

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

#### May 26, 2025 – 04:59 PM EDT

PDB ID	:	$9\mathrm{NPJ} \ / \ \mathrm{pdb} \ 00009\mathrm{npj}$
Title	:	Structural studies of reaction hijacking inhibition of a malaria parasite
		aspartyl-tRNA synthetase.
Authors	:	Khandokar, Y.; Ketprasit, K.; Tai, C.W.; Xie, S.; Tilley, L.; Griffin, M.D.W.;
		Panjikar, S.
Deposited on	:	2025-03-11
Resolution	:	2.36  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.36 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.



Motria	Whole archive	Similar resolution
wietric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	164625	$1460 \ (2.36-2.36)$
Clashscore	180529	$1571 \ (2.36-2.36)$
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	А	536	4% 	15%	6%
1	В	536	7%	13%	8%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8389 atoms, of which 8 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–tRNA ligase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	504	Total 4058	C 2603	N 681	0 748	S 26	0	0	0
1	В	494	Total 3915	C 2512	N 649	0 728	S 26	5	0	0

• Molecule 2 is 9-(5-O-{[(1R,2R)-2-amino-3-carboxy-1-hydroxypropyl]sulfamoyl}-beta-D-lyxofuranosyl)-2-chloro-9H-purin-6-amine (CCD ID: A1B0L) (formula: C<sub>14</sub>H<sub>20</sub>ClN<sub>7</sub>O<sub>9</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	А	1	Total 32	C 14	Cl 1	N 7	0 9	S 1	0	0
2	В	1	Total 32	C 14	Cl 1	- N 7	0 9	S 1	0	0

• Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	Total         C         H         O           14         3         8         3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	158	Total O 158 158	0	0
4	В	174	Total O 174 174	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–tRNA ligase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	140.04Å 140.04Å 273.02Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Bosolution (Å)	48.88 - 2.36	Depositor
Resolution (A)	48.88 - 2.36	EDS
% Data completeness	99.7 (48.88-2.36)	Depositor
(in resolution range)	99.9 (48.88-2.36)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$< I/\sigma(I) > 1$	$1.96 (at 2.37 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
P. P.	0.188 , $0.215$	Depositor
$n, n_{free}$	0.189 , $0.214$	DCC
$R_{free}$ test set	63631 reflections $(3.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	50.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $43.3$	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8389	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.

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



<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: GOL,  $\rm A1B0L$ 

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.31	0/4147	0.47	0/5595	
1	В	0.35	0/4000	0.48	0/5404	
All	All	0.33	0/8147	0.48	0/10999	

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)	H(added)	Clashes	Symm-Clashes
1	А	4058	0	3940	63	0
1	В	3915	0	3737	63	0
2	А	32	0	0	0	0
2	В	32	0	0	1	0
3	А	6	0	8	2	0
3	В	6	8	8	0	0
4	А	158	0	0	1	0
4	В	174	0	0	4	0
All	All	8381	8	7693	112	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 7.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:289:THR:HG22	1:B:291:GLU:HG2	1.45	0.97
1:B:253:ILE:H	1:B:253:ILE:HD12	1.35	0.89
1:B:124:VAL:HG11	1:B:129:MET:HE2	1.53	0.89
1:B:201:ALA:HB3	1:B:216:LEU:HB3	1.56	0.88
1:B:209:LEU:HD11	1:B:452:THR:HG21	1.57	0.86
1:A:348:GLY:O	1:A:349:GLU:HG3	1.84	0.77
1:B:124:VAL:CG1	1:B:129:MET:HE2	2.15	0.76
1:B:295:ILE:HD12	1:B:295:ILE:O	1.87	0.74
1:A:287:LYS:HG2	1:A:288:GLU:H	1.54	0.72
1:B:630:ILE:HG13	1:B:631:PRO:HA	1.72	0.72
1:B:120:SER:HA	1:B:266:LYS:HG2	1.71	0.71
1:A:486:LEU:HD13	1:A:502:MET:HE3	1.76	0.67
1:A:287:LYS:HG2	1:A:288:GLU:N	2.13	0.64
1:A:209:LEU:O	3:A:702:GOL:H12	1.98	0.64
1:A:534:MET:HE3	1:A:535:TYR:O	1.98	0.62
1:B:289:THR:CG2	1:B:291:GLU:HG2	2.25	0.62
1:A:148:LEU:HD21	1:A:180:LEU:HD11	1.81	0.62
1:A:319:PHE:CD1	1:A:621:LEU:HD13	2.35	0.61
1:A:218:ILE:HG23	1:A:228:MET:HE2	1.82	0.61
1:A:359:GLN:HG2	1:A:368:PHE:CE1	2.36	0.61
1:A:97:GLU:HG2	1:A:99:GLU:H	1.66	0.60
1:A:490:GLU:HA	1:A:493:ILE:HD11	1.83	0.60
1:B:472:THR:OG1	1:B:475:GLU:HG3	2.02	0.60
1:A:360:ILE:CG2	1:B:360:ILE:HD13	2.33	0.59
1:A:565:VAL:HG21	1:A:590:ALA:HA	1.85	0.59
1:A:360:ILE:HG22	1:B:360:ILE:HD13	1.84	0.58
1:B:496:TYR:CE2	1:B:498:MET:HA	2.40	0.56
1:B:403:TYR:C	1:B:404:ARG:HD2	2.31	0.56
1:B:360:ILE:HG22	1:B:367:GLY:C	2.30	0.56
1:B:489:LYS:HE3	1:B:491:GLU:OE2	2.06	0.56
1:B:360:ILE:HD12	1:B:361:ASN:H	1.70	0.56
1:B:194:ILE:HG13	1:B:203:ILE:HG12	1.88	0.55
1:B:320:CYS:HB3	4:B:969:HOH:O	2.07	0.54
1:B:630:ILE:HA	1:B:631:PRO:C	2.33	0.54
1:B:253:ILE:H	1:B:253:ILE:CD1	2.10	0.53
1:A:474:GLU:CD	1:A:478:LYS:HZ1	2.17	0.53
1:A:340:GLU:HB2	1:A:389:PHE:CZ	2.44	0.52
1:A:522:ILE:HG22	1:A:546:TYR:HB3	1.91	0.52
1:A:148:LEU:HD13	1:A:260:TYR:CD2	2.44	0.52
1:A:556:LEU:C	1:A:556:LEU:HD23	2.35	0.52

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:625:ASP:HB2	1:A:626:PRO:CD	2.40	0.51	
1:B:556:LEU:C	1:B:556:LEU:HD23	2.35	0.50	
1:A:490:GLU:HA	1:A:493:ILE:CD1	2.42	0.50	
1:A:330:LYS:HD3	1:B:330:LYS:HZ2	1.77	0.49	
1:B:631:PRO:HD2	4:B:926:HOH:O	2.11	0.49	
1:A:359:GLN:O	1:B:360:ILE:CD1	2.61	0.49	
1:A:330:LYS:HZ2	1:B:330:LYS:HD3	1.78	0.49	
1:A:490:GLU:O	1:A:493:ILE:HD13	2.13	0.49	
1:A:330:LYS:HZ2	1:B:330:LYS:CD	2.25	0.49	
1:A:565:VAL:HG22	1:A:589:PHE:O	2.12	0.49	
1:B:572:ILE:HG23	1:B:577:LEU:HB2	1.95	0.49	
1:A:535:TYR:HA	1:A:543:SER:HA	1.95	0.49	
1:A:546:TYR:CE1	1:A:559:SER:HA	2.48	0.48	
1:A:631:PRO:OXT	1:B:376:TYR:OH	2.21	0.48	
1:B:119:GLU:O	1:B:120:SER:HB2	2.12	0.48	
1:A:591:TYR:HA	1:B:273:THR:HG23	1.95	0.48	
1:A:273:THR:HG23	1:B:591:TYR:HA	1.96	0.48	
1:B:195:ARG:HG2	1:B:195:ARG:O	2.13	0.47	
1:B:186:TRP:CE2	1:B:243:LYS:HD2	2.50	0.47	
1:B:625:ASP:HB2	1:B:626:PRO:CD	2.45	0.47	
1:A:330:LYS:NZ	1:B:340:GLU:OE1	2.43	0.46	
1:A:121:TYR:HA	1:A:267:ILE:O	2.15	0.46	
1:A:149:MET:CE	1:A:259:LYS:H	2.27	0.46	
1:A:348:GLY:HA2	1:B:629:LEU:HD21	1.98	0.46	
1:B:195:ARG:HG2	1:B:202:PHE:HB2	1.98	0.46	
1:B:536:LYS:NZ	4:B:813:HOH:O	2.48	0.45	
1:A:523:ASN:HA	1:A:543:SER:O	2.16	0.45	
1:A:131:GLU:OE2	1:A:243:LYS:NZ	2.39	0.45	
1:A:209:LEU:C	1:A:209:LEU:HD12	2.41	0.45	
1:B:105:ALA:O	1:B:108:VAL:HG12	2.16	0.45	
1:A:255:SER:O	3:A:702:GOL:H32	2.16	0.45	
1:A:496:TYR:CZ	1:A:498:MET:HA	2.52	0.45	
1:B:192:HIS:HB2	1:B:206:ARG:HB2	1.99	0.45	
1:A:115:ASP:OD1	1:A:117:ASN:HB2	2.18	0.44	
1:B:374:GLN:HG2	1:B:532:TYR:CE2	2.52	0.44	
1:A:556:LEU:HD23	1:A:557:SER:N	2.33	0.44	
1:B:209:LEU:CD1	1:B:452:THR:HG21	2.39	0.43	
1:A:297:VAL:HG12	1:A:302:ARG:HG3	1.99	0.43	
1:A:307:CYS:SG	1:B:379:MET:HB3	2.58	0.43	
1:B:360:ILE:HD12	1:B:361:ASN:N	2.33	0.43	
1:A:535:TYR:OH	1:A:567:LEU:HD22	2.18	0.43	

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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:535:TYR:HA	1:B:543:SER:HA	2.01	0.43
1:B:286:MET:CE	1:B:295:ILE:HG12	2.48	0.43
1:A:289:THR:O	1:A:296:LYS:NZ	2.48	0.43
1:A:348:GLY:HA2	1:B:629:LEU:CD2	2.49	0.43
1:A:207:HIS:HE1	4:A:872:HOH:O	2.02	0.42
1:A:565:VAL:CG2	1:A:589:PHE:O	2.67	0.42
1:A:109:LEU:CD2	1:A:229:LYS:HG2	2.49	0.42
1:A:356:ASN:ND2	1:A:398:GLU:HG2	2.34	0.42
1:A:218:ILE:CG2	1:A:228:MET:HE2	2.49	0.42
1:A:404:ARG:HD2	1:A:553:GLU:OE1	2.19	0.42
1:A:432:MET:O	1:A:436:ILE:HG13	2.19	0.42
1:B:338:PHE:CD2	1:B:387:ARG:HB3	2.55	0.42
1:A:465:LEU:HG	1:A:516:THR:HB	2.01	0.42
1:B:124:VAL:HG12	1:B:268:PHE:HB3	2.01	0.42
1:B:123:PHE:CD1	1:B:269:CYS:HB3	2.54	0.42
1:B:295:ILE:HD12	1:B:295:ILE:C	2.43	0.42
1:B:479:MET:HE1	1:B:510:VAL:HG22	2.02	0.42
1:B:404:ARG:HB3	1:B:605:ARG:HH12	1.85	0.41
1:A:124:VAL:HG11	1:A:129:MET:SD	2.59	0.41
1:A:489:LYS:O	1:A:493:ILE:HD12	2.20	0.41
1:A:572:ILE:HG23	1:A:577:LEU:HB2	2.01	0.41
1:B:205:LEU:O	1:B:211:SER:HA	2.19	0.41
1:B:320:CYS:SG	4:B:969:HOH:O	2.61	0.41
1:A:493:ILE:HD12	1:A:493:ILE:N	2.36	0.41
1:B:126:ILE:HD13	1:B:126:ILE:HA	1.91	0.41
1:B:186:TRP:CZ2	1:B:243:LYS:HD2	2.55	0.41
1:B:629:LEU:O	1:B:629:LEU:HG	2.21	0.41
1:B:352:GLU:OE2	2:B:701:A1B0L:N06	2.54	0.41
1:B:491:GLU:H	1:B:491:GLU:CD	2.29	0.41
1:A:205:LEU:O	1:A:211:SER:HA	2.20	0.41
1:A:379:MET:HB3	1:B:307:CYS:SG	2.62	0.40

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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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	498/536~(93%)	476 (96%)	22~(4%)	0	100 100
1	В	486/536~(91%)	466 (96%)	20 (4%)	0	100 100
All	All	984/1072~(92%)	942 (96%)	42 (4%)	0	100 100

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

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	А	439/485~(90%)	432~(98%)	7 (2%)	58 71
1	В	415/485~(86%)	412 (99%)	3 (1%)	81 89
All	All	854/970~(88%)	844 (99%)	10 (1%)	67 80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	251	VAL
1	А	372	SER
1	А	499	SER
1	А	500	THR
1	А	555	ILE
1	А	556	LEU
1	А	621	LEU
1	В	113	CYS
1	В	253	ILE
1	В	500	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	221	ASN
1	А	233	ASN
1	А	299	GLN
1	А	356	ASN
1	А	401	ASN
1	А	456	GLN
1	А	583	ASN
1	В	207	HIS
1	В	361	ASN
1	В	371	GLN
1	В	425	ASN
1	В	560	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)

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).

Mal	1 Trme Chain Bes Li		T in le	Bond lengths				Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	В	702	-	$5,\!5,\!5$	0.28	0	$5,\!5,\!5$	0.53	0
2	A1B0L	В	701	-	28,34,34	4.05	11 (39%)	$33,\!51,\!51$	3.10	11 (33%)
3	GOL	А	702	-	5,5,5	0.24	0	5,5,5	0.67	0



Mal	Tuno	Chain	Res Link	Link	B	ond leng	gths	E	ond ang	gles
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	A1B0L	А	701	-	28,34,34	4.03	11 (39%)	33,51,51	2.93	9 (27%)

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	GOL	В	702	-	-	0/4/4/4	-
2	A1B0L	В	701	-	-	5/17/39/39	0/3/3/3
3	GOL	А	702	-	-	3/4/4/4	-
2	A1B0L	А	701	-	-	5/17/39/39	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	701	A1B0L	O11-S10	10.69	1.51	1.42
2	В	701	A1B0L	O12-S10	10.05	1.51	1.42
2	А	701	A1B0L	O12-S10	9.99	1.51	1.42
2	В	701	A1B0L	O11-S10	9.58	1.50	1.42
2	В	701	A1B0L	S10-N09	9.36	1.71	1.59
2	А	701	A1B0L	S10-N09	8.11	1.69	1.59
2	А	701	A1B0L	O16-C17	-6.94	1.31	1.40
2	В	701	A1B0L	O16-C17	-6.68	1.32	1.40
2	В	701	A1B0L	C29-C15	-6.60	1.36	1.53
2	А	701	A1B0L	C29-C15	-6.21	1.37	1.53
2	В	701	A1B0L	O16-C15	-4.99	1.33	1.45
2	А	701	A1B0L	O16-C15	-4.67	1.34	1.45
2	А	701	A1B0L	O32-C31	-4.00	1.33	1.43
2	В	701	A1B0L	O32-C31	-3.71	1.33	1.43
2	В	701	A1B0L	C23-N22	3.61	1.33	1.30
2	А	701	A1B0L	O13-S10	3.28	1.66	1.60
2	А	701	A1B0L	C27-N28	2.87	1.44	1.34
2	В	701	A1B0L	C27-N28	2.75	1.43	1.34
2	В	701	A1B0L	O13-S10	2.75	1.65	1.60
2	А	701	A1B0L	C23-N22	2.54	1.32	1.30
2	А	701	A1B0L	O30-C29	2.38	1.48	1.43
2	В	701	A1B0L	O30-C29	2.03	1.48	1.43

All (20) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	701	A1B0L	O12-S10-O11	-10.93	104.48	120.85
2	А	701	A1B0L	O12-S10-O11	-10.15	105.65	120.85
2	А	701	A1B0L	N22-C23-N24	-8.14	122.51	130.58
2	В	701	A1B0L	N22-C23-N24	-7.88	122.76	130.58
2	В	701	A1B0L	C23-N22-C21	5.82	118.93	114.18
2	А	701	A1B0L	C23-N22-C21	5.73	118.86	114.18
2	В	701	A1B0L	CL25-C23-N22	4.68	119.59	115.72
2	В	701	A1B0L	C23-N24-C27	3.81	121.53	116.54
2	А	701	A1B0L	CL25-C23-N22	3.65	118.74	115.72
2	В	701	A1B0L	O13-S10-N09	3.63	114.96	105.62
2	А	701	A1B0L	C23-N24-C27	3.48	121.10	116.54
2	В	701	A1B0L	C15-O16-C17	3.15	112.81	109.92
2	А	701	A1B0L	O16-C15-C29	2.67	110.45	105.15
2	В	701	A1B0L	O16-C17-N18	2.66	112.27	108.75
2	А	701	A1B0L	CL25-C23-N24	2.55	118.75	115.17
2	В	701	A1B0L	O16-C15-C29	2.45	110.01	105.15
2	В	701	A1B0L	O13-S10-O11	2.27	112.33	105.48
2	А	701	A1B0L	O13-S10-N09	2.17	111.20	105.62
2	А	701	A1B0L	C15-O16-C17	2.08	111.83	109.92
2	В	701	A1B0L	C26-C27-N24	-2.07	118.40	120.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	701	A1B0L	C04-C05-C07-O08
2	А	701	A1B0L	N06-C05-C07-O08
2	А	701	A1B0L	C05-C07-N09-S10
2	А	701	A1B0L	C07-N09-S10-O12
2	А	701	A1B0L	C07-N09-S10-O13
2	В	701	A1B0L	C04-C05-C07-O08
2	В	701	A1B0L	N06-C05-C07-O08
2	В	701	A1B0L	C05-C07-N09-S10
2	В	701	A1B0L	C07-N09-S10-O12
2	В	701	A1B0L	C07-N09-S10-O13
3	А	702	GOL	C1-C2-C3-O3
3	A	702	GOL	O2-C2-C3-O3
3	А	702	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	701	A1B0L	1	0
3	А	702	GOL	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>2		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9	
1	А	504/536~(94%)	-0.03	22 (4%)	39	46	38, 53, 83, 119	0
1	В	493/536~(91%)	0.14	35 (7%)	23	27	35, 55, 104, 116	0
All	All	997/1072~(93%)	0.05	57 (5%)	30	35	35, 54, 99, 119	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	350	SER	5.6
1	В	179	HIS	4.9
1	В	223	ASN	4.9
1	В	116	ILE	4.3
1	А	100	ASN	4.3
1	В	135	GLU	4.2
1	В	222	ASP	4.2
1	В	218	ILE	4.1
1	В	198	GLY	4.1
1	А	219	LYS	3.7
1	В	290	ASN	3.7
1	В	254	ASP	3.7
1	В	224	ASP	3.5
1	В	295	ILE	3.5
1	В	180	LEU	3.4
1	В	226	ASN	3.4
1	В	130	LYS	3.4
1	В	181	LEU	3.4
1	А	220	HIS	3.3
1	A	288	GLU	3.3
1	A	98	ARG	3.3
1	А	490	GLU	3.2
1	A	290	ASN	3.2
1	В	253	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	А	353	GLY	3.1
1	В	353	GLY	3.1
1	А	179	HIS	3.1
1	В	250	GLU	3.0
1	А	101	LEU	3.0
1	В	246	LEU	3.0
1	В	307	CYS	2.9
1	А	222	ASP	2.9
1	А	223	ASN	2.9
1	В	131	GLU	2.8
1	А	491	GLU	2.8
1	В	215	ILE	2.8
1	В	104	GLU	2.8
1	А	292	GLU	2.7
1	В	128	LYS	2.7
1	В	251	VAL	2.7
1	В	200	LEU	2.6
1	В	196	SER	2.5
1	В	182	GLN	2.4
1	А	494	LEU	2.4
1	А	349	GLU	2.3
1	В	630	ILE	2.3
1	В	487	HIS	2.3
1	А	99	GLU	2.3
1	В	261	GLU	2.2
1	В	255	SER	2.2
1	В	399	ASN	2.2
1	A	289	THR	2.2
1	A	489	LYS	2.1
1	В	114	GLU	2.1
1	А	295	ILE	2.1
1	А	291	GLU	2.0
1	В	185	ILE	2.0

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#### 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	GOL	В	702	6/6	0.63	0.16	77,94,100,113	0
3	GOL	А	702	6/6	0.88	0.11	$61,\!63,\!63,\!70$	0
2	A1B0L	А	701	32/32	0.93	0.08	41,45,47,64	0
2	A1B0L	В	701	32/32	0.95	0.08	39,43,47,65	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.

