



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:45 am GMT

PDB ID : 1KA4
Title : Structure of Pyrococcus furiosus carboxypeptidase Nat-Pb
Authors : Arndt, J.W.; Hao, B.; Ramakrishnan, V.; Cheng, T.; Chan, S.I.; Chan, M.K.
Deposited on : 2001-10-31
Resolution : 3.00 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) : recalc28949

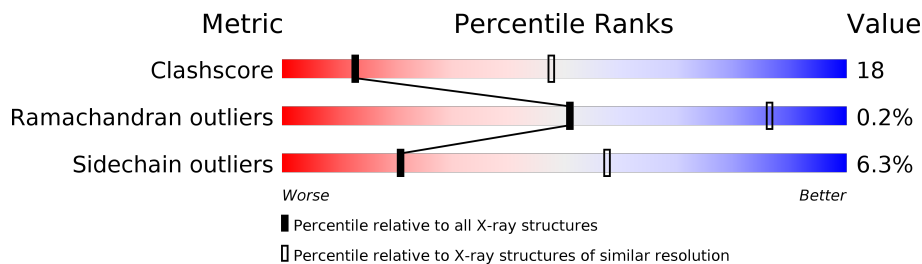
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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	499	 63% 33% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4247 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 M32 carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			4163	2700	699	755	9			

- Molecule 2 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Pb	0	0
			1	1		

- Molecule 3 is water.

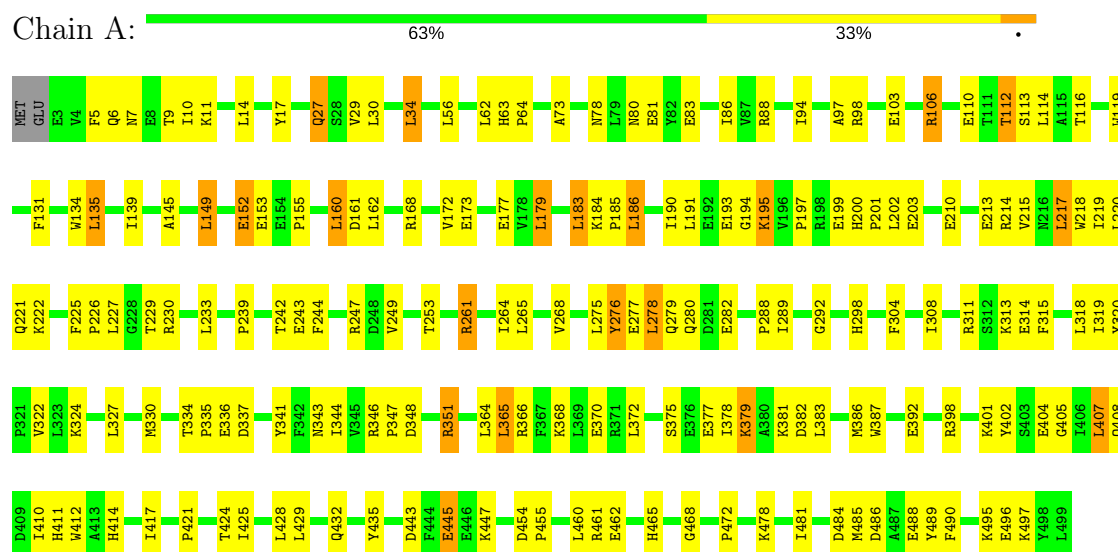
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		

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: M32 carboxypeptidase



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.30Å 67.58Å 67.19Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	19.75 – 3.00	Depositor
% Data completeness (in resolution range)	95.4 (19.75-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.236 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4247	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PB

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	0.45	0/4271	0.63	0/5770

There are no bond length outliers.

There are no bond angle outliers.

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	4163	0	4144	153	1
2	A	1	0	0	0	0
3	A	83	0	0	5	1
All	All	4247	0	4144	153	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 18.

All (153) 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:152:GLU:HG2	1:A:153:GLU:H	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:HG2	1:A:153:GLU:N	1.82	0.93
1:A:217:LEU:O	1:A:221:GLN:HG3	1.78	0.83
1:A:193:GLU:HG2	1:A:195:LYS:HE3	1.61	0.82
1:A:106:ARG:HD3	1:A:110:GLU:OE2	1.85	0.77
1:A:243:GLU:HG2	1:A:277:GLU:HG3	1.66	0.77
1:A:7:ASN:HD22	1:A:10:ILE:HG12	1.49	0.76
1:A:27:GLN:HE21	1:A:27:GLN:HA	1.52	0.74
1:A:34:LEU:HD12	1:A:34:LEU:O	1.89	0.73
1:A:173:GLU:O	1:A:177:GLU:HG3	1.87	0.73
1:A:119:TRP:CH2	1:A:410:ILE:HG12	2.23	0.72
1:A:200:HIS:HB2	1:A:344:ILE:HD11	1.71	0.71
1:A:411:HIS:CD2	1:A:411:HIS:H	2.08	0.70
1:A:230:ARG:HH21	1:A:247:ARG:HG2	1.56	0.69
1:A:243:GLU:CG	1:A:277:GLU:HG3	2.20	0.69
1:A:366:ARG:NH1	1:A:387:TRP:HH2	1.89	0.69
1:A:243:GLU:HG2	1:A:277:GLU:CG	2.23	0.68
1:A:88:ARG:NE	1:A:472:PRO:HG3	2.09	0.67
1:A:226:PRO:HB2	1:A:229:THR:CG2	2.25	0.67
1:A:103:GLU:HA	1:A:103:GLU:OE1	1.95	0.66
1:A:7:ASN:HD22	1:A:10:ILE:H	1.44	0.66
1:A:114:LEU:HB3	1:A:134:TRP:CH2	2.33	0.64
1:A:425:ILE:O	1:A:429:LEU:HD13	1.97	0.64
1:A:495:LYS:HD3	1:A:496:GLU:N	2.14	0.63
1:A:145:ALA:O	1:A:149:LEU:HD22	1.97	0.63
1:A:179:LEU:HG	1:A:183:LEU:HD12	1.80	0.63
1:A:17:TYR:CD2	1:A:288:PRO:HD3	2.34	0.62
1:A:7:ASN:HD21	1:A:9:THR:HB	1.63	0.62
1:A:152:GLU:CG	1:A:153:GLU:N	2.60	0.62
1:A:280:GLN:OE1	1:A:468:GLY:HA2	2.01	0.61
1:A:366:ARG:O	1:A:370:GLU:HG3	2.01	0.61
1:A:7:ASN:ND2	1:A:10:ILE:H	1.99	0.60
1:A:200:HIS:HD2	1:A:202:LEU:H	1.50	0.60
1:A:381:LYS:HE3	1:A:382:ASP:OD2	2.02	0.60
1:A:160:LEU:HD11	1:A:421:PRO:HG3	1.82	0.59
1:A:218:TRP:CZ2	1:A:222:LYS:HE3	2.37	0.59
1:A:432:GLN:HG3	1:A:489:TYR:CD1	2.38	0.58
1:A:218:TRP:CD2	1:A:322:VAL:HG21	2.39	0.58
1:A:34:LEU:C	1:A:34:LEU:HD12	2.24	0.57
1:A:210:GLU:HA	1:A:213:GLU:HG2	1.85	0.57
1:A:94:ILE:O	1:A:98:ARG:HG2	2.06	0.56
1:A:264:ILE:O	1:A:268:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ILE:HG22	1:A:481:ILE:O	2.06	0.56
1:A:366:ARG:NH1	1:A:387:TRP:CH2	2.73	0.55
1:A:17:TYR:CE2	1:A:288:PRO:HD3	2.42	0.55
1:A:461:ARG:HA	1:A:465:HIS:HB2	1.89	0.55
1:A:88:ARG:HE	1:A:472:PRO:HG3	1.70	0.55
1:A:225:PHE:O	1:A:227:LEU:HD22	2.08	0.54
1:A:10:ILE:HG13	1:A:83:GLU:HB3	1.89	0.54
1:A:193:GLU:CG	1:A:195:LYS:HE3	2.34	0.54
1:A:261:ARG:HD2	1:A:341:TYR:CE1	2.43	0.53
1:A:29:VAL:HA	1:A:244:PHE:CZ	2.43	0.53
1:A:200:HIS:CG	1:A:201:PRO:HD2	2.43	0.53
1:A:401:LYS:HG3	1:A:404:GLU:HG3	1.90	0.53
1:A:7:ASN:ND2	1:A:10:ILE:HG12	2.21	0.52
1:A:462:GLU:HG2	3:A:628:HOH:O	2.08	0.52
1:A:218:TRP:CE3	1:A:322:VAL:HG21	2.44	0.52
1:A:80:ASN:OD1	1:A:83:GLU:HG3	2.09	0.52
1:A:226:PRO:O	1:A:229:THR:HG22	2.09	0.52
1:A:365:LEU:HD12	1:A:365:LEU:C	2.29	0.52
1:A:304:PHE:O	1:A:308:ILE:HB	2.10	0.52
1:A:424:THR:O	1:A:428:LEU:HG	2.10	0.51
1:A:343:ASN:OD1	1:A:497:LYS:HE3	2.10	0.51
1:A:318:LEU:HG	1:A:319:ILE:HD13	1.94	0.50
1:A:379:LYS:HG3	1:A:382:ASP:OD2	2.12	0.50
1:A:313:LYS:NZ	1:A:336:GLU:HA	2.25	0.50
1:A:486:ASP:OD2	1:A:488:GLU:HB2	2.11	0.50
1:A:402:TYR:HB3	1:A:407:LEU:HD22	1.94	0.50
1:A:135:LEU:HD13	1:A:383:LEU:HD12	1.94	0.49
1:A:6:GLN:O	1:A:11:LYS:HE3	2.12	0.49
1:A:443:ASP:OD2	1:A:447:LYS:HE2	2.12	0.49
1:A:183:LEU:HD11	1:A:490:PHE:HE2	1.76	0.49
1:A:119:TRP:HB2	1:A:131:PHE:CE1	2.47	0.49
1:A:155:PRO:HD2	3:A:682:HOH:O	2.13	0.49
1:A:160:LEU:HD21	1:A:172:VAL:HG21	1.95	0.48
1:A:184:LYS:N	1:A:185:PRO:HD2	2.28	0.48
1:A:135:LEU:O	1:A:139:ILE:HG13	2.14	0.48
1:A:62:LEU:HD11	1:A:97:ALA:HB3	1.95	0.48
1:A:375:SER:OG	3:A:682:HOH:O	2.09	0.48
1:A:364:LEU:HD12	1:A:364:LEU:O	2.13	0.48
1:A:315:PHE:O	1:A:319:ILE:HG12	2.13	0.48
1:A:229:THR:HG23	1:A:230:ARG:N	2.29	0.47
1:A:210:GLU:O	1:A:214:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:NH2	1:A:282:GLU:OE2	2.48	0.47
1:A:320:TYR:CZ	1:A:335:PRO:HD3	2.49	0.47
1:A:412:TRP:CD1	1:A:417:ILE:HD13	2.48	0.47
1:A:454:ASP:N	1:A:455:PRO:HD2	2.29	0.47
1:A:5:PHE:CE2	1:A:86:ILE:HD11	2.50	0.47
1:A:327:LEU:O	1:A:330:MET:HB2	2.15	0.47
1:A:27:GLN:NE2	1:A:27:GLN:HA	2.26	0.46
1:A:348:ASP:HB3	3:A:640:HOH:O	2.15	0.46
1:A:112:THR:HG22	1:A:113:SER:N	2.29	0.46
1:A:200:HIS:CD2	1:A:201:PRO:HD2	2.50	0.46
1:A:199:GLU:HA	1:A:344:ILE:HD13	1.96	0.46
1:A:405:GLY:O	1:A:408:GLN:HG2	2.16	0.46
1:A:7:ASN:O	1:A:11:LYS:HG3	2.16	0.46
1:A:114:LEU:CB	1:A:134:TRP:CH2	2.98	0.46
1:A:411:HIS:H	1:A:411:HIS:HD2	1.59	0.45
1:A:435:TYR:CD1	1:A:489:TYR:HD2	2.34	0.45
1:A:265:LEU:HD13	1:A:311:ARG:CZ	2.46	0.45
1:A:219:ILE:HG12	1:A:319:ILE:HD12	1.99	0.45
1:A:200:HIS:CD2	1:A:202:LEU:H	2.32	0.45
1:A:5:PHE:HZ	1:A:289:ILE:HD11	1.82	0.45
1:A:249:VAL:HB	1:A:278:LEU:HD13	1.97	0.45
1:A:276:TYR:CZ	1:A:292:GLY:HA2	2.51	0.44
1:A:351:ARG:HB2	1:A:366:ARG:HH21	1.82	0.44
1:A:161:ASP:OD1	1:A:168:ARG:NH2	2.50	0.44
1:A:364:LEU:HD11	1:A:368:LYS:HE2	2.00	0.44
1:A:193:GLU:HB3	1:A:195:LYS:HG2	1.99	0.44
1:A:343:ASN:OD1	1:A:497:LYS:CE	2.65	0.44
1:A:351:ARG:HB2	1:A:366:ARG:NH2	2.33	0.44
1:A:239:PRO:HG3	1:A:253:THR:HA	1.99	0.43
1:A:377:GLU:HG3	1:A:377:GLU:O	2.18	0.43
1:A:372:LEU:HB3	1:A:378:ILE:HG13	2.00	0.43
1:A:222:LYS:HD3	1:A:222:LYS:HA	1.88	0.43
1:A:116:THR:OG1	1:A:414:HIS:HD2	2.02	0.43
1:A:478:LYS:HE3	1:A:484:ASP:OD1	2.18	0.43
1:A:214:ARG:HD3	3:A:680:HOH:O	2.19	0.43
1:A:119:TRP:HB2	1:A:131:PHE:CD1	2.54	0.43
1:A:186:LEU:O	1:A:190:ILE:HG13	2.19	0.43
1:A:334:THR:O	1:A:337:ASP:HB2	2.19	0.43
1:A:411:HIS:CD2	1:A:411:HIS:N	2.84	0.42
1:A:229:THR:CG2	1:A:230:ARG:N	2.82	0.42
1:A:314:GLU:CD	1:A:314:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:CG2	1:A:73:ALA:HB2	2.50	0.42
1:A:161:ASP:HB2	1:A:168:ARG:HH21	1.85	0.42
1:A:280:GLN:OE1	1:A:468:GLY:CA	2.67	0.42
1:A:324:LYS:HD2	1:A:330:MET:HB3	2.01	0.42
1:A:429:LEU:CD1	1:A:485:MET:SD	3.08	0.42
1:A:249:VAL:CG2	1:A:278:LEU:HD13	2.50	0.42
1:A:194:GLY:O	1:A:195:LYS:O	2.38	0.42
1:A:215:VAL:HG22	1:A:322:VAL:HG12	2.02	0.42
1:A:372:LEU:O	1:A:378:ILE:HG12	2.20	0.42
1:A:9:THR:HG22	1:A:73:ALA:HB2	2.02	0.42
1:A:103:GLU:CA	1:A:103:GLU:OE1	2.63	0.41
1:A:200:HIS:O	1:A:203:GLU:HG3	2.18	0.41
1:A:213:GLU:O	1:A:217:LEU:HB2	2.20	0.41
1:A:160:LEU:HD11	1:A:421:PRO:CG	2.50	0.41
1:A:275:LEU:O	1:A:279:GLN:HG3	2.20	0.41
1:A:383:LEU:HA	1:A:386:MET:HE3	2.03	0.41
1:A:445:GLU:H	1:A:445:GLU:HG2	1.58	0.41
1:A:63:HIS:ND1	1:A:64:PRO:HD2	2.36	0.41
1:A:378:ILE:HG22	1:A:379:LYS:N	2.36	0.41
1:A:243:GLU:HG2	1:A:277:GLU:CD	2.40	0.41
1:A:14:LEU:HD21	1:A:86:ILE:HD13	2.02	0.41
1:A:160:LEU:HA	1:A:160:LEU:HD12	1.93	0.41
1:A:481:ILE:O	1:A:481:ILE:CG2	2.69	0.41
1:A:197:PRO:O	1:A:344:ILE:HG23	2.21	0.40
1:A:314:GLU:HG2	1:A:445:GLU:O	2.21	0.40
1:A:191:LEU:HD21	1:A:347:PRO:HD3	2.04	0.40
1:A:7:ASN:HB3	1:A:10:ILE:CG1	2.51	0.40
1:A:220:LEU:HD12	1:A:233:LEU:HD22	2.03	0.40
1:A:392:GLU:OE1	1:A:398:ARG:NH1	2.53	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)
1:A:78:ASN:OD1	3:A:670:HOH:O[2_559]	1.72	0.48

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	495/499 (99%)	470 (95%)	24 (5%)	1 (0%)	51	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	LYS

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	444/446 (100%)	416 (94%)	28 (6%)	21	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	30	LEU
1	A	34	LEU
1	A	56	LEU
1	A	81	GLU
1	A	106	ARG
1	A	112	THR
1	A	135	LEU
1	A	149	LEU
1	A	152	GLU

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Mol	Chain	Res	Type
1	A	160	LEU
1	A	162	LEU
1	A	179	LEU
1	A	183	LEU
1	A	186	LEU
1	A	217	LEU
1	A	242	THR
1	A	261	ARG
1	A	276	TYR
1	A	278	LEU
1	A	298	HIS
1	A	346	ARG
1	A	351	ARG
1	A	365	LEU
1	A	379	LYS
1	A	407	LEU
1	A	445	GLU
1	A	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	GLN
1	A	27	GLN
1	A	200	HIS
1	A	411	HIS
1	A	414	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.