



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:14 PM EST

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

<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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

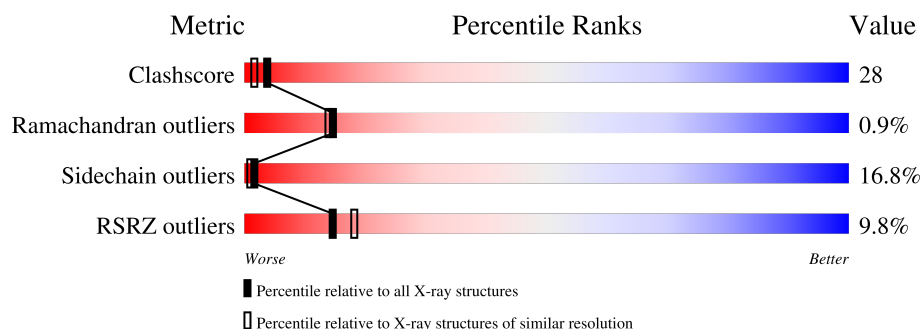
1 Overall quality at a glance

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	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	326	<div> <div>10%</div> <div>51%</div> <div>38%</div> <div>9%</div> </div>

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

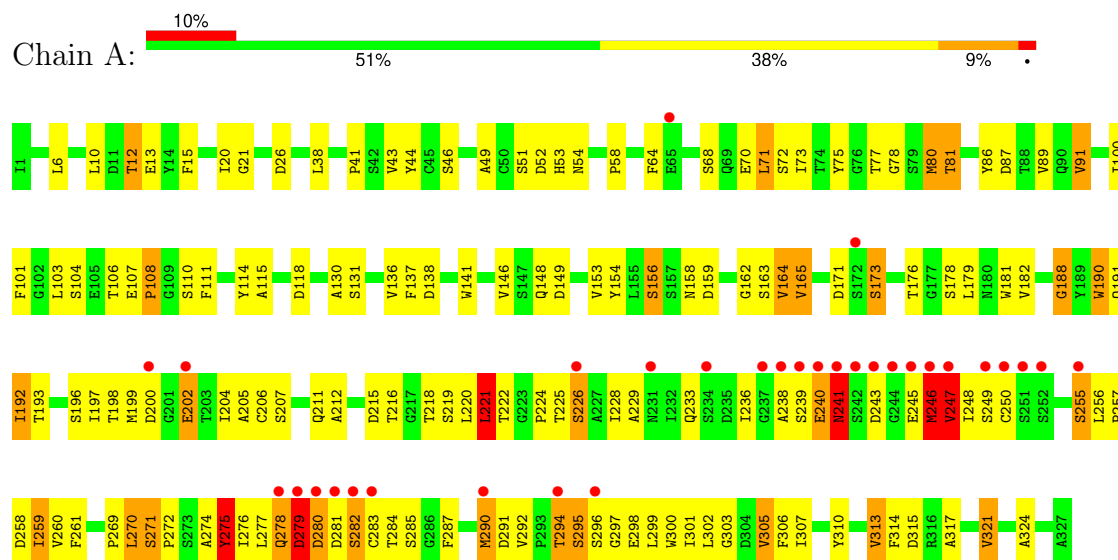
- Molecule 2 is water.

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

3 Residue-property plots [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. 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. 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	1.12	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 [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	2426	0	2253	132	0
2	A	371	0	0	6	1
All	All	2797	0	2253	132	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 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: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: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: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: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: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: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:O	1:A:100:ILE:HG23	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:HG22	1:A:275:TYR:CE1	2.50	0.47
1:A:259:ILE:CG2	1:A:275:TYR:CD1	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:C	1:A:12:THR:N	2.68	0.46
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: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:O	1:A:202:GLU:CG	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: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: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:106:THR:C	1:A:108:PRO:HD3	2.39	0.42
1:A:192:ILE:CG2	1:A:193:THR:N	2.82	0.42
1:A:241:ASN:HD22	1:A:241:ASN:C	2.22	0.42
1:A:171:ASP:C	1:A:173:SER:H	2.22	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: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: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:215:ASP:O	1:A:303:GLY:HA2	2.20	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 14

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%)	1 1

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
1	A	255	SER
1	A	259	ILE

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Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
1	A	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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

Warning: The R factor obtained from EDS is 0.2711, which does not match the depositor's R factor of 0.196. Please interpret the results in this section carefully.

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%)	0.58	32 (9%) 14 18	0, 0, 1, 1	0

All (32) 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	4.0
1	A	245	GLU	3.9
1	A	244	GLY	3.8
1	A	280	ASP	3.7
1	A	294	THR	3.5
1	A	252	SER	3.3
1	A	283	CYS	3.3
1	A	251	SER	3.3
1	A	237	GLY	3.2
1	A	234	SER	3.0
1	A	247	VAL	3.0
1	A	239	SER	2.9
1	A	200	ASP	2.9
1	A	246	MET	2.9
1	A	202	GLU	2.8
1	A	226	SER	2.8
1	A	250	CYS	2.8
1	A	231	ASN	2.8
1	A	255	SER	2.8
1	A	172	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLN	2.3
1	A	241	ASN	2.1
1	A	238	ALA	2.1
1	A	290	MET	2.1
1	A	65	GLU	2.0
1	A	249	SER	2.0
1	A	282	SER	2.0
1	A	296	SER	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 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.