



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:19 AM EDT

PDB ID : 4APE / pdb_00004ape
Title : THE ACTIVE SITE OF ASPARTIC PROTEINASES
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Deposited on : 1986-06-09
Resolution : 2.10 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

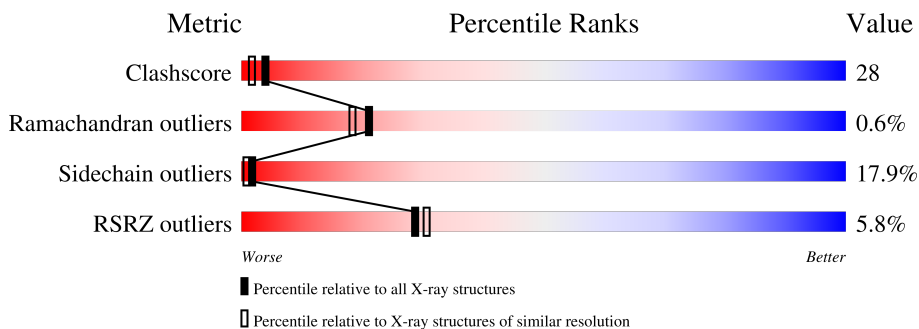
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	330	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2732 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 ENDOTHAPEPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2389	1514	366	507	2			

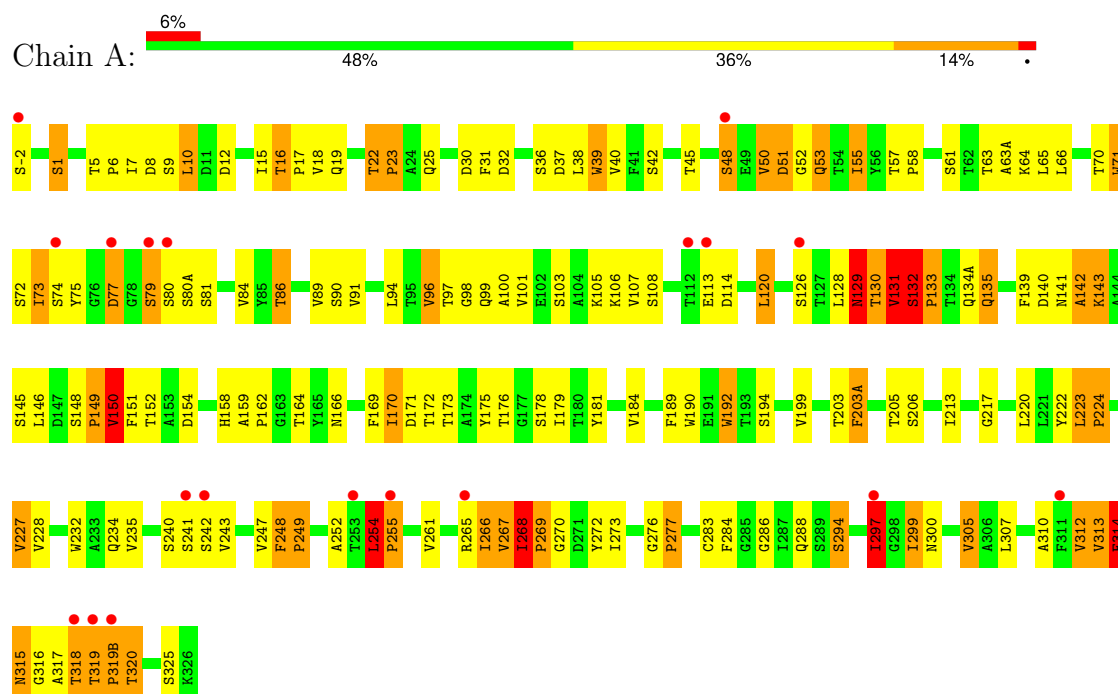
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	343	Total	O	0	0
			343	343		

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: ENDOTHAPEPSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.60Å 74.05Å 45.70Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10 50.37 – 2.11	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10) 91.6 (50.37-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.158 , (Not available) 0.257 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 0.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2732	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 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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	1.19	40/2445 (1.6%)	1.79	81/3345 (2.4%)

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	4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	THR	C-N	10.52	1.43	1.33
1	A	159	ALA	C-N	9.10	1.45	1.33
1	A	162	PRO	N-CD	8.80	1.60	1.47
1	A	16	THR	C-N	8.68	1.44	1.33
1	A	5	THR	C-N	8.39	1.43	1.33
1	A	268	ILE	C-N	8.14	1.43	1.33
1	A	254	LEU	C-N	7.76	1.43	1.33
1	A	223	LEU	C-N	7.75	1.43	1.33
1	A	248	PHE	C-N	7.63	1.43	1.33
1	A	276	GLY	C-N	7.57	1.42	1.33
1	A	133	PRO	N-CD	7.19	1.57	1.47
1	A	23	PRO	N-CD	7.10	1.57	1.47
1	A	158	HIS	CE1-NE2	7.01	1.39	1.32
1	A	158	HIS	ND1-CE1	6.89	1.39	1.32
1	A	249	PRO	N-CD	6.72	1.57	1.47
1	A	277	PRO	N-CD	6.69	1.57	1.47
1	A	17	PRO	N-CD	6.67	1.57	1.47
1	A	58	PRO	N-CD	6.61	1.57	1.47
1	A	269	PRO	N-CD	6.60	1.56	1.47
1	A	224	PRO	N-CD	6.59	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319(B)	PRO	N-CD	6.52	1.56	1.47
1	A	255	PRO	N-CD	6.50	1.56	1.47
1	A	6	PRO	N-CD	6.20	1.56	1.47
1	A	149	PRO	N-CD	5.94	1.56	1.47
1	A	71	TRP	NE1-CE2	-5.49	1.31	1.37
1	A	192	TRP	NE1-CE2	-5.49	1.31	1.37
1	A	39	TRP	NE1-CE2	-5.48	1.31	1.37
1	A	232	TRP	NE1-CE2	-5.46	1.31	1.37
1	A	190	TRP	NE1-CE2	-5.39	1.31	1.37
1	A	319	THR	C-N	5.30	1.44	1.34
1	A	135	GLN	CD-OE1	5.24	1.33	1.23
1	A	297	ILE	C-N	-5.23	1.25	1.33
1	A	288	GLN	CD-OE1	5.21	1.33	1.23
1	A	25	GLN	CD-OE1	5.20	1.33	1.23
1	A	53	GLN	CD-OE1	5.19	1.33	1.23
1	A	99	GLN	CD-OE1	5.19	1.33	1.23
1	A	134(A)	GLN	CD-OE1	5.15	1.33	1.23
1	A	19	GLN	CD-OE1	5.15	1.33	1.23
1	A	234	GLN	CD-OE1	5.15	1.33	1.23
1	A	22	THR	C-N	5.01	1.43	1.34

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	THR	CA-C-N	-18.55	102.15	120.52
1	A	5	THR	C-N-CA	-18.55	102.15	120.52
1	A	268	ILE	CA-C-N	-17.46	103.20	120.31
1	A	268	ILE	C-N-CA	-17.46	103.20	120.31
1	A	223	LEU	CA-C-N	-17.07	103.62	120.52
1	A	223	LEU	C-N-CA	-17.07	103.62	120.52
1	A	16	THR	CA-C-N	-15.26	103.97	120.14
1	A	16	THR	C-N-CA	-15.26	103.97	120.14
1	A	248	PHE	CA-C-N	-14.81	104.00	119.99
1	A	248	PHE	C-N-CA	-14.81	104.00	119.99
1	A	57	THR	CA-C-N	-14.29	103.59	120.89
1	A	57	THR	C-N-CA	-14.29	103.59	120.89
1	A	254	LEU	CA-C-N	-13.87	103.03	120.51
1	A	254	LEU	C-N-CA	-13.87	103.03	120.51
1	A	132	SER	C-N-CD	13.75	150.84	120.60
1	A	276	GLY	CA-C-N	-13.23	103.84	120.51
1	A	276	GLY	C-N-CA	-13.23	103.84	120.51
1	A	254	LEU	CA-C-O	12.60	127.48	119.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	THR	C-N-CD	11.44	145.76	120.60
1	A	57	THR	CA-C-O	11.27	128.83	119.36
1	A	319	THR	C-N-CD	9.07	147.46	128.40
1	A	22	THR	CA-C-N	-8.87	105.71	127.00
1	A	22	THR	C-N-CA	-8.87	105.71	127.00
1	A	132	SER	CA-C-N	-8.77	105.96	127.00
1	A	132	SER	C-N-CA	-8.77	105.96	127.00
1	A	148	SER	CA-C-N	-8.28	102.09	120.56
1	A	148	SER	C-N-CA	-8.28	102.09	120.56
1	A	16	THR	CA-C-O	8.00	127.54	119.86
1	A	133	PRO	N-CD-CG	-7.57	94.72	103.80
1	A	42	SER	CA-C-N	7.08	135.05	121.54
1	A	42	SER	C-N-CA	7.08	135.05	121.54
1	A	159	ALA	CA-C-N	-7.04	112.38	119.92
1	A	159	ALA	C-N-CA	-7.04	112.38	119.92
1	A	248	PHE	CA-C-O	6.63	129.25	120.16
1	A	148	SER	CA-C-O	6.53	127.84	120.46
1	A	159	ALA	CA-C-O	6.51	129.07	120.16
1	A	57	THR	C-N-CD	6.36	151.07	125.00
1	A	254	LEU	C-N-CD	6.36	151.06	125.00
1	A	276	GLY	C-N-CD	6.33	150.97	125.00
1	A	268	ILE	C-N-CD	6.33	150.93	125.00
1	A	297	ILE	O-C-N	-6.32	115.22	122.17
1	A	142	ALA	CA-C-N	6.30	129.05	120.54
1	A	142	ALA	C-N-CA	6.30	129.05	120.54
1	A	107	VAL	CA-CB-CG2	6.18	120.91	110.40
1	A	148	SER	C-N-CD	6.17	150.30	125.00
1	A	223	LEU	C-N-CD	6.16	150.26	125.00
1	A	248	PHE	C-N-CD	6.06	149.86	125.00
1	A	5	THR	CA-C-O	6.03	125.65	119.86
1	A	133	PRO	CA-N-CD	-5.93	103.19	111.50
1	A	5	THR	C-N-CD	5.84	148.93	125.00
1	A	305	VAL	CA-CB-CG2	5.82	120.29	110.40
1	A	131	VAL	CA-CB-CG2	5.75	120.18	110.40
1	A	235	VAL	CA-CB-CG2	5.74	120.15	110.40
1	A	261	VAL	CA-CB-CG1	5.74	120.15	110.40
1	A	150	VAL	CA-CB-CG1	5.70	120.08	110.40
1	A	267	VAL	CA-CB-CG2	5.67	120.04	110.40
1	A	199	VAL	CA-CB-CG2	5.63	119.98	110.40
1	A	50	VAL	CA-CB-CG2	5.62	119.96	110.40
1	A	18	VAL	CA-CB-CG2	5.62	119.95	110.40
1	A	89	VAL	CA-CB-CG2	5.62	119.96	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ILE	CA-C-O	5.62	127.48	119.95
1	A	91	VAL	CA-CB-CG2	5.62	119.94	110.40
1	A	84	VAL	CA-CB-CG2	5.59	119.90	110.40
1	A	312	VAL	CA-CB-CG2	5.59	119.90	110.40
1	A	228	VAL	CA-CB-CG2	5.58	119.89	110.40
1	A	243	VAL	CA-CB-CG2	5.58	119.88	110.40
1	A	313	VAL	CA-CB-CG2	5.57	119.86	110.40
1	A	101	VAL	CA-CB-CG2	5.56	119.86	110.40
1	A	96	VAL	CA-CB-CG2	5.50	119.75	110.40
1	A	40	VAL	CA-CB-CG2	5.50	119.75	110.40
1	A	227	VAL	CA-CB-CG2	5.45	119.66	110.40
1	A	247	VAL	CA-CB-CG2	5.34	119.48	110.40
1	A	16	THR	C-N-CD	5.34	146.88	125.00
1	A	314	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	223	LEU	CA-C-O	5.26	126.26	120.94
1	A	58	PRO	N-CD-CG	-5.17	95.44	103.20
1	A	158	HIS	CA-CB-CG	-5.17	108.64	113.80
1	A	139	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	51	ASP	CB-CA-C	-5.08	109.07	116.53
1	A	162	PRO	N-CD-CG	-5.07	95.59	103.20
1	A	277	PRO	N-CD-CG	-5.04	95.63	103.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASN	Peptide
1	A	150	VAL	Peptide
1	A	267	VAL	Peptide
1	A	318	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	2389	0	2280	131	0
2	A	343	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2732	0	2280	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (131) 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:51:ASP:CG	1:A:52:GLY:H	1.58	1.09
1:A:51:ASP:OD2	1:A:52:GLY:N	1.87	1.08
1:A:75:TYR:HD1	1:A:79:SER:HB3	1.30	0.94
1:A:315:ASN:HB2	1:A:320:THR:HG22	1.50	0.92
1:A:75:TYR:CD1	1:A:79:SER:HB3	2.06	0.89
1:A:315:ASN:CB	1:A:320:THR:HG22	2.03	0.89
1:A:10:LEU:N	1:A:10:LEU:HD23	1.87	0.88
1:A:51:ASP:CG	1:A:52:GLY:N	2.30	0.86
1:A:152:THR:HG22	1:A:313:VAL:HG22	1.59	0.84
1:A:1:SER:HB3	1:A:166:ASN:HD22	1.41	0.84
1:A:297:ILE:HG12	2:A:436:HOH:O	1.80	0.82
1:A:1:SER:HB3	1:A:166:ASN:ND2	1.96	0.79
1:A:224:PRO:HD2	1:A:227:VAL:CG2	2.13	0.78
1:A:269:PRO:HD2	1:A:272:TYR:CD1	2.20	0.76
1:A:224:PRO:HD2	1:A:227:VAL:HG23	1.71	0.73
1:A:176:THR:HG23	2:A:377:HOH:O	1.90	0.72
1:A:71:TRP:HB2	1:A:130:THR:HG22	1.73	0.70
1:A:255:PRO:HG3	2:A:507:HOH:O	1.94	0.67
1:A:314:PHE:CD1	1:A:314:PHE:N	2.62	0.67
1:A:86:THR:HG23	1:A:98:GLY:HA2	1.75	0.67
1:A:86:THR:HG22	2:A:459:HOH:O	1.95	0.66
1:A:171:ASP:OD2	1:A:173:THR:HB	1.95	0.66
1:A:299:ILE:HG12	2:A:516:HOH:O	1.95	0.66
1:A:181:TYR:HD1	1:A:320:THR:HG23	1.61	0.65
1:A:9:SER:C	1:A:10:LEU:HD23	2.22	0.65
1:A:77:ASP:OD1	1:A:79:SER:HB2	1.98	0.64
1:A:130:THR:O	1:A:130:THR:HG23	1.98	0.63
1:A:189:PHE:HB3	1:A:213:ILE:HG22	1.82	0.61
1:A:7:ILE:HG22	1:A:15:ILE:HG12	1.81	0.61
1:A:100:ALA:HB2	1:A:135:GLN:HE21	1.65	0.60
1:A:269:PRO:HD2	1:A:272:TYR:CE1	2.37	0.60
1:A:71:TRP:HB2	1:A:130:THR:CG2	2.31	0.59
1:A:173:THR:HG22	1:A:173:THR:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TYR:HB2	1:A:79:SER:CB	2.31	0.59
1:A:72:SER:H	1:A:130:THR:CG2	2.14	0.59
1:A:51:ASP:OD2	1:A:51:ASP:C	2.45	0.59
1:A:184:VAL:HB	1:A:319(B):PRO:O	2.03	0.58
1:A:71:TRP:CZ3	1:A:73:ILE:HD11	2.39	0.58
1:A:205:THR:O	1:A:205:THR:HG23	2.04	0.57
1:A:51:ASP:HB3	1:A:53:GLN:OE1	2.04	0.57
1:A:36:SER:OG	1:A:128:LEU:HB2	2.04	0.57
1:A:75:TYR:HB2	1:A:79:SER:HB2	1.87	0.56
1:A:129:ASN:HD21	1:A:131:VAL:HB	1.70	0.56
1:A:173:THR:O	1:A:173:THR:CG2	2.53	0.56
1:A:189:PHE:HB3	1:A:213:ILE:CG2	2.35	0.56
1:A:22:THR:O	1:A:61:SER:HA	2.07	0.55
1:A:150:VAL:HG21	1:A:170:ILE:HD12	1.88	0.55
1:A:96:VAL:HG11	1:A:141:ASN:HB3	1.87	0.55
1:A:10:LEU:N	1:A:10:LEU:CD2	2.59	0.55
1:A:181:TYR:CD1	1:A:320:THR:HG23	2.43	0.53
1:A:94:LEU:HD21	1:A:142:ALA:HB1	1.91	0.53
1:A:151:PHE:CE2	1:A:314:PHE:HB2	2.44	0.52
1:A:268:ILE:HG22	1:A:272:TYR:HB2	1.89	0.52
1:A:77:ASP:OD2	1:A:77:ASP:O	2.28	0.52
1:A:126:SER:HB2	1:A:140:ASP:OD1	2.09	0.52
1:A:143:LYS:HE3	1:A:316:GLY:O	2.10	0.52
1:A:315:ASN:HB2	1:A:320:THR:O	2.10	0.52
1:A:72:SER:H	1:A:130:THR:HG23	1.76	0.51
1:A:266:ILE:HG21	1:A:310:ALA:HB2	1.91	0.51
1:A:45:THR:CG2	1:A:50:VAL:HG23	2.41	0.51
1:A:77:ASP:OD2	1:A:77:ASP:C	2.53	0.51
1:A:325:SER:HB2	2:A:443:HOH:O	2.11	0.50
1:A:96:VAL:CG1	1:A:141:ASN:HB3	2.40	0.50
1:A:273:ILE:O	1:A:273:ILE:HG22	2.10	0.50
1:A:39:TRP:CD1	1:A:73:ILE:HD11	2.47	0.49
1:A:171:ASP:C	1:A:173:THR:H	2.19	0.49
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.63	0.49
1:A:164:THR:HG21	1:A:166:ASN:HD21	1.77	0.49
1:A:50:VAL:HG21	1:A:55:ILE:HD11	1.95	0.48
1:A:71:TRP:HZ3	1:A:73:ILE:HD11	1.78	0.48
1:A:170:ILE:HG22	1:A:170:ILE:O	2.13	0.48
1:A:132:SER:CB	1:A:133:PRO:HA	2.40	0.48
1:A:314:PHE:N	1:A:314:PHE:HD1	2.08	0.48
1:A:113:GLU:HB2	2:A:635:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LYS:HA	1:A:146:LEU:HD12	1.96	0.47
1:A:150:VAL:HG21	1:A:170:ILE:CD1	2.44	0.47
1:A:220:LEU:HD22	1:A:286:GLY:HA2	1.97	0.47
1:A:277:PRO:HA	1:A:283:CYS:HA	1.95	0.47
1:A:38:LEU:C	1:A:38:LEU:HD23	2.39	0.47
1:A:172:THR:HA	1:A:175:TYR:CE1	2.49	0.47
1:A:32:ASP:OD1	1:A:217:GLY:HA3	2.15	0.47
1:A:72:SER:H	1:A:130:THR:HG21	1.80	0.47
1:A:314:PHE:HD1	1:A:314:PHE:H	1.62	0.46
1:A:129:ASN:ND2	1:A:131:VAL:H	2.13	0.46
1:A:10:LEU:HB2	1:A:12:ASP:OD2	2.16	0.46
1:A:81:SER:HB2	2:A:367:HOH:O	2.16	0.46
1:A:22:THR:HA	1:A:23:PRO:HA	1.50	0.45
1:A:97:THR:HG21	2:A:616:HOH:O	2.16	0.45
1:A:220:LEU:HD11	1:A:284:PHE:HE2	1.82	0.45
1:A:45:THR:HG22	1:A:50:VAL:HG23	1.98	0.45
1:A:154:ASP:O	1:A:154:ASP:OD2	2.35	0.44
1:A:249:PRO:HD2	1:A:252:ALA:HB2	2.00	0.44
1:A:194:SER:O	1:A:206:SER:HA	2.18	0.44
1:A:189:PHE:CG	1:A:213:ILE:HG21	2.52	0.44
1:A:220:LEU:HB2	1:A:222:TYR:CE2	2.52	0.44
1:A:71:TRP:CZ3	1:A:73:ILE:CG1	3.01	0.44
1:A:7:ILE:HG13	1:A:8:ASP:OD2	2.17	0.44
1:A:154:ASP:OD2	1:A:154:ASP:C	2.61	0.44
1:A:220:LEU:HA	1:A:305:VAL:HG23	2.00	0.43
1:A:248:PHE:CZ	1:A:254:LEU:HD21	2.53	0.43
1:A:22:THR:HA	1:A:23:PRO:C	2.35	0.43
1:A:48:SER:O	1:A:48:SER:OG	2.31	0.43
1:A:181:TYR:CD1	1:A:320:THR:CG2	3.01	0.43
1:A:37:ASP:OD1	1:A:129:ASN:HA	2.18	0.43
1:A:30:ASP:HB3	1:A:120:LEU:HG	1.99	0.43
1:A:71:TRP:HZ3	1:A:73:ILE:CD1	2.32	0.43
1:A:96:VAL:HG11	1:A:141:ASN:CB	2.47	0.43
1:A:164:THR:CG2	1:A:166:ASN:HD21	2.32	0.43
1:A:294:SER:HB3	1:A:300:ASN:HD22	1.84	0.43
1:A:113:GLU:HB2	2:A:634:HOH:O	2.18	0.43
1:A:154:ASP:O	1:A:154:ASP:CG	2.62	0.43
1:A:269:PRO:HD2	1:A:272:TYR:CG	2.54	0.43
1:A:272:TYR:CD1	1:A:272:TYR:N	2.88	0.42
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.70	0.42
1:A:294:SER:CB	1:A:300:ASN:HD22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:HG3	2:A:634:HOH:O	2.20	0.41
1:A:16:THR:HB	1:A:31:PHE:CE2	2.55	0.41
1:A:166:ASN:HB3	1:A:169:PHE:CE2	2.56	0.41
1:A:192:TRP:CH2	1:A:194:SER:HB2	2.55	0.41
1:A:307:LEU:HD22	1:A:312:VAL:HG21	2.03	0.41
1:A:61:SER:HB3	1:A:63(A):ALA:HB2	2.02	0.41
1:A:-2:SER:HB3	2:A:582:HOH:O	2.20	0.41
1:A:71:TRP:HZ3	1:A:73:ILE:CG1	2.32	0.41
1:A:72:SER:N	1:A:130:THR:HG21	2.35	0.41
1:A:192:TRP:CZ3	1:A:194:SER:HA	2.56	0.41
1:A:320:THR:O	1:A:320:THR:CG2	2.67	0.41
1:A:71:TRP:CZ3	1:A:73:ILE:HG13	2.56	0.40
1:A:175:TYR:CZ	1:A:179:ILE:HD11	2.56	0.40
1:A:203(A):PHE:CB	1:A:265:ARG:NH2	2.85	0.40
1:A:270:GLY:HA2	1:A:273:ILE:HD12	2.03	0.40
1:A:71:TRP:HZ3	1:A:73:ILE:HG13	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	328/330 (99%)	311 (95%)	15 (5%)	2 (1%)	21 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ALA
1	A	319	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	263/263 (100%)	216 (82%)	47 (18%)	2 1

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	10	LEU
1	A	48	SER
1	A	55	ILE
1	A	63	THR
1	A	64	LYS
1	A	65	LEU
1	A	70	THR
1	A	73	ILE
1	A	74	SER
1	A	77	ASP
1	A	79	SER
1	A	80	SER
1	A	80(A)	SER
1	A	86	THR
1	A	90	SER
1	A	103	SER
1	A	105	LYS
1	A	106	LYS
1	A	108	SER
1	A	114	ASP
1	A	120	LEU
1	A	129	ASN
1	A	130	THR
1	A	131	VAL
1	A	132	SER
1	A	143	LYS
1	A	145	SER
1	A	149	PRO
1	A	170	ILE

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Mol	Chain	Res	Type
1	A	178	SER
1	A	203	THR
1	A	203(A)	PHE
1	A	223	LEU
1	A	240	SER
1	A	241	SER
1	A	242	SER
1	A	254	LEU
1	A	266	ILE
1	A	268	ILE
1	A	294	SER
1	A	297	ILE
1	A	299	ILE
1	A	314	PHE
1	A	315	ASN
1	A	318	THR
1	A	320	THR

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	19	GLN
1	A	99	GLN
1	A	129	ASN
1	A	134(A)	GLN
1	A	135	GLN
1	A	141	ASN
1	A	166	ASN
1	A	300	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 [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 [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	330/330 (100%)	0.50	19 (5%)	29 30	0, 0, 1, 1	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	THR	5.8
1	A	74	SER	3.5
1	A	-2	SER	3.4
1	A	255	PRO	3.3
1	A	48	SER	3.1
1	A	241	SER	3.1
1	A	297	ILE	2.9
1	A	265	ARG	2.8
1	A	113	GLU	2.7
1	A	77	ASP	2.6
1	A	253	THR	2.6
1	A	319	THR	2.5
1	A	79	SER	2.5
1	A	126	SER	2.4
1	A	311	PHE	2.4
1	A	80	SER	2.4
1	A	242	SER	2.3
1	A	112	THR	2.1
1	A	319(B)	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.