



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:29 AM UTC

PDB ID : 1AM5 / pdb_00001am5
Title : THE CRYSTAL STRUCTURE AND PROPOSED AMINO ACID SE-
SEQUENCE OF A PEPSIN FROM ATLANTIC COD (GADUS MORHUA)
Authors : Karlsen, S.; Hough, E.; Olsen, R.L.
Deposited on : 1997-06-23
Resolution : 2.16 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
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

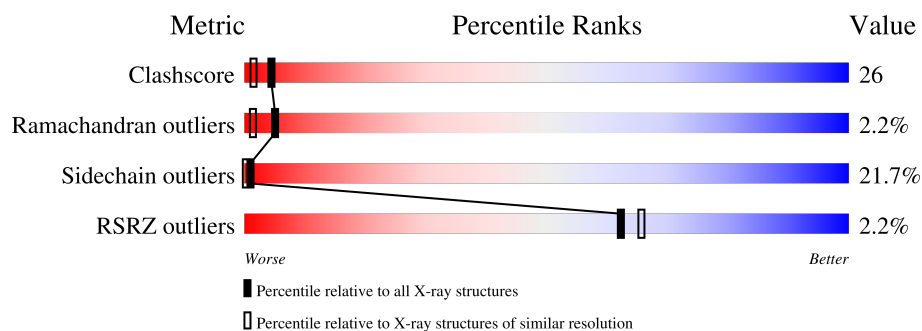
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	324	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2551 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 PEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2390	1494	394	489	13			

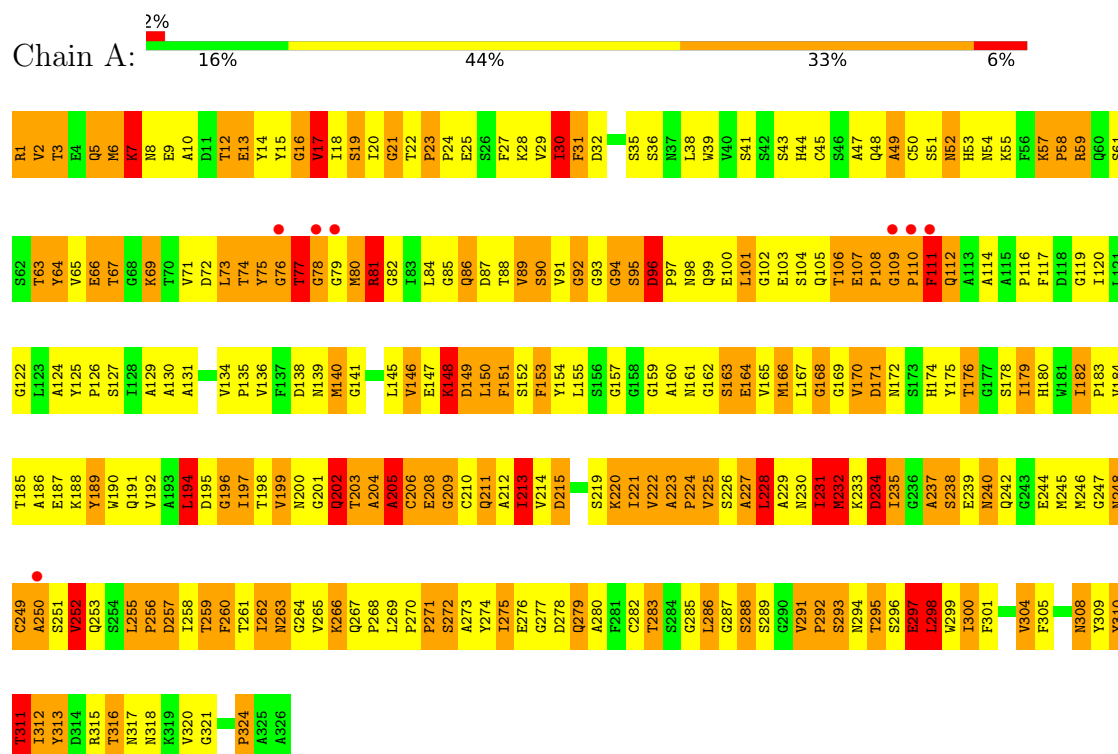
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	161	Total	O	0	0
			161	161		

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: PEPSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	35.98Å 75.40Å 108.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.16 8.00 – 2.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.16) 81.5 (8.00-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.17Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.208 , 0.224 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 145.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2551	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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	1.37	7/2441 (0.3%)	3.97	524/3318 (15.8%)

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	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLY	CA-C	8.44	1.59	1.51
1	A	78	GLY	N-CA	-5.74	1.39	1.45
1	A	157	GLY	CA-C	-5.46	1.47	1.52
1	A	32	ASP	CA-CB	5.45	1.60	1.53
1	A	16	GLY	N-CA	5.29	1.51	1.44
1	A	76	GLY	CA-C	5.14	1.59	1.51
1	A	2	VAL	N-CA	5.03	1.52	1.46

All (524) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	THR	CA-C-N	56.55	165.15	121.61
1	A	77	THR	C-N-CA	56.55	165.15	121.61
1	A	81	ARG	CD-NE-CZ	34.66	172.92	124.40
1	A	95	SER	N-CA-C	26.37	146.31	113.88
1	A	174	HIS	CA-CB-CG	-20.39	93.41	113.80
1	A	297	GLU	CA-C-O	18.08	146.36	120.51
1	A	59	ARG	CD-NE-CZ	16.59	147.63	124.40
1	A	276	GLU	CA-C-O	15.72	137.62	120.32
1	A	98	ASN	OD1-CG-ND2	-15.62	106.98	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	THR	CA-C-O	15.17	142.20	120.51
1	A	251	SER	CA-C-N	14.73	145.10	120.64
1	A	251	SER	C-N-CA	14.73	145.10	120.64
1	A	95	SER	N-CA-CB	-14.30	91.57	110.59
1	A	72	ASP	N-CA-CB	14.02	132.16	110.84
1	A	78	GLY	N-CA-C	-13.84	88.82	111.38
1	A	66	GLU	CA-C-N	13.80	142.23	122.77
1	A	66	GLU	C-N-CA	13.80	142.23	122.77
1	A	276	GLU	CB-CG-CD	13.77	136.01	112.60
1	A	73	LEU	CA-C-O	13.22	134.61	120.33
1	A	153	PHE	CA-CB-CG	13.04	126.84	113.80
1	A	234	ASP	CA-CB-CG	-12.64	99.96	112.60
1	A	77	THR	O-C-N	-12.59	105.85	122.59
1	A	146	VAL	CA-C-N	12.46	136.98	120.28
1	A	146	VAL	C-N-CA	12.46	136.98	120.28
1	A	111	PHE	CA-CB-CG	-12.12	101.68	113.80
1	A	51	SER	CB-CA-C	-11.59	89.20	110.63
1	A	169	GLY	O-C-N	-11.54	111.22	123.45
1	A	276	GLU	CB-CA-C	11.49	129.03	110.19
1	A	72	ASP	CA-C-N	-11.37	106.72	122.86
1	A	72	ASP	C-N-CA	-11.37	106.72	122.86
1	A	221	ILE	N-CA-CB	11.37	129.04	110.86
1	A	220	LYS	N-CA-CB	-11.35	92.86	110.46
1	A	169	GLY	CA-C-N	11.33	139.67	122.68
1	A	169	GLY	C-N-CA	11.33	139.67	122.68
1	A	112	GLN	O-C-N	-11.27	110.46	122.07
1	A	311	THR	N-CA-CB	-11.25	91.78	110.68
1	A	95	SER	CA-C-O	-11.15	106.64	119.24
1	A	297	GLU	CA-C-N	11.06	141.44	122.64
1	A	297	GLU	C-N-CA	11.06	141.44	122.64
1	A	278	ASP	CA-C-N	10.93	142.42	121.54
1	A	278	ASP	C-N-CA	10.93	142.42	121.54
1	A	146	VAL	CA-CB-CG2	10.91	128.95	110.40
1	A	110	PRO	N-CA-CB	10.80	109.92	102.79
1	A	294	ASN	OD1-CG-ND2	-10.75	111.85	122.60
1	A	32	ASP	CA-C-O	10.71	131.92	120.46
1	A	197	ILE	CA-C-O	10.69	132.90	120.72
1	A	55	LYS	CA-C-O	10.62	133.13	120.92
1	A	96	ASP	CB-CA-C	-10.50	94.64	110.71
1	A	53	HIS	CA-CB-CG	-10.49	103.31	113.80
1	A	213	ILE	CB-CA-C	10.49	125.58	111.21
1	A	1	ARG	NE-CZ-NH1	-10.42	111.08	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LYS	N-CA-C	10.40	125.86	110.46
1	A	21	GLY	CA-C-N	10.38	135.62	122.64
1	A	21	GLY	C-N-CA	10.38	135.62	122.64
1	A	195	ASP	CA-CB-CG	-10.37	102.23	112.60
1	A	67	THR	N-CA-CB	10.28	126.91	110.77
1	A	294	ASN	CA-C-N	10.27	141.16	121.54
1	A	294	ASN	C-N-CA	10.27	141.16	121.54
1	A	308	ASN	OD1-CG-ND2	-10.27	112.33	122.60
1	A	126	PRO	CA-C-N	10.19	133.93	120.28
1	A	126	PRO	C-N-CA	10.19	133.93	120.28
1	A	258	ILE	O-C-N	-10.10	112.84	123.14
1	A	1	ARG	CA-C-O	-10.06	103.70	120.80
1	A	36	SER	CA-C-O	-9.98	107.40	119.18
1	A	20	ILE	CA-C-O	-9.96	109.73	121.28
1	A	13	GLU	O-C-N	9.94	134.80	123.27
1	A	279	GLN	CA-C-O	9.92	134.69	120.51
1	A	258	ILE	CB-CA-C	9.76	125.64	110.81
1	A	240	ASN	CA-CB-CG	9.75	122.35	112.60
1	A	17	VAL	CA-C-N	9.73	135.25	122.51
1	A	17	VAL	C-N-CA	9.73	135.25	122.51
1	A	74	THR	N-CA-C	-9.72	93.39	109.24
1	A	110	PRO	CA-C-O	9.71	128.50	121.31
1	A	150	LEU	CB-CA-C	-9.69	88.75	110.07
1	A	111	PHE	CA-C-O	-9.67	106.68	120.51
1	A	294	ASN	O-C-N	-9.54	110.16	122.37
1	A	165	VAL	N-CA-CB	9.50	125.39	111.52
1	A	301	PHE	CA-C-O	-9.50	111.40	122.13
1	A	31	PHE	CA-CB-CG	-9.49	104.31	113.80
1	A	148	LYS	CB-CG-CD	9.43	132.98	111.30
1	A	110	PRO	CA-C-N	9.38	139.45	121.54
1	A	110	PRO	C-N-CA	9.38	139.45	121.54
1	A	230	ASN	CA-CB-CG	9.37	121.97	112.60
1	A	55	LYS	CA-CB-CG	9.29	132.68	114.10
1	A	73	LEU	CB-CA-C	9.29	124.64	110.62
1	A	5	GLN	OE1-CD-NE2	-9.20	113.40	122.60
1	A	221	ILE	N-CA-C	-9.11	95.14	108.71
1	A	238	SER	CA-CB-OG	9.11	129.31	111.10
1	A	317	ASN	OD1-CG-ND2	9.11	131.71	122.60
1	A	122	GLY	O-C-N	9.09	130.80	122.99
1	A	13	GLU	CA-C-O	-9.00	110.67	120.30
1	A	196	GLY	O-C-N	8.98	132.11	123.76
1	A	99	GLN	OE1-CD-NE2	-8.84	113.76	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLN	CB-CG-CD	8.81	127.58	112.60
1	A	267	GLN	CA-C-O	8.81	129.48	119.61
1	A	261	THR	CA-C-O	-8.80	111.38	120.54
1	A	313	TYR	CA-C-O	-8.79	110.65	120.32
1	A	179	ILE	CA-C-O	8.78	131.10	120.74
1	A	229	ALA	N-CA-CB	-8.77	95.48	109.78
1	A	3	THR	CA-CB-OG1	-8.77	96.45	109.60
1	A	24	PRO	N-CA-C	8.71	124.18	110.50
1	A	234	ASP	CA-C-O	-8.70	111.24	120.55
1	A	188	LYS	CA-C-O	8.67	132.91	120.51
1	A	266	LYS	CB-CG-CD	8.66	131.22	111.30
1	A	250	ALA	CA-C-O	-8.65	108.14	120.51
1	A	288	SER	N-CA-CB	-8.64	96.55	109.95
1	A	225	VAL	CA-C-O	-8.59	110.04	120.78
1	A	87	ASP	O-C-N	-8.57	114.26	123.26
1	A	78	GLY	O-C-N	8.54	130.89	123.37
1	A	91	VAL	CB-CA-C	-8.51	100.71	110.41
1	A	93	GLY	CA-C-N	8.51	138.09	121.41
1	A	93	GLY	C-N-CA	8.51	138.09	121.41
1	A	76	GLY	N-CA-C	-8.44	93.18	113.18
1	A	252	VAL	N-CA-C	8.41	123.82	112.04
1	A	233	LYS	O-C-N	-8.38	111.44	122.33
1	A	223	ALA	CA-C-O	8.31	129.22	120.66
1	A	17	VAL	CA-C-O	8.24	131.16	121.93
1	A	263	ASN	OD1-CG-ND2	-8.23	114.37	122.60
1	A	23	PRO	CA-N-CD	-8.20	100.02	111.50
1	A	168	GLY	CA-C-N	8.16	135.25	121.47
1	A	168	GLY	C-N-CA	8.16	135.25	121.47
1	A	189	TYR	N-CA-C	-8.14	97.74	110.36
1	A	44	HIS	N-CA-C	-8.12	102.42	113.30
1	A	294	ASN	CA-C-O	8.12	129.57	119.59
1	A	165	VAL	N-CA-C	-8.07	96.50	108.12
1	A	146	VAL	CG1-CB-CG2	-8.06	93.07	110.80
1	A	140	MET	CA-C-N	8.05	137.18	121.41
1	A	140	MET	C-N-CA	8.05	137.18	121.41
1	A	94	GLY	N-CA-C	8.03	132.22	113.18
1	A	233	LYS	CA-C-O	8.02	129.07	119.61
1	A	320	VAL	CA-C-N	-7.98	115.47	121.61
1	A	320	VAL	C-N-CA	-7.98	115.47	121.61
1	A	304	VAL	O-C-N	-7.97	113.82	121.87
1	A	228	LEU	N-CA-CB	7.95	121.91	109.82
1	A	15	TYR	CA-C-O	-7.94	111.82	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	TYR	CA-C-N	7.92	128.66	119.47
1	A	125	TYR	C-N-CA	7.92	128.66	119.47
1	A	96	ASP	OD1-CG-OD2	7.91	141.89	122.90
1	A	210	CYS	N-CA-C	-7.89	97.04	109.50
1	A	221	ILE	CA-CB-CG2	7.87	123.89	110.50
1	A	67	THR	CB-CA-C	-7.86	97.56	110.14
1	A	65	VAL	CA-C-O	-7.86	112.47	120.25
1	A	317	ASN	CA-CB-CG	-7.86	104.75	112.60
1	A	96	ASP	N-CA-C	7.85	126.16	108.74
1	A	151	PHE	CA-CB-CG	7.83	121.63	113.80
1	A	258	ILE	CA-CB-CG2	7.79	123.75	110.50
1	A	171	ASP	CA-CB-CG	7.75	120.36	112.60
1	A	81	ARG	CA-C-O	7.75	129.57	120.66
1	A	32	ASP	N-CA-C	7.71	121.64	107.99
1	A	191	GLN	CA-C-O	-7.70	112.07	120.92
1	A	48	GLN	CA-C-N	7.70	130.44	120.44
1	A	48	GLN	C-N-CA	7.70	130.44	120.44
1	A	215	ASP	N-CA-C	7.69	121.61	107.99
1	A	127	SER	O-C-N	7.69	130.27	122.12
1	A	279	GLN	N-CA-C	7.69	127.18	110.80
1	A	271	PRO	CA-C-N	7.67	131.32	120.28
1	A	271	PRO	C-N-CA	7.67	131.32	120.28
1	A	152	SER	O-C-N	7.67	131.99	123.25
1	A	17	VAL	N-CA-C	7.60	120.88	109.17
1	A	263	ASN	CB-CG-ND2	7.60	127.80	116.40
1	A	297	GLU	O-C-N	-7.56	112.53	122.59
1	A	211	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	A	52	ASN	CA-CB-CG	7.53	120.13	112.60
1	A	119	GLY	CA-C-O	7.52	128.55	121.41
1	A	171	ASP	CA-C-N	7.52	133.27	120.72
1	A	171	ASP	C-N-CA	7.52	133.27	120.72
1	A	262	ILE	CA-CB-CG1	7.50	123.14	110.40
1	A	188	LYS	O-C-N	-7.47	112.65	122.59
1	A	294	ASN	CA-CB-CG	7.47	120.07	112.60
1	A	2	VAL	N-CA-CB	7.47	123.56	111.23
1	A	261	THR	O-C-N	7.47	131.94	123.05
1	A	321	GLY	CA-C-O	-7.43	115.11	121.57
1	A	249	CYS	O-C-N	-7.37	112.78	122.59
1	A	146	VAL	O-C-N	-7.35	115.34	122.98
1	A	299	TRP	CA-C-O	-7.34	112.68	121.56
1	A	81	ARG	NE-CZ-NH1	-7.32	114.19	121.50
1	A	286	LEU	CA-C-N	-7.30	112.69	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	C-N-CA	-7.30	112.69	122.03
1	A	85	GLY	CA-C-N	7.28	133.95	122.74
1	A	85	GLY	C-N-CA	7.28	133.95	122.74
1	A	41	SER	N-CA-C	-7.26	99.70	110.23
1	A	107	GLU	CB-CA-C	-7.25	99.62	110.71
1	A	176	THR	CA-CB-CG2	7.22	122.77	110.50
1	A	32	ASP	O-C-N	-7.21	114.04	123.13
1	A	1	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	A	232	MET	O-C-N	7.18	129.46	122.07
1	A	174	HIS	N-CA-C	7.17	121.74	112.92
1	A	186	ALA	CA-C-O	7.17	128.89	120.14
1	A	186	ALA	CA-C-N	7.17	132.66	122.05
1	A	186	ALA	C-N-CA	7.17	132.66	122.05
1	A	305	PHE	CA-C-N	7.16	130.59	120.28
1	A	305	PHE	C-N-CA	7.16	130.59	120.28
1	A	276	GLU	O-C-N	-7.16	114.83	123.27
1	A	170	VAL	CA-CB-CG2	7.15	122.55	110.40
1	A	191	GLN	OE1-CD-NE2	7.14	129.74	122.60
1	A	129	ALA	CA-C-N	-7.08	110.82	120.87
1	A	129	ALA	C-N-CA	-7.08	110.82	120.87
1	A	295	THR	CA-C-N	7.07	133.63	122.74
1	A	295	THR	C-N-CA	7.07	133.63	122.74
1	A	191	GLN	CB-CA-C	-7.05	97.90	109.53
1	A	269	LEU	CA-C-N	7.03	127.62	120.38
1	A	269	LEU	C-N-CA	7.03	127.62	120.38
1	A	312	ILE	CA-C-O	-7.03	112.71	120.72
1	A	209	GLY	CA-C-O	7.01	132.77	120.57
1	A	30	ILE	CB-CG1-CD1	-7.01	99.08	113.80
1	A	165	VAL	CG1-CB-CG2	-6.99	95.42	110.80
1	A	49	ALA	CA-C-N	6.99	129.64	120.28
1	A	49	ALA	C-N-CA	6.99	129.64	120.28
1	A	94	GLY	CA-C-N	6.97	134.35	122.36
1	A	94	GLY	C-N-CA	6.97	134.35	122.36
1	A	256	PRO	N-CA-CB	6.96	109.41	103.35
1	A	294	ASN	CB-CA-C	6.90	122.75	110.81
1	A	291	VAL	CA-C-N	6.90	127.14	119.90
1	A	291	VAL	C-N-CA	6.90	127.14	119.90
1	A	148	LYS	CG-CD-CE	6.89	127.16	111.30
1	A	250	ALA	N-CA-CB	6.88	122.13	110.49
1	A	74	THR	N-CA-CB	6.88	121.65	110.43
1	A	180	HIS	CA-CB-CG	6.88	120.68	113.80
1	A	244	GLU	CA-C-O	-6.88	113.27	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	SER	CA-C-O	-6.87	113.28	120.70
1	A	100	GLU	CA-C-O	6.85	128.53	120.58
1	A	315	ARG	CA-C-N	-6.85	108.91	121.52
1	A	315	ARG	C-N-CA	-6.85	108.91	121.52
1	A	72	ASP	N-CA-C	-6.85	95.83	108.02
1	A	197	ILE	O-C-N	-6.84	116.16	123.14
1	A	159	GLY	CA-C-O	6.82	128.44	119.58
1	A	262	ILE	CB-CA-C	-6.81	102.13	110.99
1	A	300	ILE	N-CA-CB	6.81	120.81	111.41
1	A	251	SER	CA-C-O	6.81	127.22	119.18
1	A	278	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	126	PRO	CB-CA-C	-6.80	100.90	112.26
1	A	59	ARG	NE-CZ-NH1	6.80	128.30	121.50
1	A	146	VAL	CB-CA-C	6.79	121.89	110.95
1	A	309	TYR	CA-CB-CG	-6.79	101.68	113.90
1	A	273	ALA	CA-C-O	-6.78	111.58	119.78
1	A	237	ALA	CA-C-O	-6.77	114.37	121.55
1	A	199	VAL	CA-C-O	-6.77	113.43	120.27
1	A	166	MET	O-C-N	-6.76	115.32	123.29
1	A	259	THR	N-CA-CB	6.75	124.07	111.52
1	A	263	ASN	CA-CB-CG	-6.75	105.86	112.60
1	A	151	PHE	O-C-N	-6.74	115.71	123.33
1	A	316	THR	N-CA-C	-6.74	104.07	112.90
1	A	64	TYR	CA-C-O	6.73	128.72	121.05
1	A	163	SER	O-C-N	-6.72	115.37	122.96
1	A	5	GLN	CB-CA-C	6.72	120.88	109.53
1	A	13	GLU	CB-CA-C	-6.68	99.07	110.16
1	A	277	GLY	N-CA-C	-6.66	97.40	113.18
1	A	97	PRO	O-C-N	-6.65	114.75	123.13
1	A	197	ILE	N-CA-CB	6.63	123.48	111.21
1	A	12	THR	CA-C-N	6.62	132.34	123.00
1	A	12	THR	C-N-CA	6.62	132.34	123.00
1	A	81	ARG	NH1-CZ-NH2	6.62	127.90	119.30
1	A	22	THR	CA-C-O	-6.59	112.70	119.49
1	A	148	LYS	CA-CB-CG	6.58	127.27	114.10
1	A	97	PRO	CB-CA-C	6.58	120.04	110.63
1	A	30	ILE	CA-CB-CG1	6.57	121.58	110.40
1	A	160	ALA	N-CA-C	-6.57	102.33	110.41
1	A	229	ALA	N-CA-C	6.57	122.20	111.37
1	A	315	ARG	CA-C-O	-6.54	111.40	119.18
1	A	95	SER	O-C-N	-6.53	113.61	122.36
1	A	262	ILE	O-C-N	-6.53	116.00	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ALA	O-C-N	-6.53	113.91	122.59
1	A	77	THR	N-CA-CB	6.52	121.51	110.49
1	A	164	GLU	N-CA-CB	-6.52	99.46	111.13
1	A	89	VAL	CA-C-O	6.51	127.23	120.39
1	A	107	GLU	CA-C-N	6.51	127.98	119.84
1	A	107	GLU	C-N-CA	6.51	127.98	119.84
1	A	67	THR	O-C-N	-6.51	115.65	123.27
1	A	54	ASN	CA-C-O	-6.51	113.61	120.58
1	A	256	PRO	CB-CA-C	-6.50	102.91	111.23
1	A	154	TYR	CA-CB-CG	-6.50	102.21	113.90
1	A	90	SER	O-C-N	-6.49	115.63	123.29
1	A	130	ALA	CB-CA-C	6.48	120.74	109.65
1	A	199	VAL	N-CA-CB	6.48	120.64	111.82
1	A	257	ASP	OD1-CG-OD2	6.47	138.44	122.90
1	A	117	PHE	CA-C-O	-6.46	113.74	121.56
1	A	153	PHE	CA-C-O	6.46	127.49	120.32
1	A	240	ASN	CA-C-O	6.46	131.78	120.80
1	A	258	ILE	N-CA-CB	-6.45	99.28	111.21
1	A	116	PRO	N-CA-CB	6.44	108.38	101.88
1	A	54	ASN	CA-CB-CG	-6.43	106.17	112.60
1	A	63	THR	CA-CB-OG1	6.43	119.25	109.60
1	A	295	THR	CA-CB-OG1	6.43	119.25	109.60
1	A	16	GLY	CA-C-O	-6.42	115.34	121.38
1	A	66	GLU	O-C-N	-6.42	115.75	122.94
1	A	75	TYR	CB-CA-C	-6.42	100.79	111.13
1	A	208	GLU	CB-CG-CD	6.40	123.48	112.60
1	A	149	ASP	CA-C-N	6.39	132.56	122.21
1	A	149	ASP	C-N-CA	6.39	132.56	122.21
1	A	86	GLN	CB-CG-CD	6.38	123.44	112.60
1	A	19	SER	CB-CA-C	-6.37	97.20	109.37
1	A	255	LEU	CA-C-N	6.37	126.34	119.78
1	A	255	LEU	C-N-CA	6.37	126.34	119.78
1	A	58	PRO	O-C-N	-6.36	113.72	122.24
1	A	187	GLU	CA-C-N	6.36	133.69	121.54
1	A	187	GLU	C-N-CA	6.36	133.69	121.54
1	A	45	CYS	CA-C-O	6.36	127.45	120.71
1	A	296	SER	N-CA-CB	-6.32	99.88	110.80
1	A	318	ASN	CA-CB-CG	-6.31	106.29	112.60
1	A	179	ILE	O-C-N	-6.29	115.78	122.83
1	A	25	GLU	CB-CG-CD	6.28	123.28	112.60
1	A	309	TYR	N-CA-C	6.26	118.73	108.52
1	A	202	GLN	CA-CB-CG	6.26	126.61	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	THR	O-C-N	-6.25	115.72	123.04
1	A	220	LYS	CB-CA-C	-6.25	99.63	110.45
1	A	225	VAL	CA-CB-CG1	6.24	121.01	110.40
1	A	184	VAL	CA-C-N	6.24	132.63	121.66
1	A	184	VAL	C-N-CA	6.24	132.63	121.66
1	A	23	PRO	N-CA-CB	6.23	109.45	102.60
1	A	44	HIS	N-CA-CB	6.21	119.99	110.61
1	A	82	GLY	CA-C-O	6.21	129.00	121.61
1	A	105	GLN	CB-CA-C	-6.20	99.74	109.34
1	A	74	THR	CA-CB-OG1	-6.18	100.32	109.60
1	A	298	LEU	N-CA-CB	-6.18	100.56	110.63
1	A	15	TYR	CA-C-N	-6.17	110.05	121.15
1	A	15	TYR	C-N-CA	-6.17	110.05	121.15
1	A	135	PRO	CB-CA-C	6.16	119.12	111.23
1	A	90	SER	CA-C-O	6.15	127.09	120.38
1	A	165	VAL	CA-CB-CG2	6.15	120.86	110.40
1	A	199	VAL	N-CA-C	-6.14	98.68	107.77
1	A	41	SER	CA-C-O	-6.13	114.45	121.19
1	A	98	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	67	THR	CA-C-O	6.13	126.73	120.24
1	A	294	ASN	CB-CG-OD1	6.13	133.05	120.80
1	A	200	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	259	THR	CA-C-O	6.11	127.84	120.99
1	A	163	SER	CA-C-N	6.11	132.87	122.37
1	A	163	SER	C-N-CA	6.11	132.87	122.37
1	A	277	GLY	O-C-N	6.10	130.63	122.70
1	A	260	PHE	CA-C-N	-6.08	114.94	122.84
1	A	260	PHE	C-N-CA	-6.08	114.94	122.84
1	A	140	MET	CA-C-O	6.05	126.96	120.55
1	A	186	ALA	N-CA-CB	6.04	120.77	110.57
1	A	223	ALA	O-C-N	-6.03	116.23	121.35
1	A	234	ASP	OD1-CG-OD2	6.03	137.36	122.90
1	A	194	LEU	N-CA-CB	6.01	120.01	110.57
1	A	174	HIS	CA-C-N	-6.01	112.02	121.87
1	A	174	HIS	C-N-CA	-6.01	112.02	121.87
1	A	95	SER	CB-CA-C	-6.00	99.31	109.03
1	A	44	HIS	CB-CA-C	-5.99	100.04	110.17
1	A	200	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	107	GLU	CA-CB-CG	5.99	126.08	114.10
1	A	30	ILE	CB-CA-C	5.99	118.93	111.15
1	A	162	GLY	N-CA-C	-5.96	106.54	114.95
1	A	12	THR	CA-C-O	5.92	126.48	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLN	N-CA-C	-5.92	100.25	109.72
1	A	93	GLY	CA-C-O	5.90	128.03	121.31
1	A	58	PRO	CA-C-O	5.89	127.61	119.18
1	A	59	ARG	CB-CA-C	-5.89	97.68	109.99
1	A	311	THR	N-CA-C	5.89	118.50	108.90
1	A	54	ASN	CB-CA-C	5.88	120.51	110.81
1	A	54	ASN	N-CA-CB	-5.87	100.88	110.21
1	A	141	GLY	CA-C-N	5.86	128.41	120.38
1	A	141	GLY	C-N-CA	5.86	128.41	120.38
1	A	203	THR	N-CA-CB	-5.86	100.58	110.49
1	A	214	VAL	CA-C-N	5.86	131.43	123.11
1	A	214	VAL	C-N-CA	5.86	131.43	123.11
1	A	112	GLN	CA-C-N	5.85	130.49	121.19
1	A	112	GLN	C-N-CA	5.85	130.49	121.19
1	A	285	GLY	O-C-N	-5.85	115.10	122.70
1	A	191	GLN	CB-CG-CD	-5.84	102.67	112.60
1	A	44	HIS	O-C-N	5.84	129.31	122.24
1	A	220	LYS	CG-CD-CE	5.83	124.72	111.30
1	A	200	ASN	N-CA-C	5.82	119.69	112.24
1	A	263	ASN	O-C-N	-5.82	114.78	122.47
1	A	256	PRO	N-CA-C	5.81	120.45	111.21
1	A	55	LYS	O-C-N	-5.81	116.42	123.16
1	A	85	GLY	O-C-N	-5.81	117.13	123.29
1	A	285	GLY	CA-C-N	5.81	132.14	122.73
1	A	285	GLY	C-N-CA	5.81	132.14	122.73
1	A	225	VAL	O-C-N	5.81	129.83	122.57
1	A	92	GLY	N-CA-C	-5.80	105.97	114.90
1	A	51	SER	N-CA-CB	5.79	119.13	110.22
1	A	78	GLY	CA-C-O	-5.77	116.55	121.57
1	A	210	CYS	CB-CA-C	5.76	121.42	109.38
1	A	315	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	A	301	PHE	O-C-N	5.75	129.05	122.55
1	A	213	ILE	N-CA-C	-5.74	100.14	108.87
1	A	104	SER	O-C-N	5.73	129.62	122.86
1	A	231	ILE	N-CA-C	-5.72	104.94	110.72
1	A	41	SER	CA-CB-OG	5.70	122.50	111.10
1	A	111	PHE	N-CA-CB	5.69	120.10	110.49
1	A	101	LEU	CA-C-N	5.69	128.02	122.73
1	A	101	LEU	C-N-CA	5.69	128.02	122.73
1	A	264	GLY	O-C-N	-5.69	115.47	122.46
1	A	174	HIS	ND1-CE1-NE2	5.66	114.06	108.40
1	A	66	GLU	N-CA-CB	-5.65	101.42	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	LEU	CA-C-O	-5.65	114.82	120.64
1	A	272	SER	O-C-N	5.64	128.82	122.22
1	A	147	GLU	CA-C-O	5.63	126.52	120.55
1	A	102	GLY	N-CA-C	-5.63	102.10	110.71
1	A	35	SER	O-C-N	-5.62	116.84	123.25
1	A	80	MET	CA-CB-CG	5.62	125.33	114.10
1	A	58	PRO	CA-C-N	5.61	130.96	121.14
1	A	58	PRO	C-N-CA	5.61	130.96	121.14
1	A	91	VAL	CA-C-O	-5.61	115.23	120.22
1	A	96	ASP	CB-CG-OD1	-5.60	105.51	118.40
1	A	136	VAL	N-CA-C	5.60	116.06	110.23
1	A	272	SER	CB-CA-C	-5.59	100.29	110.63
1	A	167	LEU	CA-C-O	-5.59	114.32	120.36
1	A	168	GLY	O-C-N	-5.58	115.25	122.34
1	A	312	ILE	CB-CG1-CD1	5.57	125.50	113.80
1	A	149	ASP	OD1-CG-OD2	-5.57	109.53	122.90
1	A	227	ALA	CA-C-O	-5.57	112.75	119.49
1	A	251	SER	O-C-N	-5.55	115.65	122.20
1	A	109	GLY	N-CA-C	-5.55	101.03	112.34
1	A	225	VAL	CB-CA-C	-5.54	102.21	111.29
1	A	287	GLY	CA-C-N	5.53	129.41	121.50
1	A	287	GLY	C-N-CA	5.53	129.41	121.50
1	A	308	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	215	ASP	CB-CA-C	-5.53	101.78	110.79
1	A	270	PRO	CA-C-N	5.52	125.36	119.28
1	A	270	PRO	C-N-CA	5.52	125.36	119.28
1	A	278	ASP	N-CA-C	-5.51	103.83	110.44
1	A	242	GLN	CA-C-O	5.50	130.15	120.80
1	A	293	SER	CA-C-N	-5.50	113.52	122.65
1	A	293	SER	C-N-CA	-5.50	113.52	122.65
1	A	106	THR	N-CA-CB	5.49	119.65	110.59
1	A	315	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	50	CYS	CA-C-O	-5.49	114.73	120.55
1	A	296	SER	O-C-N	-5.48	116.89	123.31
1	A	136	VAL	CA-C-O	5.47	127.10	121.41
1	A	205	ALA	N-CA-C	5.47	122.45	110.80
1	A	213	ILE	O-C-N	-5.45	116.50	122.83
1	A	310	TYR	CA-CB-CG	5.45	123.71	113.90
1	A	89	VAL	O-C-N	-5.45	117.37	123.26
1	A	27	PHE	CA-C-N	5.45	129.67	122.42
1	A	27	PHE	C-N-CA	5.45	129.67	122.42
1	A	134	VAL	N-CA-CB	-5.43	103.60	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ILE	N-CA-C	-5.43	100.50	108.11
1	A	49	ALA	CA-C-O	5.43	126.53	120.82
1	A	150	LEU	CA-CB-CG	5.43	135.30	116.30
1	A	197	ILE	CA-C-N	5.41	131.49	122.73
1	A	197	ILE	C-N-CA	5.41	131.49	122.73
1	A	258	ILE	N-CA-C	-5.40	100.70	108.53
1	A	282	CYS	CA-C-O	-5.40	114.73	120.40
1	A	77	THR	CA-CB-OG1	5.39	117.69	109.60
1	A	23	PRO	CA-CB-CG	-5.38	93.77	104.00
1	A	8	ASN	CB-CG-ND2	5.38	124.47	116.40
1	A	286	LEU	N-CA-CB	5.38	120.74	111.00
1	A	185	THR	N-CA-C	-5.37	106.57	113.23
1	A	7	LYS	CA-CB-CG	5.37	124.84	114.10
1	A	100	GLU	CA-C-N	5.37	131.24	122.81
1	A	100	GLU	C-N-CA	5.37	131.24	122.81
1	A	195	ASP	OD1-CG-OD2	5.37	135.79	122.90
1	A	10	ALA	N-CA-CB	-5.37	101.42	110.49
1	A	17	VAL	O-C-N	-5.35	115.94	122.36
1	A	86	GLN	N-CA-C	5.34	117.79	108.76
1	A	252	VAL	N-CA-CB	-5.34	99.83	111.05
1	A	69	LYS	CG-CD-CE	5.33	123.57	111.30
1	A	257	ASP	CA-C-N	5.33	129.98	123.10
1	A	257	ASP	C-N-CA	5.33	129.98	123.10
1	A	30	ILE	CA-C-O	5.33	126.93	120.85
1	A	171	ASP	N-CA-CB	5.32	119.30	110.47
1	A	234	ASP	O-C-N	5.32	128.61	122.17
1	A	234	ASP	N-CA-C	5.32	117.89	111.40
1	A	106	THR	CB-CA-C	-5.32	102.47	110.24
1	A	324	PRO	N-CA-CB	5.31	108.05	103.27
1	A	161	ASN	CA-C-N	-5.30	113.87	122.30
1	A	161	ASN	C-N-CA	-5.30	113.87	122.30
1	A	295	THR	O-C-N	-5.30	115.53	122.59
1	A	265	VAL	CA-C-O	5.30	126.77	120.72
1	A	162	GLY	CA-C-O	-5.30	113.19	118.86
1	A	6	MET	CA-C-N	-5.30	113.09	122.74
1	A	6	MET	C-N-CA	-5.30	113.09	122.74
1	A	99	GLN	CG-CD-NE2	5.29	124.33	116.40
1	A	14	TYR	CA-C-O	5.28	125.94	120.40
1	A	72	ASP	CB-CA-C	-5.27	102.66	110.62
1	A	178	SER	O-C-N	5.26	128.95	123.06
1	A	283	THR	CA-CB-CG2	5.26	119.44	110.50
1	A	163	SER	CA-C-O	5.25	127.51	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	GLU	O-C-N	5.25	128.96	123.03
1	A	212	ALA	CA-C-N	-5.23	114.14	122.50
1	A	212	ALA	C-N-CA	-5.23	114.14	122.50
1	A	2	VAL	CA-CB-CG2	5.23	119.28	110.40
1	A	23	PRO	N-CD-CG	5.21	110.06	103.80
1	A	260	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	170	VAL	CA-C-O	-5.21	114.79	121.40
1	A	224	PRO	CA-C-N	5.21	131.34	121.97
1	A	224	PRO	C-N-CA	5.21	131.34	121.97
1	A	20	ILE	O-C-N	5.20	128.57	123.00
1	A	279	GLN	O-C-N	-5.20	115.68	122.59
1	A	219	SER	CA-C-N	5.19	131.66	122.67
1	A	219	SER	C-N-CA	5.19	131.66	122.67
1	A	74	THR	CB-CA-C	5.19	118.32	109.75
1	A	139	ASN	O-C-N	-5.19	116.23	122.15
1	A	20	ILE	CB-CG1-CD1	5.18	124.69	113.80
1	A	187	GLU	N-CA-CB	-5.18	104.20	110.53
1	A	313	TYR	CB-CA-C	5.18	118.69	110.19
1	A	76	GLY	O-C-N	5.18	129.43	122.70
1	A	22	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	199	VAL	CA-CB-CG1	5.15	119.16	110.40
1	A	213	ILE	N-CA-CB	5.15	117.67	110.56
1	A	175	TYR	CA-C-O	-5.14	115.95	121.45
1	A	53	HIS	CE1-NE2-CD2	5.14	114.14	109.00
1	A	245	MET	N-CA-C	-5.14	99.42	108.20
1	A	201	GLY	CA-C-N	5.13	130.63	122.94
1	A	201	GLY	C-N-CA	5.13	130.63	122.94
1	A	124	ALA	N-CA-CB	5.11	119.13	110.49
1	A	253	GLN	CG-CD-NE2	5.11	124.06	116.40
1	A	206	CYS	CA-C-O	-5.11	112.12	120.80
1	A	97	PRO	CA-C-N	5.10	129.38	122.19
1	A	97	PRO	C-N-CA	5.10	129.38	122.19
1	A	155	LEU	O-C-N	-5.08	116.62	123.23
1	A	316	THR	N-CA-CB	5.08	117.96	110.33
1	A	153	PHE	N-CA-C	5.08	117.35	108.76
1	A	6	MET	CA-C-O	-5.08	115.69	121.58
1	A	310	TYR	N-CA-C	-5.07	102.87	110.23
1	A	211	GLN	CA-CB-CG	5.07	124.24	114.10
1	A	292	PRO	N-CA-CB	5.07	107.82	103.36
1	A	3	THR	O-C-N	5.06	129.33	122.96
1	A	105	GLN	CA-CB-CG	5.06	124.22	114.10
1	A	288	SER	CA-C-O	-5.05	114.93	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLN	CG-CD-NE2	-5.03	108.86	116.40
1	A	187	GLU	OE1-CD-OE2	5.02	134.96	122.90
1	A	166	MET	CA-CB-CG	5.02	124.14	114.10
1	A	266	LYS	N-CA-CB	-5.02	102.08	110.37
1	A	48	GLN	CG-CD-OE1	5.02	130.84	120.80
1	A	174	HIS	CA-C-O	-5.01	113.70	119.56
1	A	267	GLN	CB-CA-C	5.01	115.47	109.31
1	A	89	VAL	CA-C-N	5.01	129.91	123.00
1	A	89	VAL	C-N-CA	5.01	129.91	123.00
1	A	232	MET	N-CA-CB	5.01	117.27	110.01
1	A	190	TRP	N-CA-C	-5.01	99.85	108.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	THR	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	2390	0	2267	123	1
2	A	161	0	0	3	1
All	All	2551	0	2267	123	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 26.

All (123) 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:166:MET:HE2	1:A:171:ASP:HB3	1.50	0.93
1:A:227:ALA:O	1:A:231:ILE:HD13	1.68	0.92
1:A:259:THR:HG22	1:A:268:PRO:HA	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:THR:HG23	1:A:313:TYR:HE1	1.37	0.86
1:A:3:THR:HG22	1:A:166:MET:HA	1.58	0.86
1:A:74:THR:HA	1:A:79:GLY:HA2	1.62	0.82
1:A:182:ILE:HG12	1:A:263:ASN:OD1	1.82	0.79
1:A:311:THR:HG23	1:A:313:TYR:CE1	2.16	0.79
1:A:30:ILE:CG2	1:A:120:ILE:HG12	2.13	0.79
1:A:7:LYS:HZ3	1:A:28:LYS:HE3	1.49	0.77
1:A:57:LYS:HE3	1:A:58:PRO:HD2	1.66	0.77
1:A:279:GLN:O	1:A:280:ALA:HB3	1.85	0.75
1:A:298:LEU:HB2	2:A:720:HOH:O	1.89	0.72
1:A:7:LYS:HZ3	1:A:17:VAL:HG22	1.56	0.70
1:A:57:LYS:CE	1:A:58:PRO:HD2	2.21	0.70
1:A:206:CYS:O	1:A:208:GLU:N	2.26	0.68
1:A:164:GLU:CD	1:A:166:MET:HE3	2.18	0.68
1:A:18:ILE:HD13	1:A:29:VAL:HG21	1.76	0.67
1:A:89:VAL:O	1:A:96:ASP:HB2	1.94	0.67
1:A:198:THR:HA	1:A:202:GLN:O	1.94	0.66
1:A:182:ILE:HD12	1:A:192:VAL:HB	1.76	0.66
1:A:279:GLN:O	1:A:280:ALA:CB	2.43	0.65
1:A:111:PHE:CE1	1:A:114:ALA:HB3	2.32	0.65
1:A:235:ILE:HG22	1:A:255:LEU:HG	1.79	0.65
1:A:259:THR:HG22	1:A:268:PRO:CA	2.25	0.65
1:A:39:TRP:NE1	1:A:75:TYR:OH	2.31	0.64
1:A:235:ILE:HG22	1:A:256:PRO:HD2	1.80	0.63
1:A:182:ILE:HD13	1:A:183:PRO:O	1.98	0.63
1:A:222:VAL:HG11	1:A:300:ILE:HD12	1.79	0.63
1:A:1:ARG:HG3	1:A:146:VAL:HA	1.81	0.62
1:A:166:MET:HE1	1:A:310:TYR:HE1	1.65	0.62
1:A:204:ALA:O	1:A:205:ALA:HB2	2.00	0.62
1:A:57:LYS:HE3	1:A:57:LYS:HA	1.82	0.62
1:A:164:GLU:OE1	1:A:166:MET:HE3	2.01	0.61
1:A:232:MET:HE3	1:A:237:ALA:HB3	1.82	0.61
1:A:182:ILE:HG12	1:A:183:PRO:HD2	1.83	0.60
1:A:247:GLY:HA3	2:A:644:HOH:O	2.02	0.59
1:A:153:PHE:HB2	1:A:311:THR:CG2	2.33	0.59
1:A:194:LEU:HD22	1:A:262:ILE:CD1	2.34	0.58
1:A:3:THR:HG22	1:A:166:MET:CB	2.33	0.58
1:A:148:LYS:O	1:A:168:GLY:HA2	2.05	0.57
1:A:58:PRO:HG3	1:A:103:GLU:OE1	2.04	0.57
1:A:111:PHE:HE1	1:A:114:ALA:HB3	1.69	0.57
1:A:213:ILE:CD1	1:A:215:ASP:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HG22	1:A:3:THR:H	1.70	0.57
1:A:3:THR:HG22	1:A:166:MET:CA	2.30	0.56
1:A:240:ASN:HB3	1:A:246:MET:HG3	1.87	0.56
1:A:7:LYS:NZ	1:A:17:VAL:HG22	2.20	0.56
1:A:248:ASN:C	1:A:249:CYS:O	2.43	0.56
1:A:7:LYS:NZ	1:A:16:GLY:HA2	2.20	0.55
1:A:149:ASP:HB2	1:A:316:THR:CG2	2.36	0.55
1:A:249:CYS:O	1:A:250:ALA:HB3	2.07	0.55
1:A:176:THR:O	1:A:324:PRO:HD2	2.06	0.54
1:A:196:GLY:HA2	1:A:206:CYS:HB2	1.90	0.54
1:A:49:ALA:HB3	1:A:107:GLU:O	2.07	0.54
1:A:197:ILE:CG2	1:A:205:ALA:HB3	2.37	0.54
1:A:291:VAL:O	1:A:298:LEU:HD21	2.06	0.54
1:A:81:ARG:HH11	1:A:81:ARG:HB2	1.73	0.54
1:A:19:SER:HB2	1:A:90:SER:HB3	1.91	0.53
1:A:150:LEU:O	1:A:168:GLY:N	2.31	0.52
1:A:197:ILE:HD12	1:A:260:PHE:CE2	2.44	0.52
1:A:231:ILE:O	1:A:234:ASP:HB2	2.10	0.52
1:A:213:ILE:HD11	1:A:215:ASP:HB2	1.93	0.51
1:A:222:VAL:HG13	1:A:289:SER:HA	1.92	0.51
1:A:179:ILE:CG2	1:A:312:ILE:HD12	2.42	0.50
1:A:228:LEU:HD22	1:A:232:MET:SD	2.52	0.49
1:A:2:VAL:CG1	1:A:92:GLY:O	2.61	0.49
1:A:39:TRP:CE2	1:A:75:TYR:OH	2.66	0.49
1:A:182:ILE:CG1	1:A:183:PRO:HD2	2.41	0.49
1:A:71:VAL:HG23	1:A:131:ALA:CB	2.43	0.49
1:A:271:PRO:O	1:A:275:ILE:HB	2.13	0.48
1:A:109:GLY:C	1:A:111:PHE:H	2.21	0.48
1:A:235:ILE:CG2	1:A:255:LEU:HG	2.43	0.48
1:A:166:MET:CE	1:A:310:TYR:HE1	2.26	0.48
1:A:197:ILE:O	1:A:203:THR:HA	2.14	0.47
1:A:222:VAL:HG13	1:A:289:SER:HB2	1.95	0.47
1:A:166:MET:SD	1:A:310:TYR:OH	2.67	0.47
1:A:71:VAL:HG23	1:A:131:ALA:HB2	1.96	0.46
1:A:252:VAL:HA	1:A:255:LEU:HD22	1.97	0.46
1:A:77:THR:HA	1:A:78:GLY:O	2.15	0.46
1:A:189:TYR:HB3	2:A:602:HOH:O	2.13	0.46
1:A:39:TRP:HE1	1:A:75:TYR:HE2	1.64	0.46
1:A:75:TYR:O	1:A:76:GLY:C	2.58	0.46
1:A:221:ILE:HB	1:A:304:VAL:CG2	2.45	0.46
1:A:222:VAL:HG13	1:A:289:SER:CA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG13	1:A:289:SER:CB	2.45	0.46
1:A:182:ILE:CG1	1:A:263:ASN:OD1	2.61	0.45
1:A:291:VAL:HA	1:A:292:PRO:HD3	1.75	0.45
1:A:274:TYR:HB2	1:A:286:LEU:CD1	2.47	0.45
1:A:297:GLU:HG3	1:A:298:LEU:HD23	1.99	0.44
1:A:249:CYS:O	1:A:250:ALA:CB	2.63	0.44
1:A:182:ILE:CD1	1:A:183:PRO:HD2	2.48	0.43
1:A:76:GLY:O	1:A:77:THR:C	2.60	0.43
1:A:57:LYS:HE2	1:A:58:PRO:HD2	1.97	0.43
1:A:213:ILE:HD12	1:A:215:ASP:HB2	2.00	0.43
1:A:197:ILE:HG22	1:A:205:ALA:HB3	2.00	0.43
1:A:235:ILE:O	1:A:255:LEU:HD11	2.18	0.43
1:A:30:ILE:HG21	1:A:120:ILE:HG12	1.98	0.42
1:A:80:MET:HB2	1:A:81:ARG:H	1.73	0.42
1:A:111:PHE:O	1:A:112:GLN:C	2.60	0.42
1:A:153:PHE:HB2	1:A:311:THR:HG22	2.02	0.42
1:A:5:GLN:HA	1:A:163:SER:O	2.19	0.42
1:A:64:TYR:OH	1:A:103:GLU:OE2	2.31	0.42
1:A:109:GLY:HA2	1:A:110:PRO:HD3	1.86	0.42
1:A:7:LYS:HZ2	1:A:16:GLY:HA2	1.83	0.42
1:A:149:ASP:HB2	1:A:316:THR:HG22	2.02	0.42
1:A:204:ALA:O	1:A:205:ALA:CB	2.67	0.41
1:A:31:PHE:HB3	1:A:153:PHE:HZ	1.85	0.41
1:A:203:THR:O	1:A:204:ALA:HB2	2.20	0.41
1:A:232:MET:HE3	1:A:237:ALA:CB	2.49	0.41
1:A:57:LYS:HE3	1:A:58:PRO:CD	2.44	0.41
1:A:198:THR:HG23	1:A:202:GLN:N	2.35	0.41
1:A:64:TYR:OH	1:A:66:GLU:HG2	2.20	0.41
1:A:12:THR:HG22	1:A:13:GLU:HG2	2.02	0.41
1:A:21:GLY:HA2	1:A:61:SER:OG	2.21	0.41
1:A:49:ALA:CB	1:A:107:GLU:O	2.69	0.41
1:A:164:GLU:HB3	1:A:166:MET:HE3	2.03	0.41
1:A:179:ILE:HG23	1:A:312:ILE:HD12	2.02	0.41
1:A:151:PHE:HA	1:A:166:MET:O	2.21	0.41
1:A:223:ALA:HB1	1:A:224:PRO:HD2	2.03	0.41
1:A:227:ALA:O	1:A:228:LEU:C	2.64	0.41
1:A:140:MET:HA	1:A:145:LEU:HD12	2.03	0.40
1:A:225:VAL:HG13	1:A:226:SER:N	2.36	0.40

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)
1:A:1:ARG:NH2	2:A:647:HOH:O[4_558]	1.46	0.74

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	318/324 (98%)	292 (92%)	19 (6%)	7 (2%)	5 1

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	94	GLY
1	A	205	ALA
1	A	204	ALA
1	A	43	SER
1	A	108	PRO
1	A	209	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	258/258 (100%)	202 (78%)	56 (22%)	1 0

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

Mol	Chain	Res	Type
1	A	6	MET
1	A	7	LYS
1	A	9	GLU
1	A	17	VAL
1	A	23	PRO
1	A	30	ILE
1	A	38	LEU
1	A	52	ASN
1	A	57	LYS
1	A	59	ARG
1	A	63	THR
1	A	67	THR
1	A	69	LYS
1	A	73	LEU
1	A	81	ARG
1	A	84	LEU
1	A	86	GLN
1	A	95	SER
1	A	96	ASP
1	A	101	LEU
1	A	106	THR
1	A	108	PRO
1	A	111	PHE
1	A	138	ASP
1	A	148	LYS
1	A	170	VAL
1	A	172	ASN
1	A	182	ILE
1	A	194	LEU
1	A	199	VAL
1	A	202	GLN
1	A	211	GLN
1	A	213	ILE
1	A	220	LYS
1	A	222	VAL
1	A	228	LEU
1	A	231	ILE
1	A	232	MET
1	A	234	ASP
1	A	235	ILE
1	A	238	SER
1	A	239	GLU
1	A	248	ASN

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Mol	Chain	Res	Type
1	A	252	VAL
1	A	257	ASP
1	A	266	LYS
1	A	272	SER
1	A	275	ILE
1	A	283	THR
1	A	288	SER
1	A	293	SER
1	A	295	THR
1	A	297	GLU
1	A	298	LEU
1	A	308	ASN
1	A	311	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	105	GLN
1	A	174	HIS
1	A	180	HIS
1	A	230	ASN
1	A	279	GLN
1	A	317	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 ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	240:ASN	C	242:GLN	N	3.85
1	A	206:CYS	C	208:GLU	N	3.44

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	324/324 (100%)	-0.30	7 (2%) 62 66	3, 14, 35, 46	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	GLY	4.3
1	A	111	PHE	3.5
1	A	79	GLY	2.9
1	A	78	GLY	2.6
1	A	76	GLY	2.3
1	A	250	ALA	2.1
1	A	110	PRO	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 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.