

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

### Aug 2, 2021 – 03:06 pm BST

PDB ID	:	6ZNW
$\operatorname{Title}$	:	Methanosaeta concilii ATP citrate lyase (D541A mutant) in complex with
		(3S)-citryl-CoA.
Authors	:	Verschueren, K.H.G.; Verstraete, K.
Deposited on	:	2020-07-06
$\operatorname{Resolution}$	:	2.12  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 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
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	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)	:	2.23.1

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.12 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 (#Entries)	Similar resolution $(\#Entries, resolution range(Å))$
	(// ======)	
$\mathbf{R}_{free}$	130704	6241(2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	
			41%	
1	А	421	86%	10% 5%
			13%	
2	В	631	92%	5% •



#### $6\mathrm{ZNW}$

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8294 atoms, of which 5 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 Citrate lyase, subunit 1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	402	Total 3187	$\begin{array}{c} \mathrm{C} \\ 2045 \end{array}$	N 516	O 615	S 11	0	0	0

• Molecule 2 is a protein called Methanosaeta concilii ACLY-B.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	616	Total 4731	C 3011	N 811	O 882	S 27	0	1	0

• Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 18	С 6	Н 5	O 7	5	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand



of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mg 1 1	0	0

• Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 5	0 4	Р 1	0	0

• Molecule 6 is (3S)-citryl-Coenzyme A (three-letter code: Q5B) (formula: C<sub>27</sub>H<sub>42</sub>N<sub>7</sub>O<sub>22</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Α	ton	ıs			ZeroOcc	AltConf
6	В	1	Total 60	С 27	N 7	O 22	Р 3	S 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	30	Total O 30 30	0	0
7	В	262	Total         O           262         262	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: Citrate lyase, subunit 1

# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	73.53Å $154.37$ Å $276.05$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Bosolution} \left( \overset{\wedge}{\mathbf{A}} \right)$	79.04 - 2.12	Depositor
	79.04 - 2.12	EDS
% Data completeness	99.2 (79.04-2.12)	Depositor
(in resolution range)	99.2(79.04-2.12)	EDS
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.25 (at 2.12 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
D D.	0.186 , $0.203$	Depositor
$\Pi, \Pi_{free}$	0.194 , $0.212$	DCC
$R_{free}$ test set	4490 reflections $(5.07\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 73.8	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8294	wwPDB-VP
Average B, all atoms $(Å^2)$	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.70% 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: PO4, FLC, MG, Q5B

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		
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.33	0/3257	0.54	0/4412	
2	В	0.47	0/4819	0.58	0/6507	
All	All	0.42	0/8076	0.57	0/10919	

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	3187	0	3131	29	0
2	В	4731	0	4802	19	0
3	А	13	5	5	0	0
4	А	1	0	0	0	0
5	А	5	0	0	1	0
6	В	60	0	0	0	0
7	А	30	0	0	0	0
7	В	262	0	0	0	0
All	All	8289	5	7938	46	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.



Atom 1	A tama D	Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:A:114:HIS:HB2	1:A:204:THR:HG21	1.59	0.84	
1:A:204:THR:HG22	1:A:205:PHE:H	1.51	0.75	
2:B:613:GLU:O	2:B:617:GLN:HG2	1.90	0.71	
1:A:131:ILE:HB	1:A:151:ILE:CG1	2.28	0.64	
5:A:503:PO4:O4	2:B:275:HIS:NE2	2.28	0.63	
2:B:8:LEU:HD21	2:B:136:ILE:HD11	1.81	0.62	
1:A:204:THR:HG22	1:A:205:PHE:N	2.17	0.59	
1:A:276:MET:HE1	1:A:318:THR:HA	1.85	0.59	
1:A:273:VAL:HG22	1:A:299:MET:HA	1.84	0.57	
1:A:12:LYS:HZ3	1:A:215:MET:HB2	1.70	0.56	
2:B:60:THR:CG2	2:B:337:PRO:HG3	2.37	0.55	
1:A:131:ILE:HB	1:A:151:ILE:HG12	1.91	0.52	
1:A:33:ALA:HB1	1:A:44:LEU:HD21	1.92	0.51	
1:A:311:THR:HG21	1:A:353:LYS:HE3	1.93	0.51	
2:B:21:GLN:HG3	2:B:87:PHE:CG	2.47	0.50	
1:A:35:VAL:HG21	1:A:86:LEU:HD11	1.94	0.49	
1:A:114:HIS:CB	1:A:204:THR:HG21	2.38	0.49	
1:A:335:VAL:HG11	1:A:416:ALA:HB1	1.95	0.49	
1:A:373:ILE:HB	1:A:400:ILE:HG12	1.94	0.48	
1:A:131:ILE:HB	1:A:151:ILE:HG13	1.95	0.48	
1:A:35:VAL:HG11	1:A:86:LEU:HD11	1.95	0.47	
1:A:341:ALA:HB1	2:B:184:GLU:HB2	1.96	0.47	
2:B:79:PRO:O	2:B:105:THR:OG1	2.29	0.47	
2:B:239:GLU:HA	2:B:242:ILE:HD12	1.97	0.46	
1:A:12:LYS:NZ	1:A:215:MET:HB2	2.31	0.46	
2:B:317:ASP:O	2:B:321:THR:HG23	2.15	0.46	
1:A:276:MET:HE2	1:A:321:ILE:HD12	1.98	0.45	
1:A:326:THR:HG21	1:A:365:LYS:HD3	1.99	0.45	
2:B:60:THR:HG23	2:B:337:PRO:HG3	1.97	0.45	
2:B:9:PHE:CZ	2:B:151:ILE:HD11	2.51	0.45	
1:A:344:ASN:O	2:B:156:GLY:HA2	2.17	0.45	
2:B:60:THR:HG22	2:B:337:PRO:HG3	1.99	0.45	
2:B:29:LEU:CD2	2:B:40:PRO:HB3	2.45	0.44	
1:A:134:SER:HB2	1:A:148:VAL:HG22	1.99	0.44	
1:A:35:VAL:HG11	1:A:86:LEU:HD21	1.98	0.43	
2:B:336:ILE:HG12	2:B:337:PRO:HD2	1.99	0.43	
1:A:337:LEU:HD23	1:A:374:TYR:HB2	2.00	0.43	
1:A:261:SER:O	1:A:305:TYR:HA	2.18	0.43	
1:A:204:THR:CG2	1:A:205:PHE:H	2.24	0.42	
1:A:252:LYS:NZ	1:A:264:LEU:H	2.17	0.42	

All (46) 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)
2:B:177:LYS:HD3	2:B:233:GLU:HG2	2.02	0.42
2:B:246:LEU:HD21	2:B:299:ALA:HB2	2.01	0.42
2:B:212:MET:HE2	2:B:230:CYS:HB2	2.02	0.41
2:B:522:ALA:CB	2:B:546:ILE:HD13	2.51	0.41
1:A:326:THR:OG1	1:A:365:LYS:HB3	2.21	0.41
1:A:254:ILE:HG22	1:A:262:LEU:HD13	2.02	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	396/421~(94%)	376~(95%)	19~(5%)	1 (0%)	41	40
2	В	615/631~(98%)	604 (98%)	11 (2%)	0	100	100
All	All	1011/1052~(96%)	980 (97%)	30 (3%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	173	GLY

#### 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	339/353~(96%)	332~(98%)	7(2%)	53 57		
2	В	498/510~(98%)	495~(99%)	3~(1%)	86 90		
All	All	837/863~(97%)	827~(99%)	10 (1%)	71 77		

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

Mol	Chain	Res	Type
1	А	86	LEU
1	А	159	ILE
1	А	233	GLU
1	А	234	LEU
1	А	273	VAL
1	А	304	GLU
1	А	370	ASP
2	В	227	MET
2	В	294	PHE
2	В	307	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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 length (or angles).

Mal	Type Chain Bes		Link	Bond lengths			Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	Q5B	В	701	-	48,62,62	0.64	0	60,93,93	1.05	4 (6%)
3	FLC	А	501	4	3,12,12	0.58	0	$3,\!17,\!17$	0.94	0
5	PO4	А	503	4	4,4,4	2.60	1 (25%)	6,6,6	0.55	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
6	Q5B	В	701	-	-	11/54/83/83	0/3/3/3
3	FLC	А	501	4	-	3/6/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	А	503	PO4	P-01	4.36	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	В	701	Q5B	C23-C24-C25	3.74	120.97	114.98
6	В	701	Q5B	C10-C13-N4	2.24	123.76	120.35
6	В	701	Q5B	O9-P2-O12	-2.13	101.16	109.39
6	В	701	Q5B	O8-C7-C6	2.12	117.19	111.17

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	701	Q5B	C3-O-P-O1
6	В	701	Q5B	C3-O-P-O2
6	В	701	Q5B	C4-O6-P1-O3
3	А	501	FLC	CA-CB-CG-CGC
6	В	701	Q5B	C21-C22-C23-C24



	6	1	1 5	
Mol	Chain	Res	Type	Atoms
6	В	701	Q5B	O6-C4-C5-O7
6	В	701	Q5B	O6-C4-C5-C6
6	В	701	Q5B	C4-O6-P1-O4
6	В	701	Q5B	C4-O6-P1-O5
3	А	501	FLC	CBC-CB-CG-CGC
6	В	701	Q5B	C21-C22-C23-O20
3	А	501	FLC	OHB-CB-CG-CGC
6	В	701	Q5B	C3-O-P-O3
6	В	701	Q5B	C21-C22-C23-C26

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	503	PO4	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<sup>th</sup> 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	< <b>RSRZ</b> >	#RSR	Z>2	2	$OWAB(Å^2)$	Q<0.9
1	А	402/421~(95%)	2.34	172 (42%)	0	0	71, 143, 199, 211	0
2	В	616/631~(97%)	1.08	82~(13%)	3	4	30, 78, 127, 150	0
All	All	1018/1052~(96%)	1.57	254 (24%)	0	0	30, 99, 188, 211	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	44	LEU	14.3
1	А	118	TYR	11.0
1	А	211	VAL	10.9
1	А	198	VAL	10.0
1	А	204	THR	9.8
1	А	56	LEU	9.5
1	А	75	LEU	9.3
1	А	108	ILE	9.2
1	А	182	PHE	8.9
1	А	60	PRO	8.6
1	А	32	LEU	8.1
1	А	34	LEU	8.1
1	А	200	ILE	8.1
1	А	159	ILE	7.9
1	А	241	GLY	7.6
1	А	213	LEU	7.6
1	А	161	ALA	7.5
1	А	133	PHE	7.3
1	А	27	SER	7.3
1	A	74	LEU	7.1
1	A	121	ALA	7.1
1	A	170	ALA	7.0
1	A	168	LEU	6.9
1	A	79	TRP	6.9



Mol	Chain	Res	Type	RSRZ
1	А	164	VAL	6.8
1	А	64	PHE	6.7
1	А	120	VAL	6.6
1	А	210	ILE	6.5
1	А	178	LEU	6.5
1	А	208	ARG	6.5
1	А	122	ILE	6.4
1	А	26	PHE	6.2
1	А	203	PHE	6.2
1	А	184	THR	6.1
1	А	209	GLY	6.1
1	А	183	ILE	6.1
1	А	28	TYR	5.9
1	A	111	PHE	5.9
1	A	212	PRO	5.9
1	А	197	TYR	5.9
1	А	50	TRP	5.9
1	А	14	LEU	5.8
1	А	57	VAL	5.8
1	А	179	VAL	5.7
1	А	205	PHE	5.7
1	А	151	ILE	5.7
1	А	107	LEU	5.6
1	А	186	LEU	5.6
1	А	174	ASP	5.6
1	А	16	ALA	5.6
2	В	242	ILE	5.6
2	В	294	PHE	5.6
1	А	105	TYR	5.6
1	A	116	GLU	5.5
1	A	58	VAL	5.4
1	A	86	LEU	5.3
1	A	23	LEU	5.3
1	A	51	LEU	5.3
1	A	82	ALA	5.2
1	A	286	TYR	5.1
1	A	12	LYS	5.1
1	A	103	LEU	5.1
1	A	233	GLU	5.0
1	A	119	TYR	5.0
1	A	49	PRO	5.0
1	A	217	ALA	5.0



Mol	Chain	Res	Type	RSRZ
1	А	72	LEU	4.9
1	А	85	TYR	4.9
1	А	15	LEU	4.8
1	А	73	VAL	4.8
1	А	189	PHE	4.8
1	А	175	LYS	4.7
1	А	167	LYS	4.5
1	А	55	ARG	4.5
1	А	149	ILE	4.4
1	А	45	GLU	4.4
1	А	43	GLY	4.4
1	А	52	LYS	4.4
1	А	207	GLY	4.3
1	А	96	ILE	4.3
1	А	337	LEU	4.3
1	А	240	PHE	4.3
1	А	165	GLY	4.3
1	А	413	VAL	4.2
1	А	20	PRO	4.2
1	А	297	ASP	4.1
1	А	335	VAL	4.1
1	А	94	VAL	4.0
2	В	243	ILE	4.0
2	В	273	PHE	4.0
1	А	33	ALA	4.0
1	А	70	LEU	4.0
2	В	325	VAL	4.0
1	А	9	TYR	3.9
1	А	199	GLU	3.9
1	A	216	VAL	3.9
2	В	296	GLN	3.9
1	А	18	TYR	3.9
1	A	48	ASN	3.8
1	A	19	LEU	3.8
1	A	29	LYS	3.7
1	A	117	GLU	3.7
2	В	300	TYR	3.6
1	A	59	LYS	3.6
1	А	290	ILE	3.6
1	A	22	TYR	3.6
2	В	322	ARG	3.6
1	А	374	TYR	3.6



Mol	Chain	Res	Type	RSRZ
1	А	110	PRO	3.6
2	В	258	TRP	3.6
1	А	131	ILE	3.5
2	В	271	VAL	3.5
1	А	180	GLU	3.5
1	А	83	LYS	3.5
1	А	171	GLU	3.5
2	В	283	GLU	3.5
1	А	63	LEU	3.5
1	А	236	PHE	3.3
1	А	47	GLU	3.3
1	А	293	LEU	3.3
1	А	17	ARG	3.3
1	A	416	ALA	3.3
1	А	195	PHE	3.3
2	В	280	ALA	3.2
2	В	305	PHE	3.2
1	А	412	ILE	3.2
1	А	266	ILE	3.1
2	В	254	PRO	3.1
1	А	162	LEU	3.1
2	В	256	VAL	3.1
2	В	324	ILE	3.1
1	А	267	LEU	3.0
1	А	242	ARG	3.0
1	А	172	LEU	3.0
1	А	25	ASP	3.0
1	А	92	LEU	3.0
1	А	246	LYS	2.9
2	В	229	ALA	2.9
1	A	135	MET	2.9
1	A	31	ASN	2.9
1	A	40	ASP	2.9
2	В	134	ILE	2.8
1	A	206	SER	2.8
1	A	181	GLU	2.8
2	В	278	ALA	2.8
1	A	234	LEU	2.8
2	В	231	LEU	2.8
1	A	35	VAL	2.8
2	В	270	SER	2.8
2	В	207	TYR	2.8



6ZNW
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Mol	Chain	Res	Type	RSRZ
1	А	112	THR	2.8
2	В	440	CYS	2.7
1	А	336	LEU	2.7
1	A	169	PRO	2.7
1	А	190	TYR	2.7
1	А	76	ASP	2.7
2	В	240	TYR	2.7
1	А	396	LEU	2.7
2	В	8	LEU	2.7
2	В	430	CYS	2.6
2	В	318	MET	2.6
2	В	213	LEU	2.6
1	А	187	TRP	2.6
2	В	269	ALA	2.6
1	А	176	ARG	2.6
1	А	419	GLU	2.6
1	А	106	PHE	2.6
1	А	6	ILE	2.6
1	А	231	TRP	2.6
2	В	618	CYS	2.6
2	В	299	ALA	2.5
2	В	405	ILE	2.5
1	А	249	LEU	2.5
2	В	230	CYS	2.5
1	А	408	HIS	2.5
1	А	273	VAL	2.5
1	А	215	MET	2.5
1	А	102	ARG	2.5
1	А	78	ASP	2.5
2	В	340	TYR	2.5
1	А	163	ASP	2.5
1	А	177	ALA	2.5
1	А	185	ALA	2.5
1	А	415	LEU	2.5
2	В	220	GLU	2.5
1	А	42	GLU	2.5
2	В	31	PHE	2.5
2	В	291	ASN	2.4
2	В	136	ILE	2.4
1	А	324	LEU	2.4
1	А	202	PRO	2.4
2	В	234	LEU	2.4



6ZNW
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Mol	Chain	Res	Type	RSRZ	
1	А	95	THR	2.4	
1	А	100	THR	2.4	
1	А	99	ILE	2.4	
1	А	366	LEU	2.4	
2	В	444	LEU	2.4	
2	В	247	LYS	2.4	
2	В	295	ARG	2.4	
2	В	443	LEU	2.3	
2	В	616	ILE	2.3	
1	А	7	ARG	2.3	
2	В	409	ILE	2.3	
2	В	588	ILE	2.3	
1	А	214	ASP	2.3	
1	A	244	PRO	2.3	
2	В	105	THR	2.3	
2	В	392	TRP	2.3	
2	В	158	ILE	2.2	
2	В	585	ILE	2.2	
2	В	255	LEU	2.2	
2	В	426	ILE	2.2	
1	А	134	SER	2.2	
2	В	161	ILE	2.2	
2	В	252	THR	2.2	
1	А	193	THR	2.2	
1	А	417	LEU	2.1	
2	В	217	LEU	2.1	
2	В	439	LEU	2.1	
2	В	584	LEU	2.1	
1	А	11	ALA	2.1	
1	A	113	PRO	2.1	
2	В	108	ILE	2.1	
$2^{-}$	B	359	ILE	2.1	
1	A	219	LEU	2.1	
2	В	427	VAL	2.1	
2	В	566	VAL	2.1	
2	В	106	ILE	2.1	
2	В	292	ASP	2.1	
2	В	221	ARG	2.1	
2	В	436	ILE	2.1	
2	В	141	VAL	2.1	
2	B	56	ALA	2.1	
2	В	219	TYR	2.1	



Mol	Chain	hain Res Type		RSRZ	
2	В	388	ILE	2.1	
2	В	435	LEU	2.1	
2	В	419	VAL	2.1	
1	А	362	TYR	2.1	
2	В	437	SER	2.0	
2	В	216	ILE	2.0	
2	В	185	ALA	2.0	
2	В	303	ARG	2.0	
1	А	373	ILE	2.0	
2	В	575	LEU	2.0	
2	В	172	VAL	2.0	
1	А	317	TYR	2.0	
2	В	327	LYS	2.0	
1	А	276	MET	2.0	
1	А	53	THR	2.0	
2	В	349	ILE	2.0	
2	В	374	LEU	2.0	
2	В	357	CYS	2.0	
1	A	398	VAL	2.0	
2	В	532	LYS	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	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	А	502	1/1	0.71	0.08	113,113,113,113	0
5	PO4	А	503	5/5	0.83	0.17	$106,\!107,\!107,\!107$	0
3	FLC	А	501	13/13	0.94	0.14	75,77,92,92	5



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	Q5B	В	701	60/60	0.95	0.15	$43,\!65,\!85,\!86$	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.

