



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 PM GMT

PDB ID : 5PEP
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

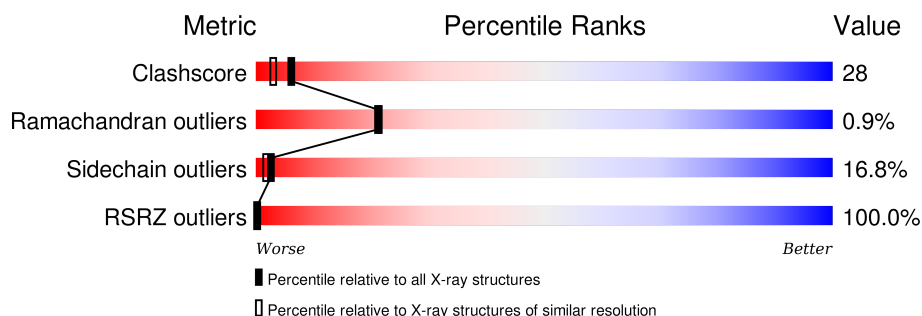
1 Overall quality at a glance

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	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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
1	A	326	Total	C	N	O	S	0	0	0
			2426	1529	366	521	10			

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

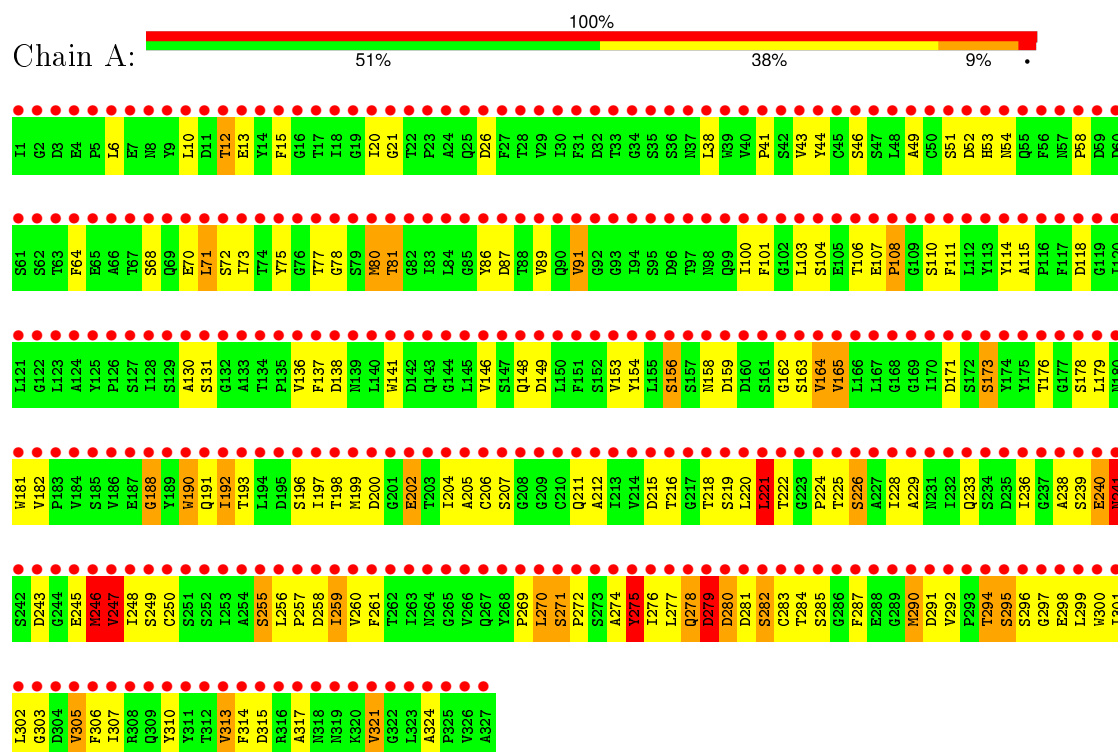
- Molecule 2 is water.

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	67.40 Å 67.40 Å 290.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.34 9.99 – 2.34	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.34) 77.1 (9.99-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.33 Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.196 , (Not available) 0.257 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	135.34 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 13330 reflections	Xtriage
F_o, F_c correlation	0.28	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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.12	5/2481 (0.2%)	1.45	32/3396 (0.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ASP	C-O	5.86	1.34	1.23
1	A	188	GLY	N-CA	5.71	1.54	1.46
1	A	241	ASN	CG-OD1	5.30	1.35	1.24
1	A	211	GLN	CD-OE1	5.28	1.35	1.24
1	A	190	TRP	NE1-CE2	-5.08	1.30	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	VAL	CA-CB-CG2	9.21	124.72	110.90
1	A	313	VAL	CA-CB-CG2	9.07	124.51	110.90
1	A	153	VAL	CA-CB-CG2	8.56	123.73	110.90
1	A	164	VAL	CA-CB-CG2	8.46	123.58	110.90
1	A	279	ASP	CA-C-N	8.38	135.63	117.20
1	A	165	VAL	CA-CB-CG2	7.63	122.35	110.90
1	A	246	MET	CG-SD-CE	7.35	111.96	100.20
1	A	247	VAL	CA-CB-CG2	6.94	121.31	110.90
1	A	321	VAL	CA-CB-CG2	6.84	121.16	110.90
1	A	221	LEU	C-N-CA	6.71	138.48	121.70
1	A	290	MET	CG-SD-CE	6.71	110.94	100.20
1	A	282	SER	C-N-CA	6.56	138.10	121.70
1	A	182	VAL	CA-CB-CG2	6.47	120.61	110.90
1	A	146	VAL	CA-CB-CG2	6.43	120.54	110.90
1	A	44	TYR	CA-CB-CG	6.20	125.19	113.40
1	A	305	VAL	CA-CB-CG2	6.10	120.05	110.90
1	A	282	SER	N-CA-CB	6.04	119.56	110.50
1	A	275	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	A	302	LEU	C-N-CA	5.91	134.70	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLY	O-C-N	5.64	131.73	122.70
1	A	44	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	A	188	GLY	N-CA-C	-5.51	99.33	113.10
1	A	15	PHE	CB-CG-CD1	5.43	124.60	120.80
1	A	279	ASP	CA-C-O	-5.43	108.69	120.10
1	A	255	SER	C-N-CA	5.37	135.13	121.70
1	A	114	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	A	198	THR	CA-C-O	5.22	131.06	120.10
1	A	26	ASP	O-C-N	5.18	130.99	122.70
1	A	218	THR	C-N-CA	5.15	134.58	121.70
1	A	80	MET	CG-SD-CE	5.12	108.39	100.20
1	A	51	SER	C-N-CA	5.12	134.50	121.70
1	A	44	TYR	CB-CG-CD1	5.00	124.00	121.00

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	2253	132	0
2	A	371	0	0	6	2
All	All	2797	0	2253	132	2

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 (132) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:71:LEU:CD1	1:A:73:ILE:HD11	2.15	0.75
1:A:238:ALA:CB	1:A:246:MET:HE2	2.18	0.74
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
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:238:ALA:HB3	1:A:246:MET:HE2	1.75	0.68
1:A:280:ASP:HB3	2:A:608:HOH:O	1.93	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:284:THR:HG22	1:A:285:SER:N	2.14	0.63
1:A:52:ASP:HB3	1:A:53:HIS:CD2	2.34	0.63
1:A:80:MET:HG2	1:A:81:THR:N	2.14	0.62
1:A:279:ASP:C	1:A:281:ASP:H	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:O	1:A:278:GLN:HG2	2.03	0.58
1:A:101:PHE:CZ	1:A:103:LEU:HD11	2.39	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:72:SER:C	1:A:73:ILE:HG13	2.25	0.55
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:238:ALA:HB1	1:A:246:MET:HE2	1.87	0.54
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:130:ALA:O	1:A:131:SER:HB2	2.08	0.53
1:A:239:SER:N	1:A:246:MET:HE3	2.23	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: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
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:290:MET:HG2	1:A:292:VAL:HG23	1.91	0.51
1:A:275:TYR:CD2	1:A:276:ILE:HG13	2.46	0.51
1:A:236:ILE:HB	1:A:256:LEU:HD21	1.93	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:89:VAL:HG12	1:A:91:VAL:CG2	2.42	0.50
1:A:100:ILE:HG23	1:A:100:ILE:O	2.11	0.50
1:A:259:ILE:HG12	1:A:261:PHE:HE2	1.76	0.50
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:238:ALA:C	1:A:246:MET:HE3	2.35	0.47
1:A:259:ILE:CG2	1:A:275:TYR:CD1	2.97	0.47
1:A:259:ILE:HG22	1:A:275:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:SER:O	1:A:229:ALA:HB3	2.15	0.46
1:A:10:LEU:C	1:A:12:THR:N	2.68	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:279:ASP:C	1:A:281:ASP:N	2.68	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:259:ILE:HG12	1:A:261:PHE:CE2	2.52	0.44
1:A:202:GLU:CG	1:A:202:GLU:O	2.63	0.44
1:A:43:VAL:HG12	1:A:43:VAL:O	2.17	0.44
1:A:38:LEU:HD23	1:A:101:PHE:HB3	1.98	0.44
1:A:202:GLU:HG2	1:A:202:GLU:O	2.17	0.44
1:A:141:TRP:CH2	1:A:149:ASP:HB2	2.53	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:281:ASP:O	1:A:282:SER:CB	2.65	0.43
1:A:190:TRP:CZ2	1:A:314:PHE:HB3	2.54	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:106:THR:C	1:A:108:PRO:HD3	2.39	0.42
1:A:241:ASN:C	1:A:241:ASN:HD22	2.22	0.42
1:A:171:ASP:C	1:A:173:SER:H	2.22	0.42
1:A:224:PRO:HB3	1:A:298:GLU:OE2	2.20	0.41
1:A:256:LEU:HA	1:A:256:LEU:HD12	1.78	0.41
1:A:190:TRP:CD2	1:A:314:PHE:HD2	2.37	0.41
1:A:225:THR:HB	1:A:291:ASP:OD2	2.20	0.41
1:A:284:THR:CG2	1:A:285:SER:N	2.83	0.41
1:A:269:PRO:HD2	1:A:310:TYR:OH	2.20	0.41
1:A:58:PRO:HB3	1:A:64:PHE:CD1	2.55	0.41
1:A:154:TYR:CD2	1:A:162:GLY:O	2.71	0.41
1:A:179:LEU:HD23	1:A:324:ALA:HB2	2.01	0.41
1:A:41:PRO:HD3	1:A:118:ASP:O	2.20	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:238:ALA:C	1:A:246:MET:CE	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ALA:HB1	1:A:246:MET:CE	2.50	0.41
1:A:277:LEU:N	1:A:277:LEU:HD12	2.36	0.41
1:A:221:LEU:HD11	1:A:306:PHE:CB	2.39	0.40
1:A:215:ASP:O	1:A:303:GLY:HA2	2.20	0.40

All (2) 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:488:HOH:O	2:A:488:HOH:O[11_555]	0.50	1.70
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%)	21 21

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%)	228 (83%)	46 (17%)	2 2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	13	GLU
1	A	46	SER
1	A	68	SER
1	A	70	GLU
1	A	71	LEU
1	A	77	THR
1	A	81	THR
1	A	91	VAL
1	A	104	SER
1	A	108	PRO
1	A	110	SER
1	A	138	ASP
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	202	GLU
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	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

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Mol	Chain	Res	Type
1	A	255	SER
1	A	259	ILE
1	A	270	LEU
1	A	271	SER
1	A	275	TYR
1	A	278	GLN
1	A	279	ASP
1	A	294	THR
1	A	295	SER
1	A	299	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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

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 carbohydrates 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%)	11.89	326 (100%) 0 0	0, 0, 1, 1	0

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	ALA	32.1
1	A	77	THR	28.4
1	A	125	TYR	26.5
1	A	232	ILE	24.8
1	A	103	LEU	24.6
1	A	203	THR	24.3
1	A	134	THR	24.3
1	A	255	SER	23.6
1	A	44	TYR	23.0
1	A	66	ALA	22.8
1	A	307	ILE	22.6
1	A	237	GLY	22.4
1	A	285	SER	22.3
1	A	123	LEU	22.3
1	A	74	THR	21.9
1	A	267	GLN	21.9
1	A	9	TYR	21.6
1	A	240	GLU	21.4
1	A	95	SER	21.3
1	A	261	PHE	20.9
1	A	172	SER	20.9
1	A	107	GLU	20.5
1	A	281	ASP	20.3
1	A	78	GLY	20.2
1	A	168	GLY	19.6
1	A	114	TYR	19.6
1	A	300	TRP	19.6

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Mol	Chain	Res	Type	RSRZ
1	A	141	TRP	19.3
1	A	128	ILE	19.1
1	A	181	TRP	19.0
1	A	165	VAL	18.5
1	A	196	SER	18.4
1	A	14	TYR	18.4
1	A	75	TYR	18.1
1	A	234	SER	18.1
1	A	158	ASN	17.8
1	A	86	TYR	17.6
1	A	98	ASN	17.6
1	A	64	PHE	17.6
1	A	274	ALA	17.5
1	A	6	LEU	17.3
1	A	135	PRO	17.2
1	A	253	ILE	17.2
1	A	257	PRO	17.2
1	A	110	SER	17.1
1	A	38	LEU	17.0
1	A	112	LEU	16.9
1	A	233	GLN	16.8
1	A	116	PRO	16.8
1	A	28	THR	16.7
1	A	199	MET	16.7
1	A	302	LEU	16.6
1	A	214	VAL	16.5
1	A	122	GLY	16.4
1	A	102	GLY	16.3
1	A	166	LEU	16.3
1	A	189	TYR	16.2
1	A	252	SER	16.1
1	A	305	VAL	16.1
1	A	48	LEU	16.0
1	A	40	VAL	16.0
1	A	310	TYR	15.9
1	A	169	GLY	15.7
1	A	33	THR	15.7
1	A	96	ASP	15.6
1	A	109	GLY	15.6
1	A	142	ASP	15.5
1	A	249	SER	15.5
1	A	224	PRO	15.4

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Mol	Chain	Res	Type	RSRZ
1	A	54	ASN	15.3
1	A	270	LEU	15.3
1	A	225	THR	15.2
1	A	32	ASP	15.1
1	A	76	GLY	15.0
1	A	198	THR	15.0
1	A	190	TRP	14.8
1	A	262	THR	14.8
1	A	210	CYS	14.8
1	A	195	ASP	14.7
1	A	143	GLN	14.7
1	A	221	LEU	14.7
1	A	235	ASP	14.7
1	A	133	ALA	14.7
1	A	213	ILE	14.6
1	A	309	GLN	14.5
1	A	73	ILE	14.5
1	A	218	THR	14.5
1	A	104	SER	14.5
1	A	284	THR	14.5
1	A	170	ILE	14.4
1	A	62	SER	14.3
1	A	238	ALA	14.2
1	A	43	VAL	14.1
1	A	150	LEU	14.1
1	A	268	TYR	14.0
1	A	206	CYS	13.9
1	A	177	GLY	13.8
1	A	1	ILE	13.8
1	A	299	LEU	13.8
1	A	153	VAL	13.8
1	A	137	PHE	13.7
1	A	220	LEU	13.7
1	A	247	VAL	13.7
1	A	70	GLU	13.7
1	A	157	SER	13.6
1	A	289	GLY	13.6
1	A	127	SER	13.4
1	A	108	PRO	13.4
1	A	301	ILE	13.4
1	A	207	SER	13.4
1	A	22	THR	13.4

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Mol	Chain	Res	Type	RSRZ
1	A	18	ILE	13.3
1	A	12	THR	13.2
1	A	258	ASP	13.2
1	A	226	SER	13.1
1	A	279	ASP	13.1
1	A	272	PRO	12.8
1	A	31	PHE	12.7
1	A	265	GLY	12.7
1	A	151	PHE	12.5
1	A	15	PHE	12.4
1	A	256	LEU	12.4
1	A	100	ILE	12.3
1	A	290	MET	12.2
1	A	236	ILE	12.1
1	A	259	ILE	12.1
1	A	266	VAL	12.1
1	A	132	GLY	12.0
1	A	192	ILE	12.0
1	A	178	SER	11.9
1	A	179	LEU	11.9
1	A	106	THR	11.9
1	A	19	GLY	11.9
1	A	24	ALA	11.9
1	A	325	PRO	11.8
1	A	94	ILE	11.8
1	A	81	THR	11.7
1	A	269	PRO	11.6
1	A	3	ASP	11.6
1	A	47	SER	11.6
1	A	45	CYS	11.6
1	A	17	THR	11.6
1	A	29	VAL	11.6
1	A	215	ASP	11.6
1	A	144	GLY	11.6
1	A	295	SER	11.5
1	A	193	THR	11.5
1	A	296	SER	11.5
1	A	164	VAL	11.5
1	A	58	PRO	11.4
1	A	145	LEU	11.4
1	A	306	PHE	11.4
1	A	208	GLY	11.4

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Mol	Chain	Res	Type	RSRZ
1	A	46	SER	11.3
1	A	250	CYS	11.3
1	A	30	ILE	11.2
1	A	314	PHE	11.2
1	A	275	TYR	11.2
1	A	183	PRO	11.0
1	A	294	THR	11.0
1	A	68	SER	10.8
1	A	173	SER	10.7
1	A	287	PHE	10.7
1	A	148	GLN	10.7
1	A	111	PHE	10.6
1	A	323	LEU	10.6
1	A	51	SER	10.5
1	A	180	ASN	10.5
1	A	271	SER	10.5
1	A	174	TYR	10.4
1	A	231	ASN	10.4
1	A	10	LEU	10.3
1	A	194	LEU	10.3
1	A	155	LEU	10.3
1	A	315	ASP	10.3
1	A	312	THR	10.3
1	A	23	PRO	10.3
1	A	197	ILE	10.3
1	A	88	THR	10.2
1	A	39	TRP	10.2
1	A	318	ASN	10.2
1	A	200	ASP	10.2
1	A	326	VAL	10.2
1	A	117	PHE	10.1
1	A	260	VAL	10.1
1	A	219	SER	10.1
1	A	313	VAL	10.1
1	A	243	ASP	10.1
1	A	311	TYR	10.1
1	A	280	ASP	10.0
1	A	50	CYS	10.0
1	A	292	VAL	10.0
1	A	56	PHE	9.9
1	A	5	PRO	9.9
1	A	79	SER	9.9

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Mol	Chain	Res	Type	RSRZ
1	A	163	SER	9.9
1	A	242	SER	9.9
1	A	16	GLY	9.9
1	A	84	LEU	9.9
1	A	37	ASN	9.8
1	A	282	SER	9.8
1	A	222	THR	9.8
1	A	115	ALA	9.7
1	A	49	ALA	9.7
1	A	60	ASP	9.7
1	A	324	ALA	9.6
1	A	187	GLU	9.6
1	A	212	ALA	9.6
1	A	322	GLY	9.6
1	A	90	GLN	9.6
1	A	239	SER	9.6
1	A	147	SER	9.5
1	A	246	MET	9.5
1	A	277	LEU	9.5
1	A	184	VAL	9.5
1	A	276	ILE	9.4
1	A	303	GLY	9.4
1	A	251	SER	9.4
1	A	149	ASP	9.4
1	A	167	LEU	9.4
1	A	216	THR	9.3
1	A	69	GLN	9.2
1	A	61	SER	9.2
1	A	42	SER	9.1
1	A	113	TYR	9.1
1	A	154	TYR	9.1
1	A	101	PHE	9.0
1	A	209	GLY	9.0
1	A	59	ASP	8.9
1	A	83	ILE	8.9
1	A	136	VAL	8.8
1	A	211	GLN	8.8
1	A	283	CYS	8.8
1	A	175	TYR	8.7
1	A	35	SER	8.7
1	A	161	SER	8.7
1	A	298	GLU	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	152	SER	8.7
1	A	126	PRO	8.6
1	A	131	SER	8.6
1	A	67	THR	8.5
1	A	278	GLN	8.5
1	A	89	VAL	8.5
1	A	241	ASN	8.5
1	A	120	ILE	8.4
1	A	185	SER	8.4
1	A	171	ASP	8.4
1	A	202	GLU	8.3
1	A	97	THR	8.3
1	A	55	GLN	8.3
1	A	160	ASP	8.3
1	A	53	HIS	8.3
1	A	186	VAL	8.3
1	A	25	GLN	8.2
1	A	320	LYS	8.2
1	A	321	VAL	8.1
1	A	80	MET	8.1
1	A	273	SER	8.1
1	A	248	ILE	8.0
1	A	121	LEU	8.0
1	A	291	ASP	7.9
1	A	205	ALA	7.9
1	A	11	ASP	7.9
1	A	93	GLY	7.9
1	A	118	ASP	7.8
1	A	4	GLU	7.8
1	A	129	SER	7.8
1	A	191	GLN	7.7
1	A	27	PHE	7.7
1	A	105	GLU	7.7
1	A	245	GLU	7.7
1	A	182	VAL	7.7
1	A	36	SER	7.7
1	A	130	ALA	7.7
1	A	34	GLY	7.7
1	A	41	PRO	7.6
1	A	7	GLU	7.5
1	A	176	THR	7.5
1	A	26	ASP	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLU	7.5
1	A	2	GLY	7.4
1	A	316	ARG	7.4
1	A	304	ASP	7.3
1	A	52	ASP	7.2
1	A	201	GLY	7.2
1	A	223	GLY	7.0
1	A	99	GLN	7.0
1	A	293	PRO	7.0
1	A	57	ASN	7.0
1	A	71	LEU	6.9
1	A	87	ASP	6.9
1	A	264	ASN	6.9
1	A	159	ASP	6.8
1	A	188	GLY	6.8
1	A	228	ILE	6.7
1	A	254	ALA	6.7
1	A	244	GLY	6.6
1	A	297	GLY	6.6
1	A	21	GLY	6.5
1	A	288	GLU	6.4
1	A	20	ILE	6.3
1	A	263	ILE	6.3
1	A	156	SER	6.3
1	A	204	ILE	6.2
1	A	139	ASN	6.1
1	A	286	GLY	6.1
1	A	317	ALA	6.1
1	A	91	VAL	5.8
1	A	13	GLU	5.8
1	A	140	LEU	5.7
1	A	217	GLY	5.7
1	A	319	ASN	5.7
1	A	124	ALA	5.6
1	A	308	ARG	5.4
1	A	162	GLY	5.3
1	A	227	ALA	5.2
1	A	229	ALA	4.9
1	A	8	ASN	4.7
1	A	146	VAL	4.2
1	A	72	SER	4.2
1	A	138	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	63	THR	3.7
1	A	92	GLY	3.3
1	A	119	GLY	3.2
1	A	85	GLY	2.8
1	A	82	GLY	2.7

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 carbohydrates 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.