

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

#### Aug 22, 2023 - 09:20 AM EDT

PDB ID	:	2RF0
Title	:	Crystal structure of human mixed lineage kinase MAP3K10 SH3 domain
Authors	:	Ugochukwu, E.; Eswaran, J.; Elkins, J.; Keates, T.; Pike, A.C.W.; Berridge,
		G.; Savitsky, P.; Sundstrom, M.; Arrowsmith, C.H.; Weigelt, J.; Edwards,
		A.M.; von Delft, F.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on		
Resolution	:	2.00 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:

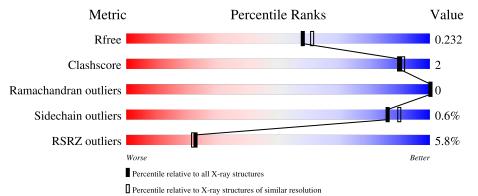
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal 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 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	89	.% •	64%	6%	30%
1	В	89	2%	61%	••	37%
1	С	89	8%	66%	•	30%
1	D	89	4%	64%	•	31%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1851 atoms, of which 0 are hydrogens and 0 are deuteriums.

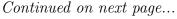
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	А	62	Total         C         N         O         S           445         286         72         86         1	0	0	0
1	В	56	Total C N O 415 267 69 79	0	0	0
1	С	62	Total         C         N         O         S           441         284         72         84         1	0	0	0
1	D	61	Total         C         N         O         S           457         289         80         87         1	0	0	0

• Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase 10.

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-10	MET	-	expression tag	UNP Q02779
А	-9	HIS	-	expression tag	UNP Q02779
А	-8	HIS	-	expression tag	UNP Q02779
А	-7	HIS	-	expression tag	UNP Q02779
А	-6	HIS	-	expression tag	UNP Q02779
A	-5	HIS	-	expression tag	UNP Q02779
А	-4	HIS	-	expression tag	UNP Q02779
А	-3	SER	-	expression tag	UNP Q02779
A	-2	SER	-	expression tag	UNP Q02779
А	-1	GLY	-	expression tag	UNP Q02779
A	0	VAL	-	expression tag	UNP Q02779
А	1	ASP	-	expression tag	UNP Q02779
А	2	LEU	-	expression tag	UNP Q02779
А	3	GLY	-	expression tag	UNP Q02779
А	4	THR	-	expression tag	UNP Q02779
A	5	GLU	-	expression tag	UNP Q02779
А	6	ASN	-	expression tag	UNP Q02779
А	7	LEU	-	expression tag	UNP Q02779
А	8	TYR	-	expression tag	UNP Q02779
А	9	PHE	-	expression tag	UNP Q02779
А	10	GLN	-	expression tag	UNP Q02779



ion tag	0111 @02115	
ion tag	UNP Q02779	

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 Chain
 Residue
 Modelled
 Actual
 Comment
 Reference

$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Chain	Residue	Modelled	Actual	Comment	Reference
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	11	SER	-	expression tag	UNP Q02779
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	12	MET	-	expression tag	UNP Q02779
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	В	-10	MET	-	expression tag	UNP Q02779
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	В	-9	HIS	-	expression tag	UNP Q02779
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	В	-8	HIS	-	expression tag	UNP Q02779
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	В	-7	HIS	-	expression tag	UNP Q02779
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	В	-6	HIS	-	expression tag	UNP Q02779
B-3SER-expression tagUNP Q02779B-2SER-expression tagUNP Q02779B-1GLY-expression tagUNP Q02779B0VAL-expression tagUNP Q02779B1ASP-expression tagUNP Q02779B2LEU-expression tagUNP Q02779B3GLY-expression tagUNP Q02779B4THR-expression tagUNP Q02779B5GLU-expression tagUNP Q02779B6ASN-expression tagUNP Q02779B7LEU-expression tagUNP Q02779B7LEU-expression tagUNP Q02779B9PHE-expression tagUNP Q02779B10GLN-expression tagUNP Q02779B10GLN-expression tagUNP Q02779C-10MET-expression tagUNP Q02779C-2HIS-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-4HIS-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-1GLY-expression tagUNP Q02779C-2SER-expression tag <t< td=""><td>В</td><td>-5</td><td>HIS</td><td>-</td><td>expression tag</td><td>UNP Q02779</td></t<>	В	-5	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	В	-4	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	В	-3	SER	-	expression tag	UNP Q02779
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	В	-2	SER	-	expression tag	UNP Q02779
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	В	-1	GLY	-	expression tag	UNP Q02779
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	В	0	VAL	-	expression tag	UNP Q02779
B3GLY-expression tagUNP Q02779B4THR-expression tagUNP Q02779B5GLU-expression tagUNP Q02779B6ASN-expression tagUNP Q02779B7LEU-expression tagUNP Q02779B8TYR-expression tagUNP Q02779B9PHE-expression tagUNP Q02779B10GLN-expression tagUNP Q02779B11SER-expression tagUNP Q02779B12MET-expression tagUNP Q02779C-10MET-expression tagUNP Q02779C-9HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-7HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-5HIS-expression tagUNP Q02779C-4HIS-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-1GLY-expression tagUNP Q02779C-1ASP-expression tagUNP Q02779C-1ASP-expression tagUNP Q02779C-1ASP-expression tag <td>В</td> <td>1</td> <td>ASP</td> <td>-</td> <td>expression tag</td> <td>UNP Q02779</td>	В	1	ASP	-	expression tag	UNP Q02779
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	В	2	LEU	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	В	3	GLY	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	В	4	THR	-	expression tag	UNP Q02779
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	В	5	GLU	-	expression tag	UNP Q02779
B8TYR-expression tagUNP Q02779B9PHE-expression tagUNP Q02779B10GLN-expression tagUNP Q02779B11SER-expression tagUNP Q02779B12MET-expression tagUNP Q02779C-10MET-expression tagUNP Q02779C-9HIS-expression tagUNP Q02779C-9HIS-expression tagUNP Q02779C-8HIS-expression tagUNP Q02779C-7HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-5HIS-expression tagUNP Q02779C-4HIS-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-1GLY-expression tagUNP Q02779C0VAL-expression tagUNP Q02779C1ASP-expression tagUNP Q02779C2LEU-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C4THR-expression tagUNP Q02779C5GLU-expression tag	В	6	ASN	-	expression tag	UNP Q02779
B9PHE-expression tagUNP $Q02779$ B10GLN-expression tagUNP $Q02779$ B11SER-expression tagUNP $Q02779$ B12MET-expression tagUNP $Q02779$ C-10MET-expression tagUNP $Q02779$ C-10MET-expression tagUNP $Q02779$ C-9HIS-expression tagUNP $Q02779$ C-8HIS-expression tagUNP $Q02779$ C-7HIS-expression tagUNP $Q02779$ C-6HIS-expression tagUNP $Q02779$ C-5HIS-expression tagUNP $Q02779$ C-4HIS-expression tagUNP $Q02779$ C-3SER-expression tagUNP $Q02779$ C-1GLY-expression tagUNP $Q02779$ C-1GLY-expression tagUNP $Q02779$ C-1GLY-expression tagUNP $Q02779$ C1ASP-expression tagUNP $Q02779$ C1ASP-expression tagUNP $Q02779$ C3GLY-expression tagUNP $Q02779$ C4THR-expression tagUNP $Q02779$ C5GLU-expression tagUNP $Q02779$ C6<	В	7	LEU	-	expression tag	UNP Q02779
B10GLN-expression tagUNP Q02779B11SER-expression tagUNP Q02779B12MET-expression tagUNP Q02779C-10MET-expression tagUNP Q02779C-9HIS-expression tagUNP Q02779C-9HIS-expression tagUNP Q02779C-8HIS-expression tagUNP Q02779C-7HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-5HIS-expression tagUNP Q02779C-5HIS-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-2SER-expression tagUNP Q02779C-1GLY-expression tagUNP Q02779C1ASP-expression tagUNP Q02779C1ASP-expression tagUNP Q02779C1ASP-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C4THR-expression tagUNP Q02779C5GLU-expression tagUNP Q02779C6ASN-expression tag	В	8	TYR	-	expression tag	UNP Q02779
B11SER-expression tagUNP Q02779B12MET-expression tagUNP Q02779C-10MET-expression tagUNP Q02779C-9HIS-expression tagUNP Q02779C-8HIS-expression tagUNP Q02779C-7HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-5HIS-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-2SER-expression tagUNP Q02779C-1GLY-expression tagUNP Q02779C0VAL-expression tagUNP Q02779C1ASP-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C4THR-expression tagUNP Q02779C5GLU-expression tagUNP Q02779C6ASN-expression tagUNP Q02779	В	9	PHE	-	expression tag	UNP Q02779
B12MET-expression tagUNP Q02779C-10MET-expression tagUNP Q02779C-9HIS-expression tagUNP Q02779C-8HIS-expression tagUNP Q02779C-7HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-6HIS-expression tagUNP Q02779C-5HIS-expression tagUNP Q02779C-4HIS-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-3SER-expression tagUNP Q02779C-1GLY-expression tagUNP Q02779C0VAL-expression tagUNP Q02779C1ASP-expression tagUNP Q02779C2LEU-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C5GLU-expression tagUNP Q02779C6ASN-expression tagUNP Q02779	В	10	GLN	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	В	11	SER	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	В	12	MET	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-10	MET	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-9	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-8	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-7	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-6	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-5	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C	-4	HIS	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-3	SER	-	expression tag	UNP Q02779
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	-2	SER	-	expression tag	UNP Q02779
C1ASP-expression tagUNP Q02779C2LEU-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C4THR-expression tagUNP Q02779C5GLU-expression tagUNP Q02779C6ASN-expression tagUNP Q02779		-1	GLY	-	expression tag	UNP Q02779
C2LEU-expression tagUNP Q02779C3GLY-expression tagUNP Q02779C4THR-expression tagUNP Q02779C5GLU-expression tagUNP Q02779C6ASN-expression tagUNP Q02779	С	0	VAL	-	expression tag	UNP Q02779
C3GLY-expression tagUNP Q02779C4THR-expression tagUNP Q02779C5GLU-expression tagUNP Q02779C6ASN-expression tagUNP Q02779	С	1	ASP	-	expression tag	UNP Q02779
C4THR-expression tagUNP Q02779C5GLU-expression tagUNP Q02779C6ASN-expression tagUNP Q02779		2	LEU	-	expression tag	UNP Q02779
C5GLU-expression tagUNP Q02779C6ASN-expression tagUNP Q02779		3	GLY	-	expression tag	UNP Q02779
C 6 ASN - expression tag UNP Q02779		4	THR	-	expression tag	•
		5	GLU	-	expression tag	
	C	6	ASN	-		UNP Q02779

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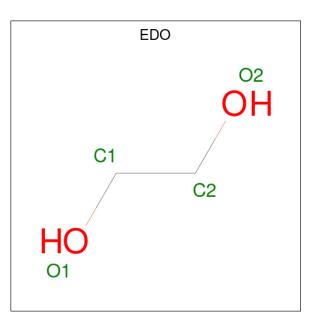


Chain	Residue	Modelled	Actual	Comment	Reference
С	7	LEU	-	expression tag	UNP Q02779
С	8	TYR	-	expression tag	UNP Q02779
С	9	PHE	-	expression tag	UNP Q02779
С	10	GLN	-	expression tag	UNP Q02779
С	11	SER	-	expression tag	UNP Q02779
С	12	MET	-	expression tag	UNP Q02779
D	-10	MET	-	expression tag	UNP Q02779
D	-9	HIS	-	expression tag	UNP Q02779
D	-8	HIS	-	expression tag	UNP Q02779
D	-7	HIS	-	expression tag	UNP Q02779
D	-6	HIS	-	expression tag	UNP Q02779
D	-5	HIS	-	expression tag	UNP Q02779
D	-4	HIS	-	expression tag	UNP Q02779
D	-3	SER	-	expression tag	UNP Q02779
D	-2	SER	-	expression tag	UNP Q02779
D	-1	GLY	-	expression tag	UNP Q02779
D	0	VAL	-	expression tag	UNP Q02779
D	1	ASP	-	expression tag	UNP Q02779
D	2	LEU	-	expression tag	UNP Q02779
D	3	GLY	-	expression tag	UNP Q02779
D	4	THR	-	expression tag	UNP Q02779
D	5	GLU	-	expression tag	UNP Q02779
D	6	ASN	-	expression tag	UNP Q02779
D	7	LEU	-	expression tag	UNP Q02779
D	8	TYR	-	expression tag	UNP Q02779
D	9	PHE	-	expression tag	UNP Q02779
D	10	GLN	-	expression tag	UNP Q02779
D	11	SER	-	expression tag	UNP Q02779
D	12	MET	-	expression tag	UNP Q02779

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





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

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	17	Total O 18 18	0	1
3	В	16	Total         O           16         16	0	0
3	С	26	Total         O           26         26	0	0
3	D	25	TotalO2525	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.

- Chain A: 64% 6% 30% • Molecule 1: Mitogen-activated protein kinase kinase kinase 10 Chain B: 61% 37% • Molecule 1: Mitogen-activated protein kinase kinase kinase 10 Chain C: 66% 30% MET HIIS HIIS HIIS HIIS HIIS SER GLY ASP GLY GLY CLEU GLY TTHR GLU GLN SER RMET TTHR GLN SER RMET TTHR PTHR • Molecule 1: Mitogen-activated protein kinase kinase kinase 10 Chain D: 64% 31%
- Molecule 1: Mitogen-activated protein kinase kinase kinase 10



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants	69.68Å $69.68$ Å $103.98$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	52.19 - 2.00	Depositor
Resolution (A)	52.19 - 2.00	EDS
% Data completeness	99.9 (52.19-2.00)	Depositor
(in resolution range)	99.9 (52.19-2.00)	EDS
R <sub>merge</sub>	0.07	Depositor
R <sub>sym</sub>	0.07	Depositor
$< I/\sigma(I) > 1$	$2.68 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
D D.	0.189 , 0.230	Depositor
$R, R_{free}$	0.194 , $0.232$	DCC
$R_{free}$ test set	1013 reflections $(5.13\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	40.6	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34,62.1	EDS
L-test for $twinning^2$	$<  L  > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1851	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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).

Mol	Chain	Boi	nd lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.76	1/458~(0.2%)	0.65	0/629	
1	В	0.82	1/427~(0.2%)	0.68	0/585	
1	С	0.64	0/454	0.66	0/624	
1	D	0.79	0/470	0.70	0/643	
All	All	0.76	2/1809~(0.1%)	0.67	0/2481	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	34	GLU	CD-OE2	7.35	1.33	1.25
1	В	34	GLU	CD-OE2	7.01	1.33	1.25

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	445	0	398	2	0
1	В	415	0	373	1	0
1	С	441	0	394	1	0
1	D	457	0	420	2	0
2	А	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4	0	6	0	0
3	А	18	0	0	0	0
3	В	16	0	0	0	0
3	С	26	0	0	0	0
3	D	25	0	0	0	0
All	All	1851	0	1597	6	0

Continued from previous page...

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 2.

All (6) 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:A:24:VAL:HG23	1:A:25:PHE:CD1	2.41	0.55
1:D:24:VAL:HG23	1:D:25:PHE:CD1	2.47	0.50
1:A:27:TYR:HB2	1:A:75:TYR:CD2	2.51	0.45
1:D:27:TYR:HB2	1:D:75:TYR:CD2	2.54	0.43
1:B:30:ALA:HB3	1:B:34:GLU:OE2	2.19	0.42
1:C:27:TYR:HB2	1:C:75:TYR:CD2	2.56	0.41

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	Percentiles	
1	А	60/89~(67%)	60 (100%)	0	0	100	100
1	В	52/89~(58%)	52 (100%)	0	0	100	100
1	$\mathbf{C}$	60/89~(67%)	60 (100%)	0	0	100	100
1	D	59/89~(66%)	58 (98%)	1 (2%)	0	100	100
All	All	231/356~(65%)	230 (100%)	1 (0%)	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 side chain 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	41/72~(57%)	41 (100%)	0	100 100		
1	В	39/72~(54%)	39 (100%)	0	100 100		
1	С	40/72~(56%)	39~(98%)	1 (2%)	47 49		
1	D	45/72~(62%)	45 (100%)	0	100 100		
All	All	165/288~(57%)	164 (99%)	1 (1%)	86 90		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	67	ARG

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)

2 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).

Mol	Type Chain I		Res	Tiple	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	EDO	А	79	-	3,3,3	0.57	0	$2,\!2,\!2$	0.08	0
2	EDO	D	79	-	3,3,3	0.60	0	$2,\!2,\!2$	0.56	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	EDO	А	79	-	-	1/1/1/1	-
2	EDO	D	79	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	79	EDO	O1-C1-C2-O2
2	А	79	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

### 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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	62/89~(69%)	0.44	1 (1%) 72 70	42, 50, 58, 63	0
1	В	56/89~(62%)	0.52	2 (3%) 42 42	44, 50, 60, 69	0
1	С	62/89~(69%)	0.66	7 (11%) 5 4	46, 51, 57, 61	0
1	D	61/89~(68%)	0.54	4 (6%) 18 17	45, 49, 66, 68	0
All	All	241/356~(67%)	0.54	14 (5%) 23 22	42, 50, 60, 69	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	CYS	4.5
1	D	51	ALA	4.5
1	С	52	VAL	4.4
1	С	68	VAL	3.2
1	А	31	GLY	2.7
1	С	64	PRO	2.6
1	С	54	GLY	2.5
1	С	66	GLY	2.4
1	С	67	ARG	2.3
1	В	31	GLY	2.2
1	С	49	ASP	2.2
1	D	52	VAL	2.1
1	D	53	SER	2.1
1	В	17	ALA	2.1

### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	EDO	А	79	4/4	0.84	0.15	55,70,72,74	0
2	EDO	D	79	4/4	0.86	0.18	52,54,56,60	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

