



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:47 PM GMT

PDB ID : 1CHG  
Title : CHYMOTRYPSINOGEN,2.5 ANGSTROMS CRYSTAL STRUCTURE,  
COMPARISON WITH ALPHA-CHYMOTRYPSIN,AND IMPLICATIONS  
FOR ZYMOGEN ACTIVATION  
Authors : Freer, S.T.; Kraut, J.; Robertus, J.D.; Wright, H.T.; Xuong, N.H.  
Deposited on : 1975-03-01  
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

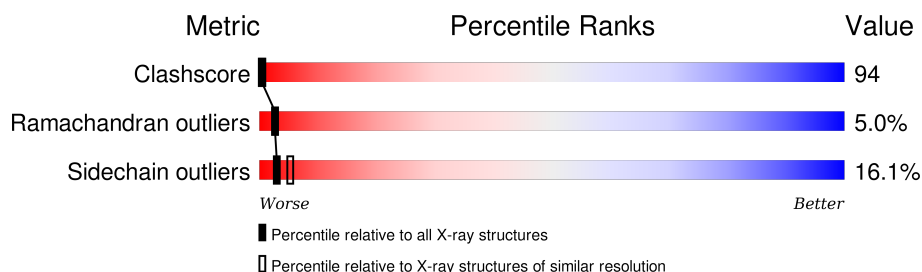
# 1 Overall quality at a glance

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	245	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1643 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 CHYMOTRYPSINOGEN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1643	1034	279	318	12	0	0	5

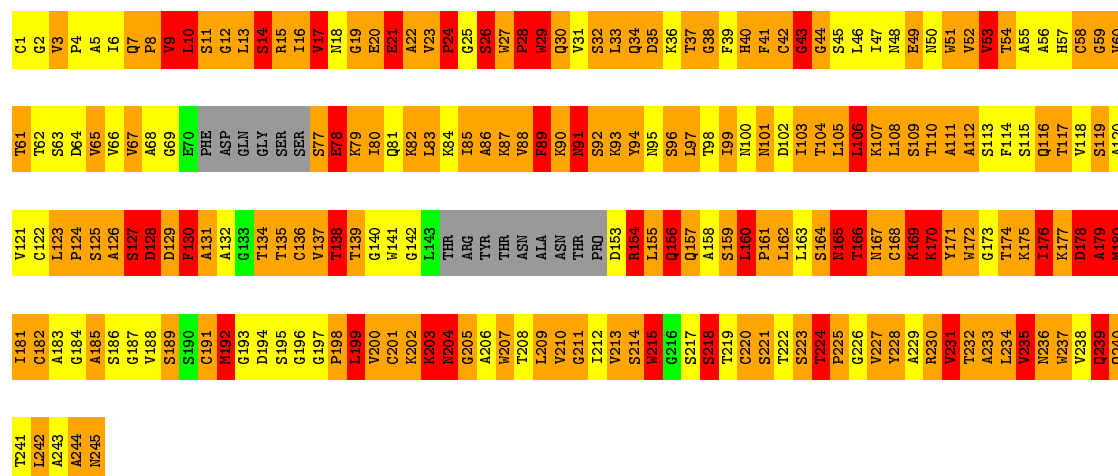
### 3 Residue-property plots

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: CHYMOTRYPSINOGEN A

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	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.00 Å 63.90 Å 77.10 Å 90.00° 90.00° 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, $R_{free}$	0.430 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1643	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	3.81	272/1673 (16.3%)	3.84	386/2277 (17.0%)

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	9

All (272) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ARG	N-CA	-20.18	1.05	1.46
1	A	127	SER	CB-OG	-17.93	1.19	1.42
1	A	43	GLY	CA-C	15.81	1.77	1.51
1	A	9	VAL	CA-CB	-14.71	1.23	1.54
1	A	141	TRP	CD2-CE2	14.29	1.58	1.41
1	A	78	GLU	CD-OE1	-14.27	1.09	1.25
1	A	20	GLU	CD-OE2	-14.13	1.10	1.25
1	A	126	ALA	N-CA	-13.65	1.19	1.46
1	A	29	TRP	CD1-NE1	13.58	1.61	1.38
1	A	51	TRP	NE1-CE2	-13.29	1.20	1.37
1	A	207	TRP	CD2-CE2	-13.23	1.25	1.41
1	A	207	TRP	NE1-CE2	-13.01	1.20	1.37
1	A	114	PHE	C-O	-12.77	0.99	1.23
1	A	128	ASP	CB-CG	12.59	1.78	1.51
1	A	9	VAL	N-CA	12.55	1.71	1.46
1	A	21	GLU	CD-OE1	12.36	1.39	1.25
1	A	54	THR	C-N	-12.34	1.05	1.34
1	A	19	GLY	CA-C	12.01	1.71	1.51
1	A	53	VAL	N-CA	-11.74	1.22	1.46
1	A	114	PHE	CG-CD1	-11.66	1.21	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	VAL	CB-CG2	-11.63	1.28	1.52
1	A	160	LEU	N-CA	11.24	1.68	1.46
1	A	218	SER	CB-OG	-11.08	1.27	1.42
1	A	125	SER	CA-C	11.06	1.81	1.52
1	A	117	THR	C-O	-10.95	1.02	1.23
1	A	241	THR	C-O	-10.55	1.03	1.23
1	A	91	ASN	N-CA	-10.52	1.25	1.46
1	A	178	ASP	CG-OD2	10.35	1.49	1.25
1	A	59	GLY	CA-C	10.30	1.68	1.51
1	A	207	TRP	C-O	-10.29	1.03	1.23
1	A	106	LEU	CA-CB	10.21	1.77	1.53
1	A	204	ASN	CG-OD1	-10.08	1.01	1.24
1	A	53	VAL	C-O	-10.02	1.04	1.23
1	A	242	LEU	N-CA	-9.88	1.26	1.46
1	A	89	PHE	CE2-CZ	9.79	1.55	1.37
1	A	38	GLY	N-CA	9.77	1.60	1.46
1	A	204	ASN	C-O	-9.71	1.04	1.23
1	A	60	VAL	C-O	-9.61	1.05	1.23
1	A	130	PHE	CE1-CZ	9.59	1.55	1.37
1	A	141	TRP	NE1-CE2	-9.59	1.25	1.37
1	A	49	GLU	CD-OE1	-9.54	1.15	1.25
1	A	89	PHE	CB-CG	9.40	1.67	1.51
1	A	142	GLY	C-O	9.39	1.38	1.23
1	A	141	TRP	CZ2-CH2	9.37	1.55	1.37
1	A	124	PRO	CA-CB	9.32	1.72	1.53
1	A	27	TRP	CD2-CE2	-9.30	1.30	1.41
1	A	194	ASP	CB-CG	9.19	1.71	1.51
1	A	128	ASP	CG-OD2	-9.05	1.04	1.25
1	A	171	TYR	CZ-OH	9.00	1.53	1.37
1	A	220	CYS	C-N	8.90	1.54	1.34
1	A	211	GLY	CA-C	8.88	1.66	1.51
1	A	77	SER	C-O	-8.88	1.06	1.23
1	A	215	TRP	CG-CD2	-8.78	1.28	1.43
1	A	112	ALA	C-N	-8.73	1.14	1.34
1	A	205	GLY	CA-C	8.72	1.65	1.51
1	A	155	LEU	C-O	-8.68	1.06	1.23
1	A	32	SER	CB-OG	8.62	1.53	1.42
1	A	64	ASP	CA-CB	-8.62	1.34	1.53
1	A	123	LEU	C-O	-8.54	1.07	1.23
1	A	3	VAL	C-O	-8.50	1.07	1.23
1	A	22	ALA	CA-CB	8.46	1.70	1.52
1	A	198	PRO	N-CD	8.43	1.59	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	CYS	C-O	8.38	1.39	1.23
1	A	12	GLY	C-O	8.33	1.36	1.23
1	A	235	VAL	CB-CG1	8.28	1.70	1.52
1	A	127	SER	C-O	-8.12	1.07	1.23
1	A	242	LEU	C-N	-8.03	1.15	1.34
1	A	194	ASP	CG-OD1	-7.93	1.07	1.25
1	A	185	ALA	C-O	-7.87	1.08	1.23
1	A	94	TYR	CZ-OH	7.83	1.51	1.37
1	A	154	ARG	CD-NE	7.81	1.59	1.46
1	A	204	ASN	CA-CB	7.80	1.73	1.53
1	A	173	GLY	N-CA	-7.75	1.34	1.46
1	A	89	PHE	CG-CD2	-7.73	1.27	1.38
1	A	19	GLY	N-CA	-7.73	1.34	1.46
1	A	224	THR	C-O	7.69	1.38	1.23
1	A	236	ASN	C-O	-7.68	1.08	1.23
1	A	131	ALA	C-N	-7.67	1.16	1.34
1	A	239	GLN	C-O	-7.65	1.08	1.23
1	A	130	PHE	N-CA	7.60	1.61	1.46
1	A	191	CYS	CB-SG	7.57	1.95	1.82
1	A	142	GLY	C-N	-7.57	1.16	1.34
1	A	164	SER	C-O	7.57	1.37	1.23
1	A	210	VAL	CB-CG1	7.55	1.68	1.52
1	A	82	LYS	CD-CE	7.55	1.70	1.51
1	A	242	LEU	C-O	7.55	1.37	1.23
1	A	203	LYS	CE-NZ	7.51	1.67	1.49
1	A	38	GLY	C-N	-7.47	1.16	1.34
1	A	9	VAL	C-N	-7.44	1.17	1.34
1	A	27	TRP	CA-CB	7.41	1.70	1.53
1	A	5	ALA	C-O	-7.41	1.09	1.23
1	A	236	ASN	N-CA	-7.38	1.31	1.46
1	A	44	GLY	C-O	-7.36	1.11	1.23
1	A	223	SER	N-CA	7.33	1.61	1.46
1	A	20	GLU	CB-CG	7.32	1.66	1.52
1	A	236	ASN	CB-CG	7.32	1.67	1.51
1	A	51	TRP	CD2-CE3	7.29	1.51	1.40
1	A	51	TRP	CD1-NE1	7.29	1.50	1.38
1	A	134	THR	N-CA	-7.27	1.31	1.46
1	A	113	SER	CA-CB	-7.23	1.42	1.52
1	A	11	SER	CB-OG	7.20	1.51	1.42
1	A	61	THR	C-O	-7.18	1.09	1.23
1	A	59	GLY	C-N	-7.17	1.17	1.34
1	A	34	GLN	CD-NE2	-7.17	1.15	1.32

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	GLN	CD-OE1	-7.13	1.08	1.24
1	A	130	PHE	CG-CD1	-7.13	1.28	1.38
1	A	160	LEU	C-N	-7.11	1.20	1.34
1	A	209	LEU	CA-C	7.11	1.71	1.52
1	A	27	TRP	CE2-CZ2	7.10	1.51	1.39
1	A	137	VAL	N-CA	7.08	1.60	1.46
1	A	245	ASN	CB-CG	7.06	1.67	1.51
1	A	57	HIS	C-O	7.05	1.36	1.23
1	A	222	THR	CB-OG1	-7.05	1.29	1.43
1	A	7	GLN	CD-NE2	7.04	1.50	1.32
1	A	104	THR	C-O	7.03	1.36	1.23
1	A	244	ALA	CA-CB	7.02	1.67	1.52
1	A	209	LEU	C-N	-7.01	1.18	1.34
1	A	93	LYS	CA-C	6.96	1.71	1.52
1	A	32	SER	C-N	-6.95	1.18	1.34
1	A	117	THR	CA-C	6.90	1.70	1.52
1	A	67	VAL	N-CA	-6.90	1.32	1.46
1	A	92	SER	C-O	-6.88	1.10	1.23
1	A	172	TRP	CD1-NE1	-6.85	1.26	1.38
1	A	218	SER	C-O	6.85	1.36	1.23
1	A	168	CYS	C-O	-6.85	1.10	1.23
1	A	59	GLY	C-O	-6.83	1.12	1.23
1	A	125	SER	C-O	-6.81	1.10	1.23
1	A	114	PHE	CA-C	6.81	1.70	1.52
1	A	156	GLN	C-O	-6.80	1.10	1.23
1	A	178	ASP	C-O	6.77	1.36	1.23
1	A	202	LYS	CB-CG	6.77	1.70	1.52
1	A	209	LEU	C-O	-6.74	1.10	1.23
1	A	30	GLN	C-O	-6.71	1.10	1.23
1	A	57	HIS	CB-CG	6.71	1.62	1.50
1	A	130	PHE	CB-CG	6.66	1.62	1.51
1	A	29	TRP	CD2-CE3	-6.63	1.30	1.40
1	A	139	THR	C-O	-6.62	1.10	1.23
1	A	52	VAL	C-O	6.62	1.35	1.23
1	A	94	TYR	C-N	-6.59	1.18	1.34
1	A	239	GLN	C-N	-6.57	1.19	1.34
1	A	20	GLU	N-CA	-6.56	1.33	1.46
1	A	205	GLY	C-N	-6.56	1.19	1.34
1	A	126	ALA	CA-CB	6.52	1.66	1.52
1	A	104	THR	C-N	-6.52	1.19	1.34
1	A	202	LYS	C-N	-6.52	1.19	1.34
1	A	132	ALA	C-O	6.51	1.35	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	CYS	CB-SG	-6.50	1.71	1.82
1	A	221	SER	CB-OG	-6.50	1.33	1.42
1	A	67	VAL	C-N	-6.49	1.19	1.34
1	A	224	THR	CB-OG1	-6.48	1.30	1.43
1	A	215	TRP	CD2-CE2	6.44	1.49	1.41
1	A	64	ASP	CB-CG	6.43	1.65	1.51
1	A	160	LEU	C-O	6.41	1.35	1.23
1	A	207	TRP	CG-CD1	-6.36	1.27	1.36
1	A	159	SER	CB-OG	-6.36	1.33	1.42
1	A	102	ASP	CA-CB	6.35	1.68	1.53
1	A	202	LYS	CE-NZ	6.34	1.65	1.49
1	A	81	GLN	N-CA	6.33	1.59	1.46
1	A	37	THR	C-O	-6.30	1.11	1.23
1	A	78	GLU	CA-CB	6.28	1.67	1.53
1	A	14	SER	CA-CB	-6.21	1.43	1.52
1	A	191	CYS	C-N	-6.17	1.19	1.34
1	A	236	ASN	CA-CB	6.17	1.69	1.53
1	A	29	TRP	CB-CG	-6.16	1.39	1.50
1	A	172	TRP	CZ3-CH2	-6.13	1.30	1.40
1	A	141	TRP	CD1-NE1	6.10	1.48	1.38
1	A	68	ALA	C-O	-6.09	1.11	1.23
1	A	1	CYS	CB-SG	6.07	1.92	1.82
1	A	226	GLY	C-O	-6.04	1.14	1.23
1	A	94	TYR	CB-CG	6.04	1.60	1.51
1	A	96	SER	CA-CB	6.03	1.61	1.52
1	A	21	GLU	CG-CD	6.02	1.60	1.51
1	A	194	ASP	C-N	-6.02	1.20	1.34
1	A	80	ILE	C-N	-5.99	1.20	1.34
1	A	207	TRP	CE2-CZ2	5.97	1.50	1.39
1	A	203	LYS	C-O	-5.96	1.12	1.23
1	A	101	ASN	N-CA	-5.93	1.34	1.46
1	A	207	TRP	CB-CG	5.93	1.60	1.50
1	A	92	SER	N-CA	-5.91	1.34	1.46
1	A	112	ALA	CA-C	5.87	1.68	1.52
1	A	201	CYS	C-O	-5.86	1.12	1.23
1	A	138	THR	C-O	-5.85	1.12	1.23
1	A	83	LEU	CA-C	5.85	1.68	1.52
1	A	43	GLY	N-CA	-5.84	1.37	1.46
1	A	113	SER	N-CA	5.83	1.58	1.46
1	A	175	LYS	C-N	-5.83	1.20	1.34
1	A	51	TRP	CA-C	5.79	1.68	1.52
1	A	27	TRP	CZ3-CH2	-5.76	1.30	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	TRP	C-N	5.76	1.43	1.33
1	A	20	GLU	C-O	-5.76	1.12	1.23
1	A	159	SER	CA-C	5.75	1.68	1.52
1	A	186	SER	CB-OG	5.73	1.49	1.42
1	A	28	PRO	CA-C	5.72	1.64	1.52
1	A	194	ASP	CA-CB	-5.71	1.41	1.53
1	A	141	TRP	CZ3-CH2	-5.71	1.30	1.40
1	A	67	VAL	CA-C	5.69	1.67	1.52
1	A	94	TYR	CD1-CE1	-5.66	1.30	1.39
1	A	85	ILE	CA-CB	5.66	1.67	1.54
1	A	41	PHE	CB-CG	5.65	1.60	1.51
1	A	165	ASN	C-N	-5.65	1.21	1.34
1	A	136	CYS	N-CA	5.64	1.57	1.46
1	A	21	GLU	CB-CG	-5.62	1.41	1.52
1	A	85	ILE	N-CA	5.59	1.57	1.46
1	A	5	ALA	N-CA	5.58	1.57	1.46
1	A	141	TRP	CD2-CE3	-5.57	1.31	1.40
1	A	141	TRP	CE2-CZ2	-5.57	1.30	1.39
1	A	221	SER	N-CA	-5.55	1.35	1.46
1	A	155	LEU	C-N	5.55	1.46	1.34
1	A	18	ASN	C-O	-5.54	1.12	1.23
1	A	78	GLU	C-O	-5.51	1.12	1.23
1	A	199	LEU	N-CA	5.51	1.57	1.46
1	A	69	GLY	CA-C	5.51	1.60	1.51
1	A	106	LEU	C-O	-5.50	1.12	1.23
1	A	24	PRO	CA-C	5.50	1.63	1.52
1	A	79	LYS	CA-CB	5.49	1.66	1.53
1	A	44	GLY	N-CA	5.49	1.54	1.46
1	A	94	TYR	CA-C	5.44	1.67	1.52
1	A	37	THR	CA-C	5.43	1.67	1.52
1	A	180	MET	C-O	-5.43	1.13	1.23
1	A	109	SER	N-CA	-5.43	1.35	1.46
1	A	32	SER	N-CA	-5.42	1.35	1.46
1	A	157	GLN	C-O	-5.41	1.13	1.23
1	A	124	PRO	CA-C	5.41	1.63	1.52
1	A	222	THR	N-CA	-5.40	1.35	1.46
1	A	68	ALA	N-CA	5.38	1.57	1.46
1	A	230	ARG	CB-CG	5.38	1.67	1.52
1	A	108	LEU	CA-CB	5.38	1.66	1.53
1	A	165	ASN	CG-ND2	-5.38	1.19	1.32
1	A	167	ASN	CG-OD1	-5.38	1.12	1.24
1	A	24	PRO	N-CD	5.38	1.55	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	THR	CB-OG1	5.36	1.53	1.43
1	A	239	GLN	CD-OE1	-5.34	1.12	1.24
1	A	64	ASP	CG-OD2	-5.34	1.13	1.25
1	A	153	ASP	C-O	-5.33	1.13	1.23
1	A	43	GLY	C-N	-5.33	1.23	1.33
1	A	33	LEU	N-CA	5.32	1.56	1.46
1	A	215	TRP	CE3-CZ3	5.31	1.47	1.38
1	A	68	ALA	CA-CB	5.30	1.63	1.52
1	A	94	TYR	CA-CB	-5.30	1.42	1.53
1	A	117	THR	N-CA	-5.28	1.35	1.46
1	A	27	TRP	C-N	-5.28	1.24	1.34
1	A	83	LEU	C-O	-5.28	1.13	1.23
1	A	210	VAL	N-CA	5.27	1.56	1.46
1	A	51	TRP	CB-CG	5.25	1.59	1.50
1	A	69	GLY	N-CA	-5.25	1.38	1.46
1	A	86	ALA	C-O	-5.25	1.13	1.23
1	A	165	ASN	C-O	5.24	1.33	1.23
1	A	113	SER	C-N	-5.23	1.22	1.34
1	A	125	SER	CB-OG	5.22	1.49	1.42
1	A	40	HIS	C-O	-5.20	1.13	1.23
1	A	91	ASN	CB-CG	5.19	1.62	1.51
1	A	18	ASN	CG-OD1	-5.19	1.12	1.24
1	A	91	ASN	CA-C	5.18	1.66	1.52
1	A	237	TRP	CD1-NE1	5.15	1.46	1.38
1	A	237	TRP	N-CA	-5.15	1.36	1.46
1	A	82	LYS	C-N	-5.15	1.22	1.34
1	A	245	ASN	CA-C	5.14	1.66	1.52
1	A	82	LYS	C-O	-5.14	1.13	1.23
1	A	27	TRP	CZ2-CH2	5.13	1.47	1.37
1	A	17	VAL	CA-CB	5.11	1.65	1.54
1	A	87	LYS	CB-CG	5.10	1.66	1.52
1	A	93	LYS	C-O	-5.10	1.13	1.23
1	A	187	GLY	C-N	-5.09	1.22	1.34
1	A	241	THR	CA-C	5.09	1.66	1.52
1	A	234	LEU	CB-CG	5.07	1.67	1.52
1	A	27	TRP	CD2-CE3	5.07	1.48	1.40
1	A	114	PHE	CD1-CE1	-5.04	1.29	1.39
1	A	107	LYS	CA-CB	-5.02	1.42	1.53
1	A	207	TRP	CZ2-CH2	-5.02	1.27	1.37
1	A	41	PHE	C-N	-5.01	1.22	1.34
1	A	37	THR	CA-CB	-5.01	1.40	1.53
1	A	163	LEU	N-CA	5.01	1.56	1.46

All (386) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	VAL	CB-CA-C	20.59	150.52	111.40
1	A	9	VAL	CA-CB-CG1	-20.23	80.55	110.90
1	A	55	ALA	CB-CA-C	16.76	135.24	110.10
1	A	94	TYR	CB-CG-CD1	-16.17	111.30	121.00
1	A	89	PHE	CZ-CE2-CD2	-14.79	102.35	120.10
1	A	215	TRP	CB-CG-CD1	-14.65	107.96	127.00
1	A	171	TYR	CB-CG-CD1	-13.78	112.73	121.00
1	A	195	SER	N-CA-CB	-13.37	90.44	110.50
1	A	55	ALA	N-CA-CB	-13.13	91.71	110.10
1	A	83	LEU	CB-CG-CD2	-13.09	88.75	111.00
1	A	132	ALA	CB-CA-C	13.06	129.69	110.10
1	A	141	TRP	CD1-NE1-CE2	12.86	120.57	109.00
1	A	215	TRP	CD1-CG-CD2	12.78	116.53	106.30
1	A	59	GLY	O-C-N	12.72	143.05	122.70
1	A	114	PHE	O-C-N	12.62	142.89	122.70
1	A	185	ALA	CB-CA-C	-12.49	91.36	110.10
1	A	94	TYR	N-CA-CB	12.49	133.08	110.60
1	A	194	ASP	CB-CG-OD1	-12.22	107.30	118.30
1	A	59	GLY	CA-C-N	-12.13	90.51	117.20
1	A	230	ARG	CA-C-N	-12.13	90.51	117.20
1	A	200	VAL	CA-CB-CG1	11.92	128.78	110.90
1	A	86	ALA	O-C-N	11.78	141.55	122.70
1	A	32	SER	N-CA-CB	11.71	128.06	110.50
1	A	34	GLN	O-C-N	11.55	141.18	122.70
1	A	89	PHE	N-CA-CB	11.28	130.91	110.60
1	A	155	LEU	CB-CG-CD2	-11.24	91.89	111.00
1	A	107	LYS	N-CA-CB	11.17	130.71	110.60
1	A	96	SER	CB-CA-C	-10.93	89.33	110.10
1	A	53	VAL	CG1-CB-CG2	-10.83	93.58	110.90
1	A	130	PHE	N-CA-CB	10.74	129.93	110.60
1	A	125	SER	O-C-N	10.59	139.65	122.70
1	A	169	LYS	CB-CA-C	10.46	131.32	110.40
1	A	159	SER	CA-C-N	-10.40	94.31	117.20
1	A	138	THR	CB-CA-C	10.36	139.57	111.60
1	A	231	VAL	CB-CA-C	10.34	131.04	111.40
1	A	27	TRP	CB-CG-CD2	10.33	140.03	126.60
1	A	123	LEU	CB-CG-CD2	10.28	128.47	111.00
1	A	17	VAL	C-N-CA	10.12	147.01	121.70
1	A	168	CYS	CA-CB-SG	-10.03	95.94	114.00
1	A	230	ARG	N-CA-C	9.98	137.95	111.00
1	A	227	VAL	CA-CB-CG2	-9.97	95.94	110.90
1	A	159	SER	O-C-N	9.96	138.63	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ALA	N-CA-CB	-9.91	96.22	110.10
1	A	130	PHE	CA-C-N	-9.86	95.52	117.20
1	A	93	LYS	N-CA-CB	9.85	128.33	110.60
1	A	32	SER	CB-CA-C	-9.77	91.53	110.10
1	A	222	THR	CA-C-N	-9.75	95.75	117.20
1	A	204	ASN	CB-CA-C	9.74	129.88	110.40
1	A	203	LYS	CA-C-N	-9.52	96.26	117.20
1	A	54	THR	N-CA-CB	9.50	128.35	110.30
1	A	29	TRP	CE3-CZ3-CH2	-9.47	110.78	121.20
1	A	68	ALA	CB-CA-C	9.47	124.31	110.10
1	A	183	ALA	CB-CA-C	-9.45	95.92	110.10
1	A	200	VAL	N-CA-CB	-9.44	90.73	111.50
1	A	207	TRP	CG-CD1-NE1	-9.37	100.73	110.10
1	A	34	GLN	CB-CG-CD	-9.27	87.50	111.60
1	A	230	ARG	CA-C-O	9.26	139.54	120.10
1	A	178	ASP	CB-CG-OD1	9.22	126.59	118.30
1	A	237	TRP	CZ3-CH2-CZ2	9.21	132.65	121.60
1	A	110	THR	CA-CB-CG2	-9.19	99.53	112.40
1	A	129	ASP	N-CA-CB	-9.18	94.07	110.60
1	A	180	MET	CB-CA-C	9.16	128.73	110.40
1	A	209	LEU	O-C-N	9.15	137.33	122.70
1	A	10	LEU	CB-CA-C	-9.09	92.93	110.20
1	A	49	GLU	CA-C-O	9.06	139.12	120.10
1	A	107	LYS	CB-CA-C	-9.00	92.39	110.40
1	A	8	PRO	C-N-CA	9.00	144.19	121.70
1	A	97	LEU	CB-CA-C	8.95	127.20	110.20
1	A	185	ALA	N-CA-CB	8.93	122.60	110.10
1	A	94	TYR	CG-CD2-CE2	-8.92	114.17	121.30
1	A	141	TRP	CG-CD2-CE3	8.89	141.90	133.90
1	A	141	TRP	CG-CD1-NE1	-8.86	101.24	110.10
1	A	61	THR	N-CA-CB	8.81	127.03	110.30
1	A	105	LEU	CB-CG-CD1	-8.76	96.11	111.00
1	A	117	THR	CA-CB-CG2	-8.70	100.22	112.40
1	A	119	SER	N-CA-CB	8.69	123.53	110.50
1	A	242	LEU	CB-CA-C	-8.69	93.70	110.20
1	A	111	ALA	N-CA-CB	-8.68	97.95	110.10
1	A	237	TRP	CE3-CZ3-CH2	-8.61	111.73	121.20
1	A	207	TRP	CG-CD2-CE3	-8.59	126.17	133.90
1	A	35	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	A	218	SER	O-C-N	-8.54	109.04	122.70
1	A	237	TRP	CE2-CD2-CG	8.52	114.12	107.30
1	A	18	ASN	CA-CB-CG	-8.52	94.65	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	VAL	CG1-CB-CG2	8.51	124.52	110.90
1	A	228	TYR	CZ-CE2-CD2	8.48	127.43	119.80
1	A	29	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	A	27	TRP	CB-CG-CD1	-8.27	116.25	127.00
1	A	241	THR	O-C-N	8.24	135.88	122.70
1	A	88	VAL	CB-CA-C	8.22	127.03	111.40
1	A	20	GLU	N-CA-CB	-8.22	95.80	110.60
1	A	112	ALA	O-C-N	8.20	135.81	122.70
1	A	194	ASP	OD1-CG-OD2	8.19	138.86	123.30
1	A	228	TYR	N-CA-CB	-8.18	95.88	110.60
1	A	215	TRP	CG-CD2-CE3	8.15	141.23	133.90
1	A	204	ASN	CA-C-N	-8.13	99.94	116.20
1	A	139	THR	CA-CB-CG2	-8.11	101.05	112.40
1	A	171	TYR	CB-CG-CD2	8.06	125.84	121.00
1	A	9	VAL	CG1-CB-CG2	8.04	123.77	110.90
1	A	112	ALA	N-CA-CB	8.04	121.35	110.10
1	A	91	ASN	N-CA-CB	-8.03	96.14	110.60
1	A	158	ALA	CB-CA-C	-8.02	98.08	110.10
1	A	94	TYR	CG-CD1-CE1	-8.01	114.89	121.30
1	A	135	THR	CA-CB-OG1	8.01	125.82	109.00
1	A	93	LYS	CB-CA-C	7.98	126.36	110.40
1	A	186	SER	CB-CA-C	7.98	125.26	110.10
1	A	88	VAL	N-CA-CB	-7.96	93.98	111.50
1	A	22	ALA	N-CA-C	7.95	132.46	111.00
1	A	161	PRO	O-C-N	-7.93	110.00	122.70
1	A	240	GLN	CB-CA-C	-7.91	94.58	110.40
1	A	174	THR	CB-CA-C	7.91	132.94	111.60
1	A	67	VAL	O-C-N	7.85	135.26	122.70
1	A	42	CYS	C-N-CA	-7.84	105.83	122.30
1	A	88	VAL	CA-CB-CG2	7.83	122.65	110.90
1	A	162	LEU	CB-CA-C	-7.83	95.32	110.20
1	A	192	MET	CA-CB-CG	7.81	126.58	113.30
1	A	171	TYR	CB-CA-C	-7.72	94.95	110.40
1	A	202	LYS	O-C-N	-7.72	110.35	122.70
1	A	199	LEU	CB-CG-CD2	-7.72	97.88	111.00
1	A	77	SER	O-C-N	7.71	135.04	122.70
1	A	162	LEU	CB-CG-CD2	7.70	124.08	111.00
1	A	179	ALA	CA-C-N	7.67	134.09	117.20
1	A	89	PHE	CG-CD1-CE1	-7.67	112.36	120.80
1	A	123	LEU	CB-CA-C	7.65	124.73	110.20
1	A	52	VAL	N-CA-C	-7.62	90.41	111.00
1	A	83	LEU	CB-CG-CD1	7.57	123.87	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	VAL	CA-C-O	-7.56	104.23	120.10
1	A	160	LEU	CB-CA-C	-7.50	95.95	110.20
1	A	177	LYS	N-CA-CB	-7.50	97.11	110.60
1	A	142	GLY	CA-C-O	-7.49	107.12	120.60
1	A	159	SER	C-N-CA	-7.49	102.98	121.70
1	A	94	TYR	CD1-CE1-CZ	7.48	126.54	119.80
1	A	124	PRO	CA-N-CD	7.46	122.15	111.70
1	A	213	VAL	CB-CA-C	-7.42	97.31	111.40
1	A	58	CYS	N-CA-CB	7.41	123.94	110.60
1	A	137	VAL	CB-CA-C	-7.41	97.33	111.40
1	A	237	TRP	CH2-CZ2-CE2	-7.40	110.00	117.40
1	A	132	ALA	N-CA-CB	-7.40	99.74	110.10
1	A	27	TRP	CB-CA-C	7.38	125.17	110.40
1	A	171	TYR	N-CA-CB	7.36	123.85	110.60
1	A	164	SER	CB-CA-C	-7.31	96.21	110.10
1	A	52	VAL	CA-C-O	7.30	135.44	120.10
1	A	214	SER	N-CA-CB	7.28	121.42	110.50
1	A	130	PHE	CZ-CE2-CD2	7.27	128.82	120.10
1	A	64	ASP	O-C-N	7.25	134.31	122.70
1	A	20	GLU	CA-CB-CG	7.21	129.27	113.40
1	A	162	LEU	O-C-N	7.21	134.23	122.70
1	A	194	ASP	CA-C-N	7.20	133.03	117.20
1	A	230	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	A	207	TRP	CA-C-O	7.12	135.05	120.10
1	A	29	TRP	CA-C-O	-7.12	105.16	120.10
1	A	166	THR	CA-CB-CG2	7.11	122.35	112.40
1	A	34	GLN	CA-C-N	-7.09	101.59	117.20
1	A	88	VAL	O-C-N	7.09	134.05	122.70
1	A	200	VAL	CB-CA-C	7.09	124.87	111.40
1	A	155	LEU	CB-CG-CD1	7.09	123.05	111.00
1	A	238	VAL	CA-CB-CG2	-7.09	100.27	110.90
1	A	138	THR	CA-CB-CG2	7.08	122.31	112.40
1	A	229	ALA	O-C-N	7.06	133.99	122.70
1	A	124	PRO	CB-CA-C	-7.04	94.39	112.00
1	A	50	ASN	N-CA-CB	-7.02	97.97	110.60
1	A	34	GLN	CA-CB-CG	7.01	128.81	113.40
1	A	134	THR	N-CA-CB	6.99	123.57	110.30
1	A	237	TRP	O-C-N	6.98	133.87	122.70
1	A	85	ILE	N-CA-CB	-6.97	94.77	110.80
1	A	181	ILE	CB-CA-C	-6.96	97.67	111.60
1	A	124	PRO	N-CA-CB	-6.96	94.94	102.60
1	A	14	SER	N-CA-CB	6.94	120.91	110.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ASN	N-CA-CB	-6.92	98.13	110.60
1	A	202	LYS	CA-C-N	6.91	132.41	117.20
1	A	240	GLN	N-CA-CB	6.91	123.03	110.60
1	A	191	CYS	O-C-N	6.89	133.73	122.70
1	A	116	GLN	CB-CA-C	-6.89	96.63	110.40
1	A	85	ILE	CA-CB-CG2	-6.87	97.17	110.90
1	A	223	SER	N-CA-CB	-6.85	100.23	110.50
1	A	220	CYS	CB-CA-C	-6.84	96.72	110.40
1	A	203	LYS	O-C-N	6.82	133.62	122.70
1	A	141	TRP	CD2-CE3-CZ3	6.82	127.66	118.80
1	A	41	PHE	CG-CD2-CE2	-6.81	113.31	120.80
1	A	89	PHE	CA-CB-CG	-6.79	97.59	113.90
1	A	206	ALA	CB-CA-C	6.75	120.22	110.10
1	A	106	LEU	CB-CA-C	-6.74	97.40	110.20
1	A	130	PHE	CD1-CE1-CZ	-6.72	112.04	120.10
1	A	244	ALA	CB-CA-C	-6.71	100.03	110.10
1	A	88	VAL	CA-CB-CG1	-6.70	100.85	110.90
1	A	89	PHE	CG-CD2-CE2	6.67	128.14	120.80
1	A	41	PHE	CB-CG-CD1	-6.66	116.14	120.80
1	A	57	HIS	CA-CB-CG	-6.65	102.30	113.60
1	A	91	ASN	CB-CA-C	-6.62	97.16	110.40
1	A	27	TRP	CG-CD2-CE3	-6.59	127.97	133.90
1	A	17	VAL	CA-CB-CG2	-6.58	101.02	110.90
1	A	108	LEU	N-CA-CB	-6.56	97.29	110.40
1	A	155	LEU	C-N-CA	-6.54	105.36	121.70
1	A	32	SER	C-N-CA	-6.53	105.38	121.70
1	A	29	TRP	CD2-CE3-CZ3	6.52	127.27	118.80
1	A	80	ILE	N-CA-CB	-6.50	95.84	110.80
1	A	159	SER	N-CA-CB	-6.48	100.79	110.50
1	A	131	ALA	O-C-N	-6.47	112.34	122.70
1	A	208	THR	N-CA-CB	-6.44	98.06	110.30
1	A	215	TRP	CB-CG-CD2	6.42	134.95	126.60
1	A	54	THR	O-C-N	6.42	132.97	122.70
1	A	23	VAL	CA-CB-CG2	6.42	120.52	110.90
1	A	53	VAL	CA-C-N	6.40	131.28	117.20
1	A	175	LYS	N-CA-CB	-6.40	99.08	110.60
1	A	229	ALA	N-CA-CB	-6.40	101.14	110.10
1	A	233	ALA	N-CA-CB	6.39	119.05	110.10
1	A	229	ALA	CA-C-N	-6.39	103.14	117.20
1	A	43	GLY	N-CA-C	-6.38	97.14	113.10
1	A	13	LEU	CB-CA-C	6.37	122.30	110.20
1	A	9	VAL	CA-C-N	6.36	131.20	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ASP	C-N-CA	-6.36	105.80	121.70
1	A	50	ASN	CB-CA-C	6.35	123.11	110.40
1	A	20	GLU	CB-CG-CD	-6.35	97.06	114.20
1	A	228	TYR	CG-CD2-CE2	-6.35	116.22	121.30
1	A	17	VAL	CA-CB-CG1	-6.34	101.39	110.90
1	A	224	THR	OG1-CB-CG2	6.34	124.58	110.00
1	A	154	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	124	PRO	CA-C-N	-6.32	103.30	117.20
1	A	27	TRP	CE3-CZ3-CH2	6.31	128.14	121.20
1	A	212	ILE	N-CA-C	-6.30	93.99	111.00
1	A	203	LYS	CA-CB-CG	-6.30	99.54	113.40
1	A	194	ASP	CA-CB-CG	6.27	127.20	113.40
1	A	29	TRP	O-C-N	6.27	132.73	122.70
1	A	234	LEU	CB-CG-CD1	-6.25	100.38	111.00
1	A	174	THR	N-CA-CB	-6.25	98.43	110.30
1	A	222	THR	CA-C-O	6.24	133.21	120.10
1	A	17	VAL	O-C-N	-6.24	112.72	122.70
1	A	162	LEU	N-CA-CB	6.23	122.86	110.40
1	A	130	PHE	CG-CD1-CE1	6.22	127.64	120.80
1	A	154	ARG	N-CA-CB	6.21	121.78	110.60
1	A	141	TRP	CD1-CG-CD2	6.21	111.27	106.30
1	A	22	ALA	O-C-N	6.20	132.63	122.70
1	A	60	VAL	N-CA-CB	-6.20	97.86	111.50
1	A	114	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	A	51	TRP	CH2-CZ2-CE2	6.17	123.57	117.40
1	A	80	ILE	O-C-N	6.17	132.58	122.70
1	A	125	SER	N-CA-CB	6.17	119.76	110.50
1	A	220	CYS	CA-CB-SG	-6.17	102.89	114.00
1	A	195	SER	CB-CA-C	6.17	121.82	110.10
1	A	61	THR	O-C-N	6.16	132.56	122.70
1	A	235	VAL	CA-CB-CG1	-6.16	101.67	110.90
1	A	53	VAL	O-C-N	-6.15	112.87	122.70
1	A	128	ASP	O-C-N	-6.15	112.87	122.70
1	A	221	SER	N-CA-CB	-6.14	101.28	110.50
1	A	87	LYS	CA-CB-CG	-6.14	99.89	113.40
1	A	160	LEU	O-C-N	-6.13	109.45	121.10
1	A	191	CYS	CA-C-O	-6.13	107.22	120.10
1	A	16	ILE	N-CA-CB	-6.13	96.70	110.80
1	A	103	ILE	CG1-CB-CG2	6.13	124.88	111.40
1	A	170	LYS	CD-CE-NZ	-6.12	97.63	111.70
1	A	242	LEU	CB-CG-CD1	6.11	121.38	111.00
1	A	234	LEU	CA-CB-CG	-6.10	101.26	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	GLN	N-CA-CB	6.09	121.57	110.60
1	A	125	SER	CA-C-O	-6.09	107.31	120.10
1	A	87	LYS	CB-CA-C	6.09	122.58	110.40
1	A	43	GLY	CA-C-N	6.08	128.36	116.20
1	A	90	LYS	O-C-N	-6.07	112.98	122.70
1	A	94	TYR	CD1-CG-CD2	6.06	124.57	117.90
1	A	154	ARG	CD-NE-CZ	-6.06	115.12	123.60
1	A	9	VAL	N-CA-C	-6.05	94.67	111.00
1	A	230	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	207	TRP	CE2-CD2-CG	6.04	112.14	107.30
1	A	169	LYS	N-CA-C	-6.02	94.74	111.00
1	A	108	LEU	CB-CA-C	6.00	121.61	110.20
1	A	8	PRO	CA-N-CD	6.00	120.10	111.70
1	A	158	ALA	CA-C-O	-6.00	107.50	120.10
1	A	237	TRP	CA-C-O	-5.99	107.52	120.10
1	A	114	PHE	CA-C-N	-5.99	104.03	117.20
1	A	131	ALA	CA-C-N	5.89	130.17	117.20
1	A	43	GLY	CA-C-O	-5.89	110.00	120.60
1	A	49	GLU	OE1-CD-OE2	5.88	130.36	123.30
1	A	207	TRP	CD1-NE1-CE2	5.87	114.29	109.00
1	A	207	TRP	CA-C-N	-5.86	104.30	117.20
1	A	99	ILE	O-C-N	-5.85	113.33	122.70
1	A	51	TRP	O-C-N	5.85	132.06	122.70
1	A	129	ASP	O-C-N	5.84	132.05	122.70
1	A	68	ALA	CA-C-N	-5.84	104.53	116.20
1	A	229	ALA	N-CA-C	5.84	126.76	111.00
1	A	237	TRP	CB-CA-C	5.83	122.05	110.40
1	A	195	SER	C-N-CA	5.82	134.52	122.30
1	A	141	TRP	NE1-CE2-CD2	-5.81	101.49	107.30
1	A	228	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	A	89	PHE	CB-CG-CD1	-5.79	116.75	120.80
1	A	178	ASP	N-CA-CB	5.79	121.01	110.60
1	A	208	THR	CA-CB-OG1	5.78	121.14	109.00
1	A	135	THR	N-CA-CB	-5.75	99.38	110.30
1	A	136	CYS	C-N-CA	-5.74	107.35	121.70
1	A	201	CYS	CA-C-N	-5.73	104.58	117.20
1	A	61	THR	C-N-CA	-5.73	107.38	121.70
1	A	104	THR	O-C-N	5.73	131.86	122.70
1	A	155	LEU	CB-CA-C	-5.70	99.36	110.20
1	A	129	ASP	CA-C-N	-5.70	104.67	117.20
1	A	244	ALA	O-C-N	5.68	131.80	122.70
1	A	29	TRP	CD2-CE2-CZ2	-5.68	115.48	122.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLU	CB-CG-CD	-5.67	98.89	114.20
1	A	97	LEU	N-CA-CB	-5.67	99.06	110.40
1	A	179	ALA	CA-C-O	-5.66	108.22	120.10
1	A	89	PHE	CD1-CG-CD2	5.65	125.65	118.30
1	A	192	MET	CA-C-O	5.64	131.96	120.10
1	A	113	SER	N-CA-CB	5.63	118.95	110.50
1	A	206	ALA	N-CA-C	-5.62	95.82	111.00
1	A	13	LEU	O-C-N	-5.61	113.73	122.70
1	A	200	VAL	CA-C-O	5.59	131.84	120.10
1	A	67	VAL	C-N-CA	-5.59	107.73	121.70
1	A	107	LYS	CA-CB-CG	5.57	125.66	113.40
1	A	130	PHE	O-C-N	5.57	131.62	122.70
1	A	33	LEU	CB-CA-C	5.56	120.77	110.20
1	A	202	LYS	CD-CE-NZ	-5.56	98.91	111.70
1	A	49	GLU	CA-C-N	-5.56	104.97	117.20
1	A	114	PHE	CG-CD1-CE1	5.55	126.91	120.80
1	A	245	ASN	CB-CA-C	5.55	121.50	110.40
1	A	31	VAL	C-N-CA	5.54	135.56	121.70
1	A	61	THR	CA-C-N	-5.54	105.01	117.20
1	A	218	SER	C-N-CA	5.54	135.55	121.70
1	A	13	LEU	C-N-CA	5.53	135.52	121.70
1	A	124	PRO	O-C-N	5.51	131.52	122.70
1	A	210	VAL	CA-CB-CG1	-5.51	102.64	110.90
1	A	93	LYS	N-CA-C	-5.50	96.14	111.00
1	A	52	VAL	CA-C-N	-5.50	105.10	117.20
1	A	194	ASP	O-C-N	-5.50	113.90	122.70
1	A	202	LYS	C-N-CA	5.49	135.41	121.70
1	A	80	ILE	CB-CA-C	5.48	122.56	111.60
1	A	138	THR	N-CA-C	-5.47	96.22	111.00
1	A	232	THR	CB-CA-C	5.46	126.35	111.60
1	A	10	LEU	CB-CG-CD2	5.46	120.28	111.00
1	A	170	LYS	N-CA-CB	-5.45	100.79	110.60
1	A	21	GLU	CG-CD-OE2	5.44	129.17	118.30
1	A	218	SER	CA-C-O	5.42	131.48	120.10
1	A	97	LEU	N-CA-C	-5.41	96.40	111.00
1	A	65	VAL	N-CA-CB	-5.38	99.67	111.50
1	A	89	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	93	LYS	CA-C-N	-5.36	105.42	117.20
1	A	244	ALA	N-CA-C	5.34	125.43	111.00
1	A	89	PHE	CE1-CZ-CE2	5.31	129.55	120.00
1	A	138	THR	CA-C-N	-5.29	105.56	117.20
1	A	194	ASP	CB-CG-OD2	-5.29	113.54	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	THR	CA-CB-OG1	5.28	120.08	109.00
1	A	176	ILE	N-CA-CB	-5.27	98.68	110.80
1	A	225	PRO	N-CA-CB	5.26	109.62	103.30
1	A	200	VAL	O-C-N	-5.26	114.28	122.70
1	A	172	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	A	111	ALA	CA-C-N	-5.24	105.66	117.20
1	A	115	SER	CB-CA-C	5.24	120.06	110.10
1	A	26	SER	O-C-N	5.24	131.08	122.70
1	A	7	GLN	N-CA-CB	-5.23	101.19	110.60
1	A	64	ASP	CA-C-O	-5.23	109.12	120.10
1	A	212	ILE	CA-CB-CG1	5.23	120.94	111.00
1	A	29	TRP	CB-CA-C	5.22	120.85	110.40
1	A	192	MET	N-CA-CB	5.22	120.00	110.60
1	A	44	GLY	O-C-N	5.22	131.05	122.70
1	A	52	VAL	CB-CA-C	5.21	121.31	111.40
1	A	230	ARG	N-CA-CB	-5.21	101.22	110.60
1	A	178	ASP	CB-CA-C	-5.21	99.98	110.40
1	A	161	PRO	CA-C-O	5.20	132.68	120.20
1	A	7	GLN	CA-C-O	5.19	130.99	120.10
1	A	203	LYS	C-N-CA	5.19	134.67	121.70
1	A	215	TRP	CE3-CZ3-CH2	-5.18	115.50	121.20
1	A	23	VAL	N-CA-CB	-5.17	100.12	111.50
1	A	189	SER	CA-C-O	5.17	130.96	120.10
1	A	191	CYS	CB-CA-C	-5.17	100.07	110.40
1	A	58	CYS	CB-CA-C	-5.16	100.07	110.40
1	A	107	LYS	CA-C-O	-5.16	109.26	120.10
1	A	82	LYS	N-CA-C	-5.15	97.08	111.00
1	A	220	CYS	O-C-N	-5.15	114.45	122.70
1	A	128	ASP	N-CA-CB	-5.15	101.33	110.60
1	A	170	LYS	CA-CB-CG	5.14	124.70	113.40
1	A	242	LEU	N-CA-CB	5.14	120.67	110.40
1	A	23	VAL	CA-CB-CG1	-5.13	103.21	110.90
1	A	53	VAL	N-CA-C	-5.12	97.17	111.00
1	A	230	ARG	CA-CB-CG	5.12	124.67	113.40
1	A	127	SER	CA-C-O	5.11	130.83	120.10
1	A	186	SER	O-C-N	5.11	131.89	123.20
1	A	54	THR	CA-C-O	-5.09	109.41	120.10
1	A	29	TRP	N-CA-CB	-5.08	101.45	110.60
1	A	176	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	A	163	LEU	CA-C-O	5.07	130.75	120.10
1	A	220	CYS	CA-C-O	5.07	130.75	120.10
1	A	237	TRP	CB-CG-CD1	5.07	133.59	127.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	THR	O-C-N	5.05	130.79	122.70
1	A	241	THR	CA-CB-CG2	-5.04	105.34	112.40
1	A	20	GLU	CA-C-O	5.03	130.67	120.10
1	A	68	ALA	O-C-N	5.03	131.74	123.20
1	A	130	PHE	CA-C-O	5.02	130.65	120.10
1	A	49	GLU	N-CA-CB	-5.02	101.56	110.60
1	A	103	ILE	CB-CA-C	5.02	121.63	111.60
1	A	231	VAL	CA-CB-CG2	5.02	118.42	110.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ARG	Sidechain
1	A	160	LEU	Mainchain
1	A	179	ALA	Mainchain
1	A	242	LEU	Mainchain
1	A	29	TRP	Mainchain
1	A	32	SER	Mainchain
1	A	43	GLY	Mainchain
1	A	53	VAL	Mainchain
1	A	9	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	1643	0	1598	304	52
All	All	1643	0	1598	304	52

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 94.

All (304) 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:106:LEU:CB	1:A:106:LEU:CA	1.77	1.55
1:A:203:LYS:NZ	1:A:203:LYS:CE	1.67	1.53
1:A:43:GLY:CA	1:A:43:GLY:C	1.77	1.51
1:A:128:ASP:CB	1:A:128:ASP:CG	1.78	1.50
1:A:160:LEU:CA	1:A:160:LEU:N	1.68	1.50
1:A:9:VAL:CA	1:A:9:VAL:N	1.71	1.50
1:A:125:SER:C	1:A:125:SER:CA	1.81	1.47
1:A:174:THR:O	1:A:177:LYS:NZ	1.58	1.34
1:A:54:THR:OG1	1:A:196:GLY:HA3	1.30	1.26
1:A:25:GLY:O	1:A:28:PRO:HD3	1.32	1.25
1:A:23:VAL:O	1:A:26:SER:CB	1.86	1.21
1:A:23:VAL:O	1:A:26:SER:HB2	0.93	1.09
1:A:162:LEU:HD13	1:A:181:ILE:HD11	1.31	1.09
1:A:34:GLN:OE1	1:A:38:GLY:HA2	1.52	1.08
1:A:136:CYS:HB3	1:A:200:VAL:O	1.50	1.08
1:A:165:ASN:O	1:A:169:LYS:HE3	1.55	1.07
1:A:35:ASP:OD1	1:A:39:PHE:HB3	1.52	1.06
1:A:2:GLY:O	1:A:4:PRO:HD3	1.56	1.05
1:A:20:GLU:O	1:A:156:GLN:HG3	1.56	1.04
1:A:239:GLN:HA	1:A:239:GLN:OE1	1.52	1.04
1:A:20:GLU:C	1:A:156:GLN:HG3	1.80	1.02
1:A:224:THR:CG2	1:A:225:PRO:HD2	1.89	1.02
1:A:224:THR:HG22	1:A:225:PRO:HD2	1.42	1.00
1:A:165:ASN:O	1:A:169:LYS:HB2	1.63	0.98
1:A:131:ALA:HB3	1:A:134:THR:OG1	1.64	0.97
1:A:87:LYS:HG2	1:A:88:VAL:H	1.30	0.97
1:A:95:ASN:O	1:A:99:ILE:N	1.98	0.97
1:A:159:SER:C	1:A:160:LEU:CA	2.33	0.96
1:A:34:GLN:HA	1:A:39:PHE:O	1.67	0.95
1:A:11:SER:OG	1:A:20:GLU:OE1	1.84	0.94
1:A:46:LEU:HD23	1:A:52:VAL:CG2	1.97	0.94
1:A:54:THR:OG1	1:A:196:GLY:CA	2.15	0.93
1:A:243:ALA:CA	1:A:244:ALA:N	2.31	0.93
1:A:172:TRP:HB2	1:A:176:ILE:CD1	1.98	0.92
1:A:27:TRP:CG	1:A:139:THR:HG21	2.05	0.91
1:A:34:GLN:HE22	1:A:82:LYS:HE3	1.35	0.90
1:A:20:GLU:O	1:A:156:GLN:CG	2.19	0.89
1:A:46:LEU:HD23	1:A:52:VAL:HG22	1.55	0.89
1:A:23:VAL:C	1:A:26:SER:HB2	1.92	0.89
1:A:171:TYR:CD2	1:A:225:PRO:HG3	2.08	0.88
1:A:16:ILE:HG22	1:A:17:VAL:HG23	1.55	0.88
1:A:87:LYS:HG2	1:A:88:VAL:N	1.86	0.86

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:O	1:A:188:VAL:HB	1.76	0.86
1:A:16:ILE:CG2	1:A:17:VAL:HG23	2.05	0.85
1:A:189:SER:O	1:A:192:MET:CE	2.23	0.85
1:A:177:LYS:O	1:A:178:ASP:C	2.13	0.85
1:A:27:TRP:CB	1:A:139:THR:HG21	2.06	0.85
1:A:34:GLN:NE2	1:A:82:LYS:HE3	1.92	0.84
1:A:25:GLY:O	1:A:28:PRO:CD	2.23	0.83
1:A:20:GLU:C	1:A:156:GLN:CG	2.46	0.83
1:A:65:VAL:HG11	1:A:82:LYS:HG2	1.61	0.82
1:A:9:VAL:N	1:A:9:VAL:CB	2.39	0.82
1:A:172:TRP:HB2	1:A:176:ILE:HD13	1.61	0.81
1:A:134:THR:O	1:A:161:PRO:HA	1.81	0.81
1:A:164:SER:HB3	1:A:167:ASN:HB2	1.63	0.80
1:A:22:ALA:HB2	1:A:157:GLN:OE1	1.82	0.80
1:A:2:GLY:C	1:A:4:PRO:HD3	2.02	0.80
1:A:54:THR:HG1	1:A:196:GLY:HA3	1.45	0.80
1:A:203:LYS:HG3	1:A:204:ASN:OD1	1.83	0.79
1:A:106:LEU:CB	1:A:106:LEU:C	2.52	0.78
1:A:44:GLY:HA2	1:A:196:GLY:O	1.82	0.78
1:A:65:VAL:CG1	1:A:82:LYS:HG2	2.12	0.78
1:A:10:LEU:HD23	1:A:10:LEU:N	1.99	0.78
1:A:100:ASN:ND2	1:A:177:LYS:HB2	1.98	0.78
1:A:108:LEU:N	1:A:108:LEU:HD12	1.99	0.77
1:A:43:GLY:N	1:A:43:GLY:C	2.37	0.76
1:A:26:SER:O	1:A:28:PRO:HD2	1.85	0.76
1:A:175:LYS:O	1:A:180:MET:SD	2.44	0.76
1:A:35:ASP:CG	1:A:39:PHE:HB3	2.06	0.75
1:A:159:SER:C	1:A:160:LEU:HA	2.06	0.75
1:A:224:THR:HG23	1:A:225:PRO:HD2	1.69	0.74
1:A:172:TRP:HB2	1:A:176:ILE:HD11	1.67	0.74
1:A:47:ILE:CA	1:A:120:ALA:HB1	2.17	0.74
1:A:11:SER:O	1:A:14:SER:HB2	1.88	0.74
1:A:235:VAL:O	1:A:239:GLN:HG2	1.87	0.74
1:A:200:VAL:HG13	1:A:207:TRP:HB3	1.68	0.73
1:A:61:THR:OG1	1:A:62:THR:N	2.19	0.73
1:A:6:ILE:HD11	1:A:116:GLN:HB3	1.70	0.73
1:A:172:TRP:CB	1:A:176:ILE:CD1	2.66	0.73
1:A:91:ASN:HB2	1:A:237:TRP:CZ2	2.24	0.73
1:A:174:THR:O	1:A:177:LYS:CE	2.37	0.72
1:A:9:VAL:N	1:A:9:VAL:C	2.42	0.72
1:A:127:SER:O	1:A:128:ASP:C	2.22	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HA	1:A:112:ALA:HB3	1.71	0.72
1:A:2:GLY:O	1:A:4:PRO:CD	2.37	0.71
1:A:160:LEU:HB3	1:A:184:GLY:HA2	1.70	0.71
1:A:164:SER:HB3	1:A:167:ASN:H	1.56	0.71
1:A:202:LYS:O	1:A:203:LYS:HB2	1.90	0.70
1:A:47:ILE:C	1:A:120:ALA:HB1	2.11	0.70
1:A:239:GLN:CA	1:A:239:GLN:OE1	2.37	0.70
1:A:85:ILE:HG21	1:A:88:VAL:CG2	2.21	0.69
1:A:164:SER:HB3	1:A:167:ASN:CB	2.22	0.69
1:A:30:GLN:NE2	1:A:198:PRO:CD	2.55	0.69
1:A:224:THR:CG2	1:A:225:PRO:CD	2.68	0.69
1:A:87:LYS:CG	1:A:88:VAL:H	2.05	0.68
1:A:181:ILE:HG23	1:A:181:ILE:O	1.93	0.68
1:A:165:ASN:O	1:A:169:LYS:CE	2.39	0.68
1:A:164:SER:CB	1:A:167:ASN:HB2	2.23	0.68
1:A:46:LEU:CD2	1:A:52:VAL:CG2	2.72	0.68
1:A:203:LYS:NZ	1:A:203:LYS:CD	2.57	0.68
1:A:26:SER:C	1:A:28:PRO:CD	2.62	0.68
1:A:176:ILE:C	1:A:177:LYS:HD3	2.15	0.67
1:A:51:TRP:HZ2	1:A:245:ASN:O	1.77	0.67
1:A:172:TRP:CB	1:A:176:ILE:HD11	2.24	0.67
1:A:98:THR:O	1:A:99:ILE:HB	1.95	0.67
1:A:7:GLN:O	1:A:9:VAL:HG23	1.96	0.67
1:A:224:THR:HG22	1:A:225:PRO:CD	2.21	0.67
1:A:136:CYS:CB	1:A:200:VAL:O	2.36	0.66
1:A:218:SER:C	1:A:220:CYS:H	1.99	0.66
1:A:125:SER:O	1:A:125:SER:CA	2.38	0.66
1:A:92:SER:C	1:A:94:TYR:H	1.98	0.66
1:A:185:ALA:HB2	1:A:225:PRO:N	2.11	0.66
1:A:162:LEU:HD13	1:A:181:ILE:CD1	2.19	0.66
1:A:45:SER:O	1:A:53:VAL:HG12	1.95	0.66
1:A:171:TYR:CD1	1:A:225:PRO:HD3	2.31	0.65
1:A:89:PHE:N	1:A:89:PHE:CD2	2.61	0.65
1:A:199:LEU:HD23	1:A:211:GLY:HA3	1.79	0.65
1:A:10:LEU:CD2	1:A:10:LEU:N	2.60	0.64
1:A:24:PRO:C	1:A:26:SER:H	2.00	0.64
1:A:178:ASP:OD2	1:A:179:ALA:HB2	1.96	0.64
1:A:228:TYR:CD1	1:A:228:TYR:N	2.66	0.64
1:A:47:ILE:HA	1:A:120:ALA:HB1	1.80	0.64
1:A:189:SER:O	1:A:192:MET:HE1	1.96	0.63
1:A:52:VAL:O	1:A:106:LEU:N	2.31	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:N	1:A:42:CYS:O	2.32	0.62
1:A:191:CYS:C	1:A:193:GLY:H	1.99	0.62
1:A:191:CYS:C	1:A:193:GLY:N	2.48	0.62
1:A:26:SER:C	1:A:28:PRO:HD2	2.20	0.62
1:A:171:TYR:CG	1:A:225:PRO:HG3	2.34	0.62
1:A:16:ILE:HG23	1:A:17:VAL:HG23	1.83	0.61
1:A:8:PRO:HB2	1:A:10:LEU:HD21	1.83	0.61
1:A:53:VAL:O	1:A:53:VAL:CG1	2.49	0.61
1:A:66:VAL:HG21	1:A:108:LEU:HD21	1.83	0.61
1:A:27:TRP:CD1	1:A:139:THR:CG2	2.84	0.61
1:A:236:ASN:HA	1:A:239:GLN:HB2	1.81	0.61
1:A:125:SER:CA	1:A:126:ALA:N	2.58	0.60
1:A:86:ALA:HB2	1:A:109:SER:HA	1.83	0.60
1:A:16:ILE:O	1:A:19:GLY:HA2	2.00	0.60
1:A:35:ASP:OD1	1:A:39:PHE:CB	2.38	0.60
1:A:53:VAL:O	1:A:53:VAL:HG13	2.00	0.60
1:A:172:TRP:CZ3	1:A:215:TRP:NE1	2.69	0.60
1:A:127:SER:O	1:A:128:ASP:O	2.19	0.60
1:A:108:LEU:CD1	1:A:108:LEU:N	2.63	0.60
1:A:178:ASP:OD2	1:A:179:ALA:N	2.35	0.60
1:A:244:ALA:HB3	1:A:245:ASN:ND2	2.17	0.60
1:A:46:LEU:HD23	1:A:52:VAL:HG23	1.79	0.59
1:A:159:SER:O	1:A:160:LEU:HA	2.02	0.59
1:A:8:PRO:HA	1:A:26:SER:OG	2.03	0.59
1:A:21:GLU:N	1:A:156:GLN:HG3	2.17	0.59
1:A:27:TRP:CG	1:A:139:THR:CG2	2.81	0.59
1:A:244:ALA:HB1	1:A:245:ASN:OD1	2.02	0.59
1:A:106:LEU:N	1:A:106:LEU:CB	2.59	0.59
1:A:39:PHE:HE2	1:A:41:PHE:HB3	1.68	0.59
1:A:125:SER:N	1:A:125:SER:C	2.55	0.59
1:A:47:ILE:C	1:A:120:ALA:CB	2.71	0.59
1:A:189:SER:O	1:A:192:MET:HE3	2.02	0.59
1:A:52:VAL:O	1:A:105:LEU:HA	2.02	0.58
1:A:67:VAL:HG22	1:A:82:LYS:HG3	1.85	0.58
1:A:140:GLY:CA	1:A:155:LEU:HD12	2.33	0.58
1:A:87:LYS:CG	1:A:88:VAL:N	2.63	0.58
1:A:25:GLY:C	1:A:28:PRO:HD3	2.20	0.58
1:A:33:LEU:O	1:A:41:PHE:CD2	2.56	0.58
1:A:6:ILE:HD12	1:A:6:ILE:N	2.18	0.57
1:A:178:ASP:CG	1:A:179:ALA:N	2.50	0.57
1:A:233:ALA:C	1:A:234:LEU:HG	2.24	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:HB	1:A:106:LEU:HG	1.86	0.57
1:A:201:CYS:SG	1:A:210:VAL:HG21	2.44	0.57
1:A:136:CYS:HB3	1:A:200:VAL:C	2.23	0.57
1:A:168:CYS:O	1:A:169:LYS:C	2.44	0.57
1:A:79:LYS:HG2	1:A:79:LYS:O	2.05	0.57
1:A:203:LYS:C	1:A:205:GLY:N	2.49	0.56
1:A:160:LEU:HA	1:A:160:LEU:N	1.98	0.56
1:A:218:SER:C	1:A:220:CYS:N	2.57	0.56
1:A:177:LYS:CD	1:A:177:LYS:N	2.67	0.56
1:A:41:PHE:HE1	1:A:58:CYS:O	1.89	0.56
1:A:66:VAL:HB	1:A:83:LEU:HB2	1.88	0.56
1:A:27:TRP:N	1:A:28:PRO:CD	2.69	0.56
1:A:91:ASN:C	1:A:91:ASN:OD1	2.44	0.56
1:A:27:TRP:HB2	1:A:139:THR:HG21	1.86	0.56
1:A:201:CYS:O	1:A:207:TRP:HA	2.04	0.56
1:A:9:VAL:HB	1:A:23:VAL:HG21	1.88	0.56
1:A:30:GLN:NE2	1:A:198:PRO:HD2	2.21	0.55
1:A:203:LYS:CG	1:A:204:ASN:OD1	2.54	0.55
1:A:127:SER:C	1:A:128:ASP:O	2.45	0.55
1:A:79:LYS:HD3	1:A:117:THR:HG21	1.89	0.55
1:A:100:ASN:HD22	1:A:177:LYS:HB2	1.70	0.55
1:A:65:VAL:HG12	1:A:82:LYS:HG2	1.89	0.54
1:A:177:LYS:HD3	1:A:177:LYS:N	2.23	0.54
1:A:217:SER:O	1:A:220:CYS:HA	2.06	0.54
1:A:43:GLY:CA	1:A:43:GLY:O	2.51	0.54
1:A:47:ILE:O	1:A:120:ALA:CB	2.57	0.53
1:A:77:SER:C	1:A:78:GLU:CG	2.76	0.53
1:A:33:LEU:HD21	1:A:106:LEU:HD11	1.90	0.53
1:A:27:TRP:CD1	1:A:139:THR:HG21	2.41	0.53
1:A:30:GLN:OE1	1:A:155:LEU:HD11	2.09	0.53
1:A:137:VAL:HG12	1:A:138:THR:N	2.24	0.52
1:A:98:THR:O	1:A:99:ILE:CB	2.57	0.52
1:A:171:TYR:CG	1:A:225:PRO:CG	2.92	0.52
1:A:95:ASN:O	1:A:99:ILE:CA	2.56	0.52
1:A:27:TRP:CD1	1:A:139:THR:HG22	2.45	0.52
1:A:107:LYS:C	1:A:108:LEU:HD12	2.30	0.52
1:A:83:LEU:CD2	1:A:110:THR:O	2.58	0.52
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.75	0.52
1:A:125:SER:CB	1:A:125:SER:C	2.73	0.51
1:A:166:THR:HA	1:A:169:LYS:HB2	1.92	0.51
1:A:244:ALA:HB3	1:A:245:ASN:CG	2.30	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:SER:C	1:A:28:PRO:HD3	2.30	0.51
1:A:8:PRO:HB3	1:A:27:TRP:CZ2	2.45	0.51
1:A:9:VAL:O	1:A:9:VAL:HG12	2.09	0.51
1:A:185:ALA:HB2	1:A:224:THR:C	2.31	0.51
1:A:230:ARG:HG3	1:A:230:ARG:NH1	2.26	0.51
1:A:218:SER:O	1:A:220:CYS:N	2.44	0.51
1:A:172:TRP:CE3	1:A:215:TRP:CZ2	2.99	0.51
1:A:125:SER:O	1:A:125:SER:N	2.44	0.50
1:A:83:LEU:HB3	1:A:108:LEU:HD23	1.92	0.50
1:A:35:ASP:N	1:A:39:PHE:O	2.43	0.50
1:A:49:GLU:O	1:A:112:ALA:N	2.39	0.50
1:A:9:VAL:CG2	1:A:9:VAL:N	2.74	0.50
1:A:181:ILE:CG2	1:A:181:ILE:O	2.60	0.50
1:A:199:LEU:HD22	1:A:228:TYR:CD2	2.47	0.50
1:A:66:VAL:O	1:A:83:LEU:N	2.43	0.50
1:A:66:VAL:HG21	1:A:108:LEU:CD2	2.42	0.49
1:A:85:ILE:HG21	1:A:88:VAL:HG23	1.92	0.49
1:A:221:SER:C	1:A:223:SER:H	1.97	0.49
1:A:87:LYS:HD3	1:A:89:PHE:CE1	2.47	0.49
1:A:140:GLY:C	1:A:155:LEU:HD12	2.33	0.49
1:A:175:LYS:O	1:A:180:MET:CE	2.61	0.49
1:A:20:GLU:C	1:A:156:GLN:HG2	2.33	0.48
1:A:230:ARG:O	1:A:233:ALA:N	2.35	0.48
1:A:200:VAL:HG22	1:A:209:LEU:HA	1.94	0.48
1:A:90:LYS:HA	1:A:104:THR:OG1	2.13	0.48
1:A:77:SER:C	1:A:78:GLU:HG2	2.33	0.48
1:A:39:PHE:C	1:A:39:PHE:CD2	2.87	0.48
1:A:235:VAL:HG13	1:A:236:ASN:N	2.27	0.48
1:A:171:TYR:CD1	1:A:225:PRO:CD	2.97	0.48
1:A:39:PHE:CE2	1:A:41:PHE:HB3	2.47	0.48
1:A:199:LEU:C	1:A:200:VAL:HG23	2.34	0.48
1:A:230:ARG:CG	1:A:230:ARG:HH11	2.27	0.48
1:A:197:GLY:O	1:A:213:VAL:HG23	2.14	0.48
1:A:34:GLN:CD	1:A:38:GLY:HA2	2.31	0.47
1:A:24:PRO:C	1:A:26:SER:N	2.65	0.47
1:A:123:LEU:HA	1:A:124:PRO:HD3	1.81	0.46
1:A:47:ILE:O	1:A:120:ALA:HB1	2.14	0.46
1:A:93:LYS:O	1:A:101:ASN:HB2	2.15	0.46
1:A:22:ALA:HB1	1:A:26:SER:HB3	1.96	0.46
1:A:235:VAL:CG1	1:A:236:ASN:N	2.78	0.46
1:A:34:GLN:HE22	1:A:82:LYS:CE	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:C	1:A:223:SER:N	2.62	0.46
1:A:197:GLY:HA2	1:A:198:PRO:HD3	1.40	0.45
1:A:182:CYS:SG	1:A:227:VAL:HG22	2.56	0.45
1:A:100:ASN:HD21	1:A:177:LYS:HB2	1.78	0.45
1:A:14:SER:HB3	1:A:159:SER:HB2	1.97	0.45
1:A:200:VAL:CG1	1:A:207:TRP:HB3	2.42	0.45
1:A:29:TRP:HB3	1:A:119:SER:O	2.17	0.45
1:A:3:VAL:HG12	1:A:3:VAL:O	2.16	0.45
1:A:22:ALA:HB1	1:A:26:SER:CB	2.47	0.45
1:A:91:ASN:HB2	1:A:237:TRP:CE2	2.52	0.45
1:A:202:LYS:O	1:A:203:LYS:CB	2.59	0.44
1:A:85:ILE:CG2	1:A:88:VAL:HG23	2.46	0.44
1:A:56:ALA:O	1:A:59:GLY:N	2.44	0.44
1:A:26:SER:O	1:A:28:PRO:CD	2.58	0.44
1:A:204:ASN:N	1:A:204:ASN:OD1	2.49	0.44
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.83	0.43
1:A:121:VAL:HG22	1:A:122:CYS:H	1.83	0.43
1:A:6:ILE:HD12	1:A:6:ILE:H	1.83	0.43
1:A:244:ALA:CB	1:A:245:ASN:CG	2.86	0.43
1:A:83:LEU:HD21	1:A:110:THR:O	2.17	0.43
1:A:20:GLU:O	1:A:156:GLN:HG2	2.11	0.43
1:A:165:ASN:HA	1:A:168:CYS:HB3	1.99	0.43
1:A:230:ARG:O	1:A:231:VAL:C	2.56	0.43
1:A:119:SER:HB2	1:A:120:ALA:H	1.51	0.43
1:A:90:LYS:HG2	1:A:91:ASN:N	2.33	0.43
1:A:95:ASN:OD1	1:A:98:THR:OG1	2.31	0.43
1:A:61:THR:HG23	1:A:63:SER:H	1.84	0.43
1:A:138:THR:O	1:A:157:GLN:HA	2.19	0.43
1:A:51:TRP:CZ2	1:A:245:ASN:O	2.66	0.43
1:A:91:ASN:O	1:A:94:TYR:N	2.52	0.43
1:A:9:VAL:HB	1:A:23:VAL:CG2	2.49	0.42
1:A:162:LEU:CD1	1:A:181:ILE:HD11	2.22	0.42
1:A:129:ASP:O	1:A:130:PHE:CG	2.72	0.42
1:A:139:THR:OG1	1:A:198:PRO:HG2	2.20	0.42
1:A:99:ILE:O	1:A:99:ILE:HG22	2.19	0.42
1:A:29:TRP:CD2	1:A:121:VAL:HB	2.55	0.42
1:A:23:VAL:HA	1:A:24:PRO:HD2	1.64	0.42
1:A:47:ILE:HG13	1:A:48:ASN:HD22	1.85	0.42
1:A:160:LEU:HD22	1:A:184:GLY:HA3	2.00	0.42
1:A:9:VAL:N	1:A:9:VAL:HG23	2.35	0.42
1:A:188:VAL:HG22	1:A:189:SER:N	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:O	1:A:235:VAL:HG21	2.19	0.42
1:A:244:ALA:CB	1:A:245:ASN:OD1	2.66	0.41
1:A:167:ASN:O	1:A:170:LYS:HB3	2.19	0.41
1:A:11:SER:HB2	1:A:12:GLY:H	1.60	0.41
1:A:172:TRP:HB3	1:A:176:ILE:CD1	2.49	0.41
1:A:199:LEU:HD22	1:A:228:TYR:CG	2.55	0.41
1:A:60:VAL:O	1:A:60:VAL:HG13	2.20	0.41
1:A:47:ILE:HG21	1:A:47:ILE:HD13	1.69	0.41
1:A:27:TRP:HA	1:A:28:PRO:HD2	1.72	0.41
1:A:235:VAL:O	1:A:239:GLN:CG	2.64	0.41
1:A:28:PRO:O	1:A:118:VAL:HA	2.20	0.41
1:A:213:VAL:CG1	1:A:214:SER:N	2.75	0.41
1:A:34:GLN:NE2	1:A:82:LYS:CE	2.75	0.40
1:A:103:ILE:HG21	1:A:234:LEU:HD13	2.03	0.40
1:A:3:VAL:HA	1:A:4:PRO:HD2	1.91	0.40
1:A:106:LEU:HB2	1:A:108:LEU:HD11	2.02	0.40

All (52) 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:36:LYS:C	1:A:174:THR:OG1[3_655]	0.73	1.47
1:A:78:GLU:OE2	1:A:99:ILE:CA[3_655]	0.89	1.31
1:A:36:LYS:O	1:A:174:THR:CA[3_655]	1.02	1.18
1:A:78:GLU:N	1:A:94:TYR:CE2[3_655]	1.05	1.15
1:A:65:VAL:CG1	1:A:175:LYS:NZ[3_655]	1.23	0.97
1:A:36:LYS:CA	1:A:174:THR:CB[3_655]	1.25	0.95
1:A:37:THR:N	1:A:174:THR:OG1[3_655]	1.26	0.94
1:A:78:GLU:CD	1:A:99:ILE:CA[3_655]	1.29	0.91
1:A:80:ILE:CD1	1:A:97:LEU:CD2[3_655]	1.30	0.90
1:A:80:ILE:CD1	1:A:97:LEU:CG[3_655]	1.33	0.87
1:A:36:LYS:C	1:A:174:THR:CB[3_655]	1.34	0.86
1:A:36:LYS:O	1:A:174:THR:CB[3_655]	1.35	0.85
1:A:78:GLU:OE1	1:A:99:ILE:C[3_655]	1.36	0.84
1:A:78:GLU:OE2	1:A:99:ILE:N[3_655]	1.41	0.79
1:A:77:SER:C	1:A:94:TYR:CD2[3_655]	1.45	0.75
1:A:36:LYS:CA	1:A:174:THR:OG1[3_655]	1.47	0.73
1:A:65:VAL:CG2	1:A:175:LYS:CE[3_655]	1.48	0.72
1:A:79:LYS:N	1:A:96:SER:OG[3_655]	1.55	0.65
1:A:78:GLU:OE1	1:A:99:ILE:CA[3_655]	1.62	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:O	1:A:174:THR:OG1[3_655]	1.70	0.50
1:A:80:ILE:CG2	1:A:96:SER:O[3_655]	1.73	0.47
1:A:77:SER:C	1:A:94:TYR:CG[3_655]	1.74	0.46
1:A:65:VAL:CB	1:A:175:LYS:NZ[3_655]	1.80	0.40
1:A:80:ILE:CG2	1:A:96:SER:C[3_655]	1.83	0.37
1:A:78:GLU:N	1:A:94:TYR:CZ[3_655]	1.84	0.36
1:A:78:GLU:OE2	1:A:99:ILE:CB[3_655]	1.84	0.36
1:A:78:GLU:CG	1:A:94:TYR:CE1[3_655]	1.84	0.36
1:A:78:GLU:N	1:A:94:TYR:CD2[3_655]	1.87	0.33
1:A:65:VAL:CG2	1:A:175:LYS:NZ[3_655]	1.87	0.33
1:A:77:SER:C	1:A:94:TYR:CE2[3_655]	1.88	0.32
1:A:77:SER:O	1:A:94:TYR:O[3_655]	1.89	0.31
1:A:78:GLU:C	1:A:96:SER:OG[3_655]	1.90	0.30
1:A:78:GLU:OE1	1:A:100:ASN:N[3_655]	1.92	0.28
1:A:78:GLU:CB	1:A:96:SER:CA[3_655]	1.92	0.28
1:A:80:ILE:CG2	1:A:97:LEU:N[3_655]	1.92	0.28
1:A:36:LYS:O	1:A:174:THR:C[3_655]	1.92	0.28
1:A:84:LYS:NZ	1:A:172:TRP:CZ3[3_655]	1.95	0.25
1:A:78:GLU:CA	1:A:96:SER:OG[3_655]	1.95	0.25
1:A:78:GLU:CD	1:A:99:ILE:C[3_655]	1.96	0.24
1:A:36:LYS:N	1:A:174:THR:OG1[3_655]	1.97	0.23
1:A:13:LEU:CD2	1:A:240:GLN:CB[2_564]	1.98	0.22
1:A:80:ILE:CG2	1:A:97:LEU:CA[3_655]	2.01	0.19
1:A:78:GLU:CD	1:A:99:ILE:N[3_655]	2.06	0.14
1:A:80:ILE:CB	1:A:96:SER:CB[3_655]	2.06	0.14
1:A:78:GLU:CD	1:A:95:ASN:O[3_655]	2.07	0.13
1:A:110:THR:OG1	1:A:218:SER:OG[3_655]	2.09	0.11
1:A:35:ASP:O	1:A:174:THR:OG1[3_655]	2.09	0.11
1:A:84:LYS:NZ	1:A:172:TRP:CE3[3_655]	2.10	0.10
1:A:36:LYS:C	1:A:174:THR:CA[3_655]	2.15	0.05
1:A:78:GLU:CG	1:A:94:TYR:CZ[3_655]	2.16	0.04
1:A:36:LYS:CA	1:A:174:THR:CG2[3_655]	2.17	0.03
1:A:17:VAL:CG2	1:A:243:ALA:CA[2_564]	2.19	0.01

## 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	222/245 (91%)	182 (82%)	29 (13%)	11 (5%)	3	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	A	128	ASP
1	A	178	ASP
1	A	17	VAL
1	A	28	PRO
1	A	170	LYS
1	A	218	SER
1	A	231	VAL
1	A	24	PRO
1	A	219	THR
1	A	235	VAL

### 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	180/200 (90%)	151 (84%)	29 (16%)	3	5

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	14	SER
1	A	21	GLU
1	A	26	SER
1	A	40	HIS
1	A	78	GLU
1	A	89	PHE
1	A	91	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	106	LEU
1	A	127	SER
1	A	130	PHE
1	A	135	THR
1	A	138	THR
1	A	154	ARG
1	A	156	GLN
1	A	160	LEU
1	A	165	ASN
1	A	166	THR
1	A	169	LYS
1	A	176	ILE
1	A	180	MET
1	A	192	MET
1	A	199	LEU
1	A	203	LYS
1	A	204	ASN
1	A	215	TRP
1	A	224	THR
1	A	232	THR
1	A	239	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	165	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [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](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

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

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