

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

#### Sep 24, 2024 – 04:11 PM EDT

PDB ID	:	8VZJ
Title	:	Crystal Structure of 2-Hydroxyacyl-CoA Lyase/Synthase DhcHACS from De-
		halococcoidia bacterium in the Complex with THDP and ADP
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		K.; Joachimiak, A.
Deposited on	:	2024-02-11
Resolution	:	2.70  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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

# 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 2.70 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
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	554	87%	10%	•••
1	В	554	85%	13%	·
1	С	554	85%	12%	•••
1	D	554	88%	10%	·



Mol	Chain	Length	Quality of chain	
1	Е	554	88%	10% •
1	F	554	85%	12% ••
1	G	554	% • 88%	9% •
1	Н	554	% 85%	11% • •



## 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 33287 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	Δ	549	Total	С	Ν	0	S	0	0	0
1	A	042	4111	2604	712	765	30	0	0	0
1	В	530	Total	С	Ν	0	S	0	0	0
1	D	009	4084	2587	705	762	30	0	0	0
1	С	549	Total	С	Ν	0	S	0	0	0
1	U	042	4102	2597	708	766	31	0	0	0
1	Л	546	Total	С	Ν	0	S	0	1	0
1	D	040	4149	2626	719	772	32		I	0
1	F	541	Total	С	Ν	0	S	0	0	0
1	Ľ	041	4104	2599	711	764	30	0	0	0
1	Б	549	Total	С	Ν	0	S	0	0	0
1	Г	042	4102	2597	708	766	31	0	0	0
1	C	540	Total	С	Ν	0	S	0	0	0
1	G	540	4090	2591	706	762	31	0	0	0
1	Ц	538	Total	С	Ν	0	S	0	0	0
	11	000	4080	2585	704	761	30	U	0	

• Molecule 1 is a protein called Oxalyl-CoA decarboxylase.

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	SER	-	expression tag	UNP A0A315XEK8
А	-1	ASN	-	expression tag	UNP A0A315XEK8
А	0	ALA	-	expression tag	UNP A0A315XEK8
В	-2	SER	-	expression tag	UNP A0A315XEK8
В	-1	ASN	-	expression tag	UNP A0A315XEK8
В	0	ALA	-	expression tag	UNP A0A315XEK8
С	-2	SER	-	expression tag	UNP A0A315XEK8
С	-1	ASN	-	expression tag	UNP A0A315XEK8
С	0	ALA	-	expression tag	UNP A0A315XEK8
D	-2	SER	-	expression tag	UNP A0A315XEK8
D	-1	ASN	-	expression tag	UNP A0A315XEK8
D	0	ALA	-	expression tag	UNP A0A315XEK8
E	-2	SER	-	expression tag	UNP A0A315XEK8



Chain	Residue	Modelled	Actual Comment		Reference
E	-1	ASN	-	expression tag	UNP A0A315XEK8
Е	0	ALA	-	expression tag	UNP A0A315XEK8
F	-2	SER	-	expression tag	UNP A0A315XEK8
F	-1	ASN	-	expression tag	UNP A0A315XEK8
F	0	ALA	-	expression tag	UNP A0A315XEK8
G	-2	SER	-	expression tag	UNP A0A315XEK8
G	-1	ASN	-	expression tag	UNP A0A315XEK8
G	0	ALA	-	expression tag	UNP A0A315XEK8
Н	-2	SER	-	expression tag	UNP A0A315XEK8
H	-1	ASN	-	expression tag	UNP A0A315XEK8
Н	0	ALA	-	expression tag	UNP A0A315XEK8

• Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	Δ	1	Total	С	Ν	0	Р	S	0	0
	Л	1	26	12	4	7	2	1	0	0
9	В	1	Total	С	Ν	0	Р	S	0	0
	D		26	12	4	7	2	1	0	0
0	C	1	Total	С	Ν	0	Р	S	0	0
	U		26	12	4	7	2	1		0
0	р	1	Total	С	Ν	0	Р	S	0	0
	1	26	12	4	7	2	1	0	0	
0	9 F	1	Total	С	Ν	0	Р	S	0	0
		1	26	12	4	7	2	1	U	U



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
0	Б	1	Total	С	Ν	Ο	Р	S	0	0
	L	26	12	4	7	2	1	0	0	
0	C	1	Total	С	Ν	Ο	Р	S	0	0
	G	L	26	12	4	7	2	1	0	0
9	ц	1	Total	С	Ν	0	Р	S	0	0
	11	L	26	12	4	7	2	1	0	0

• Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
2	Λ	1	Total	С	Ν	0	Р	0	0
0	A	L	27	10	5	10	2	0	0
9	2 D	1	Total	С	Ν	Ο	Р	0	0
0	D	L	27	10	5	10	2	0	0
9	С	1	Total	С	Ν	Ο	Р	0	0
0	C	1	27	10	5	10	2	0	0
9	р	1	Total	С	Ν	Ο	Р	0	0
0	D		27	10	5	10	2		
9	Б	1	Total	С	Ν	0	Р	0	0
0	E	1	27	10	5	10	2		0
9	Б	1	Total	С	Ν	0	Р	0	0
0	5 F	L	27	10	5	10	2	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0
0	G		27	10	5	10	2	0	0
2	ц	1	Total	С	Ν	Ο	Р	0	0
3	11		27	10	5	10	2	0	0



• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





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

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	1	Total O 1 1	0	0
7	Е	1	Total O 1 1	0	0
7	F	2	Total O 2 2	0	0
7	G	1	Total O 1 1	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: Oxalyl-CoA decarboxylase





• Molecule 1: Oxalyl-CoA decarboxylase













## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	324.22Å 77.84Å 229.55Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $134.53^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	40.53 - 2.70	Depositor
Resolution (A)	40.53 - 2.70	EDS
% Data completeness	99.6 (40.53-2.70)	Depositor
(in resolution range)	99.6 (40.53 - 2.70)	EDS
R <sub>merge</sub>	0.17	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.42 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.197 , $0.235$	Depositor
It, It <sub>free</sub>	0.197 , $0.235$	DCC
$R_{free}$ test set	5510 reflections $(4.89%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	66.0	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.32 , $44.3$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.31$	Xtriage
	0.016  for  h+2*l,k,-h-l	
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
	0.010 for -h-2*l,-k,l	
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33287	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.71% 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: EDO, MG, GOL, ADP, TPP

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	Mol Chain		Bond lengths		angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/4211	0.47	0/5722
1	В	0.25	0/4183	0.47	0/5685
1	С	0.25	0/4201	0.47	0/5709
1	D	0.25	0/4249	0.47	0/5772
1	Ε	0.24	0/4203	0.47	0/5710
1	F	0.25	0/4201	0.47	0/5709
1	G	0.24	0/4189	0.47	0/5693
1	Н	0.25	0/4179	0.47	0/5680
All	All	0.25	0/33616	0.47	0/45680

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	4111	0	4060	34	0
1	В	4084	0	4027	38	0
1	С	4102	0	4047	40	0
1	D	4149	0	4099	35	0
1	Е	4104	0	4053	30	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4102	0	4047	37	0
1	G	4090	0	4037	32	0
1	Н	4080	0	4024	35	0
2	А	26	0	16	1	0
2	В	26	0	16	1	0
2	С	26	0	16	1	0
2	D	26	0	16	1	0
2	Е	26	0	16	3	0
2	F	26	0	16	0	0
2	G	26	0	16	2	0
2	Н	26	0	16	1	0
3	А	27	0	12	1	0
3	В	27	0	12	0	0
3	С	27	0	12	1	0
3	D	27	0	12	1	0
3	Е	27	0	12	0	0
3	F	27	0	12	1	0
3	G	27	0	12	1	0
3	Н	27	0	12	0	0
4	А	6	0	8	2	0
4	В	6	0	8	1	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
5	С	1	0	0	0	0
5	D	1	0	0	0	0
5	Е	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	Н	1	0	0	0	0
6	С	4	0	6	0	0
6	F	4	0	6	0	0
6	G	4	0	6	1	0
6	Н	4	0	6	0	0
7	С	1	0	0	0	0
7	Е	1	0	0	0	0
7	F	2	0	0	0	0
7	G	1	0	0	0	0
All	All	33287	0	32658	272	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 4.

The worst 5 of 272 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:388:GLY:H	1:F:392:MET:HE2	1.63	0.62
1:H:252:ILE:HA	1:H:347:ILE:HD11	1.82	0.62
1:C:479:LEU:HD12	1:C:491:PRO:HD3	1.84	0.59
1:F:220:GLU:HG2	1:F:404:PRO:HG3	1.84	0.59
1:F:311:LEU:HB3	1:F:318:ILE:HD13	1.84	0.59

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	entiles
1	А	540/554~(98%)	524 (97%)	16 (3%)	0	100	100
1	В	537/554~(97%)	522 (97%)	15 (3%)	0	100	100
1	С	540/554~(98%)	521 (96%)	18 (3%)	1 (0%)	44	68
1	D	545/554~(98%)	530 (97%)	15 (3%)	0	100	100
1	Ε	539/554~(97%)	520 (96%)	19 (4%)	0	100	100
1	F	540/554~(98%)	525 (97%)	15 (3%)	0	100	100
1	G	538/554~(97%)	521 (97%)	17 (3%)	0	100	100
1	Н	536/554~(97%)	518 (97%)	18 (3%)	0	100	100
All	All	4315/4432 (97%)	4181 (97%)	133 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	515	LEU



#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	422/432~(98%)	415~(98%)	7~(2%)	56	81
1	В	419/432~(97%)	414 (99%)	5 (1%)	67	86
1	С	421/432~(98%)	411 (98%)	10 (2%)	44	73
1	D	426/432~(99%)	420 (99%)	6 (1%)	62	84
1	Ε	421/432~(98%)	412 (98%)	9~(2%)	48	76
1	F	421/432~(98%)	410 (97%)	11 (3%)	41	70
1	G	419/432~(97%)	414 (99%)	5 (1%)	67	86
1	Н	419/432~(97%)	405 (97%)	14 (3%)	33	62
All	All	3368/3456~(98%)	3301 (98%)	67(2%)	50	78

 $5~{\rm of}~67$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	Н	365	MET
1	Н	375	ARG
1	Н	519	LEU
1	D	390	SER
1	D	371	TYR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	А	386	ASN
1	В	386	ASN
1	F	385	GLN
1	F	422	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)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Tuno	Chain	Dog	Tink	Bo	Bond lengths			ond ang	les
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPP	Е	601	5	23,27,27	0.49	0	30,40,40	0.59	1 (3%)
2	TPP	D	601	5	23,27,27	0.47	0	30,40,40	0.58	1 (3%)
3	ADP	С	602	-	24,29,29	0.89	0	29,45,45	1.33	3 (10%)
4	GOL	А	603	-	$5,\!5,\!5$	0.91	0	$5,\!5,\!5$	1.03	0
4	GOL	В	603	-	$5,\!5,\!5$	0.93	0	$5,\!5,\!5$	1.07	0
2	TPP	F	601	5	23,27,27	0.47	0	30,40,40	0.58	1 (3%)
3	ADP	D	602	-	24,29,29	0.88	0	29,45,45	1.39	4 (13%)
2	TPP	С	601	5	23,27,27	0.47	0	30,40,40	0.58	1 (3%)
6	EDO	С	603	-	3,3,3	0.42	0	2,2,2	0.39	0
6	EDO	F	603	-	3,3,3	0.43	0	2,2,2	0.37	0
3	ADP	F	602	-	24,29,29	0.87	0	29,45,45	1.36	3 (10%)
3	ADP	В	602	-	24,29,29	0.91	0	29,45,45	1.38	4 (13%)
2	TPP	А	601	5	23,27,27	0.48	0	30,40,40	0.58	1 (3%)
6	EDO	Н	603	-	3,3,3	0.42	0	2,2,2	0.38	0
3	ADP	G	602	-	24,29,29	0.89	0	29,45,45	1.33	3 (10%)
2	TPP	G	601	5	23,27,27	0.48	0	30,40,40	0.58	1 (3%)
3	ADP	А	602	-	24,29,29	0.88	0	29,45,45	1.41	4 (13%)
3	ADP	Н	602	-	24,29,29	0.88	0	29,45,45	1.36	3 (10%)
2	TPP	В	601	5	23,27,27	0.47	0	30,40,40	0.59	1 (3%)



Mol Tyr	Turne	Chain R	Dog	Tink	Bond lengths			Bond angles		
IVIOI	туре		nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPP	Н	601	5	23,27,27	0.47	0	30,40,40	0.59	1 (3%)
3	ADP	Е	602	-	24,29,29	0.90	0	29,45,45	1.33	3 (10%)
6	EDO	G	603	-	3,3,3	0.43	0	2,2,2	0.38	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	TPP	E	601	5	-	3/16/17/17	0/2/2/2
2	TPP	D	601	5	-	1/16/17/17	0/2/2/2
3	ADP	С	602	-	-	5/12/32/32	0/3/3/3
4	GOL	А	603	-	-	2/4/4/4	-
4	GOL	В	603	-	-	0/4/4/4	-
2	TPP	F	601	5	-	1/16/17/17	0/2/2/2
3	ADP	D	602	-	-	7/12/32/32	0/3/3/3
2	TPP	С	601	5	-	2/16/17/17	0/2/2/2
6	EDO	С	603	-	-	0/1/1/1	-
6	EDO	F	603	-	-	0/1/1/1	-
3	ADP	F	602	-	-	7/12/32/32	0/3/3/3
3	ADP	В	602	-	-	6/12/32/32	0/3/3/3
2	TPP	А	601	5	-	1/16/17/17	0/2/2/2
6	EDO	Н	603	-	-	0/1/1/1	-
3	ADP	G	602	-	-	7/12/32/32	0/3/3/3
2	TPP	G	601	5	-	3/16/17/17	0/2/2/2
3	ADP	А	602	-	-	5/12/32/32	0/3/3/3
3	ADP	Н	602	-	-	8/12/32/32	0/3/3/3
2	TPP	В	601	5	-	3/16/17/17	0/2/2/2
2	TPP	Н	601	5	-	1/16/17/17	0/2/2/2
3	ADP	E	602	-	-	7/12/32/32	0/3/3/3
6	EDO	G	603	-	-	0/1/1/1	-

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	602	ADP	N3-C2-N1	-3.76	123.56	128.67



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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	Н	602	ADP	N3-C2-N1	-3.75	123.58	128.67
3	G	602	ADP	N3-C2-N1	-3.75	123.59	128.67
3	А	602	ADP	N3-C2-N1	-3.72	123.62	128.67
3	D	602	ADP	N3-C2-N1	-3.72	123.62	128.67

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	601	TPP	C4-C5-C6-C7
2	В	601	TPP	C4-C5-C6-C7
2	В	601	TPP	PA-O3A-PB-O2B
2	С	601	TPP	C4-C5-C6-C7
2	D	601	TPP	C4-C5-C6-C7

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	601	TPP	3	0
2	D	601	TPP	1	0
3	С	602	ADP	1	0
4	А	603	GOL	2	0
4	В	603	GOL	1	0
3	D	602	ADP	1	0
2	С	601	TPP	1	0
3	F	602	ADP	1	0
2	А	601	TPP	1	0
3	G	602	ADP	1	0
2	G	601	TPP	2	0
3	А	602	ADP	1	0
2	В	601	TPP	1	0
2	Н	601	TPP	1	0
6	G	603	EDO	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.









Rings

Torsions





























### 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	542/554~(97%)	-0.34	0 100 100	47, 62, 89, 124	1 (0%)
1	В	539/554~(97%)	-0.27	0 100 100	47, 69, 106, 137	0
1	С	542/554~(97%)	0.01	3 (0%) 85 85	54, 85, 119, 153	1 (0%)
1	D	546/554~(98%)	0.01	3 (0%) 87 86	47, 80, 109, 146	1 (0%)
1	Ε	541/554~(97%)	-0.05	1 (0%) 92 91	51, 76, 108, 140	0
1	$\mathbf{F}$	542/554~(97%)	0.10	0 100 100	49, 79, 118, 144	0
1	G	540/554~(97%)	0.02	4 (0%) 84 83	55, 84, 117, 158	0
1	Н	538/554~(97%)	0.08	3 (0%) 85 85	56, 85, 121, 149	0
All	All	4330/4432 (97%)	-0.05	14 (0%) 90 89	47, 77, 114, 158	3 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	35[A]	MET	2.8
1	D	515	LEU	2.6
1	С	451	VAL	2.5
1	Е	542	LYS	2.5
1	Н	448	GLY	2.5

### 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	$B-factors(Å^2)$	Q < 0.9
6	EDO	Н	603	4/4	0.64	0.18	62,63,64,66	0
6	EDO	G	603	4/4	0.76	0.14	$65,\!65,\!65,\!68$	0
6	EDO	F	603	4/4	0.79	0.10	61,61,62,62	0
4	GOL	А	603	6/6	0.80	0.13	51,52,55,55	0
6	EDO	С	603	4/4	0.86	0.11	$65,\!66,\!66,\!69$	0
5	MG	Н	604	1/1	0.88	0.11	86,86,86,86	0
4	GOL	В	603	6/6	0.90	0.08	59,61,62,66	0
3	ADP	F	602	27/27	0.91	0.09	65,68,73,75	0
3	ADP	G	602	27/27	0.91	0.08	72,74,77,79	0
3	ADP	Е	602	27/27	0.91	0.08	66,68,72,74	0
3	ADP	С	602	27/27	0.92	0.08	71,75,81,83	0
3	ADP	Н	602	27/27	0.92	0.08	70,75,81,83	0
3	ADP	D	602	27/27	0.92	0.08	68,72,79,80	0
3	ADP	В	602	27/27	0.93	0.08	62,65,67,67	0
2	TPP	F	601	26/26	0.93	0.09	66,75,86,86	0
2	TPP	С	601	26/26	0.94	0.08	63,69,81,84	0
2	TPP	Н	601	26/26	0.94	0.09	63,69,89,96	0
3	ADP	А	602	27/27	0.94	0.07	55,58,62,64	0
2	TPP	Е	601	26/26	0.94	0.09	59,65,74,76	0
5	MG	В	604	1/1	0.94	0.08	58,58,58,58	0
2	TPP	G	601	26/26	0.95	0.08	67,74,82,85	0
2	TPP	D	601	26/26	0.95	0.08	69,73,77,79	0
2	TPP	А	601	26/26	0.96	0.07	48,53,57,64	0
5	MG	D	603	1/1	0.96	0.09	72,72,72,72	0
5	MG	F	604	1/1	0.96	0.07	82,82,82,82	0
2	TPP	В	601	26/26	0.96	0.07	53,58,64,66	0
5	MG	C	604	1/1	0.97	0.05	75,75,75,75	0
5	MG	А	604	1/1	0.97	0.08	54,54,54,54	0
5	MG	G	604	1/1	0.98	0.06	80,80,80,80	0
5	MG	E	603	1/1	0.99	0.04	70,70,70,70	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.

