



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:33 AM UTC

PDB ID : 8WV2 / pdb_00008wv2
Title : Crystal structure of urethanase from *Candida parapsilosis* and structure-based Engineering to improve the catalytic activity and stability
Authors : Zhao, T.; Wu, H.
Deposited on : 2023-10-22
Resolution : 2.66 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

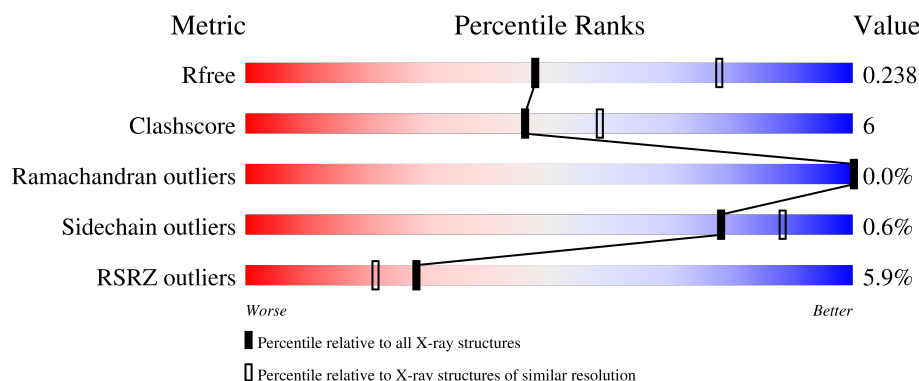
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	551	2% 88% 12%
1	B	551	2% 89% 11%
1	C	551	3% 87% 13%
1	D	551	33% 78% 21%
1	E	551	0% 89% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	551	% 87% 13%
1	G	551	2% 86% 14%
1	H	551	3% 87% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35789 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 Amidase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			
1	B	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			
1	C	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			
1	E	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			
1	F	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			
1	G	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			
1	H	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			
1	D	551	Total	C	N	O	S	0	0	0
			4354	2795	720	822	17			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	161	Total	O	0	0
			161	161		
2	B	117	Total	O	0	0
			117	117		
2	C	100	Total	O	0	0
			100	100		
2	E	148	Total	O	0	0
			148	148		
2	F	139	Total	O	0	0
			139	139		
2	G	117	Total	O	0	0
			117	117		

Continued on next page...

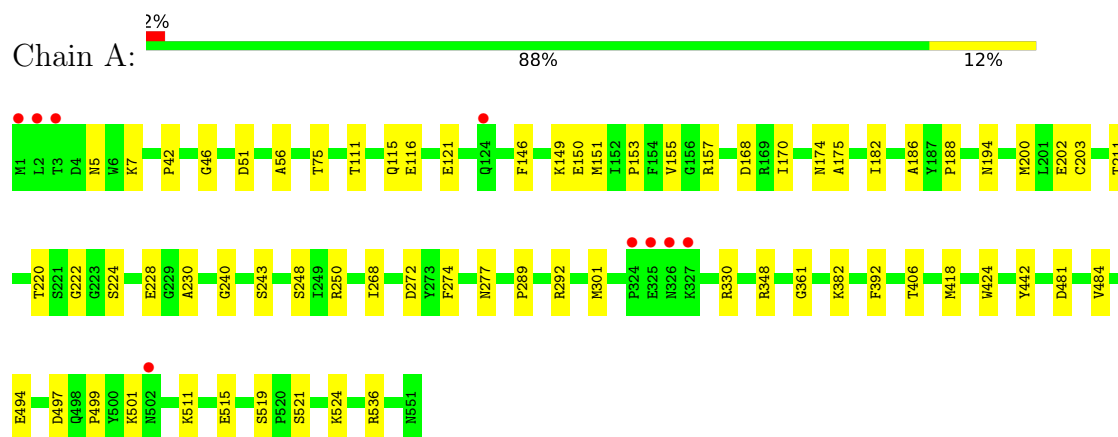
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	104	Total 104	O 104	0	0
2	D	71	Total 71	O 71	0	0

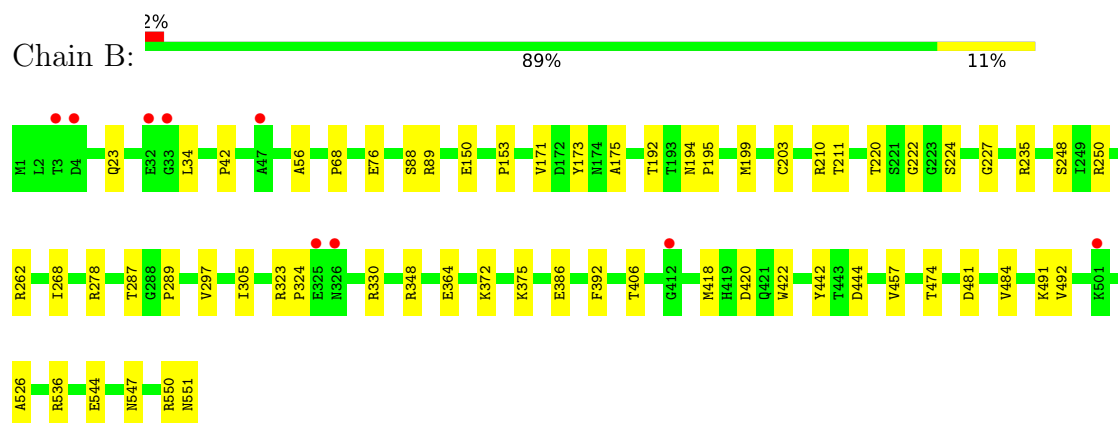
3 Residue-property plots [i](#)

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.

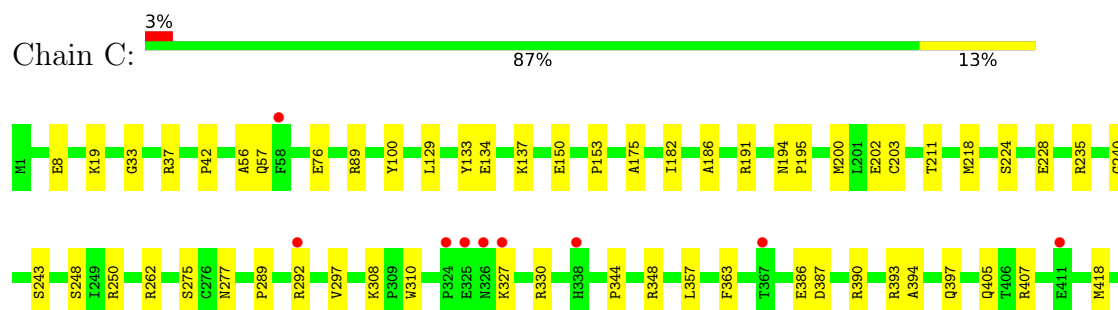
- Molecule 1: Amidase family protein

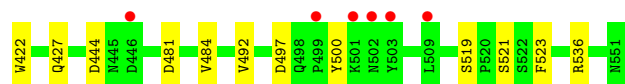


- Molecule 1: Amidase family protein

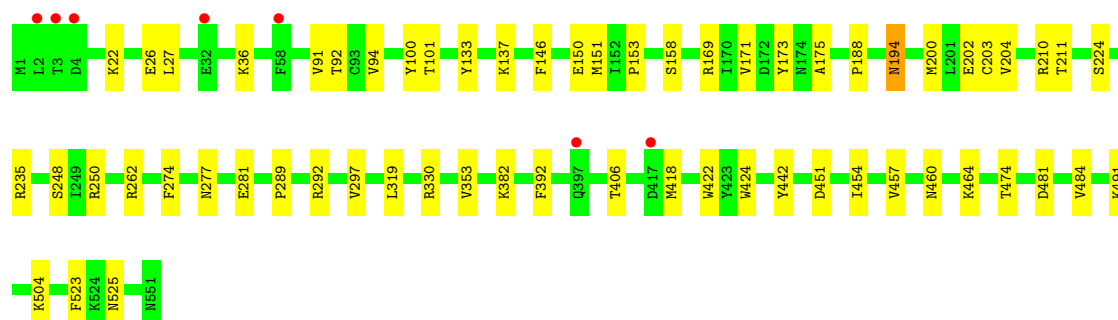
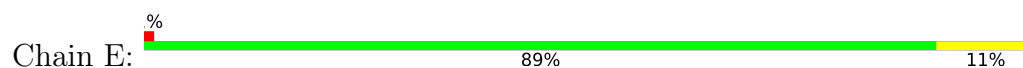


- Molecule 1: Amidase family protein

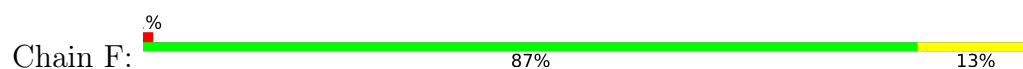




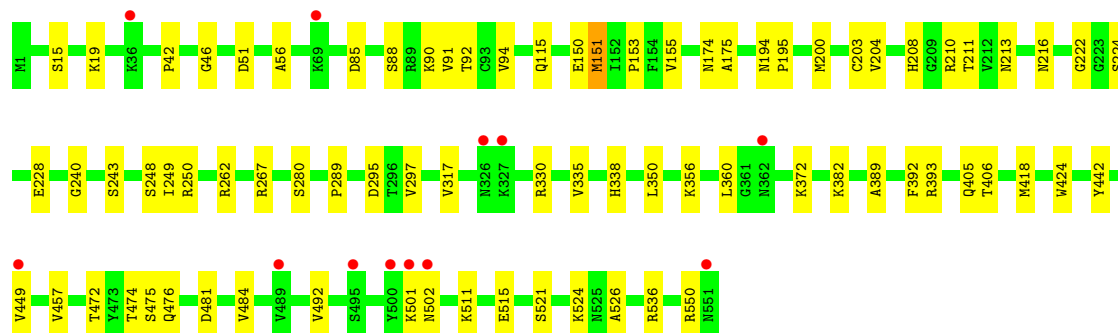
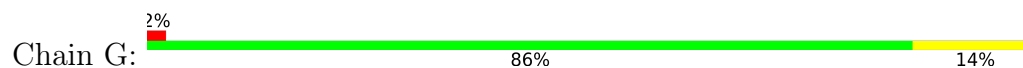
• Molecule 1: Amidase family protein



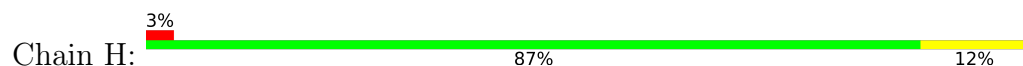
• Molecule 1: Amidase family protein

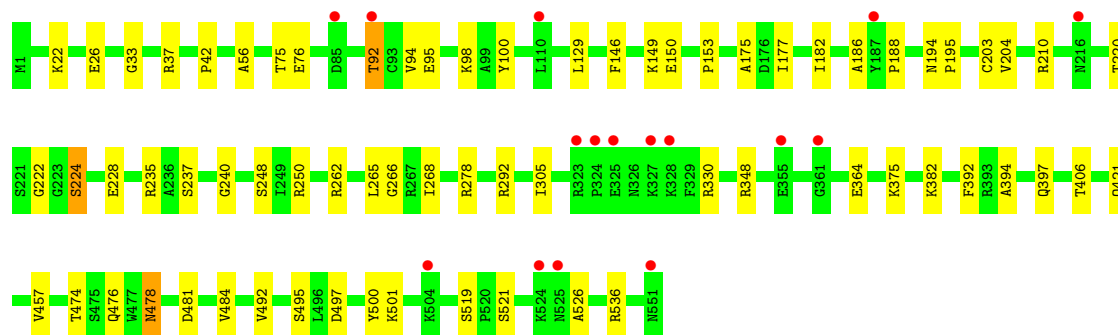


• Molecule 1: Amidase family protein

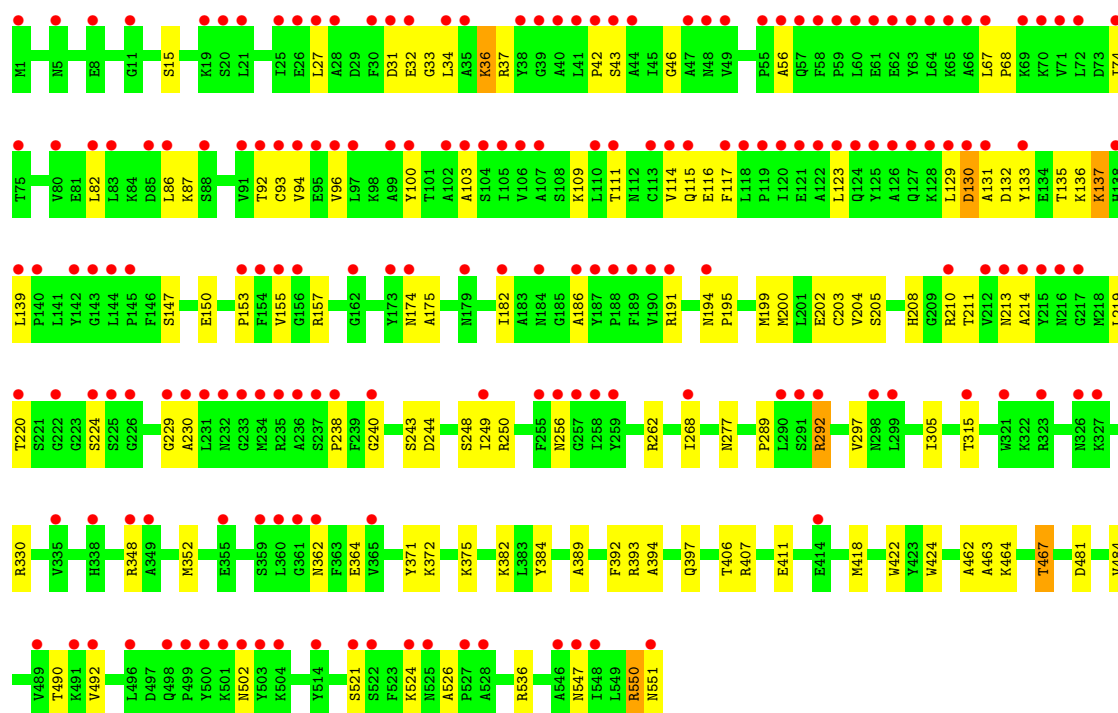
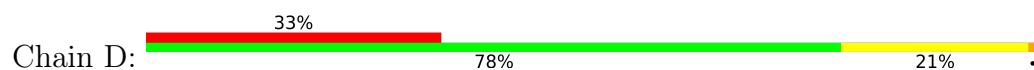


• Molecule 1: Amidase family protein





• Molecule 1: Amidase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.42Å 110.16Å 180.58Å 75.84° 83.62° 73.95°	Depositor
Resolution (Å)	48.91 – 2.66 48.91 – 2.66	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.91-2.66) 98.3 (48.91-2.66)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.204 , 0.237 0.205 , 0.238	Depositor DCC
R_{free} test set	6324 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	1.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35789	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/4460	0.48	0/6061
1	B	0.32	2/4460 (0.0%)	0.50	0/6061
1	C	0.24	0/4460	0.47	0/6061
1	D	0.37	1/4460 (0.0%)	0.54	3/6061 (0.0%)
1	E	0.25	0/4460	0.46	0/6061
1	F	0.26	0/4460	0.47	0/6061
1	G	0.36	1/4460 (0.0%)	0.51	1/6061 (0.0%)
1	H	0.31	0/4460	0.50	2/6061 (0.0%)
All	All	0.30	4/35680 (0.0%)	0.49	6/48488 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	36	LYS	CA-C	-8.25	1.44	1.53
1	B	372	LYS	C-O	-6.78	1.15	1.24
1	G	372	LYS	C-O	5.58	1.26	1.23
1	B	372	LYS	CA-C	5.35	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	LYS	N-CA-C	-8.21	103.27	113.28
1	H	478	ASN	N-CA-C	-7.89	103.26	113.12
1	D	36	LYS	N-CA-C	-5.86	103.69	111.96
1	D	130	ASP	N-CA-C	-5.81	105.68	112.89
1	G	222	GLY	N-CA-C	-5.74	104.13	112.17
1	H	500	TYR	N-CA-C	-5.14	103.69	110.43

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	4354	0	4331	51	0
1	B	4354	0	4331	41	0
1	C	4354	0	4331	52	0
1	D	4354	0	4331	89	0
1	E	4354	0	4331	43	0
1	F	4354	0	4331	51	0
1	G	4354	0	4331	44	0
1	H	4354	0	4331	45	0
2	A	161	0	0	5	0
2	B	117	0	0	9	0
2	C	100	0	0	12	0
2	D	71	0	0	6	0
2	E	148	0	0	5	0
2	F	139	0	0	6	0
2	G	117	0	0	4	0
2	H	104	0	0	6	0
All	All	35789	0	34648	406	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 6.

All (406) 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:E:171:VAL:HG13	1:E:173:TYR:CE2	2.00	0.96
1:A:111:THR:HG21	1:A:230:ALA:HB1	1.62	0.81
1:F:235:ARG:HG2	1:F:292:ARG:HD3	1.64	0.80
1:E:171:VAL:HG12	1:E:173:TYR:H	1.49	0.77
1:C:200:MET:HE2	1:C:405:GLN:HB2	1.68	0.75
1:E:171:VAL:HG13	1:E:173:TYR:CD2	2.21	0.74
1:G:330:ARG:NH2	1:G:442:TYR:O	2.20	0.74
1:A:153:PRO:HD2	1:A:175:ALA:HB2	1.70	0.74
1:B:150:GLU:HB3	1:B:194:ASN:ND2	2.03	0.74
1:G:338:HIS:NE2	2:G:602:HOH:O	2.21	0.74
1:A:268:ILE:HD13	1:A:301:MET:HE1	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ARG:HG2	1:E:292:ARG:HD3	1.70	0.73
1:G:150:GLU:HB3	1:G:194:ASN:ND2	2.03	0.73
1:D:92:THR:HG23	1:D:130:ASP:CG	2.14	0.73
1:C:224:SER:HB3	1:C:248:SER:HB3	1.70	0.72
1:G:153:PRO:HD2	1:G:175:ALA:HB2	1.71	0.72
1:F:153:PRO:HD2	1:F:175:ALA:HB2	1.71	0.71
1:E:330:ARG:NH2	1:E:442:TYR:O	2.24	0.70
1:D:362:ASN:ND2	2:D:601:HOH:O	2.23	0.70
1:D:150:GLU:HB3	1:D:194:ASN:ND2	2.07	0.70
1:E:171:VAL:CG1	1:E:173:TYR:CD2	2.75	0.69
1:G:267:ARG:NH1	2:G:604:HOH:O	2.23	0.69
1:H:330:ARG:NH1	1:H:364:GLU:OE2	2.25	0.69
1:D:132:ASP:HB3	1:D:135:THR:OG1	1.92	0.69
1:D:199:MET:SD	2:D:669:HOH:O	2.51	0.69
1:C:292:ARG:HD2	2:C:635:HOH:O	1.93	0.69
1:E:171:VAL:CG1	1:E:173:TYR:CE2	2.75	0.69
1:G:228:GLU:HG2	2:G:614:HOH:O	1.91	0.69
1:C:150:GLU:HB3	1:C:194:ASN:ND2	2.09	0.68
1:C:153:PRO:HD2	1:C:175:ALA:HB2	1.74	0.68
1:D:33:GLY:O	1:D:37:ARG:HG3	1.93	0.68
1:C:150:GLU:HB3	1:C:194:ASN:HD21	1.57	0.68
1:D:362:ASN:ND2	2:D:603:HOH:O	2.26	0.68
1:B:150:GLU:HB3	1:B:194:ASN:HD21	1.58	0.68
1:A:330:ARG:NH2	1:A:442:TYR:O	2.26	0.68
1:C:481:ASP:OD2	1:C:536:ARG:NH1	2.27	0.68
1:A:75:THR:O	1:A:292:ARG:NH2	2.25	0.67
1:F:100:TYR:OH	1:F:292:ARG:NH2	2.28	0.67
1:D:86:LEU:HD21	1:D:96:VAL:HG21	1.77	0.66
1:C:100:TYR:OH	1:C:292:ARG:NH2	2.29	0.66
1:F:292:ARG:NH1	2:F:605:HOH:O	2.28	0.66
1:C:57:GLN:HE22	1:C:218:MET:HE2	1.61	0.66
1:B:153:PRO:HD2	1:B:175:ALA:HB2	1.78	0.66
1:D:74:ILE:HG23	1:D:82:LEU:HD21	1.78	0.65
1:B:330:ARG:NH2	1:B:442:TYR:O	2.29	0.65
1:F:277:ASN:ND2	2:F:602:HOH:O	2.23	0.65
1:A:289:PRO:HD3	1:A:301:MET:HE3	1.79	0.65
1:E:100:TYR:OH	1:E:292:ARG:NH2	2.29	0.64
1:D:213:ASN:ND2	1:D:256:ASN:OD1	2.30	0.64
1:C:492:VAL:HG21	1:C:523:PHE:O	1.96	0.64
1:H:153:PRO:HD2	1:H:175:ALA:HB2	1.80	0.64
1:D:46:GLY:N	2:D:610:HOH:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:ASP:OD1	1:G:550:ARG:NH2	2.30	0.63
1:E:153:PRO:HD2	1:E:175:ALA:HB2	1.81	0.62
1:D:371:TYR:OH	1:D:372:LYS:NZ	2.33	0.62
1:C:134:GLU:OE1	1:C:137:LYS:NZ	2.26	0.62
1:H:150:GLU:HB3	1:H:194:ASN:ND2	2.15	0.62
1:F:547:ASN:OD1	1:F:550:ARG:NH1	2.32	0.61
1:A:224:SER:OG	1:A:248:SER:HB3	2.01	0.61
1:G:92:THR:HG22	1:G:94:VAL:H	1.65	0.61
1:E:36:LYS:NZ	2:E:613:HOH:O	2.28	0.61
1:D:375:LYS:NZ	2:D:612:HOH:O	2.33	0.61
1:D:407:ARG:O	1:D:411:GLU:HG2	2.00	0.61
1:G:150:GLU:HB3	1:G:194:ASN:HD21	1.66	0.60
1:G:224:SER:H	1:G:248:SER:HB3	1.66	0.60
1:D:150:GLU:HB3	1:D:194:ASN:HD21	1.66	0.60
1:G:501:LYS:HG2	1:G:502:ASN:N	2.17	0.60
1:C:235:ARG:HG2	1:C:292:ARG:HD3	1.84	0.60
1:E:92:THR:HG22	1:E:94:VAL:H	1.67	0.59
1:B:323:ARG:HG3	1:B:324:PRO:HD2	1.84	0.59
1:G:200:MET:HE2	1:G:405:GLN:HB2	1.84	0.59
1:B:420:ASP:OD2	1:C:327:LYS:NZ	2.36	0.58
1:E:200:MET:HE2	1:E:202:GLU:HB2	1.86	0.58
1:B:250:ARG:HD3	1:B:484:VAL:HB	1.84	0.58
1:E:150:GLU:HB3	1:E:194:ASN:HD21	1.68	0.58
1:D:289:PRO:HG2	1:D:297:VAL:HG13	1.86	0.58
1:H:262:ARG:HE	1:H:478:ASN:ND2	2.02	0.58
1:H:268:ILE:HD11	1:H:305:ILE:HG13	1.86	0.58
1:D:136:LYS:HB3	1:D:139:LEU:HD12	1.85	0.57
1:H:75:THR:O	1:H:292:ARG:NH2	2.37	0.57
1:B:220:THR:HG22	1:B:222:GLY:H	1.69	0.57
1:D:204:VAL:HG22	1:D:210:ARG:HG3	1.87	0.57
1:D:250:ARG:HD3	1:D:484:VAL:HB	1.87	0.57
1:D:348:ARG:NH1	2:D:609:HOH:O	2.31	0.57
1:D:330:ARG:HG2	1:D:364:GLU:HB3	1.87	0.56
1:A:494:GLU:OE2	1:A:524:LYS:HE2	2.04	0.56
1:H:92:THR:CG2	1:H:95:GLU:H	2.17	0.56
1:D:492:VAL:HG23	1:D:526:ALA:O	2.05	0.56
1:D:116:GLU:OE1	1:D:191:ARG:NH1	2.37	0.56
1:E:250:ARG:HD3	1:E:484:VAL:HB	1.87	0.56
1:E:200:MET:CE	1:E:202:GLU:HB2	2.36	0.56
1:H:204:VAL:HG22	1:H:210:ARG:HG3	1.87	0.56
1:H:224:SER:H	1:H:248:SER:HB3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:PRO:HD2	1:D:175:ALA:HB2	1.87	0.55
1:E:150:GLU:HB3	1:E:194:ASN:ND2	2.22	0.55
1:F:330:ARG:NH2	1:F:442:TYR:O	2.39	0.55
1:A:499:PRO:HB3	2:A:644:HOH:O	2.06	0.55
1:C:33:GLY:O	1:C:37:ARG:HG3	2.06	0.54
1:A:200:MET:HE3	1:A:202:GLU:HB2	1.89	0.54
1:A:224:SER:H	1:A:248:SER:HB3	1.71	0.54
1:A:42:PRO:HG2	1:A:56:ALA:HB2	1.89	0.54
1:G:382:LYS:HD2	1:G:424:TRP:NE1	2.22	0.54
1:H:33:GLY:O	1:H:37:ARG:HG3	2.07	0.54
1:D:195:PRO:HA	1:D:205:SER:HB3	1.90	0.54
1:C:89:ARG:CD	2:C:695:HOH:O	2.55	0.54
1:D:200:MET:HE2	1:D:202:GLU:HB2	1.90	0.54
1:D:87:LYS:HA	1:D:137:LYS:HG3	1.89	0.54
1:C:89:ARG:HD2	2:C:695:HOH:O	2.08	0.54
1:A:149:LYS:NZ	1:A:224:SER:OG	2.36	0.54
1:D:34:LEU:HD22	1:D:68:PRO:HD3	1.90	0.54
1:A:250:ARG:HD3	1:A:484:VAL:HB	1.90	0.54
1:B:171:VAL:HG12	1:B:173:TYR:H	1.72	0.54
1:G:250:ARG:HD3	1:G:484:VAL:HB	1.90	0.53
1:E:460:ASN:ND2	2:E:623:HOH:O	2.39	0.53
1:D:203:CYS:HB3	1:D:211:THR:HB	1.89	0.53
1:D:213:ASN:HD22	1:D:214:ALA:H	1.54	0.53
1:A:511:LYS:HE2	1:A:515:GLU:OE2	2.08	0.53
1:B:268:ILE:HD11	1:B:305:ILE:HG13	1.91	0.53
1:F:22:LYS:O	1:F:26:GLU:HG3	2.09	0.53
1:D:42:PRO:HG2	1:D:56:ALA:HB2	1.89	0.53
1:F:348:ARG:NH1	1:F:497:ASP:OD2	2.42	0.53
1:D:224:SER:H	1:D:248:SER:HB3	1.74	0.53
1:G:42:PRO:HG2	1:G:56:ALA:HB2	1.90	0.53
1:G:492:VAL:HG23	1:G:526:ALA:O	2.08	0.53
1:A:519:SER:OG	1:A:521:SER:OG	2.27	0.53
1:F:224:SER:HB3	1:F:248:SER:HB3	1.90	0.53
1:C:191:ARG:HG2	1:C:191:ARG:HH11	1.73	0.52
1:H:250:ARG:HD3	1:H:484:VAL:HB	1.91	0.52
1:F:348:ARG:NH2	1:F:490:THR:OG1	2.42	0.52
1:F:547:ASN:O	1:F:550:ARG:HG3	2.10	0.52
1:D:463:ALA:HB1	1:D:467:THR:HG22	1.91	0.52
1:F:407:ARG:O	1:F:411:GLU:HG2	2.08	0.52
1:D:93:CYS:N	1:D:130:ASP:OD1	2.29	0.52
1:D:230:ALA:HA	1:D:256:ASN:ND2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ARG:HD3	1:F:484:VAL:HB	1.91	0.52
1:H:492:VAL:HG23	1:H:526:ALA:O	2.09	0.52
1:G:195:PRO:HB3	1:G:203:CYS:HA	1.91	0.52
1:A:200:MET:CE	1:A:202:GLU:HB2	2.40	0.52
1:B:481:ASP:OD2	1:B:536:ARG:NH1	2.43	0.52
1:D:131:ALA:C	1:D:133:TYR:H	2.17	0.51
1:C:308:LYS:HG2	1:C:310:TRP:CZ2	2.45	0.51
1:C:308:LYS:NZ	2:C:618:HOH:O	2.42	0.51
1:H:476:GLN:O	1:H:476:GLN:HG3	2.09	0.51
1:D:463:ALA:HB1	1:D:467:THR:CG2	2.40	0.51
1:B:457:VAL:O	1:B:474:THR:HG23	2.10	0.51
1:C:203:CYS:HB3	1:C:211:THR:HB	1.91	0.51
1:F:42:PRO:HG2	1:F:56:ALA:HB2	1.93	0.51
1:F:492:VAL:HG23	1:F:526:ALA:O	2.09	0.51
1:B:192:THR:HB	1:B:227:GLY:HA3	1.93	0.51
1:B:550:ARG:O	1:B:551:ASN:HB2	2.11	0.51
1:A:220:THR:HG23	1:A:222:GLY:H	1.76	0.51
1:B:287:THR:HG22	2:B:646:HOH:O	2.09	0.51
1:E:133:TYR:O	1:E:137:LYS:HB2	2.11	0.51
1:A:203:CYS:HB3	1:A:211:THR:HB	1.93	0.51
1:D:87:LYS:HG3	1:D:137:LYS:HG2	1.93	0.50
1:H:348:ARG:NH1	1:H:497:ASP:OD1	2.44	0.50
1:C:289:PRO:HG2	1:C:297:VAL:HG13	1.93	0.50
1:D:67:LEU:HD11	1:D:103:ALA:HA	1.92	0.50
1:B:171:VAL:HG13	1:B:173:TYR:CD2	2.47	0.50
1:E:262:ARG:NH2	1:E:481:ASP:HA	2.27	0.50
1:D:115:GLN:OE1	1:D:208:HIS:HB3	2.12	0.50
1:C:89:ARG:HG3	2:C:695:HOH:O	2.11	0.50
1:C:200:MET:HG2	1:C:202:GLU:H	1.75	0.50
1:E:203:CYS:HB3	1:E:211:THR:HB	1.92	0.50
1:A:228:GLU:OE1	1:A:240:GLY:HA3	2.12	0.50
1:B:76:GLU:OE1	1:B:235:ARG:NH1	2.45	0.50
1:E:224:SER:H	1:E:248:SER:HB3	1.76	0.49
1:D:27:LEU:HD11	1:D:123:LEU:HB2	1.92	0.49
1:H:42:PRO:HG2	1:H:56:ALA:HB2	1.94	0.49
1:D:155:VAL:HG23	1:D:174:ASN:OD1	2.12	0.49
1:D:224:SER:OG	1:D:248:SER:HB3	2.12	0.49
1:C:387:ASP:O	1:C:390:ARG:HD3	2.11	0.49
1:F:224:SER:H	1:F:248:SER:HB3	1.77	0.49
1:H:237:SER:O	1:H:292:ARG:NH1	2.45	0.49
1:E:422:TRP:CZ3	1:F:277:ASN:HA	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:THR:CG2	1:A:230:ALA:HB1	2.39	0.49
1:C:262:ARG:NH1	1:C:481:ASP:HA	2.27	0.48
1:G:521:SER:O	1:G:524:LYS:HG3	2.13	0.48
1:D:92:THR:CG2	1:D:130:ASP:CG	2.84	0.48
1:F:182:ILE:HA	1:F:186:ALA:O	2.12	0.48
1:F:295:ASP:OD1	1:F:550:ARG:NH2	2.47	0.48
1:G:228:GLU:OE1	1:G:240:GLY:HA3	2.13	0.48
1:G:472:THR:HA	1:G:475:SER:OG	2.13	0.48
1:H:22:LYS:NZ	1:H:26:GLU:OE2	2.36	0.48
1:E:146:PHE:O	1:E:188:PRO:HA	2.14	0.48
1:E:451:ASP:O	2:E:601:HOH:O	2.20	0.48
1:H:195:PRO:HB3	1:H:203:CYS:HA	1.95	0.48
1:B:392:PHE:CZ	1:B:406:THR:HG21	2.49	0.48
1:C:277:ASN:HA	1:D:422:TRP:CZ3	2.48	0.48
1:F:386:GLU:OE2	1:F:421:GLN:NE2	2.43	0.48
1:H:497:ASP:OD1	2:H:601:HOH:O	2.20	0.48
1:B:278:ARG:HD2	2:B:603:HOH:O	2.13	0.48
1:A:220:THR:HG23	1:A:222:GLY:N	2.29	0.48
1:D:92:THR:HG23	1:D:130:ASP:OD1	2.13	0.48
1:A:150:GLU:HB3	1:A:194:ASN:HD21	1.78	0.48
1:F:220:THR:OG1	2:F:601:HOH:O	2.20	0.48
1:F:521:SER:O	1:F:524:LYS:HG3	2.14	0.47
1:A:392:PHE:CZ	1:A:406:THR:HG21	2.49	0.47
1:B:203:CYS:HB3	1:B:211:THR:HB	1.96	0.47
1:D:268:ILE:HD11	1:D:305:ILE:HG13	1.95	0.47
1:H:519:SER:OG	1:H:521:SER:OG	2.29	0.47
1:D:87:LYS:CG	1:D:137:LYS:HG2	2.44	0.47
1:E:27:LEU:HD23	1:E:101:THR:HG21	1.96	0.47
1:E:171:VAL:HG12	1:E:173:TYR:N	2.25	0.47
1:F:250:ARG:NH1	2:F:617:HOH:O	2.44	0.47
1:B:34:LEU:HD13	1:B:68:PRO:HD3	1.95	0.47
1:B:88:SER:O	2:B:601:HOH:O	2.20	0.47
1:D:262:ARG:NH2	1:D:481:ASP:HA	2.29	0.47
1:B:375:LYS:NZ	2:B:622:HOH:O	2.47	0.47
1:D:382:LYS:HG3	1:D:424:TRP:CE2	2.50	0.47
1:D:521:SER:O	1:D:524:LYS:HG3	2.15	0.47
1:F:353:VAL:HG11	1:F:454:ILE:HD13	1.97	0.46
1:H:481:ASP:OD2	1:H:536:ARG:NH1	2.48	0.46
1:B:224:SER:H	1:B:248:SER:HB3	1.80	0.46
1:H:228:GLU:OE1	1:H:240:GLY:HA3	2.15	0.46
1:E:277:ASN:HA	1:F:422:TRP:CZ3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:NH1	1:A:497:ASP:OD2	2.47	0.46
1:G:389:ALA:O	1:G:393:ARG:HG3	2.16	0.46
1:H:92:THR:HG23	1:H:95:GLU:H	1.79	0.46
1:D:243:SER:O	1:D:249:ILE:HG13	2.15	0.46
1:F:145:PRO:HB2	1:F:189:PHE:CD2	2.51	0.46
1:G:88:SER:OG	1:G:90:LYS:HG3	2.15	0.46
1:H:278:ARG:NH2	2:H:623:HOH:O	2.42	0.46
1:F:371:TYR:CZ	1:F:372:LYS:HE3	2.51	0.46
1:G:335:VAL:HA	1:G:350:LEU:HD13	1.98	0.46
1:D:133:TYR:CZ	1:D:137:LYS:HD3	2.50	0.46
1:D:220:THR:HG22	1:D:463:ALA:O	2.16	0.46
1:A:224:SER:H	1:A:248:SER:CB	2.28	0.46
1:H:182:ILE:HA	1:H:186:ALA:O	2.16	0.46
1:A:150:GLU:HB3	1:A:194:ASN:ND2	2.30	0.46
1:A:155:VAL:HG23	2:A:648:HOH:O	2.16	0.46
1:C:386:GLU:HG2	2:C:641:HOH:O	2.16	0.45
1:G:203:CYS:HB3	1:G:211:THR:HB	1.98	0.45
1:D:244:ASP:HB2	1:D:249:ILE:HB	1.98	0.45
1:A:168:ASP:C	1:A:170:ILE:HD12	2.41	0.45
1:A:277:ASN:HA	1:B:422:TRP:CZ3	2.51	0.45
1:F:224:SER:H	1:F:248:SER:CB	2.29	0.45
1:H:501:LYS:HA	1:H:501:LYS:HD2	1.57	0.45
1:A:521:SER:HB2	1:A:524:LYS:HE3	1.97	0.45
1:C:42:PRO:HG2	1:C:56:ALA:HB2	1.97	0.45
1:C:89:ARG:CG	2:C:695:HOH:O	2.65	0.45
1:D:219:LEU:HD13	1:D:462:ALA:O	2.17	0.45
1:E:319:LEU:O	2:E:602:HOH:O	2.21	0.45
1:F:262:ARG:NH2	1:F:481:ASP:HA	2.32	0.45
1:G:155:VAL:HG23	1:G:174:ASN:OD1	2.17	0.45
1:A:301:MET:HE2	1:A:301:MET:HA	1.97	0.45
1:C:8:GLU:OE1	2:C:601:HOH:O	2.21	0.45
1:C:195:PRO:HB3	1:C:203:CYS:HA	1.97	0.45
1:C:330:ARG:NH2	1:C:444:ASP:HB3	2.32	0.45
1:H:92:THR:HG22	1:H:95:GLU:HB2	1.99	0.45
1:A:157:ARG:HA	1:A:157:ARG:HD3	1.65	0.45
1:C:224:SER:H	1:C:248:SER:CB	2.29	0.45
1:H:457:VAL:O	1:H:474:THR:HG23	2.16	0.45
1:D:352:MET:HE2	1:D:490:THR:HB	1.98	0.45
1:B:195:PRO:HB3	1:B:203:CYS:HA	1.99	0.45
1:B:42:PRO:HG2	1:B:56:ALA:HB2	1.98	0.45
1:C:250:ARG:HD3	1:C:484:VAL:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:GLU:OE1	1:F:240:GLY:HA3	2.17	0.45
1:G:204:VAL:HG22	1:G:210:ARG:HG3	1.98	0.45
1:G:280:SER:O	2:G:601:HOH:O	2.20	0.45
1:A:348:ARG:NH1	1:A:497:ASP:OD1	2.50	0.44
1:D:147:SER:O	1:D:240:GLY:HA2	2.17	0.44
1:D:213:ASN:ND2	1:D:214:ALA:H	2.15	0.44
1:C:393:ARG:NH1	2:C:623:HOH:O	2.49	0.44
1:G:457:VAL:O	1:G:474:THR:HG23	2.17	0.44
1:H:392:PHE:CZ	1:H:406:THR:HG21	2.52	0.44
1:H:394:ALA:O	1:H:397:GLN:HG3	2.17	0.44
1:B:492:VAL:HG23	1:B:526:ALA:O	2.17	0.44
1:E:353:VAL:HG11	1:E:454:ILE:HD13	1.99	0.44
1:E:457:VAL:O	1:E:474:THR:HG23	2.18	0.44
1:G:262:ARG:NH1	1:G:481:ASP:HA	2.32	0.44
1:G:289:PRO:HG2	1:G:297:VAL:HG13	2.00	0.44
1:H:94:VAL:HG12	1:H:98:LYS:HE2	1.99	0.44
1:H:224:SER:H	1:H:248:SER:CB	2.31	0.44
1:D:86:LEU:HD21	1:D:96:VAL:CG2	2.44	0.44
1:A:182:ILE:HA	1:A:186:ALA:O	2.18	0.44
1:B:210:ARG:NH2	2:B:628:HOH:O	2.51	0.44
1:B:224:SER:H	1:B:248:SER:CB	2.31	0.44
1:A:382:LYS:HG3	1:A:424:TRP:CE2	2.53	0.44
1:G:511:LYS:HE2	1:G:515:GLU:OE2	2.17	0.44
1:D:481:ASP:OD2	1:D:536:ARG:NH1	2.50	0.44
1:A:155:VAL:HG13	1:A:174:ASN:OD1	2.17	0.44
1:A:243:SER:O	1:A:248:SER:HB2	2.17	0.44
1:A:250:ARG:NH1	2:A:631:HOH:O	2.50	0.44
1:E:92:THR:HG22	1:E:94:VAL:N	2.31	0.44
1:G:15:SER:HB3	1:G:19:LYS:HZ1	1.83	0.44
1:G:476:GLN:O	1:G:476:GLN:HG3	2.17	0.44
1:H:265:LEU:O	2:H:602:HOH:O	2.20	0.44
1:D:34:LEU:C	1:D:36:LYS:N	2.76	0.44
1:D:194:ASN:OD1	1:D:194:ASN:N	2.51	0.44
1:A:116:GLU:OE2	1:A:157:ARG:NH2	2.45	0.43
1:H:149:LYS:HZ1	1:H:224:SER:HB2	1.82	0.43
1:H:382:LYS:HA	2:H:631:HOH:O	2.18	0.43
1:G:356:LYS:O	1:G:360:LEU:HD22	2.17	0.43
1:A:481:ASP:OD2	1:A:536:ARG:NH1	2.51	0.43
1:C:394:ALA:O	1:C:397:GLN:HG3	2.17	0.43
1:F:155:VAL:HG23	1:F:174:ASN:OD1	2.18	0.43
1:G:481:ASP:OD2	1:G:536:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:THR:HG22	1:H:95:GLU:H	1.83	0.43
1:D:182:ILE:HA	1:D:186:ALA:O	2.18	0.43
1:F:392:PHE:CZ	1:F:406:THR:HG21	2.53	0.43
1:D:213:ASN:ND2	1:D:214:ALA:N	2.66	0.43
1:F:192:THR:HB	1:F:227:GLY:HA3	2.01	0.43
1:F:243:SER:O	1:F:249:ILE:HG13	2.19	0.43
1:E:158:SER:HA	1:E:169:ARG:O	2.18	0.43
1:H:76:GLU:OE1	1:H:235:ARG:HD2	2.19	0.43
1:D:229:GLY:C	1:D:256:ASN:HD22	2.27	0.43
1:D:521:SER:HB2	1:D:524:LYS:HE3	2.01	0.43
1:B:348:ARG:NH2	1:B:491:LYS:O	2.40	0.43
1:C:133:TYR:O	1:C:137:LYS:HB3	2.18	0.43
1:D:92:THR:HG22	1:D:94:VAL:H	1.83	0.43
1:B:330:ARG:NH1	1:B:444:ASP:HB3	2.33	0.43
1:E:224:SER:OG	1:E:248:SER:HB3	2.19	0.43
1:F:481:ASP:OD2	1:F:536:ARG:NH1	2.52	0.43
1:D:389:ALA:O	1:D:393:ARG:HG3	2.19	0.43
1:C:275:SER:HB2	2:C:627:HOH:O	2.19	0.42
1:F:220:THR:HG23	1:F:222:GLY:N	2.33	0.42
1:F:450:LEU:HD23	1:F:450:LEU:HA	1.94	0.42
1:G:151:MET:HB3	1:G:151:MET:HE2	1.75	0.42
1:H:100:TYR:OH	1:H:292:ARG:NH2	2.47	0.42
1:D:87:LYS:O	1:D:133:TYR:OH	2.36	0.42
1:C:240:GLY:O	1:C:289:PRO:HA	2.19	0.42
1:E:418:MET:HE2	1:F:418:MET:HE2	2.01	0.42
1:H:146:PHE:O	1:H:188:PRO:HA	2.19	0.42
1:D:43:SER:HB2	1:D:109:LYS:HE3	2.00	0.42
1:D:114:VAL:HG11	1:D:117:PHE:CZ	2.55	0.42
1:C:182:ILE:HA	1:C:186:ALA:O	2.20	0.42
1:C:348:ARG:NH1	1:C:497:ASP:OD1	2.52	0.42
1:D:550:ARG:O	1:D:551:ASN:HB2	2.19	0.42
1:C:243:SER:O	1:C:248:SER:HB2	2.20	0.42
1:G:115:GLN:OE1	1:G:208:HIS:HB3	2.20	0.42
1:G:392:PHE:CZ	1:G:406:THR:HG21	2.53	0.42
1:D:392:PHE:CZ	1:D:406:THR:HG21	2.55	0.42
1:F:220:THR:HG23	1:F:222:GLY:H	1.85	0.42
1:D:34:LEU:C	1:D:36:LYS:H	2.26	0.42
1:D:464:LYS:O	1:D:467:THR:HG22	2.20	0.42
1:B:536:ARG:NH2	2:B:630:HOH:O	2.52	0.42
1:E:392:PHE:CZ	1:E:406:THR:HG21	2.55	0.42
1:G:85:ASP:HB3	1:G:91:VAL:HG23	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LEU:HD22	1:D:68:PRO:CD	2.50	0.42
1:B:23:GLN:O	2:B:602:HOH:O	2.21	0.42
1:C:422:TRP:CZ3	1:D:277:ASN:HA	2.55	0.42
1:F:390:ARG:HD2	2:F:610:HOH:O	2.20	0.42
1:F:457:VAL:O	1:F:474:THR:HG23	2.20	0.42
1:G:243:SER:O	1:G:249:ILE:HG13	2.19	0.42
1:B:199:MET:O	2:B:604:HOH:O	2.22	0.42
1:C:129:LEU:HG	2:C:636:HOH:O	2.18	0.42
1:E:289:PRO:HG2	1:E:297:VAL:HG13	2.01	0.42
1:F:114:VAL:HG11	1:F:117:PHE:CZ	2.55	0.42
1:G:418:MET:HE1	1:H:421:GLN:NE2	2.35	0.42
1:A:146:PHE:O	1:A:188:PRO:HA	2.19	0.41
1:A:151:MET:HE3	1:A:274:PHE:O	2.20	0.41
1:A:272:ASP:OD1	2:A:601:HOH:O	2.21	0.41
1:E:491:LYS:NZ	1:E:525:ASN:HD22	2.18	0.41
1:G:213:ASN:HB3	1:G:216:ASN:O	2.19	0.41
1:C:228:GLU:OE1	1:C:240:GLY:HA3	2.19	0.41
1:C:357:LEU:HD22	1:C:363:PHE:CD1	2.56	0.41
1:E:22:LYS:O	1:E:26:GLU:HG3	2.20	0.41
1:F:262:ARG:HE	1:F:478:ASN:ND2	2.19	0.41
1:D:200:MET:CE	1:D:202:GLU:HB2	2.51	0.41
1:A:115:GLN:HG2	1:A:150:GLU:HG3	2.03	0.41
1:B:330:ARG:NH1	1:B:364:GLU:CD	2.79	0.41
1:E:464:LYS:HE3	1:E:523:PHE:CZ	2.55	0.41
1:D:394:ALA:O	1:D:397:GLN:HG3	2.20	0.41
1:A:5:ASN:ND2	1:A:7:LYS:HB2	2.36	0.41
1:G:46:GLY:HA3	1:G:51:ASP:O	2.20	0.41
1:A:418:MET:HE2	1:B:418:MET:HE2	2.03	0.41
1:H:495:SER:O	2:H:603:HOH:O	2.21	0.41
1:D:31:ASP:O	1:D:32:GLU:C	2.63	0.41
1:D:292:ARG:H	1:D:292:ARG:HG3	1.45	0.41
1:D:547:ASN:O	1:D:550:ARG:HG3	2.21	0.41
1:C:427:GLN:HA	2:C:602:HOH:O	2.20	0.41
1:C:224:SER:H	1:C:248:SER:HB3	1.84	0.41
1:E:382:LYS:HG3	1:E:424:TRP:CE2	2.55	0.41
1:F:339:ILE:HD11	1:F:373:PRO:HG2	2.03	0.41
1:F:501:LYS:HA	1:F:501:LYS:HD2	1.90	0.41
1:D:213:ASN:HD22	1:D:214:ALA:N	2.18	0.41
1:C:519:SER:OG	1:C:521:SER:OG	2.39	0.41
1:A:361:GLY:O	2:A:602:HOH:O	2.22	0.41
1:A:501:LYS:HA	1:A:501:LYS:HD2	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PRO:HG2	1:B:297:VAL:HG13	2.02	0.41
1:F:88:SER:OG	1:F:90:LYS:HG3	2.20	0.41
1:G:224:SER:H	1:G:248:SER:CB	2.33	0.41
1:H:177:ILE:HD12	1:H:268:ILE:CG2	2.51	0.41
1:H:262:ARG:NH2	1:H:481:ASP:HA	2.36	0.41
1:E:281:GLU:OE1	2:E:604:HOH:O	2.22	0.41
1:F:213:ASN:HB3	1:F:216:ASN:O	2.21	0.40
1:H:220:THR:HG23	1:H:222:GLY:H	1.86	0.40
1:D:137:LYS:HB3	1:D:137:LYS:HE2	1.39	0.40
1:A:46:GLY:HA3	1:A:51:ASP:O	2.21	0.40
1:A:121:GLU:OE2	1:A:157:ARG:NH1	2.54	0.40
1:B:262:ARG:NH1	1:B:481:ASP:HA	2.36	0.40
1:C:418:MET:HE2	1:D:418:MET:HE2	2.03	0.40
1:E:204:VAL:HG22	1:E:210:ARG:HG3	2.03	0.40
1:H:266:GLY:N	2:H:611:HOH:O	2.28	0.40
1:D:100:TYR:CE2	1:D:238:PRO:HG3	2.57	0.40
1:F:146:PHE:O	1:F:188:PRO:HA	2.21	0.40
1:C:344:PRO:HG3	1:C:500:TYR:CE1	2.56	0.40
1:E:151:MET:HE3	1:E:274:PHE:O	2.21	0.40
1:F:133:TYR:O	1:F:137:LYS:HB2	2.21	0.40
1:B:386:GLU:HG2	2:B:620:HOH:O	2.22	0.40
1:B:544:GLU:O	1:B:547:ASN:HB3	2.21	0.40
1:C:76:GLU:OE2	1:C:235:ARG:NH1	2.52	0.40
1:F:476:GLN:NE2	2:F:625:HOH:O	2.49	0.40
1:D:27:LEU:CD1	1:D:123:LEU:HB2	2.51	0.40
1:D:157:ARG:HB3	1:D:191:ARG:NH1	2.36	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	549/551 (100%)	535 (97%)	14 (3%)	0	100	100
1	B	549/551 (100%)	533 (97%)	16 (3%)	0	100	100
1	C	549/551 (100%)	532 (97%)	17 (3%)	0	100	100
1	D	549/551 (100%)	527 (96%)	21 (4%)	1 (0%)	43	60
1	E	549/551 (100%)	532 (97%)	17 (3%)	0	100	100
1	F	549/551 (100%)	532 (97%)	17 (3%)	0	100	100
1	G	549/551 (100%)	533 (97%)	16 (3%)	0	100	100
1	H	549/551 (100%)	533 (97%)	16 (3%)	0	100	100
All	All	4392/4408 (100%)	4257 (97%)	134 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	502	ASN

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	476/476 (100%)	476 (100%)	0	100	100
1	B	476/476 (100%)	475 (100%)	1 (0%)	87	95
1	C	476/476 (100%)	474 (100%)	2 (0%)	84	93
1	D	476/476 (100%)	468 (98%)	8 (2%)	53	73
1	E	476/476 (100%)	473 (99%)	3 (1%)	78	88
1	F	476/476 (100%)	475 (100%)	1 (0%)	87	95
1	G	476/476 (100%)	473 (99%)	3 (1%)	78	88
1	H	476/476 (100%)	472 (99%)	4 (1%)	73	85
All	All	3808/3808 (100%)	3786 (99%)	22 (1%)	78	88

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	89	ARG
1	C	19	LYS
1	C	407	ARG
1	E	91	VAL
1	E	194	ASN
1	E	504	LYS
1	F	550	ARG
1	G	151	MET
1	G	317	VAL
1	G	449	VAL
1	H	92	THR
1	H	129	LEU
1	H	224	SER
1	H	375	LYS
1	D	15	SER
1	D	111	THR
1	D	129	LEU
1	D	292	ARG
1	D	315	THR
1	D	384	TYR
1	D	467	THR
1	D	550	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	465	HIS
1	A	516	GLN
1	B	57	GLN
1	B	232	ASN
1	B	277	ASN
1	B	448	ASN
1	B	516	GLN
1	C	14	GLN
1	C	57	GLN
1	C	216	ASN
1	C	277	ASN
1	C	421	GLN
1	E	18	GLN
1	E	184	ASN
1	E	465	HIS
1	E	525	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	57	GLN
1	F	184	ASN
1	F	448	ASN
1	G	421	GLN
1	H	421	GLN
1	H	476	GLN
1	H	525	ASN
1	D	23	GLN
1	D	213	ASN
1	D	397	GLN
1	D	421	GLN
1	D	516	GLN
1	D	525	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 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 ⓘ

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	551/551 (100%)	-0.15	9 (1%) 70 66	10, 26, 50, 109	0
1	B	551/551 (100%)	0.00	9 (1%) 70 66	10, 30, 57, 110	0
1	C	551/551 (100%)	0.33	15 (2%) 56 49	15, 37, 71, 128	0
1	D	551/551 (100%)	1.55	184 (33%) 1 0	22, 56, 93, 119	0
1	E	551/551 (100%)	-0.01	7 (1%) 75 71	13, 30, 54, 101	0
1	F	551/551 (100%)	-0.06	7 (1%) 75 71	10, 30, 54, 104	0
1	G	551/551 (100%)	0.25	12 (2%) 62 56	17, 35, 64, 106	0
1	H	551/551 (100%)	0.47	16 (2%) 53 46	18, 40, 68, 107	0
All	All	4408/4408 (100%)	0.30	259 (5%) 28 21	10, 34, 72, 128	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	71	VAL	5.6
1	D	236	ALA	5.1
1	D	39	GLY	4.9
1	D	80	VAL	4.7
1	D	113	CYS	4.5
1	D	234	MET	4.5
1	D	25	ILE	4.2
1	E	2	LEU	4.1
1	D	83	LEU	4.1
1	D	257	GLY	4.1
1	D	292	ARG	4.0
1	D	38	TYR	4.0
1	D	67	LEU	3.9
1	D	96	VAL	3.9
1	G	551	ASN	3.9
1	D	42	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	69	LYS	3.8
1	B	3	THR	3.8
1	F	3	THR	3.8
1	C	326	ASN	3.8
1	D	27	LEU	3.8
1	D	126	ALA	3.7
1	D	119	PRO	3.7
1	D	86	LEU	3.7
1	D	64	LEU	3.6
1	D	125	TYR	3.6
1	D	525	ASN	3.6
1	D	348	ARG	3.6
1	D	123	LEU	3.5
1	D	56	ALA	3.5
1	D	114	VAL	3.5
1	D	237	SER	3.5
1	D	326	ASN	3.5
1	D	189	PHE	3.5
1	D	47	ALA	3.5
1	D	28	ALA	3.4
1	D	213	ASN	3.4
1	D	60	LEU	3.4
1	D	102	ALA	3.4
1	D	355	GLU	3.4
1	D	129	LEU	3.4
1	D	143	GLY	3.4
1	D	186	ALA	3.4
1	D	130	ASP	3.4
1	E	58	PHE	3.4
1	D	154	PHE	3.4
1	D	145	PRO	3.3
1	D	120	ILE	3.3
1	D	30	PHE	3.3
1	D	92	THR	3.3
1	D	111	THR	3.3
1	F	502	ASN	3.3
1	D	124	GLN	3.2
1	D	142	TYR	3.2
1	D	156	GLY	3.2
1	D	75	THR	3.2
1	D	63	TYR	3.2
1	D	94	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	215	TYR	3.2
1	D	49	VAL	3.2
1	D	91	VAL	3.1
1	F	4	ASP	3.1
1	D	58	PHE	3.1
1	D	187	TYR	3.1
1	D	72	LEU	3.1
1	D	256	ASN	3.1
1	D	131	ALA	3.1
1	D	155	VAL	3.1
1	D	190	VAL	3.1
1	D	290	LEU	3.0
1	D	184	ASN	3.0
1	G	69	LYS	3.0
1	D	188	PRO	3.0
1	D	233	GLY	3.0
1	D	240	GLY	3.0
1	D	66	ALA	3.0
1	D	299	LEU	3.0
1	D	44	ALA	3.0
1	H	327	LYS	3.0
1	D	105	ILE	3.0
1	D	327	LYS	2.9
1	C	502	ASN	2.9
1	D	547	ASN	2.9
1	D	99	ALA	2.9
1	H	324	PRO	2.9
1	D	85	ASP	2.9
1	D	212	VAL	2.9
1	D	153	PRO	2.8
1	D	214	ALA	2.8
1	D	95	GLU	2.8
1	D	238	PRO	2.8
1	D	65	LYS	2.8
1	D	93	CYS	2.8
1	D	323	ARG	2.8
1	D	82	LEU	2.8
1	G	500	TYR	2.8
1	D	127	GLN	2.8
1	D	498	GLN	2.8
1	C	327	LYS	2.8
1	D	43	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	521	SER	2.8
1	A	2	LEU	2.8
1	D	11	GLY	2.8
1	E	4	ASP	2.7
1	D	110	LEU	2.7
1	G	495	SER	2.7
1	D	546	ALA	2.7
1	G	327	LYS	2.7
1	D	1	MET	2.7
1	D	144	LEU	2.7
1	D	231	LEU	2.7
1	D	496	LEU	2.7
1	D	226	GLY	2.7
1	D	48	ASN	2.7
1	D	489	VAL	2.7
1	D	35	ALA	2.7
1	B	32	GLU	2.6
1	D	41	LEU	2.6
1	H	504	LYS	2.6
1	D	229	GLY	2.6
1	A	3	THR	2.6
1	D	117	PHE	2.6
1	D	140	PRO	2.6
1	D	220	THR	2.6
1	E	417	ASP	2.6
1	F	501	LYS	2.6
1	D	107	ALA	2.6
1	D	174	ASN	2.6
1	D	522	SER	2.5
1	D	361	GLY	2.5
1	D	122	ALA	2.5
1	D	230	ALA	2.5
1	C	503	TYR	2.5
1	D	217	GLY	2.5
1	G	449	VAL	2.5
1	A	1	MET	2.5
1	D	88	SER	2.5
1	D	34	LEU	2.5
1	D	118	LEU	2.5
1	C	411	GLU	2.5
1	C	58	PHE	2.5
1	H	551	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	70	LYS	2.5
1	C	499	PRO	2.5
1	D	191	ARG	2.4
1	D	224	SER	2.4
1	D	138	HIS	2.4
1	D	527	PRO	2.4
1	D	259	TYR	2.4
1	D	335	VAL	2.4
1	D	235	ARG	2.4
1	D	97	LEU	2.4
1	D	258	ILE	2.4
1	A	324	PRO	2.4
1	H	361	GLY	2.4
1	D	55	PRO	2.4
1	H	524	LYS	2.4
1	D	500	TYR	2.4
1	D	414	GLU	2.4
1	B	412	GLY	2.4
1	D	139	LEU	2.4
1	C	501	LYS	2.4
1	H	328	LYS	2.4
1	E	397	GLN	2.4
1	D	268	ILE	2.3
1	G	362	ASN	2.3
1	D	225	SER	2.3
1	D	162	GLY	2.3
1	B	47	ALA	2.3
1	E	3	THR	2.3
1	D	26	GLU	2.3
1	D	32	GLU	2.3
1	C	324	PRO	2.3
1	H	323	ARG	2.3
1	H	110	LEU	2.3
1	D	255	PHE	2.3
1	D	100	TYR	2.3
1	B	326	ASN	2.3
1	G	326	ASN	2.3
1	H	325	GLU	2.3
1	D	19	LYS	2.3
1	D	104	SER	2.3
1	D	74	ILE	2.3
1	D	103	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	327	LYS	2.3
1	D	173	TYR	2.3
1	D	62	GLU	2.3
1	H	525	ASN	2.3
1	D	31	ASP	2.3
1	D	291	SER	2.3
1	D	499	PRO	2.3
1	D	57	GLN	2.3
1	C	509	LEU	2.3
1	D	249	ILE	2.2
1	D	128	LYS	2.2
1	A	325	GLU	2.2
1	A	326	ASN	2.2
1	A	502	ASN	2.2
1	D	524	LYS	2.2
1	F	500	TYR	2.2
1	D	321	TRP	2.2
1	C	325	GLU	2.2
1	D	502	ASN	2.2
1	D	59	PRO	2.2
1	D	360	LEU	2.2
1	D	40	ALA	2.2
1	F	32	GLU	2.2
1	D	61	GLU	2.2
1	H	92	THR	2.2
1	D	503	TYR	2.2
1	D	106	VAL	2.2
1	D	492	VAL	2.2
1	D	349	ALA	2.1
1	E	32	GLU	2.1
1	H	355	GLU	2.1
1	G	36	LYS	2.1
1	G	501	LYS	2.1
1	D	5	ASN	2.1
1	D	501	LYS	2.1
1	B	4	ASP	2.1
1	G	489	VAL	2.1
1	H	85	ASP	2.1
1	D	182	ILE	2.1
1	D	548	ILE	2.1
1	D	528	ALA	2.1
1	B	325	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	504	LYS	2.1
1	D	514	TYR	2.1
1	D	365	VAL	2.1
1	D	20	SER	2.1
1	D	359	SER	2.1
1	C	292	ARG	2.1
1	D	21	LEU	2.1
1	D	179	ASN	2.1
1	D	216	ASN	2.1
1	D	232	ASN	2.1
1	D	551	ASN	2.1
1	B	33	GLY	2.1
1	D	338	HIS	2.1
1	C	446	ASP	2.1
1	D	210	ARG	2.1
1	B	501	LYS	2.1
1	D	491	LYS	2.1
1	C	367	THR	2.1
1	H	216	ASN	2.1
1	D	194	ASN	2.1
1	D	362	ASN	2.1
1	D	8	GLU	2.0
1	D	315	THR	2.0
1	D	115	GLN	2.0
1	D	222	GLY	2.0
1	H	187	TYR	2.0
1	D	121	GLU	2.0
1	A	124	GLN	2.0
1	C	338	HIS	2.0
1	F	326	ASN	2.0
1	G	502	ASN	2.0
1	D	298	ASN	2.0
1	D	133	TYR	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 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.