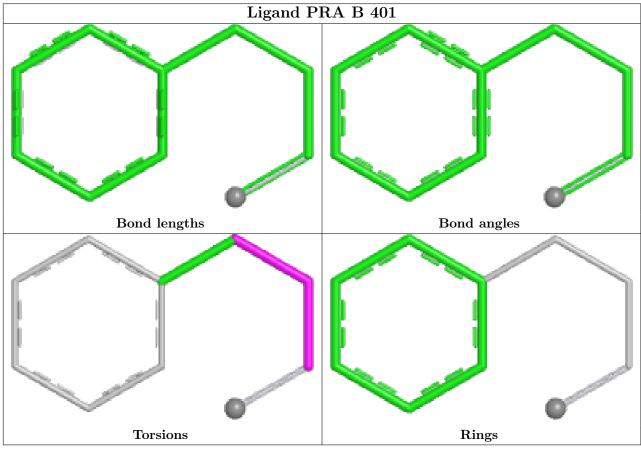
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	401	PRA	1	0
2	В	401	PRA	2	0

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	324/349 (92%)	0.34	8 (2%) 57 66	39, 60, 99, 121	0
1	В	346/349 (99%)	0.28	7 (2%) 65 74	36, 55, 99, 124	0
1	С	332/349 (95%)	0.39	13 (3%) 39 50	38, 65, 99, 122	0
All	All	1002/1047 (95%)	0.33	28 (2%) 53 63	36, 60, 99, 124	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	375	SER	4.5
1	С	130	ASP	4.0
1	В	130	ASP	3.6
1	С	38	PHE	3.4
1	В	248	LYS	3.2

### 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.

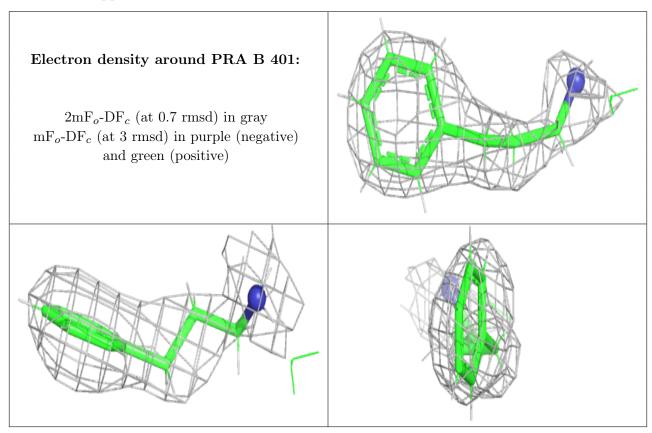
### 6.4 Ligands (i)

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
3	NA	A	402	1/1	0.86	0.26	53,53,53,53	0
2	PRA	В	401	10/10	0.87	0.27	71,79,93,94	0
2	PRA	С	401	10/10	0.88	0.43	73,80,92,93	0
2	PRA	A	401	10/10	0.90	0.22	63,70,87,90	0
4	SO4	С	402	5/5	0.98	0.13	50,51,64,73	0
4	SO4	С	403	5/5	0.99	0.11	48,51,54,57	0

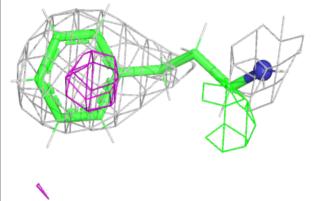
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

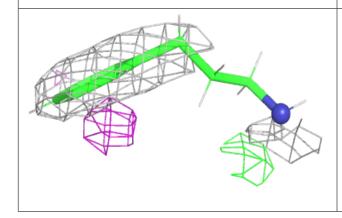


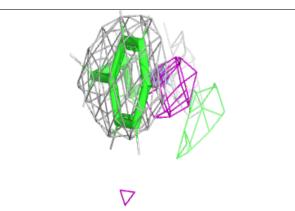


#### Electron density around PRA C 401:

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

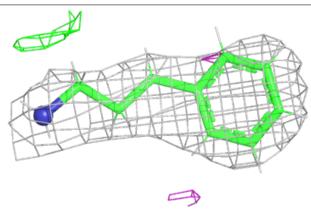


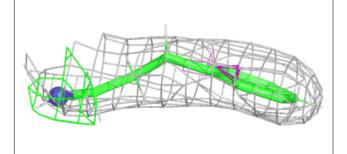


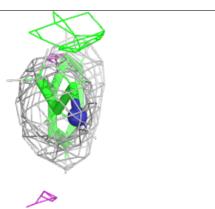


#### Electron density around PRA A 401:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (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.

