



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:13 PM GMT

PDB ID : 1SMR  
Title : The 3-d structure of mouse submaxillary renin complexed with a decapeptide inhibitor ch-66 based on the 4-16 fragment of rat angiotensinogen  
Authors : Dealwis, C.G.; Blundell, T.L.  
Deposited on : 1992-03-11  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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.

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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

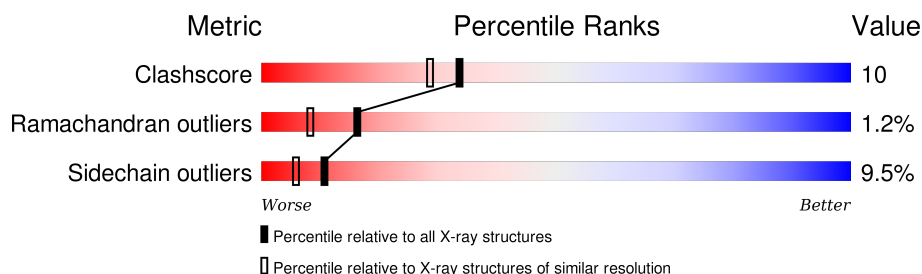
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

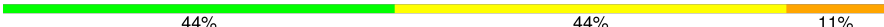
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	335	
1	C	335	
1	E	335	
1	G	335	
2	B	9	
2	D	9	
2	F	9	

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Mol	Chain	Length	Quality of chain
2	H	9	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (44%), yellow (44%), and orange (11%).

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10560 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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			
1	C	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			
1	E	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			
1	G	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLN	GLU	CONFLICT	UNP P00796
A	173	GLN	GLU	CONFLICT	UNP P00796
C	106	GLN	GLU	CONFLICT	UNP P00796
C	173	GLN	GLU	CONFLICT	UNP P00796
E	106	GLN	GLU	CONFLICT	UNP P00796
E	173	GLN	GLU	CONFLICT	UNP P00796
G	106	GLN	GLU	CONFLICT	UNP P00796
G	173	GLN	GLU	CONFLICT	UNP P00796

- Molecule 2 is a protein called INHIBITOR CH-66.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			90	65	12	13			
2	D	9	Total	C	N	O	0	0	0
			90	65	12	13			
2	F	9	Total	C	N	O	0	0	0
			90	65	12	13			
2	H	9	Total	C	N	O	0	0	0
			90	65	12	13			

- Molecule 3 is water.

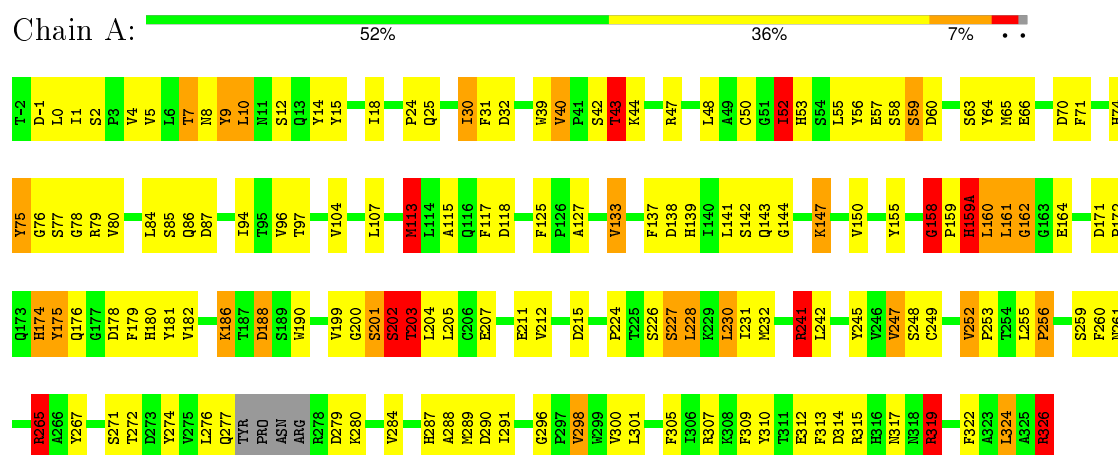
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total 148	O 148	0	0
3	B	5	Total 5	O 5	0	0
3	C	3	Total 3	O 3	0	0

### 3 Residue-property plots

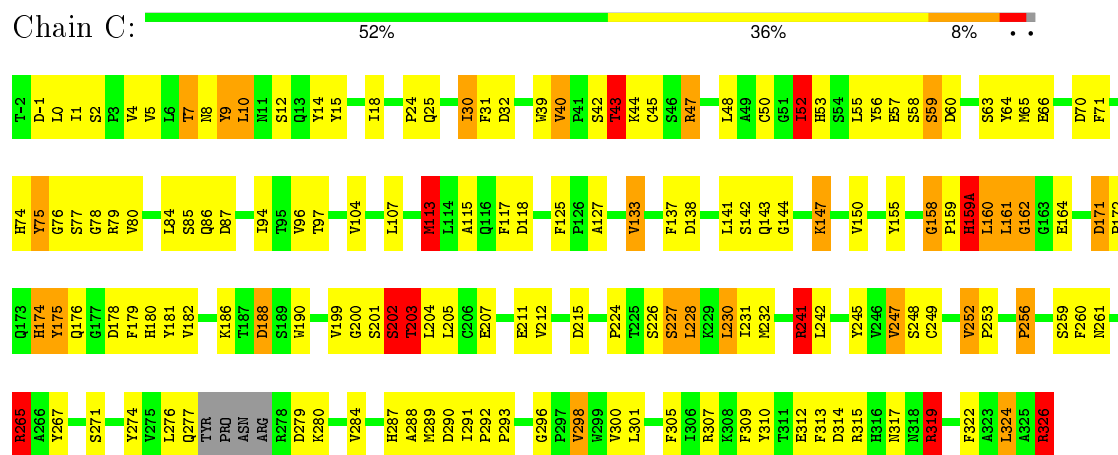
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

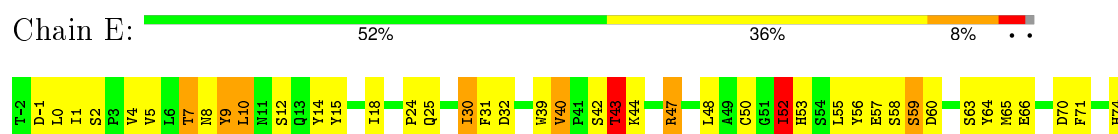
#### • Molecule 1: RENIN

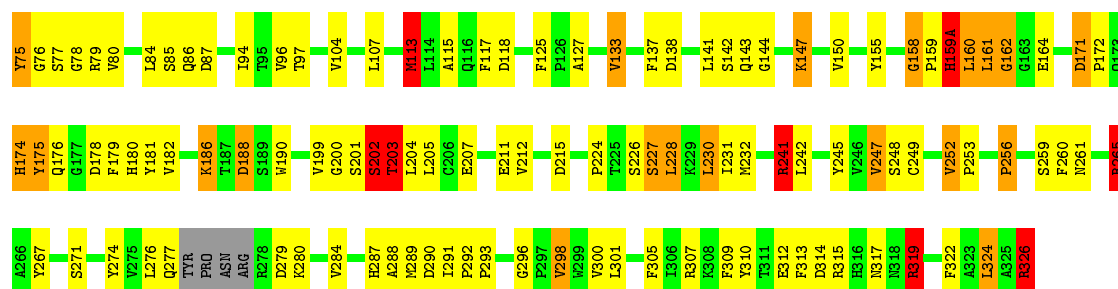


#### • Molecule 1: RENIN



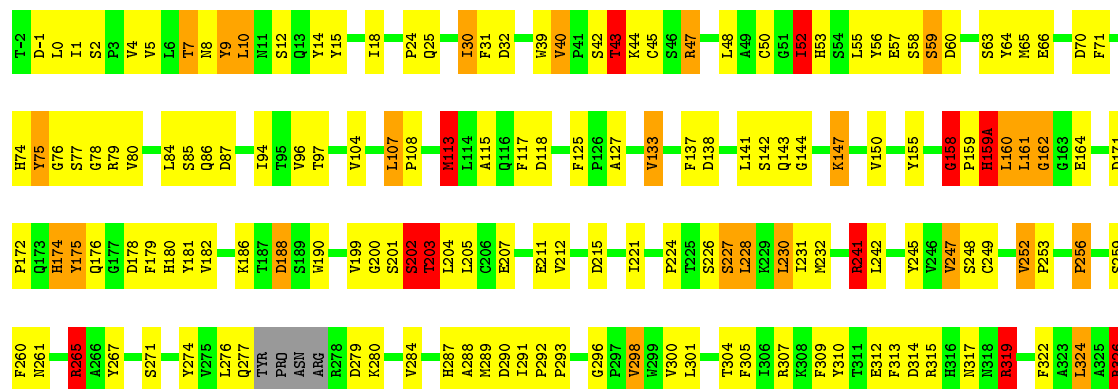
#### • Molecule 1: RENIN





• Molecule 1: RENIN

Chain G: 51% 37% 7% . .



• Molecule 2: INHIBITOR CH-66

Chain B: 44% 44% 11%



• Molecule 2: INHIBITOR CH-66

Chain D: 44% 44% 11%



• Molecule 2: INHIBITOR CH-66

Chain F: 44% 44% 11%



• Molecule 2: INHIBITOR CH-66

Chain H: 44% 44% 11%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.34Å 117.76Å 85.88Å 90.00° 101.18° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.49	18/2572 (0.7%)	2.47	178/3500 (5.1%)
1	C	1.49	18/2572 (0.7%)	2.47	179/3500 (5.1%)
1	E	1.49	18/2572 (0.7%)	2.47	178/3500 (5.1%)
1	G	1.49	18/2572 (0.7%)	2.47	179/3500 (5.1%)
2	B	1.45	0/72	2.62	6/96 (6.2%)
2	D	1.45	0/72	2.62	6/96 (6.2%)
2	F	1.45	0/72	2.62	6/96 (6.2%)
2	H	1.45	0/72	2.62	6/96 (6.2%)
All	All	1.49	72/10576 (0.7%)	2.47	738/14384 (5.1%)

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	3
1	C	0	3
1	E	0	3
1	G	0	3
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
All	All	0	20

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	42	SER	CB-OG	-19.90	1.16	1.42
1	G	42	SER	CB-OG	-19.87	1.16	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	SER	CB-OG	-19.85	1.16	1.42
1	C	42	SER	CB-OG	-19.83	1.16	1.42
1	G	43	THR	CB-OG1	-9.08	1.25	1.43
1	C	43	THR	CB-OG1	-9.07	1.25	1.43
1	A	43	THR	CB-OG1	-9.07	1.25	1.43
1	E	43	THR	CB-OG1	-9.05	1.25	1.43
1	C	326	ARG	C-OXT	7.89	1.38	1.23
1	A	326	ARG	C-OXT	7.89	1.38	1.23
1	E	326	ARG	C-OXT	7.88	1.38	1.23
1	G	326	ARG	C-OXT	7.85	1.38	1.23
1	G	164	GLU	CD-OE1	-7.24	1.17	1.25
1	A	164	GLU	CD-OE1	-7.20	1.17	1.25
1	E	164	GLU	CD-OE1	-7.20	1.17	1.25
1	C	164	GLU	CD-OE1	-7.16	1.17	1.25
1	G	39	TRP	NE1-CE2	-6.92	1.28	1.37
1	A	39	TRP	NE1-CE2	-6.91	1.28	1.37
1	C	39	TRP	NE1-CE2	-6.88	1.28	1.37
1	E	39	TRP	NE1-CE2	-6.87	1.28	1.37
1	C	248	SER	CB-OG	6.71	1.50	1.42
1	E	248	SER	CB-OG	6.70	1.50	1.42
1	A	248	SER	CB-OG	6.70	1.50	1.42
1	G	248	SER	CB-OG	6.66	1.50	1.42
1	A	305	PHE	CD1-CE1	6.14	1.51	1.39
1	C	227	SER	CB-OG	-6.12	1.34	1.42
1	C	305	PHE	CD1-CE1	6.12	1.51	1.39
1	G	305	PHE	CD1-CE1	6.12	1.51	1.39
1	E	305	PHE	CD1-CE1	6.12	1.51	1.39
1	E	227	SER	CB-OG	-6.10	1.34	1.42
1	A	227	SER	CB-OG	-6.08	1.34	1.42
1	G	227	SER	CB-OG	-6.07	1.34	1.42
1	E	78	GLY	N-CA	5.86	1.54	1.46
1	A	78	GLY	N-CA	5.85	1.54	1.46
1	C	78	GLY	N-CA	5.85	1.54	1.46
1	G	78	GLY	N-CA	5.84	1.54	1.46
1	E	15	TYR	CD1-CE1	5.64	1.47	1.39
1	G	15	TYR	CD1-CE1	5.64	1.47	1.39
1	A	15	TYR	CD1-CE1	5.64	1.47	1.39
1	C	15	TYR	CD1-CE1	5.64	1.47	1.39
1	G	85	SER	CB-OG	-5.63	1.34	1.42
1	A	85	SER	CB-OG	-5.62	1.34	1.42
1	C	85	SER	CB-OG	-5.61	1.34	1.42
1	E	85	SER	CB-OG	-5.60	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	162	GLY	CA-C	5.54	1.60	1.51
1	E	63	SER	CB-OG	5.54	1.49	1.42
1	G	162	GLY	CA-C	5.53	1.60	1.51
1	A	162	GLY	CA-C	5.53	1.60	1.51
1	C	162	GLY	CA-C	5.53	1.60	1.51
1	G	63	SER	CB-OG	5.52	1.49	1.42
1	C	63	SER	CB-OG	5.51	1.49	1.42
1	A	63	SER	CB-OG	5.51	1.49	1.42
1	C	190	TRP	NE1-CE2	-5.35	1.30	1.37
1	A	190	TRP	NE1-CE2	-5.35	1.30	1.37
1	G	190	TRP	NE1-CE2	-5.34	1.30	1.37
1	E	190	TRP	NE1-CE2	-5.34	1.30	1.37
1	G	180	HIS	CE1-NE2	5.26	1.44	1.32
1	C	180	HIS	CE1-NE2	5.26	1.44	1.32
1	A	180	HIS	CE1-NE2	5.26	1.44	1.32
1	E	180	HIS	CE1-NE2	5.26	1.44	1.32
1	G	261	ASN	CG-OD1	5.16	1.35	1.24
1	C	190	TRP	CD2-CE2	-5.15	1.35	1.41
1	A	261	ASN	CG-OD1	5.14	1.35	1.24
1	C	261	ASN	CG-OD1	5.13	1.35	1.24
1	A	190	TRP	CD2-CE2	-5.12	1.35	1.41
1	G	190	TRP	CD2-CE2	-5.12	1.35	1.41
1	E	261	ASN	CG-OD1	5.12	1.35	1.24
1	E	190	TRP	CD2-CE2	-5.10	1.35	1.41
1	A	9	TYR	CG-CD1	5.09	1.45	1.39
1	C	9	TYR	CG-CD1	5.08	1.45	1.39
1	E	9	TYR	CG-CD1	5.08	1.45	1.39
1	G	9	TYR	CG-CD1	5.07	1.45	1.39

All (738) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	LEU	O-C-N	15.66	147.76	122.70
1	A	160	LEU	O-C-N	15.65	147.74	122.70
1	C	160	LEU	O-C-N	15.65	147.74	122.70
1	G	160	LEU	O-C-N	15.65	147.74	122.70
1	G	307	ARG	NE-CZ-NH1	-14.70	112.95	120.30
1	E	307	ARG	NE-CZ-NH1	-14.70	112.95	120.30
1	A	307	ARG	NE-CZ-NH1	-14.65	112.98	120.30
1	C	307	ARG	NE-CZ-NH1	-14.63	112.98	120.30
1	C	319	ARG	CD-NE-CZ	14.44	143.81	123.60
1	E	319	ARG	CD-NE-CZ	14.44	143.82	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	319	ARG	CD-NE-CZ	14.43	143.81	123.60
1	A	319	ARG	CD-NE-CZ	14.43	143.80	123.60
1	C	326	ARG	CD-NE-CZ	12.48	141.07	123.60
1	A	326	ARG	CD-NE-CZ	12.45	141.03	123.60
1	E	326	ARG	CD-NE-CZ	12.45	141.03	123.60
1	G	326	ARG	CD-NE-CZ	12.45	141.03	123.60
2	D	7	TYR	CB-CG-CD1	-12.17	113.70	121.00
2	B	7	TYR	CB-CG-CD1	-12.17	113.70	121.00
2	F	7	TYR	CB-CG-CD1	-12.16	113.70	121.00
2	H	7	TYR	CB-CG-CD1	-12.13	113.72	121.00
1	E	160	LEU	CA-C-N	-11.83	91.17	117.20
1	G	315	ARG	NE-CZ-NH1	11.83	126.22	120.30
1	A	160	LEU	CA-C-N	-11.82	91.20	117.20
1	C	315	ARG	NE-CZ-NH1	11.81	126.21	120.30
1	G	160	LEU	CA-C-N	-11.81	91.21	117.20
1	C	160	LEU	CA-C-N	-11.80	91.24	117.20
1	A	315	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	E	315	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	G	137	PHE	CB-CG-CD1	-11.66	112.64	120.80
1	C	137	PHE	CB-CG-CD1	-11.61	112.67	120.80
1	A	137	PHE	CB-CG-CD1	-11.61	112.67	120.80
1	G	9	TYR	CB-CG-CD1	-11.60	114.04	121.00
1	E	9	TYR	CB-CG-CD1	-11.59	114.04	121.00
1	A	9	TYR	CB-CG-CD1	-11.59	114.05	121.00
1	E	137	PHE	CB-CG-CD1	-11.59	112.69	120.80
1	C	265	ARG	NE-CZ-NH2	11.58	126.09	120.30
1	G	307	ARG	NE-CZ-NH2	11.55	126.07	120.30
1	C	9	TYR	CB-CG-CD1	-11.54	114.08	121.00
1	E	15	TYR	CB-CG-CD1	-11.54	114.08	121.00
1	A	265	ARG	NE-CZ-NH2	11.52	126.06	120.30
1	C	15	TYR	CB-CG-CD1	-11.52	114.09	121.00
1	G	265	ARG	NE-CZ-NH2	11.52	126.06	120.30
1	A	15	TYR	CB-CG-CD1	-11.52	114.09	121.00
1	E	40	VAL	CA-CB-CG2	11.48	128.11	110.90
1	C	43	THR	CA-CB-OG1	11.47	133.09	109.00
1	G	43	THR	CA-CB-OG1	11.47	133.09	109.00
1	A	40	VAL	CA-CB-CG2	11.46	128.10	110.90
1	A	43	THR	CA-CB-OG1	11.46	133.08	109.00
1	C	40	VAL	CA-CB-CG2	11.47	128.10	110.90
1	G	40	VAL	CA-CB-CG2	11.46	128.09	110.90
1	G	15	TYR	CB-CG-CD1	-11.46	114.13	121.00
1	E	43	THR	CA-CB-OG1	11.45	133.05	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	A	307	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	E	265	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	E	307	ARG	NE-CZ-NH2	11.43	126.02	120.30
1	E	326	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	C	42	SER	CA-CB-OG	11.16	141.33	111.20
1	E	42	SER	CA-CB-OG	11.16	141.33	111.20
1	A	42	SER	CA-CB-OG	11.15	141.31	111.20
1	G	42	SER	CA-CB-OG	11.14	141.27	111.20
1	G	326	ARG	NE-CZ-NH1	11.13	125.87	120.30
1	A	326	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	C	113	MET	CG-SD-CE	11.07	117.91	100.20
1	C	326	ARG	NE-CZ-NH1	11.07	125.83	120.30
1	E	113	MET	CG-SD-CE	11.06	117.89	100.20
1	A	113	MET	CG-SD-CE	11.05	117.89	100.20
1	G	113	MET	CG-SD-CE	11.05	117.88	100.20
1	C	267	TYR	CB-CG-CD2	-10.96	114.42	121.00
1	A	267	TYR	CB-CG-CD2	-10.94	114.44	121.00
1	G	267	TYR	CB-CG-CD2	-10.92	114.45	121.00
1	E	267	TYR	CB-CG-CD2	-10.92	114.45	121.00
1	G	279	ASP	O-C-N	-10.26	106.28	122.70
1	E	279	ASP	O-C-N	-10.26	106.28	122.70
1	A	279	ASP	O-C-N	-10.25	106.31	122.70
1	C	279	ASP	O-C-N	-10.25	106.31	122.70
1	C	43	THR	OG1-CB-CG2	-9.98	87.05	110.00
1	A	43	THR	OG1-CB-CG2	-9.97	87.06	110.00
1	E	43	THR	OG1-CB-CG2	-9.97	87.07	110.00
1	G	43	THR	OG1-CB-CG2	-9.96	87.08	110.00
1	E	87	ASP	CB-CG-OD2	9.70	127.03	118.30
1	A	87	ASP	CB-CG-OD2	9.66	127.00	118.30
1	E	43	THR	N-CA-CB	-9.65	91.96	110.30
1	A	43	THR	N-CA-CB	-9.63	92.00	110.30
1	C	43	THR	N-CA-CB	-9.63	92.01	110.30
1	C	87	ASP	CB-CG-OD2	9.63	126.96	118.30
1	G	43	THR	N-CA-CB	-9.63	92.01	110.30
1	G	87	ASP	CB-CG-OD2	9.62	126.96	118.30
1	C	113	MET	CA-CB-CG	-9.53	97.10	113.30
1	E	113	MET	CA-CB-CG	-9.51	97.13	113.30
1	G	113	MET	CA-CB-CG	-9.50	97.14	113.30
1	A	113	MET	CA-CB-CG	-9.50	97.15	113.30
1	A	277	GLN	C-N-CA	9.49	145.41	121.70
1	G	277	GLN	C-N-CA	9.48	145.41	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	GLN	C-N-CA	9.47	145.39	121.70
1	E	277	GLN	C-N-CA	9.47	145.38	121.70
1	G	203	THR	C-N-CA	9.41	145.22	121.70
1	A	203	THR	C-N-CA	9.41	145.22	121.70
1	E	203	THR	C-N-CA	9.40	145.21	121.70
1	C	203	THR	C-N-CA	9.40	145.19	121.70
1	A	60	ASP	CB-CG-OD1	9.27	126.64	118.30
1	C	60	ASP	CB-CG-OD1	9.25	126.63	118.30
1	E	60	ASP	CB-CG-OD1	9.23	126.61	118.30
1	E	137	PHE	CB-CG-CD2	9.21	127.25	120.80
1	G	60	ASP	CB-CG-OD1	9.21	126.59	118.30
1	A	137	PHE	CB-CG-CD2	9.20	127.24	120.80
1	G	137	PHE	CB-CG-CD2	9.20	127.24	120.80
1	C	137	PHE	CB-CG-CD2	9.19	127.23	120.80
1	E	150	VAL	CA-CB-CG1	9.10	124.55	110.90
1	C	150	VAL	CA-CB-CG1	9.08	124.52	110.90
1	A	150	VAL	CA-CB-CG1	9.08	124.51	110.90
1	G	150	VAL	CA-CB-CG1	9.05	124.48	110.90
1	C	75	TYR	CG-CD2-CE2	-8.84	114.23	121.30
1	G	75	TYR	CG-CD2-CE2	-8.84	114.23	121.30
1	A	75	TYR	CG-CD2-CE2	-8.84	114.23	121.30
1	G	75	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	A	75	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	E	75	TYR	CG-CD2-CE2	-8.83	114.23	121.30
1	E	75	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	G	55	LEU	CB-CG-CD2	8.82	125.99	111.00
1	C	55	LEU	CB-CG-CD2	8.82	125.99	111.00
1	A	55	LEU	CB-CG-CD2	8.82	125.99	111.00
1	E	55	LEU	CB-CG-CD2	8.80	125.97	111.00
1	C	75	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	G	133	VAL	CA-CB-CG2	8.77	124.05	110.90
1	E	133	VAL	CA-CB-CG2	8.74	124.02	110.90
1	A	133	VAL	CA-CB-CG2	8.74	124.01	110.90
1	C	133	VAL	CA-CB-CG2	8.70	123.95	110.90
1	A	203	THR	O-C-N	8.69	136.60	122.70
1	C	203	THR	O-C-N	8.69	136.60	122.70
1	E	203	THR	O-C-N	8.68	136.59	122.70
1	G	203	THR	O-C-N	8.68	136.58	122.70
1	C	190	TRP	CG-CD1-NE1	-8.62	101.48	110.10
1	E	75	TYR	CD1-CG-CD2	8.59	127.35	117.90
1	G	75	TYR	CD1-CG-CD2	8.59	127.34	117.90
1	G	190	TRP	CG-CD1-NE1	-8.58	101.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	TYR	CD1-CG-CD2	8.58	127.34	117.90
1	A	75	TYR	CD1-CG-CD2	8.58	127.33	117.90
1	A	190	TRP	CG-CD1-NE1	-8.57	101.53	110.10
1	E	190	TRP	CG-CD1-NE1	-8.56	101.53	110.10
1	E	314	ASP	CB-CG-OD1	8.51	125.95	118.30
1	A	314	ASP	CB-CG-OD1	8.49	125.94	118.30
1	G	314	ASP	CB-CG-OD1	8.49	125.94	118.30
1	C	314	ASP	CB-CG-OD1	8.48	125.94	118.30
1	C	181	TYR	CB-CG-CD1	-8.41	115.96	121.00
1	A	181	TYR	CB-CG-CD1	-8.38	115.97	121.00
1	G	181	TYR	CB-CG-CD1	-8.38	115.97	121.00
1	C	75	TYR	CG-CD1-CE1	-8.35	114.62	121.30
1	A	75	TYR	CG-CD1-CE1	-8.33	114.64	121.30
1	E	181	TYR	CB-CG-CD1	-8.33	116.00	121.00
1	E	75	TYR	CG-CD1-CE1	-8.32	114.64	121.30
1	G	75	TYR	CG-CD1-CE1	-8.30	114.66	121.30
1	G	305	PHE	CB-CG-CD2	-8.30	114.99	120.80
1	E	305	PHE	CB-CG-CD2	-8.29	115.00	120.80
1	A	305	PHE	CB-CG-CD2	-8.27	115.01	120.80
1	C	305	PHE	CB-CG-CD2	-8.25	115.03	120.80
1	C	138	ASP	CB-CG-OD2	8.19	125.67	118.30
1	E	77	SER	C-N-CA	-8.19	105.10	122.30
1	A	77	SER	C-N-CA	-8.18	105.12	122.30
1	G	77	SER	C-N-CA	-8.18	105.12	122.30
1	E	138	ASP	CB-CG-OD2	8.17	125.65	118.30
1	C	77	SER	C-N-CA	-8.16	105.15	122.30
1	A	138	ASP	CB-CG-OD2	8.15	125.63	118.30
1	G	138	ASP	CB-CG-OD2	8.13	125.62	118.30
1	A	14	TYR	CG-CD2-CE2	-8.06	114.85	121.30
1	C	14	TYR	CG-CD2-CE2	-8.06	114.85	121.30
1	G	14	TYR	CG-CD2-CE2	-8.05	114.86	121.30
1	A	181	TYR	CG-CD2-CE2	-8.03	114.87	121.30
1	E	181	TYR	CG-CD2-CE2	-8.02	114.88	121.30
1	G	181	TYR	CG-CD2-CE2	-8.01	114.89	121.30
1	C	181	TYR	CG-CD2-CE2	-8.00	114.90	121.30
1	E	14	TYR	CG-CD2-CE2	-8.00	114.90	121.30
1	E	212	VAL	CA-CB-CG1	8.00	122.90	110.90
1	C	212	VAL	CA-CB-CG1	7.99	122.89	110.90
1	E	298	VAL	CA-CB-CG2	7.99	122.89	110.90
1	A	212	VAL	CA-CB-CG1	7.98	122.88	110.90
1	A	298	VAL	CA-CB-CG2	7.98	122.87	110.90
1	C	298	VAL	CA-CB-CG2	7.98	122.87	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	212	VAL	CA-CB-CG1	7.97	122.85	110.90
1	G	298	VAL	CA-CB-CG2	7.96	122.85	110.90
1	C	125	PHE	CG-CD2-CE2	7.96	129.55	120.80
1	G	125	PHE	CG-CD2-CE2	7.96	129.55	120.80
1	A	125	PHE	CG-CD2-CE2	7.95	129.54	120.80
1	E	125	PHE	CG-CD2-CE2	7.92	129.52	120.80
1	E	215	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	A	215	ASP	CB-CG-OD1	-7.84	111.24	118.30
1	C	215	ASP	CB-CG-OD1	-7.84	111.25	118.30
1	G	215	ASP	CB-CG-OD1	-7.83	111.25	118.30
2	B	7	TYR	CD1-CG-CD2	7.83	126.51	117.90
2	F	7	TYR	CD1-CG-CD2	7.82	126.50	117.90
2	D	7	TYR	CD1-CG-CD2	7.81	126.49	117.90
2	H	7	TYR	CD1-CG-CD2	7.78	126.46	117.90
1	G	7	THR	O-C-N	7.76	135.12	122.70
1	E	7	THR	O-C-N	7.76	135.12	122.70
1	A	7	THR	O-C-N	7.75	135.10	122.70
1	C	7	THR	O-C-N	7.72	135.06	122.70
1	G	39	TRP	CH2-CZ2-CE2	7.69	125.09	117.40
1	C	39	TRP	CH2-CZ2-CE2	7.66	125.06	117.40
1	A	39	TRP	CH2-CZ2-CE2	7.64	125.04	117.40
1	E	39	TRP	CH2-CZ2-CE2	7.60	125.00	117.40
1	C	125	PHE	CZ-CE2-CD2	-7.52	111.08	120.10
1	E	125	PHE	CZ-CE2-CD2	-7.50	111.10	120.10
1	G	125	PHE	CZ-CE2-CD2	-7.50	111.10	120.10
1	A	125	PHE	CZ-CE2-CD2	-7.50	111.11	120.10
1	C	256	PRO	CA-C-O	7.43	138.04	120.20
1	A	232	MET	CG-SD-CE	7.42	112.07	100.20
1	C	15	TYR	CD1-CE1-CZ	-7.42	113.12	119.80
1	A	256	PRO	CA-C-O	7.41	137.99	120.20
1	E	232	MET	CG-SD-CE	7.41	112.06	100.20
1	G	256	PRO	CA-C-O	7.41	137.99	120.20
1	E	256	PRO	CA-C-O	7.41	137.99	120.20
1	G	232	MET	CG-SD-CE	7.41	112.06	100.20
1	C	232	MET	CG-SD-CE	7.41	112.05	100.20
1	E	15	TYR	CD1-CE1-CZ	-7.40	113.14	119.80
1	G	15	TYR	CD1-CE1-CZ	-7.39	113.15	119.80
1	A	15	TYR	CD1-CE1-CZ	-7.38	113.16	119.80
1	C	267	TYR	CB-CG-CD1	7.32	125.39	121.00
1	E	310	TYR	O-C-N	-7.31	111.01	122.70
1	E	300	VAL	CA-CB-CG2	7.30	121.85	110.90
1	G	300	VAL	CA-CB-CG2	7.30	121.85	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	PHE	CB-CG-CD1	7.29	125.91	120.80
1	G	310	TYR	O-C-N	-7.29	111.04	122.70
1	A	310	TYR	O-C-N	-7.29	111.04	122.70
1	A	300	VAL	CA-CB-CG2	7.28	121.81	110.90
1	A	267	TYR	CB-CG-CD1	7.27	125.36	121.00
1	G	267	TYR	CB-CG-CD1	7.27	125.36	121.00
1	A	117	PHE	CB-CG-CD1	7.26	125.89	120.80
1	C	300	VAL	CA-CB-CG2	7.26	121.80	110.90
1	C	310	TYR	O-C-N	-7.26	111.08	122.70
1	C	117	PHE	CB-CG-CD1	7.24	125.87	120.80
1	E	267	TYR	CB-CG-CD1	7.24	125.34	121.00
1	G	324	LEU	CB-CG-CD1	-7.23	98.71	111.00
1	A	324	LEU	CB-CG-CD1	-7.22	98.72	111.00
1	E	324	LEU	CB-CG-CD1	-7.22	98.73	111.00
1	C	324	LEU	CB-CG-CD1	-7.21	98.74	111.00
1	E	117	PHE	CB-CG-CD1	7.21	125.84	120.80
1	E	188	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	188	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	76	GLY	O-C-N	-7.08	111.36	122.70
1	C	188	ASP	CB-CG-OD1	7.08	124.67	118.30
1	E	215	ASP	O-C-N	-7.08	111.37	122.70
1	E	76	GLY	O-C-N	-7.07	111.39	122.70
1	C	215	ASP	O-C-N	-7.07	111.39	122.70
1	G	188	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	215	ASP	O-C-N	-7.06	111.40	122.70
1	A	76	GLY	O-C-N	-7.06	111.41	122.70
1	G	215	ASP	O-C-N	-7.05	111.42	122.70
1	G	76	GLY	O-C-N	-7.04	111.44	122.70
1	C	298	VAL	CA-CB-CG1	6.98	121.37	110.90
1	G	178	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	G	298	VAL	CA-CB-CG1	6.97	121.36	110.90
1	C	9	TYR	CD1-CE1-CZ	-6.97	113.53	119.80
1	A	9	TYR	CD1-CE1-CZ	-6.97	113.53	119.80
1	E	298	VAL	CA-CB-CG1	6.97	121.35	110.90
1	A	298	VAL	CA-CB-CG1	6.96	121.35	110.90
1	G	9	TYR	CD1-CE1-CZ	-6.96	113.53	119.80
1	E	178	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	A	178	ASP	CB-CG-OD1	-6.94	112.06	118.30
1	E	9	TYR	CD1-CE1-CZ	-6.91	113.58	119.80
1	A	14	TYR	CZ-CE2-CD2	6.89	126.00	119.80
1	G	14	TYR	CZ-CE2-CD2	6.89	126.00	119.80
1	C	14	TYR	CZ-CE2-CD2	6.89	126.00	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	LEU	CB-CA-C	6.88	123.28	110.20
1	C	60	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	178	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	A	160	LEU	CB-CA-C	6.87	123.25	110.20
1	G	160	LEU	CB-CA-C	6.86	123.23	110.20
1	E	14	TYR	CZ-CE2-CD2	6.86	125.97	119.80
1	E	160	LEU	CB-CA-C	6.85	123.22	110.20
1	G	60	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	60	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	E	60	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	C	75	TYR	CB-CG-CD1	-6.77	116.94	121.00
1	E	75	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	C	32	ASP	CB-CG-OD2	6.76	124.38	118.30
1	E	32	ASP	CB-CG-OD2	6.74	124.37	118.30
1	G	75	TYR	CB-CG-CD1	-6.74	116.95	121.00
1	E	305	PHE	CD1-CE1-CZ	-6.74	112.02	120.10
1	A	75	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	G	314	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	32	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	305	PHE	CD1-CE1-CZ	-6.73	112.03	120.10
1	E	314	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	305	PHE	CD1-CE1-CZ	-6.71	112.05	120.10
1	G	47	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	G	32	ASP	CB-CG-OD2	6.70	124.33	118.30
1	G	305	PHE	CD1-CE1-CZ	-6.70	112.06	120.10
1	C	47	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	314	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	314	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	C	137	PHE	CG-CD1-CE1	-6.66	113.48	120.80
1	G	137	PHE	CG-CD1-CE1	-6.63	113.51	120.80
1	C	241	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	C	252	VAL	CA-CB-CG1	6.62	120.83	110.90
1	A	137	PHE	CG-CD1-CE1	-6.62	113.52	120.80
1	E	252	VAL	CA-CB-CG1	6.62	120.83	110.90
1	A	252	VAL	CA-CB-CG1	6.61	120.82	110.90
1	G	252	VAL	CA-CB-CG1	6.61	120.81	110.90
1	A	47	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	E	326	ARG	CB-CG-CD	6.60	128.76	111.60
1	E	14	TYR	CD1-CE1-CZ	-6.60	113.86	119.80
1	E	326	ARG	CA-CB-CG	6.60	127.92	113.40
1	C	326	ARG	CA-CB-CG	6.59	127.91	113.40
1	E	137	PHE	CG-CD1-CE1	-6.59	113.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	241	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	326	ARG	CA-CB-CG	6.59	127.90	113.40
1	A	326	ARG	CB-CG-CD	6.59	128.73	111.60
1	G	326	ARG	CA-CB-CG	6.59	127.90	113.40
1	A	14	TYR	CD1-CE1-CZ	-6.59	113.87	119.80
1	C	326	ARG	CB-CG-CD	6.59	128.73	111.60
1	A	241	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	G	14	TYR	CD1-CE1-CZ	-6.58	113.87	119.80
1	G	326	ARG	CB-CG-CD	6.58	128.71	111.60
1	E	305	PHE	CE1-CZ-CE2	6.58	131.84	120.00
1	A	305	PHE	CE1-CZ-CE2	6.55	131.79	120.00
1	G	85	SER	O-C-N	-6.55	112.22	122.70
1	C	14	TYR	CD1-CE1-CZ	-6.55	113.91	119.80
1	C	85	SER	O-C-N	-6.55	112.22	122.70
1	C	305	PHE	CE1-CZ-CE2	6.55	131.78	120.00
1	G	305	PHE	CE1-CZ-CE2	6.54	131.77	120.00
1	A	85	SER	O-C-N	-6.53	112.25	122.70
1	E	47	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	C	137	PHE	CD1-CE1-CZ	6.52	127.93	120.10
1	E	160	LEU	CA-CB-CG	-6.52	100.31	115.30
1	A	160	LEU	CA-CB-CG	-6.51	100.32	115.30
1	C	160	LEU	CA-CB-CG	-6.51	100.33	115.30
1	G	125	PHE	CD1-CE1-CZ	6.50	127.90	120.10
1	A	125	PHE	CD1-CE1-CZ	6.50	127.90	120.10
1	G	241	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	137	PHE	CD1-CE1-CZ	6.50	127.89	120.10
1	G	160	LEU	CA-CB-CG	-6.50	100.36	115.30
1	E	171	ASP	CB-CG-OD2	6.49	124.14	118.30
1	G	137	PHE	CD1-CE1-CZ	6.49	127.89	120.10
1	E	85	SER	O-C-N	-6.49	112.32	122.70
1	E	125	PHE	CD1-CE1-CZ	6.48	127.87	120.10
1	E	137	PHE	CD1-CE1-CZ	6.47	127.86	120.10
1	G	171	ASP	CB-CG-OD2	6.46	124.12	118.30
1	C	125	PHE	CD1-CE1-CZ	6.46	127.85	120.10
1	A	171	ASP	CB-CG-OD2	6.44	124.09	118.30
1	C	171	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	175	TYR	CZ-CE2-CD2	-6.39	114.05	119.80
1	G	175	TYR	CZ-CE2-CD2	-6.39	114.05	119.80
1	A	43	THR	CA-CB-CG2	6.39	121.34	112.40
1	G	43	THR	CA-CB-CG2	6.39	121.34	112.40
1	C	43	THR	CA-CB-CG2	6.38	121.33	112.40
1	A	160	LEU	C-N-CA	6.38	137.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	LEU	C-N-CA	6.38	137.64	121.70
1	E	160	LEU	C-N-CA	6.37	137.63	121.70
1	G	160	LEU	C-N-CA	6.37	137.63	121.70
1	A	175	TYR	CZ-CE2-CD2	-6.37	114.07	119.80
1	E	43	THR	CA-CB-CG2	6.36	121.31	112.40
1	E	175	TYR	CZ-CE2-CD2	-6.35	114.09	119.80
1	G	14	TYR	CG-CD1-CE1	6.34	126.37	121.30
1	G	260	PHE	CB-CG-CD1	-6.34	116.36	120.80
1	A	14	TYR	CG-CD1-CE1	6.33	126.37	121.30
1	E	260	PHE	CB-CG-CD1	-6.33	116.37	120.80
1	E	14	TYR	CG-CD1-CE1	6.32	126.36	121.30
1	C	247	VAL	CA-CB-CG2	6.31	120.37	110.90
1	A	260	PHE	CB-CG-CD1	-6.31	116.38	120.80
1	C	96	VAL	CA-CB-CG2	6.30	120.35	110.90
1	G	96	VAL	CA-CB-CG2	6.30	120.35	110.90
1	A	96	VAL	CA-CB-CG2	6.30	120.35	110.90
1	C	260	PHE	CB-CG-CD1	-6.29	116.39	120.80
1	A	247	VAL	CA-CB-CG2	6.28	120.33	110.90
1	G	247	VAL	CA-CB-CG2	6.28	120.31	110.90
1	E	144	GLY	O-C-N	-6.27	112.66	122.70
1	E	247	VAL	CA-CB-CG2	6.27	120.31	110.90
1	E	309	PHE	CB-CG-CD1	-6.27	116.41	120.80
1	A	144	GLY	O-C-N	-6.26	112.68	122.70
1	C	14	TYR	CG-CD1-CE1	6.26	126.31	121.30
1	E	96	VAL	CA-CB-CG2	6.26	120.29	110.90
1	C	144	GLY	O-C-N	-6.26	112.69	122.70
1	G	305	PHE	CD1-CG-CD2	6.25	126.43	118.30
1	G	144	GLY	O-C-N	-6.25	112.70	122.70
1	G	174	HIS	CA-CB-CG	-6.24	103.00	113.60
1	E	174	HIS	CA-CB-CG	-6.24	103.00	113.60
1	A	174	HIS	CA-CB-CG	-6.23	103.01	113.60
1	A	305	PHE	CD1-CG-CD2	6.23	126.40	118.30
1	C	309	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	A	309	PHE	CB-CG-CD1	-6.22	116.44	120.80
1	C	174	HIS	CA-CB-CG	-6.22	103.02	113.60
1	E	305	PHE	CD1-CG-CD2	6.22	126.39	118.30
2	F	7	TYR	CG-CD2-CE2	-6.21	116.33	121.30
1	C	10	LEU	CB-CG-CD2	6.20	121.55	111.00
1	G	7	THR	CA-C-O	-6.20	107.08	120.10
1	A	7	THR	CA-C-O	-6.20	107.09	120.10
1	A	10	LEU	CB-CG-CD2	6.20	121.53	111.00
2	D	7	TYR	CG-CD2-CE2	-6.20	116.34	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	VAL	CG1-CB-CG2	-6.20	100.99	110.90
2	B	7	TYR	CG-CD2-CE2	-6.20	116.34	121.30
1	E	7	THR	CA-C-O	-6.20	107.09	120.10
1	G	309	PHE	CB-CG-CD1	-6.19	116.46	120.80
1	C	284	VAL	CG1-CB-CG2	-6.19	100.99	110.90
1	C	305	PHE	CD1-CG-CD2	6.19	126.35	118.30
1	G	284	VAL	CG1-CB-CG2	-6.19	100.99	110.90
1	E	322	PHE	CZ-CE2-CD2	-6.19	112.67	120.10
1	G	10	LEU	CB-CG-CD2	6.19	121.53	111.00
1	E	10	LEU	CB-CG-CD2	6.18	121.51	111.00
1	C	7	THR	CA-C-O	-6.17	107.13	120.10
1	E	284	VAL	CG1-CB-CG2	-6.17	101.02	110.90
1	G	324	LEU	O-C-N	6.17	132.57	122.70
1	A	322	PHE	CZ-CE2-CD2	-6.15	112.72	120.10
1	A	159(A)	HIS	C-N-CA	-6.15	106.33	121.70
2	H	7	TYR	CG-CD2-CE2	-6.14	116.39	121.30
1	A	324	LEU	O-C-N	6.14	132.53	122.70
1	E	159(A)	HIS	C-N-CA	-6.14	106.35	121.70
1	A	326	ARG	CG-CD-NE	6.14	124.69	111.80
1	A	15	TYR	CD1-CG-CD2	6.13	124.64	117.90
1	C	326	ARG	CG-CD-NE	6.13	124.68	111.80
1	E	324	LEU	O-C-N	6.13	132.50	122.70
1	C	118	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	159(A)	HIS	C-N-CA	-6.12	106.39	121.70
1	G	159(A)	HIS	C-N-CA	-6.12	106.39	121.70
1	G	155	TYR	CD1-CE1-CZ	-6.12	114.29	119.80
1	G	322	PHE	CZ-CE2-CD2	-6.12	112.75	120.10
1	C	322	PHE	CZ-CE2-CD2	-6.12	112.75	120.10
1	G	326	ARG	CG-CD-NE	6.12	124.65	111.80
1	C	15	TYR	CD1-CG-CD2	6.12	124.63	117.90
1	E	326	ARG	CG-CD-NE	6.12	124.64	111.80
1	C	324	LEU	O-C-N	6.11	132.48	122.70
1	E	15	TYR	CD1-CG-CD2	6.11	124.62	117.90
1	A	118	ASP	CB-CG-OD2	6.11	123.80	118.30
1	E	171	ASP	C-N-CD	-6.11	107.17	120.60
1	G	15	TYR	CD1-CG-CD2	6.10	124.61	117.90
1	G	118	ASP	CB-CG-OD2	6.09	123.78	118.30
1	E	155	TYR	CD1-CE1-CZ	-6.09	114.32	119.80
1	A	171	ASP	C-N-CD	-6.08	107.21	120.60
1	E	118	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	147	LYS	CA-CB-CG	6.08	126.76	113.40
1	C	171	ASP	C-N-CD	-6.07	107.24	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	171	ASP	C-N-CD	-6.07	107.24	120.60
1	A	39	TRP	CD1-NE1-CE2	6.07	114.46	109.00
1	A	147	LYS	CA-CB-CG	6.07	126.75	113.40
1	C	39	TRP	CD1-NE1-CE2	6.07	114.46	109.00
1	A	155	TYR	CD1-CE1-CZ	-6.06	114.34	119.80
1	G	147	LYS	CA-CB-CG	6.06	126.74	113.40
1	C	15	TYR	CE1-CZ-CE2	6.06	129.50	119.80
2	B	4	PHE	CZ-CE2-CD2	6.05	127.37	120.10
1	C	155	TYR	CD1-CE1-CZ	-6.05	114.35	119.80
1	G	39	TRP	CD1-NE1-CE2	6.05	114.45	109.00
1	E	15	TYR	CE1-CZ-CE2	6.05	129.48	119.80
2	H	4	PHE	CZ-CE2-CD2	6.05	127.36	120.10
2	F	4	PHE	CZ-CE2-CD2	6.05	127.36	120.10
1	A	15	TYR	CE1-CZ-CE2	6.04	129.47	119.80
1	G	15	TYR	CE1-CZ-CE2	6.04	129.47	119.80
1	E	147	LYS	CA-CB-CG	6.04	126.69	113.40
2	D	4	PHE	CZ-CE2-CD2	6.03	127.33	120.10
1	A	190	TRP	CB-CG-CD1	-6.01	119.19	127.00
1	C	190	TRP	CB-CG-CD1	-6.01	119.19	127.00
1	E	39	TRP	CD1-NE1-CE2	6.00	114.40	109.00
1	G	190	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	E	190	TRP	CB-CG-CD1	-6.00	119.21	127.00
1	C	301	LEU	CB-CG-CD2	5.99	121.18	111.00
1	A	301	LEU	CB-CG-CD2	5.98	121.17	111.00
1	E	301	LEU	CB-CG-CD2	5.97	121.15	111.00
1	G	301	LEU	CB-CG-CD2	5.96	121.14	111.00
1	C	161	LEU	N-CA-CB	5.96	122.33	110.40
1	E	161	LEU	N-CA-CB	5.96	122.33	110.40
1	A	161	LEU	N-CA-CB	5.96	122.32	110.40
1	G	161	LEU	N-CA-CB	5.95	122.29	110.40
1	G	141	LEU	CB-CG-CD1	5.94	121.10	111.00
1	A	113	MET	O-C-N	-5.91	113.24	122.70
1	A	141	LEU	CB-CG-CD1	5.91	121.04	111.00
1	C	141	LEU	CB-CG-CD1	5.91	121.05	111.00
1	C	113	MET	O-C-N	-5.90	113.25	122.70
1	E	113	MET	O-C-N	-5.90	113.25	122.70
1	E	141	LEU	CB-CG-CD1	5.90	121.03	111.00
1	G	-1	ASP	CA-C-O	5.90	132.49	120.10
1	G	138	ASP	OD1-CG-OD2	-5.90	112.09	123.30
1	C	138	ASP	OD1-CG-OD2	-5.89	112.10	123.30
1	E	138	ASP	OD1-CG-OD2	-5.89	112.10	123.30
1	A	138	ASP	OD1-CG-OD2	-5.89	112.10	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	THR	O-C-N	5.89	132.13	122.70
1	G	113	MET	O-C-N	-5.89	113.27	122.70
1	A	-1	ASP	CA-C-O	5.88	132.45	120.10
1	E	-1	ASP	CA-C-O	5.88	132.45	120.10
1	E	56	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	G	97	THR	O-C-N	5.88	132.11	122.70
1	C	-1	ASP	CA-C-O	5.87	132.43	120.10
1	C	260	PHE	CG-CD1-CE1	-5.87	114.34	120.80
1	E	260	PHE	CG-CD1-CE1	-5.87	114.34	120.80
1	A	260	PHE	CG-CD1-CE1	-5.87	114.35	120.80
1	C	289	MET	CG-SD-CE	5.87	109.58	100.20
1	A	97	THR	O-C-N	5.86	132.08	122.70
1	A	289	MET	CG-SD-CE	5.86	109.58	100.20
1	A	322	PHE	CB-CG-CD1	-5.86	116.70	120.80
1	E	289	MET	CG-SD-CE	5.86	109.57	100.20
1	G	260	PHE	CG-CD1-CE1	-5.85	114.36	120.80
1	C	276	LEU	C-N-CA	5.85	136.32	121.70
1	G	265	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	G	288	ALA	O-C-N	5.85	132.06	122.70
1	G	289	MET	CG-SD-CE	5.85	109.55	100.20
1	G	276	LEU	C-N-CA	5.84	136.31	121.70
1	E	97	THR	O-C-N	5.84	132.05	122.70
1	G	322	PHE	CB-CG-CD1	-5.84	116.72	120.80
1	C	288	ALA	O-C-N	5.83	132.04	122.70
1	C	265	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	A	276	LEU	C-N-CA	5.83	136.27	121.70
1	A	288	ALA	O-C-N	5.83	132.02	122.70
1	E	276	LEU	C-N-CA	5.82	136.26	121.70
1	C	322	PHE	CB-CG-CD1	-5.82	116.73	120.80
1	E	322	PHE	CB-CG-CD1	-5.81	116.73	120.80
1	A	56	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	C	56	TYR	CB-CG-CD1	-5.79	117.52	121.00
1	E	300	VAL	CA-CB-CG1	5.79	119.58	110.90
1	A	265	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	E	288	ALA	O-C-N	5.79	131.96	122.70
1	C	309	PHE	CB-CG-CD2	5.78	124.85	120.80
1	A	300	VAL	CA-CB-CG1	5.78	119.56	110.90
1	E	309	PHE	CB-CG-CD2	5.78	124.84	120.80
1	G	300	VAL	CA-CB-CG1	5.78	119.56	110.90
1	A	309	PHE	CB-CG-CD2	5.77	124.84	120.80
1	E	265	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	C	300	VAL	CA-CB-CG1	5.77	119.55	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	HIS	O-C-N	5.76	131.92	122.70
1	G	56	TYR	CB-CG-CD1	-5.76	117.55	121.00
1	G	52	ILE	N-CA-CB	-5.76	97.56	110.80
1	A	74	HIS	O-C-N	5.75	131.91	122.70
1	A	52	ILE	N-CA-CB	-5.75	97.57	110.80
1	C	52	ILE	N-CA-CB	-5.75	97.57	110.80
1	G	309	PHE	CB-CG-CD2	5.75	124.82	120.80
1	E	52	ILE	N-CA-CB	-5.74	97.59	110.80
1	E	4	VAL	CA-CB-CG1	-5.74	102.30	110.90
1	A	10	LEU	O-C-N	5.73	131.88	122.70
1	E	84	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	G	74	HIS	O-C-N	5.73	131.87	122.70
1	E	10	LEU	O-C-N	5.73	131.87	122.70
1	E	74	HIS	O-C-N	5.73	131.87	122.70
1	C	10	LEU	O-C-N	5.73	131.87	122.70
1	C	84	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	A	84	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	A	4	VAL	CA-CB-CG1	-5.72	102.32	110.90
1	G	10	LEU	O-C-N	5.72	131.85	122.70
1	G	84	LEU	CB-CG-CD1	-5.72	101.28	111.00
1	G	4	VAL	CA-CB-CG1	-5.72	102.33	110.90
1	E	107	LEU	CB-CG-CD1	5.71	120.70	111.00
1	C	4	VAL	CA-CB-CG1	-5.70	102.34	110.90
1	A	107	LEU	CB-CG-CD1	5.70	120.69	111.00
1	G	107	LEU	CB-CG-CD1	5.70	120.68	111.00
1	C	179	PHE	CG-CD1-CE1	5.69	127.06	120.80
1	C	107	LEU	CB-CG-CD1	5.68	120.67	111.00
1	G	179	PHE	CG-CD1-CE1	5.67	127.04	120.80
1	A	179	PHE	CG-CD1-CE1	5.67	127.04	120.80
1	E	9	TYR	C-N-CA	5.66	135.85	121.70
1	E	179	PHE	CG-CD1-CE1	5.66	127.02	120.80
1	A	9	TYR	C-N-CA	5.65	135.83	121.70
1	C	39	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	G	9	TYR	C-N-CA	5.64	135.81	121.70
1	A	39	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	E	31	PHE	CZ-CE2-CD2	-5.64	113.33	120.10
1	C	9	TYR	C-N-CA	5.63	135.78	121.70
1	C	265	ARG	CA-CB-CG	5.63	125.79	113.40
1	G	265	ARG	CA-CB-CG	5.63	125.79	113.40
1	A	265	ARG	CA-CB-CG	5.63	125.78	113.40
1	C	31	PHE	CZ-CE2-CD2	-5.63	113.35	120.10
1	E	39	TRP	CG-CD1-NE1	-5.62	104.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	31	PHE	CZ-CE2-CD2	-5.62	113.36	120.10
1	G	39	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	A	31	PHE	CZ-CE2-CD2	-5.61	113.37	120.10
1	E	265	ARG	CA-CB-CG	5.61	125.74	113.40
1	E	1	ILE	O-C-N	5.61	131.68	122.70
1	E	182	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	A	1	ILE	O-C-N	5.59	131.65	122.70
1	C	1	ILE	O-C-N	5.58	131.62	122.70
1	A	182	VAL	CG1-CB-CG2	-5.57	101.98	110.90
1	E	141	LEU	CB-CG-CD2	5.57	120.47	111.00
1	G	1	ILE	O-C-N	5.57	131.62	122.70
1	A	66	GLU	O-C-N	-5.57	113.79	122.70
1	A	141	LEU	CB-CG-CD2	5.57	120.46	111.00
1	C	71	PHE	O-C-N	-5.57	113.80	122.70
1	C	182	VAL	CG1-CB-CG2	-5.57	102.00	110.90
1	E	66	GLU	O-C-N	-5.57	113.79	122.70
1	G	71	PHE	O-C-N	-5.57	113.79	122.70
1	G	66	GLU	O-C-N	-5.56	113.80	122.70
1	A	71	PHE	O-C-N	-5.56	113.80	122.70
1	G	141	LEU	CB-CG-CD2	5.56	120.44	111.00
1	G	182	VAL	CG1-CB-CG2	-5.56	102.01	110.90
1	C	141	LEU	CB-CG-CD2	5.55	120.44	111.00
1	E	71	PHE	O-C-N	-5.54	113.83	122.70
1	C	66	GLU	O-C-N	-5.54	113.83	122.70
1	C	30	ILE	CA-C-N	5.54	129.38	117.20
1	A	30	ILE	CA-C-N	5.53	129.38	117.20
1	G	30	ILE	CA-C-N	5.52	129.35	117.20
1	E	30	ILE	CA-C-N	5.52	129.35	117.20
1	E	242	LEU	CB-CG-CD1	5.52	120.39	111.00
1	G	204	LEU	O-C-N	-5.52	113.87	122.70
1	C	242	LEU	CB-CG-CD1	5.51	120.38	111.00
1	A	242	LEU	CB-CG-CD1	5.51	120.36	111.00
1	A	204	LEU	O-C-N	-5.50	113.90	122.70
1	E	204	LEU	O-C-N	-5.50	113.90	122.70
1	G	242	LEU	CB-CG-CD1	5.48	120.31	111.00
1	E	245	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	C	204	LEU	O-C-N	-5.46	113.96	122.70
1	A	245	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	G	79	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	C	79	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	C	245	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	C	15	TYR	O-C-N	-5.41	114.00	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	50	CYS	O-C-N	-5.41	114.01	123.20
1	C	50	CYS	O-C-N	-5.40	114.02	123.20
1	G	211	GLU	O-C-N	5.40	131.34	122.70
1	G	15	TYR	O-C-N	-5.40	114.02	123.20
1	E	231	ILE	O-C-N	-5.40	114.07	122.70
1	E	248	SER	CA-CB-OG	-5.40	96.63	111.20
1	A	79	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	248	SER	CA-CB-OG	-5.39	96.64	111.20
1	C	231	ILE	O-C-N	-5.39	114.07	122.70
1	E	50	CYS	O-C-N	-5.39	114.03	123.20
1	E	211	GLU	O-C-N	5.39	131.33	122.70
1	A	211	GLU	O-C-N	5.39	131.32	122.70
1	C	248	SER	CA-CB-OG	-5.39	96.66	111.20
1	A	15	TYR	O-C-N	-5.38	114.05	123.20
1	C	211	GLU	O-C-N	5.38	131.31	122.70
1	G	248	SER	CA-CB-OG	-5.38	96.66	111.20
1	A	50	CYS	O-C-N	-5.38	114.06	123.20
1	A	231	ILE	O-C-N	-5.36	114.12	122.70
1	G	245	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	E	25	GLN	CA-CB-CG	-5.36	101.62	113.40
1	E	79	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	G	231	ILE	O-C-N	-5.36	114.13	122.70
1	A	25	GLN	CA-CB-CG	-5.35	101.62	113.40
1	C	190	TRP	CD1-NE1-CE2	5.35	113.82	109.00
1	E	15	TYR	O-C-N	-5.35	114.11	123.20
1	G	175	TYR	CD1-CG-CD2	5.35	123.78	117.90
1	A	5	VAL	CA-CB-CG1	5.34	118.92	110.90
1	E	5	VAL	CA-CB-CG1	5.34	118.92	110.90
1	G	25	GLN	CA-CB-CG	-5.34	101.64	113.40
1	E	80	VAL	O-C-N	-5.34	114.15	122.70
1	E	175	TYR	CD1-CG-CD2	5.34	123.78	117.90
1	C	25	GLN	CA-CB-CG	-5.34	101.65	113.40
1	A	175	TYR	CD1-CG-CD2	5.34	123.77	117.90
1	G	5	VAL	CA-CB-CG1	5.33	118.90	110.90
1	G	224	PRO	O-C-N	-5.32	114.18	122.70
1	G	301	LEU	CA-C-O	-5.32	108.92	120.10
1	C	158	GLY	O-C-N	5.32	131.21	121.10
2	D	4	PHE	CG-CD1-CE1	5.32	126.65	120.80
1	C	5	VAL	CA-CB-CG1	5.32	118.87	110.90
1	C	175	TYR	CD1-CG-CD2	5.31	123.74	117.90
1	C	80	VAL	O-C-N	-5.31	114.20	122.70
1	E	301	LEU	CA-C-O	-5.31	108.95	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	TRP	CD1-NE1-CE2	5.31	113.78	109.00
1	G	80	VAL	O-C-N	-5.31	114.21	122.70
1	G	158	GLY	O-C-N	5.31	131.19	121.10
1	G	190	TRP	CD1-NE1-CE2	5.31	113.78	109.00
1	A	190	TRP	CD1-NE1-CE2	5.31	113.78	109.00
1	E	202	SER	C-N-CA	5.31	134.96	121.70
1	A	158	GLY	O-C-N	5.30	131.18	121.10
1	A	301	LEU	CA-C-O	-5.30	108.96	120.10
1	A	80	VAL	O-C-N	-5.30	114.22	122.70
1	E	224	PRO	O-C-N	-5.30	114.23	122.70
2	H	4	PHE	CG-CD1-CE1	5.30	126.62	120.80
1	C	301	LEU	CA-C-O	-5.29	108.98	120.10
1	C	202	SER	C-N-CA	5.29	134.94	121.70
1	A	202	SER	C-N-CA	5.29	134.92	121.70
1	A	224	PRO	O-C-N	-5.29	114.24	122.70
1	E	158	GLY	O-C-N	5.29	131.14	121.10
2	B	4	PHE	CG-CD1-CE1	5.28	126.61	120.80
1	G	202	SER	C-N-CA	5.28	134.90	121.70
1	C	224	PRO	O-C-N	-5.28	114.26	122.70
2	F	4	PHE	CG-CD1-CE1	5.27	126.60	120.80
1	C	24	PRO	CA-N-CD	5.27	119.08	111.70
1	E	144	GLY	C-N-CA	-5.27	108.52	121.70
1	E	104	VAL	CA-CB-CG1	5.27	118.80	110.90
1	G	144	GLY	C-N-CA	-5.27	108.54	121.70
1	C	70	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	144	GLY	C-N-CA	-5.26	108.54	121.70
1	C	179	PHE	CB-CG-CD1	5.26	124.48	120.80
1	G	104	VAL	CA-CB-CG1	5.25	118.78	110.90
1	C	144	GLY	C-N-CA	-5.25	108.57	121.70
1	A	24	PRO	CA-N-CD	5.25	119.05	111.70
1	G	312	GLU	O-C-N	-5.25	114.30	122.70
1	A	179	PHE	CB-CG-CD1	5.25	124.47	120.80
1	E	24	PRO	CA-N-CD	5.25	119.05	111.70
1	G	24	PRO	CA-N-CD	5.24	119.04	111.70
1	A	104	VAL	CA-CB-CG1	5.24	118.76	110.90
1	C	104	VAL	CA-CB-CG1	5.24	118.76	110.90
1	E	70	ASP	CB-CG-OD1	-5.24	113.59	118.30
2	D	2	HIS	CA-CB-CG	-5.23	104.70	113.60
1	E	312	GLU	O-C-N	-5.23	114.33	122.70
1	G	179	PHE	CB-CG-CD1	5.23	124.46	120.80
1	A	312	GLU	O-C-N	-5.23	114.33	122.70
1	G	117	PHE	CG-CD1-CE1	5.22	126.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	HIS	CA-CB-CG	-5.22	104.72	113.60
1	E	174	HIS	O-C-N	-5.22	114.35	122.70
2	F	2	HIS	CA-CB-CG	-5.22	104.73	113.60
1	A	70	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	G	182	VAL	CA-CB-CG2	5.21	118.72	110.90
1	C	182	VAL	CA-CB-CG2	5.21	118.72	110.90
1	C	312	GLU	O-C-N	-5.21	114.36	122.70
1	E	182	VAL	CA-CB-CG2	5.21	118.71	110.90
1	A	117	PHE	CG-CD1-CE1	5.20	126.52	120.80
1	A	182	VAL	CA-CB-CG2	5.20	118.71	110.90
1	G	70	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	H	2	HIS	CA-CB-CG	-5.20	104.76	113.60
1	C	18	ILE	C-N-CA	-5.20	111.38	122.30
1	C	117	PHE	CG-CD1-CE1	5.20	126.52	120.80
1	E	18	ILE	C-N-CA	-5.19	111.39	122.30
1	A	18	ILE	C-N-CA	-5.19	111.40	122.30
1	E	117	PHE	CG-CD1-CE1	5.19	126.51	120.80
1	A	174	HIS	O-C-N	-5.19	114.40	122.70
1	G	18	ILE	C-N-CA	-5.18	111.42	122.30
1	G	174	HIS	O-C-N	-5.18	114.41	122.70
1	E	179	PHE	CB-CG-CD1	5.18	124.42	120.80
1	C	174	HIS	O-C-N	-5.17	114.42	122.70
1	E	313	PHE	CG-CD2-CE2	5.16	126.47	120.80
1	G	313	PHE	CG-CD2-CE2	5.15	126.46	120.80
1	A	313	PHE	CG-CD2-CE2	5.14	126.45	120.80
1	G	175	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	C	313	PHE	CG-CD2-CE2	5.13	126.45	120.80
1	G	290	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	290	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	24	PRO	O-C-N	5.12	130.89	122.70
1	G	24	PRO	O-C-N	5.11	130.88	122.70
1	C	24	PRO	O-C-N	5.11	130.87	122.70
1	E	290	ASP	CB-CG-OD2	5.11	122.89	118.30
1	E	24	PRO	O-C-N	5.10	130.86	122.70
1	A	290	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	175	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	C	76	GLY	CA-C-N	5.07	128.35	117.20
1	C	310	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	A	228	LEU	CB-CG-CD1	5.06	119.60	111.00
1	C	175	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	C	228	LEU	CB-CG-CD1	5.06	119.60	111.00
1	G	228	LEU	CB-CG-CD1	5.06	119.60	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	76	GLY	CA-C-N	5.06	128.33	117.20
1	E	175	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	76	GLY	CA-C-N	5.05	128.31	117.20
1	E	228	LEU	CB-CG-CD1	5.05	119.58	111.00
1	G	76	GLY	CA-C-N	5.04	128.29	117.20
1	A	15	TYR	CG-CD2-CE2	-5.02	117.29	121.30
1	A	158	GLY	C-N-CD	-5.01	109.58	120.60
1	E	158	GLY	C-N-CD	-5.01	109.58	120.60
1	G	158	GLY	C-N-CD	-5.01	109.59	120.60
1	G	310	TYR	CG-CD1-CE1	-5.01	117.30	121.30
1	G	15	TYR	CG-CD2-CE2	-5.00	117.30	121.30
1	C	158	GLY	C-N-CD	-5.00	109.59	120.60
1	C	30	ILE	O-C-N	-5.00	114.70	122.70
1	E	15	TYR	CG-CD2-CE2	-5.00	117.30	121.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	319	ARG	Sidechain
2	B	6	LPL	Mainchain,Peptide
1	C	241	ARG	Sidechain
1	C	265	ARG	Sidechain
1	C	319	ARG	Sidechain
2	D	6	LPL	Mainchain,Peptide
1	E	241	ARG	Sidechain
1	E	265	ARG	Sidechain
1	E	319	ARG	Sidechain
2	F	6	LPL	Mainchain,Peptide
1	G	241	ARG	Sidechain
1	G	265	ARG	Sidechain
1	G	319	ARG	Sidechain
2	H	6	LPL	Mainchain,Peptide

## 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	2511	0	2442	53	16
1	C	2511	0	2442	51	19
1	E	2511	0	2442	53	17
1	G	2511	0	2442	53	19
2	B	90	0	86	2	0
2	D	90	0	86	2	0
2	F	90	0	86	2	0
2	H	90	0	86	2	0
3	A	148	0	0	3	1
3	B	5	0	0	0	0
3	C	3	0	0	1	0
All	All	10560	0	10112	210	36

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 10.

All (210) 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:C:199:VAL:HB	1:C:203:THR:HG23	1.44	1.00
1:E:199:VAL:HB	1:E:203:THR:HG23	1.44	1.00
1:G:199:VAL:HB	1:G:203:THR:HG23	1.44	0.99
1:A:199:VAL:HB	1:A:203:THR:HG23	1.44	0.97
1:A:199:VAL:HB	1:A:203:THR:CG2	2.00	0.92
1:E:199:VAL:HB	1:E:203:THR:CG2	2.00	0.91
1:G:199:VAL:HB	1:G:203:THR:CG2	2.00	0.91
1:C:199:VAL:HB	1:C:203:THR:CG2	2.00	0.90
1:A:65:MET:HG3	1:A:86:GLN:HE21	1.42	0.84
1:E:65:MET:HG3	1:E:86:GLN:HE21	1.42	0.82
1:G:65:MET:HG3	1:G:86:GLN:HE21	1.42	0.81
1:C:65:MET:HG3	1:C:86:GLN:HE21	1.42	0.81
1:G:8:ASN:H	1:G:160:LEU:CD2	1.94	0.81
1:C:8:ASN:H	1:C:160:LEU:CD2	1.94	0.81
1:C:159:PRO:O	1:C:159(A):HIS:CB	2.30	0.80
1:A:8:ASN:H	1:A:160:LEU:CD2	1.94	0.80
1:A:317:ASN:HB2	1:A:319:ARG:HD3	1.64	0.79
1:G:317:ASN:HB2	1:G:319:ARG:HD3	1.64	0.79
1:E:317:ASN:HB2	1:E:319:ARG:HD3	1.64	0.79
1:E:8:ASN:H	1:E:160:LEU:CD2	1.94	0.79
1:E:159:PRO:O	1:E:159(A):HIS:CB	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:O	1:A:159(A):HIS:CB	2.30	0.79
1:C:159(A):HIS:O	1:C:161:LEU:N	2.16	0.78
1:A:159(A):HIS:O	1:A:161:LEU:N	2.16	0.78
1:A:8:ASN:H	1:A:160:LEU:HD21	1.49	0.78
1:G:159:PRO:O	1:G:159(A):HIS:CB	2.30	0.78
1:C:317:ASN:HB2	1:C:319:ARG:HD3	1.64	0.77
1:C:8:ASN:H	1:C:160:LEU:HD21	1.49	0.77
1:E:8:ASN:H	1:E:160:LEU:HD21	1.49	0.77
1:G:159(A):HIS:O	1:G:161:LEU:N	2.16	0.76
1:G:8:ASN:H	1:G:160:LEU:HD21	1.49	0.75
1:E:159(A):HIS:O	1:E:161:LEU:N	2.16	0.74
1:E:43:THR:HG22	1:E:44:LYS:HD2	1.70	0.74
1:A:43:THR:HG22	1:A:44:LYS:HD2	1.70	0.73
1:C:43:THR:HG22	1:C:44:LYS:HD2	1.70	0.73
1:G:43:THR:HG22	1:G:44:LYS:HD2	1.70	0.72
1:C:203:THR:OG1	1:C:203:THR:O	2.03	0.71
1:G:203:THR:OG1	1:G:203:THR:O	2.03	0.70
1:E:203:THR:O	1:E:203:THR:OG1	2.03	0.70
1:A:48:LEU:O	1:A:48:LEU:HD23	1.92	0.69
1:C:48:LEU:HD23	1:C:48:LEU:O	1.92	0.69
1:A:317:ASN:CB	1:A:319:ARG:HD3	2.23	0.69
1:E:48:LEU:HD23	1:E:48:LEU:O	1.92	0.69
1:C:317:ASN:CB	1:C:319:ARG:HD3	2.23	0.69
1:G:48:LEU:O	1:G:48:LEU:HD23	1.92	0.68
1:A:203:THR:O	1:A:203:THR:OG1	2.03	0.68
1:E:317:ASN:CB	1:E:319:ARG:HD3	2.23	0.67
1:G:317:ASN:CB	1:G:319:ARG:HD3	2.23	0.67
1:E:160:LEU:HD23	1:E:162:GLY:N	2.10	0.67
1:A:160:LEU:HD23	1:A:162:GLY:N	2.10	0.66
1:G:160:LEU:HD23	1:G:162:GLY:N	2.10	0.66
1:C:160:LEU:HD23	1:C:162:GLY:N	2.10	0.66
1:E:200:GLY:HA2	1:E:256:PRO:HB2	1.80	0.64
1:C:57:GLU:OE2	1:C:59:SER:HB2	1.98	0.64
1:E:57:GLU:OE2	1:E:59:SER:HB2	1.98	0.64
1:G:57:GLU:OE2	1:G:59:SER:HB2	1.98	0.64
1:A:200:GLY:HA2	1:A:256:PRO:HB2	1.80	0.64
1:G:200:GLY:HA2	1:G:256:PRO:HB2	1.80	0.64
1:C:200:GLY:HA2	1:C:256:PRO:HB2	1.80	0.64
1:A:57:GLU:OE2	1:A:59:SER:HB2	1.98	0.62
1:E:174:HIS:HD2	1:E:326:ARG:OXT	1.83	0.61
1:G:200:GLY:CA	1:G:256:PRO:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLY:CA	1:A:256:PRO:HB2	2.30	0.61
1:C:200:GLY:CA	1:C:256:PRO:HB2	2.30	0.61
1:A:201:SER:HB2	3:A:460:HOH:O	1.99	0.61
1:C:174:HIS:HD2	1:C:326:ARG:OXT	1.83	0.60
1:A:174:HIS:HD2	1:A:326:ARG:OXT	1.83	0.60
1:E:200:GLY:CA	1:E:256:PRO:HB2	2.30	0.60
1:G:202:SER:C	1:G:203:THR:HG22	2.21	0.60
1:A:53:HIS:HE1	1:A:115:ALA:O	1.85	0.60
1:E:202:SER:C	1:E:203:THR:HG22	2.21	0.60
1:C:65:MET:HG3	1:C:86:GLN:NE2	2.16	0.60
1:G:174:HIS:HD2	1:G:326:ARG:OXT	1.83	0.59
1:A:202:SER:C	1:A:203:THR:HG22	2.21	0.59
1:C:202:SER:C	1:C:203:THR:HG22	2.21	0.59
1:E:53:HIS:HE1	1:E:115:ALA:O	1.85	0.59
1:G:53:HIS:HE1	1:G:115:ALA:O	1.85	0.59
1:A:65:MET:HG3	1:A:86:GLN:NE2	2.16	0.59
1:C:53:HIS:HE1	1:C:115:ALA:O	1.85	0.58
1:G:65:MET:HG3	1:G:86:GLN:NE2	2.16	0.58
1:E:65:MET:HG3	1:E:86:GLN:NE2	2.16	0.57
1:A:139:HIS:HE1	3:A:402:HOH:O	1.87	0.57
1:G:52:ILE:CD1	1:G:113:MET:HG2	2.35	0.56
1:A:249:CYS:O	1:A:252:VAL:HG23	2.06	0.56
1:A:52:ILE:CD1	1:A:113:MET:HG2	2.35	0.56
1:E:52:ILE:CD1	1:E:113:MET:HG2	2.35	0.56
1:E:249:CYS:O	1:E:252:VAL:HG23	2.06	0.56
1:C:249:CYS:O	1:C:252:VAL:HG23	2.06	0.56
1:C:52:ILE:CD1	1:C:113:MET:HG2	2.35	0.56
1:G:249:CYS:O	1:G:252:VAL:HG23	2.06	0.56
1:C:202:SER:O	1:C:203:THR:HG22	2.06	0.55
1:G:202:SER:O	1:G:203:THR:HG22	2.06	0.55
1:A:52:ILE:HG22	1:A:53:HIS:CD2	2.42	0.55
1:G:52:ILE:HG22	1:G:53:HIS:CD2	2.42	0.55
1:C:52:ILE:HG22	1:C:53:HIS:CD2	2.42	0.55
1:E:202:SER:O	1:E:203:THR:HG22	2.07	0.55
1:E:52:ILE:HG22	1:E:53:HIS:CD2	2.42	0.55
1:A:202:SER:O	1:A:203:THR:HG22	2.06	0.54
1:A:205:LEU:HD13	1:A:227:SER:HB3	1.89	0.54
1:C:205:LEU:HD13	1:C:227:SER:HB3	1.89	0.54
1:G:160:LEU:HD23	1:G:162:GLY:CA	2.38	0.54
1:E:160:LEU:HD23	1:E:162:GLY:CA	2.38	0.54
1:C:160:LEU:HD23	1:C:162:GLY:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:LEU:HD13	1:G:227:SER:HB3	1.89	0.54
1:A:160:LEU:HD23	1:A:162:GLY:CA	2.38	0.53
1:G:252:VAL:HB	1:G:253:PRO:HD3	1.91	0.53
1:E:205:LEU:HD13	1:E:227:SER:HB3	1.89	0.52
1:E:0:LEU:HD21	1:E:94:ILE:HD11	1.92	0.52
1:E:8:ASN:OD1	1:E:8:ASN:C	2.48	0.52
1:E:7:THR:HA	1:E:160:LEU:HD22	1.92	0.52
1:C:8:ASN:C	1:C:8:ASN:OD1	2.48	0.52
1:A:7:THR:HA	1:A:160:LEU:HD22	1.92	0.52
1:A:252:VAL:HB	1:A:253:PRO:HD3	1.91	0.52
1:A:0:LEU:HD21	1:A:94:ILE:HD11	1.92	0.51
1:C:252:VAL:HB	1:C:253:PRO:HD3	1.91	0.51
1:G:7:THR:HA	1:G:160:LEU:HD22	1.92	0.51
1:G:0:LEU:HD21	1:G:94:ILE:HD11	1.92	0.51
1:G:8:ASN:C	1:G:8:ASN:OD1	2.48	0.51
1:E:252:VAL:HB	1:E:253:PRO:HD3	1.91	0.51
1:A:127:ALA:HB3	1:A:188:ASP:HB3	1.93	0.51
1:C:7:THR:HA	1:C:160:LEU:HD22	1.92	0.50
1:G:58:SER:HB2	1:G:64:TYR:CD1	2.47	0.50
1:C:58:SER:HB2	1:C:64:TYR:CD1	2.47	0.50
1:C:0:LEU:HD21	1:C:94:ILE:HD11	1.92	0.50
1:G:127:ALA:HB3	1:G:188:ASP:HB3	1.93	0.50
1:E:58:SER:HB2	1:E:64:TYR:CD1	2.47	0.49
1:E:75:TYR:HA	2:F:6:LPL:O	2.12	0.49
1:A:8:ASN:C	1:A:8:ASN:OD1	2.48	0.49
1:C:127:ALA:HB3	1:C:188:ASP:HB3	1.93	0.49
1:G:75:TYR:HA	2:H:6:LPL:O	2.12	0.49
1:A:58:SER:HB2	1:A:64:TYR:CD1	2.47	0.49
1:E:127:ALA:HB3	1:E:188:ASP:HB3	1.93	0.49
1:C:75:TYR:HA	2:D:6:LPL:O	2.12	0.49
1:A:75:TYR:HA	2:B:6:LPL:O	2.12	0.48
1:C:291:ILE:O	1:C:296:GLY:HA3	2.14	0.48
1:A:291:ILE:O	1:A:296:GLY:HA3	2.14	0.48
1:G:291:ILE:O	1:G:296:GLY:HA3	2.14	0.47
1:C:48:LEU:HD23	1:C:48:LEU:C	2.34	0.47
1:C:9:TYR:CE2	1:C:10:LEU:HD12	2.49	0.47
1:A:9:TYR:CE2	1:A:10:LEU:HD12	2.49	0.47
1:G:9:TYR:CE2	1:G:10:LEU:HD12	2.49	0.47
1:E:291:ILE:O	1:E:296:GLY:HA3	2.14	0.47
1:E:9:TYR:CE2	1:E:10:LEU:HD12	2.49	0.47
1:G:199:VAL:HB	1:G:203:THR:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:SER:HB2	1:E:64:TYR:CG	2.50	0.47
1:A:58:SER:HB2	1:A:64:TYR:CG	2.50	0.47
1:A:48:LEU:C	1:A:48:LEU:HD23	2.34	0.47
1:C:58:SER:HB2	1:C:64:TYR:CG	2.50	0.47
1:G:58:SER:HB2	1:G:64:TYR:CG	2.50	0.47
1:G:48:LEU:C	1:G:48:LEU:HD23	2.34	0.47
1:A:158:GLY:HA3	1:A:159:PRO:HD2	1.27	0.46
1:E:48:LEU:C	1:E:48:LEU:HD23	2.34	0.46
1:A:199:VAL:HB	1:A:203:THR:HG21	1.94	0.46
1:C:271:SER:HA	1:C:274:TYR:CE2	2.51	0.45
1:G:271:SER:HA	1:G:274:TYR:CE2	2.51	0.45
1:A:271:SER:HA	1:A:274:TYR:CE2	2.51	0.45
1:G:8:ASN:HB2	1:G:162:GLY:CA	2.47	0.45
1:A:8:ASN:HB2	1:A:162:GLY:CA	2.47	0.45
1:E:271:SER:HA	1:E:274:TYR:CE2	2.51	0.45
1:C:292:PRO:HA	1:C:293:PRO:HD3	1.82	0.45
1:E:8:ASN:HB2	1:E:162:GLY:CA	2.47	0.45
1:E:172:PRO:HA	1:E:175:TYR:CE1	2.52	0.45
1:G:172:PRO:HA	1:G:175:TYR:CE1	2.52	0.45
1:A:172:PRO:HA	1:A:175:TYR:CE1	2.52	0.45
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.72	0.45
1:C:199:VAL:HB	1:C:203:THR:HG21	1.94	0.44
1:E:171:ASP:HA	1:E:172:PRO:HD2	1.72	0.44
1:C:172:PRO:HA	1:C:175:TYR:CE1	2.52	0.44
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.94	0.44
1:C:8:ASN:HB2	1:C:162:GLY:CA	2.47	0.44
1:C:175:TYR:HA	1:C:324:LEU:O	2.18	0.44
1:G:175:TYR:HA	1:G:324:LEU:O	2.18	0.44
1:E:292:PRO:HA	1:E:293:PRO:HD3	1.81	0.44
1:G:292:PRO:HA	1:G:293:PRO:HD3	1.81	0.44
1:A:272:THR:HG23	3:A:456:HOH:O	2.18	0.44
1:C:171:ASP:HA	1:C:172:PRO:HD2	1.72	0.44
1:E:175:TYR:HA	1:E:324:LEU:O	2.18	0.43
1:A:175:TYR:HA	1:A:324:LEU:O	2.18	0.43
1:A:12:SER:HB3	2:B:1:PIV:C3	2.48	0.43
1:E:12:SER:HB3	2:F:1:PIV:C3	2.49	0.43
1:E:199:VAL:HB	1:E:203:THR:HG21	1.94	0.43
1:G:159(A):HIS:C	1:G:160:LEU:HG	2.39	0.43
1:E:159(A):HIS:C	1:E:160:LEU:HG	2.39	0.43
1:C:12:SER:HB3	2:D:1:PIV:C3	2.48	0.43
1:C:159(A):HIS:C	1:C:160:LEU:HG	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LEU:C	3:C:329:HOH:O	2.57	0.42
1:G:158:GLY:HA3	1:G:159:PRO:HD2	1.27	0.42
1:G:230:LEU:HA	1:G:230:LEU:HD12	1.72	0.42
1:A:8:ASN:HB3	1:A:160:LEU:HD21	2.01	0.42
1:E:8:ASN:HB3	1:E:160:LEU:HD21	2.02	0.42
1:G:47:ARG:HH11	1:G:47:ARG:HD3	1.66	0.42
1:G:12:SER:HB3	2:H:1:PIV:C3	2.48	0.42
1:A:159(A):HIS:C	1:A:160:LEU:HG	2.39	0.42
1:E:161:LEU:HA	1:E:161:LEU:HD12	1.94	0.42
1:G:8:ASN:HB3	1:G:160:LEU:HD21	2.02	0.42
1:C:230:LEU:HA	1:C:230:LEU:HD12	1.72	0.42
1:A:48:LEU:CD2	1:A:48:LEU:C	2.89	0.41
1:G:107:LEU:HA	1:G:108:PRO:HD2	1.82	0.41
1:A:186:LYS:HB2	1:A:186:LYS:HE3	1.07	0.41
1:C:48:LEU:CD2	1:C:48:LEU:C	2.89	0.41
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.91	0.41
1:C:8:ASN:HB3	1:C:160:LEU:HD21	2.02	0.41
1:E:48:LEU:C	1:E:48:LEU:CD2	2.89	0.41
1:E:47:ARG:HD3	1:E:47:ARG:HH11	1.66	0.41
1:E:52:ILE:HG22	1:E:53:HIS:NE2	2.36	0.41
1:E:230:LEU:HD12	1:E:230:LEU:HA	1.72	0.41
1:G:221:ILE:HG13	1:G:304:THR:HB	2.03	0.41
1:E:186:LYS:HE3	1:E:186:LYS:HB2	1.08	0.41
1:G:48:LEU:C	1:G:48:LEU:CD2	2.89	0.40
1:G:317:ASN:HB3	1:G:319:ARG:HD3	2.03	0.40

All (36) 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:C:113:MET:CE	1:E:113:MET:CE[1_444]	0.33	1.87
1:E:326:ARG:NE	1:G:326:ARG:NH1[1_565]	0.52	1.68
1:A:326:ARG:NE	1:C:326:ARG:NH1[1_565]	0.63	1.57
1:A:326:ARG:CZ	1:C:326:ARG:CZ[1_565]	0.67	1.53
1:A:113:MET:CE	1:G:113:MET:CE[1_464]	0.69	1.51
1:E:326:ARG:NH1	1:G:326:ARG:CZ[1_565]	0.76	1.44
1:A:326:ARG:NH1	1:C:326:ARG:CZ[1_565]	0.81	1.39
1:E:326:ARG:CZ	1:G:326:ARG:NH1[1_565]	0.86	1.34
1:A:326:ARG:CZ	1:C:326:ARG:NH1[1_565]	0.87	1.33
1:E:326:ARG:CZ	1:G:326:ARG:CZ[1_565]	0.87	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:NH1	1:C:326:ARG:NE[1_565]	0.88	1.32
1:E:326:ARG:NH1	1:G:326:ARG:NE[1_565]	1.01	1.19
1:E:326:ARG:NH1	1:G:326:ARG:NH2[1_565]	1.41	0.79
1:A:326:ARG:NH1	1:C:326:ARG:NH2[1_565]	1.46	0.74
1:A:326:ARG:NE	1:C:326:ARG:CZ[1_565]	1.61	0.59
1:E:326:ARG:NE	1:G:326:ARG:CZ[1_565]	1.65	0.55
1:A:326:ARG:NH2	1:C:326:ARG:NH1[1_565]	1.70	0.50
1:A:326:ARG:CZ	1:C:326:ARG:NH2[1_565]	1.72	0.48
1:A:326:ARG:CZ	1:C:326:ARG:NE[1_565]	1.74	0.46
1:E:326:ARG:CZ	1:G:326:ARG:NH2[1_565]	1.80	0.40
1:E:326:ARG:NH2	1:G:326:ARG:NH1[1_565]	1.85	0.35
1:A:326:ARG:NH2	1:C:326:ARG:CZ[1_565]	1.89	0.31
1:E:326:ARG:CZ	1:G:326:ARG:NE[1_565]	1.90	0.30
1:E:326:ARG:CD	1:G:326:ARG:NH1[1_565]	1.92	0.28
1:C:47:ARG:NH1	1:G:45:CYS:O[1_455]	1.94	0.26
1:A:113:MET:CE	1:G:113:MET:SD[1_464]	2.00	0.20
1:C:113:MET:SD	1:E:113:MET:CE[1_444]	2.04	0.16
1:C:113:MET:CE	1:E:113:MET:SD[1_444]	2.04	0.16
1:E:326:ARG:NH1	1:G:326:ARG:NH1[1_565]	2.05	0.15
1:E:47:ARG:O	3:A:366:HOH:O[1_657]	2.06	0.14
1:A:113:MET:SD	1:G:113:MET:CE[1_464]	2.07	0.13
1:A:326:ARG:CD	1:C:326:ARG:NH1[1_565]	2.07	0.13
1:E:326:ARG:NH2	1:G:326:ARG:CZ[1_565]	2.11	0.09
1:A:326:ARG:NH1	1:C:326:ARG:NH1[1_565]	2.14	0.06
1:C:45:CYS:O	1:G:47:ARG:NH1[1_455]	2.15	0.05
1:C:45:CYS:O	1:G:47:ARG:NH2[1_455]	2.18	0.02

## 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	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	16 8
1	C	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	16 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	16	8
1	G	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	16	8
2	B	6/9 (67%)	6 (100%)	0	0	100	100
2	D	6/9 (67%)	6 (100%)	0	0	100	100
2	F	6/9 (67%)	6 (100%)	0	0	100	100
2	H	6/9 (67%)	6 (100%)	0	0	100	100
All	All	1332/1376 (97%)	1284 (96%)	32 (2%)	16 (1%)	16	8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159(A)	HIS
1	A	203	THR
1	A	280	LYS
1	C	159(A)	HIS
1	C	203	THR
1	C	280	LYS
1	E	159(A)	HIS
1	E	203	THR
1	E	280	LYS
1	G	159(A)	HIS
1	G	203	THR
1	G	280	LYS
1	A	158	GLY
1	C	158	GLY
1	E	158	GLY
1	G	158	GLY

### 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	277/287 (96%)	250 (90%)	27 (10%)	10	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	277/287 (96%)	250 (90%)	27 (10%)	10	5
1	E	277/287 (96%)	250 (90%)	27 (10%)	10	5
1	G	277/287 (96%)	250 (90%)	27 (10%)	10	5
2	B	7/7 (100%)	7 (100%)	0	100	100
2	D	7/7 (100%)	7 (100%)	0	100	100
2	F	7/7 (100%)	7 (100%)	0	100	100
2	H	7/7 (100%)	7 (100%)	0	100	100
All	All	1136/1176 (97%)	1028 (90%)	108 (10%)	11	6

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	30	ILE
1	A	40	VAL
1	A	43	THR
1	A	52	ILE
1	A	59	SER
1	A	113	MET
1	A	133	VAL
1	A	142	SER
1	A	143	GLN
1	A	147	LYS
1	A	176	GLN
1	A	186	LYS
1	A	201	SER
1	A	202	SER
1	A	203	THR
1	A	207	GLU
1	A	226	SER
1	A	228	LEU
1	A	230	LEU
1	A	241	ARG
1	A	247	VAL
1	A	259	SER
1	A	265	ARG
1	A	287	HIS
1	A	298	VAL
1	A	326	ARG
1	C	2	SER

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Mol	Chain	Res	Type
1	C	30	ILE
1	C	40	VAL
1	C	43	THR
1	C	52	ILE
1	C	59	SER
1	C	113	MET
1	C	133	VAL
1	C	142	SER
1	C	143	GLN
1	C	147	LYS
1	C	176	GLN
1	C	186	LYS
1	C	201	SER
1	C	202	SER
1	C	203	THR
1	C	207	GLU
1	C	226	SER
1	C	228	LEU
1	C	230	LEU
1	C	241	ARG
1	C	247	VAL
1	C	259	SER
1	C	265	ARG
1	C	287	HIS
1	C	298	VAL
1	C	326	ARG
1	E	2	SER
1	E	30	ILE
1	E	40	VAL
1	E	43	THR
1	E	52	ILE
1	E	59	SER
1	E	113	MET
1	E	133	VAL
1	E	142	SER
1	E	143	GLN
1	E	147	LYS
1	E	176	GLN
1	E	186	LYS
1	E	201	SER
1	E	202	SER
1	E	203	THR

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Mol	Chain	Res	Type
1	E	207	GLU
1	E	226	SER
1	E	228	LEU
1	E	230	LEU
1	E	241	ARG
1	E	247	VAL
1	E	259	SER
1	E	265	ARG
1	E	287	HIS
1	E	298	VAL
1	E	326	ARG
1	G	2	SER
1	G	30	ILE
1	G	40	VAL
1	G	43	THR
1	G	52	ILE
1	G	59	SER
1	G	113	MET
1	G	133	VAL
1	G	142	SER
1	G	143	GLN
1	G	147	LYS
1	G	176	GLN
1	G	186	LYS
1	G	201	SER
1	G	202	SER
1	G	203	THR
1	G	207	GLU
1	G	226	SER
1	G	228	LEU
1	G	230	LEU
1	G	241	ARG
1	G	247	VAL
1	G	259	SER
1	G	265	ARG
1	G	287	HIS
1	G	298	VAL
1	G	326	ARG

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



Mol	Chain	Res	Type
1	A	53	HIS
1	A	86	GLN
1	A	174	HIS
1	A	233	GLN
1	C	53	HIS
1	C	86	GLN
1	C	174	HIS
1	C	233	GLN
1	E	53	HIS
1	E	86	GLN
1	E	174	HIS
1	E	233	GLN
1	G	53	HIS
1	G	86	GLN
1	G	174	HIS
1	G	233	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PIV	B	1	2	4,5,6	1.08	0	3,7,9	0.69	0
2	LPL	B	6	2	14,15,16	1.31	2 (14%)	12,19,21	1.19	1 (8%)
2	PIV	D	1	2	4,5,6	1.09	0	3,7,9	0.70	0
2	LPL	D	6	2	14,15,16	1.31	2 (14%)	12,19,21	1.19	1 (8%)
2	PIV	F	1	2	4,5,6	1.08	0	3,7,9	0.69	0
2	LPL	F	6	2	14,15,16	1.33	2 (14%)	12,19,21	1.19	1 (8%)
2	PIV	H	1	2	4,5,6	1.07	0	3,7,9	0.69	0
2	LPL	H	6	2	14,15,16	1.30	2 (14%)	12,19,21	1.19	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIV	B	1	2	-	0/3/3/6	0/0/0/0
2	LPL	B	6	2	-	0/16/18/20	0/0/0/0
2	PIV	D	1	2	-	0/3/3/6	0/0/0/0
2	LPL	D	6	2	-	0/16/18/20	0/0/0/0
2	PIV	F	1	2	-	0/3/3/6	0/0/0/0
2	LPL	F	6	2	-	0/16/18/20	0/0/0/0
2	PIV	H	1	2	-	0/3/3/6	0/0/0/0
2	LPL	H	6	2	-	0/16/18/20	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6	LPL	CH-CA	-3.25	1.49	1.53
2	D	6	LPL	CH-CA	-3.22	1.49	1.53
2	B	6	LPL	CH-CA	-3.21	1.49	1.53
2	H	6	LPL	CH-CA	-3.16	1.50	1.53
2	F	6	LPL	CM-CA1	-2.57	1.50	1.54
2	B	6	LPL	CM-CA1	-2.51	1.50	1.54
2	H	6	LPL	CM-CA1	-2.49	1.50	1.54
2	D	6	LPL	CM-CA1	-2.47	1.50	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	LPL	OH-CH-CA	2.26	112.83	109.49
2	B	6	LPL	OH-CH-CA	2.28	112.87	109.49
2	H	6	LPL	OH-CH-CA	2.29	112.88	109.49
2	F	6	LPL	OH-CH-CA	2.30	112.90	109.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	PIV	1	0
2	B	6	LPL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	PIV	1	0
2	D	6	LPL	1	0
2	F	1	PIV	1	0
2	F	6	LPL	1	0
2	H	1	PIV	1	0
2	H	6	LPL	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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.