



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:19 AM UTC

PDB ID : 2PCD / pdb_00002pcd
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE FROM PSEUDOMONAS AERUGINOSA AT 2.15 ANGSTROMS RESOLUTION
Authors : Ohlendorf, D.H.; Orville, A.M.; Lipscomb, J.D.
Deposited on : 1994-06-21
Resolution : 2.15 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
Xtrriage (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

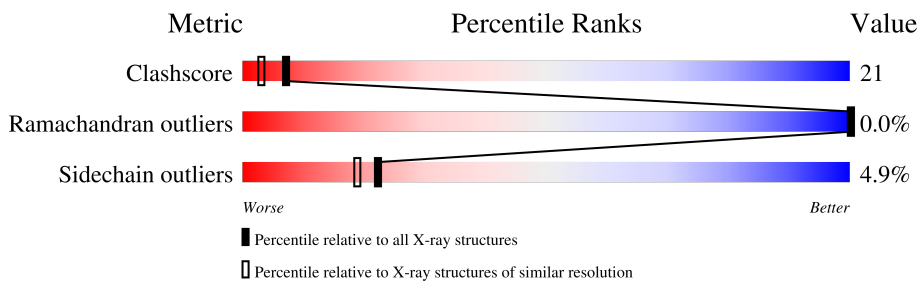
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)


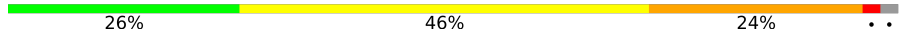

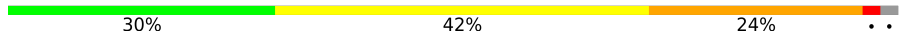
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	200	28% 51% 18% .
1	B	200	34% 46% 20%
1	C	200	26% 53% 20% .
1	D	200	32% 48% 20% .
1	E	200	25% 51% 22% .
1	F	200	27% 44% 26% .
2	M	238	30% 50% 15% . .
2	N	238	34% 48% 15% . .

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Mol	Chain	Length	Quality of chain
2	O	238	
2	P	238	
2	Q	238	
2	R	238	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21906 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 PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1571	993	276	299	3	0	0	0
1	B	200	1571	993	276	299	3	0	0	0
1	C	200	1571	993	276	299	3	0	0	0
1	D	200	1571	993	276	299	3	0	0	0
1	E	200	1571	993	276	299	3	0	0	0
1	F	200	1571	993	276	299	3	0	0	0

- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	233	1840	1171	334	328	7	0	0	0
2	N	233	1840	1171	334	328	7	0	0	0
2	O	233	1840	1171	334	328	7	0	0	0
2	P	233	1840	1171	334	328	7	0	0	0
2	Q	233	1840	1171	334	328	7	0	0	0
2	R	233	1840	1171	334	328	7	0	0	0

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	M	154	Total O 154 154	0	0
4	B	79	Total O 79 79	0	0
4	N	163	Total O 163 163	0	0
4	C	80	Total O 80 80	0	0
4	O	158	Total O 158 158	0	0
4	D	77	Total O 77 77	0	0
4	P	159	Total O 159 159	0	0
4	E	77	Total O 77 77	0	0
4	Q	163	Total O 163 163	0	0
4	F	83	Total O 83 83	0	0
4	R	158	Total O 158 158	0	0

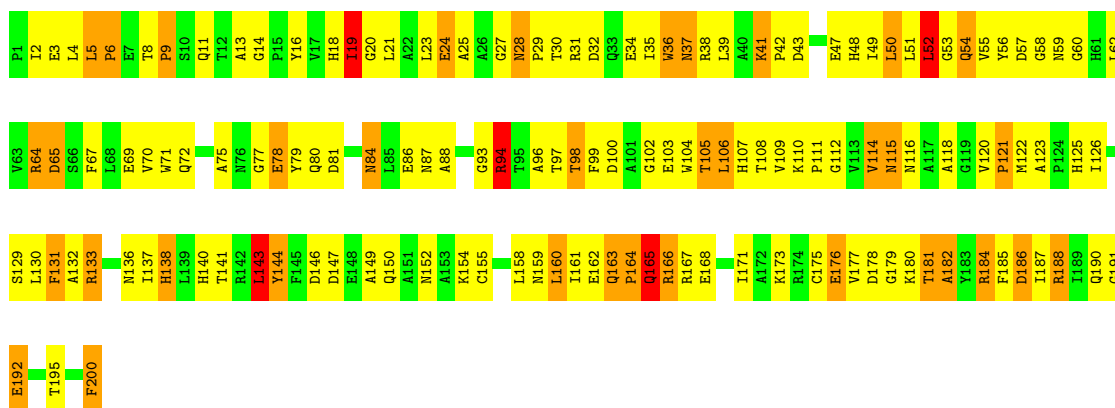
3 Residue-property plots

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.

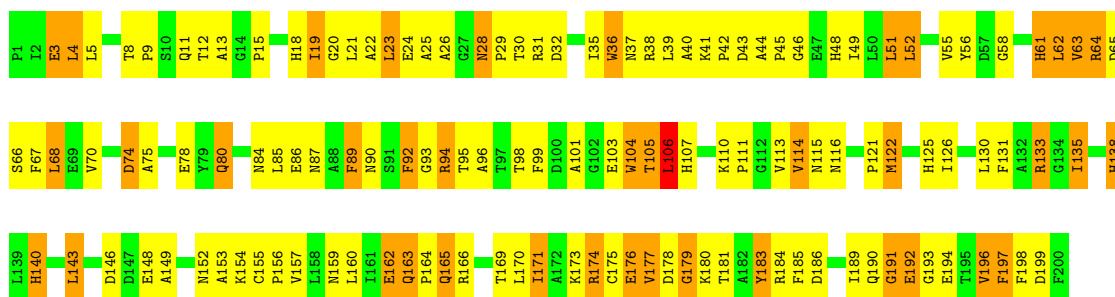
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain A: 



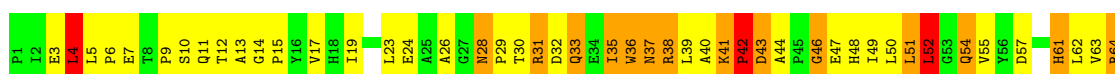
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

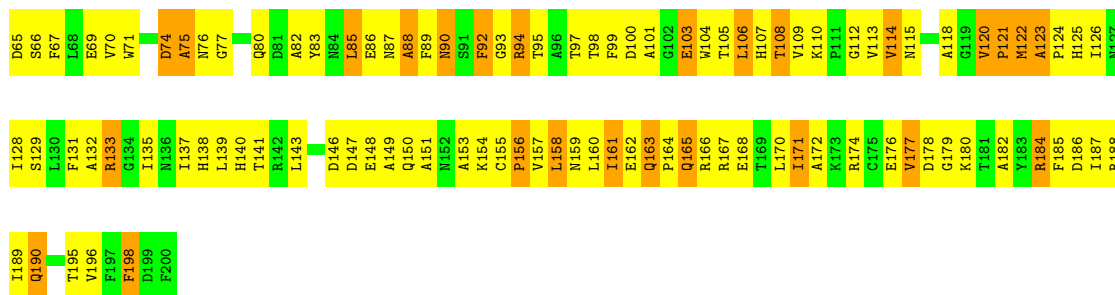
Chain B: 



- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

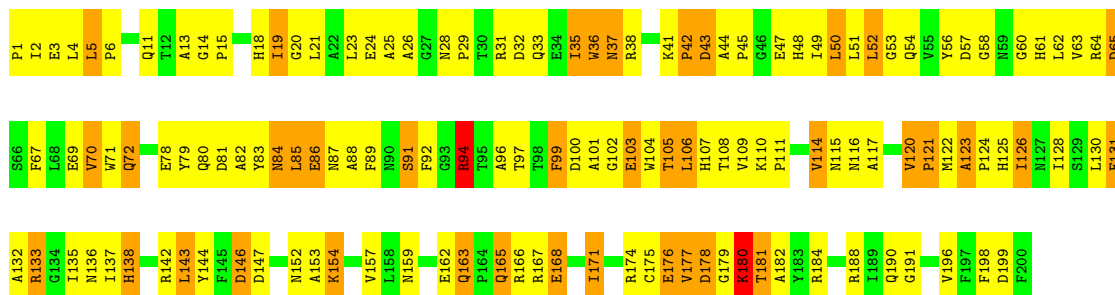
Chain C: 





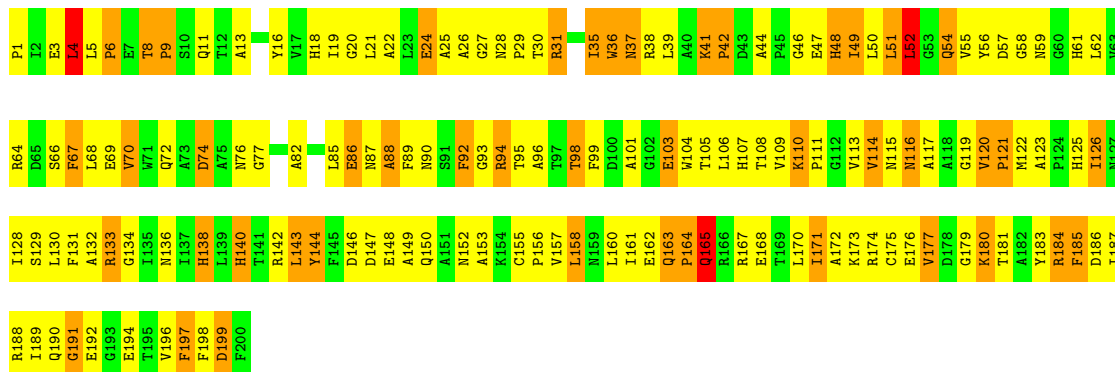
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain D: 32% 48% 20%



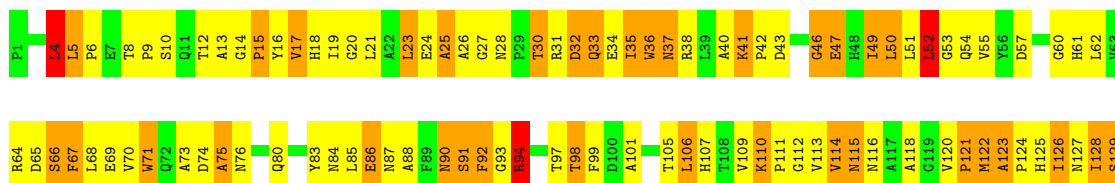
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain E: 25% 51% 22%



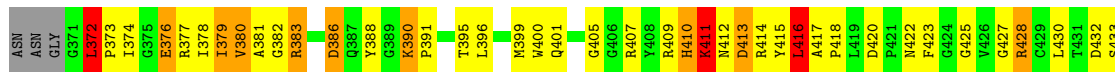
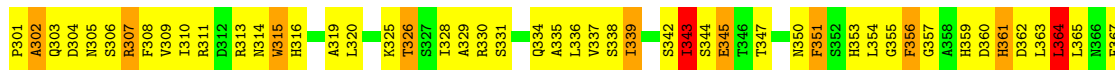
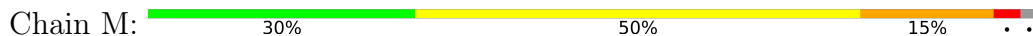
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain F: 27% 44% 26%

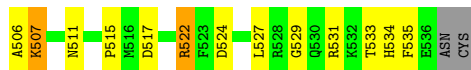
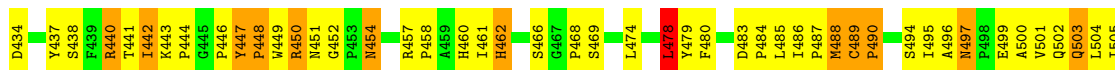
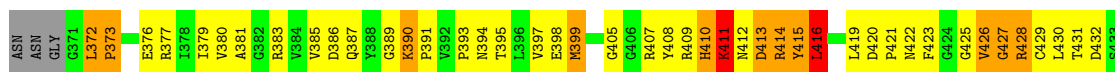




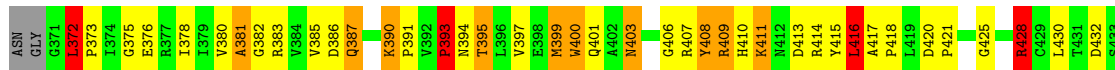
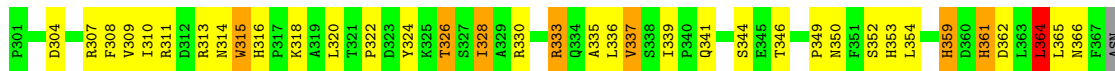
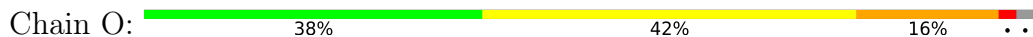
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

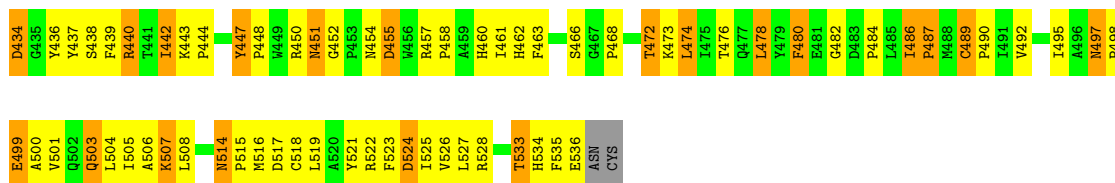


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

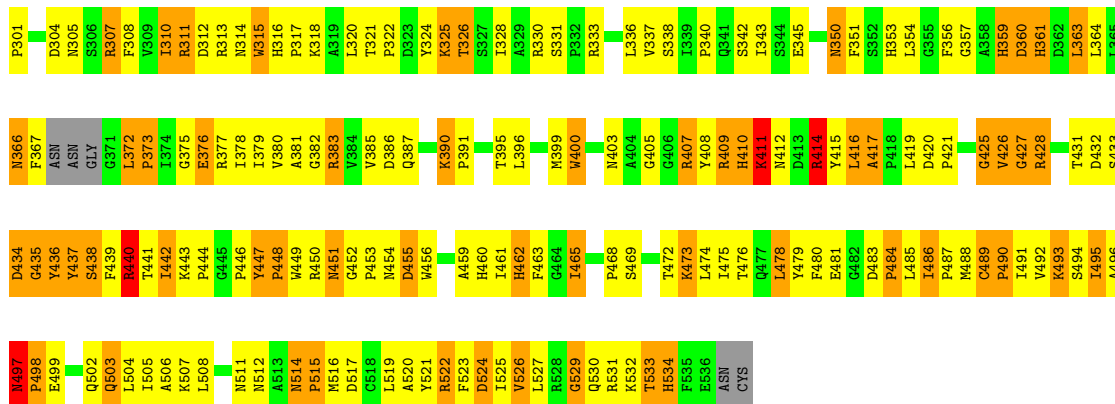
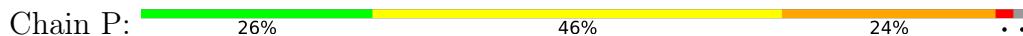


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

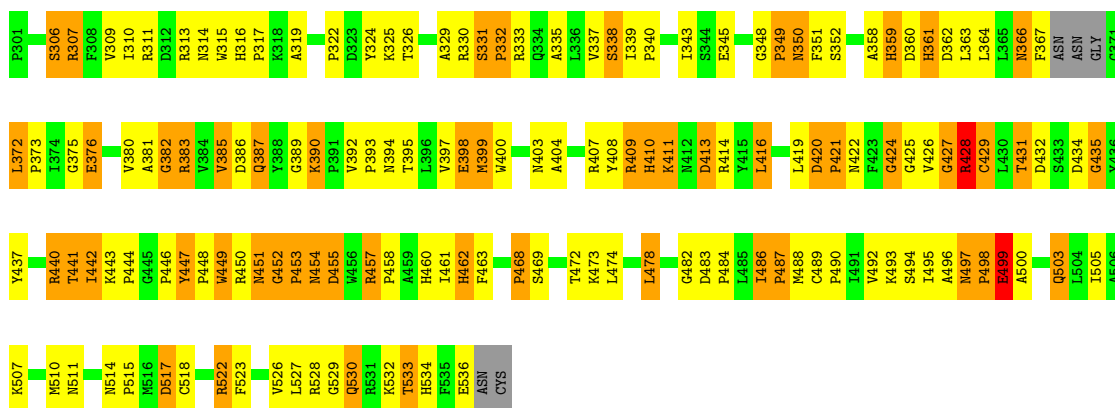




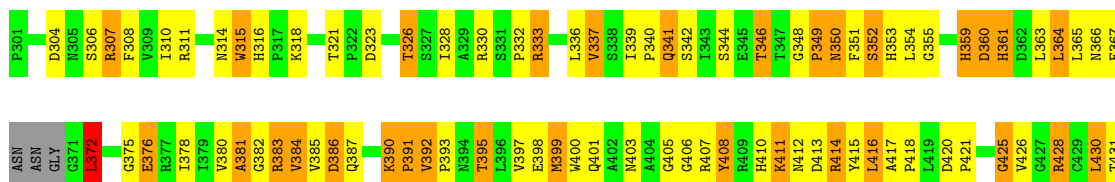
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)



D432	S433	D434	G435	Y436	Y437	S438	F439	R440	T441	I442	Y447	P448	W449	R450	N451	G452	P453	M454	P458	A459	H460	I461	H462	S466	G467	P468	S469	I470	A471	T472	K473	L474	I475	I476	Q477	L478	Y479	F480	E481	G482	D483	P484	I485	I486	P487	M488	C489	P490	I491	V492	K493	S494	I495	A496	M497	P498
E499	A500	V501	Q502	Q503	L504	L505	A506	K507	L508	D509	M510	M511	M514	P515	M516	D517	C518	L519	A520	Y521	R522	F523	D524	I525	V526	L527	R528	G529	Q530	R531	K532	T533	H534	F535	E536	ASN	CYS																			

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.17Å 127.03Å 134.18Å 90.00° 97.64° 90.00°	Depositor
Resolution (Å)	5.00 – 2.15	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	21906	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	2.53	116/1611 (7.2%)	2.20	64/2195 (2.9%)
1	B	2.54	95/1611 (5.9%)	2.11	60/2195 (2.7%)
1	C	2.40	89/1611 (5.5%)	2.23	75/2195 (3.4%)
1	D	2.55	104/1611 (6.5%)	2.16	52/2195 (2.4%)
1	E	2.58	118/1611 (7.3%)	2.17	69/2195 (3.1%)
1	F	2.42	91/1611 (5.6%)	2.20	54/2195 (2.5%)
2	M	2.47	106/1895 (5.6%)	2.21	70/2580 (2.7%)
2	N	2.54	120/1895 (6.3%)	2.15	65/2580 (2.5%)
2	O	2.41	96/1895 (5.1%)	2.12	63/2580 (2.4%)
2	P	2.54	115/1895 (6.1%)	2.23	76/2580 (2.9%)
2	Q	2.50	119/1895 (6.3%)	2.19	86/2580 (3.3%)
2	R	2.45	106/1895 (5.6%)	2.17	77/2580 (3.0%)
All	All	2.49	1275/21036 (6.1%)	2.18	811/28650 (2.8%)

All (1275) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	486	ILE	CA-CB	-10.85	1.48	1.54
2	Q	392	VAL	CA-CB	-10.83	1.44	1.54
2	P	460	HIS	CE1-NE2	-10.62	1.22	1.32
2	N	440	ARG	CD-NE	-10.41	1.31	1.46
1	E	133	ARG	NE-CZ	-10.37	1.21	1.33
1	D	36	TRP	CA-C	-10.31	1.43	1.53
1	A	94	ARG	CD-NE	-10.08	1.32	1.46
2	N	339	ILE	CA-C	-9.93	1.44	1.52
1	B	94	ARG	CD-NE	-9.65	1.32	1.46
1	D	48	HIS	CE1-NE2	-9.56	1.23	1.32
1	A	125	HIS	CE1-NE2	-9.53	1.23	1.32
1	E	133	ARG	CD-NE	-9.45	1.33	1.46
1	D	94	ARG	CD-NE	-9.44	1.33	1.46
1	F	38	ARG	CA-CB	-9.24	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	191	GLY	CA-C	-9.23	1.41	1.52
1	D	175	CYS	CA-CB	-9.23	1.41	1.54
2	P	428	ARG	CD-NE	-9.22	1.33	1.46
2	M	428	ARG	CD-NE	-9.19	1.33	1.46
1	E	119	GLY	C-N	-8.97	1.23	1.33
1	E	82	ALA	CA-CB	-8.89	1.41	1.52
2	P	331	SER	CA-C	-8.75	1.45	1.52
1	F	163	GLN	CA-C	-8.53	1.43	1.52
2	O	316	HIS	CE1-NE2	-8.45	1.24	1.32
1	E	70	VAL	CA-C	-8.40	1.42	1.52
2	N	416	LEU	CA-C	-8.40	1.41	1.52
2	O	521	TYR	C-N	-8.40	1.22	1.33
2	M	350	ASN	C-N	-8.28	1.23	1.33
2	M	379	ILE	C-N	-8.28	1.23	1.33
2	M	468	PRO	N-CA	-8.27	1.36	1.47
2	N	338	SER	C-N	-8.26	1.25	1.33
2	Q	462	HIS	CD2-NE2	-8.23	1.28	1.37
1	C	42	PRO	CA-CB	-8.08	1.42	1.53
1	A	138	HIS	CE1-NE2	-8.06	1.24	1.32
1	E	51	LEU	C-N	-8.05	1.23	1.33
1	A	48	HIS	CE1-NE2	-8.04	1.24	1.32
2	Q	511	ASN	N-CA	-8.02	1.36	1.46
2	R	311	ARG	NE-CZ	-7.98	1.24	1.33
1	E	11	GLN	C-N	-7.92	1.23	1.33
1	E	48	HIS	CA-C	-7.90	1.42	1.52
1	E	61	HIS	CA-C	-7.90	1.42	1.52
1	C	163	GLN	CA-C	-7.89	1.44	1.52
1	D	107	HIS	CG-CD2	-7.88	1.27	1.35
1	A	175	CYS	CA-CB	-7.86	1.43	1.53
2	R	314	ASN	CA-CB	-7.85	1.42	1.54
1	D	109	VAL	N-CA	-7.85	1.37	1.46
2	P	381	ALA	C-N	-7.84	1.25	1.33
1	D	138	HIS	CE1-NE2	-7.82	1.24	1.32
2	N	505	ILE	CA-C	-7.82	1.43	1.52
1	F	57	ASP	C-N	-7.82	1.24	1.33
1	A	80	GLN	CA-C	-7.80	1.43	1.53
1	D	125	HIS	CE1-NE2	-7.79	1.24	1.32
1	E	175	CYS	CA-CB	-7.78	1.44	1.54
2	R	381	ALA	CA-C	-7.78	1.43	1.52
2	Q	427	GLY	C-N	-7.77	1.23	1.33
1	B	31	ARG	C-N	-7.76	1.24	1.33
1	B	9	PRO	N-CA	-7.75	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	ALA	CA-C	-7.73	1.44	1.52
2	N	428	ARG	CD-NE	-7.73	1.35	1.46
2	M	383	ARG	C-N	-7.72	1.23	1.33
2	P	436	TYR	N-CA	-7.72	1.35	1.46
2	Q	324	TYR	CA-CB	-7.72	1.43	1.53
1	C	52	LEU	CA-CB	-7.71	1.40	1.53
2	O	359	HIS	CE1-NE2	-7.70	1.24	1.32
1	D	107	HIS	C-N	-7.70	1.25	1.33
1	B	18	HIS	CG-ND1	-7.69	1.29	1.38
1	E	9	PRO	N-CA	-7.67	1.37	1.47
2	N	352	SER	N-CA	-7.67	1.36	1.46
2	R	359	HIS	CG-CD2	-7.64	1.27	1.35
2	R	515	PRO	CA-C	-7.64	1.43	1.52
2	P	307	ARG	CD-NE	-7.64	1.35	1.46
1	D	18	HIS	C-N	-7.59	1.24	1.34
2	M	325	LYS	CA-C	-7.57	1.42	1.52
2	M	433	SER	C-N	-7.56	1.23	1.33
1	E	58	GLY	CA-C	-7.55	1.42	1.52
1	F	40	ALA	CA-C	-7.55	1.43	1.52
2	O	450	ARG	CA-C	-7.54	1.44	1.53
2	R	433	SER	CA-C	-7.54	1.42	1.52
2	N	517	ASP	CA-C	-7.53	1.42	1.52
1	D	50	LEU	N-CA	-7.52	1.36	1.46
2	N	394	ASN	CA-C	-7.50	1.43	1.53
2	N	333	ARG	CA-CB	-7.50	1.43	1.54
1	A	18	HIS	C-N	-7.50	1.25	1.34
2	P	382	GLY	CA-C	-7.49	1.44	1.52
1	E	197	PHE	C-N	-7.48	1.22	1.33
1	E	183	TYR	C-N	-7.46	1.23	1.33
2	P	475	ILE	C-N	-7.42	1.24	1.33
1	F	140	HIS	CE1-NE2	-7.42	1.25	1.32
2	Q	505	ILE	CA-C	-7.41	1.43	1.52
1	B	114	VAL	C-O	-7.40	1.16	1.24
2	P	359	HIS	C-N	-7.40	1.24	1.34
1	E	156	PRO	CA-CB	-7.40	1.42	1.53
1	A	138	HIS	CG-CD2	-7.39	1.27	1.35
2	Q	440	ARG	CA-CB	-7.38	1.39	1.53
1	A	109	VAL	N-CA	-7.38	1.37	1.46
2	Q	416	LEU	CA-C	-7.37	1.42	1.52
1	B	148	GLU	C-N	-7.35	1.24	1.33
2	N	441	THR	C-O	-7.33	1.18	1.24
1	C	171	ILE	CA-C	-7.33	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	167	ARG	CZ-NH2	-7.33	1.24	1.33
2	P	519	LEU	CA-C	-7.32	1.43	1.53
1	D	65	ASP	C-N	-7.32	1.23	1.33
2	Q	529	GLY	C-O	-7.31	1.17	1.24
1	B	183	TYR	C-N	-7.31	1.23	1.33
1	D	105	THR	C-N	-7.31	1.23	1.33
1	E	186	ASP	CA-CB	-7.29	1.42	1.53
2	P	379	ILE	C-N	-7.28	1.24	1.33
2	O	439	PHE	C-N	-7.28	1.23	1.33
1	A	108	THR	CA-C	-7.28	1.43	1.52
2	O	450	ARG	C-N	-7.28	1.24	1.34
2	P	520	ALA	N-CA	-7.27	1.37	1.46
1	B	179	GLY	CA-C	-7.26	1.44	1.51
2	M	331	SER	CA-C	-7.25	1.47	1.52
1	E	22	ALA	CA-CB	-7.24	1.46	1.53
1	F	118	ALA	C-N	-7.24	1.23	1.33
1	F	182	ALA	CA-C	-7.24	1.43	1.52
2	Q	426	VAL	CA-C	-7.24	1.43	1.52
2	M	469	SER	C-O	-7.23	1.15	1.23
2	R	518	CYS	CA-C	-7.22	1.43	1.52
1	D	108	THR	CA-C	-7.21	1.44	1.53
1	B	140	HIS	CD2-NE2	-7.21	1.29	1.37
1	F	150	GLN	C-O	-7.20	1.15	1.24
2	P	465	ILE	CA-C	-7.19	1.43	1.52
1	B	103	GLU	CA-C	-7.19	1.44	1.52
2	R	352	SER	CA-C	-7.18	1.43	1.52
2	N	335	ALA	C-N	-7.17	1.24	1.33
2	M	529	GLY	CA-C	-7.16	1.45	1.52
2	O	428	ARG	C-N	-7.16	1.24	1.33
1	E	62	LEU	C-N	-7.13	1.24	1.33
2	P	433	SER	C-N	-7.13	1.23	1.33
1	A	53	GLY	CA-C	-7.12	1.43	1.51
2	N	413	ASP	CA-CB	-7.11	1.43	1.53
1	F	101	ALA	CA-C	-7.11	1.44	1.52
2	R	418	PRO	N-CA	-7.11	1.39	1.46
1	C	151	ALA	C-O	-7.10	1.15	1.24
2	M	522	ARG	C-N	-7.09	1.24	1.33
2	P	383	ARG	C-N	-7.08	1.24	1.33
2	N	410	HIS	CD2-NE2	-7.08	1.30	1.37
1	F	167	ARG	CZ-NH2	-7.08	1.24	1.33
1	A	20	GLY	CA-C	-7.08	1.42	1.51
2	P	476	THR	CA-C	-7.08	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	409	ARG	CA-CB	-7.07	1.43	1.52
1	E	173	LYS	CA-CB	-7.07	1.43	1.53
1	A	99	PHE	CA-CB	-7.07	1.41	1.53
2	O	314	ASN	CA-CB	-7.07	1.43	1.54
2	N	366	ASN	CA-C	-7.06	1.43	1.52
1	F	171	ILE	CA-C	-7.06	1.43	1.52
1	D	29	PRO	N-CD	-7.06	1.37	1.47
1	E	105	THR	CA-C	-7.05	1.44	1.52
2	Q	517	ASP	CA-C	-7.05	1.43	1.52
2	Q	394	ASN	CA-C	-7.05	1.44	1.53
1	E	103	GLU	CA-C	-7.05	1.44	1.52
1	B	18	HIS	CD2-NE2	-7.04	1.30	1.37
2	N	361	HIS	CD2-NE2	-7.04	1.30	1.37
1	C	187	ILE	N-CA	-7.04	1.37	1.46
2	R	473	LYS	CA-CB	-7.04	1.42	1.53
1	E	61	HIS	CD2-NE2	-7.03	1.30	1.37
2	O	518	CYS	CA-C	-7.03	1.43	1.52
1	A	191	GLY	CA-C	-7.02	1.42	1.51
2	Q	316	HIS	ND1-CE1	-7.02	1.25	1.32
2	N	534	HIS	CG-ND1	-7.01	1.30	1.38
1	C	185	PHE	N-CA	-7.00	1.37	1.47
2	O	353	HIS	N-CA	-7.00	1.37	1.46
2	M	475	ILE	C-N	-6.99	1.25	1.33
1	E	49	ILE	C-N	-6.99	1.24	1.33
1	E	170	LEU	N-CA	-6.99	1.36	1.46
1	A	188	ARG	C-N	-6.97	1.25	1.33
2	P	462	HIS	CG-CD2	-6.97	1.28	1.35
2	N	340	PRO	N-CA	-6.97	1.38	1.47
2	Q	317	PRO	N-CA	-6.96	1.38	1.47
2	R	323	ASP	CA-C	-6.95	1.43	1.52
2	P	353	HIS	CG-ND1	-6.95	1.30	1.38
2	Q	358	ALA	C-N	-6.94	1.23	1.33
1	B	22	ALA	CA-CB	-6.94	1.46	1.53
2	M	326	THR	C-O	-6.94	1.15	1.24
1	F	61	HIS	C-N	-6.93	1.24	1.33
1	A	114	VAL	CA-CB	-6.92	1.44	1.55
1	D	54	GLN	C-N	-6.92	1.24	1.33
2	P	320	LEU	C-N	-6.92	1.25	1.33
1	B	185	PHE	C-N	-6.92	1.23	1.33
2	Q	352	SER	N-CA	-6.91	1.37	1.46
2	R	393	PRO	C-N	-6.90	1.24	1.33
1	D	138	HIS	CG-CD2	-6.90	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	ALA	CA-C	-6.90	1.44	1.52
2	P	441	THR	CA-C	-6.90	1.44	1.53
2	N	325	LYS	N-CA	-6.90	1.38	1.46
1	C	92	PHE	CA-C	-6.90	1.44	1.52
1	A	54	GLN	C-N	-6.90	1.24	1.33
1	E	37	ASN	C-N	-6.89	1.23	1.33
2	P	468	PRO	N-CA	-6.89	1.38	1.47
2	M	460	HIS	CE1-NE2	-6.89	1.25	1.32
2	Q	483	ASP	CA-C	-6.87	1.44	1.52
2	O	437	TYR	N-CA	-6.87	1.37	1.45
1	E	123	ALA	CA-CB	-6.85	1.42	1.53
1	F	155	CYS	CA-C	-6.85	1.44	1.52
1	D	48	HIS	CG-ND1	-6.84	1.30	1.38
2	P	386	ASP	CA-CB	-6.84	1.43	1.53
2	R	315	TRP	NE1-CE2	-6.84	1.29	1.37
2	M	492	VAL	CA-CB	-6.84	1.46	1.54
2	M	381	ALA	C-N	-6.83	1.26	1.33
2	O	526	VAL	CA-CB	-6.83	1.45	1.54
2	N	438	SER	CA-CB	-6.83	1.42	1.53
2	R	477	GLN	C-O	-6.83	1.15	1.23
2	R	386	ASP	CA-C	-6.81	1.43	1.53
1	B	48	HIS	CD2-NE2	-6.81	1.30	1.37
2	O	523	PHE	C-N	-6.81	1.23	1.33
1	F	52	LEU	CA-CB	-6.80	1.41	1.53
1	F	31	ARG	NE-CZ	-6.80	1.25	1.33
2	M	515	PRO	N-CA	-6.80	1.39	1.47
1	B	48	HIS	CA-C	-6.80	1.43	1.52
2	N	345	GLU	CA-C	-6.79	1.43	1.52
1	F	123	ALA	C-N	-6.78	1.25	1.33
2	M	320	LEU	CA-C	-6.78	1.44	1.52
1	C	168	GLU	N-CA	-6.78	1.38	1.46
2	Q	322	PRO	N-CA	-6.77	1.38	1.47
2	M	320	LEU	C-N	-6.76	1.25	1.33
2	N	490	PRO	CA-CB	-6.75	1.44	1.53
1	C	120	VAL	CA-C	-6.75	1.47	1.52
1	D	128	ILE	N-CA	-6.75	1.38	1.46
2	N	314	ASN	C-N	-6.75	1.24	1.33
1	D	69	GLU	CA-C	-6.75	1.44	1.52
2	M	441	THR	CA-C	-6.75	1.45	1.53
1	B	15	PRO	C-N	-6.75	1.25	1.33
1	C	15	PRO	N-CA	-6.74	1.38	1.47
1	E	190	GLN	CA-C	-6.74	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	450	ARG	C-N	-6.74	1.24	1.33
2	R	528	ARG	C-N	-6.74	1.26	1.33
2	R	439	PHE	C-N	-6.74	1.24	1.33
2	O	330	ARG	CA-C	-6.73	1.44	1.53
1	A	144	TYR	C-N	-6.73	1.24	1.33
1	F	34	GLU	C-N	-6.72	1.24	1.33
1	F	147	ASP	CA-CB	-6.72	1.43	1.53
2	O	460	HIS	C-O	-6.72	1.15	1.23
1	D	49	ILE	CA-C	-6.71	1.44	1.52
2	O	515	PRO	CA-C	-6.71	1.44	1.52
1	E	5	LEU	C-N	-6.71	1.25	1.33
2	Q	399	MET	C-N	-6.70	1.25	1.33
2	Q	329	ALA	CA-C	-6.70	1.43	1.52
1	E	175	CYS	C-O	-6.69	1.19	1.24
1	A	87	ASN	C-N	-6.69	1.24	1.34
2	M	454	ASN	CA-CB	-6.69	1.44	1.53
1	B	116	ASN	CA-CB	-6.68	1.43	1.53
2	M	309	VAL	CA-CB	-6.68	1.47	1.54
1	B	8	THR	CA-C	-6.68	1.46	1.53
1	F	43	ASP	CA-C	-6.68	1.43	1.52
2	M	307	ARG	CD-NE	-6.67	1.36	1.46
2	N	426	VAL	CA-C	-6.67	1.44	1.52
1	F	177	VAL	CA-C	-6.66	1.45	1.52
2	N	306	SER	CB-OG	-6.65	1.28	1.42
1	C	32	ASP	C-N	-6.65	1.24	1.33
1	B	42	PRO	C-N	-6.65	1.24	1.33
1	F	173	LYS	CA-C	-6.65	1.44	1.52
2	O	430	LEU	C-N	-6.65	1.24	1.33
1	A	185	PHE	CA-C	-6.65	1.45	1.53
1	A	23	LEU	C-N	-6.64	1.25	1.33
1	D	2	ILE	C-N	-6.64	1.24	1.33
1	D	120	VAL	C-O	-6.63	1.16	1.24
1	F	148	GLU	CA-C	-6.63	1.42	1.52
1	B	156	PRO	CA-CB	-6.63	1.44	1.53
2	N	343	ILE	C-N	-6.63	1.24	1.34
1	B	157	VAL	CA-C	-6.62	1.43	1.52
1	D	63	VAL	C-N	-6.61	1.25	1.33
2	P	493	LYS	CA-C	-6.61	1.43	1.52
2	Q	411	LYS	N-CA	-6.60	1.38	1.46
2	O	524	ASP	CA-CB	-6.60	1.43	1.53
1	D	79	TYR	N-CA	-6.60	1.38	1.46
2	R	384	VAL	C-N	-6.60	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	359	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	29	PRO	N-CD	-6.59	1.38	1.47
2	O	535	PHE	C-N	-6.59	1.24	1.33
1	E	18	HIS	CE1-NE2	-6.59	1.25	1.32
1	E	61	HIS	ND1-CE1	-6.59	1.25	1.32
1	E	69	GLU	N-CA	-6.59	1.38	1.46
2	Q	317	PRO	C-N	-6.59	1.24	1.33
1	E	85	LEU	C-N	-6.58	1.24	1.33
1	B	61	HIS	ND1-CE1	-6.57	1.25	1.32
2	Q	307	ARG	C-N	-6.57	1.24	1.33
1	D	99	PHE	CA-CB	-6.57	1.42	1.53
2	M	359	HIS	C-N	-6.57	1.25	1.33
2	N	451	ASN	CA-CB	-6.57	1.44	1.53
1	E	157	VAL	CA-C	-6.57	1.43	1.52
1	F	121	PRO	N-CA	-6.57	1.39	1.47
1	B	122	MET	C-N	-6.55	1.23	1.33
1	B	11	GLN	C-N	-6.55	1.25	1.33
1	B	74	ASP	CA-CB	-6.55	1.43	1.53
2	M	534	HIS	CG-CD2	-6.55	1.28	1.35
2	P	507	LYS	C-N	-6.54	1.24	1.33
2	M	465	ILE	CA-C	-6.54	1.44	1.52
1	D	70	VAL	N-CA	-6.54	1.38	1.46
2	P	479	TYR	C-N	-6.53	1.24	1.33
1	B	169	THR	CA-C	-6.53	1.43	1.52
2	R	521	TYR	C-N	-6.53	1.24	1.33
1	C	106	LEU	CA-CB	-6.52	1.42	1.53
2	R	450	ARG	CA-C	-6.52	1.45	1.53
2	R	342	SER	C-N	-6.51	1.26	1.34
1	A	48	HIS	CG-ND1	-6.51	1.31	1.38
1	C	94	ARG	CD-NE	-6.51	1.37	1.46
1	D	32	ASP	N-CA	-6.51	1.38	1.46
2	N	332	PRO	N-CD	-6.50	1.38	1.47
2	N	397	VAL	C-N	-6.50	1.24	1.33
2	Q	413	ASP	CA-CB	-6.50	1.44	1.53
2	Q	429	CYS	C-N	-6.49	1.24	1.33
2	M	307	ARG	CA-C	-6.49	1.44	1.52
1	C	118	ALA	C-N	-6.49	1.24	1.33
1	B	35	ILE	CA-C	-6.49	1.45	1.52
2	N	444	PRO	N-CA	-6.49	1.39	1.46
2	R	393	PRO	N-CA	-6.48	1.39	1.46
1	B	75	ALA	C-N	-6.48	1.25	1.33
2	R	466	SER	CA-C	-6.48	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	399	MET	C-O	-6.47	1.16	1.23
1	D	87	ASN	N-CA	-6.47	1.38	1.46
2	R	346	THR	CA-C	-6.47	1.43	1.52
1	B	171	ILE	C-O	-6.47	1.17	1.24
1	D	57	ASP	CA-CB	-6.46	1.43	1.53
2	P	420	ASP	C-O	-6.46	1.17	1.24
2	R	359	HIS	CE1-NE2	-6.46	1.26	1.32
2	P	322	PRO	CA-C	-6.46	1.41	1.52
1	B	197	PHE	C-N	-6.45	1.24	1.33
1	F	184	ARG	CA-C	-6.45	1.44	1.52
2	Q	332	PRO	CA-CB	-6.45	1.45	1.53
2	Q	349	PRO	N-CA	-6.44	1.39	1.47
2	M	452	GLY	C-N	-6.43	1.26	1.33
2	Q	343	ILE	C-N	-6.43	1.25	1.34
2	Q	340	PRO	N-CA	-6.43	1.39	1.47
2	Q	421	PRO	CA-C	-6.43	1.43	1.52
2	Q	449	TRP	CA-C	-6.42	1.44	1.52
2	M	339	ILE	N-CA	-6.42	1.38	1.46
1	B	186	ASP	CA-CB	-6.42	1.43	1.53
1	E	142	ARG	C-O	-6.42	1.15	1.23
1	B	190	GLN	CA-C	-6.41	1.44	1.52
2	O	504	LEU	N-CA	-6.41	1.37	1.46
1	B	48	HIS	ND1-CE1	-6.41	1.26	1.32
2	R	506	ALA	CA-CB	-6.40	1.43	1.53
1	C	6	PRO	CA-C	-6.40	1.44	1.52
1	F	17	VAL	CA-C	-6.40	1.44	1.52
2	R	490	PRO	C-N	-6.40	1.25	1.33
1	B	143	LEU	C-O	-6.40	1.16	1.24
2	N	380	VAL	CA-CB	-6.40	1.46	1.54
2	O	487	PRO	C-N	-6.40	1.24	1.33
1	A	107	HIS	CE1-NE2	-6.39	1.26	1.32
1	C	28	ASN	CA-CB	-6.39	1.44	1.53
2	O	382	GLY	C-N	-6.39	1.24	1.33
2	P	410	HIS	ND1-CE1	-6.39	1.26	1.32
2	M	481	GLU	CA-C	-6.39	1.44	1.52
2	N	409	ARG	CA-CB	-6.39	1.44	1.52
2	N	450	ARG	N-CA	-6.38	1.38	1.46
2	Q	393	PRO	CA-CB	-6.38	1.45	1.53
2	R	308	PHE	CA-C	-6.38	1.44	1.52
2	M	344	SER	CA-C	-6.38	1.44	1.52
2	O	506	ALA	CA-CB	-6.38	1.43	1.53
1	E	31	ARG	C-N	-6.38	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	339	ILE	CA-C	-6.38	1.46	1.52
1	A	49	ILE	CA-C	-6.38	1.45	1.52
1	A	161	ILE	C-O	-6.38	1.17	1.23
2	N	427	GLY	C-N	-6.38	1.25	1.33
1	E	140	HIS	CD2-NE2	-6.38	1.30	1.37
2	P	489	CYS	CA-C	-6.37	1.45	1.52
2	Q	366	ASN	CA-C	-6.37	1.43	1.52
2	M	361	HIS	CA-C	-6.37	1.43	1.52
2	Q	451	ASN	CA-CB	-6.37	1.44	1.53
1	D	100	ASP	CA-C	-6.37	1.44	1.52
1	E	104	TRP	N-CA	-6.36	1.38	1.45
2	M	342	SER	C-N	-6.36	1.26	1.34
2	P	525	ILE	CA-C	-6.36	1.44	1.52
2	P	529	GLY	CA-C	-6.35	1.45	1.52
2	P	310	ILE	CA-C	-6.35	1.44	1.52
1	B	89	PHE	C-O	-6.35	1.16	1.23
2	O	439	PHE	N-CA	-6.35	1.37	1.45
2	N	440	ARG	CA-CB	-6.35	1.41	1.53
1	D	92	PHE	N-CA	-6.35	1.38	1.46
1	B	49	ILE	N-CA	-6.34	1.39	1.46
1	C	23	LEU	CA-C	-6.34	1.44	1.52
2	R	375	GLY	C-N	-6.34	1.24	1.33
2	O	381	ALA	CA-C	-6.34	1.44	1.52
2	R	328	ILE	C-N	-6.34	1.24	1.33
1	C	90	ASN	C-N	-6.33	1.25	1.33
1	C	167	ARG	CA-C	-6.33	1.44	1.52
2	P	417	ALA	C-O	-6.33	1.16	1.24
1	F	10	SER	C-N	-6.33	1.25	1.33
2	R	316	HIS	CG-ND1	-6.33	1.31	1.38
2	R	507	LYS	CA-CB	-6.33	1.43	1.53
1	A	173	LYS	C-N	-6.33	1.25	1.33
2	M	524	ASP	C-N	-6.33	1.24	1.33
2	N	327	SER	C-N	-6.33	1.25	1.33
2	O	399	MET	CA-C	-6.33	1.45	1.52
2	N	407	ARG	C-O	-6.33	1.16	1.24
2	Q	511	ASN	C-N	-6.33	1.24	1.33
2	P	314	ASN	C-O	-6.32	1.16	1.24
2	P	410	HIS	CG-CD2	-6.32	1.28	1.35
1	B	104	TRP	C-N	-6.32	1.25	1.33
1	B	184	ARG	CA-CB	-6.32	1.44	1.53
2	P	396	LEU	C-N	-6.32	1.25	1.33
2	P	312	ASP	C-O	-6.31	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	428	ARG	NE-CZ	-6.31	1.26	1.33
2	Q	469	SER	CA-C	-6.31	1.44	1.52
2	Q	498	PRO	CA-C	-6.31	1.42	1.52
2	R	382	GLY	C-N	-6.31	1.25	1.33
2	N	502	GLN	N-CA	-6.31	1.38	1.46
1	C	54	GLN	CA-C	-6.31	1.45	1.52
1	B	24	GLU	CA-C	-6.30	1.44	1.52
2	P	449	TRP	NE1-CE2	-6.30	1.30	1.37
2	Q	431	THR	CA-C	-6.30	1.44	1.53
1	C	137	ILE	CA-CB	-6.30	1.46	1.54
1	C	35	ILE	CA-CB	-6.29	1.46	1.54
2	O	341	GLN	C-N	-6.29	1.24	1.33
2	O	365	LEU	N-CA	-6.29	1.37	1.45
2	O	466	SER	CA-C	-6.29	1.45	1.52
1	D	188	ARG	C-N	-6.29	1.25	1.33
2	P	331	SER	C-N	-6.29	1.25	1.33
2	P	311	ARG	N-CA	-6.28	1.38	1.46
1	A	65	ASP	C-N	-6.28	1.24	1.33
1	B	37	ASN	C-N	-6.28	1.23	1.33
2	P	534	HIS	C-N	-6.28	1.24	1.33
1	D	196	VAL	CA-CB	-6.27	1.46	1.54
1	A	57	ASP	CA-CB	-6.27	1.44	1.53
2	P	366	ASN	C-N	-6.27	1.24	1.33
2	Q	461	ILE	CA-CB	-6.26	1.46	1.54
1	F	76	ASN	CA-C	-6.26	1.42	1.52
2	P	440	ARG	CD-NE	-6.25	1.37	1.46
1	B	189	ILE	C-N	-6.25	1.25	1.33
1	C	113	VAL	N-CA	-6.25	1.39	1.46
1	D	78	GLU	CA-C	-6.24	1.45	1.52
1	F	137	ILE	CA-CB	-6.24	1.46	1.54
2	R	341	GLN	C-N	-6.23	1.24	1.33
2	M	308	PHE	C-N	-6.23	1.26	1.33
2	M	382	GLY	CA-C	-6.23	1.45	1.52
1	B	95	THR	C-N	-6.23	1.25	1.33
2	N	332	PRO	C-N	-6.23	1.25	1.33
1	D	101	ALA	N-CA	-6.23	1.39	1.46
2	Q	444	PRO	N-CA	-6.23	1.39	1.47
2	O	528	ARG	C-N	-6.22	1.27	1.33
2	Q	310	ILE	N-CA	-6.22	1.38	1.46
2	R	514	ASN	CA-CB	-6.21	1.43	1.53
2	M	479	TYR	C-N	-6.21	1.25	1.33
2	N	489	CYS	C-N	-6.21	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	18	HIS	CG-ND1	-6.21	1.31	1.38
2	O	437	TYR	C-N	-6.21	1.25	1.33
2	Q	462	HIS	CA-C	-6.21	1.44	1.52
1	B	46	GLY	C-N	-6.20	1.24	1.33
2	P	409	ARG	CD-NE	-6.20	1.37	1.46
2	R	535	PHE	C-N	-6.20	1.24	1.33
2	R	332	PRO	CA-C	-6.20	1.44	1.52
1	A	13	ALA	CA-CB	-6.20	1.43	1.53
2	O	507	LYS	CA-CB	-6.19	1.43	1.53
1	E	126	ILE	C-O	-6.19	1.17	1.24
1	E	68	LEU	CA-C	-6.19	1.45	1.52
2	R	430	LEU	C-N	-6.19	1.25	1.33
2	P	440	ARG	C-N	-6.18	1.27	1.33
2	Q	440	ARG	CD-NE	-6.18	1.37	1.46
2	R	330	ARG	NE-CZ	-6.18	1.26	1.33
1	A	186	ASP	C-N	-6.18	1.25	1.33
2	M	425	GLY	CA-C	-6.18	1.43	1.51
1	E	164	PRO	C-N	-6.18	1.25	1.34
1	C	198	PHE	C-N	-6.17	1.25	1.33
2	O	375	GLY	C-N	-6.17	1.24	1.33
1	C	9	PRO	CA-C	-6.17	1.44	1.52
1	D	159	ASN	C-N	-6.17	1.25	1.33
1	E	185	PHE	C-N	-6.16	1.24	1.33
2	P	340	PRO	N-CD	-6.16	1.39	1.47
2	R	391	PRO	N-CA	-6.15	1.39	1.47
1	B	106	LEU	C-N	-6.15	1.24	1.33
2	N	316	HIS	ND1-CE1	-6.15	1.26	1.32
2	N	529	GLY	C-O	-6.15	1.17	1.23
2	P	524	ASP	C-N	-6.15	1.25	1.33
1	D	157	VAL	N-CA	-6.15	1.39	1.46
2	R	365	LEU	N-CA	-6.15	1.36	1.45
1	F	129	SER	C-O	-6.15	1.17	1.24
2	M	328	ILE	CA-C	-6.14	1.45	1.52
1	C	139	LEU	C-O	-6.14	1.16	1.24
2	O	516	MET	N-CA	-6.14	1.37	1.46
1	D	20	GLY	CA-C	-6.14	1.43	1.51
1	A	32	ASP	N-CA	-6.13	1.39	1.46
1	E	181	THR	C-N	-6.13	1.25	1.33
2	P	498	PRO	N-CA	-6.13	1.39	1.47
1	C	36	TRP	CA-CB	-6.13	1.45	1.54
2	P	484	PRO	CA-CB	-6.13	1.44	1.53
2	N	419	LEU	C-N	-6.12	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	531	ARG	NE-CZ	-6.12	1.26	1.33
1	F	106	LEU	CA-CB	-6.12	1.43	1.53
2	O	359	HIS	CG-CD2	-6.12	1.29	1.35
1	D	152	ASN	C-N	-6.12	1.25	1.34
2	P	435	GLY	CA-C	-6.12	1.43	1.51
2	O	519	LEU	C-N	-6.11	1.25	1.33
2	P	376	GLU	CA-C	-6.11	1.44	1.52
2	R	436	TYR	CA-C	-6.11	1.45	1.52
2	N	353	HIS	CG-CD2	-6.11	1.29	1.35
1	E	16	TYR	CA-C	-6.11	1.43	1.52
1	D	29	PRO	CA-CB	-6.11	1.45	1.53
1	C	87	ASN	CA-CB	-6.11	1.43	1.53
1	E	155	CYS	C-N	-6.11	1.26	1.34
2	Q	490	PRO	CA-CB	-6.11	1.45	1.53
1	B	193	GLY	CA-C	-6.10	1.42	1.51
1	A	121	PRO	N-CD	-6.10	1.39	1.47
1	C	123	ALA	C-N	-6.10	1.26	1.33
2	O	460	HIS	CE1-NE2	-6.10	1.26	1.32
2	P	427	GLY	CA-C	-6.10	1.45	1.51
1	A	29	PRO	C-N	-6.09	1.25	1.33
2	Q	454	ASN	CA-C	-6.09	1.45	1.53
1	C	10	SER	C-N	-6.09	1.25	1.33
2	O	344	SER	C-N	-6.09	1.25	1.33
1	E	59	ASN	N-CA	-6.09	1.38	1.46
2	O	395	THR	CA-C	-6.09	1.45	1.52
2	P	503	GLN	CA-CB	-6.09	1.42	1.53
1	E	48	HIS	ND1-CE1	-6.09	1.26	1.32
2	Q	434	ASP	CA-C	-6.09	1.44	1.52
1	B	90	ASN	C-O	-6.09	1.16	1.24
2	R	364	LEU	CA-C	-6.09	1.44	1.52
1	F	128	ILE	C-O	-6.08	1.17	1.24
2	P	350	ASN	C-N	-6.08	1.25	1.33
2	R	390	LYS	CA-C	-6.08	1.45	1.53
2	P	425	GLY	CA-C	-6.08	1.43	1.51
1	A	166	ARG	C-N	-6.08	1.25	1.34
1	D	47	GLU	CA-C	-6.08	1.45	1.52
1	D	123	ALA	CA-C	-6.08	1.46	1.53
1	F	120	VAL	CA-C	-6.08	1.47	1.52
2	P	363	LEU	CA-C	-6.07	1.44	1.52
2	P	492	VAL	CA-CB	-6.07	1.46	1.54
2	Q	452	GLY	C-N	-6.07	1.26	1.34
1	B	30	THR	CA-C	-6.07	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	152	ASN	CA-C	-6.06	1.45	1.52
2	M	311	ARG	N-CA	-6.05	1.38	1.46
2	M	378	ILE	CA-C	-6.05	1.45	1.52
1	B	149	ALA	CA-CB	-6.05	1.44	1.53
2	Q	404	ALA	CA-C	-6.05	1.44	1.52
2	M	410	HIS	ND1-CE1	-6.05	1.26	1.32
2	R	531	ARG	CA-CB	-6.05	1.43	1.53
2	O	436	TYR	CA-C	-6.04	1.44	1.52
2	P	377	ARG	C-N	-6.04	1.25	1.33
1	A	154	LYS	CA-C	-6.04	1.44	1.52
2	M	440	ARG	CD-NE	-6.04	1.37	1.46
1	B	105	THR	CA-C	-6.04	1.45	1.52
2	R	440	ARG	NE-CZ	-6.04	1.26	1.33
2	P	421	PRO	N-CD	-6.03	1.39	1.47
2	N	529	GLY	C-N	-6.03	1.25	1.33
2	O	352	SER	CA-C	-6.03	1.44	1.52
1	E	13	ALA	C-N	-6.03	1.24	1.33
2	Q	359	HIS	CD2-NE2	-6.03	1.31	1.37
2	Q	468	PRO	C-N	-6.03	1.25	1.33
2	R	470	ILE	CA-C	-6.03	1.45	1.52
1	C	31	ARG	NE-CZ	-6.03	1.26	1.33
1	F	64	ARG	N-CA	-6.02	1.39	1.46
1	F	135	ILE	C-N	-6.02	1.25	1.34
2	M	319	ALA	CA-CB	-6.02	1.43	1.53
2	R	527	LEU	CA-CB	-6.02	1.44	1.53
1	C	154	LYS	N-CA	-6.01	1.38	1.46
1	D	111	PRO	CA-C	-6.01	1.45	1.52
2	O	428	ARG	CD-NE	-6.01	1.37	1.46
1	F	67	PHE	C-O	-5.99	1.17	1.23
2	R	326	THR	C-N	-5.99	1.25	1.33
1	B	176	GLU	C-N	-5.99	1.26	1.33
1	F	113	VAL	N-CA	-5.99	1.39	1.46
1	D	45	PRO	N-CA	-5.98	1.39	1.47
2	M	507	LYS	C-N	-5.98	1.25	1.33
2	N	306	SER	CA-C	-5.98	1.45	1.52
1	D	35	ILE	C-N	-5.98	1.28	1.33
1	E	192	GLU	CA-C	-5.97	1.44	1.52
1	C	189	ILE	C-O	-5.97	1.17	1.24
1	E	153	ALA	C-N	-5.97	1.25	1.33
1	A	141	THR	C-N	-5.96	1.25	1.33
1	B	101	ALA	C-N	-5.96	1.23	1.33
1	B	155	CYS	C-N	-5.96	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	49	ILE	N-CA	-5.96	1.39	1.46
1	F	12	THR	CA-C	-5.96	1.45	1.53
1	C	80	GLN	CA-CB	-5.95	1.45	1.53
1	E	64	ARG	CA-C	-5.95	1.45	1.53
2	P	340	PRO	CA-CB	-5.95	1.45	1.53
1	E	156	PRO	N-CD	-5.95	1.39	1.47
2	P	307	ARG	CA-C	-5.95	1.45	1.52
1	E	187	ILE	CA-C	-5.95	1.45	1.52
1	C	150	GLN	C-O	-5.95	1.17	1.24
2	Q	457	ARG	NE-CZ	-5.94	1.26	1.33
2	R	486	ILE	CA-C	-5.94	1.46	1.52
1	B	62	LEU	C-N	-5.94	1.25	1.33
2	O	361	HIS	CE1-NE2	-5.94	1.26	1.32
1	D	72	GLN	C-N	-5.94	1.25	1.33
2	Q	447	TYR	C-N	-5.94	1.25	1.33
1	F	73	ALA	CA-C	-5.93	1.45	1.53
2	Q	529	GLY	C-N	-5.93	1.25	1.33
2	M	442	ILE	N-CA	-5.93	1.39	1.46
2	O	354	LEU	C-N	-5.93	1.24	1.33
1	B	41	LYS	CA-CB	-5.93	1.43	1.53
1	B	70	VAL	CA-C	-5.92	1.45	1.52
1	E	55	VAL	CA-C	-5.92	1.45	1.52
1	E	99	PHE	C-N	-5.92	1.25	1.33
1	A	131	PHE	N-CA	-5.92	1.38	1.45
2	M	415	TYR	C-N	-5.92	1.24	1.33
1	A	184	ARG	N-CA	-5.92	1.38	1.46
2	P	444	PRO	CA-CB	-5.92	1.45	1.53
2	M	531	ARG	CA-C	-5.92	1.45	1.52
1	C	164	PRO	N-CA	-5.92	1.39	1.47
2	N	462	HIS	CD2-NE2	-5.92	1.31	1.37
2	M	386	ASP	CA-CB	-5.91	1.44	1.53
1	B	56	TYR	N-CA	-5.91	1.38	1.46
2	M	532	LYS	C-N	-5.91	1.25	1.33
2	N	468	PRO	C-N	-5.91	1.25	1.33
1	A	52	LEU	C-N	-5.91	1.25	1.33
2	Q	427	GLY	N-CA	-5.90	1.39	1.45
1	B	61	HIS	CA-C	-5.90	1.45	1.52
1	F	143	LEU	CA-CB	-5.90	1.44	1.53
1	E	61	HIS	CB-CG	-5.90	1.41	1.50
1	E	122	MET	C-N	-5.90	1.24	1.33
1	E	68	LEU	CB-CG	-5.90	1.41	1.53
1	F	164	PRO	N-CA	-5.90	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	310	ILE	N-CA	-5.89	1.38	1.46
2	M	497	ASN	C-N	-5.89	1.26	1.33
1	D	71	TRP	CA-C	-5.89	1.45	1.52
2	P	311	ARG	C-N	-5.89	1.23	1.33
1	F	47	GLU	C-N	-5.89	1.25	1.33
1	B	173	LYS	CA-CB	-5.89	1.45	1.53
2	M	449	TRP	NE1-CE2	-5.88	1.30	1.37
1	E	148	GLU	C-N	-5.88	1.26	1.33
2	M	374	ILE	N-CA	-5.88	1.39	1.46
2	O	380	VAL	C-N	-5.88	1.25	1.33
1	E	42	PRO	C-N	-5.88	1.25	1.33
2	R	519	LEU	N-CA	-5.88	1.38	1.45
1	D	117	ALA	CA-C	-5.88	1.44	1.52
2	R	437	TYR	C-N	-5.88	1.26	1.33
2	N	451	ASN	C-O	-5.88	1.17	1.24
2	M	446	PRO	N-CD	-5.87	1.39	1.47
2	N	422	ASN	N-CA	-5.87	1.39	1.46
1	E	95	THR	C-N	-5.87	1.26	1.33
1	F	42	PRO	CA-CB	-5.87	1.45	1.53
2	N	359	HIS	CG-ND1	-5.87	1.31	1.38
1	C	121	PRO	N-CA	-5.87	1.40	1.47
2	Q	350	ASN	CA-CB	-5.87	1.44	1.53
2	M	472	THR	C-O	-5.86	1.16	1.24
2	P	448	PRO	CA-C	-5.86	1.45	1.52
1	B	64	ARG	CA-C	-5.86	1.44	1.52
1	A	192	GLU	C-N	-5.86	1.26	1.33
2	R	340	PRO	CA-C	-5.85	1.45	1.52
2	M	345	GLU	N-CA	-5.85	1.38	1.46
1	B	5	LEU	CB-CG	-5.85	1.41	1.53
2	M	444	PRO	CA-CB	-5.84	1.45	1.53
2	M	462	HIS	CG-CD2	-5.84	1.29	1.35
1	D	107	HIS	CE1-NE2	-5.84	1.26	1.32
1	F	54	GLN	CA-C	-5.84	1.45	1.52
1	F	167	ARG	CA-C	-5.84	1.44	1.52
2	R	420	ASP	C-N	-5.84	1.26	1.33
1	B	49	ILE	C-N	-5.83	1.25	1.33
1	E	46	GLY	C-N	-5.83	1.25	1.33
1	A	3	GLU	CA-CB	-5.83	1.42	1.53
2	N	340	PRO	C-N	-5.83	1.25	1.33
2	P	481	GLU	CA-C	-5.83	1.45	1.52
2	O	346	THR	C-N	-5.83	1.25	1.33
1	B	153	ALA	C-N	-5.82	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	458	PRO	C-N	-5.82	1.25	1.33
2	Q	338	SER	N-CA	-5.82	1.38	1.46
2	Q	324	TYR	C-N	-5.82	1.26	1.33
1	B	107	HIS	CG-ND1	-5.82	1.31	1.38
1	A	130	LEU	CA-C	-5.82	1.45	1.52
1	D	166	ARG	C-N	-5.82	1.26	1.34
2	P	521	TYR	CA-C	-5.81	1.45	1.52
2	N	422	ASN	C-N	-5.81	1.25	1.33
1	F	94	ARG	CZ-NH1	-5.80	1.24	1.32
2	R	481	GLU	N-CA	-5.80	1.38	1.46
2	N	466	SER	C-N	-5.80	1.24	1.33
2	R	349	PRO	N-CA	-5.80	1.40	1.47
2	N	535	PHE	CA-C	-5.79	1.45	1.52
2	Q	515	PRO	C-N	-5.79	1.25	1.33
2	R	353	HIS	N-CA	-5.79	1.39	1.46
1	D	130	LEU	CA-C	-5.79	1.45	1.52
1	B	181	THR	C-O	-5.78	1.17	1.23
2	P	360	ASP	CA-CB	-5.78	1.43	1.53
1	E	66	SER	CA-C	-5.78	1.44	1.53
2	N	474	LEU	C-O	-5.78	1.16	1.23
1	E	171	ILE	C-O	-5.78	1.17	1.24
2	Q	375	GLY	CA-C	-5.77	1.46	1.52
2	R	376	GLU	CA-CB	-5.77	1.45	1.53
2	O	328	ILE	C-N	-5.77	1.24	1.33
1	D	184	ARG	CZ-NH2	-5.77	1.25	1.33
2	Q	373	PRO	N-CA	-5.77	1.40	1.47
1	D	168	GLU	CA-C	-5.76	1.44	1.52
2	M	495	ILE	C-O	-5.76	1.17	1.23
2	M	377	ARG	C-N	-5.76	1.26	1.33
2	N	448	PRO	N-CA	-5.76	1.40	1.46
1	F	174	ARG	N-CA	-5.76	1.39	1.46
2	M	530	GLN	N-CA	-5.75	1.39	1.46
1	B	111	PRO	C-O	-5.75	1.17	1.23
1	E	136	ASN	CA-C	-5.75	1.45	1.52
1	E	189	ILE	C-N	-5.75	1.26	1.33
2	R	505	ILE	C-N	-5.75	1.25	1.33
2	R	503	GLN	CA-C	-5.75	1.44	1.52
1	E	184	ARG	CA-CB	-5.75	1.45	1.53
2	Q	496	ALA	C-N	-5.74	1.24	1.33
2	R	304	ASP	N-CA	-5.74	1.39	1.46
1	E	46	GLY	CA-C	-5.73	1.46	1.52
1	C	133	ARG	C-N	-5.73	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	324	TYR	C-O	-5.72	1.15	1.23
2	R	499	GLU	CA-C	-5.72	1.45	1.52
1	D	42	PRO	CA-C	-5.72	1.44	1.52
1	D	177	VAL	CA-CB	-5.72	1.46	1.54
1	A	60	GLY	C-N	-5.72	1.25	1.33
1	D	82	ALA	C-N	-5.72	1.25	1.33
1	A	163	GLN	C-N	-5.72	1.25	1.33
1	C	160	LEU	C-N	-5.72	1.25	1.33
2	Q	316	HIS	CB-CG	-5.72	1.42	1.50
1	A	25	ALA	CA-C	-5.72	1.45	1.52
1	A	152	ASN	C-N	-5.72	1.26	1.34
1	F	36	TRP	NE1-CE2	-5.71	1.31	1.37
1	A	192	GLU	N-CA	-5.71	1.38	1.46
1	E	117	ALA	N-CA	-5.71	1.39	1.46
1	A	5	LEU	C-N	-5.71	1.26	1.33
1	A	24	GLU	CA-CB	-5.71	1.44	1.53
2	N	393	PRO	CA-CB	-5.71	1.46	1.54
2	P	325	LYS	CA-C	-5.71	1.45	1.52
1	E	8	THR	CA-C	-5.71	1.47	1.53
1	E	86	GLU	CA-CB	-5.71	1.44	1.53
2	Q	332	PRO	N-CD	-5.71	1.39	1.47
1	C	195	THR	CA-C	-5.71	1.45	1.52
2	N	515	PRO	CA-CB	-5.70	1.45	1.53
1	D	60	GLY	C-N	-5.70	1.25	1.33
2	O	514	ASN	CA-CB	-5.70	1.44	1.53
1	F	168	GLU	C-O	-5.70	1.17	1.24
1	D	6	PRO	N-CD	-5.70	1.39	1.47
1	F	168	GLU	N-CA	-5.70	1.39	1.46
1	C	159	ASN	N-CA	-5.69	1.38	1.46
2	O	480	PHE	CA-C	-5.69	1.45	1.52
2	P	446	PRO	N-CD	-5.69	1.39	1.47
1	F	46	GLY	C-O	-5.69	1.17	1.23
2	P	508	LEU	CA-CB	-5.68	1.44	1.53
1	F	36	TRP	CA-CB	-5.68	1.45	1.53
1	A	81	ASP	N-CA	-5.68	1.38	1.46
2	N	324	TYR	C-N	-5.68	1.27	1.33
2	P	345	GLU	N-CA	-5.68	1.38	1.46
1	A	36	TRP	CA-C	-5.67	1.45	1.52
2	Q	306	SER	CA-C	-5.67	1.46	1.52
2	M	311	ARG	C-N	-5.67	1.24	1.33
2	M	472	THR	N-CA	-5.67	1.38	1.46
1	D	28	ASN	C-O	-5.67	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	394	ASN	N-CA	-5.67	1.38	1.46
2	M	523	PHE	CA-C	-5.66	1.46	1.52
2	P	505	ILE	N-CA	-5.66	1.39	1.46
2	N	429	CYS	N-CA	-5.66	1.39	1.46
1	A	96	ALA	C-O	-5.66	1.17	1.23
2	P	361	HIS	CA-C	-5.66	1.44	1.52
1	B	125	HIS	ND1-CE1	-5.65	1.26	1.32
2	R	432	ASP	CA-C	-5.65	1.45	1.53
2	M	338	SER	CA-C	-5.65	1.45	1.52
2	Q	333	ARG	CA-CB	-5.65	1.44	1.53
1	F	52	LEU	CA-C	-5.65	1.45	1.52
1	D	103	GLU	N-CA	-5.65	1.39	1.46
2	P	373	PRO	CA-CB	-5.65	1.46	1.53
2	Q	375	GLY	C-O	-5.65	1.18	1.23
2	Q	515	PRO	CA-CB	-5.65	1.46	1.53
2	Q	351	PHE	C-N	-5.65	1.26	1.33
2	R	344	SER	C-N	-5.65	1.25	1.33
2	M	326	THR	N-CA	-5.64	1.38	1.46
1	A	112	GLY	C-N	-5.64	1.26	1.33
1	C	135	ILE	C-N	-5.64	1.26	1.33
2	M	313	ARG	CA-C	-5.63	1.44	1.52
2	M	390	LYS	CA-CB	-5.63	1.43	1.53
2	P	415	TYR	C-N	-5.63	1.26	1.33
2	Q	528	ARG	CA-C	-5.63	1.45	1.52
1	C	147	ASP	CA-CB	-5.63	1.44	1.53
2	R	380	VAL	C-N	-5.63	1.26	1.33
1	B	70	VAL	C-O	-5.63	1.18	1.24
2	N	461	ILE	CA-CB	-5.63	1.47	1.54
2	N	534	HIS	CD2-NE2	-5.63	1.31	1.37
2	N	411	LYS	N-CA	-5.62	1.39	1.46
2	N	524	ASP	CA-C	-5.62	1.45	1.52
1	A	100	ASP	CA-C	-5.62	1.45	1.52
1	E	101	ALA	C-N	-5.62	1.25	1.33
2	Q	450	ARG	N-CA	-5.62	1.39	1.46
1	A	2	ILE	C-N	-5.62	1.25	1.33
1	A	50	LEU	C-N	-5.62	1.25	1.33
2	P	530	GLN	C-N	-5.62	1.25	1.33
2	M	437	TYR	CA-C	-5.62	1.45	1.52
1	B	99	PHE	C-N	-5.62	1.26	1.33
2	O	455	ASP	C-O	-5.61	1.17	1.24
2	O	320	LEU	C-O	-5.61	1.17	1.24
2	O	407	ARG	CD-NE	-5.61	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	501	VAL	CA-C	-5.61	1.45	1.52
2	O	501	VAL	C-N	-5.61	1.26	1.34
1	D	48	HIS	N-CA	-5.61	1.39	1.46
1	D	162	GLU	C-O	-5.61	1.17	1.24
1	E	94	ARG	CD-NE	-5.61	1.38	1.46
1	E	96	ALA	CA-C	-5.61	1.46	1.52
1	E	185	PHE	CA-CB	-5.60	1.44	1.52
1	B	181	THR	C-N	-5.60	1.26	1.33
1	F	137	ILE	C-N	-5.60	1.26	1.33
2	O	406	GLY	C-N	-5.60	1.25	1.33
2	Q	376	GLU	C-N	-5.60	1.25	1.33
2	Q	447	TYR	CA-C	-5.60	1.45	1.52
2	O	403	ASN	CA-CB	-5.59	1.45	1.53
2	O	461	ILE	C-O	-5.59	1.18	1.24
1	B	51	LEU	C-N	-5.59	1.26	1.33
1	A	50	LEU	N-CA	-5.59	1.39	1.46
2	P	504	LEU	CA-C	-5.59	1.44	1.52
2	Q	518	CYS	C-N	-5.58	1.25	1.33
1	C	157	VAL	C-N	-5.58	1.26	1.33
2	R	495	ILE	CA-C	-5.58	1.46	1.52
2	P	486	ILE	N-CA	-5.58	1.39	1.46
2	P	531	ARG	CA-C	-5.58	1.45	1.52
1	E	5	LEU	CB-CG	-5.58	1.42	1.53
1	F	114	VAL	CA-C	-5.58	1.46	1.52
2	P	515	PRO	C-N	-5.57	1.25	1.33
2	P	495	ILE	C-O	-5.57	1.17	1.23
1	F	181	THR	N-CA	-5.57	1.39	1.46
2	P	315	TRP	C-O	-5.57	1.17	1.23
2	R	337	VAL	C-O	-5.56	1.18	1.24
2	N	309	VAL	C-N	-5.56	1.26	1.33
2	N	531	ARG	CD-NE	-5.56	1.38	1.46
2	Q	482	GLY	CA-C	-5.55	1.43	1.51
1	A	16	TYR	C-N	-5.55	1.26	1.34
2	O	476	THR	C-O	-5.55	1.18	1.24
2	N	448	PRO	C-N	-5.54	1.26	1.33
1	E	74	ASP	CA-CB	-5.54	1.45	1.53
2	Q	419	LEU	C-N	-5.54	1.24	1.33
1	F	156	PRO	N-CA	-5.54	1.40	1.47
1	D	91	SER	C-N	-5.54	1.25	1.33
2	Q	510	MET	CA-C	-5.54	1.45	1.52
2	R	494	SER	CA-CB	-5.54	1.43	1.53
1	E	1	PRO	N-CD	-5.54	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	VAL	C-O	-5.54	1.18	1.24
2	Q	314	ASN	C-N	-5.54	1.26	1.33
2	N	337	VAL	CA-C	-5.53	1.45	1.52
2	O	315	TRP	CA-C	-5.53	1.45	1.53
1	D	37	ASN	N-CA	-5.53	1.39	1.46
2	M	442	ILE	C-O	-5.53	1.18	1.24
2	R	408	TYR	CA-C	-5.53	1.45	1.52
1	D	87	ASN	C-N	-5.53	1.25	1.33
1	C	36	TRP	NE1-CE2	-5.53	1.31	1.37
1	D	11	GLN	CA-CB	-5.53	1.44	1.53
1	A	6	PRO	CA-CB	-5.52	1.46	1.53
1	B	85	LEU	C-N	-5.52	1.25	1.33
2	O	457	ARG	C-N	-5.52	1.26	1.33
1	A	6	PRO	N-CD	-5.52	1.40	1.47
1	F	15	PRO	CA-C	-5.52	1.42	1.52
1	D	89	PHE	CA-CB	-5.52	1.42	1.53
1	D	138	HIS	CA-C	-5.52	1.45	1.52
1	A	5	LEU	C-O	-5.52	1.16	1.24
2	M	310	ILE	CA-C	-5.52	1.45	1.52
1	B	18	HIS	CA-C	-5.52	1.45	1.52
1	F	25	ALA	CA-CB	-5.52	1.44	1.53
1	A	133	ARG	CZ-NH1	-5.51	1.25	1.32
1	C	61	HIS	C-N	-5.51	1.26	1.33
2	M	345	GLU	C-O	-5.51	1.17	1.24
1	B	199	ASP	C-N	-5.51	1.25	1.33
2	O	387	GLN	N-CA	-5.51	1.39	1.46
1	E	19	ILE	CA-C	-5.51	1.44	1.52
1	E	67	PHE	N-CA	-5.51	1.39	1.46
2	Q	473	LYS	CA-C	-5.51	1.46	1.52
2	M	376	GLU	CA-C	-5.50	1.45	1.52
1	C	57	ASP	C-N	-5.50	1.26	1.33
2	N	307	ARG	N-CA	-5.50	1.39	1.46
2	P	472	THR	N-CA	-5.50	1.38	1.46
2	Q	337	VAL	CA-C	-5.50	1.45	1.52
1	C	184	ARG	CA-C	-5.50	1.46	1.52
1	B	61	HIS	CB-CG	-5.49	1.42	1.50
2	N	496	ALA	CA-C	-5.49	1.45	1.52
1	C	62	LEU	CA-CB	-5.49	1.44	1.53
2	P	532	LYS	C-N	-5.49	1.26	1.33
1	C	97	THR	C-N	-5.49	1.26	1.33
1	D	5	LEU	C-O	-5.49	1.16	1.24
1	B	174	ARG	C-O	-5.49	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	319	ALA	CA-C	-5.49	1.46	1.52
2	R	487	PRO	N-CA	-5.49	1.40	1.47
2	O	438	SER	CA-C	-5.48	1.45	1.52
1	D	107	HIS	ND1-CE1	-5.48	1.27	1.32
2	N	410	HIS	CG-ND1	-5.48	1.32	1.38
2	P	439	PHE	CA-C	-5.48	1.46	1.52
1	E	24	GLU	CA-C	-5.48	1.45	1.52
1	E	94	ARG	C-N	-5.48	1.26	1.33
2	Q	487	PRO	CA-C	-5.47	1.42	1.52
2	Q	534	HIS	CG-ND1	-5.47	1.32	1.38
2	P	502	GLN	C-N	-5.47	1.26	1.33
2	Q	443	LYS	CA-C	-5.47	1.46	1.52
1	A	9	PRO	N-CD	-5.47	1.40	1.47
2	N	363	LEU	C-N	-5.47	1.26	1.33
1	C	108	THR	C-O	-5.47	1.19	1.24
1	A	195	THR	C-N	-5.47	1.27	1.33
2	N	431	THR	CA-C	-5.47	1.45	1.52
1	D	23	LEU	C-N	-5.46	1.27	1.33
1	E	146	ASP	CA-CB	-5.46	1.44	1.53
2	O	390	LYS	CA-C	-5.46	1.46	1.53
1	D	38	ARG	C-N	-5.46	1.26	1.34
1	A	168	GLU	C-N	-5.46	1.26	1.33
2	Q	488	MET	N-CA	-5.46	1.38	1.46
1	A	70	VAL	N-CA	-5.46	1.39	1.46
2	Q	432	ASP	N-CA	-5.46	1.39	1.45
2	O	447	TYR	C-O	-5.45	1.18	1.24
2	Q	532	LYS	CA-CB	-5.45	1.44	1.53
1	B	48	HIS	CB-CG	-5.45	1.42	1.50
1	C	82	ALA	CA-C	-5.45	1.45	1.52
1	C	188	ARG	CZ-NH2	-5.45	1.26	1.33
1	E	172	ALA	CA-CB	-5.45	1.45	1.53
2	R	525	ILE	C-N	-5.45	1.26	1.33
1	A	98	THR	C-N	-5.45	1.26	1.34
1	C	140	HIS	CE1-NE2	-5.45	1.27	1.32
2	O	385	VAL	C-N	-5.45	1.25	1.33
1	C	88	ALA	C-N	-5.45	1.26	1.33
2	P	526	VAL	C-N	-5.45	1.25	1.33
2	R	406	GLY	C-N	-5.44	1.26	1.33
1	A	37	ASN	CA-C	-5.44	1.43	1.52
2	Q	410	HIS	CG-ND1	-5.44	1.32	1.38
2	M	329	ALA	N-CA	-5.44	1.38	1.46
2	N	447	TYR	CA-C	-5.44	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	156	PRO	N-CA	-5.44	1.40	1.47
2	O	451	ASN	CA-C	5.44	1.55	1.52
1	D	167	ARG	CA-CB	-5.44	1.44	1.53
2	P	428	ARG	N-CA	-5.44	1.39	1.46
1	E	48	HIS	CB-CG	-5.44	1.42	1.50
1	F	115	ASN	C-N	-5.44	1.26	1.33
1	F	179	GLY	C-N	-5.44	1.25	1.33
1	E	107	HIS	CD2-NE2	-5.44	1.31	1.37
2	N	305	ASN	CA-CB	-5.44	1.45	1.54
1	E	18	HIS	CD2-NE2	-5.43	1.31	1.37
2	N	356	PHE	C-O	-5.43	1.17	1.23
1	D	115	ASN	C-O	-5.43	1.17	1.23
1	B	61	HIS	CD2-NE2	-5.43	1.31	1.37
2	N	432	ASP	N-CA	-5.43	1.39	1.46
2	Q	330	ARG	CZ-NH1	-5.43	1.25	1.32
1	B	68	LEU	CA-C	-5.42	1.46	1.52
2	N	480	PHE	C-N	-5.42	1.26	1.33
2	O	391	PRO	N-CA	-5.42	1.40	1.47
1	A	105	THR	C-N	-5.42	1.25	1.33
2	M	484	PRO	CA-CB	-5.42	1.45	1.53
1	D	18	HIS	ND1-CE1	-5.42	1.27	1.32
1	D	174	ARG	CA-CB	-5.42	1.44	1.53
2	O	364	LEU	CA-C	-5.41	1.45	1.52
1	D	125	HIS	C-N	-5.41	1.26	1.33
2	Q	422	ASN	C-N	-5.41	1.26	1.33
2	N	434	ASP	CA-C	-5.41	1.44	1.52
2	R	533	THR	C-N	-5.41	1.26	1.33
2	Q	440	ARG	N-CA	5.41	1.52	1.46
1	B	19	ILE	CA-C	-5.41	1.44	1.52
1	D	56	TYR	C-N	-5.41	1.25	1.33
1	A	69	GLU	CA-C	-5.40	1.46	1.52
1	A	146	ASP	CA-C	-5.40	1.45	1.52
2	Q	503	GLN	C-N	-5.40	1.25	1.33
1	A	164	PRO	CA-CB	-5.40	1.46	1.53
2	Q	435	GLY	N-CA	-5.40	1.36	1.45
2	Q	453	PRO	CA-CB	-5.40	1.45	1.53
1	F	187	ILE	C-N	-5.40	1.24	1.33
2	N	449	TRP	CA-C	-5.40	1.45	1.52
1	C	186	ASP	CA-C	-5.40	1.45	1.52
2	Q	463	PHE	C-O	-5.40	1.17	1.23
2	R	532	LYS	N-CA	5.39	1.52	1.45
2	P	345	GLU	CD-OE1	-5.39	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	THR	C-O	-5.39	1.17	1.23
2	M	420	ASP	C-O	-5.39	1.18	1.24
1	C	43	ASP	CA-C	-5.39	1.44	1.52
1	E	104	TRP	C-N	-5.39	1.26	1.33
1	C	93	GLY	C-O	-5.39	1.18	1.23
1	E	116	ASN	CA-CB	-5.39	1.45	1.53
2	Q	407	ARG	C-O	-5.39	1.17	1.24
1	F	186	ASP	CA-C	-5.39	1.46	1.52
2	M	412	ASN	CA-C	-5.38	1.45	1.52
2	M	512	ASN	C-N	-5.38	1.26	1.33
1	D	25	ALA	CA-C	-5.38	1.45	1.52
1	E	111	PRO	C-N	-5.38	1.25	1.33
2	R	417	ALA	CA-CB	-5.38	1.42	1.53
1	A	147	ASP	N-CA	-5.38	1.39	1.46
2	N	377	ARG	CD-NE	-5.38	1.38	1.46
2	R	425	GLY	N-CA	-5.38	1.37	1.45
2	R	496	ALA	N-CA	-5.38	1.39	1.46
2	P	438	SER	N-CA	-5.38	1.40	1.46
2	Q	515	PRO	N-CD	-5.38	1.40	1.47
1	E	6	PRO	CA-CB	-5.37	1.48	1.54
1	F	142	ARG	C-N	-5.37	1.26	1.33
1	C	129	SER	C-O	-5.37	1.18	1.24
2	Q	432	ASP	C-N	-5.37	1.26	1.33
1	C	94	ARG	NE-CZ	-5.37	1.27	1.33
2	M	438	SER	N-CA	-5.36	1.40	1.46
2	N	351	PHE	CA-C	-5.36	1.44	1.52
1	E	125	HIS	ND1-CE1	-5.36	1.27	1.32
1	A	107	HIS	CG-CD2	-5.36	1.29	1.35
2	N	488	MET	N-CA	-5.36	1.38	1.46
1	A	37	ASN	N-CA	-5.36	1.39	1.46
1	F	15	PRO	N-CA	-5.36	1.40	1.47
1	A	19	ILE	CA-CB	-5.36	1.46	1.54
1	D	48	HIS	CG-CD2	-5.36	1.29	1.35
1	E	18	HIS	CA-C	-5.36	1.45	1.52
1	F	50	LEU	CA-C	-5.36	1.46	1.52
2	R	420	ASP	CA-CB	-5.36	1.46	1.53
1	A	47	GLU	CA-C	-5.35	1.46	1.52
1	F	6	PRO	CA-C	-5.35	1.45	1.52
1	A	131	PHE	C-N	-5.35	1.27	1.33
2	N	414	ARG	CA-CB	-5.35	1.46	1.53
2	M	504	LEU	CA-C	-5.35	1.45	1.52
2	N	446	PRO	C-N	-5.35	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	450	ARG	CA-C	-5.35	1.47	1.53
1	C	3	GLU	C-N	-5.34	1.25	1.33
1	A	42	PRO	N-CA	-5.34	1.40	1.47
1	A	14	GLY	C-O	-5.34	1.16	1.24
2	M	491	ILE	C-N	-5.34	1.27	1.33
1	E	56	TYR	N-CA	-5.34	1.39	1.46
1	E	121	PRO	CA-C	-5.34	1.45	1.52
2	Q	413	ASP	C-N	-5.34	1.26	1.33
1	F	130	LEU	C-O	-5.34	1.17	1.24
1	B	23	LEU	CA-CB	-5.33	1.45	1.53
2	O	393	PRO	C-N	-5.33	1.26	1.33
1	F	161	ILE	C-N	-5.33	1.27	1.33
1	A	177	VAL	CA-CB	-5.33	1.46	1.54
2	N	531	ARG	CZ-NH2	-5.33	1.26	1.33
1	F	32	ASP	C-N	-5.33	1.26	1.33
1	D	97	THR	CA-C	-5.33	1.46	1.52
2	P	490	PRO	N-CA	-5.33	1.40	1.47
2	N	485	LEU	C-N	-5.33	1.27	1.33
1	A	29	PRO	CA-CB	-5.33	1.46	1.53
1	A	94	ARG	NE-CZ	-5.33	1.27	1.33
2	N	469	SER	CA-C	-5.33	1.45	1.52
2	R	483	ASP	CA-CB	-5.33	1.43	1.53
2	M	505	ILE	N-CA	-5.32	1.39	1.46
1	D	53	GLY	CA-C	-5.32	1.45	1.51
1	D	80	GLN	CA-C	-5.32	1.46	1.52
1	D	176	GLU	CA-C	-5.32	1.46	1.52
2	O	486	ILE	C-N	-5.32	1.28	1.34
1	B	107	HIS	CD2-NE2	-5.32	1.32	1.37
1	D	85	LEU	CA-CB	-5.32	1.44	1.53
2	Q	428	ARG	CA-C	-5.32	1.46	1.52
2	R	524	ASP	CA-CB	-5.32	1.45	1.53
2	M	448	PRO	CA-C	-5.31	1.45	1.52
2	P	454	ASN	C-N	-5.31	1.25	1.33
2	P	405	GLY	C-N	-5.31	1.26	1.33
2	M	314	ASN	N-CA	-5.31	1.39	1.46
2	Q	499	GLU	N-CA	-5.31	1.39	1.46
1	C	155	CYS	CA-C	-5.31	1.47	1.52
1	F	83	TYR	CA-C	-5.30	1.46	1.52
2	N	504	LEU	CA-CB	-5.30	1.44	1.53
1	C	64	ARG	C-N	-5.30	1.25	1.34
2	P	403	ASN	C-N	-5.30	1.26	1.33
2	P	527	LEU	C-N	-5.30	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	492	VAL	C-N	-5.30	1.26	1.33
2	M	500	ALA	C-N	-5.30	1.27	1.34
2	N	338	SER	N-CA	-5.30	1.39	1.46
2	P	469	SER	C-O	-5.30	1.17	1.23
2	R	321	THR	C-O	-5.30	1.18	1.24
2	O	432	ASP	CA-C	-5.30	1.46	1.53
2	M	365	LEU	CA-C	-5.30	1.45	1.52
2	P	378	ILE	CA-C	-5.30	1.46	1.52
2	P	455	ASP	CA-CB	-5.30	1.45	1.53
1	B	122	MET	SD-CE	-5.29	1.66	1.79
1	E	191	GLY	N-CA	-5.29	1.37	1.45
1	A	28	ASN	C-O	-5.29	1.17	1.24
2	N	334	GLN	CA-C	-5.29	1.46	1.52
2	N	428	ARG	CA-C	-5.29	1.46	1.52
2	N	432	ASP	C-N	-5.29	1.26	1.34
2	O	393	PRO	CA-C	-5.29	1.46	1.52
2	Q	474	LEU	C-N	-5.29	1.26	1.33
2	P	523	PHE	CA-C	-5.29	1.46	1.52
1	A	34	GLU	CA-C	-5.29	1.46	1.52
2	O	499	GLU	CA-CB	-5.29	1.44	1.53
1	F	187	ILE	N-CA	-5.29	1.40	1.46
1	A	182	ALA	N-CA	-5.29	1.39	1.45
1	B	113	VAL	CA-C	-5.29	1.46	1.52
2	O	336	LEU	C-O	-5.29	1.17	1.23
1	D	88	ALA	CA-CB	-5.29	1.44	1.53
1	A	143	LEU	CA-C	-5.28	1.46	1.52
1	C	86	GLU	C-N	-5.28	1.26	1.33
2	O	311	ARG	CD-NE	-5.28	1.38	1.46
2	R	421	PRO	N-CA	-5.28	1.40	1.47
2	N	389	GLY	C-O	-5.28	1.17	1.24
2	R	447	TYR	CA-CB	-5.28	1.46	1.54
1	C	106	LEU	CB-CG	-5.28	1.43	1.53
2	M	531	ARG	NE-CZ	-5.27	1.27	1.33
2	P	301	PRO	N-CD	-5.27	1.40	1.47
2	M	316	HIS	CE1-NE2	-5.27	1.27	1.32
2	O	315	TRP	NE1-CE2	-5.27	1.31	1.37
1	E	129	SER	CA-CB	-5.27	1.43	1.53
1	B	106	LEU	N-CA	-5.27	1.39	1.46
1	C	122	MET	CA-C	-5.27	1.46	1.52
1	A	104	TRP	CA-C	-5.27	1.45	1.53
1	E	35	ILE	CA-C	-5.27	1.46	1.52
2	M	396	LEU	C-N	-5.26	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	VAL	C-N	-5.26	1.25	1.33
1	F	189	ILE	CA-C	-5.26	1.46	1.52
2	Q	380	VAL	CA-CB	-5.26	1.47	1.54
1	F	14	GLY	CA-C	-5.26	1.44	1.51
1	F	71	TRP	NE1-CE2	-5.26	1.31	1.37
1	A	21	LEU	N-CA	-5.26	1.38	1.45
2	N	353	HIS	ND1-CE1	-5.25	1.27	1.32
2	O	503	GLN	CA-C	-5.25	1.45	1.52
2	P	515	PRO	N-CA	-5.25	1.41	1.47
2	Q	345	GLU	CA-C	-5.25	1.45	1.52
2	N	316	HIS	CD2-NE2	-5.24	1.32	1.37
1	D	124	PRO	C-N	-5.24	1.27	1.33
2	Q	453	PRO	C-N	-5.24	1.27	1.33
1	A	31	ARG	CA-C	-5.24	1.46	1.53
1	F	140	HIS	C-O	-5.24	1.17	1.24
2	M	339	ILE	C-O	-5.24	1.17	1.24
2	N	399	MET	C-N	-5.24	1.27	1.33
1	F	62	LEU	CA-CB	-5.24	1.44	1.53
2	M	466	SER	N-CA	-5.23	1.39	1.46
1	E	143	LEU	C-O	-5.23	1.17	1.24
2	Q	534	HIS	C-O	-5.23	1.17	1.23
2	O	391	PRO	C-N	-5.23	1.27	1.33
1	C	7	GLU	N-CA	-5.23	1.39	1.46
2	O	316	HIS	C-N	-5.23	1.27	1.33
1	F	146	ASP	C-N	-5.23	1.27	1.33
2	Q	455	ASP	N-CA	-5.23	1.39	1.46
2	O	472	THR	C-N	-5.22	1.26	1.33
1	A	56	TYR	C-N	-5.22	1.25	1.33
2	O	318	LYS	CA-C	-5.22	1.45	1.53
1	F	147	ASP	C-N	-5.22	1.26	1.33
1	A	118	ALA	CA-C	-5.22	1.45	1.52
1	B	92	PHE	C-N	-5.22	1.26	1.33
2	R	307	ARG	NE-CZ	-5.22	1.27	1.33
1	D	81	ASP	N-CA	-5.22	1.39	1.46
1	B	156	PRO	N-CD	-5.21	1.40	1.47
1	A	79	TYR	N-CA	-5.21	1.39	1.46
2	M	364	LEU	CB-CG	-5.21	1.43	1.53
2	M	488	MET	CA-C	-5.21	1.45	1.52
1	B	140	HIS	CG-ND1	-5.21	1.32	1.38
2	O	361	HIS	CG-CD2	-5.21	1.30	1.35
1	C	74	ASP	C-N	-5.21	1.26	1.33
1	C	114	VAL	C-N	-5.21	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ASP	C-N	-5.20	1.27	1.33
1	B	62	LEU	N-CA	-5.20	1.39	1.46
2	P	473	LYS	C-N	-5.20	1.27	1.33
1	A	125	HIS	CG-CD2	-5.20	1.30	1.35
1	C	77	GLY	N-CA	-5.20	1.38	1.45
2	N	416	LEU	CA-CB	-5.19	1.44	1.53
2	P	342	SER	C-O	-5.19	1.16	1.23
1	E	113	VAL	CA-C	-5.19	1.46	1.52
2	N	373	PRO	N-CA	-5.19	1.40	1.47
1	D	121	PRO	C-N	-5.19	1.26	1.33
1	D	125	HIS	CG-ND1	-5.19	1.32	1.38
1	E	108	THR	CA-CB	5.19	1.60	1.54
1	D	86	GLU	CA-C	-5.19	1.45	1.52
2	O	326	THR	C-N	-5.19	1.26	1.33
2	Q	329	ALA	C-N	-5.19	1.27	1.33
2	N	377	ARG	CZ-NH2	-5.18	1.26	1.33
1	F	16	TYR	N-CA	-5.18	1.40	1.46
2	M	417	ALA	C-O	-5.18	1.17	1.24
2	N	391	PRO	N-CD	-5.18	1.40	1.47
2	N	534	HIS	C-O	-5.18	1.17	1.23
1	C	75	ALA	CA-CB	-5.18	1.44	1.53
2	O	304	ASP	CA-C	-5.18	1.46	1.53
1	F	28	ASN	CA-CB	-5.18	1.47	1.54
1	F	158	LEU	CA-C	-5.18	1.46	1.52
2	M	462	HIS	ND1-CE1	-5.18	1.27	1.32
2	Q	441	THR	CA-CB	5.17	1.60	1.53
2	O	309	VAL	C-N	-5.17	1.27	1.33
1	E	134	GLY	C-N	-5.17	1.26	1.33
2	R	507	LYS	CA-C	-5.17	1.46	1.52
2	R	509	ASP	C-O	-5.17	1.17	1.23
1	D	102	GLY	CA-C	-5.17	1.43	1.51
1	D	184	ARG	C-O	-5.17	1.17	1.24
1	C	83	TYR	N-CA	-5.17	1.39	1.46
1	F	93	GLY	C-O	-5.17	1.17	1.23
2	O	444	PRO	C-O	-5.17	1.17	1.23
1	E	98	THR	CA-C	-5.16	1.46	1.52
1	C	190	GLN	C-O	-5.16	1.17	1.23
2	O	408	TYR	CA-C	-5.16	1.46	1.52
2	Q	325	LYS	N-CA	-5.16	1.40	1.46
2	P	342	SER	C-N	-5.16	1.27	1.34
1	F	86	GLU	C-N	-5.16	1.26	1.33
1	A	186	ASP	N-CA	-5.16	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	LEU	CA-CB	-5.16	1.44	1.53
1	D	180	LYS	CA-CB	-5.15	1.44	1.53
2	M	519	LEU	CB-CG	-5.15	1.43	1.53
2	Q	410	HIS	CE1-NE2	-5.15	1.27	1.32
1	E	66	SER	C-N	-5.15	1.26	1.33
2	M	482	GLY	N-CA	-5.15	1.36	1.45
1	B	13	ALA	C-N	-5.15	1.25	1.33
2	P	409	ARG	CZ-NH2	-5.15	1.26	1.33
2	P	437	TYR	CA-C	-5.15	1.46	1.52
2	M	315	TRP	C-O	-5.15	1.18	1.24
1	D	146	ASP	CA-C	-5.14	1.45	1.52
1	D	42	PRO	N-CA	-5.14	1.40	1.47
1	E	92	PHE	C-N	-5.14	1.26	1.33
2	N	322	PRO	CA-CB	-5.14	1.46	1.53
2	N	329	ALA	C-N	-5.14	1.26	1.33
2	O	337	VAL	C-N	-5.14	1.26	1.33
2	P	400	TRP	C-N	-5.14	1.26	1.33
1	A	178	ASP	CA-C	-5.13	1.46	1.53
2	O	313	ARG	NE-CZ	-5.13	1.27	1.33
2	P	426	VAL	N-CA	-5.13	1.40	1.46
1	E	95	THR	CA-C	-5.13	1.46	1.52
1	A	149	ALA	C-N	-5.13	1.27	1.33
1	D	62	LEU	C-O	-5.13	1.17	1.23
1	C	100	ASP	N-CA	-5.12	1.39	1.46
2	M	336	LEU	C-N	-5.12	1.24	1.33
2	M	520	ALA	N-CA	-5.12	1.39	1.46
2	P	522	ARG	N-CA	-5.12	1.40	1.46
2	R	428	ARG	C-N	-5.12	1.27	1.33
2	R	417	ALA	C-N	-5.12	1.27	1.33
2	M	355	GLY	CA-C	-5.12	1.44	1.51
2	N	506	ALA	N-CA	-5.12	1.39	1.46
1	E	30	THR	CA-C	-5.12	1.46	1.53
1	B	162	GLU	N-CA	-5.11	1.40	1.46
2	N	347	THR	C-O	-5.11	1.17	1.23
1	B	192	GLU	CD-OE2	-5.11	1.15	1.25
1	C	149	ALA	CA-C	-5.11	1.45	1.52
1	B	45	PRO	N-CD	-5.11	1.40	1.47
2	N	312	ASP	C-N	-5.11	1.25	1.33
2	O	418	PRO	N-CA	-5.11	1.41	1.47
2	R	336	LEU	C-N	-5.11	1.26	1.33
2	M	418	PRO	N-CD	-5.11	1.40	1.47
1	D	13	ALA	CA-C	-5.11	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	75	ALA	CA-CB	-5.10	1.44	1.53
1	B	138	HIS	ND1-CE1	-5.10	1.27	1.32
1	D	32	ASP	CA-C	-5.10	1.46	1.52
1	C	147	ASP	C-N	-5.10	1.26	1.33
2	P	452	GLY	C-N	-5.09	1.27	1.34
1	B	55	VAL	CA-CB	-5.09	1.48	1.54
1	E	58	GLY	N-CA	-5.09	1.38	1.45
1	E	160	LEU	CB-CG	-5.09	1.43	1.53
1	F	138	HIS	C-O	-5.09	1.17	1.23
2	R	501	VAL	C-O	-5.09	1.18	1.24
1	F	66	SER	C-O	-5.09	1.17	1.23
2	R	479	TYR	CA-CB	-5.09	1.45	1.53
2	R	511	ASN	CA-C	-5.09	1.45	1.52
2	N	342	SER	CA-CB	-5.09	1.45	1.53
2	P	407	ARG	CA-C	-5.09	1.46	1.52
1	A	59	ASN	CG-ND2	-5.09	1.22	1.33
1	F	55	VAL	N-CA	-5.09	1.39	1.46
2	N	494	SER	C-N	-5.08	1.26	1.33
1	D	24	GLU	CA-CB	-5.08	1.45	1.53
1	C	172	ALA	C-N	-5.08	1.26	1.33
2	O	533	THR	CA-C	-5.08	1.46	1.52
2	R	360	ASP	CA-C	-5.08	1.45	1.52
2	O	508	LEU	C-O	-5.08	1.17	1.23
2	R	493	LYS	N-CA	-5.08	1.39	1.46
1	A	11	GLN	CD-OE1	-5.07	1.14	1.23
1	F	60	GLY	CA-C	-5.07	1.44	1.51
1	A	129	SER	N-CA	-5.07	1.40	1.46
2	R	508	LEU	C-N	-5.07	1.26	1.33
1	C	161	ILE	CA-CB	-5.07	1.48	1.54
1	D	114	VAL	CA-CB	-5.07	1.46	1.54
1	A	152	ASN	N-CA	-5.07	1.40	1.46
2	N	358	ALA	C-N	-5.07	1.27	1.33
1	E	72	GLN	CA-C	-5.07	1.46	1.52
2	M	515	PRO	C-N	-5.06	1.26	1.33
1	C	174	ARG	C-N	-5.06	1.27	1.33
2	R	330	ARG	C-N	-5.06	1.26	1.33
2	R	361	HIS	ND1-CE1	-5.06	1.27	1.32
2	R	460	HIS	CA-C	-5.06	1.46	1.52
1	A	141	THR	CA-C	-5.05	1.46	1.52
2	Q	306	SER	CB-OG	-5.05	1.32	1.42
1	A	176	GLU	CA-CB	-5.05	1.43	1.54
2	N	511	ASN	C-N	-5.05	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	ARG	CD-NE	-5.05	1.39	1.46
1	E	109	VAL	CA-CB	-5.05	1.46	1.55
1	A	72	GLN	N-CA	-5.05	1.39	1.45
2	O	417	ALA	CA-CB	-5.05	1.43	1.53
2	R	440	ARG	CD-NE	-5.05	1.39	1.46
1	A	16	TYR	CA-C	-5.05	1.46	1.52
1	C	17	VAL	C-N	-5.05	1.27	1.34
2	O	418	PRO	C-O	-5.05	1.17	1.23
2	R	336	LEU	C-O	-5.05	1.17	1.23
2	N	412	ASN	C-N	-5.04	1.26	1.33
1	C	17	VAL	CA-C	-5.04	1.45	1.52
1	C	153	ALA	CA-C	-5.04	1.45	1.52
2	Q	309	VAL	CA-C	-5.04	1.45	1.52
1	D	143	LEU	CA-C	-5.04	1.46	1.52
2	O	378	ILE	C-O	-5.04	1.18	1.23
2	P	336	LEU	CB-CG	-5.04	1.43	1.53
1	F	92	PHE	CA-C	-5.04	1.46	1.52
2	R	351	PHE	N-CA	-5.04	1.39	1.46
2	M	476	THR	C-N	-5.04	1.26	1.33
1	E	41	LYS	CA-CB	-5.04	1.46	1.53
1	A	150	GLN	CA-CB	-5.04	1.45	1.53
2	M	407	ARG	CA-C	-5.03	1.46	1.52
2	N	359	HIS	CB-CG	-5.03	1.43	1.50
2	Q	392	VAL	N-CA	5.03	1.50	1.46
2	R	447	TYR	C-O	-5.03	1.18	1.24
1	E	167	ARG	C-N	-5.03	1.27	1.34
2	Q	397	VAL	C-N	-5.03	1.26	1.33
1	A	78	GLU	CA-C	-5.03	1.46	1.52
1	A	106	LEU	CA-C	-5.02	1.46	1.52
1	B	191	GLY	N-CA	-5.02	1.38	1.45
1	C	115	ASN	C-N	-5.02	1.26	1.33
2	M	388	TYR	CA-CB	-5.02	1.44	1.53
1	A	107	HIS	C-N	-5.02	1.27	1.33
2	R	495	ILE	C-N	-5.01	1.27	1.33
2	R	333	ARG	C-O	-5.01	1.17	1.24
1	A	184	ARG	C-N	-5.01	1.27	1.33
2	N	379	ILE	CA-CB	-5.01	1.48	1.54
1	A	136	ASN	C-N	-5.01	1.26	1.33
1	F	55	VAL	C-N	-5.01	1.26	1.33
2	N	372	LEU	CB-CG	-5.01	1.43	1.53
2	Q	383	ARG	CZ-NH2	-5.01	1.26	1.33
1	E	199	ASP	C-N	-5.00	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	ASN	N-CA	-5.00	1.39	1.46

All (811) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	38	ARG	CD-NE-CZ	19.08	151.11	124.40
1	A	94	ARG	CD-NE-CZ	15.77	146.48	124.40
2	N	434	ASP	CA-CB-CG	-15.02	97.58	112.60
2	N	440	ARG	NE-CZ-NH2	-14.03	106.58	119.20
1	C	94	ARG	CD-NE-CZ	13.27	142.97	124.40
1	D	84	ASN	CA-CB-CG	12.43	125.03	112.60
1	D	94	ARG	CD-NE-CZ	11.92	141.08	124.40
2	Q	440	ARG	NE-CZ-NH2	-11.81	108.58	119.20
1	A	133	ARG	CD-NE-CZ	11.48	140.48	124.40
1	E	133	ARG	CD-NE-CZ	11.39	140.35	124.40
2	M	434	ASP	CA-CB-CG	-11.19	101.41	112.60
2	P	452	GLY	N-CA-C	-11.04	98.52	112.10
2	M	440	ARG	NE-CZ-NH2	-10.82	109.46	119.20
2	R	434	ASP	CA-CB-CG	-10.79	101.81	112.60
2	O	434	ASP	CA-CB-CG	-10.73	101.87	112.60
1	A	178	ASP	CA-CB-CG	-10.44	102.17	112.60
2	M	452	GLY	N-CA-C	-10.30	99.43	112.10
1	D	133	ARG	CD-NE-CZ	10.27	138.77	124.40
2	N	361	HIS	CA-CB-CG	-10.20	103.60	113.80
2	P	372	LEU	CB-CA-C	10.01	122.59	108.68
1	D	178	ASP	CA-CB-CG	-9.94	102.66	112.60
2	Q	434	ASP	CA-CB-CG	-9.73	102.87	112.60
2	Q	361	HIS	CA-CB-CG	-9.72	104.08	113.80
1	D	94	ARG	NE-CZ-NH2	-9.71	110.46	119.20
2	Q	522	ARG	NE-CZ-NH1	-9.68	111.82	121.50
2	P	353	HIS	CA-CB-CG	-9.58	104.22	113.80
1	F	38	ARG	CA-CB-CG	9.55	133.21	114.10
2	Q	452	GLY	N-CA-C	-9.55	100.35	112.10
2	P	440	ARG	NE-CZ-NH2	-9.29	110.84	119.20
2	O	339	ILE	O-C-N	9.28	127.54	121.69
1	E	37	ASN	N-CA-C	9.19	123.22	112.93
2	N	333	ARG	NE-CZ-NH1	-9.18	112.32	121.50
2	R	336	LEU	CA-C-O	-9.07	111.67	121.56
2	M	489	CYS	O-C-N	9.06	129.01	121.31
2	Q	325	LYS	N-CA-C	9.03	121.95	111.11
1	C	94	ARG	CA-CB-CG	9.02	132.14	114.10
2	M	353	HIS	CA-CB-CG	-8.99	104.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	359	HIS	CA-CB-CG	-8.94	104.86	113.80
1	D	43	ASP	CA-CB-CG	-8.87	103.73	112.60
2	M	354	LEU	CB-CA-C	8.87	124.81	109.65
1	B	176	GLU	CB-CG-CD	8.79	127.54	112.60
1	F	46	GLY	CA-C-O	-8.74	116.16	122.45
2	O	353	HIS	CA-CB-CG	-8.71	105.09	113.80
2	R	407	ARG	NE-CZ-NH2	-8.62	111.45	119.20
1	E	133	ARG	N-CA-C	-8.58	98.68	110.35
2	N	447	TYR	O-C-N	8.53	128.48	121.83
1	D	177	VAL	CB-CA-C	8.50	121.89	110.42
2	N	452	GLY	N-CA-C	-8.47	101.68	112.10
2	R	440	ARG	NE-CZ-NH2	-8.44	111.61	119.20
2	P	314	ASN	N-CA-C	-8.33	103.26	113.50
2	P	483	ASP	CA-CB-CG	8.32	120.92	112.60
1	B	37	ASN	N-CA-C	8.27	122.94	113.02
2	N	419	LEU	N-CA-C	-8.21	99.46	110.55
1	D	163	GLN	CA-C-O	8.20	125.39	119.32
2	Q	454	ASN	CA-C-O	-8.19	114.06	121.67
1	B	94	ARG	CG-CD-NE	8.18	129.99	112.00
1	E	133	ARG	NE-CZ-NH2	-8.17	111.85	119.20
2	P	481	GLU	CB-CG-CD	8.13	126.42	112.60
1	B	24	GLU	CA-CB-CG	8.13	130.36	114.10
1	C	87	ASN	CA-CB-CG	8.12	120.72	112.60
2	M	514	ASN	O-C-N	8.09	128.79	121.19
2	R	353	HIS	CA-CB-CG	-8.06	105.74	113.80
2	O	458	PRO	CB-CA-C	-8.01	100.46	110.95
2	P	333	ARG	CD-NE-CZ	-7.99	113.21	124.40
1	D	166	ARG	NE-CZ-NH2	-7.98	112.02	119.20
2	R	497	ASN	N-CA-C	7.95	120.29	109.24
1	E	88	ALA	N-CA-C	-7.95	103.04	112.89
2	N	441	THR	N-CA-CB	-7.94	99.24	110.51
2	Q	451	ASN	O-C-N	7.94	126.71	120.83
2	O	350	ASN	CA-C-O	-7.94	111.59	120.32
1	D	131	PHE	CA-CB-CG	7.94	121.74	113.80
1	E	46	GLY	N-CA-C	-7.93	103.95	112.04
1	E	133	ARG	NE-CZ-NH1	7.92	129.43	121.50
2	Q	383	ARG	CD-NE-CZ	-7.92	113.31	124.40
2	O	428	ARG	CD-NE-CZ	7.92	135.49	124.40
2	N	385	VAL	CA-C-O	-7.91	113.29	121.67
1	C	46	GLY	CA-C-O	-7.90	114.44	122.26
1	D	176	GLU	CB-CG-CD	7.87	125.98	112.60
1	E	52	LEU	CB-CA-C	7.86	126.69	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	HIS	CA-CB-CG	-7.84	105.96	113.80
2	O	353	HIS	CA-C-O	-7.83	110.39	119.56
2	N	350	ASN	CA-CB-CG	-7.81	104.79	112.60
2	O	330	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	A	3	GLU	CB-CG-CD	7.77	125.81	112.60
1	A	64	ARG	CD-NE-CZ	-7.75	113.55	124.40
2	Q	489	CYS	CA-C-O	7.74	125.42	119.46
1	C	29	PRO	CA-C-O	-7.72	112.54	121.34
1	F	155	CYS	O-C-N	7.72	128.03	121.31
2	O	516	MET	CA-C-O	-7.72	111.22	120.32
1	F	37	ASN	N-CA-C	7.71	122.08	113.21
1	C	133	ARG	CD-NE-CZ	7.68	135.15	124.40
1	C	167	ARG	CD-NE-CZ	-7.67	113.66	124.40
2	P	451	ASN	O-C-N	7.64	126.48	120.83
2	O	447	TYR	O-C-N	7.64	127.20	121.85
2	R	383	ARG	NE-CZ-NH1	-7.63	113.87	121.50
2	R	524	ASP	CA-CB-CG	7.61	120.21	112.60
2	R	458	PRO	CB-CA-C	-7.61	100.99	110.95
1	A	52	LEU	CB-CA-C	7.60	126.13	109.94
1	E	5	LEU	N-CA-C	-7.60	99.59	110.08
2	N	483	ASP	O-C-N	7.59	127.91	121.31
1	D	159	ASN	CA-CB-CG	-7.59	105.01	112.60
2	M	494	SER	N-CA-C	-7.58	103.29	112.54
2	O	514	ASN	CA-CB-CG	7.57	120.17	112.60
1	D	142	ARG	NE-CZ-NH1	-7.57	113.93	121.50
2	Q	441	THR	N-CA-CB	-7.53	99.22	110.97
1	C	122	MET	CA-C-O	-7.52	112.48	121.66
2	R	352	SER	O-C-N	7.51	130.08	122.12
1	F	176	GLU	CB-CG-CD	7.50	125.35	112.60
1	F	107	HIS	CA-CB-CG	-7.49	106.31	113.80
2	P	483	ASP	CA-C-O	7.48	126.10	119.59
1	C	133	ARG	N-CA-C	-7.43	100.25	110.35
2	Q	385	VAL	CA-C-O	-7.43	113.87	121.67
1	A	115	ASN	CA-CB-CG	7.40	120.00	112.60
1	A	64	ARG	NE-CZ-NH1	-7.37	114.13	121.50
2	M	512	ASN	CA-CB-CG	-7.33	105.28	112.60
2	M	391	PRO	CA-C-O	-7.32	113.07	121.56
1	E	174	ARG	CD-NE-CZ	-7.32	114.16	124.40
2	P	380	VAL	CA-C-O	-7.28	112.74	120.53
2	Q	446	PRO	N-CA-C	-7.28	101.03	111.22
2	N	496	ALA	N-CA-C	7.25	119.26	111.36
1	E	19	ILE	CA-C-O	-7.25	112.64	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	PHE	N-CA-C	-7.23	103.40	111.28
2	Q	419	LEU	N-CA-C	-7.23	99.78	110.48
1	C	38	ARG	CD-NE-CZ	-7.22	114.29	124.40
1	A	14	GLY	CA-C-N	7.22	126.85	119.56
1	A	14	GLY	C-N-CA	7.22	126.85	119.56
2	R	360	ASP	O-C-N	7.21	130.66	122.22
2	P	350	ASN	N-CA-CB	7.20	121.89	110.65
1	C	148	GLU	CA-C-O	-7.19	112.98	121.32
1	F	133	ARG	N-CA-C	-7.18	99.81	110.23
1	D	96	ALA	N-CA-CB	-7.18	100.65	111.56
2	O	492	VAL	N-CA-C	-7.16	103.32	110.62
1	B	103	GLU	CA-C-O	-7.11	112.69	120.36
1	E	120	VAL	N-CA-CB	-7.10	101.27	111.21
1	E	57	ASP	CA-C-N	7.10	129.01	120.14
1	E	57	ASP	C-N-CA	7.10	129.01	120.14
2	P	428	ARG	CG-CD-NE	7.09	127.61	112.00
1	C	37	ASN	N-CA-C	7.09	121.36	113.21
1	C	133	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	A	21	LEU	N-CA-CB	-7.08	101.12	110.88
1	B	36	TRP	CB-CA-C	7.08	124.50	110.42
1	E	54	GLN	OE1-CD-NE2	7.06	129.66	122.60
1	B	192	GLU	CB-CA-C	-7.06	100.00	110.16
2	N	440	ARG	NE-CZ-NH1	7.04	128.54	121.50
2	Q	496	ALA	N-CA-C	7.04	119.03	111.36
2	N	524	ASP	CA-C-O	-7.02	113.00	121.28
2	P	367	PHE	CA-C-O	-7.01	108.88	120.80
1	F	180	LYS	O-C-N	7.00	131.79	123.33
1	E	38	ARG	NE-CZ-NH2	-6.99	112.91	119.20
1	F	177	VAL	CB-CA-C	6.99	118.85	111.09
1	C	94	ARG	NE-CZ-NH1	6.99	128.49	121.50
1	C	110	LYS	N-CA-C	-6.98	100.85	109.65
2	O	452	GLY	N-CA-C	-6.98	103.52	112.10
1	A	165	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	F	99	PHE	N-CA-C	-6.96	103.70	111.71
1	A	47	GLU	CB-CG-CD	6.96	124.43	112.60
1	B	43	ASP	CB-CA-C	6.95	121.81	111.17
1	D	94	ARG	NE-CZ-NH1	6.95	128.45	121.50
1	A	94	ARG	NE-CZ-NH2	-6.93	112.96	119.20
2	M	428	ARG	CD-NE-CZ	6.92	134.09	124.40
2	P	361	HIS	O-C-N	6.92	130.64	122.34
2	M	450	ARG	NE-CZ-NH1	6.90	128.40	121.50
2	N	367	PHE	CA-C-O	-6.89	109.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	428	ARG	CD-NE-CZ	6.89	134.05	124.40
1	F	167	ARG	CD-NE-CZ	-6.89	114.75	124.40
1	A	133	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	B	94	ARG	CB-CG-CD	6.87	127.09	111.30
2	O	333	ARG	N-CA-C	-6.87	105.06	113.50
2	R	411	LYS	CB-CA-C	-6.86	100.01	110.92
2	O	320	LEU	CA-C-N	6.86	131.59	123.16
2	O	320	LEU	C-N-CA	6.86	131.59	123.16
1	B	38	ARG	NE-CZ-NH2	-6.85	113.03	119.20
1	C	150	GLN	OE1-CD-NE2	6.83	129.43	122.60
2	R	417	ALA	N-CA-C	-6.83	101.46	109.93
2	N	339	ILE	O-C-N	6.83	127.64	121.57
1	F	126	ILE	O-C-N	6.83	130.63	123.26
2	O	409	ARG	NE-CZ-NH2	6.82	125.34	119.20
1	A	171	ILE	N-CA-C	6.82	117.94	107.99
2	Q	367	PHE	CA-C-O	-6.82	109.21	120.80
2	M	356	PHE	CA-CB-CG	6.81	120.61	113.80
1	D	31	ARG	CA-C-O	-6.80	113.59	121.82
1	A	187	ILE	CA-C-O	-6.79	113.28	120.48
2	O	474	LEU	N-CA-CB	-6.79	98.89	111.52
1	E	52	LEU	CA-CB-CG	6.78	140.03	116.30
2	P	357	GLY	N-CA-C	-6.78	103.86	112.54
2	O	308	PHE	CA-CB-CG	-6.78	107.02	113.80
1	A	184	ARG	NE-CZ-NH2	-6.77	113.10	119.20
1	C	108	THR	CA-CB-OG1	-6.77	99.44	109.60
2	P	380	VAL	N-CA-C	-6.77	97.99	107.80
1	B	46	GLY	N-CA-C	-6.76	104.16	112.33
1	A	112	GLY	CA-C-N	6.75	130.30	120.91
1	A	112	GLY	C-N-CA	6.75	130.30	120.91
1	C	30	THR	CA-CB-OG1	-6.75	99.48	109.60
2	Q	447	TYR	O-C-N	6.74	126.57	121.85
1	D	166	ARG	NE-CZ-NH1	6.74	128.24	121.50
2	P	428	ARG	CB-CG-CD	6.74	126.80	111.30
1	E	187	ILE	CA-C-O	-6.74	113.04	120.72
2	R	483	ASP	CA-CB-CG	6.73	119.33	112.60
2	R	492	VAL	N-CA-C	-6.72	103.30	110.36
1	B	3	GLU	CA-C-O	-6.71	113.11	120.36
1	C	103	GLU	CB-CG-CD	6.70	124.00	112.60
1	E	171	ILE	CB-CA-C	6.70	120.16	110.98
1	B	87	ASN	CA-CB-CG	6.69	119.29	112.60
2	R	454	ASN	OD1-CG-ND2	-6.69	115.91	122.60
2	N	451	ASN	CA-C-O	-6.69	115.96	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	354	LEU	N-CA-C	-6.68	100.39	110.28
1	C	95	THR	CA-C-O	-6.68	114.28	121.36
1	E	70	VAL	CA-C-O	-6.67	112.51	121.32
2	R	454	ASN	CA-CB-CG	6.67	119.27	112.60
2	M	417	ALA	CA-C-O	-6.66	113.83	119.76
1	F	125	HIS	CA-CB-CG	-6.66	107.14	113.80
2	R	361	HIS	CA-CB-CG	-6.66	107.14	113.80
2	M	338	SER	CA-C-O	-6.62	113.51	121.05
2	M	314	ASN	N-CA-C	-6.60	105.38	113.50
2	O	409	ARG	NE-CZ-NH1	-6.60	114.90	121.50
2	O	440	ARG	NE-CZ-NH2	-6.59	113.27	119.20
2	R	311	ARG	O-C-N	6.59	130.40	122.96
2	M	307	ARG	CA-C-O	-6.58	113.41	121.11
1	B	63	VAL	CB-CA-C	6.57	120.51	111.31
2	P	447	TYR	O-C-N	6.56	126.44	121.85
1	A	167	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	D	171	ILE	N-CA-CB	-6.55	103.54	111.21
1	F	4	LEU	N-CA-CB	-6.55	99.97	110.39
1	C	151	ALA	N-CA-C	-6.55	104.22	111.36
1	B	5	LEU	N-CA-C	-6.55	101.04	110.08
2	R	383	ARG	NH1-CZ-NH2	6.54	127.81	119.30
2	P	496	ALA	CA-C-O	-6.54	112.45	119.97
2	Q	483	ASP	CA-CB-CG	6.54	119.14	112.60
1	E	171	ILE	N-CA-CB	-6.53	103.57	111.21
2	Q	390	LYS	CA-C-N	6.53	126.44	119.85
2	Q	390	LYS	C-N-CA	6.53	126.44	119.85
2	O	411	LYS	N-CA-C	6.52	118.94	111.11
2	P	512	ASN	CA-CB-CG	-6.51	106.08	112.60
2	Q	484	PRO	CB-CA-C	6.51	121.19	111.68
2	R	328	ILE	N-CA-C	6.51	116.67	110.42
2	Q	394	ASN	CA-CB-CG	-6.50	106.10	112.60
2	M	463	PHE	O-C-N	6.50	131.23	123.24
2	N	458	PRO	N-CA-C	-6.50	101.67	111.41
1	C	150	GLN	N-CA-CB	6.49	119.77	110.16
2	N	322	PRO	N-CA-C	6.49	123.22	113.81
2	R	494	SER	N-CA-C	-6.49	104.63	112.54
1	C	120	VAL	CA-C-O	6.48	123.40	119.19
1	B	184	ARG	NE-CZ-NH2	-6.48	113.37	119.20
2	Q	458	PRO	N-CA-C	-6.47	101.70	111.41
2	M	428	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	C	76	ASN	CA-CB-CG	-6.45	106.15	112.60
1	D	120	VAL	CA-C-N	6.45	126.21	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	120	VAL	C-N-CA	6.45	126.21	119.76
2	Q	420	ASP	CB-CA-C	6.44	117.19	109.85
1	A	41	LYS	N-CA-C	-6.44	100.84	110.24
2	Q	426	VAL	CA-C-O	-6.43	113.64	120.39
1	A	177	VAL	CB-CA-C	6.43	117.74	110.41
1	C	107	HIS	CA-CB-CG	-6.43	107.37	113.80
1	E	38	ARG	CA-C-O	-6.43	113.20	121.11
1	D	32	ASP	O-C-N	6.42	128.71	122.03
1	D	162	GLU	N-CA-CB	6.42	119.58	109.82
1	A	137	ILE	CB-CA-C	6.41	119.69	110.33
1	C	13	ALA	N-CA-C	-6.40	104.73	112.54
2	P	326	THR	CA-C-O	-6.40	111.51	119.38
2	N	357	GLY	N-CA-C	-6.39	102.57	112.85
2	P	506	ALA	CA-C-O	-6.38	114.01	121.16
2	M	503	GLN	OE1-CD-NE2	6.38	128.98	122.60
1	D	94	ARG	CB-CG-CD	6.37	125.95	111.30
2	R	333	ARG	N-CA-C	-6.36	105.68	113.50
1	D	181	THR	O-C-N	6.36	130.97	122.96
2	M	417	ALA	N-CA-C	-6.35	101.65	109.65
1	D	116	ASN	CA-CB-CG	6.35	118.95	112.60
2	R	383	ARG	N-CA-CB	-6.34	99.74	111.53
1	A	87	ASN	CA-CB-CG	6.34	118.94	112.60
2	R	533	THR	N-CA-C	-6.34	102.00	110.55
1	F	122	MET	CA-C-O	-6.33	113.81	121.28
2	Q	451	ASN	CA-C-O	-6.33	116.16	119.77
2	P	366	ASN	N-CA-C	6.33	121.00	113.16
1	B	178	ASP	CB-CA-C	6.32	121.81	112.09
1	A	30	THR	CA-CB-OG1	-6.31	100.13	109.60
1	E	138	HIS	CA-CB-CG	-6.31	107.49	113.80
1	B	11	GLN	N-CA-CB	6.30	123.24	111.52
2	N	353	HIS	CA-CB-CG	-6.30	107.50	113.80
2	O	440	ARG	NH1-CZ-NH2	6.30	127.49	119.30
1	A	118	ALA	CA-C-O	-6.30	111.66	119.28
2	R	536	GLU	CB-CG-CD	6.29	123.30	112.60
1	E	28	ASN	O-C-N	6.29	127.67	121.57
1	C	57	ASP	CA-CB-CG	6.29	118.89	112.60
2	O	383	ARG	NE-CZ-NH1	-6.29	115.21	121.50
2	R	412	ASN	CA-CB-CG	6.28	118.88	112.60
2	O	454	ASN	OD1-CG-ND2	-6.26	116.34	122.60
2	R	350	ASN	OD1-CG-ND2	-6.26	116.34	122.60
2	R	516	MET	CA-C-O	-6.26	112.94	120.32
2	P	359	HIS	CA-CB-CG	-6.25	107.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	177	VAL	O-C-N	6.24	128.76	122.71
2	P	324	TYR	CA-C-N	6.24	128.93	120.38
2	P	324	TYR	C-N-CA	6.24	128.93	120.38
2	Q	311	ARG	CD-NE-CZ	6.24	133.14	124.40
1	A	75	ALA	CB-CA-C	6.24	122.65	110.67
2	Q	534	HIS	CA-CB-CG	6.23	120.03	113.80
1	B	152	ASN	CA-CB-CG	6.23	118.83	112.60
1	A	192	GLU	CB-CA-C	-6.23	101.40	110.06
2	M	359	HIS	CA-CB-CG	-6.22	107.58	113.80
2	O	428	ARG	CB-CG-CD	6.22	125.61	111.30
2	M	526	VAL	O-C-N	6.22	129.64	122.99
1	C	28	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	P	440	ARG	NE-CZ-NH1	6.21	127.71	121.50
1	F	23	LEU	CB-CA-C	6.20	120.78	110.92
1	B	38	ARG	CA-C-O	-6.20	113.49	121.11
2	R	339	ILE	O-C-N	6.20	126.06	121.72
2	O	489	CYS	CA-C-N	6.19	126.09	119.28
2	O	489	CYS	C-N-CA	6.19	126.09	119.28
1	F	106	LEU	N-CA-CB	-6.19	100.00	111.52
2	M	367	PHE	CA-C-O	-6.19	110.28	120.80
2	M	337	VAL	N-CA-CB	-6.19	103.98	110.72
2	Q	392	VAL	CA-C-O	6.18	125.08	120.88
1	C	55	VAL	CA-C-O	-6.18	113.90	120.39
1	A	116	ASN	CA-CB-CG	6.17	118.77	112.60
2	N	522	ARG	CD-NE-CZ	6.17	133.03	124.40
2	Q	514	ASN	CA-CB-CG	6.16	118.76	112.60
2	R	514	ASN	CA-CB-CG	6.16	118.76	112.60
2	M	422	ASN	CA-CB-CG	-6.16	106.44	112.60
2	Q	383	ARG	N-CA-CB	-6.15	100.17	111.37
1	B	80	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	B	28	ASN	O-C-N	6.13	127.52	121.57
1	C	43	ASP	CA-CB-CG	6.13	118.73	112.60
1	F	180	LYS	CA-C-O	-6.13	113.24	120.60
2	Q	522	ARG	CD-NE-CZ	-6.13	115.82	124.40
2	M	302	ALA	N-CA-C	6.11	118.67	110.35
2	N	440	ARG	CB-CG-CD	-6.11	97.24	111.30
1	E	64	ARG	NE-CZ-NH1	6.11	127.61	121.50
2	P	361	HIS	CA-CB-CG	-6.11	107.69	113.80
2	M	306	SER	N-CA-CB	-6.11	101.45	110.85
2	M	357	GLY	N-CA-C	-6.10	103.17	112.51
2	N	309	VAL	O-C-N	6.10	129.32	122.67
1	E	187	ILE	O-C-N	6.10	129.37	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	304	ASP	CA-CB-CG	-6.10	106.50	112.60
2	Q	533	THR	CA-C-O	-6.10	114.80	121.87
1	E	162	GLU	CA-CB-CG	6.09	126.28	114.10
2	Q	469	SER	O-C-N	6.09	130.10	123.10
2	N	446	PRO	N-CA-C	-6.08	102.70	111.22
2	R	350	ASN	CA-C-O	-6.08	113.80	120.30
2	R	473	LYS	CA-CB-CG	6.07	126.24	114.10
2	M	415	TYR	N-CA-C	-6.07	102.10	110.35
1	E	4	LEU	CA-C-O	-6.07	114.48	121.82
2	Q	443	LYS	O-C-N	6.04	126.80	121.18
1	F	109	VAL	O-C-N	6.04	129.44	122.97
2	P	415	TYR	N-CA-C	-6.03	102.14	110.35
1	A	171	ILE	N-CA-CB	-6.03	104.15	111.21
2	M	450	ARG	NE-CZ-NH2	-6.03	113.78	119.20
1	A	200	PHE	CA-CB-CG	6.00	119.80	113.80
2	R	474	LEU	N-CA-CB	-6.00	100.36	111.52
1	E	38	ARG	CD-NE-CZ	-6.00	116.00	124.40
2	M	474	LEU	N-CA-CB	-5.99	100.38	111.53
2	R	392	VAL	O-C-N	5.99	127.93	121.10
1	A	136	ASN	N-CA-C	5.99	117.89	111.36
1	B	99	PHE	N-CA-C	-5.99	104.08	111.33
2	R	440	ARG	CB-CG-CD	-5.98	97.54	111.30
2	N	314	ASN	N-CA-CB	5.97	119.43	110.53
2	Q	313	ARG	CB-CA-C	5.97	122.09	110.57
1	F	126	ILE	CA-C-O	-5.97	114.12	120.39
1	B	28	ASN	N-CA-C	-5.97	100.97	110.10
1	B	64	ARG	CD-NE-CZ	-5.97	116.04	124.40
1	E	165	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	F	98	THR	CA-CB-OG1	-5.97	100.65	109.60
2	N	428	ARG	CG-CD-NE	5.96	125.11	112.00
1	E	113	VAL	N-CA-CB	-5.95	102.11	110.26
2	Q	348	GLY	CA-C-N	5.95	125.86	119.85
2	Q	348	GLY	C-N-CA	5.95	125.86	119.85
1	C	112	GLY	N-CA-C	-5.95	103.28	112.85
2	Q	528	ARG	CA-C-N	5.95	126.73	120.43
2	Q	528	ARG	C-N-CA	5.95	126.73	120.43
1	F	180	LYS	N-CA-C	-5.94	98.96	109.06
2	R	367	PHE	CA-C-O	-5.93	110.71	120.80
2	P	533	THR	CA-CB-OG1	-5.93	100.70	109.60
1	B	95	THR	CA-CB-OG1	-5.93	100.71	109.60
1	A	143	LEU	O-C-N	5.93	130.26	123.27
1	F	99	PHE	CB-CA-C	5.92	121.58	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	517	ASP	CA-CB-CG	5.92	118.52	112.60
1	F	138	HIS	N-CA-C	5.92	118.39	110.35
2	O	457	ARG	CA-CB-CG	5.91	125.93	114.10
1	F	150	GLN	N-CA-CB	5.91	118.54	109.91
1	D	64	ARG	CA-C-O	-5.91	112.75	119.78
1	E	161	ILE	CB-CA-C	5.91	117.61	111.23
2	O	536	GLU	CA-C-O	-5.91	110.76	120.80
1	C	94	ARG	CB-CG-CD	5.90	124.87	111.30
1	E	142	ARG	CA-C-O	-5.90	114.21	121.11
1	C	28	ASN	O-C-N	5.90	127.29	121.57
2	N	457	ARG	N-CA-C	-5.89	102.62	109.93
1	E	19	ILE	O-C-N	5.89	128.46	121.80
1	C	171	ILE	CB-CA-C	5.89	119.04	110.98
1	C	177	VAL	O-C-N	5.89	128.74	123.03
1	B	163	GLN	N-CA-C	5.88	119.28	108.69
2	P	494	SER	N-CA-C	-5.88	105.36	112.54
2	N	535	PHE	CA-CB-CG	5.88	119.68	113.80
1	C	129	SER	CA-C-O	-5.88	114.01	120.30
1	F	41	LYS	N-CA-C	-5.87	102.19	110.29
1	C	85	LEU	CB-CA-C	5.87	122.58	110.31
2	P	354	LEU	CB-CA-C	5.87	119.69	109.65
2	R	536	GLU	CA-C-O	-5.87	110.82	120.80
1	A	140	HIS	CA-CB-CG	5.87	119.67	113.80
2	M	413	ASP	CB-CA-C	5.87	120.57	110.77
2	P	414	ARG	CA-C-O	-5.87	112.67	119.59
1	F	109	VAL	CA-C-O	-5.86	114.83	121.75
2	P	532	LYS	N-CA-C	-5.86	102.64	110.55
1	E	142	ARG	NE-CZ-NH2	-5.86	113.92	119.20
1	C	4	LEU	N-CA-CB	-5.86	101.53	110.49
1	C	40	ALA	O-C-N	5.86	130.81	123.19
1	F	101	ALA	O-C-N	5.85	130.85	123.12
1	E	110	LYS	O-C-N	5.85	126.62	121.18
1	B	159	ASN	CB-CG-ND2	5.85	125.17	116.40
2	N	316	HIS	O-C-N	5.85	127.80	121.60
1	D	181	THR	CA-C-O	-5.84	113.81	120.58
1	F	43	ASP	CA-CB-CG	-5.84	106.76	112.60
2	P	497	ASN	OD1-CG-ND2	-5.84	116.76	122.60
2	Q	440	ARG	CD-NE-CZ	5.82	132.55	124.40
2	M	497	ASN	CA-C-O	5.82	123.62	119.32
1	E	177	VAL	CA-C-O	-5.82	114.08	120.48
2	R	428	ARG	CG-CD-NE	5.82	124.80	112.00
2	Q	530	GLN	CA-C-O	-5.82	114.04	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	497	ASN	CA-C-N	5.81	125.67	119.28
2	Q	497	ASN	C-N-CA	5.81	125.67	119.28
2	Q	316	HIS	O-C-N	5.81	127.75	121.60
2	Q	457	ARG	N-CA-C	-5.81	102.73	109.93
2	M	475	ILE	N-CA-C	-5.80	100.12	108.48
2	P	380	VAL	O-C-N	5.80	129.89	123.10
2	M	351	PHE	CA-CB-CG	5.80	119.60	113.80
2	O	401	GLN	CA-C-O	-5.80	114.93	121.25
1	A	163	GLN	N-CA-C	5.79	117.85	109.04
1	C	11	GLN	N-CA-CB	5.79	122.31	111.53
2	R	321	THR	CA-C-N	5.79	126.19	119.47
2	R	321	THR	C-N-CA	5.79	126.19	119.47
2	M	533	THR	CA-CB-OG1	-5.79	100.91	109.60
2	Q	382	GLY	O-C-N	5.79	130.28	123.62
1	B	8	THR	N-CA-C	-5.79	102.48	109.83
1	D	37	ASN	N-CA-C	5.78	119.40	112.93
2	P	497	ASN	CA-C-O	5.78	123.60	119.32
2	R	407	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	C	99	PHE	CB-CA-C	5.77	120.37	110.79
1	E	70	VAL	O-C-N	5.76	129.08	123.03
1	B	116	ASN	CA-CB-CG	5.76	118.36	112.60
2	Q	457	ARG	CA-CB-CG	5.76	125.62	114.10
1	E	197	PHE	N-CA-C	-5.75	100.02	109.40
2	P	463	PHE	O-C-N	5.75	130.31	123.24
2	N	457	ARG	NE-CZ-NH2	-5.75	114.03	119.20
2	N	478	LEU	N-CA-CB	-5.75	101.03	110.52
2	M	411	LYS	CB-CA-C	-5.75	98.98	110.42
2	P	474	LEU	N-CA-CB	-5.75	100.83	111.52
1	F	192	GLU	CA-C-O	-5.75	114.37	120.92
1	B	133	ARG	N-CA-C	-5.75	101.90	110.23
2	R	420	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	162	GLU	N-CA-CB	5.74	119.48	109.72
1	A	181	THR	O-C-N	5.74	130.08	123.02
2	P	503	GLN	OE1-CD-NE2	5.74	128.34	122.60
2	M	313	ARG	NE-CZ-NH1	5.74	127.24	121.50
2	Q	311	ARG	NE-CZ-NH2	-5.73	114.04	119.20
2	N	415	TYR	CB-CA-C	5.73	119.87	109.62
1	D	44	ALA	N-CA-C	-5.73	102.41	110.31
1	B	162	GLU	CA-CB-CG	5.72	125.55	114.10
1	B	103	GLU	O-C-N	5.72	130.11	123.30
1	F	5	LEU	N-CA-C	-5.72	102.19	110.08
2	O	440	ARG	CB-CG-CD	-5.72	98.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	350	ASN	CA-CB-CG	-5.72	106.88	112.60
1	D	184	ARG	CD-NE-CZ	-5.71	116.40	124.40
1	F	30	THR	CA-CB-CG2	5.71	120.20	110.50
2	M	380	VAL	N-CA-C	-5.70	99.42	107.75
2	R	497	ASN	CA-C-N	5.70	126.08	119.47
2	R	497	ASN	C-N-CA	5.70	126.08	119.47
1	E	36	TRP	N-CA-C	5.70	115.93	108.07
2	Q	440	ARG	CB-CG-CD	-5.70	98.20	111.30
1	A	3	GLU	CA-CB-CG	5.70	125.49	114.10
1	F	105	THR	CA-CB-OG1	-5.69	101.06	109.60
1	B	175	CYS	CA-CB-SG	5.69	127.48	114.40
2	O	463	PHE	O-C-N	5.69	130.24	123.24
2	M	502	GLN	CA-C-O	5.68	126.58	120.55
1	B	44	ALA	CA-C-N	5.68	125.63	119.78
1	B	44	ALA	C-N-CA	5.68	125.63	119.78
1	E	190	GLN	N-CA-CB	-5.68	100.95	111.52
2	Q	522	ARG	NH1-CZ-NH2	5.68	126.69	119.30
1	C	157	VAL	CB-CA-C	5.68	119.46	112.02
1	D	31	ARG	CA-C-N	5.68	128.15	120.65
1	D	31	ARG	C-N-CA	5.68	128.15	120.65
1	C	155	CYS	O-C-N	5.68	127.44	121.42
2	P	461	ILE	O-C-N	5.68	129.39	123.26
2	Q	424	GLY	CA-C-N	5.68	129.32	121.26
2	Q	424	GLY	C-N-CA	5.68	129.32	121.26
2	Q	462	HIS	CA-C-O	-5.68	114.39	120.92
2	O	372	LEU	N-CA-CB	-5.67	103.17	110.03
2	P	514	ASN	O-C-N	5.67	127.58	121.12
2	R	489	CYS	CA-C-N	5.67	125.52	119.28
2	R	489	CYS	C-N-CA	5.67	125.52	119.28
2	O	484	PRO	CB-CA-C	5.67	119.95	111.68
1	E	130	LEU	CB-CA-C	5.67	119.58	109.38
2	Q	316	HIS	N-CA-C	-5.67	102.04	110.20
2	N	381	ALA	N-CA-CB	-5.66	101.84	111.69
2	O	416	LEU	CB-CA-C	5.66	121.72	110.17
1	D	83	TYR	CB-CA-C	5.66	118.95	109.89
2	R	440	ARG	NH1-CZ-NH2	5.66	126.66	119.30
2	Q	382	GLY	CA-C-O	-5.66	115.44	121.38
1	B	19	ILE	CA-C-O	-5.65	114.36	120.47
1	B	133	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	C	195	THR	CA-CB-OG1	-5.65	101.13	109.60
2	M	430	LEU	CA-C-O	-5.64	114.28	120.43
2	Q	409	ARG	NE-CZ-NH2	5.64	124.28	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	LEU	CA-C-N	5.64	130.78	123.00
1	F	139	LEU	C-N-CA	5.64	130.78	123.00
2	Q	381	ALA	N-CA-CB	-5.63	101.89	111.69
2	P	517	ASP	CB-CA-C	5.63	121.63	110.42
1	A	18	HIS	N-CA-C	5.63	117.42	111.28
2	N	308	PHE	CB-CA-C	5.63	119.52	109.38
2	M	376	GLU	CA-C-O	-5.63	114.05	120.58
2	R	352	SER	CA-C-O	-5.63	114.55	120.63
2	Q	311	ARG	NE-CZ-NH1	5.63	127.13	121.50
2	O	407	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	A	97	THR	CA-C-O	-5.62	114.76	121.11
1	C	67	PHE	CA-C-O	-5.62	114.08	120.32
2	O	386	ASP	CB-CA-C	5.62	120.17	110.45
2	O	361	HIS	CA-CB-CG	-5.61	108.19	113.80
1	C	38	ARG	CB-CA-C	-5.61	102.20	111.51
2	Q	389	GLY	N-CA-C	-5.61	107.53	115.43
1	F	112	GLY	N-CA-C	-5.60	103.58	112.66
2	O	394	ASN	CA-C-O	-5.60	115.34	121.84
2	O	359	HIS	CA-CB-CG	-5.60	108.20	113.80
1	C	36	TRP	N-CA-C	5.60	115.79	108.07
1	C	32	ASP	CA-CB-CG	5.59	118.19	112.60
2	P	527	LEU	N-CA-C	-5.59	101.93	110.14
2	N	428	ARG	CB-CG-CD	5.58	124.13	111.30
2	N	430	LEU	CA-C-O	-5.58	114.24	120.54
1	D	106	LEU	N-CA-CB	-5.57	101.15	111.13
1	E	116	ASN	CA-C-O	-5.56	115.60	121.88
2	R	473	LYS	CG-CD-CE	5.56	124.09	111.30
2	O	324	TYR	N-CA-C	-5.56	98.18	108.24
1	D	137	ILE	CB-CA-C	5.56	118.44	110.33
1	C	94	ARG	CA-C-O	-5.55	114.61	121.11
2	R	307	ARG	N-CA-C	-5.55	100.73	109.50
1	E	28	ASN	N-CA-C	-5.55	101.61	110.10
2	R	348	GLY	O-C-N	5.54	127.31	121.77
1	E	192	GLU	CA-CB-CG	5.54	125.18	114.10
2	N	479	TYR	CA-C-O	-5.54	114.98	121.46
1	A	23	LEU	CB-CA-C	5.54	121.43	110.42
1	A	94	ARG	CB-CG-CD	5.53	124.03	111.30
1	E	76	ASN	CA-CB-CG	-5.53	107.07	112.60
1	C	41	LYS	N-CA-C	-5.53	102.81	109.72
2	M	303	GLN	N-CA-C	5.52	117.95	109.07
2	O	505	ILE	CB-CA-C	5.52	117.64	110.96
1	E	163	GLN	N-CA-C	5.52	117.43	109.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	THR	N-CA-C	-5.51	102.85	110.35
2	O	408	TYR	O-C-N	5.51	129.24	123.06
2	R	497	ASN	N-CA-CB	-5.51	103.01	110.23
2	O	364	LEU	N-CA-C	-5.50	106.07	112.89
2	M	476	THR	CA-CB-CG2	5.50	119.85	110.50
1	C	128	ILE	N-CA-C	5.49	116.39	108.48
2	M	447	TYR	O-C-N	5.48	126.11	121.83
2	Q	332	PRO	N-CA-CB	5.48	108.42	103.33
1	C	5	LEU	N-CA-C	-5.47	102.53	110.08
2	Q	503	GLN	OE1-CD-NE2	-5.47	117.13	122.60
2	P	475	ILE	N-CA-C	-5.47	100.61	108.48
1	A	80	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	64	ARG	NE-CZ-NH2	-5.46	114.28	119.20
2	P	372	LEU	CA-C-O	5.46	125.27	120.19
2	P	491	ILE	N-CA-CB	5.46	117.56	110.57
1	E	198	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	48	HIS	CA-CB-CG	-5.45	108.35	113.80
2	P	417	ALA	CA-C-N	5.45	125.43	120.03
2	P	417	ALA	C-N-CA	5.45	125.43	120.03
1	B	140	HIS	CB-CA-C	-5.45	100.32	109.48
1	B	19	ILE	O-C-N	5.44	127.95	121.80
2	N	415	TYR	N-CA-C	-5.44	102.95	110.35
1	A	168	GLU	CB-CG-CD	5.44	121.85	112.60
2	O	350	ASN	OD1-CG-ND2	-5.44	117.16	122.60
2	O	503	GLN	O-C-N	5.44	129.72	122.43
2	M	326	THR	CA-C-O	-5.44	112.69	119.38
2	N	358	ALA	N-CA-C	5.43	117.96	111.71
2	M	512	ASN	N-CA-CB	-5.43	102.46	110.49
2	P	325	LYS	N-CA-C	5.42	117.89	111.33
1	A	160	LEU	N-CA-C	-5.42	106.17	112.89
1	C	71	TRP	CB-CA-C	5.42	118.16	110.24
1	C	166	ARG	CD-NE-CZ	5.42	131.99	124.40
2	R	533	THR	CA-CB-OG1	-5.42	101.47	109.60
2	N	333	ARG	NH1-CZ-NH2	5.42	126.34	119.30
1	D	84	ASN	CB-CA-C	5.42	119.04	109.89
1	A	31	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	C	141	THR	CA-C-O	-5.41	115.62	121.36
2	N	383	ARG	CG-CD-NE	-5.41	100.10	112.00
2	N	390	LYS	CA-C-N	5.41	125.35	119.78
2	N	390	LYS	C-N-CA	5.41	125.35	119.78
2	M	314	ASN	CA-C-O	-5.41	113.19	119.14
2	Q	331	SER	CA-C-N	5.40	125.31	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	331	SER	C-N-CA	5.40	125.31	119.85
2	M	401	GLN	N-CA-CB	-5.40	101.99	111.49
2	P	450	ARG	CA-C-N	5.39	129.07	121.79
2	P	450	ARG	C-N-CA	5.39	129.07	121.79
2	M	316	HIS	O-C-N	5.39	127.31	121.60
1	F	52	LEU	CB-CA-C	5.39	122.04	110.45
2	R	308	PHE	CA-CB-CG	-5.37	108.43	113.80
1	E	90	ASN	CA-CB-CG	5.37	117.97	112.60
1	D	32	ASP	CA-C-O	-5.37	115.36	121.00
2	N	460	HIS	CA-CB-CG	-5.37	108.44	113.80
1	D	135	ILE	N-CA-CB	-5.37	104.91	111.67
1	B	152	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	C	52	LEU	CB-CA-C	5.36	121.98	110.45
1	A	96	ALA	N-CA-CB	-5.36	102.56	111.57
2	N	454	ASN	CA-C-O	-5.36	114.22	122.32
2	Q	398	GLU	CA-C-O	-5.36	115.05	121.11
2	R	496	ALA	CA-C-N	5.36	129.06	121.61
2	R	496	ALA	C-N-CA	5.36	129.06	121.61
2	M	361	HIS	CA-CB-CG	-5.35	108.45	113.80
2	O	527	LEU	CA-C-O	-5.35	115.13	121.66
1	A	144	TYR	N-CA-C	-5.35	102.28	110.14
1	C	188	ARG	CA-C-N	5.35	128.02	120.42
1	C	188	ARG	C-N-CA	5.35	128.02	120.42
2	P	512	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	E	8	THR	CA-CB-CG2	5.35	119.59	110.50
2	Q	349	PRO	N-CA-CB	5.35	108.31	103.33
1	B	196	VAL	O-C-N	5.35	128.44	122.61
2	O	415	TYR	CA-C-O	-5.34	115.74	121.56
2	O	514	ASN	OD1-CG-ND2	-5.34	117.26	122.60
2	P	428	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	C	33	GLN	OE1-CD-NE2	-5.34	117.26	122.60
2	P	326	THR	O-C-N	5.34	129.58	122.43
1	A	84	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	198	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	55	VAL	CB-CA-C	5.33	118.52	110.63
2	M	503	GLN	CG-CD-NE2	-5.33	108.41	116.40
2	P	407	ARG	NE-CZ-NH2	5.33	123.99	119.20
2	N	325	LYS	CA-C-N	5.32	127.94	120.28
2	N	325	LYS	C-N-CA	5.32	127.94	120.28
2	N	457	ARG	O-C-N	5.32	128.87	121.64
2	M	313	ARG	CD-NE-CZ	5.32	131.84	124.40
1	C	167	ARG	O-C-N	5.31	128.43	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	495	ILE	CA-C-O	-5.31	114.28	120.75
1	B	68	LEU	O-C-N	5.30	129.76	123.24
1	D	41	LYS	CA-C-N	5.30	126.47	119.84
1	D	41	LYS	C-N-CA	5.30	126.47	119.84
1	E	130	LEU	N-CA-CB	-5.30	102.15	110.69
1	E	140	HIS	CB-CA-C	-5.30	100.57	109.48
1	B	135	ILE	CA-C-N	5.30	127.81	120.29
1	B	135	ILE	C-N-CA	5.30	127.81	120.29
1	B	171	ILE	CB-CA-C	5.30	117.37	110.96
2	O	397	VAL	CA-C-O	-5.30	114.86	120.48
1	F	90	ASN	N-CA-C	-5.29	100.77	109.40
2	R	372	LEU	N-CA-CB	-5.29	101.38	110.11
2	P	372	LEU	N-CA-CB	-5.29	101.38	110.11
2	Q	313	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	96	ALA	O-C-N	5.29	128.81	123.26
2	N	333	ARG	N-CA-C	-5.29	107.20	113.97
2	M	517	ASP	N-CA-CB	-5.28	101.56	110.49
2	P	503	GLN	CG-CD-NE2	-5.28	108.47	116.40
1	F	38	ARG	NE-CZ-NH1	5.28	126.78	121.50
2	R	352	SER	CA-CB-OG	-5.28	100.53	111.10
1	E	196	VAL	O-C-N	5.28	128.43	122.67
1	E	46	GLY	CA-C-O	-5.28	118.65	122.45
1	B	162	GLU	CA-C-O	-5.28	115.25	120.90
2	N	451	ASN	N-CA-C	-5.28	100.07	108.30
1	C	76	ASN	OD1-CG-ND2	5.28	127.88	122.60
1	F	97	THR	N-CA-CB	5.28	120.55	111.00
2	R	401	GLN	CA-C-O	-5.28	115.50	121.25
1	B	174	ARG	CD-NE-CZ	-5.27	117.02	124.40
1	C	14	GLY	O-C-N	5.27	127.04	121.77
2	Q	522	ARG	CA-C-O	-5.27	114.63	120.38
2	O	352	SER	CA-C-O	-5.27	114.15	120.10
2	Q	494	SER	N-CA-C	-5.26	106.55	112.87
2	R	340	PRO	CA-C-O	-5.26	115.34	122.08
1	D	14	GLY	CA-C-N	5.26	124.87	119.56
1	D	14	GLY	C-N-CA	5.26	124.87	119.56
1	F	110	LYS	CA-C-O	5.25	124.69	119.49
2	M	326	THR	CA-CB-OG1	-5.25	101.72	109.60
1	E	35	ILE	O-C-N	5.25	130.48	122.76
1	D	23	LEU	CB-CA-C	5.25	120.87	110.42
2	P	390	LYS	N-CA-CB	-5.25	103.20	110.29
2	Q	428	ARG	O-C-N	5.25	129.26	123.33
1	C	114	VAL	N-CA-C	-5.25	100.77	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	333	ARG	CB-CA-C	5.25	120.22	109.67
1	E	8	THR	N-CA-C	-5.25	102.98	109.64
1	A	32	ASP	CA-C-O	-5.24	115.32	120.82
1	D	81	ASP	CA-C-O	-5.24	113.61	119.79
1	E	66	SER	N-CA-CB	5.24	118.84	110.46
1	E	158	LEU	CB-CA-C	5.24	119.49	110.79
1	C	42	PRO	CB-CA-C	5.24	120.20	111.56
2	R	526	VAL	N-CA-CB	-5.24	104.83	111.64
2	M	446	PRO	N-CA-C	-5.23	103.85	111.33
1	D	199	ASP	CA-C-O	-5.23	114.51	120.32
2	Q	333	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	121	PRO	N-CA-CB	5.22	108.20	103.34
2	M	343	ILE	CA-C-N	5.22	127.28	120.28
2	M	343	ILE	C-N-CA	5.22	127.28	120.28
2	O	322	PRO	N-CA-CB	5.22	108.73	103.25
2	N	313	ARG	CB-CA-C	5.22	120.40	110.27
1	C	95	THR	CA-CB-CG2	5.22	119.37	110.50
2	N	511	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	C	69	GLU	CB-CA-C	5.21	119.67	109.35
2	P	451	ASN	CB-CG-ND2	5.21	124.22	116.40
2	R	476	THR	CA-CB-CG2	5.21	119.36	110.50
1	F	99	PHE	O-C-N	5.21	128.31	122.22
2	Q	431	THR	N-CA-CB	5.20	117.80	110.36
1	B	130	LEU	N-CA-CB	-5.20	101.94	110.68
2	P	416	LEU	CB-CA-C	5.20	121.18	110.31
1	A	120	VAL	CA-C-N	5.20	124.96	119.76
1	A	120	VAL	C-N-CA	5.20	124.96	119.76
1	D	132	ALA	O-C-N	5.20	128.15	123.26
1	F	146	ASP	CA-CB-CG	5.19	117.79	112.60
2	R	321	THR	CA-CB-OG1	-5.19	101.81	109.60
2	Q	372	LEU	N-CA-CB	-5.19	98.78	110.56
1	C	158	LEU	N-CA-CB	-5.19	102.50	110.12
1	D	126	ILE	O-C-N	5.19	128.86	123.26
2	R	500	ALA	N-CA-C	-5.19	105.71	111.36
2	O	383	ARG	NH1-CZ-NH2	5.19	126.04	119.30
1	F	13	ALA	N-CA-C	-5.19	106.46	112.89
2	Q	441	THR	CA-CB-OG1	-5.18	101.82	109.60
2	R	450	ARG	NE-CZ-NH1	-5.18	116.31	121.50
2	M	372	LEU	CB-CA-C	5.18	116.54	108.61
2	O	330	ARG	CD-NE-CZ	-5.18	117.14	124.40
2	R	514	ASN	O-C-N	5.18	126.06	121.19
2	N	333	ARG	CD-NE-CZ	-5.18	117.15	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	THR	O-C-N	5.18	130.03	122.94
2	P	377	ARG	CD-NE-CZ	-5.18	117.15	124.40
2	N	341	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	E	50	LEU	CA-C-O	-5.17	114.74	120.38
2	M	481	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	107	HIS	CA-C-O	-5.17	114.63	120.32
1	F	35	ILE	N-CA-CB	-5.17	105.11	111.00
1	D	3	GLU	CA-C-O	-5.17	115.12	120.70
1	A	78	GLU	CB-CG-CD	-5.17	103.82	112.60
1	D	136	ASN	CA-C-O	5.17	125.89	120.42
2	M	519	LEU	O-C-N	5.16	128.60	122.20
1	B	41	LYS	N-CA-C	-5.16	103.44	110.36
2	O	497	ASN	N-CA-C	5.16	117.06	109.42
1	A	71	TRP	CA-CB-CG	5.16	123.40	113.60
2	N	405	GLY	CA-C-N	5.16	129.35	121.51
2	N	405	GLY	C-N-CA	5.16	129.35	121.51
1	D	176	GLU	CA-CB-CG	5.15	124.40	114.10
2	Q	403	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	F	33	GLN	OE1-CD-NE2	-5.15	117.45	122.60
2	R	401	GLN	CB-CG-CD	5.15	121.35	112.60
2	P	307	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	B	196	VAL	N-CA-C	-5.14	102.95	109.58
2	P	446	PRO	N-CA-C	-5.14	104.03	111.22
1	A	62	LEU	CA-C-N	5.14	130.29	123.10
1	A	62	LEU	C-N-CA	5.14	130.29	123.10
1	C	126	ILE	O-C-N	5.14	128.81	123.26
2	M	306	SER	N-CA-C	5.13	118.10	110.14
2	O	489	CYS	N-CA-C	5.13	116.12	109.65
2	P	311	ARG	CG-CD-NE	-5.13	100.70	112.00
2	P	420	ASP	CB-CA-C	5.13	116.05	110.15
1	E	38	ARG	NH1-CZ-NH2	5.13	125.97	119.30
2	N	426	VAL	CA-C-O	-5.13	114.93	120.67
1	C	54	GLN	CA-CB-CG	-5.12	103.85	114.10
2	R	451	ASN	N-CA-C	-5.12	99.89	110.80
1	B	110	LYS	O-C-N	5.12	126.40	121.28
1	F	113	VAL	N-CA-CB	-5.12	103.49	110.56
1	F	60	GLY	CA-C-O	-5.12	113.17	119.06
2	M	519	LEU	CA-C-O	-5.12	115.63	121.82
2	Q	468	PRO	N-CA-C	5.12	121.18	114.27
1	A	133	ARG	NH1-CZ-NH2	-5.11	112.65	119.30
1	B	177	VAL	CB-CA-C	5.11	117.31	110.42
1	C	123	ALA	N-CA-C	-5.11	102.73	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	ILE	O-C-N	5.11	128.72	123.20
1	E	69	GLU	CB-CG-CD	5.11	121.28	112.60
1	D	57	ASP	CA-CB-CG	5.10	117.70	112.60
2	M	376	GLU	CA-C-N	5.10	128.09	120.95
2	M	376	GLU	C-N-CA	5.10	128.09	120.95
1	F	60	GLY	N-CA-C	-5.09	108.25	115.43
1	A	37	ASN	N-CA-C	5.09	118.63	112.93
2	N	522	ARG	CA-C-O	-5.09	114.88	120.43
2	O	482	GLY	N-CA-C	5.09	122.12	115.40
2	Q	486	ILE	CB-CA-C	-5.09	108.86	113.70
1	A	187	ILE	CB-CG1-CD1	5.09	124.49	113.80
2	O	463	PHE	CA-CB-CG	5.09	118.89	113.80
1	D	21	LEU	N-CA-CB	-5.09	102.58	110.98
1	E	29	PRO	CA-C-O	-5.09	115.61	121.36
2	N	325	LYS	N-CA-C	5.09	119.71	111.37
2	P	321	THR	N-CA-CB	-5.09	104.74	111.40
2	N	443	LYS	O-C-N	5.08	126.36	121.28
2	P	483	ASP	CB-CA-C	5.08	117.28	109.60
2	M	416	LEU	CB-CA-C	5.08	119.76	110.11
2	P	338	SER	CA-C-O	-5.08	115.26	121.05
1	E	181	THR	N-CA-CB	5.08	117.41	109.85
2	Q	431	THR	O-C-N	5.07	128.57	122.79
2	R	452	GLY	CA-C-N	5.07	124.73	119.56
2	R	452	GLY	C-N-CA	5.07	124.73	119.56
1	C	168	GLU	CA-C-O	-5.07	115.17	120.55
1	B	58	GLY	CA-C-O	-5.07	112.42	119.01
2	P	351	PHE	CA-CB-CG	5.07	118.87	113.80
2	P	411	LYS	CB-CA-C	-5.07	100.34	110.42
1	F	148	GLU	CA-C-O	-5.06	115.94	121.20
2	M	478	LEU	O-C-N	5.06	129.11	123.19
2	N	442	ILE	CA-CB-CG2	5.06	119.10	110.50
2	Q	505	ILE	O-C-N	5.05	129.10	122.94
2	Q	413	ASP	CB-CA-C	5.05	118.86	110.78
2	M	383	ARG	NH1-CZ-NH2	5.05	125.86	119.30
2	R	461	ILE	CA-C-O	-5.04	115.01	120.36
1	A	123	ALA	CA-C-N	5.04	125.04	119.90
1	A	123	ALA	C-N-CA	5.04	125.04	119.90
2	Q	474	LEU	N-CA-CB	-5.04	102.15	111.52
2	N	507	LYS	CA-CB-CG	5.03	124.17	114.10
1	E	55	VAL	O-C-N	5.03	128.70	123.26
1	F	142	ARG	CA-C-N	-5.03	116.05	123.00
1	F	142	ARG	C-N-CA	-5.03	116.05	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	403	ASN	OD1-CG-ND2	-5.03	117.57	122.60
2	O	508	LEU	CA-C-O	-5.03	115.66	121.19
1	E	30	THR	CA-CB-CG2	5.03	119.05	110.50
2	N	497	ASN	CB-CA-C	5.03	116.62	109.38
2	N	505	ILE	CA-C-O	-5.02	114.92	120.74
2	Q	366	ASN	CA-CB-CG	5.02	117.62	112.60
2	Q	497	ASN	N-CA-CB	-5.02	103.66	110.23
1	B	90	ASN	CA-C-O	-5.02	114.94	120.36
2	O	400	TRP	CA-C-O	-5.02	115.37	120.99
2	R	414	ARG	CD-NE-CZ	-5.01	117.38	124.40
1	E	152	ASN	OD1-CG-ND2	-5.01	117.59	122.60
2	P	459	ALA	N-CA-C	-5.01	102.96	110.23
1	E	144	TYR	CA-CB-CG	5.01	122.92	113.90
1	E	3	GLU	CA-C-O	-5.01	114.95	120.36
2	O	455	ASP	CB-CA-C	5.01	118.01	109.80
2	O	346	THR	N-CA-C	5.00	119.08	112.92
2	Q	387	GLN	CB-CG-CD	-5.00	104.09	112.60
2	Q	440	ARG	NH1-CZ-NH2	5.00	125.80	119.30

There are no chirality outliers.

There are no planarity outliers.

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	1571	0	1499	61	0
1	B	1571	0	1499	72	0
1	C	1571	0	1499	75	0
1	D	1571	0	1499	50	0
1	E	1571	0	1499	69	0
1	F	1571	0	1499	101	0
2	M	1840	0	1793	85	0
2	N	1840	0	1793	62	0
2	O	1840	0	1793	64	0
2	P	1840	0	1793	93	0
2	Q	1840	0	1793	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1840	0	1793	104	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	A	83	0	0	2	0
4	B	79	0	0	3	0
4	C	80	0	0	4	0
4	D	77	0	0	1	0
4	E	77	0	0	1	0
4	F	83	0	0	4	0
4	M	154	0	0	5	0
4	N	163	0	0	6	0
4	O	158	0	0	7	0
4	P	159	0	0	4	0
4	Q	163	0	0	8	0
4	R	158	0	0	8	0
All	All	21906	0	19752	838	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 21.

All (838) 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:E:165:GLN:H	1:E:165:GLN:NE2	1.32	1.26
1:E:165:GLN:HE21	1:E:165:GLN:N	1.38	1.20
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.64	1.12
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.34	1.07
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.34	1.06
1:B:165:GLN:H	1:B:165:GLN:NE2	1.59	1.00
1:B:176:GLU:HG3	1:B:180:LYS:O	1.62	0.99
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.30	0.96
1:C:163:GLN:HB3	1:C:165:GLN:HE21	1.32	0.93
1:F:176:GLU:CG	1:F:179:GLY:HA2	1.99	0.93
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.69	0.93
2:O:522:ARG:NH1	4:O:673:HOH:O	2.01	0.92
2:R:411:LYS:O	2:R:414:ARG:NH1	2.02	0.92
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.07	0.89
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.88	0.89
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.55	0.89
1:B:176:GLU:HG3	1:B:180:LYS:C	1.97	0.89
2:Q:411:LYS:HE2	2:Q:411:LYS:H	1.38	0.86
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.41	0.86
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.11	0.86
2:R:497:ASN:ND2	2:R:499:GLU:H	1.75	0.85
2:P:411:LYS:CE	2:P:411:LYS:H	1.91	0.83
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.43	0.83
1:C:44:ALA:O	1:C:48:HIS:NE2	2.12	0.82
2:Q:411:LYS:H	2:Q:411:LYS:CE	1.92	0.82
1:D:180:LYS:HG3	1:D:181:THR:N	1.93	0.82
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.61	0.82
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.15	0.81
2:O:497:ASN:HD22	2:O:499:GLU:H	1.28	0.81
2:N:497:ASN:ND2	2:N:499:GLU:HB2	1.96	0.81
2:N:361:HIS:CD2	2:N:361:HIS:H	1.97	0.81
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	1.96	0.80
2:M:497:ASN:ND2	2:M:499:GLU:H	1.79	0.80
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.96	0.80
1:F:177:VAL:O	1:F:180:LYS:HB3	1.82	0.79
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.17	0.79
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.63	0.78
2:R:497:ASN:C	2:R:497:ASN:HD22	1.91	0.78
2:P:411:LYS:O	2:P:414:ARG:NH1	2.17	0.78
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.66	0.78
2:R:361:HIS:H	2:R:361:HIS:CD2	1.99	0.77
1:A:176:GLU:HG3	1:A:180:LYS:O	1.84	0.77
2:N:522:ARG:NH1	4:N:673:HOH:O	2.17	0.77
1:F:165:GLN:NE2	1:F:165:GLN:H	1.83	0.77
2:Q:411:LYS:HE2	2:Q:411:LYS:N	1.99	0.77
2:P:497:ASN:HD22	2:P:499:GLU:H	1.29	0.77
1:C:26:ALA:O	2:O:411:LYS:NZ	2.16	0.76
2:M:522:ARG:NH1	4:M:661:HOH:O	2.17	0.76
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.11	0.76
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.10	0.76
2:O:497:ASN:ND2	2:O:499:GLU:H	1.84	0.75
2:M:361:HIS:H	2:M:361:HIS:CD2	2.05	0.74
1:C:143:LEU:HD23	1:C:143:LEU:C	2.11	0.74
1:B:65:ASP:OD2	1:B:133:ARG:HD3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.21	0.74
1:A:65:ASP:OD2	1:A:133:ARG:HD3	1.88	0.74
2:R:411:LYS:H	2:R:411:LYS:CE	2.01	0.73
1:F:23:LEU:O	1:F:26:ALA:HB3	1.87	0.73
2:N:411:LYS:CE	2:N:411:LYS:H	2.02	0.73
1:B:39:LEU:HD13	1:B:106:LEU:HD21	1.70	0.73
2:P:497:ASN:ND2	2:P:499:GLU:H	1.85	0.73
2:O:413:ASP:C	2:O:414:ARG:HD2	2.12	0.73
2:M:411:LYS:O	2:M:414:ARG:NH1	2.22	0.72
1:B:165:GLN:H	1:B:165:GLN:HE21	1.38	0.72
2:N:361:HIS:H	2:N:361:HIS:HD2	1.35	0.72
2:N:411:LYS:H	2:N:411:LYS:HE2	1.55	0.72
2:N:497:ASN:HD22	2:N:499:GLU:H	1.37	0.71
2:P:411:LYS:H	2:P:411:LYS:HE2	1.53	0.71
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.72	0.71
2:Q:522:ARG:NH1	4:Q:1072:HOH:O	2.24	0.71
1:C:35:ILE:HG22	1:C:94:ARG:HD3	1.73	0.71
1:F:133:ARG:HG3	2:R:326:THR:HG21	1.71	0.70
1:F:50:LEU:HD12	1:F:51:LEU:N	2.06	0.70
1:B:176:GLU:HA	1:B:180:LYS:O	1.92	0.70
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.19	0.70
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.07	0.70
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.38	0.70
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.39	0.69
2:M:497:ASN:HD22	2:M:499:GLU:H	1.40	0.69
1:C:165:GLN:NE2	1:C:165:GLN:H	1.91	0.69
2:R:497:ASN:HD22	2:R:499:GLU:H	1.40	0.69
2:P:376:GLU:O	2:P:442:ILE:HA	1.92	0.69
2:O:411:LYS:H	2:O:411:LYS:CE	2.06	0.68
1:C:52:LEU:HD23	1:C:103:GLU:CD	2.19	0.68
2:Q:376:GLU:OE1	4:Q:1021:HOH:O	2.09	0.68
2:R:361:HIS:H	2:R:361:HIS:HD2	1.41	0.68
2:R:522:ARG:NH1	4:R:1311:HOH:O	2.25	0.68
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.28	0.68
2:P:325:LYS:HD3	2:Q:335:ALA:HB1	1.75	0.68
1:E:133:ARG:HG3	2:Q:326:THR:HG21	1.76	0.68
2:P:414:ARG:NE	2:P:414:ARG:HA	2.08	0.68
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.09	0.68
2:Q:306:SER:OG	2:Q:530:GLN:NE2	2.22	0.67
1:F:53:GLY:HA3	1:F:185:PHE:O	1.94	0.67
2:R:497:ASN:HD22	2:R:498:PRO:N	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ALA:O	1:E:48:HIS:NE2	2.21	0.67
2:M:411:LYS:H	2:M:411:LYS:HD3	1.59	0.67
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.77	0.67
1:C:4:LEU:HB3	2:O:387:GLN:HB3	1.76	0.67
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.76	0.67
2:M:411:LYS:H	2:M:411:LYS:CD	2.08	0.66
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.91	0.66
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.29	0.66
2:M:413:ASP:O	2:M:414:ARG:NH1	2.28	0.66
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.93	0.66
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.76	0.66
1:C:103:GLU:OE2	1:C:184:ARG:NH1	2.25	0.66
2:R:390:LYS:HE2	4:R:1433:HOH:O	1.96	0.66
1:C:64:ARG:O	1:C:98:THR:HA	1.95	0.66
2:M:390:LYS:HD2	4:M:637:HOH:O	1.96	0.66
1:B:39:LEU:HD13	1:B:106:LEU:CD2	2.26	0.66
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.13	0.66
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.97	0.65
1:C:41:LYS:O	1:C:43:ASP:N	2.29	0.65
1:E:26:ALA:O	2:Q:411:LYS:NZ	2.24	0.65
2:R:410:HIS:ND1	2:R:411:LYS:HE2	2.10	0.65
2:Q:454:ASN:HB2	2:R:310:ILE:HG13	1.78	0.65
2:Q:497:ASN:ND2	2:Q:499:GLU:HB2	2.11	0.65
2:M:376:GLU:OE1	4:M:632:HOH:O	2.13	0.65
2:Q:359:HIS:O	2:Q:366:ASN:HB3	1.96	0.65
2:M:376:GLU:O	2:M:442:ILE:HA	1.97	0.65
1:D:176:GLU:HA	1:D:180:LYS:O	1.97	0.65
1:C:35:ILE:CG2	1:C:94:ARG:HD3	2.26	0.65
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.62	0.65
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.79	0.64
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.61	0.64
2:R:392:VAL:HG12	2:R:395:THR:HB	1.79	0.64
2:P:361:HIS:H	2:P:361:HIS:CD2	2.14	0.64
2:O:361:HIS:H	2:O:361:HIS:CD2	2.15	0.64
1:F:26:ALA:O	2:R:411:LYS:NZ	2.27	0.64
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.78	0.64
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.32	0.64
1:F:176:GLU:HG3	1:F:180:LYS:H	1.62	0.64
1:F:190:GLN:HG3	2:R:333:ARG:HG2	1.80	0.64
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.62	0.63
2:R:411:LYS:H	2:R:411:LYS:HE2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:536:GLU:HB2	4:Q:1116:HOH:O	1.97	0.63
1:A:84:ASN:OD1	1:A:86:GLU:HB2	1.99	0.63
1:B:26:ALA:O	2:N:411:LYS:NZ	2.22	0.63
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.63	0.63
2:M:363:LEU:HD11	2:M:427:GLY:HA3	1.81	0.63
1:D:165:GLN:H	1:D:165:GLN:HE21	1.44	0.63
1:E:24:GLU:O	1:E:27:GLY:N	2.28	0.62
2:Q:411:LYS:O	2:Q:414:ARG:NH1	2.31	0.62
2:R:399:MET:HA	2:R:462:HIS:O	1.98	0.62
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.82	0.62
1:C:163:GLN:HB3	1:C:165:GLN:HE22	1.57	0.62
1:D:26:ALA:O	2:P:411:LYS:NZ	2.30	0.62
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.06	0.62
2:O:326:THR:HG22	2:O:326:THR:O	1.99	0.62
2:O:362:ASP:OD1	2:O:440:ARG:HD3	2.00	0.62
1:E:47:GLU:O	1:E:49:ILE:HG23	2.00	0.62
2:R:410:HIS:CE1	2:R:411:LYS:HE2	2.34	0.62
2:O:376:GLU:O	2:O:442:ILE:HA	1.98	0.62
1:F:176:GLU:HG3	1:F:180:LYS:N	2.15	0.62
1:F:147:ASP:OD2	1:F:174:ARG:CD	2.47	0.62
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.35	0.61
1:B:165:GLN:H	1:B:165:GLN:CD	2.06	0.61
1:F:143:LEU:C	1:F:143:LEU:HD23	2.25	0.61
1:B:19:ILE:O	2:N:426:VAL:HG21	2.00	0.61
2:N:478:LEU:C	2:N:478:LEU:HD23	2.25	0.61
1:E:176:GLU:HA	1:E:180:LYS:O	1.99	0.61
1:B:176:GLU:HG3	1:B:180:LYS:N	2.15	0.61
1:B:176:GLU:OE2	1:B:179:GLY:C	2.43	0.61
2:Q:386:ASP:HA	2:Q:527:LEU:O	2.00	0.61
2:R:318:LYS:HE2	4:R:1430:HOH:O	2.00	0.61
1:D:35:ILE:HG22	1:D:94:ARG:HG3	1.82	0.61
1:D:165:GLN:H	1:D:165:GLN:NE2	1.99	0.60
2:O:414:ARG:HD2	2:O:414:ARG:N	2.16	0.60
2:P:414:ARG:HA	2:P:414:ARG:HE	1.66	0.60
2:M:414:ARG:HD2	2:M:414:ARG:N	2.16	0.60
2:M:361:HIS:H	2:M:361:HIS:HD2	1.43	0.60
1:F:174:ARG:HD2	1:F:183:TYR:CE2	2.36	0.60
1:A:36:TRP:HA	1:A:36:TRP:CE3	2.35	0.60
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.82	0.60
1:B:23:LEU:N	1:B:23:LEU:HD12	2.17	0.60
1:F:74:ASP:HB2	4:F:1285:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HB2	4:A:278:HOH:O	2.02	0.60
2:N:359:HIS:O	2:N:366:ASN:HB3	2.01	0.60
1:E:149:ALA:O	4:E:254:HOH:O	2.17	0.60
1:F:36:TRP:CG	1:F:37:ASN:H	2.20	0.59
1:A:176:GLU:HA	1:A:180:LYS:O	2.02	0.59
1:B:176:GLU:CG	1:B:180:LYS:N	2.65	0.59
1:E:164:PRO:N	1:E:165:GLN:NE2	2.50	0.59
2:Q:390:LYS:HE2	4:Q:1154:HOH:O	2.02	0.59
1:A:155:CYS:O	1:A:159:ASN:ND2	2.32	0.59
1:C:31:ARG:NH1	2:O:428:ARG:HG2	2.18	0.59
2:M:304:ASP:HB2	2:M:343:ILE:HG13	1.84	0.59
2:M:497:ASN:HD22	2:M:498:PRO:N	2.00	0.59
2:R:408:TYR:HE2	2:R:447:TYR:CZ	2.20	0.59
1:A:36:TRP:CG	1:A:37:ASN:H	2.20	0.59
1:D:177:VAL:O	1:D:180:LYS:N	2.34	0.59
2:O:315:TRP:HZ2	2:O:503:GLN:NE2	2.00	0.59
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.01	0.59
2:O:411:LYS:H	2:O:411:LYS:HE2	1.66	0.59
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.38	0.59
2:P:315:TRP:HZ2	2:P:503:GLN:NE2	2.01	0.59
1:F:80:GLN:O	1:F:91:SER:HB2	2.02	0.59
1:F:163:GLN:HB3	1:F:165:GLN:HE21	1.66	0.59
1:A:165:GLN:CD	1:A:165:GLN:H	2.11	0.58
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.18	0.58
2:N:411:LYS:HE2	2:N:411:LYS:N	2.18	0.58
1:E:54:GLN:OE1	1:E:184:ARG:NH2	2.36	0.58
1:D:33:GLN:HG2	1:D:85:LEU:HD12	1.85	0.58
1:B:165:GLN:NE2	1:B:165:GLN:N	2.43	0.58
2:N:497:ASN:ND2	2:N:499:GLU:H	2.00	0.58
1:E:143:LEU:HD12	1:E:185:PHE:CB	2.33	0.58
2:R:405:GLY:HA3	4:R:1277:HOH:O	2.04	0.58
1:C:41:LYS:O	1:C:42:PRO:C	2.47	0.58
2:P:522:ARG:NH1	4:P:674:HOH:O	2.30	0.58
2:O:497:ASN:HD22	2:O:497:ASN:C	2.12	0.58
1:E:31:ARG:HH12	2:Q:428:ARG:HG2	1.69	0.58
1:F:157:VAL:O	1:F:160:LEU:HB2	2.03	0.58
1:C:64:ARG:HH11	1:C:64:ARG:HG2	1.67	0.58
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.37	0.58
1:E:143:LEU:HD12	1:E:185:PHE:CG	2.39	0.57
1:E:165:GLN:NE2	1:E:165:GLN:N	2.17	0.57
1:A:50:LEU:O	1:A:182:ALA:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.51	0.57
1:B:74:ASP:OD2	1:B:80:GLN:NE2	2.37	0.57
2:P:411:LYS:HE2	2:P:411:LYS:N	2.19	0.57
1:F:4:LEU:HB3	2:R:387:GLN:HB3	1.86	0.57
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.23	0.57
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.86	0.57
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.70	0.57
1:B:51:LEU:HD11	1:B:126:ILE:HD12	1.86	0.56
2:N:356:PHE:HD2	2:N:428:ARG:HD3	1.70	0.56
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.87	0.56
1:F:24:GLU:O	1:F:27:GLY:N	2.36	0.56
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.70	0.56
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.30	0.56
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.40	0.56
1:F:165:GLN:H	1:F:165:GLN:CD	2.13	0.56
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.88	0.56
1:E:116:ASN:C	1:E:116:ASN:OD1	2.49	0.56
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.54	0.56
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.87	0.56
2:N:386:ASP:HA	2:N:527:LEU:O	2.06	0.56
1:C:41:LYS:O	1:C:44:ALA:N	2.37	0.56
2:P:411:LYS:H	2:P:411:LYS:NZ	2.03	0.56
2:N:484:PRO:O	2:N:488:MET:HE3	2.06	0.56
1:F:176:GLU:HA	1:F:180:LYS:O	2.06	0.56
2:R:411:LYS:H	2:R:411:LYS:CD	2.18	0.56
1:C:64:ARG:HG2	1:C:64:ARG:NH1	2.21	0.56
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.06	0.56
2:N:414:ARG:NE	2:N:414:ARG:HA	2.21	0.56
1:A:188:ARG:HG3	1:A:188:ARG:HH11	1.71	0.55
1:A:64:ARG:O	1:A:98:THR:HA	2.07	0.55
1:B:94:ARG:NH2	2:N:398:GLU:OE2	2.38	0.55
1:C:146:ASP:HB3	1:C:171:ILE:HG22	1.88	0.55
2:N:360:ASP:OD2	2:N:428:ARG:HD2	2.06	0.55
1:E:94:ARG:NH2	2:Q:398:GLU:OE2	2.36	0.55
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.05	0.55
1:C:163:GLN:CB	1:C:165:GLN:NE2	2.54	0.55
2:Q:429:CYS:SG	4:Q:1122:HOH:O	2.06	0.55
2:Q:437:TYR:CD1	2:Q:437:TYR:C	2.84	0.55
2:R:413:ASP:C	2:R:414:ARG:HD2	2.31	0.55
1:F:178:ASP:O	1:F:179:GLY:C	2.49	0.55
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.88	0.55
2:R:359:HIS:O	2:R:366:ASN:HB3	2.07	0.55
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.42	0.55
2:R:414:ARG:HD2	2:R:414:ARG:N	2.21	0.55
2:P:363:LEU:HD11	2:P:427:GLY:HA3	1.89	0.54
1:B:176:GLU:HG2	1:B:179:GLY:CA	2.36	0.54
1:C:190:GLN:HG3	2:O:333:ARG:HG2	1.89	0.54
2:O:400:TRP:HA	2:O:425:GLY:O	2.07	0.54
1:E:188:ARG:HG3	1:E:188:ARG:NH1	2.23	0.54
2:R:400:TRP:HA	2:R:425:GLY:O	2.07	0.54
1:D:51:LEU:O	1:D:105:THR:HA	2.06	0.54
2:P:361:HIS:H	2:P:361:HIS:HD2	1.54	0.54
2:Q:411:LYS:H	2:Q:411:LYS:CD	2.20	0.54
2:N:450:ARG:HG3	4:N:639:HOH:O	2.08	0.54
2:O:381:ALA:O	2:O:522:ARG:HA	2.08	0.54
1:E:177:VAL:O	1:E:180:LYS:HB3	2.07	0.54
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.55	0.54
2:R:364:LEU:HB2	2:R:440:ARG:HD3	1.90	0.54
1:D:110:LYS:NZ	1:D:147:ASP:OD1	2.40	0.54
1:D:153:ALA:C	1:D:154:LYS:HE3	2.32	0.54
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.08	0.54
2:P:443:LYS:HE2	2:P:480:PHE:CG	2.43	0.54
2:P:484:PRO:O	2:P:487:PRO:HD2	2.08	0.54
1:A:143:LEU:C	1:A:143:LEU:HD23	2.32	0.54
2:N:363:LEU:HD23	2:N:425:GLY:HA2	1.89	0.54
1:F:50:LEU:HD12	1:F:51:LEU:H	1.73	0.54
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.38	0.54
2:R:478:LEU:C	2:R:478:LEU:HD23	2.33	0.54
1:C:114:VAL:HG22	4:C:234:HOH:O	2.07	0.54
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.89	0.54
1:F:47:GLU:O	1:F:49:ILE:HG23	2.08	0.53
2:R:486:ILE:N	2:R:487:PRO:CD	2.71	0.53
2:Q:497:ASN:HD21	2:Q:499:GLU:HB2	1.73	0.53
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.90	0.53
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.09	0.53
1:E:131:PHE:O	1:E:132:ALA:HB2	2.07	0.53
1:F:33:GLN:NE2	2:R:355:GLY:HA3	2.23	0.53
1:F:84:ASN:O	1:F:90:ASN:ND2	2.31	0.53
2:O:486:ILE:N	2:O:487:PRO:CD	2.72	0.53
1:C:36:TRP:CG	1:C:37:ASN:H	2.26	0.53
1:F:51:LEU:HD11	1:F:126:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:390:LYS:HE2	4:O:730:HOH:O	2.07	0.53
1:E:92:PHE:CD1	2:Q:349:PRO:HG3	2.44	0.53
2:M:434:ASP:HB3	2:M:436:TYR:CE2	2.44	0.53
2:M:448:PRO:HD3	2:M:456:TRP:CZ3	2.44	0.53
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.72	0.52
2:R:376:GLU:O	2:R:442:ILE:HA	2.10	0.52
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.90	0.52
1:B:39:LEU:CD1	1:B:106:LEU:HD21	2.38	0.52
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.58	0.52
1:B:40:ALA:HB2	1:B:89:PHE:HD1	1.75	0.52
1:B:170:LEU:HD21	1:B:196:VAL:HB	1.92	0.52
2:N:399:MET:HA	2:N:462:HIS:O	2.09	0.52
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.91	0.52
1:D:36:TRP:CG	1:D:37:ASN:H	2.27	0.52
2:Q:414:ARG:HD2	2:Q:414:ARG:N	2.24	0.52
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.90	0.52
1:F:52:LEU:HD21	1:F:184:ARG:NH1	2.24	0.52
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.75	0.52
1:F:176:GLU:CG	1:F:179:GLY:CA	2.81	0.52
2:R:361:HIS:CD2	2:R:361:HIS:N	2.68	0.52
1:B:4:LEU:HB3	2:N:387:GLN:HB3	1.92	0.52
2:N:361:HIS:CD2	2:N:361:HIS:N	2.65	0.52
1:C:177:VAL:O	1:C:180:LYS:HB3	2.09	0.52
1:D:19:ILE:O	2:P:426:VAL:HG21	2.10	0.52
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.07	0.52
2:M:411:LYS:H	2:M:411:LYS:CE	2.23	0.52
2:M:416:LEU:C	2:M:416:LEU:HD23	2.35	0.52
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.40	0.52
2:O:390:LYS:CD	4:O:730:HOH:O	2.57	0.52
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.90	0.52
1:F:70:VAL:HA	1:F:127:ASN:O	2.10	0.52
1:F:123:ALA:O	1:F:124:PRO:C	2.51	0.52
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.10	0.52
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.45	0.51
1:E:20:GLY:O	1:E:21:LEU:HD23	2.10	0.51
2:M:413:ASP:C	2:M:414:ARG:HD2	2.35	0.51
2:M:497:ASN:HD22	2:M:497:ASN:C	2.17	0.51
2:P:399:MET:HA	2:P:462:HIS:O	2.10	0.51
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.91	0.51
1:F:94:ARG:NH2	2:R:398:GLU:OE2	2.41	0.51
1:B:165:GLN:HE21	1:B:165:GLN:N	2.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:THR:OG1	1:C:109:VAL:N	2.39	0.51
1:D:52:LEU:HD23	1:D:103:GLU:CD	2.35	0.51
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	1.93	0.51
1:D:26:ALA:O	2:P:411:LYS:CE	2.58	0.51
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.76	0.51
2:R:360:ASP:HB3	2:R:428:ARG:HG3	1.92	0.51
1:B:92:PHE:CD1	2:N:349:PRO:HG3	2.46	0.51
2:Q:382:GLY:HA3	2:Q:523:PHE:O	2.11	0.51
1:F:198:PHE:HA	2:R:337:VAL:O	2.10	0.51
1:C:41:LYS:C	1:C:43:ASP:N	2.69	0.51
2:P:497:ASN:HD22	2:P:497:ASN:C	2.18	0.51
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.41	0.51
2:N:307:ARG:CG	2:N:533:THR:HG22	2.38	0.51
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.11	0.51
1:A:51:LEU:O	1:A:105:THR:HA	2.11	0.50
1:B:74:ASP:HB2	4:B:329:HOH:O	2.11	0.50
2:P:497:ASN:HD22	2:P:499:GLU:N	2.04	0.50
2:R:306:SER:CB	2:R:530:GLN:HE21	2.22	0.50
2:R:460:HIS:HB3	2:R:479:TYR:CD1	2.46	0.50
2:R:472:THR:HG22	2:R:528:ARG:HB2	1.93	0.50
2:P:313:ARG:O	2:P:318:LYS:HE3	2.10	0.50
2:O:359:HIS:O	2:O:366:ASN:HB3	2.12	0.50
2:P:310:ILE:HD12	2:R:453:PRO:HB2	1.93	0.50
2:O:315:TRP:CZ2	2:O:503:GLN:NE2	2.80	0.50
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.46	0.50
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.77	0.50
2:O:390:LYS:CE	4:O:730:HOH:O	2.60	0.50
1:F:176:GLU:HG2	1:F:179:GLY:CA	2.25	0.50
2:R:408:TYR:HE2	2:R:447:TYR:CE2	2.29	0.50
2:N:376:GLU:O	2:N:442:ILE:HA	2.12	0.50
2:P:497:ASN:HD22	2:P:498:PRO:N	2.10	0.50
1:A:188:ARG:HG3	1:A:188:ARG:NH1	2.26	0.50
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.93	0.50
2:R:306:SER:OG	2:R:530:GLN:NE2	2.37	0.50
2:N:360:ASP:O	2:N:427:GLY:HA2	2.12	0.49
2:N:413:ASP:C	2:N:414:ARG:HD2	2.37	0.49
1:F:18:HIS:CE1	1:F:98:THR:HG22	2.47	0.49
2:R:483:ASP:HB2	4:R:1379:HOH:O	2.11	0.49
1:A:52:LEU:O	1:A:184:ARG:HA	2.13	0.49
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.93	0.49
1:D:143:LEU:C	1:D:143:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:356:PHE:HD1	2:P:428:ARG:HD3	1.77	0.49
1:E:165:GLN:H	1:E:165:GLN:HE21	0.59	0.49
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.48	0.49
1:E:6:PRO:HG2	2:Q:503:GLN:NE2	2.27	0.49
2:Q:410:HIS:ND1	2:Q:411:LYS:HE2	2.28	0.49
2:M:410:HIS:CE1	2:M:411:LYS:HZ1	2.30	0.49
1:B:143:LEU:C	1:B:143:LEU:HD23	2.37	0.49
1:C:89:PHE:CE1	1:C:109:VAL:HG22	2.47	0.49
2:R:390:LYS:HD3	4:R:1393:HOH:O	2.11	0.49
2:R:400:TRP:CD2	2:R:462:HIS:HB2	2.48	0.49
1:B:177:VAL:O	1:B:180:LYS:HB3	2.12	0.49
1:E:41:LYS:O	1:E:44:ALA:N	2.41	0.49
2:R:363:LEU:N	2:R:363:LEU:HD12	2.27	0.49
2:M:453:PRO:HB2	2:N:310:ILE:HD12	1.95	0.49
2:O:411:LYS:H	2:O:411:LYS:CD	2.25	0.49
2:O:478:LEU:HD23	2:O:478:LEU:C	2.38	0.49
2:P:478:LEU:C	2:P:478:LEU:HD23	2.38	0.49
2:Q:390:LYS:HD2	4:Q:1033:HOH:O	2.12	0.49
2:M:386:ASP:HA	2:M:527:LEU:O	2.13	0.49
2:M:515:PRO:HB3	2:P:453:PRO:O	2.13	0.49
2:R:383:ARG:HA	2:R:435:GLY:O	2.13	0.49
1:A:163:GLN:CB	1:A:165:GLN:HE22	2.26	0.49
1:F:19:ILE:O	2:R:426:VAL:HG21	2.12	0.49
1:B:23:LEU:N	1:B:23:LEU:CD1	2.75	0.49
1:C:47:GLU:O	1:C:49:ILE:HG23	2.13	0.49
2:R:473:LYS:HD2	2:R:474:LEU:N	2.28	0.49
1:C:143:LEU:C	1:C:143:LEU:CD2	2.85	0.48
2:R:484:PRO:O	2:R:488:MET:HE3	2.12	0.48
1:C:39:LEU:N	1:C:39:LEU:HD12	2.28	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.47	0.48
1:B:23:LEU:CD1	1:B:23:LEU:H	2.26	0.48
2:R:354:LEU:HD21	2:R:428:ARG:NH2	2.29	0.48
2:N:328:ILE:HD12	2:O:335:ALA:HB2	1.96	0.48
2:P:359:HIS:O	2:P:366:ASN:HB3	2.14	0.48
2:O:495:ILE:CG2	2:O:500:ALA:HB3	2.44	0.48
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.43	0.48
1:E:74:ASP:C	1:E:74:ASP:OD1	2.54	0.48
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.13	0.48
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.28	0.48
1:B:63:VAL:HG12	1:B:66:SER:HB3	1.95	0.48
1:B:68:LEU:HD12	1:B:68:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:304:ASP:HA	4:P:740:HOH:O	2.12	0.48
2:M:373:PRO:HB3	2:M:423:PHE:HB2	1.95	0.48
2:M:410:HIS:ND1	2:M:411:LYS:HE2	2.28	0.48
2:O:451:ASN:HB3	2:O:455:ASP:OD2	2.14	0.48
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.80	0.48
2:P:305:ASN:N	4:P:740:HOH:O	2.41	0.48
1:E:163:GLN:C	1:E:165:GLN:NE2	2.72	0.48
1:F:52:LEU:C	1:F:52:LEU:HD22	2.38	0.48
1:F:146:ASP:HB3	1:F:171:ILE:CG2	2.44	0.48
1:A:180:LYS:CG	1:A:181:THR:N	2.76	0.48
2:O:390:LYS:HD3	4:O:730:HOH:O	2.13	0.48
2:O:408:TYR:HE1	2:O:447:TYR:CE2	2.30	0.48
2:P:409:ARG:HA	2:P:419:LEU:HD21	1.95	0.48
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.96	0.48
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.69	0.48
1:D:123:ALA:HB3	1:D:144:TYR:CE2	2.49	0.48
1:D:177:VAL:O	1:D:180:LYS:HB3	2.14	0.48
2:P:485:LEU:HA	2:P:488:MET:HE3	1.96	0.48
2:P:497:ASN:ND2	2:P:499:GLU:OE1	2.40	0.48
2:Q:493:LYS:C	2:Q:495:ILE:N	2.68	0.48
2:R:363:LEU:HD23	2:R:425:GLY:HA2	1.96	0.48
2:R:397:VAL:O	2:R:428:ARG:HA	2.14	0.48
1:D:1:PRO:HG2	2:R:488:MET:HE2	1.95	0.47
1:D:61:HIS:CD2	1:E:165:GLN:OE1	2.67	0.47
1:F:71:TRP:CZ3	1:F:91:SER:HB3	2.49	0.47
2:R:442:ILE:O	2:R:442:ILE:HG13	2.13	0.47
1:A:52:LEU:HD23	1:A:103:GLU:CD	2.40	0.47
2:M:478:LEU:HD23	2:M:478:LEU:C	2.39	0.47
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.69	0.47
1:F:41:LYS:HE3	1:F:85:LEU:O	2.14	0.47
2:N:478:LEU:HD23	2:N:478:LEU:O	2.14	0.47
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.49	0.47
2:P:383:ARG:NH2	2:P:391:PRO:HG3	2.28	0.47
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.13	0.47
2:Q:493:LYS:C	2:Q:495:ILE:H	2.21	0.47
2:R:522:ARG:NH2	2:R:524:ASP:OD1	2.46	0.47
1:C:131:PHE:O	1:C:132:ALA:HB2	2.14	0.47
1:D:26:ALA:O	2:P:411:LYS:HE3	2.14	0.47
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.94	0.47
2:Q:468:PRO:HD2	2:Q:472:THR:OG1	2.15	0.47
1:F:174:ARG:HE	1:F:181:THR:HG21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:GLU:OE2	1:F:179:GLY:C	2.57	0.47
2:O:307:ARG:HG2	2:O:533:THR:HG22	1.96	0.47
2:O:410:HIS:ND1	2:O:411:LYS:N	2.61	0.47
1:D:52:LEU:HA	1:D:104:TRP:O	2.15	0.47
1:E:41:LYS:HD2	1:E:87:ASN:O	2.14	0.47
2:Q:460:HIS:HA	2:Q:478:LEU:O	2.14	0.47
1:C:35:ILE:HG22	1:C:94:ARG:CD	2.44	0.47
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.14	0.47
1:D:1:PRO:HG2	2:R:488:MET:CE	2.45	0.47
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.14	0.47
2:N:437:TYR:CD2	2:N:437:TYR:C	2.92	0.47
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.50	0.47
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.96	0.47
1:F:36:TRP:CD1	1:F:37:ASN:OD1	2.67	0.47
1:C:198:PHE:HA	2:O:337:VAL:O	2.15	0.47
1:B:51:LEU:O	1:B:105:THR:HA	2.14	0.47
2:P:326:THR:HG22	2:P:330:ARG:HD2	1.96	0.47
1:B:84:ASN:OD1	1:B:86:GLU:HB2	2.15	0.47
1:B:140:HIS:O	1:B:197:PHE:HA	2.14	0.47
2:N:447:TYR:HB2	2:N:448:PRO:HD2	1.97	0.47
1:C:63:VAL:HG12	1:C:66:SER:HB3	1.96	0.47
1:C:92:PHE:CG	2:O:349:PRO:HG3	2.50	0.47
2:P:308:PHE:HA	2:P:529:GLY:O	2.15	0.47
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.50	0.47
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.15	0.47
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.97	0.47
2:R:366:ASN:OD1	2:R:366:ASN:C	2.56	0.47
2:O:473:LYS:HD2	2:O:474:LEU:N	2.30	0.46
1:A:78:GLU:OE1	2:M:301:PRO:HG3	2.13	0.46
2:N:350:ASN:OD1	2:N:350:ASN:C	2.58	0.46
1:D:15:PRO:HB3	1:D:133:ARG:HD2	1.97	0.46
2:P:411:LYS:HE2	2:P:411:LYS:HB2	1.67	0.46
1:F:24:GLU:O	1:F:25:ALA:C	2.57	0.46
2:R:378:ILE:HA	2:R:519:LEU:O	2.15	0.46
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.72	0.46
1:A:110:LYS:HG3	1:A:111:PRO:HD2	1.97	0.46
1:A:166:ARG:CZ	2:M:334:GLN:HG3	2.45	0.46
1:C:120:VAL:CG1	1:C:156:PRO:HG3	2.45	0.46
2:P:316:HIS:HB3	2:P:317:PRO:HD2	1.97	0.46
1:E:36:TRP:CG	1:E:37:ASN:H	2.33	0.46
1:F:131:PHE:CD2	1:F:138:HIS:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:432:ASP:OD1	2:M:432:ASP:C	2.58	0.46
2:O:403:ASN:HB2	4:O:613:HOH:O	2.15	0.46
2:R:381:ALA:O	2:R:522:ARG:HA	2.15	0.46
2:R:385:VAL:O	2:R:526:VAL:HA	2.15	0.46
2:M:302:ALA:HB1	2:M:347:THR:CG2	2.45	0.46
1:B:146:ASP:HB3	1:B:171:ILE:HG22	1.98	0.46
1:D:51:LEU:HD12	1:D:106:LEU:HD23	1.97	0.46
2:P:350:ASN:OD1	2:P:350:ASN:C	2.59	0.46
2:P:410:HIS:HA	2:P:411:LYS:NZ	2.31	0.46
1:F:66:SER:HA	1:F:132:ALA:HB2	1.97	0.46
1:B:78:GLU:HB3	2:N:301:PRO:HB3	1.97	0.46
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.46	0.46
2:Q:360:ASP:O	2:Q:427:GLY:HA2	2.14	0.46
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.15	0.46
1:A:35:ILE:HG22	1:A:94:ARG:HG3	1.97	0.46
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.46
1:E:140:HIS:O	1:E:197:PHE:HA	2.16	0.46
2:Q:364:LEU:HD13	2:Q:441:THR:HA	1.98	0.46
2:R:350:ASN:OD1	2:R:352:SER:HB2	2.15	0.46
2:P:410:HIS:HA	2:P:411:LYS:HZ1	1.81	0.46
2:M:305:ASN:O	2:M:533:THR:HG23	2.16	0.45
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.52	0.45
2:Q:409:ARG:HD2	2:Q:424:GLY:HA2	1.98	0.45
1:B:12:THR:HA	1:B:135:ILE:O	2.17	0.45
1:B:52:LEU:C	1:B:52:LEU:HD12	2.41	0.45
2:Q:399:MET:HA	2:Q:462:HIS:O	2.15	0.45
1:E:41:LYS:HB2	1:E:88:ALA:HA	1.98	0.45
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.46	0.45
2:M:399:MET:HA	2:M:462:HIS:O	2.16	0.45
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.99	0.45
2:P:318:LYS:HA	2:P:318:LYS:HD3	1.68	0.45
1:F:90:ASN:HB2	4:F:1427:HOH:O	2.16	0.45
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.52	0.45
2:O:443:LYS:HE3	2:O:480:PHE:CG	2.51	0.45
2:R:383:ARG:NE	2:R:434:ASP:O	2.36	0.45
2:R:497:ASN:ND2	2:R:497:ASN:C	2.61	0.45
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.97	0.45
1:C:41:LYS:N	1:C:88:ALA:O	2.40	0.45
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.78	0.45
2:R:364:LEU:HD13	2:R:441:THR:HA	1.99	0.45
2:R:437:TYR:CD1	2:R:437:TYR:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:517:ASP:C	2:M:517:ASP:OD1	2.60	0.45
2:M:508:LEU:CD2	2:P:488:MET:HE1	2.44	0.45
2:N:454:ASN:HB2	2:O:310:ILE:HG13	1.98	0.45
2:O:409:ARG:HG3	2:O:409:ARG:HH11	1.82	0.45
2:O:486:ILE:N	2:O:487:PRO:HD2	2.32	0.45
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.76	0.45
1:E:77:GLY:O	1:E:114:VAL:HG12	2.17	0.45
2:R:416:LEU:C	2:R:416:LEU:HD23	2.42	0.45
2:R:432:ASP:OD1	2:R:432:ASP:C	2.59	0.45
1:F:174:ARG:HE	1:F:181:THR:CG2	2.30	0.45
1:A:163:GLN:HG3	1:C:61:HIS:CE1	2.51	0.45
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.85	0.45
2:M:405:GLY:HA3	4:M:641:HOH:O	2.16	0.45
2:M:483:ASP:HB3	2:M:486:ILE:CD1	2.47	0.45
2:N:411:LYS:H	2:N:411:LYS:CD	2.29	0.45
2:N:495:ILE:CG2	2:N:500:ALA:HB3	2.47	0.45
1:C:66:SER:HA	1:C:132:ALA:HB2	1.99	0.45
1:D:51:LEU:HD11	1:D:126:ILE:HD12	1.98	0.45
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.17	0.45
2:R:386:ASP:HA	2:R:527:LEU:O	2.17	0.45
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.52	0.45
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.68	0.44
2:M:510:MET:HE1	2:P:456:TRP:CD1	2.52	0.44
2:O:514:ASN:O	2:O:517:ASP:HB3	2.17	0.44
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.17	0.44
1:F:70:VAL:HG21	1:F:106:LEU:HD11	1.99	0.44
1:A:176:GLU:HG3	1:A:180:LYS:C	2.41	0.44
2:N:390:LYS:HE2	4:N:730:HOH:O	2.17	0.44
2:O:372:LEU:HA	2:O:373:PRO:HD3	1.72	0.44
2:O:416:LEU:C	2:O:416:LEU:HD23	2.43	0.44
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.31	0.44
2:P:522:ARG:NE	2:P:524:ASP:OD1	2.49	0.44
1:E:35:ILE:HG22	1:E:94:ARG:HG3	2.00	0.44
1:F:36:TRP:CD1	1:F:37:ASN:H	2.34	0.44
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.98	0.44
2:R:468:PRO:HD2	2:R:472:THR:HG21	1.99	0.44
1:C:163:GLN:CB	1:C:165:GLN:HE22	2.23	0.44
1:D:58:GLY:CA	1:D:190:GLN:HB3	2.47	0.44
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.50	0.44
2:P:407:ARG:HD3	2:P:417:ALA:O	2.17	0.44
1:E:115:ASN:HA	1:E:121:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:GLU:HG3	1:F:180:LYS:O	2.18	0.44
2:M:434:ASP:HB3	2:M:436:TYR:HD2	1.81	0.44
2:N:364:LEU:HB2	2:N:440:ARG:HD3	1.99	0.44
1:F:131:PHE:O	1:F:132:ALA:HB2	2.17	0.44
1:F:147:ASP:OD2	1:F:174:ARG:CZ	2.66	0.44
1:F:158:LEU:HD12	1:F:158:LEU:HA	1.77	0.44
2:R:458:PRO:HD3	2:R:489:CYS:HB2	1.98	0.44
2:M:372:LEU:HA	2:M:373:PRO:HD3	1.84	0.44
2:M:448:PRO:HB2	2:P:516:MET:HA	1.98	0.44
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.80	0.44
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.52	0.44
2:P:372:LEU:HA	2:P:373:PRO:HD3	1.72	0.44
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.75	0.44
1:F:69:GLU:OE2	1:F:94:ARG:HD3	2.18	0.44
1:F:110:LYS:HA	1:F:111:PRO:HD2	1.73	0.44
1:D:176:GLU:OE2	1:D:179:GLY:C	2.61	0.44
2:Q:449:TRP:CE2	2:Q:457:ARG:HD2	2.53	0.44
2:R:411:LYS:HE2	2:R:411:LYS:N	2.31	0.44
2:R:447:TYR:HB2	2:R:448:PRO:HD2	1.99	0.44
1:B:62:LEU:HD12	1:B:64:ARG:NH2	2.33	0.44
2:O:409:ARG:HG3	2:O:409:ARG:NH1	2.32	0.44
1:F:86:GLU:O	1:F:87:ASN:C	2.57	0.44
2:R:415:TYR:CE1	2:R:416:LEU:CD2	3.00	0.44
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.99	0.44
2:M:410:HIS:CE1	2:M:411:LYS:CE	3.00	0.44
2:O:409:ARG:HH11	2:O:409:ARG:CG	2.31	0.44
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.74	0.44
2:O:497:ASN:HD22	2:O:498:PRO:N	2.16	0.44
2:P:385:VAL:O	2:P:526:VAL:HA	2.18	0.44
1:E:39:LEU:O	1:E:89:PHE:HA	2.17	0.44
1:E:52:LEU:HD23	1:E:103:GLU:OE1	2.18	0.44
1:C:165:GLN:H	1:C:165:GLN:CD	2.25	0.44
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.46	0.44
2:M:379:ILE:HA	2:M:439:PHE:O	2.17	0.43
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.50	0.43
2:O:399:MET:HA	2:O:462:HIS:O	2.17	0.43
2:P:390:LYS:HE2	4:P:754:HOH:O	2.16	0.43
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.79	0.43
1:F:36:TRP:CG	1:F:37:ASN:N	2.86	0.43
1:A:51:LEU:HD11	1:A:126:ILE:HD12	1.98	0.43
1:A:115:ASN:HA	1:A:121:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:CYS:HB3	1:A:158:LEU:HB2	2.00	0.43
1:C:176:GLU:HG2	1:C:179:GLY:HA2	1.99	0.43
2:M:448:PRO:CB	2:P:516:MET:HA	2.49	0.43
2:N:390:LYS:CD	4:N:648:HOH:O	2.65	0.43
1:D:177:VAL:O	1:D:178:ASP:C	2.61	0.43
2:Q:449:TRP:NE1	2:Q:457:ARG:HD2	2.33	0.43
1:F:52:LEU:O	1:F:184:ARG:HA	2.18	0.43
1:F:116:ASN:OD1	1:F:116:ASN:C	2.61	0.43
1:F:154:LYS:HZ3	1:F:154:LYS:HG3	1.72	0.43
2:M:302:ALA:HB1	2:M:347:THR:HG21	2.01	0.43
1:B:176:GLU:OE2	1:B:179:GLY:O	2.36	0.43
2:O:390:LYS:HD2	4:O:649:HOH:O	2.16	0.43
1:D:114:VAL:HG23	1:D:122:MET:HE3	2.01	0.43
2:N:486:ILE:HB	2:N:487:PRO:HD3	2.00	0.43
1:C:46:GLY:HA3	1:C:75:ALA:HB2	2.00	0.43
1:C:170:LEU:HD21	1:C:196:VAL:HB	2.00	0.43
1:E:39:LEU:HD11	1:E:93:GLY:HA3	2.00	0.43
2:Q:360:ASP:HB3	2:Q:428:ARG:HG3	2.00	0.43
2:Q:398:GLU:OE2	4:Q:1171:HOH:O	2.21	0.43
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.36	0.43
2:Q:517:ASP:OD1	2:Q:517:ASP:C	2.60	0.43
2:R:410:HIS:ND1	2:R:411:LYS:N	2.66	0.43
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.51	0.43
1:A:39:LEU:HD11	1:A:93:GLY:HA3	2.00	0.43
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.47	0.43
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.99	0.43
1:E:164:PRO:N	1:E:165:GLN:HE21	2.16	0.43
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.81	0.43
1:A:8:THR:HA	1:A:9:PRO:HD3	1.85	0.43
2:M:405:GLY:HA2	2:P:375:GLY:C	2.43	0.43
1:F:35:ILE:HG21	1:F:92:PHE:CE2	2.54	0.43
1:A:24:GLU:O	1:A:27:GLY:N	2.47	0.43
1:B:52:LEU:HA	1:B:104:TRP:O	2.19	0.43
2:N:415:TYR:CE1	2:N:416:LEU:HD23	2.53	0.43
1:D:146:ASP:HB3	1:D:171:ILE:HG22	2.00	0.43
2:P:383:ARG:HA	2:P:435:GLY:O	2.18	0.43
2:P:414:ARG:NE	2:P:414:ARG:CA	2.81	0.43
2:Q:386:ASP:C	2:Q:386:ASP:OD1	2.60	0.43
1:F:5:LEU:O	2:R:387:GLN:HG2	2.17	0.43
1:F:35:ILE:HG21	1:F:92:PHE:HE2	1.84	0.43
1:F:70:VAL:HG11	1:F:106:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:HA	1:B:164:PRO:HD2	1.65	0.43
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.76	0.43
2:P:328:ILE:HD12	2:Q:335:ALA:HB2	2.01	0.43
1:F:24:GLU:C	1:F:26:ALA:N	2.74	0.43
1:F:32:ASP:HB2	4:R:1405:HOH:O	2.19	0.43
1:F:122:MET:HA	1:F:156:PRO:HD2	2.01	0.43
2:R:390:LYS:HG2	4:R:1433:HOH:O	2.19	0.43
2:R:431:THR:HG22	2:R:437:TYR:HB3	2.01	0.43
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.62	0.43
2:M:411:LYS:HE2	2:M:411:LYS:N	2.34	0.43
1:B:163:GLN:O	1:B:166:ARG:N	2.50	0.43
2:N:411:LYS:HE2	2:N:411:LYS:HB2	1.64	0.43
2:R:395:THR:O	2:R:430:LEU:HA	2.19	0.43
1:A:54:GLN:HG2	1:A:102:GLY:O	2.19	0.42
2:M:380:VAL:O	2:M:438:SER:HA	2.18	0.42
2:N:315:TRP:HZ2	2:N:503:GLN:NE2	2.15	0.42
1:C:74:ASP:C	1:C:74:ASP:OD1	2.59	0.42
2:Q:350:ASN:C	2:Q:350:ASN:OD1	2.61	0.42
1:F:68:LEU:HA	1:F:129:SER:O	2.18	0.42
2:M:410:HIS:CE1	2:M:411:LYS:NZ	2.87	0.42
1:C:123:ALA:O	1:C:124:PRO:C	2.61	0.42
1:C:51:LEU:O	1:C:105:THR:HA	2.20	0.42
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.81	0.42
1:E:24:GLU:O	1:E:25:ALA:C	2.61	0.42
1:E:191:GLY:O	1:E:194:GLU:HB2	2.20	0.42
2:Q:408:TYR:HE1	2:Q:447:TYR:CE2	2.37	0.42
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.67	0.42
2:R:408:TYR:CE2	2:R:447:TYR:CE2	3.07	0.42
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.67	0.42
2:P:400:TRP:HA	2:P:425:GLY:O	2.20	0.42
1:E:48:HIS:C	1:E:49:ILE:CG2	2.92	0.42
1:E:86:GLU:O	1:E:87:ASN:C	2.63	0.42
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.19	0.42
1:A:93:GLY:C	1:A:94:ARG:HG2	2.43	0.42
2:P:411:LYS:CE	2:P:411:LYS:N	2.72	0.42
1:F:68:LEU:HD23	1:F:128:ILE:CG2	2.49	0.42
1:F:115:ASN:HA	1:F:121:PRO:HA	2.01	0.42
1:F:149:ALA:HB1	4:F:1353:HOH:O	2.19	0.42
2:R:364:LEU:HD11	2:R:442:ILE:HG23	2.02	0.42
1:A:165:GLN:NE2	1:C:61:HIS:NE2	2.68	0.42
1:E:25:ALA:HB1	1:E:98:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:GLU:HG2	1:E:179:GLY:HA2	2.02	0.42
2:Q:451:ASN:HB3	2:Q:452:GLY:H	1.67	0.42
1:A:131:PHE:O	1:A:132:ALA:HB2	2.19	0.42
2:M:450:ARG:HG3	4:M:629:HOH:O	2.18	0.42
2:N:341:GLN:HB3	2:N:346:THR:CG2	2.50	0.42
1:C:163:GLN:OE1	1:C:165:GLN:NE2	2.46	0.42
2:O:468:PRO:HD2	2:O:472:THR:HG21	2.02	0.42
1:D:5:LEU:O	2:P:387:GLN:HG2	2.20	0.42
2:P:514:ASN:O	2:P:515:PRO:C	2.62	0.42
1:E:70:VAL:HG12	1:E:128:ILE:HG12	2.02	0.42
2:R:341:GLN:HB3	2:R:346:THR:CG2	2.50	0.42
1:B:28:ASN:O	1:B:29:PRO:C	2.63	0.42
1:B:115:ASN:HA	1:B:121:PRO:HA	2.02	0.42
2:O:524:ASP:C	2:O:525:ILE:HG13	2.45	0.42
1:A:200:PHE:CG	2:M:345:GLU:HG2	2.54	0.42
1:B:191:GLY:O	1:B:194:GLU:HB2	2.20	0.42
1:C:161:ILE:HD13	1:C:196:VAL:HG21	2.00	0.42
2:P:437:TYR:CD1	2:P:437:TYR:C	2.98	0.42
2:P:489:CYS:O	2:P:493:LYS:HG3	2.20	0.42
2:Q:383:ARG:HA	2:Q:435:GLY:O	2.20	0.42
1:F:50:LEU:O	1:F:182:ALA:HA	2.20	0.42
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.81	0.42
1:C:28:ASN:HB3	4:C:270:HOH:O	2.19	0.42
2:P:432:ASP:OD1	2:P:432:ASP:C	2.63	0.42
2:P:484:PRO:O	2:P:488:MET:CE	2.68	0.42
2:Q:331:SER:HA	2:Q:332:PRO:HD3	1.90	0.42
2:Q:390:LYS:CE	4:Q:1154:HOH:O	2.66	0.42
2:N:360:ASP:HB3	2:N:428:ARG:HG3	2.02	0.41
1:C:177:VAL:O	1:C:178:ASP:C	2.62	0.41
1:E:199:ASP:O	2:Q:338:SER:HA	2.20	0.41
1:A:200:PHE:CD1	2:M:345:GLU:HG2	2.55	0.41
2:M:326:THR:HG22	2:M:330:ARG:HD2	2.02	0.41
2:M:400:TRP:CE2	2:M:462:HIS:HB2	2.54	0.41
1:C:52:LEU:HA	1:C:104:TRP:O	2.20	0.41
2:O:411:LYS:HE2	2:O:411:LYS:HB2	1.83	0.41
1:D:50:LEU:O	1:D:182:ALA:HA	2.19	0.41
2:P:431:THR:HG22	2:P:437:TYR:HB3	2.02	0.41
1:E:41:LYS:O	1:E:42:PRO:C	2.64	0.41
1:F:46:GLY:HA3	1:F:75:ALA:HB2	2.02	0.41
2:R:384:VAL:HA	2:R:525:ILE:O	2.20	0.41
2:R:497:ASN:ND2	2:R:499:GLU:N	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.76	0.41
2:N:390:LYS:HD3	4:N:648:HOH:O	2.19	0.41
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.60	0.41
1:C:74:ASP:HB2	4:C:238:HOH:O	2.20	0.41
1:E:39:LEU:CD1	1:E:106:LEU:HD11	2.50	0.41
1:F:8:THR:HA	1:F:9:PRO:HD3	1.87	0.41
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.55	0.41
1:B:64:ARG:O	1:B:98:THR:HA	2.20	0.41
1:B:176:GLU:HG2	1:B:179:GLY:C	2.46	0.41
1:B:176:GLU:CG	1:B:179:GLY:C	2.94	0.41
2:N:390:LYS:CE	4:N:730:HOH:O	2.67	0.41
1:C:35:ILE:CG2	1:C:94:ARG:CD	2.97	0.41
2:P:408:TYR:HE2	2:P:447:TYR:CE2	2.39	0.41
2:R:364:LEU:HD13	2:R:441:THR:CA	2.50	0.41
1:A:28:ASN:HB3	4:A:271:HOH:O	2.21	0.41
2:N:408:TYR:HE2	2:N:447:TYR:CZ	2.39	0.41
1:C:39:LEU:HB3	1:C:90:ASN:O	2.20	0.41
1:C:162:GLU:HG3	4:C:257:HOH:O	2.20	0.41
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	2.02	0.41
1:F:176:GLU:CD	1:F:179:GLY:HA2	2.45	0.41
1:C:41:LYS:HB2	1:C:88:ALA:HA	2.02	0.41
1:D:43:ASP:O	1:D:43:ASP:CG	2.63	0.41
1:D:84:ASN:OD1	1:D:86:GLU:HB2	2.21	0.41
1:E:54:GLN:HG3	1:E:103:GLU:HG3	2.03	0.41
2:Q:447:TYR:HB2	2:Q:448:PRO:HD2	2.02	0.41
2:M:410:HIS:CE1	2:M:411:LYS:HE2	2.56	0.41
2:N:386:ASP:OD1	2:N:386:ASP:C	2.64	0.41
2:N:420:ASP:HA	2:N:421:PRO:HD2	1.88	0.41
2:O:517:ASP:C	2:O:517:ASP:OD1	2.63	0.41
1:D:99:PHE:CD2	2:P:412:ASN:OD1	2.74	0.41
1:E:31:ARG:HH11	2:Q:428:ARG:HG2	1.83	0.41
1:B:174:ARG:HB2	1:B:183:TYR:CE2	2.55	0.41
4:D:720:HOH:O	2:P:311:ARG:HB2	2.20	0.41
2:R:372:LEU:HD12	2:R:372:LEU:HA	1.94	0.41
1:A:54:GLN:O	1:A:186:ASP:HA	2.21	0.41
1:A:58:GLY:HA2	1:A:190:GLN:O	2.21	0.41
2:M:383:ARG:HA	2:M:435:GLY:O	2.21	0.41
2:M:453:PRO:O	2:P:515:PRO:HB3	2.20	0.41
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.65	0.41
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.36	0.41
1:B:114:VAL:HG22	4:B:319:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:333:ARG:HH11	2:N:333:ARG:HD3	1.39	0.41
2:O:326:THR:O	2:O:326:THR:CG2	2.69	0.41
2:O:393:PRO:O	2:O:393:PRO:HG2	2.19	0.41
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.56	0.41
2:P:412:ASN:N	2:P:412:ASN:HD22	2.19	0.41
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.90	0.41
1:F:23:LEU:O	1:F:26:ALA:N	2.54	0.41
1:F:41:LYS:HD2	1:F:87:ASN:O	2.21	0.41
1:F:94:ARG:HH22	2:R:398:GLU:CD	2.27	0.41
2:M:497:ASN:HD22	2:M:498:PRO:CD	2.34	0.41
1:B:20:GLY:O	1:B:21:LEU:HD23	2.22	0.41
2:O:411:LYS:CD	2:O:411:LYS:N	2.83	0.41
1:D:72:GLN:O	1:D:91:SER:OG	2.30	0.41
2:P:465:ILE:O	2:P:473:LYS:HA	2.21	0.41
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.51	0.41
1:F:20:GLY:O	1:F:21:LEU:HD23	2.20	0.41
1:A:77:GLY:O	1:A:114:VAL:HG12	2.21	0.40
1:A:160:LEU:HD12	2:M:339:ILE:HG22	2.04	0.40
1:B:25:ALA:HB1	1:B:98:THR:HG21	2.03	0.40
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.67	0.40
1:F:121:PRO:HG2	4:F:1368:HOH:O	2.21	0.40
1:A:5:LEU:HA	1:A:6:PRO:HD3	1.91	0.40
1:A:36:TRP:CG	1:A:37:ASN:N	2.87	0.40
2:M:362:ASP:OD2	2:M:440:ARG:NH1	2.54	0.40
2:O:447:TYR:HA	2:O:448:PRO:HD3	1.94	0.40
1:E:8:THR:HA	1:E:9:PRO:HD3	1.70	0.40
1:F:92:PHE:CG	2:R:349:PRO:HG3	2.56	0.40
2:M:409:ARG:NH1	2:M:409:ARG:HG3	2.36	0.40
1:B:19:ILE:HG21	2:N:410:HIS:HB2	2.03	0.40
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.89	0.40
2:Q:478:LEU:HD12	2:Q:523:PHE:CG	2.57	0.40
2:M:307:ARG:HD3	2:M:307:ARG:HA	1.92	0.40
2:M:447:TYR:HB2	2:M:448:PRO:HD2	2.03	0.40
1:B:36:TRP:CE3	1:B:36:TRP:HA	2.55	0.40
1:B:162:GLU:HG3	4:B:400:HOH:O	2.21	0.40
2:N:373:PRO:HB3	2:N:423:PHE:HB2	2.04	0.40
1:C:85:LEU:HD23	1:C:85:LEU:HA	1.89	0.40
2:P:317:PRO:HD3	2:P:495:ILE:HG12	2.04	0.40
1:E:144:TYR:CE2	1:E:158:LEU:HD13	2.55	0.40
1:D:36:TRP:CG	1:D:37:ASN:N	2.89	0.40
1:D:198:PHE:HA	2:P:337:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:447:TYR:HB2	2:P:448:PRO:HD2	2.04	0.40
2:P:516:MET:HB3	2:P:516:MET:HE3	1.61	0.40
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.36	0.40
1:F:146:ASP:OD1	1:F:174:ARG:HB2	2.21	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	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	C	198/200 (99%)	192 (97%)	5 (2%)	1 (0%)	24	20
1	D	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	185 (93%)	13 (7%)	0	100	100
2	M	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	N	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	O	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	P	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	Q	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	R	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
All	All	2562/2628 (98%)	2463 (96%)	98 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	152 (94%)	10 (6%)	16	12
1	B	162/163 (99%)	155 (96%)	7 (4%)	26	24
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	24
1	D	162/163 (99%)	154 (95%)	8 (5%)	22	19
1	E	162/163 (99%)	157 (97%)	5 (3%)	35	37
1	F	162/163 (99%)	152 (94%)	10 (6%)	16	12
2	M	196/202 (97%)	186 (95%)	10 (5%)	21	18
2	N	196/202 (97%)	188 (96%)	8 (4%)	27	26
2	O	196/202 (97%)	185 (94%)	11 (6%)	19	15
2	P	196/202 (97%)	183 (93%)	13 (7%)	15	10
2	Q	196/202 (97%)	188 (96%)	8 (4%)	27	26
2	R	196/202 (97%)	188 (96%)	8 (4%)	27	26
All	All	2148/2190 (98%)	2043 (95%)	105 (5%)	22	19

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	38	ARG
1	A	43	ASP
1	A	52	LEU
1	A	94	ARG
1	A	106	LEU
1	A	143	LEU
1	A	165	GLN
1	A	192	GLU

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Mol	Chain	Res	Type
2	M	343	ILE
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	411	LYS
2	M	416	LEU
2	M	434	ASP
2	M	478	LEU
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	32	ASP
1	B	52	LEU
1	B	106	LEU
1	B	154	LYS
1	B	165	GLN
1	B	192	GLU
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	411	LYS
2	N	416	LEU
2	N	478	LEU
2	N	503	GLN
2	N	507	LYS
1	C	4	LEU
1	C	19	ILE
1	C	24	GLU
1	C	38	ARG
1	C	52	LEU
1	C	158	LEU
1	C	165	GLN
2	O	364	LEU
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP
2	O	442	ILE
2	O	478	LEU
2	O	507	LYS

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Mol	Chain	Res	Type
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	42	PRO
1	D	52	LEU
1	D	94	ARG
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	343	ILE
2	P	395	THR
2	P	411	LYS
2	P	414	ARG
2	P	416	LEU
2	P	434	ASP
2	P	438	SER
2	P	440	ARG
2	P	442	ILE
2	P	478	LEU
2	P	497	ASN
2	P	511	ASN
2	P	534	HIS
1	E	4	LEU
1	E	52	LEU
1	E	150	GLN
1	E	165	GLN
1	E	180	LYS
2	Q	372	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	442	ILE
2	Q	478	LEU
2	Q	499	GLU
2	Q	507	LYS
1	F	4	LEU
1	F	30	THR
1	F	49	ILE
1	F	52	LEU
1	F	91	SER
1	F	94	ARG
1	F	114	VAL

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Mol	Chain	Res	Type
1	F	165	GLN
1	F	176	GLU
1	F	181	THR
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	473	LYS
2	R	497	ASN
2	R	499	GLU
2	R	507	LYS
2	R	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	165	GLN
2	M	359	HIS
2	M	361	HIS
2	M	412	ASN
2	M	422	ASN
2	M	497	ASN
2	M	503	GLN
2	M	530	GLN
1	B	107	HIS
1	B	140	HIS
1	B	163	GLN
1	B	165	GLN
2	N	361	HIS
2	N	412	ASN
2	N	422	ASN
2	N	497	ASN
2	N	503	GLN
1	C	11	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
2	O	511	ASN
2	O	530	GLN
1	D	59	ASN

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Mol	Chain	Res	Type
1	D	163	GLN
1	D	165	GLN
2	P	361	HIS
2	P	394	ASN
2	P	412	ASN
2	P	497	ASN
2	P	511	ASN
1	E	59	ASN
1	E	107	HIS
1	E	165	GLN
2	Q	305	ASN
2	Q	334	GLN
2	Q	361	HIS
2	Q	394	ASN
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
1	F	127	ASN
1	F	136	ASN
1	F	165	GLN
2	R	334	GLN
2	R	361	HIS
2	R	422	ASN
2	R	497	ASN
2	R	503	GLN
2	R	530	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.