

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

Sep 7, 2023 - 01:48 pm BST

:	8BUE
:	Structure of DDB1 bound to Z11-engaged CDK12-cyclin K
:	Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.
:	2022-11-30
:	3.25  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	:	2.35
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)	:	2.35

# 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 3.25 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	
			10%	
1	А	840	87%	11% •
			8%	
1	D	840	88%	11% •
			9%	
1	G	840	87%	11% •
			15%	
2	В	344	83%	12% • •
			8%	
2	E	344	83%	11% • 6%



Mol	Chain	Length	Quality of chain	
2	Н	344	9%	12% • •
3	С	271	<u>6%</u> 85%	6% 8%
3	F	271	<b>4%</b> 86%	• • 8%
3	Ι	271	<mark>6%</mark> 87%	• 8%

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
4	SO4	F	301	-	-	-	Х



#### 8BUE

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 67598 atoms, of which 33625 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			Aton	ns			ZeroOcc	AltConf	Trace
1	Λ	826	Total	С	Η	Ν	Ο	$\mathbf{S}$	6450	0	0
	820	12937	4105	6450	1094	1252	36	0430	0	0	
1	л	897	Total	С	Н	Ν	Ο	S	6462	0	0
	021	12957	4111	6462	1095	1253	36	0402	0	U	
1	1 C	200	Total	С	Н	Ν	Ο	S	6452	0	0
I G	820	12938	4106	6452	1093	1251	36	0432	0	0	

• Molecule 1 is a protein called DNA damage-binding protein 1.

1 1	There are 39	discrepancies	between	the	modelled	and	reference	sequences:
-----	--------------	---------------	---------	-----	----------	-----	-----------	------------

Chain	Residue	Modelled	Actual	Comment	Reference
А	-3	GLY	-	expression tag	UNP Q16531
А	-2	GLY	-	expression tag	UNP Q16531
А	-1	GLY	-	expression tag	UNP Q16531
А	0	ARG	-	expression tag	UNP Q16531
А	700	GLY	-	linker	UNP Q16531
А	701	ASN	-	linker	UNP Q16531
А	702	GLY	-	linker	UNP Q16531
А	703	ASN	-	linker	UNP Q16531
А	704	SER	-	linker	UNP Q16531
А	705	GLY	-	linker	UNP Q16531
А	706	GLU	-	linker	UNP Q16531
А	707	ILE	-	linker	UNP Q16531
А	708	GLN	-	linker	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531



8BUE	
------	--

Chain	Decidure	Medallad	Actual	Commont	Defenence
Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLU	-	linker	UNP Q16531
D	707	ILE	-	linker	UNP Q16531
D	708	GLN	-	linker	UNP Q16531
G	-3	GLY	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531
G	706	GLU	-	linker	UNP Q16531
G	707	ILE	-	linker	UNP Q16531
G	708	GLN	-	linker	UNP Q16531

• Molecule 2 is a protein called Cyclin-dependent kinase 12.

Mol	Chain	Residues			Ato	$\mathbf{ms}$				ZeroOcc	AltConf	Trace
0	В	220	Total	С	Η	Ν	0	Р	S	2607	0	0
	D	529	5384	1723	2697	454	492	1	17	2097	0	0
0	Б	295	Total	С	Н	Ν	0	Р	S	2662	0	0
	2 E 325	5309	1695	2663	447	486	1	17	2005	0	0	
0	0 II 200	Total	С	Η	Ν	0	Р	S	2607	0	0	
2 H	329	5384	1723	2697	454	492	1	17	2097	U	U	

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	709	GLY	- expression tag		UNP Q9NYV4
В	710	GLY	-	expression tag	UNP Q9NYV4
В	711	GLY	-	expression tag	UNP Q9NYV4
В	965	ARG	LYS	engineered mutation	UNP Q9NYV4
В	1052	GLN	-	expression tag	UNP Q9NYV4
Е	709	GLY	-	expression tag	UNP Q9NYV4
E	710	GLY	-	expression tag	UNP Q9NYV4
Е	711	GLY	-	expression tag	UNP Q9NYV4
E	965	ARG	LYS	engineered mutation	UNP Q9NYV4
Е	1052	GLN	-	expression tag	UNP Q9NYV4
Н	709	GLY	-	expression tag	UNP Q9NYV4
Н	710	GLY	-	expression tag	UNP Q9NYV4



Chain	Residue	Modelled	Actual	Comment	Reference
Η	711	GLY	-	expression tag	UNP Q9NYV4
Н	965	ARG	LYS	engineered mutation	UNP Q9NYV4
Н	1052	GLN	-	expression tag	UNP Q9NYV4

• Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
2 0	248	Total	С	Η	Ν	0	S	2048	0	0	
5	3 0	240	4111	1341	2048	346	363	13	2040	0	0
2	E Q	248	Total	С	Η	Ν	0	S	2048	0	0
0	Г	240	4111	1341	2048	346	363	13	2040		
2	т	248	Total	С	Н	Ν	0	S	2048	0	0
5	3 1	240	4111	1341	2048	346	363	13	2048		0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-3	GLY	-	expression tag	UNP 075909
С	-2	GLY	-	expression tag	UNP 075909
С	-1	GLY	-	expression tag	UNP 075909
С	0	ARG	-	expression tag	UNP 075909
F	-3	GLY	-	expression tag	UNP 075909
F	-2	GLY	-	expression tag	UNP 075909
F	-1	GLY	-	expression tag	UNP 075909
F	0	ARG	-	expression tag	UNP 075909
Ι	-3	GLY	-	expression tag	UNP 075909
Ι	-2	GLY	-	expression tag	UNP 075909
Ι	-1	GLY	-	expression tag	UNP 075909
Ι	0	ARG	-	expression tag	UNP 075909

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S	0	0
		-	5 4 1		
4	D	1	Total O S $5 4 1$	0	0
			Total O S		
4	D	1	5 4 1	0	0
4	D	1	Total O S	0	0
			Total O S		
4	D	1	5 4 1	0	0
4	D	1	Total O S	0	0
			5 4 1 Total O S		
4	D	1	5 $4$ $1$	0	0
4	D	1	Total O S	0	0
			5 4 1 Total O S		-
4	Ε	1	5 4 1	0	0
4	E	1	Total O S	0	0
		1	5 $4$ $1$	0	0
4	F	1	$\begin{array}{ccc} 1 \text{ otal } \mathbf{O} \ \mathbf{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	F	1	Total O S	0	0
4	Ľ	1	5 4 1	0	0
4	F	1	Total O S	0	0
			$\begin{array}{ccc} 5 & 4 & 1 \\ \hline Total & O & S \end{array}$		
4	F	1	5 4 1	0	0
4	G	1	Total O S	0	0
	~		5 $4$ $1$		
4	G	1	$\begin{array}{cccc} 10tal & O & S \\ 5 & 4 & 1 \end{array}$	0	0
1	С	1	Total O S	0	0
	G		5 4 1	0	0
4	G	1	$\begin{array}{c ccc} 1 & \text{Otal} & \text{O} & \text{S} \\ \hline 5 & 4 & 1 \end{array}$	0	0
4	C	1	Total O S	0	0
4	G		5 4 1	0	U
4	G	1	Total O S	0	0
			Total O S		
4	G	1		0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
4	Ι	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 5 is {N}-(1 {H}-benzimidazol-2-yl)-1-(2-methoxy-5-methyl-phenyl)-5-oxidanylide ne-pyrrolidine-3-carboxamide (three-letter code: RVU) (formula:  $C_{20}H_{20}N_4O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
5	В	1	Total	С	Η	Ν	0	20	0	
5 В	1	47	20	20	4	3	20	0		
5	F	1	Total	С	Η	Ν	Ο	20	0	
0	5 E	1	47	20	20	4	3	20	0	



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	Ц	1	Total	С	Η	Ν	0	20	0
5	11	1	47	20	20	4	3	20	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: DNA damage-binding protein 1

• Molecule 1: DNA damage-binding protein 1





# VI028 V817 V1028 Y828 V1036 Y828 F1039 Y828 V1036 Y828 V1036 Y828 V1036 Y828 V1049 Y828 V1046 Y849 V1046 Y849 V1046 Y849 V1046 Y861 V1047 Y861 V1048 Y861 V1049 Y861 V1049 Y861 V1049 Y861 V114 Y908 Y114 Y908 Y1149 Y916 Y1149 Y916 Y1140 Y916 Y9104 Y9104 Y9104 Y1004 Y1005 Y1004 Y9106 Y1004 <td

• Molecule 1: DNA damage-binding protein 1











# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	249.33Å 249.33Å 218.68Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	60.41 - 3.25	Depositor
Resolution (A)	$215.93 \ - \ 3.25$	EDS
% Data completeness	79.3 (60.41-3.25)	Depositor
(in resolution range)	$79.3\ (215.93‐3.25)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.51 (at 3.26 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.184 , $0.213$	Depositor
$\Pi, \Pi_{free}$	0.202 , $0.225$	DCC
$R_{free}$ test set	4845 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	134.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.32 , $92.7$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	67598	wwPDB-VP
Average B, all atoms $(Å^2)$	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.60% 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: RVU, SO4, 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	Bond	lengths	Bo	ond angles
MIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.36	0/6604	0.61	0/8931
1	D	0.34	0/6612	0.60	0/8942
1	G	0.36	0/6603	0.60	0/8930
2	В	0.36	0/2737	0.60	0/3691
2	Е	0.35	0/2693	0.61	0/3630
2	Н	0.36	0/2737	0.62	1/3691~(0.0%)
3	С	0.36	0/2120	0.53	0/2868
3	F	0.37	0/2120	0.58	0/2868
3	Ι	0.35	0/2120	0.56	0/2868
All	All	0.35	0/34346	$0.\overline{60}$	1/46419~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	876	ALA	N-CA-C	5.43	125.65	111.00

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	6487	6450	6451	52	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6495	6462	6464	49	0
1	G	6486	6452	6454	56	0
2	В	2687	2697	2697	26	0
2	Е	2646	2663	2663	25	0
2	Н	2687	2697	2697	27	0
3	С	2063	2048	2048	8	0
3	F	2063	2048	2048	7	0
3	Ι	2063	2048	2048	6	0
4	А	35	0	0	1	0
4	В	10	0	0	0	0
4	С	15	0	0	0	0
4	D	50	0	0	0	0
4	Е	10	0	0	1	0
4	F	20	0	0	0	0
4	G	40	0	0	0	0
4	Н	20	0	0	0	0
4	Ι	15	0	0	0	0
5	В	27	20	0	0	0
5	Е	27	20	0	1	0
5	Н	27	20	0	0	0
All	All	33973	33625	33570	244	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 244 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)
3:F:231:TYR:OH	3:F:236:GLU:OE1	1.95	0.85
1:A:1022:THR:HB	1:A:1023:PRO:HD2	1.75	0.69
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.61	0.64
2:E:867:LEU:HD21	2:E:1031:PRO:HG3	1.78	0.64
2:H:828:LEU:O	2:H:1034:PRO:HD2	1.98	0.63

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	822/840~(98%)	799~(97%)	23 (3%)	0	100	100
1	D	823/840~(98%)	801~(97%)	22 (3%)	0	100	100
1	G	822/840~(98%)	802~(98%)	20 (2%)	0	100	100
2	В	326/344~(95%)	315~(97%)	11 (3%)	0	100	100
2	Е	322/344~(94%)	312~(97%)	10 (3%)	0	100	100
2	Н	326/344~(95%)	317~(97%)	9(3%)	0	100	100
3	С	246/271~(91%)	244 (99%)	2 (1%)	0	100	100
3	F	246/271~(91%)	244 (99%)	2 (1%)	0	100	100
3	Ι	246/271 (91%)	244 (99%)	2 (1%)	0	100	100
All	All	4179/4365~(96%)	4078 (98%)	101 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	721/728~(99%)	716~(99%)	5 (1%)	84	90	
1	D	722/728~(99%)	719 (100%)	3 (0%)	91	94	
1	G	721/728~(99%)	715~(99%)	6 (1%)	81	89	
2	В	296/308~(96%)	292~(99%)	4 (1%)	67	81	
2	Е	292/308~(95%)	288~(99%)	4 (1%)	67	81	



Mol	Chain	Analysed	Rotameric	Rotameric Outliers		Percentiles		
2	Н	296/308~(96%)	294~(99%)	2(1%)	84	90		
3	С	223/242~(92%)	220~(99%)	3 (1%)	69	82		
3	F	223/242~(92%)	219~(98%)	4 (2%)	59	77		
3	Ι	223/242~(92%)	221~(99%)	2(1%)	78	87		
All	All	3717/3834~(97%)	3684~(99%)	33~(1%)	78	87		

Continued from previous page...

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	G	1140	HIS
2	Н	829	VAL
3	Ι	231	TYR
1	D	746	SER
3	С	257	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
2	В	999	HIS
1	D	261	HIS
2	Н	999	HIS
1	G	370	GLN
2	В	944	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)

3 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).



Mol Type	Turne	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Dea Link	Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2					
2	TPO	Е	893	2	8,10,11	1.70	1 (12%)	10,14,16	1.36	2 (20%)					
2	TPO	В	893	2	8,10,11	1.19	0	10,14,16	1.49	2 (20%)					
2	TPO	Н	893	2	8,10,11	1.48	1 (12%)	10,14,16	1.13	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	Res	Link	Chirals	Torsions	Rings
2	TPO	Е	893	2	-	6/9/11/13	-
2	TPO	В	893	2	-	0/9/11/13	-
2	TPO	Н	893	2	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ε	893	TPO	P-01P	3.45	1.61	1.50
2	Н	893	TPO	P-OG1	2.51	1.64	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	893	TPO	P-OG1-CB	-3.14	113.72	123.21
2	Е	893	TPO	P-OG1-CB	-2.46	115.79	123.21
2	Е	893	TPO	CG2-CB-CA	-2.41	108.41	113.16
2	Н	893	TPO	CG2-CB-CA	-2.39	108.45	113.16
2	В	893	TPO	CG2-CB-CA	-2.04	109.13	113.16

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	893	TPO	N-CA-CB-CG2
2	Е	893	TPO	N-CA-CB-OG1
2	Е	893	TPO	C-CA-CB-CG2
2	Е	893	TPO	O-C-CA-CB
2	Е	893	TPO	CG2-CB-OG1-P

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	893	TPO	1	0

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

46 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	Dec	Link	Bo	ond leng	ths	В	ond ang	gles
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	D	1207	-	4,4,4	0.18	0	$6,\!6,\!6$	0.09	0
4	SO4	F	304	-	4,4,4	0.18	0	$6,\!6,\!6$	0.16	0
4	SO4	D	1206	-	4,4,4	0.22	0	$6,\!6,\!6$	0.08	0
4	SO4	А	1204	-	4,4,4	0.24	0	$6,\!6,\!6$	0.13	0
4	SO4	G	1202	-	4,4,4	0.19	0	$6,\!6,\!6$	0.04	0
4	SO4	G	1207	-	4,4,4	0.20	0	$6,\!6,\!6$	0.09	0
4	SO4	D	1201	-	4,4,4	0.19	0	$6,\!6,\!6$	0.05	0
4	SO4	G	1205	-	4,4,4	0.22	0	$6,\!6,\!6$	0.10	0
4	SO4	G	1204	-	4,4,4	0.21	0	$6,\!6,\!6$	0.07	0
4	SO4	D	1205	-	4,4,4	0.23	0	$6,\!6,\!6$	0.06	0
4	SO4	D	1204	-	4,4,4	0.25	0	$6,\!6,\!6$	0.05	0
4	SO4	А	1202	-	4,4,4	0.20	0	$6,\!6,\!6$	0.08	0
4	SO4	F	302	-	4,4,4	0.21	0	$6,\!6,\!6$	0.07	0
4	SO4	G	1208	-	4,4,4	0.25	0	$6,\!6,\!6$	0.06	0
4	SO4	С	303	-	4,4,4	0.22	0	$6,\!6,\!6$	0.13	0
4	SO4	D	1208	-	4,4,4	0.25	0	$6,\!6,\!6$	0.08	0
4	SO4	Н	1103	-	4,4,4	0.25	0	$6,\!6,\!6$	0.07	0
4	SO4	G	1203	-	4,4,4	0.19	0	$6,\!6,\!6$	0.08	0
4	SO4	D	1209	-	4,4,4	0.27	0	$6,\!6,\!6$	0.06	0
4	SO4	А	1201	-	4,4,4	0.21	0	$6,\!6,\!6$	0.05	0
4	SO4	А	1206	-	4,4,4	0.20	0	$6,\!6,\!6$	0.08	0
4	SO4	Н	1105	-	4,4,4	0.23	0	$6,\!6,\!6$	0.07	0



Mal	Tuno	Chain	Dog	Tink	Bo	ond leng	$\operatorname{ths}$	В	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	SO4	D	1210	-	4,4,4	0.19	0	$6,\!6,\!6$	0.08	0
4	SO4	G	1201	-	4,4,4	0.21	0	$6,\!6,\!6$	0.07	0
4	SO4	D	1202	-	4,4,4	0.20	0	$6,\!6,\!6$	0.07	0
4	SO4	А	1207	-	4,4,4	0.19	0	$6,\!6,\!6$	0.09	0
4	SO4	Е	1103	-	4,4,4	0.22	0	$6,\!6,\!6$	0.08	0
4	SO4	F	301	-	4,4,4	0.22	0	$6,\!6,\!6$	0.10	0
4	SO4	В	1102	-	4,4,4	0.24	0	$6,\!6,\!6$	0.08	0
4	SO4	Н	1104	-	4,4,4	0.23	0	$6,\!6,\!6$	0.07	0
4	SO4	А	1205	-	4,4,4	0.22	0	$6,\!6,\!6$	0.07	0
4	SO4	А	1203	-	4,4,4	0.22	0	$6,\!6,\!6$	0.12	0
4	SO4	В	1103	-	4,4,4	0.23	0	$6,\!6,\!6$	0.07	0
4	SO4	D	1203	-	4,4,4	0.19	0	$6,\!6,\!6$	0.07	0
4	SO4	С	301	-	4,4,4	0.20	0	$6,\!6,\!6$	0.05	0
4	SO4	Н	1102	-	4,4,4	0.22	0	$6,\!6,\!6$	0.05	0
5	RVU	В	1101	-	30,30,30	0.76	0	32,43,43	1.06	3 (9%)
5	RVU	Н	1101	-	30,30,30	0.75	0	32,43,43	1.09	3 (9%)
4	SO4	F	303	-	4,4,4	0.16	0	$6,\!6,\!6$	0.06	0
4	SO4	Ι	303	-	4,4,4	0.22	0	$6,\!6,\!6$	0.12	0
4	SO4	Е	1102	-	4,4,4	0.25	0	$6,\!6,\!6$	0.09	0
5	RVU	Е	1101	-	30,30,30	0.73	0	32,43,43	1.11	2 (6%)
4	SO4	Ι	301	-	4,4,4	0.22	0	$6,\!6,\!6$	0.06	0
4	SO4	С	302	-	4,4,4	0.23	0	$6,\!6,\!6$	0.07	0
4	SO4	G	1206	-	4,4,4	0.25	0	$6,\!6,\!6$	0.07	0
4	SO4	Ι	302	-	4,4,4	0.16	0	6,6,6	0.09	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
5	RVU	В	1101	-	-	2/12/26/26	0/4/4/4
5	RVU	Н	1101	-	-	2/12/26/26	0/4/4/4
5	RVU	Е	1101	-	-	2/12/26/26	0/4/4/4

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Е	1101	RVU	C3-N1-C2	-3.22	125.41	130.28



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Н	1101	RVU	C3-N1-C2	-2.68	126.22	130.28
5	Е	1101	RVU	C18-C17-C15	-2.37	116.68	120.08
5	В	1101	RVU	C3-N1-C2	-2.30	126.80	130.28
5	Н	1101	RVU	C18-C17-C15	-2.29	116.79	120.08

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	1101	RVU	C4-C1-C2-N1
5	В	1101	RVU	C4-C1-C2-O3
5	Е	1101	RVU	C4-C1-C2-N1
5	Е	1101	RVU	C4-C1-C2-O3
5	Н	1101	RVU	C4-C1-C2-N1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	1203	SO4	1	0
4	Е	1102	SO4	1	0
5	Е	1101	RVU	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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	826/840~(98%)	0.63	81 (9%) 7 7	105, 141, 210, 292	0
1	D	827/840~(98%)	0.55	70 (8%) 10 10	96, 135, 201, 269	0
1	G	826/840~(98%)	0.55	74 (8%) 9 10	103, 142, 213, 308	0
2	В	328/344~(95%)	0.77	52 (15%) 1 2	112, 146, 215, 239	0
2	Е	324/344~(94%)	0.71	29 (8%) 9 10	105, 137, 203, 240	0
2	Н	328/344~(95%)	0.76	30 (9%) 9 10	91, 122, 199, 270	0
3	С	248/271~(91%)	0.60	16 (6%) 18 18	109, 135, 173, 246	0
3	F	248/271~(91%)	0.62	10 (4%) 38 35	92, 118, 155, 229	0
3	Ι	248/271~(91%)	0.64	15 (6%) 21 21	97, 121, 162, 236	0
All	All	$420\overline{3}/4365~(96\%)$	0.62	377 (8%) 9 10	91, 136, 206, 308	0

The worst 5 of 377 RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	1016	ASN	10.1
2	Н	1039	CYS	7.6
2	Н	1043	TRP	7.5
1	А	1017	LEU	6.5
2	В	1035	HIS	6.4

# 6.2 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	$B-factors(Å^2)$	Q<0.9
2	TPO	Е	893	11/12	0.87	0.15	183,196,237,239	6
2	TPO	Н	893	11/12	0.87	0.24	141,159,191,194	6
2	TPO	В	893	11/12	0.89	0.15	188,204,247,248	6

## 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	SO4	Ι	303	5/5	0.68	0.19	161,162,166,192	0
4	SO4	D	1205	5/5	0.73	0.13	159,162,177,199	0
4	SO4	D	1207	5/5	0.74	0.26	146,154,156,189	0
4	SO4	Е	1102	5/5	0.75	0.21	163,172,176,208	0
4	SO4	D	1206	5/5	0.76	0.29	146,157,159,198	0
4	SO4	С	302	5/5	0.77	0.14	154,161,170,190	0
4	SO4	F	304	5/5	0.78	0.19	152,153,156,182	0
4	SO4	А	1205	5/5	0.78	0.26	163,170,174,206	0
4	SO4	F	301	5/5	0.79	0.44	144,161,163,193	0
4	SO4	D	1208	5/5	0.81	0.17	162,163,168,196	0
4	SO4	Н	1105	5/5	0.81	0.16	156,162,169,200	0
4	SO4	F	302	5/5	0.81	0.14	157,162,166,193	0
4	SO4	D	1203	5/5	0.82	0.23	141,153,161,193	0
4	SO4	G	1207	5/5	0.83	0.20	149,157,163,195	0
4	SO4	С	303	5/5	0.83	0.11	161,169,170,194	0
4	SO4	D	1204	5/5	0.83	0.20	153,156,174,194	0
4	SO4	G	1208	5/5	0.84	0.37	168,170,176,201	0
4	SO4	G	1206	5/5	0.84	0.09	177,177,183,211	0
4	SO4	G	1204	5/5	0.84	0.14	150,160,164,190	0
4	SO4	А	1204	5/5	0.85	0.16	175,176,179,204	0
4	SO4	D	1210	5/5	0.86	0.16	141,144,154,163	0
4	SO4	G	1201	5/5	0.86	0.17	144,147,151,162	0
4	SO4	A	1201	5/5	0.87	0.16	147,153,155,171	0
4	SO4	A	1202	5/5	0.87	0.16	140,147,147,173	0
4	SO4	A	1203	5/5	0.88	0.30	141,151,170,188	0
4	SO4	D	1202	5/5	0.88	0.19	140,152,161,184	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
4	SO4	D	1201	5/5	0.89	0.18	135,140,149,151	0
4	SO4	D	1209	5/5	0.89	0.21	180,182,187,212	0
4	SO4	G	1203	5/5	0.89	0.19	132,138,153,163	0
4	SO4	С	301	5/5	0.90	0.23	137,139,150,158	0
4	SO4	А	1206	5/5	0.90	0.15	144,148,152,167	0
4	SO4	G	1205	5/5	0.90	0.17	155,170,181,201	0
4	SO4	А	1207	5/5	0.90	0.14	134,153,171,184	0
4	SO4	G	1202	5/5	0.91	0.14	146,150,156,177	0
4	SO4	Н	1103	5/5	0.91	0.10	158,161,177,199	0
4	SO4	Е	1103	5/5	0.92	0.12	158,164,167,194	0
4	SO4	В	1102	5/5	0.92	0.12	165,169,173,200	0
4	SO4	Ι	301	5/5	0.92	0.13	147,154,168,185	0
4	SO4	Н	1102	5/5	0.92	0.16	164,164,179,195	0
4	SO4	Ι	302	5/5	0.93	0.20	124,124,146,147	0
4	SO4	Н	1104	5/5	0.93	0.11	150,156,171,190	0
5	RVU	Н	1101	27/27	0.94	0.51	102,122,147,148	20
5	RVU	В	1101	27/27	0.95	0.47	111,130,156,159	20
5	RVU	Е	1101	27/27	0.95	0.48	104,122,148,158	20
4	SO4	В	1103	5/5	0.95	0.11	163,164,175,200	0
4	SO4	F	303	5/5	0.96	0.17	116,120,136,138	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.

