Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:57 PM EDT

PDB ID	:	1AM5
Title	:	THE CRYSTAL STRUCTURE AND PROPOSED AMINO ACID 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

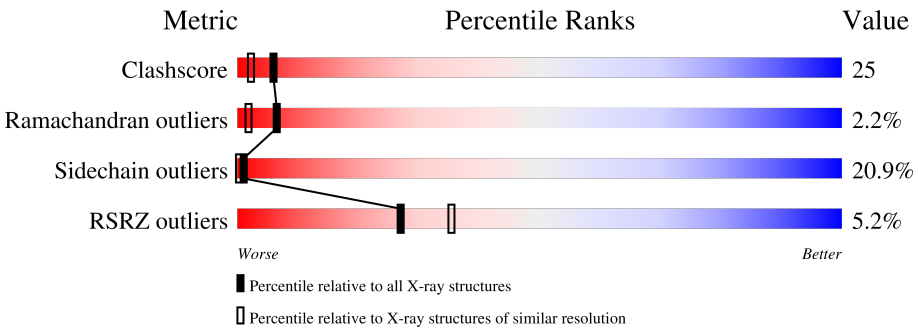
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 <=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	5% 36% 36% 22% 6%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	324	2390	1494	394	489	13	0	0	0

- Molecule 2 is water.

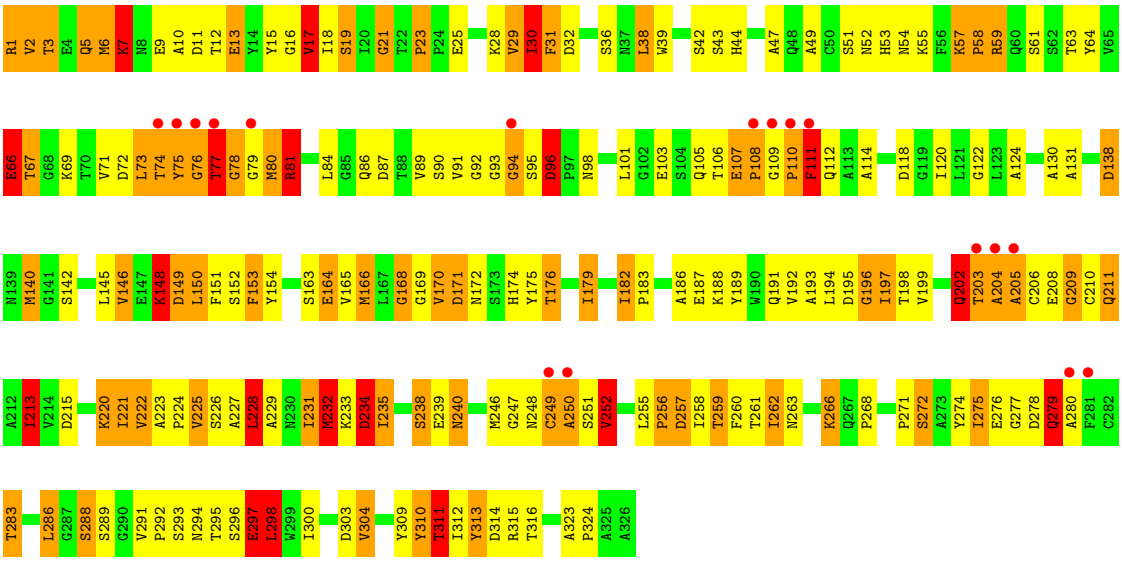
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	161	161	161	0	0

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: PEPSIN

Chain A: 5% 36% 36% 22% 6%



4 Data and refinement statistics (i)

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 24.48 – 2.16	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.16) 83.7 (24.48-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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)	0.31 , 157.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	1.03	1/2441 (0.0%)	2.93	241/3318 (7.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	CD-OE2	5.51	1.31	1.25

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	ARG	CD-NE-CZ	35.23	172.92	123.60
1	A	77	THR	C-N-CA	20.41	165.15	122.30
1	A	1	ARG	NE-CZ-NH1	-18.45	111.08	120.30
1	A	59	ARG	CD-NE-CZ	17.17	147.63	123.60
1	A	59	ARG	NE-CZ-NH1	15.99	128.30	120.30
1	A	96	ASP	CB-CG-OD1	-14.21	105.51	118.30
1	A	315	ARG	NE-CZ-NH1	13.91	127.26	120.30
1	A	95	SER	N-CA-C	13.08	146.31	111.00
1	A	95	SER	N-CA-CB	-12.62	91.57	110.50
1	A	297	GLU	CA-C-O	12.50	146.36	120.10
1	A	81	ARG	NE-CZ-NH1	-12.23	114.19	120.30
1	A	315	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	146	VAL	CA-CB-CG2	12.03	128.95	110.90
1	A	72	ASP	N-CA-CB	11.97	132.16	110.60
1	A	174	HIS	CA-CB-CG	-11.88	93.41	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	TYR	CB-CG-CD2	11.50	127.90	121.00
1	A	150	LEU	CB-CA-C	-11.29	88.75	110.20
1	A	146	VAL	CG1-CB-CG2	-11.14	93.07	110.90
1	A	51	SER	CB-CA-C	-11.00	89.20	110.10
1	A	11	ASP	CB-CG-OD1	10.77	128.00	118.30
1	A	1	ARG	NE-CZ-NH2	10.73	125.66	120.30
1	A	257	ASP	CB-CG-OD2	-10.60	108.76	118.30
1	A	77	THR	CA-C-O	10.53	142.20	120.10
1	A	229	ALA	N-CA-CB	-10.44	95.48	110.10
1	A	95	SER	CA-C-N	10.25	139.75	117.20
1	A	77	THR	O-C-N	-10.21	105.85	123.20
1	A	138	ASP	CB-CG-OD2	10.09	127.38	118.30
1	A	220	LYS	N-CA-CB	-9.85	92.86	110.60
1	A	96	ASP	OD1-CG-OD2	9.78	141.89	123.30
1	A	311	THR	N-CA-CB	-9.75	91.78	110.30
1	A	78	GLY	N-CA-C	-9.71	88.82	113.10
1	A	187	GLU	OE1-CD-OE2	9.71	134.96	123.30
1	A	165	VAL	CG1-CB-CG2	-9.68	95.42	110.90
1	A	195	ASP	CB-CG-OD2	-9.46	109.79	118.30
1	A	149	ASP	CB-CG-OD1	9.41	126.77	118.30
1	A	251	SER	C-N-CA	9.36	145.10	121.70
1	A	276	GLU	CB-CA-C	9.31	129.03	110.40
1	A	288	SER	N-CA-CB	-9.30	96.55	110.50
1	A	314	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	A	55	LYS	CA-CB-CG	8.77	132.68	113.40
1	A	67	THR	N-CA-CB	8.74	126.91	110.30
1	A	154	TYR	CB-CG-CD2	-8.74	115.75	121.00
1	A	150	LEU	CA-CB-CG	8.70	135.30	115.30
1	A	250	ALA	N-CA-CB	8.59	122.13	110.10
1	A	234	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	1	ARG	CA-C-N	8.37	135.62	117.20
1	A	276	GLU	CA-C-O	8.34	137.62	120.10
1	A	32	ASP	CB-CG-OD2	8.33	125.79	118.30
1	A	278	ASP	C-N-CA	8.29	142.42	121.70
1	A	148	LYS	CB-CG-CD	8.22	132.98	111.60
1	A	66	GLU	C-N-CA	8.21	142.23	121.70
1	A	23	PRO	CA-N-CD	-8.20	100.02	111.50
1	A	276	GLU	CB-CG-CD	8.08	136.01	114.20
1	A	76	GLY	N-CA-C	-7.97	93.18	113.10
1	A	257	ASP	OD1-CG-OD2	7.97	138.44	123.30
1	A	221	ILE	N-CA-CB	7.93	129.04	110.80
1	A	297	GLU	C-N-CA	7.90	141.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	ASP	CB-CA-C	-7.88	94.64	110.40
1	A	294	ASN	O-C-N	-7.83	110.16	122.70
1	A	1	ARG	CA-C-O	-7.81	103.70	120.10
1	A	294	ASN	C-N-CA	7.78	141.16	121.70
1	A	170	VAL	CA-CB-CG2	7.77	122.55	110.90
1	A	81	ARG	NH1-CZ-NH2	7.73	127.90	119.40
1	A	112	GLN	O-C-N	-7.65	110.46	122.70
1	A	94	GLY	N-CA-C	7.65	132.22	113.10
1	A	186	ALA	N-CA-CB	7.62	120.77	110.10
1	A	73	LEU	CB-CA-C	7.60	124.64	110.20
1	A	13	GLU	O-C-N	7.56	134.80	122.70
1	A	266	LYS	CB-CG-CD	7.54	131.22	111.60
1	A	93	GLY	C-N-CA	7.52	138.09	122.30
1	A	176	THR	CA-CB-CG2	7.41	122.77	112.40
1	A	234	ASP	OD1-CG-OD2	7.40	137.36	123.30
1	A	297	GLU	CA-C-N	-7.32	101.10	117.20
1	A	59	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	298	LEU	CA-CB-CG	7.31	132.12	115.30
1	A	303	ASP	CB-CG-OD1	-7.28	111.74	118.30
1	A	234	ASP	CB-CG-OD1	-7.25	111.78	118.30
1	A	149	ASP	OD1-CG-OD2	-7.25	109.53	123.30
1	A	259	THR	N-CA-CB	7.25	124.07	110.30
1	A	169	GLY	C-N-CA	7.19	139.67	121.70
1	A	169	GLY	O-C-N	-7.17	111.22	122.70
1	A	154	TYR	CB-CG-CD1	7.11	125.26	121.00
1	A	111	PHE	CA-C-N	7.10	132.82	117.20
1	A	110	PRO	C-N-CA	7.10	139.45	121.70
1	A	130	ALA	CB-CA-C	7.09	120.74	110.10
1	A	140	MET	C-N-CA	7.09	137.18	122.30
1	A	296	SER	N-CA-CB	-7.08	99.88	110.50
1	A	80	MET	CA-CB-CG	7.08	125.33	113.30
1	A	233	LYS	O-C-N	-7.04	111.44	122.70
1	A	258	ILE	CB-CA-C	7.02	125.64	111.60
1	A	213	ILE	CB-CA-C	6.99	125.58	111.60
1	A	249	CYS	CA-C-N	6.98	132.55	117.20
1	A	279	GLN	CA-C-O	6.95	134.69	120.10
1	A	73	LEU	CA-C-O	6.91	134.61	120.10
1	A	73	LEU	CA-C-N	-6.82	102.20	117.20
1	A	19	SER	CB-CA-C	-6.79	97.20	110.10
1	A	209	GLY	CA-C-O	6.76	132.77	120.60
1	A	225	VAL	CA-CB-CG1	6.74	121.01	110.90
1	A	238	SER	CA-CB-OG	6.71	129.31	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	A	165	VAL	CA-CB-CG2	6.64	120.86	110.90
1	A	221	ILE	CG1-CB-CG2	-6.58	96.92	111.40
1	A	195	ASP	OD1-CG-OD2	6.57	135.79	123.30
1	A	74	THR	N-CA-C	-6.52	93.39	111.00
1	A	221	ILE	CA-CB-CG2	6.49	123.89	110.90
1	A	98	ASN	OD1-CG-ND2	-6.49	106.98	121.90
1	A	124	ALA	N-CA-CB	6.45	119.13	110.10
1	A	75	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	A	258	ILE	CA-CB-CG2	6.42	123.75	110.90
1	A	95	SER	CA-C-O	-6.41	106.64	120.10
1	A	118	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	262	ILE	CA-CB-CG1	6.39	123.14	111.00
1	A	111	PHE	CA-C-O	-6.39	106.68	120.10
1	A	166	MET	CA-CB-CG	6.38	124.14	113.30
1	A	323	ALA	N-CA-CB	6.37	119.02	110.10
1	A	171	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	59	ARG	CB-CA-C	-6.36	97.68	110.40
1	A	297	GLU	O-C-N	-6.35	112.53	122.70
1	A	96	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	165	VAL	N-CA-CB	6.31	125.39	111.50
1	A	148	LYS	CA-CB-CG	6.30	127.27	113.40
1	A	188	LYS	O-C-N	-6.28	112.65	122.70
1	A	277	GLY	N-CA-C	-6.28	97.40	113.10
1	A	191	GLN	CB-CA-C	-6.25	97.90	110.40
1	A	55	LYS	CA-C-O	6.21	133.13	120.10
1	A	10	ALA	N-CA-CB	-6.20	101.42	110.10
1	A	249	CYS	O-C-N	-6.20	112.78	122.70
1	A	164	GLU	N-CA-CB	-6.19	99.46	110.60
1	A	294	ASN	CB-CA-C	6.18	122.75	110.40
1	A	309	TYR	CA-CB-CG	-6.17	101.68	113.40
1	A	168	GLY	C-N-CA	6.17	135.25	122.30
1	A	258	ILE	O-C-N	-6.16	112.84	122.70
1	A	211	GLN	CB-CG-CD	6.15	127.58	111.60
1	A	146	VAL	C-N-CA	6.11	136.98	121.70
1	A	234	ASP	CA-CB-CG	-6.11	99.96	113.40
1	A	257	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	A	188	LYS	CA-C-O	6.10	132.91	120.10
1	A	197	ILE	CA-C-O	6.10	132.90	120.10
1	A	42	SER	N-CA-CB	6.08	119.63	110.50
1	A	53	HIS	CA-CB-CG	-6.05	103.31	113.60
1	A	36	SER	CA-C-O	-6.05	107.40	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	GLN	CA-CB-CG	6.00	126.61	113.40
1	A	72	ASP	C-N-CA	-5.99	106.72	121.70
1	A	279	GLN	N-CA-C	5.99	127.18	111.00
1	A	149	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	3	THR	CA-CB-OG1	-5.98	96.45	109.00
1	A	74	THR	N-CA-CB	5.97	121.65	110.30
1	A	77	THR	N-CA-CB	5.90	121.51	110.30
1	A	154	TYR	CA-CB-CG	-5.89	102.21	113.40
1	A	196	GLY	O-C-N	5.88	132.11	122.70
1	A	221	ILE	N-CA-C	-5.88	95.14	111.00
1	A	15	TYR	C-N-CA	-5.83	110.05	122.30
1	A	31	PHE	CZ-CE2-CD2	5.82	127.09	120.10
1	A	152	SER	O-C-N	5.81	131.99	122.70
1	A	261	THR	O-C-N	5.77	131.94	122.70
1	A	107	GLU	CA-CB-CG	5.76	126.08	113.40
1	A	228	LEU	N-CA-CB	5.75	121.91	110.40
1	A	51	SER	N-CA-CB	5.75	119.13	110.50
1	A	25	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	A	112	GLN	CA-C-N	5.74	129.82	117.20
1	A	294	ASN	CB-CG-OD1	5.73	133.05	121.60
1	A	250	ALA	CA-C-O	-5.70	108.14	120.10
1	A	11	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	95	SER	O-C-N	-5.68	113.61	122.70
1	A	95	SER	CB-CA-C	-5.68	99.31	110.10
1	A	13	GLU	CB-CA-C	-5.67	99.07	110.40
1	A	15	TYR	CB-CG-CD1	5.65	124.39	121.00
1	A	32	ASP	CA-C-O	5.63	131.92	120.10
1	A	91	VAL	CB-CA-C	-5.63	100.71	111.40
1	A	47	ALA	N-CA-CB	-5.62	102.23	110.10
1	A	72	ASP	N-CA-C	-5.62	95.83	111.00
1	A	96	ASP	N-CA-C	5.62	126.16	111.00
1	A	58	PRO	O-C-N	-5.61	113.72	122.70
1	A	2	VAL	CA-CB-CG2	5.59	119.28	110.90
1	A	6	MET	CA-CB-CG	5.58	122.78	113.30
1	A	21	GLY	C-N-CA	5.57	135.62	121.70
1	A	30	ILE	CA-CB-CG1	5.57	121.58	111.00
1	A	240	ASN	CA-C-O	5.56	131.78	120.10
1	A	304	VAL	O-C-N	-5.55	113.82	122.70
1	A	193	ALA	N-CA-CB	5.53	117.84	110.10
1	A	110	PRO	N-CA-CB	5.52	109.92	103.30
1	A	146	VAL	CB-CA-C	5.52	121.89	111.40
1	A	197	ILE	N-CA-CB	5.51	123.48	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	CYS	CB-CA-C	5.51	121.42	110.40
1	A	199	VAL	CA-CB-CG1	5.50	119.16	110.90
1	A	220	LYS	N-CA-C	5.50	125.86	111.00
1	A	47	ALA	O-C-N	-5.49	113.91	122.70
1	A	2	VAL	N-CA-CB	5.48	123.56	111.50
1	A	175	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	38	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	250	ALA	CA-C-N	5.45	129.19	117.20
1	A	310	TYR	CA-CB-CG	5.43	123.71	113.40
1	A	17	VAL	C-N-CA	5.42	135.25	121.70
1	A	32	ASP	O-C-N	-5.41	114.04	122.70
1	A	54	ASN	N-CA-CB	-5.40	100.88	110.60
1	A	153	PHE	CA-CB-CG	5.39	126.84	113.90
1	A	238	SER	N-CA-CB	5.39	118.59	110.50
1	A	107	GLU	CB-CA-C	-5.39	99.62	110.40
1	A	23	PRO	CA-CB-CG	-5.38	93.77	104.00
1	A	220	LYS	CB-CA-C	-5.38	99.63	110.40
1	A	165	VAL	N-CA-C	-5.37	96.50	111.00
1	A	105	GLN	CB-CA-C	-5.33	99.74	110.40
1	A	77	THR	CA-CB-CG2	-5.32	104.96	112.40
1	A	252	VAL	N-CA-CB	-5.31	99.83	111.50
1	A	30	ILE	CB-CG1-CD1	-5.29	99.08	113.90
1	A	31	PHE	CG-CD2-CE2	-5.29	114.99	120.80
1	A	111	PHE	N-CA-CB	5.28	120.10	110.60
1	A	87	ASP	O-C-N	-5.28	114.26	122.70
1	A	17	VAL	CA-C-O	5.26	131.16	120.10
1	A	32	ASP	OD1-CG-OD2	-5.26	113.30	123.30
1	A	10	ALA	CB-CA-C	-5.26	102.22	110.10
1	A	5	GLN	CB-CA-C	5.24	120.88	110.40
1	A	179	ILE	CA-C-O	5.24	131.10	120.10
1	A	30	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	A	44	HIS	N-CA-CB	5.21	119.99	110.60
1	A	7	LYS	CA-CB-CG	5.20	124.84	113.40
1	A	67	THR	CB-CA-C	-5.20	97.56	111.60
1	A	232	MET	CG-SD-CE	5.19	108.50	100.20
1	A	44	HIS	CB-CA-C	-5.18	100.04	110.40
1	A	210	CYS	N-CA-C	-5.17	97.04	111.00
1	A	286	LEU	N-CA-CB	5.17	120.74	110.40
1	A	272	SER	CB-CA-C	-5.17	100.29	110.10
1	A	23	PRO	N-CA-CB	5.13	109.45	103.30
1	A	29	VAL	CG1-CB-CG2	-5.13	102.70	110.90
1	A	315	ARG	C-N-CA	-5.12	108.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	THR	N-CA-CB	-5.11	100.58	110.30
1	A	66	GLU	N-CA-CB	-5.10	101.42	110.60
1	A	111	PHE	CA-CB-CG	-5.09	101.68	113.90
1	A	256	PRO	N-CA-CB	5.09	109.41	103.30
1	A	313	TYR	CG-CD1-CE1	5.09	125.37	121.30
1	A	148	LYS	CG-CD-CE	5.09	127.16	111.90
1	A	195	ASP	CA-CB-CG	-5.08	102.23	113.40
1	A	122	GLY	O-C-N	5.07	130.80	122.70
1	A	94	GLY	C-N-CA	5.06	134.35	121.70
1	A	54	ASN	CB-CA-C	5.06	120.51	110.40
1	A	283	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	2	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	81	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	258	ILE	N-CA-CB	-5.01	99.28	110.80
1	A	76	GLY	CA-C-N	-5.01	106.18	117.20
1	A	309	TYR	CB-CG-CD2	5.01	124.00	121.00

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 (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	2390	0	2264	116	1
2	A	161	0	0	3	1
All	All	2551	0	2264	116	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 25.

All (116) 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: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
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:HZ1	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:HZ1	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: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: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: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: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:166:MET:HE1	1:A:310:TYR:HE1	1.68	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ASN:C	1:A:249:CYS:O	2.43	0.56
1:A:7:LYS:NZ	1:A:17:VAL:HG22	2.20	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:166:MET:HE1	1:A:310:TYR:CE1	2.44	0.51
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: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: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:249:CYS:O	1:A:250:ALA:CB	2.63	0.47
1:A:222:VAL:HG13	1:A:289:SER:HB2	1.95	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: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
1:A:222:VAL:HG13	1:A:289:SER:CB	2.45	0.46
1:A:166:MET:CE	1:A:171:ASP:HB3	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:HG3	1:A:298:LEU:HD23	1.99	0.44
1:A:109:GLY:C	1:A:111:PHE:H	2.21	0.44
1:A:182:ILE:CD1	1:A:183:PRO:HD2	2.48	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: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:HZ3	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:166:MET:SD	1:A:310:TYR:OH	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:57:LYS:HE3	1:A:58:PRO:CD	2.44	0.41
1:A:75:TYR:O	1:A:76:GLY:C	2.58	0.41
1:A:198:THR:HG23	1:A:202:GLN:N	2.35	0.41
1:A:164:GLU:OE1	1:A:166:MET:HE2	2.20	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: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:164:GLU:HB3	1:A:166:MET:HE3	2.02	0.40
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%)	6 2

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%)	204 (79%)	54 (21%)	1 0

All (54) 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

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Mol	Chain	Res	Type
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	66	GLU
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	96	ASP
1	A	101	LEU
1	A	106	THR
1	A	108	PRO
1	A	111	PHE
1	A	138	ASP
1	A	142	SER
1	A	148	LYS
1	A	170	VAL
1	A	172	ASN
1	A	182	ILE
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	252	VAL
1	A	257	ASP
1	A	266	LYS
1	A	272	SER
1	A	275	ILE

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Mol	Chain	Res	Type
1	A	279	GLN
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	311	THR

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	86	GLN
1	A	294	ASN
1	A	318	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 monosaccharides 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%)	0.10	17 (5%) 27 35	3, 14, 35, 46	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	TYR	5.0
1	A	94	GLY	4.5
1	A	204	ALA	4.3
1	A	110	PRO	3.7
1	A	205	ALA	3.4
1	A	76	GLY	3.1
1	A	77	THR	3.0
1	A	111	PHE	3.0
1	A	109	GLY	2.9
1	A	79	GLY	2.7
1	A	203	THR	2.6
1	A	280	ALA	2.5
1	A	108	PRO	2.5
1	A	250	ALA	2.4
1	A	249	CYS	2.3
1	A	74	THR	2.2
1	A	281	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.