



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:40 PM GMT

PDB ID : 1BVZ  
Title : ALPHA-AMYLASE II (TVAII) FROM THERMOACTINOMYCES VULGARIS R-47  
Authors : Kamitori, S.; Kondo, S.; Okuyama, K.; Yokota, T.; Shimura, Y.; Tonozuka, T.; Sakano, Y.  
Deposited on : 1998-09-22  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

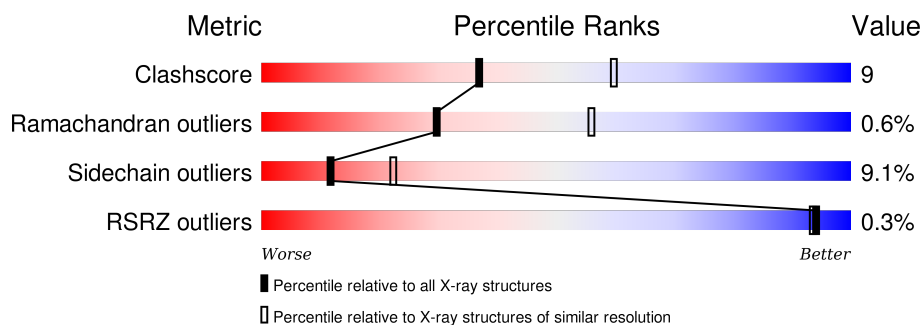
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10030 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 PROTEIN (ALPHA-AMYLASE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	831	874	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	831	874	15			

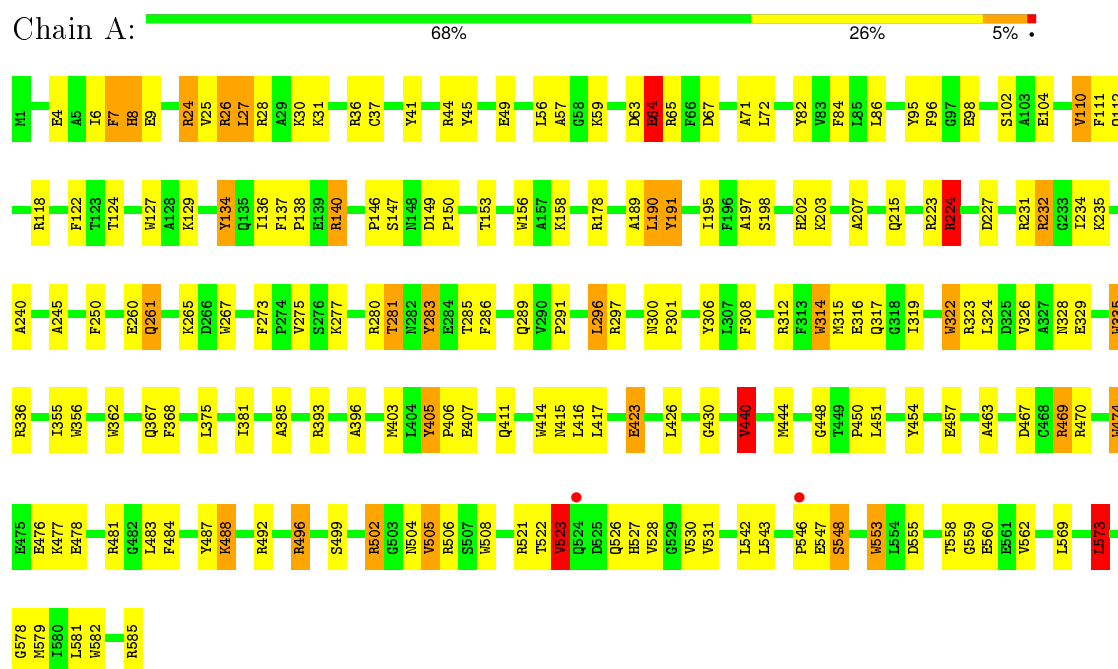
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	267	Total	O	0	0
			267	267		
2	B	211	Total	O	0	0
			211	211		

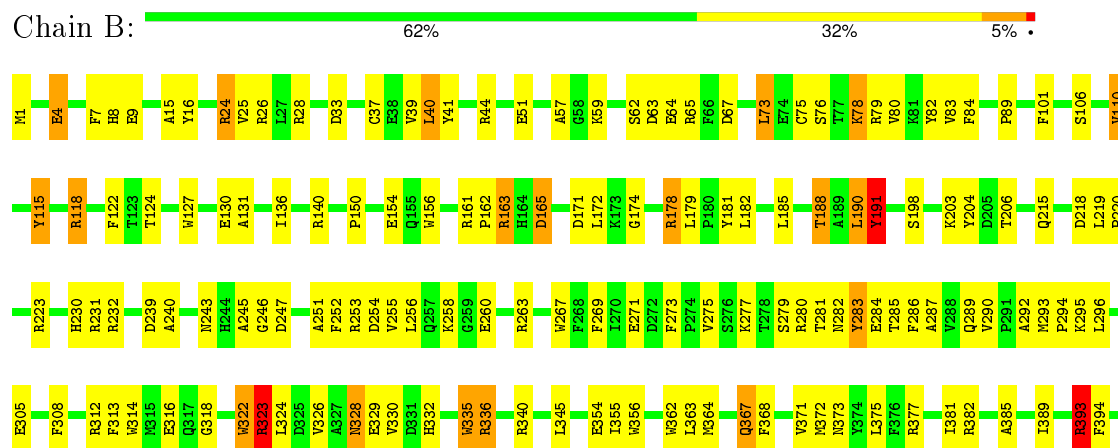
### 3 Residue-property plots

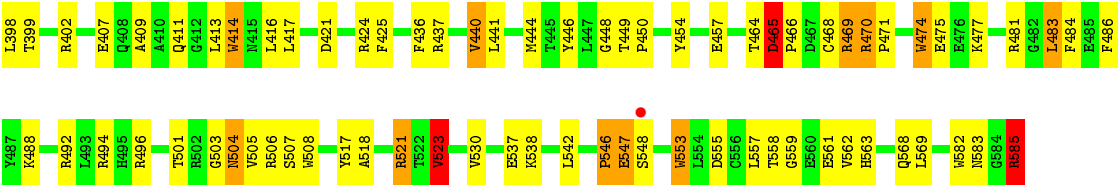
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: PROTEIN (ALPHA-AMYLASE II)



#### • Molecule 1: PROTEIN (ALPHA-AMYLASE II)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.60Å 117.90Å 114.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60 7.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.0 (7.00-2.60) 85.0 (7.00-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.196 , 0.272 0.192 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 133.1	EDS
Estimated twinning fraction	0.038 for k,h,-l 0.042 for -h,-l,-k 0.036 for l,-k,h 0.025 for k,l,h 0.025 for l,h,k	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 38661 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.85	0/4906	1.50	64/6641 (1.0%)
1	B	0.84	0/4906	1.51	75/6641 (1.1%)
All	All	0.85	0/9812	1.51	139/13282 (1.0%)

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	24
1	B	0	26
All	All	0	50

There are no bond length outliers.

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	TRP	CD1-CG-CD2	11.27	115.32	106.30
1	B	232	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	474	TRP	CD1-CG-CD2	9.32	113.76	106.30
1	B	335	TRP	CD1-CG-CD2	9.29	113.73	106.30
1	B	156	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	A	508	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	B	362	TRP	CD1-CG-CD2	8.99	113.49	106.30
1	B	127	TRP	CD1-CG-CD2	8.92	113.44	106.30
1	A	335	TRP	CD1-CG-CD2	8.91	113.43	106.30
1	A	582	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	A	322	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	414	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	B	356	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	B	582	TRP	CD1-CG-CD2	8.47	113.08	106.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	TRP	CD1-CG-CD2	8.47	113.07	106.30
1	A	558	THR	N-CA-C	8.41	133.71	111.00
1	B	474	TRP	CE2-CD2-CG	-8.40	100.58	107.30
1	A	362	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	B	508	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	314	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	B	474	TRP	CG-CD1-NE1	-8.17	101.93	110.10
1	B	322	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	B	335	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	B	267	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	B	314	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	A	267	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	B	161	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	191	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	B	558	THR	N-CA-C	7.67	131.69	111.00
1	B	127	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	B	156	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	B	382	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	314	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	127	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	B	414	TRP	CD1-CG-CD2	7.58	112.37	106.30
1	A	335	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	B	267	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	B	356	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	582	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	191	TYR	CB-CG-CD2	-7.39	116.56	121.00
1	A	356	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	A	156	TRP	CD1-CG-CD2	7.32	112.16	106.30
1	B	314	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	B	553	TRP	CD1-CG-CD2	7.31	112.15	106.30
1	B	362	TRP	CE2-CD2-CG	-7.29	101.46	107.30
1	A	508	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	322	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	B	582	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	A	267	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	B	414	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A	474	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B	446	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	A	523	VAL	O-C-N	-7.02	111.47	122.70
1	A	362	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	B	553	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	B	322	TRP	CE2-CD2-CG	-6.85	101.82	107.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	356	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	A	156	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	A	414	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	B	508	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	A	474	TRP	CG-CD1-NE1	-6.71	103.39	110.10
1	A	508	TRP	CG-CD1-NE1	-6.60	103.50	110.10
1	B	336	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	405	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	B	367	GLN	N-CA-C	6.45	128.42	111.00
1	B	118	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	127	TRP	CG-CD1-NE1	-6.41	103.69	110.10
1	A	336	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	26	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	553	TRP	CE2-CD2-CG	-6.33	102.24	107.30
1	B	474	TRP	CG-CD2-CE3	6.28	139.55	133.90
1	B	437	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	156	TRP	CG-CD1-NE1	-6.23	103.87	110.10
1	A	322	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	A	553	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	B	474	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	B	267	TRP	CG-CD2-CE3	5.92	139.23	133.90
1	B	267	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	B	393	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	558	THR	N-CA-CB	-5.91	99.07	110.30
1	B	287	ALA	N-CA-C	5.85	126.81	111.00
1	A	553	TRP	CD1-CG-CD2	5.84	110.97	106.30
1	B	546	PRO	N-CA-C	5.83	127.25	112.10
1	A	127	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	B	127	TRP	CB-CG-CD1	-5.79	119.48	127.00
1	B	110	VAL	CA-CB-CG1	5.77	119.55	110.90
1	A	335	TRP	CB-CG-CD1	-5.75	119.52	127.00
1	B	399	THR	CA-CB-CG2	-5.74	104.36	112.40
1	B	362	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	523	VAL	CA-C-N	5.72	129.79	117.20
1	A	362	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	B	65	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	582	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	A	440	VAL	CA-CB-CG2	5.64	119.36	110.90
1	B	506	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	335	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	232	ARG	NE-CZ-NH2	-5.57	117.51	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	MET	CA-CB-CG	-5.54	103.88	113.30
1	B	322	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	B	558	THR	CA-C-N	5.49	127.18	116.20
1	A	64	GLU	CA-CB-CG	-5.49	101.33	113.40
1	A	530	VAL	CA-CB-CG2	-5.49	102.67	110.90
1	B	523	VAL	O-C-N	-5.47	113.95	122.70
1	B	340	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	335	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	24	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	557	LEU	O-C-N	-5.43	114.02	122.70
1	B	582	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	B	585	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	59	LYS	CB-CG-CD	-5.39	97.59	111.60
1	A	488	LYS	CB-CG-CD	-5.38	97.60	111.60
1	B	465	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	314	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	B	218	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	335	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	A	560	GLU	N-CA-C	5.28	125.25	111.00
1	A	267	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	286	PHE	CA-C-N	5.26	128.77	117.20
1	B	356	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	A	127	TRP	CB-CG-CD1	-5.21	120.23	127.00
1	B	508	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	B	547	GLU	N-CA-C	5.20	125.03	111.00
1	A	191	TYR	CB-CG-CD1	5.19	124.11	121.00
1	B	335	TRP	CB-CG-CD1	-5.18	120.27	127.00
1	A	558	THR	O-C-N	-5.18	114.40	123.20
1	B	481	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	323	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	558	THR	CA-C-N	5.12	126.44	116.20
1	A	41	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	B	79	ARG	N-CA-C	-5.08	97.28	111.00
1	B	172	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	335	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	A	356	TRP	CG-CD1-NE1	-5.08	105.03	110.10
1	B	555	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	573	LEU	CA-CB-CG	5.07	126.96	115.30
1	B	188	THR	CA-CB-CG2	5.07	119.50	112.40
1	A	289	GLN	N-CA-C	-5.01	97.47	111.00
1	A	362	TRP	CB-CG-CD1	-5.01	120.49	127.00

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	TYR	Sidechain
1	A	140	ARG	Sidechain
1	A	191	TYR	Sidechain
1	A	224	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	28	ARG	Sidechain
1	A	283	TYR	Sidechain
1	A	323	ARG	Sidechain
1	A	367	GLN	Mainchain
1	A	405	TYR	Sidechain
1	A	45	TYR	Sidechain
1	A	469	ARG	Sidechain
1	A	481	ARG	Sidechain
1	A	487	TYR	Sidechain
1	A	492	ARG	Sidechain
1	A	496	ARG	Sidechain
1	A	502	ARG	Sidechain
1	A	506	ARG	Sidechain
1	A	523	VAL	Peptide
1	A	7	PHE	Sidechain
1	A	8	HIS	Peptide
1	A	96	PHE	Sidechain
1	B	115	TYR	Sidechain
1	B	16	TYR	Sidechain
1	B	163	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	181	TYR	Sidechain
1	B	191	TYR	Sidechain
1	B	204	TYR	Sidechain
1	B	24	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	280	ARG	Sidechain
1	B	283	TYR	Sidechain
1	B	323	ARG	Sidechain
1	B	377	ARG	Sidechain
1	B	393	ARG	Sidechain
1	B	394	PHE	Sidechain
1	B	402	ARG	Sidechain
1	B	454	TYR	Sidechain
1	B	469	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	470	ARG	Sidechain
1	B	492	ARG	Sidechain
1	B	517	TYR	Sidechain
1	B	521	ARG	Sidechain
1	B	523	VAL	Peptide
1	B	559	GLY	Peptide
1	B	63	ASP	Mainchain
1	B	82	TYR	Sidechain

## 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	4776	0	4607	84	0
1	B	4776	0	4607	95	0
2	A	267	0	0	2	0
2	B	211	0	0	0	0
All	All	10030	0	9214	177	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 9.

All (177) 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:B:281:THR:H	1:B:289:GLN:HE22	1.28	0.79
1:A:136:ILE:HD12	1:A:190:LEU:HG	1.67	0.76
1:B:136:ILE:HD12	1:B:190:LEU:HG	1.66	0.76
1:B:75:CYS:SG	1:B:80:VAL:HB	2.27	0.75
1:B:290:VAL:HG11	1:B:293:MET:SD	2.29	0.73
1:B:185:LEU:HA	1:B:488:LYS:HG2	1.71	0.73
1:A:297:ARG:HG2	1:A:300:ASN:HB2	1.73	0.71
1:A:27:LEU:HD22	1:A:37:CYS:SG	2.33	0.69
1:B:363:LEU:HD21	1:B:371:VAL:HG13	1.75	0.69
1:A:417:LEU:HD11	1:A:440:VAL:HG12	1.75	0.67
1:A:328:ASN:ND2	1:A:355:ILE:HG23	2.10	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:HZ	1:A:9:GLU:HG3	1.60	0.67
1:A:484:PHE:CE2	1:A:488:LYS:HE3	2.30	0.66
1:B:583:ASN:ND2	1:B:585:ARG:HB2	2.10	0.66
1:A:224:ARG:NH2	1:A:227:ASP:HB3	2.10	0.66
1:B:256:LEU:HD21	1:B:277:LYS:HD3	1.78	0.65
1:A:6:ILE:HD13	1:A:86:LEU:HD13	1.78	0.65
1:B:131:ALA:HA	1:B:188:THR:HG21	1.79	0.65
1:B:40:LEU:HD12	1:B:83:VAL:HG13	1.77	0.64
1:A:328:ASN:HD22	1:A:355:ILE:HG23	1.64	0.62
1:B:363:LEU:HD12	1:B:409:ALA:HB1	1.81	0.62
1:B:484:PHE:CE2	1:B:488:LYS:HD2	2.34	0.62
1:A:523:VAL:O	1:A:526:GLN:HB3	2.00	0.61
1:B:245:ALA:HB2	1:B:296:LEU:HD13	1.83	0.60
1:A:423:GLU:HB3	1:A:463:ALA:HA	1.84	0.60
1:B:178:ARG:HG3	1:B:474:TRP:CZ2	2.37	0.59
1:B:140:ARG:HH21	1:B:162:PRO:HB3	1.66	0.59
1:A:7:PHE:CZ	1:A:9:GLU:HG3	2.37	0.59
1:A:261:GLN:HE21	1:A:261:GLN:H	1.50	0.59
1:A:44:ARG:HG2	1:A:112:GLN:HE21	1.68	0.58
1:B:198:SER:HB3	1:B:203:LYS:HD2	1.85	0.58
1:B:503:GLY:HA2	1:B:523:VAL:HG23	1.86	0.57
1:B:8:HIS:HE1	1:B:25:VAL:HG23	1.69	0.57
1:A:546:PRO:HG3	1:A:553:TRP:CH2	2.39	0.57
1:A:407:GLU:O	1:A:411:GLN:HG3	2.05	0.57
1:B:8:HIS:CE1	1:B:25:VAL:HG23	2.39	0.57
1:B:253:ARG:HA	1:B:256:LEU:HD12	1.86	0.56
1:A:98:GLU:HB2	1:A:110:VAL:O	2.04	0.56
1:B:542:LEU:HD22	1:B:568:GLN:HB3	1.86	0.56
1:B:583:ASN:HD21	1:B:585:ARG:HB2	1.71	0.56
1:B:163:ARG:NH2	1:B:165:ASP:HB2	2.22	0.55
1:A:314:TRP:HB3	1:A:319:ILE:HD13	1.89	0.55
1:A:36:ARG:HG2	1:A:56:LEU:HD11	1.89	0.55
1:A:30:LYS:HG3	1:B:4:GLU:HG3	1.88	0.55
1:A:499:SER:OG	1:A:526:GLN:HG2	2.07	0.54
1:A:260:GLU:HA	1:A:265:LYS:HD3	1.89	0.54
1:B:389:ILE:HB	1:B:393:ARG:HB3	1.89	0.54
1:B:1:MET:HA	1:B:33:ASP:HB3	1.90	0.53
1:A:573:LEU:HD13	1:A:579:MET:SD	2.48	0.53
1:B:130:GLU:HB3	1:B:501:THR:HG21	1.91	0.52
1:B:174:GLY:O	1:B:178:ARG:HG2	2.09	0.52
1:B:7:PHE:CZ	1:B:9:GLU:HG3	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:CD2	1:B:277:LYS:HD3	2.40	0.52
1:B:269:PHE:HB2	1:B:284:GLU:HB2	1.92	0.52
1:B:323:ARG:HH12	1:B:354:GLU:CD	2.13	0.52
1:A:281:THR:HG21	1:A:285:THR:HG23	1.91	0.52
1:A:178:ARG:HG3	1:A:474:TRP:CZ2	2.45	0.51
1:B:416:LEU:H	1:B:416:LEU:HD23	1.75	0.51
1:B:444:MET:O	1:B:494:ARG:HD2	2.09	0.51
1:A:277:LYS:NZ	2:A:751:HOH:O	2.44	0.51
1:A:543:LEU:HD12	1:A:569:LEU:HD23	1.93	0.51
1:B:246:GLY:HA2	1:B:292:ALA:O	2.12	0.50
1:B:230:HIS:HE1	1:B:318:GLY:O	1.93	0.50
1:B:332:HIS:O	1:B:336:ARG:HB2	2.12	0.50
1:B:78:LYS:O	1:B:115:TYR:HA	2.12	0.50
1:A:57:ALA:HA	1:A:71:ALA:HB2	1.94	0.50
1:A:82:TYR:CE2	1:A:111:PHE:HB2	2.47	0.49
1:A:281:THR:HG22	1:A:283:TYR:H	1.76	0.49
1:A:542:LEU:HA	1:A:569:LEU:O	2.11	0.49
1:B:546:PRO:HD2	1:B:553:TRP:CZ2	2.47	0.49
1:B:243:ASN:OD1	1:B:295:LYS:NZ	2.45	0.49
1:B:483:LEU:O	1:B:486:PHE:HB3	2.13	0.49
1:A:261:GLN:NE2	1:A:261:GLN:H	2.11	0.48
1:A:484:PHE:HE2	1:A:488:LYS:HE3	1.77	0.48
1:B:37:CYS:HB3	1:B:57:ALA:HB3	1.94	0.48
1:B:324:LEU:HD13	1:B:335:TRP:CZ3	2.48	0.48
1:A:415:ASN:ND2	1:A:448:GLY:HA3	2.28	0.48
1:B:281:THR:N	1:B:289:GLN:HE22	2.05	0.48
1:A:281:THR:HG21	1:A:285:THR:CG2	2.43	0.48
1:B:470:ARG:HG3	1:B:471:PRO:HD2	1.94	0.48
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.49	0.48
1:B:372:MET:SD	1:B:414:TRP:HE3	2.37	0.47
1:A:505:VAL:HG13	1:A:521:ARG:HD3	1.95	0.47
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.97	0.47
1:B:150:PRO:HD3	1:B:215:GLN:HG3	1.96	0.47
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.50	0.47
1:B:468:CYS:SG	1:B:469:ARG:HG3	2.55	0.47
1:A:138:PRO:HG2	1:A:195:ILE:HG22	1.97	0.47
1:B:24:ARG:HD2	1:B:407:GLU:OE1	2.15	0.47
1:A:527:HIS:HE1	1:A:548:SER:HB3	1.80	0.47
1:A:30:LYS:HG2	1:A:31:LYS:N	2.30	0.46
1:B:256:LEU:HD23	1:B:275:VAL:HG23	1.97	0.46
1:B:275:VAL:HA	1:B:282:ASN:HD21	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:PRO:HG2	1:B:470:ARG:HA	1.97	0.46
1:A:202:HIS:ND1	1:A:202:HIS:O	2.48	0.46
1:B:363:LEU:HD12	1:B:409:ALA:CB	2.43	0.46
1:B:240:ALA:HB2	1:B:322:TRP:CE3	2.51	0.46
1:A:232:ARG:HB2	1:A:234:ILE:HD12	1.98	0.46
1:B:33:ASP:O	1:B:89:PRO:HD3	2.15	0.46
1:A:197:ALA:O	1:A:207:ALA:HB3	2.15	0.46
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.98	0.46
1:A:416:LEU:HB3	1:A:451:LEU:HD23	1.97	0.46
1:A:553:TRP:HB3	1:A:581:LEU:HB3	1.98	0.46
1:B:449:THR:HA	1:B:450:PRO:HD3	1.86	0.46
1:A:198:SER:HB3	1:A:203:LYS:HD2	1.98	0.45
1:B:39:VAL:HG22	1:B:84:PHE:CD1	2.51	0.45
1:A:265:LYS:HB2	1:A:273:PHE:HZ	1.81	0.45
1:B:283:TYR:CE1	1:B:294:PRO:HB3	2.51	0.45
1:B:286:PHE:HE1	1:B:326:VAL:HG21	1.82	0.45
1:A:312:ARG:O	1:A:316:GLU:HG2	2.16	0.45
1:B:381:ILE:O	1:B:385:ALA:HB3	2.16	0.45
1:A:245:ALA:HB2	1:A:296:LEU:HD11	1.99	0.45
1:A:444:MET:HE2	1:A:450:PRO:HB3	1.99	0.44
1:A:189:ALA:HA	1:A:235:LYS:H	1.82	0.44
1:B:417:LEU:HD11	1:B:440:VAL:HG12	1.99	0.44
1:B:371:VAL:H	1:B:413:LEU:HD23	1.83	0.44
1:A:300:ASN:HA	1:A:301:PRO:HD3	1.90	0.44
1:A:308:PHE:O	1:A:312:ARG:HG3	2.18	0.44
1:B:328:ASN:HB3	1:B:355:ILE:CG1	2.48	0.44
1:B:15:ALA:HA	1:B:24:ARG:O	2.17	0.44
1:B:328:ASN:HB3	1:B:355:ILE:HG13	2.00	0.44
1:B:372:MET:SD	1:B:414:TRP:CE3	3.11	0.43
1:B:355:ILE:HD11	1:B:368:PHE:HE2	1.83	0.43
1:B:163:ARG:HH22	1:B:165:ASP:HB2	1.83	0.43
1:B:425:PHE:HB3	1:B:436:PHE:HE1	1.82	0.43
1:B:219:LEU:HD21	1:B:313:PHE:HZ	1.82	0.43
1:A:124:THR:HB	2:A:706:HOH:O	2.18	0.43
1:B:260:GLU:HB3	1:B:273:PHE:CD2	2.54	0.43
1:A:64:GLU:H	1:A:396:ALA:HB1	1.83	0.43
1:A:467:ASP:O	1:A:470:ARG:HG3	2.18	0.43
1:B:179:LEU:HD23	1:B:182:LEU:HD12	1.98	0.43
1:B:41:TYR:CD1	1:B:73:LEU:HG	2.54	0.43
1:B:465:ASP:HA	1:B:466:PRO:HA	1.66	0.43
1:B:448:GLY:O	1:B:494:ARG:NH2	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:CD	1:A:478:GLU:HG3	2.49	0.42
1:A:240:ALA:HB2	1:A:322:TRP:HE3	1.84	0.42
1:A:149:ASP:HB3	1:A:153:THR:OG1	2.19	0.42
1:A:129:LYS:HB2	1:A:502:ARG:HH21	1.84	0.42
1:B:424:ARG:HD3	1:B:424:ARG:HH11	1.65	0.42
1:B:75:CYS:SG	1:B:80:VAL:CB	3.02	0.42
1:A:527:HIS:CE1	1:A:548:SER:HB3	2.54	0.42
1:A:137:PHE:CZ	1:A:469:ARG:HD3	2.55	0.42
1:B:285:THR:HB	1:B:290:VAL:O	2.19	0.42
1:A:250:PHE:HE2	1:A:306:TYR:CE2	2.38	0.42
1:B:518:ALA:HA	1:B:530:VAL:O	2.19	0.42
1:B:477:LYS:HB3	1:B:477:LYS:HZ3	1.85	0.41
1:A:297:ARG:HG2	1:A:300:ASN:CB	2.48	0.41
1:A:526:GLN:HA	1:A:585:ARG:HB2	2.02	0.41
1:A:150:PRO:HG3	1:A:215:GLN:HG2	2.02	0.41
1:A:65:ARG:HH12	1:B:101:PHE:HD2	1.67	0.41
1:A:26:ARG:HD2	1:A:403:MET:SD	2.60	0.41
1:B:251:ALA:O	1:B:255:VAL:HG23	2.21	0.41
1:A:8:HIS:CD2	1:A:26:ARG:O	2.73	0.41
1:B:504:ASN:O	1:B:521:ARG:HA	2.21	0.41
1:A:102:SER:HB3	1:A:104:GLU:O	2.20	0.41
1:B:373:ASN:HB2	1:B:413:LEU:HB3	2.03	0.41
1:A:531:VAL:O	1:A:578:GLY:HA2	2.20	0.41
1:B:247:ASP:HA	1:B:252:PHE:CD2	2.55	0.41
1:A:522:THR:HA	1:A:526:GLN:O	2.21	0.41
1:B:381:ILE:HD13	1:B:425:PHE:HE1	1.85	0.41
1:B:381:ILE:HD13	1:B:425:PHE:CE1	2.56	0.41
1:B:563:HIS:O	1:B:569:LEU:HA	2.20	0.41
1:B:308:PHE:O	1:B:312:ARG:HG3	2.21	0.41
1:A:476:GLU:HB2	1:A:477:LYS:HE2	2.03	0.41
1:B:230:HIS:CE1	1:B:318:GLY:O	2.72	0.41
1:B:505:VAL:HG22	1:B:521:ARG:CD	2.51	0.41
1:A:134:TYR:OH	1:A:454:TYR:HA	2.21	0.41
1:A:555:ASP:HB3	1:A:559:GLY:H	1.86	0.41
1:A:381:ILE:O	1:A:385:ALA:HB3	2.20	0.41
1:A:84:PHE:O	1:A:95:TYR:HA	2.21	0.41
1:A:146:PRO:HA	1:A:149:ASP:OD1	2.21	0.41
1:B:44:ARG:HD3	1:B:44:ARG:HH11	1.73	0.41
1:A:190:LEU:HD13	1:A:234:ILE:HG21	2.02	0.40
1:B:240:ALA:HB3	1:B:324:LEU:HD23	2.04	0.40
1:A:355:ILE:HD11	1:A:368:PHE:HE2	1.86	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:HA	1:A:150:PRO:HD3	1.86	0.40
1:B:59:LYS:NZ	1:B:67:ASP:CG	2.74	0.40

There are no symmetry-related clashes.

## 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	583/585 (100%)	534 (92%)	45 (8%)	4 (1%)	26	51
1	B	583/585 (100%)	534 (92%)	46 (8%)	3 (0%)	34	60
All	All	1166/1170 (100%)	1068 (92%)	91 (8%)	7 (1%)	30	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	VAL
1	A	64	GLU
1	B	562	VAL
1	A	430	GLY
1	B	118	ARG
1	B	345	LEU
1	A	275	VAL

### 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	493/493 (100%)	458 (93%)	35 (7%)	18	36
1	B	493/493 (100%)	438 (89%)	55 (11%)	7	13
All	All	986/986 (100%)	896 (91%)	90 (9%)	12	22

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	25	VAL
1	A	27	LEU
1	A	49	GLU
1	A	63	ASP
1	A	67	ASP
1	A	72	LEU
1	A	110	VAL
1	A	118	ARG
1	A	122	PHE
1	A	147	SER
1	A	190	LEU
1	A	223	ARG
1	A	224	ARG
1	A	261	GLN
1	A	280	ARG
1	A	281	THR
1	A	291	PRO
1	A	296	LEU
1	A	317	GLN
1	A	375	LEU
1	A	393	ARG
1	A	406	PRO
1	A	423	GLU
1	A	426	LEU
1	A	440	VAL
1	A	457	GLU
1	A	483	LEU
1	A	496	ARG
1	A	504	ASN
1	A	505	VAL
1	A	528	VAL
1	A	547	GLU
1	A	548	SER
1	A	573	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	4	GLU
1	B	40	LEU
1	B	51	GLU
1	B	62	SER
1	B	64	GLU
1	B	73	LEU
1	B	76	SER
1	B	78	LYS
1	B	106	SER
1	B	110	VAL
1	B	122	PHE
1	B	124	THR
1	B	154	GLU
1	B	165	ASP
1	B	171	ASP
1	B	190	LEU
1	B	191	TYR
1	B	206	THR
1	B	220	PRO
1	B	223	ARG
1	B	231	ARG
1	B	239	ASP
1	B	254	ASP
1	B	258	LYS
1	B	263	ARG
1	B	271	GLU
1	B	279	SER
1	B	305	GLU
1	B	316	GLU
1	B	328	ASN
1	B	329	GLU
1	B	330	VAL
1	B	364	MET
1	B	375	LEU
1	B	393	ARG
1	B	398	LEU
1	B	411	GLN
1	B	421	ASP
1	B	440	VAL
1	B	441	LEU
1	B	457	GLU
1	B	464	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	465	ASP
1	B	475	GLU
1	B	483	LEU
1	B	496	ARG
1	B	504	ASN
1	B	507	SER
1	B	523	VAL
1	B	537	GLU
1	B	538	LYS
1	B	547	GLU
1	B	548	SER
1	B	561	GLU
1	B	585	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	112	GLN
1	A	261	GLN
1	A	328	ASN
1	A	332	HIS
1	A	443	GLN
1	A	504	ASN
1	A	527	HIS
1	B	244	HIS
1	B	289	GLN
1	B	317	GLN
1	B	332	HIS
1	B	367	GLN
1	B	504	ASN
1	B	509	HIS
1	B	534	ASN

### 5.3.3 RNA ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	585/585 (100%)	-0.73	2 (0%) 94 93	8, 26, 45, 55	0
1	B	585/585 (100%)	-0.62	1 (0%) 95 95	7, 29, 47, 60	0
All	All	1170/1170 (100%)	-0.67	3 (0%) 94 93	7, 28, 46, 60	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	PRO	4.6
1	B	548	SER	3.4
1	A	524	GLN	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.