



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:08 PM GMT

PDB ID : 1SBT  
Title : ATOMIC COORDINATES FOR SUBTILISIN BPN (OR NOVO)  
Authors : Alden, R.A.; Birktoft, J.J.; Kraut, J.; Robertus, J.D.; Wright, C.S.  
Deposited on : 1972-08-11  
Resolution : 2.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

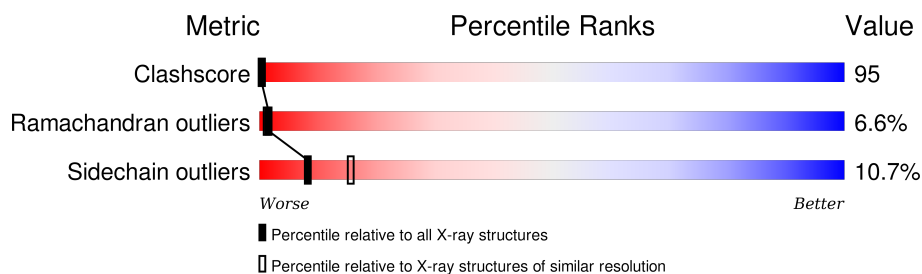
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1955 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 SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			1938	1204	335	394	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	PRO	ASN	CONFLICT	UNP P00782
A	57	ASN	PRO	CONFLICT	UNP P00782
A	61	ASP	ASN	CONFLICT	UNP P00782
A	88	SER	ALA	CONFLICT	UNP P00782
A	89	ALA	SER	CONFLICT	UNP P00782
A	98	ASP	ALA	CONFLICT	UNP P00782
A	99	ALA	ASP	CONFLICT	UNP P00782
A	158	SER	THR	CONFLICT	UNP P00782
A	159	THR	SER	CONFLICT	UNP P00782
A	251	GLN	GLU	CONFLICT	UNP P00782

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		

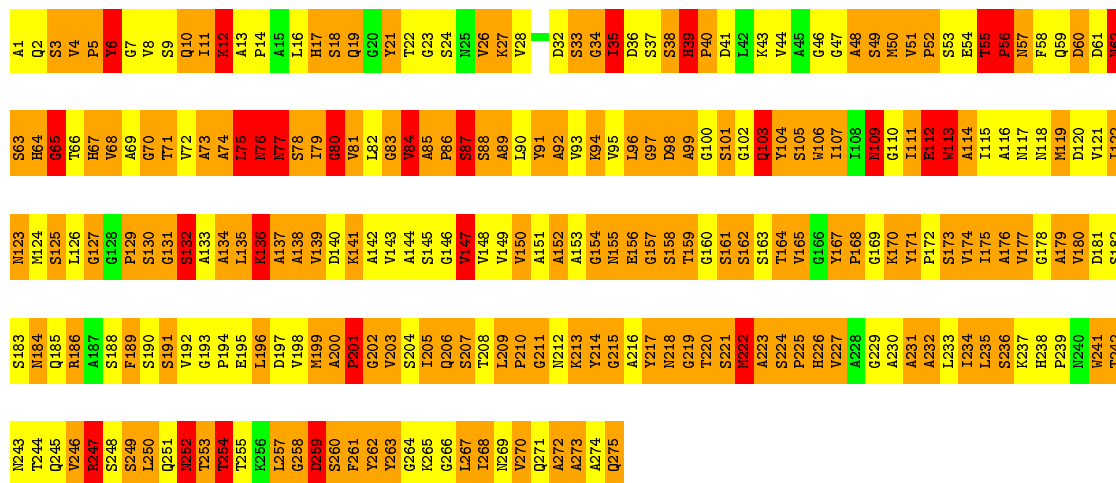
### 3 Residue-property plots

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.

Note EDS was not executed.

#### • Molecule 1: SUBTILISIN BPN'

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.70 Å 54.40 Å 62.90 Å 90.00° 91.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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	13.30	367/1976 (18.6%)	3.24	289/2697 (10.7%)

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	19

All (367) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	ASN	CG-OD1	561.54	13.59	1.24
1	A	76	ASN	CB-CG	45.28	2.55	1.51
1	A	112	GLU	CG-CD	-19.62	1.22	1.51
1	A	101	SER	CB-OG	-18.06	1.18	1.42
1	A	168	PRO	N-CD	16.35	1.70	1.47
1	A	156	GLU	CD-OE1	16.34	1.43	1.25
1	A	79	ILE	C-N	16.26	1.62	1.33
1	A	76	ASN	CG-ND2	15.63	1.72	1.32
1	A	189	PHE	CG-CD1	15.09	1.61	1.38
1	A	186	ARG	CZ-NH1	14.41	1.51	1.33
1	A	106	TRP	CD1-NE1	14.15	1.62	1.38
1	A	112	GLU	CB-CG	14.01	1.78	1.52
1	A	112	GLU	CD-OE1	13.46	1.40	1.25
1	A	91	TYR	CG-CD1	13.22	1.56	1.39
1	A	6	TYR	CG-CD2	12.97	1.56	1.39
1	A	111	ILE	CA-CB	12.69	1.84	1.54
1	A	87	SER	CA-CB	12.64	1.72	1.52
1	A	163	SER	C-O	-12.58	0.99	1.23
1	A	136	LYS	CD-CE	12.45	1.82	1.51
1	A	201	PRO	N-CA	-12.41	1.26	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLY	N-CA	-12.21	1.27	1.46
1	A	85	ALA	C-N	-12.05	1.11	1.34
1	A	7	GLY	CA-C	11.99	1.71	1.51
1	A	167	TYR	CG-CD1	11.73	1.54	1.39
1	A	57	ASN	CG-ND2	11.66	1.62	1.32
1	A	197	ASP	CB-CG	-11.63	1.27	1.51
1	A	130	SER	CB-OG	11.57	1.57	1.42
1	A	201	PRO	CA-C	11.26	1.75	1.52
1	A	147	VAL	C-O	11.22	1.44	1.23
1	A	112	GLU	CD-OE2	11.16	1.38	1.25
1	A	178	GLY	CA-C	11.07	1.69	1.51
1	A	201	PRO	N-CD	10.99	1.63	1.47
1	A	217	TYR	CG-CD2	10.98	1.53	1.39
1	A	26	VAL	C-N	10.80	1.58	1.34
1	A	113	TRP	CB-CG	10.73	1.69	1.50
1	A	263	TYR	C-N	-10.57	1.14	1.33
1	A	84	VAL	CA-CB	10.37	1.76	1.54
1	A	182	SER	CB-OG	-10.27	1.28	1.42
1	A	86	PRO	N-CD	10.11	1.62	1.47
1	A	194	PRO	N-CD	10.11	1.62	1.47
1	A	123	ASN	CB-CG	10.08	1.74	1.51
1	A	219	GLY	N-CA	10.02	1.61	1.46
1	A	151	ALA	C-O	-9.99	1.04	1.23
1	A	106	TRP	CZ3-CH2	-9.94	1.24	1.40
1	A	71	THR	C-O	9.93	1.42	1.23
1	A	87	SER	C-O	9.93	1.42	1.23
1	A	91	TYR	C-O	9.93	1.42	1.23
1	A	113	TRP	CG-CD1	-9.88	1.23	1.36
1	A	34	GLY	CA-C	-9.85	1.36	1.51
1	A	189	PHE	CE2-CZ	9.82	1.56	1.37
1	A	126	LEU	CA-CB	-9.80	1.31	1.53
1	A	49	SER	C-O	9.75	1.41	1.23
1	A	91	TYR	CZ-OH	-9.75	1.21	1.37
1	A	261	PHE	CG-CD2	-9.74	1.24	1.38
1	A	262	TYR	CE2-CZ	9.67	1.51	1.38
1	A	167	TYR	CB-CG	-9.63	1.37	1.51
1	A	60	ASP	CA-CB	9.61	1.75	1.53
1	A	96	LEU	CA-C	9.61	1.77	1.52
1	A	197	ASP	N-CA	9.51	1.65	1.46
1	A	219	GLY	C-N	-9.48	1.12	1.34
1	A	113	TRP	CD2-CE3	9.37	1.54	1.40
1	A	21	TYR	CB-CG	9.35	1.65	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	SER	CB-OG	9.35	1.54	1.42
1	A	182	SER	C-O	9.19	1.40	1.23
1	A	226	HIS	CE1-NE2	9.17	1.53	1.32
1	A	6	TYR	CE1-CZ	9.15	1.50	1.38
1	A	71	THR	CB-OG1	-9.15	1.25	1.43
1	A	127	GLY	C-O	9.15	1.38	1.23
1	A	216	ALA	CA-CB	9.13	1.71	1.52
1	A	102	GLY	C-O	8.92	1.38	1.23
1	A	129	PRO	N-CD	-8.92	1.35	1.47
1	A	146	GLY	C-O	8.92	1.38	1.23
1	A	259	ASP	N-CA	-8.92	1.28	1.46
1	A	139	VAL	C-N	8.85	1.54	1.34
1	A	132	SER	CB-OG	8.84	1.53	1.42
1	A	262	TYR	CB-CG	8.74	1.64	1.51
1	A	224	SER	C-O	-8.74	1.06	1.23
1	A	140	ASP	N-CA	-8.72	1.28	1.46
1	A	118	ASN	C-N	-8.71	1.14	1.34
1	A	196	LEU	C-N	-8.71	1.14	1.34
1	A	262	TYR	CG-CD1	8.69	1.50	1.39
1	A	150	VAL	CB-CG1	8.66	1.71	1.52
1	A	106	TRP	CE3-CZ3	8.61	1.53	1.38
1	A	36	ASP	N-CA	8.60	1.63	1.46
1	A	134	ALA	N-CA	8.60	1.63	1.46
1	A	4	VAL	C-N	-8.59	1.18	1.34
1	A	180	VAL	C-N	8.56	1.53	1.34
1	A	193	GLY	C-O	-8.54	1.09	1.23
1	A	167	TYR	CD2-CE2	8.51	1.52	1.39
1	A	55	THR	C-O	-8.49	1.07	1.23
1	A	76	ASN	C-O	-8.49	1.07	1.23
1	A	173	SER	C-O	-8.49	1.07	1.23
1	A	145	SER	CB-OG	-8.49	1.31	1.42
1	A	182	SER	CA-CB	8.48	1.65	1.52
1	A	195	GLU	CA-CB	8.43	1.72	1.53
1	A	218	ASN	C-N	-8.40	1.18	1.33
1	A	171	TYR	CE2-CZ	8.38	1.49	1.38
1	A	65	GLY	N-CA	8.34	1.58	1.46
1	A	172	PRO	CA-CB	8.30	1.70	1.53
1	A	53	SER	N-CA	8.29	1.62	1.46
1	A	207	SER	CA-C	8.19	1.74	1.52
1	A	224	SER	CA-C	8.19	1.74	1.52
1	A	176	ALA	CA-CB	8.15	1.69	1.52
1	A	218	ASN	CG-OD1	8.15	1.41	1.24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	GLY	N-CA	-8.12	1.33	1.46
1	A	151	ALA	CA-CB	8.01	1.69	1.52
1	A	129	PRO	CA-CB	8.01	1.69	1.53
1	A	154	GLY	C-O	-7.97	1.10	1.23
1	A	155	ASN	N-CA	-7.95	1.30	1.46
1	A	113	TRP	CZ3-CH2	-7.95	1.27	1.40
1	A	156	GLU	C-N	-7.93	1.18	1.33
1	A	177	VAL	C-N	-7.93	1.18	1.33
1	A	264	GLY	N-CA	7.92	1.57	1.46
1	A	65	GLY	CA-C	7.88	1.64	1.51
1	A	56	PRO	C-N	7.85	1.52	1.34
1	A	179	ALA	N-CA	7.83	1.62	1.46
1	A	195	GLU	CD-OE1	-7.80	1.17	1.25
1	A	131	GLY	C-O	7.78	1.36	1.23
1	A	181	ASP	CB-CG	7.78	1.68	1.51
1	A	82	LEU	CA-CB	7.77	1.71	1.53
1	A	158	SER	C-N	-7.76	1.16	1.34
1	A	76	ASN	N-CA	7.67	1.61	1.46
1	A	119	MET	N-CA	7.67	1.61	1.46
1	A	275	GLN	C-OXT	7.67	1.38	1.23
1	A	109	ASN	CG-OD1	7.66	1.40	1.24
1	A	38	SER	CA-C	7.63	1.72	1.52
1	A	104	TYR	CE1-CZ	7.61	1.48	1.38
1	A	97	GLY	CA-C	-7.57	1.39	1.51
1	A	60	ASP	N-CA	-7.57	1.31	1.46
1	A	113	TRP	N-CA	-7.57	1.31	1.46
1	A	174	VAL	N-CA	-7.57	1.31	1.46
1	A	35	ILE	N-CA	7.52	1.61	1.46
1	A	105	SER	CA-C	7.52	1.72	1.52
1	A	190	SER	CA-C	7.52	1.72	1.52
1	A	218	ASN	N-CA	7.52	1.61	1.46
1	A	27	LYS	CB-CG	7.50	1.72	1.52
1	A	227	VAL	CA-CB	7.48	1.70	1.54
1	A	54	GLU	CD-OE2	7.47	1.33	1.25
1	A	167	TYR	CE1-CZ	-7.42	1.28	1.38
1	A	98	ASP	C-N	7.42	1.51	1.34
1	A	182	SER	C-N	-7.38	1.17	1.34
1	A	82	LEU	N-CA	-7.38	1.31	1.46
1	A	190	SER	CB-OG	7.33	1.51	1.42
1	A	202	GLY	CA-C	7.31	1.63	1.51
1	A	26	VAL	C-O	7.29	1.37	1.23
1	A	258	GLY	N-CA	7.28	1.56	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	ASN	C-N	7.28	1.50	1.34
1	A	147	VAL	CB-CG1	7.25	1.68	1.52
1	A	180	VAL	CB-CG1	7.25	1.68	1.52
1	A	198	VAL	CB-CG1	7.25	1.68	1.52
1	A	171	TYR	CD1-CE1	-7.22	1.28	1.39
1	A	225	PRO	N-CA	-7.21	1.34	1.47
1	A	210	PRO	N-CD	7.20	1.57	1.47
1	A	129	PRO	CA-C	7.17	1.67	1.52
1	A	33	SER	CA-CB	-7.15	1.42	1.52
1	A	261	PHE	CG-CD1	7.13	1.49	1.38
1	A	97	GLY	N-CA	-7.13	1.35	1.46
1	A	200	ALA	C-O	7.10	1.36	1.23
1	A	91	TYR	CE1-CZ	7.08	1.47	1.38
1	A	217	TYR	CE1-CZ	7.08	1.47	1.38
1	A	122	ILE	CA-C	7.07	1.71	1.52
1	A	213	LYS	CA-C	7.07	1.71	1.52
1	A	55	THR	CA-CB	-7.06	1.34	1.53
1	A	163	SER	CA-CB	7.06	1.63	1.52
1	A	265	LYS	C-N	-7.00	1.20	1.33
1	A	57	ASN	N-CA	-7.00	1.32	1.46
1	A	72	VAL	N-CA	-7.00	1.32	1.46
1	A	154	GLY	C-N	6.99	1.50	1.34
1	A	6	TYR	CD2-CE2	-6.96	1.28	1.39
1	A	189	PHE	CE1-CZ	-6.95	1.24	1.37
1	A	215	GLY	CA-C	6.92	1.62	1.51
1	A	174	VAL	CA-CB	6.91	1.69	1.54
1	A	12	LYS	C-O	6.90	1.36	1.23
1	A	17	HIS	C-O	6.90	1.36	1.23
1	A	19	GLN	C-O	6.90	1.36	1.23
1	A	93	VAL	C-O	6.90	1.36	1.23
1	A	65	GLY	C-O	-6.89	1.12	1.23
1	A	185	GLN	CG-CD	6.88	1.66	1.51
1	A	162	SER	CA-CB	6.86	1.63	1.52
1	A	213	LYS	CB-CG	6.85	1.71	1.52
1	A	78	SER	C-N	-6.83	1.18	1.34
1	A	214	TYR	CE1-CZ	6.82	1.47	1.38
1	A	263	TYR	CE2-CZ	6.82	1.47	1.38
1	A	78	SER	N-CA	6.74	1.59	1.46
1	A	212	ASN	CA-C	6.73	1.70	1.52
1	A	232	ALA	CA-CB	6.73	1.66	1.52
1	A	191	SER	C-N	6.69	1.49	1.34
1	A	220	THR	C-N	6.69	1.49	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	ASN	CG-ND2	-6.66	1.16	1.32
1	A	77	ASN	CA-CB	6.65	1.70	1.53
1	A	124	MET	C-N	-6.64	1.18	1.34
1	A	147	VAL	C-N	-6.64	1.18	1.34
1	A	106	TRP	CA-CB	-6.62	1.39	1.53
1	A	91	TYR	CG-CD2	6.62	1.47	1.39
1	A	219	GLY	C-O	6.62	1.34	1.23
1	A	52	PRO	C-O	6.61	1.36	1.23
1	A	113	TRP	CD1-NE1	6.57	1.49	1.38
1	A	249	SER	CB-OG	6.56	1.50	1.42
1	A	58	PHE	CA-CB	6.56	1.68	1.53
1	A	92	ALA	C-N	6.55	1.49	1.34
1	A	263	TYR	CD1-CE1	6.51	1.49	1.39
1	A	181	ASP	CA-CB	-6.46	1.39	1.53
1	A	185	GLN	CA-CB	-6.46	1.39	1.53
1	A	129	PRO	C-N	-6.46	1.19	1.34
1	A	215	GLY	C-N	-6.46	1.19	1.34
1	A	189	PHE	CA-CB	6.42	1.68	1.53
1	A	66	THR	CB-OG1	-6.40	1.30	1.43
1	A	201	PRO	C-O	-6.40	1.10	1.23
1	A	214	TYR	CG-CD2	-6.40	1.30	1.39
1	A	177	VAL	CB-CG2	6.40	1.66	1.52
1	A	260	SER	CA-C	6.39	1.69	1.52
1	A	258	GLY	C-O	6.38	1.33	1.23
1	A	154	GLY	CA-C	6.35	1.62	1.51
1	A	157	GLY	CA-C	6.35	1.62	1.51
1	A	169	GLY	CA-C	6.35	1.62	1.51
1	A	198	VAL	C-O	6.32	1.35	1.23
1	A	214	TYR	C-O	-6.31	1.11	1.23
1	A	165	VAL	C-N	-6.31	1.21	1.33
1	A	224	SER	CB-OG	6.31	1.50	1.42
1	A	99	ALA	CA-CB	6.30	1.65	1.52
1	A	171	TYR	CE1-CZ	6.30	1.46	1.38
1	A	254	THR	C-N	-6.28	1.19	1.34
1	A	172	PRO	CA-C	6.26	1.65	1.52
1	A	140	ASP	CG-OD1	6.25	1.39	1.25
1	A	186	ARG	CZ-NH2	6.24	1.41	1.33
1	A	217	TYR	CD2-CE2	-6.19	1.30	1.39
1	A	158	SER	CB-OG	-6.16	1.34	1.42
1	A	221	SER	CB-OG	-6.16	1.34	1.42
1	A	83	GLY	C-O	6.15	1.33	1.23
1	A	100	GLY	N-CA	-6.14	1.36	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	GLY	N-CA	-6.14	1.36	1.46
1	A	62	ASN	CG-ND2	-6.14	1.17	1.32
1	A	123	ASN	CG-OD1	-6.14	1.10	1.24
1	A	222	MET	CA-CB	-6.14	1.40	1.53
1	A	39	HIS	C-O	6.12	1.34	1.23
1	A	177	VAL	C-O	6.12	1.34	1.23
1	A	36	ASP	C-N	6.11	1.48	1.34
1	A	261	PHE	CD1-CE1	6.10	1.51	1.39
1	A	19	GLN	C-N	6.07	1.44	1.33
1	A	103	GLN	N-CA	-6.05	1.34	1.46
1	A	156	GLU	N-CA	-6.05	1.34	1.46
1	A	224	SER	N-CA	-6.05	1.34	1.46
1	A	24	SER	CB-OG	6.05	1.50	1.42
1	A	224	SER	CA-CB	6.04	1.62	1.52
1	A	262	TYR	CE1-CZ	6.04	1.46	1.38
1	A	185	GLN	N-CA	5.95	1.58	1.46
1	A	119	MET	CB-CG	-5.93	1.32	1.51
1	A	155	ASN	CA-C	5.93	1.68	1.52
1	A	158	SER	CA-C	5.93	1.68	1.52
1	A	119	MET	C-O	5.93	1.34	1.23
1	A	106	TRP	CD2-CE2	-5.92	1.34	1.41
1	A	33	SER	C-N	5.88	1.43	1.33
1	A	101	SER	C-N	5.88	1.43	1.33
1	A	38	SER	CB-OG	-5.87	1.34	1.42
1	A	78	SER	CB-OG	-5.87	1.34	1.42
1	A	104	TYR	N-CA	-5.87	1.34	1.46
1	A	168	PRO	C-O	5.87	1.34	1.23
1	A	218	ASN	CA-CB	-5.86	1.38	1.53
1	A	196	LEU	C-O	-5.84	1.12	1.23
1	A	113	TRP	CZ2-CH2	5.83	1.48	1.37
1	A	172	PRO	N-CD	5.83	1.56	1.47
1	A	158	SER	CA-CB	5.83	1.61	1.52
1	A	104	TYR	CB-CG	-5.82	1.43	1.51
1	A	83	GLY	CA-C	-5.80	1.42	1.51
1	A	161	SER	N-CA	5.79	1.57	1.46
1	A	164	THR	N-CA	5.79	1.57	1.46
1	A	241	TRP	CD1-NE1	5.77	1.47	1.38
1	A	241	TRP	NE1-CE2	-5.76	1.30	1.37
1	A	141	LYS	CB-CG	5.75	1.68	1.52
1	A	18	SER	C-O	5.73	1.34	1.23
1	A	28	VAL	C-N	-5.73	1.20	1.34
1	A	49	SER	C-N	-5.73	1.20	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	LEU	C-O	5.73	1.34	1.23
1	A	84	VAL	C-O	5.73	1.34	1.23
1	A	85	ALA	C-O	5.73	1.34	1.23
1	A	105	SER	C-N	-5.73	1.20	1.34
1	A	125	SER	C-O	5.73	1.34	1.23
1	A	161	SER	C-O	5.73	1.34	1.23
1	A	186	ARG	C-O	5.73	1.34	1.23
1	A	218	ASN	C-O	5.73	1.34	1.23
1	A	67	HIS	CB-CG	-5.73	1.39	1.50
1	A	64	HIS	CG-ND1	-5.73	1.26	1.38
1	A	40	PRO	N-CA	5.72	1.56	1.47
1	A	152	ALA	CA-CB	5.72	1.64	1.52
1	A	32	ASP	CG-OD2	-5.69	1.12	1.25
1	A	61	ASP	CG-OD2	-5.69	1.12	1.25
1	A	2	GLN	CD-OE1	5.69	1.36	1.24
1	A	1	ALA	N-CA	-5.68	1.34	1.46
1	A	198	VAL	CB-CG2	5.67	1.64	1.52
1	A	186	ARG	CD-NE	-5.66	1.36	1.46
1	A	4	VAL	CA-CB	5.63	1.66	1.54
1	A	257	LEU	C-N	-5.62	1.23	1.33
1	A	36	ASP	CB-CG	5.62	1.63	1.51
1	A	113	TRP	CE3-CZ3	-5.62	1.28	1.38
1	A	186	ARG	NE-CZ	-5.62	1.25	1.33
1	A	3	SER	C-O	-5.61	1.12	1.23
1	A	184	ASN	C-O	-5.61	1.12	1.23
1	A	231	ALA	CA-CB	5.58	1.64	1.52
1	A	146	GLY	N-CA	5.57	1.54	1.46
1	A	52	PRO	C-N	-5.55	1.21	1.34
1	A	211	GLY	C-N	-5.55	1.21	1.34
1	A	64	HIS	C-O	5.54	1.33	1.23
1	A	106	TRP	CG-CD2	-5.54	1.34	1.43
1	A	226	HIS	C-O	5.54	1.33	1.23
1	A	148	VAL	CB-CG1	5.53	1.64	1.52
1	A	67	HIS	CE1-NE2	5.53	1.45	1.32
1	A	107	ILE	N-CA	-5.50	1.35	1.46
1	A	96	LEU	C-N	5.49	1.43	1.33
1	A	210	PRO	N-CA	-5.48	1.38	1.47
1	A	183	SER	CA-C	5.47	1.67	1.52
1	A	209	LEU	CA-C	5.47	1.67	1.52
1	A	66	THR	N-CA	5.47	1.57	1.46
1	A	175	ILE	N-CA	5.47	1.57	1.46
1	A	201	PRO	CA-CB	5.46	1.64	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	HIS	CG-CD2	5.45	1.45	1.35
1	A	206	GLN	CG-CD	5.43	1.63	1.51
1	A	141	LYS	CD-CE	5.41	1.64	1.51
1	A	104	TYR	CD2-CE2	5.38	1.47	1.39
1	A	137	ALA	C-N	-5.37	1.21	1.34
1	A	226	HIS	C-N	-5.37	1.21	1.34
1	A	186	ARG	CG-CD	5.37	1.65	1.51
1	A	150	VAL	CA-C	5.36	1.66	1.52
1	A	167	TYR	CA-C	5.36	1.66	1.52
1	A	257	LEU	CB-CG	5.36	1.68	1.52
1	A	24	SER	N-CA	5.31	1.56	1.46
1	A	117	ASN	N-CA	5.31	1.56	1.46
1	A	158	SER	N-CA	5.31	1.56	1.46
1	A	226	HIS	N-CA	5.31	1.56	1.46
1	A	273	ALA	N-CA	5.31	1.56	1.46
1	A	210	PRO	CA-CB	-5.31	1.43	1.53
1	A	37	SER	CB-OG	-5.30	1.35	1.42
1	A	246	VAL	CA-CB	-5.30	1.43	1.54
1	A	94	LYS	CG-CD	5.29	1.70	1.52
1	A	53	SER	CA-CB	-5.29	1.45	1.52
1	A	1	ALA	CA-CB	5.28	1.63	1.52
1	A	9	SER	CB-OG	5.28	1.49	1.42
1	A	18	SER	CB-OG	5.28	1.49	1.42
1	A	207	SER	CB-OG	5.28	1.49	1.42
1	A	248	SER	CB-OG	5.28	1.49	1.42
1	A	95	VAL	CB-CG1	-5.23	1.41	1.52
1	A	264	GLY	C-O	5.21	1.31	1.23
1	A	145	SER	C-N	-5.17	1.23	1.33
1	A	67	HIS	CG-ND1	5.17	1.50	1.38
1	A	241	TRP	CB-CG	5.14	1.59	1.50
1	A	191	SER	C-O	5.14	1.33	1.23
1	A	200	ALA	CA-CB	5.14	1.63	1.52
1	A	86	PRO	C-O	5.12	1.33	1.23
1	A	10	GLN	CB-CG	5.12	1.66	1.52
1	A	8	VAL	CB-CG1	5.09	1.63	1.52
1	A	165	VAL	CB-CG1	5.09	1.63	1.52
1	A	159	THR	CA-CB	5.09	1.66	1.53
1	A	111	ILE	CA-C	-5.08	1.39	1.52
1	A	257	LEU	CA-C	-5.08	1.39	1.52
1	A	195	GLU	CD-OE2	5.06	1.31	1.25
1	A	43	LYS	CE-NZ	5.06	1.61	1.49
1	A	263	TYR	CG-CD2	5.04	1.45	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	TYR	CZ-OH	-5.04	1.29	1.37
1	A	120	ASP	C-N	-5.01	1.22	1.34
1	A	160	GLY	C-N	-5.01	1.22	1.34
1	A	212	ASN	C-N	-5.01	1.22	1.34
1	A	72	VAL	CA-C	5.01	1.66	1.52
1	A	116	ALA	CA-C	5.01	1.66	1.52
1	A	181	ASP	CA-C	5.01	1.66	1.52
1	A	272	ALA	CA-C	5.01	1.66	1.52
1	A	6	TYR	CA-CB	-5.01	1.43	1.53
1	A	54	GLU	CA-CB	-5.01	1.43	1.53
1	A	61	ASP	CA-CB	-5.01	1.43	1.53

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH2	19.12	129.86	120.30
1	A	232	ALA	O-C-N	18.35	152.05	122.70
1	A	261	PHE	CB-CG-CD1	-17.97	108.22	120.80
1	A	76	ASN	OD1-CG-ND2	-16.36	84.26	121.90
1	A	213	LYS	CB-CA-C	-14.79	80.81	110.40
1	A	158	SER	N-CA-CB	-13.97	89.55	110.50
1	A	58	PHE	CB-CG-CD1	13.10	129.97	120.80
1	A	79	ILE	N-CA-CB	12.55	139.66	110.80
1	A	188	SER	CB-CA-C	-12.41	86.52	110.10
1	A	89	ALA	CB-CA-C	12.38	128.66	110.10
1	A	214	TYR	CB-CG-CD1	-12.13	113.72	121.00
1	A	74	ALA	N-CA-CB	-11.79	93.59	110.10
1	A	183	SER	N-CA-CB	11.68	128.01	110.50
1	A	263	TYR	CG-CD1-CE1	-11.66	111.97	121.30
1	A	263	TYR	CD1-CE1-CZ	11.35	130.01	119.80
1	A	76	ASN	CB-CG-OD1	11.09	143.78	121.60
1	A	75	LEU	CB-CA-C	-11.06	89.18	110.20
1	A	210	PRO	C-N-CA	10.82	145.03	122.30
1	A	104	TYR	CZ-CE2-CD2	10.73	129.46	119.80
1	A	182	SER	CA-C-O	-10.66	97.72	120.10
1	A	163	SER	N-CA-CB	-10.64	94.54	110.50
1	A	106	TRP	NE1-CE2-CZ2	-10.60	118.74	130.40
1	A	113	TRP	CD1-NE1-CE2	-10.41	99.63	109.00
1	A	217	TYR	CD1-CE1-CZ	-10.23	110.59	119.80
1	A	113	TRP	CE3-CZ3-CH2	10.22	132.45	121.20
1	A	61	ASP	CB-CG-OD2	10.13	127.42	118.30
1	A	263	TYR	CB-CG-CD2	-10.13	114.92	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	TYR	CD1-CE1-CZ	10.12	128.91	119.80
1	A	58	PHE	CB-CG-CD2	-10.07	113.75	120.80
1	A	112	GLU	OE1-CD-OE2	-9.98	111.33	123.30
1	A	247	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	A	214	TYR	CD1-CE1-CZ	9.89	128.70	119.80
1	A	232	ALA	CA-C-N	-9.89	95.44	117.20
1	A	84	VAL	CB-CA-C	-9.82	92.75	111.40
1	A	195	GLU	OE1-CD-OE2	-9.80	111.54	123.30
1	A	262	TYR	CB-CG-CD1	-9.64	115.21	121.00
1	A	261	PHE	CB-CG-CD2	9.63	127.54	120.80
1	A	224	SER	CA-C-O	9.59	140.24	120.10
1	A	140	ASP	CB-CG-OD2	9.59	126.93	118.30
1	A	182	SER	CA-C-N	9.49	138.07	117.20
1	A	63	SER	CB-CA-C	9.47	128.09	110.10
1	A	197	ASP	CB-CA-C	9.42	129.24	110.40
1	A	96	LEU	CA-C-N	-9.35	97.50	116.20
1	A	139	VAL	O-C-N	-9.20	107.98	122.70
1	A	6	TYR	CB-CG-CD1	9.20	126.52	121.00
1	A	189	PHE	CB-CG-CD2	9.17	127.22	120.80
1	A	164	THR	CA-CB-CG2	-9.06	99.71	112.40
1	A	161	SER	N-CA-CB	-9.05	96.92	110.50
1	A	199	MET	O-C-N	-9.04	108.24	122.70
1	A	141	LYS	O-C-N	-8.98	108.32	122.70
1	A	26	VAL	C-N-CA	-8.96	99.30	121.70
1	A	60	ASP	CB-CG-OD1	8.96	126.36	118.30
1	A	96	LEU	O-C-N	8.94	138.39	123.20
1	A	216	ALA	N-CA-CB	-8.92	97.62	110.10
1	A	215	GLY	O-C-N	8.86	136.88	122.70
1	A	214	TYR	CG-CD1-CE1	-8.85	114.22	121.30
1	A	151	ALA	CA-C-N	-8.81	97.82	117.20
1	A	189	PHE	CB-CG-CD1	-8.80	114.64	120.80
1	A	102	GLY	CA-C-O	-8.77	104.81	120.60
1	A	54	GLU	OE1-CD-OE2	-8.73	112.82	123.30
1	A	189	PHE	CG-CD1-CE1	-8.71	111.22	120.80
1	A	66	THR	CA-CB-CG2	-8.71	100.21	112.40
1	A	156	GLU	OE1-CD-OE2	-8.64	112.93	123.30
1	A	7	GLY	O-C-N	8.63	136.51	122.70
1	A	147	VAL	CA-CB-CG1	-8.63	97.95	110.90
1	A	262	TYR	CZ-CE2-CD2	-8.61	112.06	119.80
1	A	232	ALA	N-CA-CB	-8.57	98.10	110.10
1	A	163	SER	CA-C-N	-8.53	98.43	117.20
1	A	262	TYR	CG-CD2-CE2	8.41	128.03	121.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	O-C-N	8.39	136.12	122.70
1	A	111	ILE	CA-CB-CG2	-8.37	94.16	110.90
1	A	106	TRP	CD1-NE1-CE2	-8.33	101.51	109.00
1	A	164	THR	N-CA-CB	-8.29	94.54	110.30
1	A	125	SER	N-CA-CB	8.29	122.93	110.50
1	A	84	VAL	CA-CB-CG1	-8.24	98.54	110.90
1	A	217	TYR	CG-CD1-CE1	8.23	127.89	121.30
1	A	63	SER	N-CA-CB	-8.18	98.22	110.50
1	A	189	PHE	CZ-CE2-CD2	-8.16	110.31	120.10
1	A	262	TYR	CG-CD1-CE1	-8.16	114.78	121.30
1	A	208	THR	N-CA-CB	8.14	125.76	110.30
1	A	65	GLY	N-CA-C	-8.09	92.87	113.10
1	A	92	ALA	O-C-N	-8.08	109.77	122.70
1	A	104	TYR	CG-CD2-CE2	-8.06	114.85	121.30
1	A	263	TYR	CG-CD2-CE2	-8.02	114.88	121.30
1	A	259	ASP	CB-CG-OD1	7.97	125.48	118.30
1	A	106	TRP	CH2-CZ2-CE2	-7.96	109.44	117.40
1	A	106	TRP	CB-CG-CD1	-7.95	116.67	127.00
1	A	167	TYR	CD1-CE1-CZ	7.87	126.88	119.80
1	A	126	LEU	CB-CG-CD2	7.82	124.30	111.00
1	A	194	PRO	O-C-N	7.82	135.21	122.70
1	A	210	PRO	N-CA-CB	7.68	112.51	103.30
1	A	85	ALA	CB-CA-C	7.62	121.54	110.10
1	A	106	TRP	CE2-CD2-CG	7.59	113.37	107.30
1	A	186	ARG	CD-NE-CZ	7.53	134.14	123.60
1	A	102	GLY	CA-C-N	7.50	133.71	117.20
1	A	137	ALA	O-C-N	7.41	134.55	122.70
1	A	71	THR	CA-CB-CG2	-7.40	102.03	112.40
1	A	195	GLU	CG-CD-OE1	7.39	133.08	118.30
1	A	170	LYS	N-CA-CB	-7.35	97.37	110.60
1	A	151	ALA	O-C-N	7.34	134.45	122.70
1	A	190	SER	CA-C-N	-7.34	101.05	117.20
1	A	163	SER	O-C-N	7.33	134.43	122.70
1	A	104	TYR	CE1-CZ-CE2	-7.32	108.09	119.80
1	A	141	LYS	CB-CG-CD	-7.30	92.63	111.60
1	A	246	VAL	N-CA-C	7.27	130.62	111.00
1	A	96	LEU	CB-CG-CD1	-7.22	98.73	111.00
1	A	263	TYR	CD1-CG-CD2	7.17	125.78	117.90
1	A	130	SER	CA-C-O	7.15	135.11	120.10
1	A	203	VAL	CA-C-O	7.15	135.11	120.10
1	A	261	PHE	CG-CD2-CE2	7.13	128.65	120.80
1	A	91	TYR	CD1-CE1-CZ	7.09	126.18	119.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	TYR	CE1-CZ-CE2	-6.96	108.66	119.80
1	A	68	VAL	CA-CB-CG1	-6.96	100.46	110.90
1	A	106	TRP	CD2-CE2-CZ2	6.95	130.64	122.30
1	A	227	VAL	CA-CB-CG2	-6.94	100.49	110.90
1	A	7	GLY	CA-C-O	-6.93	108.12	120.60
1	A	186	ARG	NH1-CZ-NH2	-6.93	111.78	119.40
1	A	94	LYS	O-C-N	-6.90	111.66	122.70
1	A	193	GLY	CA-C-O	6.89	133.01	120.60
1	A	133	ALA	O-C-N	-6.88	111.70	122.70
1	A	177	VAL	C-N-CA	6.87	136.73	122.30
1	A	88	SER	CA-C-O	6.86	134.51	120.10
1	A	10	GLN	O-C-N	6.85	133.66	122.70
1	A	171	TYR	CD1-CE1-CZ	6.84	125.96	119.80
1	A	148	VAL	CA-CB-CG2	6.84	121.16	110.90
1	A	181	ASP	C-N-CA	-6.84	104.61	121.70
1	A	8	VAL	CG1-CB-CG2	-6.82	99.99	110.90
1	A	247	ARG	N-CA-C	-6.79	92.67	111.00
1	A	113	TRP	NE1-CE2-CZ2	-6.76	122.97	130.40
1	A	90	LEU	CB-CA-C	6.76	123.04	110.20
1	A	259	ASP	C-N-CA	6.69	138.43	121.70
1	A	78	SER	CA-C-O	-6.68	106.08	120.10
1	A	194	PRO	CA-C-N	-6.67	102.53	117.20
1	A	224	SER	O-C-N	-6.65	108.46	121.10
1	A	241	TRP	NE1-CE2-CZ2	-6.65	123.09	130.40
1	A	88	SER	O-C-N	-6.64	112.07	122.70
1	A	90	LEU	N-CA-CB	-6.62	97.16	110.40
1	A	34	GLY	CA-C-O	6.59	132.46	120.60
1	A	92	ALA	CA-C-O	6.59	133.93	120.10
1	A	176	ALA	N-CA-CB	-6.57	100.91	110.10
1	A	214	TYR	CZ-CE2-CD2	6.57	125.71	119.80
1	A	6	TYR	CG-CD2-CE2	6.56	126.55	121.30
1	A	62	ASN	CB-CG-OD1	-6.52	108.56	121.60
1	A	62	ASN	OD1-CG-ND2	6.50	136.84	121.90
1	A	130	SER	CA-C-N	-6.49	103.22	116.20
1	A	241	TRP	CE3-CZ3-CH2	6.47	128.32	121.20
1	A	94	LYS	CA-C-N	6.47	131.43	117.20
1	A	81	VAL	N-CA-C	6.46	128.44	111.00
1	A	11	ILE	CA-CB-CG2	-6.39	98.13	110.90
1	A	215	GLY	CA-C-O	-6.35	109.16	120.60
1	A	117	ASN	CB-CA-C	6.34	123.09	110.40
1	A	28	VAL	CB-CA-C	6.34	123.45	111.40
1	A	113	TRP	CG-CD1-NE1	6.32	116.42	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	THR	N-CA-C	-6.29	94.01	111.00
1	A	77	ASN	O-C-N	6.26	132.72	122.70
1	A	88	SER	N-CA-CB	-6.26	101.11	110.50
1	A	89	ALA	N-CA-C	-6.24	94.14	111.00
1	A	218	ASN	CB-CA-C	6.24	122.88	110.40
1	A	199	MET	CA-C-N	6.22	130.89	117.20
1	A	91	TYR	CG-CD1-CE1	-6.22	116.32	121.30
1	A	252	ASN	N-CA-C	6.21	127.76	111.00
1	A	257	LEU	CB-CG-CD1	-6.20	100.46	111.00
1	A	201	PRO	N-CA-CB	6.20	110.74	103.30
1	A	57	ASN	N-CA-CB	-6.19	99.46	110.60
1	A	85	ALA	N-CA-CB	6.15	118.71	110.10
1	A	50	MET	N-CA-CB	-6.13	99.57	110.60
1	A	260	SER	CB-CA-C	-6.12	98.47	110.10
1	A	220	THR	N-CA-CB	6.11	121.91	110.30
1	A	152	ALA	CB-CA-C	-6.08	100.98	110.10
1	A	82	LEU	CB-CA-C	-6.08	98.66	110.20
1	A	189	PHE	CG-CD2-CE2	6.04	127.44	120.80
1	A	139	VAL	CA-C-O	6.02	132.75	120.10
1	A	197	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	70	GLY	O-C-N	6.00	132.31	122.70
1	A	35	ILE	O-C-N	5.98	132.27	122.70
1	A	91	TYR	CA-CB-CG	-5.98	102.03	113.40
1	A	135	LEU	O-C-N	5.98	132.27	122.70
1	A	5	PRO	N-CD-CG	5.96	112.14	103.20
1	A	247	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	58	PHE	CB-CA-C	-5.93	98.53	110.40
1	A	64	HIS	CA-CB-CG	5.92	123.66	113.60
1	A	106	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	A	28	VAL	CA-C-N	5.91	130.19	117.20
1	A	213	LYS	CA-CB-CG	-5.88	100.47	113.40
1	A	37	SER	N-CA-CB	-5.87	101.69	110.50
1	A	70	GLY	C-N-CA	-5.87	107.02	121.70
1	A	62	ASN	N-CA-C	5.86	126.83	111.00
1	A	214	TYR	CE1-CZ-OH	5.86	135.91	120.10
1	A	84	VAL	CA-C-O	-5.85	107.81	120.10
1	A	196	LEU	O-C-N	5.82	132.02	122.70
1	A	263	TYR	CE1-CZ-CE2	-5.81	110.50	119.80
1	A	189	PHE	O-C-N	-5.79	113.43	122.70
1	A	222	MET	O-C-N	5.79	131.97	122.70
1	A	167	TYR	CA-C-O	-5.77	107.98	120.10
1	A	163	SER	CB-CA-C	5.77	121.06	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	VAL	CB-CA-C	-5.76	100.45	111.40
1	A	98	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	217	TYR	CA-C-N	-5.76	104.53	117.20
1	A	177	VAL	CB-CA-C	5.76	122.34	111.40
1	A	124	MET	CA-C-O	-5.74	108.04	120.10
1	A	171	TYR	CG-CD2-CE2	5.74	125.89	121.30
1	A	267	LEU	CA-C-N	-5.73	104.59	117.20
1	A	162	SER	N-CA-C	-5.72	95.55	111.00
1	A	122	ILE	N-CA-CB	5.72	123.95	110.80
1	A	61	ASP	CB-CA-C	5.71	121.81	110.40
1	A	121	VAL	CA-CB-CG1	5.70	119.44	110.90
1	A	197	ASP	N-CA-CB	-5.68	100.38	110.60
1	A	116	ALA	C-N-CA	-5.67	107.53	121.70
1	A	157	GLY	C-N-CA	-5.67	107.53	121.70
1	A	234	ILE	N-CA-C	-5.65	95.74	111.00
1	A	36	ASP	CA-CB-CG	-5.64	100.99	113.40
1	A	99	ALA	N-CA-CB	5.63	117.99	110.10
1	A	58	PHE	CA-C-N	-5.63	104.81	117.20
1	A	106	TRP	CG-CD2-CE3	-5.60	128.86	133.90
1	A	73	ALA	N-CA-C	5.59	126.09	111.00
1	A	113	TRP	CD2-CE2-CZ2	5.59	129.00	122.30
1	A	259	ASP	OD1-CG-OD2	-5.59	112.69	123.30
1	A	207	SER	N-CA-CB	-5.56	102.16	110.50
1	A	3	SER	CB-CA-C	-5.56	99.54	110.10
1	A	263	TYR	CZ-CE2-CD2	5.55	124.79	119.80
1	A	217	TYR	CA-CB-CG	-5.53	102.89	113.40
1	A	133	ALA	CA-C-O	5.53	131.71	120.10
1	A	223	ALA	N-CA-CB	-5.51	102.38	110.10
1	A	185	GLN	CB-CA-C	5.50	121.40	110.40
1	A	167	TYR	O-C-N	5.48	131.51	121.10
1	A	155	ASN	N-CA-CB	-5.48	100.74	110.60
1	A	182	SER	N-CA-CB	-5.47	102.29	110.50
1	A	194	PRO	C-N-CA	5.46	135.35	121.70
1	A	32	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	71	THR	CA-C-N	5.45	129.19	117.20
1	A	27	LYS	CA-CB-CG	-5.44	101.44	113.40
1	A	10	GLN	N-CA-CB	-5.43	100.83	110.60
1	A	28	VAL	CG1-CB-CG2	5.42	119.56	110.90
1	A	54	GLU	CB-CA-C	5.41	121.22	110.40
1	A	179	ALA	O-C-N	5.41	131.36	122.70
1	A	75	LEU	C-N-CA	5.39	135.17	121.70
1	A	21	TYR	CD1-CG-CD2	5.38	123.81	117.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASN	CB-CG-ND2	-5.37	103.80	116.70
1	A	171	TYR	CA-CB-CG	5.36	123.58	113.40
1	A	78	SER	CB-CA-C	5.35	120.27	110.10
1	A	165	VAL	CA-CB-CG1	-5.35	102.88	110.90
1	A	36	ASP	N-CA-CB	-5.34	100.99	110.60
1	A	246	VAL	CB-CA-C	-5.34	101.25	111.40
1	A	114	ALA	N-CA-CB	5.32	117.55	110.10
1	A	119	MET	CB-CA-C	5.32	121.05	110.40
1	A	151	ALA	N-CA-CB	-5.32	102.66	110.10
1	A	105	SER	CB-CA-C	-5.30	100.02	110.10
1	A	132	SER	N-CA-CB	-5.30	102.55	110.50
1	A	154	GLY	CA-C-O	5.29	130.12	120.60
1	A	79	ILE	N-CA-C	-5.25	96.83	111.00
1	A	76	ASN	CB-CA-C	5.24	120.89	110.40
1	A	174	VAL	N-CA-C	5.23	125.13	111.00
1	A	246	VAL	CA-CB-CG1	5.23	118.74	110.90
1	A	96	LEU	C-N-CA	-5.21	111.36	122.30
1	A	113	TRP	CE2-CD2-CG	5.21	111.47	107.30
1	A	124	MET	N-CA-CB	5.20	119.96	110.60
1	A	109	ASN	CB-CG-ND2	5.19	129.16	116.70
1	A	21	TYR	CB-CG-CD1	-5.17	117.89	121.00
1	A	64	HIS	N-CA-CB	-5.17	101.29	110.60
1	A	227	VAL	CA-CB-CG1	5.17	118.65	110.90
1	A	79	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	A	91	TYR	N-CA-CB	5.14	119.85	110.60
1	A	38	SER	N-CA-C	-5.14	97.13	111.00
1	A	71	THR	N-CA-C	-5.13	97.14	111.00
1	A	163	SER	C-N-CA	-5.13	108.86	121.70
1	A	241	TRP	NE1-CE2-CD2	5.13	112.43	107.30
1	A	205	ILE	N-CA-C	-5.12	97.18	111.00
1	A	132	SER	CA-C-O	5.11	130.84	120.10
1	A	78	SER	O-C-N	5.11	130.87	122.70
1	A	257	LEU	CA-CB-CG	-5.11	103.56	115.30
1	A	261	PHE	CB-CA-C	-5.09	100.22	110.40
1	A	91	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	207	SER	O-C-N	5.08	130.83	122.70
1	A	106	TRP	N-CA-CB	5.08	119.74	110.60
1	A	64	HIS	C-N-CA	5.08	132.96	122.30
1	A	82	LEU	O-C-N	5.08	131.83	123.20
1	A	138	ALA	N-CA-CB	-5.07	103.00	110.10
1	A	152	ALA	N-CA-CB	-5.07	103.01	110.10
1	A	199	MET	CA-CB-CG	-5.07	104.69	113.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	VAL	CA-C-N	-5.05	106.08	117.20
1	A	1	ALA	CB-CA-C	-5.05	102.52	110.10
1	A	65	GLY	CA-C-N	-5.04	106.10	117.20
1	A	84	VAL	CA-C-N	5.04	128.29	117.20
1	A	164	THR	CA-C-O	-5.04	109.51	120.10
1	A	232	ALA	N-CA-C	5.03	124.58	111.00
1	A	171	TYR	CB-CG-CD2	5.01	124.01	121.00
1	A	194	PRO	N-CA-CB	5.01	109.32	103.30
1	A	109	ASN	N-CA-CB	5.00	119.61	110.60
1	A	71	THR	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLN	Mainchain
1	A	109	ASN	Mainchain
1	A	136	LYS	Mainchain
1	A	147	VAL	Mainchain
1	A	157	GLY	Mainchain
1	A	196	LEU	Mainchain
1	A	247	ARG	Sidechain
1	A	261	PHE	Sidechain
1	A	266	GLY	Mainchain
1	A	39	HIS	Sidechain
1	A	44	VAL	Mainchain
1	A	51	VAL	Mainchain
1	A	56	PRO	Mainchain
1	A	62	ASN	Sidechain,Mainchain
1	A	76	ASN	Sidechain
1	A	78	SER	Mainchain
1	A	80	GLY	Mainchain
1	A	84	VAL	Mainchain

## 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	1938	0	1875	364	5
2	A	17	0	0	2	0
All	All	1955	0	1875	364	5

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 95.

All (364) 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:60:ASP:CB	1:A:60:ASP:CA	1.75	1.58
1:A:112:GLU:CB	1:A:112:GLU:CG	1.78	1.54
1:A:84:VAL:CB	1:A:84:VAL:CA	1.76	1.54
1:A:201:PRO:C	1:A:201:PRO:CA	1.75	1.53
1:A:111:ILE:CB	1:A:111:ILE:CA	1.84	1.51
1:A:136:LYS:CD	1:A:136:LYS:CE	1.82	1.51
1:A:96:LEU:CA	1:A:96:LEU:C	1.77	1.49
1:A:76:ASN:ND2	1:A:76:ASN:CG	1.71	1.42
1:A:168:PRO:CD	1:A:168:PRO:N	1.70	1.39
1:A:41:ASP:OD1	1:A:75:LEU:HG	1.28	1.34
1:A:22:THR:CB	1:A:87:SER:HG	1.42	1.32
1:A:233:LEU:HA	1:A:236:SER:OG	1.34	1.25
1:A:22:THR:CB	1:A:87:SER:OG	1.81	1.23
1:A:41:ASP:HB3	1:A:75:LEU:CD1	1.70	1.22
1:A:41:ASP:CG	1:A:75:LEU:HG	1.64	1.17
1:A:104:TYR:HE1	2:A:281:HOH:O	1.28	1.14
1:A:19:GLN:NE2	1:A:237:LYS:HZ2	1.48	1.12
1:A:75:LEU:CD2	1:A:79:ILE:O	1.99	1.11
1:A:75:LEU:N	1:A:75:LEU:HD12	1.65	1.10
1:A:274:ALA:O	1:A:275:GLN:HB2	1.45	1.10
1:A:41:ASP:HB3	1:A:75:LEU:HD12	1.14	1.07
1:A:253:THR:HG23	1:A:272:ALA:HB3	1.33	1.07
1:A:41:ASP:CB	1:A:75:LEU:CD1	2.35	1.03
1:A:57:ASN:ND2	1:A:92:ALA:O	1.92	1.03
1:A:97:GLY:HA3	1:A:101:SER:CB	1.88	1.02
1:A:253:THR:HG23	1:A:272:ALA:CB	1.89	1.02
1:A:253:THR:CG2	1:A:272:ALA:HB3	1.90	1.02
1:A:97:GLY:HA3	1:A:101:SER:HB2	1.40	1.01
1:A:41:ASP:CG	1:A:75:LEU:CG	2.29	0.99
1:A:56:PRO:HB2	1:A:59:GLN:CG	1.92	0.99
1:A:19:GLN:HG2	1:A:21:TYR:CE2	1.97	0.99
1:A:85:ALA:CB	1:A:233:LEU:HD11	1.94	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:THR:HB	1:A:87:SER:OG	1.64	0.96
1:A:19:GLN:HG2	1:A:21:TYR:HE2	1.27	0.96
1:A:75:LEU:HD21	1:A:79:ILE:O	1.65	0.93
1:A:84:VAL:C	1:A:86:PRO:HD3	1.89	0.93
1:A:97:GLY:CA	1:A:101:SER:HB2	1.98	0.93
1:A:233:LEU:HA	1:A:236:SER:HG	1.25	0.93
1:A:33:SER:O	1:A:94:LYS:HE3	1.68	0.93
1:A:242:THR:O	1:A:246:VAL:HG23	1.69	0.92
1:A:204:SER:N	1:A:218:ASN:OD1	2.00	0.92
1:A:84:VAL:HG12	1:A:84:VAL:C	1.90	0.92
1:A:253:THR:HG21	1:A:273:ALA:N	1.84	0.92
1:A:41:ASP:CG	1:A:75:LEU:CD1	2.37	0.92
1:A:84:VAL:CG1	1:A:84:VAL:C	2.39	0.91
1:A:97:GLY:HA3	1:A:101:SER:OG	1.70	0.91
1:A:112:GLU:CD	1:A:112:GLU:CB	2.39	0.90
1:A:135:LEU:O	1:A:139:VAL:HG23	1.71	0.90
1:A:84:VAL:CB	1:A:84:VAL:C	2.39	0.90
1:A:75:LEU:N	1:A:75:LEU:CD1	2.35	0.89
1:A:19:GLN:HE21	1:A:237:LYS:HZ2	1.00	0.88
1:A:274:ALA:O	1:A:275:GLN:CB	2.22	0.88
1:A:11:ILE:O	1:A:12:LYS:HB2	1.71	0.88
1:A:22:THR:OG1	1:A:87:SER:OG	1.62	0.88
1:A:14:PRO:HA	1:A:17:HIS:HB2	1.57	0.87
1:A:254:THR:HG22	1:A:268:ILE:HA	1.53	0.87
1:A:84:VAL:CG1	1:A:84:VAL:CA	2.53	0.87
1:A:19:GLN:NE2	1:A:237:LYS:NZ	2.22	0.87
1:A:16:LEU:HD22	1:A:270:VAL:HG12	1.57	0.87
1:A:233:LEU:CA	1:A:236:SER:OG	2.21	0.86
1:A:104:TYR:CE1	2:A:281:HOH:O	2.12	0.86
1:A:16:LEU:HD21	1:A:274:ALA:HB2	1.58	0.86
1:A:254:THR:HB	1:A:267:LEU:O	1.75	0.86
1:A:41:ASP:CG	1:A:75:LEU:HD11	1.97	0.85
1:A:111:ILE:CG2	1:A:111:ILE:CA	2.56	0.84
1:A:56:PRO:HB2	1:A:59:GLN:HG3	1.60	0.84
1:A:238:HIS:HB3	1:A:241:TRP:CD1	2.12	0.84
1:A:41:ASP:CB	1:A:75:LEU:HD11	2.06	0.84
1:A:75:LEU:HD23	1:A:79:ILE:O	1.75	0.83
1:A:122:ILE:HD12	1:A:147:VAL:HG11	1.61	0.83
1:A:56:PRO:HB2	1:A:59:GLN:HG2	1.60	0.83
1:A:62:ASN:OD1	1:A:98:ASP:HA	1.80	0.82
1:A:97:GLY:N	1:A:101:SER:HB2	1.94	0.82

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:SER:O	1:A:94:LYS:CE	2.28	0.82
1:A:96:LEU:CA	1:A:97:GLY:N	2.42	0.82
1:A:84:VAL:O	1:A:86:PRO:HD3	1.80	0.81
1:A:242:THR:OG1	1:A:245:GLN:HB2	1.81	0.81
1:A:142:ALA:O	1:A:147:VAL:HB	1.81	0.81
1:A:22:THR:HG1	1:A:87:SER:CB	1.95	0.79
1:A:255:THR:N	1:A:267:LEU:O	2.16	0.79
1:A:34:GLY:O	1:A:35:ILE:CG1	2.30	0.79
1:A:199:MET:HG2	1:A:263:TYR:O	1.83	0.79
1:A:122:ILE:CD1	1:A:147:VAL:HG11	2.11	0.78
1:A:174:VAL:O	1:A:247:ARG:NH1	2.17	0.78
1:A:222:MET:C	1:A:225:PRO:HD2	2.03	0.78
1:A:60:ASP:N	1:A:60:ASP:CB	2.45	0.78
1:A:167:TYR:C	1:A:168:PRO:CD	2.52	0.78
1:A:199:MET:CG	1:A:263:TYR:O	2.32	0.78
1:A:41:ASP:OD1	1:A:75:LEU:CG	2.22	0.77
1:A:254:THR:CB	1:A:267:LEU:O	2.33	0.76
1:A:56:PRO:CB	1:A:59:GLN:HG3	2.15	0.76
1:A:253:THR:CG2	1:A:272:ALA:CB	2.58	0.76
1:A:209:LEU:HD12	1:A:214:TYR:C	2.07	0.75
1:A:76:ASN:CB	1:A:76:ASN:CG	2.55	0.75
1:A:111:ILE:CG1	1:A:111:ILE:CA	2.66	0.74
1:A:55:THR:HB	1:A:56:PRO:CD	2.18	0.74
1:A:71:THR:HG21	1:A:226:HIS:CE1	2.23	0.73
1:A:75:LEU:HD12	1:A:75:LEU:H	1.51	0.73
1:A:84:VAL:CG2	1:A:84:VAL:CA	2.64	0.73
1:A:97:GLY:H	1:A:101:SER:HB2	1.54	0.73
1:A:68:VAL:O	1:A:70:GLY:N	2.22	0.72
1:A:3:SER:O	1:A:5:PRO:HD3	1.89	0.72
1:A:56:PRO:HG2	1:A:59:GLN:HG3	1.72	0.72
1:A:85:ALA:HA	1:A:233:LEU:HD11	1.71	0.71
1:A:136:LYS:CG	1:A:136:LYS:CE	2.69	0.71
1:A:56:PRO:CG	1:A:59:GLN:HG3	2.20	0.71
1:A:201:PRO:CA	1:A:202:GLY:N	2.52	0.71
1:A:40:PRO:HB2	1:A:79:ILE:HD11	1.73	0.71
1:A:13:ALA:N	1:A:14:PRO:HD2	2.05	0.71
1:A:85:ALA:HB2	1:A:233:LEU:HD11	1.74	0.70
1:A:238:HIS:HE1	1:A:275:GLN:HB2	1.55	0.70
1:A:153:ALA:HB1	1:A:165:VAL:HG22	1.72	0.70
1:A:179:ALA:HA	1:A:200:ALA:O	1.92	0.69
1:A:22:THR:C	1:A:87:SER:OG	2.30	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:CA	1:A:112:GLU:CG	2.69	0.69
1:A:84:VAL:O	1:A:86:PRO:CD	2.41	0.69
1:A:56:PRO:CB	1:A:59:GLN:CG	2.70	0.69
1:A:11:ILE:O	1:A:12:LYS:CB	2.41	0.69
1:A:254:THR:HG22	1:A:268:ILE:CA	2.23	0.68
1:A:233:LEU:N	1:A:233:LEU:HD12	2.07	0.68
1:A:34:GLY:O	1:A:35:ILE:HG13	1.94	0.68
1:A:48:ALA:H	1:A:57:ASN:ND2	1.92	0.68
1:A:258:GLY:O	1:A:263:TYR:HB2	1.93	0.67
1:A:34:GLY:O	1:A:35:ILE:HG12	1.93	0.67
1:A:55:THR:HG22	1:A:56:PRO:N	2.10	0.67
1:A:85:ALA:HB1	1:A:233:LEU:HD11	1.74	0.67
1:A:253:THR:O	1:A:253:THR:HG23	1.95	0.67
1:A:103:GLN:HB3	1:A:106:TRP:CD2	2.30	0.67
1:A:201:PRO:N	1:A:201:PRO:C	2.43	0.66
1:A:55:THR:CB	1:A:56:PRO:CD	2.74	0.66
1:A:60:ASP:OD1	1:A:63:SER:N	2.20	0.66
1:A:167:TYR:HD2	1:A:171:TYR:CZ	2.14	0.66
1:A:254:THR:CA	1:A:267:LEU:O	2.44	0.66
1:A:85:ALA:N	1:A:86:PRO:CD	2.60	0.65
1:A:73:ALA:HA	1:A:83:GLY:HA3	1.79	0.65
1:A:67:HIS:CD2	1:A:217:TYR:CD2	2.84	0.65
1:A:177:VAL:HG21	1:A:227:VAL:HG11	1.79	0.64
1:A:60:ASP:C	1:A:60:ASP:CB	2.63	0.64
1:A:253:THR:HG23	1:A:272:ALA:HB1	1.80	0.63
1:A:33:SER:HB3	1:A:96:LEU:HB2	1.80	0.63
1:A:13:ALA:N	1:A:14:PRO:CD	2.61	0.63
1:A:219:GLY:C	1:A:221:SER:N	2.50	0.63
1:A:22:THR:HG1	1:A:87:SER:HG	0.63	0.63
1:A:22:THR:CA	1:A:87:SER:OG	2.46	0.62
1:A:174:VAL:HG12	1:A:175:ILE:N	2.13	0.62
1:A:238:HIS:CG	1:A:241:TRP:CE2	2.87	0.62
1:A:223:ALA:C	1:A:225:PRO:HD2	2.19	0.62
1:A:96:LEU:C	1:A:96:LEU:CB	2.66	0.61
1:A:110:GLY:O	1:A:111:ILE:C	2.36	0.61
1:A:74:ALA:HB1	1:A:75:LEU:HD13	1.81	0.61
1:A:16:LEU:HD22	1:A:76:ASN:OD1	2.01	0.61
1:A:74:ALA:C	1:A:75:LEU:HD12	2.20	0.61
1:A:232:ALA:HB3	1:A:233:LEU:HD12	1.82	0.61
1:A:253:THR:O	1:A:253:THR:CG2	2.48	0.61
1:A:84:VAL:CB	1:A:84:VAL:N	2.61	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:CB	1:A:233:LEU:CD1	2.75	0.61
1:A:112:GLU:OE1	1:A:115:ILE:HD12	2.01	0.61
1:A:75:LEU:HD21	1:A:79:ILE:C	2.21	0.61
1:A:237:LYS:O	1:A:239:PRO:CD	2.49	0.61
1:A:253:THR:HG21	1:A:273:ALA:H	1.61	0.61
1:A:174:VAL:CG1	1:A:175:ILE:N	2.64	0.61
1:A:85:ALA:HB2	1:A:233:LEU:CD1	2.31	0.60
1:A:252:ASN:OD1	1:A:252:ASN:N	2.35	0.60
1:A:201:PRO:HG2	1:A:226:HIS:CD2	2.36	0.60
1:A:22:THR:OG1	1:A:87:SER:CB	2.46	0.60
1:A:125:SER:HB3	1:A:221:SER:HB2	1.81	0.60
1:A:235:LEU:O	1:A:239:PRO:CA	2.49	0.60
1:A:237:LYS:C	1:A:239:PRO:HD3	2.22	0.60
1:A:48:ALA:N	1:A:57:ASN:ND2	2.48	0.60
1:A:199:MET:HG3	1:A:263:TYR:O	2.02	0.60
1:A:156:GLU:HB2	1:A:164:THR:HB	1.84	0.60
1:A:74:ALA:HB1	1:A:75:LEU:CD1	2.32	0.60
1:A:235:LEU:O	1:A:239:PRO:HA	2.01	0.60
1:A:219:GLY:C	1:A:221:SER:H	2.04	0.60
1:A:68:VAL:C	1:A:70:GLY:H	2.05	0.59
1:A:152:ALA:HB1	1:A:220:THR:HG23	1.83	0.59
1:A:238:HIS:HB3	1:A:241:TRP:CG	2.36	0.59
1:A:209:LEU:HD11	1:A:215:GLY:HA3	1.84	0.59
1:A:154:GLY:H	1:A:220:THR:HG21	1.68	0.59
1:A:232:ALA:HB3	1:A:233:LEU:CD1	2.32	0.59
1:A:229:GLY:O	1:A:233:LEU:HD13	2.03	0.59
1:A:177:VAL:HG11	1:A:227:VAL:HG21	1.85	0.59
1:A:12:LYS:NZ	1:A:269:ASN:OD1	2.36	0.59
1:A:180:VAL:HG13	1:A:199:MET:HB3	1.84	0.59
1:A:211:GLY:O	1:A:213:LYS:HG3	2.03	0.58
1:A:179:ALA:HB1	1:A:202:GLY:HA3	1.85	0.58
1:A:111:ILE:O	1:A:114:ALA:HB3	2.03	0.58
1:A:209:LEU:O	1:A:213:LYS:HB2	2.02	0.58
1:A:237:LYS:O	1:A:239:PRO:HD2	2.04	0.58
1:A:80:GLY:HA3	1:A:214:TYR:CE2	2.38	0.58
1:A:207:SER:O	1:A:215:GLY:N	2.31	0.58
1:A:84:VAL:C	1:A:86:PRO:CD	2.67	0.57
1:A:167:TYR:CD2	1:A:171:TYR:CZ	2.91	0.57
1:A:127:GLY:CA	1:A:167:TYR:O	2.53	0.57
1:A:38:SER:O	1:A:40:PRO:HD3	2.03	0.57
1:A:122:ILE:CG1	1:A:147:VAL:HG11	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:MET:O	1:A:225:PRO:HD2	2.03	0.57
1:A:98:ASP:O	1:A:99:ALA:HB3	2.05	0.57
1:A:233:LEU:N	1:A:233:LEU:CD1	2.68	0.56
1:A:127:GLY:HA2	1:A:167:TYR:O	2.04	0.56
1:A:71:THR:HG21	1:A:226:HIS:ND1	2.20	0.56
1:A:136:LYS:HB2	1:A:171:TYR:CE1	2.40	0.56
1:A:136:LYS:HB2	1:A:171:TYR:CZ	2.41	0.56
1:A:184:ASN:HB3	1:A:257:LEU:HD13	1.85	0.56
1:A:109:ASN:O	1:A:112:GLU:HB2	2.05	0.56
1:A:85:ALA:N	1:A:86:PRO:HD3	2.14	0.56
1:A:177:VAL:CG1	1:A:227:VAL:HG21	2.35	0.56
1:A:253:THR:HG21	1:A:272:ALA:HB3	1.83	0.56
1:A:122:ILE:HD12	1:A:149:VAL:HG22	1.88	0.56
1:A:232:ALA:CB	1:A:233:LEU:HD12	2.36	0.56
1:A:41:ASP:OD2	1:A:75:LEU:HD11	2.05	0.56
1:A:143:VAL:HA	1:A:147:VAL:O	2.06	0.56
1:A:12:LYS:NZ	1:A:269:ASN:CG	2.60	0.56
1:A:74:ALA:C	1:A:75:LEU:CD1	2.74	0.55
1:A:238:HIS:HE1	1:A:274:ALA:O	1.89	0.55
1:A:119:MET:O	1:A:147:VAL:HG22	2.07	0.55
1:A:136:LYS:CD	1:A:136:LYS:NZ	2.66	0.55
1:A:209:LEU:CD1	1:A:215:GLY:HA3	2.35	0.55
1:A:229:GLY:O	1:A:230:ALA:C	2.44	0.55
1:A:97:GLY:CA	1:A:101:SER:CB	2.69	0.55
1:A:75:LEU:HB3	1:A:77:ASN:ND2	2.22	0.55
1:A:177:VAL:HG11	1:A:227:VAL:CG2	2.37	0.54
1:A:23:GLY:HA2	1:A:236:SER:HB3	1.89	0.54
1:A:60:ASP:CG	1:A:60:ASP:CA	2.67	0.54
1:A:111:ILE:CB	1:A:111:ILE:C	2.67	0.54
1:A:268:ILE:HG13	1:A:268:ILE:O	2.06	0.54
1:A:258:GLY:O	1:A:259:ASP:C	2.46	0.54
1:A:27:LYS:HG2	1:A:89:ALA:HB3	1.89	0.54
1:A:74:ALA:O	1:A:75:LEU:O	2.26	0.54
1:A:16:LEU:HD11	1:A:271:GLN:HA	1.90	0.53
1:A:134:ALA:O	1:A:137:ALA:N	2.41	0.53
1:A:154:GLY:CA	1:A:220:THR:HG21	2.38	0.53
1:A:131:GLY:O	1:A:132:SER:HB2	2.07	0.53
1:A:209:LEU:HD12	1:A:215:GLY:N	2.24	0.53
1:A:242:THR:OG1	1:A:245:GLN:OE1	2.27	0.53
1:A:34:GLY:C	1:A:35:ILE:HG13	2.28	0.53
1:A:33:SER:O	1:A:94:LYS:HE2	2.07	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLY:N	1:A:220:THR:HG21	2.23	0.53
1:A:238:HIS:CB	1:A:241:TRP:CE2	2.92	0.52
1:A:159:THR:O	1:A:159:THR:HG23	2.08	0.52
1:A:62:ASN:O	1:A:63:SER:HB3	2.09	0.52
1:A:84:VAL:HG12	1:A:84:VAL:O	2.10	0.52
1:A:255:THR:HB	1:A:267:LEU:HB3	1.90	0.52
1:A:186:ARG:HD2	1:A:262:TYR:HB3	1.90	0.52
1:A:237:LYS:C	1:A:239:PRO:CD	2.77	0.52
1:A:136:LYS:HB2	1:A:171:TYR:CE2	2.44	0.52
1:A:210:PRO:O	1:A:213:LYS:HD2	2.09	0.52
1:A:67:HIS:CG	1:A:217:TYR:HD2	2.27	0.52
1:A:23:GLY:O	1:A:88:SER:HA	2.10	0.52
1:A:55:THR:HB	1:A:56:PRO:HD3	1.91	0.52
1:A:27:LYS:HD3	1:A:91:TYR:CE1	2.45	0.52
1:A:189:PHE:C	1:A:189:PHE:CD1	2.83	0.52
1:A:167:TYR:CZ	1:A:170:LYS:HD3	2.45	0.51
1:A:224:SER:N	1:A:225:PRO:CD	2.72	0.51
1:A:177:VAL:O	1:A:220:THR:OG1	2.28	0.51
1:A:16:LEU:CD2	1:A:270:VAL:HG12	2.34	0.51
1:A:234:ILE:HD12	1:A:250:LEU:HD21	1.93	0.51
1:A:270:VAL:O	1:A:274:ALA:HB2	2.11	0.51
1:A:179:ALA:CB	1:A:202:GLY:HA3	2.41	0.50
1:A:249:SER:OG	1:A:273:ALA:O	2.28	0.50
1:A:64:HIS:O	1:A:68:VAL:HG23	2.11	0.50
1:A:41:ASP:OD1	1:A:79:ILE:HG13	2.11	0.50
1:A:237:LYS:O	1:A:239:PRO:HD3	2.11	0.50
1:A:125:SER:CB	1:A:221:SER:HB2	2.42	0.50
1:A:19:GLN:HE22	1:A:237:LYS:NZ	2.09	0.50
1:A:103:GLN:HG2	1:A:105:SER:OG	2.12	0.49
1:A:154:GLY:C	1:A:191:SER:HG	2.15	0.49
1:A:206:GLN:OE1	1:A:215:GLY:C	2.51	0.49
1:A:55:THR:HB	1:A:56:PRO:HD2	1.92	0.49
1:A:204:SER:CA	1:A:218:ASN:OD1	2.59	0.49
1:A:186:ARG:CD	1:A:262:TYR:HB3	2.43	0.49
1:A:13:ALA:HB3	1:A:14:PRO:HD3	1.95	0.48
1:A:84:VAL:CG1	1:A:84:VAL:O	2.61	0.48
1:A:222:MET:C	1:A:225:PRO:CD	2.78	0.48
1:A:55:THR:CB	1:A:56:PRO:HD3	2.42	0.48
1:A:186:ARG:HH21	1:A:192:VAL:CG1	2.26	0.48
1:A:47:GLY:HA3	1:A:92:ALA:O	2.14	0.48
1:A:184:ASN:HB3	1:A:257:LEU:CD1	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:HIS:CE1	1:A:274:ALA:O	2.66	0.48
1:A:244:THR:O	1:A:245:GLN:C	2.51	0.48
1:A:103:GLN:HB3	1:A:106:TRP:CE3	2.48	0.48
1:A:111:ILE:N	1:A:111:ILE:CB	2.69	0.48
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.59	0.48
1:A:155:ASN:OD1	1:A:220:THR:HG22	2.14	0.47
1:A:41:ASP:OD2	1:A:80:GLY:HA3	2.14	0.47
1:A:122:ILE:HG13	1:A:147:VAL:HG11	1.95	0.47
1:A:201:PRO:HG2	1:A:226:HIS:CG	2.48	0.47
1:A:22:THR:C	1:A:233:LEU:HG	2.35	0.47
1:A:39:HIS:ND1	1:A:40:PRO:HD2	2.29	0.47
1:A:235:LEU:O	1:A:239:PRO:N	2.47	0.47
1:A:46:GLY:O	1:A:92:ALA:N	2.47	0.47
1:A:85:ALA:CA	1:A:233:LEU:HD11	2.40	0.47
1:A:134:ALA:O	1:A:135:LEU:C	2.52	0.47
1:A:12:LYS:HZ1	1:A:269:ASN:CG	2.19	0.46
1:A:139:VAL:HG12	1:A:173:SER:OG	2.14	0.46
1:A:113:TRP:CD2	1:A:113:TRP:O	2.69	0.46
1:A:125:SER:HB3	1:A:221:SER:CB	2.44	0.46
1:A:122:ILE:HD12	1:A:147:VAL:CG1	2.41	0.46
1:A:68:VAL:HG13	1:A:225:PRO:HG3	1.97	0.46
1:A:17:HIS:HE2	1:A:86:PRO:CD	2.29	0.46
1:A:13:ALA:O	1:A:17:HIS:N	2.49	0.45
1:A:51:VAL:HA	1:A:52:PRO:HD2	1.62	0.45
1:A:6:TYR:OH	1:A:203:VAL:O	2.12	0.45
1:A:17:HIS:NE2	1:A:86:PRO:CD	2.80	0.45
1:A:104:TYR:CD1	1:A:107:ILE:HD12	2.50	0.45
1:A:238:HIS:HB3	1:A:241:TRP:CE2	2.51	0.45
1:A:67:HIS:CD2	1:A:217:TYR:HD2	2.34	0.45
1:A:250:LEU:HD13	1:A:250:LEU:HA	1.80	0.45
1:A:141:LYS:O	1:A:142:ALA:C	2.54	0.45
1:A:177:VAL:CG1	1:A:200:ALA:HB3	2.46	0.45
1:A:71:THR:O	1:A:84:VAL:N	2.44	0.45
1:A:219:GLY:HA3	1:A:222:MET:SD	2.57	0.45
1:A:159:THR:CG2	1:A:159:THR:O	2.65	0.45
1:A:233:LEU:H	1:A:233:LEU:CD1	2.30	0.45
1:A:47:GLY:O	1:A:48:ALA:HB2	2.17	0.45
1:A:41:ASP:O	1:A:75:LEU:N	2.42	0.45
1:A:26:VAL:HG21	1:A:232:ALA:O	2.16	0.45
1:A:17:HIS:HE2	1:A:86:PRO:HD2	1.81	0.44
1:A:74:ALA:HB3	1:A:83:GLY:N	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:C	1:A:35:ILE:CG1	2.84	0.44
1:A:34:GLY:O	1:A:65:GLY:HA3	2.18	0.44
1:A:19:GLN:HG2	1:A:21:TYR:CD2	2.51	0.44
1:A:55:THR:CG2	1:A:56:PRO:N	2.78	0.44
1:A:238:HIS:ND1	1:A:241:TRP:CZ2	2.85	0.44
1:A:85:ALA:C	1:A:87:SER:H	2.21	0.44
1:A:67:HIS:CE1	1:A:217:TYR:HB2	2.53	0.44
1:A:200:ALA:O	1:A:202:GLY:N	2.51	0.44
1:A:55:THR:CG2	1:A:56:PRO:HD3	2.48	0.44
1:A:4:VAL:HA	1:A:5:PRO:HD2	1.64	0.44
1:A:68:VAL:C	1:A:70:GLY:N	2.70	0.44
1:A:209:LEU:CD1	1:A:215:GLY:N	2.81	0.43
1:A:201:PRO:HB2	1:A:226:HIS:CE1	2.53	0.43
1:A:49:SER:O	1:A:50:MET:HE1	2.18	0.43
1:A:19:GLN:CG	1:A:21:TYR:HE2	2.13	0.43
1:A:222:MET:O	1:A:225:PRO:HG2	2.18	0.43
1:A:224:SER:HB3	1:A:225:PRO:HD3	2.01	0.43
1:A:84:VAL:CA	1:A:86:PRO:HD3	2.49	0.42
1:A:39:HIS:ND1	1:A:39:HIS:C	2.72	0.42
1:A:113:TRP:C	1:A:113:TRP:CD2	2.92	0.42
1:A:6:TYR:CD1	1:A:6:TYR:C	2.93	0.42
1:A:85:ALA:C	1:A:87:SER:N	2.72	0.42
1:A:34:GLY:HA3	1:A:60:ASP:HB2	2.02	0.42
1:A:11:ILE:O	1:A:12:LYS:NZ	2.33	0.42
1:A:142:ALA:O	1:A:147:VAL:N	2.44	0.42
1:A:96:LEU:HD23	1:A:101:SER:O	2.20	0.42
1:A:41:ASP:CB	1:A:75:LEU:HG	2.43	0.42
1:A:238:HIS:CB	1:A:241:TRP:CD2	3.03	0.41
1:A:12:LYS:HZ2	1:A:12:LYS:HB2	1.85	0.41
1:A:207:SER:O	1:A:214:TYR:HA	2.19	0.41
1:A:6:TYR:CZ	1:A:203:VAL:O	2.73	0.41
1:A:231:ALA:O	1:A:232:ALA:C	2.58	0.41
1:A:153:ALA:HB2	1:A:176:ALA:HB1	2.02	0.41
1:A:6:TYR:CZ	1:A:205:ILE:CD1	3.03	0.41
1:A:270:VAL:O	1:A:274:ALA:CB	2.69	0.41
1:A:199:MET:HG3	1:A:263:TYR:HA	2.02	0.41
1:A:223:ALA:C	1:A:225:PRO:CD	2.87	0.41
1:A:84:VAL:O	1:A:86:PRO:HD2	2.21	0.41
1:A:111:ILE:HG21	1:A:111:ILE:HD13	1.92	0.41
1:A:135:LEU:HA	1:A:135:LEU:HD12	1.83	0.41
1:A:201:PRO:C	1:A:201:PRO:CB	2.81	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ALA:O	1:A:139:VAL:C	2.59	0.40
1:A:49:SER:O	1:A:50:MET:CE	2.69	0.40
1:A:123:ASN:HA	1:A:150:VAL:O	2.21	0.40
1:A:67:HIS:CG	1:A:217:TYR:CD2	3.09	0.40

All (5) 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:55:THR:CG2	1:A:144:ALA:O[4_546]	0.95	1.25
1:A:6:TYR:CB	1:A:161:SER:OG[4_545]	1.90	0.30
1:A:18:SER:CB	1:A:162:SER:OG[3_545]	2.06	0.14
1:A:55:THR:CG2	1:A:144:ALA:C[4_546]	2.14	0.06
1:A:18:SER:OG	1:A:162:SER:OG[3_545]	2.14	0.06

## 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	273/275 (99%)	212 (78%)	43 (16%)	18 (7%)	 

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	35	ILE
1	A	55	THR
1	A	69	ALA
1	A	75	LEU
1	A	77	ASN
1	A	132	SER
1	A	48	ALA

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	76	ASN
1	A	81	VAL
1	A	112	GLU
1	A	113	TRP
1	A	259	ASP
1	A	260	SER
1	A	254	THR
1	A	201	PRO
1	A	65	GLY
1	A	80	GLY

### 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	205/205 (100%)	183 (89%)	22 (11%)	<b>8</b> <b>15</b>

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

Mol	Chain	Res	Type
1	A	6	TYR
1	A	75	LEU
1	A	76	ASN
1	A	77	ASN
1	A	87	SER
1	A	103	GLN
1	A	109	ASN
1	A	129	PRO
1	A	130	SER
1	A	158	SER
1	A	222	MET
1	A	235	LEU
1	A	236	SER
1	A	242	THR
1	A	243	ASN
1	A	247	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	250	LEU
1	A	251	GLN
1	A	252	ASN
1	A	253	THR
1	A	268	ILE
1	A	270	VAL

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	19	GLN
1	A	57	ASN
1	A	67	HIS
1	A	77	ASN
1	A	238	HIS
1	A	245	GLN

### 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 ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.