

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

#### Oct 15, 2023 – 06:23 AM EDT

PDB ID	:	7SH1
Title	:	Class II UvrA protein - Ecm16
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Deposited on	:	2021-10-07
Resolution	:	2.04  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 2.04 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.



Motria	Whole archive	Similar resolution
wietric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	812	3% 69%	7%	23%			
1	В	812	70%	7%	23%			



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10007 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	Atoms				ZeroOcc	AltConf	Trace	
1	А	626	Total 4650	C 2892	N 842	O 896	S 20	0	1	0
1	В	626	Total 4626	C 2870	N 837	O 899	S 20	0	0	0

• Molecule 1 is a protein called Excinuclease ABC subunit UvrA.

Chain	Residue	Modelled	Actual	Actual Comment	
А	-19	MET	-	initiating methionine	UNP Q0X0A9
А	-18	GLY	-	expression tag	UNP Q0X0A9
А	-17	SER	-	expression tag	UNP Q0X0A9
А	-16	SER	-	expression tag	UNP Q0X0A9
А	-15	HIS	-	expression tag	UNP Q0X0A9
А	-14	HIS	-	expression tag	UNP Q0X0A9
А	-13	HIS	-	expression tag	UNP Q0X0A9
A	-12	HIS	-	expression tag	UNP Q0X0A9
А	-11	HIS	-	expression tag	UNP Q0X0A9
А	-10	HIS	-	expression tag	UNP Q0X0A9
А	-9	SER	-	expression tag	UNP Q0X0A9
А	-8	SER	-	expression tag	UNP Q0X0A9
А	-7	GLY	-	expression tag	UNP Q0X0A9
А	-6	LEU	-	expression tag	UNP Q0X0A9
А	-5	VAL	-	expression tag	UNP Q0X0A9
А	-4	PRO	-	expression tag	UNP Q0X0A9
А	-3	ARG	-	expression tag	UNP Q0X0A9
А	-2	GLY	-	expression tag	UNP Q0X0A9
А	-1	SER	-	expression tag	UNP Q0X0A9
А	0	HIS	-	expression tag	UNP Q0X0A9
В	-19	MET	-	initiating methionine	UNP Q0X0A9
В	-18	GLY	-	expression tag	UNP Q0X0A9
В	-17	SER	-	expression tag	UNP Q0X0A9
В	-16	SER	-	expression tag	UNP Q0X0A9
В	-15	HIS	-	expression tag	UNP Q0X0A9

There are 40 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
В	-14	HIS	-	expression tag	UNP Q0X0A9
В	-13	HIS	-	expression tag	UNP Q0X0A9
В	-12	HIS	-	expression tag	UNP Q0X0A9
В	-11	HIS	-	expression tag	UNP Q0X0A9
В	-10	HIS	-	expression tag	UNP Q0X0A9
В	-9	SER	-	expression tag	UNP Q0X0A9
В	-8	SER	-	expression tag	UNP Q0X0A9
В	-7	GLY	-	expression tag	UNP Q0X0A9
В	-6	LEU	-	expression tag	UNP Q0X0A9
В	-5	VAL	-	expression tag	UNP Q0X0A9
В	-4	PRO	-	expression tag	UNP Q0X0A9
В	-3	ARG	-	expression tag	UNP Q0X0A9
В	-2	GLY	-	expression tag	UNP Q0X0A9
В	-1	SER	-	expression tag	UNP Q0X0A9
В	0	HIS	-	expression tag	UNP Q0X0A9

• Molecule 2 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	Atoms				ZeroOcc	AltConf	
9	Δ	1	Total	С	Ν	Ο	Р	0	0
	Л	1	27	10	5	10	2	0	0
0	۸	1	Total	С	Ν	Ο	Р	0	0
	A	1	27	10	5	10	2	0	0
0	P	1	Total	С	Ν	0	Р	0	0
	D	1	27	10	5	10	2	0	0



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
2	В	1	Total 27	C 10	N 5	O 10	Р 2	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Zn 2 2	0	0
3	В	2	Total Zn 2 2	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	3	Total Cl 3 3	0	0
4	В	2	Total Cl 2 2	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	309	Total O 309 309	0	0
6	В	303	Total O 303 303	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: Excinuclease ABC subunit UvrA





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	141.13Å 141.13Å 173.61Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	122.22 - 2.04	Depositor
Resolution (A)	122.22 - 2.04	EDS
% Data completeness	100.0 (122.22-2.04)	Depositor
(in resolution range)	$100.0\ (122.22-2.04)$	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.19 (at 2.03 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
P. P.	0.198 , $0.239$	Depositor
$\Pi, \Pi_{free}$	0.205 , $0.244$	DCC
$R_{free}$ test set	6157 reflections $(4.85%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.5	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , $48.3$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10007	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.24% 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: ZN, CL, MG, ADP

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	B	ond angles
Moi Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.97	1/4715~(0.0%)	0.98	8/6385~(0.1%)
1	В	0.96	1/4691~(0.0%)	0.99	9/6355~(0.1%)
All	All	0.97	2/9406~(0.0%)	0.98	17/12740~(0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	В	779	SER	CB-OG	5.18	1.49	1.42
1	А	708	GLU	CD-OE2	5.04	1.31	1.25

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	690	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	В	619	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	А	504	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	А	440	ASP	CB-CG-OD2	6.65	124.28	118.30
1	А	366	ASP	CB-CG-OD1	6.31	123.98	118.30
1	В	445	LEU	CA-CB-CG	-5.97	101.58	115.30
1	В	421	ASP	CB-CG-OD1	5.93	123.64	118.30
1	В	690	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	В	487	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	В	487	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	А	567	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	А	420	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	В	761	ASP	CB-CG-OD1	5.24	123.02	118.30
1	А	474	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	А	420	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	В	128	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	В	723	ARG	NE-CZ-NH1	5.06	122.83	120.30

All (17) bond angle outliers are listed below:



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	4650	0	4683	30	0
1	В	4626	0	4651	30	0
2	А	54	0	24	1	0
2	В	54	0	24	0	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
4	А	3	0	0	0	0
4	В	2	0	0	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
6	А	309	0	0	6	0
6	В	303	0	0	5	1
All	All	10007	0	9382	59	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (59) 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:B:22:MET:HE2	1:B:39:GLU:HB3	1.67	0.76	
1:A:488:GLN:O	6:A:901:HOH:O	2.09	0.71	
1:A:325:GLN:HE22	1:A:760:HIS:H	1.39	0.71	
1:A:699:GLY:O	6:A:902:HOH:O	2.09	0.70	
1:A:723:ARG:NH2	1:B:478:ASP:OD1	2.25	0.70	
1:A:139:ILE:O	6:A:903:HOH:O	2.13	0.67	
1:A:26:HIS:HB2	1:A:94:VAL:HG13	1.75	0.67	
1:A:357:GLN:O	1:A:411:ARG:HD2	1.95	0.66	
1:B:640:MET:HE3	1:B:645:ALA:HB2	1.78	0.65	
1:B:358:ILE:HD11	1:B:360:LEU:HD12	1.84	0.60	
1:A:70:ARG:NH1	1:A:74:GLU:OE2	2.35	0.59	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:592:CYS:SG	1:A:593:LYS:N	2.75	0.58	
1:B:595:ALA:HB2	1:B:619:ARG:CG	2.33	0.58	
1:B:595:ALA:HB2	1:B:619:ARG:HG2	1.86	0.57	
1:B:595:ALA:HB1	1:B:617:GLY:HA2	1.87	0.56	
1:B:591:THR:HG21	1:B:614:ASP:OD2	2.06	0.55	
1:A:338:ASP:OD1	1:A:340:SER:HB3	2.07	0.54	
1:A:595:ALA:HB2	1:A:619:ARG:CG	2.38	0.54	
1:A:640:MET:HE1	1:A:645:ALA:HA	1.90	0.54	
1:B:767:PHE:CD2	1:B:774:LEU:HD13	2.44	0.52	
1:B:26:HIS:HB2	1:B:94:VAL:HB	1.92	0.52	
1:A:592:CYS:O	1:A:593:LYS:NZ	2.39	0.52	
1:A:583:PRO:HB3	1:A:593:LYS:HD2	1.92	0.51	
1:A:121:THR:HG21	1:A:355:PHE:HZ	1.76	0.50	
1:A:595:ALA:HB2	1:A:619:ARG:HG3	1.93	0.50	
1:A:435:THR:O	1:A:438:ILE:HG12	2.11	0.50	
1:B:451:THR:HG21	6:B:918:HOH:O	2.11	0.50	
1:B:608:VAL:HG23	1:B:609:ALA:H	1.77	0.49	
1:B:24:ARG:NH1	6:B:905:HOH:O	2.29	0.49	
1:A:682:THR:HG21	2:A:801:ADP:N6	2.28	0.49	
1:A:42:LYS:HE3	1:A:97:GLY:O	2.12	0.48	
1:B:358:ILE:HD12	1:B:379:ARG:HB3	1.96	0.48	
1:A:432:LYS:NZ	6:A:922:HOH:O	2.47	0.48	
1:B:640:MET:HE3	1:B:645:ALA:CB	2.44	0.47	
1:B:592:CYS:SG	1:B:593:LYS:N	2.88	0.47	
1:B:26:HIS:HB3	6:B:940:HOH:O	2.15	0.46	
1:B:435:THR:O	1:B:438:ILE:HG12	2.17	0.45	
1:B:595:ALA:HB2	1:B:619:ARG:HG3	1.97	0.45	
1:A:668:GLU:OE2	1:A:727:ARG:NH2	2.40	0.45	
1:A:303:ARG:HD2	6:A:1006:HOH:O	2.16	0.45	
1:A:442:VAL:HG11	1:A:465:LEU:HD22	1.99	0.44	
1:A:592:CYS:O	1:A:593:LYS:CE	2.65	0.44	
1:B:358:ILE:HG22	1:B:415:LEU:HD13	2.00	0.44	
1:B:654:ALA:O	1:B:655:ARG:C	2.56	0.44	
1:A:80:ILE:O	1:A:81:GLN:HB2	2.18	0.44	
1:B:89:ARG:N	6:B:929:HOH:O	2.50	0.44	
1:B:70:ARG:NH1	1:B:74:GLU:OE2	2.51	0.43	
1:A:131:PHE:HB3	1:A:145:PHE:CE2	2.53	0.43	
1:A:595:ALA:HB2	1:A:619:ARG:HG2	1.99	0.43	
1:B:593:LYS:N	1:B:593:LYS:HD3	2.33	0.43	
1:B:358:ILE:HG22	1:B:415:LEU:CD1	2.49	0.43	
1:B:358:ILE:HD11	1:B:360:LEU:CD1	2.48	0.42	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:HIS:HD2	6:A:1177:HOH:O	2.02	0.42
1:A:102:ILE:HD12	1:A:393:VAL:HG11	2.02	0.42
1:B:95:LEU:HD22	1:B:98:LEU:HD21	2.03	0.41
1:A:471:VAL:O	1:A:475:HIS:HD2	2.03	0.41
1:B:121:THR:HG21	1:B:355:PHE:HZ	1.86	0.41
1:B:89:ARG:N	6:B:933:HOH:O	2.53	0.40
1:B:781:LEU:HD23	1:B:781:LEU:HA	1.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
6:B:1103:HOH:O	6:B:1123:HOH:O[6_765]	1.81	0.39	

### 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	615/812~(76%)	597 (97%)	17 (3%)	1 (0%)	47	39
1	В	616/812~(76%)	596 (97%)	19 (3%)	1 (0%)	47	39
All	All	1231/1624~(76%)	1193 (97%)	36 (3%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	700	ALA
1	А	593	LYS



#### 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	Percentiles		
1	А	498/650~(77%)	482~(97%)	16 (3%)	39 32		
1	В	497/650~(76%)	481 (97%)	16 (3%)	39 32		
All	All	995/1300~(76%)	963~(97%)	32 (3%)	39 32		

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	81	GLN
1	А	87	LEU
1	А	94	VAL
1	А	95	LEU
1	А	114	ARG
1	А	172	VAL
1	А	182	ILE
1	А	343	THR
1	А	406	PRO
1	А	432	LYS
1	А	492	VAL
1	А	572	LYS
1	А	598	ILE
1	А	608	VAL
1	А	621	GLN
1	А	635	SER
1	В	15	CYS
1	В	96	ASP
1	В	109	MET
1	В	111	THR
1	В	115	SER
1	В	149	VAL
1	В	296	CYS
1	В	351	THR
1	В	368	SER
1	В	445	LEU
1	В	479	ARG



Continued from previous page...

Mol	Chain	Res	Type
1	В	538	ASP
1	В	549	LYS
1	В	562	MET
1	В	586	GLU
1	В	611	THR

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	81	GLN
1	А	148	ASN
1	А	325	GLN
1	А	720	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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



Mal	Type	Chain	Dec	Tiple	Bo	ond leng	$\mathbf{ths}$	B	ond ang	les
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	ADP	В	802	-	24,29,29	1.14	1 (4%)	29,45,45	1.46	3 (10%)
2	ADP	А	802	-	24,29,29	1.24	4 (16%)	29,45,45	1.37	7 (24%)
2	ADP	В	801	5	24,29,29	1.60	5 (20%)	29,45,45	1.74	5 (17%)
2	ADP	А	801	5	24,29,29	1.39	2 (8%)	29,45,45	1.32	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	В	802	-	-	1/12/32/32	0/3/3/3
2	ADP	А	802	-	-	0/12/32/32	0/3/3/3
2	ADP	В	801	5	-	1/12/32/32	0/3/3/3
2	ADP	А	801	5	-	3/12/32/32	0/3/3/3

Mol	Chain	$\mathbf{Res}$	Type	Atoms	$\mathbf{Z}$	Observed(A)	Ideal(Å)
2	А	801	ADP	C2'-C1'	-4.52	1.46	1.53
2	В	801	ADP	C2-N3	3.73	1.38	1.32
2	В	802	ADP	C2'-C1'	-3.10	1.49	1.53
2	В	801	ADP	C5-C4	3.07	1.49	1.40
2	А	802	ADP	O4'-C4'	-2.45	1.39	1.45
2	А	802	ADP	PB-O3B	-2.32	1.45	1.54
2	А	801	ADP	O4'-C4'	-2.29	1.39	1.45
2	А	802	ADP	C2-N3	2.18	1.35	1.32
2	А	802	ADP	C5-C4	2.16	1.46	1.40
2	В	801	ADP	C2'-C1'	-2.08	1.50	1.53
2	В	801	ADP	C5-N7	-2.06	1.32	1.39
2	В	801	ADP	O3'-C3'	2.06	1.47	1.43

All (12) bond length outliers are listed below:

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
2	В	801	ADP	N3-C2-N1	-4.68	121.37	128.68
2	В	802	ADP	N3-C2-N1	-4.32	121.93	128.68
2	А	801	ADP	N3-C2-N1	-3.90	122.58	128.68
2	В	801	ADP	O3B-PB-O2B	3.51	121.07	107.64
2	В	801	ADP	O2A-PA-O1A	3.43	129.21	112.24
2	В	801	ADP	C2-N1-C6	3.41	124.59	118.75



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	802	ADP	C2-N1-C6	3.22	124.27	118.75
2	В	801	ADP	N6-C6-N1	2.84	124.46	118.57
2	А	802	ADP	C1'-N9-C4	-2.65	121.99	126.64
2	А	802	ADP	N3-C2-N1	-2.47	124.83	128.68
2	А	801	ADP	O3B-PB-O2B	2.30	116.43	107.64
2	А	801	ADP	N6-C6-N1	2.29	123.33	118.57
2	А	802	ADP	O2'-C2'-C1'	2.21	119.01	110.85
2	В	802	ADP	PA-O3A-PB	-2.15	125.45	132.83
2	А	802	ADP	PA-O3A-PB	-2.12	125.54	132.83
2	А	802	ADP	O4'-C4'-C3'	2.11	109.29	105.11
2	А	802	ADP	O3B-PB-O2B	2.09	115.64	107.64
2	A	802	ADP	O3B-PB-O1B	2.07	118.77	110.68
2	А	801	ADP	O2A-PA-O1A	2.00	122.14	112.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	801	ADP	PA-O3A-PB-O3B
2	А	801	ADP	C5'-O5'-PA-O1A
2	В	802	ADP	PA-O3A-PB-O3B
2	В	801	ADP	PA-O3A-PB-O3B
2	А	801	ADP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	801	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers (i)

There are no such residues in this entry.



## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	626/812~(77%)	0.21	24 (3%) 40 44	26, 44, 81, 105	0
1	В	626/812~(77%)	0.07	4 (0%) 89 91	26, 43, 71, 101	0
All	All	1252/1624~(77%)	0.14	28 (2%) 62 66	26, 43, 78, 105	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	87	LEU	5.0
1	А	581	PHE	4.0
1	А	570	PHE	3.5
1	А	616	GLY	3.4
1	А	566	ILE	3.3
1	А	575	GLY	3.1
1	А	79	PHE	3.1
1	А	580	LEU	3.1
1	В	792	ALA	3.0
1	А	613	GLU	2.9
1	А	571	ALA	2.9
1	А	583	PRO	2.8
1	А	173	GLY	2.6
1	А	792	ALA	2.5
1	А	573	ALA	2.5
1	В	150	ALA	2.4
1	А	586	GLU	2.4
1	А	654	ALA	2.4
1	А	576	VAL	2.4
1	А	579	ALA	2.4
1	А	677	GLY	2.3
1	А	553	ARG	2.2
1	В	111	THR	2.2
1	А	551	SER	2.1



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	В	151	SER	2.0
1	А	80	ILE	2.0
1	А	612	CYS	2.0
1	А	614	ASP	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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	CL	А	807	1/1	0.89	0.05	88,88,88,88	0
4	CL	В	805	1/1	0.90	0.15	58, 58, 58, 58	0
4	CL	А	805	1/1	0.92	0.10	49,49,49,49	0
4	CL	А	806	1/1	0.93	0.15	$63,\!63,\!63,\!63$	0
5	MG	В	807	1/1	0.93	0.05	49,49,49,49	0
3	ZN	А	804	1/1	0.94	0.12	67,67,67,67	0
4	CL	В	806	1/1	0.95	0.10	58, 58, 58, 58	0
5	MG	А	808	1/1	0.97	0.04	59, 59, 59, 59, 59	0
3	ZN	В	804	1/1	0.98	0.13	$65,\!65,\!65,\!65$	0
3	ZN	А	803	1/1	0.98	0.05	$65,\!65,\!65,\!65$	0
2	ADP	В	802	27/27	0.98	0.12	$29,\!38,\!45,\!47$	0
3	ZN	В	803	1/1	0.98	0.16	48,48,48,48	0
2	ADP	А	801	27/27	0.99	0.14	24,36,49,53	0
2	ADP	A	802	27/27	0.99	0.12	24,33,39,40	0
2	ADP	В	801	27/27	0.99	0.13	24,30,43,48	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.

