



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:18 AM UTC

PDB ID : 5PEP / pdb_00005pep
Title : X-RAY ANALYSES OF ASPARTIC PROTEASES. II. THREE-DIMENSIONAL STRUCTURE OF THE HEXAGONAL CRYSTAL FORM OF PORCINE PEPSIN AT 2.3 ANGSTROMS RESOLUTION
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Deposited on : 1990-05-30
Resolution : 2.34 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

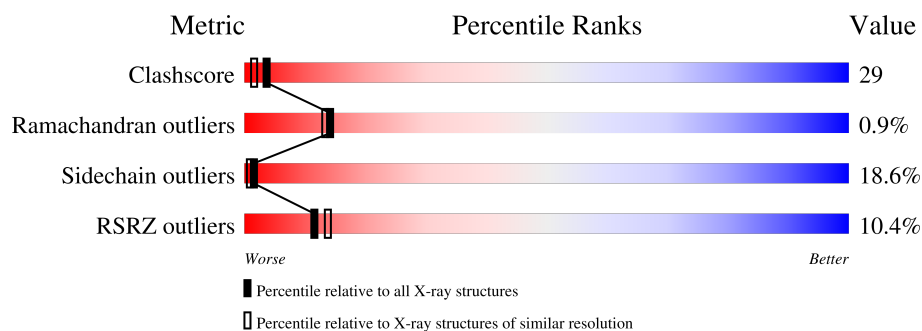
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	326	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2797 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	326	2426	1529	366	521	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P00791
A	254	ALA	ASP	conflict	UNP P00791

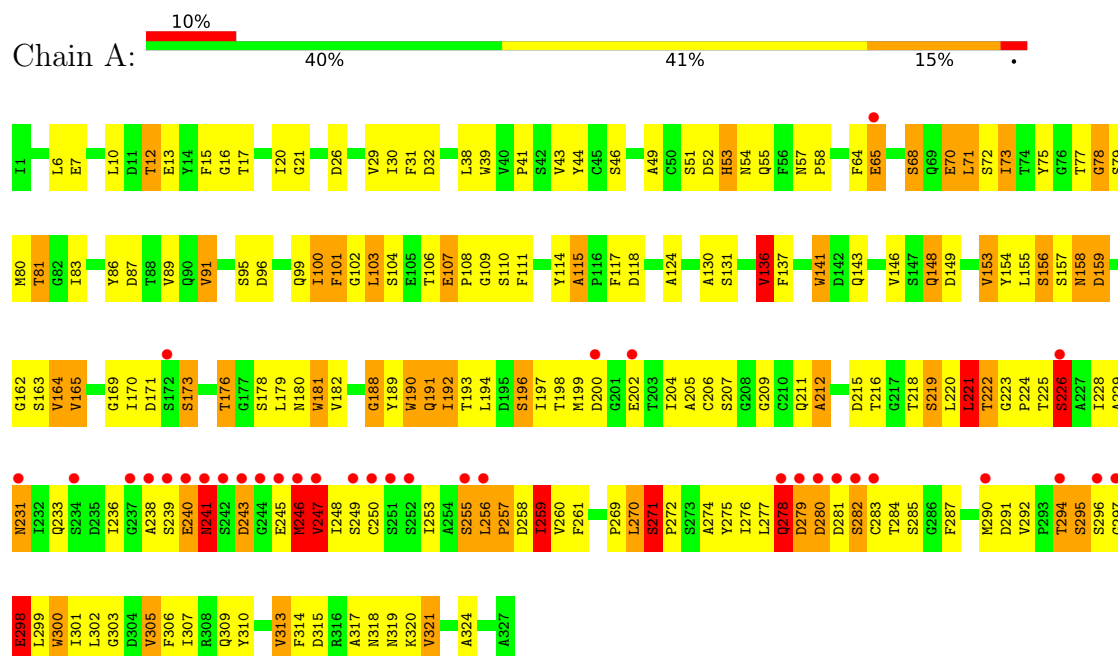
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	371	Total	O	0	0
			371	371		

3 Residue-property plots

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 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	67.40Å 67.40Å 290.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.34 10.00 – 2.34	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.34) 76.0 (10.00-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.33Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.196 , (Not available) 0.269 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 18.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2797	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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	1.40	30/2481 (1.2%)	1.98	117/3396 (3.4%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ASP	C-O	8.55	1.34	1.24
1	A	189	TYR	C-N	-7.30	1.23	1.33
1	A	103	LEU	C-N	-6.86	1.24	1.33
1	A	218	THR	C-N	-6.83	1.24	1.33
1	A	53	HIS	ND1-CE1	6.59	1.39	1.32
1	A	221	LEU	C-N	-6.44	1.24	1.33
1	A	188	GLY	N-CA	6.38	1.54	1.45
1	A	241	ASN	CG-OD1	6.35	1.35	1.23
1	A	211	GLN	CD-OE1	6.32	1.35	1.23
1	A	212	ALA	C-N	5.99	1.42	1.33
1	A	190	TRP	NE1-CE2	-5.92	1.30	1.37
1	A	39	TRP	NE1-CE2	-5.79	1.31	1.37
1	A	300	TRP	NE1-CE2	-5.77	1.31	1.37
1	A	278	GLN	CD-OE1	5.76	1.34	1.23
1	A	279	ASP	C-N	-5.55	1.25	1.33
1	A	100	ILE	C-N	-5.54	1.26	1.33
1	A	158	ASN	CG-OD1	5.51	1.34	1.23
1	A	181	TRP	NE1-CE2	-5.48	1.31	1.37
1	A	99	GLN	CD-OE1	5.47	1.33	1.23
1	A	53	HIS	CE1-NE2	5.43	1.38	1.32
1	A	143	GLN	CD-OE1	5.30	1.33	1.23
1	A	148	GLN	CD-OE1	5.25	1.33	1.23
1	A	319	ASN	CG-OD1	5.25	1.33	1.23
1	A	318	ASN	CG-OD1	5.19	1.33	1.23
1	A	55	GLN	CD-OE1	5.12	1.33	1.23
1	A	309	GLN	CD-OE1	5.11	1.33	1.23
1	A	155	LEU	C-N	-5.09	1.26	1.33
1	A	141	TRP	NE1-CE2	-5.07	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ASN	CG-OD1	5.07	1.33	1.23
1	A	95	SER	C-N	-5.03	1.27	1.33

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ASP	CA-C-O	-11.34	108.69	120.71
1	A	282	SER	CA-C-N	11.28	138.10	122.19
1	A	282	SER	C-N-CA	11.28	138.10	122.19
1	A	221	LEU	CA-C-N	10.62	138.48	122.65
1	A	221	LEU	C-N-CA	10.62	138.48	122.65
1	A	218	THR	CA-C-N	10.06	134.58	120.29
1	A	218	THR	C-N-CA	10.06	134.58	120.29
1	A	302	LEU	CA-C-N	9.23	134.70	121.96
1	A	302	LEU	C-N-CA	9.23	134.70	121.96
1	A	212	ALA	CA-C-N	-8.52	109.90	122.68
1	A	212	ALA	C-N-CA	-8.52	109.90	122.68
1	A	241	ASN	CA-CB-CG	8.47	121.07	112.60
1	A	260	VAL	CA-CB-CG2	8.42	124.72	110.40
1	A	68	SER	CA-C-N	8.34	132.62	120.95
1	A	68	SER	C-N-CA	8.34	132.62	120.95
1	A	313	VAL	CA-CB-CG2	8.30	124.51	110.40
1	A	198	THR	CA-C-O	8.21	131.06	121.46
1	A	194	LEU	CA-C-O	-8.18	111.72	120.80
1	A	153	VAL	CA-CB-CG2	7.84	123.73	110.40
1	A	115	ALA	CA-C-O	7.84	128.71	120.25
1	A	164	VAL	CA-CB-CG2	7.75	123.58	110.40
1	A	51	SER	CA-C-N	7.63	134.50	121.14
1	A	51	SER	C-N-CA	7.63	134.50	121.14
1	A	226	SER	CA-C-N	7.48	130.64	120.54
1	A	226	SER	C-N-CA	7.48	130.64	120.54
1	A	31	PHE	CA-CB-CG	-7.17	106.62	113.80
1	A	26	ASP	O-C-N	7.08	130.99	123.06
1	A	17	THR	CA-C-O	7.04	129.59	121.28
1	A	165	VAL	CA-CB-CG2	7.03	122.35	110.40
1	A	101	PHE	CA-C-O	-7.01	113.48	121.40
1	A	188	GLY	O-C-N	6.94	131.73	122.70
1	A	300	TRP	O-C-N	-6.93	115.32	123.22
1	A	31	PHE	CA-C-N	6.92	131.62	122.42
1	A	31	PHE	C-N-CA	6.92	131.62	122.42
1	A	319	ASN	CA-CB-CG	-6.83	105.77	112.60
1	A	146	VAL	CA-C-N	6.80	129.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	VAL	C-N-CA	6.80	129.40	120.28
1	A	53	HIS	CA-CB-CG	-6.79	107.01	113.80
1	A	29	VAL	O-C-N	6.67	130.44	123.04
1	A	253	ILE	CA-C-N	6.60	129.02	120.44
1	A	253	ILE	C-N-CA	6.60	129.02	120.44
1	A	114	TYR	CA-C-N	6.54	129.78	120.49
1	A	114	TYR	C-N-CA	6.54	129.78	120.49
1	A	117	PHE	CA-C-O	6.54	128.55	121.16
1	A	243	ASP	CA-CB-CG	-6.51	106.09	112.60
1	A	259	ILE	CA-C-O	-6.43	113.12	120.65
1	A	247	VAL	CA-CB-CG2	6.42	121.31	110.40
1	A	222	THR	CA-C-O	6.38	127.88	120.80
1	A	279	ASP	O-C-N	-6.38	115.11	123.21
1	A	209	GLY	N-CA-C	6.37	120.04	112.33
1	A	155	LEU	CA-C-N	6.36	130.93	120.94
1	A	155	LEU	C-N-CA	6.36	130.93	120.94
1	A	95	SER	CA-C-O	-6.35	114.12	120.98
1	A	321	VAL	CA-CB-CG2	6.33	121.16	110.40
1	A	44	TYR	CA-CB-CG	6.27	125.19	113.90
1	A	191	GLN	CA-C-O	6.27	127.76	120.49
1	A	70	GLU	CA-C-O	-6.19	114.11	121.66
1	A	136	VAL	CB-CA-C	-6.12	104.14	111.97
1	A	271	SER	CA-C-N	6.09	125.98	119.28
1	A	271	SER	C-N-CA	6.09	125.98	119.28
1	A	107	GLU	O-C-N	6.03	126.11	121.23
1	A	103	LEU	CA-C-O	-6.02	114.08	120.40
1	A	182	VAL	CA-CB-CG2	6.00	120.61	110.40
1	A	146	VAL	CA-CB-CG2	5.97	120.54	110.40
1	A	241	ASN	CA-C-N	5.95	132.90	121.54
1	A	241	ASN	C-N-CA	5.95	132.90	121.54
1	A	196	SER	CA-C-N	5.94	131.75	122.84
1	A	196	SER	C-N-CA	5.94	131.75	122.84
1	A	141	TRP	CA-C-N	5.89	128.18	120.28
1	A	141	TRP	C-N-CA	5.89	128.18	120.28
1	A	188	GLY	N-CA-C	-5.85	99.33	113.18
1	A	176	THR	CA-C-O	-5.79	114.62	121.16
1	A	15	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	157	SER	CA-C-O	-5.75	114.61	121.56
1	A	170	ILE	CA-C-O	-5.71	114.31	120.36
1	A	124	ALA	CA-C-N	5.70	128.58	120.49
1	A	124	ALA	C-N-CA	5.70	128.58	120.49
1	A	305	VAL	CA-CB-CG2	5.67	120.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	TYR	CA-C-O	-5.64	115.00	121.82
1	A	190	TRP	CA-C-N	5.63	129.88	121.72
1	A	190	TRP	C-N-CA	5.63	129.88	121.72
1	A	103	LEU	CA-C-N	5.58	129.17	120.75
1	A	103	LEU	C-N-CA	5.58	129.17	120.75
1	A	65	GLU	CA-C-N	5.57	133.36	121.45
1	A	65	GLU	C-N-CA	5.57	133.36	121.45
1	A	196	SER	CA-C-O	-5.51	115.54	121.38
1	A	102	GLY	CA-C-N	5.50	131.10	123.07
1	A	102	GLY	C-N-CA	5.50	131.10	123.07
1	A	180	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	218	THR	CA-C-O	-5.46	114.45	120.30
1	A	255	SER	CA-C-N	5.46	135.13	121.80
1	A	255	SER	C-N-CA	5.46	135.13	121.80
1	A	241	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	78	GLY	CA-C-N	5.41	131.09	122.59
1	A	78	GLY	C-N-CA	5.41	131.09	122.59
1	A	282	SER	N-CA-CB	5.37	119.56	110.49
1	A	320	LYS	O-C-N	5.28	129.56	123.17
1	A	32	ASP	O-C-N	-5.28	116.60	122.93
1	A	190	TRP	O-C-N	5.21	129.65	122.83
1	A	223	GLY	CA-C-N	5.20	125.45	119.83
1	A	223	GLY	C-N-CA	5.20	125.45	119.83
1	A	159	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	318	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	16	GLY	O-C-N	-5.16	117.98	123.45
1	A	44	TYR	O-C-N	5.15	128.68	122.35
1	A	298	GLU	CA-C-N	5.14	128.16	120.87
1	A	298	GLU	C-N-CA	5.14	128.16	120.87
1	A	109	GLY	O-C-N	5.10	129.28	123.21
1	A	211	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	96	ASP	CA-C-N	5.07	128.41	120.75
1	A	96	ASP	C-N-CA	5.07	128.41	120.75
1	A	57	ASN	CA-C-O	-5.05	115.59	119.99
1	A	169	GLY	CA-C-N	5.04	129.99	122.99
1	A	169	GLY	C-N-CA	5.04	129.99	122.99
1	A	246	MET	CG-SD-CE	5.03	111.96	100.90
1	A	219	SER	CA-C-O	-5.01	115.11	120.42
1	A	73	ILE	CA-C-O	5.00	126.26	120.76

There are no chirality outliers.

There are no planarity outliers.

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	2426	0	2256	136	0
2	A	371	0	0	6	1
All	All	2797	0	2256	136	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 29.

All (136) 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:71:LEU:HD11	1:A:73:ILE:HD11	1.39	1.04
1:A:240:GLU:HG2	1:A:246:MET:HG2	1.49	0.95
1:A:278:GLN:HB2	1:A:283:CYS:SG	2.12	0.90
1:A:221:LEU:HD11	1:A:306:PHE:HB2	1.57	0.87
1:A:248:ILE:HD11	1:A:276:ILE:CG2	2.05	0.87
1:A:248:ILE:HD11	1:A:276:ILE:HG21	1.57	0.86
1:A:71:LEU:HD11	1:A:73:ILE:CD1	2.07	0.84
1:A:86:TYR:CZ	1:A:100:ILE:HD12	2.12	0.83
1:A:238:ALA:CB	1:A:246:MET:HE2	2.11	0.81
1:A:240:GLU:HG2	1:A:246:MET:CG	2.12	0.80
1:A:86:TYR:CE2	1:A:100:ILE:HD12	2.16	0.80
1:A:221:LEU:HD12	1:A:305:VAL:HB	1.63	0.79
1:A:222:THR:HG21	1:A:301:ILE:HD12	1.65	0.78
1:A:179:LEU:HD13	1:A:181:TRP:CZ2	2.18	0.78
1:A:238:ALA:HB1	1:A:246:MET:HE2	1.67	0.77
1:A:71:LEU:CD1	1:A:73:ILE:HD11	2.15	0.75
1:A:294:THR:HG22	1:A:296:SER:N	2.03	0.74
1:A:224:PRO:HG3	1:A:298:GLU:HG2	1.70	0.73
1:A:259:ILE:HD13	1:A:287:PHE:CZ	2.24	0.73
1:A:192:ILE:HD11	1:A:321:VAL:CG2	2.17	0.73
1:A:240:GLU:HG3	2:A:590:HOH:O	1.87	0.72
1:A:81:THR:HB	1:A:106:THR:OG1	1.91	0.70
1:A:222:THR:CG2	1:A:301:ILE:HD12	2.21	0.70
1:A:294:THR:HG22	1:A:296:SER:H	1.57	0.69
1:A:294:THR:CG2	1:A:296:SER:H	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASP:O	1:A:281:ASP:N	2.25	0.69
1:A:6:LEU:HD11	1:A:165:VAL:HG23	1.75	0.68
1:A:280:ASP:HB3	2:A:608:HOH:O	1.93	0.67
1:A:279:ASP:C	1:A:281:ASP:H	2.01	0.67
1:A:284:THR:HG22	1:A:285:SER:H	1.60	0.67
1:A:240:GLU:HA	1:A:245:GLU:O	1.95	0.66
1:A:247:VAL:HG12	1:A:283:CYS:O	1.96	0.66
1:A:233:GLN:HB3	1:A:238:ALA:HB3	1.78	0.65
1:A:239:SER:O	1:A:246:MET:HA	1.97	0.65
1:A:259:ILE:HG22	1:A:275:TYR:CD1	2.32	0.64
1:A:49:ALA:O	1:A:53:HIS:HD2	1.81	0.64
1:A:259:ILE:HD13	1:A:287:PHE:HZ	1.63	0.63
1:A:192:ILE:HD11	1:A:321:VAL:HG21	1.78	0.63
1:A:52:ASP:HB3	1:A:53:HIS:CD2	2.34	0.63
1:A:284:THR:HG22	1:A:285:SER:N	2.14	0.63
1:A:80:MET:HG2	1:A:81:THR:N	2.14	0.62
1:A:192:ILE:CD1	1:A:321:VAL:HG21	2.30	0.62
1:A:278:GLN:CB	1:A:283:CYS:SG	2.87	0.61
1:A:72:SER:C	1:A:73:ILE:HG13	2.25	0.60
1:A:248:ILE:CD1	1:A:276:ILE:HD13	2.32	0.60
1:A:171:ASP:OD2	1:A:173:SER:HB2	2.02	0.60
1:A:53:HIS:HE1	1:A:115:ALA:O	1.85	0.59
1:A:238:ALA:HB3	1:A:246:MET:HE2	1.85	0.59
1:A:101:PHE:CZ	1:A:103:LEU:HD11	2.39	0.58
1:A:278:GLN:O	1:A:278:GLN:HG2	2.03	0.58
1:A:20:ILE:HG12	1:A:89:VAL:HG22	1.86	0.57
1:A:248:ILE:HD11	1:A:276:ILE:HG23	1.83	0.57
1:A:80:MET:HG2	1:A:81:THR:H	1.71	0.56
1:A:202:GLU:HB3	2:A:466:HOH:O	2.04	0.56
1:A:111:PHE:HD2	2:A:412:HOH:O	1.89	0.55
1:A:107:GLU:N	1:A:108:PRO:HD3	2.22	0.55
1:A:258:ASP:OD1	1:A:272:PRO:HD3	2.07	0.55
1:A:75:TYR:HB2	1:A:78:GLY:O	2.07	0.54
1:A:294:THR:HG23	1:A:295:SER:N	2.23	0.54
1:A:238:ALA:C	1:A:246:MET:HE3	2.33	0.53
1:A:6:LEU:HD11	1:A:165:VAL:CG2	2.38	0.53
1:A:238:ALA:CB	1:A:246:MET:CE	2.86	0.53
1:A:89:VAL:HG12	1:A:91:VAL:HG22	1.91	0.53
1:A:130:ALA:O	1:A:131:SER:HB2	2.08	0.52
1:A:199:MET:O	1:A:200:ASP:HB2	2.08	0.52
1:A:290:MET:HG2	1:A:292:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:MET:HE2	1:A:257:PRO:HG2	1.92	0.52
1:A:216:THR:HG22	1:A:307:ILE:HD13	1.91	0.52
1:A:197:ILE:HG13	1:A:206:CYS:HB3	1.92	0.52
1:A:199:MET:HB3	1:A:204:ILE:HG21	1.92	0.51
1:A:239:SER:N	1:A:246:MET:HE3	2.25	0.51
1:A:290:MET:HG2	1:A:292:VAL:HG23	1.91	0.51
1:A:236:ILE:HB	1:A:256:LEU:HD21	1.93	0.51
1:A:275:TYR:CD2	1:A:276:ILE:HG13	2.46	0.51
1:A:71:LEU:HD21	1:A:80:MET:HE1	1.91	0.51
1:A:136:VAL:HG12	1:A:137:PHE:N	2.26	0.51
1:A:154:TYR:HB3	1:A:164:VAL:HG12	1.92	0.51
1:A:154:TYR:HD2	1:A:162:GLY:O	1.94	0.51
1:A:294:THR:CG2	1:A:295:SER:N	2.74	0.50
1:A:10:LEU:C	1:A:12:THR:N	2.68	0.50
1:A:89:VAL:HG12	1:A:91:VAL:CG2	2.42	0.50
1:A:259:ILE:HG12	1:A:261:PHE:HE2	1.76	0.50
1:A:100:ILE:O	1:A:100:ILE:HG23	2.11	0.49
1:A:315:ASP:OD1	1:A:317:ALA:HB3	2.12	0.49
1:A:212:ALA:HA	1:A:300:TRP:O	2.12	0.49
1:A:49:ALA:O	1:A:53:HIS:CD2	2.64	0.48
1:A:141:TRP:CZ2	1:A:149:ASP:HB2	2.48	0.48
1:A:240:GLU:HG2	1:A:246:MET:SD	2.53	0.47
1:A:106:THR:C	1:A:108:PRO:HD3	2.39	0.47
1:A:171:ASP:C	1:A:173:SER:H	2.22	0.47
1:A:241:ASN:HD22	1:A:241:ASN:C	2.22	0.47
1:A:259:ILE:HG22	1:A:275:TYR:CE1	2.50	0.47
1:A:259:ILE:CG2	1:A:275:TYR:CD1	2.97	0.47
1:A:226:SER:O	1:A:229:ALA:HB3	2.15	0.46
1:A:199:MET:HB3	1:A:204:ILE:CG2	2.45	0.46
1:A:297:GLY:HA3	2:A:474:HOH:O	2.15	0.46
1:A:156:SER:HB2	1:A:163:SER:OG	2.16	0.46
1:A:204:ILE:O	1:A:205:ALA:HB2	2.15	0.46
1:A:259:ILE:HG23	1:A:270:LEU:CB	2.46	0.45
1:A:181:TRP:CH2	1:A:313:VAL:HG11	2.51	0.45
1:A:41:PRO:HG2	1:A:54:ASN:O	2.17	0.45
1:A:238:ALA:C	1:A:246:MET:CE	2.89	0.45
1:A:111:PHE:CD1	1:A:111:PHE:C	2.95	0.44
1:A:259:ILE:HG12	1:A:261:PHE:CE2	2.52	0.44
1:A:202:GLU:O	1:A:202:GLU:CG	2.63	0.44
1:A:43:VAL:O	1:A:43:VAL:HG12	2.17	0.44
1:A:38:LEU:HD23	1:A:101:PHE:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TRP:CH2	1:A:149:ASP:HB2	2.53	0.44
1:A:202:GLU:O	1:A:202:GLU:HG2	2.17	0.44
1:A:271:SER:O	1:A:274:ALA:HB3	2.18	0.44
1:A:21:GLY:HA2	1:A:87:ASP:OD2	2.18	0.44
1:A:190:TRP:CZ2	1:A:314:PHE:HB3	2.54	0.43
1:A:294:THR:O	1:A:295:SER:C	2.59	0.43
1:A:80:MET:CG	1:A:81:THR:N	2.80	0.43
1:A:148:GLN:HG2	2:A:426:HOH:O	2.18	0.43
1:A:53:HIS:HB3	1:A:118:ASP:OD1	2.18	0.42
1:A:248:ILE:HG13	1:A:283:CYS:HB3	2.01	0.42
1:A:192:ILE:CG2	1:A:193:THR:N	2.82	0.42
1:A:281:ASP:O	1:A:282:SER:CB	2.65	0.42
1:A:190:TRP:CD2	1:A:314:PHE:HD2	2.37	0.41
1:A:224:PRO:HB3	1:A:298:GLU:OE2	2.20	0.41
1:A:225:THR:HB	1:A:291:ASP:OD2	2.20	0.41
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.78	0.41
1:A:58:PRO:HB3	1:A:64:PHE:CD1	2.55	0.41
1:A:269:PRO:HD2	1:A:310:TYR:OH	2.20	0.41
1:A:284:THR:CG2	1:A:285:SER:N	2.83	0.41
1:A:154:TYR:CD2	1:A:162:GLY:O	2.71	0.41
1:A:41:PRO:HD3	1:A:118:ASP:O	2.20	0.41
1:A:179:LEU:HD23	1:A:324:ALA:HB2	2.01	0.41
1:A:222:THR:HG23	1:A:290:MET:HB3	2.03	0.41
1:A:224:PRO:HD2	1:A:300:TRP:CE2	2.54	0.41
1:A:277:LEU:HD12	1:A:277:LEU:N	2.36	0.41
1:A:221:LEU:HD11	1:A:306:PHE:CB	2.39	0.40
1:A:238:ALA:HB3	1:A:246:MET:CE	2.50	0.40
1:A:215:ASP:O	1:A:303:GLY:HA2	2.20	0.40
1:A:246:MET:HE2	1:A:246:MET:HB3	2.00	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)
2:A:676:HOH:O	2:A:676:HOH:O[11_455]	0.68	1.52

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	324/326 (99%)	304 (94%)	17 (5%)	3 (1%)	14 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ASP
1	A	188	GLY
1	A	257	PRO

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	274/274 (100%)	223 (81%)	51 (19%)	1 1

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

Mol	Chain	Res	Type
1	A	7	GLU
1	A	12	THR
1	A	13	GLU
1	A	30	ILE
1	A	46	SER
1	A	65	GLU
1	A	68	SER
1	A	70	GLU

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Mol	Chain	Res	Type
1	A	71	LEU
1	A	77	THR
1	A	79	SER
1	A	81	THR
1	A	83	ILE
1	A	91	VAL
1	A	104	SER
1	A	110	SER
1	A	136	VAL
1	A	153	VAL
1	A	156	SER
1	A	158	ASN
1	A	159	ASP
1	A	173	SER
1	A	176	THR
1	A	178	SER
1	A	191	GLN
1	A	192	ILE
1	A	196	SER
1	A	207	SER
1	A	219	SER
1	A	220	LEU
1	A	221	LEU
1	A	226	SER
1	A	228	ILE
1	A	231	ASN
1	A	240	GLU
1	A	241	ASN
1	A	243	ASP
1	A	246	MET
1	A	247	VAL
1	A	249	SER
1	A	250	CYS
1	A	255	SER
1	A	256	LEU
1	A	259	ILE
1	A	270	LEU
1	A	271	SER
1	A	278	GLN
1	A	294	THR
1	A	295	SER
1	A	298	GLU

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Mol	Chain	Res	Type
1	A	299	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	143	GLN
1	A	158	ASN
1	A	191	GLN
1	A	211	GLN
1	A	241	ASN
1	A	264	ASN
1	A	278	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](#)

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	326/326 (100%)	0.68	34 (10%)	11 14	0, 0, 1, 1	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	SER	7.4
1	A	243	ASP	5.4
1	A	240	GLU	5.3
1	A	279	ASP	4.7
1	A	281	ASP	4.1
1	A	245	GLU	3.9
1	A	244	GLY	3.9
1	A	280	ASP	3.7
1	A	294	THR	3.6
1	A	283	CYS	3.4
1	A	252	SER	3.4
1	A	251	SER	3.3
1	A	237	GLY	3.3
1	A	247	VAL	3.1
1	A	234	SER	3.1
1	A	239	SER	3.0
1	A	200	ASP	3.0
1	A	246	MET	3.0
1	A	250	CYS	2.9
1	A	226	SER	2.9
1	A	231	ASN	2.9
1	A	255	SER	2.9
1	A	202	GLU	2.9
1	A	172	SER	2.6
1	A	278	GLN	2.4
1	A	241	ASN	2.2
1	A	238	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	290	MET	2.1
1	A	249	SER	2.1
1	A	282	SER	2.1
1	A	296	SER	2.1
1	A	65	GLU	2.1
1	A	297	GLY	2.0
1	A	256	LEU	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.