

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

#### Nov 22, 2023 – 07:53 PM JST

PDB ID	:	7YSE
Title	:	Crystal structure of E. coli heterotetrameric GlyRS in complex with tRNA
Authors	:	Han, L.; Ju, Y.; Zhou, H.
Deposited on	:	2022-08-12
Resolution	:	2.91  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 (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
$\mathrm{EDS}$	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	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)	:	2.36

#### Overall quality at a glance (i) 1

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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.



Percentile relative to X-ray structures of similar resolution	on
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Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	303	% 91%	5	3% •
1	В	303	93%		5%•
2	С	697	% 	6%	8%
2	D	697	80%	11% •	8%



Mol	Chain	Length		Quality of chain		
3	Е	76	6	7%	30%	•
3	F	76	33%	42%	9%	16%



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17368 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	208	Total	С	Ν	0	$\mathbf{S}$	0	0	0
1	Л	290	2386	1531	395	448	12	0	0	0
1	р	200	Total	С	Ν	0	S	0	0	0
1	D	299	2385	1528	394	451	12	0	0	0

• Molecule 1 is a protein called Glycine–tRNA ligase alpha subunit.

• Molecule 2 is a protein called Glycine–tRNA ligase beta subunit.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	C	641	Total	С	Ν	0	$\mathbf{S}$	0	0	0
		041	4941	3134	856	934	17	0	0	
0	Л	642	Total	С	Ν	0	S	0	0	0
		043	4628	2908	818	887	15	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	690	LEU	-	expression tag	UNP P00961
С	691	GLU	-	expression tag	UNP P00961
С	692	HIS	-	expression tag	UNP P00961
С	693	HIS	-	expression tag	UNP P00961
С	694	HIS	-	expression tag	UNP P00961
С	695	HIS	-	expression tag	UNP P00961
С	696	HIS	-	expression tag	UNP P00961
С	697	HIS	-	expression tag	UNP P00961
D	690	LEU	-	expression tag	UNP P00961
D	691	GLU	-	expression tag	UNP P00961
D	692	HIS	-	expression tag	UNP P00961
D	693	HIS	-	expression tag	UNP P00961
D	694	HIS	-	expression tag	UNP P00961
D	695	HIS	-	expression tag	UNP P00961
D	696	HIS	-	expression tag	UNP P00961
D	697	HIS	-	expression tag	UNP P00961





Mol	Chain	Residues		At	toms			ZeroOcc	AltConf	Trace
9	Б	76	Total	С	Ν	0	Р	0	0	0
5	Ľ	70	1608	714	285	533	76	0	0	0
2	Б	64	Total	С	Ν	0	Р	0	0	0
ა	ЭГ	04	1344	594	242	444	64	0	0	0

 $\bullet\,$  Molecule 3 is a RNA chain called RNA (76-MER).

• Molecule 4 is [(2R,3S,4R,5R)-5-(6-azanyl-2-chloranyl-purin-9-yl)-3,4-bis(oxidanyl) oxolan-2-yl]methyl N-(2-azanylethanoyl)sulfamate (three-letter code: JPO) (formula: C<sub>12</sub>H<sub>16</sub>ClN<sub>7</sub>O<sub>7</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		A	tom	IS			ZeroOcc	AltConf
4	Δ	1	Total	С	Cl	Ν	0	$\mathbf{S}$	0	0
4	4 A	1	28	12	1	7	7	1	0	0
4	р	1	Total	С	Cl	Ν	0	S	0	0
4	4 B	L	28	12	1	7	7	1	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Mg 1 1	0	0
5	В	1	Total Mg 1 1	0	0
5	С	2	Total Mg 2 2	0	0
5	D	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	1	Total Mg 1 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	2	Total O 2 2	0	0
6	С	5	Total O 5 5	0	0
6	D	3	Total O 3 3	0	0
6	Ε	4	$\begin{array}{cc} \text{Total} & \text{O} \\ 4 & 4 \end{array}$	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.



 $\bullet$  Molecule 1: Glycine–tRNA ligase alpha subunit







S686 L687 L687 GLN GLN HIS HIS HIS HIS HIS HIS

• Molecule 3: RNA (76-MER)







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants	72.71Å 162.12Å 324.09Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	50.01 - 2.91	Depositor
Resolution (A)	162.12 - 2.91	EDS
% Data completeness	99.9 (50.01-2.91)	Depositor
(in resolution range)	99.9(162.12-2.91)	EDS
R <sub>merge</sub>	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.20 (at 2.91 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
B B.	0.230 , $0.260$	Depositor
II, II, <i>free</i>	0.234 , $0.263$	DCC
$R_{free}$ test set	4395 reflections $(5.15%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	72.2	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $54.2$	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	17368	wwPDB-VP
Average B, all atoms $(Å^2)$	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.97% 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: JPO, MG

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
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.64	0/2450	0.73	0/3337
1	В	0.64	0/2449	0.73	0/3339
2	С	0.65	0/5027	0.75	0/6824
2	D	0.69	0/4705	0.77	0/6419
3	Е	0.39	0/1795	0.68	0/2796
3	F	0.29	0/1498	0.69	0/2328
All	All	0.62	0/17924	0.74	0/25043

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	2386	0	2284	12	0
1	В	2385	0	2264	8	0
2	С	4941	0	4889	22	0
2	D	4628	0	4250	50	0
3	Е	1608	0	814	7	0
3	F	1344	0	682	18	0
4	А	28	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	28	0	0	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
5	С	2	0	0	0	0
5	D	1	0	0	0	0
5	Ε	1	0	0	0	0
6	А	2	0	0	0	0
6	С	5	0	0	0	0
6	D	3	0	0	0	0
6	Е	4	0	0	0	0
All	All	17368	0	15183	106	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 3.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ( m \AA)$	overlap (Å)
2:D:634:TYR:HD1	2:D:682:VAL:HG22	1.17	1.08
2:D:634:TYR:CD1	2:D:682:VAL:HG22	2.04	0.92
2:D:629:PHE:HE1	2:D:682:VAL:HG23	1.52	0.74
2:D:414:MET:CB	2:D:431:ASN:HD21	2.10	0.65
2:D:659:VAL:HG21	2:D:664:LEU:HB2	1.80	0.64
2:D:545:THR:HG22	2:D:564:MET:SD	2.39	0.63
2:C:658:MET:HE3	2:C:669:LEU:HD21	1.85	0.59
2:D:17:PRO:O	2:D:253:SER:HB2	2.02	0.59
1:B:242:LEU:HB2	1:B:243:PRO:HD3	1.86	0.57
3:F:44:G:H2'	3:F:45:G:O4'	2.05	0.56
1:A:242:LEU:HB2	1:A:243:PRO:HD3	1.88	0.56
2:D:629:PHE:CE1	2:D:682:VAL:HG23	2.37	0.55
2:D:406:THR:HG21	3:F:74:C:H2'	1.89	0.55
2:D:629:PHE:HE1	2:D:682:VAL:CG2	2.18	0.54
2:D:531:ARG:NH1	3:F:70:C:OP2	2.41	0.54
2:D:366:ASP:OD1	2:D:367:ARG:N	2.41	0.53
2:D:585:ARG:HA	3:F:37:A:O5'	2.08	0.53
2:D:601:VAL:HG21	2:D:671:MET:HG2	1.91	0.53
3:F:43:G:H2'	3:F:44:G:C8	2.44	0.53
1:B:126:LEU:HA	1:B:280:THR:HG21	1.90	0.53
2:C:233:ALA:HB1	2:C:262:THR:CG2	2.38	0.53
3:F:67:U:H2'	3:F:68:C:C6	2.44	0.53
2:D:324:ARG:HB2	2:D:325:PRO:HD3	1.91	0.52



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:458:MET:HE1	2:C:487:VAL:HG11	1.91	0.52	
2:C:396:ASP:OD1	2:C:409:GLN:O	2.27	0.52	
2:D:264:LYS:HA	2:D:300:ASN:HA	1.92	0.52	
1:A:126:LEU:HA	1:A:280:THR:HG21	1.92	0.52	
2:D:545:THR:HG23	2:D:567:VAL:HB	1.90	0.52	
3:F:51:G:H2'	3:F:51:G:N3	2.25	0.51	
2:D:613:LYS:O	2:D:617:GLN:HG2	2.10	0.51	
2:D:601:VAL:HG21	2:D:671:MET:CG	2.40	0.51	
2:C:481:ARG:HD2	3:E:71:G:OP2	2.11	0.51	
2:D:50:ALA:HB1	2:D:256:GLU:HG2	1.94	0.50	
2:C:517:ASN:O	2:C:520:VAL:HG23	2.11	0.50	
2:D:636:ASP:O	2:D:640:GLU:HG2	2.12	0.50	
2:D:346:LEU:N	2:D:347:PRO:HD2	2.28	0.49	
3:E:33:U:H4'	3:E:34:G:OP1	2.12	0.49	
1:A:134:GLU:HB2	1:A:141:GLU:HG3	1.96	0.48	
2:C:626:GLU:HB3	2:C:627:PRO:HD3	1.95	0.48	
2:D:53:ARG:NH1	2:D:256:GLU:OE2	2.47	0.48	
2:D:548:ALA:HB1	2:D:683:ALA:HB1	1.95	0.48	
1:A:215:ASP:OD1	1:A:218:PHE:HB2	2.15	0.47	
2:D:612:ILE:O	2:D:616:MET:HG3	2.14	0.47	
3:F:51:G:O2'	3:F:52:A:OP2	2.31	0.47	
2:C:585:ARG:HG3	3:E:36:C:O2	2.15	0.47	
2:C:553:ARG:N	2:C:554:PRO:HD3	2.30	0.47	
2:D:553:ARG:O	2:D:555:THR:N	2.48	0.46	
2:D:27:PHE:HB2	2:D:142:LEU:HD21	1.98	0.46	
2:C:26:SER:OG	2:C:143:PRO:HD3	2.16	0.45	
2:C:277:LEU:HD23	2:C:327:LEU:HD22	1.97	0.45	
2:C:524:VAL:O	2:C:528:MET:HG3	2.16	0.45	
2:D:458:MET:HE1	2:D:487:VAL:HG21	1.98	0.45	
2:D:543:VAL:HG11	3:F:12:U:H5'	1.99	0.45	
3:F:65:U:H2'	3:F:66:U:C6	2.51	0.45	
1:A:63:ARG:NH2	1:B:246:GLU:OE2	2.50	0.45	
2:D:616:MET:HB2	2:D:617:GLN:HE21	1.81	0.45	
3:F:68:C:H2'	3:F:69:C:C6	2.51	0.45	
1:B:206:GLN:O	1:B:210:ASN:ND2	2.49	0.45	
2:C:571:ARG:HD3	2:C:688:LEU:HD13	1.97	0.45	
2:D:606:LEU:HD23	2:D:667:ASN:HD21	1.81	0.45	
1:A:202:ASN:O	1:A:206:GLN:HB2	2.17	0.44	
2:D:11:GLY:HA3	2:D:163:THR:HB	1.99	0.44	
1:A:91:PRO:HD2	1:A:94:ILE:HD12	1.98	0.44	
2:D:656:MET:O	2:D:659:VAL:HG13	2.18	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:F:62:U:H2'	3:F:63:C:C6	2.52	0.44	
2:D:49:ALA:O	2:D:222:ARG:NH2	2.48	0.44	
2:D:53:ARG:NH2	2:D:187:ARG:O	2.51	0.44	
3:F:28:G:N2	3:F:43:G:C4	2.86	0.44	
1:A:117:VAL:HG21	1:A:136:TRP:CD2	2.53	0.43	
2:C:346:LEU:N	2:C:347:PRO:CD	2.81	0.43	
2:C:324:ARG:HB3	2:C:325:PRO:HD3	1.99	0.43	
1:A:64:ARG:NH2	4:A:401:JPO:O1	2.50	0.43	
1:B:135:VAL:HB	1:B:143:THR:HB	2.00	0.43	
2:D:563:ARG:O	2:D:567:VAL:HG23	2.19	0.43	
3:E:30:C:H2'	3:E:31:C:O4'	2.19	0.43	
2:C:210:ARG:NH2	2:C:221:GLU:OE2	2.51	0.42	
2:C:526:ASP:OD1	2:C:553:ARG:NH1	2.51	0.42	
2:D:453:ALA:O	2:D:457:LYS:HG3	2.20	0.42	
2:D:552:ARG:O	2:D:553:ARG:C	2.58	0.42	
2:C:8:VAL:HA	2:C:165:THR:O	2.20	0.42	
2:D:543:VAL:HG11	3:F:12:U:C5'	2.50	0.42	
1:B:64:ARG:NH1	3:F:76:A:C8	2.87	0.42	
2:D:634:TYR:HD1	2:D:682:VAL:CG2	2.07	0.42	
3:F:44:G:C6	3:F:45:G:C5	3.08	0.42	
2:D:414:MET:CB	2:D:431:ASN:ND2	2.80	0.41	
2:D:57:LYS:NZ	2:D:205:TYR:O	2.53	0.41	
2:D:374:TRP:CZ2	2:D:502:THR:HB	2.55	0.41	
1:A:76:ARG:C	1:A:77:LEU:HD12	2.41	0.41	
3:E:10:G:H2'	3:E:10:G:N3	2.34	0.41	
1:A:115:ARG:HD3	2:C:306:ASN:HB2	2.02	0.41	
1:B:169:ARG:O	1:B:172:MET:HB2	2.20	0.41	
2:C:233:ALA:HB1	2:C:262:THR:HG21	2.01	0.41	
2:D:278:VAL:O	2:D:282:LYS:N	2.52	0.41	
2:D:437:ARG:O	2:D:482:ARG:HD3	2.20	0.41	
3:F:52:A:H2'	3:F:53:G:O4'	2.21	0.41	
1:A:118:GLU:OE2	2:C:159:ARG:NH2	2.53	0.40	
2:D:381:ALA:O	2:D:382:ASP:C	2.59	0.40	
3:E:64:G:H2'	3:E:65:U:O4'	2.20	0.40	
3:F:36:C:H2'	3:F:37:A:C5	2.56	0.40	
2:D:626:GLU:N	2:D:627:PRO:HD2	2.37	0.40	
3:E:62:U:H2'	3:E:63:C:H6	1.86	0.40	
2:C:47:TRP:HA	2:C:56:LEU:HD23	2.03	0.40	
2:D:184:ARG:O	2:D:198:THR:HA	2.21	0.40	
2:D:374:TRP:HZ2	2:D:502:THR:HB	1.87	0.40	
1:B:83:PHE:HB2	1:B:167:LEU:HD21	2.04	0.40	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:616:MET:HB2	2:D:617:GLN:NE2	2.37	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	А	296/303~(98%)	288 (97%)	8 (3%)	0	100	100
1	В	297/303~(98%)	285~(96%)	12 (4%)	0	100	100
2	С	637/697~(91%)	618 (97%)	18 (3%)	1 (0%)	47	78
2	D	639/697~(92%)	561 (88%)	71 (11%)	7 (1%)	14	42
All	All	1869/2000~(94%)	1752 (94%)	109 (6%)	8 (0%)	34	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
2	D	382	ASP
2	С	409	GLN
2	D	409	GLN
2	D	439	ALA
2	D	544	ASP
2	D	553	ARG
2	D	682	VAL
2	D	618	VAL

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Rotameric	Outliers	F	Perce	ntiles
1	А	250/261~(96%)	247~(99%)	3~(1%)		71	91
1	В	249/261~(95%)	247~(99%)	2(1%)		81	94
2	С	506/574~(88%)	500 (99%)	6 (1%)		71	91
2	D	417/574~(73%)	395~(95%)	22~(5%)		22	54
All	All	1422/1670~(85%)	1389 (98%)	33 (2%)		50	80

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

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	69	ARG
1	А	145	PHE
1	А	278	THR
1	В	145	PHE
1	В	247	ARG
2	С	34	GLU
2	С	65	GLN
2	С	348	ARG
2	С	406	THR
2	С	645	ARG
2	С	656	MET
2	D	3	GLU
2	D	210	ARG
2	D	219	TYR
2	D	237	ILE
2	D	248	LEU
2	D	255	VAL
2	D	261	LEU
2	D	268	LYS
2	D	314	GLN
2	D	326	ARG
2	D	406	THR
2	D	531	ARG
2	D	532	PHE
2	D	535	TRP
2	D	552	ARG
2	D	560	PHE
2	D	579	LEU
2	D	601	VAL
2	D	613	LYS



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Mol	Chain	Res	Type
2	D	624	LYS
2	D	636	ASP
2	D	640	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such side chains are listed below:

Mol	Chain	Res	Type
1	А	202	ASN
1	А	206	GLN
1	В	75	ASN
1	В	123	ASN
2	С	285	GLN
2	С	319	ASN
2	D	240	ASN
2	D	431	ASN
2	D	435	GLN
2	D	617	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	Ε	75/76~(98%)	16 (21%)	1 (1%)
3	F	60/76~(78%)	26 (43%)	0
All	All	135/152~(88%)	42 (31%)	1 (0%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	Е	14	А
3	Е	16	U
3	Е	17	U
3	Е	18	G
3	Е	19	G
3	Е	20	U
3	Е	21	А
3	Ε	22	G
3	Е	32	U
3	Е	33	U
3	E	34	G
3	Е	45	G



Mol	Chain	Res	Type
3	Е	46	G
3	Е	47	U
3	Е	48	С
3	Е	75	С
3	F	9	А
3	F	10	G
3	F	13	C
3	F	14	А
3	F	15	G
3	F	19	G
3	F	20	U
3	F	21	A
3	F	22	G
3	$\mathbf{F}$	24	G
3	F	28	G
3	F	37	А
3	F	38	А
3	F	39	G
3	F	40	G
3	F	41	U
3	F	42	С
3	F	43	G
3	F	45	G
3	F	52	A
3	F	53	G
3	F	57	G
3	F	59	G
3	F	60	U
3	F	74	С
3	F	75	С

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All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	Ε	46	G

#### 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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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 Trupa		Chain	Chain	Chain	Chain	Chain	Chain	Dec	Dea Link	Bo	Bond lengths			Bond angles		
INIOI	туре	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2						
4	JPO	А	401	-	26,30,30	0.86	1 (3%)	29,45,45	1.32	4 (13%)						
4	JPO	В	401	-	26,30,30	0.83	1 (3%)	29,45,45	1.35	4 (13%)						

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
4	JPO	А	401	-	-	4/12/33/33	0/3/3/3
4	JPO	В	401	-	-	6/12/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(\text{\AA})$	Ideal(Å)
4	А	401	JPO	C8-N6	3.13	1.32	1.30
4	В	401	JPO	C8-N6	2.92	1.32	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	401	JPO	C8-N6-C9	-4.21	110.76	114.09
4	В	401	JPO	C8-N6-C9	-4.09	110.86	114.09
4	В	401	JPO	C1-N1-S	3.31	129.67	124.30
4	В	401	JPO	C6-C7-N5	-3.29	118.85	121.01



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
4	А	401	JPO	C1-N1-S	3.25	129.56	124.30
4	А	401	JPO	C6-C7-N5	-3.20	118.91	121.01
4	А	401	JPO	C6-C7-N4	2.30	123.85	120.35
4	В	401	JPO	C6-C7-N4	2.29	123.83	120.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	401	JPO	O3-C2-C3-C11
4	А	401	JPO	C1-N1-S-O2
4	В	401	JPO	N-C-C1-N1
4	В	401	JPO	O3-C2-C3-C11
4	В	401	JPO	C1-N1-S-O1
4	В	401	JPO	C1-N1-S-O2
4	А	401	JPO	O3-C2-C3-O4
4	В	401	JPO	N-C-C1-O
4	В	401	JPO	O3-C2-C3-O4
4	А	401	JPO	C1-N1-S-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	401	JPO	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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	298/303~(98%)	0.61	4 (1%) 77 77	45, 61, 89, 118	0
1	В	299/303~(98%)	0.58	14 (4%) 31 28	53, 75, 100, 119	0
2	С	641/697~(91%)	0.48	7 (1%) 80 80	45, 65, 88, 143	0
2	D	643/697~(92%)	0.67	72 (11%) 5 4	74, 115, 146, 163	0
3	Е	76/76~(100%)	0.66	0 100 100	43, 76, 147, 168	0
3	F	64/76~(84%)	1.06	9 (14%) 2 2	74, 135, 182, 198	0
All	All	2021/2152~(93%)	0.60	106 (5%) 27 23	43, 76, 141, 198	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	611	GLU	4.9
2	D	605	THR	4.4
2	D	487	VAL	4.4
2	D	614	LEU	4.4
2	D	375	ILE	4.2
3	F	59	G	4.0
2	D	465	PHE	3.9
3	F	9	А	3.7
2	D	450	CYS	3.7
2	D	615	ALA	3.6
2	D	433	GLN	3.6
2	D	606	LEU	3.5
2	D	508	VAL	3.5
2	D	402	VAL	3.4
3	F	8	U	3.4
3	F	60	U	3.3
2	D	371	LEU	3.3
2	D	548	ALA	3.3
2	D	469	GLN	3.3



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Mol	Chain	Res	Type	RSRZ				
2	D	570	PHE	3.2				
1	В	137	LEU	3.2				
2	D	589	ILE	3.2				
2	D	457	LYS	3.1				
2	D	651	PHE	3.1				
2	D	634	TYR	3.0				
2	D	461	LEU	3.0				
1	А	195	TYR	2.9				
2	D	686	SER	2.9				
2	D	168	LEU	2.9				
2	D	167	LEU	2.9				
1	В	12	LEU	2.9				
1	А	185	TRP	2.8				
2	D	607	LYS	2.7				
1	В	126	LEU	2.7				
2	D	395	CYS	2.7				
1	В	75	ASN	2.7				
2	С	147	LEU	2.6				
2	D	280	THR	2.6				
2	D	527	PHE	2.6				
2	D	4	LYS	2.6				
2	D	138	SER	2.6				
3	F	21	А	2.5				
2	D	200	ASP	2.5				
2	D	368	ILE	2.5				
2	D	532	PHE	2.5				
2	С	54	LEU	2.5				
2	D	144	ILE	2.5				
1	А	99	LEU	2.4				
2	D	557	PRO	2.4				
2	D	602	ASN	2.4				
2	D	566	ALA	2.4				
2	D	685	ILE	2.4				
1	В	45	CYS	2.4				
2	D	265	PHE	2.4				
1	В	131	LEU	2.4				
2	D	232	GLU	2.4				
2	D	302	ILE	2.4				
3	F	27	С	2.4				
2	D	604	SER	2.3				
2	С	372	ALA	2.3				
1	В	129	TRP	2.3				



Mol	Chain	Res	Type	RSRZ
2	D	641	LEU	2.3
2	D	158	VAL	2.3
1	В	170	LEU	2.3
2	D	453	ALA	2.3
1	В	145	PHE	2.3
2	С	402	VAL	2.3
2	D	139	LEU	2.2
2	D	408	THR	2.2
2	D	564	MET	2.2
2	D	666	ILE	2.2
3	F	58	А	2.2
2	D	687	LEU	2.2
2	D	618	VAL	2.2
2	D	54	LEU	2.2
2	D	510	LEU	2.2
2	D	334	PHE	2.2
2	D	648	VAL	2.2
2	D	372	ALA	2.2
2	D	45	VAL	2.2
2	D	536	TYR	2.2
2	D	389	ALA	2.1
2	D	156	HIS	2.1
2	D	642	ALA	2.1
2	D	149	ARG	2.1
2	D	452	LEU	2.1
2	D	577	ALA	2.1
2	D	398	MET	2.1
1	В	180	VAL	2.1
2	С	549	VAL	2.1
2	D	199	ILE	2.1
1	В	254	SER	2.1
2	C	658	MET	2.1
3	F	44	G	2.1
2	С	576	ALA	2.1
2	D	234	ALA	2.1
2	D	58	VAL	2.1
2	D	480	LEU	2.0
2	D	492	VAL	2.0
1	В	210	ASN	2.0
1	А	129	TRP	2.0
2	D	31	PHE	2.0
1	В	77	LEU	2.0



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Mol	Chain	Res	Type	RSRZ
2	D	488	LEU	2.0
1	В	259	ASP	2.0
3	F	38	А	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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
5	MG	С	701	1/1	0.89	0.37	75,75,75,75	0
5	MG	А	402	1/1	0.90	0.31	$58,\!58,\!58,\!58$	0
5	MG	D	701	1/1	0.93	0.14	84,84,84,84	0
5	MG	В	402	1/1	0.94	0.20	$65,\!65,\!65,\!65$	0
4	JPO	В	401	28/28	0.95	0.25	76,84,86,97	0
4	JPO	А	401	28/28	0.96	0.26	62,71,76,84	0
5	MG	Е	101	1/1	0.96	0.36	68,68,68,68	0
5	MG	С	702	1/1	0.97	0.33	64,64,64,64	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.

