



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 02:32 AM EST

PDB ID : 4APE
Title : THE ACTIVE SITE OF ASPARTIC PROTEINASES
Authors : Pearl, L.H.; Sewell, B.T.; Jenkins, J.A.; Cooper, J.B.; Blundell, T.L.
Deposited on : unknown
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

<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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

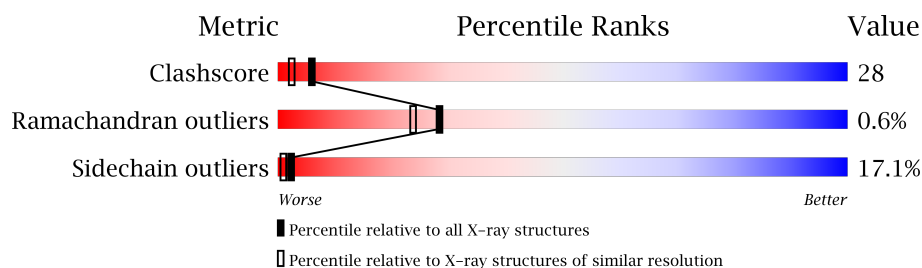
1 Overall quality at a glance

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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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 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.

Note EDS was not executed.

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.

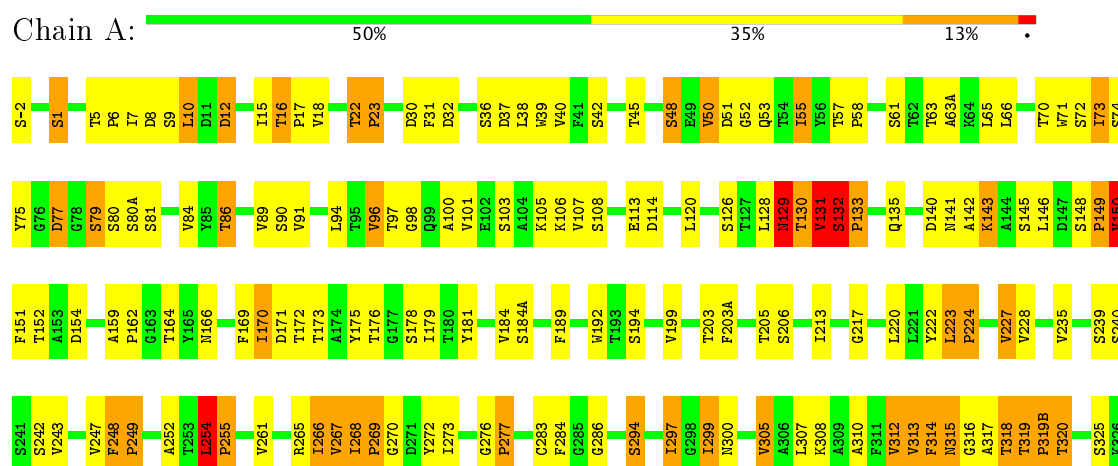
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	343	Total	O	0	0
			343	343		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

• Molecule 1: ENDOTHIAPEPSIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.60 Å 74.05 Å 45.70 Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2732	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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	0.95	18/2445 (0.7%)	1.21	41/3345 (1.2%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	PRO	N-CD	8.73	1.60	1.47
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	249	PRO	N-CD	6.65	1.57	1.47
1	A	277	PRO	N-CD	6.62	1.57	1.47
1	A	17	PRO	N-CD	6.60	1.57	1.47
1	A	58	PRO	N-CD	6.54	1.57	1.47
1	A	269	PRO	N-CD	6.53	1.56	1.47
1	A	224	PRO	N-CD	6.52	1.56	1.47
1	A	319(B)	PRO	N-CD	6.45	1.56	1.47
1	A	255	PRO	N-CD	6.43	1.56	1.47
1	A	6	PRO	N-CD	6.13	1.56	1.47
1	A	149	PRO	N-CD	5.87	1.56	1.47
1	A	159	ALA	C-N	5.71	1.45	1.34
1	A	319	THR	C-N	5.30	1.44	1.34
1	A	16	THR	C-N	5.26	1.44	1.34
1	A	5	THR	C-N	5.05	1.43	1.34
1	A	22	THR	C-N	5.01	1.43	1.34

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	THR	C-N-CD	10.79	151.07	128.40
1	A	254	LEU	C-N-CD	10.79	151.06	128.40
1	A	276	GLY	C-N-CD	10.75	150.97	128.40
1	A	268	ILE	C-N-CD	10.73	150.93	128.40
1	A	132	SER	C-N-CD	10.69	150.84	128.40
1	A	148	SER	C-N-CD	10.43	150.30	128.40
1	A	223	LEU	C-N-CD	10.41	150.26	128.40
1	A	248	PHE	C-N-CD	10.22	149.86	128.40
1	A	5	THR	C-N-CD	9.78	148.93	128.40
1	A	319	THR	C-N-CD	9.07	147.46	128.40
1	A	16	THR	C-N-CD	8.80	146.88	128.40
1	A	22	THR	C-N-CD	8.27	145.76	128.40
1	A	107	VAL	CA-CB-CG2	6.67	120.91	110.90
1	A	305	VAL	CA-CB-CG2	6.26	120.29	110.90
1	A	131	VAL	CA-CB-CG2	6.18	120.18	110.90
1	A	235	VAL	CA-CB-CG2	6.17	120.15	110.90
1	A	261	VAL	CA-CB-CG1	6.17	120.15	110.90
1	A	150	VAL	CA-CB-CG1	6.12	120.08	110.90
1	A	267	VAL	CA-CB-CG2	6.09	120.04	110.90
1	A	199	VAL	CA-CB-CG2	6.05	119.98	110.90
1	A	50	VAL	CA-CB-CG2	6.04	119.96	110.90
1	A	89	VAL	CA-CB-CG2	6.04	119.96	110.90
1	A	18	VAL	CA-CB-CG2	6.04	119.95	110.90
1	A	91	VAL	CA-CB-CG2	6.03	119.94	110.90
1	A	84	VAL	CA-CB-CG2	6.00	119.90	110.90
1	A	312	VAL	CA-CB-CG2	6.00	119.90	110.90
1	A	228	VAL	CA-CB-CG2	5.99	119.89	110.90
1	A	243	VAL	CA-CB-CG2	5.99	119.88	110.90
1	A	313	VAL	CA-CB-CG2	5.98	119.86	110.90
1	A	101	VAL	CA-CB-CG2	5.97	119.86	110.90
1	A	133	PRO	CA-N-CD	-5.93	103.19	111.50
1	A	96	VAL	CA-CB-CG2	5.90	119.75	110.90
1	A	40	VAL	CA-CB-CG2	5.90	119.75	110.90
1	A	227	VAL	CA-CB-CG2	5.84	119.66	110.90
1	A	247	VAL	CA-CB-CG2	5.72	119.48	110.90
1	A	159	ALA	C-N-CD	5.67	140.30	128.40
1	A	133	PRO	N-CD-CG	-5.65	94.72	103.20
1	A	42	SER	C-N-CA	5.34	135.05	121.70
1	A	58	PRO	N-CD-CG	-5.17	95.44	103.20
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	129	0
2	A	343	0	0	12	0
All	All	2732	0	2280	129	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 (129) 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:OD2	1:A:52:GLY:N	1.87	1.08
1:A:51:ASP:CG	1:A:52:GLY:H	1.58	1.05
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: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:51:ASP:CG	1:A:52:GLY:N	2.30	0.74
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:314:PHE:CD1	2.62	0.67
1:A:86:THR:HG23	1:A:98:GLY:HA2	1.75	0.67
1:A:171:ASP:OD2	1:A:173:THR:HB	1.95	0.66
1:A:86:THR:HG22	2:A:459:HOH:O	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:77:ASP:OD1	1:A:79:SER:HB2	1.98	0.64
1:A:130:THR:HG23	1:A:130:THR:O	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:9:SER:C	1:A:10:LEU:HD23	2.22	0.60
1:A:269:PRO:HD2	1:A:272:TYR:CE1	2.37	0.60
1:A:173:THR:O	1:A:173:THR:HG22	2.00	0.59
1:A:71:TRP:HB2	1:A:130:THR:CG2	2.31	0.59
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: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:126:SER:HB2	1:A:140:ASP:OD1	2.09	0.52
1:A:77:ASP:O	1:A:77:ASP:OD2	2.28	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:266:ILE:HG21	1:A:310:ALA:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:H	1:A:130:THR:HG23	1.76	0.51
1:A:45:THR:CG2	1:A:50:VAL:HG23	2.41	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: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:51:ASP:C	1:A:51:ASP:OD2	2.45	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
1:A:71:TRP:HH2	1:A:80(A):SER:HG	1.60	0.47
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: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:H	1:A:314:PHE:HD1	1.62	0.46
1:A:77:ASP:C	1:A:77:ASP:OD2	2.53	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:171:ASP:C	1:A:173:THR:H	2.19	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:248:PHE:CZ	1:A:254:LEU:HD21	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HA	1:A:305:VAL:HG23	2.00	0.43
1:A:181:TYR:CD1	1:A:320:THR:CG2	3.01	0.43
1:A:48:SER:O	1:A:48:SER:OG	2.31	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:269:PRO:HD2	1:A:272:TYR:CG	2.54	0.43
1:A:38:LEU:C	1:A:38:LEU:HD23	2.39	0.42
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
1:A:113:GLU:HG3	2:A:634:HOH:O	2.20	0.41
1:A:166:ASN:HB3	1:A:169:PHE:CE2	2.56	0.41
1:A:16:THR:HB	1:A:31:PHE:CE2	2.55	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%)	28	24

All (2) Ramachandran outliers are listed below:

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

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	263/263 (100%)	218 (83%)	45 (17%)	2	1

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	10	LEU
1	A	12	ASP
1	A	48	SER
1	A	55	ILE
1	A	63	THR
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	86	THR
1	A	90	SER
1	A	103	SER
1	A	105	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	106	LYS
1	A	108	SER
1	A	114	ASP
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
1	A	178	SER
1	A	184(A)	SER
1	A	203	THR
1	A	223	LEU
1	A	239	SER
1	A	240	SER
1	A	242	SER
1	A	254	LEU
1	A	266	ILE
1	A	294	SER
1	A	297	ILE
1	A	299	ILE
1	A	308	LYS
1	A	314	PHE
1	A	315	ASN
1	A	318	THR
1	A	320	THR

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

Mol	Chain	Res	Type
1	A	28	ASN
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 [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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.