



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 AM UTC

PDB ID : 1PPO / pdb_00001ppo
Title : DETERMINATION OF THE STRUCTURE OF PAPAYA PROTEASE OMEGA
Authors : Pickersgill, R.W.; Rizkallah, P.J.; Harris, G.W.; Goodenough, P.W.
Deposited on : 1991-07-12
Resolution : 1.80 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
Xtrriage (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

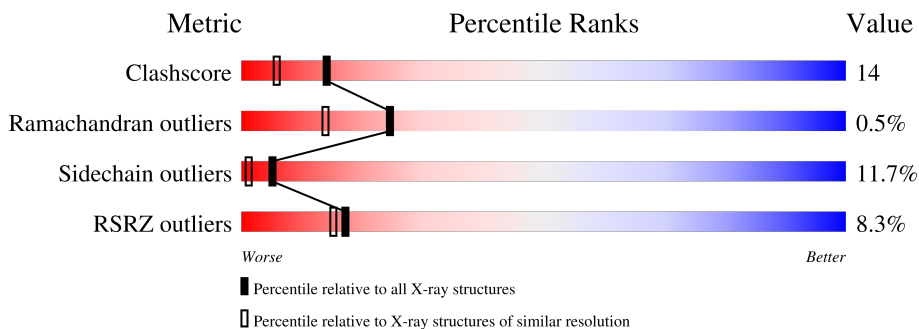
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	216	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1775 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 PROTEASE OMEGA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1641	1037	300	297	7	0	0	0

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Hg	0	0
			1	1		

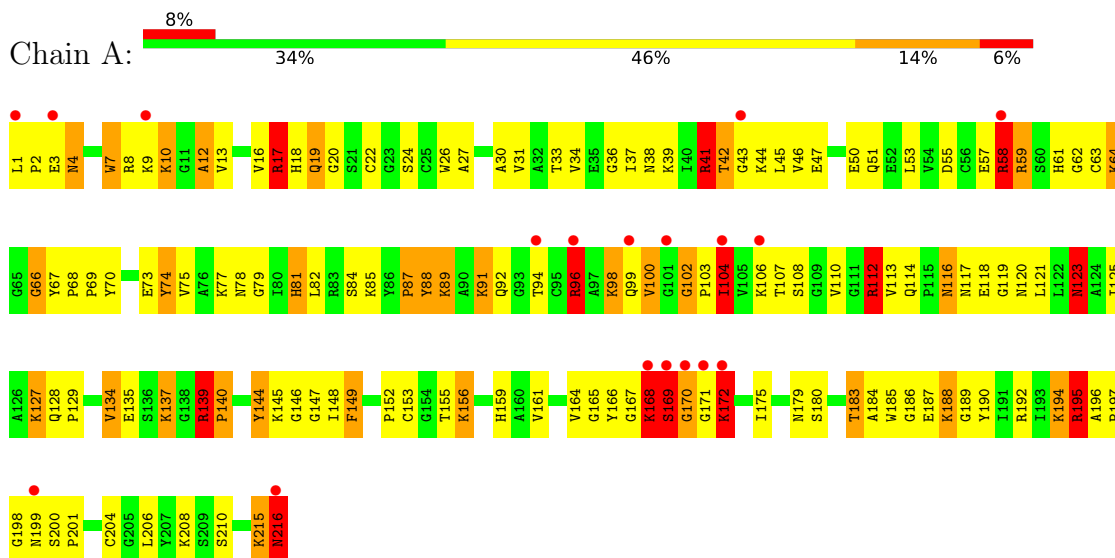
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total	O	0	0
			133	133		

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: PROTEASE OMEGA



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	74.11Å 74.11Å 77.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.80 64.18 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.80) 79.8 (64.18-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 1.80Å)	Xtrriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.155 , (Not available) 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.1	Xtrriage
Anisotropy	0.190	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1775	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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 i

5.1 Standard geometry i

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

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	1.89	34/1680 (2.0%)	3.01	208/2266 (9.2%)

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	A	2	8

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	GLY	N-CA	8.95	1.56	1.44
1	A	61	HIS	CE1-NE2	8.43	1.41	1.32
1	A	114	GLN	CD-OE1	7.36	1.37	1.23
1	A	159	HIS	ND1-CE1	7.26	1.39	1.32
1	A	120	ASN	CG-OD1	6.98	1.36	1.23
1	A	185	TRP	NE1-CE2	-6.78	1.29	1.37
1	A	53	LEU	N-CA	6.76	1.54	1.46
1	A	18	HIS	ND1-CE1	6.69	1.39	1.32
1	A	79	GLY	C-N	-6.58	1.26	1.33
1	A	18	HIS	CE1-NE2	6.46	1.39	1.32
1	A	92	GLN	CD-OE1	6.46	1.35	1.23
1	A	146	GLY	N-CA	6.39	1.51	1.45
1	A	99	GLN	CD-OE1	6.15	1.35	1.23
1	A	61	HIS	ND1-CE1	6.00	1.38	1.32
1	A	215	LYS	CA-C	5.93	1.59	1.52
1	A	78	ASN	CG-OD1	5.89	1.34	1.23
1	A	104	ILE	CA-CB	-5.89	1.47	1.54
1	A	139	ARG	NE-CZ	5.88	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLN	CA-C	5.80	1.60	1.52
1	A	216	ASN	CG-OD1	5.78	1.34	1.23
1	A	96	ARG	NE-CZ	5.74	1.39	1.33
1	A	31	VAL	CA-CB	-5.69	1.48	1.54
1	A	38	ASN	CA-CB	-5.62	1.44	1.53
1	A	61	HIS	CG-CD2	5.62	1.42	1.35
1	A	129	PRO	CA-CB	-5.56	1.46	1.53
1	A	2	PRO	CA-CB	-5.47	1.46	1.53
1	A	81	HIS	ND1-CE1	5.41	1.38	1.32
1	A	87	PRO	CA-CB	5.40	1.61	1.53
1	A	144	TYR	CA-C	-5.37	1.45	1.52
1	A	116	ASN	CG-OD1	5.28	1.33	1.23
1	A	7	TRP	NE1-CE2	-5.17	1.31	1.37
1	A	216	ASN	C-OXT	5.17	1.33	1.23
1	A	128	GLN	CD-OE1	5.14	1.33	1.23
1	A	4	ASN	CG-OD1	5.07	1.33	1.23

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASN	CA-CB-CG	19.00	131.60	112.60
1	A	102	GLY	CA-C-N	13.32	136.49	119.84
1	A	102	GLY	C-N-CA	13.32	136.49	119.84
1	A	139	ARG	CD-NE-CZ	-12.73	106.58	124.40
1	A	179	ASN	OD1-CG-ND2	-12.33	110.27	122.60
1	A	8	ARG	O-C-N	12.30	137.40	122.27
1	A	110	VAL	CA-C-N	11.80	133.41	122.20
1	A	110	VAL	C-N-CA	11.80	133.41	122.20
1	A	164	VAL	CA-C-O	11.28	131.19	119.35
1	A	42	THR	N-CA-C	10.56	126.33	113.23
1	A	8	ARG	CA-C-O	-9.90	108.58	119.97
1	A	165	GLY	O-C-N	-9.74	112.31	123.61
1	A	43	GLY	CA-C-N	-9.40	109.73	122.99
1	A	43	GLY	C-N-CA	-9.40	109.73	122.99
1	A	102	GLY	N-CA-C	-9.30	93.36	112.34
1	A	104	ILE	CB-CA-C	9.25	122.38	110.91
1	A	165	GLY	CA-C-O	9.24	130.41	121.63
1	A	169	SER	CA-C-O	-9.19	107.80	120.21
1	A	45	LEU	CB-CA-C	8.82	124.75	110.29
1	A	169	SER	O-C-N	8.77	134.23	123.44
1	A	116	ASN	OD1-CG-ND2	-8.76	113.84	122.60
1	A	100	VAL	CA-CB-CG2	8.76	125.29	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	TYR	CA-C-N	8.74	135.09	122.94
1	A	190	TYR	C-N-CA	8.74	135.09	122.94
1	A	164	VAL	CA-CB-CG2	8.72	125.22	110.40
1	A	96	ARG	CG-CD-NE	8.72	131.18	112.00
1	A	216	ASN	OD1-CG-ND2	-8.69	113.92	122.60
1	A	33	THR	CA-C-N	8.63	131.61	120.56
1	A	33	THR	C-N-CA	8.63	131.61	120.56
1	A	216	ASN	N-CA-CB	8.61	125.14	110.50
1	A	172	LYS	CA-C-O	-8.59	111.26	120.80
1	A	17	ARG	CA-C-N	8.50	134.99	123.00
1	A	17	ARG	C-N-CA	8.50	134.99	123.00
1	A	34	VAL	N-CA-CB	8.48	121.42	110.57
1	A	84	SER	CA-C-O	-8.41	109.86	119.79
1	A	188	LYS	N-CA-CB	-8.41	99.59	111.62
1	A	123	ASN	O-C-N	-8.39	113.23	122.12
1	A	164	VAL	O-C-N	-8.19	114.71	122.16
1	A	59	ARG	CA-C-O	-8.10	110.12	119.60
1	A	179	ASN	CA-CB-CG	-8.07	104.53	112.60
1	A	175	ILE	CA-C-N	8.05	133.98	121.99
1	A	175	ILE	C-N-CA	8.05	133.98	121.99
1	A	127	LYS	O-C-N	-8.00	111.00	122.36
1	A	194	LYS	CA-C-O	-7.98	112.18	120.80
1	A	74	TYR	CA-C-N	7.97	131.38	120.46
1	A	74	TYR	C-N-CA	7.97	131.38	120.46
1	A	69	PRO	O-C-N	-7.96	112.68	122.23
1	A	37	ILE	CA-C-N	7.84	132.59	120.82
1	A	37	ILE	C-N-CA	7.84	132.59	120.82
1	A	75	VAL	CA-C-O	-7.83	112.81	120.95
1	A	91	LYS	O-C-N	7.77	131.73	123.42
1	A	44	LYS	N-CA-C	-7.69	96.36	108.90
1	A	102	GLY	C-N-CD	-7.69	93.48	125.00
1	A	106	LYS	O-C-N	-7.63	113.95	123.27
1	A	145	LYS	CA-C-N	-7.58	109.87	121.62
1	A	145	LYS	C-N-CA	-7.58	109.87	121.62
1	A	183	THR	CA-C-N	7.55	131.15	120.28
1	A	183	THR	C-N-CA	7.55	131.15	120.28
1	A	128	GLN	O-C-N	7.49	129.93	121.32
1	A	134	VAL	CA-CB-CG1	7.44	123.04	110.40
1	A	197	PRO	O-C-N	7.42	132.66	122.64
1	A	81	HIS	CA-CB-CG	-7.41	106.39	113.80
1	A	92	GLN	CA-CB-CG	-7.40	99.29	114.10
1	A	198	GLY	CA-C-N	-7.31	113.05	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	GLY	C-N-CA	-7.31	113.05	122.77
1	A	116	ASN	CB-CG-ND2	7.30	127.34	116.40
1	A	159	HIS	CE1-NE2-CD2	7.27	116.27	109.00
1	A	172	LYS	CA-C-N	7.19	128.06	120.43
1	A	172	LYS	C-N-CA	7.19	128.06	120.43
1	A	208	LYS	CA-CB-CG	-7.19	99.73	114.10
1	A	19	GLN	CG-CD-NE2	7.17	127.16	116.40
1	A	24	SER	O-C-N	-7.13	113.76	122.25
1	A	30	ALA	CA-C-O	-7.00	113.47	120.82
1	A	78	ASN	CA-C-O	-6.98	111.37	119.05
1	A	19	GLN	N-CA-C	6.95	120.86	112.38
1	A	192	ARG	CG-CD-NE	-6.95	96.70	112.00
1	A	38	ASN	N-CA-CB	6.92	121.06	109.78
1	A	159	HIS	ND1-CE1-NE2	-6.89	101.51	108.40
1	A	67	TYR	CA-C-O	-6.87	114.23	119.59
1	A	79	GLY	O-C-N	-6.87	113.77	122.70
1	A	31	VAL	CA-C-N	6.84	129.77	120.54
1	A	31	VAL	C-N-CA	6.84	129.77	120.54
1	A	196	ALA	O-C-N	-6.83	113.47	121.32
1	A	184	ALA	N-CA-C	6.83	119.56	111.71
1	A	92	GLN	O-C-N	6.78	131.27	122.93
1	A	194	LYS	CA-CB-CG	-6.75	100.60	114.10
1	A	88	TYR	O-C-N	-6.74	114.73	123.02
1	A	96	ARG	N-CA-C	-6.70	104.41	112.59
1	A	146	GLY	N-CA-C	-6.67	103.02	110.96
1	A	106	LYS	CA-C-O	6.65	128.30	120.66
1	A	62	GLY	O-C-N	6.63	131.32	122.70
1	A	66	GLY	CA-C-N	-6.63	113.68	122.56
1	A	66	GLY	C-N-CA	-6.63	113.68	122.56
1	A	153	CYS	O-C-N	6.63	130.51	123.42
1	A	38	ASN	CA-C-N	6.57	131.81	120.58
1	A	38	ASN	C-N-CA	6.57	131.81	120.58
1	A	146	GLY	CA-C-N	6.57	131.59	122.06
1	A	146	GLY	C-N-CA	6.57	131.59	122.06
1	A	168	LYS	CA-C-N	-6.57	110.46	121.89
1	A	168	LYS	C-N-CA	-6.57	110.46	121.89
1	A	47	GLU	CA-CB-CG	-6.56	100.99	114.10
1	A	189	GLY	CA-C-O	-6.55	111.73	119.07
1	A	108	SER	O-C-N	-6.54	114.56	122.48
1	A	104	ILE	N-CA-CB	6.53	117.84	110.72
1	A	123	ASN	N-CA-CB	-6.50	100.30	110.06
1	A	55	ASP	O-C-N	-6.46	113.67	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	PRO	O-C-N	-6.42	113.89	121.46
1	A	137	LYS	CA-C-N	6.39	126.05	119.92
1	A	137	LYS	C-N-CA	6.39	126.05	119.92
1	A	135	GLU	CA-CB-CG	-6.38	101.35	114.10
1	A	81	HIS	CA-C-N	6.37	131.49	121.56
1	A	81	HIS	C-N-CA	6.37	131.49	121.56
1	A	170	GLY	CA-C-N	6.32	135.01	121.18
1	A	170	GLY	C-N-CA	6.32	135.01	121.18
1	A	134	VAL	CG1-CB-CG2	-6.31	96.92	110.80
1	A	215	LYS	CA-C-O	-6.29	114.72	121.45
1	A	73	GLU	CA-CB-CG	-6.20	101.69	114.10
1	A	4	ASN	CB-CG-ND2	6.16	125.64	116.40
1	A	172	LYS	O-C-N	6.16	130.40	123.19
1	A	104	ILE	O-C-N	-6.16	115.93	122.95
1	A	92	GLN	CA-C-O	-6.09	113.80	120.81
1	A	73	GLU	CA-C-O	-6.04	114.48	120.82
1	A	161	VAL	N-CA-CB	-6.02	105.39	112.32
1	A	152	PRO	CA-N-CD	6.02	119.92	111.50
1	A	96	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	A	116	ASN	CA-CB-CG	-5.98	106.62	112.60
1	A	31	VAL	CB-CA-C	5.96	119.33	111.70
1	A	112	ARG	CA-C-O	-5.96	113.77	120.32
1	A	140	PRO	CA-C-N	5.96	128.54	120.44
1	A	140	PRO	C-N-CA	5.96	128.54	120.44
1	A	155	THR	N-CA-C	-5.96	104.67	112.41
1	A	137	LYS	CA-CB-CG	-5.95	102.20	114.10
1	A	78	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	77	LYS	CA-C-N	5.92	131.67	122.26
1	A	77	LYS	C-N-CA	5.92	131.67	122.26
1	A	127	LYS	N-CA-C	5.90	120.60	113.41
1	A	20	GLY	CA-C-O	5.89	130.25	122.06
1	A	128	GLN	CA-C-O	-5.86	112.13	120.16
1	A	59	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	A	102	GLY	CA-C-O	-5.82	113.20	121.52
1	A	195	ARG	O-C-N	-5.79	114.96	122.77
1	A	34	VAL	CA-C-O	-5.76	114.66	121.05
1	A	187	GLU	O-C-N	5.72	129.87	122.43
1	A	18	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	17	ARG	N-CA-C	-5.71	101.47	109.69
1	A	46	VAL	O-C-N	-5.69	116.73	123.04
1	A	73	GLU	CB-CG-CD	-5.66	102.98	112.60
1	A	134	VAL	N-CA-CB	5.66	122.37	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ILE	CA-C-O	-5.64	114.50	120.48
1	A	68	PRO	CB-CA-C	5.52	117.66	110.92
1	A	187	GLU	N-CA-CB	-5.52	102.33	110.49
1	A	64	LYS	N-CA-CB	-5.49	102.24	110.91
1	A	13	VAL	O-C-N	-5.45	117.51	123.18
1	A	166	TYR	CA-C-O	-5.43	115.64	121.45
1	A	27	ALA	O-C-N	-5.42	115.97	122.15
1	A	125	ILE	N-CA-CB	5.42	117.91	110.54
1	A	159	HIS	O-C-N	-5.42	116.77	123.44
1	A	149	PHE	O-C-N	-5.40	116.38	123.02
1	A	125	ILE	O-C-N	5.39	127.10	121.87
1	A	69	PRO	CA-C-N	5.39	127.44	120.44
1	A	69	PRO	C-N-CA	5.39	127.44	120.44
1	A	119	GLY	N-CA-C	-5.37	105.80	113.86
1	A	46	VAL	CA-C-N	-5.37	114.66	122.65
1	A	46	VAL	C-N-CA	-5.37	114.66	122.65
1	A	171	GLY	N-CA-C	5.35	123.00	115.30
1	A	94	THR	CA-C-N	-5.35	113.85	121.50
1	A	94	THR	C-N-CA	-5.35	113.85	121.50
1	A	159	HIS	CG-CD2-NE2	-5.30	101.90	107.20
1	A	24	SER	N-CA-C	-5.29	106.05	112.88
1	A	12	ALA	N-CA-CB	5.28	118.31	110.49
1	A	16	VAL	O-C-N	-5.28	117.03	122.63
1	A	9	LYS	CA-C-N	5.28	131.87	121.58
1	A	9	LYS	C-N-CA	5.28	131.87	121.58
1	A	36	GLY	CA-C-O	-5.26	115.00	120.90
1	A	4	ASN	O-C-N	-5.26	116.94	123.36
1	A	22	CYS	CA-C-N	5.25	131.69	121.41
1	A	22	CYS	C-N-CA	5.25	131.69	121.41
1	A	172	LYS	CB-CA-C	-5.22	100.70	109.48
1	A	75	VAL	O-C-N	5.22	126.93	121.87
1	A	30	ALA	CA-C-N	5.21	127.60	120.77
1	A	30	ALA	C-N-CA	5.21	127.60	120.77
1	A	53	LEU	CA-C-O	-5.21	115.03	120.55
1	A	38	ASN	CB-CG-ND2	5.20	124.19	116.40
1	A	58	ARG	CD-NE-CZ	5.19	131.67	124.40
1	A	184	ALA	N-CA-CB	5.19	118.21	110.22
1	A	10	LYS	N-CA-CB	5.17	119.10	110.41
1	A	98	LYS	N-CA-CB	5.16	119.09	110.32
1	A	159	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	A	201	PRO	N-CA-C	-5.14	107.44	113.86
1	A	147	GLY	O-C-N	-5.13	116.78	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	CA-CB-CG	-5.13	103.84	114.10
1	A	85	LYS	N-CA-CB	-5.13	102.44	110.44
1	A	67	TYR	CB-CG-CD1	-5.12	113.12	120.80
1	A	41	ARG	CA-C-N	5.11	130.65	121.66
1	A	41	ARG	C-N-CA	5.11	130.65	121.66
1	A	7	TRP	CA-CB-CG	-5.10	103.91	113.60
1	A	78	ASN	N-CA-CB	5.10	118.14	110.65
1	A	112	ARG	O-C-N	5.09	129.27	123.27
1	A	88	TYR	CG-CD2-CE2	-5.09	113.57	121.20
1	A	139	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	47	GLU	CB-CG-CD	-5.05	104.02	112.60
1	A	8	ARG	CG-CD-NE	-5.04	100.92	112.00
1	A	107	THR	CA-C-N	5.03	130.37	122.11
1	A	107	THR	C-N-CA	5.03	130.37	122.11
1	A	121	LEU	O-C-N	-5.03	116.79	122.12
1	A	145	LYS	CA-C-O	5.02	124.71	119.03
1	A	99	GLN	O-C-N	5.02	128.12	122.20
1	A	94	THR	O-C-N	5.01	128.55	122.94

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	58	ARG	CA
1	A	216	ASN	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	123	ASN	Mainchain
1	A	139	ARG	Sidechain
1	A	169	SER	Peptide
1	A	17	ARG	Sidechain
1	A	195	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	58	ARG	Sidechain

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	A	1641	0	1654	47	0
2	A	1	0	0	0	0
3	A	133	0	0	11	1
All	All	1775	0	1654	47	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (47) 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:89:LYS:HD2	3:A:301:HOH:O	1.45	1.14
1:A:1:LEU:HB2	3:A:283:HOH:O	1.71	0.88
1:A:81:HIS:CD2	1:A:100:VAL:HG23	2.14	0.82
1:A:216:ASN:OXT	3:A:349:HOH:O	2.00	0.78
1:A:168:LYS:HE3	3:A:341:HOH:O	1.86	0.74
1:A:7:TRP:CZ3	1:A:10:LYS:HD2	2.26	0.70
1:A:1:LEU:HD11	1:A:123:ASN:CA	2.27	0.64
1:A:81:HIS:CG	1:A:100:VAL:HG23	2.32	0.64
1:A:89:LYS:HE3	3:A:301:HOH:O	1.98	0.62
1:A:12:ALA:HA	1:A:39:LYS:HG2	1.81	0.61
1:A:183:THR:O	1:A:188:LYS:HA	2.01	0.61
1:A:41:ARG:HD2	1:A:216:ASN:OD1	2.03	0.58
1:A:1:LEU:HD11	1:A:123:ASN:HA	1.84	0.57
1:A:88:TYR:HB2	3:A:271:HOH:O	2.04	0.57
1:A:4:ASN:HD22	1:A:167:GLY:HA3	1.69	0.56
1:A:89:LYS:HE2	1:A:96:ARG:NH2	2.22	0.55
1:A:17:ARG:NH1	1:A:50:GLU:OE2	2.35	0.54
1:A:89:LYS:CE	3:A:301:HOH:O	2.50	0.53
1:A:144:TYR:CD2	1:A:186:GLY:HA2	2.43	0.53
1:A:134:VAL:HG12	1:A:206:LEU:HD13	1.91	0.51
1:A:89:LYS:CD	3:A:301:HOH:O	2.23	0.51
1:A:139:ARG:HB3	1:A:140:PRO:HD3	1.92	0.51
1:A:116:ASN:HA	1:A:200:SER:O	2.10	0.51
1:A:134:VAL:HG12	1:A:206:LEU:CD1	2.41	0.50
1:A:113:VAL:HB	1:A:210:SER:HB2	1.94	0.49
1:A:1:LEU:HD11	1:A:123:ASN:N	2.27	0.48
1:A:169:SER:OG	3:A:291:HOH:O	2.19	0.48
1:A:63:CYS:SG	1:A:91:LYS:HA	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:HIS:CG	1:A:100:VAL:CG2	2.97	0.47
1:A:104:ILE:HD12	1:A:104:ILE:HG21	1.66	0.46
1:A:117:ASN:HB2	1:A:199:ASN:ND2	2.31	0.45
1:A:1:LEU:HD12	3:A:283:HOH:O	2.16	0.45
1:A:1:LEU:HD21	1:A:123:ASN:HA	1.99	0.45
1:A:26:TRP:CG	1:A:66:GLY:HA3	2.53	0.44
1:A:102:GLY:HA2	1:A:103:PRO:HD3	1.49	0.43
1:A:26:TRP:CD2	1:A:66:GLY:HA3	2.55	0.42
1:A:19:GLN:HG3	1:A:180:SER:O	2.20	0.42
1:A:51:GLN:HB2	1:A:88:TYR:HA	2.01	0.42
1:A:118:GLU:OE2	1:A:195:ARG:HD2	2.19	0.42
1:A:215:LYS:HG2	1:A:216:ASN:N	2.35	0.42
1:A:149:PHE:HE1	1:A:204:CYS:SG	2.43	0.42
1:A:148:ILE:HD12	1:A:172:LYS:HG3	2.02	0.41
1:A:59:ARG:HB3	1:A:70:TYR:CD2	2.55	0.41
1:A:74:TYR:CD1	1:A:74:TYR:C	2.98	0.41
1:A:156:LYS:HE2	3:A:288:HOH:O	2.20	0.41
1:A:89:LYS:HE2	1:A:96:ARG:HH21	1.85	0.41
1:A:4:ASN:HD22	1:A:167:GLY:CA	2.32	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:329:HOH:O	3:A:329:HOH:O[6_565]	1.58	0.62

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	214/216 (99%)	203 (95%)	10 (5%)	1 (0%)	24 14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	GLY

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	171/171 (100%)	151 (88%)	20 (12%)	5 1

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	42	THR
1	A	57	GLU
1	A	58	ARG
1	A	64	LYS
1	A	82	LEU
1	A	87	PRO
1	A	89	LYS
1	A	96	ARG
1	A	98	LYS
1	A	104	ILE
1	A	112	ARG
1	A	127	LYS
1	A	137	LYS
1	A	156	LYS
1	A	168	LYS
1	A	169	SER
1	A	172	LYS
1	A	194	LYS
1	A	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	116	ASN
1	A	142	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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	216/216 (100%)	0.48	18 (8%) 17 15	0, 0, 0, 1	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ASN	8.3
1	A	170	GLY	6.2
1	A	171	GLY	4.9
1	A	58	ARG	4.3
1	A	99	GLN	3.8
1	A	169	SER	3.6
1	A	172	LYS	2.9
1	A	96	ARG	2.8
1	A	3	GLU	2.8
1	A	168	LYS	2.7
1	A	106	LYS	2.6
1	A	1	LEU	2.5
1	A	104	ILE	2.5
1	A	94	THR	2.4
1	A	101	GLY	2.4
1	A	199	ASN	2.4
1	A	9	LYS	2.2
1	A	43	GLY	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 oligosaccharides 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, 95th 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(\AA^2)	Q<0.9
2	HG	A	217	1/1	1.00	0.01	0,0,0,0	1

6.5 Other polymers [i](#)

There are no such residues in this entry.