

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

Dec 18, 2023 - 09:32 am GMT

PDB ID	:	2WTV
Title	:	Aurora-A Inhibitor Structure
Authors	:	Kosmopoulou, M.; Bayliss, R.
Deposited on	:	2009-09-22
Resolution	:	2.40  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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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

# 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 2.40 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.



Motrie	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	А	287	Х	-	-	-
1	TPO	В	287	Х	-	-	-
1	TPO	С	287	Х	-	-	-
1	TPO	D	287	X	-	-	-
3	EDO	В	1399	-	-	Х	-
4	ACT	С	1393	-	-	Х	-



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9657 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.

• Molecule 1 is a protein called SERINE/THREONINE-PROTEIN KINASE 6 AURORA/IPL1-RELATED KINASE 1, BREAST TUMOR-AMPLIFIED KINASE, AURORA-A, AURORA-RELATED KINASE 1, HARK1.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Δ	265	Total	С	Ν	0	Р	S	0	1	0
	A	205	2190	1400	385	396	2	7	0	1	U
1	В	264	Total	С	Ν	0	Р	S	0	0	0
1	D	204	2158	1383	375	391	2	7	0		
1	C	264	Total	С	Ν	0	Р	S	0	1	0
1		204	2170	1390	376	395	2	7	0	1	0
1	л	265	Total	С	Ν	0	Р	S	0	0	0
1	D	205	2172	1390	378	395	2	7	U	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	215	ARG	LEU	engineered mutation	UNP 014965
А	217	GLU	THR	engineered mutation	UNP 014965
А	220	LYS	ARG	engineered mutation	UNP 014965
В	215	ARG	LEU	engineered mutation	UNP 014965
В	217	GLU	THR	engineered mutation	UNP 014965
В	220	LYS	ARG	engineered mutation	UNP 014965
С	215	ARG	LEU	engineered mutation	UNP 014965
С	217	GLU	THR	engineered mutation	UNP 014965
С	220	LYS	ARG	engineered mutation	UNP 014965
D	215	ARG	LEU	engineered mutation	UNP 014965
D	217	GLU	THR	engineered mutation	UNP 014965
D	220	LYS	ARG	engineered mutation	UNP 014965

• Molecule 2 is 4-{[9-CHLORO-7-(2,6-DIFLUOROPHENYL)-5H-PYRIMIDO[5,4-D] [2]BENZAZEPIN-2-YL]AMINO}BENZOIC ACID (three-letter code: ZZL) (formula: C<sub>25</sub>H<sub>15</sub>ClF<sub>2</sub>N<sub>4</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Λ	1	Total C Cl F N O	0	0
	Л	T	34  25  1  2  4  2	0	0
9	В	1	Total C Cl F N O	0	0
	D		34  25  1  2  4  2	0	0
9	С	1	Total C Cl F N O	0	0
	U	T	34  25  1  2  4  2	0	0
9	Л	1	Total C Cl F N O	0	0
	D	L	34  25  1  2  4  2	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





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

• Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	А	1	Total 4	C 2	O 2	0	0

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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	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

• Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total C 4 2	0 1	${f S}$ 1	0	0
5	В	1	Total C 4 2	0 1	S 1	0	0

• Molecule 6 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	165	Total O 165 165	0	0
6	В	197	Total O 197 197	0	0
6	С	197	Total O 197 197	0	0
6	D	184	Total O 184 184	0	0

SEQUENCE-PLOTS INFOmissingINFO



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants	118.71Å 118.71Å 135.89Å	Deneiten
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	19.78 - 2.40	Depositor
Resolution (A)	56.68 - 2.40	EDS
% Data completeness	94.7 (19.78-2.40)	Depositor
(in resolution range)	99.5(56.68-2.40)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.98 (at 2.40 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
P. P.	0.164 , $0.211$	Depositor
$\Pi, \Pi_{free}$	0.164 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	27.0	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, $35.1$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
	0.018 for -h,-k,l	
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
	0.018 for -k,-h,-l	
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9657	wwPDB-VP
Average B, all atoms $(Å^2)$	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.25% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: CME, EDO, DMS, ZZL, ACT, TPO

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		Bo	nd lengths	Bond angles		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.33	0/2211	0.50	0/2984	
1	В	0.42	1/2178~(0.0%)	0.50	1/2941~(0.0%)	
1	С	0.43	1/2190~(0.0%)	0.51	1/2956~(0.0%)	
1	D	0.33	0/2192	0.51	0/2960	
All	All	0.38	2/8771~(0.0%)	0.51	2/11841~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	1	0
1	В	1	0
1	С	1	0
1	D	1	0
All	All	4	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	126	ARG	NE-CZ	13.07	1.50	1.33
1	В	126	ARG	NE-CZ	12.99	1.50	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	126	ARG	CD-NE-CZ	-9.38	110.46	123.60
1	С	126	ARG	CD-NE-CZ	-7.96	112.45	123.60



Mol	Chain	Res	Type	Atom
1	А	287	TPO	CB
1	В	287	TPO	CB
1	С	287	TPO	CB
1	D	287	TPO	CB

All (4) chirality outliers are listed below:

There are no planarity outliers.

#### 4.2 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	2190	0	2171	33	0
1	В	2158	0	2133	45	0
1	С	2170	0	2142	42	0
1	D	2172	0	2147	43	0
2	А	34	0	15	0	0
2	В	34	0	15	1	0
2	С	34	0	15	0	0
2	D	34	0	15	0	0
3	А	4	0	6	1	0
3	В	24	0	36	7	0
3	С	12	0	18	2	0
3	D	4	0	6	0	0
4	А	8	0	6	0	0
4	В	12	0	9	0	0
4	С	8	0	6	3	0
4	D	8	0	6	1	0
5	А	4	0	6	0	0
5	В	4	0	6	0	0
6	А	165	0	0	3	0
6	В	197	0	0	6	0
6	С	197	0	0	5	0
6	D	184	0	0	5	0
All	All	9657	0	8758	163	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 9.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HH21	1:B:340:ARG:HG3	0.94	1.03
1:D:286:ARG:HD3	1:D:291:GLY:HA2	1.40	1.02
1:B:340:ARG:HG3	1:B:340:ARG:NH2	1.67	1.00
1:A:286:ARG:HD3	1:A:291:GLY:HA2	1.46	0.93
1:B:340:ARG:HH21	1:B:340:ARG:CG	1.82	0.90

The worst 5 of 163 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

There are no symmetry-related clashes.

#### 4.3 Torsion angles (i)

#### 4.3.1 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	261/285~(92%)	253~(97%)	8(3%)	0	100	100
1	В	259/285~(91%)	254 (98%)	5 (2%)	0	100	100
1	С	260/285~(91%)	253~(97%)	7 (3%)	0	100	100
1	D	260/285~(91%)	254 (98%)	6 (2%)	0	100	100
All	All	1040/1140~(91%)	1014 (98%)	26~(2%)	0	100	100

There are no Ramachandran outliers to report.

#### 4.3.2 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	Perce	entiles
1	А	229/248~(92%)	215~(94%)	14 (6%)	18	30
1	В	225/248~(91%)	215~(96%)	10 (4%)	28	45
1	С	226/248~(91%)	215~(95%)	11 (5%)	25	40
1	D	226/248~(91%)	212 (94%)	14 (6%)	18	29
All	All	906/992~(91%)	857~(95%)	49 (5%)	22	36

5 of 49 residues with a non-rotameric side chain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	С	253	ILE
1	D	130	LEU
1	С	271	LYS
1	С	343	ARG
1	D	175	GLU

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

Mol	Chain	Res	Type
1	А	223	GLN
1	В	231	GLN
1	С	231	GLN
1	D	223	GLN

#### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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



Mal	Type	Chain	Dog	Link	B	ond leng	$\operatorname{gths}$	Bond angles		
MOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
1	TPO	A	288	1	8,10,11	0.77	0	$10,\!14,\!16$	1.21	0
1	TPO	В	288	1	8,10,11	0.87	0	$10,\!14,\!16$	0.92	0
1	CME	D	290	1	8,9,10	0.81	0	5, 9, 11	1.14	0
1	CME	А	290	1	8,9,10	0.82	0	5, 9, 11	1.27	0
1	CME	В	290	1	8,9,10	0.83	0	5, 9, 11	0.90	0
1	TPO	С	288	1	8,10,11	0.92	0	10,14,16	0.81	0
1	TPO	С	287	1	8,10,11	0.81	0	10,14,16	1.26	1 (10%)
1	TPO	D	287	1	8,10,11	0.67	0	10,14,16	1.40	0
1	TPO	D	288	1	8,10,11	0.73	0	10,14,16	1.23	1 (10%)
1	CME	С	290	1	8,9,10	0.81	0	5, 9, 11	0.82	0
1	TPO	А	287	1	8,10,11	0.71	0	$10,\!14,\!16$	1.44	0
1	TPO	В	287	1	8,10,11	0.82	0	10,14,16	1.31	1 (10%)

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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
1	TPO	А	288	1	-	1/9/11/13	-
1	TPO	В	288	1	-	1/9/11/13	-
1	CME	D	290	1	-	2/5/8/10	-
1	CME	А	290	1	-	1/5/8/10	-
1	TPO	D	287	1	1/1/3/4	4/9/11/13	-
1	CME	В	290	1	-	2/5/8/10	-
1	TPO	С	287	1	1/1/3/4	4/9/11/13	-
1	TPO	С	288	1	-	1/9/11/13	-
1	TPO	D	288	1	-	3/9/11/13	-
1	CME	С	290	1	-	1/5/8/10	-
1	TPO	А	287	1	1/1/3/4	4/9/11/13	-
1	TPO	В	287	1	1/1/3/4	6/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	D	288	TPO	O3P-P-O2P	2.49	117.14	107.64
1	В	287	TPO	CG2-CB-CA	-2.18	108.86	113.16
1	С	287	TPO	CB-CA-N	-2.04	101.02	114.41



Mol	Chain	Res	Type	Atom
1	А	287	TPO	CB
1	В	287	TPO	CB
1	С	287	TPO	CB
1	D	287	TPO	CB

All (4) chirality outliers are listed below:

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	287	TPO	N-CA-CB-OG1
1	А	287	TPO	C-CA-CB-CG2
1	А	287	TPO	O-C-CA-CB
1	А	290	CME	SD-CE-CZ-OH
1	В	287	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	290	CME	1	0
1	С	290	CME	1	0

#### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

26 ligands are modelled in this entry.

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

Mal	Turne	Chain		Tink	Bond lengths			Bond angles		
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	ZZL	С	1392	-	35,38,38	1.63	7 (20%)	45,55,55	2.41	10 (22%)



Mal	Tuno	Chain	Dog	Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	ACT	А	1393	-	$3,\!3,\!3$	1.39	1 (33%)	3,3,3	0.89	0	
5	DMS	А	1394	-	3,3,3	0.78	0	3,3,3	1.52	1 (33%)	
4	ACT	С	1393	-	3,3,3	1.39	1 (33%)	3,3,3	0.78	0	
3	EDO	В	1399	-	3,3,3	0.51	0	2,2,2	0.67	0	
3	EDO	С	1391	-	3,3,3	0.49	0	2,2,2	0.75	0	
3	EDO	В	1398	-	3,3,3	0.46	0	2,2,2	0.80	0	
3	EDO	С	1390	-	3,3,3	0.50	0	2,2,2	0.78	0	
2	ZZL	D	1390	-	35,38,38	1.59	8 (22%)	45,55,55	2.32	11 (24%)	
3	EDO	В	1396	-	3,3,3	0.49	0	2,2,2	0.67	0	
4	ACT	В	1393	-	3,3,3	1.41	1 (33%)	3,3,3	0.71	0	
2	ZZL	В	1390	-	35,38,38	1.61	8 (22%)	45,55,55	2.42	11 (24%)	
2	ZZL	А	1390	-	35,38,38	1.54	5 (14%)	45,55,55	2.41	11 (24%)	
3	EDO	А	1391	-	3,3,3	0.49	0	2,2,2	0.71	0	
3	EDO	В	1397	-	3,3,3	0.48	0	2,2,2	1.01	0	
4	ACT	В	1392	-	$3,\!3,\!3$	1.50	1 (33%)	3,3,3	0.97	0	
4	ACT	А	1392	-	3,3,3	1.42	1 (33%)	3,3,3	0.92	0	
5	DMS	В	1391	-	3,3,3	0.78	0	3,3,3	1.58	1 (33%)	
3	EDO	D	1391	-	3,3,3	0.48	0	2,2,2	0.76	0	
4	ACT	D	1392	-	3,3,3	1.43	1 (33%)	3,3,3	0.83	0	
3	EDO	С	1395	-	3,3,3	0.48	0	2,2,2	0.76	0	
3	EDO	В	1394	-	3,3,3	0.48	0	2,2,2	0.73	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	ZZL	С	1392	-	-	2/12/25/25	0/4/5/5
2	ZZL	D	1390	-	-	2/12/25/25	0/4/5/5
3	EDO	В	1396	-	-	1/1/1/1	-
3	EDO	D	1391	-	-	1/1/1/1	-
2	ZZL	В	1390	-	-	2/12/25/25	0/4/5/5
2	ZZL	А	1390	-	-	2/12/25/25	0/4/5/5
3	EDO	В	1399	-	-	1/1/1/1	-
3	EDO	А	1391	-	-	0/1/1/1	-
3	EDO	C	1395	-	-	0/1/1/1	-
3	EDO	C	1391	-	-	0/1/1/1	-
3	EDO	В	1394	-	-	1/1/1/1	-

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The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	С	1392	ZZL	C09-N08	3.96	1.44	1.36
2	D	1390	ZZL	C09-N08	3.79	1.44	1.36
2	В	1390	ZZL	C09-N08	3.74	1.44	1.36
2	А	1390	ZZL	C09-N08	3.72	1.44	1.36
2	В	1390	ZZL	C09-N10	3.38	1.39	1.34

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1390	ZZL	C13-N14-C15	9.98	128.80	117.48
2	С	1392	ZZL	C13-N14-C15	9.87	128.68	117.48
2	А	1390	ZZL	C13-N14-C15	9.07	127.77	117.48
2	D	1390	ZZL	C13-N14-C15	8.04	126.60	117.48
2	А	1390	ZZL	C24-C15-C16	-7.06	109.91	118.10

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	1398	EDO	O1-C1-C2-O2
3	D	1391	EDO	O1-C1-C2-O2
3	С	1390	EDO	O1-C1-C2-O2
3	В	1394	EDO	O1-C1-C2-O2
3	В	1399	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	1393	ACT	3	0
3	В	1399	EDO	5	0
3	В	1398	EDO	1	0
3	С	1390	EDO	2	0
2	В	1390	ZZL	1	0

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Chain Torsions Mol Type  $\mathbf{Res}$ Link Chirals Rings EDO 3 В 1398 1/1/1/1\_ \_ \_ 3 EDO В 1397 1/1/1/1---3 EDO С 1/1/1/11390\_ \_ \_

		1	1 0		
$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
3	А	1391	EDO	1	0
3	В	1397	EDO	1	0
4	D	1392	ACT	1	0
3	В	1394	EDO	1	0

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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 similar 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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	262/285~(91%)	-0.56	0 100 100	15, 27, 51, 69	0
1	В	261/285~(91%)	-0.55	1 (0%) 92 91	16, 27, 49, 71	0
1	С	261/285~(91%)	-0.58	1 (0%) 92 91	16, 27, 50, 72	0
1	D	262/285~(91%)	-0.54	0 100 100	13, 28, 50, 68	0
All	All	1046/1140~(91%)	-0.56	2 (0%) 95 94	13, 27, 51, 72	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	253	ILE	2.3
1	С	253	ILE	2.2

### 5.2 Non-standard residues in protein, DNA, RNA chains (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
1	CME	А	290	10/11	0.95	0.09	$27,\!42,\!65,\!67$	0
1	TPO	А	287	11/12	0.96	0.14	34,47,68,71	0
1	TPO	С	287	11/12	0.96	0.13	21,32,60,61	0
1	CME	D	290	10/11	0.96	0.11	31,40,69,70	0
1	TPO	D	287	11/12	0.97	0.11	37,48,67,69	0
1	TPO	А	288	11/12	0.98	0.13	29,37,48,53	0
1	CME	С	290	10/11	0.98	0.10	18,25,30,34	0
1	TPO	В	287	11/12	0.98	0.13	20,25,61,70	0
1	TPO	D	288	11/12	0.98	0.12	32,39,48,52	0
1	CME	В	290	10/11	0.98	0.09	$15,\!25,\!30,\!37$	0

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Mol	Type	Chain	Res	Atoms	RSCC	$\mathbf{RSR}$	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
1	TPO	В	288	11/12	0.99	0.11	14,22,23,24	0
1	TPO	С	288	11/12	0.99	0.13	16,20,27,28	0

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#### 5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.4 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
5	DMS	В	1391	4/4	0.80	0.14	18,24,35,74	0
4	ACT	В	1393	4/4	0.89	0.24	34,65,72,77	0
3	EDO	В	1397	4/4	0.91	0.17	46,49,50,58	0
4	ACT	В	1392	4/4	0.93	0.12	31,34,48,59	0
3	EDO	В	1398	4/4	0.93	0.15	39,49,50,53	0
5	DMS	А	1394	4/4	0.93	0.12	16,28,32,67	0
3	EDO	С	1395	4/4	0.93	0.12	38,41,50,74	0
4	ACT	В	1400	4/4	0.94	0.15	44,50,51,53	0
4	ACT	С	1394	4/4	0.94	0.18	40,46,61,70	0
3	EDO	В	1399	4/4	0.95	0.15	31,40,44,51	0
3	EDO	В	1396	4/4	0.96	0.15	39,44,47,61	0
4	ACT	С	1393	4/4	0.96	0.10	42,45,48,52	0
4	ACT	А	1392	4/4	0.96	0.09	43,52,56,59	0
3	EDO	В	1394	4/4	0.96	0.13	41,54,55,58	0
3	EDO	С	1390	4/4	0.96	0.17	36,43,46,53	0
3	EDO	В	1395	4/4	0.97	0.14	34,46,54,66	0
4	ACT	D	1392	4/4	0.97	0.20	46,52,59,68	0
4	ACT	D	1393	4/4	0.97	0.10	38,42,44,45	0
4	ACT	А	1393	4/4	0.97	0.09	34,37,43,52	0
3	EDO	D	1391	4/4	0.97	0.15	50,51,59,61	0
2	ZZL	D	1390	34/34	0.98	0.13	10,18,29,45	0
3	EDO	С	1391	4/4	0.98	0.35	30,32,36,38	0
3	EDO	A	1391	4/4	0.98	0.14	31,38,48,56	0
2	ZZL	В	1390	34/34	0.98	0.11	15,22,46,67	0
2	ZZL	С	1392	34/34	0.98	0.10	14,21,41,66	0
2	ZZL	А	1390	34/34	0.99	0.12	11,18,31,38	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.











## 5.5 Other polymers (i)

There are no such residues in this entry.

