



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:50 AM UTC

PDB ID : 1U5I / pdb_00001u5i
Title : Crystal Structure analysis of rat m-calpain mutant Lys10 Thr
Authors : Hosfield, C.M.; Pal, G.P.; Elce, J.S.; Jia, Z.
Deposited on : 2004-07-27
Resolution : 2.86 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

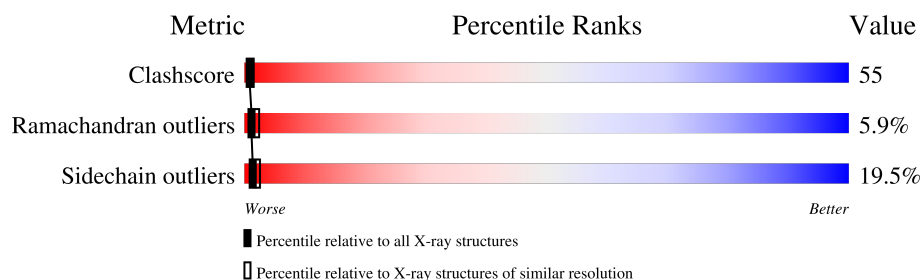
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)

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	700	
2	B	184	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6706 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 Calpain 2, large [catalytic] subunit precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4980	3176	836	945	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	THR	LYS	engineered mutation	UNP Q07009
A	105	SER	CYS	engineered mutation	UNP Q07009

- Molecule 2 is a protein called Calpain small subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1427	897	246	274	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q64537

- Molecule 3 is water.

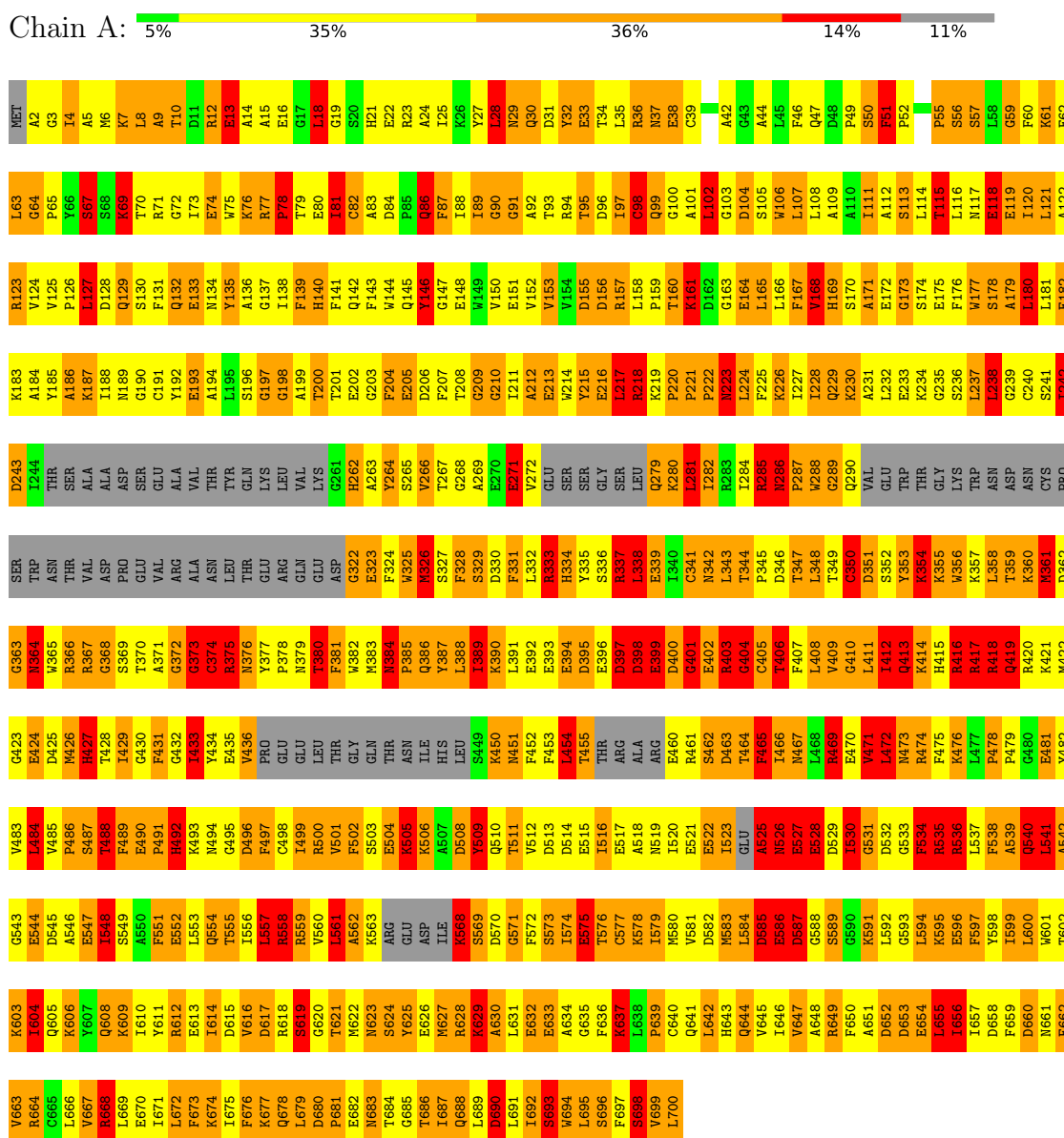
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		
3	B	52	Total	O	0	0
			52	52		

3 Residue-property plots

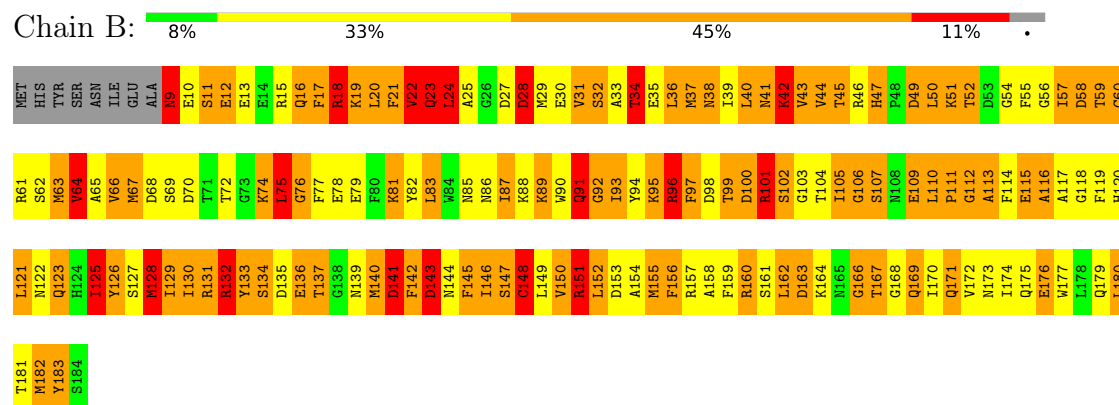
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Calpain 2, large [catalytic] subunit precursor



- Molecule 2: Calpain small subunit 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.66Å 156.52Å 64.23Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	25.00 – 2.86	Depositor
% Data completeness (in resolution range)	90.1 (25.00-2.86)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6706	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	3.80	789/5083 (15.5%)	2.62	381/6854 (5.6%)
2	B	3.42	189/1454 (13.0%)	2.42	90/1955 (4.6%)
All	All	3.72	978/6537 (15.0%)	2.57	471/8809 (5.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
2	B	0	2
All	All	0	21

All (978) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	ASP	C-N	38.72	1.90	1.33
1	A	402	GLU	C-N	38.24	1.87	1.33
1	A	521	GLU	C-N	24.21	1.64	1.33
1	A	527	GLU	C-N	-22.08	1.02	1.33
1	A	522	GLU	C-N	21.55	1.58	1.33
1	A	699	VAL	CA-CB	20.71	1.82	1.54
1	A	627	MET	SD-CE	-19.61	1.30	1.79
1	A	527	GLU	C-O	16.58	1.44	1.24
2	B	137	THR	CA-CB	16.35	1.82	1.53
2	B	151	ARG	CA-C	-15.73	1.32	1.52
1	A	548	ILE	CA-CB	-15.69	1.34	1.54
1	A	660	ASP	C-O	-15.06	1.06	1.24
1	A	13	GLU	CA-C	14.41	1.71	1.52
1	A	326	MET	SD-CE	14.33	2.15	1.79
1	A	422	MET	C-O	14.13	1.41	1.23
1	A	512	VAL	CA-CB	13.95	1.71	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	LEU	C-O	-13.95	1.07	1.24
1	A	401	GLY	C-N	-13.93	1.15	1.33
1	A	89	ILE	CA-CB	13.87	1.70	1.54
1	A	628	ARG	CZ-NH2	13.85	1.51	1.33
1	A	98	CYS	CA-C	-13.80	1.35	1.52
1	A	142	GLN	C-O	13.71	1.41	1.23
1	A	364	ASN	N-CA	-13.61	1.28	1.45
2	B	18	ARG	CA-C	13.55	1.71	1.52
1	A	334	HIS	N-CA	13.52	1.62	1.46
1	A	148	GLU	C-O	13.12	1.40	1.23
1	A	675	ILE	C-O	-13.06	1.08	1.24
1	A	640	CYS	CA-C	13.00	1.70	1.52
1	A	578	LYS	C-O	12.98	1.39	1.24
1	A	382	TRP	C-O	12.89	1.40	1.24
1	A	125	VAL	C-O	-12.83	1.08	1.24
1	A	608	GLN	C-O	-12.73	1.07	1.24
1	A	685	GLY	C-O	-12.71	1.06	1.24
1	A	414	LYS	C-O	-12.66	1.07	1.23
1	A	140	HIS	C-O	-12.54	1.08	1.23
2	B	182	MET	SD-CE	-12.47	1.48	1.79
1	A	663	VAL	CA-CB	12.46	1.70	1.54
1	A	668	ARG	NE-CZ	12.43	1.46	1.33
2	B	129	ILE	C-O	12.32	1.38	1.24
1	A	237	LEU	C-O	-12.17	1.09	1.23
1	A	518	ALA	C-O	-12.15	1.09	1.23
1	A	403	ARG	C-N	12.05	1.51	1.33
1	A	604	ILE	CA-CB	-11.99	1.40	1.54
2	B	130	ILE	CA-CB	11.99	1.68	1.54
1	A	417	ARG	CG-CD	11.96	1.88	1.52
1	A	428	THR	CA-C	-11.89	1.38	1.52
2	B	62	SER	C-O	11.89	1.38	1.24
1	A	322	GLY	C-O	11.83	1.38	1.24
2	B	183	TYR	CA-C	11.76	1.66	1.53
1	A	489	PHE	C-O	11.64	1.37	1.24
1	A	150	VAL	C-O	-11.62	1.11	1.24
1	A	577	CYS	CA-C	-11.61	1.37	1.52
1	A	605	GLN	CA-C	-11.58	1.38	1.52
1	A	136	ALA	CA-C	-11.53	1.39	1.53
2	B	167	THR	CA-C	-11.33	1.38	1.52
2	B	129	ILE	CA-CB	-11.31	1.40	1.54
2	B	162	LEU	CA-C	11.23	1.68	1.52
1	A	7	LYS	CD-CE	11.19	1.86	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	THR	N-CA	11.17	1.59	1.46
1	A	656	ILE	CA-CB	11.10	1.68	1.54
1	A	44	ALA	CA-CB	-11.07	1.34	1.53
1	A	465	PHE	N-CA	-10.98	1.32	1.46
1	A	692	ILE	CG1-CD1	10.97	1.94	1.51
1	A	606	LYS	CA-C	10.92	1.68	1.52
1	A	218	ARG	CG-CD	10.85	1.84	1.52
1	A	466	ILE	CA-C	-10.80	1.43	1.52
1	A	604	ILE	C-O	-10.75	1.11	1.24
1	A	107	LEU	CA-C	-10.75	1.38	1.52
1	A	692	ILE	CA-CB	10.66	1.68	1.54
1	A	634	ALA	CA-CB	-10.64	1.35	1.53
1	A	629	LYS	N-CA	-10.61	1.33	1.46
1	A	540	GLN	CB-CG	10.60	1.84	1.52
1	A	211	ILE	CA-C	-10.60	1.39	1.52
1	A	515	GLU	CA-C	10.56	1.66	1.52
1	A	95	THR	C-O	-10.55	1.10	1.23
1	A	131	PHE	N-CA	10.51	1.59	1.46
1	A	422	MET	CG-SD	-10.48	1.54	1.80
1	A	24	ALA	CA-CB	10.48	1.70	1.53
1	A	155	ASP	C-O	10.48	1.37	1.23
1	A	8	LEU	C-O	-10.41	1.11	1.24
1	A	410	GLY	C-O	10.38	1.38	1.23
1	A	243	ASP	CA-C	10.36	1.66	1.52
1	A	99	GLN	C-O	-10.36	1.11	1.23
1	A	226	LYS	CD-CE	10.34	1.83	1.52
1	A	681	PRO	C-O	-10.34	1.10	1.24
1	A	225	PHE	CA-C	-10.33	1.39	1.52
1	A	681	PRO	CA-C	-10.33	1.36	1.52
1	A	667	VAL	CA-CB	10.32	1.65	1.54
2	B	125	ILE	CA-CB	-10.31	1.42	1.54
1	A	146	TYR	N-CA	-10.29	1.30	1.46
1	A	18	LEU	CA-CB	-10.26	1.38	1.53
2	B	97	PHE	C-O	10.23	1.36	1.24
1	A	406	THR	C-O	10.21	1.36	1.24
1	A	227	ILE	C-O	10.20	1.36	1.24
1	A	97	ILE	CA-C	-10.19	1.41	1.52
1	A	31	ASP	N-CA	-10.17	1.33	1.46
1	A	511	THR	C-O	-10.16	1.11	1.23
1	A	466	ILE	CG1-CD1	10.12	1.91	1.51
1	A	539	ALA	CA-CB	10.10	1.69	1.53
1	A	333	ARG	CA-C	-10.08	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	ILE	CA-CB	-10.05	1.39	1.55
1	A	374	CYS	N-CA	-10.04	1.33	1.46
1	A	14	ALA	N-CA	-10.03	1.34	1.46
1	A	692	ILE	CA-C	-10.02	1.40	1.52
1	A	186	ALA	CA-CB	9.99	1.69	1.53
1	A	689	LEU	N-CA	-9.95	1.33	1.46
1	A	453	PHE	C-O	9.95	1.36	1.24
2	B	74	LYS	C-O	9.88	1.36	1.23
1	A	497	PHE	C-O	-9.84	1.12	1.23
1	A	347	THR	C-O	-9.83	1.12	1.24
1	A	469	ARG	CA-C	-9.82	1.39	1.52
1	A	627	MET	CA-C	-9.82	1.40	1.52
2	B	60	CYS	CA-C	9.82	1.65	1.52
1	A	369	SER	C-O	-9.81	1.11	1.24
1	A	161	LYS	CB-CG	9.79	1.81	1.52
1	A	7	LYS	CE-NZ	9.79	1.78	1.49
1	A	478	PRO	C-O	-9.78	1.16	1.25
2	B	158	ALA	C-O	-9.76	1.11	1.24
1	A	52	PRO	C-O	9.75	1.36	1.23
2	B	96	ARG	CA-C	9.74	1.65	1.52
1	A	12	ARG	C-O	-9.72	1.12	1.24
1	A	87	PHE	C-O	9.72	1.35	1.24
1	A	138	ILE	N-CA	-9.68	1.35	1.46
1	A	214	TRP	C-O	-9.68	1.11	1.23
2	B	66	VAL	CA-CB	-9.67	1.41	1.54
1	A	32	TYR	CA-CB	-9.64	1.38	1.53
1	A	197	GLY	C-O	9.64	1.36	1.23
1	A	326	MET	CG-SD	9.63	2.04	1.80
2	B	33	ALA	CA-C	-9.63	1.39	1.52
1	A	331	PHE	C-O	9.63	1.35	1.24
1	A	375	ARG	CG-CD	9.59	1.81	1.52
1	A	408	LEU	C-O	9.57	1.35	1.24
1	A	150	VAL	CA-CB	9.57	1.66	1.54
1	A	232	LEU	C-O	-9.57	1.12	1.24
1	A	695	LEU	C-O	-9.51	1.12	1.24
1	A	14	ALA	C-O	9.47	1.35	1.24
1	A	606	LYS	CG-CD	9.47	1.80	1.52
2	B	157	ARG	C-O	9.45	1.35	1.24
2	B	42	LYS	CA-C	-9.42	1.40	1.52
2	B	140	MET	N-CA	-9.41	1.35	1.46
1	A	133	GLU	C-O	9.40	1.35	1.24
1	A	555	THR	C-O	9.38	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	641	GLN	C-O	9.35	1.35	1.24
1	A	220	PRO	CA-C	9.31	1.60	1.52
1	A	686	THR	CA-CB	-9.30	1.37	1.53
1	A	123	ARG	NE-CZ	9.29	1.43	1.33
1	A	670	GLU	CA-CB	-9.20	1.38	1.53
1	A	574	ILE	CA-CB	9.19	1.66	1.54
1	A	373	GLY	C-O	-9.19	1.11	1.23
1	A	426	MET	SD-CE	-9.18	1.56	1.79
2	B	66	VAL	CA-C	-9.17	1.41	1.52
1	A	454	LEU	C-O	9.14	1.35	1.24
1	A	644	GLN	CA-C	9.13	1.64	1.52
1	A	14	ALA	CA-CB	-9.12	1.38	1.53
1	A	467	ASN	C-O	9.12	1.35	1.24
1	A	153	VAL	C-O	9.11	1.33	1.24
1	A	474	ARG	CA-CB	-9.09	1.40	1.53
1	A	181	LEU	CG-CD2	-9.08	1.22	1.52
1	A	510	GLN	CD-NE2	9.08	1.52	1.33
2	B	141	ASP	CA-C	9.07	1.65	1.52
1	A	642	LEU	C-O	9.06	1.35	1.24
1	A	500	ARG	C-N	-9.05	1.21	1.33
1	A	666	LEU	CA-C	-9.03	1.41	1.52
1	A	69	LYS	C-O	9.00	1.35	1.24
2	B	153	ASP	CA-CB	8.99	1.67	1.53
1	A	414	LYS	CA-C	8.98	1.65	1.53
2	B	85	ASN	C-O	-8.92	1.13	1.24
1	A	76	LYS	N-CA	-8.91	1.34	1.45
2	B	155	MET	CG-SD	8.91	2.03	1.80
1	A	352	SER	CA-C	8.89	1.64	1.52
1	A	669	LEU	CA-CB	-8.88	1.39	1.53
1	A	391	LEU	C-O	8.85	1.35	1.23
1	A	358	LEU	C-O	-8.85	1.12	1.24
1	A	644	GLN	C-O	8.83	1.34	1.24
1	A	464	THR	CA-C	8.83	1.64	1.52
1	A	674	LYS	CE-NZ	8.83	1.75	1.49
1	A	674	LYS	CA-C	-8.82	1.41	1.52
1	A	360	LYS	N-CA	-8.80	1.34	1.45
1	A	9	ALA	C-O	-8.80	1.13	1.24
1	A	168	VAL	CA-C	-8.77	1.43	1.52
1	A	344	THR	CA-C	-8.77	1.41	1.53
1	A	631	LEU	N-CA	-8.77	1.35	1.46
1	A	10	THR	C-O	8.76	1.34	1.24
1	A	174	SER	CA-C	8.73	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	574	ILE	N-CA	-8.73	1.34	1.46
2	B	171	GLN	C-O	-8.72	1.14	1.24
1	A	364	ASN	CB-CG	-8.70	1.30	1.52
1	A	86	GLN	CA-C	8.70	1.63	1.52
1	A	471	VAL	CA-C	-8.70	1.42	1.52
2	B	58	ASP	CB-CG	8.69	1.73	1.52
1	A	636	PHE	C-O	8.69	1.35	1.24
1	A	667	VAL	C-O	8.68	1.33	1.24
1	A	409	VAL	N-CA	-8.68	1.35	1.46
2	B	77	PHE	C-O	-8.67	1.14	1.24
1	A	361	MET	CG-SD	8.65	2.02	1.80
1	A	179	ALA	CA-CB	8.64	1.67	1.53
1	A	548	ILE	CA-C	-8.62	1.42	1.52
1	A	285	ARG	C-O	-8.61	1.12	1.23
1	A	663	VAL	CA-C	-8.60	1.41	1.52
1	A	429	ILE	N-CA	-8.58	1.35	1.46
1	A	105	SER	CA-CB	8.56	1.68	1.53
1	A	390	LYS	CG-CD	8.56	1.78	1.52
1	A	634	ALA	CA-C	-8.56	1.39	1.52
2	B	128	MET	CG-SD	8.54	2.02	1.80
1	A	151	GLU	N-CA	-8.51	1.35	1.46
2	B	57	ILE	CA-C	8.51	1.63	1.52
2	B	156	PHE	CG-CD2	8.51	1.56	1.38
2	B	180	LEU	CA-C	8.50	1.64	1.52
1	A	123	ARG	CA-C	-8.49	1.40	1.52
1	A	76	LYS	C-O	-8.47	1.13	1.23
1	A	156	ASP	CG-OD1	8.47	1.41	1.25
1	A	399	GLU	N-CA	8.47	1.57	1.46
1	A	455	THR	CB-CG2	8.46	1.80	1.52
1	A	202	GLU	N-CA	-8.45	1.36	1.46
1	A	651	ALA	CA-C	-8.45	1.42	1.52
1	A	13	GLU	C-O	8.44	1.33	1.24
1	A	118	GLU	CA-CB	8.44	1.66	1.53
1	A	190	GLY	C-O	-8.43	1.12	1.24
1	A	651	ALA	C-O	8.42	1.34	1.23
2	B	40	LEU	CA-C	8.42	1.64	1.52
2	B	159	PHE	N-CA	-8.40	1.36	1.46
1	A	98	CYS	C-O	-8.38	1.13	1.23
1	A	611	TYR	CA-C	8.38	1.64	1.52
1	A	351	ASP	CA-C	8.37	1.64	1.52
1	A	383	MET	C-O	-8.37	1.12	1.24
1	A	629	LYS	C-O	8.37	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	ASP	N-CA	8.33	1.56	1.45
1	A	30	GLN	C-O	-8.32	1.14	1.23
1	A	138	ILE	CA-CB	-8.32	1.43	1.54
1	A	614	ILE	C-O	-8.31	1.13	1.24
1	A	475	PHE	CA-C	8.31	1.62	1.52
1	A	689	LEU	CA-C	8.26	1.62	1.52
1	A	229	GLN	N-CA	-8.26	1.36	1.46
1	A	192	TYR	CA-C	8.25	1.63	1.52
1	A	386	GLN	CD-NE2	8.25	1.50	1.33
1	A	676	PHE	C-O	-8.25	1.14	1.24
1	A	82	CYS	CA-C	8.24	1.63	1.52
2	B	152	LEU	CA-C	-8.23	1.42	1.52
1	A	356	TRP	CZ3-CH2	-8.23	1.19	1.40
2	B	96	ARG	C-O	8.22	1.34	1.24
1	A	579	ILE	C-O	8.22	1.33	1.24
1	A	605	GLN	C-O	-8.21	1.14	1.24
1	A	284	ILE	C-O	-8.21	1.15	1.24
1	A	639	PRO	CA-C	-8.20	1.43	1.52
1	A	28	LEU	N-CA	8.20	1.57	1.46
1	A	500	ARG	CA-C	-8.18	1.42	1.52
1	A	628	ARG	CG-CD	8.16	1.76	1.52
1	A	474	ARG	C-O	-8.15	1.14	1.24
1	A	33	GLU	CA-C	8.12	1.63	1.52
1	A	356	TRP	C-O	-8.12	1.13	1.23
1	A	476	LYS	CG-CD	8.12	1.76	1.52
1	A	496	ASP	CA-C	-8.11	1.43	1.52
1	A	61	LYS	N-CA	8.10	1.56	1.46
1	A	491	PRO	CA-C	-8.09	1.43	1.52
1	A	229	GLN	CA-C	-8.07	1.42	1.52
2	B	177	TRP	CD2-CE3	-8.06	1.27	1.40
2	B	128	MET	SD-CE	8.05	1.99	1.79
1	A	657	ILE	C-O	8.04	1.33	1.24
2	B	133	TYR	CD2-CE2	8.04	1.62	1.38
2	B	173	ASN	CA-C	8.03	1.64	1.53
1	A	226	LYS	CE-NZ	8.00	1.73	1.49
1	A	384	ASN	C-O	-7.99	1.13	1.23
1	A	49	PRO	C-O	-7.98	1.14	1.24
1	A	539	ALA	C-O	7.97	1.33	1.24
2	B	134	SER	CA-C	-7.96	1.42	1.53
1	A	76	LYS	CA-C	7.95	1.62	1.52
1	A	205	GLU	CD-OE2	-7.95	1.10	1.25
1	A	503	SER	CA-C	7.92	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	LEU	CG-CD1	-7.90	1.26	1.52
1	A	652	ASP	CA-C	-7.90	1.42	1.53
1	A	487	SER	CA-C	-7.89	1.43	1.52
1	A	417	ARG	NE-CZ	7.89	1.41	1.33
2	B	95	LYS	N-CA	7.89	1.55	1.46
1	A	9	ALA	CA-CB	-7.84	1.40	1.53
1	A	111	ILE	CA-CB	7.83	1.64	1.54
1	A	454	LEU	N-CA	7.82	1.56	1.46
1	A	39	CYS	CA-C	7.81	1.62	1.52
1	A	214	TRP	N-CA	7.81	1.55	1.46
1	A	161	LYS	N-CA	7.79	1.55	1.46
1	A	35	LEU	CA-CB	-7.78	1.41	1.53
1	A	161	LYS	CG-CD	7.76	1.75	1.52
1	A	188	ILE	C-O	-7.76	1.12	1.24
1	A	618	ARG	NE-CZ	7.74	1.41	1.33
2	B	65	ALA	C-O	7.74	1.33	1.24
2	B	75	LEU	C-N	-7.69	1.23	1.33
1	A	15	ALA	CA-CB	-7.68	1.40	1.53
1	A	385	PRO	CA-CB	-7.67	1.44	1.53
2	B	51	LYS	CA-C	-7.64	1.43	1.52
1	A	141	PHE	C-O	-7.62	1.14	1.24
1	A	358	LEU	CA-C	-7.62	1.43	1.52
2	B	156	PHE	C-O	-7.61	1.14	1.24
1	A	558	ARG	NE-CZ	7.59	1.41	1.33
1	A	180	LEU	CA-C	7.59	1.63	1.52
2	B	18	ARG	C-O	7.59	1.33	1.24
1	A	412	ILE	CA-CB	-7.59	1.44	1.54
1	A	686	THR	N-CA	-7.59	1.36	1.46
1	A	597	PHE	C-O	-7.58	1.14	1.24
1	A	666	LEU	C-O	-7.58	1.15	1.24
1	A	674	LYS	CD-CE	7.58	1.75	1.52
1	A	212	ALA	N-CA	7.57	1.55	1.46
1	A	409	VAL	CA-C	-7.57	1.43	1.52
1	A	559	ARG	N-CA	7.57	1.55	1.46
1	A	699	VAL	CB-CG1	7.57	1.77	1.52
1	A	238	LEU	CA-C	-7.56	1.43	1.52
1	A	530	ILE	CA-C	7.54	1.62	1.52
2	B	174	ILE	CA-CB	7.54	1.65	1.54
1	A	84	ASP	N-CA	-7.54	1.37	1.46
1	A	469	ARG	CD-NE	-7.54	1.35	1.46
2	B	181	THR	CA-C	-7.53	1.42	1.52
1	A	142	GLN	CA-CB	7.53	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	ASP	C-O	-7.53	1.14	1.24
1	A	377	TYR	N-CA	7.52	1.55	1.46
1	A	168	VAL	CA-CB	-7.52	1.45	1.54
1	A	280	LYS	N-CA	7.50	1.56	1.46
1	A	74	GLU	CD-OE2	7.50	1.39	1.25
1	A	289	GLY	C-O	7.50	1.33	1.23
1	A	198	GLY	C-O	-7.50	1.13	1.23
1	A	499	ILE	CA-CB	-7.50	1.45	1.54
1	A	506	LYS	CG-CD	7.48	1.74	1.52
1	A	160	THR	CA-C	-7.47	1.43	1.52
2	B	174	ILE	C-N	-7.47	1.23	1.33
1	A	218	ARG	CB-CG	7.46	1.74	1.52
2	B	90	TRP	CA-C	-7.46	1.42	1.52
1	A	153	VAL	CB-CG2	-7.45	1.27	1.52
2	B	119	PHE	C-O	7.45	1.33	1.24
1	A	184	ALA	CA-C	7.44	1.62	1.52
2	B	135	ASP	N-CA	7.42	1.54	1.46
1	A	656	ILE	CG1-CD1	-7.42	1.22	1.51
1	A	624	SER	N-CA	7.41	1.55	1.46
1	A	686	THR	C-O	-7.41	1.14	1.23
1	A	398	ASP	CA-C	7.41	1.62	1.52
1	A	462	SER	N-CA	7.40	1.55	1.46
1	A	201	THR	C-O	-7.39	1.14	1.24
1	A	579	ILE	CB-CG1	-7.36	1.38	1.53
1	A	635	GLY	N-CA	7.36	1.55	1.45
1	A	37	ASN	CA-C	7.36	1.62	1.52
1	A	389	ILE	CA-CB	-7.36	1.45	1.54
1	A	469	ARG	CZ-NH1	7.36	1.43	1.32
1	A	264	TYR	CA-C	-7.34	1.43	1.52
2	B	70	ASP	N-CA	-7.33	1.36	1.46
1	A	219	LYS	C-O	7.33	1.32	1.23
2	B	70	ASP	CB-CG	-7.33	1.33	1.52
1	A	101	ALA	N-CA	-7.32	1.36	1.46
2	B	175	GLN	CG-CD	7.32	1.70	1.52
1	A	230	LYS	C-O	7.31	1.32	1.24
1	A	134	ASN	C-O	-7.31	1.14	1.24
1	A	501	VAL	CA-CB	7.31	1.64	1.54
2	B	112	GLY	C-O	7.31	1.33	1.23
1	A	136	ALA	C-O	-7.29	1.16	1.24
1	A	603	LYS	CA-C	-7.28	1.43	1.52
1	A	132	GLN	N-CA	-7.26	1.36	1.46
1	A	409	VAL	CB-CG1	7.26	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	ARG	CZ-NH1	7.25	1.43	1.32
1	A	598	TYR	N-CA	7.25	1.55	1.46
1	A	623	ASN	CA-C	7.24	1.62	1.52
2	B	37	MET	CA-C	7.24	1.62	1.52
1	A	552	GLU	C-O	7.23	1.32	1.24
1	A	405	CYS	N-CA	7.23	1.55	1.46
1	A	582	ASP	N-CA	7.21	1.55	1.46
2	B	76	GLY	CA-C	7.21	1.59	1.52
1	A	370	THR	C-O	7.21	1.33	1.24
1	A	649	ARG	CD-NE	7.21	1.56	1.46
1	A	526	ASN	CA-C	7.19	1.62	1.52
1	A	668	ARG	N-CA	7.16	1.54	1.46
2	B	131	ARG	NE-CZ	7.16	1.41	1.33
2	B	160	ARG	CG-CD	7.16	1.74	1.52
1	A	28	LEU	CA-C	-7.15	1.41	1.52
1	A	353	TYR	N-CA	7.15	1.54	1.46
1	A	481	GLU	N-CA	-7.14	1.37	1.46
1	A	205	GLU	N-CA	7.13	1.55	1.46
1	A	191	CYS	CA-C	7.13	1.61	1.52
1	A	495	GLY	CA-C	-7.13	1.44	1.51
2	B	168	GLY	N-CA	7.12	1.55	1.45
1	A	399	GLU	C-N	-7.12	1.22	1.33
1	A	137	GLY	C-O	-7.12	1.13	1.24
2	B	20	LEU	C-O	7.12	1.32	1.24
1	A	171	ALA	C-O	-7.11	1.15	1.24
1	A	243	ASP	C-O	7.10	1.32	1.23
2	B	145	PHE	N-CA	-7.10	1.37	1.46
1	A	38	GLU	N-CA	-7.10	1.37	1.46
2	B	147	SER	C-O	7.09	1.32	1.24
1	A	263	ALA	CA-CB	7.09	1.64	1.53
1	A	610	ILE	C-O	7.09	1.32	1.24
1	A	184	ALA	N-CA	7.09	1.55	1.46
2	B	25	ALA	CA-CB	7.07	1.64	1.54
1	A	672	LEU	N-CA	7.07	1.55	1.46
1	A	221	PRO	C-O	7.06	1.32	1.24
1	A	73	ILE	C-O	-7.06	1.16	1.24
1	A	139	PHE	C-O	-7.04	1.14	1.23
1	A	587	ASP	CA-C	7.04	1.62	1.52
2	B	87	ILE	CA-CB	-7.04	1.44	1.54
1	A	676	PHE	CE2-CZ	7.03	1.59	1.38
2	B	153	ASP	N-CA	7.02	1.54	1.46
1	A	364	ASN	C-N	7.02	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	146	ILE	N-CA	-7.02	1.38	1.46
1	A	678	GLN	N-CA	-7.01	1.38	1.46
1	A	425	ASP	N-CA	7.01	1.57	1.46
1	A	506	LYS	CB-CG	7.00	1.73	1.52
1	A	371	ALA	N-CA	-7.00	1.37	1.46
1	A	509	TYR	C-O	-7.00	1.15	1.23
1	A	157	ARG	CZ-NH1	-6.99	1.23	1.32
1	A	697	PHE	N-CA	6.99	1.54	1.46
1	A	23	ARG	CB-CG	-6.98	1.31	1.52
2	B	163	ASP	CA-C	6.98	1.63	1.53
1	A	208	THR	N-CA	6.97	1.54	1.46
1	A	502	PHE	C-N	-6.96	1.24	1.33
1	A	120	ILE	C-N	-6.96	1.25	1.33
1	A	692	ILE	C-O	-6.95	1.16	1.24
2	B	128	MET	CA-C	-6.95	1.43	1.52
1	A	571	GLY	CA-C	6.94	1.61	1.51
1	A	418	ARG	CA-C	-6.94	1.43	1.52
1	A	475	PHE	C-O	6.93	1.32	1.23
1	A	363	GLY	CA-C	6.93	1.59	1.51
1	A	338	LEU	CA-C	6.93	1.60	1.52
2	B	177	TRP	CE3-CZ3	6.91	1.59	1.38
1	A	629	LYS	CB-CG	6.90	1.73	1.52
2	B	67	MET	CG-SD	-6.89	1.63	1.80
2	B	107	SER	C-O	6.88	1.32	1.24
1	A	73	ILE	CA-C	-6.88	1.44	1.52
1	A	271	GLU	CA-C	6.87	1.62	1.53
1	A	143	PHE	CA-C	-6.87	1.44	1.52
1	A	204	PHE	C-O	-6.86	1.15	1.24
1	A	228	ILE	C-O	6.86	1.32	1.24
2	B	125	ILE	C-O	6.86	1.31	1.24
1	A	431	PHE	CG-CD2	-6.85	1.24	1.38
1	A	586	GLU	CA-C	-6.85	1.43	1.52
1	A	513	ASP	CG-OD1	6.85	1.38	1.25
2	B	62	SER	CA-C	-6.83	1.44	1.52
1	A	49	PRO	N-CA	6.82	1.56	1.47
1	A	462	SER	CA-C	6.81	1.61	1.52
1	A	177	TRP	C-O	6.80	1.32	1.24
1	A	18	LEU	CA-C	-6.79	1.43	1.52
1	A	371	ALA	CA-C	6.79	1.61	1.52
1	A	474	ARG	CG-CD	6.79	1.72	1.52
1	A	172	GLU	CA-C	-6.79	1.43	1.52
1	A	644	GLN	CD-OE1	6.78	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	LEU	C-O	6.78	1.31	1.24
2	B	63	MET	C-O	6.77	1.32	1.24
1	A	120	ILE	CB-CG1	6.77	1.67	1.53
1	A	140	HIS	CA-C	-6.77	1.44	1.52
1	A	408	LEU	CA-C	6.77	1.60	1.52
1	A	690	ASP	N-CA	-6.76	1.37	1.45
1	A	34	THR	CA-C	-6.76	1.44	1.52
1	A	95	THR	CA-C	-6.76	1.44	1.52
1	A	344	THR	C-N	-6.75	1.25	1.33
2	B	148	CYS	N-CA	6.75	1.54	1.46
1	A	433	ILE	CB-CG1	-6.75	1.40	1.53
1	A	577	CYS	N-CA	6.75	1.54	1.46
2	B	143	ASP	CA-C	6.75	1.61	1.52
2	B	68	ASP	CG-OD1	6.75	1.38	1.25
2	B	27	ASP	CA-C	6.74	1.61	1.52
1	A	121	LEU	CA-C	-6.74	1.43	1.52
2	B	183	TYR	C-O	6.74	1.31	1.23
1	A	143	PHE	C-O	-6.74	1.15	1.23
1	A	57	SER	N-CA	-6.73	1.37	1.46
1	A	671	ILE	C-O	6.73	1.31	1.24
1	A	547	GLU	CA-C	6.72	1.60	1.52
1	A	671	ILE	CA-CB	6.72	1.63	1.54
2	B	64	VAL	C-O	6.71	1.31	1.24
1	A	157	ARG	CZ-NH2	-6.70	1.24	1.33
1	A	683	ASN	C-O	6.70	1.32	1.23
1	A	175	GLU	C-O	6.70	1.32	1.24
1	A	288	TRP	CA-C	6.70	1.61	1.52
1	A	469	ARG	NE-CZ	6.70	1.40	1.33
1	A	215	TYR	N-CA	6.69	1.54	1.46
1	A	582	ASP	C-O	-6.69	1.15	1.24
1	A	282	ILE	CA-CB	6.68	1.62	1.54
1	A	412	ILE	C-O	-6.68	1.16	1.24
2	B	137	THR	N-CA	6.68	1.55	1.46
1	A	113	SER	CA-C	-6.68	1.43	1.52
1	A	124	VAL	N-CA	6.68	1.53	1.46
1	A	29	ASN	CA-CB	-6.67	1.43	1.53
1	A	106	TRP	CD2-CE3	6.67	1.50	1.40
2	B	143	ASP	C-O	6.67	1.32	1.24
1	A	151	GLU	CA-C	-6.67	1.44	1.52
1	A	189	ASN	CA-C	6.66	1.61	1.52
1	A	220	PRO	CA-CB	-6.66	1.44	1.54
1	A	25	ILE	C-O	-6.65	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	81	LYS	CB-CG	6.65	1.72	1.52
1	A	129	GLN	CA-C	-6.64	1.44	1.52
1	A	645	VAL	N-CA	-6.64	1.38	1.46
1	A	63	LEU	CA-CB	-6.63	1.43	1.53
1	A	341	CYS	C-O	-6.63	1.16	1.23
1	A	183	LYS	N-CA	-6.62	1.38	1.46
1	A	116	LEU	N-CA	-6.62	1.38	1.46
1	A	559	ARG	NE-CZ	6.60	1.40	1.33
1	A	435	GLU	C-O	-6.60	1.15	1.23
1	A	289	GLY	CA-C	6.59	1.63	1.52
1	A	669	LEU	CG-CD2	6.59	1.74	1.52
1	A	674	LYS	CB-CG	6.59	1.72	1.52
1	A	28	LEU	C-O	-6.58	1.13	1.24
1	A	529	ASP	CA-C	6.58	1.61	1.52
1	A	368	GLY	C-O	-6.58	1.16	1.24
1	A	666	LEU	N-CA	-6.58	1.38	1.46
2	B	133	TYR	CA-C	6.56	1.61	1.52
1	A	434	TYR	CB-CG	-6.55	1.37	1.51
1	A	530	ILE	N-CA	6.55	1.54	1.46
1	A	141	PHE	CG-CD2	6.54	1.52	1.38
1	A	427	HIS	CG-ND1	-6.53	1.31	1.38
1	A	148	GLU	CD-OE1	6.53	1.37	1.25
1	A	219	LYS	CA-C	-6.53	1.45	1.52
1	A	675	ILE	CA-CB	-6.52	1.46	1.54
2	B	32	SER	CA-CB	-6.52	1.43	1.53
1	A	455	THR	CA-CB	6.51	1.72	1.54
1	A	484	LEU	CA-CB	-6.51	1.44	1.53
2	B	116	ALA	CA-CB	6.51	1.63	1.53
1	A	578	LYS	CE-NZ	6.50	1.68	1.49
1	A	348	LEU	CA-C	-6.50	1.44	1.52
1	A	677	LYS	CD-CE	6.49	1.72	1.52
2	B	158	ALA	CA-C	6.49	1.61	1.52
1	A	200	THR	CA-C	-6.48	1.43	1.52
2	B	50	LEU	CA-C	6.48	1.60	1.52
1	A	649	ARG	C-O	-6.48	1.15	1.24
2	B	146	ILE	CA-C	6.47	1.60	1.52
1	A	377	TYR	CA-CB	-6.47	1.44	1.53
1	A	595	LYS	CE-NZ	6.47	1.68	1.49
1	A	390	LYS	CA-C	-6.46	1.45	1.52
1	A	422	MET	CA-CB	6.46	1.64	1.53
1	A	576	THR	C-O	-6.46	1.16	1.24
2	B	77	PHE	CA-C	-6.46	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	625	TYR	C-O	6.46	1.32	1.24
1	A	135	TYR	C-O	-6.45	1.15	1.24
1	A	27	TYR	CZ-OH	-6.45	1.24	1.38
1	A	689	LEU	C-O	6.45	1.31	1.23
1	A	237	LEU	CG-CD2	-6.44	1.31	1.52
1	A	328	PHE	C-O	-6.44	1.15	1.24
1	A	608	GLN	CA-C	-6.44	1.43	1.52
1	A	514	ASP	C-O	6.44	1.31	1.24
1	A	538	PHE	CA-C	6.43	1.61	1.52
1	A	688	GLN	CA-CB	-6.43	1.41	1.53
1	A	668	ARG	CD-NE	6.42	1.55	1.46
1	A	130	SER	C-O	-6.42	1.17	1.24
1	A	19	GLY	CA-C	6.41	1.60	1.51
1	A	372	GLY	C-O	-6.41	1.15	1.23
2	B	168	GLY	C-O	-6.41	1.15	1.23
1	A	46	PHE	CB-CG	6.41	1.65	1.50
1	A	102	LEU	N-CA	6.40	1.53	1.45
1	A	350	CYS	CA-C	6.40	1.61	1.52
1	A	374	CYS	CB-SG	-6.40	1.60	1.81
1	A	197	GLY	N-CA	6.40	1.54	1.45
1	A	492	HIS	CA-CB	-6.40	1.42	1.53
1	A	55	PRO	C-O	6.40	1.32	1.24
1	A	661	ASN	C-N	-6.39	1.25	1.33
1	A	692	ILE	CB-CG1	6.39	1.66	1.53
2	B	173	ASN	N-CA	-6.39	1.38	1.46
1	A	493	LYS	CA-C	6.39	1.60	1.52
2	B	113	ALA	C-O	-6.38	1.16	1.24
1	A	144	TRP	CA-CB	-6.37	1.44	1.53
1	A	653	ASP	C-N	-6.37	1.25	1.33
2	B	75	LEU	CB-CG	-6.37	1.40	1.53
1	A	73	ILE	N-CA	6.36	1.54	1.46
1	A	695	LEU	C-N	-6.36	1.25	1.33
1	A	125	VAL	CA-C	-6.36	1.46	1.52
1	A	138	ILE	CA-C	6.34	1.60	1.52
1	A	654	GLU	N-CA	6.34	1.54	1.46
2	B	29	MET	CA-C	6.34	1.61	1.53
1	A	60	PHE	C-O	-6.33	1.16	1.24
1	A	10	THR	CA-CB	6.32	1.63	1.53
1	A	535	ARG	C-O	6.32	1.31	1.24
1	A	540	GLN	CG-CD	6.32	1.67	1.52
1	A	56	SER	N-CA	6.31	1.54	1.46
1	A	552	GLU	CA-CB	6.31	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	86	ASN	C-O	6.31	1.32	1.24
1	A	557	LEU	C-O	6.29	1.31	1.24
1	A	417	ARG	CB-CG	6.28	1.71	1.52
1	A	364	ASN	C-O	-6.28	1.16	1.23
1	A	658	ASP	CG-OD1	6.28	1.37	1.25
1	A	392	GLU	C-O	-6.28	1.16	1.24
1	A	79	THR	CA-C	6.27	1.61	1.52
2	B	75	LEU	C-O	-6.26	1.16	1.24
1	A	426	MET	CB-CG	-6.25	1.33	1.52
1	A	80	GLU	C-O	-6.25	1.15	1.23
1	A	488	THR	CB-CG2	-6.25	1.31	1.52
1	A	536	ARG	CA-CB	6.25	1.63	1.53
1	A	637	LYS	CD-CE	6.24	1.71	1.52
1	A	699	VAL	CA-C	6.24	1.60	1.52
1	A	27	TYR	CE2-CZ	-6.24	1.23	1.38
2	B	21	PHE	N-CA	6.24	1.54	1.46
1	A	504	GLU	N-CA	6.24	1.53	1.46
2	B	22	VAL	CA-C	6.23	1.60	1.52
1	A	385	PRO	C-O	6.23	1.30	1.23
1	A	67	SER	C-O	6.23	1.31	1.23
1	A	559	ARG	CA-C	6.19	1.60	1.52
2	B	81	LYS	N-CA	-6.19	1.39	1.46
1	A	462	SER	C-O	6.18	1.31	1.24
1	A	147	GLY	C-N	-6.18	1.25	1.33
1	A	217	LEU	CA-C	6.18	1.61	1.52
1	A	349	THR	CB-CG2	6.18	1.73	1.52
1	A	99	GLN	N-CA	6.17	1.53	1.45
1	A	639	PRO	C-O	-6.16	1.16	1.23
1	A	488	THR	CA-CB	6.16	1.63	1.53
1	A	81	ILE	C-O	-6.16	1.16	1.24
1	A	614	ILE	CA-C	-6.16	1.43	1.52
1	A	684	THR	N-CA	6.15	1.54	1.46
2	B	67	MET	CA-C	6.15	1.60	1.52
1	A	159	PRO	CA-CB	-6.14	1.45	1.53
1	A	576	THR	CA-CB	6.14	1.63	1.53
1	A	99	GLN	CD-OE1	6.13	1.35	1.23
1	A	152	VAL	CA-CB	6.13	1.64	1.55
1	A	653	ASP	CA-C	-6.13	1.44	1.53
1	A	562	ALA	C-O	6.11	1.31	1.24
2	B	136	GLU	CA-CB	-6.10	1.43	1.53
1	A	29	ASN	CG-ND2	6.10	1.46	1.33
1	A	118	GLU	CG-CD	6.10	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	661	ASN	CA-C	-6.09	1.44	1.52
2	B	133	TYR	CE1-CZ	6.08	1.52	1.38
1	A	102	LEU	C-N	-6.07	1.24	1.33
1	A	359	THR	CB-CG2	-6.07	1.32	1.52
1	A	362	ASP	CB-CG	-6.07	1.36	1.52
1	A	518	ALA	N-CA	6.07	1.55	1.46
2	B	51	LYS	CA-CB	6.07	1.62	1.53
1	A	234	LYS	N-CA	6.07	1.54	1.46
1	A	146	TYR	CE2-CZ	-6.06	1.23	1.38
1	A	81	ILE	C-N	-6.06	1.26	1.33
1	A	400	ASP	C-O	6.06	1.31	1.23
1	A	158	LEU	C-N	-6.05	1.25	1.33
2	B	64	VAL	N-CA	6.05	1.53	1.46
1	A	133	GLU	N-CA	6.05	1.53	1.46
2	B	156	PHE	CA-C	-6.04	1.44	1.52
2	B	45	THR	C-O	6.04	1.31	1.23
1	A	513	ASP	CG-OD2	6.04	1.36	1.25
2	B	61	ARG	CZ-NH2	6.03	1.41	1.33
1	A	600	LEU	N-CA	-6.03	1.39	1.46
1	A	516	ILE	C-O	6.01	1.31	1.24
1	A	645	VAL	CA-C	6.01	1.60	1.52
1	A	42	ALA	C-O	-6.01	1.16	1.24
1	A	399	GLU	CA-C	6.01	1.60	1.52
1	A	10	THR	N-CA	-6.01	1.38	1.46
1	A	286	ASN	C-O	-6.00	1.16	1.24
1	A	6	MET	CG-SD	6.00	1.95	1.80
1	A	180	LEU	CG-CD1	-6.00	1.32	1.52
2	B	74	LYS	CE-NZ	6.00	1.67	1.49
1	A	450	LYS	CE-NZ	5.99	1.67	1.49
1	A	146	TYR	C-O	5.98	1.31	1.23
1	A	128	ASP	CG-OD1	5.98	1.36	1.25
1	A	577	CYS	C-N	-5.98	1.26	1.33
1	A	597	PHE	CA-CB	-5.97	1.43	1.53
1	A	473	ASN	N-CA	-5.97	1.38	1.46
1	A	47	GLN	C-O	-5.97	1.17	1.23
1	A	608	GLN	CA-CB	-5.97	1.44	1.53
1	A	142	GLN	CB-CG	-5.96	1.34	1.52
1	A	171	ALA	N-CA	5.96	1.53	1.46
1	A	167	PHE	CB-CG	5.95	1.64	1.50
2	B	134	SER	CA-CB	-5.95	1.44	1.53
2	B	172	VAL	C-O	5.94	1.30	1.24
1	A	114	LEU	CA-C	-5.93	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	156	PHE	CD1-CE1	5.93	1.56	1.38
1	A	424	GLU	CA-CB	-5.92	1.44	1.53
2	B	20	LEU	N-CA	-5.92	1.38	1.46
2	B	158	ALA	CA-CB	-5.92	1.43	1.53
2	B	160	ARG	CB-CG	5.92	1.70	1.52
1	A	164	GLU	C-O	-5.91	1.16	1.24
1	A	557	LEU	CG-CD2	5.91	1.72	1.52
1	A	64	GLY	CA-C	5.91	1.60	1.51
1	A	183	LYS	CE-NZ	-5.91	1.31	1.49
1	A	347	THR	CA-CB	5.90	1.62	1.53
1	A	99	GLN	CA-C	-5.89	1.45	1.52
1	A	668	ARG	CB-CG	5.89	1.70	1.52
1	A	366	ARG	C-O	-5.89	1.17	1.23
2	B	145	PHE	C-O	5.89	1.31	1.24
1	A	96	ASP	CB-CG	-5.88	1.37	1.52
1	A	654	GLU	CD-OE2	5.88	1.36	1.25
1	A	130	SER	CA-C	-5.88	1.45	1.52
1	A	473	ASN	CA-C	-5.87	1.45	1.52
1	A	354	LYS	CG-CD	5.87	1.70	1.52
2	B	182	MET	C-O	-5.87	1.17	1.24
1	A	104	ASP	C-N	-5.86	1.25	1.33
2	B	44	VAL	CA-CB	5.86	1.61	1.54
2	B	70	ASP	CA-C	5.86	1.60	1.52
1	A	569	SER	C-O	5.85	1.31	1.23
1	A	387	TYR	C-O	-5.85	1.16	1.23
1	A	159	PRO	N-CD	-5.84	1.39	1.47
1	A	640	CYS	N-CA	5.84	1.53	1.46
1	A	114	LEU	CA-CB	5.83	1.62	1.53
1	A	652	ASP	CA-CB	-5.83	1.44	1.53
2	B	21	PHE	CA-C	-5.83	1.45	1.52
1	A	576	THR	CA-C	5.83	1.60	1.52
1	A	75	TRP	N-CA	-5.82	1.38	1.46
1	A	144	TRP	C-O	-5.82	1.16	1.24
1	A	336	SER	C-O	-5.82	1.16	1.24
1	A	491	PRO	CG-CD	-5.82	1.30	1.50
2	B	122	ASN	N-CA	-5.82	1.38	1.46
1	A	428	THR	CB-OG1	5.80	1.53	1.43
1	A	135	TYR	CA-C	-5.80	1.45	1.52
1	A	381	PHE	CA-CB	-5.80	1.44	1.53
1	A	413	GLN	CA-C	-5.79	1.45	1.52
1	A	115	THR	CA-CB	5.79	1.63	1.53
1	A	342	ASN	C-O	-5.79	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	526	ASN	C-O	5.79	1.31	1.24
2	B	132	ARG	CG-CD	5.79	1.69	1.52
1	A	230	LYS	N-CA	5.78	1.53	1.46
1	A	118	GLU	CB-CG	5.78	1.69	1.52
1	A	147	GLY	C-O	-5.78	1.16	1.24
1	A	184	ALA	CA-CB	-5.78	1.44	1.53
1	A	94	ARG	C-O	-5.76	1.17	1.24
1	A	281	LEU	N-CA	-5.76	1.39	1.46
2	B	57	ILE	N-CA	5.76	1.53	1.46
1	A	112	ALA	C-O	5.75	1.30	1.24
1	A	356	TRP	CE2-CZ2	-5.75	1.27	1.39
1	A	510	GLN	CG-CD	5.75	1.66	1.52
1	A	21	HIS	N-CA	5.75	1.53	1.46
1	A	81	ILE	CA-CB	5.75	1.62	1.54
1	A	612	ARG	CZ-NH1	5.75	1.40	1.32
1	A	419	GLN	CG-CD	-5.74	1.37	1.52
1	A	242	ILE	C-O	-5.74	1.18	1.24
1	A	501	VAL	C-O	5.73	1.30	1.24
1	A	367	ARG	CA-CB	5.72	1.62	1.53
1	A	419	GLN	N-CA	5.72	1.53	1.46
1	A	329	SER	CA-C	-5.72	1.44	1.52
1	A	599	ILE	C-N	-5.71	1.26	1.33
2	B	181	THR	CB-CG2	-5.71	1.33	1.52
2	B	61	ARG	CZ-NH1	5.71	1.40	1.32
1	A	237	LEU	CA-CB	-5.71	1.44	1.53
2	B	153	ASP	C-O	5.71	1.30	1.24
1	A	42	ALA	CA-C	5.70	1.60	1.52
1	A	605	GLN	CB-CG	5.70	1.69	1.52
1	A	6	MET	SD-CE	5.69	1.93	1.79
1	A	193	GLU	N-CA	-5.68	1.38	1.46
1	A	204	PHE	C-N	-5.68	1.26	1.33
1	A	69	LYS	CA-C	5.68	1.60	1.52
1	A	435	GLU	CD-OE1	5.68	1.36	1.25
1	A	491	PRO	C-N	-5.68	1.25	1.33
1	A	483	VAL	C-O	5.68	1.30	1.24
1	A	500	ARG	NE-CZ	5.67	1.39	1.33
1	A	541	LEU	CG-CD2	5.67	1.71	1.52
1	A	485	VAL	CA-CB	-5.66	1.46	1.54
2	B	163	ASP	N-CA	-5.66	1.39	1.46
1	A	384	ASN	CA-CB	-5.66	1.45	1.53
2	B	67	MET	SD-CE	-5.66	1.65	1.79
2	B	96	ARG	N-CA	-5.66	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	661	ASN	N-CA	5.65	1.53	1.46
2	B	20	LEU	CA-C	5.65	1.60	1.52
1	A	352	SER	C-O	5.65	1.31	1.24
1	A	89	ILE	N-CA	5.65	1.53	1.46
1	A	471	VAL	N-CA	-5.65	1.39	1.46
1	A	156	ASP	C-N	-5.64	1.25	1.33
1	A	226	LYS	C-O	5.63	1.31	1.24
1	A	610	ILE	CA-C	-5.63	1.46	1.52
1	A	24	ALA	N-CA	-5.63	1.38	1.45
1	A	591	LYS	CB-CG	5.63	1.69	1.52
2	B	81	LYS	CA-C	-5.63	1.45	1.52
1	A	469	ARG	CZ-NH2	5.62	1.40	1.33
1	A	621	THR	C-O	5.62	1.30	1.23
1	A	434	TYR	C-N	5.62	1.41	1.33
1	A	280	LYS	CA-CB	5.61	1.60	1.53
1	A	211	ILE	C-O	5.61	1.30	1.24
2	B	9	ASN	C-O	5.60	1.34	1.23
1	A	117	ASN	CA-C	-5.59	1.46	1.52
1	A	266	VAL	CA-CB	-5.59	1.47	1.54
1	A	660	ASP	N-CA	5.59	1.52	1.46
1	A	93	THR	N-CA	5.58	1.53	1.45
1	A	388	LEU	N-CA	5.58	1.52	1.46
2	B	182	MET	CB-CG	-5.58	1.35	1.52
1	A	406	THR	CA-C	5.58	1.59	1.52
1	A	179	ALA	CA-C	5.57	1.60	1.52
2	B	95	LYS	CE-NZ	5.57	1.66	1.49
1	A	21	HIS	CA-CB	-5.57	1.44	1.53
1	A	80	GLU	CA-C	-5.57	1.46	1.53
1	A	431	PHE	CD2-CE2	-5.57	1.22	1.38
2	B	102	SER	CA-C	5.57	1.60	1.52
1	A	568	LYS	CG-CD	5.57	1.69	1.52
1	A	224	LEU	C-O	5.56	1.30	1.24
2	B	47	HIS	C-N	5.56	1.39	1.33
1	A	6	MET	CA-C	5.55	1.60	1.52
1	A	65	PRO	N-CA	-5.55	1.40	1.46
1	A	161	LYS	CE-NZ	5.55	1.66	1.49
1	A	529	ASP	C-O	5.55	1.30	1.24
1	A	389	ILE	CG1-CD1	5.54	1.73	1.51
1	A	211	ILE	CA-CB	5.54	1.61	1.54
1	A	482	TYR	C-N	-5.54	1.26	1.33
1	A	674	LYS	CG-CD	5.54	1.69	1.52
2	B	88	LYS	C-O	-5.54	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	PRO	CB-CG	5.53	1.77	1.49
1	A	32	TYR	CA-C	-5.52	1.46	1.52
1	A	203	GLY	C-O	-5.52	1.17	1.23
1	A	476	LYS	CA-C	-5.52	1.46	1.52
2	B	159	PHE	CG-CD2	-5.51	1.27	1.38
1	A	152	VAL	C-O	-5.51	1.18	1.24
1	A	365	TRP	CG-CD1	-5.51	1.23	1.36
1	A	486	PRO	C-O	-5.51	1.16	1.24
1	A	133	GLU	CA-C	5.50	1.60	1.52
1	A	198	GLY	CA-C	-5.50	1.43	1.52
1	A	187	LYS	CA-CB	5.50	1.62	1.53
2	B	170	ILE	CA-C	-5.50	1.46	1.52
1	A	325	TRP	CE2-CZ2	5.50	1.51	1.39
2	B	129	ILE	CA-C	5.49	1.59	1.52
1	A	8	LEU	CG-CD2	5.48	1.70	1.52
2	B	69	SER	CA-CB	-5.48	1.44	1.53
1	A	239	GLY	C-O	-5.48	1.16	1.23
2	B	131	ARG	CD-NE	5.47	1.53	1.46
1	A	411	LEU	CG-CD1	5.47	1.70	1.52
1	A	143	PHE	CA-CB	-5.47	1.44	1.53
1	A	587	ASP	C-O	-5.47	1.17	1.24
2	B	87	ILE	CB-CG2	5.47	1.70	1.52
1	A	472	LEU	CA-C	5.46	1.59	1.52
1	A	632	GLU	CG-CD	5.46	1.65	1.52
1	A	668	ARG	C-O	-5.45	1.17	1.24
1	A	365	TRP	CD2-CE2	-5.45	1.32	1.41
1	A	51	PHE	CA-C	-5.45	1.46	1.52
2	B	82	TYR	N-CA	5.45	1.53	1.46
2	B	72	THR	CA-CB	-5.44	1.46	1.54
1	A	394	GLU	C-O	-5.44	1.17	1.23
2	B	69	SER	CB-OG	-5.44	1.31	1.42
1	A	519	ASN	C-N	-5.43	1.26	1.33
1	A	219	LYS	CB-CG	5.43	1.68	1.52
1	A	678	GLN	CD-OE1	5.43	1.33	1.23
2	B	75	LEU	N-CA	5.43	1.53	1.46
1	A	125	VAL	CB-CG2	5.42	1.70	1.52
1	A	341	CYS	CA-C	-5.42	1.47	1.53
1	A	375	ARG	NE-CZ	5.42	1.39	1.33
1	A	396	GLU	CA-C	5.42	1.59	1.52
1	A	148	GLU	CA-C	5.41	1.59	1.52
1	A	33	GLU	C-O	5.41	1.30	1.24
1	A	390	LYS	CD-CE	5.41	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	601	TRP	CG-CD2	-5.41	1.34	1.43
1	A	686	THR	CB-CG2	-5.41	1.34	1.52
2	B	29	MET	CG-SD	5.40	1.94	1.80
1	A	127	LEU	CA-C	-5.40	1.45	1.52
1	A	156	ASP	CA-C	5.39	1.60	1.52
1	A	673	PHE	CG-CD2	-5.39	1.27	1.38
2	B	33	ALA	C-O	-5.39	1.17	1.24
1	A	49	PRO	CA-CB	-5.39	1.46	1.53
2	B	161	SER	N-CA	-5.39	1.39	1.46
1	A	2	ALA	C-O	-5.38	1.12	1.23
2	B	52	THR	CA-CB	5.38	1.62	1.53
1	A	192	TYR	CE1-CZ	-5.38	1.25	1.38
1	A	186	ALA	N-CA	5.38	1.52	1.46
1	A	3	GLY	CA-C	-5.37	1.44	1.51
1	A	673	PHE	CE1-CZ	-5.37	1.22	1.38
2	B	23	GLN	CG-CD	5.37	1.65	1.52
1	A	636	PHE	CA-C	5.37	1.59	1.52
1	A	466	ILE	CA-CB	-5.37	1.45	1.55
1	A	218	ARG	CD-NE	5.36	1.53	1.46
1	A	59	GLY	C-O	-5.36	1.18	1.23
1	A	536	ARG	CA-C	5.36	1.59	1.52
1	A	271	GLU	N-CA	5.36	1.52	1.45
1	A	604	ILE	CB-CG2	-5.35	1.34	1.52
2	B	154	ALA	C-O	-5.35	1.17	1.24
2	B	54	GLY	N-CA	5.34	1.51	1.45
1	A	46	PHE	CE1-CZ	5.34	1.54	1.38
1	A	201	THR	C-N	5.34	1.41	1.33
1	A	35	LEU	CA-C	5.33	1.59	1.52
1	A	268	GLY	C-O	-5.33	1.18	1.23
1	A	163	GLY	C-O	5.33	1.31	1.24
2	B	151	ARG	CZ-NH1	5.32	1.40	1.32
1	A	490	GLU	CD-OE2	5.32	1.35	1.25
1	A	693	SER	CA-C	-5.32	1.45	1.52
1	A	135	TYR	CG-CD1	-5.31	1.28	1.39
1	A	611	TYR	C-O	5.31	1.30	1.24
1	A	55	PRO	CG-CD	5.31	1.68	1.50
1	A	279	GLN	N-CA	5.31	1.56	1.46
2	B	49	ASP	N-CA	5.31	1.53	1.46
1	A	694	TRP	C-O	5.30	1.30	1.24
1	A	151	GLU	CD-OE2	5.30	1.35	1.25
2	B	96	ARG	CA-CB	5.30	1.62	1.53
2	B	177	TRP	CA-CB	-5.30	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	608	GLN	C-N	-5.29	1.27	1.33
1	A	333	ARG	NE-CZ	5.29	1.38	1.33
1	A	109	ALA	C-O	5.29	1.30	1.24
1	A	177	TRP	CA-CB	-5.28	1.45	1.53
1	A	597	PHE	CD1-CE1	5.28	1.54	1.38
1	A	87	PHE	CG-CD1	-5.28	1.27	1.38
1	A	280	LYS	C-O	5.28	1.30	1.24
1	A	508	ASP	C-O	-5.27	1.17	1.23
1	A	126	PRO	C-O	5.27	1.30	1.24
2	B	153	ASP	CG-OD1	5.27	1.35	1.25
2	B	91	GLN	N-CA	5.27	1.52	1.46
1	A	497	PHE	CB-CG	-5.26	1.38	1.50
1	A	169	HIS	N-CA	5.26	1.52	1.46
1	A	359	THR	C-O	5.26	1.30	1.23
1	A	619	SER	CA-C	5.26	1.62	1.52
2	B	101	ARG	C-O	5.26	1.30	1.24
1	A	224	LEU	C-N	5.25	1.40	1.33
1	A	416	ARG	CA-CB	5.25	1.61	1.53
1	A	535	ARG	NE-CZ	5.25	1.38	1.33
1	A	90	GLY	C-O	5.25	1.31	1.23
1	A	534	PHE	CA-CB	5.24	1.62	1.53
2	B	31	VAL	CA-CB	-5.24	1.47	1.54
1	A	452	PHE	CA-C	-5.24	1.46	1.53
1	A	65	PRO	C-O	5.24	1.29	1.23
1	A	123	ARG	CG-CD	-5.24	1.36	1.52
1	A	383	MET	SD-CE	-5.24	1.66	1.79
1	A	78	PRO	CG-CD	5.24	1.68	1.50
1	A	346	ASP	C-O	-5.23	1.17	1.24
1	A	612	ARG	CA-C	5.23	1.59	1.52
1	A	526	ASN	C-N	5.23	1.41	1.33
1	A	220	PRO	C-N	-5.22	1.27	1.33
1	A	203	GLY	C-N	-5.22	1.26	1.33
1	A	334	HIS	CB-CG	5.22	1.57	1.50
1	A	659	PHE	CE1-CZ	-5.22	1.23	1.38
2	B	95	LYS	CD-CE	5.22	1.68	1.52
1	A	152	VAL	C-N	-5.22	1.26	1.33
1	A	614	ILE	N-CA	-5.22	1.39	1.46
1	A	241	SER	CA-C	-5.21	1.45	1.52
1	A	131	PHE	CG-CD1	-5.21	1.27	1.38
1	A	513	ASP	CA-C	-5.21	1.46	1.52
1	A	402	GLU	C-O	5.20	1.29	1.24
1	A	226	LYS	N-CA	5.20	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	THR	CA-C	-5.19	1.46	1.52
1	A	266	VAL	C-O	5.19	1.29	1.24
2	B	51	LYS	CB-CG	5.19	1.68	1.52
1	A	375	ARG	CA-C	5.19	1.59	1.52
1	A	662	PHE	CD2-CE2	5.19	1.54	1.38
1	A	178	SER	C-N	-5.19	1.26	1.34
1	A	55	PRO	CA-CB	5.18	1.61	1.53
1	A	505	LYS	C-O	-5.18	1.16	1.23
2	B	43	VAL	CA-C	5.18	1.60	1.52
1	A	52	PRO	CA-C	5.18	1.58	1.52
2	B	62	SER	N-CA	-5.18	1.40	1.46
1	A	592	LEU	C-O	-5.18	1.17	1.24
1	A	561	LEU	CA-CB	5.18	1.62	1.53
1	A	663	VAL	C-N	-5.18	1.27	1.33
2	B	179	GLN	C-O	5.18	1.30	1.24
1	A	7	LYS	C-O	-5.17	1.17	1.24
1	A	166	LEU	C-O	-5.17	1.17	1.24
1	A	413	GLN	C-O	-5.17	1.17	1.24
1	A	508	ASP	CA-C	-5.17	1.46	1.52
1	A	673	PHE	CA-C	-5.17	1.46	1.52
1	A	143	PHE	N-CA	-5.16	1.39	1.45
1	A	231	ALA	C-O	5.16	1.30	1.24
1	A	89	ILE	CB-CG1	5.16	1.63	1.53
1	A	411	LEU	CA-C	-5.15	1.46	1.52
1	A	213	GLU	CD-OE1	5.15	1.35	1.25
1	A	357	LYS	CD-CE	5.14	1.67	1.52
1	A	417	ARG	C-O	-5.14	1.17	1.24
1	A	183	LYS	CG-CD	-5.14	1.37	1.52
1	A	141	PHE	N-CA	5.14	1.53	1.46
2	B	25	ALA	CA-C	5.14	1.59	1.52
1	A	35	LEU	CG-CD2	5.13	1.69	1.52
1	A	272	VAL	N-CA	5.13	1.52	1.46
1	A	155	ASP	CA-C	5.13	1.59	1.52
1	A	111	ILE	CA-C	5.12	1.59	1.52
2	B	19	LYS	CB-CG	5.12	1.67	1.52
1	A	206	ASP	CG-OD2	-5.12	1.15	1.25
1	A	204	PHE	CD2-CE2	-5.12	1.23	1.38
1	A	207	PHE	CA-C	-5.11	1.45	1.52
1	A	659	PHE	C-N	-5.11	1.27	1.33
1	A	647	VAL	C-N	-5.11	1.27	1.33
1	A	379	ASN	CG-ND2	5.11	1.44	1.33
2	B	82	TYR	CG-CD1	-5.11	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	119	PHE	CA-C	-5.11	1.46	1.52
2	B	182	MET	N-CA	5.10	1.52	1.46
1	A	212	ALA	CA-CB	-5.10	1.46	1.53
2	B	9	ASN	N-CA	5.10	1.55	1.46
1	A	510	GLN	CA-CB	-5.10	1.45	1.53
2	B	126	TYR	CA-CB	-5.09	1.45	1.53
1	A	335	TYR	CA-CB	-5.09	1.45	1.53
1	A	339	GLU	C-O	-5.09	1.18	1.24
1	A	637	LYS	CE-NZ	5.08	1.64	1.49
1	A	285	ARG	CG-CD	-5.08	1.37	1.52
1	A	325	TRP	N-CA	5.08	1.52	1.45
1	A	646	ILE	CB-CG2	-5.08	1.35	1.52
2	B	24	LEU	N-CA	5.08	1.52	1.46
1	A	361	MET	C-O	-5.08	1.17	1.24
2	B	180	LEU	N-CA	-5.08	1.39	1.46
1	A	576	THR	CB-CG2	-5.07	1.35	1.52
2	B	54	GLY	CA-C	5.07	1.58	1.51
1	A	181	LEU	C-O	5.07	1.30	1.24
1	A	534	PHE	C-O	5.07	1.30	1.24
1	A	387	TYR	CE2-CZ	5.06	1.50	1.38
1	A	551	PHE	CA-C	5.06	1.59	1.52
2	B	38	ASN	C-N	-5.05	1.26	1.33
1	A	651	ALA	N-CA	5.05	1.52	1.45
2	B	155	MET	N-CA	-5.05	1.39	1.46
2	B	151	ARG	CD-NE	5.04	1.53	1.46
1	A	199	ALA	N-CA	5.04	1.51	1.45
1	A	451	ASN	CG-ND2	-5.04	1.22	1.33
2	B	182	MET	CA-C	5.03	1.59	1.52
1	A	326	MET	C-O	5.03	1.30	1.23
1	A	570	ASP	CA-CB	5.03	1.60	1.52
2	B	110	LEU	C-O	5.03	1.30	1.24
1	A	280	LYS	CE-NZ	-5.02	1.34	1.49
1	A	72	GLY	N-CA	-5.02	1.38	1.45
1	A	357	LYS	CA-C	5.02	1.58	1.52
2	B	79	GLU	CA-C	-5.01	1.46	1.52
1	A	235	GLY	C-O	-5.01	1.17	1.23
1	A	233	GLU	CD-OE1	5.00	1.34	1.25
1	A	692	ILE	CB-CG2	5.00	1.69	1.52

All (471) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ILE	CA-C-O	26.97	152.56	120.74
1	A	400	ASP	CA-C-N	-24.90	72.61	121.41
1	A	400	ASP	C-N-CA	-24.90	72.61	121.41
1	A	400	ASP	O-C-N	19.55	147.06	122.43
1	A	399	GLU	CA-C-N	18.92	156.13	122.64
1	A	399	GLU	C-N-CA	18.92	156.13	122.64
1	A	404	GLY	CA-C-N	-15.93	98.62	121.72
1	A	404	GLY	C-N-CA	-15.93	98.62	121.72
1	A	525	ALA	O-C-N	-15.11	102.50	122.59
1	A	522	GLU	CA-C-N	-13.10	103.46	121.80
1	A	522	GLU	C-N-CA	-13.10	103.46	121.80
1	A	559	ARG	N-CA-C	12.64	125.06	111.28
1	A	526	ASN	CA-C-N	12.60	145.60	121.54
1	A	526	ASN	C-N-CA	12.60	145.60	121.54
1	A	619	SER	N-CA-C	12.00	127.43	113.15
2	B	64	VAL	N-CA-C	11.41	121.36	110.30
2	B	58	ASP	N-CA-C	-10.87	99.44	111.07
1	A	29	ASN	N-CA-C	10.58	125.78	112.24
1	A	100	GLY	N-CA-C	-10.43	96.77	112.41
1	A	222	PRO	N-CA-C	-10.40	96.65	111.22
1	A	403	ARG	CA-C-O	10.07	134.92	120.51
1	A	23	ARG	NE-CZ-NH1	10.07	131.57	121.50
1	A	525	ALA	CA-C-N	9.88	140.41	121.54
1	A	525	ALA	C-N-CA	9.88	140.41	121.54
1	A	469	ARG	N-CA-C	9.86	123.04	111.71
1	A	526	ASN	O-C-N	-9.84	109.50	122.59
1	A	402	GLU	O-C-N	-9.79	111.91	123.27
2	B	90	TRP	N-CA-C	-9.77	101.35	113.18
2	B	83	LEU	CA-C-N	9.76	133.72	120.54
2	B	83	LEU	C-N-CA	9.76	133.72	120.54
1	A	418	ARG	CA-C-N	-9.69	110.25	122.84
1	A	418	ARG	C-N-CA	-9.69	110.25	122.84
1	A	520	ILE	CA-C-N	-9.59	106.83	121.02
1	A	520	ILE	C-N-CA	-9.59	106.83	121.02
1	A	628	ARG	NE-CZ-NH1	-9.52	111.98	121.50
1	A	399	GLU	O-C-N	-9.47	109.99	122.59
1	A	419	GLN	N-CA-C	-9.38	92.15	108.20
1	A	59	GLY	CA-C-O	9.37	130.69	121.60
1	A	23	ARG	NE-CZ-NH2	-9.07	111.03	119.20
1	A	94	ARG	N-CA-C	9.02	120.16	108.34
1	A	455	THR	OG1-CB-CG2	-8.99	91.31	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	VAL	CA-C-N	-8.86	115.86	122.33
1	A	409	VAL	C-N-CA	-8.86	115.86	122.33
1	A	520	ILE	O-C-N	8.83	132.45	123.18
1	A	130	SER	N-CA-C	8.78	120.26	107.88
1	A	516	ILE	CB-CA-C	-8.74	99.78	111.15
1	A	359	THR	OG1-CB-CG2	-8.68	91.94	109.30
1	A	403	ARG	O-C-N	8.61	134.04	122.59
1	A	364	ASN	N-CA-C	8.60	122.56	109.23
2	B	167	THR	CA-C-O	-8.59	111.71	121.15
1	A	10	THR	N-CA-C	-8.44	101.31	111.69
1	A	9	ALA	N-CA-C	-8.43	101.33	111.69
1	A	322	GLY	N-CA-C	-8.38	97.94	110.42
1	A	361	MET	CG-SD-CE	8.36	119.29	100.90
1	A	221	PRO	CB-CA-C	-8.36	100.73	110.92
1	A	264	TYR	N-CA-C	-8.31	96.72	109.85
1	A	396	GLU	N-CA-C	8.24	121.89	110.35
1	A	597	PHE	N-CA-C	-8.16	102.77	112.89
1	A	635	GLY	N-CA-C	-8.10	103.56	115.63
1	A	134	ASN	N-CA-C	-8.09	103.87	112.93
1	A	452	PHE	CA-C-O	-8.07	112.66	121.94
1	A	610	ILE	CA-C-N	-8.06	107.71	120.60
1	A	610	ILE	C-N-CA	-8.06	107.71	120.60
1	A	196	SER	CA-C-N	-8.00	105.72	121.41
1	A	196	SER	C-N-CA	-8.00	105.72	121.41
1	A	342	ASN	N-CA-C	8.00	122.01	110.10
2	B	168	GLY	CA-C-N	7.99	135.15	122.21
2	B	168	GLY	C-N-CA	7.99	135.15	122.21
1	A	89	ILE	CB-CA-C	-7.98	101.30	110.96
1	A	102	LEU	O-C-N	-7.94	114.05	123.03
1	A	105	SER	N-CA-C	-7.94	103.61	113.38
1	A	203	GLY	N-CA-C	-7.94	102.73	113.37
1	A	118	GLU	CB-CG-CD	7.93	126.07	112.60
1	A	583	MET	N-CA-C	7.90	119.97	111.36
2	B	130	ILE	N-CA-C	-7.88	102.85	110.42
1	A	628	ARG	NE-CZ-NH2	7.80	126.22	119.20
1	A	182	GLU	N-CA-C	-7.72	102.50	112.23
1	A	212	ALA	N-CA-C	7.70	121.20	108.96
2	B	152	LEU	CB-CG-CD2	-7.65	87.75	110.70
2	B	134	SER	CA-C-O	-7.65	112.03	121.67
1	A	367	ARG	NE-CZ-NH2	7.64	126.08	119.20
1	A	198	GLY	CA-C-O	-7.64	111.46	122.62
1	A	380	THR	OG1-CB-CG2	-7.63	94.04	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	GLU	N-CA-C	7.61	120.90	109.25
1	A	681	PRO	CB-CA-C	-7.61	99.41	112.64
1	A	428	THR	CA-C-O	-7.59	112.46	120.58
1	A	523	ILE	CB-CA-C	7.57	119.94	111.08
1	A	493	LYS	CA-C-O	7.53	128.50	120.36
1	A	521	GLU	CB-CA-C	7.51	120.98	110.16
1	A	284	ILE	CB-CA-C	-7.47	101.84	110.73
1	A	69	LYS	CD-CE-NZ	-7.41	88.18	111.90
1	A	397	ASP	N-CA-C	7.41	121.44	110.48
1	A	603	LYS	N-CA-C	-7.41	102.90	110.97
2	B	22	VAL	CA-C-N	-7.38	109.81	120.29
2	B	22	VAL	C-N-CA	-7.38	109.81	120.29
1	A	697	PHE	O-C-N	7.34	129.90	122.12
2	B	151	ARG	CA-CB-CG	-7.30	99.50	114.10
1	A	683	ASN	CB-CA-C	-7.29	101.53	111.89
1	A	653	ASP	CA-C-N	-7.29	112.19	125.02
1	A	653	ASP	C-N-CA	-7.29	112.19	125.02
1	A	528	GLU	N-CA-C	-7.28	95.29	110.80
1	A	376	ASN	CA-C-N	-7.27	114.22	123.16
1	A	376	ASN	C-N-CA	-7.27	114.22	123.16
1	A	483	VAL	N-CA-CB	-7.20	102.78	111.21
1	A	515	GLU	N-CA-C	-7.18	100.38	110.50
1	A	86	GLN	O-C-N	-7.17	114.81	123.19
1	A	329	SER	N-CA-C	-7.14	104.70	113.41
1	A	488	THR	N-CA-C	-7.13	100.25	110.59
2	B	47	HIS	CB-CA-C	7.12	121.57	109.82
1	A	538	PHE	N-CA-C	7.11	120.06	111.82
1	A	61	LYS	CA-CB-CG	7.10	128.30	114.10
1	A	385	PRO	N-CD-CG	-7.09	92.57	103.20
1	A	367	ARG	N-CA-C	-7.08	99.41	109.96
1	A	671	ILE	N-CA-C	-7.07	103.97	110.82
1	A	89	ILE	N-CA-C	7.05	119.01	108.23
1	A	542	ALA	O-C-N	7.04	129.58	122.12
1	A	488	THR	N-CA-CB	-7.02	99.75	110.42
1	A	173	GLY	CA-C-N	-6.96	110.96	122.79
1	A	173	GLY	C-N-CA	-6.96	110.96	122.79
1	A	355	LYS	N-CA-C	6.95	120.35	110.14
1	A	465	PHE	N-CA-C	-6.93	93.75	107.69
2	B	153	ASP	CA-C-O	6.93	127.89	120.55
2	B	150	VAL	CA-C-N	6.92	129.44	120.44
2	B	150	VAL	C-N-CA	6.92	129.44	120.44
2	B	164	LYS	N-CA-C	-6.91	103.52	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	THR	OG1-CB-CG2	-6.86	95.58	109.30
1	A	515	GLU	CA-CB-CG	6.83	127.77	114.10
2	B	46	ARG	N-CA-C	-6.83	103.76	111.14
1	A	91	GLY	N-CA-C	-6.82	106.57	114.69
1	A	404	GLY	O-C-N	-6.82	113.84	122.70
1	A	224	LEU	N-CA-C	6.79	119.26	111.11
1	A	655	LEU	CA-C-N	-6.77	114.37	123.10
1	A	655	LEU	C-N-CA	-6.77	114.37	123.10
1	A	487	SER	N-CA-C	6.77	117.52	108.38
1	A	483	VAL	N-CA-C	6.77	117.87	107.99
1	A	562	ALA	N-CA-C	-6.76	103.09	111.75
1	A	528	GLU	CB-CA-C	6.76	123.86	110.42
1	A	529	ASP	CA-C-N	6.76	134.13	121.97
1	A	529	ASP	C-N-CA	6.76	134.13	121.97
2	B	167	THR	N-CA-C	-6.75	100.73	110.24
1	A	676	PHE	CA-C-O	-6.72	113.67	121.07
1	A	333	ARG	N-CA-C	-6.71	104.13	112.72
1	A	551	PHE	N-CA-CB	-6.69	100.23	110.07
1	A	405	CYS	N-CA-C	6.68	119.48	109.25
1	A	603	LYS	CA-C-N	-6.68	111.11	120.53
1	A	603	LYS	C-N-CA	-6.68	111.11	120.53
1	A	464	THR	CA-C-O	6.66	130.04	120.51
1	A	576	THR	CA-C-N	6.64	134.23	121.54
1	A	576	THR	C-N-CA	6.64	134.23	121.54
2	B	125	ILE	CB-CA-C	-6.64	103.32	112.02
1	A	127	LEU	CA-C-N	-6.62	112.04	122.23
1	A	127	LEU	C-N-CA	-6.62	112.04	122.23
1	A	157	ARG	NE-CZ-NH2	6.62	125.15	119.20
1	A	471	VAL	N-CA-C	-6.60	98.68	108.85
1	A	73	ILE	N-CA-C	6.60	118.28	109.37
1	A	578	LYS	CG-CD-CE	6.60	126.47	111.30
2	B	89	LYS	CD-CE-NZ	-6.59	90.81	111.90
1	A	548	ILE	CB-CA-C	-6.58	100.80	110.81
2	B	81	LYS	N-CA-C	-6.56	104.06	111.14
1	A	104	ASP	CA-C-O	6.55	129.47	121.87
1	A	33	GLU	CA-CB-CG	6.51	127.12	114.10
2	B	66	VAL	CA-C-N	-6.51	111.73	122.08
2	B	66	VAL	C-N-CA	-6.51	111.73	122.08
1	A	29	ASN	N-CA-CB	-6.49	102.43	112.30
1	A	629	LYS	CD-CE-NZ	-6.49	91.13	111.90
1	A	427	HIS	ND1-CG-CD2	-6.48	99.62	106.10
1	A	403	ARG	CB-CA-C	-6.48	97.53	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	LEU	CA-C-N	6.46	131.63	120.58
1	A	8	LEU	C-N-CA	6.46	131.63	120.58
1	A	548	ILE	N-CA-C	6.46	117.90	108.53
1	A	378	PRO	CA-C-O	-6.44	110.78	118.90
2	B	162	LEU	CA-C-O	6.44	126.84	119.18
2	B	115	GLU	N-CA-C	-6.44	104.69	112.54
2	B	85	ASN	O-C-N	-6.43	115.44	122.07
1	A	604	ILE	CB-CA-C	-6.43	103.62	112.04
1	A	649	ARG	NE-CZ-NH2	6.42	124.98	119.20
1	A	609	LYS	CA-C-N	6.40	129.16	120.77
1	A	609	LYS	C-N-CA	6.40	129.16	120.77
1	A	614	ILE	N-CA-C	-6.39	103.10	111.09
1	A	161	LYS	CD-CE-NZ	6.39	132.35	111.90
2	B	23	GLN	N-CA-C	-6.37	104.42	111.36
2	B	118	GLY	CA-C-N	-6.37	114.30	122.77
2	B	118	GLY	C-N-CA	-6.37	114.30	122.77
2	B	109	GLU	CA-C-O	6.36	126.98	119.67
1	A	28	LEU	N-CA-CB	-6.34	102.58	112.41
1	A	698	SER	CA-CB-OG	6.33	123.76	111.10
1	A	501	VAL	CB-CA-C	-6.33	101.09	110.33
1	A	420	ARG	CA-C-O	-6.31	111.89	119.27
1	A	487	SER	CB-CA-C	-6.30	98.93	111.91
1	A	485	VAL	CB-CA-C	-6.29	99.90	111.36
1	A	683	ASN	N-CA-C	6.29	120.06	111.39
1	A	42	ALA	O-C-N	-6.27	113.72	122.37
1	A	174	SER	CA-C-N	6.27	130.81	121.72
1	A	174	SER	C-N-CA	6.27	130.81	121.72
1	A	111	ILE	N-CA-C	6.26	117.01	110.62
1	A	322	GLY	O-C-N	6.26	130.87	123.61
1	A	113	SER	N-CA-CB	6.25	119.84	110.22
1	A	272	VAL	N-CA-C	6.23	122.30	109.34
1	A	360	LYS	N-CA-CB	-6.23	100.85	111.69
1	A	203	GLY	O-C-N	-6.22	115.50	122.28
1	A	19	GLY	CA-C-O	6.20	126.02	119.07
2	B	18	ARG	CA-CB-CG	-6.19	101.72	114.10
1	A	201	THR	OG1-CB-CG2	-6.18	96.93	109.30
2	B	134	SER	CA-CB-OG	-6.18	98.75	111.10
1	A	210	GLY	CA-C-O	-6.17	116.11	122.28
1	A	264	TYR	CA-C-O	-6.17	114.24	121.46
1	A	219	LYS	CB-CA-C	-6.17	102.90	111.41
2	B	85	ASN	CB-CA-C	6.15	120.53	110.88
1	A	667	VAL	N-CA-C	6.15	116.27	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ARG	CG-CD-NE	-6.15	98.48	112.00
1	A	156	ASP	O-C-N	-6.14	114.26	122.43
1	A	222	PRO	CA-C-O	-6.14	113.66	122.31
1	A	653	ASP	N-CA-C	-6.12	102.44	110.33
1	A	641	GLN	N-CA-C	-6.11	104.17	111.69
2	B	161	SER	O-C-N	6.11	129.78	122.27
1	A	377	TYR	O-C-N	6.11	126.86	121.37
1	A	331	PHE	O-C-N	6.10	129.59	122.20
2	B	93	ILE	N-CA-C	-6.10	103.75	112.35
1	A	243	ASP	CB-CA-C	6.09	119.58	109.53
1	A	36	ARG	CG-CD-NE	-6.09	98.61	112.00
1	A	83	ALA	CA-C-N	-6.08	115.68	123.16
1	A	83	ALA	C-N-CA	-6.08	115.68	123.16
1	A	511	THR	O-C-N	-6.07	115.85	123.01
2	B	60	CYS	CB-CA-C	6.07	120.48	110.90
1	A	679	LEU	N-CA-CB	6.06	121.00	110.39
1	A	82	CYS	O-C-N	-6.05	116.87	123.52
1	A	576	THR	CA-CB-OG1	6.05	118.67	109.60
1	A	636	PHE	CA-C-O	6.04	127.22	120.70
1	A	86	GLN	N-CA-CB	-6.04	100.56	110.52
1	A	418	ARG	CB-CA-C	-6.04	101.70	111.06
1	A	547	GLU	OE1-CD-OE2	-6.03	108.43	122.90
1	A	699	VAL	CA-CB-CG1	6.03	120.65	110.40
1	A	608	GLN	N-CA-C	-6.01	105.03	112.90
1	A	417	ARG	NE-CZ-NH2	6.01	124.61	119.20
2	B	106	GLY	N-CA-C	-6.00	103.38	111.54
1	A	432	GLY	O-C-N	-6.00	117.85	123.25
2	B	81	LYS	CB-CG-CD	-6.00	97.50	111.30
1	A	681	PRO	CA-C-O	-5.98	109.74	119.84
1	A	661	ASN	N-CA-C	5.97	123.51	110.80
2	B	120	HIS	N-CA-C	5.97	118.64	108.02
1	A	56	SER	CA-CB-OG	-5.94	99.22	111.10
1	A	581	VAL	CB-CA-C	-5.93	104.40	111.81
2	B	152	LEU	N-CA-C	-5.92	104.83	111.28
1	A	12	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	165	LEU	N-CA-CB	5.91	118.72	109.69
1	A	497	PHE	CA-C-N	5.90	131.82	122.74
1	A	497	PHE	C-N-CA	5.90	131.82	122.74
1	A	374	CYS	N-CA-C	-5.88	98.26	110.80
1	A	375	ARG	CB-CG-CD	5.88	124.81	111.30
1	A	337	ARG	CB-CG-CD	5.86	124.79	111.30
1	A	606	LYS	CB-CG-CD	5.86	124.78	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ILE	CB-CA-C	-5.86	101.96	110.63
1	A	138	ILE	CA-C-N	-5.85	112.59	123.01
1	A	138	ILE	C-N-CA	-5.85	112.59	123.01
1	A	624	SER	CB-CA-C	-5.85	101.03	110.74
1	A	547	GLU	CA-C-N	-5.84	115.56	123.10
1	A	547	GLU	C-N-CA	-5.84	115.56	123.10
1	A	262	HIS	CB-CA-C	5.83	119.87	109.38
2	B	132	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	A	119	GLU	N-CA-C	-5.82	105.02	111.71
2	B	107	SER	N-CA-C	5.81	123.19	110.80
2	B	37	MET	N-CA-C	-5.81	104.86	111.07
1	A	606	LYS	O-C-N	-5.79	115.45	122.11
2	B	160	ARG	N-CA-C	-5.79	105.10	111.82
1	A	33	GLU	CG-CD-OE1	-5.78	105.10	118.40
2	B	111	PRO	N-CA-C	-5.78	106.00	113.57
2	B	41	ASN	CB-CA-C	5.77	118.95	111.50
1	A	389	ILE	CB-CA-C	-5.77	103.08	110.98
1	A	395	ASP	CB-CA-C	-5.77	98.94	110.42
2	B	34	THR	OG1-CB-CG2	-5.77	97.76	109.30
1	A	453	PHE	N-CA-CB	5.77	120.23	110.49
2	B	61	ARG	NH1-CZ-NH2	5.76	126.79	119.30
1	A	70	THR	O-C-N	-5.76	115.26	122.35
1	A	416	ARG	CG-CD-NE	-5.76	99.33	112.00
1	A	401	GLY	CA-C-N	5.76	131.12	123.00
1	A	401	GLY	C-N-CA	5.76	131.12	123.00
1	A	287	PRO	CB-CA-C	-5.75	103.23	112.21
1	A	450	LYS	CB-CG-CD	5.75	124.53	111.30
1	A	668	ARG	CB-CA-C	-5.75	101.61	110.81
1	A	146	TYR	N-CA-C	-5.75	103.46	111.39
1	A	102	LEU	CA-C-N	-5.74	110.16	121.41
1	A	102	LEU	C-N-CA	-5.74	110.16	121.41
1	A	373	GLY	N-CA-C	5.74	126.79	113.18
2	B	57	ILE	N-CA-C	5.72	117.14	110.62
1	A	426	MET	O-C-N	-5.71	115.67	122.63
1	A	171	ALA	CA-C-O	-5.70	114.38	120.42
2	B	170	ILE	N-CA-C	-5.69	99.59	108.81
1	A	199	ALA	O-C-N	-5.69	115.99	123.16
2	B	49	ASP	CA-C-N	5.68	131.29	121.64
2	B	49	ASP	C-N-CA	5.68	131.29	121.64
1	A	478	PRO	N-CA-C	-5.67	105.03	110.47
1	A	631	LEU	N-CA-CB	-5.67	101.79	110.12
1	A	341	CYS	CA-C-N	5.66	128.81	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	CYS	C-N-CA	5.66	128.81	120.82
1	A	37	ASN	CA-C-O	5.66	126.75	120.63
1	A	208	THR	CA-C-O	5.66	125.67	118.54
1	A	223	ASN	N-CA-C	5.66	122.33	113.72
1	A	134	ASN	CA-C-N	5.66	132.35	121.54
1	A	134	ASN	C-N-CA	5.66	132.35	121.54
1	A	657	ILE	N-CA-CB	-5.65	104.78	111.90
1	A	689	LEU	CA-C-O	5.63	127.36	120.60
1	A	666	LEU	CA-C-O	-5.62	114.59	120.55
1	A	455	THR	N-CA-C	-5.61	95.29	111.00
1	A	157	ARG	NH1-CZ-NH2	-5.61	112.01	119.30
2	B	169	GLN	N-CA-C	5.60	117.70	109.24
1	A	664	ARG	CG-CD-NE	5.58	124.27	112.00
1	A	339	GLU	CA-C-N	-5.58	115.36	123.06
1	A	339	GLU	C-N-CA	-5.58	115.36	123.06
1	A	325	TRP	CA-C-O	-5.57	115.07	121.47
1	A	325	TRP	N-CA-CB	5.56	118.75	110.29
2	B	41	ASN	N-CA-C	-5.56	103.80	111.81
1	A	575	GLU	CB-CA-C	-5.55	102.12	110.90
1	A	225	PHE	CB-CA-C	-5.55	101.58	110.79
1	A	474	ARG	O-C-N	-5.55	117.00	123.27
1	A	578	LYS	N-CA-C	5.54	117.00	111.07
1	A	159	PRO	N-CA-C	5.53	119.88	111.19
1	A	453	PHE	N-CA-C	5.53	122.58	110.80
1	A	632	GLU	N-CA-C	-5.53	105.15	111.07
1	A	70	THR	OG1-CB-CG2	-5.53	98.24	109.30
1	A	690	ASP	N-CA-C	-5.53	101.16	109.95
1	A	50	SER	CA-CB-OG	-5.53	100.05	111.10
1	A	555	THR	OG1-CB-CG2	-5.52	98.26	109.30
1	A	94	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	A	197	GLY	CA-C-N	-5.52	113.17	121.01
1	A	197	GLY	C-N-CA	-5.52	113.17	121.01
1	A	49	PRO	N-CD-CG	-5.51	94.94	103.20
2	B	18	ARG	CA-C-N	5.50	129.79	120.88
2	B	18	ARG	C-N-CA	5.50	129.79	120.88
2	B	136	GLU	N-CA-C	-5.50	105.29	111.28
1	A	382	TRP	N-CA-C	5.50	119.46	112.87
1	A	451	ASN	N-CA-C	5.49	118.19	110.23
1	A	82	CYS	CA-C-N	-5.47	111.37	120.68
1	A	82	CYS	C-N-CA	-5.47	111.37	120.68
1	A	127	LEU	N-CA-C	-5.47	106.10	112.89
2	B	29	MET	O-C-N	-5.47	115.73	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	THR	CA-CB-OG1	5.45	117.78	109.60
1	A	360	LYS	CG-CD-CE	-5.44	98.80	111.30
2	B	162	LEU	N-CA-C	5.43	119.90	113.28
2	B	137	THR	CA-CB-OG1	5.43	117.74	109.60
1	A	522	GLU	CA-C-O	5.42	128.97	122.41
1	A	8	LEU	N-CA-C	-5.42	105.45	111.36
1	A	378	PRO	N-CA-C	-5.42	106.95	114.27
1	A	680	ASP	CA-C-N	5.42	125.50	119.32
1	A	680	ASP	C-N-CA	5.42	125.50	119.32
1	A	630	ALA	N-CA-CB	-5.41	100.95	109.78
1	A	337	ARG	CG-CD-NE	-5.41	100.10	112.00
2	B	59	THR	CA-C-O	5.41	126.47	120.63
1	A	646	ILE	CA-C-O	-5.41	115.44	121.17
2	B	64	VAL	CB-CA-C	-5.40	105.06	111.81
1	A	136	ALA	CA-C-O	5.39	124.74	119.08
1	A	219	LYS	O-C-N	5.39	125.73	121.20
1	A	540	GLN	CB-CG-CD	5.39	121.76	112.60
2	B	151	ARG	CB-CG-CD	5.38	123.67	111.30
1	A	433	ILE	CG1-CB-CG2	-5.37	94.58	110.70
2	B	144	ASN	N-CA-C	5.37	117.83	111.33
1	A	544	GLU	N-CA-C	5.37	118.93	112.38
1	A	466	ILE	CA-CB-CG2	-5.36	101.38	110.50
1	A	656	ILE	CA-CB-CG1	-5.36	101.28	110.40
1	A	687	ILE	CB-CA-C	-5.36	103.52	111.19
1	A	14	ALA	CA-C-O	5.36	126.10	120.42
2	B	43	VAL	CA-C-N	-5.36	116.15	122.36
2	B	43	VAL	C-N-CA	-5.36	116.15	122.36
2	B	58	ASP	CA-C-O	5.36	126.44	120.82
1	A	232	LEU	CA-C-O	-5.35	114.20	120.20
1	A	262	HIS	CA-CB-CG	5.35	119.15	113.80
1	A	505	LYS	CA-C-O	-5.34	114.94	121.78
1	A	123	ARG	N-CA-C	-5.34	106.02	112.54
1	A	649	ARG	CB-CG-CD	5.34	123.58	111.30
1	A	36	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	A	455	THR	CA-CB-CG2	5.34	119.58	110.50
1	A	329	SER	CA-C-N	5.33	129.70	120.58
1	A	329	SER	C-N-CA	5.33	129.70	120.58
1	A	156	ASP	N-CA-C	5.33	119.27	112.87
1	A	650	PHE	CA-C-N	-5.33	114.23	122.59
1	A	650	PHE	C-N-CA	-5.33	114.23	122.59
1	A	166	LEU	CD1-CG-CD2	-5.32	99.09	110.80
1	A	625	TYR	O-C-N	5.32	129.31	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	THR	OG1-CB-CG2	-5.32	98.65	109.30
1	A	423	GLY	CA-C-O	-5.32	112.94	119.69
2	B	182	MET	N-CA-CB	5.32	118.00	110.13
1	A	475	PHE	N-CA-CB	-5.31	102.59	111.20
1	A	515	GLU	N-CA-CB	-5.31	102.52	110.17
1	A	527	GLU	CB-CA-C	5.31	120.99	110.42
2	B	176	GLU	N-CA-C	-5.31	105.57	111.36
2	B	60	CYS	N-CA-CB	-5.31	102.37	110.07
1	A	681	PRO	N-CD-CG	-5.31	95.24	103.20
1	A	700	LEU	CA-CB-CG	5.30	134.84	116.30
1	A	71	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	241	SER	CA-C-N	-5.29	115.76	123.06
1	A	241	SER	C-N-CA	-5.29	115.76	123.06
2	B	21	PHE	N-CA-CB	5.29	119.43	110.49
1	A	209	GLY	N-CA-C	-5.29	107.98	115.43
1	A	118	GLU	CA-CB-CG	5.28	124.65	114.10
1	A	595	LYS	CA-C-O	5.27	126.14	120.55
1	A	225	PHE	O-C-N	5.27	127.70	122.12
1	A	375	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	65	PRO	N-CA-C	-5.26	103.57	111.57
2	B	28	ASP	CB-CG-OD2	5.26	130.50	118.40
2	B	175	GLN	N-CA-C	-5.25	105.63	111.36
1	A	386	GLN	N-CA-CB	-5.25	102.44	110.85
1	A	415	HIS	N-CA-C	5.25	118.41	110.64
1	A	466	ILE	CA-C-O	-5.25	117.53	121.68
1	A	682	GLU	CB-CA-C	-5.25	100.44	110.57
1	A	470	GLU	CA-C-O	-5.24	114.64	120.66
2	B	43	VAL	CA-C-O	5.22	126.34	120.03
1	A	630	ALA	N-CA-C	5.21	119.97	111.37
2	B	88	LYS	N-CA-C	-5.21	106.07	112.90
1	A	213	GLU	N-CA-C	-5.21	100.90	109.40
1	A	469	ARG	O-C-N	5.21	128.32	122.22
1	A	164	GLU	CA-C-O	-5.20	114.45	120.49
1	A	612	ARG	N-CA-C	-5.20	105.26	111.03
1	A	50	SER	N-CA-CB	-5.19	102.97	110.70
1	A	647	VAL	N-CA-C	-5.19	105.34	111.00
1	A	285	ARG	N-CA-C	5.18	118.19	110.52
1	A	174	SER	CA-CB-OG	-5.18	100.73	111.10
1	A	414	LYS	O-C-N	-5.18	117.14	122.94
2	B	65	ALA	CA-C-O	-5.17	114.97	121.02
1	A	610	ILE	N-CA-C	-5.17	104.85	110.23
1	A	613	GLU	CA-CB-CG	-5.17	103.76	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	THR	CA-C-O	5.16	124.72	119.05
1	A	502	PHE	N-CA-C	-5.15	101.29	109.59
1	A	514	ASP	CA-C-N	5.15	129.03	120.94
1	A	514	ASP	C-N-CA	5.15	129.03	120.94
1	A	122	ALA	N-CA-C	-5.15	105.84	111.82
1	A	181	LEU	CD1-CG-CD2	-5.14	99.48	110.80
1	A	493	LYS	O-C-N	-5.14	117.18	123.30
1	A	77	ARG	CA-C-O	-5.14	115.36	120.96
1	A	653	ASP	O-C-N	-5.14	116.62	122.68
2	B	58	ASP	CA-C-N	-5.12	113.36	120.38
2	B	58	ASP	C-N-CA	-5.12	113.36	120.38
1	A	374	CYS	CA-CB-SG	-5.12	102.63	114.40
1	A	207	PHE	N-CA-C	-5.12	106.72	113.17
1	A	196	SER	O-C-N	-5.11	115.79	122.59
1	A	271	GLU	N-CA-C	5.11	117.45	110.55
1	A	281	LEU	N-CA-CB	-5.11	102.23	110.71
1	A	418	ARG	N-CA-C	5.11	118.34	112.57
1	A	478	PRO	O-C-N	5.11	123.66	121.31
1	A	543	GLY	N-CA-C	-5.11	101.08	113.18
1	A	266	VAL	N-CA-CB	-5.11	105.03	111.46
1	A	8	LEU	CA-C-O	-5.10	115.01	120.42
2	B	115	GLU	CA-C-N	5.10	127.53	120.29
2	B	115	GLU	C-N-CA	5.10	127.53	120.29
1	A	225	PHE	CA-C-O	-5.09	115.16	120.55
1	A	104	ASP	CB-CG-OD2	5.09	130.10	118.40
1	A	610	ILE	O-C-N	5.09	127.45	121.96
1	A	279	GLN	CA-C-N	5.08	129.59	121.66
1	A	279	GLN	C-N-CA	5.08	129.59	121.66
1	A	157	ARG	CB-CA-C	-5.08	102.84	110.16
1	A	7	LYS	N-CA-C	-5.07	105.88	111.71
1	A	132	GLN	N-CA-C	-5.06	106.80	113.12
1	A	333	ARG	CA-C-O	-5.06	113.89	119.81
1	A	427	HIS	ND1-CE1-NE2	-5.06	103.34	108.40
1	A	138	ILE	CA-CB-CG2	5.06	119.10	110.50
2	B	34	THR	N-CA-C	-5.05	105.77	111.28
1	A	407	PHE	CA-C-N	-5.05	115.61	122.93
1	A	407	PHE	C-N-CA	-5.05	115.61	122.93
1	A	633	GLU	CA-C-N	-5.05	113.87	122.56
1	A	633	GLU	C-N-CA	-5.05	113.87	122.56
1	A	216	GLU	CB-CG-CD	-5.05	104.02	112.60
1	A	271	GLU	O-C-N	-5.05	117.10	122.85
1	A	450	LYS	CG-CD-CE	-5.05	99.69	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	674	LYS	CA-C-N	-5.04	113.55	120.46
1	A	674	LYS	C-N-CA	-5.04	113.55	120.46
2	B	115	GLU	CB-CG-CD	5.04	121.16	112.60
2	B	86	ASN	CA-C-N	-5.03	112.52	120.47
2	B	86	ASN	C-N-CA	-5.03	112.52	120.47
1	A	678	GLN	CB-CG-CD	-5.03	104.05	112.60
2	B	118	GLY	N-CA-C	-5.03	107.61	114.64
1	A	419	GLN	CG-CD-NE2	-5.01	108.88	116.40
2	B	103	GLY	O-C-N	5.01	128.80	122.43
1	A	629	LYS	CB-CG-CD	5.00	122.80	111.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	A	18	LEU	Mainchain
1	A	197	GLY	Peptide
1	A	373	GLY	Mainchain
1	A	384	ASN	Mainchain
1	A	399	GLU	Mainchain,Peptide
1	A	401	GLY	Mainchain,Peptide
1	A	403	ARG	Mainchain,Peptide
1	A	404	GLY	Mainchain
1	A	427	HIS	Sidechain,Mainchain
1	A	525	ALA	Mainchain,Peptide
1	A	527	GLU	Mainchain
1	A	9	ALA	Mainchain
1	A	98	CYS	Mainchain
2	B	142	PHE	Peptide
2	B	64	VAL	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4980	0	4809	539	10

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1427	0	1375	167	9
3	A	247	0	0	67	0
3	B	52	0	0	23	0
All	All	6706	0	6184	697	10

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 55.

All (697) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:CG	1:A:218:ARG:CB	1.74	1.66
1:A:409:VAL:CB	1:A:409:VAL:CG1	1.76	1.64
1:A:628:ARG:CD	1:A:628:ARG:CG	1.76	1.63
1:A:699:VAL:CB	1:A:699:VAL:CG1	1.77	1.62
1:A:455:THR:CB	1:A:455:THR:CG2	1.80	1.60
1:A:161:LYS:CB	1:A:161:LYS:CG	1.81	1.58
1:A:674:LYS:CE	1:A:674:LYS:CD	1.75	1.58
1:A:699:VAL:CB	1:A:699:VAL:CA	1.82	1.57
1:A:390:LYS:CD	1:A:390:LYS:CG	1.78	1.57
1:A:161:LYS:CG	1:A:161:LYS:CD	1.75	1.57
1:A:375:ARG:CD	1:A:375:ARG:CG	1.81	1.55
1:A:476:LYS:CD	1:A:476:LYS:CG	1.76	1.55
1:A:506:LYS:CD	1:A:506:LYS:CG	1.74	1.55
1:A:540:GLN:CG	1:A:540:GLN:CB	1.84	1.53
1:A:606:LYS:CD	1:A:606:LYS:CG	1.80	1.53
2:B:137:THR:CB	2:B:137:THR:CA	1.82	1.53
1:A:226:LYS:CE	1:A:226:LYS:CD	1.83	1.52
1:A:578:LYS:CE	1:A:578:LYS:NZ	1.68	1.52
1:A:7:LYS:CE	1:A:7:LYS:CD	1.86	1.51
1:A:595:LYS:CE	1:A:595:LYS:NZ	1.68	1.51
1:A:218:ARG:CG	1:A:218:ARG:CD	1.85	1.49
1:A:417:ARG:CD	1:A:417:ARG:CG	1.88	1.48
1:A:226:LYS:CE	1:A:226:LYS:NZ	1.73	1.48
1:A:674:LYS:CE	1:A:674:LYS:NZ	1.75	1.48
1:A:466:ILE:CD1	1:A:466:ILE:CG1	1.91	1.48
2:B:128:MET:SD	2:B:128:MET:CG	2.02	1.47
2:B:155:MET:SD	2:B:155:MET:CG	2.03	1.47
1:A:361:MET:SD	1:A:361:MET:CG	2.02	1.47
1:A:326:MET:SD	1:A:326:MET:CG	2.04	1.45
1:A:692:ILE:CD1	1:A:692:ILE:CG1	1.94	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:CE	1:A:7:LYS:NZ	1.78	1.44
1:A:222:PRO:CG	1:A:222:PRO:CB	1.77	1.42
1:A:326:MET:SD	1:A:326:MET:CE	2.15	1.35
1:A:400:ASP:C	1:A:401:GLY:CA	2.01	1.33
1:A:402:GLU:C	1:A:403:ARG:N	1.87	1.30
1:A:400:ASP:C	1:A:401:GLY:N	1.90	1.29
1:A:69:LYS:HB3	1:A:69:LYS:NZ	1.28	1.26
1:A:402:GLU:CA	1:A:403:ARG:N	2.04	1.21
1:A:402:GLU:HA	1:A:403:ARG:N	1.56	1.21
1:A:400:ASP:C	1:A:401:GLY:HA2	1.58	1.20
2:B:106:GLY:HA2	2:B:139:ASN:ND2	1.55	1.19
1:A:238:LEU:HD12	1:A:238:LEU:N	1.61	1.15
1:A:699:VAL:O	1:A:700:LEU:HD23	1.46	1.12
2:B:20:LEU:O	2:B:24:LEU:HG	1.47	1.10
1:A:69:LYS:NZ	1:A:69:LYS:CB	1.99	1.09
2:B:106:GLY:HA2	2:B:139:ASN:HD22	0.98	1.09
1:A:290:GLN:N	1:A:322:GLY:N	2.03	1.06
1:A:653:ASP:O	1:A:654:GLU:HG2	1.53	1.06
2:B:47:HIS:HB3	2:B:49:ASP:OD1	1.57	1.02
1:A:462:SER:CB	3:A:809:HOH:O	2.07	1.02
1:A:33:GLU:OE1	3:A:812:HOH:O	1.76	1.02
1:A:69:LYS:CB	1:A:69:LYS:HZ2	1.62	1.02
1:A:115:THR:HG21	3:A:759:HOH:O	1.59	1.00
1:A:220:PRO:HG3	3:A:870:HOH:O	1.62	0.99
1:A:286:ASN:C	1:A:286:ASN:HD22	1.68	0.98
1:A:226:LYS:O	1:A:230:LYS:HG3	1.61	0.98
1:A:530:ILE:HB	1:A:535:ARG:NH1	1.80	0.97
1:A:534:PHE:O	1:A:537:LEU:HB3	1.66	0.96
1:A:416:ARG:HG3	1:A:416:ARG:NH1	1.79	0.95
2:B:9:ASN:N	2:B:9:ASN:HD22	1.64	0.94
2:B:45:THR:O	3:B:218:HOH:O	1.86	0.94
1:A:69:LYS:HB3	1:A:69:LYS:HZ3	1.21	0.93
1:A:629:LYS:HG3	3:A:827:HOH:O	1.65	0.93
1:A:517:GLU:OE1	1:A:637:LYS:NZ	2.00	0.92
1:A:530:ILE:HB	1:A:535:ARG:HH12	1.31	0.92
1:A:224:LEU:HD21	1:A:228:ILE:HD11	1.52	0.91
1:A:373:GLY:H	1:A:384:ASN:HD21	0.99	0.90
1:A:238:LEU:HD12	1:A:238:LEU:H	1.27	0.90
1:A:226:LYS:NZ	3:A:712:HOH:O	2.04	0.89
1:A:168:VAL:HG12	1:A:179:ALA:HA	1.53	0.89
1:A:400:ASP:CA	1:A:401:GLY:N	2.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ALA:O	3:A:791:HOH:O	1.91	0.88
1:A:523:ILE:C	1:A:525:ALA:HB2	1.98	0.88
1:A:561:LEU:HD12	1:A:571:GLY:HA2	1.53	0.88
1:A:398:ASP:N	1:A:398:ASP:OD1	2.07	0.88
1:A:286:ASN:ND2	1:A:288:TRP:H	1.69	0.88
1:A:36:ARG:HH21	1:A:37:ASN:HD21	1.23	0.86
1:A:694:TRP:O	1:A:698:SER:OG	1.92	0.86
2:B:106:GLY:CA	2:B:139:ASN:HD22	1.87	0.86
1:A:558:ARG:HH11	1:A:558:ARG:HB3	1.38	0.86
2:B:146:ILE:O	2:B:150:VAL:HG23	1.76	0.85
1:A:406:THR:OG1	1:A:476:LYS:HG3	1.76	0.85
1:A:281:LEU:HD22	1:A:325:TRP:HE3	1.41	0.85
1:A:409:VAL:CG1	1:A:409:VAL:CG2	2.54	0.84
1:A:286:ASN:C	1:A:286:ASN:ND2	2.32	0.84
1:A:243:ASP:HB2	3:A:724:HOH:O	1.75	0.84
1:A:286:ASN:HD21	1:A:288:TRP:H	1.21	0.84
1:A:466:ILE:HG22	1:A:467:ASN:N	1.92	0.84
1:A:668:ARG:HD2	3:A:749:HOH:O	1.76	0.84
1:A:398:ASP:HB3	3:A:805:HOH:O	1.78	0.84
2:B:81:LYS:NZ	3:B:219:HOH:O	2.11	0.84
1:A:361:MET:HG2	1:A:509:TYR:CE1	2.13	0.83
1:A:544:GLU:OE2	3:A:845:HOH:O	1.95	0.83
1:A:216:GLU:HG3	3:A:941:HOH:O	1.77	0.83
1:A:193:GLU:HG3	1:A:193:GLU:O	1.78	0.83
2:B:107:SER:HB2	3:B:201:HOH:O	1.76	0.83
1:A:653:ASP:O	1:A:654:GLU:CG	2.26	0.83
1:A:238:LEU:N	1:A:238:LEU:CD1	2.36	0.83
1:A:522:GLU:CG	1:A:522:GLU:CA	2.56	0.83
1:A:530:ILE:O	1:A:531:GLY:C	2.21	0.82
2:B:19:LYS:O	3:B:209:HOH:O	1.96	0.82
1:A:403:ARG:O	1:A:478:PRO:HA	1.80	0.82
1:A:4:ILE:HD13	2:B:180:LEU:HD23	1.60	0.82
1:A:416:ARG:HG3	1:A:416:ARG:HH11	1.40	0.81
1:A:545:ASP:OD1	1:A:591:LYS:NZ	2.13	0.81
2:B:100:ASP:OD2	2:B:102:SER:OG	1.98	0.81
1:A:69:LYS:HB3	1:A:69:LYS:HZ2	1.01	0.81
1:A:523:ILE:C	1:A:525:ALA:CB	2.54	0.81
1:A:350:CYS:HB3	1:A:353:TYR:HB2	1.62	0.81
2:B:20:LEU:O	2:B:24:LEU:CG	2.28	0.81
1:A:523:ILE:O	1:A:525:ALA:CB	2.29	0.80
2:B:56:GLY:HA3	3:B:195:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HD12	1:A:571:GLY:CA	2.11	0.79
1:A:699:VAL:O	1:A:700:LEU:CD2	2.30	0.79
2:B:132:ARG:CG	2:B:132:ARG:HH11	1.96	0.79
1:A:69:LYS:CB	1:A:69:LYS:HZ3	1.66	0.79
1:A:373:GLY:N	1:A:384:ASN:HD21	1.79	0.78
1:A:286:ASN:HD22	1:A:287:PRO:N	1.82	0.78
1:A:400:ASP:HB3	1:A:401:GLY:N	1.99	0.78
2:B:18:ARG:O	2:B:22:VAL:HG23	1.84	0.78
1:A:530:ILE:O	1:A:531:GLY:O	2.02	0.78
1:A:395:ASP:OD2	1:A:476:LYS:HE3	1.83	0.78
1:A:587:ASP:OD2	1:A:589:SER:OG	2.01	0.78
2:B:145:PHE:CZ	2:B:149:LEU:HD11	2.20	0.77
1:A:286:ASN:ND2	1:A:288:TRP:N	2.31	0.77
1:A:290:GLN:O	3:A:730:HOH:O	2.02	0.77
1:A:455:THR:CG2	1:A:455:THR:OG1	2.32	0.77
1:A:271:GLU:HA	1:A:279:GLN:O	1.84	0.77
2:B:156:PHE:CZ	2:B:160:ARG:HD3	2.20	0.77
2:B:151:ARG:HH11	2:B:151:ARG:HB3	1.49	0.76
1:A:89:ILE:HG22	1:A:90:GLY:O	1.86	0.75
1:A:104:ASP:HB2	3:A:879:HOH:O	1.86	0.75
2:B:142:PHE:O	2:B:143:ASP:C	2.28	0.75
1:A:573:SER:HG	1:A:576:THR:HG1	1.31	0.75
1:A:281:LEU:HD23	1:A:326:MET:O	1.86	0.75
1:A:236:SER:O	1:A:238:LEU:HD11	1.87	0.75
1:A:218:ARG:CG	1:A:218:ARG:CA	2.64	0.75
1:A:668:ARG:NH2	2:B:182:MET:O	2.19	0.74
1:A:129:GLN:HE22	1:A:140:HIS:H	1.35	0.74
2:B:132:ARG:NH1	2:B:132:ARG:HG3	2.01	0.74
2:B:148:CYS:O	2:B:152:LEU:HD23	1.87	0.74
1:A:523:ILE:O	1:A:525:ALA:HB3	1.88	0.74
1:A:386:GLN:HE22	1:A:451:ASN:H	1.35	0.74
1:A:558:ARG:HB3	1:A:558:ARG:NH1	2.03	0.74
2:B:137:THR:CA	2:B:137:THR:HB	2.15	0.73
1:A:408:LEU:HD22	1:A:472:LEU:HD21	1.70	0.73
1:A:554:GLN:HG3	1:A:574:ILE:HD13	1.70	0.73
1:A:30:GLN:HE22	1:A:187:LYS:HZ1	1.37	0.73
1:A:476:LYS:CD	1:A:476:LYS:CB	2.64	0.73
1:A:290:GLN:C	1:A:322:GLY:CA	2.62	0.73
2:B:134:SER:HB2	3:B:206:HOH:O	1.87	0.73
1:A:409:VAL:CG1	1:A:409:VAL:CA	2.66	0.72
1:A:30:GLN:HE22	1:A:187:LYS:NZ	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLN:HE21	1:A:554:GLN:C	1.97	0.72
1:A:375:ARG:HD3	1:A:376:ASN:HD22	1.54	0.72
2:B:113:ALA:O	2:B:116:ALA:HB3	1.89	0.72
1:A:373:GLY:H	1:A:384:ASN:ND2	1.82	0.71
2:B:132:ARG:HH11	2:B:132:ARG:HG3	1.55	0.71
1:A:398:ASP:CB	3:A:805:HOH:O	2.37	0.71
1:A:628:ARG:CD	1:A:628:ARG:CB	2.69	0.71
2:B:17:PHE:O	2:B:19:LYS:N	2.24	0.71
1:A:226:LYS:NZ	1:A:400:ASP:OD2	2.21	0.71
2:B:20:LEU:HD11	3:B:194:HOH:O	1.90	0.71
1:A:281:LEU:HD21	1:A:326:MET:H	1.56	0.71
1:A:506:LYS:HG3	3:A:831:HOH:O	1.91	0.70
1:A:539:ALA:CB	3:A:893:HOH:O	2.38	0.70
1:A:476:LYS:CG	1:A:476:LYS:CE	2.69	0.70
1:A:286:ASN:HD21	1:A:288:TRP:N	1.87	0.70
1:A:213:GLU:OE1	1:A:474:ARG:HD2	1.91	0.70
1:A:653:ASP:C	1:A:654:GLU:HG2	2.17	0.70
1:A:523:ILE:C	1:A:525:ALA:N	2.49	0.70
1:A:400:ASP:CB	1:A:401:GLY:N	2.56	0.69
1:A:585:ASP:O	1:A:586:GLU:HB2	1.91	0.69
1:A:226:LYS:NZ	1:A:400:ASP:CG	2.50	0.69
1:A:686:THR:HG23	1:A:686:THR:O	1.93	0.69
1:A:216:GLU:CG	3:A:941:HOH:O	2.37	0.69
1:A:617:ASP:OD1	1:A:619:SER:HB2	1.91	0.69
1:A:576:THR:HA	1:A:664:ARG:HD3	1.75	0.69
1:A:585:ASP:OD1	1:A:587:ASP:OD1	2.11	0.69
1:A:216:GLU:CD	3:A:941:HOH:O	2.35	0.68
1:A:410:GLY:O	1:A:499:ILE:HA	1.94	0.68
1:A:500:ARG:HD3	3:A:945:HOH:O	1.93	0.68
2:B:105:ILE:HG22	2:B:110:LEU:HD12	1.76	0.68
2:B:163:ASP:OD1	2:B:167:THR:O	2.11	0.68
1:A:342:ASN:HD22	1:A:356:TRP:HE1	1.39	0.68
1:A:678:GLN:O	1:A:681:PRO:HD3	1.94	0.68
1:A:466:ILE:HG22	1:A:467:ASN:H	1.59	0.68
1:A:403:ARG:HD2	1:A:478:PRO:HB3	1.76	0.68
1:A:64:GLY:C	3:A:795:HOH:O	2.37	0.68
1:A:64:GLY:O	1:A:67:SER:HB3	1.93	0.67
1:A:285:ARG:HD3	1:A:286:ASN:N	2.10	0.67
1:A:679:LEU:C	1:A:681:PRO:HD2	2.19	0.67
1:A:364:ASN:ND2	1:A:644:GLN:HE22	1.93	0.67
1:A:523:ILE:HD13	1:A:602:THR:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:ILE:CD1	2:B:117:ALA:HA	2.24	0.67
1:A:223:ASN:HD22	1:A:226:LYS:HE2	1.60	0.67
1:A:56:SER:OG	3:A:804:HOH:O	2.13	0.66
1:A:418:ARG:NH1	3:A:731:HOH:O	2.28	0.66
1:A:562:ALA:HA	1:A:569:SER:O	1.95	0.66
2:B:20:LEU:HD13	2:B:39:ILE:HG23	1.78	0.66
1:A:224:LEU:HD21	1:A:228:ILE:CD1	2.25	0.66
1:A:541:LEU:HG	1:A:556:ILE:CD1	2.26	0.66
1:A:548:ILE:HG22	1:A:552:GLU:CB	2.26	0.66
1:A:652:ASP:OD2	1:A:656:ILE:HG23	1.96	0.66
1:A:699:VAL:CA	1:A:699:VAL:HB	2.18	0.66
1:A:164:GLU:OE1	3:A:903:HOH:O	2.14	0.66
1:A:539:ALA:HB1	3:A:893:HOH:O	1.96	0.65
1:A:472:LEU:HG	3:A:791:HOH:O	1.96	0.65
1:A:517:GLU:OE1	1:A:637:LYS:CE	2.44	0.65
2:B:137:THR:CB	2:B:137:THR:HA	2.13	0.65
1:A:688:GLN:HB2	3:A:928:HOH:O	1.95	0.65
1:A:387:TYR:OH	3:A:741:HOH:O	2.14	0.65
1:A:578:LYS:NZ	1:A:578:LYS:CD	2.58	0.65
1:A:226:LYS:HZ2	1:A:400:ASP:CG	2.04	0.65
1:A:343:LEU:HG	1:A:347:THR:HG21	1.79	0.65
1:A:374:CYS:HB2	1:A:489:PHE:O	1.96	0.64
1:A:463:ASP:C	1:A:464:THR:OG1	2.41	0.64
1:A:699:VAL:CG1	1:A:699:VAL:CG2	2.74	0.64
1:A:527:GLU:HA	1:A:527:GLU:OE2	1.97	0.64
1:A:328:PHE:O	1:A:332:LEU:HD13	1.98	0.64
1:A:668:ARG:CG	3:A:848:HOH:O	2.45	0.64
2:B:38:ASN:O	2:B:42:LYS:HG3	1.98	0.64
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.62	0.64
2:B:75:LEU:C	2:B:75:LEU:HD12	2.23	0.64
1:A:472:LEU:HD13	1:A:472:LEU:C	2.23	0.64
2:B:31:VAL:HG12	2:B:32:SER:O	1.98	0.64
1:A:424:GLU:HB2	3:A:782:HOH:O	1.97	0.63
1:A:469:ARG:HD2	3:A:946:HOH:O	1.98	0.63
2:B:133:TYR:HB2	2:B:140:MET:HE2	1.80	0.63
1:A:364:ASN:HD21	1:A:644:GLN:HE22	1.46	0.63
1:A:463:ASP:O	1:A:464:THR:OG1	2.17	0.63
1:A:536:ARG:HH11	1:A:536:ARG:CG	2.11	0.63
1:A:500:ARG:CD	3:A:945:HOH:O	2.45	0.63
1:A:680:ASP:N	1:A:681:PRO:HD2	2.13	0.63
1:A:281:LEU:HD23	1:A:282:ILE:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ILE:CD1	1:A:471:VAL:HG22	2.29	0.62
2:B:34:THR:HB	3:B:222:HOH:O	1.99	0.62
1:A:694:TRP:C	1:A:698:SER:HG	2.01	0.62
2:B:34:THR:O	2:B:37:MET:HB3	1.98	0.62
2:B:96:ARG:NH1	2:B:97:PHE:CZ	2.68	0.62
1:A:344:THR:HB	1:A:345:PRO:HD2	1.79	0.62
2:B:18:ARG:O	2:B:18:ARG:HG3	1.99	0.62
1:A:145:GLN:O	1:A:146:TYR:C	2.43	0.62
1:A:289:GLY:C	1:A:322:GLY:N	2.58	0.62
1:A:488:THR:HG22	1:A:490:GLU:O	2.00	0.62
1:A:373:GLY:HA3	1:A:487:SER:HB2	1.80	0.62
1:A:472:LEU:HD13	1:A:473:ASN:N	2.14	0.62
2:B:32:SER:HB3	2:B:35:GLU:HG3	1.80	0.62
2:B:105:ILE:CG2	2:B:110:LEU:HD12	2.30	0.62
1:A:368:GLY:O	1:A:624:SER:HB3	2.00	0.61
1:A:523:ILE:O	1:A:525:ALA:HB2	1.96	0.61
2:B:58:ASP:O	2:B:59:THR:C	2.41	0.61
2:B:63:MET:HG2	2:B:83:LEU:HD11	1.81	0.61
1:A:331:PHE:C	1:A:333:ARG:H	2.07	0.61
1:A:525:ALA:HB1	1:A:526:ASN:CA	2.24	0.61
2:B:162:LEU:HD11	2:B:180:LEU:HD11	1.80	0.61
1:A:609:LYS:O	1:A:612:ARG:CB	2.49	0.61
2:B:110:LEU:HD22	2:B:130:ILE:HD12	1.83	0.61
1:A:86:GLN:OE1	1:A:132:GLN:NE2	2.33	0.61
1:A:224:LEU:HD23	1:A:224:LEU:C	2.25	0.61
1:A:535:ARG:O	1:A:536:ARG:C	2.44	0.61
1:A:167:PHE:HB3	1:A:182:GLU:OE1	2.00	0.61
2:B:60:CYS:HA	2:B:63:MET:HE3	1.83	0.61
1:A:326:MET:HE2	1:A:330:ASP:HB3	1.83	0.61
1:A:99:GLN:HE21	1:A:168:VAL:HG23	1.66	0.60
2:B:9:ASN:N	2:B:9:ASN:ND2	2.39	0.60
1:A:361:MET:CG	1:A:509:TYR:CE1	2.84	0.60
1:A:404:GLY:CA	1:A:476:LYS:HG2	2.32	0.60
1:A:680:ASP:N	1:A:681:PRO:CD	2.64	0.60
1:A:421:LYS:NZ	3:A:796:HOH:O	2.33	0.60
2:B:50:LEU:HD12	2:B:52:THR:HG22	1.83	0.60
2:B:132:ARG:CG	2:B:132:ARG:NH1	2.60	0.60
1:A:375:ARG:HD3	1:A:376:ASN:ND2	2.15	0.60
1:A:551:PHE:O	1:A:552:GLU:C	2.45	0.60
1:A:557:LEU:HD23	1:A:572:PHE:HD2	1.66	0.60
1:A:217:LEU:O	1:A:220:PRO:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ALA:CB	1:A:282:ILE:HG22	2.32	0.59
1:A:411:LEU:HB3	1:A:471:VAL:HG23	1.84	0.59
1:A:541:LEU:HG	1:A:556:ILE:HD13	1.84	0.59
2:B:121:LEU:HA	3:B:192:HOH:O	2.02	0.59
1:A:63:LEU:N	1:A:63:LEU:HD12	2.17	0.59
1:A:13:GLU:OE2	1:A:13:GLU:HA	2.02	0.59
1:A:89:ILE:HB	3:A:798:HOH:O	2.01	0.59
1:A:606:LYS:CG	1:A:606:LYS:CE	2.76	0.59
2:B:106:GLY:HA3	3:B:199:HOH:O	2.03	0.59
1:A:216:GLU:OE2	3:A:941:HOH:O	2.15	0.59
1:A:281:LEU:HD21	1:A:325:TRP:HB3	1.84	0.59
1:A:395:ASP:N	1:A:404:GLY:O	2.36	0.59
1:A:237:LEU:C	1:A:238:LEU:HD12	2.26	0.59
1:A:620:GLY:O	1:A:621:THR:HG23	2.01	0.59
2:B:40:LEU:O	2:B:44:VAL:HG22	2.03	0.59
2:B:50:LEU:HD12	2:B:52:THR:CG2	2.33	0.59
1:A:384:ASN:HB3	1:A:385:PRO:CD	2.33	0.58
1:A:285:ARG:HD3	1:A:286:ASN:C	2.28	0.58
1:A:77:ARG:NH1	1:A:156:ASP:OD2	2.36	0.58
1:A:363:GLY:HA3	1:A:497:PHE:CZ	2.38	0.58
1:A:548:ILE:HG22	1:A:552:GLU:HB2	1.85	0.58
1:A:361:MET:HE3	1:A:387:TYR:HB3	1.84	0.58
1:A:558:ARG:HH12	1:A:559:ARG:HH11	1.50	0.58
2:B:36:LEU:HD22	2:B:75:LEU:HD23	1.85	0.58
1:A:516:ILE:HG12	1:A:639:PRO:HD3	1.85	0.58
1:A:538:PHE:CZ	1:A:594:LEU:N	2.71	0.58
1:A:394:GLU:CD	1:A:403:ARG:HB2	2.29	0.57
1:A:525:ALA:HB1	1:A:526:ASN:HA	1.86	0.57
1:A:342:ASN:HD22	1:A:356:TRP:NE1	2.02	0.57
2:B:16:GLN:O	2:B:17:PHE:C	2.47	0.57
2:B:123:GLN:HB3	3:B:204:HOH:O	2.04	0.57
1:A:95:THR:OG1	1:A:97:ILE:HG12	2.05	0.57
1:A:373:GLY:O	1:A:374:CYS:CB	2.51	0.57
1:A:289:GLY:HA3	3:A:926:HOH:O	2.04	0.57
2:B:17:PHE:O	2:B:20:LEU:HB2	2.04	0.57
2:B:47:HIS:CB	2:B:49:ASP:OD1	2.45	0.57
1:A:402:GLU:HA	1:A:403:ARG:CA	2.33	0.57
1:A:629:LYS:HB3	3:A:721:HOH:O	2.05	0.57
1:A:394:GLU:OE1	1:A:403:ARG:HB2	2.05	0.57
1:A:404:GLY:HA3	1:A:476:LYS:HE2	1.86	0.57
1:A:417:ARG:HG3	3:B:191:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLN:H	1:A:322:GLY:N	1.96	0.57
1:A:394:GLU:HA	1:A:405:CYS:SG	2.44	0.57
1:A:404:GLY:HA2	1:A:476:LYS:HG2	1.86	0.57
1:A:603:LYS:O	1:A:604:ILE:C	2.46	0.57
1:A:367:ARG:CZ	1:A:655:LEU:HD21	2.35	0.57
1:A:676:PHE:CD1	1:A:687:ILE:HD13	2.39	0.57
1:A:200:THR:O	1:A:204:PHE:HB2	2.06	0.56
2:B:96:ARG:NH1	2:B:97:PHE:CE1	2.74	0.56
2:B:110:LEU:HB3	2:B:130:ILE:HD11	1.87	0.56
1:A:615:ASP:O	1:A:616:VAL:C	2.48	0.56
1:A:353:TYR:HD1	1:A:353:TYR:O	1.89	0.56
1:A:460:GLU:N	3:A:770:HOH:O	2.38	0.56
2:B:169:GLN:NE2	3:B:207:HOH:O	2.38	0.56
1:A:599:ILE:O	1:A:600:LEU:C	2.40	0.56
1:A:600:LEU:HD11	1:A:604:ILE:HD11	1.88	0.56
1:A:549:SER:OG	1:A:551:PHE:HB2	2.06	0.56
1:A:596:GLU:HG3	3:A:764:HOH:O	2.05	0.56
1:A:690:ASP:OD1	1:A:693:SER:OG	2.18	0.56
1:A:88:ILE:CG2	1:A:88:ILE:O	2.54	0.56
2:B:87:ILE:O	2:B:87:ILE:HG22	2.05	0.56
2:B:105:ILE:CG2	2:B:109:GLU:HB2	2.36	0.55
2:B:126:TYR:C	2:B:128:MET:H	2.15	0.55
1:A:290:GLN:C	1:A:322:GLY:N	2.65	0.55
1:A:639:PRO:HD2	1:A:642:LEU:HD12	1.88	0.55
1:A:668:ARG:HB3	2:B:182:MET:HE1	1.89	0.55
1:A:686:THR:O	1:A:686:THR:CG2	2.50	0.55
1:A:56:SER:HB2	3:A:703:HOH:O	2.05	0.55
1:A:236:SER:O	1:A:238:LEU:CD1	2.54	0.55
1:A:530:ILE:CB	1:A:535:ARG:HH12	2.13	0.55
1:A:269:ALA:HA	1:A:282:ILE:HG22	1.88	0.55
2:B:39:ILE:CD1	3:B:235:HOH:O	2.55	0.55
1:A:367:ARG:H	1:A:494:ASN:HD21	1.55	0.55
1:A:542:ALA:HB1	1:A:547:GLU:N	2.21	0.55
2:B:63:MET:HG2	2:B:83:LEU:CD1	2.36	0.55
1:A:36:ARG:HH21	1:A:37:ASN:ND2	2.00	0.55
1:A:463:ASP:O	1:A:464:THR:C	2.50	0.55
1:A:533:GLY:O	1:A:537:LEU:HB2	2.07	0.55
1:A:575:GLU:N	3:A:786:HOH:O	2.29	0.55
1:A:568:LYS:NZ	1:A:608:GLN:HG2	2.21	0.54
1:A:394:GLU:HG2	1:A:479:PRO:HD3	1.89	0.54
1:A:98:CYS:SG	1:A:169:HIS:CE1	3.00	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ARG:CD	3:A:927:HOH:O	2.54	0.54
1:A:226:LYS:HG2	1:A:230:LYS:HG3	1.89	0.54
1:A:492:HIS:HD2	1:A:625:TYR:OH	1.91	0.54
1:A:538:PHE:CD2	1:A:594:LEU:HD23	2.43	0.54
1:A:699:VAL:HG23	1:A:700:LEU:CD2	2.38	0.54
2:B:99:THR:O	2:B:101:ARG:N	2.40	0.54
1:A:338:LEU:HD22	1:A:339:GLU:N	2.23	0.54
1:A:331:PHE:C	1:A:333:ARG:N	2.63	0.54
1:A:386:GLN:NE2	1:A:451:ASN:H	2.04	0.54
2:B:23:GLN:N	3:B:209:HOH:O	2.41	0.54
1:A:350:CYS:CB	1:A:353:TYR:HB2	2.34	0.53
1:A:554:GLN:CG	1:A:574:ILE:HD13	2.37	0.53
2:B:41:ASN:O	2:B:45:THR:HG21	2.07	0.53
1:A:584:LEU:HD23	1:A:600:LEU:HB2	1.90	0.53
1:A:622:MET:HE1	1:A:662:PHE:CE1	2.44	0.53
1:A:337:ARG:NH1	1:A:337:ARG:HG2	2.24	0.53
1:A:408:LEU:CD2	1:A:472:LEU:HD21	2.38	0.53
1:A:548:ILE:HG22	1:A:552:GLU:HB3	1.90	0.53
2:B:110:LEU:O	2:B:114:PHE:N	2.41	0.53
2:B:93:ILE:HD13	2:B:117:ALA:HA	1.91	0.53
1:A:367:ARG:H	1:A:494:ASN:ND2	2.06	0.53
2:B:92:GLY:O	2:B:96:ARG:HB3	2.08	0.53
2:B:107:SER:CB	3:B:201:HOH:O	2.47	0.53
1:A:119:GLU:HB2	1:A:348:LEU:HD23	1.91	0.53
1:A:290:GLN:CA	1:A:322:GLY:N	2.72	0.53
1:A:620:GLY:O	1:A:621:THR:CG2	2.56	0.53
1:A:81:ILE:O	1:A:82:CYS:HB2	2.08	0.53
1:A:281:LEU:HD23	1:A:282:ILE:H	1.72	0.53
1:A:390:LYS:HB2	1:A:481:GLU:HG2	1.90	0.52
1:A:427:HIS:CD2	3:A:725:HOH:O	2.61	0.52
2:B:99:THR:C	2:B:101:ARG:H	2.16	0.52
1:A:337:ARG:NH1	1:A:339:GLU:OE2	2.43	0.52
1:A:99:GLN:NE2	1:A:168:VAL:HG23	2.23	0.52
1:A:358:LEU:HD13	1:A:502:PHE:CZ	2.44	0.52
1:A:467:ASN:CG	1:A:467:ASN:O	2.52	0.52
1:A:281:LEU:CD2	1:A:326:MET:O	2.56	0.52
1:A:402:GLU:C	1:A:403:ARG:CA	2.80	0.52
1:A:242:ILE:HG12	1:A:334:HIS:O	2.10	0.52
1:A:583:MET:HG2	1:A:584:LEU:HD13	1.90	0.52
1:A:414:LYS:NZ	1:A:498:CYS:HB2	2.24	0.52
2:B:16:GLN:O	2:B:19:LYS:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:CD2	1:A:228:ILE:CD1	2.88	0.52
1:A:676:PHE:CE1	1:A:687:ILE:HG23	2.45	0.52
2:B:32:SER:CB	2:B:35:GLU:HG3	2.40	0.52
2:B:95:LYS:O	2:B:97:PHE:N	2.42	0.52
2:B:123:GLN:CB	3:B:204:HOH:O	2.58	0.52
1:A:217:LEU:HD22	1:A:337:ARG:N	2.25	0.51
1:A:398:ASP:CG	3:A:805:HOH:O	2.52	0.51
2:B:166:GLY:O	2:B:167:THR:C	2.53	0.51
1:A:281:LEU:CD2	1:A:282:ILE:N	2.73	0.51
2:B:126:TYR:O	2:B:128:MET:N	2.43	0.51
2:B:83:LEU:O	2:B:87:ILE:HG13	2.10	0.51
1:A:106:TRP:CD1	1:A:198:GLY:HA3	2.45	0.51
1:A:361:MET:HE3	1:A:387:TYR:CB	2.40	0.51
1:A:267:THR:CG2	1:A:285:ARG:HB2	2.40	0.51
1:A:393:GLU:HB3	1:A:505:LYS:HG2	1.91	0.51
1:A:609:LYS:O	1:A:612:ARG:N	2.42	0.51
1:A:264:TYR:CD2	1:A:286:ASN:HB2	2.46	0.51
1:A:497:PHE:CD2	1:A:497:PHE:C	2.89	0.51
1:A:81:ILE:HD12	1:A:165:LEU:CD2	2.41	0.51
1:A:120:ILE:O	1:A:121:LEU:C	2.50	0.51
1:A:129:GLN:NE2	1:A:139:PHE:HA	2.26	0.51
1:A:209:GLY:O	1:A:500:ARG:NH2	2.44	0.51
1:A:366:ARG:HA	1:A:494:ASN:ND2	2.26	0.51
1:A:380:THR:O	1:A:381:PHE:C	2.53	0.51
1:A:155:ASP:OD2	1:A:155:ASP:C	2.54	0.50
1:A:412:ILE:HD11	1:A:469:ARG:HD3	1.92	0.50
2:B:98:ASP:OD2	2:B:104:THR:O	2.28	0.50
1:A:402:GLU:CA	1:A:403:ARG:CA	2.88	0.50
1:A:436:VAL:C	3:A:944:HOH:O	2.53	0.50
2:B:109:GLU:C	2:B:111:PRO:HD2	2.37	0.50
2:B:75:LEU:HD12	2:B:76:GLY:N	2.26	0.50
2:B:96:ARG:HG2	2:B:97:PHE:CE1	2.45	0.50
1:A:62:GLU:C	1:A:63:LEU:HD12	2.37	0.50
1:A:354:LYS:NZ	3:A:844:HOH:O	2.37	0.50
2:B:96:ARG:HG2	2:B:96:ARG:HH11	1.77	0.50
1:A:204:PHE:HZ	1:A:237:LEU:HD12	1.77	0.50
2:B:41:ASN:HD21	2:B:55:PHE:N	2.08	0.50
1:A:168:VAL:CG1	1:A:179:ALA:HA	2.34	0.50
1:A:216:GLU:OE1	1:A:337:ARG:HG3	2.12	0.50
1:A:262:HIS:CE1	3:A:740:HOH:O	2.64	0.50
2:B:50:LEU:HD21	2:B:94:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:HB2	1:A:348:LEU:CD2	2.42	0.50
1:A:400:ASP:O	1:A:401:GLY:HA2	2.08	0.50
1:A:226:LYS:HZ3	1:A:400:ASP:CG	2.20	0.50
1:A:285:ARG:HA	1:A:323:GLU:HA	1.94	0.50
1:A:395:ASP:OD1	1:A:504:GLU:HG3	2.12	0.50
1:A:409:VAL:HG11	1:A:484:LEU:HD21	1.93	0.50
1:A:12:ARG:O	1:A:16:GLU:HG3	2.12	0.49
1:A:281:LEU:HD21	1:A:326:MET:N	2.23	0.49
1:A:414:LYS:HZ1	1:A:498:CYS:HB2	1.76	0.49
1:A:527:GLU:C	1:A:528:GLU:O	2.50	0.49
1:A:699:VAL:HG23	1:A:700:LEU:HD23	1.94	0.49
1:A:97:ILE:HA	1:A:170:SER:HA	1.92	0.49
1:A:332:LEU:HD23	3:A:870:HOH:O	2.11	0.49
1:A:337:ARG:HD2	3:A:724:HOH:O	2.11	0.49
1:A:416:ARG:HH11	1:A:416:ARG:CG	2.18	0.49
1:A:427:HIS:HD2	3:A:725:HOH:O	1.96	0.49
2:B:60:CYS:O	2:B:64:VAL:HG23	2.12	0.49
2:B:123:GLN:N	2:B:123:GLN:HE21	2.10	0.49
1:A:240:CYS:HA	1:A:337:ARG:O	2.12	0.49
2:B:151:ARG:HB3	2:B:151:ARG:NH1	2.23	0.49
1:A:557:LEU:HD23	1:A:572:PHE:CD2	2.46	0.49
1:A:87:PHE:O	1:A:177:TRP:HD1	1.96	0.49
1:A:373:GLY:O	1:A:374:CYS:HB2	2.12	0.49
2:B:28:ASP:OD1	2:B:28:ASP:N	2.37	0.49
1:A:22:GLU:CD	1:A:22:GLU:H	2.21	0.49
1:A:210:GLY:C	1:A:500:ARG:HH22	2.20	0.49
1:A:344:THR:CB	1:A:345:PRO:HD2	2.40	0.49
2:B:96:ARG:HG3	2:B:96:ARG:O	2.13	0.49
1:A:193:GLU:O	1:A:193:GLU:CG	2.52	0.48
2:B:42:LYS:HD3	3:B:194:HOH:O	2.12	0.48
2:B:78:GLU:HA	2:B:81:LYS:HE2	1.95	0.48
1:A:4:ILE:CD1	2:B:180:LEU:HD23	2.35	0.48
1:A:88:ILE:CD1	1:A:121:LEU:HD21	2.43	0.48
1:A:228:ILE:HD12	1:A:328:PHE:HE1	1.78	0.48
2:B:87:ILE:O	2:B:87:ILE:CG2	2.60	0.48
1:A:561:LEU:C	1:A:563:LYS:N	2.68	0.48
1:A:88:ILE:HD11	1:A:121:LEU:HD21	1.94	0.48
1:A:269:ALA:HB2	1:A:282:ILE:HG22	1.95	0.48
1:A:399:GLU:O	1:A:399:GLU:HG2	2.08	0.48
1:A:532:ASP:OD1	1:A:536:ARG:NH2	2.46	0.48
1:A:647:VAL:HG13	1:A:648:ALA:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TYR:N	1:A:387:TYR:CD1	2.82	0.48
1:A:573:SER:OG	1:A:576:THR:OG1	2.07	0.48
1:A:541:LEU:HG	1:A:556:ILE:HD11	1.96	0.48
1:A:542:ALA:CB	1:A:546:ALA:HA	2.43	0.48
1:A:63:LEU:N	1:A:63:LEU:CD1	2.76	0.48
1:A:402:GLU:C	1:A:403:ARG:HG2	2.38	0.48
1:A:620:GLY:C	1:A:621:THR:HG23	2.38	0.48
1:A:673:PHE:O	1:A:677:LYS:HG3	2.14	0.48
1:A:372:GLY:O	1:A:491:PRO:HB3	2.14	0.48
1:A:629:LYS:O	1:A:630:ALA:C	2.55	0.48
2:B:39:ILE:HD11	3:B:235:HOH:O	2.14	0.47
1:A:331:PHE:O	1:A:333:ARG:N	2.47	0.47
1:A:568:LYS:HZ3	1:A:608:GLN:HG2	1.78	0.47
2:B:17:PHE:O	2:B:20:LEU:N	2.47	0.47
2:B:148:CYS:O	2:B:152:LEU:CD2	2.59	0.47
1:A:558:ARG:HD2	3:A:927:HOH:O	2.12	0.47
1:A:609:LYS:O	1:A:612:ARG:HB3	2.14	0.47
1:A:617:ASP:CG	1:A:619:SER:HB2	2.39	0.47
1:A:678:GLN:NE2	3:A:807:HOH:O	2.47	0.47
2:B:100:ASP:C	2:B:102:SER:N	2.72	0.47
1:A:285:ARG:HG3	1:A:285:ARG:NH1	2.28	0.47
1:A:536:ARG:HH11	1:A:536:ARG:HG3	1.79	0.47
1:A:7:LYS:HD2	3:A:854:HOH:O	2.14	0.47
1:A:238:LEU:H	1:A:238:LEU:CD1	2.09	0.47
1:A:389:ILE:HA	1:A:389:ILE:HD13	1.62	0.47
1:A:413:GLN:OE1	1:A:426:MET:HG3	2.14	0.47
1:A:421:LYS:HB3	1:A:424:GLU:HG3	1.96	0.47
1:A:99:GLN:OE1	1:A:103:GLY:HA3	2.15	0.47
1:A:127:LEU:O	1:A:129:GLN:N	2.48	0.47
1:A:327:SER:HB3	1:A:330:ASP:OD2	2.14	0.47
1:A:596:GLU:CG	3:A:764:HOH:O	2.62	0.47
1:A:674:LYS:CE	1:A:674:LYS:CG	2.83	0.47
2:B:11:SER:O	2:B:13:GLU:N	2.48	0.47
2:B:123:GLN:N	2:B:123:GLN:NE2	2.63	0.47
1:A:37:ASN:O	1:A:38:GLU:C	2.53	0.47
1:A:88:ILE:O	1:A:88:ILE:HG23	2.14	0.47
1:A:397:ASP:C	1:A:398:ASP:OD1	2.58	0.47
1:A:419:GLN:NE2	1:A:424:GLU:O	2.48	0.47
1:A:417:ARG:CG	3:B:191:HOH:O	2.63	0.47
1:A:699:VAL:CA	1:A:699:VAL:CG2	2.83	0.47
2:B:22:VAL:O	2:B:23:GLN:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:HIS:HE2	1:A:288:TRP:HE3	1.62	0.46
1:A:359:THR:O	1:A:501:VAL:N	2.36	0.46
1:A:373:GLY:HA3	1:A:487:SER:CB	2.45	0.46
1:A:374:CYS:CB	1:A:489:PHE:O	2.63	0.46
2:B:41:ASN:O	2:B:45:THR:CG2	2.63	0.46
2:B:41:ASN:C	2:B:45:THR:HG22	2.40	0.46
2:B:89:LYS:C	2:B:91:GLN:N	2.68	0.46
2:B:93:ILE:HD13	2:B:117:ALA:CA	2.45	0.46
1:A:28:LEU:HD23	1:A:50:SER:HB2	1.97	0.46
1:A:156:ASP:O	1:A:157:ARG:C	2.52	0.46
1:A:506:LYS:CG	1:A:506:LYS:CE	2.83	0.46
1:A:573:SER:OG	1:A:660:ASP:OD2	2.24	0.46
1:A:652:ASP:C	1:A:653:ASP:O	2.53	0.46
2:B:59:THR:HG23	2:B:147:SER:HB2	1.97	0.46
1:A:429:ILE:HD12	1:A:471:VAL:HG22	1.97	0.46
2:B:41:ASN:C	2:B:45:THR:CG2	2.89	0.46
2:B:110:LEU:HD22	2:B:130:ILE:CD1	2.45	0.46
1:A:177:TRP:CG	1:A:178:SER:N	2.84	0.46
1:A:430:GLY:HA3	1:A:465:PHE:CZ	2.51	0.46
1:A:81:ILE:O	1:A:82:CYS:CB	2.59	0.46
1:A:561:LEU:O	1:A:562:ALA:C	2.59	0.46
1:A:692:ILE:O	1:A:696:SER:OG	2.34	0.46
1:A:91:GLY:O	1:A:92:ALA:C	2.56	0.46
1:A:433:ILE:HG12	1:A:484:LEU:HD22	1.98	0.46
2:B:20:LEU:CD1	3:B:194:HOH:O	2.57	0.46
1:A:106:TRP:NE1	1:A:198:GLY:HA3	2.31	0.46
1:A:269:ALA:CA	1:A:282:ILE:HG22	2.46	0.46
2:B:50:LEU:CD1	2:B:52:THR:HG22	2.46	0.46
2:B:126:TYR:C	2:B:128:MET:N	2.74	0.46
1:A:426:MET:O	1:A:427:HIS:C	2.58	0.45
1:A:74:GLU:O	1:A:160:THR:OG1	2.27	0.45
1:A:229:GLN:CD	3:A:846:HOH:O	2.59	0.45
1:A:486:PRO:O	1:A:486:PRO:HG2	2.15	0.45
1:A:586:GLU:C	1:A:588:GLY:H	2.24	0.45
2:B:17:PHE:C	2:B:19:LYS:H	2.23	0.45
1:A:4:ILE:CD1	2:B:180:LEU:HA	2.47	0.45
1:A:412:ILE:HG12	1:A:413:GLN:N	2.31	0.45
2:B:20:LEU:CD1	2:B:39:ILE:HG23	2.46	0.45
1:A:78:PRO:HG3	1:A:176:PHE:CD2	2.51	0.45
1:A:527:GLU:OE2	1:A:527:GLU:CA	2.63	0.45
1:A:626:GLU:HA	3:A:827:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:O	1:A:324:PHE:HB3	2.16	0.45
1:A:530:ILE:HD12	1:A:535:ARG:HH12	1.80	0.45
1:A:632:GLU:O	1:A:633:GLU:C	2.56	0.45
2:B:11:SER:C	2:B:13:GLU:N	2.73	0.45
1:A:537:LEU:O	1:A:541:LEU:HB2	2.17	0.45
1:A:118:GLU:OE1	1:A:119:GLU:HA	2.17	0.45
2:B:55:PHE:HA	2:B:143:ASP:OD2	2.17	0.45
2:B:57:ILE:HG23	2:B:58:ASP:N	2.32	0.45
1:A:30:GLN:NE2	1:A:187:LYS:NZ	2.62	0.45
1:A:173:GLY:HA2	3:A:915:HOH:O	2.16	0.45
1:A:281:LEU:CD2	1:A:281:LEU:C	2.90	0.45
2:B:145:PHE:CZ	2:B:149:LEU:CD1	2.97	0.45
1:A:551:PHE:HA	1:A:554:GLN:HB2	1.99	0.44
1:A:586:GLU:C	1:A:588:GLY:N	2.75	0.44
1:A:115:THR:CG2	3:A:759:HOH:O	2.38	0.44
1:A:593:GLY:O	1:A:594:LEU:C	2.59	0.44
1:A:694:TRP:C	1:A:698:SER:OG	2.57	0.44
1:A:699:VAL:CG1	1:A:699:VAL:HB	2.19	0.44
2:B:24:LEU:HD11	2:B:39:ILE:HD11	1.99	0.44
1:A:403:ARG:O	1:A:478:PRO:CA	2.59	0.44
2:B:112:GLY:O	2:B:116:ALA:HB2	2.18	0.44
1:A:113:SER:HB3	1:A:237:LEU:HD13	1.99	0.44
1:A:557:LEU:O	1:A:561:LEU:HB2	2.17	0.44
1:A:584:LEU:O	1:A:585:ASP:O	2.35	0.44
1:A:628:ARG:HA	1:A:643:HIS:HE1	1.83	0.44
1:A:649:ARG:NH2	1:A:668:ARG:HH12	2.14	0.44
1:A:649:ARG:HB2	2:B:183:TYR:HD1	1.80	0.44
2:B:151:ARG:HH11	2:B:151:ARG:CB	2.23	0.44
2:B:151:ARG:O	2:B:152:LEU:C	2.58	0.44
1:A:361:MET:HG2	1:A:509:TYR:HE1	1.79	0.44
2:B:47:HIS:N	2:B:47:HIS:CD2	2.86	0.44
2:B:98:ASP:O	2:B:99:THR:C	2.61	0.44
2:B:163:ASP:CG	2:B:167:THR:O	2.61	0.44
1:A:32:TYR:O	1:A:33:GLU:C	2.59	0.44
2:B:100:ASP:C	2:B:102:SER:H	2.24	0.44
1:A:51:PHE:CE1	1:A:57:SER:HB3	2.53	0.44
1:A:213:GLU:HG2	1:A:215:TYR:CE1	2.53	0.44
2:B:11:SER:O	2:B:12:GLU:C	2.60	0.44
1:A:180:LEU:HA	1:A:180:LEU:HD12	1.70	0.43
1:A:221:PRO:HB2	1:A:222:PRO:O	2.18	0.43
1:A:345:PRO:HB3	1:A:356:TRP:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PHE:O	1:A:542:ALA:N	2.47	0.43
1:A:649:ARG:HB2	2:B:183:TYR:CD1	2.53	0.43
1:A:553:LEU:O	1:A:554:GLN:C	2.60	0.43
1:A:51:PHE:HB2	1:A:187:LYS:HE3	1.99	0.43
1:A:290:GLN:O	1:A:322:GLY:HA2	2.18	0.43
1:A:628:ARG:CG	1:A:628:ARG:NE	2.67	0.43
1:A:668:ARG:HG2	3:A:848:HOH:O	2.14	0.43
2:B:105:ILE:HG23	2:B:109:GLU:HB2	2.00	0.43
1:A:171:ALA:HB2	3:A:826:HOH:O	2.19	0.43
1:A:194:ALA:HA	1:A:421:LYS:HG3	2.01	0.43
1:A:238:LEU:HB2	1:A:266:VAL:HB	2.01	0.43
1:A:668:ARG:CD	3:A:848:HOH:O	2.66	0.43
2:B:50:LEU:CD1	2:B:52:THR:CG2	2.96	0.43
1:A:8:LEU:O	1:A:12:ARG:HG3	2.19	0.43
1:A:267:THR:HG23	1:A:285:ARG:HB2	2.01	0.43
1:A:628:ARG:HA	1:A:643:HIS:CE1	2.54	0.43
2:B:125:ILE:O	2:B:128:MET:N	2.51	0.43
2:B:30:GLU:HB3	2:B:74:LYS:HB3	2.00	0.43
2:B:125:ILE:O	2:B:128:MET:HB2	2.18	0.43
1:A:102:LEU:CD1	1:A:102:LEU:N	2.81	0.43
1:A:224:LEU:HD22	1:A:328:PHE:CZ	2.53	0.43
1:A:364:ASN:ND2	1:A:644:GLN:NE2	2.64	0.43
1:A:419:GLN:HE21	1:A:419:GLN:HA	1.83	0.43
1:A:59:GLY:HA3	1:A:63:LEU:O	2.19	0.43
1:A:431:PHE:CD1	1:A:431:PHE:N	2.87	0.43
2:B:110:LEU:HB3	2:B:130:ILE:CD1	2.47	0.43
1:A:120:ILE:O	1:A:123:ARG:N	2.49	0.42
1:A:386:GLN:C	1:A:387:TYR:CD1	2.97	0.42
1:A:534:PHE:O	1:A:535:ARG:C	2.62	0.42
2:B:133:TYR:HB2	2:B:140:MET:CE	2.47	0.42
2:B:129:ILE:HG21	2:B:129:ILE:HD13	1.62	0.42
1:A:541:LEU:CD1	1:A:556:ILE:HD11	2.49	0.42
1:A:700:LEU:HD13	2:B:128:MET:HB3	2.01	0.42
2:B:111:PRO:O	2:B:115:GLU:HG3	2.19	0.42
2:B:146:ILE:O	2:B:147:SER:C	2.61	0.42
1:A:61:LYS:O	1:A:62:GLU:C	2.61	0.42
1:A:488:THR:CG2	1:A:490:GLU:O	2.65	0.42
2:B:31:VAL:HG11	2:B:36:LEU:HB2	2.02	0.42
1:A:579:ILE:HG13	1:A:580:MET:N	2.33	0.42
1:A:690:ASP:O	1:A:691:LEU:C	2.61	0.42
2:B:55:PHE:HD2	2:B:143:ASP:OD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:883:HOH:O	2:B:171:GLN:HG2	2.19	0.42
2:B:31:VAL:HG13	2:B:35:GLU:HB2	2.01	0.42
1:A:210:GLY:O	1:A:500:ARG:NH2	2.38	0.42
1:A:545:ASP:O	1:A:546:ALA:HB3	2.20	0.42
1:A:585:ASP:OD1	1:A:585:ASP:C	2.62	0.42
1:A:56:SER:CB	3:A:703:HOH:O	2.66	0.42
2:B:38:ASN:O	2:B:39:ILE:C	2.62	0.42
1:A:4:ILE:HD12	1:A:5:ALA:N	2.35	0.42
1:A:62:GLU:HB3	1:A:193:GLU:OE1	2.20	0.42
1:A:236:SER:HB3	1:A:341:CYS:O	2.20	0.42
1:A:412:ILE:HG13	1:A:469:ARG:O	2.19	0.42
2:B:24:LEU:CD1	3:B:235:HOH:O	2.67	0.42
1:A:496:ASP:HB3	3:A:739:HOH:O	2.19	0.41
2:B:110:LEU:N	2:B:111:PRO:CD	2.83	0.41
1:A:223:ASN:ND2	1:A:226:LYS:HE2	2.32	0.41
1:A:264:TYR:CE2	1:A:286:ASN:HB2	2.55	0.41
1:A:364:ASN:HB3	1:A:496:ASP:OD2	2.20	0.41
1:A:553:LEU:O	1:A:557:LEU:HD13	2.21	0.41
1:A:185:TYR:O	1:A:186:ALA:C	2.62	0.41
1:A:265:SER:HB3	3:A:887:HOH:O	2.20	0.41
1:A:472:LEU:C	1:A:472:LEU:CD1	2.91	0.41
1:A:622:MET:HG2	1:A:623:ASN:N	2.35	0.41
1:A:221:PRO:C	1:A:222:PRO:O	2.56	0.41
1:A:492:HIS:CD2	1:A:625:TYR:OH	2.71	0.41
2:B:66:VAL:HG23	2:B:67:MET:HG2	2.02	0.41
1:A:429:ILE:HD12	1:A:471:VAL:CG2	2.50	0.41
1:A:454:LEU:O	3:A:787:HOH:O	2.22	0.41
1:A:327:SER:OG	1:A:330:ASP:N	2.51	0.41
1:A:491:PRO:HB2	1:A:492:HIS:CD2	2.55	0.41
1:A:558:ARG:NH1	1:A:559:ARG:HH11	2.18	0.41
1:A:583:MET:SD	1:A:667:VAL:HG13	2.61	0.41
2:B:19:LYS:O	2:B:23:GLN:N	2.42	0.41
2:B:39:ILE:HG13	3:B:235:HOH:O	2.20	0.41
1:A:614:ILE:C	1:A:616:VAL:H	2.29	0.41
1:A:627:MET:O	1:A:630:ALA:HB3	2.21	0.41
1:A:629:LYS:NZ	3:A:755:HOH:O	2.45	0.41
2:B:19:LYS:C	2:B:21:PHE:N	2.79	0.41
2:B:96:ARG:O	2:B:96:ARG:CG	2.69	0.41
1:A:129:GLN:HE22	1:A:140:HIS:N	2.11	0.40
1:A:393:GLU:HB3	1:A:505:LYS:CG	2.51	0.40
1:A:597:PHE:CD2	1:A:597:PHE:C	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:HA	1:A:695:LEU:HD23	1.92	0.40
1:A:63:LEU:HB2	1:A:193:GLU:HB2	2.03	0.40
1:A:386:GLN:HE22	1:A:451:ASN:N	2.11	0.40
1:A:224:LEU:HD22	1:A:328:PHE:HZ	1.87	0.40
2:B:10:GLU:O	2:B:11:SER:C	2.65	0.40
2:B:97:PHE:CG	2:B:113:ALA:HB2	2.56	0.40
1:A:12:ARG:HH11	2:B:176:GLU:CD	2.29	0.40
1:A:523:ILE:HD13	1:A:602:THR:CG2	2.46	0.40
1:A:556:ILE:O	1:A:557:LEU:C	2.58	0.40
1:A:654:GLU:C	1:A:655:LEU:HD22	2.46	0.40
2:B:109:GLU:O	2:B:110:LEU:C	2.61	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLU:OE1	2:B:19:LYS:CE[1_554]	0.67	1.53
1:A:527:GLU:CD	2:B:19:LYS:CE[1_554]	0.84	1.36
1:A:527:GLU:CD	2:B:19:LYS:NZ[1_554]	1.15	1.05
1:A:527:GLU:OE1	2:B:19:LYS:CD[1_554]	1.29	0.91
1:A:527:GLU:OE2	2:B:19:LYS:NZ[1_554]	1.33	0.87
1:A:527:GLU:OE2	2:B:19:LYS:CE[1_554]	1.59	0.61
1:A:527:GLU:OE1	2:B:19:LYS:NZ[1_554]	1.75	0.45
1:A:527:GLU:OE1	2:B:19:LYS:CG[1_554]	2.10	0.10
1:A:38:GLU:OE2	1:A:490:GLU:OE2[1_455]	2.17	0.03
1:A:527:GLU:CG	2:B:19:LYS:NZ[1_554]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	609/700 (87%)	506 (83%)	70 (12%)	33 (5%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	174/184 (95%)	130 (75%)	31 (18%)	13 (8%)	1	1
All	All	783/884 (89%)	636 (81%)	101 (13%)	46 (6%)	1	2

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	351	ASP
1	A	354	LYS
1	A	373	GLY
1	A	399	GLU
1	A	403	ARG
1	A	427	HIS
1	A	461	ARG
1	A	526	ASN
1	A	527	GLU
1	A	585	ASP
2	B	18	ARG
2	B	96	ARG
2	B	127	SER
2	B	143	ASP
1	A	81	ILE
1	A	375	ARG
1	A	454	LEU
1	A	528	GLU
1	A	531	GLY
1	A	573	SER
1	A	587	ASP
1	A	616	VAL
1	A	617	ASP
2	B	100	ASP
2	B	101	ARG
2	B	141	ASP
1	A	135	TYR
1	A	218	ARG
1	A	350	CYS
1	A	463	ASP
1	A	492	HIS
2	B	99	THR
1	A	398	ASP
1	A	534	PHE
1	A	586	GLU

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Mol	Chain	Res	Type
2	B	17	PHE
2	B	166	GLY
1	A	530	ILE
1	A	535	ARG
1	A	577	CYS
2	B	28	ASP
1	A	374	CYS
2	B	42	LYS
2	B	92	GLY
1	A	51	PHE

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	522/603 (87%)	417 (80%)	105 (20%)	1	2
2	B	155/162 (96%)	128 (83%)	27 (17%)	2	3
All	All	677/765 (88%)	545 (80%)	132 (20%)	1	2

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	10	THR
1	A	13	GLU
1	A	18	LEU
1	A	28	LEU
1	A	29	ASN
1	A	55	PRO
1	A	67	SER
1	A	69	LYS
1	A	76	LYS
1	A	78	PRO
1	A	81	ILE
1	A	86	GLN

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Mol	Chain	Res	Type
1	A	102	LEU
1	A	107	LEU
1	A	108	LEU
1	A	111	ILE
1	A	115	THR
1	A	118	GLU
1	A	127	LEU
1	A	153	VAL
1	A	161	LYS
1	A	168	VAL
1	A	180	LEU
1	A	205	GLU
1	A	217	LEU
1	A	223	ASN
1	A	238	LEU
1	A	242	ILE
1	A	271	GLU
1	A	280	LYS
1	A	281	LEU
1	A	285	ARG
1	A	286	ASN
1	A	323	GLU
1	A	326	MET
1	A	329	SER
1	A	333	ARG
1	A	337	ARG
1	A	338	LEU
1	A	343	LEU
1	A	354	LYS
1	A	355	LYS
1	A	360	LYS
1	A	361	MET
1	A	364	ASN
1	A	375	ARG
1	A	380	THR
1	A	388	LEU
1	A	389	ILE
1	A	397	ASP
1	A	399	GLU
1	A	403	ARG
1	A	406	THR
1	A	412	ILE

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Mol	Chain	Res	Type
1	A	413	GLN
1	A	416	ARG
1	A	417	ARG
1	A	418	ARG
1	A	419	GLN
1	A	433	ILE
1	A	436	VAL
1	A	450	LYS
1	A	465	PHE
1	A	469	ARG
1	A	471	VAL
1	A	472	LEU
1	A	484	LEU
1	A	488	THR
1	A	505	LYS
1	A	508	ASP
1	A	509	TYR
1	A	511	THR
1	A	527	GLU
1	A	535	ARG
1	A	536	ARG
1	A	540	GLN
1	A	541	LEU
1	A	548	ILE
1	A	554	GLN
1	A	555	THR
1	A	557	LEU
1	A	558	ARG
1	A	560	VAL
1	A	561	LEU
1	A	568	LYS
1	A	575	GLU
1	A	584	LEU
1	A	589	SER
1	A	594	LEU
1	A	596	GLU
1	A	604	ILE
1	A	619	SER
1	A	629	LYS
1	A	637	LYS
1	A	655	LEU
1	A	656	ILE

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Mol	Chain	Res	Type
1	A	663	VAL
1	A	668	ARG
1	A	672	LEU
1	A	683	ASN
1	A	690	ASP
1	A	693	SER
1	A	696	SER
1	A	698	SER
2	B	9	ASN
2	B	11	SER
2	B	12	GLU
2	B	15	ARG
2	B	16	GLN
2	B	18	ARG
2	B	22	VAL
2	B	23	GLN
2	B	24	LEU
2	B	34	THR
2	B	36	LEU
2	B	43	VAL
2	B	51	LYS
2	B	75	LEU
2	B	91	GLN
2	B	96	ARG
2	B	105	ILE
2	B	121	LEU
2	B	123	GLN
2	B	125	ILE
2	B	128	MET
2	B	131	ARG
2	B	132	ARG
2	B	136	GLU
2	B	141	ASP
2	B	148	CYS
2	B	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	37	ASN
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	129	GLN
1	A	142	GLN
1	A	169	HIS
1	A	189	ASN
1	A	223	ASN
1	A	286	ASN
1	A	342	ASN
1	A	364	ASN
1	A	376	ASN
1	A	379	ASN
1	A	384	ASN
1	A	386	GLN
1	A	413	GLN
1	A	419	GLN
1	A	451	ASN
1	A	492	HIS
1	A	494	ASN
1	A	540	GLN
1	A	554	GLN
1	A	608	GLN
1	A	683	ASN
2	B	23	GLN
2	B	47	HIS
2	B	123	GLN
2	B	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	400:ASP	C	401:GLY	N	1.90
1	A	402:GLU	C	403:ARG	N	1.87
1	A	521:GLU	C	522:GLU	N	1.64
1	A	401:GLY	C	402:GLU	N	1.15
1	A	527:GLU	C	528:GLU	N	1.02

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.