



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:05 PM UTC

PDB ID : 5TTR / pdb_00005ttr
Title : LEU 55 PRO TRANSTHYRETIN CRYSTAL STRUCTURE
Authors : Sebastiao, M.P.; Saraiva, M.J.; Damas, A.M.
Deposited on : 1998-04-30
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

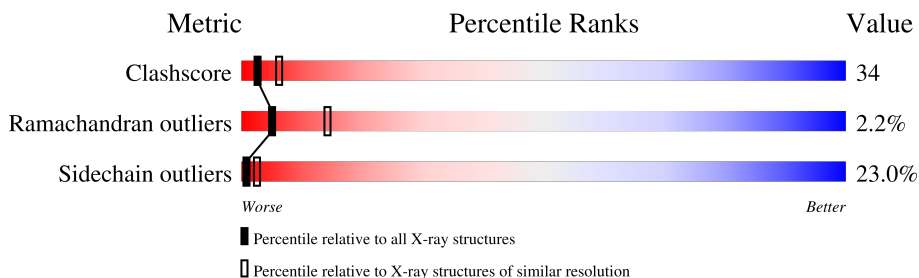
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	
1	C	127	
1	D	127	
1	E	127	
1	F	127	
1	G	127	
1	H	127	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7147 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 TRANSTHYRETIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	4	0	0
			895	572	147	174	2			
1	B	116	Total	C	N	O	S	18	0	0
			890	569	145	174	2			
1	C	116	Total	C	N	O	S	7	0	0
			895	572	147	174	2			
1	D	116	Total	C	N	O	S	0	0	0
			891	570	147	172	2			
1	E	116	Total	C	N	O	S	11	0	0
			895	572	147	174	2			
1	F	116	Total	C	N	O	S	0	0	0
			895	572	147	174	2			
1	G	116	Total	C	N	O	S	7	0	0
			891	570	147	172	2			
1	H	116	Total	C	N	O	S	4	0	0
			895	572	147	174	2			

There are 8 discrepancies between the modelled and reference sequences:

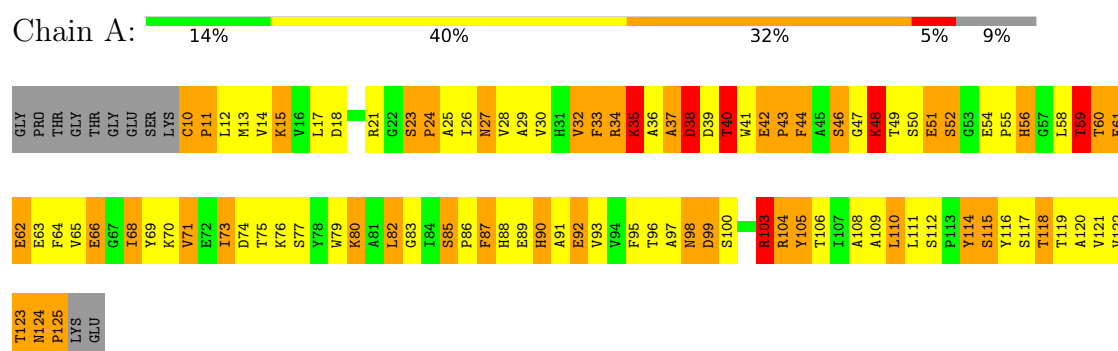
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	PRO	LEU	engineered mutation	UNP P02766
B	55	PRO	LEU	engineered mutation	UNP P02766
C	55	PRO	LEU	engineered mutation	UNP P02766
D	55	PRO	LEU	engineered mutation	UNP P02766
E	55	PRO	LEU	engineered mutation	UNP P02766
F	55	PRO	LEU	engineered mutation	UNP P02766
G	55	PRO	LEU	engineered mutation	UNP P02766
H	55	PRO	LEU	engineered mutation	UNP P02766

3 Residue-property plots [i](#)

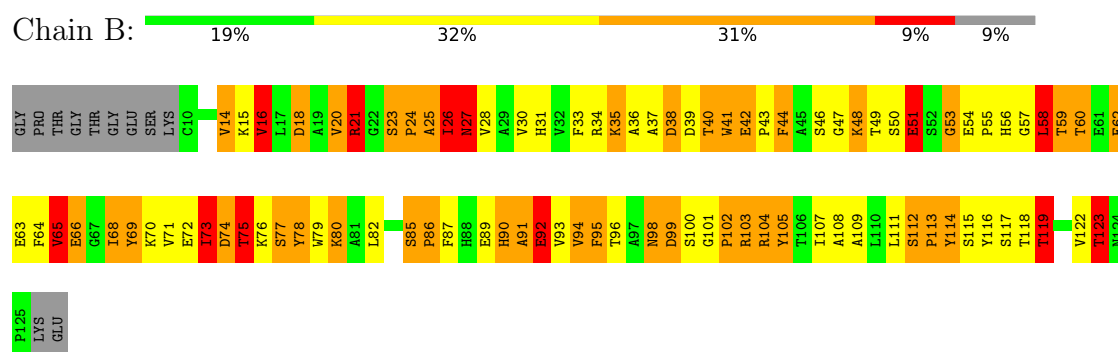
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

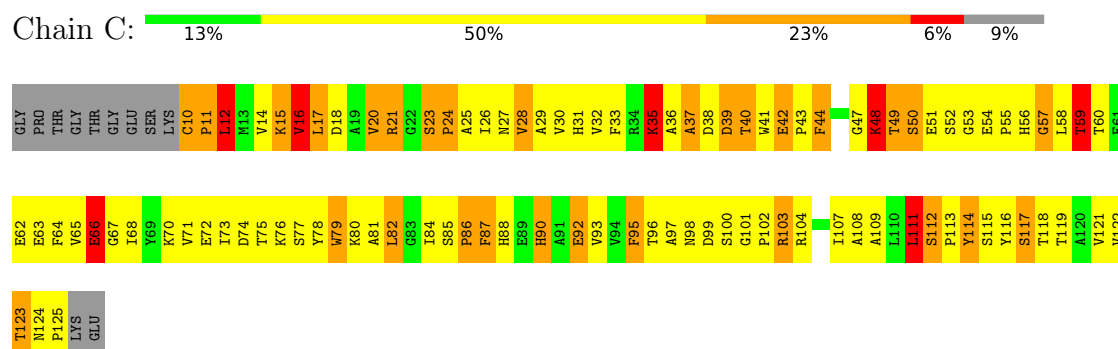
• Molecule 1: TRANSTHYRETIN



• Molecule 1: TRANSTHYRETIN

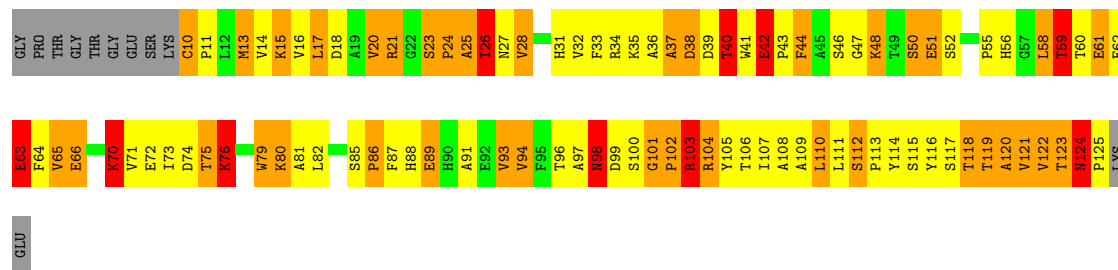


• Molecule 1: TRANSTHYRETIN

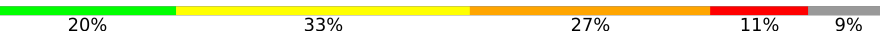


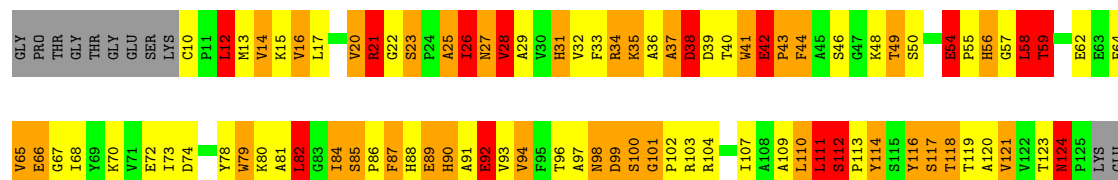
- Molecule 1: TRANSTHYRETIN

Chain D: 

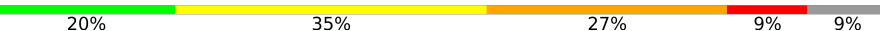


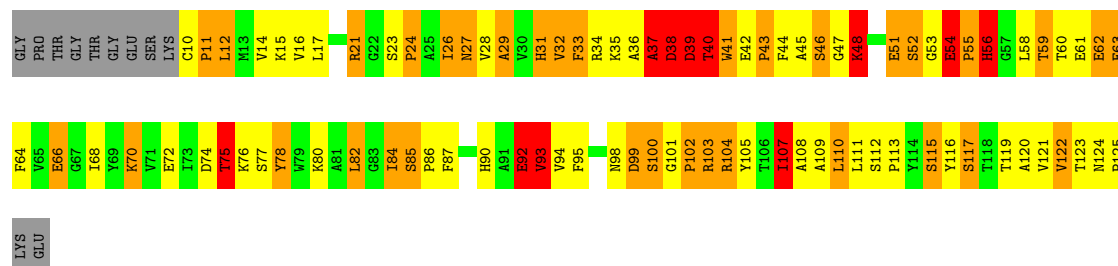
- Molecule 1: TRANSTHYRETIN

Chain E: 



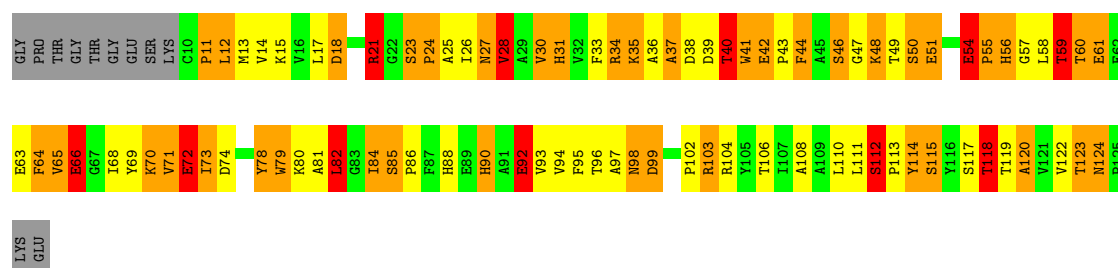
- Molecule 1: TRANSTHYRETIN

Chain F: 

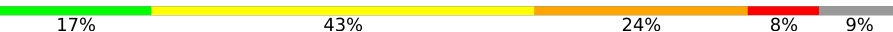


- Molecule 1: TRANSTHYRETIN

Chain G: 



- Molecule 1: TRANSTHYRETIN

Chain H: 

GLY	PRO	THR	GLY	THR	GLY	GLU	SER	LYS	C10	P11			V14	K15	V16	L17	D18	A19	V20	R21	G22	S23	P24	A25	I26	N27	V28	A29	V30	H31	V32	F33	R34	K35	A36	A37	D38	D39	T40	W41	E42	P43	F44	A45	S46	G47	K48	T49	S50	E51	S52	G53	E54	P55	H56	G57	L58	T59	T60	E61
E62	E63	F64	V65	E66	G67	I68	Y69	K70	V71	E72	I73	D74	T75	K76	S77	Y78	W79		S85	P86	F87	H88	E89	H90	A91	E92	V93	V94	F95	T96	A97	N98	D99		P102	R103	R104	Y105		A108	A109	L110	L111	S112	P113	Y114	S115	Y116	S117	T118	T119		V122	T123	N124	P125	LYS	GLU		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.99Å 78.74Å 98.95Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (8.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	1.47	4/920 (0.4%)	3.36	134/1257 (10.7%)
1	B	1.44	4/914 (0.4%)	3.25	151/1249 (12.1%)
1	C	1.71	3/920 (0.3%)	3.40	164/1257 (13.0%)
1	D	1.35	2/916 (0.2%)	3.23	153/1252 (12.2%)
1	E	1.39	3/920 (0.3%)	3.24	137/1257 (10.9%)
1	F	1.31	1/920 (0.1%)	3.21	139/1257 (11.1%)
1	G	1.36	3/916 (0.3%)	4.01	152/1252 (12.1%)
1	H	1.39	3/920 (0.3%)	3.35	142/1257 (11.3%)
All	All	1.43	23/7346 (0.3%)	3.39	1172/10038 (11.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0
1	E	0	1
1	G	0	1
All	All	1	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	PRO	CA-C	26.54	2.08	1.52
1	B	123	THR	C-N	17.06	1.68	1.33
1	G	124	ASN	C-N	12.91	1.55	1.34
1	G	39	ASP	C-O	8.43	1.34	1.24
1	F	39	ASP	C-O	7.97	1.34	1.24
1	H	39	ASP	C-O	6.89	1.32	1.24
1	A	110	LEU	CA-CB	-6.67	1.43	1.53
1	C	39	ASP	C-O	6.44	1.32	1.24
1	C	30	VAL	C-N	-6.05	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	SER	N-CA	-5.95	1.38	1.45
1	E	109	ALA	C-O	-5.77	1.16	1.24
1	B	79	TRP	CA-CB	5.59	1.62	1.53
1	E	39	ASP	C-O	5.54	1.32	1.24
1	H	39	ASP	C-N	-5.49	1.25	1.33
1	B	16	VAL	C-O	-5.34	1.18	1.24
1	D	70	LYS	C-O	-5.23	1.18	1.24
1	D	65	VAL	C-O	-5.23	1.17	1.24
1	A	119	THR	C-O	-5.21	1.17	1.23
1	E	67	GLY	N-CA	5.20	1.50	1.45
1	A	110	LEU	C-O	-5.15	1.18	1.24
1	B	21	ARG	C-N	-5.14	1.27	1.33
1	H	38	ASP	C-O	-5.05	1.18	1.23
1	G	111	LEU	CA-CB	5.00	1.61	1.53

All (1172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	124	ASN	O-C-N	-75.39	25.90	121.64
1	A	21	ARG	CD-NE-CZ	39.60	179.85	124.40
1	H	27	ASN	CA-CB-CG	29.78	142.38	112.60
1	G	35	LYS	CG-CD-CE	28.84	177.63	111.30
1	C	54	GLU	CA-CB-CG	18.93	151.96	114.10
1	G	42	GLU	CB-CG-CD	18.82	144.60	112.60
1	H	37	ALA	CA-C-N	-17.81	96.78	123.14
1	H	37	ALA	C-N-CA	-17.81	96.78	123.14
1	G	66	GLU	CB-CG-CD	17.51	142.37	112.60
1	F	54	GLU	CB-CG-CD	17.49	142.33	112.60
1	E	92	GLU	CB-CG-CD	17.21	141.86	112.60
1	F	107	ILE	CB-CA-C	16.82	135.89	110.83
1	C	125	PRO	CB-CA-C	16.23	140.94	110.10
1	F	21	ARG	CD-NE-CZ	15.76	146.47	124.40
1	D	21	ARG	NE-CZ-NH2	14.97	132.67	119.20
1	G	124	ASN	CA-C-O	-14.43	105.78	120.64
1	D	103	ARG	NE-CZ-NH2	-14.32	106.31	119.20
1	A	21	ARG	CG-CD-NE	14.25	143.34	112.00
1	C	12	LEU	N-CA-CB	14.18	134.50	110.68
1	G	59	THR	CA-C-N	13.98	142.01	122.72
1	G	59	THR	C-N-CA	13.98	142.01	122.72
1	B	38	ASP	CA-CB-CG	13.95	126.55	112.60
1	E	21	ARG	NE-CZ-NH2	-13.72	106.86	119.20
1	C	44	PHE	CA-CB-CG	13.55	127.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	ARG	NE-CZ-NH1	13.52	135.02	121.50
1	H	38	ASP	CA-CB-CG	-13.50	99.10	112.60
1	F	14	VAL	CA-C-O	-13.37	106.36	120.39
1	C	56	HIS	CA-CB-CG	-13.23	100.57	113.80
1	D	33	PHE	CA-CB-CG	-13.02	100.78	113.80
1	E	90	HIS	CA-CB-CG	-13.00	100.80	113.80
1	A	55	PRO	CA-C-O	-12.95	105.94	121.48
1	A	98	ASN	CA-CB-CG	-12.94	99.66	112.60
1	D	75	THR	N-CA-CB	-12.90	90.98	110.20
1	B	59	THR	N-CA-CB	12.75	131.38	111.24
1	D	27	ASN	OD1-CG-ND2	12.58	135.18	122.60
1	C	125	PRO	CA-C-O	-12.52	81.44	119.00
1	E	59	THR	N-CA-CB	12.45	132.10	111.31
1	H	38	ASP	N-CA-CB	12.44	131.48	110.46
1	H	21	ARG	CD-NE-CZ	12.22	141.51	124.40
1	F	47	GLY	O-C-N	12.21	136.23	123.29
1	D	75	THR	CA-CB-OG1	-12.17	91.35	109.60
1	B	62	GLU	N-CA-CB	11.94	128.32	110.53
1	C	28	VAL	CB-CA-C	11.94	127.57	111.21
1	D	117	SER	CA-C-O	-11.88	107.68	121.11
1	E	121	VAL	N-CA-CB	11.75	126.71	111.90
1	B	21	ARG	NE-CZ-NH2	11.74	129.76	119.20
1	F	99	ASP	N-CA-CB	-11.61	92.64	109.94
1	B	34	ARG	NE-CZ-NH1	11.59	133.09	121.50
1	C	55	PRO	CA-C-O	-11.55	107.61	121.48
1	F	115	SER	CA-CB-OG	-11.53	88.03	111.10
1	C	93	VAL	CA-C-O	-11.28	108.08	120.48
1	H	15	LYS	CA-C-O	-11.22	108.29	120.30
1	C	21	ARG	NE-CZ-NH1	-11.20	110.30	121.50
1	H	103	ARG	CD-NE-CZ	11.17	140.03	124.40
1	E	68	ILE	CB-CA-C	-11.16	97.46	110.96
1	F	48	LYS	CA-CB-CG	11.15	136.39	114.10
1	D	34	ARG	NE-CZ-NH2	-11.07	109.23	119.20
1	A	118	THR	CA-CB-OG1	-11.06	93.00	109.60
1	C	103	ARG	CA-C-O	-11.04	109.14	121.51
1	D	33	PHE	CA-C-O	-10.92	108.34	121.11
1	E	16	VAL	CA-C-O	-10.90	108.94	120.39
1	A	48	LYS	CA-C-O	10.90	132.42	120.32
1	H	108	ALA	CA-C-O	-10.71	108.76	120.43
1	H	56	HIS	CA-CB-CG	-10.70	103.10	113.80
1	C	90	HIS	CA-CB-CG	-10.64	103.16	113.80
1	D	107	ILE	CA-CB-CG1	10.61	128.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	GLY	CA-C-O	-10.60	106.88	119.06
1	B	73	ILE	CA-CB-CG1	10.59	128.40	110.40
1	B	69	TYR	CA-C-O	-10.58	109.15	121.11
1	E	23	SER	CA-C-O	-10.58	105.67	120.16
1	G	104	ARG	CB-CA-C	-10.57	92.86	110.19
1	E	27	ASN	CA-CB-CG	-10.53	102.07	112.60
1	A	115	SER	CB-CA-C	-10.46	87.96	110.45
1	E	79	TRP	CA-C-O	-10.46	108.63	120.24
1	F	103	ARG	CD-NE-CZ	10.46	139.04	124.40
1	C	31	HIS	CA-C-O	-10.44	109.00	120.38
1	D	63	GLU	CB-CG-CD	-10.43	94.88	112.60
1	A	43	PRO	CA-C-O	-10.42	109.96	121.32
1	A	98	ASN	N-CA-CB	-10.41	96.85	112.78
1	G	111	LEU	N-CA-C	10.39	126.90	110.17
1	C	35	LYS	N-CA-CB	10.38	125.57	109.69
1	F	26	ILE	CB-CG1-CD1	10.36	135.55	113.80
1	H	68	ILE	N-CA-CB	10.35	123.32	111.21
1	G	98	ASN	CA-CB-CG	-10.27	102.33	112.60
1	F	119	THR	CA-CB-OG1	-10.24	94.25	109.60
1	C	59	THR	N-CA-CB	10.22	128.18	111.62
1	B	99	ASP	N-CA-CB	-10.20	94.32	109.82
1	B	34	ARG	NH1-CZ-NH2	-10.12	106.14	119.30
1	G	24	PRO	CA-C-O	-10.10	109.84	121.56
1	H	61	GLU	CB-CG-CD	-10.05	95.52	112.60
1	E	110	LEU	CB-CA-C	-10.02	93.52	110.16
1	A	13	MET	CA-C-O	-10.01	109.20	120.32
1	H	124	ASN	OD1-CG-ND2	9.95	132.55	122.60
1	B	98	ASN	OD1-CG-ND2	9.90	132.50	122.60
1	E	99	ASP	N-CA-CB	-9.90	94.77	109.82
1	E	42	GLU	CA-CB-CG	9.90	133.90	114.10
1	H	102	PRO	CA-C-O	9.88	133.17	121.31
1	C	54	GLU	CB-CA-C	9.85	122.25	108.76
1	B	26	ILE	CB-CA-C	9.83	125.20	111.63
1	E	23	SER	O-C-N	9.82	132.62	121.32
1	C	14	VAL	CA-C-O	-9.82	110.08	120.48
1	C	31	HIS	CA-CB-CG	-9.81	103.99	113.80
1	F	70	LYS	CA-C-O	-9.75	109.86	120.30
1	C	74	ASP	CA-CB-CG	-9.75	102.85	112.60
1	H	55	PRO	CB-CA-C	9.73	124.57	110.85
1	G	14	VAL	CA-C-O	-9.70	110.21	120.39
1	A	86	PRO	O-C-N	-9.69	111.42	123.04
1	E	27	ASN	OD1-CG-ND2	9.64	132.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	PRO	CB-CA-C	-9.59	99.24	111.71
1	B	62	GLU	CB-CG-CD	-9.58	96.32	112.60
1	C	33	PHE	CA-C-O	-9.54	110.42	121.68
1	A	110	LEU	CA-CB-CG	9.53	149.67	116.30
1	B	56	HIS	CA-C-O	9.53	132.53	121.28
1	G	104	ARG	NE-CZ-NH1	-9.51	111.99	121.50
1	D	98	ASN	OD1-CG-ND2	9.51	132.11	122.60
1	C	41	TRP	N-CA-CB	9.48	125.88	110.42
1	B	65	VAL	N-CA-CB	9.48	126.87	111.23
1	C	80	LYS	O-C-N	-9.45	112.11	122.12
1	A	54	GLU	CA-C-O	-9.35	109.30	120.05
1	H	47	GLY	O-C-N	9.32	134.42	123.61
1	B	117	SER	CA-C-O	-9.31	110.59	121.11
1	G	79	TRP	CA-C-O	-9.30	108.81	119.79
1	G	85	SER	CA-C-N	9.30	129.43	120.31
1	G	85	SER	C-N-CA	9.30	129.43	120.31
1	G	119	THR	CA-C-O	-9.29	109.46	120.60
1	G	104	ARG	NH1-CZ-NH2	9.26	131.34	119.30
1	B	118	THR	CA-C-O	-9.25	110.02	120.66
1	E	74	ASP	CA-CB-CG	-9.21	103.39	112.60
1	G	117	SER	CA-C-O	-9.18	110.79	120.70
1	G	18	ASP	CA-CB-CG	9.16	121.76	112.60
1	F	48	LYS	CB-CA-C	9.13	125.63	109.65
1	E	48	LYS	CA-C-O	-9.12	109.06	120.28
1	B	103	ARG	CD-NE-CZ	-9.10	111.66	124.40
1	D	86	PRO	CA-C-O	-9.10	110.94	122.13
1	C	84	ILE	O-C-N	-9.08	112.01	122.72
1	H	46	SER	CB-CA-C	-9.05	95.15	109.72
1	D	75	THR	OG1-CB-CG2	9.01	127.33	109.30
1	D	108	ALA	O-C-N	-9.00	113.10	123.27
1	E	70	LYS	CA-C-O	-8.97	110.86	120.46
1	H	104	ARG	CD-NE-CZ	8.97	136.96	124.40
1	B	15	LYS	CA-C-O	-8.96	110.72	120.30
1	D	70	LYS	CA-C-O	-8.90	111.05	120.40
1	H	98	ASN	N-CA-CB	-8.85	98.71	112.08
1	H	33	PHE	CA-CB-CG	-8.85	104.95	113.80
1	G	123	THR	CB-CA-C	8.84	127.33	109.38
1	F	98	ASN	N-CA-CB	-8.83	99.12	112.28
1	B	103	ARG	NE-CZ-NH2	8.83	127.15	119.20
1	F	103	ARG	NE-CZ-NH1	8.82	130.32	121.50
1	A	80	LYS	O-C-N	-8.80	111.44	122.27
1	B	102	PRO	N-CA-CB	8.79	111.09	103.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	ARG	NE-CZ-NH1	-8.78	112.72	121.50
1	E	21	ARG	CD-NE-CZ	8.78	136.69	124.40
1	E	54	GLU	N-CA-CB	-8.78	95.02	109.94
1	C	103	ARG	N-CA-CB	-8.77	97.41	111.62
1	B	23	SER	CA-C-O	-8.76	113.09	120.71
1	A	74	ASP	CB-CG-OD1	8.70	138.41	118.40
1	G	12	LEU	CA-C-O	-8.70	110.75	120.32
1	D	52	SER	N-CA-C	-8.67	102.13	112.89
1	C	39	ASP	O-C-N	-8.65	111.08	122.59
1	C	42	GLU	CA-C-O	8.64	129.29	119.61
1	E	109	ALA	CA-C-O	-8.62	111.39	120.70
1	C	84	ILE	CA-CB-CG1	8.61	125.04	110.40
1	D	51	GLU	CB-CG-CD	8.61	127.23	112.60
1	H	117	SER	CA-C-O	-8.57	110.80	120.66
1	E	68	ILE	N-CA-CB	8.57	120.77	111.00
1	F	63	GLU	N-CA-CB	-8.57	97.47	110.33
1	D	93	VAL	CA-CB-CG1	8.56	124.95	110.40
1	E	28	VAL	CB-CA-C	8.56	123.05	110.98
1	G	28	VAL	CB-CA-C	8.56	122.93	111.21
1	B	42	GLU	CB-CA-C	-8.55	98.79	109.31
1	F	21	ARG	CA-CB-CG	8.55	131.19	114.10
1	A	59	THR	N-CA-CB	8.53	125.04	111.56
1	G	38	ASP	CA-CB-CG	8.53	121.13	112.60
1	C	116	TYR	CA-CB-CG	8.52	129.23	113.90
1	E	42	GLU	CB-CG-CD	8.51	127.07	112.60
1	F	93	VAL	CA-C-O	-8.50	111.55	120.39
1	A	21	ARG	CB-CA-C	8.50	124.28	110.09
1	E	42	GLU	CA-C-N	8.50	129.02	119.93
1	E	42	GLU	C-N-CA	8.50	129.02	119.93
1	G	98	ASN	N-CA-CB	-8.50	99.24	112.41
1	D	80	LYS	O-C-N	-8.49	111.82	122.27
1	B	20	VAL	CA-CB-CG2	-8.48	95.98	110.40
1	E	79	TRP	O-C-N	8.45	133.21	122.23
1	H	68	ILE	CB-CG1-CD1	-8.45	96.06	113.80
1	A	115	SER	CA-CB-OG	-8.43	94.25	111.10
1	C	54	GLU	N-CA-CB	-8.41	93.04	110.45
1	D	116	TYR	CA-CB-CG	8.41	129.04	113.90
1	B	54	GLU	CA-CB-CG	8.41	130.91	114.10
1	C	74	ASP	CB-CA-C	-8.40	98.39	111.83
1	F	122	VAL	N-CA-CB	-8.38	99.84	111.41
1	H	70	LYS	CA-C-O	-8.38	111.36	120.24
1	A	18	ASP	CB-CG-OD1	8.37	137.65	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GLU	CB-CG-CD	8.34	126.78	112.60
1	H	55	PRO	CA-C-O	8.34	131.48	121.48
1	E	26	ILE	CB-CG1-CD1	8.33	131.30	113.80
1	F	117	SER	CA-C-O	-8.31	111.72	121.11
1	C	82	LEU	CB-CA-C	-8.23	96.26	110.17
1	C	40	THR	CA-C-O	-8.22	112.01	121.47
1	F	68	ILE	N-CA-CB	8.22	120.83	111.21
1	B	79	TRP	N-CA-CB	8.21	122.30	110.16
1	C	116	TYR	CA-C-O	-8.20	111.80	120.99
1	F	111	LEU	N-CA-CB	-8.20	96.99	110.52
1	B	44	PHE	CB-CA-C	8.20	121.92	109.13
1	D	27	ASN	CB-CG-ND2	-8.17	104.15	116.40
1	A	33	PHE	CA-CB-CG	-8.16	105.64	113.80
1	C	66	GLU	CA-C-O	-8.16	112.90	121.55
1	C	96	THR	CA-C-O	-8.16	111.53	120.43
1	A	117	SER	CA-C-O	-8.15	111.89	121.11
1	E	110	LEU	CA-C-O	-8.15	111.58	120.30
1	F	34	ARG	NE-CZ-NH2	8.14	126.52	119.20
1	B	51	GLU	CB-CG-CD	8.13	126.43	112.60
1	B	60	THR	O-C-N	8.13	133.41	123.16
1	F	104	ARG	NE-CZ-NH1	8.12	129.62	121.50
1	B	107	ILE	CA-C-O	-8.11	111.88	120.48
1	B	39	ASP	CA-C-N	8.10	133.00	121.42
1	B	39	ASP	C-N-CA	8.10	133.00	121.42
1	E	80	LYS	CA-CB-CG	-8.10	97.91	114.10
1	G	70	LYS	CA-C-O	-8.08	111.61	120.33
1	E	98	ASN	CA-C-N	8.07	132.01	120.79
1	E	98	ASN	C-N-CA	8.07	132.01	120.79
1	B	40	THR	CB-CA-C	-8.07	95.90	109.53
1	G	54	GLU	CB-CG-CD	8.07	126.31	112.60
1	G	42	GLU	CG-CD-OE1	8.06	136.94	118.40
1	A	83	GLY	O-C-N	-8.06	113.01	122.60
1	A	116	TYR	CA-CB-CG	8.05	128.39	113.90
1	H	85	SER	CB-CA-C	8.05	118.14	110.17
1	A	93	VAL	CA-C-O	-8.05	112.14	120.27
1	E	119	THR	N-CA-CB	8.05	126.50	111.53
1	C	27	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	H	75	THR	CA-CB-OG1	-8.04	97.54	109.60
1	E	44	PHE	N-CA-CB	-8.04	96.91	110.49
1	C	12	LEU	O-C-N	8.03	132.85	123.30
1	H	48	LYS	CA-CB-CG	-8.03	98.05	114.10
1	C	124	ASN	O-C-N	8.00	130.24	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	TYR	CA-C-N	8.00	131.64	120.29
1	B	78	TYR	C-N-CA	8.00	131.64	120.29
1	C	71	VAL	N-CA-CB	7.99	120.56	111.21
1	F	12	LEU	N-CA-CB	7.99	124.10	110.68
1	F	21	ARG	NE-CZ-NH1	7.97	129.47	121.50
1	F	78	TYR	CA-C-O	-7.96	111.98	120.42
1	G	56	HIS	CA-CB-CG	-7.95	105.86	113.80
1	C	16	VAL	CB-CA-C	7.94	122.38	110.63
1	F	33	PHE	CB-CA-C	-7.93	95.44	109.71
1	B	60	THR	CA-C-O	-7.92	112.20	121.16
1	D	111	LEU	N-CA-C	7.92	122.76	109.76
1	B	18	ASP	CA-CB-CG	7.92	120.52	112.60
1	D	76	LYS	CG-CD-CE	7.91	129.50	111.30
1	C	21	ARG	CD-NE-CZ	-7.91	113.33	124.40
1	B	74	ASP	CA-C-O	7.91	130.44	121.58
1	E	79	TRP	N-CA-CB	7.87	121.93	110.20
1	A	15	LYS	CA-C-O	-7.87	111.88	120.30
1	A	74	ASP	CB-CG-OD2	-7.87	100.30	118.40
1	A	111	LEU	N-CA-C	7.86	122.83	110.17
1	F	24	PRO	CA-C-O	-7.84	112.40	121.34
1	H	119	THR	CA-CB-OG1	-7.84	97.84	109.60
1	H	66	GLU	CA-C-O	-7.83	112.98	121.44
1	C	21	ARG	NH1-CZ-NH2	7.82	129.47	119.30
1	F	75	THR	N-CA-CB	-7.82	98.73	110.07
1	G	13	MET	CA-C-O	-7.81	111.92	120.36
1	D	41	TRP	CA-C-O	-7.81	111.69	120.43
1	F	39	ASP	CA-C-O	-7.80	109.36	120.51
1	B	103	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	C	81	ALA	O-C-N	-7.77	112.09	122.43
1	G	59	THR	CA-C-O	7.77	130.59	121.58
1	B	21	ARG	CD-NE-CZ	-7.76	113.53	124.40
1	H	40	THR	CA-CB-OG1	-7.75	97.97	109.60
1	G	50	SER	CB-CA-C	-7.75	95.81	113.33
1	G	80	LYS	O-C-N	-7.75	113.31	122.15
1	F	121	VAL	N-CA-C	-7.75	96.44	107.75
1	B	24	PRO	N-CA-CB	7.75	110.53	103.33
1	B	33	PHE	CA-CB-CG	-7.73	106.07	113.80
1	G	112	SER	N-CA-CB	7.73	122.15	111.25
1	D	112	SER	CA-CB-OG	-7.72	95.65	111.10
1	H	85	SER	CA-C-N	7.72	127.88	120.31
1	H	85	SER	C-N-CA	7.72	127.88	120.31
1	D	38	ASP	CA-CB-CG	7.72	120.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	GLU	N-CA-C	7.70	121.64	109.64
1	C	67	GLY	CA-C-O	-7.66	114.14	121.96
1	D	115	SER	CA-C-O	-7.66	112.41	120.99
1	E	23	SER	CB-CA-C	-7.65	95.11	110.17
1	G	123	THR	CA-C-O	7.64	129.77	120.60
1	A	99	ASP	CA-CB-CG	-7.63	104.97	112.60
1	G	79	TRP	CA-CB-CG	-7.63	99.10	113.60
1	E	49	THR	O-C-N	-7.63	113.58	122.89
1	E	10	CYS	CB-CA-C	7.61	124.56	110.10
1	F	92	GLU	CB-CG-CD	7.61	125.53	112.60
1	G	82	LEU	N-CA-C	-7.60	103.11	113.30
1	A	104	ARG	CA-C-O	-7.60	112.10	120.38
1	E	82	LEU	N-CA-CB	7.60	122.50	110.73
1	H	23	SER	CB-CA-C	-7.59	99.98	110.37
1	E	54	GLU	CA-C-N	7.58	128.04	119.92
1	E	54	GLU	C-N-CA	7.58	128.04	119.92
1	B	95	PHE	O-C-N	-7.57	114.01	123.17
1	C	24	PRO	CB-CA-C	-7.56	101.70	111.46
1	F	47	GLY	CA-C-O	-7.56	112.77	121.46
1	F	16	VAL	CA-C-O	-7.54	112.55	120.39
1	D	33	PHE	CB-CA-C	-7.53	93.64	109.38
1	D	74	ASP	CB-CA-C	-7.53	98.99	111.41
1	F	42	GLU	CB-CG-CD	-7.52	99.81	112.60
1	F	74	ASP	N-CA-CB	7.51	121.61	110.49
1	A	90	HIS	CA-CB-CG	-7.50	106.30	113.80
1	E	44	PHE	CB-CA-C	7.50	125.34	110.42
1	C	102	PRO	N-CA-CB	7.50	109.96	103.36
1	E	14	VAL	CA-C-O	-7.48	112.53	120.39
1	A	91	ALA	CA-C-O	-7.48	112.62	120.70
1	A	75	THR	CA-C-N	7.48	130.64	120.54
1	A	75	THR	C-N-CA	7.48	130.64	120.54
1	G	21	ARG	CD-NE-CZ	7.47	134.86	124.40
1	G	71	VAL	CA-C-N	-7.47	112.46	122.99
1	G	71	VAL	C-N-CA	-7.47	112.46	122.99
1	B	26	ILE	CA-C-N	7.46	132.71	122.19
1	B	26	ILE	C-N-CA	7.46	132.71	122.19
1	F	28	VAL	N-CA-CB	7.45	120.84	110.56
1	F	102	PRO	CB-CA-C	-7.45	102.26	111.64
1	H	102	PRO	O-C-N	-7.44	114.17	123.10
1	H	52	SER	CB-CA-C	-7.43	97.14	110.37
1	H	79	TRP	CB-CG-CD2	7.43	137.20	126.80
1	A	111	LEU	N-CA-CB	-7.42	98.53	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLU	CB-CG-CD	7.42	125.21	112.60
1	D	122	VAL	CB-CA-C	7.42	122.89	110.95
1	E	119	THR	CA-CB-CG2	7.42	123.11	110.50
1	H	75	THR	N-CA-CB	-7.41	99.33	110.07
1	B	78	TYR	CA-C-O	-7.39	112.59	120.42
1	B	99	ASP	CA-CB-CG	-7.38	105.22	112.60
1	B	109	ALA	CA-C-O	-7.38	112.39	120.36
1	H	28	VAL	CB-CA-C	7.38	121.83	110.83
1	E	112	SER	O-C-N	-7.37	116.69	121.85
1	F	33	PHE	CA-CB-CG	-7.36	106.44	113.80
1	F	48	LYS	O-C-N	-7.34	114.41	123.36
1	C	122	VAL	CA-C-O	7.33	128.25	120.48
1	H	40	THR	N-CA-CB	-7.33	99.00	110.06
1	B	20	VAL	CB-CA-C	-7.32	102.45	112.04
1	H	111	LEU	N-CA-C	7.32	121.77	109.76
1	E	96	THR	CA-C-O	-7.31	112.46	120.43
1	A	71	VAL	CA-C-N	-7.31	112.69	123.00
1	A	71	VAL	C-N-CA	-7.31	112.69	123.00
1	B	55	PRO	N-CA-CB	7.31	109.43	103.36
1	E	15	LYS	CB-CA-C	7.30	123.07	109.71
1	D	60	THR	CA-CB-OG1	-7.30	98.65	109.60
1	B	35	LYS	N-CA-CB	7.29	120.94	109.71
1	G	49	THR	CA-C-N	7.29	133.89	121.86
1	G	49	THR	C-N-CA	7.29	133.89	121.86
1	G	23	SER	CA-C-N	7.29	127.29	119.78
1	G	23	SER	C-N-CA	7.29	127.29	119.78
1	B	116	TYR	CA-CB-CG	7.29	127.01	113.90
1	C	48	LYS	CA-CB-CG	7.29	128.67	114.10
1	D	51	GLU	CA-CB-CG	7.28	128.66	114.10
1	H	124	ASN	N-CA-CB	7.27	123.31	110.37
1	B	85	SER	O-C-N	7.27	128.53	120.83
1	E	57	GLY	CA-C-N	7.27	130.32	120.44
1	E	57	GLY	C-N-CA	7.27	130.32	120.44
1	C	40	THR	CA-C-N	-7.27	113.11	122.77
1	C	40	THR	C-N-CA	-7.27	113.11	122.77
1	B	20	VAL	CA-CB-CG1	-7.26	98.05	110.40
1	F	108	ALA	CA-C-O	-7.26	112.33	120.32
1	C	23	SER	CA-C-N	7.25	127.23	119.76
1	C	23	SER	C-N-CA	7.25	127.23	119.76
1	G	99	ASP	CA-CB-CG	-7.23	105.37	112.60
1	D	34	ARG	NH1-CZ-NH2	7.23	128.70	119.30
1	E	104	ARG	CA-CB-CG	-7.23	99.64	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	ASP	CB-CA-C	-7.23	99.43	110.92
1	A	79	TRP	CA-C-O	-7.22	110.35	119.31
1	G	94	VAL	O-C-N	-7.22	113.44	122.97
1	C	59	THR	CB-CA-C	-7.22	94.57	110.67
1	E	74	ASP	CB-CG-OD1	7.22	135.00	118.40
1	A	28	VAL	N-CA-CB	7.21	118.58	110.72
1	D	121	VAL	CB-CA-C	7.21	121.00	110.77
1	A	83	GLY	CA-C-O	7.20	127.14	119.07
1	B	96	THR	N-CA-CB	7.19	122.25	110.17
1	H	114	TYR	CB-CG-CD1	-7.19	110.01	120.80
1	H	88	HIS	CG-CD2-NE2	7.18	114.38	107.20
1	E	28	VAL	CA-C-O	7.17	129.16	120.84
1	F	107	ILE	CA-CB-CG2	7.17	122.68	110.50
1	C	38	ASP	CA-C-O	-7.16	112.85	122.44
1	F	55	PRO	N-CA-CB	7.14	110.74	103.25
1	B	108	ALA	CA-C-O	-7.13	113.15	120.71
1	D	107	ILE	CB-CG1-CD1	-7.13	98.83	113.80
1	A	115	SER	N-CA-CB	7.13	123.56	111.66
1	G	31	HIS	CB-CA-C	-7.13	97.39	109.72
1	D	43	PRO	CA-C-O	-7.12	113.56	121.32
1	E	50	SER	CA-C-O	7.12	130.64	121.67
1	C	88	HIS	CA-C-O	-7.12	112.74	120.92
1	C	107	ILE	N-CA-CB	-7.11	102.89	111.21
1	D	59	THR	N-CA-CB	7.10	123.12	111.62
1	G	18	ASP	CB-CA-C	7.10	122.14	110.78
1	G	12	LEU	CB-CA-C	-7.09	98.56	110.19
1	H	88	HIS	ND1-CG-CD2	-7.09	99.01	106.10
1	B	79	TRP	CA-C-O	-7.08	112.91	120.42
1	E	43	PRO	N-CA-CB	7.08	109.56	103.19
1	D	97	ALA	CA-C-N	7.07	132.43	122.46
1	D	97	ALA	C-N-CA	7.07	132.43	122.46
1	C	21	ARG	CB-CG-CD	-7.04	95.10	111.30
1	C	49	THR	CA-C-N	7.04	137.63	123.20
1	C	49	THR	C-N-CA	7.04	137.63	123.20
1	B	99	ASP	OD1-CG-OD2	7.02	139.74	122.90
1	A	42	GLU	CA-C-O	7.01	126.71	120.19
1	E	49	THR	N-CA-CB	-7.00	99.69	109.97
1	E	118	THR	N-CA-CB	6.99	123.03	111.08
1	F	53	GLY	O-C-N	6.98	130.61	122.45
1	E	100	SER	CA-C-O	6.97	128.25	119.12
1	G	25	ALA	CA-C-O	6.97	128.04	120.58
1	D	52	SER	N-CA-CB	6.97	121.75	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	PHE	CA-C-O	-6.96	113.53	121.40
1	H	38	ASP	CA-C-O	6.95	128.62	120.70
1	G	35	LYS	N-CA-CB	6.95	120.41	109.71
1	C	28	VAL	N-CA-C	-6.94	98.32	108.87
1	A	25	ALA	CA-C-N	6.94	131.24	121.66
1	A	25	ALA	C-N-CA	6.94	131.24	121.66
1	A	51	GLU	CA-CB-CG	6.93	127.95	114.10
1	H	110	LEU	CA-C-O	-6.92	113.05	120.46
1	C	98	ASN	N-CA-CB	-6.92	101.97	112.28
1	G	74	ASP	CA-CB-CG	-6.92	105.68	112.60
1	H	51	GLU	CB-CG-CD	6.92	124.36	112.60
1	C	113	PRO	O-C-N	-6.91	113.31	122.64
1	C	117	SER	N-CA-CB	6.91	123.58	111.55
1	D	46	SER	CB-CA-C	-6.91	97.42	109.86
1	H	28	VAL	N-CA-C	-6.91	98.50	108.17
1	G	30	VAL	CA-CB-CG1	-6.90	98.67	110.40
1	B	38	ASP	N-CA-CB	-6.90	98.83	110.49
1	A	12	LEU	CA-C-O	-6.89	112.91	120.36
1	E	28	VAL	O-C-N	-6.89	115.62	122.93
1	H	99	ASP	CA-CB-CG	-6.89	105.71	112.60
1	D	98	ASN	CA-CB-CG	6.88	119.48	112.60
1	F	107	ILE	O-C-N	-6.87	115.97	123.18
1	A	63	GLU	CB-CG-CD	6.87	124.27	112.60
1	F	48	LYS	CB-CG-CD	6.86	127.08	111.30
1	D	42	GLU	CB-CG-CD	6.86	124.26	112.60
1	A	77	SER	CA-CB-OG	-6.85	97.39	111.10
1	E	44	PHE	CA-CB-CG	-6.85	106.95	113.80
1	B	99	ASP	CB-CA-C	-6.85	100.03	110.92
1	B	80	LYS	O-C-N	-6.85	114.86	122.12
1	D	103	ARG	CA-CB-CG	-6.84	100.42	114.10
1	D	65	VAL	CA-C-O	6.84	129.33	120.78
1	H	67	GLY	CA-C-O	-6.84	114.90	121.87
1	E	21	ARG	NH1-CZ-NH2	6.83	128.17	119.30
1	G	99	ASP	CA-C-O	-6.82	113.19	120.42
1	H	109	ALA	CA-C-N	6.82	132.79	123.11
1	H	109	ALA	C-N-CA	6.82	132.79	123.11
1	H	93	VAL	CA-CB-CG2	-6.82	98.81	110.40
1	D	79	TRP	CA-CB-CG	-6.81	100.65	113.60
1	E	10	CYS	CA-C-N	6.81	126.06	118.97
1	E	10	CYS	C-N-CA	6.81	126.06	118.97
1	E	116	TYR	CA-CB-CG	6.80	126.15	113.90
1	B	34	ARG	CB-CA-C	6.80	120.61	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	56	HIS	CA-C-O	-6.80	110.79	120.51
1	F	117	SER	CB-CA-C	-6.79	95.94	109.33
1	B	64	PHE	CA-C-N	-6.78	109.76	121.97
1	B	64	PHE	C-N-CA	-6.78	109.76	121.97
1	C	90	HIS	N-CA-CB	6.78	123.42	111.49
1	B	100	SER	N-CA-CB	-6.77	99.45	110.42
1	A	115	SER	CA-C-O	-6.77	114.02	121.33
1	A	51	GLU	CA-C-N	6.76	132.01	120.72
1	A	51	GLU	C-N-CA	6.76	132.01	120.72
1	H	39	ASP	CA-C-N	6.76	131.08	121.42
1	H	39	ASP	C-N-CA	6.76	131.08	121.42
1	H	32	VAL	CB-CA-C	6.75	121.08	110.81
1	E	20	VAL	CA-C-O	6.73	128.52	121.05
1	C	57	GLY	N-CA-C	6.73	129.13	113.18
1	G	118	THR	N-CA-CB	6.73	123.18	111.00
1	A	124	ASN	OD1-CG-ND2	6.72	129.32	122.60
1	G	95	PHE	CA-C-O	6.72	128.59	121.33
1	D	101	GLY	CA-C-N	6.71	126.95	119.90
1	D	101	GLY	C-N-CA	6.71	126.95	119.90
1	C	111	LEU	O-C-N	-6.71	115.37	123.16
1	C	39	ASP	CA-C-N	6.71	132.52	121.39
1	C	39	ASP	C-N-CA	6.71	132.52	121.39
1	B	93	VAL	N-CA-CB	-6.70	102.93	111.64
1	D	21	ARG	NE-CZ-NH1	-6.70	114.80	121.50
1	F	74	ASP	CA-C-N	6.70	129.55	120.44
1	F	74	ASP	C-N-CA	6.70	129.55	120.44
1	A	120	ALA	CA-C-O	6.70	127.81	120.71
1	D	65	VAL	O-C-N	-6.69	114.21	122.57
1	F	48	LYS	N-CA-C	-6.67	96.87	108.69
1	E	15	LYS	CA-C-O	-6.67	113.16	120.36
1	E	82	LEU	N-CA-C	-6.67	104.28	112.88
1	F	110	LEU	CA-C-N	6.66	132.58	122.65
1	F	110	LEU	C-N-CA	6.66	132.58	122.65
1	A	118	THR	CA-C-O	-6.65	113.33	121.11
1	D	80	LYS	CB-CA-C	6.65	123.43	110.67
1	H	114	TYR	CB-CG-CD2	6.65	130.77	120.80
1	G	112	SER	O-C-N	-6.64	116.80	121.65
1	A	18	ASP	CB-CG-OD2	-6.64	103.12	118.40
1	E	111	LEU	N-CA-C	6.64	120.28	109.59
1	G	92	GLU	N-CA-CB	-6.64	98.98	111.00
1	F	72	GLU	CB-CG-CD	-6.64	101.32	112.60
1	H	98	ASN	CB-CG-ND2	6.64	126.35	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	41	TRP	CA-C-O	-6.63	113.00	120.43
1	H	64	PHE	CA-C-O	6.63	130.44	122.41
1	B	98	ASN	CA-CB-CG	-6.63	105.97	112.60
1	C	51	GLU	CA-CB-CG	6.63	127.36	114.10
1	A	46	SER	CB-CA-C	-6.63	98.53	109.80
1	H	123	THR	N-CA-CB	-6.62	98.95	110.87
1	F	115	SER	CB-CA-C	-6.62	96.23	110.45
1	D	121	VAL	CA-C-O	-6.61	113.52	120.39
1	C	28	VAL	CA-CB-CG2	6.61	121.63	110.40
1	H	64	PHE	O-C-N	-6.60	113.67	122.38
1	H	89	GLU	CA-C-O	6.60	127.56	119.97
1	D	89	GLU	CB-CG-CD	-6.60	101.38	112.60
1	F	109	ALA	CA-C-O	-6.58	113.74	120.71
1	B	75	THR	CA-CB-OG1	-6.58	99.73	109.60
1	D	73	ILE	CA-CB-CG1	6.58	121.58	110.40
1	B	69	TYR	O-C-N	6.57	131.73	123.19
1	A	110	LEU	O-C-N	-6.56	115.66	123.27
1	B	44	PHE	O-C-N	-6.56	115.15	122.10
1	C	85	SER	O-C-N	6.55	127.77	120.83
1	C	85	SER	CA-CB-OG	-6.55	98.00	111.10
1	C	88	HIS	O-C-N	6.55	130.76	123.16
1	E	58	LEU	N-CA-C	6.54	118.21	111.14
1	B	27	ASN	CA-CB-CG	6.54	119.14	112.60
1	C	52	SER	N-CA-CB	-6.54	100.44	110.44
1	G	55	PRO	CA-C-O	-6.54	113.58	121.03
1	D	107	ILE	CA-CB-CG2	-6.53	99.39	110.50
1	B	79	TRP	CA-CB-CG	-6.53	101.19	113.60
1	C	92	GLU	CA-CB-CG	6.53	127.16	114.10
1	E	88	HIS	CA-CB-CG	6.53	120.33	113.80
1	A	125	PRO	N-CA-CB	6.53	110.18	103.00
1	D	70	LYS	CB-CG-CD	-6.53	96.29	111.30
1	A	59	THR	CB-CA-C	-6.52	96.28	111.09
1	B	75	THR	N-CA-CB	-6.52	100.61	110.07
1	D	72	GLU	OE1-CD-OE2	6.52	138.55	122.90
1	E	68	ILE	CA-C-O	-6.52	113.02	120.65
1	A	34	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	D	109	ALA	O-C-N	-6.52	115.55	123.30
1	B	116	TYR	CA-C-O	-6.51	113.70	120.99
1	H	69	TYR	CB-CA-C	6.51	121.42	109.71
1	H	21	ARG	CB-CA-C	-6.50	99.73	110.72
1	D	72	GLU	CG-CD-OE1	-6.50	103.45	118.40
1	F	24	PRO	CB-CA-C	-6.50	103.08	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	31	HIS	CA-CB-CG	-6.50	107.31	113.80
1	F	124	ASN	CA-C-O	-6.49	115.07	119.29
1	B	119	THR	CA-C-O	-6.49	112.81	120.60
1	D	47	GLY	CA-C-O	-6.49	114.80	121.61
1	G	64	PHE	CA-CB-CG	6.48	120.28	113.80
1	B	33	PHE	N-CA-CB	6.48	120.77	111.05
1	E	72	GLU	CB-CG-CD	6.48	123.62	112.60
1	E	43	PRO	CB-CA-C	-6.47	103.42	111.64
1	H	57	GLY	N-CA-C	6.47	128.53	113.18
1	A	38	ASP	N-CA-CB	-6.47	99.55	110.49
1	C	88	HIS	ND1-CE1-NE2	-6.47	101.93	108.40
1	A	116	TYR	CA-C-O	-6.47	113.77	120.89
1	B	18	ASP	CB-CG-OD2	-6.47	103.52	118.40
1	A	121	VAL	CB-CA-C	6.46	119.14	111.32
1	D	25	ALA	N-CA-CB	6.46	119.97	110.35
1	H	45	ALA	N-CA-CB	6.46	121.76	111.56
1	D	110	LEU	CB-CA-C	6.45	121.12	110.74
1	G	90	HIS	CA-CB-CG	-6.45	107.35	113.80
1	H	55	PRO	N-CA-C	-6.45	100.30	111.32
1	E	67	GLY	CA-C-O	-6.44	115.26	121.83
1	G	31	HIS	CA-CB-CG	-6.44	107.36	113.80
1	H	113	PRO	CB-CA-C	6.44	123.85	112.64
1	E	41	TRP	N-CA-CB	-6.44	99.97	110.21
1	F	77	SER	CA-CB-OG	-6.44	98.22	111.10
1	G	31	HIS	N-CA-C	6.44	119.43	109.07
1	G	104	ARG	CA-C-O	-6.43	113.24	120.32
1	A	34	ARG	CD-NE-CZ	-6.43	115.39	124.40
1	A	55	PRO	N-CA-CB	6.43	109.30	103.19
1	D	123	THR	N-CA-CB	-6.43	99.57	111.53
1	F	41	TRP	CB-CA-C	-6.43	100.20	110.81
1	H	118	THR	CA-CB-CG2	6.42	121.42	110.50
1	C	111	LEU	N-CA-C	6.42	120.74	109.96
1	A	30	VAL	CB-CA-C	-6.41	101.66	110.77
1	E	25	ALA	CA-C-O	-6.41	113.35	120.60
1	D	109	ALA	CB-CA-C	6.41	121.43	109.71
1	H	52	SER	O-C-N	6.40	130.65	122.39
1	C	97	ALA	O-C-N	6.40	131.55	123.23
1	A	21	ARG	CA-CB-CG	6.40	126.90	114.10
1	G	117	SER	CB-CA-C	-6.39	97.16	109.37
1	F	72	GLU	OE1-CD-OE2	6.39	138.24	122.90
1	C	33	PHE	CA-CB-CG	-6.39	107.41	113.80
1	C	101	GLY	CA-C-N	6.39	126.61	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	GLY	C-N-CA	6.39	126.61	119.90
1	F	58	LEU	N-CA-CB	-6.38	100.81	110.07
1	B	66	GLU	N-CA-CB	6.37	119.41	110.04
1	G	54	GLU	CA-C-N	6.34	126.56	119.90
1	G	54	GLU	C-N-CA	6.34	126.56	119.90
1	F	101	GLY	CA-C-N	6.34	126.67	119.83
1	F	101	GLY	C-N-CA	6.34	126.67	119.83
1	D	76	LYS	CD-CE-NZ	6.33	132.17	111.90
1	A	32	VAL	O-C-N	-6.33	116.53	123.18
1	A	103	ARG	N-CA-CB	-6.33	101.37	111.43
1	F	115	SER	O-C-N	6.33	130.47	123.25
1	G	81	ALA	N-CA-CB	-6.33	99.28	110.42
1	A	68	ILE	N-CA-CB	6.33	119.43	111.46
1	D	104	ARG	O-C-N	-6.31	115.82	123.27
1	H	40	THR	OG1-CB-CG2	6.31	121.92	109.30
1	C	109	ALA	CA-C-O	-6.31	113.55	120.36
1	H	39	ASP	O-C-N	-6.30	114.21	122.59
1	H	43	PRO	N-CA-CB	6.30	109.87	103.25
1	C	97	ALA	CA-C-O	-6.30	113.90	120.70
1	E	114	TYR	CA-CB-CG	-6.30	102.56	113.90
1	F	75	THR	CA-CB-OG1	-6.30	100.16	109.60
1	C	121	VAL	CB-CA-C	6.29	118.22	110.73
1	H	73	ILE	CB-CG1-CD1	6.29	127.00	113.80
1	D	80	LYS	CA-C-O	-6.29	112.74	119.97
1	B	122	VAL	N-CA-CB	6.29	120.92	110.86
1	E	117	SER	CA-CB-OG	-6.29	98.53	111.10
1	F	100	SER	CB-CA-C	-6.28	100.57	110.94
1	B	33	PHE	CB-CA-C	-6.28	98.44	110.24
1	D	56	HIS	CA-C-N	6.28	133.71	121.41
1	D	56	HIS	C-N-CA	6.28	133.71	121.41
1	A	123	THR	CA-CB-OG1	-6.27	100.19	109.60
1	C	32	VAL	CA-C-O	-6.27	113.57	120.72
1	B	105	TYR	CA-C-O	6.27	127.36	120.71
1	E	65	VAL	CA-CB-CG1	-6.26	99.75	110.40
1	G	114	TYR	CA-C-O	-6.26	112.24	119.56
1	E	111	LEU	O-C-N	-6.26	115.26	123.21
1	H	79	TRP	CB-CG-CD1	-6.26	117.51	126.90
1	E	38	ASP	CA-C-O	-6.25	111.56	120.51
1	B	74	ASP	N-CA-CB	6.25	119.74	110.49
1	E	29	ALA	N-CA-CB	-6.25	99.86	110.16
1	B	31	HIS	CA-C-O	-6.24	113.62	120.36
1	C	54	GLU	CA-C-N	6.24	126.73	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	GLU	C-N-CA	6.24	126.73	119.99
1	F	24	PRO	CA-C-N	6.24	130.71	122.42
1	F	24	PRO	C-N-CA	6.24	130.71	122.42
1	B	41	TRP	N-CA-CB	-6.23	100.30	110.21
1	D	15	LYS	CA-C-O	-6.23	113.63	120.30
1	H	123	THR	CA-CB-OG1	-6.23	100.25	109.60
1	E	119	THR	CA-CB-OG1	-6.22	100.27	109.60
1	C	103	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	F	68	ILE	N-CA-C	-6.21	98.92	107.99
1	H	74	ASP	CB-CA-C	-6.21	101.89	111.83
1	B	24	PRO	CA-C-O	-6.21	114.10	121.67
1	G	111	LEU	CA-C-O	-6.21	113.96	121.28
1	D	14	VAL	CA-C-O	-6.21	113.94	120.39
1	D	27	ASN	N-CA-C	6.20	120.18	112.24
1	A	108	ALA	CA-C-O	-6.20	113.50	120.32
1	A	11	PRO	O-C-N	6.20	129.98	122.23
1	E	34	ARG	CB-CA-C	6.20	120.92	109.70
1	D	46	SER	CA-C-O	-6.20	113.12	120.43
1	A	24	PRO	N-CD-CG	-6.19	93.91	103.20
1	G	27	ASN	N-CA-C	6.19	120.17	112.24
1	G	61	GLU	N-CA-CB	-6.19	99.04	110.18
1	B	72	GLU	CB-CG-CD	-6.19	102.08	112.60
1	D	73	ILE	CB-CG1-CD1	6.18	126.78	113.80
1	E	84	ILE	CB-CA-C	-6.18	102.74	111.21
1	A	73	ILE	CB-CA-C	6.18	119.25	110.84
1	F	110	LEU	O-C-N	-6.18	114.97	123.12
1	F	59	THR	OG1-CB-CG2	6.18	121.65	109.30
1	H	68	ILE	CA-C-O	-6.18	113.86	120.59
1	F	11	PRO	N-CA-CB	6.17	110.12	103.33
1	H	112	SER	N-CA-CB	6.17	121.67	111.17
1	H	29	ALA	CB-CA-C	-6.17	99.78	109.84
1	C	122	VAL	O-C-N	-6.16	116.71	123.18
1	B	87	PHE	N-CA-CB	-6.16	101.01	110.13
1	C	43	PRO	CA-C-O	-6.16	114.64	121.23
1	G	34	ARG	CB-CG-CD	6.15	125.45	111.30
1	B	114	TYR	CA-CB-CG	-6.15	102.83	113.90
1	H	74	ASP	CA-C-N	6.15	128.80	120.44
1	H	74	ASP	C-N-CA	6.15	128.80	120.44
1	B	68	ILE	O-C-N	6.15	130.44	122.94
1	C	10	CYS	CA-C-N	6.14	125.86	119.05
1	C	10	CYS	C-N-CA	6.14	125.86	119.05
1	F	52	SER	CA-C-O	6.14	125.80	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	98	ASN	CA-C-N	6.14	128.83	120.54
1	F	98	ASN	C-N-CA	6.14	128.83	120.54
1	C	93	VAL	CB-CA-C	-6.13	103.02	110.99
1	F	27	ASN	CA-CB-CG	-6.13	106.47	112.60
1	D	72	GLU	CB-CG-CD	-6.13	102.18	112.60
1	B	91	ALA	CA-C-O	-6.12	113.75	120.36
1	C	58	LEU	N-CA-C	6.12	117.61	111.07
1	A	124	ASN	CA-CB-CG	-6.11	106.49	112.60
1	B	98	ASN	CB-CA-C	-6.11	101.40	111.36
1	H	63	GLU	CG-CD-OE2	-6.11	104.35	118.40
1	E	99	ASP	CA-CB-CG	-6.11	106.49	112.60
1	B	43	PRO	CA-C-O	-6.11	114.66	121.32
1	G	78	TYR	CA-C-O	-6.10	113.95	120.42
1	H	36	ALA	CA-C-O	6.10	129.10	121.66
1	G	124	ASN	CB-CG-ND2	6.10	125.55	116.40
1	D	46	SER	O-C-N	6.09	130.42	123.48
1	A	71	VAL	CB-CA-C	6.09	119.85	110.96
1	F	29	ALA	CA-C-O	-6.09	113.75	120.69
1	H	109	ALA	O-C-N	-6.09	115.31	123.23
1	A	29	ALA	CA-C-O	-6.08	113.76	120.69
1	A	44	PHE	N-CA-CB	-6.08	101.82	110.81
1	E	15	LYS	CA-CB-CG	-6.07	101.95	114.10
1	E	111	LEU	CA-C-O	6.07	127.15	120.71
1	G	46	SER	N-CA-C	6.07	117.63	108.46
1	E	118	THR	CB-CA-C	-6.07	97.37	109.33
1	B	21	ARG	N-CA-CB	6.07	119.77	110.61
1	D	18	ASP	CB-CA-C	-6.07	101.08	110.78
1	A	52	SER	CA-C-O	6.05	126.82	119.38
1	G	72	GLU	CA-C-O	-6.04	113.83	120.36
1	E	55	PRO	N-CA-CB	6.03	109.06	103.39
1	C	112	SER	N-CA-CB	6.03	119.15	110.77
1	B	15	LYS	N-CA-CB	-6.03	101.25	110.65
1	E	99	ASP	CA-C-O	6.03	127.70	121.07
1	G	24	PRO	N-CA-CB	6.03	108.59	103.35
1	D	70	LYS	CA-CB-CG	-6.02	102.06	114.10
1	E	98	ASN	CB-CA-C	-6.02	102.21	111.66
1	D	124	ASN	N-CA-CB	6.01	118.79	110.01
1	E	13	MET	CA-C-O	-6.01	112.88	120.28
1	A	33	PHE	CB-CA-C	-6.01	98.94	110.24
1	D	26	ILE	N-CA-CB	6.01	121.00	110.49
1	D	104	ARG	CA-C-O	6.01	126.93	120.32
1	D	89	GLU	OE1-CD-OE2	6.01	137.31	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	GLY	N-CA-C	-6.00	101.48	110.42
1	C	48	LYS	CG-CD-CE	6.00	125.11	111.30
1	G	69	TYR	CA-CB-CG	-6.00	103.10	113.90
1	E	59	THR	CA-C-O	6.00	128.06	121.40
1	H	115	SER	N-CA-CB	-6.00	102.26	111.56
1	D	32	VAL	CA-C-N	6.00	131.98	122.62
1	D	32	VAL	C-N-CA	6.00	131.98	122.62
1	H	118	THR	O-C-N	-5.99	115.96	123.27
1	E	101	GLY	CA-C-N	5.99	126.93	119.98
1	E	101	GLY	C-N-CA	5.99	126.93	119.98
1	H	26	ILE	CA-C-N	5.99	130.66	122.34
1	H	26	ILE	C-N-CA	5.99	130.66	122.34
1	B	90	HIS	ND1-CE1-NE2	-5.99	102.41	108.40
1	E	59	THR	CB-CA-C	-5.99	97.29	111.65
1	E	111	LEU	N-CA-CB	-5.98	101.06	110.69
1	A	27	ASN	CA-CB-CG	5.98	118.58	112.60
1	F	54	GLU	CG-CD-OE1	5.98	132.16	118.40
1	G	114	TYR	CB-CG-CD1	-5.98	111.83	120.80
1	A	80	LYS	CB-CA-C	5.98	122.14	110.67
1	G	21	ARG	CB-CA-C	-5.98	97.66	109.67
1	H	77	SER	CB-CA-C	5.97	121.00	110.85
1	B	74	ASP	CA-C-N	5.97	128.56	120.44
1	B	74	ASP	C-N-CA	5.97	128.56	120.44
1	C	52	SER	O-C-N	-5.97	114.13	122.37
1	G	27	ASN	CA-CB-CG	-5.97	106.63	112.60
1	H	105	TYR	CA-C-O	5.97	127.03	120.71
1	B	114	TYR	CB-CA-C	-5.96	100.64	110.72
1	H	20	VAL	O-C-N	-5.96	114.15	121.90
1	G	24	PRO	O-C-N	5.96	130.40	123.01
1	D	62	GLU	CA-C-N	-5.96	111.96	122.26
1	D	62	GLU	C-N-CA	-5.96	111.96	122.26
1	D	94	VAL	CA-CB-CG2	-5.96	100.28	110.40
1	B	117	SER	CB-CA-C	-5.96	97.60	109.33
1	D	121	VAL	CA-C-N	-5.95	113.76	122.68
1	D	121	VAL	C-N-CA	-5.95	113.76	122.68
1	G	21	ARG	CB-CG-CD	5.95	124.97	111.30
1	C	20	VAL	N-CA-C	-5.94	105.06	110.82
1	F	37	ALA	CA-C-N	-5.94	113.26	122.05
1	F	37	ALA	C-N-CA	-5.94	113.26	122.05
1	G	66	GLU	CB-CA-C	5.94	120.48	109.54
1	H	44	PHE	CA-C-O	-5.94	112.84	119.67
1	B	43	PRO	N-CA-CB	5.94	108.53	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	46	SER	O-C-N	5.94	130.35	123.41
1	H	42	GLU	CA-C-O	5.93	126.87	120.05
1	D	116	TYR	CA-C-O	-5.93	113.25	120.54
1	F	75	THR	CA-C-N	5.93	128.54	120.54
1	F	75	THR	C-N-CA	5.93	128.54	120.54
1	G	43	PRO	CA-C-O	-5.92	114.86	121.32
1	G	55	PRO	N-CA-CB	5.92	108.56	103.36
1	A	96	THR	N-CA-CB	5.91	119.91	110.16
1	A	106	THR	N-CA-CB	5.91	119.86	110.65
1	G	95	PHE	O-C-N	-5.90	116.52	123.25
1	F	34	ARG	CA-C-O	-5.90	113.77	120.32
1	F	122	VAL	CA-CB-CG1	-5.90	100.36	110.40
1	E	117	SER	CA-C-O	-5.90	114.21	121.11
1	C	87	PHE	CA-C-N	5.89	130.81	122.09
1	C	87	PHE	C-N-CA	5.89	130.81	122.09
1	D	55	PRO	N-CA-C	-5.89	101.95	111.14
1	A	88	HIS	CA-CB-CG	5.89	119.69	113.80
1	C	95	PHE	CA-C-O	5.89	128.10	121.51
1	D	20	VAL	CB-CA-C	5.88	119.63	111.92
1	B	111	LEU	N-CA-C	5.88	119.41	109.76
1	A	109	ALA	N-CA-CB	5.88	121.06	110.83
1	B	92	GLU	CB-CG-CD	-5.88	102.61	112.60
1	E	88	HIS	CA-C-N	5.88	129.24	120.31
1	E	88	HIS	C-N-CA	5.88	129.24	120.31
1	H	124	ASN	CA-CB-CG	-5.88	106.72	112.60
1	G	74	ASP	CA-C-N	5.87	128.43	120.44
1	G	74	ASP	C-N-CA	5.87	128.43	120.44
1	F	10	CYS	CA-C-N	5.87	125.56	119.05
1	F	10	CYS	C-N-CA	5.87	125.56	119.05
1	F	62	GLU	O-C-N	5.87	130.69	122.36
1	B	123	THR	CA-C-O	-5.87	114.36	120.70
1	D	61	GLU	CA-CB-CG	5.87	125.83	114.10
1	B	44	PHE	N-CA-C	-5.86	107.11	114.56
1	F	46	SER	CA-C-N	-5.86	110.97	121.93
1	F	46	SER	C-N-CA	-5.86	110.97	121.93
1	B	54	GLU	CA-C-N	5.86	126.75	120.13
1	B	54	GLU	C-N-CA	5.86	126.75	120.13
1	C	57	GLY	O-C-N	-5.86	115.08	122.70
1	C	27	ASN	CA-CB-CG	5.86	118.46	112.60
1	G	103	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	D	35	LYS	N-CA-CB	5.85	118.72	109.71
1	G	42	GLU	CB-CA-C	5.85	116.50	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ASP	CA-C-O	5.84	127.50	121.07
1	B	122	VAL	CA-C-O	5.84	127.62	120.84
1	G	96	THR	CA-C-N	-5.84	114.46	122.93
1	G	96	THR	C-N-CA	-5.84	114.46	122.93
1	G	80	LYS	CA-CB-CG	-5.84	102.43	114.10
1	B	66	GLU	CB-CG-CD	5.83	122.52	112.60
1	H	56	HIS	N-CA-CB	-5.82	101.17	109.85
1	F	40	THR	N-CA-CB	5.82	119.77	110.46
1	A	40	THR	CA-C-O	-5.81	114.42	121.28
1	G	42	GLU	OE1-CD-OE2	-5.81	108.95	122.90
1	D	28	VAL	N-CA-C	-5.81	101.31	109.21
1	D	35	LYS	CD-CE-NZ	5.81	130.48	111.90
1	E	92	GLU	CG-CD-OE1	5.81	131.75	118.40
1	C	15	LYS	CA-C-O	-5.80	114.09	120.36
1	B	46	SER	CA-C-O	-5.80	114.72	121.10
1	C	70	LYS	CA-C-O	-5.80	114.09	120.30
1	D	36	ALA	O-C-N	5.80	129.51	122.96
1	H	87	PHE	CA-C-N	5.80	129.72	121.42
1	H	87	PHE	C-N-CA	5.80	129.72	121.42
1	F	12	LEU	CB-CA-C	-5.80	99.10	109.71
1	B	70	LYS	CA-C-O	-5.79	114.10	120.24
1	C	124	ASN	CA-CB-CG	-5.79	106.81	112.60
1	G	41	TRP	N-CA-CB	5.79	119.89	110.17
1	C	11	PRO	N-CA-CB	5.79	109.69	103.33
1	D	52	SER	CA-C-O	-5.78	112.14	119.31
1	A	75	THR	O-C-N	-5.78	115.18	122.17
1	A	86	PRO	CA-C-N	5.78	134.28	121.80
1	A	86	PRO	C-N-CA	5.78	134.28	121.80
1	G	86	PRO	CA-C-O	-5.78	114.96	122.12
1	E	50	SER	O-C-N	-5.77	114.18	121.74
1	C	98	ASN	N-CA-C	5.77	119.62	112.47
1	G	48	LYS	CA-C-O	-5.77	113.19	120.28
1	F	55	PRO	N-CA-C	-5.76	100.60	112.47
1	F	115	SER	CA-C-O	-5.76	115.11	121.33
1	E	21	ARG	N-CA-CB	-5.76	101.95	110.53
1	H	61	GLU	N-CA-C	5.76	119.92	113.01
1	E	89	GLU	CA-C-O	5.76	126.59	119.97
1	D	34	ARG	CD-NE-CZ	5.75	132.46	124.40
1	D	71	VAL	CA-C-N	-5.75	115.00	123.05
1	D	71	VAL	C-N-CA	-5.75	115.00	123.05
1	D	16	VAL	CA-CB-CG2	-5.75	100.62	110.40
1	D	89	GLU	CA-CB-CG	-5.75	102.61	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	TYR	CA-CB-CG	-5.75	103.56	113.90
1	D	21	ARG	CD-NE-CZ	-5.75	116.36	124.40
1	E	124	ASN	OD1-CG-ND2	-5.75	116.86	122.60
1	H	21	ARG	CA-C-O	-5.74	112.81	119.59
1	B	20	VAL	CG1-CB-CG2	-5.74	98.18	110.80
1	G	12	LEU	O-C-N	5.74	130.04	123.27
1	F	82	LEU	N-CA-C	-5.73	105.95	113.17
1	G	120	ALA	N-CA-CB	5.73	120.02	110.85
1	G	78	TYR	CB-CG-CD2	-5.73	112.21	120.80
1	B	119	THR	O-C-N	5.72	130.25	123.33
1	D	121	VAL	N-CA-C	-5.72	99.40	107.75
1	F	122	VAL	CB-CA-C	5.72	119.09	110.63
1	E	93	VAL	CA-C-O	-5.71	114.71	120.31
1	D	23	SER	CB-CA-C	-5.71	103.79	110.76
1	A	42	GLU	CA-C-N	5.70	126.03	119.93
1	A	42	GLU	C-N-CA	5.70	126.03	119.93
1	B	16	VAL	N-CA-CB	5.70	119.28	111.41
1	G	44	PHE	CA-CB-CG	5.70	119.50	113.80
1	D	96	THR	O-C-N	-5.70	116.72	123.22
1	B	26	ILE	O-C-N	-5.68	115.60	122.59
1	D	102	PRO	CB-CA-C	-5.68	104.59	111.46
1	C	96	THR	N-CA-CB	5.68	119.69	110.43
1	A	35	LYS	CA-CB-CG	-5.68	102.74	114.10
1	B	122	VAL	CB-CA-C	-5.68	102.97	110.98
1	H	56	HIS	O-C-N	-5.68	115.95	122.93
1	G	65	VAL	N-CA-CB	-5.67	101.88	111.23
1	D	23	SER	N-CA-CB	-5.66	105.47	111.29
1	G	15	LYS	CA-C-O	-5.65	114.26	120.36
1	C	55	PRO	CA-C-N	-5.65	109.46	121.32
1	C	55	PRO	C-N-CA	-5.65	109.46	121.32
1	G	112	SER	N-CA-C	-5.65	101.70	108.25
1	D	117	SER	CB-CA-C	-5.64	98.22	109.33
1	F	62	GLU	CB-CG-CD	5.64	122.19	112.60
1	C	25	ALA	N-CA-CB	5.64	118.42	110.24
1	F	64	PHE	N-CA-CB	-5.64	102.45	110.46
1	H	49	THR	N-CA-CB	-5.64	101.69	109.97
1	H	24	PRO	O-C-N	-5.63	116.21	123.03
1	B	43	PRO	CA-C-N	-5.63	113.46	122.08
1	B	43	PRO	C-N-CA	-5.63	113.46	122.08
1	F	41	TRP	CA-CB-CG	-5.63	102.90	113.60
1	F	43	PRO	CB-CA-C	-5.63	102.27	111.56
1	G	39	ASP	O-C-N	-5.63	115.11	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	92	GLU	O-C-N	-5.63	116.40	123.27
1	D	119	THR	CA-CB-CG2	-5.62	100.94	110.50
1	A	49	THR	O-C-N	-5.62	116.17	122.75
1	C	118	THR	CA-CB-OG1	-5.62	101.17	109.60
1	A	46	SER	N-CA-C	5.62	118.59	108.48
1	A	50	SER	CA-CB-OG	-5.62	99.87	111.10
1	D	32	VAL	O-C-N	-5.62	116.98	122.93
1	H	75	THR	OG1-CB-CG2	5.62	120.53	109.30
1	C	29	ALA	CB-CA-C	-5.61	100.69	109.84
1	F	38	ASP	N-CA-CB	5.61	117.38	110.53
1	F	103	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
1	D	37	ALA	CA-C-O	5.61	128.53	120.51
1	E	102	PRO	CA-C-O	-5.61	115.38	121.27
1	H	19	ALA	CA-C-N	5.61	128.76	120.74
1	H	19	ALA	C-N-CA	5.61	128.76	120.74
1	A	66	GLU	N-CA-CB	5.61	118.24	110.17
1	E	85	SER	CA-CB-OG	5.61	122.31	111.10
1	F	125	PRO	N-CA-CB	5.61	109.17	103.00
1	H	31	HIS	CA-C-O	-5.61	114.31	120.36
1	G	63	GLU	CB-CA-C	5.60	119.49	109.29
1	H	104	ARG	N-CA-C	-5.60	100.05	109.07
1	H	88	HIS	CA-CB-CG	5.60	119.40	113.80
1	D	59	THR	OG1-CB-CG2	5.60	120.50	109.30
1	E	74	ASP	N-CA-CB	5.60	118.64	110.58
1	A	37	ALA	CB-CA-C	5.59	121.55	110.42
1	G	73	ILE	CA-C-O	5.59	126.55	120.57
1	E	21	ARG	O-C-N	-5.59	115.10	122.42
1	E	124	ASN	N-CA-CB	5.59	120.31	110.37
1	A	11	PRO	N-CA-CB	5.58	109.69	103.44
1	B	21	ARG	CA-C-N	5.58	132.45	121.06
1	B	21	ARG	C-N-CA	5.58	132.45	121.06
1	C	86	PRO	CB-CA-C	5.58	118.27	110.95
1	H	52	SER	CA-CB-OG	-5.58	99.94	111.10
1	C	20	VAL	N-CA-CB	5.58	118.55	110.52
1	D	98	ASN	CB-CG-OD1	-5.58	109.65	120.80
1	F	119	THR	CA-CB-CG2	5.57	119.98	110.50
1	C	50	SER	CA-C-O	-5.57	114.05	121.46
1	D	40	THR	N-CA-CB	5.57	118.91	110.45
1	D	106	THR	CA-C-O	-5.57	114.50	120.46
1	B	54	GLU	N-CA-C	5.56	118.22	108.82
1	D	43	PRO	N-CA-CB	5.56	108.20	103.19
1	E	27	ASN	N-CA-C	5.56	119.25	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	69	TYR	CA-CB-CG	5.56	123.91	113.90
1	D	44	PHE	CA-C-O	-5.55	113.03	119.64
1	E	109	ALA	CA-C-N	5.55	130.83	123.00
1	E	109	ALA	C-N-CA	5.55	130.83	123.00
1	E	34	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	D	27	ASN	CA-CB-CG	-5.55	107.05	112.60
1	D	91	ALA	O-C-N	-5.55	116.70	123.30
1	D	88	HIS	N-CA-CB	5.54	118.12	109.97
1	F	78	TYR	O-C-N	5.54	128.47	122.15
1	C	77	SER	O-C-N	-5.54	115.46	122.27
1	G	106	THR	CA-CB-CG2	5.54	119.92	110.50
1	F	51	GLU	CA-C-O	5.54	126.37	119.12
1	B	16	VAL	CA-C-O	-5.53	114.58	120.39
1	E	22	GLY	O-C-N	5.53	128.18	122.54
1	D	24	PRO	CA-C-N	5.53	130.54	122.41
1	D	24	PRO	C-N-CA	5.53	130.54	122.41
1	G	112	SER	CA-C-N	5.53	126.75	119.84
1	G	112	SER	C-N-CA	5.53	126.75	119.84
1	C	93	VAL	N-CA-CB	5.53	118.86	111.90
1	F	66	GLU	N-CA-CB	-5.53	101.48	109.83
1	G	108	ALA	O-C-N	-5.52	116.77	123.29
1	H	110	LEU	CA-CB-CG	5.52	135.62	116.30
1	F	111	LEU	O-C-N	-5.52	116.73	123.19
1	H	14	VAL	CA-C-O	-5.52	114.63	120.48
1	A	106	THR	CA-C-O	-5.52	114.40	120.30
1	G	80	LYS	CD-CE-NZ	5.52	129.55	111.90
1	C	122	VAL	CA-C-N	5.51	130.61	123.00
1	C	122	VAL	C-N-CA	5.51	130.61	123.00
1	G	27	ASN	N-CA-CB	-5.51	103.92	112.30
1	G	86	PRO	CB-CA-C	-5.51	103.00	110.60
1	G	13	MET	CB-CG-SD	5.50	129.21	112.70
1	F	27	ASN	N-CA-C	5.50	119.16	111.90
1	B	96	THR	CA-CB-OG1	5.50	117.85	109.60
1	C	12	LEU	CA-C-O	-5.50	114.42	120.36
1	B	86	PRO	CA-C-O	-5.50	115.30	122.12
1	C	11	PRO	CA-C-N	-5.50	115.24	122.99
1	C	11	PRO	C-N-CA	-5.50	115.24	122.99
1	C	62	GLU	OE1-CD-OE2	5.50	136.09	122.90
1	E	17	LEU	N-CA-CB	5.49	120.47	111.08
1	G	70	LYS	CA-C-N	-5.49	116.02	122.93
1	G	70	LYS	C-N-CA	-5.49	116.02	122.93
1	B	14	VAL	CB-CA-C	5.48	118.74	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	PRO	N-CA-CB	5.48	108.19	103.31
1	C	124	ASN	N-CA-CB	5.48	119.36	110.05
1	D	66	GLU	OE1-CD-OE2	5.48	136.04	122.90
1	A	105	TYR	CB-CG-CD2	5.47	129.01	120.80
1	A	10	CYS	CA-C-N	5.47	124.81	118.85
1	A	10	CYS	C-N-CA	5.47	124.81	118.85
1	B	28	VAL	N-CA-C	-5.47	100.56	108.87
1	B	99	ASP	CA-C-N	5.46	132.87	121.94
1	B	99	ASP	C-N-CA	5.46	132.87	121.94
1	E	87	PHE	CA-C-O	5.46	126.54	120.80
1	F	24	PRO	O-C-N	-5.46	116.42	123.03
1	G	40	THR	CA-CB-OG1	-5.46	101.40	109.60
1	C	44	PHE	CA-C-O	-5.46	113.14	119.64
1	F	31	HIS	CA-C-O	-5.46	114.46	120.30
1	H	91	ALA	CB-CA-C	5.46	119.80	109.37
1	A	87	PHE	O-C-N	-5.46	114.94	122.30
1	C	65	VAL	CA-CB-CG2	5.46	119.67	110.40
1	G	103	ARG	CA-CB-CG	-5.45	103.19	114.10
1	H	23	SER	CA-C-N	5.45	125.37	119.76
1	H	23	SER	C-N-CA	5.45	125.37	119.76
1	G	63	GLU	CB-CG-CD	-5.45	103.34	112.60
1	E	34	ARG	CG-CD-NE	-5.44	100.04	112.00
1	D	112	SER	CA-C-O	-5.43	114.68	120.28
1	F	45	ALA	N-CA-CB	5.43	119.83	111.46
1	G	114	TYR	CB-CG-CD2	5.43	128.95	120.80
1	B	42	GLU	OE1-CD-OE2	5.43	135.94	122.90
1	D	104	ARG	CD-NE-CZ	5.43	132.00	124.40
1	C	119	THR	CA-CB-CG2	5.43	119.72	110.50
1	C	82	LEU	N-CA-CB	5.42	118.80	110.61
1	F	56	HIS	CA-C-N	5.42	132.03	121.41
1	F	56	HIS	C-N-CA	5.42	132.03	121.41
1	A	117	SER	CB-CA-C	-5.42	98.65	109.33
1	H	72	GLU	CB-CG-CD	-5.42	103.39	112.60
1	B	44	PHE	N-CA-CB	5.42	118.21	111.00
1	G	40	THR	N-CA-CB	-5.42	101.58	110.41
1	A	85	SER	CB-CA-C	-5.42	104.81	110.17
1	G	42	GLU	CA-CB-CG	5.42	124.93	114.10
1	F	26	ILE	CA-C-N	5.41	130.04	122.08
1	F	26	ILE	C-N-CA	5.41	130.04	122.08
1	H	68	ILE	CB-CA-C	-5.41	103.57	110.98
1	C	111	LEU	CA-C-O	5.41	127.14	120.92
1	G	11	PRO	N-CA-CB	5.41	109.28	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	LYS	CA-C-O	5.40	126.67	120.90
1	D	110	LEU	N-CA-CB	-5.39	102.13	110.65
1	D	76	LYS	O-C-N	-5.39	116.48	122.09
1	B	112	SER	N-CA-CB	5.39	120.89	111.19
1	C	62	GLU	CA-C-N	-5.38	113.67	122.54
1	C	62	GLU	C-N-CA	-5.38	113.67	122.54
1	D	16	VAL	N-CA-CB	5.38	118.56	111.25
1	G	47	GLY	CA-C-O	-5.37	115.97	121.61
1	H	17	LEU	CA-C-N	5.37	129.83	122.84
1	H	17	LEU	C-N-CA	5.37	129.83	122.84
1	H	118	THR	OG1-CB-CG2	-5.37	98.55	109.30
1	H	114	TYR	CA-CB-CG	-5.37	104.23	113.90
1	C	72	GLU	CA-CB-CG	-5.37	103.37	114.10
1	H	96	THR	O-C-N	-5.37	116.96	123.13
1	B	77	SER	O-C-N	-5.36	115.67	122.27
1	A	82	LEU	CA-CB-CG	5.36	135.06	116.30
1	F	54	GLU	OE1-CD-OE2	-5.36	110.05	122.90
1	F	116	TYR	CA-C-N	5.35	131.22	122.81
1	F	116	TYR	C-N-CA	5.35	131.22	122.81
1	C	79	TRP	CA-C-O	-5.35	114.75	120.42
1	A	24	PRO	CA-C-O	-5.35	115.36	121.56
1	C	66	GLU	CG-CD-OE2	5.35	130.69	118.40
1	C	48	LYS	CB-CA-C	5.34	118.89	109.80
1	C	81	ALA	CA-C-O	5.34	125.83	119.10
1	G	59	THR	O-C-N	-5.34	115.63	122.94
1	B	113	PRO	CA-N-CD	5.34	119.47	112.00
1	E	12	LEU	CA-C-O	-5.34	114.56	120.38
1	D	120	ALA	CA-C-N	-5.33	116.01	123.10
1	D	120	ALA	C-N-CA	-5.33	116.01	123.10
1	C	55	PRO	CB-CA-C	-5.33	103.34	110.85
1	B	58	LEU	CB-CA-C	5.32	121.02	110.42
1	E	110	LEU	N-CA-CB	5.32	118.95	110.65
1	G	124	ASN	CA-C-N	-5.32	96.00	122.60
1	G	124	ASN	C-N-CA	-5.32	96.00	122.60
1	D	63	GLU	CA-CB-CG	-5.32	103.47	114.10
1	F	63	GLU	O-C-N	5.31	129.90	122.36
1	H	20	VAL	CA-CB-CG2	5.31	119.43	110.40
1	H	10	CYS	N-CA-CB	5.31	119.52	110.50
1	H	68	ILE	CA-CB-CG2	5.31	119.52	110.50
1	C	121	VAL	CA-CB-CG1	5.30	119.42	110.40
1	D	27	ASN	N-CA-CB	-5.30	104.24	112.30
1	E	65	VAL	N-CA-CB	5.30	118.11	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	78	TYR	N-CA-CB	-5.30	102.32	110.16
1	F	84	ILE	CA-CB-CG2	-5.30	101.49	110.50
1	A	52	SER	CA-CB-OG	5.30	121.69	111.10
1	A	79	TRP	CA-C-N	-5.29	112.26	120.31
1	A	79	TRP	C-N-CA	-5.29	112.26	120.31
1	C	70	LYS	CG-CD-CE	5.29	123.47	111.30
1	G	55	PRO	CA-C-N	-5.29	114.27	122.09
1	G	55	PRO	C-N-CA	-5.29	114.27	122.09
1	H	23	SER	N-CA-C	5.28	114.22	108.14
1	C	17	LEU	CA-C-N	5.28	129.44	122.42
1	C	17	LEU	C-N-CA	5.28	129.44	122.42
1	F	21	ARG	N-CA-CB	5.27	118.27	110.53
1	F	26	ILE	O-C-N	-5.27	116.11	122.59
1	H	42	GLU	CA-C-N	5.27	126.42	119.84
1	H	42	GLU	C-N-CA	5.27	126.42	119.84
1	E	104	ARG	NE-CZ-NH2	-5.26	114.46	119.20
1	B	73	ILE	O-C-N	-5.26	117.19	123.03
1	G	78	TYR	CB-CG-CD1	5.26	128.69	120.80
1	H	94	VAL	O-C-N	-5.26	116.94	123.10
1	G	31	HIS	CA-C-O	-5.25	114.66	120.38
1	G	38	ASP	CA-C-O	-5.24	113.01	120.51
1	A	114	TYR	CB-CG-CD1	-5.24	112.94	120.80
1	D	23	SER	CA-C-N	5.24	125.18	119.78
1	D	23	SER	C-N-CA	5.24	125.18	119.78
1	H	88	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
1	G	123	THR	CA-C-N	5.24	135.84	120.97
1	G	123	THR	C-N-CA	5.24	135.84	120.97
1	D	21	ARG	NH1-CZ-NH2	-5.23	112.50	119.30
1	G	60	THR	N-CA-CB	-5.23	101.91	110.43
1	C	111	LEU	N-CA-CB	-5.22	101.77	110.23
1	F	104	ARG	N-CA-CB	5.22	118.75	110.55
1	H	55	PRO	O-C-N	-5.22	116.48	123.06
1	H	60	THR	CA-C-N	-5.21	110.86	121.18
1	H	60	THR	C-N-CA	-5.21	110.86	121.18
1	E	124	ASN	CA-C-O	-5.21	113.02	120.16
1	B	101	GLY	N-CA-C	-5.21	101.71	112.34
1	C	85	SER	CB-CA-C	-5.21	105.02	110.33
1	F	70	LYS	N-CA-CB	5.21	118.78	110.65
1	B	31	HIS	CA-CB-CG	-5.21	108.59	113.80
1	G	88	HIS	CA-C-N	5.21	127.68	120.29
1	G	88	HIS	C-N-CA	5.21	127.68	120.29
1	B	89	GLU	CA-C-O	5.20	125.94	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	GLU	CG-CD-OE1	-5.20	106.44	118.40
1	H	92	GLU	CG-CD-OE1	-5.20	106.44	118.40
1	A	121	VAL	CA-CB-CG2	5.20	119.24	110.40
1	F	110	LEU	CA-C-O	-5.20	114.94	120.40
1	G	34	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	D	24	PRO	N-CA-CB	5.20	107.87	103.35
1	G	47	GLY	O-C-N	5.19	129.46	123.44
1	B	25	ALA	CA-C-O	5.18	126.13	120.58
1	A	11	PRO	CA-C-O	-5.17	112.24	119.74
1	F	54	GLU	CA-CB-CG	5.17	124.44	114.10
1	F	55	PRO	CA-N-CD	-5.17	104.76	112.00
1	G	104	ARG	CG-CD-NE	-5.17	100.62	112.00
1	B	38	ASP	CB-CA-C	-5.17	100.14	110.42
1	F	42	GLU	CA-C-N	5.16	126.29	119.84
1	F	42	GLU	C-N-CA	5.16	126.29	119.84
1	C	72	GLU	OE1-CD-OE2	5.16	135.29	122.90
1	F	99	ASP	O-C-N	-5.16	116.72	122.09
1	G	79	TRP	CB-CA-C	-5.16	99.85	110.38
1	B	53	GLY	N-CA-C	-5.16	108.11	115.64
1	C	40	THR	O-C-N	5.16	128.79	122.96
1	D	50	SER	CA-CB-OG	-5.16	100.79	111.10
1	F	74	ASP	CB-CA-C	-5.15	103.03	111.68
1	A	110	LEU	CA-C-N	5.15	131.39	122.64
1	A	110	LEU	C-N-CA	5.15	131.39	122.64
1	B	79	TRP	O-C-N	5.14	128.01	122.15
1	C	20	VAL	CA-CB-CG2	5.14	119.14	110.40
1	C	53	GLY	N-CA-C	-5.14	108.53	115.21
1	H	52	SER	N-CA-C	5.13	119.18	113.02
1	C	54	GLU	CB-CG-CD	5.13	121.32	112.60
1	D	59	THR	CA-C-O	5.13	127.25	121.51
1	H	35	LYS	N-CA-C	-5.13	102.32	109.96
1	A	13	MET	CA-CB-CG	-5.12	103.85	114.10
1	C	96	THR	CA-CB-OG1	-5.12	101.92	109.60
1	C	16	VAL	CA-C-O	-5.12	115.01	120.39
1	E	31	HIS	CB-CA-C	-5.12	100.86	109.72
1	E	16	VAL	CA-CB-CG2	-5.12	101.70	110.40
1	A	56	HIS	CB-CA-C	-5.11	100.77	109.51
1	B	56	HIS	CA-C-N	5.11	130.69	120.77
1	B	56	HIS	C-N-CA	5.11	130.69	120.77
1	G	63	GLU	N-CA-CB	-5.11	103.02	110.53
1	C	47	GLY	CA-C-O	-5.11	116.56	121.41
1	A	23	SER	CA-C-N	5.11	125.04	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	SER	C-N-CA	5.11	125.04	119.78
1	A	92	GLU	CB-CG-CD	-5.11	103.92	112.60
1	G	72	GLU	OE1-CD-OE2	5.11	135.15	122.90
1	E	104	ARG	CD-NE-CZ	5.10	131.54	124.40
1	D	55	PRO	CB-CA-C	5.10	118.04	111.46
1	E	56	HIS	CA-CB-CG	-5.10	108.70	113.80
1	C	40	THR	CA-CB-CG2	5.10	119.17	110.50
1	G	78	TYR	CB-CA-C	5.10	119.51	110.85
1	D	26	ILE	CB-CA-C	-5.09	104.61	111.63
1	E	35	LYS	N-CA-CB	5.09	117.55	109.71
1	B	23	SER	O-C-N	5.09	125.86	121.54
1	H	103	ARG	CG-CD-NE	-5.09	100.81	112.00
1	C	72	GLU	CB-CG-CD	-5.08	103.96	112.60
1	A	60	THR	CA-CB-OG1	-5.08	101.98	109.60
1	B	80	LYS	CA-CB-CG	5.08	124.25	114.10
1	B	27	ASN	N-CA-C	5.07	118.59	111.74
1	A	103	ARG	CD-NE-CZ	5.07	131.50	124.40
1	B	59	THR	CA-C-O	5.07	126.73	121.31
1	D	58	LEU	CA-C-N	5.07	130.47	122.36
1	D	58	LEU	C-N-CA	5.07	130.47	122.36
1	G	68	ILE	CA-CB-CG1	-5.07	101.78	110.40
1	F	21	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
1	A	112	SER	CA-C-O	-5.05	114.86	119.76
1	D	103	ARG	CD-NE-CZ	5.05	131.48	124.40
1	G	92	GLU	CB-CG-CD	-5.05	104.01	112.60
1	A	85	SER	CA-C-N	5.05	125.52	120.52
1	A	85	SER	C-N-CA	5.05	125.52	120.52
1	A	96	THR	CA-C-O	-5.05	114.84	120.54
1	A	48	LYS	CB-CA-C	5.04	118.83	109.70
1	D	66	GLU	CB-CG-CD	-5.04	104.03	112.60
1	A	42	GLU	CB-CG-CD	5.04	121.16	112.60
1	A	106	THR	CA-CB-CG2	5.04	119.06	110.50
1	C	77	SER	CA-C-N	5.04	127.79	120.79
1	C	77	SER	C-N-CA	5.04	127.79	120.79
1	E	123	THR	CA-C-N	5.04	134.09	121.80
1	E	123	THR	C-N-CA	5.04	134.09	121.80
1	H	68	ILE	N-CA-C	-5.04	100.64	107.99
1	D	124	ASN	O-C-N	5.03	126.95	121.36
1	B	25	ALA	CB-CA-C	5.03	119.11	110.81
1	C	108	ALA	CA-C-O	-5.03	114.90	120.38
1	E	23	SER	N-CA-CB	-5.03	101.42	110.37
1	C	52	SER	CA-C-O	5.03	125.36	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	SER	CA-CB-OG	-5.03	101.05	111.10
1	D	37	ALA	N-CA-CB	-5.03	102.00	110.49
1	F	58	LEU	CA-C-O	-5.02	115.53	120.70
1	A	119	THR	CB-CA-C	-5.02	99.73	109.68
1	C	42	GLU	CB-CA-C	5.02	115.49	109.31
1	F	32	VAL	CA-C-N	5.02	131.76	122.92
1	F	32	VAL	C-N-CA	5.02	131.76	122.92
1	F	41	TRP	N-CA-CB	-5.02	102.22	110.21
1	G	71	VAL	N-CA-CB	5.02	117.02	110.99
1	D	13	MET	CA-CB-CG	-5.01	104.07	114.10
1	H	61	GLU	OE1-CD-OE2	5.01	134.92	122.90
1	H	62	GLU	CA-C-O	-5.01	113.74	119.60
1	C	103	ARG	CB-CG-CD	5.01	122.81	111.30
1	G	106	THR	CA-CB-OG1	-5.00	102.09	109.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	125	PRO	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	124	ASN	Peptide
1	G	124	ASN	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	895	0	865	69	0
1	B	890	0	860	75	0
1	C	895	0	864	52	0
1	D	891	0	861	74	0
1	E	895	0	865	59	0
1	F	895	0	865	52	0
1	G	891	0	860	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	895	0	865	56	0
All	All	7147	0	6905	470	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (470) 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:D:26:ILE:CD1	1:D:51:GLU:HA	1.24	1.62
1:C:21:ARG:NH2	1:C:82:LEU:HD11	1.29	1.48
1:C:21:ARG:NH2	1:C:82:LEU:CD1	1.82	1.42
1:F:44:PHE:CZ	1:F:59:THR:HG21	1.63	1.33
1:C:44:PHE:CZ	1:C:59:THR:HG21	1.63	1.32
1:B:18:ASP:OD1	1:B:20:VAL:CG2	1.77	1.30
1:C:21:ARG:HH22	1:C:82:LEU:CD2	1.54	1.19
1:C:44:PHE:CZ	1:C:59:THR:CG2	2.26	1.18
1:D:26:ILE:CD1	1:D:51:GLU:CA	2.21	1.17
1:D:26:ILE:HD12	1:D:51:GLU:HA	1.20	1.17
1:A:40:THR:HG22	1:A:42:GLU:OE2	1.42	1.16
1:A:40:THR:CG2	1:A:42:GLU:OE2	1.93	1.15
1:C:21:ARG:HH21	1:C:82:LEU:CD1	1.49	1.14
1:G:44:PHE:CZ	1:G:59:THR:HG21	1.83	1.13
1:G:44:PHE:HZ	1:G:59:THR:HG21	1.01	1.13
1:C:90:HIS:CE1	1:C:92:GLU:OE2	2.01	1.12
1:D:26:ILE:HD13	1:D:51:GLU:HA	1.28	1.10
1:F:15:LYS:HE2	1:F:17:LEU:HD21	1.14	1.10
1:A:103:ARG:HG2	1:A:122:VAL:CG1	1.82	1.08
1:A:34:ARG:HH12	1:A:65:VAL:HG22	1.17	1.08
1:H:123:THR:HG22	1:H:125:PRO:CD	1.82	1.08
1:H:10:CYS:SG	1:H:11:PRO:HD2	1.94	1.07
1:G:44:PHE:CZ	1:G:59:THR:CG2	2.39	1.05
1:C:21:ARG:HH22	1:C:82:LEU:HD21	1.20	1.04
1:B:18:ASP:OD1	1:B:20:VAL:HG22	1.56	1.02
1:B:20:VAL:HG23	1:B:21:ARG:H	1.24	1.02
1:G:40:THR:HG22	1:G:42:GLU:OE1	1.60	1.02
1:H:123:THR:CG2	1:H:125:PRO:HD3	1.89	1.01
1:D:26:ILE:HD11	1:D:51:GLU:HA	1.40	1.01
1:G:56:HIS:ND1	1:G:57:GLY:N	2.08	1.00
1:B:36:ALA:HB3	1:B:40:THR:HB	1.40	1.00
1:B:18:ASP:OD1	1:B:20:VAL:HG23	1.58	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:LYS:HE2	1:G:92:GLU:CD	1.86	0.99
1:E:26:ILE:HG12	1:E:27:ASN:N	1.77	0.99
1:D:44:PHE:CZ	1:D:59:THR:HG21	1.96	0.99
1:H:25:ALA:O	1:H:49:THR:HG21	1.64	0.98
1:H:123:THR:HG22	1:H:125:PRO:HD3	1.00	0.98
1:B:20:VAL:HG23	1:B:21:ARG:N	1.77	0.97
1:B:42:GLU:OE1	1:B:44:PHE:HE2	1.46	0.96
1:C:90:HIS:HE1	1:C:92:GLU:OE2	1.40	0.95
1:G:44:PHE:HZ	1:G:59:THR:CG2	1.73	0.95
1:D:76:LYS:NZ	1:D:80:LYS:NZ	2.16	0.94
1:A:34:ARG:NH1	1:A:65:VAL:HG22	1.84	0.92
1:C:44:PHE:HZ	1:C:59:THR:HG21	1.12	0.92
1:B:26:ILE:HG21	1:B:51:GLU:HA	1.48	0.92
1:E:66:GLU:OE1	1:E:99:ASP:HA	1.69	0.92
1:H:68:ILE:N	1:H:68:ILE:HD12	1.85	0.91
1:A:103:ARG:HG2	1:A:122:VAL:HG13	1.50	0.91
1:D:11:PRO:HA	1:D:104:ARG:HG2	1.53	0.90
1:D:101:GLY:O	1:D:103:ARG:HD2	1.71	0.90
1:A:89:GLU:HB2	1:B:94:VAL:HG22	1.54	0.90
1:G:11:PRO:HB2	1:G:64:PHE:CD2	2.06	0.89
1:B:98:ASN:OD1	1:B:102:PRO:HA	1.72	0.89
1:D:103:ARG:NH2	1:D:124:ASN:HB3	1.86	0.89
1:F:44:PHE:CE2	1:F:59:THR:HG21	2.09	0.87
1:C:21:ARG:NH2	1:C:82:LEU:HD13	1.89	0.86
1:C:21:ARG:NH2	1:C:82:LEU:CD2	2.36	0.86
1:B:26:ILE:CG2	1:B:51:GLU:HA	2.06	0.86
1:D:76:LYS:HZ1	1:D:80:LYS:NZ	1.73	0.86
1:F:102:PRO:O	1:F:103:ARG:HD3	1.76	0.86
1:A:40:THR:HG21	1:A:42:GLU:OE2	1.75	0.85
1:B:21:ARG:HH21	1:D:81:ALA:HA	1.39	0.85
1:G:11:PRO:HB2	1:G:64:PHE:HD2	1.38	0.85
1:B:104:ARG:NH1	1:B:104:ARG:HB3	1.92	0.85
1:H:10:CYS:SG	1:H:11:PRO:CD	2.65	0.85
1:D:26:ILE:HD12	1:D:51:GLU:CA	1.96	0.84
1:G:70:LYS:HE2	1:G:92:GLU:OE1	1.77	0.84
1:A:48:LYS:HD3	1:A:48:LYS:N	1.92	0.84
1:H:16:VAL:O	1:H:17:LEU:HD23	1.77	0.84
1:A:11:PRO:HG3	1:A:61:GLU:HG2	1.57	0.84
1:H:35:LYS:HD3	1:H:39:ASP:HA	1.59	0.84
1:H:25:ALA:O	1:H:49:THR:CG2	2.25	0.83
1:B:21:ARG:NH2	1:D:81:ALA:HA	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HH12	1:A:65:VAL:CG2	1.91	0.82
1:A:34:ARG:NH1	1:A:65:VAL:CG2	2.42	0.81
1:C:21:ARG:NH2	1:C:82:LEU:CG	2.43	0.81
1:F:15:LYS:CE	1:F:17:LEU:HD21	2.06	0.80
1:A:105:TYR:CD1	1:A:122:VAL:HG22	2.16	0.80
1:D:103:ARG:HH21	1:D:124:ASN:HB3	1.46	0.79
1:C:21:ARG:NH2	1:C:82:LEU:HD21	1.95	0.79
1:H:37:ALA:O	1:H:38:ASP:OD1	1.99	0.79
1:D:76:LYS:NZ	1:D:80:LYS:HZ2	1.79	0.77
1:G:70:LYS:CE	1:G:92:GLU:CD	2.57	0.77
1:D:76:LYS:NZ	1:D:80:LYS:HZ3	1.81	0.77
1:H:123:THR:HG22	1:H:124:ASN:N	2.00	0.76
1:H:123:THR:CG2	1:H:124:ASN:N	2.48	0.76
1:C:44:PHE:CZ	1:C:59:THR:HG23	2.15	0.76
1:C:44:PHE:CE2	1:C:59:THR:HG23	2.20	0.75
1:B:65:VAL:O	1:B:69:TYR:OH	2.04	0.75
1:C:21:ARG:HH22	1:C:82:LEU:CG	2.00	0.75
1:E:79:TRP:HB3	1:E:84:ILE:HB	1.67	0.75
1:G:28:VAL:HG23	1:G:78:TYR:CD1	2.22	0.74
1:G:44:PHE:CZ	1:G:59:THR:HG23	2.22	0.74
1:F:44:PHE:HZ	1:F:59:THR:HG21	1.45	0.73
1:D:70:LYS:HG3	1:D:94:VAL:HG22	1.70	0.73
1:F:54:GLU:OE1	1:F:55:PRO:HD2	1.88	0.73
1:C:18:ASP:OD2	1:C:78:TYR:OH	2.05	0.72
1:D:24:PRO:HG2	1:D:51:GLU:O	1.89	0.72
1:E:34:ARG:HH21	1:E:65:VAL:HG23	1.54	0.72
1:A:11:PRO:HB2	1:A:64:PHE:CD2	2.25	0.71
1:D:76:LYS:HZ3	1:D:80:LYS:NZ	1.87	0.71
1:D:103:ARG:HG3	1:D:105:TYR:OH	1.91	0.71
1:A:36:ALA:HB2	1:A:42:GLU:CG	2.20	0.71
1:F:33:PHE:HD2	1:F:41:TRP:HB3	1.55	0.71
1:G:93:VAL:CG2	1:G:118:THR:HG21	2.21	0.71
1:F:56:HIS:H	1:F:56:HIS:CD2	2.08	0.70
1:H:68:ILE:HD12	1:H:68:ILE:H	1.56	0.70
1:D:103:ARG:HG3	1:D:105:TYR:CZ	2.26	0.70
1:H:28:VAL:H	1:H:49:THR:HB	1.56	0.70
1:B:104:ARG:HB3	1:B:104:ARG:HH11	1.57	0.70
1:F:44:PHE:CZ	1:F:59:THR:CG2	2.59	0.69
1:F:56:HIS:CD2	1:F:56:HIS:N	2.61	0.69
1:C:16:VAL:HG23	1:C:111:LEU:HD23	1.74	0.69
1:C:21:ARG:HH21	1:C:82:LEU:HD11	0.61	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:C	1:A:48:LYS:HD3	2.17	0.68
1:A:44:PHE:CZ	1:A:59:THR:HG21	2.29	0.68
1:H:98:ASN:OD1	1:H:102:PRO:HA	1.94	0.68
1:D:26:ILE:HD13	1:D:51:GLU:CA	2.10	0.68
1:F:60:THR:OG1	1:F:63:GLU:HG3	1.93	0.68
1:B:26:ILE:CG2	1:B:51:GLU:CA	2.73	0.67
1:C:48:LYS:O	1:C:48:LYS:HD3	1.94	0.67
1:H:74:ASP:OD2	1:H:77:SER:HB2	1.95	0.67
1:B:42:GLU:OE1	1:B:44:PHE:CE2	2.37	0.67
1:A:26:ILE:N	1:A:26:ILE:HD12	2.10	0.67
1:E:32:VAL:HG21	1:E:58:LEU:HD12	1.77	0.66
1:D:13:MET:CE	1:D:104:ARG:HH12	2.09	0.66
1:E:21:ARG:HG2	1:E:21:ARG:O	1.93	0.66
1:D:44:PHE:CE1	1:D:59:THR:HG21	2.31	0.66
1:F:23:SER:HB2	1:F:24:PRO:HD2	1.78	0.66
1:D:26:ILE:HG23	1:D:50:SER:C	2.22	0.65
1:B:26:ILE:HG23	1:B:50:SER:O	1.96	0.65
1:C:16:VAL:HG23	1:C:111:LEU:CD2	2.26	0.65
1:G:18:ASP:OD2	1:G:21:ARG:CB	2.44	0.65
1:G:18:ASP:OD2	1:G:21:ARG:HB2	1.96	0.65
1:A:44:PHE:HZ	1:A:59:THR:HG21	1.61	0.65
1:G:11:PRO:CB	1:G:64:PHE:HD2	2.10	0.65
1:B:35:LYS:N	1:B:41:TRP:CZ3	2.65	0.65
1:A:70:LYS:HE2	1:A:92:GLU:OE2	1.96	0.64
1:G:40:THR:CG2	1:G:42:GLU:OE1	2.41	0.64
1:E:14:VAL:O	1:E:54:GLU:HG2	1.97	0.64
1:B:74:ASP:OD2	1:B:77:SER:HB2	1.97	0.64
1:F:29:ALA:HA	1:F:48:LYS:HE3	1.80	0.64
1:A:32:VAL:CG2	1:A:58:LEU:HD13	2.28	0.63
1:A:36:ALA:HB2	1:A:42:GLU:HG2	1.80	0.63
1:C:16:VAL:CG1	1:C:49:THR:HG21	2.28	0.63
1:H:50:SER:OG	1:H:54:GLU:O	2.16	0.63
1:D:103:ARG:HA	1:D:125:PRO:HD3	1.81	0.63
1:G:93:VAL:HG22	1:G:118:THR:HG21	1.80	0.63
1:B:16:VAL:HG13	1:B:49:THR:HG21	1.80	0.63
1:D:79:TRP:HA	1:D:79:TRP:CE3	2.31	0.63
1:G:70:LYS:NZ	1:G:92:GLU:CD	2.57	0.63
1:C:23:SER:HB2	1:C:24:PRO:HD2	1.80	0.63
1:A:36:ALA:HB2	1:A:42:GLU:HG3	1.80	0.63
1:B:75:THR:HB	1:B:90:HIS:HA	1.79	0.62
1:H:102:PRO:O	1:H:103:ARG:HD3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ILE:HB	1:B:91:ALA:HB3	1.81	0.61
1:D:121:VAL:HG21	1:F:17:LEU:HD13	1.82	0.61
1:H:35:LYS:HD3	1:H:39:ASP:CA	2.29	0.61
1:E:32:VAL:CG2	1:E:58:LEU:HD12	2.31	0.61
1:B:26:ILE:CG2	1:B:50:SER:C	2.74	0.61
1:C:11:PRO:HB2	1:C:64:PHE:CD2	2.36	0.61
1:D:10:CYS:O	1:D:104:ARG:NH1	2.33	0.61
1:H:16:VAL:C	1:H:17:LEU:HD23	2.25	0.61
1:A:40:THR:HG22	1:A:42:GLU:CD	2.24	0.61
1:B:76:LYS:HG2	1:B:80:LYS:HD2	1.83	0.60
1:A:41:TRP:CH2	1:A:68:ILE:HG22	2.36	0.60
1:C:12:LEU:O	1:C:12:LEU:HD23	2.02	0.60
1:B:41:TRP:HA	1:B:41:TRP:CE3	2.37	0.60
1:G:33:PHE:HB3	1:G:41:TRP:HB3	1.82	0.60
1:B:102:PRO:C	1:B:103:ARG:HG2	2.27	0.60
1:A:105:TYR:CE1	1:A:122:VAL:HG22	2.36	0.60
1:E:31:HIS:HB3	1:E:33:PHE:CE1	2.37	0.60
1:G:120:ALA:HB2	1:H:87:PHE:CE2	2.37	0.59
1:G:28:VAL:HG22	1:G:78:TYR:HB2	1.84	0.59
1:E:78:TYR:O	1:E:82:LEU:HD22	2.02	0.59
1:B:57:GLY:O	1:B:58:LEU:C	2.43	0.59
1:H:10:CYS:CB	1:H:11:PRO:HD2	2.31	0.59
1:B:20:VAL:CG2	1:B:21:ARG:N	2.58	0.59
1:B:36:ALA:CB	1:B:40:THR:HB	2.24	0.59
1:A:24:PRO:O	1:A:26:ILE:HD12	2.02	0.59
1:A:70:LYS:HE2	1:A:92:GLU:CD	2.28	0.59
1:B:76:LYS:O	1:B:80:LYS:HD3	2.03	0.59
1:F:44:PHE:CE2	1:F:59:THR:CG2	2.83	0.58
1:H:123:THR:CG2	1:H:125:PRO:CD	2.64	0.58
1:B:26:ILE:CG2	1:B:51:GLU:N	2.66	0.58
1:C:23:SER:HA	1:E:121:VAL:HG13	1.84	0.58
1:G:70:LYS:NZ	1:G:92:GLU:OE2	2.35	0.58
1:G:84:ILE:HG13	1:G:85:SER:N	2.17	0.58
1:E:28:VAL:O	1:E:49:THR:HG23	2.04	0.58
1:F:33:PHE:CD2	1:F:41:TRP:HB3	2.38	0.58
1:F:66:GLU:OE2	1:F:99:ASP:HA	2.04	0.58
1:E:33:PHE:N	1:E:33:PHE:CD1	2.68	0.58
1:D:79:TRP:HB2	1:D:86:PRO:HG3	1.85	0.58
1:E:66:GLU:CD	1:E:99:ASP:HA	2.28	0.58
1:D:44:PHE:CE1	1:D:59:THR:CG2	2.87	0.57
1:A:99:ASP:OD1	1:A:99:ASP:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LYS:HG3	1:D:94:VAL:CG2	2.33	0.57
1:H:38:ASP:OD1	1:H:39:ASP:N	2.38	0.57
1:A:41:TRP:HH2	1:A:68:ILE:HG22	1.70	0.57
1:B:21:ARG:NH2	1:D:81:ALA:CA	2.65	0.57
1:F:102:PRO:O	1:F:103:ARG:CD	2.51	0.57
1:B:26:ILE:HG21	1:B:51:GLU:CA	2.29	0.57
1:E:35:LYS:HE3	1:E:41:TRP:CE2	2.40	0.56
1:A:70:LYS:CE	1:A:92:GLU:OE2	2.53	0.56
1:B:21:ARG:HH22	1:D:81:ALA:C	2.13	0.56
1:G:44:PHE:CE1	1:G:59:THR:OG1	2.59	0.56
1:G:114:TYR:N	1:G:114:TYR:CD1	2.73	0.56
1:H:36:ALA:O	1:H:37:ALA:C	2.49	0.56
1:C:20:VAL:HG22	1:C:79:TRP:CH2	2.41	0.56
1:H:28:VAL:CG1	1:H:49:THR:HB	2.36	0.56
1:A:23:SER:HB2	1:A:24:PRO:HD2	1.88	0.56
1:E:73:ILE:HB	1:E:91:ALA:HB3	1.87	0.56
1:G:97:ALA:O	1:G:98:ASN:HB2	2.04	0.56
1:F:35:LYS:HE2	1:F:39:ASP:O	2.06	0.56
1:G:115:SER:HB2	1:H:118:THR:O	2.06	0.56
1:F:75:THR:HB	1:F:90:HIS:HA	1.89	0.55
1:C:123:THR:O	1:C:123:THR:HG22	2.06	0.55
1:A:97:ALA:O	1:A:98:ASN:HB2	2.07	0.55
1:E:26:ILE:HG12	1:E:27:ASN:H	1.71	0.55
1:G:72:GLU:O	1:G:72:GLU:HG3	2.06	0.55
1:A:103:ARG:HG2	1:A:122:VAL:HG11	1.84	0.55
1:B:26:ILE:HG23	1:B:50:SER:C	2.31	0.55
1:D:121:VAL:HG13	1:F:23:SER:HA	1.89	0.55
1:E:90:HIS:NE2	1:F:94:VAL:HG21	2.22	0.55
1:H:28:VAL:HG13	1:H:49:THR:CB	2.37	0.55
1:B:66:GLU:HG3	1:B:98:ASN:O	2.07	0.55
1:E:87:PHE:CE2	1:F:120:ALA:HB2	2.42	0.55
1:E:41:TRP:CE3	1:E:41:TRP:HA	2.42	0.54
1:E:35:LYS:NZ	1:E:41:TRP:NE1	2.55	0.54
1:G:66:GLU:HA	1:G:97:ALA:O	2.07	0.54
1:A:34:ARG:HD3	1:A:69:TYR:CE2	2.42	0.54
1:E:26:ILE:HD11	1:E:27:ASN:OD1	2.07	0.54
1:F:105:TYR:CD2	1:F:122:VAL:HG22	2.42	0.54
1:C:48:LYS:HD3	1:C:48:LYS:C	2.33	0.54
1:F:27:ASN:ND2	1:F:48:LYS:HG3	2.22	0.54
1:A:23:SER:HB2	1:A:24:PRO:CD	2.38	0.54
1:A:100:SER:O	1:F:103:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LYS:HE3	1:C:35:LYS:N	2.23	0.53
1:E:14:VAL:O	1:E:54:GLU:CG	2.56	0.53
1:E:32:VAL:C	1:E:33:PHE:CD1	2.86	0.53
1:G:99:ASP:OD1	1:G:99:ASP:N	2.42	0.53
1:H:123:THR:CG2	1:H:124:ASN:H	2.20	0.53
1:B:35:LYS:HE2	1:B:68:ILE:HD12	1.89	0.53
1:E:36:ALA:O	1:E:37:ALA:C	2.51	0.53
1:D:20:VAL:HA	1:E:113:PRO:HG2	1.90	0.53
1:E:35:LYS:HZ2	1:E:41:TRP:NE1	2.07	0.53
1:G:31:HIS:HB2	1:G:72:GLU:HG2	1.91	0.53
1:H:16:VAL:CG1	1:H:111:LEU:HD22	2.39	0.53
1:B:27:ASN:O	1:B:48:LYS:NZ	2.42	0.53
1:B:114:TYR:N	1:B:114:TYR:CD1	2.76	0.53
1:D:44:PHE:HZ	1:D:59:THR:HG21	1.63	0.53
1:E:32:VAL:C	1:E:33:PHE:HD1	2.17	0.53
1:F:33:PHE:CD1	1:F:33:PHE:N	2.75	0.52
1:C:75:THR:HG21	1:C:111:LEU:HD11	1.91	0.52
1:E:32:VAL:CG2	1:E:58:LEU:CD1	2.87	0.52
1:H:95:PHE:CE2	1:H:97:ALA:HB2	2.45	0.52
1:F:38:ASP:O	1:F:40:THR:N	2.42	0.52
1:G:31:HIS:HB3	1:G:33:PHE:CE1	2.44	0.52
1:C:16:VAL:CG2	1:C:111:LEU:HD23	2.39	0.52
1:D:13:MET:HE2	1:D:104:ARG:NH1	2.24	0.52
1:E:79:TRP:HZ2	1:E:111:LEU:HB3	1.73	0.52
1:A:26:ILE:HD12	1:A:26:ILE:H	1.75	0.52
1:G:18:ASP:OD2	1:G:21:ARG:HB3	2.09	0.52
1:A:103:ARG:HH22	1:F:100:SER:HB3	1.75	0.52
1:B:112:SER:HB3	1:B:113:PRO:HD2	1.92	0.52
1:H:95:PHE:HE2	1:H:97:ALA:HB2	1.74	0.52
1:D:20:VAL:HG21	1:D:113:PRO:HD3	1.92	0.52
1:C:17:LEU:HD23	1:C:24:PRO:HA	1.91	0.51
1:G:70:LYS:HZ1	1:G:92:GLU:CD	2.18	0.51
1:H:26:ILE:HG13	1:H:26:ILE:O	2.10	0.51
1:A:11:PRO:HB2	1:A:64:PHE:HD2	1.71	0.51
1:F:104:ARG:HG3	1:F:104:ARG:HH11	1.75	0.51
1:A:73:ILE:O	1:A:90:HIS:HB2	2.11	0.51
1:A:103:ARG:HG3	1:A:123:THR:O	2.11	0.51
1:F:102:PRO:C	1:F:103:ARG:HG2	2.36	0.51
1:G:28:VAL:O	1:G:48:LYS:HA	2.10	0.51
1:A:36:ALA:O	1:A:37:ALA:C	2.53	0.51
1:A:44:PHE:CZ	1:A:59:THR:CG2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:LYS:CD	1:H:17:LEU:HD21	2.41	0.51
1:E:89:GLU:O	1:E:90:HIS:HB3	2.11	0.50
1:C:99:ASP:N	1:C:99:ASP:OD1	2.45	0.50
1:A:35:LYS:HB2	1:A:41:TRP:CZ3	2.46	0.50
1:F:11:PRO:HA	1:F:104:ARG:HG2	1.94	0.50
1:C:73:ILE:O	1:C:90:HIS:HB2	2.11	0.50
1:D:103:ARG:HH21	1:D:124:ASN:CB	2.22	0.50
1:A:38:ASP:OD1	1:A:40:THR:HB	2.11	0.50
1:B:18:ASP:OD2	1:B:21:ARG:HD3	2.11	0.50
1:G:17:LEU:HB2	1:G:110:LEU:HD12	1.94	0.50
1:G:114:TYR:N	1:G:114:TYR:HD1	2.09	0.49
1:F:23:SER:HB2	1:F:24:PRO:CD	2.41	0.49
1:G:23:SER:HB2	1:G:24:PRO:CD	2.42	0.49
1:A:32:VAL:HG21	1:A:58:LEU:HD13	1.93	0.49
1:F:29:ALA:CA	1:F:48:LYS:HE3	2.42	0.49
1:C:16:VAL:HG11	1:C:49:THR:HG21	1.95	0.49
1:E:16:VAL:CG1	1:E:111:LEU:HD22	2.42	0.49
1:E:34:ARG:HD3	1:E:42:GLU:OE2	2.13	0.49
1:A:65:VAL:O	1:A:69:TYR:OH	2.21	0.49
1:E:32:VAL:HG23	1:E:58:LEU:CD1	2.43	0.49
1:A:24:PRO:O	1:A:26:ILE:CD1	2.61	0.49
1:B:77:SER:HA	1:B:80:LYS:HD3	1.94	0.49
1:C:11:PRO:HB2	1:C:64:PHE:HD2	1.78	0.49
1:F:33:PHE:HB2	1:F:70:LYS:HB3	1.95	0.49
1:E:38:ASP:OD1	1:E:38:ASP:N	2.45	0.49
1:G:102:PRO:C	1:G:103:ARG:HG3	2.37	0.49
1:D:76:LYS:HZ1	1:D:80:LYS:HZ3	1.43	0.48
1:A:17:LEU:N	1:A:17:LEU:HD22	2.27	0.48
1:G:73:ILE:O	1:G:90:HIS:HB2	2.14	0.48
1:D:13:MET:HE2	1:D:104:ARG:HH12	1.78	0.48
1:F:93:VAL:HG21	1:F:107:ILE:HD11	1.93	0.48
1:H:90:HIS:ND1	1:H:90:HIS:C	2.72	0.48
1:E:101:GLY:O	1:E:103:ARG:HD3	2.14	0.48
1:G:44:PHE:HE1	1:G:59:THR:OG1	1.95	0.48
1:A:87:PHE:HE1	1:B:105:TYR:HD2	1.62	0.48
1:C:20:VAL:HG22	1:C:79:TRP:HH2	1.76	0.48
1:E:114:TYR:CD1	1:E:114:TYR:N	2.82	0.48
1:H:28:VAL:HG12	1:H:49:THR:HB	1.95	0.48
1:D:23:SER:HB2	1:D:24:PRO:HD2	1.96	0.47
1:F:11:PRO:HG3	1:F:61:GLU:HG3	1.96	0.47
1:A:32:VAL:HG13	1:A:71:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ALA:HB2	1:B:42:GLU:OE2	2.14	0.47
1:E:25:ALA:HB1	1:E:28:VAL:HG11	1.96	0.47
1:D:99:ASP:OD1	1:D:99:ASP:N	2.45	0.47
1:E:94:VAL:HG11	1:F:90:HIS:CE1	2.50	0.47
1:B:59:THR:HB	1:B:60:THR:H	1.28	0.47
1:B:104:ARG:HB3	1:B:104:ARG:CZ	2.43	0.47
1:E:79:TRP:CZ2	1:E:111:LEU:HB3	2.49	0.47
1:F:36:ALA:O	1:F:37:ALA:C	2.57	0.47
1:G:65:VAL:HG22	1:G:66:GLU:H	1.79	0.47
1:A:103:ARG:CG	1:A:122:VAL:CG1	2.74	0.47
1:E:28:VAL:HG13	1:E:49:THR:HG21	1.97	0.47
1:H:10:CYS:SG	1:H:11:PRO:N	2.87	0.47
1:H:93:VAL:HG22	1:H:118:THR:HG21	1.96	0.47
1:B:26:ILE:HG23	1:B:51:GLU:HA	1.93	0.47
1:E:35:LYS:N	1:E:41:TRP:CZ3	2.83	0.47
1:E:92:GLU:OE2	1:F:90:HIS:NE2	2.48	0.47
1:D:59:THR:HG22	1:D:63:GLU:OE1	2.15	0.46
1:D:48:LYS:HB3	1:D:48:LYS:HE3	1.54	0.46
1:H:32:VAL:HG13	1:H:45:ALA:HB3	1.96	0.46
1:B:23:SER:HB2	1:B:24:PRO:HD2	1.97	0.46
1:D:98:ASN:HB3	1:D:102:PRO:HA	1.95	0.46
1:D:118:THR:C	1:D:119:THR:CG2	2.88	0.46
1:E:79:TRP:CD1	1:E:86:PRO:HB3	2.50	0.46
1:E:87:PHE:HB2	1:E:114:TYR:CD2	2.49	0.46
1:G:65:VAL:HG22	1:G:66:GLU:N	2.30	0.46
1:B:26:ILE:HG23	1:B:51:GLU:CA	2.44	0.46
1:A:104:ARG:HH11	1:A:104:ARG:HB3	1.80	0.46
1:B:102:PRO:C	1:B:103:ARG:CG	2.88	0.46
1:B:36:ALA:CB	1:B:42:GLU:OE2	2.63	0.46
1:C:115:SER:HB2	1:D:119:THR:CB	2.46	0.46
1:H:75:THR:HB	1:H:90:HIS:HA	1.97	0.46
1:B:18:ASP:OD2	1:B:78:TYR:OH	2.26	0.46
1:B:75:THR:HG22	1:B:76:LYS:N	2.29	0.46
1:H:28:VAL:CG1	1:H:49:THR:CB	2.94	0.46
1:B:18:ASP:OD2	1:B:21:ARG:CD	2.64	0.45
1:H:28:VAL:HG13	1:H:49:THR:HB	1.98	0.45
1:B:16:VAL:HG22	1:B:25:ALA:HB3	1.98	0.45
1:A:105:TYR:CE1	1:A:122:VAL:CG2	3.00	0.45
1:D:42:GLU:O	1:D:42:GLU:HG2	2.16	0.45
1:D:13:MET:CE	1:D:104:ARG:NH1	2.75	0.45
1:D:21:ARG:HH11	1:D:21:ARG:HD2	1.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:ILE:HG22	1:F:85:SER:N	2.31	0.45
1:H:112:SER:HB3	1:H:113:PRO:HD2	1.99	0.45
1:B:66:GLU:HA	1:B:98:ASN:HB2	1.99	0.45
1:B:105:TYR:N	1:B:105:TYR:CD1	2.85	0.45
1:C:35:LYS:HE3	1:C:35:LYS:CA	2.47	0.45
1:C:68:ILE:HD13	1:D:89:GLU:OE2	2.17	0.45
1:G:21:ARG:O	1:G:21:ARG:HG2	2.16	0.45
1:H:25:ALA:O	1:H:49:THR:HG22	2.11	0.44
1:D:76:LYS:HZ1	1:D:80:LYS:HZ2	1.48	0.44
1:E:12:LEU:HD12	1:E:64:PHE:CE1	2.53	0.44
1:G:56:HIS:CG	1:G:57:GLY:N	2.85	0.44
1:G:84:ILE:CG1	1:G:85:SER:N	2.80	0.44
1:A:123:THR:CG2	1:A:124:ASN:N	2.80	0.44
1:C:115:SER:OG	1:D:119:THR:HG22	2.17	0.44
1:D:38:ASP:O	1:D:40:THR:N	2.49	0.44
1:E:44:PHE:CZ	1:E:59:THR:HG21	2.52	0.44
1:A:42:GLU:HA	1:A:43:PRO:HD3	1.72	0.44
1:D:11:PRO:HB2	1:D:64:PHE:HD2	1.82	0.44
1:C:36:ALA:O	1:C:37:ALA:C	2.60	0.44
1:D:93:VAL:HG13	1:D:118:THR:HG21	1.99	0.44
1:A:97:ALA:O	1:A:98:ASN:CB	2.64	0.44
1:A:124:ASN:O	1:A:125:PRO:C	2.61	0.44
1:F:78:TYR:O	1:F:82:LEU:HD13	2.18	0.44
1:B:27:ASN:C	1:B:48:LYS:HZ1	2.24	0.44
1:H:15:LYS:HE3	1:H:15:LYS:HB2	1.42	0.44
1:A:33:PHE:CD1	1:A:33:PHE:N	2.86	0.44
1:E:32:VAL:O	1:E:33:PHE:HD1	2.01	0.44
1:E:42:GLU:HA	1:E:43:PRO:HD2	1.84	0.44
1:G:23:SER:HB2	1:G:24:PRO:HD2	1.98	0.43
1:G:26:ILE:HG12	1:G:51:GLU:HA	2.01	0.43
1:B:71:VAL:HG23	1:B:95:PHE:HE1	1.82	0.43
1:E:66:GLU:HA	1:E:97:ALA:O	2.19	0.43
1:G:112:SER:O	1:G:113:PRO:C	2.59	0.43
1:B:25:ALA:HB1	1:B:78:TYR:CE1	2.53	0.43
1:D:26:ILE:HD12	1:D:51:GLU:N	2.33	0.43
1:F:61:GLU:CD	1:F:104:ARG:HH22	2.25	0.43
1:C:66:GLU:OE1	1:C:99:ASP:HA	2.18	0.43
1:B:18:ASP:OD1	1:B:20:VAL:HG21	2.01	0.43
1:D:26:ILE:HD11	1:D:51:GLU:CA	2.24	0.43
1:A:115:SER:OG	1:B:119:THR:HG23	2.19	0.43
1:B:63:GLU:OE1	1:B:63:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HD3	1:A:92:GLU:OE2	2.19	0.43
1:F:23:SER:CB	1:F:24:PRO:CD	2.95	0.43
1:A:41:TRP:HH2	1:A:68:ILE:CG2	2.31	0.43
1:G:28:VAL:CG2	1:G:78:TYR:CD1	2.97	0.43
1:D:76:LYS:HZ3	1:D:80:LYS:HZ2	1.51	0.42
1:G:36:ALA:O	1:G:37:ALA:C	2.61	0.42
1:A:99:ASP:OD1	1:A:100:SER:N	2.51	0.42
1:E:112:SER:O	1:E:113:PRO:C	2.60	0.42
1:H:123:THR:HG23	1:H:124:ASN:H	1.84	0.42
1:C:115:SER:HB2	1:D:119:THR:HB	2.01	0.42
1:F:112:SER:O	1:F:113:PRO:C	2.60	0.42
1:B:24:PRO:HB2	1:B:53:GLY:CA	2.50	0.42
1:D:113:PRO:HD2	1:E:20:VAL:HA	2.02	0.42
1:G:23:SER:CB	1:G:24:PRO:CD	2.95	0.42
1:H:75:THR:HG22	1:H:76:LYS:N	2.35	0.42
1:E:113:PRO:HB2	1:E:114:TYR:HD1	1.85	0.42
1:E:92:GLU:OE2	1:F:92:GLU:HG2	2.18	0.42
1:A:26:ILE:N	1:A:26:ILE:CD1	2.82	0.42
1:D:118:THR:O	1:D:119:THR:HG22	2.19	0.42
1:C:87:PHE:HB2	1:C:114:TYR:CD2	2.55	0.42
1:E:87:PHE:HB2	1:E:114:TYR:CE2	2.55	0.42
1:F:56:HIS:N	1:F:56:HIS:HD2	2.13	0.42
1:B:26:ILE:HG22	1:B:50:SER:C	2.43	0.42
1:C:36:ALA:HB2	1:C:42:GLU:HG2	2.02	0.42
1:G:54:GLU:HA	1:G:55:PRO:HD3	1.86	0.42
1:H:19:ALA:HB2	1:H:110:LEU:HD22	2.01	0.42
1:B:92:GLU:OE2	1:B:94:VAL:HG12	2.20	0.42
1:H:44:PHE:HZ	1:H:59:THR:HG1	1.65	0.42
1:A:38:ASP:O	1:A:40:THR:N	2.54	0.41
1:A:87:PHE:HB2	1:A:114:TYR:CD2	2.54	0.41
1:B:18:ASP:CG	1:B:21:ARG:HD2	2.45	0.41
1:F:12:LEU:HD21	1:F:95:PHE:HZ	1.85	0.41
1:G:56:HIS:ND1	1:G:56:HIS:C	2.72	0.41
1:G:122:VAL:HG12	1:G:123:THR:N	2.35	0.41
1:H:71:VAL:O	1:H:92:GLU:HA	2.19	0.41
1:G:90:HIS:CD2	1:G:90:HIS:C	2.98	0.41
1:H:28:VAL:HG13	1:H:49:THR:OG1	2.20	0.41
1:C:95:PHE:CD1	1:C:95:PHE:N	2.88	0.41
1:D:25:ALA:HB1	1:D:28:VAL:CG2	2.50	0.41
1:F:102:PRO:C	1:F:103:ARG:CG	2.92	0.41
1:H:114:TYR:N	1:H:114:TYR:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:PRO:HB2	1:D:64:PHE:CD2	2.55	0.41
1:D:44:PHE:CZ	1:D:59:THR:CG2	2.84	0.41
1:D:103:ARG:HE	1:D:103:ARG:HB3	1.30	0.41
1:B:36:ALA:HB2	1:B:42:GLU:HG3	2.03	0.41
1:B:92:GLU:OE2	1:B:94:VAL:CG1	2.69	0.41
1:B:104:ARG:CZ	1:B:104:ARG:CB	2.99	0.41
1:D:87:PHE:HB2	1:D:114:TYR:CD2	2.56	0.41
1:B:58:LEU:HA	1:B:58:LEU:HD23	1.78	0.41
1:D:38:ASP:O	1:D:38:ASP:CG	2.62	0.41
1:G:79:TRP:CE3	1:G:82:LEU:HD11	2.56	0.41
1:B:57:GLY:O	1:B:59:THR:N	2.53	0.41
1:C:10:CYS:O	1:C:104:ARG:HD2	2.19	0.41
1:C:87:PHE:CE2	1:D:120:ALA:HB2	2.56	0.41
1:D:58:LEU:HD23	1:D:58:LEU:HA	1.75	0.41
1:F:31:HIS:ND1	1:F:46:SER:OG	2.38	0.41
1:G:70:LYS:CE	1:G:92:GLU:OE2	2.69	0.41
1:H:32:VAL:HG22	1:H:44:PHE:HD1	1.85	0.41
1:A:10:CYS:HA	1:A:11:PRO:HD3	1.92	0.40
1:C:12:LEU:HD23	1:C:12:LEU:C	2.46	0.40
1:E:31:HIS:HB3	1:E:33:PHE:HE1	1.83	0.40
1:E:81:ALA:C	1:E:82:LEU:HD13	2.46	0.40
1:A:36:ALA:CB	1:A:42:GLU:CG	2.95	0.40
1:E:64:PHE:CE2	1:E:98:ASN:ND2	2.88	0.40
1:E:120:ALA:HB2	1:F:87:PHE:CE2	2.56	0.40
1:H:50:SER:O	1:H:51:GLU:C	2.63	0.40
1:B:103:ARG:HB3	1:B:123:THR:O	2.21	0.40
1:D:17:LEU:HD12	1:D:24:PRO:HA	2.04	0.40
1:H:79:TRP:HB2	1:H:86:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	114/127 (90%)	107 (94%)	4 (4%)	3 (3%)	4	11
1	B	114/127 (90%)	105 (92%)	5 (4%)	4 (4%)	3	6
1	C	114/127 (90%)	109 (96%)	2 (2%)	3 (3%)	4	11
1	D	114/127 (90%)	108 (95%)	4 (4%)	2 (2%)	6	18
1	E	114/127 (90%)	103 (90%)	8 (7%)	3 (3%)	4	11
1	F	114/127 (90%)	105 (92%)	7 (6%)	2 (2%)	6	18
1	G	114/127 (90%)	106 (93%)	7 (6%)	1 (1%)	14	35
1	H	114/127 (90%)	109 (96%)	3 (3%)	2 (2%)	6	18
All	All	912/1016 (90%)	852 (93%)	40 (4%)	20 (2%)	5	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	37	ALA
1	H	37	ALA
1	D	39	ASP
1	E	56	HIS
1	F	37	ALA
1	F	39	ASP
1	A	38	ASP
1	A	39	ASP
1	A	51	GLU
1	B	38	ASP
1	C	39	ASP
1	D	37	ALA
1	B	37	ALA
1	B	58	LEU
1	C	37	ALA
1	B	51	GLU
1	C	57	GLY
1	E	124	ASN
1	H	39	ASP
1	E	37	ALA

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	97/105 (92%)	76 (78%)	21 (22%)	1	3
1	B	96/105 (91%)	74 (77%)	22 (23%)	1	2
1	C	97/105 (92%)	77 (79%)	20 (21%)	1	3
1	D	96/105 (91%)	70 (73%)	26 (27%)	0	1
1	E	97/105 (92%)	72 (74%)	25 (26%)	0	2
1	F	97/105 (92%)	73 (75%)	24 (25%)	1	2
1	G	96/105 (91%)	71 (74%)	25 (26%)	0	2
1	H	97/105 (92%)	82 (84%)	15 (16%)	2	7
All	All	773/840 (92%)	595 (77%)	178 (23%)	1	2

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	15	LYS
1	A	27	ASN
1	A	35	LYS
1	A	40	THR
1	A	46	SER
1	A	48	LYS
1	A	52	SER
1	A	56	HIS
1	A	59	THR
1	A	60	THR
1	A	61	GLU
1	A	62	GLU
1	A	66	GLU
1	A	76	LYS
1	A	80	LYS
1	A	82	LEU
1	A	85	SER
1	A	103	ARG
1	A	110	LEU
1	A	118	THR
1	B	14	VAL
1	B	16	VAL
1	B	21	ARG

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Mol	Chain	Res	Type
1	B	26	ILE
1	B	27	ASN
1	B	30	VAL
1	B	48	LYS
1	B	51	GLU
1	B	62	GLU
1	B	65	VAL
1	B	73	ILE
1	B	75	THR
1	B	82	LEU
1	B	85	SER
1	B	86	PRO
1	B	92	GLU
1	B	94	VAL
1	B	99	ASP
1	B	104	ARG
1	B	115	SER
1	B	119	THR
1	B	123	THR
1	C	12	LEU
1	C	15	LYS
1	C	16	VAL
1	C	26	ILE
1	C	28	VAL
1	C	35	LYS
1	C	40	THR
1	C	48	LYS
1	C	50	SER
1	C	59	THR
1	C	60	THR
1	C	63	GLU
1	C	66	GLU
1	C	76	LYS
1	C	86	PRO
1	C	103	ARG
1	C	111	LEU
1	C	112	SER
1	C	117	SER
1	C	123	THR
1	D	10	CYS
1	D	15	LYS
1	D	17	LEU

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Mol	Chain	Res	Type
1	D	26	ILE
1	D	40	THR
1	D	42	GLU
1	D	48	LYS
1	D	59	THR
1	D	61	GLU
1	D	63	GLU
1	D	65	VAL
1	D	66	GLU
1	D	70	LYS
1	D	75	THR
1	D	76	LYS
1	D	82	LEU
1	D	85	SER
1	D	98	ASN
1	D	100	SER
1	D	103	ARG
1	D	110	LEU
1	D	112	SER
1	D	118	THR
1	D	122	VAL
1	D	123	THR
1	D	124	ASN
1	E	12	LEU
1	E	21	ARG
1	E	23	SER
1	E	26	ILE
1	E	28	VAL
1	E	38	ASP
1	E	40	THR
1	E	42	GLU
1	E	54	GLU
1	E	58	LEU
1	E	59	THR
1	E	62	GLU
1	E	66	GLU
1	E	82	LEU
1	E	85	SER
1	E	92	GLU
1	E	94	VAL
1	E	100	SER
1	E	107	ILE

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Mol	Chain	Res	Type
1	E	110	LEU
1	E	111	LEU
1	E	112	SER
1	E	116	TYR
1	E	117	SER
1	E	118	THR
1	F	21	ARG
1	F	26	ILE
1	F	32	VAL
1	F	38	ASP
1	F	40	THR
1	F	43	PRO
1	F	48	LYS
1	F	51	GLU
1	F	52	SER
1	F	54	GLU
1	F	56	HIS
1	F	62	GLU
1	F	75	THR
1	F	76	LYS
1	F	80	LYS
1	F	85	SER
1	F	86	PRO
1	F	92	GLU
1	F	93	VAL
1	F	107	ILE
1	F	110	LEU
1	F	115	SER
1	F	117	SER
1	F	123	THR
1	G	12	LEU
1	G	21	ARG
1	G	27	ASN
1	G	28	VAL
1	G	30	VAL
1	G	34	ARG
1	G	35	LYS
1	G	40	THR
1	G	46	SER
1	G	50	SER
1	G	51	GLU
1	G	54	GLU

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Mol	Chain	Res	Type
1	G	58	LEU
1	G	59	THR
1	G	60	THR
1	G	61	GLU
1	G	66	GLU
1	G	71	VAL
1	G	72	GLU
1	G	82	LEU
1	G	84	ILE
1	G	92	GLU
1	G	112	SER
1	G	115	SER
1	G	118	THR
1	H	15	LYS
1	H	21	ARG
1	H	26	ILE
1	H	28	VAL
1	H	32	VAL
1	H	35	LYS
1	H	38	ASP
1	H	50	SER
1	H	63	GLU
1	H	65	VAL
1	H	66	GLU
1	H	72	GLU
1	H	92	GLU
1	H	111	LEU
1	H	122	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	C	56	HIS
1	C	90	HIS
1	D	56	HIS
1	D	88	HIS
1	D	98	ASN
1	E	56	HIS
1	E	124	ASN
1	F	27	ASN
1	F	56	HIS

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Mol	Chain	Res	Type
1	G	27	ASN
1	G	90	HIS
1	H	88	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	123:THR	C	124:ASN	N	1.68

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.