



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 AM GMT

PDB ID : 2Q05  
Title : Crystal structure of tyr/ser protein phosphatase from Vaccinia virus WR  
Authors : Osipiuk, J.; Skarina, T.; Kagan, O.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2007-05-18  
Resolution : 2.57 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

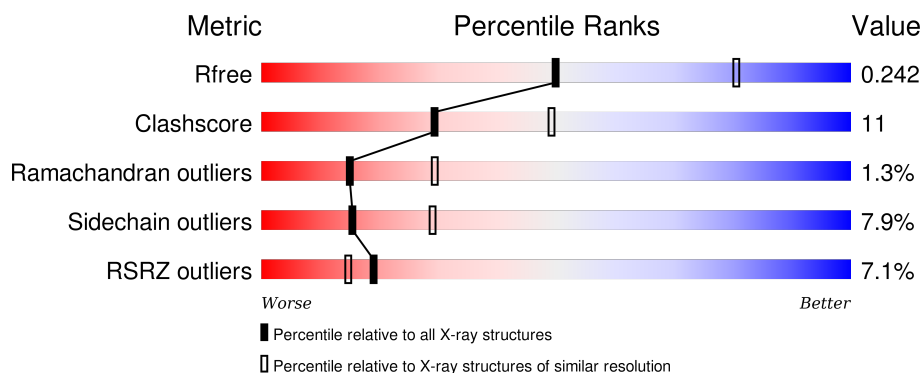
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	A	195	<div> <div>13%</div> <div>68% 18% 6% 7%</div> </div>
1	B	195	<div> <div>3%</div> <div>69% 18% 5% 8%</div> </div>
1	C	195	<div> <div>5%</div> <div>68% 18% 12%</div> </div>
1	D	195	<div> <div>5%</div> <div>69% 21% 7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5825 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 Dual specificity protein phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	Se	0	1	0
			1458	933	246	268	2	9			
1	B	179	Total	C	N	O	S	Se	0	0	0
			1453	929	245	268	2	9			
1	C	172	Total	C	N	O	S	Se	0	1	0
			1393	890	235	257	2	9			
1	D	181	Total	C	N	O	S	Se	0	2	0
			1458	932	247	267	2	10			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	CLONING ARTIFACT	UNP P07239
A	-20	GLY	-	CLONING ARTIFACT	UNP P07239
A	-19	SER	-	CLONING ARTIFACT	UNP P07239
A	-18	SER	-	CLONING ARTIFACT	UNP P07239
A	-17	HIS	-	CLONING ARTIFACT	UNP P07239
A	-16	HIS	-	CLONING ARTIFACT	UNP P07239
A	-15	HIS	-	CLONING ARTIFACT	UNP P07239
A	-14	HIS	-	CLONING ARTIFACT	UNP P07239
A	-13	HIS	-	CLONING ARTIFACT	UNP P07239
A	-12	HIS	-	CLONING ARTIFACT	UNP P07239
A	-11	SER	-	CLONING ARTIFACT	UNP P07239
A	-10	SER	-	CLONING ARTIFACT	UNP P07239
A	-9	GLY	-	CLONING ARTIFACT	UNP P07239
A	-8	ARG	-	CLONING ARTIFACT	UNP P07239
A	-7	GLU	-	CLONING ARTIFACT	UNP P07239
A	-6	ASN	-	CLONING ARTIFACT	UNP P07239
A	-5	LEU	-	CLONING ARTIFACT	UNP P07239
A	-4	TYR	-	CLONING ARTIFACT	UNP P07239
A	-3	PHE	-	CLONING ARTIFACT	UNP P07239
A	-2	GLN	-	CLONING ARTIFACT	UNP P07239
A	-1	GLY	-	CLONING ARTIFACT	UNP P07239

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	CLONING ARTIFACT	UNP P07239
A	1	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	18	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	20	ARG	LYS	SEE REMARK 999	UNP P07239
A	27	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	43	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	60	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	120	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	126	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	135	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	145	MSE	MET	MODIFIED RESIDUE	UNP P07239
A	172	GLY	-	CLONING ARTIFACT	UNP P07239
A	173	SER	-	CLONING ARTIFACT	UNP P07239
B	-21	MSE	-	CLONING ARTIFACT	UNP P07239
B	-20	GLY	-	CLONING ARTIFACT	UNP P07239
B	-19	SER	-	CLONING ARTIFACT	UNP P07239
B	-18	SER	-	CLONING ARTIFACT	UNP P07239
B	-17	HIS	-	CLONING ARTIFACT	UNP P07239
B	-16	HIS	-	CLONING ARTIFACT	UNP P07239
B	-15	HIS	-	CLONING ARTIFACT	UNP P07239
B	-14	HIS	-	CLONING ARTIFACT	UNP P07239
B	-13	HIS	-	CLONING ARTIFACT	UNP P07239
B	-12	HIS	-	CLONING ARTIFACT	UNP P07239
B	-11	SER	-	CLONING ARTIFACT	UNP P07239
B	-10	SER	-	CLONING ARTIFACT	UNP P07239
B	-9	GLY	-	CLONING ARTIFACT	UNP P07239
B	-8	ARG	-	CLONING ARTIFACT	UNP P07239
B	-7	GLU	-	CLONING ARTIFACT	UNP P07239
B	-6	ASN	-	CLONING ARTIFACT	UNP P07239
B	-5	LEU	-	CLONING ARTIFACT	UNP P07239
B	-4	TYR	-	CLONING ARTIFACT	UNP P07239
B	-3	PHE	-	CLONING ARTIFACT	UNP P07239
B	-2	GLN	-	CLONING ARTIFACT	UNP P07239
B	-1	GLY	-	CLONING ARTIFACT	UNP P07239
B	0	HIS	-	CLONING ARTIFACT	UNP P07239
B	1	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	18	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	20	ARG	LYS	SEE REMARK 999	UNP P07239
B	27	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	43	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	60	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	120	MSE	MET	MODIFIED RESIDUE	UNP P07239

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Chain	Residue	Modelled	Actual	Comment	Reference
B	126	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	135	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	145	MSE	MET	MODIFIED RESIDUE	UNP P07239
B	172	GLY	-	CLONING ARTIFACT	UNP P07239
B	173	SER	-	CLONING ARTIFACT	UNP P07239
C	-21	MSE	-	CLONING ARTIFACT	UNP P07239
C	-20	GLY	-	CLONING ARTIFACT	UNP P07239
C	-19	SER	-	CLONING ARTIFACT	UNP P07239
C	-18	SER	-	CLONING ARTIFACT	UNP P07239
C	-17	HIS	-	CLONING ARTIFACT	UNP P07239
C	-16	HIS	-	CLONING ARTIFACT	UNP P07239
C	-15	HIS	-	CLONING ARTIFACT	UNP P07239
C	-14	HIS	-	CLONING ARTIFACT	UNP P07239
C	-13	HIS	-	CLONING ARTIFACT	UNP P07239
C	-12	HIS	-	CLONING ARTIFACT	UNP P07239
C	-11	SER	-	CLONING ARTIFACT	UNP P07239
C	-10	SER	-	CLONING ARTIFACT	UNP P07239
C	-9	GLY	-	CLONING ARTIFACT	UNP P07239
C	-8	ARG	-	CLONING ARTIFACT	UNP P07239
C	-7	GLU	-	CLONING ARTIFACT	UNP P07239
C	-6	ASN	-	CLONING ARTIFACT	UNP P07239
C	-5	LEU	-	CLONING ARTIFACT	UNP P07239
C	-4	TYR	-	CLONING ARTIFACT	UNP P07239
C	-3	PHE	-	CLONING ARTIFACT	UNP P07239
C	-2	GLN	-	CLONING ARTIFACT	UNP P07239
C	-1	GLY	-	CLONING ARTIFACT	UNP P07239
C	0	HIS	-	CLONING ARTIFACT	UNP P07239
C	1	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	18	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	20	ARG	LYS	SEE REMARK 999	UNP P07239
C	27	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	43	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	60	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	120	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	126	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	135	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	145	MSE	MET	MODIFIED RESIDUE	UNP P07239
C	172	GLY	-	CLONING ARTIFACT	UNP P07239
C	173	SER	-	CLONING ARTIFACT	UNP P07239
D	-21	MSE	-	CLONING ARTIFACT	UNP P07239
D	-20	GLY	-	CLONING ARTIFACT	UNP P07239
D	-19	SER	-	CLONING ARTIFACT	UNP P07239

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	SER	-	CLONING ARTIFACT	UNP P07239
D	-17	HIS	-	CLONING ARTIFACT	UNP P07239
D	-16	HIS	-	CLONING ARTIFACT	UNP P07239
D	-15	HIS	-	CLONING ARTIFACT	UNP P07239
D	-14	HIS	-	CLONING ARTIFACT	UNP P07239
D	-13	HIS	-	CLONING ARTIFACT	UNP P07239
D	-12	HIS	-	CLONING ARTIFACT	UNP P07239
D	-11	SER	-	CLONING ARTIFACT	UNP P07239
D	-10	SER	-	CLONING ARTIFACT	UNP P07239
D	-9	GLY	-	CLONING ARTIFACT	UNP P07239
D	-8	ARG	-	CLONING ARTIFACT	UNP P07239
D	-7	GLU	-	CLONING ARTIFACT	UNP P07239
D	-6	ASN	-	CLONING ARTIFACT	UNP P07239
D	-5	LEU	-	CLONING ARTIFACT	UNP P07239
D	-4	TYR	-	CLONING ARTIFACT	UNP P07239
D	-3	PHE	-	CLONING ARTIFACT	UNP P07239
D	-2	GLN	-	CLONING ARTIFACT	UNP P07239
D	-1	GLY	-	CLONING ARTIFACT	UNP P07239
D	0	HIS	-	CLONING ARTIFACT	UNP P07239
D	1	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	18	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	20	ARG	LYS	SEE REMARK 999	UNP P07239
D	27	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	43	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	60	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	120	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	126	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	135	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	145	MSE	MET	MODIFIED RESIDUE	UNP P07239
D	172	GLY	-	CLONING ARTIFACT	UNP P07239
D	173	SER	-	CLONING ARTIFACT	UNP P07239

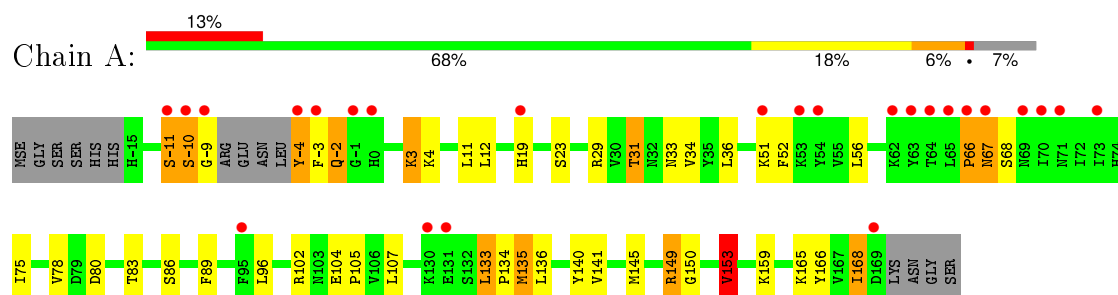
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	16	Total O 16 16	0	0
2	C	10	Total O 10 10	0	0
2	D	23	Total O 23 23	0	0

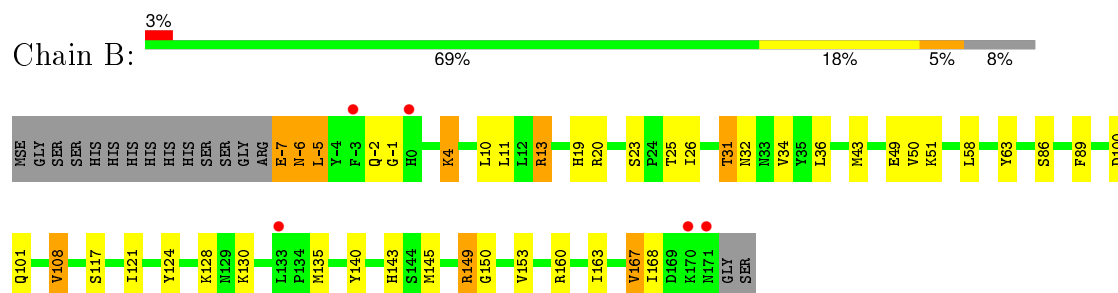
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

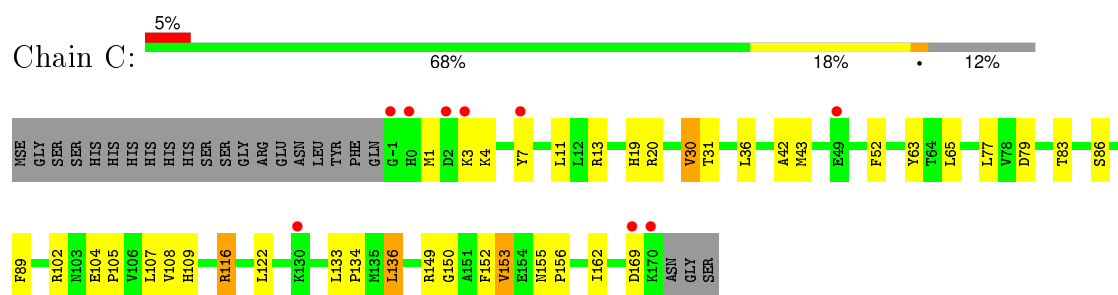
#### • Molecule 1: Dual specificity protein phosphatase



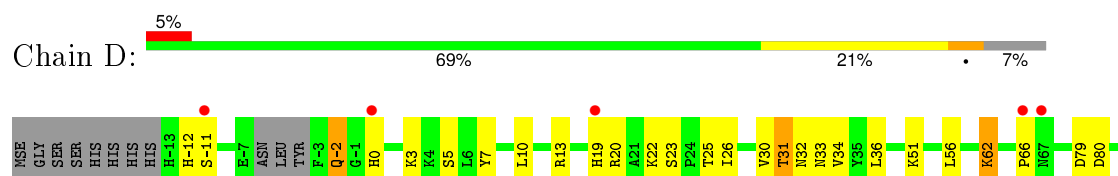
#### • Molecule 1: Dual specificity protein phosphatase

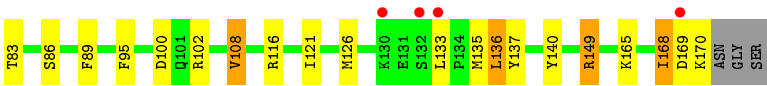


#### • Molecule 1: Dual specificity protein phosphatase



#### • Molecule 1: Dual specificity protein phosphatase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.25Å 169.25Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.57 39.89 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.57) 99.7 (39.89-2.57)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.218 0.220 , 0.242	Depositor DCC
$R_{free}$ test set	2610 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.6	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 51352 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5825	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.92	3/1483 (0.2%)	0.78	3/1986 (0.2%)
1	B	0.78	0/1475	0.82	3/1977 (0.2%)
1	C	0.65	0/1415	0.74	0/1894
1	D	0.69	1/1485 (0.1%)	0.75	2/1987 (0.1%)
All	All	0.77	4/5858 (0.1%)	0.77	8/7844 (0.1%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	LYS	CE-NZ	20.79	2.01	1.49
1	A	3	LYS	CD-CE	11.69	1.80	1.51
1	A	-9	GLY	C-O	9.62	1.39	1.23
1	D	-12	HIS	CB-CG	-5.09	1.40	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	CD-CE-NZ	-11.36	85.58	111.70
1	D	149	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	B	149	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	D	149	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	A	149	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	133	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	149	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	B	13	ARG	NE-CZ-NH1	-5.13	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	-1	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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	A	1458	0	1458	43	0
1	B	1453	0	1462	42	0
1	C	1393	0	1411	25	0
1	D	1458	0	1467	37	0
2	A	14	0	0	3	0
2	B	16	0	0	1	0
2	C	10	0	0	2	0
2	D	23	0	0	5	0
All	All	5825	0	5798	131	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 11.

All (131) 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:3:LYS:CD	1:A:3:LYS:CE	1.80	1.57
1:A:3:LYS:NZ	1:A:3:LYS:CE	2.01	1.22
1:D:31:THR:HG22	1:D:34:VAL:H	1.14	1.11
1:B:-6:ASN:N	1:B:-6:ASN:HD22	1.62	0.98
1:B:31:THR:HG22	1:B:34:VAL:H	1.37	0.90
1:B:-5:LEU:HD23	1:B:-5:LEU:H	1.36	0.87
1:A:31:THR:HG22	1:A:34:VAL:H	1.43	0.82
1:A:4:LYS:HG3	1:B:168:ILE:HD12	1.65	0.78
1:A:3:LYS:CG	1:A:3:LYS:CE	2.62	0.77
1:D:79:ASP:HB2	1:D:116:ARG:HD2	1.67	0.76
1:B:-2:GLN:HA	1:B:-2:GLN:NE2	1.99	0.75
1:D:31:THR:HG22	1:D:34:VAL:N	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ASP:HB2	1:C:116:ARG:HD2	1.70	0.74
1:C:136:LEU:HD11	1:D:135[B]:MSE:SE	2.39	0.72
1:B:31:THR:HG21	1:B:100:ASP:OD2	1.90	0.71
1:D:80:ASP:OD1	1:D:83:THR:HG23	1.91	0.70
1:D:31:THR:HG21	1:D:100:ASP:OD2	1.92	0.69
1:C:133:LEU:HD21	1:D:7:TYR:CE1	2.29	0.68
1:A:135:MSE:SE	1:B:135:MSE:HE3	2.43	0.67
1:B:19:HIS:HE1	1:B:150:GLY:O	1.77	0.67
1:B:-7:GLU:C	1:B:-6:ASN:HD22	1.98	0.67
1:B:-6:ASN:N	1:B:-6:ASN:ND2	2.36	0.67
1:A:3:LYS:CD	1:A:3:LYS:NZ	2.59	0.65
1:B:13:ARG:HG2	1:B:143:HIS:CG	2.32	0.65
1:D:7:TYR:HE2	1:D:136:LEU:HD21	1.62	0.64
1:A:31:THR:CG2	1:A:34:VAL:H	2.11	0.63
1:C:134:PRO:HA	2:C:182:HOH:O	1.98	0.62
1:C:3:LYS:HB3	1:C:7:TYR:CE2	2.35	0.61
1:A:86:SER:HA	1:A:89:PHE:CD2	2.36	0.61
1:A:149:ARG:HD3	2:A:177:HOH:O	2.02	0.60
1:C:36:LEU:HD23	1:C:149:ARG:HD2	1.85	0.59
1:A:86:SER:HA	1:A:89:PHE:CE2	2.38	0.58
1:C:133:LEU:HD21	1:D:7:TYR:HE1	1.67	0.57
1:A:135:MSE:HG2	1:B:11:LEU:HD21	1.85	0.57
1:B:149:ARG:HD3	2:B:176:HOH:O	2.04	0.57
1:D:36:LEU:HD23	1:D:149:ARG:HD2	1.85	0.57
1:B:124:TYR:CZ	1:B:128:LYS:HE2	2.39	0.57
1:C:11:LEU:HD11	1:D:135[A]:MSE:HG2	1.87	0.57
1:B:31:THR:CG2	1:B:100:ASP:OD2	2.53	0.57
1:C:149:ARG:HD3	2:C:177:HOH:O	2.04	0.56
1:A:19[A]:HIS:HE1	1:A:150:GLY:O	1.89	0.56
1:B:13:ARG:HG2	1:B:143:HIS:ND1	2.21	0.56
1:A:36:LEU:HD23	1:A:149:ARG:HD2	1.88	0.56
1:D:62:LYS:HE3	2:D:185:HOH:O	2.04	0.55
1:A:-11:SER:OG	1:A:-10:SER:N	2.39	0.55
1:D:31:THR:CG2	1:D:33:ASN:H	2.19	0.55
1:A:31:THR:HG22	1:A:34:VAL:N	2.17	0.54
1:C:11:LEU:HD21	1:D:135[B]:MSE:HG3	1.88	0.54
1:A:31:THR:HG23	1:A:33:ASN:H	1.71	0.54
1:A:136:LEU:HB2	1:B:135:MSE:HE1	1.90	0.54
1:D:149:ARG:HD3	2:D:180:HOH:O	2.08	0.54
1:D:116:ARG:HD3	2:D:174:HOH:O	2.07	0.53
1:A:80:ASP:OD1	1:A:83:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG22	1:A:34:VAL:HB	1.89	0.53
1:B:163:ILE:HA	1:B:167:VAL:HG13	1.90	0.52
1:A:67:ASN:H	1:A:67:ASN:HD22	1.56	0.52
1:B:36:LEU:HD23	1:B:149:ARG:HD2	1.92	0.51
1:D:-2:GLN:O	1:D:-2:GLN:HG2	2.11	0.50
1:D:133:LEU:HB3	1:D:135[A]:MSE:HE2	1.93	0.50
1:A:-4:TYR:HE1	2:A:183:HOH:O	1.95	0.50
1:D:31:THR:CG2	1:D:100:ASP:OD2	2.60	0.49
1:B:-5:LEU:N	1:B:-5:LEU:HD23	2.17	0.49
1:B:31:THR:HG23	1:B:32:ASN:N	2.28	0.49
1:A:-4:TYR:C	1:A:-2:GLN:H	2.16	0.48
1:C:77:LEU:HB2	1:C:116:ARG:HG2	1.95	0.48
1:B:31:THR:HG22	1:B:34:VAL:N	2.16	0.48
1:A:67:ASN:H	1:A:67:ASN:ND2	2.12	0.48
1:C:52:PHE:HA	1:C:105:PRO:HB2	1.95	0.48
1:D:26:ILE:O	1:D:149:ARG:NH1	2.46	0.48
1:B:49:GLU:HA	1:B:49:GLU:OE2	2.13	0.48
1:A:78:VAL:HB	1:A:83:THR:HG21	1.96	0.48
1:D:19[B]:HIS:HD2	2:D:186:HOH:O	1.96	0.48
1:B:-7:GLU:HB3	1:B:-6:ASN:HD22	1.78	0.48
1:A:52:PHE:HA	1:A:105:PRO:HB2	1.96	0.47
1:C:122:LEU:HD23	1:C:162:ILE:HD13	1.95	0.47
1:C:3:LYS:HB3	1:C:7:TYR:HE2	1.76	0.47
1:B:26:ILE:O	1:B:149:ARG:NH1	2.47	0.47
1:D:19[B]:HIS:CD2	2:D:186:HOH:O	2.68	0.47
1:D:126:MSE:HE1	1:D:137:TYR:CE2	2.50	0.47
1:D:126:MSE:HE1	1:D:137:TYR:CD2	2.50	0.47
1:D:10:LEU:HD21	1:D:140:TYR:HA	1.97	0.47
1:C:136:LEU:CD1	1:D:135[B]:MSE:SE	3.11	0.46
1:D:20:ARG:NH1	1:D:22:LYS:HE3	2.30	0.46
1:B:-7:GLU:OE1	1:B:145:MSE:HE1	2.16	0.45
1:D:31:THR:HG22	1:D:33:ASN:H	1.81	0.45
1:A:66:PRO:HB2	1:A:67:ASN:H	1.56	0.45
1:D:56:LEU:HD11	1:D:95:PHE:CE2	2.52	0.45
1:C:4:LYS:HB2	1:D:168:ILE:HG23	1.98	0.45
1:B:86:SER:HA	1:B:89:PHE:CD2	2.52	0.45
1:D:31:THR:HG23	1:D:32:ASN:N	2.31	0.44
1:D:3:LYS:HG2	1:D:7:TYR:CE1	2.52	0.44
1:A:31:THR:CG2	1:A:34:VAL:HB	2.47	0.44
1:C:102:ARG:NH2	1:C:104:GLU:OE2	2.50	0.44
1:D:33:ASN:HB2	1:D:100:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HD12	1:B:117:SER:HA	2.00	0.44
1:B:-7:GLU:HB3	1:B:-6:ASN:H	1.31	0.44
1:B:-2:GLN:HE21	1:B:-2:GLN:HA	1.81	0.44
1:A:153:VAL:HG22	1:A:159:LYS:HG3	1.99	0.44
1:A:168:ILE:HG13	1:B:4:LYS:HA	1.99	0.44
1:A:12:LEU:HD11	1:B:160:ARG:HG3	2.00	0.44
1:A:165:LYS:HG2	1:A:166:TYR:CE2	2.53	0.43
1:D:31:THR:HG23	1:D:33:ASN:H	1.83	0.43
1:A:11:LEU:CD1	1:B:167:VAL:HG21	2.48	0.43
1:A:141:VAL:O	1:A:145:MSE:HB2	2.18	0.43
1:D:108:VAL:HG13	1:D:121:ILE:HD11	2.00	0.43
1:C:42:ALA:HB2	1:C:109:HIS:CD2	2.53	0.43
1:A:56:LEU:HD11	1:A:75:ILE:HD12	2.01	0.43
1:B:43:MSE:HE1	1:B:63:TYR:CD2	2.54	0.43
1:C:30:VAL:HG23	1:C:31:THR:HG23	2.01	0.43
1:B:-7:GLU:CA	1:B:-6:ASN:HD22	2.32	0.42
1:A:102:ARG:O	1:A:104:GLU:HG3	2.19	0.42
1:C:155:ASN:HA	1:C:156:PRO:HD2	1.91	0.42
1:A:133:LEU:HA	1:A:134:PRO:HD3	1.82	0.42
1:A:-10:SER:HB2	1:A:29:ARG:O	2.19	0.42
1:B:-5:LEU:CD2	1:B:-5:LEU:H	2.10	0.41
1:B:10:LEU:HD21	1:B:140:TYR:HA	2.01	0.41
1:C:19:HIS:HE1	1:C:150:GLY:O	2.03	0.41
1:C:1:MSE:HE2	1:C:1:MSE:HB2	1.87	0.41
1:C:86:SER:HA	1:C:89:PHE:CD2	2.55	0.41
1:D:86:SER:HA	1:D:89:PHE:CD2	2.55	0.41
1:A:31:THR:HG22	1:A:34:VAL:CB	2.51	0.41
1:A:168:ILE:HG13	1:B:4:LYS:HB2	2.03	0.41
1:C:43:MSE:HE1	1:C:63:TYR:CD2	2.56	0.41
1:B:108:VAL:HG13	1:B:121:ILE:HD11	2.02	0.41
1:A:145:MSE:CE	2:A:175:HOH:O	2.67	0.41
1:C:152:PHE:O	1:C:153:VAL:C	2.58	0.41
1:B:145:MSE:HE2	1:B:145:MSE:HB2	1.80	0.41
1:A:11:LEU:HD11	1:B:167:VAL:HG21	2.03	0.41
1:A:-4:TYR:HE2	1:A:140:TYR:HE2	1.70	0.40
1:D:89:PHE:HD2	1:D:165:LYS:HD3	1.86	0.40
1:B:130:LYS:HD3	1:B:130:LYS:HA	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	A	178/195 (91%)	161 (90%)	13 (7%)	4 (2%)	8	15
1	B	177/195 (91%)	163 (92%)	13 (7%)	1 (1%)	30	54
1	C	171/195 (88%)	160 (94%)	10 (6%)	1 (1%)	30	54
1	D	179/195 (92%)	164 (92%)	12 (7%)	3 (2%)	11	22
All	All	705/780 (90%)	648 (92%)	48 (7%)	9 (1%)	15	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	153	VAL
1	D	0	HIS
1	A	-3	PHE
1	A	-11	SER
1	D	168	ILE
1	B	153	VAL
1	C	153	VAL
1	D	66	PRO

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/167 (97%)	149 (92%)	13 (8%)	15	28
1	B	164/167 (98%)	151 (92%)	13 (8%)	15	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	158/167 (95%)	148 (94%)	10 (6%)	22	43
1	D	163/167 (98%)	148 (91%)	15 (9%)	11	21
All	All	647/668 (97%)	596 (92%)	51 (8%)	15	29

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-10	SER
1	A	-4	TYR
1	A	-2	GLN
1	A	23	SER
1	A	31	THR
1	A	51	LYS
1	A	67	ASN
1	A	68	SER
1	A	96	LEU
1	A	107	LEU
1	A	135	MSE
1	A	153	VAL
1	A	168	ILE
1	B	-7	GLU
1	B	-6	ASN
1	B	-5	LEU
1	B	4	LYS
1	B	20	ARG
1	B	23	SER
1	B	25	THR
1	B	31	THR
1	B	50	VAL
1	B	51	LYS
1	B	101	GLN
1	B	108	VAL
1	B	167	VAL
1	C	13	ARG
1	C	20	ARG
1	C	30	VAL
1	C	65	LEU
1	C	83	THR
1	C	107	LEU
1	C	108	VAL
1	C	116	ARG

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Mol	Chain	Res	Type
1	C	136	LEU
1	C	169	ASP
1	D	-11	SER
1	D	-2	GLN
1	D	5	SER
1	D	13	ARG
1	D	23	SER
1	D	25	THR
1	D	30	VAL
1	D	31	THR
1	D	51	LYS
1	D	62	LYS
1	D	102	ARG
1	D	108	VAL
1	D	136	LEU
1	D	169	ASP
1	D	170	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	GLN
1	A	67	ASN
1	B	-6	ASN
1	B	-2	GLN
1	B	0	HIS
1	B	19	HIS
1	C	19	HIS
1	C	69	ASN
1	D	-2	GLN
1	D	32	ASN
1	D	103	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	172/195 (88%)	0.82	25 (14%) <b>3</b> <b>2</b>	10, 43, 61, 64	0
1	B	170/195 (87%)	0.21	5 (2%) 55 51	17, 27, 52, 68	0
1	C	163/195 (83%)	0.19	9 (5%) 29 24	19, 34, 58, 77	0
1	D	172/195 (88%)	0.26	9 (5%) 31 26	18, 31, 60, 79	0
All	All	677/780 (86%)	0.37	48 (7%) 19 15	10, 33, 60, 79	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	PHE	7.1
1	B	171	ASN	5.1
1	D	66	PRO	4.8
1	A	0	HIS	4.7
1	A	66	PRO	4.6
1	A	130	LYS	4.5
1	D	67	ASN	4.3
1	A	70	ILE	4.1
1	A	67	ASN	4.1
1	A	-11	SER	3.9
1	A	65	LEU	3.9
1	A	51	LYS	3.8
1	B	0	HIS	3.6
1	C	170	LYS	3.5
1	A	-9	GLY	3.4
1	D	130	LYS	3.4
1	A	169	ASP	3.4
1	C	7	TYR	3.3
1	C	130	LYS	3.3
1	D	169	ASP	3.3
1	A	62	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	54	TYR	3.0
1	C	0	HIS	2.9
1	B	170	LYS	2.9
1	A	69	ASN	2.8
1	A	131	GLU	2.8
1	C	-1	GLY	2.8
1	D	133	LEU	2.7
1	D	0	HIS	2.7
1	A	71	ASN	2.6
1	A	95	PHE	2.6
1	A	-10	SER	2.5
1	A	63	TYR	2.5
1	C	169	ASP	2.4
1	A	-1	GLY	2.4
1	A	53	LYS	2.4
1	A	-4	TYR	2.3
1	D	132	SER	2.3
1	C	3	LYS	2.3
1	A	64	THR	2.2
1	B	-3	PHE	2.2
1	D	-11	SER	2.2
1	A	19[A]	HIS	2.1
1	B	133	LEU	2.1
1	C	49	GLU	2.1
1	D	19[A]	HIS	2.1
1	A	73	ILE	2.0
1	C	2	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.