



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:04 AM UTC

PDB ID : 2Q05 / pdb_00002q05
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

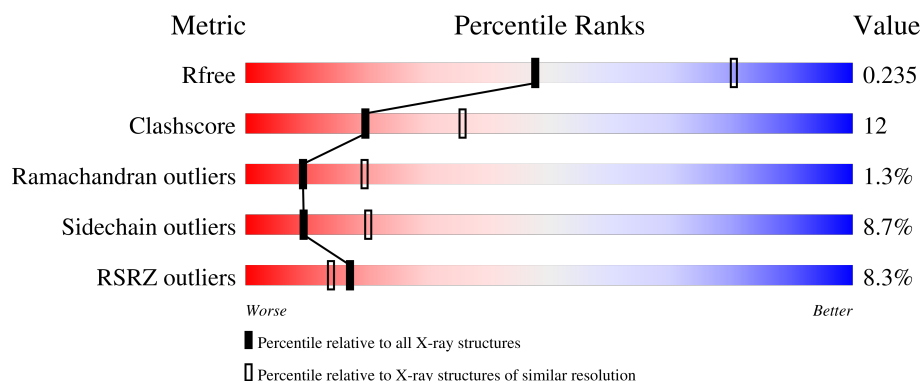
1 Overall quality at a glance ⓘ

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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 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 $\leq 5\%$. 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	11% 65% 22% 5% 7%
1	B	195	6% 69% 18% 5% 8%
1	C	195	4% 67% 18% • 12%
1	D	195	8% 68% 21% 5% 7%

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
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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

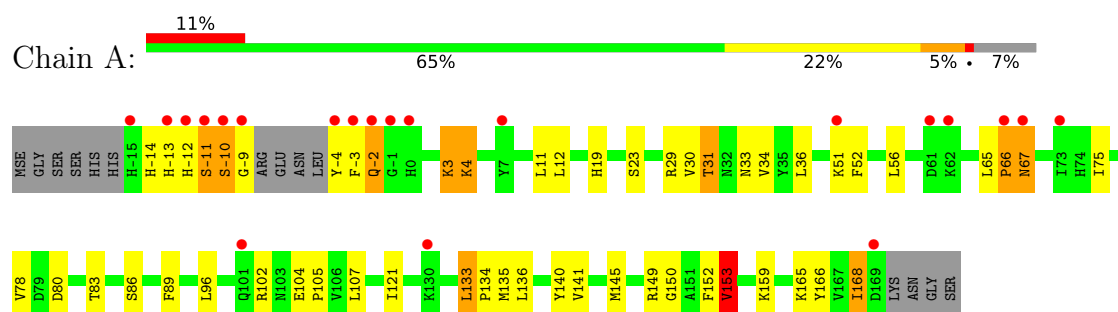
- Molecule 2 is water.

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

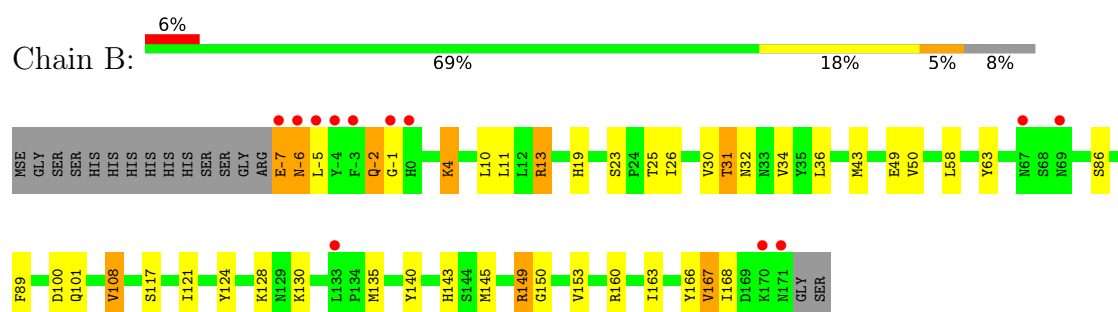
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

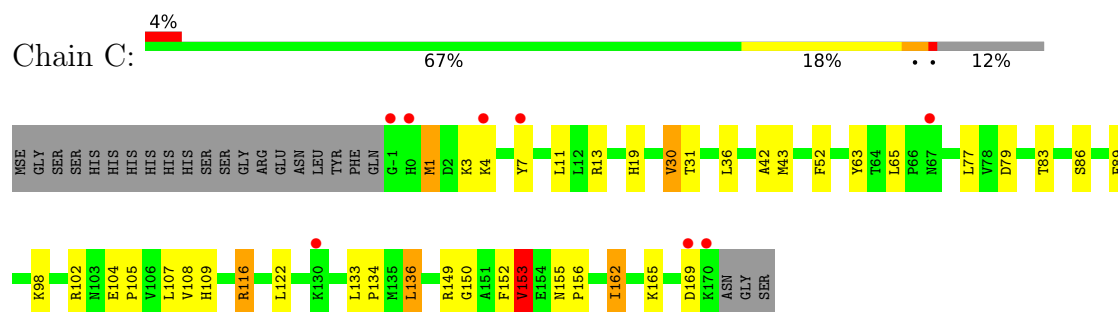
- Molecule 1: Dual specificity protein phosphatase



- Molecule 1: Dual specificity protein phosphatase

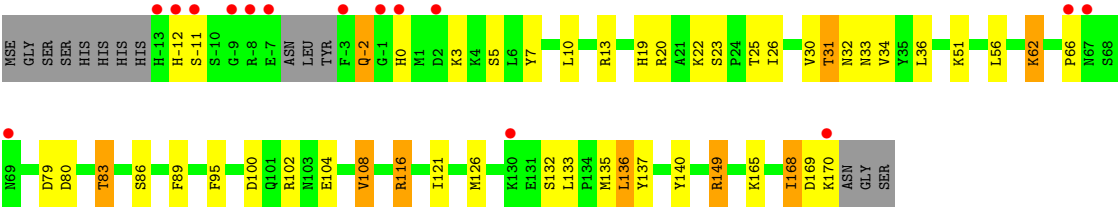


- Molecule 1: Dual specificity protein phosphatase



- 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, α , β , γ	169.25Å 169.25Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.57 40.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.57) 99.6 (40.00-2.57)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.218 0.213 , 0.235	Depositor DCC
R_{free} test set	2610 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5825	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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	0.95	6/1483 (0.4%)	1.02	6/1986 (0.3%)
1	B	0.91	0/1475	1.05	3/1977 (0.2%)
1	C	0.80	0/1415	0.93	1/1894 (0.1%)
1	D	0.83	1/1485 (0.1%)	0.95	1/1987 (0.1%)
All	All	0.87	7/5858 (0.1%)	0.99	11/7844 (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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	LYS	CE-NZ	17.22	2.01	1.49
1	A	3	LYS	CD-CE	9.34	1.80	1.52
1	A	-9	GLY	C-O	7.75	1.39	1.23
1	D	-12	HIS	CB-CG	-6.61	1.40	1.50
1	A	-14	HIS	CB-CG	-6.44	1.41	1.50
1	A	-13	HIS	CB-CG	-5.76	1.42	1.50
1	A	-12	HIS	CB-CG	-5.71	1.42	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	CD-CE-NZ	-8.23	85.58	111.90
1	A	133	LEU	CA-C-N	8.04	128.48	119.32
1	A	133	LEU	C-N-CA	8.04	128.48	119.32
1	A	-13	HIS	CA-CB-CG	-6.51	107.29	113.80
1	B	166	TYR	CA-C-N	-5.84	116.63	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	TYR	C-N-CA	-5.84	116.63	122.77
1	C	1	MSE	CB-CA-C	-5.77	107.18	114.40
1	D	149	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	65	LEU	CA-C-N	5.23	126.38	119.84
1	A	65	LEU	C-N-CA	5.23	126.38	119.84
1	B	149	ARG	NE-CZ-NH1	-5.18	116.32	121.50

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	44	0
1	B	1453	0	1462	42	0
1	C	1393	0	1411	25	0
1	D	1458	0	1467	38	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	133	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 12.

All (133) 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:CE	1:A:3:LYS:NZ	2.01	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:THR:HG22	1:D:34:VAL:H	1.14	1.11
1:B:-6:ASN:HD22	1:B:-6:ASN:N	1.62	0.98
1:B:31:THR:HG22	1:B:34:VAL:H	1.37	0.90
1:B:-5:LEU:H	1:B:-5:LEU:HD23	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:CE	1:A:3:LYS:CG	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
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:-7:GLU:C	1:B:-6:ASN:HD22	1.98	0.71
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:-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:A:36:LEU:HD23	1:A:149:ARG:HD2	1.88	0.56
1:B:13:ARG:HG2	1:B:143:HIS:ND1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:-4:TYR:C	1:A:-2:GLN:H	2.16	0.53
1:A:80:ASP:OD1	1:A:83:THR:HG23	2.08	0.53
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:B:-5:LEU:HD23	1:B:-5:LEU:N	2.17	0.49
1:D:31:THR:CG2	1:D:100:ASP:OD2	2.60	0.49
1:B:31:THR:HG23	1:B:32:ASN:N	2.28	0.49
1:C:77:LEU:HB2	1:C:116:ARG:HG2	1.95	0.48
1:A:67:ASN:H	1:A:67:ASN:ND2	2.12	0.48
1:B:31:THR:HG22	1:B:34:VAL:N	2.16	0.48
1:C:52:PHE:HA	1:C:105:PRO:HB2	1.95	0.48
1:B:49:GLU:OE2	1:B:49:GLU:HA	2.13	0.48
1:D:26:ILE:O	1:D:149:ARG:NH1	2.46	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:B:26:ILE:O	1:B:149:ARG:NH1	2.47	0.47
1:C:3:LYS:HB3	1:C:7:TYR:HE2	1.76	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:10:LEU:HD21	1:D:140:TYR:HA	1.97	0.47
1:D:126:MSE:HE1	1:D:137:TYR:CD2	2.50	0.47
1:C:136:LEU:CD1	1:D:135[B]:MSE:SE	3.11	0.46
1:C:152:PHE:O	1:C:153:VAL:C	2.58	0.46
1:D:20:ARG:NH1	1:D:22:LYS:HE3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:86:SER:HA	1:B:89:PHE:CD2	2.52	0.45
1:C:4:LYS:HB2	1:D:168:ILE:HG23	1.98	0.45
1:D:3:LYS:HG2	1:D:7:TYR:CE1	2.52	0.44
1:D:31:THR:HG23	1:D:32:ASN:N	2.31	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:B:58:LEU:HD12	1:B:117:SER:HA	2.00	0.44
1:D:33:ASN:HB2	1:D:100:ASP:OD1	2.18	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:B:-7:GLU:HB3	1:B:-6:ASN:H	1.31	0.44
1:B:-2:GLN:HA	1:B:-2:GLN:HE21	1.81	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: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:31:THR:HG23	1:D:33:ASN:H	1.83	0.43
1:D:108:VAL:HG13	1:D:121:ILE:HD11	2.00	0.43
1:A:56:LEU:HD11	1:A:75:ILE:HD12	2.01	0.43
1:C:42:ALA:HB2	1:C:109:HIS:CD2	2.53	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:A:102:ARG:O	1:A:104:GLU:HG3	2.19	0.42
1:B:-7:GLU:CA	1:B:-6:ASN:HD22	2.32	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:H	1:B:-5:LEU:CD2	2.10	0.41
1:B:10:LEU:HD21	1:B:140:TYR:HA	2.01	0.41
1:C:1:MSE:HE2	1:C:1:MSE:HB2	1.87	0.41
1:C:19:HIS:HE1	1:C:150:GLY:O	2.03	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:D:102:ARG:HH21	1:D:104:GLU:CD	2.28	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:B:108:VAL:HG13	1:B:121:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:MSE:HE1	1:C:63:TYR:CD2	2.56	0.41
1:A:145:MSE:CE	2:A:175:HOH:O	2.67	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:B:130:LYS:HA	1:B:130:LYS:HD3	1.88	0.40
1:D:89:PHE:HD2	1:D:165:LYS:HD3	1.86	0.40
1:A:152:PHE:O	1:A:153:VAL:C	2.64	0.40

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	A	178/195 (91%)	161 (90%)	13 (7%)	4 (2%)	5	9
1	B	177/195 (91%)	163 (92%)	13 (7%)	1 (1%)	21	39
1	C	171/195 (88%)	160 (94%)	10 (6%)	1 (1%)	21	39
1	D	179/195 (92%)	164 (92%)	12 (7%)	3 (2%)	7	14
All	All	705/780 (90%)	648 (92%)	48 (7%)	9 (1%)	9	19

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

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Mol	Chain	Res	Type
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%)	11	24
1	B	164/167 (98%)	151 (92%)	13 (8%)	11	24
1	C	158/167 (95%)	145 (92%)	13 (8%)	10	23
1	D	163/167 (98%)	146 (90%)	17 (10%)	7	13
All	All	647/668 (97%)	591 (91%)	56 (9%)	9	20

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-10	SER
1	A	-2	GLN
1	A	4	LYS
1	A	23	SER
1	A	30	VAL
1	A	31	THR
1	A	51	LYS
1	A	67	ASN
1	A	96	LEU
1	A	107	LEU
1	A	121	ILE
1	A	153	VAL
1	A	168	ILE
1	B	-7	GLU
1	B	-6	ASN
1	B	-2	GLN
1	B	4	LYS
1	B	13	ARG
1	B	23	SER

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Mol	Chain	Res	Type
1	B	25	THR
1	B	30	VAL
1	B	31	THR
1	B	50	VAL
1	B	101	GLN
1	B	108	VAL
1	B	167	VAL
1	C	13	ARG
1	C	30	VAL
1	C	65	LEU
1	C	83	THR
1	C	98	LYS
1	C	107	LEU
1	C	108	VAL
1	C	116	ARG
1	C	136	LEU
1	C	153	VAL
1	C	162	ILE
1	C	165	LYS
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	83	THR
1	D	108	VAL
1	D	116	ARG
1	D	132	SER
1	D	136	LEU
1	D	169	ASP
1	D	170	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	GLN

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Mol	Chain	Res	Type
1	A	67	ASN
1	A	71	ASN
1	A	129	ASN
1	B	-6	ASN
1	B	-2	GLN
1	B	0	HIS
1	B	19	HIS
1	C	0	HIS
1	C	19	HIS
1	C	32	ASN
1	C	33	ASN
1	C	69	ASN
1	D	32	ASN
1	D	103	ASN
1	D	129	ASN

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 oligosaccharides 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, 95th 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	A	172/195 (88%)	0.73	21 (12%) 8 7	10, 43, 61, 64	1 (0%)
1	B	170/195 (87%)	-0.01	12 (7%) 22 18	17, 27, 52, 68	0
1	C	163/195 (83%)	0.14	8 (4%) 35 30	19, 34, 58, 77	1 (0%)
1	D	172/195 (88%)	0.27	15 (8%) 16 13	16, 31, 60, 79	1 (0%)
All	All	677/780 (86%)	0.28	56 (8%) 17 14	10, 33, 60, 79	3 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	PHE	8.4
1	A	-11	SER	7.8
1	D	-3	PHE	6.2
1	A	-9	GLY	6.1
1	D	-13	HIS	6.0
1	B	0	HIS	5.1
1	C	-1	GLY	5.1
1	D	-8	ARG	4.9
1	A	-10	SER	4.8
1	A	0	HIS	4.5
1	C	0	HIS	4.3
1	D	-11	SER	4.0
1	B	-6	ASN	4.0
1	A	-4	TYR	3.8
1	C	170	LYS	3.8
1	A	-1	GLY	3.5
1	D	66	PRO	3.4
1	B	-3	PHE	3.4
1	B	67	ASN	3.3
1	C	7	TYR	3.3
1	D	-7	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	4	LYS	3.3
1	B	171	ASN	3.2
1	B	-4	TYR	3.2
1	D	-1	GLY	3.2
1	D	-9	GLY	3.1
1	A	169	ASP	3.1
1	D	-12	HIS	3.1
1	B	-5	LEU	3.0
1	A	130	LYS	2.9
1	D	130	LYS	2.9
1	A	66	PRO	2.8
1	C	130	LYS	2.8
1	A	67	ASN	2.7
1	B	-7	GLU	2.7
1	C	169	ASP	2.6
1	A	-2	GLN	2.6
1	A	-12	HIS	2.6
1	D	0	HIS	2.5
1	A	-13	HIS	2.5
1	C	67	ASN	2.5
1	D	170	LYS	2.4
1	B	133	LEU	2.4
1	A	51	LYS	2.3
1	D	2	ASP	2.3
1	D	67	ASN	2.3
1	B	170	LYS	2.3
1	A	62	LYS	2.2
1	A	73	ILE	2.2
1	A	61	ASP	2.1
1	A	-15	HIS	2.1
1	A	101	GLN	2.1
1	D	69	ASN	2.1
1	A	7	TYR	2.1
1	B	69	ASN	2.0
1	B	-1	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.