

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

#### Oct 3, 2023 – 06:10 AM EDT

PDB ID	:	6U6C
Title	:	Crystal structure of tryptophan synthase from M. tuberculosis - aminoacrylate-
		and GSK2-bound form
Authors	:	Chang, C.; Michalska, K.; Maltseva, N.I.; Jedrzejczak, R.; McCarren, P.; Nag,
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		(CSGID)
Deposited on	:	2019-08-29
Resolution	:	2.40  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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



# 2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 21418 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		Ate	oms			ZeroOcc	AltConf	Trace
	240	Total	С	Ν	0	$\mathbf{S}$	0	1	0	
	A	249	1807	1134	324	343	6	0	Ţ	0
1	С	240	Total	С	Ν	0	S	0	1	0
		249	1811	1136	324	345	6	0	1	0
1	F	245	Total	С	Ν	0	S	0	1	0
	E	240	1784	1120	320	338	6	0	1	0
1	С	240	Total	С	Ν	0	S	0	2	0
I G	249	1818	1140	328	344	6	U	2	0	

• Molecule 1 is a protein called Tryptophan synthase alpha chain.

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	271	HIS	-	expression tag	UNP P9WFY1
А	272	HIS	-	expression tag	UNP P9WFY1
А	273	HIS	-	expression tag	UNP P9WFY1
А	274	HIS	-	expression tag	UNP P9WFY1
А	275	HIS	-	expression tag	UNP P9WFY1
А	276	HIS	-	expression tag	UNP P9WFY1
С	271	HIS	-	expression tag	UNP P9WFY1
С	272	HIS	-	expression tag	UNP P9WFY1
С	273	HIS	-	expression tag	UNP P9WFY1
С	274	HIS	-	expression tag	UNP P9WFY1
С	275	HIS	-	expression tag	UNP P9WFY1
С	276	HIS	-	expression tag	UNP P9WFY1
Е	271	HIS	-	expression tag	UNP P9WFY1
Е	272	HIS	-	expression tag	UNP P9WFY1
Е	273	HIS	-	expression tag	UNP P9WFY1
Е	274	HIS	-	expression tag	UNP P9WFY1
Е	275	HIS	-	expression tag	UNP P9WFY1
Е	276	HIS	-	expression tag	UNP P9WFY1
G	271	HIS	-	expression tag	UNP P9WFY1
G	272	HIS	-	expression tag	UNP P9WFY1
G	273	HIS	-	expression tag	UNP P9WFY1



Chain	Residue	Modelled	Actual	Comment	Reference			
G	274	HIS	-	expression tag	UNP P9WFY1			
G	275	HIS	-	expression tag	UNP P9WFY1			
G	276	HIS	-	expression tag	UNP P9WFY1			

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• Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
0	р	405	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	D	405	3083	1919	565	586	13	0	0	0
0	П	404	Total	С	Ν	0	S	0	4	0
	D	404	3046	1901	553	579	13	0	4	U
0	Б	404	Total	С	Ν	0	S	0	2	0
	Г	404	3036	1896	551	576	13	0	5	0
0	ц	404	Total	С	Ν	0	S	0	12	0
	п	404	3106	1940	564	588	14	U	61	0

• Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \overline{\text{Total}} & \mathcal{C} & \mathcal{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{c ccc} \hline Total & C & O \\ \hline 3 & 1 & 2 \end{array}$	0	0
3	В	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 3 & 1 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 3 & 1 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 3 & 1 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	Н	1	$\begin{array}{c ccc} \hline Total & C & O \\ \hline 3 & 1 & 2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 3  1  2 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 3 & 1 & 2 \end{array}$	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	Ε	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0

• Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
5	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 6 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
6	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
6	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
6	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0
6	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 3 & 4 \end{array}$	0	0

• Molecule 7 is 1-(2-fluorobenzene-1-carbonyl)-N-methyl-2,3-dihydro-1H-indole-5-sulfonam ide (three-letter code: PZV) (formula: C<sub>16</sub>H<sub>15</sub>FN<sub>2</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Atoms						AltConf
7	7 B	1	Total	С	F	Ν	0	S	0	0
	1	23	16	1	2	3	1	0	0	
7	Л	1	Total	С	F	Ν	0	S	0	0
1		1	23	16	1	2	3	1		0
7	Б	1	Total	С	F	Ν	0	S	0	0
	1	23	16	1	2	3	1	0	0	
7	7 H	1	Total	С	F	Ν	Ο	S	0	0
1			23	16	1	2	3	1	0	0

• Molecule 8 is 2-[({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PY



RIDIN-4-YL}METHYL)AMINO]ACRYLIC ACID (three-letter code: P1T) (formula:  $C_{11}H_{15}N_2O_7P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
0	Р	1	Total	С	Ν	0	Р	0	0
0	о Б	L	21	11	2	7	1	0	0
0	Л	1	Total	С	Ν	0	Р	0	0
0	8 D	1	21	11	2	7	1		
0	Б	1	Total	С	Ν	0	Р	0	0
0 F	1	21	11	2	7	1	0	0	
8 H	1	Total	С	Ν	Ο	Р	0	0	
	п	1	21	11	2	7	1	U	

• Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
9	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
9	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
9	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	Total K 1 1	0	0
10	С	1	Total K 1 1	0	0
10	D	3	Total K 3 3	0	0
10	F	1	Total K 1 1	0	0
10	G	1	Total K 1 1	0	0
10	Н	1	Total K 1 1	0	0

• Molecule 11 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	В	1	Total	С	Ν	0	$\mathbf{S}$	0	0
		T	15	8	2	4	1	0	0
11	В	1	Total	С	Ν	0	$\mathbf{S}$	0	0
		T	15	8	2	4	1		
11	Г	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
11		1	15	8	2	4	1	0	0
11	11 H	1	Total	С	Ν	0	S	0	0
			15	8	2	4	1		0





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	Е	1	Total 5	С 3	N 1	0 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	F	1	Total C O   10 6 4	0	0
13	F	1	Total C O   10 6 4	0	0

• Molecule 14 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total Na 1 1	0	0

• Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	А	107	Total O 107 107	0	0
15	В	201	Total O 201 201	0	0
15	С	113	Total O 113 113	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	202	Total O   202 202	0	0
15	Е	71	Total O 71 71	0	0
15	F	181	Total O 181 181	0	0
15	G	124	Total O 124 124	0	0
15	Н	196	Total O 196 196	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	135.11Å $159.23$ Å $164.97$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	29.88 - 2.40	Depositor
% Data completeness	99.5 (29.88-2.40)	Depositor
(in resolution range)	55.5 (25.00-2.40)	Depositor
R <sub>merge</sub>	0.31	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.14 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
$R, R_{free}$	0.153 , $0.195$	Depositor
Wilson B-factor $(Å^2)$	27.7	Xtriage
Anisotropy	0.514	Xtriage
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
Total number of atoms	21418	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.41% 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.

# 4 Model quality (i)

## 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 4.6 Ligand geometry (i)

Of 155 ligands modelled in this entry, 9 are monoatomic - leaving 146 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



					De	nd long	tha	D	Bond angles			
Mol	Type	Chain	Res	Link	Counts   RMSZ   $\# Z  > 2$		Counts	BMSZ	# Z  > 2			
3	FMT	F	810	_	2.2.2	0.70	0	1.1.1	0.22	0		
4	EDO	D	511	_	3.3.3	0.47	0	2.2.2	0.31	0		
5	ACT	F	818	-	3.3.3	1.20	0	3,3,3	1.53	0		
9	PEG	G	309	-	6.6.6	0.14	0	5.5.5	0.12	0		
3	FMT	В	513	-	2,2,2	0.70	0	1,1,1	0.19	0		
3	FMT	В	528	_	2,2,2	0.73	0	1,1,1	0.28	0		
7	PZV	В	501	-	24,25,25	1.86	7 (29%)	32,37,37	<b>3.03</b>	8 (25%)		
3	FMT	С	305	-	2,2,2	0.70	0	1,1,1	0.21	0		
4	EDO	F	822	-	3,3,3	0.47	0	2,2,2	0.32	0		
3	FMT	F	816	_	2,2,2	0.69	0	1,1,1	0.18	0		
3	FMT	G	302	_	2,2,2	0.69	0	1,1,1	0.18	0		
3	FMT	В	514	_	2,2,2	0.70	0	1,1,1	0.24	0		
3	FMT	F	815	-	2,2,2	0.70	0	1,1,1	0.23	0		
3	FMT	D	509	-	2,2,2	0.72	0	1,1,1	0.26	0		
3	FMT	D	515	-	2,2,2	0.68	0	1,1,1	0.23	0		
3	FMT	F	813	-	2,2,2	0.68	0	1,1,1	0.14	0		
3	FMT	D	508	-	2,2,2	0.71	0	1,1,1	0.23	0		
4	EDO	В	529	-	3,3,3	0.49	0	2,2,2	0.08	0		
4	EDO	Н	533	-	3,3,3	0.51	0	2,2,2	0.12	0		
8	P1T	В	502	-	20,21,21	2.35	2 (10%)	28,30,30	1.73	4 (14%)		
3	FMT	D	514	-	2,2,2	0.70	0	1,1,1	0.24	0		
3	FMT	С	309	-	2,2,2	0.70	0	1,1,1	0.13	0		
4	EDO	Н	521	-	3,3,3	0.46	0	2,2,2	0.34	0		
3	FMT	С	302	-	2,2,2	0.70	0	1,1,1	0.17	0		
3	FMT	D	506	-	2,2,2	0.67	0	1,1,1	0.21	0		
3	FMT	D	504	-	2,2,2	0.68	0	1,1,1	0.17	0		
3	FMT	Н	514	-	$2,\!2,\!2$	0.68	0	1,1,1	0.16	0		
4	EDO	В	511	-	3,3,3	0.48	0	2,2,2	0.25	0		
3	FMT	В	504	-	2,2,2	0.69	0	1,1,1	0.18	0		
3	FMT	Н	526	-	2,2,2	0.69	0	1,1,1	0.17	0		
6	MLI	E	302	-	6,6,6	1.33	0	7,7,7	0.93	0		
3	FMT	В	521	-	2,2,2	0.69	0	1,1,1	0.21	0		
12	ALA	E	301	-	3,4,5	0.67	0	2,4,6	0.80	0		
8	P1T	D	505	-	20,21,21	2.30	2 (10%)	28,30,30	1.85	4 (14%)		
6	MLI	F	827	-	6,6,6	1.34	0	7,7,7	0.95	0		
13	PGE	F	809	-	9,9,9	0.33	0	8,8,8	0.28	0		
3	FMT	Н	518	-	2,2,2	0.72	0	1,1,1	0.21	0		
3	FMT	В	524	-	2,2,2	0.70	0	1,1,1	0.21	0		
9	PEG	В	506	-	6,6,6	0.12	0	5,5,5	0.10	0		

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).



N.T. 1	<b>T</b>		D	T ! 1.	Bo	ond leng	$\mathbf{ths}$	Bond angles		
IVI01	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	FMT	G	306	-	2,2,2	0.66	0	1,1,1	0.16	0
4	EDO	А	304	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	С	303	10	3,3,3	0.42	0	2,2,2	0.35	0
3	FMT	В	519	-	2,2,2	0.71	0	1,1,1	0.23	0
6	MLI	Н	530	-	6,6,6	1.31	0	7,7,7	1.00	0
3	FMT	А	308	-	2,2,2	0.70	0	1,1,1	0.29	0
4	EDO	F	812	-	3,3,3	0.44	0	2,2,2	0.34	0
3	FMT	G	307	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	Н	516	-	2,2,2	0.70	0	1,1,1	0.21	0
3	FMT	Е	304	-	2,2,2	0.72	0	1,1,1	0.24	0
3	FMT	Н	517	-	2,2,2	0.69	0	1,1,1	0.17	0
3	FMT	Н	501	-	2,2,2	0.64	0	1,1,1	0.13	0
3	FMT	G	305	-	2,2,2	0.72	0	1,1,1	0.25	0
3	FMT	D	502	-	2,2,2	0.67	0	1,1,1	0.18	0
3	FMT	В	512	-	2,2,2	0.71	0	1,1,1	0.23	0
3	FMT	D	513	-	2,2,2	0.69	0	1,1,1	0.21	0
4	EDO	Е	305	-	3,3,3	0.48	0	2,2,2	0.29	0
3	FMT	А	307	-	2,2,2	0.72	0	1,1,1	0.25	0
3	FMT	В	518	-	2,2,2	0.68	0	1,1,1	0.20	0
4	EDO	В	526	-	3,3,3	0.48	0	2,2,2	0.26	0
11	EPE	В	530	-	15,15,15	1.76	1 (6%)	18,20,20	1.69	3 (16%)
3	FMT	Н	529	-	2,2,2	0.71	0	1,1,1	0.23	0
4	EDO	G	310	-	3,3,3	0.54	0	2,2,2	0.14	0
3	FMT	Н	511	-	2,2,2	0.69	0	1,1,1	0.21	0
5	ACT	Н	506	-	3,3,3	1.36	1 (33%)	3,3,3	1.50	0
3	FMT	D	510	-	2,2,2	0.71	0	1,1,1	0.23	0
4	EDO	С	306	10	3,3,3	0.47	0	2,2,2	0.20	0
3	FMT	В	507	-	2,2,2	0.72	0	1,1,1	0.29	0
3	FMT	F	803	-	2,2,2	0.70	0	1,1,1	0.24	0
3	FMT	D	521	-	2,2,2	0.73	0	1,1,1	0.29	0
3	FMT	В	522	-	2,2,2	0.70	0	1,1,1	0.20	0
4	EDO	D	520	-	3,3,3	0.47	0	2,2,2	0.28	0
3	FMT	G	303	-	2,2,2	0.71	0	1,1,1	0.21	0
3	FMT	Н	519	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	E	303	-	2,2,2	0.67	0	1,1,1	0.15	0
3	FMT	G	308	-	$2,\!2,\!2$	0.70	0	$1,\!1,\!1$	0.22	0
4	EDO	В	509		3,3,3	0.46	0	2,2,2	0.33	0
8	P1T	F	805	-	20,21,21	2.47	2(10%)	28,30,30	1.68	4 (14%)
6	MLI	А	311	-	$6,\!6,\!6$	1.36	0	7,7,7	0.97	0
3	FMT	A	309	-	2,2,2	0.69	0	1,1,1	0.24	0
3	FMT	F	811	-	2,2,2	0.67	0	1,1,1	0.14	0
5	ACT	А	312	-	3,3,3	1.40	1 (33%)	3,3,3	1.31	0



	<b>—</b>		D	т •1.	Bo	ond leng	$\mathbf{ths}$	Bond angles		
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	EDO	G	312	-	3,3,3	0.59	0	2,2,2	0.19	0
3	FMT	В	531	-	2,2,2	0.72	0	1,1,1	0.24	0
3	FMT	В	508	-	2,2,2	0.70	0	1,1,1	0.23	0
4	EDO	Н	512	-	3,3,3	0.52	0	2,2,2	0.02	0
3	FMT	В	523	-	2,2,2	0.68	0	1,1,1	0.19	0
9	PEG	F	829	-	6,6,6	0.12	0	$5,\!5,\!5$	0.09	0
4	EDO	F	819	-	3,3,3	0.48	0	2,2,2	0.25	0
3	FMT	G	301	-	2,2,2	0.68	0	1,1,1	0.16	0
3	FMT	В	520	-	2,2,2	0.69	0	1,1,1	0.14	0
11	EPE	F	830	-	$15,\!15,\!15$	2.02	1 (6%)	18,20,20	1.54	3 (16%)
3	FMT	Н	507	-	2,2,2	0.70	0	1,1,1	0.18	0
3	FMT	Н	524	-	2,2,2	0.68	0	1,1,1	0.19	0
3	FMT	А	301	-	2,2,2	0.70	0	1,1,1	0.19	0
3	FMT	D	516	-	$2,\!2,\!2$	0.70	0	$1,\!1,\!1$	0.20	0
3	FMT	Н	522	-	2,2,2	0.70	0	1,1,1	0.18	0
5	ACT	А	310	-	3,3,3	1.35	0	3,3,3	1.52	0
3	FMT	Н	508	-	2,2,2	0.68	0	1,1,1	0.14	0
11	EPE	В	527	-	$15,\!15,\!15$	1.99	1 (6%)	18,20,20	1.13	1 (5%)
3	FMT	F	814	-	2,2,2	0.66	0	1,1,1	0.13	0
3	FMT	Н	503	-	2,2,2	0.69	0	1,1,1	0.19	0
3	FMT	Н	523	-	2,2,2	0.68	0	1,1,1	0.16	0
6	MLI	G	311	-	6,6,6	1.31	0	7,7,7	0.97	0
3	FMT	D	517	-	2,2,2	0.70	0	1,1,1	0.23	0
3	FMT	D	512	-	2,2,2	0.70	0	1,1,1	0.16	0
7	PZV	F	802	-	24,25,25	1.85	5 (20%)	32,37,37	3.01	7 (21%)
11	EPE	Н	532	-	$15,\!15,\!15$	1.90	1 (6%)	18,20,20	1.17	3 (16%)
4	EDO	В	510	-	3,3,3	0.51	0	2,2,2	0.15	0
3	FMT	F	817	-	2,2,2	0.69	0	1,1,1	0.21	0
3	FMT	Н	509	-	2,2,2	0.69	0	1,1,1	0.20	0
3	FMT	F	806	-	2,2,2	0.74	0	1,1,1	0.31	0
4	EDO	В	503	-	3,3,3	0.43	0	2,2,2	0.44	0
4	EDO	С	301	-	3,3,3	0.49	0	2,2,2	0.16	0
6	MLI	С	307	-	6,6,6	1.33	0	7,7,7	1.04	0
3	FMT	B	505	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	F	828	-	2,2,2	0.68	0	1,1,1	0.20	0
3	FMT	B	515	-	2,2,2	0.68	0	1,1,1	0.20	0
3	FMT	F'	807	-	2,2,2	0.68	0	1,1,1	0.16	0
3	FMT	A	306	-	2,2,2	0.70	0	1,1,1	0.22	0
7	PZV	D	501	-	24,25,25	1.83	4 (16%)	32,37,37	2.97	9 (28%)
3	FMT	G	304	-	2,2,2	0.70	0	1,1,1	0.19	0
4	EDO	Н	520	-	3,3,3	0.54	0	2,2,2	0.03	0
3	FMT	A	302	-	2,2,2	0.68	0	1,1,1	0.18	0



Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FMT	F	823	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	А	305	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	Н	525	-	2,2,2	0.68	0	1,1,1	0.22	0
3	FMT	F	824	-	2,2,2	0.69	0	1,1,1	0.21	0
4	EDO	Н	505	-	3,3,3	0.47	0	2,2,2	0.29	0
3	FMT	D	503	-	2,2,2	0.68	0	1,1,1	0.16	0
3	FMT	Н	528	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	А	303	-	2,2,2	0.67	0	1,1,1	0.16	0
3	FMT	F	820	-	2,2,2	0.71	0	1,1,1	0.25	0
3	FMT	Н	515	-	2,2,2	0.67	0	1,1,1	0.14	0
13	PGE	F	801	-	9,9,9	0.33	0	8,8,8	0.47	0
7	PZV	Н	502	-	24,25,25	1.83	4 (16%)	32,37,37	<mark>3.30</mark>	8 (25%)
3	FMT	В	517	-	2,2,2	0.72	0	1,1,1	0.22	0
4	EDO	В	516	-	3,3,3	0.45	0	2,2,2	0.42	0
3	FMT	Н	510	-	2,2,2	0.68	0	1,1,1	0.19	0
5	ACT	F	808	-	3,3,3	1.33	0	3,3,3	1.50	0
3	FMT	D	507	-	2,2,2	0.71	0	1,1,1	0.26	0
3	FMT	С	304	-	2,2,2	0.71	0	1,1,1	0.25	0
3	FMT	F	804	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	Н	527	-	2,2,2	0.68	0	$1,\!1,\!1$	0.23	0
8	P1T	Н	504	-	20,21,21	2.39	2 (10%)	28,30,30	1.73	4 (14%)
3	FMT	F	821	-	2,2,2	0.69	0	1,1,1	0.19	0
9	PEG	Н	513	-	6,6,6	0.12	0	$5,\!5,\!5$	0.08	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
4	EDO	G	310	-	-	1/1/1/1	-
11	EPE	Н	532	-	-	6/9/19/19	0/1/1/1
4	EDO	В	510	-	-	0/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	С	306	10	-	0/1/1/1	-
9	PEG	G	309	-	-	0/4/4/4	-
12	ALA	E	301	-	-	0/0/2/4	-
8	P1T	D	505	-	-	$\frac{5/14/15/15}{5}$	0/1/1/1
6	MLI	F	827	-	-	4/4/4/4	-
7	PZV	В	501	-	-	0/17/26/26	0/3/3/3
4	EDO	F	822	-	-	0/1/1/1	-



6	U	6	С
0	$\sim$	0	$\sim$

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PGE	F	809	-	-	6/7/7/7	-
4	EDO	D	520	_	_	0/1/1/1	-
4	EDO	В	503	-	-	0/1/1/1	-
4	EDO	С	301	-	-	0/1/1/1	-
6	MLI	С	307	-	-	0/4/4/4	-
9	PEG	В	506	-	-	0/4/4/4	-
8	P1T	F	805	-	-	5/14/15/15	0/1/1/1
4	EDO	В	509	-	-	0/1/1/1	-
4	EDO	В	529	-	-	0/1/1/1	-
6	MLI	А	311	-	-	2/4/4/4	-
7	PZV	D	501	-	-	0/17/26/26	0/3/3/3
4	EDO	Н	533	-	-	1/1/1/1	-
8	P1T	В	502	-	-	5/14/15/15	0/1/1/1
4	EDO	А	304	-	-	0/1/1/1	-
4	EDO	Н	520	-	-	0/1/1/1	-
4	EDO	С	303	10	-	0/1/1/1	-
4	EDO	Н	505	-	-	0/1/1/1	-
6	MLI	Н	530	-	-	$\frac{4}{4}/\frac{4}{4}$	-
4	EDO	G	312	-	-	0/1/1/1	-
4	EDO	F	812	-	-	0/1/1/1	-
4	EDO	Н	512	-	-	0/1/1/1	-
4	EDO	Н	521	-	-	1/1/1/1	-
9	PEG	F	829	-	-	1/4/4/4	-
4	EDO	F	819	-	-	0/1/1/1	-
11	EPE	F	830	-	-	2/9/19/19	0/1/1/1
13	PGE	F	801	-	-	3/7/7/7	-
7	PZV	Н	502	-	-	0/17/26/26	0/3/3/3
4	EDO	В	516	-	-	1/1/1/1	-
4	EDO	В	511	-	-	0/1/1/1	-
11	EPE	В	527	-	-	5/9/19/19	0/1/1/1
8	P1T	Н	504	-	-	5/14/15/15	0/1/1/1
4	EDO	Е	305	-	-	0/1/1/1	-
6	MLI	E	302	-	-	2/4/4/4	-
4	EDO	В	526	-	-	0/1/1/1	-
11	EPE	В	530	-	-	3/9/19/19	0/1/1/1
6	MLI	G	311	-	-	0/4/4/4	-
9	PEG	Н	513	-	-	1/4/4/4	-
7	PZV	F	802	-	-	$0/17/\overline{26/26}$	0/3/3/3

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All (34) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
8	F	805	P1T	CA-C	-10.65	1.34	1.49
8	Н	504	P1T	CA-C	-10.30	1.34	1.49
8	В	502	P1T	CA-C	-10.11	1.34	1.49
8	D	505	P1T	CA-C	-9.89	1.35	1.49
11	F	830	EPE	C10-S	-7.55	1.66	1.77
11	В	527	EPE	C10-S	-7.35	1.67	1.77
11	Н	532	EPE	C10-S	-7.02	1.67	1.77
11	В	530	EPE	C10-S	-6.41	1.68	1.77
7	Н	502	PZV	C15-N12	5.28	1.45	1.36
7	D	501	PZV	C15-N12	5.24	1.45	1.36
7	F	802	PZV	C15-N12	5.10	1.44	1.36
7	В	501	PZV	C15-N12	5.07	1.44	1.36
7	F	802	PZV	C09-N12	4.65	1.48	1.39
7	В	501	PZV	C09-N12	4.48	1.48	1.39
7	D	501	PZV	C09-N12	4.39	1.48	1.39
7	Н	502	PZV	C09-N12	4.30	1.48	1.39
7	Н	502	PZV	O04-S03	2.96	1.46	1.43
7	В	501	PZV	O04-S03	2.89	1.46	1.43
7	D	501	PZV	O05-S03	2.78	1.46	1.43
7	D	501	PZV	O04-S03	2.70	1.46	1.43
7	F	802	PZV	O05-S03	2.67	1.46	1.43
7	F	802	PZV	O04-S03	2.61	1.46	1.43
8	В	502	P1T	O-C	-2.41	1.23	1.30
8	Н	504	P1T	O-C	-2.41	1.23	1.30
8	F	805	P1T	O-C	-2.40	1.23	1.30
8	D	505	P1T	O-C	-2.34	1.23	1.30
7	В	501	PZV	C06-S03	2.33	1.80	1.76
7	Н	502	PZV	O05-S03	2.22	1.46	1.43
7	В	501	PZV	O05-S03	2.22	1.46	1.43
7	F	802	PZV	C06-S03	2.19	1.79	1.76
7	В	501	PZV	C13-C14	-2.13	1.50	1.53
5	А	312	ACT	CH3-C	2.06	1.57	1.49
7	В	501	PZV	O16-C15	-2.02	1.18	1.22
5	Н	506	ACT	CH3-C	2.01	1.57	1.49

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	Н	502	PZV	O05-S03-O04	-14.27	102.00	119.55
7	В	501	PZV	O05-S03-O04	-13.02	103.55	119.55
7	F	802	PZV	O05-S03-O04	-12.99	103.58	119.55
7	D	501	PZV	O05-S03-O04	-12.32	104.41	119.55
7	D	501	PZV	O05-S03-N02	6.26	114.14	107.08



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	F	802	PZV	O04-S03-N02	6.15	114.01	107.08
7	Н	502	PZV	O04-S03-N02	5.99	113.84	107.08
8	D	505	P1T	CB-CA-N	-5.76	111.93	125.91
7	Н	502	PZV	O05-S03-N02	5.64	113.45	107.08
7	В	501	PZV	O05-S03-N02	5.58	113.37	107.08
8	F	805	P1T	CB-CA-N	-5.51	112.54	125.91
8	В	502	P1T	CB-CA-N	-5.51	112.54	125.91
8	Н	504	P1T	CB-CA-N	-5.22	113.24	125.91
7	F	802	PZV	O05-S03-N02	5.18	112.93	107.08
8	D	505	P1T	C-CA-N	4.98	124.73	112.45
7	В	501	PZV	C08-C09-N12	-4.65	107.11	109.66
7	В	501	PZV	O04-S03-N02	4.61	112.28	107.08
7	Н	502	PZV	C08-C09-N12	-4.42	107.24	109.66
7	Н	502	PZV	C18-C17-C22	4.33	121.59	116.67
7	D	501	PZV	O04-S03-N02	4.31	111.94	107.08
8	В	502	P1T	C-CA-N	4.29	123.05	112.45
7	В	501	PZV	C18-C17-C22	4.25	121.50	116.67
8	D	505	P1T	CB-CA-C	-4.24	109.56	120.72
11	В	530	EPE	O1S-S-C10	4.17	111.93	106.92
8	F	805	P1T	C-CA-N	4.09	122.55	112.45
8	Н	504	P1T	C-CA-N	3.92	122.12	112.45
7	D	501	PZV	C18-C17-C22	3.91	121.12	116.67
8	В	502	P1T	CB-CA-C	-3.85	110.59	120.72
7	D	501	PZV	C08-C09-N12	-3.78	107.59	109.66
7	F	802	PZV	C18-C17-C22	3.75	120.93	116.67
8	Н	504	P1T	CB-CA-C	-3.73	110.90	120.72
11	В	530	EPE	O3S-S-C10	3.73	111.80	105.77
8	F	805	P1T	CB-CA-C	-3.68	111.05	120.72
7	F	802	PZV	C08-C09-N12	-3.46	107.76	109.66
11	F	830	EPE	O1S-S-C10	3.29	110.88	106.92
7	D	501	PZV	C21-C22-C17	-3.16	119.67	123.11
8	Н	504	P1T	O-C-CA	3.00	120.63	114.14
11	В	527	EPE	O2S-S-C10	2.82	110.32	106.92
11	Н	532	EPE	O1S-S-C10	2.80	110.29	106.92
11	F	830	EPE	02S-S-C10	2.70	110.16	106.92
11	F	830	EPE	C2-C3-N4	-2.67	105.17	110.64
7	Н	502	PZV	O04-S03-C06	2.63	111.20	107.97
8	D	505	P1T	O-C-CA	2.58	119.72	114.14
7	D	501	PZV	C07-C08-C09	-2.42	118.83	120.54
11	H	532	EPE	O2S-S-C10	2.30	109.69	106.92
7	Н	502	PZV	$C21-\overline{C22}-\overline{C17}$	-2.27	120.64	123.11
7	F	802	PZV	C07-C08-C09	-2.25	118.95	120.54

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	D	501	PZV	C06-S03-N02	2.22	110.62	107.56
8	В	502	P1T	O-C-CA	2.17	118.84	114.14
7	D	501	PZV	C11-C06-C07	2.14	123.25	120.62
11	Н	532	EPE	O3S-S-C10	2.13	109.21	105.77
7	F	802	PZV	C21-C22-C17	-2.13	120.80	123.11
7	В	501	PZV	C21-C22-C17	-2.06	120.87	123.11
11	В	530	EPE	C3-C2-N1	2.05	114.86	110.64
8	F	805	P1T	O-C-CA	2.03	118.53	114.14
7	Н	502	PZV	C11-C06-C07	2.03	123.11	120.62
7	B	501	PZV	C06-S03-N02	2.01	110.34	107.56
7	В	501	PZV	C07-C08-C09	-2.01	119.12	120.54

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There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	В	502	P1T	C5-C4-C4A-N
8	D	505	P1T	C5-C4-C4A-N
8	D	505	P1T	C3-C4-C4A-N
8	F	805	P1T	C5-C4-C4A-N
8	Н	504	P1T	C5-C4-C4A-N
11	В	527	EPE	C10-C9-N1-C6
11	В	527	EPE	C8-C7-N4-C3
11	F	830	EPE	C10-C9-N1-C2
11	Н	532	EPE	C10-C9-N1-C2
11	Н	532	EPE	C10-C9-N1-C6
11	Н	532	EPE	S-C10-C9-N1
11	Н	532	EPE	C9-C10-S-O1S
11	Н	532	EPE	C9-C10-S-O3S
13	F	801	PGE	C4-C3-O2-C2
9	Н	513	PEG	C4-C3-O2-C2
4	В	516	EDO	O1-C1-C2-O2
11	В	527	EPE	N4-C7-C8-O8
11	F	830	EPE	N4-C7-C8-O8
8	F	805	P1T	C3-C4-C4A-N
6	Е	302	MLI	C3-C1-C2-O7
6	F	827	MLI	C3-C1-C2-O7
6	Н	530	MLI	C3-C1-C2-O7
6	Н	530	MLI	C2-C1-C3-O8
6	Н	530	MLI	C2-C1-C3-O9
13	F	809	PGE	O2-C3-C4-O3
8	В	502	P1T	C-CA-N-C4A



Mol	Chain	Res	Type	Atoms	
8	D	505	P1T	C-CA-N-C4A	
8	F	805	P1T	C-CA-N-C4A	
8	Н	504	P1T	C-CA-N-C4A	
13	F	809	PGE	O3-C5-C6-O4	
13	F	809	PGE	O1-C1-C2-O2	
6	Е	302	MLI	C3-C1-C2-O6	
11	В	527	EPE	C10-C9-N1-C2	
11	В	530	EPE	C10-C9-N1-C6	
11	В	530	EPE	N4-C7-C8-O8	
6	Н	530	MLI	C3-C1-C2-O6	
4	G	310	EDO	O1-C1-C2-O2	
13	F	801	PGE	O2-C3-C4-O3	
13	F	801	PGE	O1-C1-C2-O2	
6	F	827	MLI	C3-C1-C2-O6	
13	F	809	PGE	C3-C4-O3-C5	
8	В	502	P1T	O-C-CA-CB	
8	В	502	P1T	OXT-C-CA-CB	
8	D	505	P1T	O-C-CA-CB	
8	D	505	P1T	OXT-C-CA-CB	
8	F	805	P1T	O-C-CA-CB	
8	F	805	P1T	OXT-C-CA-CB	
13	F	809	PGE	C4-C3-O2-C2	
11	Н	532	EPE	C9-C10-S-O2S	
13	F	809	PGE	C6-C5-O3-C4	
6	F	827	MLI	C2-C1-C3-O9	
8	В	502	P1T	C3-C4-C4A-N	
8	Н	504	P1T	C3-C4-C4A-N	
11	В	530	EPE	C10-C9-N1-C2	
6	А	311	MLI	C2-C1-C3-O9	
6	F	827	MLI	C2-C1-C3-O8	
6	А	311	MLI	C2-C1-C3-O8	
8	Н	504	P1T	O-C-CA-CB	
8	Н	504	P1T	OXT-C-CA-CB	
9	F	829	PEG	C4-C3-O2-C2	
4	Н	521	EDO	O1-C1-C2-O2	
4	Н	533	EDO	O1-C1-C2-O2	
11	В	527	EPE	C8-C7-N4-C5	

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There are no ring outliers.

No monomer is involved in short contacts.

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.



























## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

## 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

## 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

