



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:07 AM UTC

PDB ID : 1GPA / pdb_00001gpa
Title : STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE
CONTROL BY PHOSPHORYLATION AND AMP
Authors : Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on : 1990-11-13
Resolution : 2.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

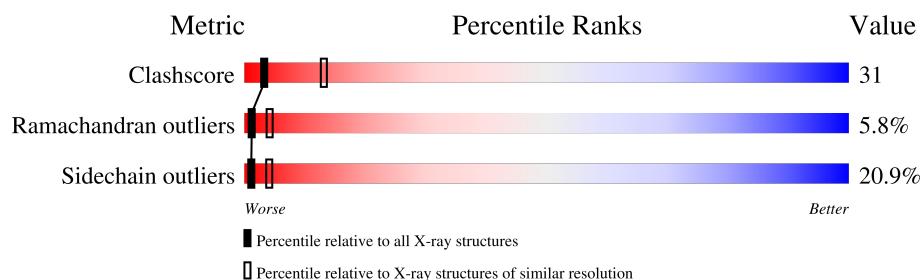
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	842	25% 40% 26% 8% .
1	B	842	26% 42% 23% 7% .
1	C	842	26% 38% 28% 7% .
1	D	842	22% 38% 30% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27029 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 GLYCOGEN PHOSPHORYLASE A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	P	S	44	0	0
			6732	4287	1190	1224	1	30			
1	B	827	Total	C	N	O	P	S	24	0	0
			6733	4286	1189	1227	1	30			
1	C	828	Total	C	N	O	P	S	0	0	0
			6732	4287	1190	1224	1	30			
1	D	828	Total	C	N	O	P	S	0	0	0
			6732	4287	1190	1224	1	30			

There are 4 discrepancies between the modelled and reference sequences:

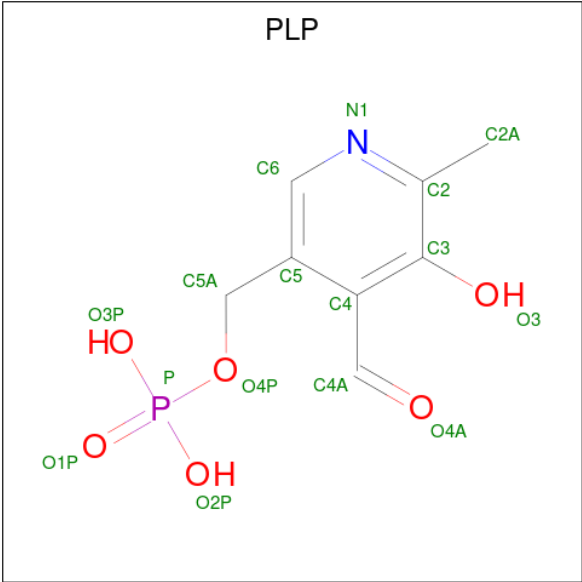
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



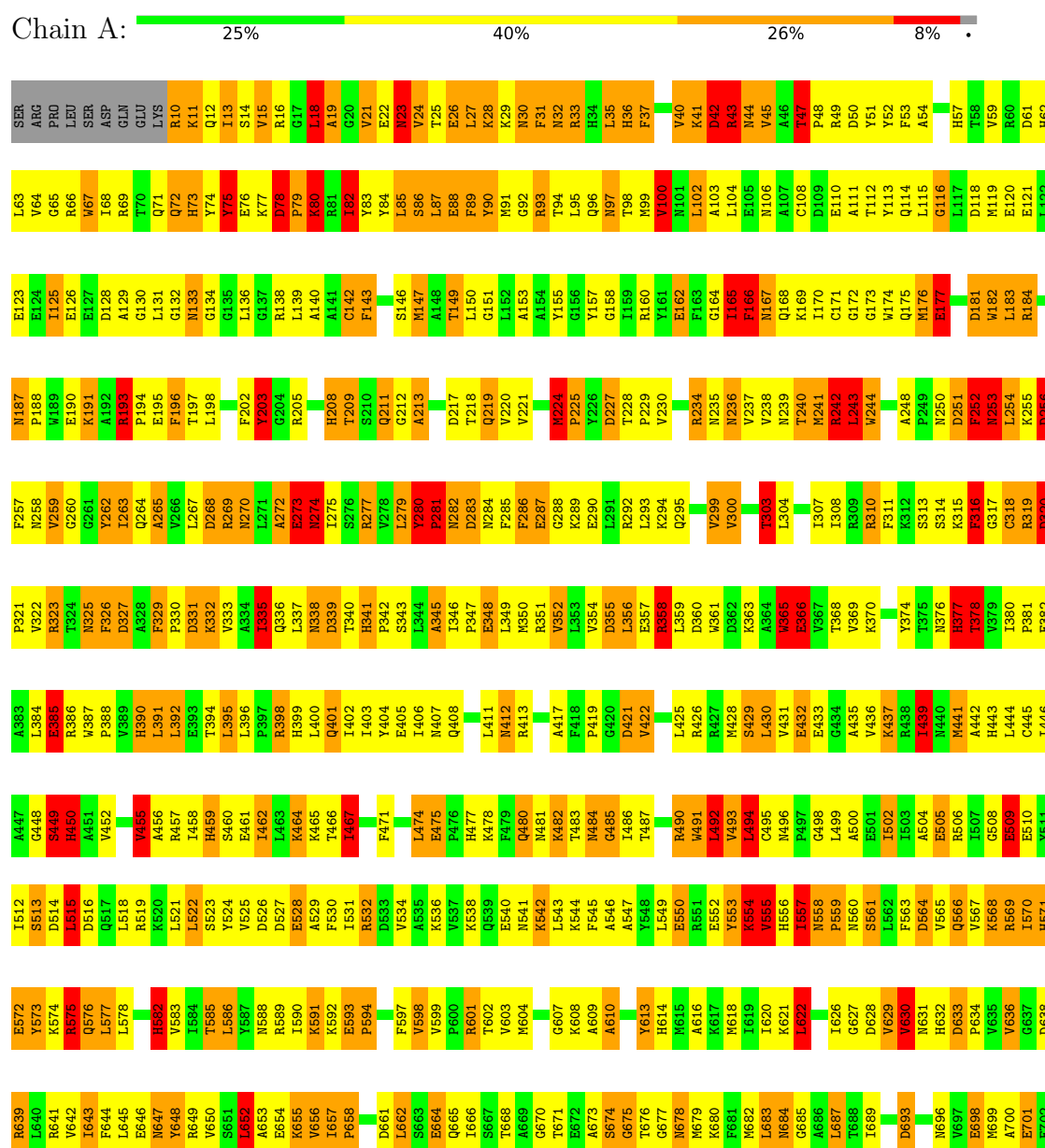
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

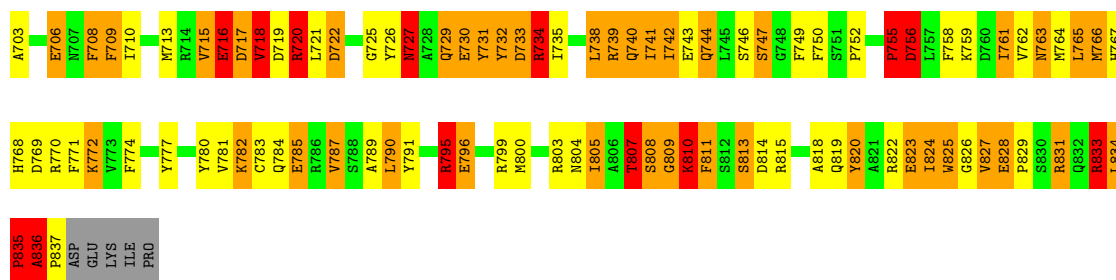
3 Residue-property plots

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.

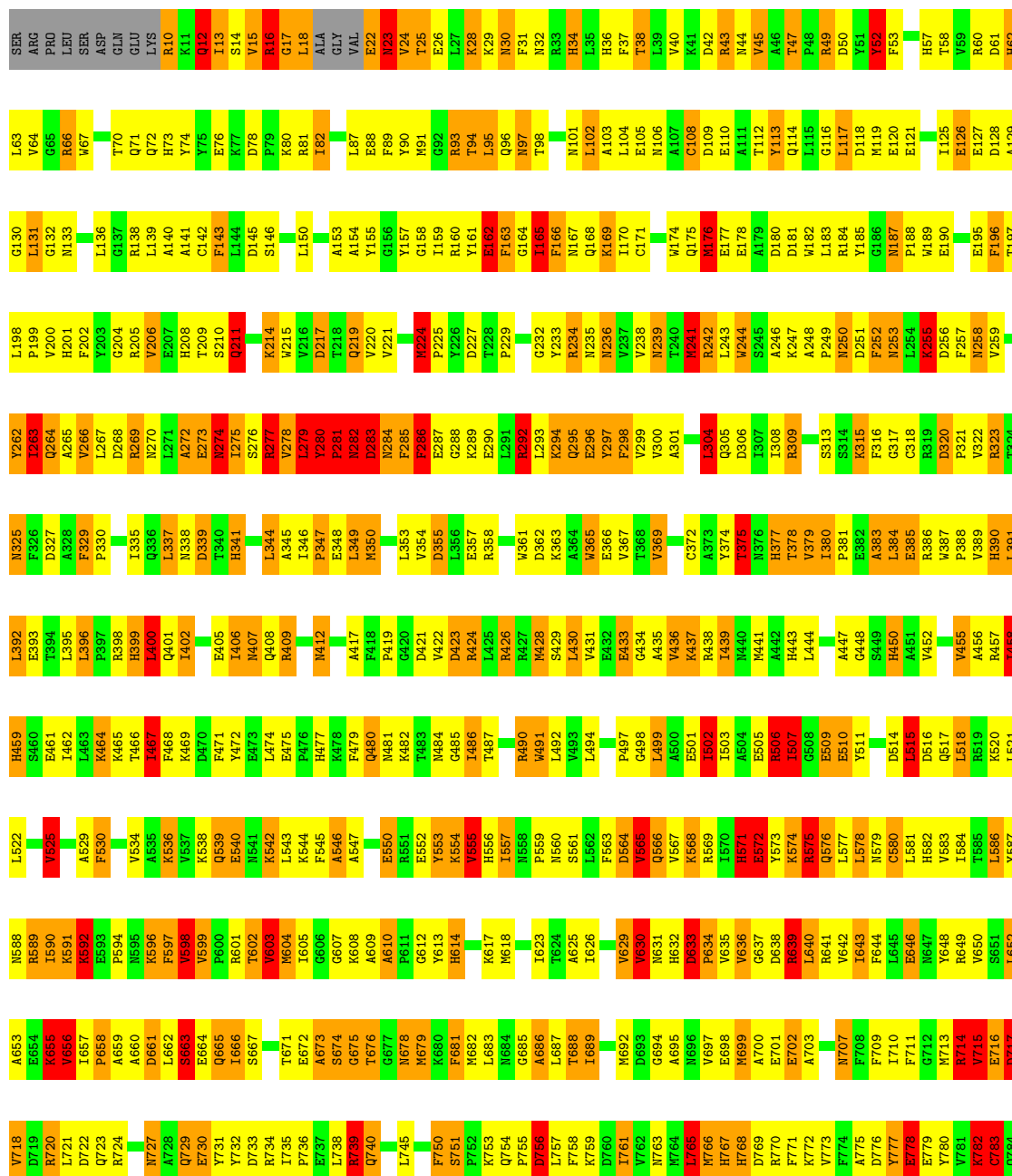
• Molecule 1: GLYCOGEN PHOSPHORYLASE A





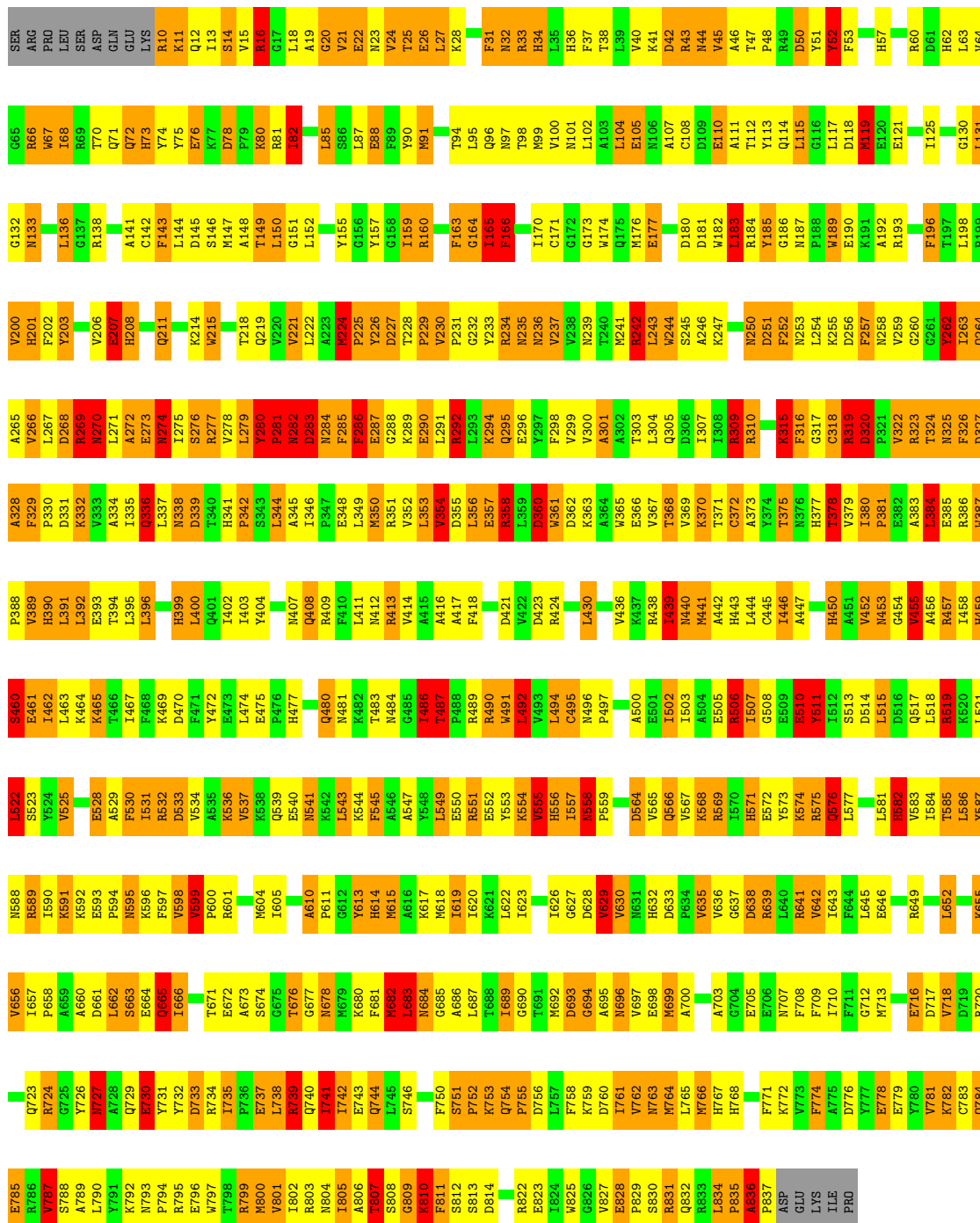
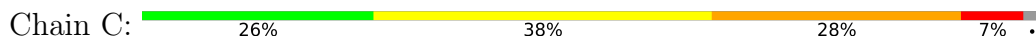
• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain B: 26% 42% 23% 7% .

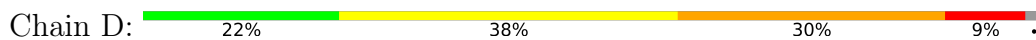




• Molecule 1: GLYCOGEN PHOSPHORYLASE A



• Molecule 1: GLYCOGEN PHOSPHORYLASE A



A818	L757	V697	V635	E572	E510	I446	V379	S314	D251	E190	D128	V64	SER
Q819	F758	E698	V636	V673	Y511	I446	I380	X315	F252	K191	A129	W67	ARG
Y820	K759	M699		K574	I512	S449	A383	G316	Y253	K192	G130	W67	PRO
A821	D760	A700	R639	R575	S513	H450	A384	G317	L253	R193	L131	I68	LEU
R822	F761	E701	L640	O576	D514	A451	E385	C318	K255	P194	G132	R69	SER
E823	V762	E702	R641	L577	L515	V452	R386	R319	D256	E195	N133	T70	ASP
I823	K763	A703	V642	L578	D516	R453	R387	D320	F257	F196	Q71	Q71	GLN
K825	K764	G704	L643	N579	Q517	G454	W388	P321	N258	L197	L136	Q72	GLU
	L765	E705	F644		L518	V455	P388	V322	V259	L198	G137	H73	LYS
E828	M766	E706	L645	H582	R519	A456	V389	R323	G260	P199	R138	Y74	R10
P829	K767	N707	E646	V583	K520	R457	H390	T324	G261	V200	L139	Y75	K11
S830	H768	F708	N647	I584	L521	I458	L391	N325	Y262	H201	A140	E76	Q12
R831	D769	F709	V648	T586	L522	H459	L392	F326	I263	F202	A141	K77	I13
Q832	K770	L710	R649	L586	S523	S460		D327	Q264	Y203	C142	D78	S14
R833	F771	F711	V650	V587	Y524	E461	L395	A328	A255	G204	F143	P79	V15
L834	K772	G712	S651	N588	V525	I462	L396	F329	D268	R205	L144	K80	R16
P835	V773	M713	L652	R589	D526	L463	P397	P330	R269	E207	D145	R81	G17
A836	F774	R714	A653	I590	D527	K464	R398	D331	K270	H208	M147	I82	
P837	A775	V715	E654	K591	E528	K465	H399	K332	L271	T209	A148	Y84	Y83
	D776	E716	K655	K592	A529	T466	L400		A272	S210	T149	L85	V21
GLU	Y777	D717	V656	E593	F530	I467	Q401	I335	E273	Q211	L150	S86	E22
LYS	E778	D718	P657	P594	R532	F468	I402	Q336	N274	G212	G151	L87	N23
ILE	E779	D719	P658	N595	R533	K469	I403	L337		A213	L152	V24	N24
PRO	Y780	L720	A659	V598	Y534	D470	E405	N338	R277	K214	A153	F88	T25
	K781	D722	D661	V599	A535	Y472	I406	T340	V276	W215	A154	Y90	K28
	K782	Q723	L662	P600	K536	E473	N407	H341	L279	V216	Y155	M91	K29
	G783	R724	S663	R601	V537	L474	Q408	P342	Y280	D217	G156		N30
	E785	G725	E664	T602	K538	E475	R409	S343	P281	T218	Y157	T94	F31
	R786	Y726	Q665	V603	Q539	P476	F410	L344	N282	G158	G157	L95	N32
	V787	N727	L666	N604	E540	H477	L411		D283	I159	R160	Q96	R33
	S788	A728	S667	L605	N541	K478	N412	E348	N284	R160	Y161	N97	H34
	A789	Q729	T668	R608	K542		R413	L349	F285	E162	F163	T98	L35
	L790	E730	A609	K544	L543	T483	V414	M350	F286	R351	P225	M99	H36
	Y791	V731		F545	F544	N484	A417	V352	E287	Y226	G164	V100	
	K792	D732	E672	A610	K544	G485		L353	G288	L227	I165	N101	L39
	N793	D733	A673	P611	F545	G486		V354	K289	D227	I166	L102	V40
	V794	R734	S674	G612	L549	T487	D421	D355	E290	T228	F166	A103	K41
	R795	L735	S675	H613	E550	P488		L356	L291	P229	M167	L104	D42
	E796	P736	T676	R614	R551	R489		D356	R292	V230	Q168	E105	R43
	V797	E737	G677	N615	E552	R490	R424	E357	L293	P231	K169	N106	N44
	L798	L738	N678	A616	Y553	W491	R426	R358	K294	G232	I170	A107	V45
	R799	R739	N679	K617	K554	L492	R427	L359	Q295	Y233	C108	A46	A46
	H800	Q740	K680	N618	V555	V493	M428	D360	F296	R234	D109	T47	T47
	V801	L741	F681	L619	H556	L494	S429	W361	Y297	N235	W174	E110	P48
	I802	L742	M682	L620	E557	C495	L430	A364	F298	N236	Q175	A111	R49
	R803	E743	L683	K621	N558	N496	V431		V299	V237	M176	T112	D50
	N804	Q744	N684	L622	P559	P497	E432			V238	E177	Y113	Y51
	T805	L745	G685	T623	N560	G498	E433			N239	A179	Q114	Y52
	A806	S746	L686	T624	S561	L499	G434			T240	D180		F53
	T807	S747	L687	K625	L562	A500	A435	T368	T303	M241	D181	D118	A54
	S808	V748	T688	L626	F563	E501	V436	K370	Q305	R242	D181		L55
	G809	F749	L689	G627	D564	I502	K437	T371	D306	L243	W182	E121	A56
	K810	F750	G690	D628	V585	I503	R438	C372	I307	W244	L183	E122	H57
	F811	S751	T691	V629	O566	A504	I439	A373	I308	S245	R184	L122	T58
	S812	V752	M692	V630	V567	E505	N440	Y374	R309	A246	Y185	E123	V59
	S813	K753	S693	N631	K586	R506		T376	R310	K247	G186	E124	K60
	D814	Q754	G694	H632	R569	I507	H443	N376	F311	A248	R157	I125	D61
	R815	P755	A695	L444	L570	L444	K377	P249	K312	P188	E126	E126	H62
		D756	N696	P634	H571	E509	C445	T378	S313	N250	W189	E127	L63

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	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27029	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, SEP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.44	53/6873 (0.8%)	2.51	530/9300 (5.7%)
1	B	1.37	43/6873 (0.6%)	2.46	464/9298 (5.0%)
1	C	1.49	49/6873 (0.7%)	2.47	487/9300 (5.2%)
1	D	1.40	48/6873 (0.7%)	2.66	513/9300 (5.5%)
All	All	1.43	193/27492 (0.7%)	2.53	1994/37198 (5.4%)

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	11
1	B	0	11
1	C	0	9
1	D	0	15
All	All	0	46

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	VAL	C-N	48.27	1.95	1.33
1	A	47	THR	N-CA	-15.37	1.22	1.45
1	A	756	ASP	N-CA	14.51	1.77	1.46
1	A	543	LEU	N-CA	9.77	1.59	1.46
1	A	262	TYR	CA-C	9.34	1.63	1.52
1	B	836	ALA	CA-C	-8.81	1.41	1.52
1	D	82	ILE	CA-CB	8.62	1.64	1.54
1	B	209	THR	CA-CB	8.60	1.65	1.53
1	D	281	PRO	CA-C	-8.50	1.40	1.52
1	D	525	VAL	CA-CB	8.44	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	837	PRO	CA-C	-8.29	1.40	1.52
1	D	229	PRO	CA-CB	-8.13	1.44	1.54
1	C	225	PRO	CA-CB	-8.10	1.43	1.53
1	C	341	HIS	CD2-NE2	-7.91	1.29	1.37
1	B	502	ILE	CA-CB	7.87	1.65	1.54
1	B	837	PRO	N-CA	-7.82	1.37	1.47
1	D	507	ILE	CA-CB	7.79	1.66	1.54
1	B	165	ILE	CA-CB	7.69	1.65	1.54
1	B	341	HIS	CD2-NE2	-7.58	1.29	1.37
1	A	829	PRO	CA-C	-7.55	1.45	1.52
1	C	571	HIS	CD2-NE2	-7.49	1.29	1.37
1	B	82	ILE	CA-CB	7.48	1.65	1.54
1	D	459	HIS	CD2-NE2	-7.41	1.29	1.37
1	B	201	HIS	CD2-NE2	-7.31	1.29	1.37
1	B	278	VAL	CA-CB	7.29	1.62	1.54
1	D	377	HIS	CD2-NE2	-7.28	1.29	1.37
1	D	209	THR	CA-CB	7.25	1.65	1.53
1	C	230	VAL	CA-CB	7.20	1.60	1.54
1	D	200	VAL	CA-CB	-7.11	1.45	1.54
1	D	557	ILE	CA-CB	7.10	1.64	1.54
1	A	100	VAL	CA-CB	7.10	1.62	1.54
1	C	73	HIS	CD2-NE2	-7.05	1.30	1.37
1	D	450	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	165	ILE	CA-CB	7.04	1.63	1.54
1	A	657	ILE	CA-CB	7.01	1.58	1.54
1	C	414	VAL	CA-CB	7.01	1.63	1.54
1	A	642	VAL	CA-CB	-6.99	1.45	1.54
1	B	73	HIS	CD2-NE2	-6.95	1.30	1.37
1	A	630	VAL	CA-CB	6.93	1.63	1.54
1	D	556	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	341	HIS	CD2-NE2	-6.87	1.30	1.37
1	D	324	THR	CA-CB	6.85	1.64	1.53
1	C	582	HIS	CD2-NE2	-6.84	1.30	1.37
1	D	45	VAL	CA-CB	6.83	1.62	1.54
1	D	630	VAL	CA-CB	6.82	1.62	1.54
1	B	450	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	459	HIS	CD2-NE2	-6.79	1.30	1.37
1	C	393	GLU	CA-CB	-6.78	1.42	1.53
1	A	582	HIS	CD2-NE2	-6.78	1.30	1.37
1	C	399	HIS	CG-ND1	-6.77	1.30	1.38
1	C	450	HIS	CG-ND1	-6.76	1.30	1.38
1	C	354	VAL	CA-CB	6.75	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	THR	CA-CB	6.75	1.64	1.53
1	C	34	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	565	VAL	CA-CB	6.72	1.63	1.54
1	A	729	GLN	CA-CB	-6.71	1.44	1.52
1	C	676	THR	CA-CB	-6.66	1.43	1.53
1	B	208	HIS	CD2-NE2	-6.61	1.30	1.37
1	C	325	ASN	CA-C	-6.61	1.44	1.52
1	D	571	HIS	CD2-NE2	-6.60	1.30	1.37
1	C	477	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	36	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	632	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	36	HIS	CG-ND1	-6.46	1.31	1.38
1	D	24	VAL	C-N	-6.44	1.24	1.33
1	A	571	HIS	CD2-NE2	-6.44	1.30	1.37
1	B	399	HIS	CG-ND1	-6.39	1.31	1.38
1	A	559	PRO	CA-CB	-6.36	1.44	1.53
1	B	280	TYR	N-CA	6.33	1.55	1.46
1	C	62	HIS	CD2-NE2	-6.33	1.30	1.37
1	B	399	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	632	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	459	HIS	CD2-NE2	-6.30	1.30	1.37
1	C	377	HIS	CD2-NE2	-6.30	1.30	1.37
1	D	614	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	582	HIS	CD2-NE2	-6.23	1.30	1.37
1	B	279	LEU	CA-C	6.22	1.61	1.53
1	D	443	HIS	CD2-NE2	-6.22	1.31	1.37
1	C	768	HIS	CD2-NE2	-6.21	1.31	1.37
1	D	16	ARG	CA-C	-6.20	1.44	1.52
1	D	57	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	467	ILE	CA-CB	6.16	1.62	1.54
1	A	316	PHE	CA-CB	-6.16	1.44	1.53
1	C	483	THR	CA-CB	6.14	1.62	1.53
1	A	57	HIS	CD2-NE2	-6.13	1.31	1.37
1	D	201	HIS	CD2-NE2	-6.12	1.31	1.37
1	D	768	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	556	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	16	ARG	C-N	-6.07	1.26	1.34
1	A	594	PRO	CA-CB	-6.05	1.45	1.53
1	A	341	HIS	CG-ND1	-6.04	1.31	1.38
1	B	477	HIS	CD2-NE2	-6.03	1.31	1.37
1	D	165	ILE	CA-CB	6.02	1.61	1.55
1	A	734	ARG	CA-C	6.02	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	HIS	CD2-NE2	-6.01	1.31	1.37
1	C	94	THR	CA-CB	-6.01	1.45	1.53
1	C	245	SER	CA-CB	-5.99	1.44	1.53
1	D	710	ILE	CA-CB	-5.96	1.48	1.54
1	A	443	HIS	CD2-NE2	-5.95	1.31	1.37
1	C	475	GLU	CA-CB	5.95	1.60	1.53
1	C	215	TRP	CA-CB	-5.94	1.45	1.53
1	C	459	HIS	CD2-NE2	-5.92	1.31	1.37
1	D	62	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	390	HIS	CD2-NE2	-5.90	1.31	1.37
1	D	341	HIS	CD2-NE2	-5.89	1.31	1.37
1	B	571	HIS	CD2-NE2	-5.88	1.31	1.37
1	D	237	VAL	CA-CB	5.85	1.62	1.54
1	B	62	HIS	CD2-NE2	-5.84	1.31	1.37
1	D	626	ILE	CA-CB	5.79	1.61	1.54
1	C	208	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	709	PHE	CA-CB	-5.79	1.45	1.52
1	A	614	HIS	CD2-NE2	-5.78	1.31	1.37
1	D	571	HIS	CG-ND1	-5.77	1.31	1.38
1	C	614	HIS	CD2-NE2	-5.76	1.31	1.37
1	B	786	ARG	NE-CZ	5.73	1.39	1.33
1	D	582	HIS	CD2-NE2	-5.72	1.31	1.37
1	C	283	ASP	C-N	-5.69	1.25	1.33
1	C	342	PRO	CA-CB	-5.69	1.45	1.53
1	D	16	ARG	C-N	-5.69	1.25	1.33
1	A	787	VAL	CA-CB	5.69	1.61	1.54
1	A	647	ASN	CA-C	-5.67	1.47	1.53
1	C	73	HIS	CG-ND1	-5.65	1.32	1.38
1	A	450	HIS	CG-ND1	-5.63	1.32	1.38
1	D	676	THR	CA-CB	-5.63	1.45	1.53
1	A	556	HIS	CD2-NE2	-5.62	1.31	1.37
1	C	450	HIS	CD2-NE2	-5.61	1.31	1.37
1	B	24	VAL	C-N	5.61	1.41	1.34
1	D	443	HIS	CG-ND1	-5.59	1.32	1.38
1	D	767	HIS	CD2-NE2	-5.59	1.31	1.37
1	D	36	HIS	CG-ND1	-5.58	1.32	1.38
1	A	79	PRO	CA-C	-5.58	1.46	1.52
1	A	450	HIS	CD2-NE2	-5.57	1.31	1.37
1	C	744	GLN	CA-CB	-5.56	1.44	1.53
1	A	768	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	436	VAL	CA-CB	5.55	1.62	1.54
1	C	62	HIS	CG-ND1	-5.55	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	HIS	CG-ND1	-5.54	1.32	1.38
1	C	556	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	613	TYR	CA-CB	-5.52	1.45	1.53
1	A	208	HIS	CD2-NE2	-5.51	1.31	1.37
1	B	630	VAL	CA-CB	5.49	1.61	1.54
1	D	189	TRP	CG-CD2	-5.48	1.33	1.43
1	D	501	GLU	CA-CB	5.48	1.62	1.53
1	A	323	ARG	CA-CB	5.47	1.61	1.53
1	C	767	HIS	CD2-NE2	-5.47	1.31	1.37
1	C	443	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	73	HIS	CD2-NE2	-5.44	1.31	1.37
1	C	632	HIS	CD2-NE2	-5.43	1.31	1.37
1	C	307	ILE	CA-CB	5.42	1.61	1.54
1	A	556	HIS	CB-CG	5.42	1.57	1.50
1	A	477	HIS	CD2-NE2	-5.41	1.31	1.37
1	D	208	HIS	CB-CG	5.39	1.57	1.50
1	B	57	HIS	CD2-NE2	-5.34	1.31	1.37
1	D	282	ASN	N-CA	-5.30	1.39	1.46
1	D	34	HIS	CD2-NE2	-5.29	1.32	1.37
1	B	36	HIS	CD2-NE2	-5.29	1.32	1.37
1	C	57	HIS	CD2-NE2	-5.27	1.32	1.37
1	B	443	HIS	CD2-NE2	-5.25	1.32	1.37
1	C	98	THR	CA-CB	-5.25	1.44	1.53
1	C	571	HIS	CA-C	-5.25	1.46	1.52
1	B	17	GLY	C-N	-5.23	1.26	1.33
1	A	824	ILE	CA-CB	5.22	1.61	1.54
1	B	215	TRP	NE1-CE2	-5.20	1.31	1.37
1	C	378	THR	CA-CB	5.20	1.59	1.53
1	C	201	HIS	CD2-NE2	-5.20	1.32	1.37
1	B	49	ARG	NE-CZ	5.19	1.38	1.33
1	B	490	ARG	CZ-NH1	5.19	1.40	1.32
1	B	390	HIS	CD2-NE2	-5.18	1.32	1.37
1	C	787	VAL	CA-CB	5.18	1.60	1.54
1	A	661	ASP	CA-CB	-5.18	1.45	1.53
1	B	768	HIS	CD2-NE2	-5.17	1.32	1.37
1	D	36	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	197	THR	CA-CB	-5.16	1.45	1.53
1	B	296	GLU	CA-CB	-5.14	1.45	1.53
1	C	208	HIS	CG-ND1	-5.14	1.32	1.38
1	B	354	VAL	CA-CB	-5.12	1.47	1.54
1	A	459	HIS	CG-ND1	-5.10	1.32	1.38
1	D	682	MET	CA-CB	5.08	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	380	ILE	CA-CB	5.08	1.60	1.54
1	C	556	HIS	CB-CG	5.06	1.57	1.50
1	D	567	VAL	CA-CB	5.06	1.61	1.54
1	A	181	ASP	CA-C	-5.05	1.47	1.53
1	C	36	HIS	CD2-NE2	-5.05	1.32	1.37
1	B	487	THR	CA-CB	5.05	1.60	1.53
1	B	754	GLN	CA-CB	5.04	1.61	1.53
1	D	309	ARG	CA-CB	5.04	1.61	1.53
1	D	377	HIS	ND1-CE1	-5.04	1.27	1.32
1	D	242	ARG	CA-CB	-5.02	1.46	1.53
1	A	82	ILE	CA-CB	5.02	1.60	1.53
1	B	244	TRP	CG-CD2	-5.02	1.34	1.43
1	C	477	HIS	CG-ND1	-5.01	1.32	1.38
1	C	460	SER	CA-CB	-5.01	1.44	1.53
1	B	467	ILE	CA-CB	5.00	1.59	1.54

All (1994) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	ASP	CA-CB-CG	57.27	169.87	112.60
1	D	24	VAL	O-C-N	42.80	165.09	121.87
1	D	250	ASN	CA-CB-CG	25.95	138.55	112.60
1	D	24	VAL	CA-C-N	-21.88	79.76	121.54
1	D	24	VAL	C-N-CA	-21.88	79.76	121.54
1	C	24	VAL	O-C-N	20.62	148.35	122.57
1	D	281	PRO	O-C-N	20.28	150.02	122.64
1	D	533	ASP	CA-CB-CG	17.69	130.29	112.60
1	A	262	TYR	CA-C-O	16.73	138.45	120.71
1	D	262	TYR	N-CA-C	15.04	134.17	108.76
1	C	597	PHE	CA-CB-CG	-14.36	99.44	113.80
1	B	274	ASN	CA-CB-CG	14.13	126.73	112.60
1	B	771	PHE	CA-CB-CG	-13.85	99.95	113.80
1	A	256	ASP	CA-CB-CG	13.80	126.40	112.60
1	A	541	ASN	OD1-CG-ND2	-13.60	109.00	122.60
1	C	264	GLN	N-CA-C	-13.54	96.85	113.50
1	C	676	THR	CA-CB-OG1	-13.19	89.82	109.60
1	B	598	VAL	N-CA-CB	-13.08	95.30	110.99
1	A	47	THR	CA-C-O	-12.83	107.50	120.97
1	D	530	PHE	CA-CB-CG	-12.80	101.00	113.80
1	B	105	GLU	N-CA-C	12.65	124.60	111.07
1	A	541	ASN	CB-CG-ND2	12.64	135.37	116.40
1	D	514	ASP	CA-CB-CG	12.48	125.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	652	LEU	N-CA-C	-12.43	98.24	113.41
1	A	281	PRO	O-C-N	12.37	139.33	122.64
1	B	264	GLN	N-CA-C	-12.31	94.31	112.04
1	C	733	ASP	CA-CB-CG	-12.19	100.41	112.60
1	C	281	PRO	O-C-N	12.18	139.09	122.64
1	D	208	HIS	CA-CB-CG	12.11	125.91	113.80
1	B	262	TYR	N-CA-C	12.10	129.63	109.06
1	D	631	ASN	CA-CB-CG	12.03	124.63	112.60
1	C	318	CYS	N-CA-C	-12.02	97.69	111.03
1	A	262	TYR	CB-CA-C	11.99	130.97	109.38
1	C	320	ASP	CA-CB-CG	11.79	124.39	112.60
1	A	24	VAL	O-C-N	11.76	133.74	121.87
1	B	609	ALA	N-CA-C	11.65	125.23	111.02
1	B	253	ASN	CA-CB-CG	11.60	124.20	112.60
1	A	181	ASP	CA-CB-CG	11.40	124.00	112.60
1	C	270	ASN	CA-CB-CG	-11.38	101.22	112.60
1	D	264	GLN	N-CA-C	-11.37	99.89	113.88
1	B	564	ASP	CA-CB-CG	11.35	123.95	112.60
1	D	561	SER	N-CA-C	11.34	125.29	110.43
1	C	24	VAL	CA-C-N	-11.31	105.73	120.44
1	C	24	VAL	C-N-CA	-11.31	105.73	120.44
1	A	331	ASP	CA-CB-CG	11.31	123.91	112.60
1	C	638	ASP	CA-C-O	11.28	130.57	119.97
1	B	836	ALA	O-C-N	11.16	134.15	121.32
1	C	739	ARG	N-CA-C	-11.11	99.19	111.07
1	D	733	ASP	CA-CB-CG	-11.08	101.52	112.60
1	D	44	ASN	CA-CB-CG	11.05	123.65	112.60
1	A	257	PHE	CA-CB-CG	-10.96	102.84	113.80
1	D	496	ASN	OD1-CG-ND2	-10.90	111.70	122.60
1	D	303	THR	CA-CB-OG1	-10.88	93.28	109.60
1	B	317	GLY	N-CA-C	-10.82	99.95	112.50
1	D	286	PHE	O-C-N	10.78	140.18	122.93
1	A	286	PHE	O-C-N	10.77	140.16	122.93
1	A	575	ARG	N-CA-C	10.76	125.81	112.47
1	D	91	MET	N-CA-C	10.73	125.47	112.38
1	C	286	PHE	O-C-N	10.68	140.01	122.93
1	B	180	ASP	CA-CB-CG	10.67	123.27	112.60
1	D	792	LYS	N-CA-C	-10.67	97.62	112.45
1	B	765	LEU	N-CA-C	-10.61	99.25	111.03
1	D	180	ASP	CA-CB-CG	10.60	123.19	112.60
1	B	511	TYR	N-CA-C	10.55	122.86	111.36
1	C	514	ASP	CA-CB-CG	10.54	123.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	TYR	N-CA-C	10.51	126.73	108.75
1	A	656	VAL	N-CA-C	10.46	120.37	110.53
1	A	477	HIS	CA-CB-CG	10.44	124.24	113.80
1	B	777	TYR	N-CA-C	10.39	122.18	111.07
1	D	811	PHE	CA-CB-CG	-10.37	103.43	113.80
1	B	804	ASN	CA-CB-CG	-10.37	102.23	112.60
1	D	455	VAL	N-CA-CB	-10.26	98.61	111.94
1	D	626	ILE	O-C-N	10.26	131.94	121.89
1	D	782	LYS	CA-CB-CG	10.21	134.51	114.10
1	C	390	HIS	CA-CB-CG	10.16	123.96	113.80
1	B	623	ILE	CA-C-O	-10.15	110.72	121.27
1	B	763	ASN	OD1-CG-ND2	-10.09	112.51	122.60
1	B	167	ASN	CB-CG-ND2	10.08	131.52	116.40
1	A	264	GLN	N-CA-C	-10.07	97.54	112.04
1	C	228	THR	CA-C-O	-10.07	110.26	120.63
1	D	560	ASN	OD1-CG-ND2	-10.07	112.53	122.60
1	C	455	VAL	N-CA-CB	-10.06	94.63	111.23
1	B	530	PHE	CA-CB-CG	-10.06	103.74	113.80
1	B	638	ASP	CA-CB-CG	10.06	122.66	112.60
1	A	577	LEU	CA-C-O	-10.05	110.35	120.70
1	C	211	GLN	OE1-CD-NE2	-10.03	112.58	122.60
1	C	553	TYR	O-C-N	-10.02	112.74	123.26
1	A	731	TYR	N-CA-C	-10.00	99.38	112.68
1	D	142	CYS	CA-CB-SG	-9.97	91.47	114.40
1	D	531	ILE	N-CA-CB	-9.97	98.89	110.55
1	D	311	PHE	N-CA-C	-9.91	100.03	111.03
1	C	272	ALA	N-CA-C	-9.89	100.76	113.12
1	C	814	ASP	CA-CB-CG	9.88	122.48	112.60
1	D	152	LEU	N-CA-C	9.84	124.31	109.25
1	C	784	GLN	CG-CD-NE2	9.83	131.14	116.40
1	B	268	ASP	CA-CB-CG	9.78	122.38	112.60
1	A	676	THR	N-CA-CB	-9.77	97.91	110.90
1	D	184	ARG	N-CA-C	-9.76	90.01	110.80
1	A	676	THR	CA-CB-OG1	-9.71	95.03	109.60
1	D	32	ASN	CA-CB-CG	-9.70	102.90	112.60
1	B	561	SER	N-CA-C	9.68	123.11	110.43
1	A	740	GLN	OE1-CD-NE2	-9.67	112.93	122.60
1	A	836	ALA	CA-C-O	9.67	133.41	120.16
1	A	316	PHE	N-CA-C	9.65	128.08	113.61
1	D	764	MET	N-CA-C	-9.57	98.89	111.24
1	D	217	ASP	CA-CB-CG	9.57	122.17	112.60
1	B	769	ASP	CA-CB-CG	9.55	122.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	HIS	CA-CB-CG	9.53	123.33	113.80
1	A	44	ASN	CA-CB-CG	9.48	122.08	112.60
1	B	487	THR	N-CA-C	-9.48	97.23	110.31
1	A	560	ASN	CA-CB-CG	-9.47	103.13	112.60
1	D	785	GLU	CB-CG-CD	9.47	128.70	112.60
1	A	68	ILE	N-CA-C	-9.46	101.13	110.30
1	C	44	ASN	CA-CB-CG	9.42	122.02	112.60
1	D	282	ASN	O-C-N	9.40	133.45	121.79
1	D	329	PHE	CA-CB-CG	9.38	123.18	113.80
1	C	211	GLN	CB-CG-CD	9.37	128.53	112.60
1	C	362	ASP	CA-CB-CG	-9.36	103.24	112.60
1	A	541	ASN	CA-CB-CG	9.30	121.91	112.60
1	C	571	HIS	CB-CG-CD2	-9.26	119.17	131.20
1	D	450	HIS	CB-CG-CD2	-9.23	119.19	131.20
1	D	283	ASP	O-C-N	9.21	134.75	122.41
1	B	281	PRO	O-C-N	9.21	135.07	122.64
1	B	406	ILE	N-CA-C	-9.20	101.42	110.72
1	C	20	GLY	N-CA-C	-9.19	101.11	115.73
1	A	654	GLU	N-CA-C	-9.16	101.19	111.82
1	D	639	ARG	CA-CB-CG	-9.15	95.79	114.10
1	B	811	PHE	CA-CB-CG	-9.13	104.67	113.80
1	C	581	LEU	N-CA-C	-9.12	99.47	111.24
1	B	836	ALA	N-CA-C	9.12	129.97	109.81
1	A	252	PHE	N-CA-C	9.12	130.22	110.80
1	D	315	LYS	CA-CB-CG	-9.11	95.89	114.10
1	D	244	TRP	CG-CD2-CE3	9.11	143.01	133.90
1	B	823	GLU	N-CA-C	9.09	120.95	111.14
1	B	782	LYS	N-CA-C	-9.07	101.08	110.97
1	D	253	ASN	OD1-CG-ND2	-9.07	113.53	122.60
1	A	449	SER	N-CA-C	9.06	124.16	109.85
1	B	663	SER	CA-CB-OG	9.04	129.19	111.10
1	C	784	GLN	OE1-CD-NE2	-9.04	113.56	122.60
1	A	272	ALA	N-CA-C	-9.03	100.92	112.93
1	B	12	GLN	N-CA-C	-9.02	100.40	111.40
1	A	480	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	B	286	PHE	O-C-N	9.01	136.21	122.87
1	C	678	ASN	CA-CB-CG	9.01	121.61	112.60
1	A	406	ILE	N-CA-C	-9.00	101.78	110.42
1	C	676	THR	CA-CB-CG2	9.00	125.80	110.50
1	D	12	GLN	N-CA-C	-8.99	101.39	111.82
1	A	341	HIS	CB-CG-CD2	-8.94	119.58	131.20
1	C	294	LYS	CA-C-O	-8.93	110.33	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	688	THR	N-CA-C	8.90	122.47	108.67
1	B	274	ASN	CB-CG-ND2	8.88	129.72	116.40
1	D	565	VAL	CB-CA-C	-8.87	97.61	110.83
1	A	763	ASN	CA-CB-CG	-8.85	103.75	112.60
1	D	750	PHE	CA-CB-CG	8.84	122.64	113.80
1	B	119	MET	CA-C-O	-8.82	111.81	120.90
1	A	678	ASN	CB-CG-ND2	8.82	129.63	116.40
1	A	238	VAL	N-CA-C	-8.81	94.73	107.77
1	C	446	ILE	CB-CA-C	-8.79	100.72	111.97
1	B	597	PHE	O-C-N	8.78	134.24	122.82
1	A	244	TRP	N-CA-C	8.77	123.72	109.59
1	B	295	GLN	OE1-CD-NE2	-8.77	113.83	122.60
1	B	97	ASN	OD1-CG-ND2	-8.76	113.84	122.60
1	B	739	ARG	N-CA-C	-8.73	101.34	111.03
1	B	783	CYS	CA-CB-SG	-8.73	94.33	114.40
1	D	163	PHE	CA-CB-CG	-8.71	105.09	113.80
1	C	251	ASP	CA-CB-CG	8.71	121.31	112.60
1	B	702	GLU	N-CA-C	8.69	120.52	111.14
1	A	644	PHE	CA-CB-CG	-8.67	105.13	113.80
1	C	149	THR	O-C-N	-8.66	112.82	122.08
1	D	72	GLN	OE1-CD-NE2	-8.66	113.94	122.60
1	B	146	SER	CA-C-O	-8.65	111.25	120.42
1	B	50	ASP	CA-CB-CG	8.64	121.24	112.60
1	A	543	LEU	CA-C-O	-8.61	109.19	119.27
1	C	660	ALA	O-C-N	8.61	132.71	123.06
1	C	440	ASN	OD1-CG-ND2	-8.60	114.00	122.60
1	A	167	ASN	CA-CB-CG	-8.59	104.01	112.60
1	D	550	GLU	CB-CG-CD	8.59	127.21	112.60
1	C	783	CYS	CA-CB-SG	-8.58	94.66	114.40
1	B	598	VAL	CB-CA-C	8.58	122.50	110.84
1	B	707	ASN	CA-CB-CG	-8.58	104.02	112.60
1	D	264	GLN	OE1-CD-NE2	-8.56	114.04	122.60
1	C	46	ALA	N-CA-C	8.54	122.29	110.24
1	D	810	LYS	N-CA-C	-8.54	102.30	112.89
1	C	574	LYS	CA-C-O	8.53	129.54	119.56
1	C	286	PHE	CA-CB-CG	-8.53	105.27	113.80
1	A	251	ASP	CA-CB-CG	8.52	121.12	112.60
1	B	286	PHE	CA-CB-CG	-8.51	105.29	113.80
1	A	450	HIS	CA-CB-CG	8.51	122.31	113.80
1	B	455	VAL	N-CA-CB	-8.51	97.79	112.08
1	C	327	ASP	CA-CB-CG	8.50	121.10	112.60
1	D	541	ASN	OD1-CG-ND2	-8.49	114.11	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	ASN	OD1-CG-ND2	-8.48	114.12	122.60
1	A	224	MET	CA-C-N	8.46	129.13	119.99
1	A	224	MET	C-N-CA	8.46	129.13	119.99
1	A	678	ASN	OD1-CG-ND2	-8.45	114.15	122.60
1	B	571	HIS	CB-CG-CD2	-8.45	120.21	131.20
1	C	236	ASN	OD1-CG-ND2	-8.44	114.16	122.60
1	D	676	THR	CA-CB-OG1	-8.43	96.95	109.60
1	C	446	ILE	N-CA-CB	8.42	120.41	110.55
1	D	744	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	D	262	TYR	CA-C-O	8.41	129.65	120.32
1	C	283	ASP	O-C-N	8.40	133.77	122.59
1	A	482	LYS	O-C-N	-8.40	115.77	123.50
1	B	727	ASN	OD1-CG-ND2	-8.40	114.20	122.60
1	C	385	GLU	N-CA-C	8.40	122.68	110.42
1	C	211	GLN	CG-CD-NE2	8.40	129.00	116.40
1	A	45	VAL	N-CA-CB	-8.39	97.98	112.08
1	A	813	SER	CA-C-O	-8.38	110.63	120.10
1	A	242	ARG	N-CA-C	-8.37	95.59	109.24
1	C	183	LEU	N-CA-C	-8.37	95.65	108.96
1	A	286	PHE	CA-CB-CG	-8.37	105.43	113.80
1	A	23	ASN	CA-CB-CG	8.37	120.97	112.60
1	C	325	ASN	O-C-N	8.36	133.09	122.89
1	B	603	VAL	N-CA-CB	-8.36	100.78	111.64
1	A	477	HIS	N-CA-C	8.35	123.19	112.34
1	A	376	ASN	OD1-CG-ND2	-8.35	114.25	122.60
1	A	341	HIS	CA-CB-CG	-8.34	105.46	113.80
1	D	91	MET	CA-CB-CG	-8.34	97.42	114.10
1	A	782	LYS	CA-C-O	-8.34	108.59	120.51
1	C	143	PHE	N-CA-C	-8.33	102.14	111.14
1	B	163	PHE	N-CA-C	8.30	123.59	112.88
1	A	835	PRO	N-CA-C	8.29	129.55	112.47
1	C	771	PHE	N-CA-C	8.29	123.62	113.17
1	B	754	GLN	N-CA-C	-8.29	91.50	109.81
1	B	754	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	A	831	ARG	CA-CB-CG	8.28	130.67	114.10
1	A	583	VAL	CB-CA-C	-8.28	100.97	112.14
1	C	266	VAL	N-CA-C	-8.27	102.37	110.72
1	D	283	ASP	N-CA-C	-8.26	100.59	111.74
1	B	751	SER	CA-CB-OG	8.25	127.61	111.10
1	C	378	THR	CA-C-O	8.25	129.12	120.54
1	D	739	ARG	N-CA-C	-8.24	101.99	110.97
1	B	258	ASN	OD1-CG-ND2	-8.23	114.37	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	591	LYS	O-C-N	8.23	133.81	122.46
1	B	731	TYR	N-CA-C	-8.22	101.90	111.03
1	C	750	PHE	CA-CB-CG	-8.21	105.59	113.80
1	C	639	ARG	CA-CB-CG	-8.21	97.69	114.10
1	D	533	ASP	CB-CA-C	-8.20	97.01	110.79
1	C	387	TRP	CA-C-O	-8.20	112.19	120.63
1	D	268	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	450	HIS	CB-CG-CD2	-8.19	120.55	131.20
1	D	699	MET	N-CA-C	-8.19	101.41	111.40
1	B	638	ASP	CA-C-O	8.19	127.66	119.97
1	D	572	GLU	N-CA-C	8.19	119.98	111.14
1	C	180	ASP	CA-CB-CG	8.18	120.78	112.60
1	B	672	GLU	CA-C-O	8.18	130.02	120.69
1	A	236	ASN	CA-CB-CG	-8.18	104.42	112.60
1	B	682	MET	N-CA-C	-8.17	102.45	111.36
1	D	256	ASP	CA-CB-CG	8.16	120.76	112.60
1	A	28	LYS	N-CA-C	-8.16	102.33	111.14
1	A	78	ASP	CA-CB-CG	8.14	120.74	112.60
1	B	832	GLN	N-CA-C	8.14	122.18	109.07
1	B	509	GLU	O-C-N	8.14	134.22	123.07
1	B	280	TYR	CA-C-N	8.13	130.01	119.84
1	B	280	TYR	C-N-CA	8.13	130.01	119.84
1	C	325	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	B	560	ASN	CA-CB-CG	-8.13	104.47	112.60
1	C	94	THR	CA-CB-OG1	-8.12	97.42	109.60
1	B	30	ASN	CA-C-O	-8.11	110.94	120.10
1	A	227	ASP	CA-CB-CG	8.10	120.70	112.60
1	D	303	THR	CA-CB-CG2	8.10	124.27	110.50
1	A	665	GLN	OE1-CD-NE2	-8.10	114.50	122.60
1	A	700	ALA	N-CA-C	-8.09	100.80	111.24
1	B	325	ASN	CA-C-O	8.06	130.19	121.16
1	C	807	THR	N-CA-CB	-8.06	98.25	111.06
1	D	175	GLN	OE1-CD-NE2	-8.04	114.56	122.60
1	C	256	ASP	CA-CB-CG	8.03	120.63	112.60
1	D	365	TRP	CG-CD2-CE3	8.03	141.93	133.90
1	A	391	LEU	N-CA-C	-8.00	102.15	111.03
1	A	366	GLU	N-CA-C	-7.99	101.27	111.02
1	D	306	ASP	N-CA-C	-7.99	102.52	111.14
1	D	761	ILE	N-CA-C	-7.99	103.02	110.53
1	B	268	ASP	N-CA-C	-7.97	102.18	111.03
1	D	335	ILE	O-C-N	-7.97	113.92	122.45
1	A	89	PHE	CA-CB-CG	-7.97	105.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	523	SER	CA-CB-OG	7.96	127.03	111.10
1	A	217	ASP	CA-CB-CG	7.96	120.56	112.60
1	D	807	THR	N-CA-CB	-7.95	97.57	110.14
1	D	12	GLN	OE1-CD-NE2	-7.94	114.66	122.60
1	B	270	ASN	O-C-N	-7.94	113.81	122.38
1	B	491	TRP	N-CA-C	7.94	123.00	113.16
1	C	564	ASP	CA-CB-CG	7.93	120.53	112.60
1	B	309	ARG	N-CA-C	-7.93	102.58	111.07
1	D	630	VAL	CB-CA-C	-7.93	101.82	111.97
1	D	236	ASN	N-CA-C	7.91	122.37	112.24
1	B	355	ASP	N-CA-C	7.91	119.54	111.07
1	D	183	LEU	N-CA-C	-7.90	98.11	109.96
1	B	457	ARG	N-CA-C	7.88	120.57	111.11
1	B	339	ASP	O-C-N	-7.87	112.12	122.59
1	C	98	THR	CA-CB-OG1	-7.86	97.81	109.60
1	A	333	VAL	O-C-N	-7.85	114.36	123.00
1	B	274	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	C	556	HIS	CA-CB-CG	7.85	121.65	113.80
1	D	575	ARG	NE-CZ-NH1	7.85	129.35	121.50
1	C	700	ALA	CA-C-O	-7.84	112.62	120.70
1	C	793	ASN	CA-CB-CG	7.83	120.43	112.60
1	C	360	ASP	N-CA-C	-7.83	98.88	110.46
1	D	286	PHE	CA-CB-CG	-7.82	105.98	113.80
1	A	316	PHE	CA-CB-CG	-7.81	105.99	113.80
1	C	696	ASN	CB-CG-ND2	7.81	128.12	116.40
1	A	412	ASN	CA-CB-CG	-7.81	104.79	112.60
1	A	268	ASP	CA-CB-CG	7.80	120.40	112.60
1	C	336	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	C	596	LYS	CA-C-N	-7.78	110.37	121.50
1	C	596	LYS	C-N-CA	-7.78	110.37	121.50
1	D	540	GLU	N-CA-C	-7.77	99.00	111.04
1	C	255	LYS	N-CA-C	7.77	121.76	110.42
1	B	686	ALA	N-CA-C	-7.76	96.28	109.24
1	D	767	HIS	N-CA-C	7.76	124.53	114.75
1	B	644	PHE	CA-CB-CG	-7.75	106.05	113.80
1	B	507	ILE	N-CA-C	7.74	123.68	113.07
1	B	327	ASP	CA-CB-CG	7.73	120.33	112.60
1	C	785	GLU	CB-CG-CD	7.73	125.74	112.60
1	B	127	GLU	CA-CB-CG	7.72	129.54	114.10
1	A	106	ASN	CA-CB-CG	7.72	120.32	112.60
1	D	743	GLU	N-CA-C	7.70	120.42	111.02
1	A	183	LEU	N-CA-C	-7.70	95.98	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	LEU	N-CA-C	7.69	120.79	108.41
1	D	224	MET	CA-C-N	7.69	129.45	119.84
1	D	224	MET	C-N-CA	7.69	129.45	119.84
1	D	326	PHE	CA-CB-CG	-7.69	106.11	113.80
1	C	219	GLN	N-CA-C	-7.68	97.80	110.17
1	B	24	VAL	O-C-N	7.68	129.32	121.87
1	B	145	ASP	CA-CB-CG	7.68	120.28	112.60
1	D	486	ILE	O-C-N	-7.67	114.97	123.03
1	A	348	GLU	CB-CG-CD	7.67	125.63	112.60
1	D	503	ILE	N-CA-CB	-7.67	102.00	110.51
1	B	788	SER	CA-C-O	7.65	128.75	119.49
1	C	513	SER	N-CA-C	-7.64	103.93	113.18
1	D	325	ASN	N-CA-CB	7.64	121.18	110.17
1	C	166	PHE	N-CA-C	7.64	127.07	110.80
1	A	738	LEU	N-CA-C	-7.63	102.56	111.03
1	A	532	ARG	CA-CB-CG	7.62	129.34	114.10
1	D	317	GLY	N-CA-C	-7.62	104.94	114.16
1	A	44	ASN	OD1-CG-ND2	-7.62	114.98	122.60
1	C	699	MET	N-CA-C	-7.62	102.91	111.14
1	B	625	ALA	N-CA-C	7.61	119.66	111.36
1	D	595	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	B	514	ASP	CA-CB-CG	7.59	120.19	112.60
1	C	31	PHE	N-CA-C	-7.59	103.90	113.01
1	C	143	PHE	CA-C-O	-7.59	112.88	120.70
1	A	582	HIS	CA-C-O	-7.59	111.70	120.20
1	A	676	THR	CA-CB-CG2	7.58	123.39	110.50
1	D	181	ASP	N-CA-CB	7.58	119.78	110.53
1	B	275	ILE	N-CA-C	-7.57	102.77	113.07
1	A	421	ASP	O-C-N	7.57	131.83	123.13
1	D	244	TRP	CB-CG-CD1	-7.56	115.55	126.90
1	A	211	GLN	OE1-CD-NE2	-7.56	115.04	122.60
1	C	443	HIS	N-CA-C	-7.56	103.12	111.36
1	A	614	HIS	CA-CB-CG	7.54	121.34	113.80
1	D	572	GLU	CA-CB-CG	-7.54	99.02	114.10
1	A	311	PHE	CA-C-O	-7.53	112.79	121.07
1	C	201	HIS	CA-CB-CG	7.52	121.32	113.80
1	D	782	LYS	N-CA-CB	-7.52	99.03	110.16
1	C	181	ASP	CA-CB-CG	7.51	120.11	112.60
1	D	650	VAL	N-CA-CB	7.51	119.34	110.55
1	D	836	ALA	N-CA-C	7.51	126.40	109.81
1	B	431	VAL	CB-CA-C	-7.50	100.76	111.19
1	B	408	GLN	N-CA-C	-7.50	103.10	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LEU	N-CA-C	7.50	120.88	108.96
1	B	455	VAL	N-CA-C	7.50	120.25	112.83
1	B	723	GLN	CA-CB-CG	-7.49	99.12	114.10
1	A	269	ARG	CA-CB-CG	7.48	129.07	114.10
1	B	424	ARG	N-CA-C	-7.48	103.06	111.07
1	A	571	HIS	CB-CG-CD2	-7.47	121.48	131.20
1	D	281	PRO	CA-C-N	7.47	133.55	121.74
1	D	281	PRO	C-N-CA	7.47	133.55	121.74
1	C	295	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	A	224	MET	CA-C-O	-7.46	113.12	119.76
1	C	131	LEU	N-CA-CB	-7.46	100.97	110.90
1	C	781	VAL	O-C-N	-7.46	113.25	122.57
1	B	771	PHE	N-CA-C	7.45	122.55	113.38
1	C	494	LEU	N-CA-CB	-7.45	99.09	110.20
1	B	553	TYR	CA-CB-CG	7.45	127.31	113.90
1	A	739	ARG	CA-C-O	-7.44	112.93	120.90
1	A	804	ASN	N-CA-C	7.43	121.26	111.75
1	C	785	GLU	N-CA-C	-7.42	103.21	111.82
1	B	250	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	A	377	HIS	CA-CB-CG	7.42	121.22	113.80
1	D	541	ASN	CB-CG-ND2	7.42	127.52	116.40
1	D	341	HIS	O-C-N	-7.41	113.74	120.71
1	D	834	LEU	CA-C-N	7.41	129.11	119.84
1	D	834	LEU	C-N-CA	7.41	129.11	119.84
1	A	557	ILE	CB-CA-C	7.40	120.78	111.15
1	D	630	VAL	N-CA-CB	7.40	119.21	110.55
1	A	92	GLY	CA-C-O	-7.39	112.52	121.83
1	B	467	ILE	CB-CG1-CD1	7.39	129.32	113.80
1	D	450	HIS	CB-CG-ND1	7.38	133.77	122.70
1	A	795	ARG	N-CA-C	-7.38	102.62	111.69
1	D	526	ASP	N-CA-C	7.37	121.19	111.75
1	B	639	ARG	N-CA-CB	-7.37	99.70	110.53
1	D	813	SER	N-CA-C	-7.37	103.18	111.07
1	C	42	ASP	CA-CB-CG	7.37	119.97	112.60
1	D	708	PHE	N-CA-C	7.37	120.61	109.63
1	B	777	TYR	O-C-N	-7.36	114.49	122.07
1	D	80	LYS	O-C-N	7.36	131.70	123.01
1	B	711	PHE	N-CA-C	7.36	117.59	107.73
1	D	268	ASP	N-CA-C	-7.36	103.20	111.07
1	A	727	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	D	32	ASN	N-CA-C	7.35	120.34	111.82
1	C	656	VAL	CA-CB-CG2	-7.34	97.93	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ASP	CA-CB-CG	7.33	119.93	112.60
1	A	405	GLU	CB-CG-CD	7.33	125.06	112.60
1	D	252	PHE	N-CA-C	7.32	122.76	111.56
1	B	642	VAL	CA-C-O	-7.31	112.78	120.39
1	A	505	GLU	CA-CB-CG	7.31	128.72	114.10
1	C	834	LEU	N-CA-C	-7.31	100.86	110.07
1	A	88	GLU	O-C-N	-7.30	115.16	123.40
1	C	274	ASN	CA-CB-CG	7.30	119.90	112.60
1	D	281	PRO	CA-N-CD	-7.29	101.79	112.00
1	C	693	ASP	N-CA-C	7.29	121.12	109.24
1	D	443	HIS	CA-CB-CG	7.29	121.09	113.80
1	D	749	PHE	CA-CB-CG	7.29	121.09	113.80
1	A	502	ILE	CA-C-O	-7.29	113.37	120.95
1	A	739	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	D	639	ARG	CB-CG-CD	7.28	128.05	111.30
1	D	325	ASN	N-CA-C	-7.28	100.24	110.50
1	A	676	THR	N-CA-C	-7.27	104.93	114.31
1	B	597	PHE	CA-CB-CG	-7.26	106.54	113.80
1	D	61	ASP	O-C-N	7.26	129.65	122.09
1	D	595	ASN	CB-CG-ND2	7.26	127.29	116.40
1	A	593	GLU	O-C-N	-7.25	112.98	121.32
1	B	187	ASN	O-C-N	-7.25	115.42	121.44
1	D	769	ASP	CA-CB-CG	7.24	119.84	112.60
1	B	506	ARG	CB-CG-CD	7.24	127.94	111.30
1	C	12	GLN	OE1-CD-NE2	-7.24	115.36	122.60
1	A	449	SER	CA-CB-OG	-7.23	96.63	111.10
1	C	165	ILE	N-CA-C	-7.23	94.30	109.34
1	A	450	HIS	CB-CG-ND1	7.22	133.53	122.70
1	B	652	LEU	N-CA-C	-7.22	103.08	112.68
1	A	303	THR	CA-C-O	-7.22	109.41	120.16
1	A	45	VAL	N-CA-C	7.21	119.97	112.83
1	C	723	GLN	OE1-CD-NE2	-7.21	115.39	122.60
1	A	570	ILE	O-C-N	-7.20	113.58	122.57
1	B	162	GLU	N-CA-C	-7.19	103.52	111.36
1	C	597	PHE	O-C-N	7.19	131.46	123.04
1	D	274	ASN	N-CA-CB	-7.19	100.14	110.57
1	A	143	PHE	CA-C-O	-7.19	112.93	120.55
1	A	191	LYS	CA-C-O	7.18	127.94	120.40
1	D	166	PHE	N-CA-C	7.18	126.09	110.80
1	A	740	GLN	CG-CD-NE2	7.17	127.16	116.40
1	C	257	PHE	CA-CB-CG	-7.17	106.63	113.80
1	A	582	HIS	CB-CG-CD2	-7.17	121.88	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	GLU	N-CA-C	-7.17	103.40	111.14
1	B	540	GLU	CA-CB-CG	7.17	128.43	114.10
1	A	810	LYS	CA-CB-CG	7.16	128.43	114.10
1	D	78	ASP	N-CA-C	7.16	125.63	109.81
1	D	97	ASN	N-CA-C	-7.16	103.41	111.14
1	A	500	ALA	O-C-N	7.15	129.44	122.07
1	C	730	GLU	N-CA-C	-7.15	95.56	110.80
1	C	807	THR	CB-CA-C	7.14	120.07	109.29
1	D	626	ILE	CA-C-N	7.13	127.86	119.94
1	D	626	ILE	C-N-CA	7.13	127.86	119.94
1	D	830	SER	N-CA-C	7.13	120.34	110.35
1	B	93	ARG	N-CA-C	7.13	120.33	110.35
1	B	390	HIS	CA-CB-CG	7.13	120.93	113.80
1	C	16	ARG	N-CA-C	7.13	125.98	110.80
1	A	197	THR	N-CA-CB	-7.12	100.17	110.36
1	B	623	ILE	N-CA-CB	7.12	118.41	110.51
1	B	673	ALA	CA-C-O	-7.12	113.57	120.90
1	D	208	HIS	CB-CA-C	-7.12	98.13	109.80
1	A	323	ARG	CA-CB-CG	7.11	128.33	114.10
1	C	789	ALA	O-C-N	7.11	129.69	122.08
1	D	379	VAL	N-CA-CB	-7.11	101.26	112.07
1	B	325	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	D	272	ALA	N-CA-C	-7.11	95.67	110.80
1	D	324	THR	N-CA-C	-7.11	101.88	111.54
1	A	140	ALA	N-CA-C	-7.10	103.15	111.03
1	B	341	HIS	CB-CG-CD2	-7.10	121.97	131.20
1	B	559	PRO	N-CA-C	-7.10	105.68	114.20
1	A	761	ILE	CB-CG1-CD1	-7.09	98.91	113.80
1	C	494	LEU	N-CA-C	7.09	120.41	111.69
1	D	283	ASP	CB-CA-C	7.09	121.79	111.73
1	C	338	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	C	525	VAL	CB-CA-C	-7.08	102.76	112.04
1	A	648	TYR	CA-C-O	-7.08	113.40	121.19
1	A	543	LEU	N-CA-C	-7.08	104.45	113.23
1	B	200	VAL	N-CA-C	-7.08	97.32	108.86
1	D	505	GLU	N-CA-C	-7.08	103.57	111.71
1	A	696	ASN	CA-CB-CG	-7.08	105.52	112.60
1	A	385	GLU	N-CA-C	7.08	120.65	110.10
1	C	388	PRO	CA-C-O	-7.08	112.99	121.48
1	D	434	GLY	O-C-N	7.08	131.90	122.70
1	A	352	VAL	CA-C-O	-7.07	113.00	120.57
1	A	716	GLU	CB-CG-CD	7.07	124.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	LEU	N-CA-C	7.07	119.84	111.71
1	D	622	LEU	N-CA-C	-7.07	103.51	111.07
1	A	627	GLY	CA-C-O	-7.06	113.77	121.05
1	A	568	LYS	CB-CG-CD	7.06	127.54	111.30
1	D	824	ILE	CA-CB-CG2	-7.06	98.49	110.50
1	A	263	ILE	CA-CB-CG1	7.06	122.40	110.40
1	B	224	MET	CA-CB-CG	7.06	128.21	114.10
1	A	485	GLY	O-C-N	-7.05	115.97	123.45
1	A	645	LEU	CA-C-O	7.05	127.91	120.36
1	A	509	GLU	CB-CG-CD	7.05	124.58	112.60
1	C	339	ASP	CA-CB-CG	-7.03	105.57	112.60
1	D	97	ASN	CA-C-O	-7.03	113.46	120.70
1	A	429	SER	CA-CB-OG	7.03	125.16	111.10
1	B	754	GLN	CA-CB-CG	7.03	128.16	114.10
1	C	315	LYS	CA-CB-CG	-7.03	100.05	114.10
1	D	372	CYS	N-CA-C	7.02	121.48	110.32
1	A	42	ASP	CA-C-N	7.02	130.01	120.54
1	A	42	ASP	C-N-CA	7.02	130.01	120.54
1	C	727	ASN	CB-CG-ND2	7.02	126.93	116.40
1	C	744	GLN	CA-CB-CG	-7.02	100.07	114.10
1	B	263	ILE	CA-C-O	7.02	129.55	120.78
1	B	666	ILE	N-CA-C	7.01	123.93	109.34
1	A	583	VAL	N-CA-CB	7.01	120.08	110.54
1	B	47	THR	N-CA-CB	-7.01	100.11	109.78
1	D	808	SER	O-C-N	-7.01	113.27	122.59
1	C	252	PHE	N-CA-C	7.01	120.93	112.38
1	C	221	VAL	O-C-N	-7.00	113.30	122.47
1	C	595	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	D	807	THR	N-CA-C	7.00	120.71	111.75
1	C	455	VAL	CB-CA-C	6.99	122.76	111.29
1	A	554	LYS	N-CA-C	6.99	119.79	109.24
1	D	18	LEU	N-CA-C	6.99	121.66	113.20
1	A	495	CYS	CA-CB-SG	6.98	130.45	114.40
1	D	781	VAL	O-C-N	6.98	128.92	121.94
1	A	253	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	C	629	VAL	CA-CB-CG2	-6.98	98.53	110.40
1	D	676	THR	N-CA-CB	-6.97	101.32	110.59
1	A	238	VAL	O-C-N	-6.97	115.94	123.18
1	B	545	PHE	CA-CB-CG	-6.97	106.83	113.80
1	D	684	ASN	CA-C-O	6.96	127.86	119.78
1	D	405	GLU	CA-CB-CG	6.96	128.01	114.10
1	C	329	PHE	CA-CB-CG	6.95	120.75	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ARG	CB-CG-CD	6.95	127.28	111.30
1	C	268	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	402	ILE	N-CA-CB	-6.95	103.05	110.62
1	A	676	THR	CB-CA-C	6.95	120.69	109.02
1	C	834	LEU	CB-CA-C	6.95	118.66	108.87
1	B	447	ALA	N-CA-C	6.94	119.87	111.82
1	B	62	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	C	26	GLU	CA-C-O	-6.92	113.62	120.89
1	B	566	GLN	N-CA-C	-6.91	95.59	107.61
1	A	18	LEU	O-C-N	6.91	131.07	123.13
1	C	510	GLU	N-CA-C	-6.91	96.09	110.80
1	B	583	VAL	CB-CA-C	-6.90	103.04	111.88
1	C	355	ASP	CA-CB-CG	6.90	119.50	112.60
1	B	341	HIS	O-C-N	-6.90	113.38	121.32
1	A	234	ARG	N-CA-C	6.90	120.68	111.30
1	C	350	MET	CG-SD-CE	-6.89	85.73	100.90
1	D	223	ALA	CA-C-O	-6.89	113.16	120.40
1	C	810	LYS	CA-CB-CG	6.89	127.89	114.10
1	D	263	ILE	O-C-N	6.89	130.36	122.99
1	B	49	ARG	CA-CB-CG	6.88	127.86	114.10
1	D	745	LEU	N-CA-CB	6.87	122.11	110.49
1	D	644	PHE	CA-CB-CG	-6.87	106.94	113.80
1	A	390	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	A	45	VAL	CA-CB-CG2	-6.86	98.74	110.40
1	C	550	GLU	CB-CG-CD	6.85	124.25	112.60
1	D	437	LYS	CB-CG-CD	-6.85	95.54	111.30
1	C	727	ASN	OD1-CG-ND2	-6.85	115.75	122.60
1	D	505	GLU	N-CA-CB	6.85	120.77	110.22
1	B	250	ASN	O-C-N	6.85	129.90	122.64
1	C	50	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	73	HIS	CB-CG-CD2	-6.85	122.30	131.20
1	B	815	ARG	N-CA-C	-6.85	103.05	111.40
1	D	496	ASN	CB-CG-ND2	6.84	126.67	116.40
1	B	552	GLU	CA-C-N	6.84	134.61	121.54
1	B	552	GLU	C-N-CA	6.84	134.61	121.54
1	A	313	SER	N-CA-C	6.84	122.61	113.72
1	B	656	VAL	N-CA-C	6.84	123.57	109.34
1	D	233	TYR	O-C-N	6.84	131.00	123.13
1	D	211	GLN	CG-CD-NE2	6.83	126.65	116.40
1	B	365	TRP	CG-CD2-CE3	6.83	140.73	133.90
1	A	317	GLY	N-CA-C	-6.83	104.54	112.73
1	A	366	GLU	CA-C-O	-6.83	113.56	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	HIS	CB-CG-CD2	-6.82	122.33	131.20
1	D	533	ASP	CA-C-O	6.82	127.85	120.55
1	B	325	ASN	N-CA-C	-6.82	100.19	110.28
1	B	28	LYS	CB-CG-CD	-6.82	95.62	111.30
1	D	745	LEU	CB-CA-C	-6.82	96.86	110.42
1	A	280	TYR	CA-C-N	6.81	128.36	119.84
1	A	280	TYR	C-N-CA	6.81	128.36	119.84
1	A	243	LEU	N-CA-CB	-6.81	98.67	111.00
1	C	114	GLN	CA-CB-CG	-6.81	100.48	114.10
1	C	316	PHE	N-CA-C	6.80	121.59	113.16
1	A	823	GLU	N-CA-C	6.80	120.67	112.38
1	B	639	ARG	CB-CA-C	6.80	121.66	109.29
1	A	572	GLU	O-C-N	-6.79	115.03	122.09
1	B	210	SER	CA-CB-OG	6.79	124.68	111.10
1	A	263	ILE	CA-CB-CG2	-6.79	98.96	110.50
1	C	263	ILE	CA-CB-CG2	-6.78	98.97	110.50
1	B	604	MET	O-C-N	-6.78	115.38	123.31
1	C	440	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	283	ASP	O-C-N	6.78	131.60	122.59
1	B	178	GLU	O-C-N	-6.77	115.07	122.79
1	C	45	VAL	N-CA-CB	-6.77	97.41	111.76
1	C	244	TRP	CG-CD2-CE3	6.77	140.67	133.90
1	C	724	ARG	CA-CB-CG	6.77	127.64	114.10
1	B	278	VAL	N-CA-CB	-6.76	102.87	110.99
1	C	663	SER	N-CA-C	-6.76	99.20	109.95
1	B	283	ASP	O-C-N	6.76	131.58	122.59
1	C	280	TYR	CA-C-N	6.76	128.29	119.84
1	C	280	TYR	C-N-CA	6.76	128.29	119.84
1	C	553	TYR	CA-CB-CG	6.76	126.07	113.90
1	D	187	ASN	CA-C-N	6.76	126.72	119.28
1	D	187	ASN	C-N-CA	6.76	126.72	119.28
1	A	677	GLY	O-C-N	6.75	128.67	122.19
1	B	602	THR	N-CA-C	-6.75	97.36	108.76
1	D	650	VAL	N-CA-C	-6.75	103.94	110.42
1	A	684	ASN	N-CA-C	6.74	121.58	112.88
1	C	480	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	B	540	GLU	N-CA-C	-6.74	103.02	111.11
1	A	555	VAL	O-C-N	-6.73	114.15	122.57
1	D	139	LEU	CA-C-O	-6.73	113.75	120.82
1	A	631	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	740	GLN	CB-CG-CD	6.73	124.04	112.60
1	A	807	THR	N-CA-C	6.73	121.08	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	ASN	CA-CB-CG	6.73	119.33	112.60
1	C	571	HIS	CB-CG-ND1	6.72	132.78	122.70
1	A	566	GLN	CA-C-O	-6.71	113.08	120.33
1	D	812	SER	CA-CB-OG	-6.71	97.67	111.10
1	D	320	ASP	CA-CB-CG	6.71	119.31	112.60
1	D	628	ASP	N-CA-C	-6.71	103.66	110.97
1	A	498	GLY	CA-C-O	-6.71	113.55	120.66
1	B	814	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	47	THR	CA-C-O	-6.70	113.73	120.63
1	A	805	ILE	CA-C-O	-6.70	113.03	120.46
1	B	219	GLN	O-C-N	-6.70	115.39	123.16
1	B	516	ASP	CA-CB-CG	6.70	119.30	112.60
1	B	433	GLU	CA-CB-CG	6.69	127.49	114.10
1	B	658	PRO	CB-CA-C	6.69	121.15	111.04
1	A	208	HIS	N-CA-C	6.69	120.34	108.24
1	C	370	LYS	CB-CG-CD	-6.69	95.92	111.30
1	C	274	ASN	N-CA-C	6.68	125.03	110.80
1	A	664	GLU	N-CA-CB	-6.68	100.96	110.58
1	A	514	ASP	CA-C-O	6.68	126.83	120.09
1	C	390	HIS	CB-CG-CD2	-6.67	122.52	131.20
1	A	37	PHE	N-CA-C	6.67	119.38	111.71
1	D	531	ILE	O-C-N	-6.67	115.37	121.91
1	A	248	ALA	CA-C-O	-6.67	113.43	120.70
1	A	491	TRP	CG-CD2-CE3	6.67	140.57	133.90
1	A	239	ASN	OD1-CG-ND2	-6.67	115.94	122.60
1	A	421	ASP	CA-C-O	6.67	127.89	120.43
1	A	554	LYS	CA-C-O	-6.65	113.88	121.40
1	B	715	VAL	CA-C-O	-6.65	114.03	120.95
1	C	375	THR	O-C-N	-6.65	114.58	123.23
1	C	292	ARG	CA-CB-CG	-6.65	100.80	114.10
1	C	662	LEU	O-C-N	-6.65	115.46	123.10
1	A	93	ARG	O-C-N	-6.64	115.42	123.19
1	A	480	GLN	CG-CD-NE2	6.64	126.37	116.40
1	C	177	GLU	CA-CB-CG	6.64	127.39	114.10
1	D	560	ASN	CB-CG-ND2	6.63	126.35	116.40
1	B	131	LEU	N-CA-CB	-6.63	96.72	111.10
1	B	349	LEU	N-CA-C	-6.63	103.98	111.07
1	D	292	ARG	CA-CB-CG	-6.63	100.85	114.10
1	A	405	GLU	N-CA-C	-6.62	104.68	112.89
1	B	630	VAL	O-C-N	-6.62	115.45	121.87
1	A	646	GLU	CA-C-O	6.62	128.02	120.54
1	C	610	ALA	N-CA-CB	6.62	122.15	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	732	TYR	O-C-N	6.62	129.13	122.12
1	B	623	ILE	CB-CA-C	-6.62	103.41	111.88
1	C	507	ILE	N-CA-C	6.62	123.10	109.34
1	A	698	GLU	CA-CB-CG	-6.61	100.87	114.10
1	D	688	THR	N-CA-C	6.61	117.86	108.54
1	C	48	PRO	CA-N-CD	-6.61	102.75	112.00
1	A	646	GLU	N-CA-C	6.61	120.43	109.46
1	A	814	ASP	CA-CB-CG	6.61	119.20	112.60
1	B	196	PHE	N-CA-C	6.60	121.03	112.92
1	C	390	HIS	CB-CG-ND1	6.60	132.60	122.70
1	D	792	LYS	N-CA-CB	6.59	120.08	110.26
1	D	31	PHE	N-CA-C	-6.58	104.18	111.82
1	C	716	GLU	CB-CG-CD	6.58	123.79	112.60
1	D	323	ARG	CA-CB-CG	6.57	127.25	114.10
1	C	52	TYR	N-CA-C	-6.57	104.16	111.71
1	D	643	ILE	N-CA-CB	-6.57	103.10	111.64
1	D	509	GLU	O-C-N	6.57	131.32	122.59
1	C	613	TYR	N-CA-C	-6.56	97.91	109.06
1	A	331	ASP	CB-CA-C	-6.56	100.58	110.88
1	C	532	ARG	CA-CB-CG	6.56	127.22	114.10
1	D	664	GLU	O-C-N	-6.56	114.70	122.96
1	B	529	ALA	N-CA-C	-6.56	100.88	111.04
1	C	554	LYS	N-CA-C	6.55	120.20	109.06
1	D	533	ASP	N-CA-CB	6.55	119.82	110.13
1	C	676	THR	N-CA-CB	-6.54	100.92	110.47
1	A	405	GLU	CA-CB-CG	6.54	127.18	114.10
1	B	114	GLN	N-CA-C	-6.54	104.23	111.36
1	D	263	ILE	CA-CB-CG2	-6.54	99.38	110.50
1	C	778	GLU	N-CA-C	6.54	118.28	111.03
1	C	300	VAL	CA-C-O	-6.53	113.61	121.18
1	B	597	PHE	CB-CA-C	-6.53	99.87	110.77
1	C	552	GLU	CA-C-N	6.52	132.95	121.80
1	C	552	GLU	C-N-CA	6.52	132.95	121.80
1	D	123	GLU	O-C-N	-6.52	115.21	122.12
1	B	727	ASN	CB-CG-ND2	6.51	126.17	116.40
1	D	336	GLN	N-CA-C	6.51	120.23	107.98
1	B	837	PRO	CA-C-N	-6.51	113.11	122.36
1	B	837	PRO	C-N-CA	-6.51	113.11	122.36
1	D	506	ARG	CB-CG-CD	6.51	126.27	111.30
1	D	316	PHE	CA-CB-CG	-6.51	107.29	113.80
1	B	634	PRO	N-CA-C	6.51	122.01	114.20
1	D	744	GLN	N-CA-C	-6.50	104.11	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	ARG	CA-CB-CG	6.50	127.09	114.10
1	B	555	VAL	CA-CB-CG1	-6.50	99.36	110.40
1	C	323	ARG	CA-CB-CG	6.49	127.08	114.10
1	A	211	GLN	CG-CD-NE2	6.49	126.13	116.40
1	D	365	TRP	CB-CG-CD1	-6.48	117.17	126.90
1	B	383	ALA	N-CA-C	6.48	120.39	112.23
1	B	626	ILE	N-CA-C	-6.48	103.49	110.23
1	B	450	HIS	CA-CB-CG	6.47	120.27	113.80
1	D	411	LEU	N-CA-C	-6.47	104.31	111.82
1	C	762	VAL	N-CA-C	-6.47	103.50	110.23
1	C	452	VAL	N-CA-C	-6.46	98.73	108.17
1	B	16	ARG	N-CA-C	6.46	124.56	110.80
1	D	295	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	B	571	HIS	CB-CG-ND1	6.45	132.37	122.70
1	C	47	THR	CA-C-N	6.45	127.90	119.84
1	C	47	THR	C-N-CA	6.45	127.90	119.84
1	C	53	PHE	CA-CB-CG	-6.45	107.35	113.80
1	B	479	PHE	CA-CB-CG	-6.45	107.36	113.80
1	D	412	ASN	CA-CB-CG	-6.45	106.16	112.60
1	D	451	ALA	N-CA-C	6.44	118.82	107.61
1	D	754	GLN	CB-CG-CD	-6.44	101.65	112.60
1	A	722	ASP	N-CA-C	-6.43	104.19	111.14
1	C	118	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	255	LYS	O-C-N	6.43	131.15	122.59
1	B	646	GLU	N-CA-C	6.43	120.00	110.48
1	B	808	SER	N-CA-C	6.43	124.49	110.80
1	C	628	ASP	CA-CB-CG	6.43	119.03	112.60
1	D	322	VAL	CA-C-N	6.43	133.81	121.54
1	D	322	VAL	C-N-CA	6.43	133.81	121.54
1	A	455	VAL	N-CA-CB	-6.42	100.63	111.23
1	A	717	ASP	CA-CB-CG	6.42	119.03	112.60
1	B	464	LYS	CB-CG-CD	6.42	126.07	111.30
1	B	575	ARG	N-CA-C	6.42	120.43	112.47
1	D	162	GLU	CA-C-O	6.42	127.23	120.42
1	B	426	ARG	CA-CB-CG	6.42	126.94	114.10
1	D	446	ILE	O-C-N	-6.41	115.61	121.89
1	A	561	SER	N-CA-C	6.41	118.99	110.53
1	A	31	PHE	N-CA-C	-6.41	103.81	111.69
1	A	219	GLN	N-CA-C	-6.41	100.08	110.20
1	C	186	GLY	O-C-N	6.41	129.65	123.05
1	C	761	ILE	CA-C-O	-6.41	113.96	120.69
1	D	790	LEU	N-CA-C	6.41	119.95	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	C	32	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	A	466	THR	CA-C-N	6.39	133.48	121.97
1	A	466	THR	C-N-CA	6.39	133.48	121.97
1	A	649	ARG	CG-CD-NE	-6.39	97.94	112.00
1	D	181	ASP	CB-CA-C	-6.39	102.53	112.12
1	A	741	ILE	CA-C-O	-6.39	113.36	120.96
1	C	421	ASP	CA-CB-CG	6.39	118.99	112.60
1	D	28	LYS	CA-CB-CG	-6.39	101.33	114.10
1	D	730	GLU	N-CA-C	-6.39	97.20	110.80
1	A	205	ARG	CA-CB-CG	6.38	126.86	114.10
1	B	275	ILE	CA-CB-CG2	-6.38	99.66	110.50
1	A	149	THR	N-CA-CB	-6.38	99.71	110.49
1	C	475	GLU	N-CA-C	6.38	118.80	109.30
1	A	382	GLU	CA-CB-CG	6.37	126.85	114.10
1	B	350	MET	N-CA-C	6.37	120.16	112.38
1	D	73	HIS	CA-CB-CG	6.37	120.17	113.80
1	A	602	THR	N-CA-C	-6.37	96.88	108.02
1	C	731	TYR	N-CA-C	-6.37	104.26	111.14
1	D	502	ILE	CB-CA-C	-6.37	103.70	112.04
1	D	502	ILE	N-CA-C	6.37	117.88	110.62
1	B	714	ARG	N-CA-C	-6.36	101.37	110.59
1	C	292	ARG	O-C-N	6.36	128.62	122.07
1	A	268	ASP	N-CA-C	-6.35	104.27	111.07
1	B	385	GLU	N-CA-C	6.35	119.56	110.10
1	C	486	ILE	CA-CB-CG1	-6.35	99.60	110.40
1	C	196	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	255	LYS	CA-C-N	6.33	133.64	121.54
1	A	255	LYS	C-N-CA	6.33	133.64	121.54
1	B	273	GLU	O-C-N	-6.33	115.41	122.12
1	D	778	GLU	CA-C-O	-6.33	114.12	120.90
1	A	275	ILE	N-CA-C	-6.33	102.96	111.44
1	C	115	LEU	N-CA-C	-6.32	105.67	113.19
1	B	636	VAL	N-CA-CB	-6.32	103.49	110.51
1	C	173	GLY	N-CA-C	-6.32	106.40	114.37
1	C	836	ALA	N-CA-C	6.32	123.78	109.81
1	A	716	GLU	CA-CB-CG	6.32	126.74	114.10
1	B	72	GLN	CA-CB-CG	6.32	126.74	114.10
1	C	439	ILE	N-CA-C	-6.32	99.37	108.53
1	A	677	GLY	CA-C-N	6.32	131.23	121.19
1	A	677	GLY	C-N-CA	6.32	131.23	121.19
1	B	166	PHE	N-CA-C	6.31	124.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	286	PHE	CA-C-N	6.31	133.60	121.54
1	D	286	PHE	C-N-CA	6.31	133.60	121.54
1	C	517	GLN	CA-CB-CG	-6.31	101.47	114.10
1	C	336	GLN	CG-CD-NE2	6.31	125.86	116.40
1	C	586	LEU	O-C-N	6.31	128.81	122.12
1	D	657	ILE	CA-CB-CG1	-6.30	99.68	110.40
1	D	457	ARG	CA-CB-CG	-6.30	101.49	114.10
1	A	80	LYS	N-CA-C	-6.29	101.16	110.48
1	A	259	VAL	O-C-N	6.29	129.71	122.97
1	A	286	PHE	CA-C-N	6.29	133.56	121.54
1	A	286	PHE	C-N-CA	6.29	133.56	121.54
1	B	597	PHE	N-CA-CB	6.29	120.00	109.94
1	C	72	GLN	CG-CD-NE2	6.29	125.83	116.40
1	B	269	ARG	N-CA-C	6.29	119.80	111.75
1	D	527	ASP	CA-C-O	6.28	127.58	120.80
1	A	808	SER	N-CA-C	6.27	120.50	112.34
1	A	666	ILE	N-CA-C	6.27	122.38	109.34
1	B	292	ARG	CA-C-O	-6.27	114.24	120.82
1	A	300	VAL	CA-CB-CG2	-6.27	99.74	110.40
1	B	542	LYS	CB-CG-CD	6.27	125.71	111.30
1	D	287	GLU	CB-CA-C	6.27	122.89	110.42
1	C	37	PHE	N-CA-C	6.26	124.14	110.80
1	B	167	ASN	CA-CB-CG	6.26	118.86	112.60
1	C	555	VAL	CA-CB-CG1	-6.25	99.77	110.40
1	D	424	ARG	CA-CB-CG	6.25	126.61	114.10
1	C	779	GLU	CA-CB-CG	-6.25	101.60	114.10
1	A	441	MET	CA-C-O	-6.25	111.93	119.49
1	B	78	ASP	CA-C-O	6.24	125.29	120.48
1	D	417	ALA	N-CA-C	6.24	117.88	111.14
1	C	226	TYR	O-C-N	-6.24	116.01	123.31
1	D	253	ASN	CB-CG-ND2	6.24	125.76	116.40
1	D	219	GLN	N-CA-C	-6.24	102.29	110.53
1	D	309	ARG	CA-CB-CG	6.24	126.58	114.10
1	A	534	VAL	O-C-N	-6.24	115.70	121.94
1	C	629	VAL	CA-CB-CG1	6.24	121.00	110.40
1	C	811	PHE	CA-C-N	-6.24	113.89	122.93
1	C	811	PHE	C-N-CA	-6.24	113.89	122.93
1	A	564	ASP	CA-C-O	-6.23	114.25	120.98
1	A	622	LEU	N-CA-C	-6.23	104.40	111.07
1	D	177	GLU	N-CA-C	6.23	118.85	108.20
1	D	253	ASN	CA-CB-CG	6.23	118.83	112.60
1	D	569	ARG	CA-C-O	-6.23	114.18	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	C	368	THR	CA-CB-OG1	-6.22	100.27	109.60
1	D	529	ALA	CA-C-O	-6.22	113.89	120.55
1	A	494	LEU	CA-C-O	-6.22	112.41	120.00
1	C	610	ALA	N-CA-C	-6.22	96.06	109.81
1	B	357	GLU	N-CA-C	-6.21	97.56	110.80
1	A	390	HIS	CA-CB-CG	6.21	120.01	113.80
1	C	360	ASP	O-C-N	6.21	130.04	122.84
1	D	565	VAL	N-CA-CB	6.21	119.70	111.25
1	C	533	ASP	N-CA-C	-6.21	104.14	111.03
1	B	355	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	71	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	B	42	ASP	CA-C-N	6.20	128.59	120.28
1	B	42	ASP	C-N-CA	6.20	128.59	120.28
1	A	789	ALA	CA-C-O	-6.20	114.32	120.70
1	C	258	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	D	57	HIS	CA-C-O	-6.20	113.85	120.42
1	B	25	THR	N-CA-C	-6.20	104.63	111.82
1	B	676	THR	CB-CA-C	6.20	121.14	110.23
1	A	664	GLU	N-CA-C	6.19	119.30	108.52
1	B	109	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	221	VAL	N-CA-C	-6.19	99.45	108.11
1	B	201	HIS	CA-CB-CG	6.18	119.98	113.80
1	A	325	ASN	CA-C-O	6.18	128.10	121.05
1	A	763	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	C	630	VAL	CG1-CB-CG2	-6.18	97.20	110.80
1	C	200	VAL	CA-C-O	6.18	126.36	120.31
1	A	217	ASP	N-CA-C	6.17	120.17	111.52
1	A	196	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	263	ILE	CA-C-O	6.17	128.50	120.78
1	A	436	VAL	O-C-N	-6.17	115.93	123.03
1	B	181	ASP	CA-CB-CG	6.17	118.77	112.60
1	D	649	ARG	CB-CG-CD	6.17	125.49	111.30
1	C	250	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	D	399	HIS	CA-C-N	6.17	128.46	120.44
1	D	399	HIS	C-N-CA	6.17	128.46	120.44
1	C	237	VAL	CA-CB-CG1	-6.16	99.93	110.40
1	D	244	TRP	CE2-CD2-CG	-6.16	99.81	107.20
1	A	356	LEU	N-CA-C	6.16	117.99	111.28
1	B	72	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	B	165	ILE	N-CA-C	-6.15	96.54	109.34
1	A	343	SER	CA-CB-OG	6.15	123.40	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	820	TYR	N-CA-C	-6.15	104.50	111.14
1	C	286	PHE	CA-C-N	6.15	133.28	121.54
1	C	286	PHE	C-N-CA	6.15	133.28	121.54
1	C	381	PRO	N-CA-C	6.15	125.13	112.47
1	C	760	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	32	ASN	N-CA-C	6.15	118.06	111.36
1	D	332	LYS	CB-CG-CD	6.15	125.44	111.30
1	A	64	VAL	CA-C-O	-6.14	114.34	120.85
1	A	167	ASN	N-CA-C	6.14	120.09	110.32
1	A	558	ASN	CA-CB-CG	6.14	118.74	112.60
1	C	262	TYR	CA-C-O	6.14	128.09	120.54
1	D	111	ALA	CA-C-O	-6.14	114.04	120.92
1	A	267	LEU	CA-C-O	-6.14	113.91	120.42
1	B	514	ASP	CA-C-O	6.14	127.08	120.63
1	B	671	THR	N-CA-CB	6.14	118.75	110.59
1	A	408	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	B	347	PRO	CA-C-O	-6.14	110.36	120.05
1	B	720	ARG	CB-CG-CD	6.14	125.41	111.30
1	C	358	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	D	210	SER	N-CA-C	6.13	117.66	110.97
1	D	454	GLY	N-CA-C	-6.13	102.72	112.66
1	D	189	TRP	CE2-CD2-CE3	6.13	124.93	118.80
1	C	307	ILE	CA-C-O	-6.13	113.12	120.78
1	C	799	ARG	N-CA-C	-6.13	104.51	112.23
1	C	440	ASN	CB-CG-ND2	6.12	125.59	116.40
1	D	808	SER	N-CA-C	6.12	123.84	110.80
1	D	181	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	32	ASN	CA-CB-CG	-6.12	106.48	112.60
1	B	436	VAL	CA-CB-CG2	-6.12	100.00	110.40
1	C	224	MET	CA-C-N	6.12	126.63	120.14
1	C	224	MET	C-N-CA	6.12	126.63	120.14
1	D	583	VAL	CA-CB-CG2	-6.12	100.00	110.40
1	C	146	SER	N-CA-C	-6.11	105.78	113.18
1	D	88	GLU	N-CA-C	-6.10	97.80	110.80
1	C	718	VAL	O-C-N	6.10	129.83	121.90
1	D	335	ILE	N-CA-C	6.10	116.03	107.37
1	A	160	ARG	CB-CG-CD	-6.09	97.28	111.30
1	A	177	GLU	O-C-N	-6.09	115.19	122.63
1	B	341	HIS	CB-CG-ND1	6.09	131.84	122.70
1	D	647	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	B	52	TYR	N-CA-C	-6.08	104.34	110.97
1	A	11	LYS	N-CA-C	6.08	119.96	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	HIS	CB-CG-ND1	6.08	131.82	122.70
1	A	558	ASN	CA-C-N	6.08	127.44	119.84
1	A	558	ASN	C-N-CA	6.08	127.44	119.84
1	C	696	ASN	CA-C-O	-6.08	114.07	120.63
1	A	341	HIS	CB-CG-ND1	6.07	131.81	122.70
1	C	642	VAL	N-CA-C	-6.07	99.41	108.46
1	A	709	PHE	N-CA-C	6.07	119.12	110.68
1	A	693	ASP	CA-CB-CG	6.07	118.67	112.60
1	D	95	LEU	CA-C-O	-6.07	111.83	120.51
1	D	112	THR	CA-C-N	6.07	128.41	120.28
1	D	112	THR	C-N-CA	6.07	128.41	120.28
1	A	740	GLN	CA-CB-CG	6.06	126.22	114.10
1	B	275	ILE	CA-CB-CG1	6.06	120.70	110.40
1	D	650	VAL	CA-C-O	-6.06	114.75	121.17
1	A	52	TYR	N-CA-C	-6.06	104.60	111.14
1	A	804	ASN	CB-CA-C	-6.06	98.71	110.46
1	B	405	GLU	CB-CG-CD	6.06	122.90	112.60
1	C	771	PHE	CA-CB-CG	-6.05	107.75	113.80
1	C	807	THR	CA-C-N	6.05	129.00	120.28
1	C	807	THR	C-N-CA	6.05	129.00	120.28
1	C	275	ILE	N-CA-C	-6.05	103.52	111.09
1	C	828	GLU	O-C-N	-6.05	115.50	121.19
1	A	45	VAL	CA-CB-CG1	6.05	120.69	110.40
1	C	657	ILE	CA-C-N	6.05	125.93	119.28
1	C	657	ILE	C-N-CA	6.05	125.93	119.28
1	A	260	GLY	O-C-N	6.05	130.56	122.70
1	A	320	ASP	CA-C-N	6.05	127.40	119.84
1	A	320	ASP	C-N-CA	6.05	127.40	119.84
1	D	804	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	C	290	GLU	O-C-N	-6.04	114.53	122.39
1	B	126	GLU	N-CA-C	-6.04	101.54	110.48
1	C	553	TYR	N-CA-C	-6.04	99.78	108.60
1	D	359	LEU	N-CA-C	-6.04	100.96	109.96
1	D	814	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	375	THR	CA-CB-OG1	-6.04	100.54	109.60
1	D	215	TRP	N-CA-C	-6.04	94.45	107.49
1	D	665	GLN	OE1-CD-NE2	-6.04	116.56	122.60
1	D	666	ILE	O-C-N	-6.04	115.02	122.57
1	D	679	MET	CG-SD-CE	-6.04	87.62	100.90
1	A	831	ARG	N-CA-C	-6.04	97.94	110.80
1	C	804	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	325	ASN	CA-CB-CG	6.03	118.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	A	639	ARG	N-CA-CB	-6.03	100.38	110.39
1	B	491	TRP	CB-CG-CD1	-6.03	117.85	126.90
1	B	214	LYS	N-CA-C	-6.03	99.97	109.50
1	B	800	MET	CA-CB-CG	6.03	126.16	114.10
1	D	211	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	C	82	ILE	N-CA-CB	-6.03	103.76	110.99
1	A	257	PHE	O-C-N	6.02	130.67	123.33
1	C	567	VAL	CA-C-O	6.02	128.30	120.78
1	C	111	ALA	CA-C-O	-6.02	114.45	121.07
1	C	316	PHE	O-C-N	-6.02	114.07	122.37
1	D	575	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	D	810	LYS	O-C-N	-6.01	114.16	122.46
1	B	412	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	C	260	GLY	N-CA-C	-6.01	98.94	113.18
1	C	744	GLN	O-C-N	6.00	128.48	122.12
1	C	145	ASP	CA-C-O	5.99	126.89	120.24
1	D	835	PRO	N-CA-C	5.99	124.81	112.47
1	D	246	ALA	CA-C-O	5.99	127.81	120.92
1	A	836	ALA	N-CA-C	5.99	123.04	109.81
1	D	614	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	A	274	ASN	CA-C-O	5.99	127.82	119.80
1	C	45	VAL	CA-CB-CG2	-5.99	100.23	110.40
1	D	733	ASP	CA-C-O	-5.98	113.60	120.24
1	D	689	ILE	N-CA-C	5.98	117.01	108.93
1	B	49	ARG	N-CA-C	-5.98	104.09	111.33
1	D	249	PRO	N-CA-C	-5.98	101.27	110.95
1	C	11	LYS	N-CA-C	5.97	118.58	111.71
1	C	645	LEU	CA-C-O	5.97	127.73	120.62
1	A	780	TYR	N-CA-C	-5.97	104.69	111.14
1	C	566	GLN	CB-CG-CD	5.97	122.75	112.60
1	C	443	HIS	CA-CB-CG	5.97	119.77	113.80
1	B	561	SER	N-CA-CB	-5.97	101.73	110.26
1	B	795	ARG	CB-CG-CD	5.97	125.03	111.30
1	C	423	ASP	CA-CB-CG	-5.97	106.63	112.60
1	D	348	GLU	CB-CG-CD	5.97	122.74	112.60
1	D	810	LYS	CA-CB-CG	5.97	126.03	114.10
1	C	576	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	D	747	SER	O-C-N	5.96	128.29	122.09
1	C	601	ARG	N-CA-C	5.96	118.76	109.52
1	A	761	ILE	CA-C-O	-5.96	114.33	120.71
1	C	346	ILE	O-C-N	-5.96	114.31	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PHE	N-CA-C	-5.96	104.78	111.28
1	A	490	ARG	NE-CZ-NH1	5.95	127.45	121.50
1	D	729	GLN	N-CA-C	-5.95	98.12	110.80
1	D	227	ASP	O-C-N	-5.95	116.44	123.22
1	D	705	GLU	CA-C-N	5.95	128.18	120.44
1	D	705	GLU	C-N-CA	5.95	128.18	120.44
1	B	401	GLN	CA-C-O	-5.95	114.57	120.82
1	D	193	ARG	N-CA-C	5.95	118.17	109.30
1	B	613	TYR	CA-C-O	-5.95	114.73	120.92
1	C	36	HIS	N-CA-C	-5.95	98.13	110.80
1	C	832	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	B	828	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	493	VAL	CA-C-O	-5.94	114.46	121.05
1	B	16	ARG	CB-CA-C	-5.94	98.61	110.42
1	B	169	LYS	N-CA-C	-5.94	99.72	109.40
1	B	279	LEU	O-C-N	-5.94	115.41	122.65
1	D	228	THR	N-CA-C	-5.93	101.36	110.32
1	A	556	HIS	N-CA-C	-5.93	95.09	107.37
1	B	565	VAL	CA-C-N	5.93	130.72	121.76
1	B	565	VAL	C-N-CA	5.93	130.72	121.76
1	D	184	ARG	CA-CB-CG	5.93	125.96	114.10
1	A	394	THR	CA-CB-OG1	-5.93	100.70	109.60
1	D	281	PRO	CB-CA-C	5.93	121.34	111.56
1	B	516	ASP	O-C-N	-5.93	115.44	122.20
1	D	387	TRP	O-C-N	-5.93	116.70	121.80
1	D	501	GLU	CB-CG-CD	5.93	122.67	112.60
1	D	676	THR	CA-CB-CG2	5.92	120.57	110.50
1	B	547	ALA	CA-C-O	-5.92	114.58	120.80
1	D	213	ALA	N-CA-C	-5.92	100.64	110.17
1	D	557	ILE	CG1-CB-CG2	-5.92	92.94	110.70
1	B	804	ASN	CA-C-O	-5.92	114.81	120.90
1	D	206	VAL	N-CA-C	5.91	116.32	107.51
1	B	465	LYS	CA-C-O	-5.91	112.55	119.05
1	A	378	THR	CA-CB-OG1	-5.91	100.74	109.60
1	D	727	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	D	686	ALA	CA-C-O	5.90	128.02	121.11
1	A	76	GLU	CB-CG-CD	5.90	122.64	112.60
1	A	632	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	D	294	LYS	N-CA-C	-5.90	104.44	111.69
1	D	556	HIS	CA-CB-CG	5.90	119.70	113.80
1	A	15	VAL	CB-CA-C	-5.90	100.20	111.40
1	A	335	ILE	N-CA-CB	-5.89	103.98	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	PRO	CA-C-N	5.89	132.79	121.54
1	C	281	PRO	C-N-CA	5.89	132.79	121.54
1	A	33	ARG	CB-CA-C	-5.89	101.56	110.92
1	A	431	VAL	CB-CA-C	-5.89	102.06	110.83
1	B	143	PHE	CA-CB-CG	5.88	119.69	113.80
1	D	353	LEU	N-CA-C	5.88	117.37	111.07
1	A	225	PRO	CA-N-CD	-5.88	103.77	112.00
1	A	435	ALA	CA-C-N	5.88	131.74	122.33
1	A	435	ALA	C-N-CA	5.88	131.74	122.33
1	D	608	LYS	N-CA-C	-5.88	101.50	110.14
1	A	559	PRO	CA-CB-CG	-5.88	93.34	104.50
1	D	677	GLY	N-CA-C	-5.88	105.68	112.73
1	A	407	ASN	CA-C-N	5.87	128.08	120.44
1	A	407	ASN	C-N-CA	5.87	128.08	120.44
1	A	455	VAL	N-CA-C	5.87	121.56	109.34
1	C	615	MET	N-CA-C	-5.87	104.96	111.36
1	D	365	TRP	CE2-CD2-CG	-5.87	100.15	107.20
1	A	281	PRO	CA-C-N	5.87	132.75	121.54
1	A	281	PRO	C-N-CA	5.87	132.75	121.54
1	C	263	ILE	CA-CB-CG1	5.87	120.38	110.40
1	D	240	THR	CA-C-O	5.87	126.65	120.54
1	B	675	GLY	O-C-N	5.87	130.33	122.70
1	D	712	GLY	O-C-N	5.87	130.33	122.70
1	D	824	ILE	CB-CG1-CD1	5.87	126.12	113.80
1	D	237	VAL	N-CA-C	-5.87	99.88	108.97
1	D	243	LEU	CA-C-O	-5.86	114.29	120.80
1	D	511	TYR	CA-C-O	-5.86	114.33	120.55
1	A	281	PRO	CB-CA-C	5.86	121.23	111.56
1	C	85	LEU	CB-CA-C	-5.86	100.43	110.22
1	D	513	SER	O-C-N	-5.86	115.15	122.24
1	B	610	ALA	N-CA-C	-5.86	96.86	109.81
1	B	205	ARG	O-C-N	-5.86	116.56	123.41
1	D	677	GLY	O-C-N	5.86	127.81	122.19
1	C	319	ARG	N-CA-C	5.86	119.94	113.21
1	A	594	PRO	N-CA-C	5.85	124.53	112.47
1	A	197	THR	CA-CB-OG1	-5.85	100.83	109.60
1	C	119	MET	CA-C-O	-5.85	114.35	120.55
1	A	274	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	552	GLU	CA-C-N	5.85	132.71	121.54
1	A	552	GLU	C-N-CA	5.85	132.71	121.54
1	B	195	GLU	CB-CA-C	-5.85	101.09	110.79
1	C	322	VAL	N-CA-CB	-5.85	101.58	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ARG	CB-CG-CD	-5.84	97.86	111.30
1	B	439	ILE	CB-CA-C	5.84	119.33	110.62
1	C	491	TRP	CE2-CD2-CG	-5.84	100.19	107.20
1	D	439	ILE	N-CA-CB	-5.84	103.98	110.99
1	A	71	GLN	N-CA-C	-5.84	104.99	111.36
1	D	576	GLN	CG-CD-NE2	5.84	125.16	116.40
1	A	33	ARG	CA-CB-CG	5.84	125.78	114.10
1	A	747	SER	CA-CB-OG	5.84	122.78	111.10
1	B	31	PHE	O-C-N	-5.84	116.02	122.09
1	C	598	VAL	O-C-N	5.84	129.04	123.03
1	B	316	PHE	CA-CB-CG	-5.83	107.97	113.80
1	B	722	ASP	O-C-N	5.83	128.39	122.09
1	C	545	PHE	CA-C-O	-5.83	114.24	120.42
1	B	770	ARG	CA-CB-CG	5.83	125.76	114.10
1	C	82	ILE	CB-CA-C	5.83	118.77	110.84
1	C	393	GLU	CB-CG-CD	-5.83	102.69	112.60
1	A	176	MET	CA-CB-CG	-5.82	102.45	114.10
1	C	160	ARG	NE-CZ-NH2	-5.82	113.96	119.20
1	C	316	PHE	CA-CB-CG	-5.82	107.98	113.80
1	C	477	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	D	744	GLN	CG-CD-NE2	5.82	125.12	116.40
1	C	328	ALA	N-CA-C	5.82	120.00	113.02
1	B	236	ASN	CB-CG-ND2	-5.81	107.68	116.40
1	D	810	LYS	CA-C-O	5.81	126.52	119.31
1	B	777	TYR	CA-C-O	-5.81	114.72	120.82
1	D	438	ARG	CG-CD-NE	-5.81	99.22	112.00
1	D	824	ILE	CA-CB-CG1	5.81	120.28	110.40
1	A	236	ASN	CA-C-O	-5.81	112.20	120.51
1	C	657	ILE	N-CA-CB	-5.81	103.08	111.21
1	A	326	PHE	CA-C-N	5.80	128.05	120.28
1	A	326	PHE	C-N-CA	5.80	128.05	120.28
1	D	47	THR	CA-C-O	-5.80	115.17	120.50
1	B	355	ASP	CA-C-O	5.80	126.91	120.82
1	D	669	ALA	N-CA-C	5.80	119.22	110.64
1	B	375	THR	CA-CB-CG2	5.79	120.35	110.50
1	B	365	TRP	CB-CG-CD1	-5.79	118.21	126.90
1	C	196	PHE	CA-C-N	5.79	129.10	120.87
1	C	196	PHE	C-N-CA	5.79	129.10	120.87
1	D	433	GLU	CB-CA-C	-5.79	101.15	109.84
1	B	365	TRP	N-CA-C	-5.79	104.57	111.69
1	C	490	ARG	O-C-N	5.79	128.26	122.12
1	B	613	TYR	O-C-N	-5.79	115.33	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	377	HIS	O-C-N	-5.79	115.19	122.19
1	A	248	ALA	CA-C-N	5.79	126.12	119.93
1	A	248	ALA	C-N-CA	5.79	126.12	119.93
1	C	754	GLN	CA-CB-CG	5.79	125.67	114.10
1	D	192	ALA	CA-C-O	-5.78	115.16	121.87
1	A	558	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	B	642	VAL	O-C-N	-5.78	117.07	123.20
1	A	173	GLY	N-CA-C	-5.78	106.74	114.25
1	B	429	SER	N-CA-C	5.78	118.86	110.42
1	C	830	SER	N-CA-C	5.78	118.21	110.35
1	B	837	PRO	O-C-N	5.78	130.44	122.64
1	B	437	LYS	N-CA-CB	-5.77	101.25	109.85
1	D	575	ARG	N-CA-C	5.77	119.52	111.90
1	A	365	TRP	CE2-CD2-CG	-5.77	100.28	107.20
1	A	641	ARG	CG-CD-NE	-5.77	99.31	112.00
1	D	377	HIS	O-C-N	-5.77	115.94	122.23
1	C	763	ASN	OD1-CG-ND2	-5.76	116.83	122.60
1	D	641	ARG	NE-CZ-NH1	5.76	127.27	121.50
1	C	104	LEU	CA-C-O	-5.76	112.81	119.61
1	C	533	ASP	CA-CB-CG	5.76	118.36	112.60
1	D	595	ASN	N-CA-C	-5.76	98.53	110.80
1	A	529	ALA	CA-C-O	-5.76	114.77	120.70
1	D	138	ARG	CG-CD-NE	5.76	124.67	112.00
1	D	175	GLN	CG-CD-NE2	5.76	125.04	116.40
1	A	527	ASP	CA-C-O	5.76	127.10	120.60
1	A	720	ARG	CB-CG-CD	5.76	124.54	111.30
1	B	211	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	D	445	CYS	CA-C-O	-5.76	114.96	121.00
1	A	26	GLU	N-CA-C	-5.75	105.09	111.36
1	A	146	SER	CA-C-O	-5.75	114.96	121.00
1	C	805	ILE	N-CA-C	5.75	117.18	110.62
1	A	733	ASP	CA-CB-CG	-5.75	106.85	112.60
1	D	759	LYS	O-C-N	5.75	129.34	122.27
1	C	255	LYS	O-C-N	5.75	129.55	123.11
1	D	800	MET	CA-C-O	5.75	127.05	120.90
1	A	190	GLU	N-CA-C	5.75	119.46	110.32
1	B	90	TYR	CA-CB-CG	5.75	124.24	113.90
1	C	110	GLU	O-C-N	5.75	129.15	122.20
1	C	656	VAL	CA-CB-CG1	5.75	120.17	110.40
1	D	825	TRP	CG-CD2-CE3	5.75	139.65	133.90
1	B	400	LEU	N-CA-C	-5.75	104.94	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	ASP	CA-C-O	5.75	127.05	120.90
1	D	771	PHE	CA-CB-CG	-5.75	108.06	113.80
1	C	774	PHE	CA-C-O	-5.74	114.75	120.90
1	B	71	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	B	97	ASN	CA-CB-CG	-5.74	106.86	112.60
1	B	304	LEU	N-CA-C	-5.74	106.12	113.23
1	A	496	ASN	CA-C-N	5.73	126.12	119.47
1	A	496	ASN	C-N-CA	5.73	126.12	119.47
1	B	325	ASN	O-C-N	5.73	129.88	122.89
1	A	385	GLU	O-C-N	-5.73	115.84	122.95
1	D	623	ILE	CA-C-O	-5.73	115.09	121.05
1	B	295	GLN	CA-C-O	5.73	126.99	120.00
1	A	78	ASP	CA-C-N	5.73	126.19	120.52
1	A	78	ASP	C-N-CA	5.73	126.19	120.52
1	B	176	MET	CA-C-N	-5.73	114.70	122.95
1	B	176	MET	C-N-CA	-5.73	114.70	122.95
1	D	530	PHE	CB-CA-C	-5.73	101.65	110.81
1	B	253	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	103	ALA	O-C-N	-5.72	114.85	122.00
1	A	236	ASN	N-CA-C	5.72	122.98	110.80
1	D	466	THR	N-CA-C	-5.72	98.62	110.80
1	A	243	LEU	O-C-N	-5.72	116.29	123.27
1	C	219	GLN	CG-CD-NE2	5.72	124.98	116.40
1	B	12	GLN	CA-C-O	-5.72	114.43	120.55
1	C	257	PHE	O-C-N	5.71	129.88	122.40
1	C	325	ASN	N-CA-CB	5.71	118.37	109.97
1	D	299	VAL	CA-CB-CG2	-5.71	100.69	110.40
1	B	281	PRO	CA-N-CD	-5.71	104.01	112.00
1	C	481	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	D	790	LEU	N-CA-CB	-5.71	101.12	110.14
1	A	655	LYS	CA-CB-CG	5.71	125.51	114.10
1	C	327	ASP	N-CA-C	-5.71	104.26	111.11
1	A	675	GLY	N-CA-C	-5.70	99.66	113.18
1	A	522	LEU	N-CA-CB	-5.70	101.74	110.12
1	B	553	TYR	N-CA-CB	5.70	120.12	110.49
1	C	529	ALA	N-CA-C	-5.70	102.20	111.04
1	C	303	THR	O-C-N	-5.70	116.08	122.12
1	A	412	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	B	239	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	C	219	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	265	ALA	N-CA-C	5.69	122.92	110.80
1	A	514	ASP	CB-CA-C	-5.69	104.38	111.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	326	PHE	N-CA-CB	-5.69	100.88	110.49
1	D	34	HIS	O-C-N	5.69	128.01	122.09
1	C	741	ILE	CA-CB-CG2	-5.68	100.84	110.50
1	A	583	VAL	CG1-CB-CG2	-5.68	98.30	110.80
1	C	663	SER	CA-CB-OG	5.68	122.47	111.10
1	A	401	GLN	CA-CB-CG	5.68	125.46	114.10
1	C	744	GLN	N-CA-C	5.68	118.20	111.33
1	D	698	GLU	N-CA-C	5.68	119.73	112.34
1	A	282	ASN	O-C-N	5.68	130.14	122.59
1	B	206	VAL	N-CA-C	5.68	115.97	107.51
1	A	59	VAL	N-CA-C	-5.68	104.81	111.00
1	C	67	TRP	CG-CD1-NE1	-5.68	102.82	110.20
1	D	21	VAL	O-C-N	5.68	129.67	122.57
1	C	75	TYR	O-C-N	5.67	128.14	122.12
1	D	224	MET	N-CA-C	5.67	119.41	109.48
1	B	517	GLN	CB-CG-CD	-5.67	102.95	112.60
1	A	586	LEU	CB-CA-C	-5.67	100.14	110.63
1	C	80	LYS	N-CA-C	-5.67	101.25	110.20
1	A	715	VAL	CA-C-O	-5.67	115.52	121.41
1	C	97	ASN	CA-CB-CG	-5.67	106.93	112.60
1	D	319	ARG	CA-CB-CG	5.67	125.43	114.10
1	C	207	GLU	O-C-N	-5.67	116.33	123.01
1	C	277	ARG	CB-CG-CD	5.66	124.33	111.30
1	C	525	VAL	N-CA-CB	5.66	117.55	110.47
1	D	96	GLN	CA-CB-CG	-5.66	102.77	114.10
1	A	228	THR	CA-C-N	5.66	125.57	119.85
1	A	228	THR	C-N-CA	5.66	125.57	119.85
1	C	514	ASP	N-CA-CB	5.66	119.66	110.32
1	D	125	ILE	N-CA-C	-5.66	105.07	113.39
1	A	10	ARG	CA-C-O	-5.66	111.18	120.80
1	C	453	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	93	ARG	N-CA-C	5.66	119.03	109.76
1	D	329	PHE	CA-C-O	-5.66	112.41	120.16
1	D	760	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	277	ARG	CD-NE-CZ	5.65	132.31	124.40
1	B	780	TYR	CA-C-O	-5.65	114.88	120.70
1	A	770	ARG	CG-CD-NE	5.65	124.43	112.00
1	B	205	ARG	N-CA-CB	-5.65	100.91	111.13
1	D	165	ILE	O-C-N	-5.65	118.06	122.97
1	A	198	LEU	O-C-N	-5.64	116.01	121.94
1	A	45	VAL	CA-C-O	5.64	126.31	119.54
1	A	167	ASN	CA-C-O	5.64	128.13	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	581	LEU	CA-C-O	-5.64	114.88	120.80
1	D	271	LEU	CA-C-O	5.64	125.41	119.03
1	A	241	MET	CA-CB-CG	-5.64	102.82	114.10
1	A	597	PHE	CA-C-O	5.64	126.41	120.54
1	B	61	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	717	ASP	CA-CB-CG	5.64	118.24	112.60
1	D	427	ARG	CA-C-O	5.64	124.98	118.55
1	B	282	ASN	O-C-N	5.64	130.09	122.59
1	B	298	PHE	CA-CB-CG	5.64	119.44	113.80
1	C	768	HIS	CA-C-O	5.64	125.27	119.97
1	B	60	ARG	CA-C-O	-5.64	113.98	120.24
1	C	684	ASN	CA-C-O	5.64	126.52	119.59
1	D	530	PHE	N-CA-CB	5.64	118.34	109.94
1	A	582	HIS	CB-CG-ND1	5.63	131.15	122.70
1	C	16	ARG	O-C-N	5.63	130.08	122.59
1	A	553	TYR	N-CA-C	-5.63	98.80	110.80
1	C	723	GLN	CG-CD-NE2	5.63	124.85	116.40
1	C	108	CYS	CA-CB-SG	-5.63	101.45	114.40
1	D	150	LEU	CB-CA-C	5.63	118.14	111.22
1	A	267	LEU	N-CA-C	5.63	117.49	111.36
1	B	63	LEU	CB-CA-C	-5.63	101.34	110.79
1	C	712	GLY	O-C-N	5.62	128.70	122.68
1	D	610	ALA	N-CA-C	-5.62	97.38	109.81
1	A	491	TRP	N-CA-C	5.62	118.93	112.97
1	B	189	TRP	CE2-CD2-CE3	5.62	124.42	118.80
1	B	263	ILE	CB-CA-C	-5.62	102.07	111.29
1	D	756	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	767	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	253	ASN	CB-CG-ND2	5.61	124.82	116.40
1	C	327	ASP	CB-CA-C	-5.61	101.83	110.81
1	A	183	LEU	O-C-N	5.61	129.89	123.27
1	A	332	LYS	N-CA-C	5.61	120.12	112.88
1	B	475	GLU	CA-C-N	5.61	125.28	119.05
1	B	475	GLU	C-N-CA	5.61	125.28	119.05
1	C	487	THR	CA-CB-CG2	5.61	120.04	110.50
1	D	706	GLU	CB-CA-C	-5.61	102.07	110.88
1	A	43	ARG	CG-CD-NE	5.61	124.34	112.00
1	A	12	GLN	CB-CG-CD	5.61	122.13	112.60
1	B	106	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	B	597	PHE	CA-C-N	5.61	129.99	122.93
1	B	597	PHE	C-N-CA	5.61	129.99	122.93
1	A	338	ASN	OD1-CG-ND2	-5.60	117.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	MET	CA-CB-CG	-5.60	102.89	114.10
1	C	202	PHE	N-CA-C	5.60	118.83	110.14
1	B	439	ILE	N-CA-C	-5.60	100.41	108.48
1	A	785	GLU	CA-CB-CG	-5.60	102.90	114.10
1	A	553	TYR	CA-CB-CG	5.60	123.98	113.90
1	B	177	GLU	N-CA-C	5.60	119.40	107.70
1	B	377	HIS	CA-CB-CG	5.60	119.40	113.80
1	C	107	ALA	O-C-N	-5.60	116.04	122.09
1	C	344	LEU	CA-C-N	5.60	128.55	120.38
1	C	344	LEU	C-N-CA	5.60	128.55	120.38
1	C	387	TRP	CA-C-N	5.60	126.03	119.99
1	C	387	TRP	C-N-CA	5.60	126.03	119.99
1	C	539	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	C	685	GLY	O-C-N	5.60	129.97	122.70
1	C	776	ASP	CA-CB-CG	-5.60	107.00	112.60
1	D	654	GLU	CB-CG-CD	5.60	122.11	112.60
1	A	142	CYS	N-CA-C	-5.59	104.67	112.45
1	B	409	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	C	416	ALA	N-CA-C	-5.59	105.08	111.07
1	D	338	ASN	OD1-CG-ND2	-5.59	117.00	122.60
1	D	202	PHE	CA-CB-CG	-5.59	108.21	113.80
1	B	34	HIS	CA-C-O	-5.59	114.50	120.42
1	C	344	LEU	CA-C-O	-5.59	113.01	119.61
1	D	322	VAL	N-CA-CB	-5.59	102.01	111.23
1	D	768	HIS	CB-CG-CD2	-5.59	123.94	131.20
1	B	94	THR	N-CA-CB	-5.59	102.30	110.40
1	B	257	PHE	CA-C-O	5.59	128.50	120.51
1	D	365	TRP	N-CA-C	-5.59	104.68	112.45
1	D	543	LEU	O-C-N	5.59	127.82	122.07
1	C	282	ASN	O-C-N	5.58	130.02	122.59
1	C	452	VAL	CA-C-O	-5.58	114.35	120.43
1	C	582	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	B	467	ILE	O-C-N	-5.57	116.37	121.94
1	C	341	HIS	CB-CG-ND1	5.57	131.06	122.70
1	D	582	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	D	72	GLN	CG-CD-NE2	5.57	124.75	116.40
1	A	647	ASN	O-C-N	5.57	130.39	123.32
1	A	675	GLY	O-C-N	-5.57	115.46	122.70
1	B	608	LYS	CA-C-O	-5.57	114.71	121.28
1	D	319	ARG	CA-C-N	5.57	130.36	121.62
1	D	319	ARG	C-N-CA	5.57	130.36	121.62
1	D	742	ILE	N-CA-C	-5.57	104.13	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	531	ILE	CB-CA-C	5.56	119.09	111.97
1	B	564	ASP	CB-CA-C	-5.56	100.93	110.22
1	B	154	ALA	N-CA-C	5.56	117.47	108.41
1	C	365	TRP	CG-CD2-CE3	5.56	139.46	133.90
1	C	327	ASP	N-CA-CB	5.56	118.22	109.94
1	D	192	ALA	CA-C-N	5.56	128.76	122.59
1	D	192	ALA	C-N-CA	5.56	128.76	122.59
1	C	163	PHE	CA-CB-CG	-5.56	108.24	113.80
1	B	168	GLN	CA-CB-CG	5.55	125.21	114.10
1	B	582	HIS	CA-CB-CG	-5.55	108.25	113.80
1	C	281	PRO	CB-CA-C	5.55	120.72	111.56
1	A	273	GLU	CB-CA-C	5.55	120.06	110.84
1	B	362	ASP	CA-CB-CG	-5.55	107.05	112.60
1	B	236	ASN	OD1-CG-ND2	5.55	128.15	122.60
1	B	491	TRP	CE2-CD2-CG	-5.55	100.54	107.20
1	B	175	GLN	CA-CB-CG	-5.55	103.01	114.10
1	D	68	ILE	CA-C-O	-5.54	114.90	121.05
1	A	86	SER	N-CA-C	5.54	118.45	108.48
1	C	33	ARG	N-CA-C	-5.54	104.88	111.69
1	A	82	ILE	N-CA-CB	-5.54	104.92	111.90
1	C	782	LYS	N-CA-C	-5.54	104.09	111.24
1	D	81	ARG	O-C-N	-5.54	115.81	123.01
1	A	569	ARG	CD-NE-CZ	-5.54	116.65	124.40
1	B	117	LEU	N-CA-C	-5.54	100.75	109.50
1	B	16	ARG	CA-C-N	-5.54	110.56	121.41
1	B	16	ARG	C-N-CA	-5.54	110.56	121.41
1	C	76	GLU	CB-CG-CD	5.54	122.01	112.60
1	C	767	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	D	652	LEU	N-CA-CB	5.54	118.83	110.30
1	D	824	ILE	CB-CA-C	-5.54	102.21	111.29
1	A	165	ILE	N-CA-C	-5.53	100.09	108.17
1	A	671	THR	CA-CB-OG1	-5.53	101.30	109.60
1	C	133	ASN	O-C-N	-5.53	115.23	122.59
1	B	580	CYS	CB-CA-C	-5.53	101.45	110.85
1	C	641	ARG	N-CA-CB	5.53	121.32	111.69
1	D	274	ASN	CA-CB-CG	5.53	118.13	112.60
1	D	30	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	C	185	TYR	N-CA-C	-5.53	104.08	111.87
1	D	470	ASP	CA-CB-CG	-5.53	107.07	112.60
1	D	554	LYS	O-C-N	5.53	129.25	122.84
1	B	64	VAL	CA-C-N	5.53	126.07	119.94
1	B	64	VAL	C-N-CA	5.53	126.07	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	GLU	N-CA-CB	-5.52	101.21	110.99
1	A	30	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	796	GLU	N-CA-C	5.52	119.19	112.23
1	D	664	GLU	CB-CG-CD	5.52	121.99	112.60
1	B	689	ILE	O-C-N	-5.52	117.08	122.93
1	C	355	ASP	N-CA-C	5.52	117.10	111.14
1	D	436	VAL	CA-C-N	5.52	130.21	121.99
1	D	436	VAL	C-N-CA	5.52	130.21	121.99
1	B	509	GLU	CA-C-O	5.52	126.76	120.80
1	D	516	ASP	N-CA-C	5.52	118.05	111.71
1	A	500	ALA	CA-C-N	5.51	128.45	120.79
1	A	500	ALA	C-N-CA	5.51	128.45	120.79
1	D	168	GLN	OE1-CD-NE2	-5.51	117.08	122.60
1	A	516	ASP	O-C-N	-5.51	114.86	122.46
1	B	184	ARG	CA-CB-CG	5.51	125.12	114.10
1	B	813	SER	CA-C-O	-5.51	114.71	120.55
1	C	368	THR	CA-CB-CG2	5.51	119.87	110.50
1	C	741	ILE	CA-C-O	-5.51	113.90	120.78
1	A	494	LEU	N-CA-C	5.51	120.11	112.45
1	B	266	VAL	N-CA-C	-5.51	104.21	111.09
1	C	148	ALA	N-CA-C	-5.51	105.19	111.14
1	D	520	LYS	CA-CB-CG	5.51	125.11	114.10
1	D	605	ILE	CA-CB-CG2	-5.50	101.14	110.50
1	D	688	THR	N-CA-CB	-5.50	100.69	110.60
1	B	116	GLY	O-C-N	5.50	128.15	122.54
1	B	267	LEU	CA-C-O	-5.50	112.49	119.31
1	D	211	GLN	CB-CG-CD	5.50	121.96	112.60
1	A	527	ASP	N-CA-C	-5.50	100.14	108.67
1	D	526	ASP	O-C-N	5.50	128.47	122.20
1	A	504	ALA	CA-C-O	-5.50	114.72	120.55
1	D	557	ILE	CB-CG1-CD1	5.50	125.35	113.80
1	C	712	GLY	CA-C-N	5.50	128.91	121.05
1	C	712	GLY	C-N-CA	5.50	128.91	121.05
1	A	439	ILE	CA-C-O	5.50	127.51	120.97
1	C	412	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	D	398	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	495	CYS	O-C-N	-5.49	115.52	122.27
1	C	796	GLU	CA-C-O	-5.49	114.60	120.42
1	C	831	ARG	CA-CB-CG	5.49	125.08	114.10
1	D	792	LYS	CB-CA-C	-5.49	99.73	110.11
1	A	811	PHE	N-CA-CB	-5.49	102.22	110.73
1	C	768	HIS	CB-CG-CD2	-5.49	124.06	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	358	ARG	CA-CB-CG	-5.49	103.12	114.10
1	B	113	TYR	O-C-N	5.49	128.41	122.15
1	D	264	GLN	CG-CD-NE2	5.49	124.63	116.40
1	D	709	PHE	O-C-N	5.49	127.61	122.18
1	D	331	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	241	MET	N-CA-C	-5.48	98.29	107.99
1	B	525	VAL	N-CA-C	5.48	120.74	109.34
1	D	90	TYR	N-CA-CB	-5.48	104.05	110.35
1	A	329	PHE	CA-C-O	-5.48	112.65	120.16
1	A	491	TRP	CE2-CD2-CG	-5.48	100.63	107.20
1	A	601	ARG	CB-CG-CD	5.48	123.90	111.30
1	C	543	LEU	N-CA-C	-5.48	105.22	111.14
1	A	252	PHE	N-CA-CB	-5.48	101.23	110.49
1	A	807	THR	CA-CB-OG1	-5.48	101.38	109.60
1	D	738	LEU	O-C-N	5.48	128.40	122.15
1	D	461	GLU	N-CA-C	-5.48	105.39	111.36
1	D	646	GLU	CA-C-O	5.47	127.17	121.15
1	B	761	ILE	O-C-N	5.47	127.27	121.91
1	C	558	ASN	CA-C-N	5.47	126.68	119.84
1	C	558	ASN	C-N-CA	5.47	126.68	119.84
1	A	97	ASN	CA-C-O	-5.47	113.92	120.10
1	B	515	LEU	CA-C-O	-5.47	112.69	120.51
1	A	182	TRP	CG-CD1-NE1	-5.47	103.09	110.20
1	C	105	GLU	CB-CG-CD	5.47	121.90	112.60
1	C	244	TRP	CA-C-O	-5.47	115.23	120.92
1	B	716	GLU	CB-CG-CD	5.47	121.89	112.60
1	C	661	ASP	O-C-N	-5.47	115.74	122.19
1	A	718	VAL	N-CA-C	-5.46	105.39	110.53
1	C	686	ALA	O-C-N	5.46	129.50	123.33
1	D	263	ILE	CA-C-O	5.46	126.49	120.48
1	B	255	LYS	O-C-N	5.46	129.65	122.93
1	B	679	MET	CG-SD-CE	-5.46	88.89	100.90
1	C	486	ILE	CA-CB-CG2	5.46	119.78	110.50
1	A	78	ASP	N-CA-CB	-5.46	100.65	110.37
1	A	177	GLU	N-CA-C	5.46	118.16	107.57
1	B	273	GLU	CB-CG-CD	5.46	121.88	112.60
1	B	547	ALA	N-CA-C	-5.46	104.20	111.24
1	C	346	ILE	CA-C-O	-5.46	112.64	119.95
1	A	270	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	366	GLU	CA-CB-CG	5.46	125.01	114.10
1	A	555	VAL	CB-CA-C	-5.46	102.34	111.29
1	B	91	MET	N-CA-C	5.46	118.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	SER	N-CA-C	5.46	116.92	110.97
1	D	492	LEU	N-CA-CB	5.46	119.71	110.49
1	B	572	GLU	N-CA-C	5.46	122.42	110.80
1	B	660	ALA	O-C-N	5.46	129.37	123.10
1	C	222	LEU	N-CA-C	-5.45	100.01	108.90
1	C	696	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	D	34	HIS	N-CA-C	5.45	117.65	111.11
1	D	313	SER	CA-C-O	-5.45	112.71	120.51
1	D	421	ASP	N-CA-C	-5.45	98.86	108.23
1	B	256	ASP	CA-CB-CG	5.45	118.05	112.60
1	C	447	ALA	O-C-N	-5.45	115.13	122.43
1	C	536	LYS	CA-CB-CG	5.45	125.00	114.10
1	C	228	THR	OG1-CB-CG2	5.45	120.19	109.30
1	C	632	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	C	203	TYR	CB-CA-C	-5.44	109.31	115.79
1	D	631	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	C	78	ASP	N-CA-C	5.44	121.84	109.81
1	A	310	ARG	O-C-N	5.44	127.97	122.09
1	D	510	GLU	N-CA-C	-5.44	99.21	110.80
1	B	42	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	256	ASP	CA-C-O	5.44	124.44	119.00
1	A	91	MET	N-CA-CB	-5.43	101.86	110.28
1	A	193	ARG	N-CA-C	5.43	121.81	109.81
1	A	422	VAL	N-CA-CB	-5.43	103.02	110.68
1	B	603	VAL	CA-C-O	-5.43	114.74	120.39
1	A	785	GLU	N-CA-C	-5.43	105.44	111.36
1	B	224	MET	CA-C-N	5.43	126.57	120.66
1	B	224	MET	C-N-CA	5.43	126.57	120.66
1	B	546	ALA	CA-C-O	5.43	126.01	119.61
1	D	315	LYS	N-CA-C	5.43	122.36	110.80
1	D	613	TYR	N-CA-C	-5.42	101.34	109.15
1	D	721	LEU	N-CA-C	-5.42	106.64	113.20
1	A	36	HIS	O-C-N	-5.42	116.52	122.38
1	B	44	ASN	CB-CA-C	-5.42	99.16	109.95
1	C	90	TYR	N-CA-C	-5.42	101.49	109.62
1	C	521	LEU	N-CA-C	-5.42	106.70	113.15
1	D	55	LEU	CA-C-O	-5.42	115.13	120.82
1	A	597	PHE	CA-C-N	5.42	129.76	122.93
1	A	597	PHE	C-N-CA	5.42	129.76	122.93
1	C	394	THR	N-CA-C	5.42	116.87	111.07
1	B	437	LYS	CB-CG-CD	-5.42	98.85	111.30
1	D	178	GLU	CA-CB-CG	5.42	124.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	LEU	N-CA-CB	5.41	118.14	110.13
1	B	372	CYS	N-CA-C	5.41	118.55	109.95
1	C	583	VAL	N-CA-C	-5.41	105.33	110.42
1	D	196	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	72	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	A	407	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	B	639	ARG	CA-C-O	5.41	125.09	119.14
1	A	351	ARG	N-CA-C	-5.41	105.30	111.14
1	A	833	ARG	CA-CB-CG	5.41	124.91	114.10
1	B	639	ARG	N-CA-C	-5.41	106.85	113.50
1	D	336	GLN	CG-CD-NE2	5.41	124.51	116.40
1	D	359	LEU	N-CA-CB	5.41	118.05	109.51
1	A	437	LYS	N-CA-CB	-5.41	101.80	109.85
1	A	763	ASN	N-CA-C	5.41	117.87	111.33
1	B	38	THR	CA-CB-OG1	-5.41	101.49	109.60
1	D	73	HIS	N-CA-C	-5.40	105.29	111.07
1	A	30	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	300	VAL	N-CA-CB	-5.40	101.54	110.56
1	B	511	TYR	CA-C-N	5.40	131.69	121.97
1	B	511	TYR	C-N-CA	5.40	131.69	121.97
1	A	593	GLU	CA-CB-CG	5.40	124.90	114.10
1	A	777	TYR	CA-C-O	-5.40	115.33	121.00
1	D	428	MET	CA-CB-CG	-5.40	103.30	114.10
1	C	491	TRP	N-CA-C	5.40	119.17	112.59
1	D	514	ASP	CA-C-O	5.39	126.29	120.63
1	A	166	PHE	N-CA-C	5.39	122.29	110.80
1	A	274	ASN	N-CA-C	5.39	118.69	112.97
1	B	390	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	D	342	PRO	O-C-N	-5.39	115.36	122.64
1	B	468	PHE	CA-CB-CG	5.39	119.19	113.80
1	C	20	GLY	O-C-N	5.39	130.29	122.26
1	C	399	HIS	CA-CB-CG	-5.39	108.41	113.80
1	D	467	ILE	O-C-N	-5.39	115.83	122.57
1	A	281	PRO	N-CA-CB	-5.39	97.59	103.25
1	C	281	PRO	N-CA-CB	-5.39	97.59	103.25
1	D	232	GLY	O-C-N	-5.39	115.73	122.84
1	A	561	SER	O-C-N	-5.39	116.65	122.79
1	B	501	GLU	CB-CA-C	-5.39	102.67	110.96
1	D	658	PRO	O-C-N	-5.39	115.27	122.22
1	D	682	MET	CG-SD-CE	5.38	112.75	100.90
1	A	116	GLY	O-C-N	-5.38	116.60	122.41
1	B	574	LYS	CA-CB-CG	5.38	124.86	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	661	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	801	VAL	N-CA-C	5.38	116.76	110.62
1	B	614	HIS	N-CA-C	5.38	119.33	112.34
1	C	215	TRP	N-CA-C	-5.38	99.00	108.20
1	C	323	ARG	O-C-N	5.38	129.31	122.91
1	A	491	TRP	CB-CG-CD1	-5.38	118.83	126.90
1	A	211	GLN	CB-CG-CD	5.37	121.74	112.60
1	A	300	VAL	CA-CB-CG1	5.37	119.53	110.40
1	C	522	LEU	CA-C-O	5.37	126.11	120.42
1	C	269	ARG	CA-CB-CG	5.37	124.83	114.10
1	C	506	ARG	CB-CG-CD	5.37	123.64	111.30
1	B	580	CYS	N-CA-CB	5.36	118.10	110.16
1	B	568	LYS	O-C-N	-5.36	116.20	122.96
1	C	51	TYR	CA-C-O	-5.36	114.74	120.42
1	A	729	GLN	CA-C-N	5.36	131.77	121.54
1	A	729	GLN	C-N-CA	5.36	131.77	121.54
1	B	458	ILE	CA-CB-CG2	-5.36	101.39	110.50
1	C	511	TYR	O-C-N	-5.36	115.47	122.59
1	A	327	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	76	GLU	CB-CG-CD	5.36	121.70	112.60
1	C	536	LYS	O-C-N	5.35	127.80	122.12
1	A	727	ASN	CB-CG-ND2	5.35	124.43	116.40
1	D	582	HIS	O-C-N	-5.35	115.96	122.22
1	A	65	GLY	O-C-N	-5.35	115.74	122.70
1	B	782	LYS	CA-C-O	-5.35	115.38	121.00
1	B	335	ILE	N-CA-C	-5.35	100.62	108.11
1	A	513	SER	CA-C-O	-5.35	113.01	119.27
1	D	507	ILE	N-CA-C	5.35	118.55	111.17
1	A	182	TRP	CE2-CD2-CG	-5.35	100.78	107.20
1	A	833	ARG	N-CA-C	-5.34	103.08	110.35
1	B	57	HIS	CB-CG-CD2	-5.34	124.25	131.20
1	A	308	ILE	N-CA-CB	-5.34	104.58	110.51
1	B	778	GLU	CA-C-O	-5.34	114.31	120.24
1	D	464	LYS	CB-CG-CD	5.34	123.59	111.30
1	A	825	TRP	CG-CD2-CE3	5.34	139.24	133.90
1	D	376	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	C	365	TRP	CE2-CD2-CG	-5.34	100.80	107.20
1	C	465	LYS	N-CA-C	-5.34	106.45	113.12
1	C	491	TRP	CG-CD1-NE1	-5.34	103.26	110.20
1	C	638	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	766	MET	N-CA-C	5.33	117.78	111.33
1	D	806	ALA	CA-C-N	5.33	128.17	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	806	ALA	C-N-CA	5.33	128.17	120.38
1	A	24	VAL	N-CA-C	-5.33	104.39	111.05
1	A	610	ALA	N-CA-CB	5.33	119.85	110.37
1	A	834	LEU	N-CA-C	-5.33	99.81	108.82
1	D	528	GLU	CA-CB-CG	-5.33	103.44	114.10
1	C	278	VAL	N-CA-C	5.33	116.33	108.45
1	D	665	GLN	N-CA-C	-5.33	99.76	109.56
1	C	595	ASN	N-CA-C	-5.33	99.45	110.80
1	A	244	TRP	CE2-CD2-CG	-5.32	100.81	107.20
1	A	466	THR	O-C-N	5.32	129.67	122.59
1	A	565	VAL	O-C-N	-5.32	117.43	123.18
1	B	25	THR	CA-C-O	-5.32	113.85	119.97
1	C	639	ARG	N-CA-CB	-5.32	102.28	110.16
1	A	515	LEU	N-CA-C	5.32	122.13	110.80
1	A	585	THR	CA-CB-OG1	-5.32	101.62	109.60
1	B	633	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	281	PRO	CA-N-CD	-5.32	104.56	112.00
1	A	575	ARG	N-CA-CB	-5.32	104.36	112.28
1	A	628	ASP	CB-CA-C	-5.32	101.81	110.85
1	D	455	VAL	CB-CA-C	5.32	119.64	112.36
1	D	667	SER	CA-C-O	-5.32	114.81	120.92
1	D	679	MET	CA-C-O	-5.32	115.43	120.90
1	A	66	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	B	588	ASN	CB-CG-ND2	-5.31	108.43	116.40
1	D	118	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	459	HIS	CB-CG-CD2	-5.31	124.29	131.20
1	D	650	VAL	CB-CA-C	-5.31	105.17	111.97
1	D	699	MET	CG-SD-CE	-5.31	89.21	100.90
1	C	574	LYS	N-CA-C	-5.31	106.39	112.92
1	A	332	LYS	CG-CD-CE	-5.31	99.09	111.30
1	A	546	ALA	O-C-N	5.31	128.22	122.11
1	B	365	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	D	742	ILE	CB-CG1-CD1	5.31	124.95	113.80
1	D	494	LEU	CA-C-O	-5.31	114.80	120.42
1	A	575	ARG	O-C-N	-5.30	112.09	122.11
1	B	828	GLU	N-CA-CB	-5.30	102.27	110.01
1	C	491	TRP	CB-CG-CD1	-5.30	118.94	126.90
1	C	804	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	A	274	ASN	N-CA-CB	-5.30	103.12	110.65
1	A	744	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	A	785	GLU	CB-CG-CD	5.30	121.61	112.60
1	C	597	PHE	N-CA-CB	5.30	118.17	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	740	GLN	CA-CB-CG	5.30	124.70	114.10
1	C	236	ASN	CA-C-N	-5.30	114.11	122.64
1	C	236	ASN	C-N-CA	-5.30	114.11	122.64
1	D	165	ILE	N-CA-C	-5.30	100.57	107.88
1	D	226	TYR	CA-C-O	-5.30	114.49	120.32
1	B	530	PHE	CB-CA-C	-5.30	101.95	110.74
1	C	274	ASN	N-CA-CB	-5.30	101.54	110.49
1	A	815	ARG	CA-C-N	5.29	128.76	120.82
1	A	815	ARG	C-N-CA	5.29	128.76	120.82
1	B	553	TYR	N-CA-C	-5.29	99.53	110.80
1	C	263	ILE	O-C-N	5.29	129.87	122.20
1	A	542	LYS	CA-C-N	-5.29	112.35	121.66
1	A	542	LYS	C-N-CA	-5.29	112.35	121.66
1	B	60	ARG	CB-CG-CD	-5.29	99.13	111.30
1	A	661	ASP	O-C-N	-5.29	114.85	122.36
1	B	12	GLN	CA-CB-CG	-5.29	103.52	114.10
1	D	643	ILE	N-CA-C	5.29	115.47	107.75
1	D	821	ALA	O-C-N	5.29	127.52	122.07
1	D	753	LYS	CG-CD-CE	5.29	123.46	111.30
1	A	744	GLN	N-CA-C	-5.29	105.10	112.45
1	C	281	PRO	CA-N-CD	-5.28	104.60	112.00
1	D	292	ARG	CG-CD-NE	-5.28	100.38	112.00
1	D	390	HIS	CA-CB-CG	5.28	119.08	113.80
1	D	695	ALA	CA-C-O	-5.28	113.56	120.00
1	B	700	ALA	O-C-N	-5.28	116.52	122.12
1	A	729	GLN	CG-CD-NE2	-5.28	108.48	116.40
1	C	171	CYS	CA-CB-SG	-5.28	102.26	114.40
1	C	354	VAL	CG1-CB-CG2	-5.28	99.18	110.80
1	D	193	ARG	CB-CA-C	-5.28	104.12	111.41
1	D	723	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	A	94	THR	CA-C-O	-5.28	113.32	118.97
1	C	267	LEU	CA-C-O	-5.28	113.90	119.97
1	C	583	VAL	CA-C-O	-5.28	115.06	121.18
1	D	784	GLN	CA-CB-CG	-5.28	103.54	114.10
1	D	180	ASP	O-C-N	-5.28	115.42	122.38
1	D	530	PHE	O-C-N	5.28	127.58	122.09
1	A	133	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	C	632	HIS	CB-CG-ND1	5.27	130.61	122.70
1	B	756	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	682	MET	N-CA-C	-5.27	99.57	110.80
1	A	171	CYS	CA-C-O	5.27	126.92	120.60
1	C	689	ILE	N-CA-C	-5.27	100.86	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	676	THR	N-CA-CB	-5.27	98.39	110.83
1	B	767	HIS	O-C-N	-5.27	116.34	121.93
1	C	591	LYS	N-CA-C	5.27	119.42	112.89
1	D	155	TYR	N-CA-C	-5.27	101.29	109.72
1	B	699	MET	CG-SD-CE	-5.27	89.31	100.90
1	A	591	LYS	N-CA-C	5.26	117.93	111.82
1	C	505	GLU	CA-C-N	5.26	131.59	121.54
1	C	505	GLU	C-N-CA	5.26	131.59	121.54
1	C	610	ALA	CB-CA-C	-5.26	99.80	110.17
1	D	244	TRP	CD1-CG-CD2	5.26	114.72	106.30
1	A	378	THR	CA-CB-CG2	5.26	119.45	110.50
1	B	247	LYS	CB-CG-CD	5.26	123.40	111.30
1	B	249	PRO	CA-C-N	-5.26	115.12	123.12
1	B	249	PRO	C-N-CA	-5.26	115.12	123.12
1	C	787	VAL	CA-CB-CG1	5.26	119.34	110.40
1	A	90	TYR	CA-C-O	5.26	129.21	122.64
1	A	345	ALA	CA-C-O	-5.26	114.16	120.10
1	C	142	CYS	N-CA-C	-5.26	105.14	112.45
1	B	235	ASN	CB-CG-ND2	5.26	124.29	116.40
1	D	280	TYR	CA-C-N	5.26	126.41	119.84
1	D	280	TYR	C-N-CA	5.26	126.41	119.84
1	C	492	LEU	CD1-CG-CD2	-5.26	99.23	110.80
1	B	393	GLU	CA-CB-CG	5.25	124.61	114.10
1	D	241	MET	N-CA-C	-5.25	100.61	108.96
1	B	582	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	B	839	GLU	CA-C-O	-5.25	111.87	120.80
1	A	41	LYS	CB-CG-CD	-5.25	99.23	111.30
1	D	554	LYS	CA-CB-CG	5.25	124.60	114.10
1	A	244	TRP	CB-CG-CD1	-5.25	119.03	126.90
1	A	732	TYR	CA-CB-CG	5.25	123.35	113.90
1	C	620	ILE	N-CA-C	-5.25	105.60	110.53
1	A	633	ASP	CA-C-N	5.24	124.75	119.19
1	A	633	ASP	C-N-CA	5.24	124.75	119.19
1	D	69	ARG	O-C-N	5.24	127.69	122.08
1	C	242	ARG	CA-CB-CG	5.24	124.58	114.10
1	B	402	ILE	N-CA-C	-5.24	105.27	110.62
1	B	408	GLN	CB-CG-CD	5.24	121.51	112.60
1	B	423	ASP	CA-CB-CG	-5.24	107.36	112.60
1	C	413	ARG	O-C-N	-5.24	116.67	122.07
1	C	441	MET	CG-SD-CE	5.24	112.43	100.90
1	B	278	VAL	CB-CA-C	5.24	117.96	110.84
1	C	655	LYS	CA-CB-CG	5.24	124.57	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ALA	N-CA-C	-5.23	102.45	110.14
1	D	550	GLU	O-C-N	-5.23	115.63	122.59
1	B	217	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	433	GLU	N-CA-CB	5.23	117.92	110.44
1	A	75	TYR	N-CA-C	-5.23	99.66	110.80
1	B	256	ASP	N-CA-CB	-5.23	108.21	114.17
1	D	763	ASN	CA-CB-CG	5.23	117.83	112.60
1	C	224	MET	CA-CB-CG	5.23	124.55	114.10
1	C	325	ASN	CA-C-O	5.23	127.01	121.16
1	A	437	LYS	CA-CB-CG	5.22	124.55	114.10
1	B	258	ASN	CA-CB-CG	5.22	117.82	112.60
1	D	608	LYS	O-C-N	-5.22	115.71	122.97
1	A	253	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	487	THR	CA-C-N	5.22	124.89	119.56
1	A	487	THR	C-N-CA	5.22	124.89	119.56
1	C	505	GLU	O-C-N	5.22	128.33	122.22
1	A	652	LEU	CB-CA-C	-5.22	102.69	110.88
1	C	62	HIS	O-C-N	5.22	127.65	122.12
1	D	413	ARG	O-C-N	5.22	127.65	122.12
1	A	421	ASP	CA-C-N	5.22	128.84	122.63
1	A	421	ASP	C-N-CA	5.22	128.84	122.63
1	C	310	ARG	N-CA-C	-5.21	105.60	111.28
1	D	780	TYR	CB-CG-CD2	-5.21	112.98	120.80
1	A	182	TRP	CD1-CG-CD2	5.21	114.64	106.30
1	B	43	ARG	CA-CB-CG	5.21	124.52	114.10
1	A	254	LEU	CB-CA-C	-5.21	100.06	110.42
1	B	374	TYR	O-C-N	-5.21	117.11	123.30
1	C	486	ILE	CA-C-O	-5.21	115.83	121.19
1	C	787	VAL	CA-CB-CG2	-5.21	101.55	110.40
1	D	478	LYS	N-CA-C	-5.21	106.95	113.72
1	D	677	GLY	CA-C-N	5.21	128.63	120.82
1	D	677	GLY	C-N-CA	5.21	128.63	120.82
1	A	181	ASP	CA-C-O	5.20	128.01	122.13
1	B	515	LEU	N-CA-C	5.20	121.88	110.80
1	B	718	VAL	CA-CB-CG1	5.20	119.25	110.40
1	D	412	ASN	CB-CA-C	-5.20	102.15	110.79
1	D	405	GLU	CB-CG-CD	5.20	121.44	112.60
1	D	633	ASP	CA-C-O	5.20	123.17	119.32
1	B	374	TYR	N-CA-C	5.20	117.37	108.90
1	D	618	MET	CB-CG-SD	-5.20	97.12	112.70
1	D	257	PHE	O-C-N	5.19	128.99	122.55
1	B	578	LEU	N-CA-C	-5.19	105.31	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	ASN	CB-CG-ND2	5.19	124.19	116.40
1	C	244	TRP	CB-CG-CD1	-5.19	119.11	126.90
1	D	487	THR	CA-CB-OG1	-5.19	101.81	109.60
1	B	329	PHE	N-CA-C	-5.19	105.69	112.75
1	B	592	LYS	CG-CD-CE	5.19	123.23	111.30
1	A	325	ASN	O-C-N	5.19	129.13	123.01
1	A	545	PHE	CA-C-O	-5.19	115.36	120.70
1	C	574	LYS	O-C-N	-5.19	116.11	122.34
1	D	722	ASP	CA-C-O	-5.19	115.35	120.80
1	B	297	TYR	N-CA-C	-5.18	106.22	112.54
1	B	400	LEU	CB-CA-C	-5.18	102.71	110.90
1	A	475	GLU	CA-C-N	5.18	126.32	119.84
1	A	475	GLU	C-N-CA	5.18	126.32	119.84
1	B	750	PHE	N-CA-CB	-5.18	103.05	110.57
1	C	392	LEU	CA-C-O	5.18	125.54	119.06
1	D	610	ALA	N-CA-CB	5.18	119.59	110.37
1	C	131	LEU	CA-C-O	5.18	124.52	118.77
1	C	795	ARG	CB-CG-CD	5.18	123.22	111.30
1	A	766	MET	O-C-N	-5.18	116.63	122.12
1	C	57	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	D	718	VAL	CA-C-O	-5.18	115.30	121.05
1	C	442	ALA	O-C-N	-5.18	116.25	122.15
1	C	470	ASP	CA-C-O	5.18	125.92	119.97
1	A	673	ALA	CA-C-O	-5.17	115.57	121.00
1	C	587	TYR	O-C-N	5.17	127.62	122.08
1	D	758	PHE	CA-C-N	5.17	128.18	120.31
1	D	758	PHE	C-N-CA	5.17	128.18	120.31
1	C	131	LEU	CB-CA-C	5.17	117.71	109.02
1	A	464	LYS	CA-C-N	-5.17	114.01	122.54
1	A	464	LYS	C-N-CA	-5.17	114.01	122.54
1	B	461	GLU	N-CA-C	-5.17	105.71	112.23
1	D	409	ARG	CA-CB-CG	-5.17	103.76	114.10
1	A	120	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	837	PRO	CB-CA-C	5.17	119.92	110.10
1	B	387	TRP	CG-CD1-NE1	-5.17	103.48	110.20
1	C	408	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	B	241	MET	CG-SD-CE	5.17	112.27	100.90
1	C	454	GLY	N-CA-C	-5.17	104.73	112.89
1	D	157	TYR	CA-C-N	5.17	129.43	121.37
1	D	157	TYR	C-N-CA	5.17	129.43	121.37
1	C	342	PRO	N-CD-CG	-5.17	95.45	103.20
1	A	54	ALA	CA-C-O	-5.16	113.13	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	589	ARG	CB-CG-CD	5.16	123.18	111.30
1	D	50	ASP	CA-CB-CG	-5.16	107.44	112.60
1	D	520	LYS	CG-CD-CE	5.16	123.17	111.30
1	B	367	VAL	CA-C-O	-5.16	115.59	120.95
1	B	809	GLY	N-CA-C	5.16	118.88	112.64
1	C	698	GLU	CB-CG-CD	-5.16	103.83	112.60
1	D	263	ILE	CA-CB-CG1	5.16	119.17	110.40
1	A	827	VAL	CB-CA-C	-5.16	104.63	111.80
1	C	180	ASP	CA-C-N	-5.15	114.10	122.34
1	C	180	ASP	C-N-CA	-5.15	114.10	122.34
1	C	639	ARG	CB-CG-CD	5.15	123.15	111.30
1	D	805	ILE	CA-C-O	-5.15	115.69	121.05
1	C	639	ARG	CB-CA-C	5.15	119.60	110.85
1	C	241	MET	N-CA-C	-5.15	99.71	108.26
1	D	208	HIS	N-CA-CB	5.15	118.66	110.16
1	A	234	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	D	16	ARG	N-CA-C	5.15	121.77	110.80
1	B	235	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	B	739	ARG	CG-CD-NE	5.14	123.32	112.00
1	C	227	ASP	CA-CB-CG	5.14	117.75	112.60
1	D	299	VAL	CA-CB-CG1	5.14	119.14	110.40
1	D	469	LYS	O-C-N	-5.14	116.20	122.22
1	A	23	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	B	658	PRO	N-CA-C	-5.14	107.34	114.27
1	D	193	ARG	CB-CG-CD	-5.14	99.49	111.30
1	B	539	GLN	N-CA-C	-5.13	105.31	112.45
1	C	665	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	D	396	LEU	CA-C-N	5.13	125.17	119.32
1	D	396	LEU	C-N-CA	5.13	125.17	119.32
1	A	649	ARG	CA-C-O	-5.13	115.51	121.26
1	B	45	VAL	N-CA-CB	-5.13	102.76	111.23
1	B	238	VAL	O-C-N	-5.13	117.61	123.10
1	C	782	LYS	CA-C-N	5.13	127.87	120.38
1	C	782	LYS	C-N-CA	5.13	127.87	120.38
1	B	108	CYS	O-C-N	5.13	127.63	122.09
1	C	617	LYS	O-C-N	5.13	128.58	122.27
1	B	44	ASN	CA-CB-CG	5.13	117.73	112.60
1	B	67	TRP	CG-CD1-NE1	-5.13	103.53	110.20
1	C	717	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	380	ILE	CA-C-N	5.13	124.82	119.64
1	D	380	ILE	C-N-CA	5.13	124.82	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	GLU	CB-CG-CD	-5.12	103.89	112.60
1	C	807	THR	O-C-N	5.12	127.36	121.93
1	C	455	VAL	CG1-CB-CG2	5.12	122.07	110.80
1	D	237	VAL	CB-CA-C	-5.12	103.58	111.31
1	A	12	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	A	538	LYS	CB-CG-CD	5.12	123.08	111.30
1	B	286	PHE	CA-C-N	5.12	131.31	121.54
1	B	286	PHE	C-N-CA	5.12	131.31	121.54
1	B	681	PHE	N-CA-C	-5.12	105.78	112.23
1	C	318	CYS	CA-CB-SG	5.12	126.17	114.40
1	D	426	ARG	N-CA-C	-5.12	106.79	112.57
1	D	663	SER	CA-CB-OG	5.12	121.33	111.10
1	D	378	THR	CA-C-O	5.12	126.94	121.16
1	A	471	PHE	N-CA-C	-5.12	105.40	111.69
1	C	36	HIS	CB-CG-ND1	5.11	130.37	122.70
1	D	193	ARG	O-C-N	-5.11	116.91	121.20
1	B	828	GLU	CB-CA-C	5.11	115.68	109.85
1	A	295	GLN	CB-CA-C	-5.11	102.83	110.90
1	A	752	PRO	N-CA-CB	5.11	108.72	103.15
1	B	400	LEU	N-CA-CB	5.11	117.48	110.07
1	B	386	ARG	O-C-N	-5.11	117.04	123.27
1	A	277	ARG	CB-CA-C	-5.11	100.82	110.01
1	A	574	LYS	CA-C-O	5.11	125.81	119.12
1	A	768	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	435	ALA	CA-C-N	5.11	131.16	121.97
1	B	435	ALA	C-N-CA	5.11	131.16	121.97
1	B	292	ARG	NE-CZ-NH2	-5.11	114.61	119.20
1	C	541	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	B	459	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	35	LEU	N-CA-C	-5.10	105.61	111.07
1	C	239	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	C	585	THR	CA-CB-OG1	-5.10	101.95	109.60
1	D	605	ILE	CB-CA-C	-5.10	104.36	110.99
1	B	431	VAL	N-CA-CB	5.10	118.09	111.67
1	B	825	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	D	379	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	C	325	ASN	CB-CG-ND2	5.09	124.04	116.40
1	C	771	PHE	N-CA-CB	-5.09	102.95	110.49
1	B	544	LYS	N-CA-C	-5.09	105.73	111.28
1	A	33	ARG	N-CA-CB	5.09	117.56	109.82
1	A	432	GLU	CB-CA-C	-5.09	103.18	111.68
1	A	687	LEU	N-CA-C	-5.09	102.94	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	745	LEU	CA-C-O	-5.09	115.02	120.42
1	C	658	PRO	CA-N-CD	-5.09	104.87	112.00
1	D	374	TYR	N-CA-CB	-5.09	102.00	110.80
1	D	493	VAL	CA-C-N	-5.09	113.06	120.29
1	D	493	VAL	C-N-CA	-5.09	113.06	120.29
1	A	205	ARG	N-CA-CB	-5.09	102.07	111.53
1	A	828	GLU	O-C-N	5.08	129.93	121.59
1	C	487	THR	CA-CB-OG1	-5.08	101.97	109.60
1	A	264	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	387	TRP	CA-C-N	5.08	124.99	119.76
1	A	387	TRP	C-N-CA	5.08	124.99	119.76
1	B	105	GLU	CA-CB-CG	-5.08	103.94	114.10
1	B	509	GLU	CA-C-N	5.08	131.25	121.54
1	B	509	GLU	C-N-CA	5.08	131.25	121.54
1	C	507	ILE	CA-C-O	-5.08	114.43	120.78
1	B	113	TYR	CA-CB-CG	5.08	123.04	113.90
1	B	178	GLU	CA-C-O	-5.08	115.98	121.87
1	B	305	GLN	CA-C-N	5.08	127.08	120.28
1	B	305	GLN	C-N-CA	5.08	127.08	120.28
1	C	462	ILE	CA-CB-CG2	-5.08	101.87	110.50
1	B	409	ARG	CA-C-O	-5.08	113.97	120.31
1	B	653	ALA	N-CA-C	-5.08	104.83	111.02
1	D	262	TYR	CA-CB-CG	-5.08	104.76	113.90
1	D	534	VAL	CA-CB-CG2	-5.08	101.77	110.40
1	A	807	THR	N-CA-CB	-5.07	101.51	110.39
1	C	683	LEU	N-CA-C	5.07	121.61	110.80
1	D	383	ALA	N-CA-C	5.07	119.34	113.20
1	D	506	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	D	545	PHE	N-CA-C	-5.07	106.25	112.90
1	D	804	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	164	GLY	O-C-N	5.07	129.55	122.55
1	C	830	SER	O-C-N	-5.07	116.57	122.81
1	B	815	ARG	CA-C-O	-5.07	115.12	120.55
1	C	171	CYS	N-CA-CB	-5.07	102.15	110.21
1	D	574	LYS	CA-CB-CG	5.07	124.24	114.10
1	A	803	ARG	N-CA-C	-5.07	105.45	110.97
1	A	809	GLY	N-CA-C	5.07	119.01	112.83
1	B	306	ASP	O-C-N	-5.07	116.75	122.12
1	B	457	ARG	O-C-N	-5.07	116.82	122.09
1	D	11	LYS	N-CA-C	5.07	121.59	110.80
1	D	16	ARG	CA-C-N	-5.07	111.48	121.41
1	D	16	ARG	C-N-CA	-5.07	111.48	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	519	ARG	N-CA-C	-5.06	105.89	111.71
1	B	564	ASP	N-CA-CB	5.06	118.67	110.17
1	C	189	TRP	CG-CD2-CE3	5.06	138.96	133.90
1	B	378	THR	CB-CA-C	-5.06	100.98	109.48
1	D	462	ILE	CB-CA-C	-5.06	105.31	112.14
1	A	227	ASP	N-CA-C	5.06	116.65	108.41
1	A	761	ILE	CB-CA-C	-5.06	105.47	112.24
1	B	636	VAL	CA-C-O	-5.05	116.01	121.27
1	C	394	THR	CA-CB-OG1	-5.05	102.02	109.60
1	D	168	GLN	CG-CD-NE2	5.05	123.98	116.40
1	A	772	LYS	CG-CD-CE	5.05	122.92	111.30
1	C	174	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	A	668	THR	CA-CB-OG1	-5.05	102.02	109.60
1	C	660	ALA	CA-C-O	-5.05	115.30	121.36
1	D	536	LYS	CA-C-N	5.05	127.39	120.77
1	D	536	LYS	C-N-CA	5.05	127.39	120.77
1	A	610	ALA	CB-CA-C	-5.05	100.22	110.17
1	D	536	LYS	CA-C-O	-5.05	115.50	120.90
1	A	71	GLN	CB-CG-CD	5.05	121.18	112.60
1	B	643	ILE	CB-CA-C	-5.05	102.96	110.33
1	C	628	ASP	N-CA-CB	-5.05	101.96	110.49
1	D	159	ILE	CG1-CB-CG2	-5.04	95.56	110.70
1	A	10	ARG	O-C-N	-5.04	114.93	123.00
1	B	477	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	C	417	ALA	N-CA-C	5.04	119.14	112.89
1	D	353	LEU	CA-C-O	-5.04	115.53	120.82
1	D	745	LEU	CA-CB-CG	5.04	133.96	116.30
1	B	294	LYS	O-C-N	-5.04	115.67	122.43
1	B	401	GLN	CB-CA-C	-5.04	102.97	110.88
1	D	440	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	749	PHE	CA-C-O	-5.04	115.53	120.82
1	B	750	PHE	O-C-N	-5.04	113.27	122.34
1	C	515	LEU	N-CA-C	5.04	117.66	111.82
1	A	404	TYR	N-CA-C	5.04	116.85	111.36
1	B	23	ASN	CA-C-O	-5.04	115.47	121.16
1	A	528	GLU	CB-CG-CD	-5.04	104.04	112.60
1	D	148	ALA	N-CA-C	-5.04	100.07	110.80
1	D	506	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	A	352	VAL	O-C-N	-5.03	116.79	121.87
1	B	407	ASN	CA-C-N	5.03	127.03	120.28
1	B	407	ASN	C-N-CA	5.03	127.03	120.28
1	C	384	LEU	N-CA-CB	-5.03	101.98	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	389	VAL	CA-C-O	-5.03	115.19	120.57
1	B	316	PHE	CA-C-O	5.03	124.58	119.05
1	A	128	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	365	TRP	CB-CG-CD1	-5.03	119.36	126.90
1	A	339	ASP	CA-CB-CG	-5.03	107.57	112.60
1	D	804	ASN	N-CA-C	-5.03	105.71	111.14
1	C	726	TYR	N-CA-C	5.03	118.14	110.20
1	D	467	ILE	CB-CG1-CD1	5.03	124.36	113.80
1	B	452	VAL	N-CA-C	-5.03	101.24	108.53
1	C	125	ILE	CA-C-O	5.03	125.05	119.42
1	C	189	TRP	CB-CG-CD1	-5.03	119.36	126.90
1	C	230	VAL	CA-C-N	5.03	124.94	119.76
1	C	230	VAL	C-N-CA	5.03	124.94	119.76
1	D	76	GLU	CA-C-O	-5.03	115.09	120.42
1	D	90	TYR	CA-CB-CG	5.02	122.94	113.90
1	B	571	HIS	CA-C-O	-5.02	114.94	120.36
1	A	402	ILE	N-CA-C	5.02	115.17	110.30
1	B	250	ASN	CB-CG-ND2	5.02	123.93	116.40
1	B	405	GLU	CA-CB-CG	5.02	124.14	114.10
1	C	301	ALA	O-C-N	5.02	127.44	122.12
1	D	502	ILE	CB-CG1-CD1	-5.02	103.26	113.80
1	D	505	GLU	CA-CB-CG	5.02	124.13	114.10
1	D	577	LEU	CA-C-N	5.02	126.96	120.44
1	D	577	LEU	C-N-CA	5.02	126.96	120.44
1	B	301	ALA	CB-CA-C	-5.02	102.32	110.85
1	A	67	TRP	CA-CB-CG	5.01	123.13	113.60
1	A	390	HIS	CB-CG-ND1	5.01	130.22	122.70
1	B	236	ASN	N-CA-C	5.01	121.34	113.72
1	D	260	GLY	N-CA-C	-5.01	101.30	113.18
1	C	666	ILE	N-CA-C	5.01	119.77	109.34
1	B	817	ILE	CA-C-O	-5.01	115.49	121.05
1	D	118	ASP	CA-C-O	-5.01	115.26	121.02
1	C	344	LEU	O-C-N	5.01	128.84	122.33
1	D	164	GLY	O-C-N	5.01	129.21	122.70
1	D	820	TYR	O-C-N	5.01	127.43	122.12
1	B	189	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	C	445	CYS	N-CA-C	5.01	116.74	111.28
1	A	556	HIS	CA-CB-CG	5.00	118.80	113.80
1	B	167	ASN	CB-CG-OD1	-5.00	110.80	120.80

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	203	TYR	Sidechain
1	A	320	ASP	Peptide
1	A	380	ILE	Peptide
1	A	421	ASP	Mainchain
1	A	51	TYR	Sidechain
1	A	569	ARG	Sidechain
1	A	573	TYR	Sidechain
1	A	820	TYR	Sidechain
1	A	833	ARG	Sidechain
1	A	836	ALA	Peptide
1	B	277	ARG	Sidechain
1	B	292	ARG	Sidechain
1	B	320	ASP	Peptide
1	B	52	TYR	Sidechain
1	B	573	TYR	Sidechain
1	B	599	VAL	Peptide
1	B	639	ARG	Sidechain
1	B	777	TYR	Sidechain
1	B	820	TYR	Sidechain
1	B	834	LEU	Peptide
1	B	836	ALA	Peptide
1	C	309	ARG	Sidechain
1	C	320	ASP	Peptide
1	C	33	ARG	Sidechain
1	C	358	ARG	Sidechain
1	C	52	TYR	Sidechain
1	C	569	ARG	Sidechain
1	C	599	VAL	Peptide
1	C	751	SER	Peptide
1	C	836	ALA	Peptide
1	D	155	TYR	Sidechain
1	D	185	TYR	Sidechain
1	D	226	TYR	Sidechain
1	D	320	ASP	Peptide
1	D	51	TYR	Sidechain
1	D	52	TYR	Sidechain
1	D	524	TYR	Sidechain
1	D	60	ARG	Sidechain
1	D	648	TYR	Sidechain
1	D	649	ARG	Sidechain
1	D	777	TYR	Sidechain
1	D	791	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	795	ARG	Sidechain
1	D	836	ALA	Peptide
1	D	84	TYR	Sidechain

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	6732	0	6675	427	1
1	B	6733	0	6667	382	0
1	C	6732	0	6674	412	0
1	D	6732	0	6674	462	1
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
3	C	15	0	7	1	0
3	D	15	0	6	0	0
All	All	27029	0	26717	1646	1

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 31.

All (1646) 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:756:ASP:N	1:A:756:ASP:CA	1.77	1.46
1:C:279:LEU:HD22	1:C:281:PRO:CD	1.62	1.28
1:C:24:VAL:C	1:C:25:THR:N	1.95	1.24
1:C:279:LEU:HD22	1:C:281:PRO:CG	1.70	1.22
1:B:283:ASP:OD2	1:B:383:ALA:HB1	1.39	1.21
1:C:283:ASP:OD2	1:C:383:ALA:HB1	1.37	1.19
1:A:555:VAL:HG21	1:A:643:ILE:CD1	1.71	1.19
1:D:279:LEU:HD22	1:D:281:PRO:CD	1.71	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CD2	1:A:303:THR:CG2	2.26	1.18
1:B:283:ASP:OD2	1:B:383:ALA:CB	1.92	1.18
1:D:279:LEU:CD2	1:D:281:PRO:HD2	1.72	1.17
1:D:251:ASP:OD1	1:D:255:LYS:HE2	1.40	1.17
1:D:251:ASP:OD1	1:D:255:LYS:HG3	1.46	1.15
1:C:279:LEU:CD2	1:C:281:PRO:CD	2.24	1.15
1:C:196:PHE:HB3	1:C:309:ARG:HH12	1.09	1.15
1:A:42:ASP:OD1	1:A:43:ARG:N	1.82	1.11
1:A:299:VAL:O	1:A:303:THR:OG1	1.69	1.09
1:D:502:ILE:HG22	1:D:506:ARG:HH21	1.13	1.09
1:B:402:ILE:O	1:B:406:ILE:HG13	1.52	1.09
1:C:280:TYR:N	1:C:281:PRO:HD2	1.62	1.09
1:C:24:VAL:HG12	1:C:28:LYS:HE2	1.29	1.08
1:C:279:LEU:CD2	1:C:281:PRO:HD3	1.88	1.04
1:D:509:GLU:OE1	1:D:510:GLU:N	1.91	1.03
1:A:555:VAL:HG21	1:A:643:ILE:HD11	1.41	1.02
1:C:283:ASP:OD2	1:C:383:ALA:CB	2.05	1.02
1:A:21:VAL:HG11	1:A:23:ASN:ND2	1.74	1.02
1:A:157:TYR:CD2	1:A:303:THR:HG22	1.91	1.02
1:D:692:MET:SD	1:D:710:ILE:HD13	2.01	1.00
1:A:274:ASN:HA	1:A:277:ARG:HG3	1.44	1.00
1:C:196:PHE:HB3	1:C:309:ARG:NH1	1.77	0.99
1:D:274:ASN:HA	1:D:277:ARG:HG3	1.43	0.98
1:A:316:PHE:CE2	1:A:332:LYS:NZ	2.32	0.98
1:B:280:TYR:N	1:B:281:PRO:HD2	1.77	0.98
1:D:279:LEU:HD22	1:D:281:PRO:HD2	0.99	0.97
1:D:251:ASP:OD1	1:D:255:LYS:CE	2.14	0.95
1:B:280:TYR:CE2	1:B:289:LYS:HE3	2.02	0.95
1:B:280:TYR:HE2	1:B:289:LYS:HE3	1.30	0.94
1:C:198:LEU:HD22	1:C:305:GLN:OE1	1.67	0.94
1:D:279:LEU:CD2	1:D:281:PRO:CD	2.40	0.94
1:B:363:LYS:NZ	1:B:366:GLU:OE1	2.01	0.93
1:D:424:ARG:HH22	1:D:473:GLU:CD	1.77	0.93
1:D:315:LYS:HG2	1:D:318:CYS:SG	2.10	0.92
1:D:502:ILE:HG22	1:D:506:ARG:NH2	1.82	0.92
1:D:251:ASP:OD1	1:D:255:LYS:CG	2.18	0.92
1:C:692:MET:SD	1:C:710:ILE:HD13	2.10	0.91
1:C:279:LEU:HD22	1:C:281:PRO:HG3	1.51	0.91
1:A:386:ARG:NE	1:A:432:GLU:OE2	2.02	0.90
1:C:15:VAL:O	1:C:18:LEU:CD2	2.20	0.90
1:A:316:PHE:CZ	1:A:332:LYS:HE2	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:VAL:HG21	1:A:643:ILE:HD12	1.53	0.90
1:B:566:GLN:HB2	1:B:664:GLU:HB2	1.53	0.90
1:B:18:LEU:N	1:B:18:LEU:HD22	1.87	0.89
1:A:549:LEU:HD23	1:A:557:ILE:HG12	1.54	0.88
1:C:115:LEU:HD23	1:D:12:GLN:HB3	1.53	0.88
1:C:350:MET:O	1:C:354:VAL:HG23	1.74	0.88
1:D:720:ARG:HG3	1:D:720:ARG:HH11	1.39	0.88
1:C:284:ASN:ND2	1:C:285:PHE:H	1.70	0.88
1:D:754:GLN:NE2	1:D:757:LEU:CD1	2.36	0.87
1:B:283:ASP:OD2	1:B:383:ALA:HB2	1.76	0.86
1:C:322:VAL:O	1:C:325:ASN:HB2	1.75	0.86
1:C:15:VAL:O	1:C:18:LEU:HD23	1.75	0.86
1:D:112:THR:HA	1:D:115:LEU:HD12	1.55	0.85
1:A:21:VAL:CG1	1:A:23:ASN:ND2	2.39	0.85
1:A:21:VAL:CB	1:A:23:ASN:HD22	1.88	0.85
1:C:280:TYR:H	1:C:281:PRO:HD2	1.37	0.85
1:D:577:LEU:HD13	1:D:765:LEU:HD11	1.58	0.85
1:C:224:MET:HG2	1:C:247:LYS:HD2	1.57	0.84
1:D:558:ASN:HD21	1:D:560:ASN:HB2	1.39	0.84
1:A:75:TYR:HE1	1:A:315:LYS:HG3	1.41	0.84
1:A:316:PHE:HE2	1:A:332:LYS:NZ	1.74	0.84
1:C:280:TYR:N	1:C:281:PRO:CD	2.39	0.84
1:D:21:VAL:HG12	1:D:22:GLU:H	1.42	0.84
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.59	0.84
1:A:42:ASP:OD1	1:A:42:ASP:C	2.21	0.83
1:A:433:GLU:OE2	1:A:437:LYS:NZ	2.11	0.83
1:A:446:ILE:HG23	1:A:452:VAL:HG21	1.59	0.83
1:A:24:VAL:HG13	1:A:111:ALA:HA	1.60	0.83
1:B:18:LEU:HD22	1:B:18:LEU:H	1.43	0.82
1:B:402:ILE:HG22	1:B:406:ILE:HD11	1.62	0.82
1:D:734:ARG:HB2	1:D:735:ILE:HD12	1.61	0.82
1:C:491:TRP:HA	1:C:495:CYS:SG	2.19	0.82
1:B:284:ASN:ND2	1:B:285:PHE:H	1.77	0.81
1:C:21:VAL:HG12	1:C:22:GLU:HG2	1.62	0.81
1:C:279:LEU:HD22	1:C:281:PRO:HD3	1.53	0.81
1:B:283:ASP:CG	1:B:383:ALA:HB1	2.04	0.81
1:C:24:VAL:N	1:C:25:THR:N	2.29	0.81
1:D:219:GLN:NE2	1:D:268:ASP:CG	2.39	0.81
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.62	0.81
1:C:400:LEU:HD22	1:C:404:TYR:CE2	2.16	0.81
1:D:707:ASN:HA	1:D:800:MET:SD	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:766:MET:HE3	1:D:774:PHE:HE2	1.46	0.81
1:D:510:GLU:HB3	1:D:517:GLN:HE22	1.45	0.80
1:A:157:TYR:HD2	1:A:303:THR:CG2	1.86	0.80
1:A:274:ASN:CA	1:A:277:ARG:HG3	2.12	0.79
1:B:766:MET:HA	1:B:766:MET:HE2	1.63	0.79
1:D:491:TRP:HA	1:D:495:CYS:SG	2.22	0.79
1:C:284:ASN:ND2	1:C:285:PHE:N	2.30	0.79
1:A:555:VAL:HB	1:A:557:ILE:HD13	1.64	0.79
1:D:21:VAL:HG12	1:D:22:GLU:N	1.98	0.79
1:B:280:TYR:OH	1:B:289:LYS:NZ	2.14	0.78
1:D:279:LEU:HD22	1:D:281:PRO:CG	2.13	0.78
1:D:754:GLN:NE2	1:D:757:LEU:HD13	1.98	0.78
1:C:284:ASN:CG	1:C:285:PHE:H	1.91	0.78
1:D:661:ASP:HB3	1:D:797:TRP:HH2	1.48	0.78
1:D:690:GLY:O	1:D:710:ILE:HA	1.83	0.78
1:A:256:ASP:HB3	1:A:258:ASN:ND2	1.97	0.78
1:A:326:PHE:HA	1:A:329:PHE:HB2	1.65	0.78
1:A:398:ARG:HA	1:A:401:GLN:HG3	1.64	0.78
1:A:102:LEU:HD23	1:A:104:LEU:HD21	1.65	0.78
1:B:88:GLU:HG3	1:B:132:GLY:HA2	1.66	0.78
1:A:294:LYS:HE2	1:A:395:LEU:HD21	1.63	0.77
1:A:157:TYR:CD2	1:A:303:THR:HG23	2.20	0.77
1:B:456:ALA:HB2	1:B:674:SER:HB2	1.67	0.77
1:C:279:LEU:HD23	1:C:281:PRO:CD	2.11	0.77
1:D:645:LEU:HD11	1:D:656:VAL:HG21	1.66	0.77
1:C:235:ASN:H	1:C:235:ASN:HD22	1.32	0.77
1:C:349:LEU:O	1:C:353:LEU:HG	1.83	0.77
1:C:196:PHE:CB	1:C:309:ARG:HH12	1.93	0.77
1:A:21:VAL:HB	1:A:23:ASN:HD22	1.50	0.77
1:C:284:ASN:O	1:C:285:PHE:CB	2.32	0.77
1:C:282:ASN:O	1:C:284:ASN:N	2.17	0.77
1:D:284:ASN:ND2	1:D:285:PHE:H	1.81	0.77
1:D:510:GLU:HB3	1:D:517:GLN:NE2	2.00	0.77
1:A:319:ARG:HD3	1:A:332:LYS:NZ	2.00	0.76
1:C:279:LEU:HD23	1:C:281:PRO:HD3	1.65	0.76
1:C:279:LEU:CD2	1:C:281:PRO:HD2	2.14	0.76
1:D:455:VAL:H	1:D:459:HIS:HD2	1.33	0.76
1:C:766:MET:HE3	1:C:774:PHE:HE2	1.50	0.76
1:C:547:ALA:O	1:C:551:ARG:HB2	1.85	0.75
1:D:280:TYR:N	1:D:281:PRO:HD2	2.01	0.75
1:A:555:VAL:HB	1:A:557:ILE:CD1	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:GLY:H	1:D:617:LYS:HE2	1.51	0.75
1:A:685:GLY:HA2	1:A:805:ILE:HD11	1.68	0.75
1:A:718:VAL:HG22	1:A:772:LYS:HE2	1.68	0.75
1:A:765:LEU:HG	1:A:774:PHE:HE1	1.51	0.75
1:C:24:VAL:CA	1:C:25:THR:N	2.49	0.75
1:D:519:ARG:HA	1:D:806:ALA:HB1	1.68	0.75
1:B:284:ASN:ND2	1:B:285:PHE:N	2.33	0.75
1:C:790:LEU:HD21	1:C:800:MET:HE3	1.68	0.75
1:A:557:ILE:HD11	1:A:643:ILE:HD11	1.68	0.75
1:B:284:ASN:CG	1:B:285:PHE:H	1.94	0.75
1:A:703:ALA:HB2	1:A:807:THR:HG21	1.68	0.75
1:D:251:ASP:CG	1:D:255:LYS:HE2	2.12	0.75
1:D:692:MET:HB2	1:D:714:ARG:HD2	1.67	0.75
1:B:486:ILE:HD13	1:B:679:MET:HB2	1.69	0.75
1:D:284:ASN:O	1:D:285:PHE:CB	2.35	0.74
1:B:282:ASN:O	1:B:284:ASN:N	2.19	0.74
1:A:221:VAL:HG13	1:A:272:ALA:HB1	1.67	0.74
1:D:373:ALA:HA	1:D:449:SER:HB3	1.69	0.74
1:C:357:GLU:O	1:C:358:ARG:HD3	1.87	0.74
1:D:219:GLN:HE21	1:D:268:ASP:CG	1.95	0.74
1:B:22:GLU:OE1	1:B:62:HIS:CD2	2.41	0.74
1:C:19:ALA:C	1:C:21:VAL:H	1.89	0.74
1:C:319:ARG:HD3	1:C:332:LYS:HE2	1.70	0.74
1:D:279:LEU:CD2	1:D:281:PRO:CG	2.66	0.74
1:A:74:TYR:OH	1:A:153:ALA:HA	1.88	0.73
1:A:316:PHE:HZ	1:A:332:LYS:HE2	1.53	0.73
1:C:23:ASN:C	1:C:25:THR:N	2.46	0.73
1:A:648:TYR:HA	1:A:652:LEU:HD12	1.68	0.73
1:A:756:ASP:O	1:A:759:LYS:HB2	1.88	0.73
1:C:32:ASN:HD21	1:D:13:ILE:HA	1.53	0.73
1:D:64:VAL:HG12	1:D:67:TRP:CE3	2.23	0.73
1:D:279:LEU:HD13	1:D:281:PRO:HG2	1.69	0.73
1:D:565:VAL:HG21	1:D:681:PHE:HE1	1.54	0.73
1:B:379:VAL:HG12	1:B:380:ILE:HG23	1.71	0.72
1:C:677:GLY:HA2	1:C:680:LYS:HE2	1.70	0.72
1:D:129:ALA:HB1	1:D:131:LEU:HD23	1.71	0.72
1:A:139:LEU:HD11	1:A:484:ASN:ND2	2.04	0.72
1:D:183:LEU:HD23	1:D:187:ASN:HB3	1.71	0.72
1:A:316:PHE:CZ	1:A:332:LYS:CE	2.73	0.72
1:A:482:LYS:HE3	1:A:819:GLN:O	1.89	0.72
1:B:369:VAL:O	1:B:450:HIS:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:CE2	1:A:332:LYS:CE	2.72	0.72
1:A:413:ARG:NH2	1:A:475:GLU:HG3	2.05	0.71
1:D:98:THR:O	1:D:102:LEU:HB2	1.90	0.71
1:D:251:ASP:OD1	1:D:255:LYS:CD	2.37	0.71
1:B:506:ARG:HG2	1:B:530:PHE:CE1	2.25	0.71
1:D:713:MET:HG2	1:D:718:VAL:HG23	1.70	0.71
1:A:555:VAL:CG2	1:A:643:ILE:CD1	2.63	0.71
1:C:530:PHE:HE1	1:C:802:ILE:HG12	1.56	0.71
1:D:64:VAL:HG12	1:D:67:TRP:HE3	1.56	0.71
1:A:157:TYR:HD2	1:A:303:THR:HG23	1.53	0.71
1:A:157:TYR:CE2	1:A:303:THR:HG22	2.25	0.71
1:D:280:TYR:H	1:D:281:PRO:HD2	1.56	0.71
1:D:279:LEU:CD1	1:D:281:PRO:HG2	2.21	0.71
1:D:284:ASN:CG	1:D:285:PHE:H	1.99	0.71
1:D:350:MET:O	1:D:354:VAL:HG23	1.90	0.71
1:C:336:GLN:NE2	1:C:825:TRP:HE1	1.89	0.71
1:B:81:ARG:HD3	1:B:155:TYR:CE1	2.26	0.71
1:B:164:GLY:O	1:B:279:LEU:HB2	1.90	0.71
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.72	0.70
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.73	0.70
1:C:280:TYR:H	1:C:281:PRO:CD	2.03	0.70
1:B:81:ARG:HG2	1:B:153:ALA:HB1	1.74	0.70
1:B:284:ASN:O	1:B:285:PHE:CB	2.37	0.70
1:A:422:VAL:HA	1:A:425:LEU:HD12	1.73	0.70
1:A:653:ALA:HA	1:A:656:VAL:HG12	1.73	0.70
1:A:168:GLN:OE1	1:A:608:LYS:HA	1.92	0.70
1:A:319:ARG:HD3	1:A:332:LYS:HZ2	1.54	0.70
1:A:601:ARG:HH22	1:A:784:GLN:HE22	1.40	0.70
1:C:729:GLN:HA	1:C:732:TYR:HB3	1.72	0.69
1:D:341:HIS:HB2	1:D:342:PRO:HD3	1.74	0.69
1:D:386:ARG:HG3	1:D:440:ASN:HA	1.73	0.69
1:A:162:GLU:OE2	1:A:277:ARG:NH2	2.25	0.69
1:C:70:THR:HG22	1:C:74:TYR:CZ	2.28	0.69
1:D:204:GLY:HA2	1:D:217:ASP:O	1.93	0.69
1:A:698:GLU:HA	1:A:701:GLU:HG3	1.74	0.69
1:B:17:GLY:H	1:B:18:LEU:HD22	1.56	0.69
1:C:315:LYS:HE2	1:C:318:CYS:SG	2.33	0.69
1:D:284:ASN:ND2	1:D:285:PHE:N	2.40	0.69
1:D:758:PHE:HD1	1:D:761:ILE:HD11	1.56	0.69
1:A:316:PHE:CZ	1:A:332:LYS:NZ	2.57	0.69
1:B:18:LEU:H	1:B:18:LEU:CD2	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LEU:O	1:B:521:LEU:HB3	1.92	0.68
1:A:42:ASP:OD1	1:A:44:ASN:N	2.26	0.68
1:A:27:LEU:HD21	1:A:62:HIS:HE1	1.58	0.68
1:A:86:SER:HB3	1:A:89:PHE:HE1	1.58	0.68
1:D:235:ASN:HB2	1:D:833:ARG:HA	1.75	0.68
1:C:360:ASP:N	1:C:360:ASP:OD1	2.25	0.68
1:D:24:VAL:HG12	1:D:28:LYS:HE2	1.76	0.68
1:D:661:ASP:HB3	1:D:797:TRP:CH2	2.29	0.68
1:B:102:LEU:HB3	1:B:104:LEU:HD13	1.74	0.68
1:D:713:MET:HG3	1:D:717:ASP:HB2	1.75	0.68
1:A:99:MET:HE1	1:A:119:MET:SD	2.34	0.68
1:B:515:LEU:HB3	1:B:809:GLY:HA2	1.74	0.68
1:D:688:THR:HB	1:D:708:PHE:CE1	2.28	0.68
1:B:280:TYR:N	1:B:281:PRO:CD	2.53	0.68
1:B:286:PHE:O	1:B:287:GLU:HG2	1.94	0.68
1:A:27:LEU:HD21	1:A:62:HIS:CE1	2.29	0.67
1:A:307:ILE:HD13	1:A:335:ILE:HD11	1.77	0.67
1:A:732:TYR:CE1	1:A:739:ARG:HG2	2.29	0.67
1:B:459:HIS:HB2	1:B:673:ALA:O	1.94	0.67
1:B:502:ILE:HA	1:B:505:GLU:HB2	1.74	0.67
1:C:320:ASP:HA	1:C:324:THR:HA	1.77	0.67
1:A:522:LEU:O	1:A:525:VAL:HG23	1.93	0.67
1:A:629:VAL:HG11	1:A:750:PHE:HE1	1.59	0.67
1:B:22:GLU:OE2	1:B:104:LEU:HD11	1.93	0.67
1:B:70:THR:HG22	1:B:74:TYR:CE2	2.29	0.67
1:B:273:GLU:HG2	1:B:277:ARG:HH21	1.58	0.67
1:D:88:GLU:OE1	1:D:133:ASN:N	2.27	0.67
1:D:322:VAL:O	1:D:325:ASN:HB2	1.95	0.67
1:A:110:GLU:HG3	1:A:114:GLN:NE2	2.10	0.67
1:C:136:LEU:HD11	1:C:338:ASN:OD1	1.94	0.67
1:B:93:ARG:HG2	1:B:126:GLU:HB3	1.77	0.67
1:C:737:GLU:O	1:C:740:GLN:HB3	1.95	0.67
1:A:550:GLU:HA	1:A:554:LYS:HA	1.77	0.67
1:C:283:ASP:CG	1:C:383:ALA:HB1	2.20	0.67
1:D:571:HIS:ND1	1:D:573:TYR:HD1	1.91	0.67
1:A:194:PRO:HA	1:A:224:MET:SD	2.35	0.66
1:C:592:LYS:HG3	1:C:593:GLU:HG3	1.77	0.66
1:D:688:THR:HB	1:D:708:PHE:HE1	1.60	0.66
1:C:525:VAL:HG12	1:C:799:ARG:HD2	1.77	0.66
1:D:138:ARG:HH11	1:D:138:ARG:HG3	1.60	0.66
1:C:131:LEU:HD21	1:C:243:LEU:HD21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:ASN:ND2	1:C:695:ALA:HB3	2.10	0.66
1:A:347:PRO:HD3	1:A:444:LEU:HD21	1.77	0.66
1:C:252:PHE:CZ	1:C:269:ARG:HB3	2.30	0.66
1:C:323:ARG:CZ	1:C:323:ARG:HB3	2.26	0.66
1:D:138:ARG:NH1	1:D:142:CYS:SG	2.68	0.66
1:C:663:SER:HB3	1:C:681:PHE:CD1	2.30	0.66
1:D:88:GLU:HG2	1:D:132:GLY:HA2	1.76	0.66
1:B:522:LEU:HD13	1:B:806:ALA:HB3	1.77	0.66
1:D:17:GLY:C	1:D:18:LEU:HD13	2.20	0.66
1:C:742:ILE:HD11	1:C:774:PHE:HZ	1.60	0.66
1:D:74:TYR:HD1	1:D:79:PRO:HG3	1.60	0.66
1:D:68:ILE:HG22	1:D:72:GLN:OE1	1.96	0.65
1:A:115:LEU:HD22	1:B:13:ILE:HG13	1.78	0.65
1:A:381:PRO:HB3	1:A:467:ILE:HD12	1.77	0.65
1:B:263:ILE:HG21	1:B:266:VAL:HG23	1.79	0.65
1:D:738:LEU:HA	1:D:741:ILE:HG12	1.78	0.65
1:C:91:MET:HE1	1:C:144:LEU:HD12	1.77	0.65
1:D:756:ASP:O	1:D:759:LYS:HB2	1.96	0.65
1:D:395:LEU:HD23	1:D:396:LEU:HD22	1.78	0.65
1:B:455:VAL:HG12	1:B:674:SER:HB3	1.79	0.65
1:C:534:VAL:O	1:C:537:VAL:HB	1.96	0.65
1:D:796:GLU:HA	1:D:799:ARG:HG3	1.78	0.65
1:A:136:LEU:HG	1:A:338:ASN:HD21	1.61	0.65
1:C:143:PHE:HB3	1:C:147:MET:HE2	1.77	0.65
1:A:102:LEU:HD23	1:A:104:LEU:CD2	2.26	0.65
1:D:721:LEU:HG	1:D:726:TYR:HB2	1.79	0.65
1:C:459:HIS:CE1	1:C:463:LEU:HD21	2.32	0.64
1:C:480:GLN:HE22	1:C:823:GLU:HB3	1.62	0.64
1:D:351:ARG:O	1:D:355:ASP:HB2	1.97	0.64
1:A:23:ASN:HB3	1:A:25:THR:HB	1.79	0.64
1:D:410:PHE:O	1:D:414:VAL:HG23	1.96	0.64
1:A:337:LEU:HG	1:A:342:PRO:HB2	1.78	0.64
1:B:229:PRO:HA	1:B:239:ASN:O	1.98	0.64
1:B:455:VAL:H	1:B:459:HIS:HD2	1.44	0.64
1:C:21:VAL:CG1	1:C:22:GLU:HG2	2.27	0.64
1:B:139:LEU:HD11	1:B:143:PHE:CE1	2.33	0.64
1:D:103:ALA:HA	1:D:234:ARG:HH21	1.62	0.64
1:A:505:GLU:OE1	1:A:506:ARG:NH2	2.27	0.64
1:B:34:HIS:HA	1:B:38:THR:HB	1.78	0.64
1:A:87:LEU:HD22	1:A:341:HIS:HB3	1.80	0.64
1:B:138:ARG:NH1	1:B:491:TRP:HE1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:ASN:ND2	1:B:796:GLU:HB2	2.12	0.64
1:D:21:VAL:CG1	1:D:22:GLU:H	1.93	0.64
1:D:290:GLU:O	1:D:294:LYS:HB2	1.98	0.64
1:B:678:ASN:HB3	1:B:699:MET:HE1	1.79	0.64
1:B:24:VAL:HG21	1:B:110:GLU:HG2	1.79	0.63
1:B:133:ASN:ND2	1:B:281:PRO:HB3	2.14	0.63
1:B:630:VAL:HG23	1:B:636:VAL:HG11	1.79	0.63
1:D:502:ILE:HG13	1:D:503:ILE:H	1.62	0.63
1:D:603:VAL:HG23	1:D:641:ARG:O	1.98	0.63
1:C:326:PHE:HA	1:C:329:PHE:HB2	1.80	0.63
1:B:81:ARG:HD3	1:B:155:TYR:HE1	1.63	0.63
1:C:133:ASN:OD1	1:C:165:ILE:HG21	1.97	0.63
1:D:682:MET:HG2	1:D:808:SER:OG	1.99	0.63
1:A:209:THR:HG23	1:A:212:GLY:H	1.63	0.63
1:C:20:GLY:HA3	1:C:26:GLU:HG3	1.80	0.63
1:C:316:PHE:HA	1:C:319:ARG:HB2	1.80	0.63
1:C:718:VAL:HG13	1:C:772:LYS:HE2	1.81	0.63
1:D:735:ILE:HG22	1:D:738:LEU:H	1.63	0.63
1:A:269:ARG:NH2	1:A:273:GLU:OE1	2.31	0.63
1:D:502:ILE:HG13	1:D:503:ILE:N	2.14	0.63
1:B:793:ASN:HD21	1:B:796:GLU:HB2	1.62	0.63
1:C:24:VAL:CG1	1:C:28:LYS:HE2	2.17	0.63
1:C:588:ASN:HD21	1:C:744:GLN:HE22	1.44	0.63
1:D:390:HIS:CE1	1:D:391:LEU:HD12	2.33	0.63
1:A:78:ASP:OD2	1:A:332:LYS:NZ	2.31	0.63
1:D:555:VAL:HB	1:D:557:ILE:HD13	1.79	0.63
1:D:558:ASN:ND2	1:D:560:ASN:HB2	2.13	0.63
1:A:74:TYR:HD1	1:A:79:PRO:HG3	1.63	0.62
1:B:133:ASN:ND2	1:B:281:PRO:CG	2.62	0.62
1:B:170:ILE:HG12	1:B:646:GLU:HG3	1.82	0.62
1:D:281:PRO:HD3	1:D:292:ARG:HH12	1.64	0.62
1:D:629:VAL:HG12	1:D:630:VAL:N	2.12	0.62
1:D:631:ASN:HD21	1:D:642:VAL:H	1.45	0.62
1:A:21:VAL:HG11	1:A:23:ASN:HD21	1.62	0.62
1:B:12:GLN:HA	1:B:16:ARG:NH2	2.14	0.62
1:C:70:THR:HG22	1:C:74:TYR:CE2	2.34	0.62
1:D:74:TYR:CD1	1:D:79:PRO:HG3	2.33	0.62
1:A:32:ASN:ND2	1:B:13:ILE:HA	2.14	0.62
1:D:582:HIS:HA	1:D:585:THR:OG1	1.99	0.62
1:C:19:ALA:C	1:C:21:VAL:N	2.50	0.62
1:D:284:ASN:OD1	1:D:610:ALA:HB1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:LEU:O	1:D:399:HIS:HB2	1.99	0.62
1:B:515:LEU:HD22	1:B:812:SER:HB2	1.81	0.62
1:C:130:GLY:O	1:C:164:GLY:HA2	2.00	0.62
1:C:317:GLY:HA2	1:C:320:ASP:HB2	1.82	0.62
1:B:729:GLN:HA	1:B:732:TYR:HB3	1.81	0.62
1:C:224:MET:HE3	1:C:226:TYR:CE1	2.34	0.62
1:C:687:LEU:HD12	1:C:797:TRP:CZ2	2.35	0.62
1:B:204:GLY:HA2	1:B:217:ASP:O	2.00	0.62
1:C:64:VAL:HG12	1:C:67:TRP:HE3	1.64	0.62
1:C:615:MET:HE1	1:C:761:ILE:HG12	1.81	0.62
1:A:115:LEU:HD22	1:B:13:ILE:CG1	2.29	0.62
1:A:721:LEU:HD21	1:A:726:TYR:CD1	2.35	0.62
1:B:590:ILE:HG22	1:B:636:VAL:HG22	1.81	0.62
1:D:75:TYR:OH	1:D:315:LYS:HG3	2.00	0.62
1:D:662:LEU:HD22	1:D:689:ILE:HG22	1.81	0.62
1:C:284:ASN:HD22	1:C:285:PHE:N	1.96	0.62
1:C:335:ILE:HG13	1:C:371:THR:HG22	1.82	0.62
1:D:486:ILE:HG12	1:D:680:LYS:HG3	1.83	0.61
1:B:133:ASN:ND2	1:B:281:PRO:CB	2.64	0.61
1:B:685:GLY:HA2	1:B:801:VAL:HG13	1.81	0.61
1:C:196:PHE:HB3	1:C:309:ARG:CZ	2.29	0.61
1:D:732:TYR:HB2	1:D:766:MET:HE1	1.82	0.61
1:A:430:LEU:N	1:A:430:LEU:CD2	2.62	0.61
1:B:739:ARG:HG3	1:B:739:ARG:HH11	1.64	0.61
1:C:133:ASN:OD1	1:C:165:ILE:CG2	2.48	0.61
1:D:219:GLN:NE2	1:D:268:ASP:OD1	2.33	0.61
1:A:67:TRP:CZ3	1:A:229:PRO:HG3	2.36	0.61
1:A:316:PHE:CE2	1:A:332:LYS:HE2	2.34	0.61
1:C:379:VAL:HG11	1:C:671:THR:O	1.99	0.61
1:A:21:VAL:C	1:A:22:GLU:HG2	2.26	0.61
1:A:568:LYS:O	1:A:607:GLY:HA3	2.01	0.61
1:B:251:ASP:HB3	1:B:255:LYS:HB2	1.82	0.61
1:C:235:ASN:OD1	1:C:237:VAL:HG22	2.00	0.61
1:D:326:PHE:O	1:D:330:PRO:HD3	1.99	0.61
1:D:678:ASN:HB3	1:D:699:MET:HE1	1.82	0.61
1:A:181:ASP:O	1:A:184:ARG:HB2	2.00	0.61
1:A:459:HIS:O	1:A:462:ILE:HG12	2.00	0.61
1:A:515:LEU:HB3	1:A:809:GLY:HA2	1.83	0.61
1:B:506:ARG:HG2	1:B:530:PHE:HE1	1.65	0.61
1:C:193:ARG:HD2	1:C:196:PHE:HE2	1.65	0.61
1:B:17:GLY:N	1:B:18:LEU:HD22	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LEU:HG	1:C:683:LEU:HD22	1.83	0.61
1:C:522:LEU:O	1:C:525:VAL:HG23	2.01	0.61
1:B:251:ASP:HB3	1:B:255:LYS:HG3	1.83	0.61
1:C:24:VAL:C	1:C:25:THR:CA	2.73	0.61
1:C:689:ILE:HA	1:C:709:PHE:HB2	1.82	0.61
1:C:588:ASN:HD21	1:C:744:GLN:NE2	1.99	0.61
1:C:678:ASN:O	1:C:681:PHE:HB2	2.01	0.61
1:A:119:MET:O	1:A:123:GLU:HG3	2.01	0.60
1:B:233:TYR:CZ	1:B:234:ARG:HD3	2.36	0.60
1:C:486:ILE:O	1:C:812:SER:HA	2.01	0.60
1:D:711:PHE:CE2	1:D:780:TYR:HB2	2.36	0.60
1:A:18:LEU:HD22	1:A:18:LEU:N	2.15	0.60
1:A:157:TYR:CD2	1:A:303:THR:HG21	2.33	0.60
1:C:456:ALA:O	1:C:460:SER:HB2	2.00	0.60
1:D:280:TYR:HE2	1:D:289:LYS:CE	2.15	0.60
1:D:552:GLU:O	1:D:553:TYR:CD1	2.54	0.60
1:D:575:ARG:HB3	1:D:578:LEU:HB2	1.82	0.60
1:D:583:VAL:HG21	1:D:603:VAL:HG21	1.82	0.60
1:A:21:VAL:CG1	1:A:23:ASN:HD22	2.09	0.60
1:C:70:THR:O	1:C:73:HIS:HB3	2.02	0.60
1:D:458:ILE:HD11	1:D:694:GLY:HA2	1.84	0.60
1:A:322:VAL:O	1:A:325:ASN:HB2	2.01	0.60
1:A:336:GLN:NE2	1:A:825:TRP:HE1	2.00	0.60
1:B:280:TYR:H	1:B:281:PRO:HD2	1.60	0.60
1:A:765:LEU:HG	1:A:774:PHE:CE1	2.33	0.60
1:B:284:ASN:HD22	1:B:285:PHE:N	2.00	0.60
1:B:761:ILE:HG22	1:B:765:LEU:HD22	1.84	0.60
1:C:590:ILE:HD13	1:C:639:ARG:HB3	1.84	0.60
1:C:280:TYR:HE2	1:C:289:LYS:CE	2.15	0.60
1:C:678:ASN:HD22	1:C:699:MET:HE1	1.67	0.60
1:D:504:ALA:HA	1:D:508:GLY:H	1.66	0.60
1:A:721:LEU:HD21	1:A:726:TYR:HD1	1.66	0.60
1:B:138:ARG:NH1	1:B:142:CYS:SG	2.75	0.60
1:B:262:TYR:HB3	1:B:264:GLN:OE1	2.02	0.60
1:D:256:ASP:HB3	1:D:258:ASN:ND2	2.16	0.60
1:D:716:GLU:O	1:D:720:ARG:HG2	2.02	0.60
1:C:262:TYR:HB3	1:C:264:GLN:OE1	2.02	0.59
1:B:581:LEU:HD13	1:B:738:LEU:HD11	1.84	0.59
1:C:682:MET:SD	1:C:699:MET:HG2	2.42	0.59
1:B:161:TYR:HE1	1:B:295:GLN:HE22	1.50	0.59
1:B:227:ASP:OD1	1:B:242:ARG:HD3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:HB2	1:B:234:ARG:HE	1.66	0.59
1:B:294:LYS:HG3	1:B:395:LEU:HD21	1.84	0.59
1:B:499:LEU:O	1:B:503:ILE:HG13	2.02	0.59
1:D:24:VAL:HG13	1:D:111:ALA:HA	1.84	0.59
1:D:754:GLN:NE2	1:D:757:LEU:HD11	2.15	0.59
1:C:555:VAL:HG21	1:C:643:ILE:HD12	1.83	0.59
1:C:687:LEU:HD12	1:C:797:TRP:CE2	2.38	0.59
1:C:699:MET:HB3	1:C:708:PHE:HE2	1.67	0.59
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.02	0.59
1:A:203:TYR:O	1:A:218:THR:HG22	2.03	0.59
1:B:12:GLN:HA	1:B:16:ARG:HH22	1.68	0.59
1:B:49:ARG:O	1:B:52:TYR:HB3	2.02	0.59
1:A:110:GLU:HG3	1:A:114:GLN:HE21	1.66	0.59
1:A:730:GLU:O	1:A:734:ARG:CD	2.50	0.59
1:B:665:GLN:CD	1:B:678:ASN:OD1	2.46	0.59
1:C:389:VAL:HG12	1:C:439:ILE:HG13	1.84	0.59
1:D:21:VAL:HA	1:D:62:HIS:HE2	1.68	0.59
1:A:23:ASN:HB3	1:A:26:GLU:H	1.67	0.59
1:B:507:ILE:HD13	1:B:521:LEU:HB2	1.85	0.59
1:C:387:TRP:CD1	1:C:441:MET:HE2	2.38	0.59
1:D:348:GLU:O	1:D:352:VAL:HG23	2.03	0.59
1:A:322:VAL:HG21	1:A:327:ASP:OD2	2.02	0.59
1:B:171:CYS:O	1:B:174:TRP:HB2	2.03	0.59
1:C:152:LEU:HD22	1:C:827:VAL:HG21	1.85	0.59
1:C:761:ILE:O	1:C:765:LEU:HB2	2.02	0.58
1:B:196:PHE:HB3	1:B:309:ARG:NH2	2.17	0.58
1:B:258:ASN:OD1	1:B:259:VAL:HG22	2.02	0.58
1:C:730:GLU:O	1:C:734:ARG:HG3	2.01	0.58
1:B:687:LEU:HD21	1:B:800:MET:HB3	1.83	0.58
1:C:381:PRO:HD3	1:C:467:ILE:HD12	1.84	0.58
1:C:751:SER:N	1:C:752:PRO:HD2	2.18	0.58
1:A:158:GLY:O	1:A:243:LEU:HA	2.03	0.58
1:D:18:LEU:HD13	1:D:18:LEU:N	2.18	0.58
1:D:636:VAL:O	1:D:639:ARG:HB2	2.02	0.58
1:D:665:GLN:NE2	1:D:678:ASN:HA	2.18	0.58
1:A:746:SER:HB3	1:A:762:VAL:HG21	1.85	0.58
1:B:685:GLY:HA2	1:B:801:VAL:CG1	2.34	0.58
1:B:833:ARG:HB2	1:B:833:ARG:CZ	2.33	0.58
1:C:280:TYR:HE2	1:C:289:LYS:HE3	1.67	0.58
1:D:22:GLU:OE1	1:D:22:GLU:HA	2.03	0.58
1:A:24:VAL:O	1:A:28:LYS:N	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ARG:HG3	1:C:806:ALA:O	2.03	0.58
1:D:53:PHE:HE1	1:D:188:PRO:HD3	1.69	0.58
1:D:594:PRO:O	1:D:639:ARG:NH2	2.36	0.58
1:D:810:LYS:HG3	1:D:811:PHE:CE1	2.39	0.58
1:A:430:LEU:N	1:A:430:LEU:HD23	2.18	0.58
1:C:573:TYR:CE2	1:C:672:GLU:OE1	2.57	0.58
1:B:96:GLN:HG2	1:B:494:LEU:HD11	1.84	0.58
1:B:136:LEU:HD11	1:B:338:ASN:HD21	1.69	0.58
1:C:23:ASN:HB2	1:C:26:GLU:H	1.68	0.58
1:D:110:GLU:HA	1:D:113:TYR:HD2	1.68	0.58
1:A:48:PRO:HB2	1:A:125:ILE:HD12	1.85	0.58
1:D:430:LEU:O	1:D:439:ILE:HA	2.01	0.58
1:A:366:GLU:HG2	1:A:370:LYS:HD2	1.86	0.58
1:C:742:ILE:HD11	1:C:774:PHE:CZ	2.38	0.58
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.68	0.57
1:C:10:ARG:N	1:C:13:ILE:HD12	2.20	0.57
1:D:279:LEU:HD22	1:D:281:PRO:HG2	1.87	0.57
1:D:700:ALA:HB2	1:D:710:ILE:HD11	1.86	0.57
1:A:486:ILE:HD13	1:A:679:MET:HB2	1.86	0.57
1:C:15:VAL:O	1:C:18:LEU:HD22	2.03	0.57
1:A:326:PHE:CD1	1:A:359:LEU:HD11	2.39	0.57
1:D:280:TYR:O	1:D:281:PRO:O	2.22	0.57
1:D:645:LEU:CD1	1:D:656:VAL:HG21	2.34	0.57
1:A:136:LEU:HG	1:A:338:ASN:ND2	2.19	0.57
1:B:555:VAL:HG11	1:B:643:ILE:CD1	2.34	0.57
1:B:703:ALA:HB2	1:B:807:THR:HG21	1.87	0.57
1:D:225:PRO:HB3	1:D:244:TRP:CZ3	2.40	0.57
1:A:18:LEU:HD22	1:A:18:LEU:H	1.68	0.57
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.39	0.57
1:A:236:ASN:HB2	1:A:834:LEU:O	2.05	0.57
1:A:348:GLU:O	1:A:352:VAL:HG23	2.05	0.57
1:C:196:PHE:HB3	1:C:309:ARG:HH22	1.70	0.57
1:D:60:ARG:HD2	1:D:189:TRP:HA	1.86	0.57
1:D:235:ASN:HA	1:D:833:ARG:HG3	1.87	0.57
1:A:13:ILE:HD11	1:B:117:LEU:HD11	1.87	0.57
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.69	0.57
1:A:590:ILE:HG21	1:A:636:VAL:HG13	1.87	0.57
1:C:96:GLN:HA	1:C:99:MET:HE3	1.87	0.57
1:C:279:LEU:O	1:C:280:TYR:HD1	1.88	0.57
1:D:778:GLU:HB3	1:D:782:LYS:NZ	2.20	0.57
1:D:102:LEU:HB3	1:D:104:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ILE:HD11	1:A:598:VAL:HG21	1.87	0.56
1:A:727:ASN:O	1:A:730:GLU:HG2	2.05	0.56
1:B:133:ASN:HD22	1:B:281:PRO:HB3	1.68	0.56
1:D:662:LEU:HD11	1:D:784:GLN:HE22	1.69	0.56
1:D:575:ARG:HG2	1:D:578:LEU:HD22	1.87	0.56
1:A:274:ASN:HA	1:A:277:ARG:CG	2.27	0.56
1:B:233:TYR:CE2	1:B:234:ARG:HD3	2.39	0.56
1:B:323:ARG:HG2	1:B:325:ASN:HB2	1.87	0.56
1:B:566:GLN:HB2	1:B:664:GLU:CB	2.30	0.56
1:B:592:LYS:O	1:B:594:PRO:HD3	2.04	0.56
1:B:612:GLY:H	1:B:617:LYS:HE2	1.69	0.56
1:B:716:GLU:O	1:B:720:ARG:HG2	2.05	0.56
1:C:21:VAL:HG12	1:C:22:GLU:CG	2.33	0.56
1:C:351:ARG:HD3	1:C:399:HIS:CE1	2.40	0.56
1:C:574:LYS:HB2	1:C:576:GLN:NE2	2.20	0.56
1:D:549:LEU:HD23	1:D:557:ILE:HG12	1.86	0.56
1:D:781:VAL:O	1:D:784:GLN:HB2	2.06	0.56
1:B:280:TYR:HE2	1:B:289:LYS:CE	2.11	0.56
1:C:515:LEU:HB3	1:C:809:GLY:HA2	1.86	0.56
1:C:636:VAL:O	1:C:639:ARG:HD3	2.05	0.56
1:C:801:VAL:O	1:C:805:ILE:HG13	2.06	0.56
1:B:10:ARG:N	1:B:13:ILE:HD12	2.21	0.56
1:B:365:TRP:O	1:B:369:VAL:HG12	2.06	0.56
1:C:390:HIS:CD2	1:C:436:VAL:HG21	2.40	0.56
1:C:407:ASN:O	1:C:411:LEU:HG	2.06	0.56
1:A:357:GLU:O	1:A:358:ARG:HB2	2.06	0.56
1:A:629:VAL:HG12	1:A:630:VAL:N	2.21	0.56
1:D:563:PHE:HD2	1:D:659:ALA:O	1.87	0.56
1:D:707:ASN:OD1	1:D:800:MET:SD	2.64	0.56
1:B:138:ARG:CZ	1:B:142:CYS:SG	2.94	0.56
1:C:21:VAL:HG12	1:C:22:GLU:N	2.20	0.56
1:C:455:VAL:HG22	1:C:484:ASN:OD1	2.06	0.56
1:A:755:PRO:C	1:A:756:ASP:CA	2.72	0.56
1:B:689:ILE:HA	1:B:709:PHE:O	2.06	0.56
1:C:196:PHE:HB3	1:C:309:ARG:NH2	2.20	0.56
1:D:370:LYS:HA	1:D:450:HIS:HD2	1.70	0.56
1:D:542:LYS:HE3	1:D:563:PHE:CE2	2.41	0.56
1:A:155:TYR:CE1	1:A:240:THR:HB	2.41	0.56
1:B:293:LEU:HD21	1:B:392:LEU:HD12	1.88	0.56
1:C:43:ARG:HG3	1:D:13:ILE:O	2.05	0.56
1:D:279:LEU:CD2	1:D:281:PRO:HG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:TYR:HB2	1:D:640:LEU:HD12	1.88	0.56
1:D:587:TYR:O	1:D:591:LYS:HG2	2.06	0.56
1:A:88:GLU:HG2	1:A:132:GLY:CA	2.36	0.55
1:B:390:HIS:CE1	1:B:391:LEU:HD12	2.41	0.55
1:B:550:GLU:HA	1:B:554:LYS:HA	1.88	0.55
1:A:521:LEU:HD21	1:A:530:PHE:HZ	1.70	0.55
1:A:636:VAL:O	1:A:639:ARG:HB2	2.07	0.55
1:C:32:ASN:ND2	1:D:13:ILE:HA	2.19	0.55
1:C:192:ALA:HA	1:C:226:TYR:HA	1.88	0.55
1:C:399:HIS:O	1:C:403:ILE:HG13	2.07	0.55
1:D:85:LEU:HD22	1:D:342:PRO:HB3	1.89	0.55
1:D:739:ARG:HH11	1:D:739:ARG:HG3	1.71	0.55
1:A:235:ASN:OD1	1:A:237:VAL:HG22	2.07	0.55
1:A:609:ALA:HB2	1:A:620:ILE:CD1	2.36	0.55
1:C:280:TYR:O	1:C:281:PRO:O	2.25	0.55
1:D:489:ARG:HD3	1:D:489:ARG:N	2.22	0.55
1:D:509:GLU:OE1	1:D:510:GLU:CA	2.54	0.55
1:A:428:MET:HE1	1:A:474:LEU:HD12	1.89	0.55
1:C:263:ILE:HB	1:C:266:VAL:HG23	1.88	0.55
1:C:573:TYR:HE2	1:C:672:GLU:OE1	1.88	0.55
1:D:499:LEU:O	1:D:503:ILE:HD12	2.07	0.55
1:D:545:PHE:CZ	1:D:656:VAL:HG23	2.41	0.55
1:B:171:CYS:SG	1:B:176:MET:HG2	2.46	0.55
1:B:322:VAL:HG22	1:B:323:ARG:NH1	2.22	0.55
1:A:129:ALA:HA	1:A:182:TRP:CZ3	2.42	0.55
1:A:720:ARG:HG3	1:A:720:ARG:HH11	1.72	0.55
1:B:766:MET:HA	1:B:766:MET:CE	2.36	0.55
1:A:83:TYR:OH	1:A:310:ARG:HD2	2.06	0.55
1:A:731:TYR:HA	1:A:734:ARG:HD3	1.89	0.55
1:B:30:ASN:HB2	1:B:58:THR:HG23	1.88	0.55
1:D:455:VAL:HG22	1:D:484:ASN:OD1	2.06	0.55
1:D:513:SER:C	1:D:831:ARG:HH21	2.14	0.55
1:A:139:LEU:HD21	1:A:484:ASN:HD21	1.72	0.54
1:A:388:PRO:HB2	1:A:390:HIS:CD2	2.43	0.54
1:B:466:THR:OG1	1:B:467:ILE:HD13	2.07	0.54
1:B:530:PHE:CE2	1:B:534:VAL:HG23	2.41	0.54
1:D:24:VAL:O	1:D:25:THR:O	2.24	0.54
1:A:461:GLU:HB3	1:A:465:LYS:NZ	2.23	0.54
1:B:15:VAL:O	1:B:17:GLY:N	2.38	0.54
1:D:279:LEU:HD22	1:D:280:TYR:N	2.22	0.54
1:D:562:LEU:HB3	1:D:601:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:OG1	1:A:385:GLU:HB2	2.07	0.54
1:A:459:HIS:HA	1:A:462:ILE:HD11	1.89	0.54
1:A:613:TYR:CD2	1:A:616:ALA:HB2	2.43	0.54
1:C:23:ASN:O	1:C:26:GLU:N	2.40	0.54
1:C:378:THR:O	1:C:459:HIS:HE1	1.91	0.54
1:D:237:VAL:HG12	1:D:834:LEU:HD13	1.88	0.54
1:A:165:ILE:HD12	1:A:166:PHE:CD1	2.43	0.54
1:C:366:GLU:HG2	1:C:370:LYS:HE2	1.88	0.54
1:C:605:ILE:HG21	1:C:623:ILE:HD13	1.89	0.54
1:B:555:VAL:HG11	1:B:643:ILE:HD11	1.88	0.54
1:B:756:ASP:O	1:B:759:LYS:HB2	2.06	0.54
1:D:280:TYR:O	1:D:281:PRO:C	2.50	0.54
1:D:390:HIS:CE1	1:D:391:LEU:CD1	2.90	0.54
1:D:489:ARG:HD3	1:D:489:ARG:H	1.71	0.54
1:D:713:MET:HG3	1:D:717:ASP:CB	2.38	0.54
1:C:584:ILE:HD11	1:C:626:ILE:HD11	1.89	0.54
1:A:740:GLN:O	1:A:744:GLN:HG3	2.07	0.54
1:B:402:ILE:C	1:B:406:ILE:HG13	2.30	0.54
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.56	0.54
1:A:761:ILE:HG22	1:A:765:LEU:HD22	1.89	0.54
1:C:177:GLU:OE2	1:C:611:PRO:HB3	2.08	0.54
1:D:322:VAL:HG13	1:D:325:ASN:HB3	1.90	0.54
1:D:626:ILE:HG22	1:D:642:VAL:HG11	1.90	0.54
1:D:804:ASN:O	1:D:807:THR:HB	2.07	0.54
1:A:350:MET:HE2	1:A:365:TRP:CE3	2.43	0.54
1:A:682:MET:SD	1:A:699:MET:HG2	2.48	0.54
1:B:97:ASN:HD22	1:B:494:LEU:HD22	1.72	0.54
1:B:118:ASP:HB3	1:B:121:GLU:HB2	1.90	0.54
1:B:381:PRO:HB3	1:B:467:ILE:HG23	1.90	0.54
1:C:519:ARG:O	1:C:522:LEU:N	2.41	0.54
1:D:10:ARG:N	1:D:13:ILE:HD12	2.22	0.54
1:D:477:HIS:CD2	1:D:477:HIS:O	2.61	0.54
1:D:545:PHE:HD1	1:D:549:LEU:HD22	1.73	0.54
1:A:174:TRP:CH2	1:D:435:ALA:HA	2.43	0.54
1:A:316:PHE:CE1	1:A:319:ARG:HB3	2.43	0.54
1:A:385:GLU:O	1:A:386:ARG:HG3	2.08	0.54
1:B:578:LEU:O	1:B:581:LEU:N	2.41	0.54
1:B:707:ASN:HA	1:B:800:MET:SD	2.48	0.54
1:C:487:THR:HG23	1:C:489:ARG:HB2	1.89	0.54
1:D:565:VAL:CG2	1:D:660:ALA:HB1	2.38	0.54
1:A:13:ILE:HA	1:B:32:ASN:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:TYR:O	1:A:739:ARG:NH1	2.42	0.53
1:C:279:LEU:C	1:C:281:PRO:HD2	2.31	0.53
1:C:592:LYS:O	1:C:594:PRO:HD3	2.08	0.53
1:C:615:MET:HE2	1:C:764:MET:HG2	1.90	0.53
1:D:67:TRP:CE3	1:D:229:PRO:HB3	2.43	0.53
1:B:631:ASN:OD1	1:B:641:ARG:HA	2.08	0.53
1:C:369:VAL:O	1:C:450:HIS:HB3	2.07	0.53
1:A:555:VAL:HG21	1:A:557:ILE:HD11	1.89	0.53
1:A:687:LEU:HD13	1:A:709:PHE:HE1	1.73	0.53
1:B:196:PHE:HB3	1:B:309:ARG:HH22	1.73	0.53
1:B:698:GLU:O	1:B:702:GLU:HG2	2.08	0.53
1:C:387:TRP:HD1	1:C:441:MET:HE2	1.72	0.53
1:C:716:GLU:O	1:C:720:ARG:HG2	2.08	0.53
1:A:37:PHE:CZ	1:B:18:LEU:HB2	2.44	0.53
1:B:287:GLU:O	1:B:289:LYS:N	2.41	0.53
1:C:42:ASP:OD1	1:C:44:ASN:HB2	2.08	0.53
1:C:280:TYR:O	1:C:281:PRO:C	2.51	0.53
1:C:568:LYS:HE2	3:C:999:PLP:O3P	2.08	0.53
1:D:173:GLY:O	1:D:624:THR:HG21	2.08	0.53
1:D:424:ARG:NH2	1:D:473:GLU:CD	2.58	0.53
1:A:48:PRO:HB2	1:A:125:ILE:CD1	2.38	0.53
1:D:455:VAL:H	1:D:459:HIS:CD2	2.22	0.53
1:D:793:ASN:ND2	1:D:796:GLU:HB2	2.24	0.53
1:A:253:ASN:O	1:A:259:VAL:HG23	2.08	0.53
1:C:511:TYR:CD2	1:C:518:LEU:HD11	2.44	0.53
1:D:424:ARG:HA	1:D:427:ARG:HB2	1.90	0.53
1:D:515:LEU:HB3	1:D:809:GLY:HA2	1.91	0.53
1:B:296:GLU:O	1:B:299:VAL:HG12	2.08	0.53
1:B:640:LEU:HD23	1:B:641:ARG:H	1.74	0.53
1:C:13:ILE:HG23	1:D:32:ASN:ND2	2.23	0.53
1:C:319:ARG:NH2	1:C:328:ALA:HB1	2.23	0.53
1:C:323:ARG:HH21	1:C:325:ASN:ND2	2.06	0.53
1:D:164:GLY:O	1:D:279:LEU:HB2	2.09	0.53
1:A:11:LYS:HA	1:B:43:ARG:NH1	2.23	0.53
1:B:661:ASP:O	1:B:686:ALA:HA	2.08	0.53
1:D:555:VAL:HG12	1:D:556:HIS:H	1.74	0.53
1:D:621:LYS:HG3	1:D:758:PHE:HZ	1.72	0.53
1:A:174:TRP:CH2	1:A:618:MET:HE1	2.44	0.53
1:A:287:GLU:O	1:A:289:LYS:N	2.42	0.53
1:A:374:TYR:CD2	1:A:445:CYS:HB3	2.44	0.53
1:B:133:ASN:OD1	1:B:165:ILE:HG21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:SER:HB3	1:C:762:VAL:HG21	1.91	0.53
1:D:10:ARG:N	1:D:10:ARG:HD2	2.24	0.53
1:D:36:HIS:O	1:D:40:VAL:HA	2.08	0.53
1:D:450:HIS:HE1	1:D:824:ILE:HG22	1.74	0.53
1:D:720:ARG:HG3	1:D:720:ARG:NH1	2.12	0.53
1:A:525:VAL:O	1:A:531:ILE:HD11	2.09	0.52
1:C:316:PHE:CD1	1:C:319:ARG:HB3	2.44	0.52
1:C:720:ARG:HG3	1:C:720:ARG:NH1	2.24	0.52
1:D:198:LEU:HD11	1:D:309:ARG:NH2	2.24	0.52
1:D:338:ASN:OD1	1:D:377:HIS:HE1	1.93	0.52
1:B:133:ASN:ND2	1:B:281:PRO:HG3	2.24	0.52
1:B:423:ASP:O	1:B:426:ARG:HG3	2.09	0.52
1:C:224:MET:HE2	1:C:247:LYS:HE2	1.90	0.52
1:C:591:LYS:HD3	1:C:635:VAL:HB	1.91	0.52
1:D:713:MET:HE1	1:D:775:ALA:HB3	1.91	0.52
1:A:75:TYR:CE1	1:A:315:LYS:HG3	2.32	0.52
1:A:456:ALA:HA	1:A:483:THR:OG1	2.10	0.52
1:A:459:HIS:HA	1:A:462:ILE:CD1	2.39	0.52
1:B:381:PRO:HD3	1:B:467:ILE:HD12	1.91	0.52
1:B:396:LEU:HB3	1:B:399:HIS:CD2	2.45	0.52
1:B:503:ILE:HG23	1:B:507:ILE:HD11	1.90	0.52
1:B:703:ALA:CA	1:B:807:THR:HG21	2.39	0.52
1:B:707:ASN:HB3	1:B:800:MET:SD	2.50	0.52
1:C:24:VAL:O	1:C:28:LYS:N	2.32	0.52
1:D:284:ASN:HD22	1:D:285:PHE:N	2.05	0.52
1:A:316:PHE:CZ	1:A:319:ARG:HB3	2.44	0.52
1:A:601:ARG:HH22	1:A:784:GLN:NE2	2.06	0.52
1:B:52:TYR:HE1	1:B:95:LEU:HD12	1.74	0.52
1:C:10:ARG:O	1:C:13:ILE:HB	2.09	0.52
1:C:286:PHE:O	1:C:287:GLU:HG2	2.09	0.52
1:C:496:ASN:ND2	1:C:541:ASN:OD1	2.42	0.52
1:C:587:TYR:CD1	1:C:630:VAL:HG12	2.45	0.52
1:D:47:THR:HG22	1:D:48:PRO:HD2	1.92	0.52
1:D:740:GLN:O	1:D:744:GLN:HG3	2.08	0.52
1:B:586:LEU:HD23	1:B:640:LEU:HD11	1.91	0.52
1:D:379:VAL:HG12	1:D:380:ILE:HG12	1.91	0.52
1:B:732:TYR:O	1:B:739:ARG:NH1	2.42	0.52
1:C:11:LYS:HA	1:D:43:ARG:NH1	2.24	0.52
1:C:196:PHE:CB	1:C:309:ARG:HH22	2.23	0.52
1:D:160:ARG:HB2	1:D:243:LEU:HB3	1.91	0.52
1:D:590:ILE:HD11	1:D:598:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:THR:HA	1:D:679:MET:HE2	1.91	0.52
1:D:718:VAL:HG13	1:D:772:LYS:HE2	1.92	0.52
1:A:588:ASN:HD21	1:A:741:ILE:HG22	1.75	0.52
1:A:742:ILE:HD11	1:A:774:PHE:HZ	1.74	0.52
1:B:346:ILE:HB	1:B:347:PRO:HD2	1.91	0.52
1:B:131:LEU:HD11	1:B:243:LEU:HD23	1.91	0.52
1:C:138:ARG:O	1:C:138:ARG:HG3	2.10	0.52
1:C:599:VAL:HG11	1:C:788:SER:O	2.10	0.52
1:C:614:HIS:O	1:C:618:MET:HB2	2.10	0.52
1:D:224:MET:HG2	1:D:247:LYS:HD2	1.92	0.52
1:D:486:ILE:HD11	1:D:680:LYS:HE3	1.92	0.52
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.10	0.52
1:C:23:ASN:O	1:C:24:VAL:C	2.51	0.52
1:C:133:ASN:CG	1:C:165:ILE:HG21	2.35	0.52
1:C:279:LEU:HD23	1:C:281:PRO:HD2	1.85	0.52
1:C:282:ASN:C	1:C:284:ASN:N	2.65	0.52
1:C:361:TRP:CZ3	1:C:409:ARG:HD2	2.44	0.52
1:A:411:LEU:HD21	1:A:429:SER:HA	1.91	0.52
1:D:24:VAL:O	1:D:25:THR:C	2.44	0.52
1:A:11:LYS:HA	1:B:43:ARG:HH11	1.75	0.51
1:A:398:ARG:O	1:A:401:GLN:HB2	2.10	0.51
1:A:708:PHE:HB3	1:A:710:ILE:CD1	2.40	0.51
1:B:24:VAL:O	1:B:28:LYS:HG3	2.10	0.51
1:B:586:LEU:H	1:B:586:LEU:HD22	1.75	0.51
1:D:498:GLY:O	1:D:501:GLU:N	2.43	0.51
1:D:567:VAL:HG23	1:D:567:VAL:O	2.10	0.51
1:D:732:TYR:O	1:D:739:ARG:NH1	2.43	0.51
1:A:270:ASN:OD1	1:B:269:ARG:HD3	2.10	0.51
1:B:713:MET:HE1	1:B:772:LYS:HD3	1.92	0.51
1:B:727:ASN:O	1:B:730:GLU:HB3	2.11	0.51
1:C:203:TYR:O	1:C:215:TRP:CZ2	2.62	0.51
1:C:678:ASN:CB	1:C:699:MET:HE1	2.40	0.51
1:D:328:ALA:O	1:D:331:ASP:HB2	2.09	0.51
1:D:533:ASP:O	1:D:537:VAL:HG23	2.11	0.51
1:D:571:HIS:ND1	1:D:572:GLU:N	2.58	0.51
1:A:96:GLN:O	1:A:100:VAL:HG13	2.10	0.51
1:A:513:SER:C	1:A:831:ARG:HH21	2.18	0.51
1:A:609:ALA:HB2	1:A:620:ILE:HD11	1.92	0.51
1:B:284:ASN:CG	1:B:285:PHE:N	2.64	0.51
1:C:283:ASP:OD2	1:C:383:ALA:HB2	2.03	0.51
1:C:790:LEU:CD2	1:C:800:MET:HE3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:THR:HG21	1:D:238:VAL:H	1.74	0.51
1:D:549:LEU:HB3	1:D:557:ILE:HG12	1.92	0.51
1:A:790:LEU:O	1:A:790:LEU:HG	2.11	0.51
1:B:274:ASN:HA	1:B:277:ARG:HG3	1.91	0.51
1:C:80:LYS:HE2	1:C:825:TRP:O	2.11	0.51
1:C:200:VAL:HG22	1:C:301:ALA:HB3	1.92	0.51
1:C:323:ARG:C	1:C:325:ASN:N	2.68	0.51
1:D:627:GLY:O	1:D:631:ASN:HB2	2.10	0.51
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.76	0.51
1:B:481:ASN:O	1:B:482:LYS:HG2	2.10	0.51
1:B:714:ARG:HG3	1:B:714:ARG:HH11	1.75	0.51
1:B:834:LEU:HD23	1:B:835:PRO:HD2	1.92	0.51
1:D:138:ARG:HD3	1:D:491:TRP:HZ2	1.75	0.51
1:D:428:MET:HE3	1:D:470:ASP:HB3	1.91	0.51
1:D:495:CYS:O	1:D:658:PRO:HG2	2.11	0.51
1:D:822:ARG:NH1	1:D:828:GLU:HG3	2.26	0.51
1:A:378:THR:O	1:A:459:HIS:HE1	1.94	0.51
1:A:502:ILE:HA	1:A:505:GLU:HB2	1.91	0.51
1:B:161:TYR:CE2	1:B:279:LEU:HG	2.46	0.51
1:B:161:TYR:O	1:B:182:TRP:HZ2	1.93	0.51
1:C:67:TRP:O	1:C:71:GLN:HG2	2.10	0.51
1:C:144:LEU:HD13	1:C:230:VAL:HG11	1.91	0.51
1:C:379:VAL:HG13	1:C:380:ILE:HG12	1.93	0.51
1:D:138:ARG:NH2	1:D:490:ARG:HD3	2.26	0.51
1:C:13:ILE:HG23	1:D:32:ASN:HD21	1.74	0.51
1:D:631:ASN:ND2	1:D:642:VAL:H	2.08	0.51
1:D:735:ILE:HD12	1:D:735:ILE:H	1.75	0.51
1:A:719:ASP:O	1:A:722:ASP:HB2	2.11	0.51
1:B:280:TYR:H	1:B:281:PRO:CD	2.20	0.51
1:B:767:HIS:HB2	1:B:768:HIS:CE1	2.45	0.51
1:C:184:ARG:HD2	1:C:185:TYR:CE2	2.46	0.51
1:C:665:GLN:HB3	1:C:696:ASN:HD21	1.75	0.51
1:A:174:TRP:HH2	1:A:618:MET:HE1	1.75	0.51
1:A:316:PHE:HE2	1:A:332:LYS:CE	2.16	0.51
1:A:354:VAL:O	1:A:358:ARG:HA	2.10	0.51
1:B:161:TYR:HA	1:B:276:SER:O	2.10	0.51
1:C:34:HIS:HD2	1:C:38:THR:OG1	1.94	0.51
1:C:491:TRP:C	1:C:495:CYS:SG	2.94	0.51
1:D:741:ILE:HG22	1:D:744:GLN:NE2	2.26	0.51
1:B:480:GLN:HG2	1:B:482:LYS:HE2	1.92	0.50
1:B:567:VAL:HB	1:B:648:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:LEU:HG	1:B:797:TRP:HD1	1.76	0.50
1:D:281:PRO:HD3	1:D:292:ARG:NH1	2.25	0.50
1:D:698:GLU:HA	1:D:701:GLU:CG	2.41	0.50
1:A:384:LEU:HB2	1:A:386:ARG:HH12	1.76	0.50
1:A:492:LEU:HG	1:A:683:LEU:HD22	1.92	0.50
1:A:519:ARG:O	1:A:522:LEU:HB2	2.10	0.50
1:A:588:ASN:ND2	1:A:741:ILE:HG22	2.26	0.50
1:B:455:VAL:HG13	1:B:484:ASN:CG	2.36	0.50
1:C:13:ILE:HA	1:D:32:ASN:OD1	2.11	0.50
1:C:735:ILE:HG22	1:C:738:LEU:H	1.75	0.50
1:D:108:CYS:O	1:D:112:THR:HG23	2.11	0.50
1:D:601:ARG:NH2	1:D:784:GLN:OE1	2.45	0.50
1:C:375:THR:HG23	1:C:453:ASN:ND2	2.27	0.50
1:D:59:VAL:O	1:D:62:HIS:HB2	2.12	0.50
1:D:489:ARG:HA	1:D:493:VAL:HG23	1.93	0.50
1:D:536:LYS:O	1:D:540:GLU:N	2.45	0.50
1:D:662:LEU:CD1	1:D:784:GLN:HE22	2.24	0.50
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.93	0.50
1:B:428:MET:HE3	1:B:471:PHE:HA	1.93	0.50
1:B:789:ALA:O	1:B:792:LYS:NZ	2.41	0.50
1:A:656:VAL:HG13	1:A:657:ILE:N	2.26	0.50
1:B:584:ILE:HD13	1:B:750:PHE:CE2	2.46	0.50
1:C:291:LEU:O	1:C:295:GLN:HG3	2.12	0.50
1:C:349:LEU:O	1:C:353:LEU:CG	2.58	0.50
1:D:168:GLN:HE21	1:D:647:ASN:H	1.59	0.50
1:D:504:ALA:HA	1:D:508:GLY:N	2.27	0.50
1:D:754:GLN:HE22	1:D:757:LEU:HD11	1.77	0.50
1:A:33:ARG:HH22	1:B:30:ASN:HD21	1.60	0.50
1:A:202:PHE:O	1:A:218:THR:HB	2.12	0.50
1:A:480:GLN:NE2	1:A:823:GLU:HB3	2.27	0.50
1:A:708:PHE:HB3	1:A:710:ILE:HD12	1.94	0.50
1:D:24:VAL:O	1:D:28:LYS:HG3	2.11	0.50
1:D:450:HIS:O	1:D:478:LYS:HG3	2.12	0.50
1:D:721:LEU:HD21	1:D:726:TYR:CD1	2.47	0.50
1:D:754:GLN:HE21	1:D:757:LEU:CD1	2.24	0.50
1:A:509:GLU:CG	1:A:512:ILE:HD12	2.42	0.50
1:C:193:ARG:HD2	1:C:196:PHE:CE2	2.47	0.50
1:C:206:VAL:HA	1:C:214:LYS:O	2.11	0.50
1:C:207:GLU:HB3	1:C:214:LYS:HB2	1.93	0.50
1:C:221:VAL:HG13	1:C:272:ALA:HB1	1.94	0.50
1:C:233:TYR:OH	1:C:234:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:MET:O	1:D:152:LEU:HB2	2.11	0.50
1:D:505:GLU:OE1	1:D:506:ARG:NH2	2.45	0.50
1:D:784:GLN:O	1:D:787:VAL:HG12	2.12	0.50
1:A:21:VAL:O	1:A:22:GLU:CB	2.59	0.50
1:B:93:ARG:O	1:B:490:ARG:NH2	2.45	0.50
1:B:378:THR:HG21	1:B:384:LEU:HD13	1.92	0.50
1:C:391:LEU:O	1:C:391:LEU:HD23	2.12	0.50
1:C:458:ILE:HD11	1:C:694:GLY:HA2	1.93	0.50
1:C:790:LEU:HB3	1:C:797:TRP:CD1	2.47	0.50
1:D:502:ILE:HA	1:D:505:GLU:HB2	1.93	0.50
1:D:538:LYS:NZ	1:D:660:ALA:O	2.45	0.50
1:D:549:LEU:HD23	1:D:557:ILE:CG1	2.42	0.50
1:D:599:VAL:HG21	1:D:788:SER:O	2.11	0.50
1:A:352:VAL:HA	1:A:356:LEU:HD23	1.93	0.50
1:C:491:TRP:CA	1:C:495:CYS:SG	2.98	0.50
1:C:741:ILE:HA	1:C:744:GLN:HB2	1.93	0.50
1:A:706:GLU:H	1:A:706:GLU:CD	2.20	0.49
1:A:716:GLU:O	1:A:719:ASP:HB2	2.11	0.49
1:C:599:VAL:HG21	1:C:788:SER:HB3	1.93	0.49
1:C:626:ILE:HG22	1:C:642:VAL:HG21	1.94	0.49
1:C:727:ASN:C	1:C:727:ASN:HD22	2.20	0.49
1:D:284:ASN:CG	1:D:285:PHE:N	2.70	0.49
1:D:565:VAL:HG21	1:D:681:PHE:CE1	2.42	0.49
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.46	0.49
1:A:168:GLN:HB3	1:A:647:ASN:HA	1.93	0.49
1:A:563:PHE:CD2	1:A:604:MET:HE1	2.47	0.49
1:B:280:TYR:CE2	1:B:289:LYS:CE	2.87	0.49
1:B:783:CYS:SG	1:B:786:ARG:NH2	2.85	0.49
1:C:784:GLN:O	1:C:787:VAL:HG12	2.12	0.49
1:D:279:LEU:HD21	1:D:281:PRO:CG	2.41	0.49
1:A:74:TYR:CD1	1:A:79:PRO:HG3	2.47	0.49
1:B:687:LEU:HD13	1:B:709:PHE:HE1	1.77	0.49
1:D:80:LYS:HG2	1:D:332:LYS:O	2.12	0.49
1:D:588:ASN:HD21	1:D:744:GLN:NE2	2.10	0.49
1:D:759:LYS:NZ	1:D:763:ASN:OD1	2.40	0.49
1:A:349:LEU:HD23	1:A:368:THR:HG23	1.93	0.49
1:B:101:ASN:HB3	1:B:232:GLY:O	2.12	0.49
1:C:23:ASN:O	1:C:27:LEU:N	2.46	0.49
1:C:315:LYS:O	1:C:319:ARG:HB2	2.12	0.49
1:C:720:ARG:HG3	1:C:720:ARG:HH11	1.76	0.49
1:D:287:GLU:O	1:D:289:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:HD11	1:A:429:SER:HB2	1.93	0.49
1:A:733:ASP:C	1:A:739:ARG:HH12	2.20	0.49
1:B:546:ALA:O	1:B:550:GLU:HB2	2.12	0.49
1:B:835:PRO:O	1:B:836:ALA:HB3	2.12	0.49
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.95	0.49
1:C:363:LYS:O	1:C:367:VAL:HG23	2.12	0.49
1:C:464:LYS:HG2	1:C:472:TYR:CD2	2.47	0.49
1:C:545:PHE:HE2	1:C:604:MET:SD	2.35	0.49
1:A:742:ILE:CD1	1:A:774:PHE:HZ	2.26	0.49
1:B:252:PHE:CZ	1:B:269:ARG:HB3	2.48	0.49
1:B:522:LEU:HD13	1:B:806:ALA:CB	2.42	0.49
1:B:629:VAL:HG12	1:B:630:VAL:N	2.28	0.49
1:C:591:LYS:CD	1:C:635:VAL:HB	2.43	0.49
1:C:455:VAL:H	1:C:459:HIS:HD2	1.60	0.49
1:D:70:THR:O	1:D:73:HIS:HB3	2.11	0.49
1:D:742:ILE:HD11	1:D:774:PHE:CE1	2.48	0.49
1:A:42:ASP:OD1	1:A:43:ARG:CA	2.60	0.49
1:A:322:VAL:O	1:A:322:VAL:HG22	2.12	0.49
1:B:350:MET:HE1	1:B:361:TRP:CE2	2.47	0.49
1:C:733:ASP:HA	1:C:739:ARG:HH12	1.77	0.49
1:A:481:ASN:O	1:A:482:LYS:HG2	2.13	0.49
1:A:834:LEU:HD23	1:A:835:PRO:HD2	1.95	0.49
1:B:23:ASN:OD1	1:B:25:THR:N	2.46	0.49
1:D:170:ILE:HD13	1:D:175:GLN:HA	1.95	0.49
1:D:565:VAL:HG21	1:D:660:ALA:HB1	1.95	0.49
1:D:736:PRO:O	1:D:740:GLN:HB3	2.13	0.49
1:D:73:HIS:ND1	1:D:834:LEU:HD11	2.28	0.49
1:D:703:ALA:CA	1:D:807:THR:HG21	2.43	0.49
1:A:319:ARG:HD3	1:A:332:LYS:HZ3	1.78	0.48
1:A:680:LYS:O	1:A:684:ASN:HB2	2.13	0.48
1:B:269:ARG:O	1:B:273:GLU:HB2	2.12	0.48
1:B:350:MET:HE1	1:B:361:TRP:NE1	2.28	0.48
1:B:574:LYS:HA	1:B:667:SER:OG	2.12	0.48
1:C:91:MET:CE	1:C:144:LEU:HD12	2.42	0.48
1:D:319:ARG:O	1:D:321:PRO:HD3	2.13	0.48
1:D:338:ASN:OD1	1:D:377:HIS:CE1	2.66	0.48
1:D:522:LEU:O	1:D:525:VAL:HG23	2.13	0.48
1:B:89:PHE:CE1	1:B:140:ALA:HB1	2.48	0.48
1:C:352:VAL:HG13	1:C:356:LEU:HD23	1.95	0.48
1:D:458:ILE:O	1:D:462:ILE:HG12	2.14	0.48
1:A:403:ILE:CG2	1:A:439:ILE:HD13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASN:C	1:B:284:ASN:N	2.66	0.48
1:D:140:ALA:O	1:D:144:LEU:HG	2.13	0.48
1:D:630:VAL:HG23	1:D:631:ASN:N	2.28	0.48
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.63	0.48
1:A:564:ASP:HB3	1:A:603:VAL:HA	1.94	0.48
1:B:94:THR:HG22	1:B:98:THR:OG1	2.13	0.48
1:B:503:ILE:O	1:B:507:ILE:HG12	2.13	0.48
1:C:732:TYR:HE1	1:C:739:ARG:HA	1.77	0.48
1:D:483:THR:HB	1:D:815:ARG:HH22	1.78	0.48
1:A:23:ASN:C	1:A:25:THR:N	2.64	0.48
1:A:139:LEU:HD11	1:A:484:ASN:HD21	1.78	0.48
1:B:246:ALA:HB2	1:B:298:PHE:CZ	2.48	0.48
1:C:23:ASN:HB3	1:C:25:THR:HB	1.95	0.48
1:C:68:ILE:O	1:C:72:GLN:HG2	2.13	0.48
1:C:82:ILE:HA	1:C:334:ALA:HB3	1.94	0.48
1:C:352:VAL:HG13	1:C:356:LEU:CD2	2.42	0.48
1:C:589:ARG:O	1:C:592:LYS:HB3	2.13	0.48
1:C:709:PHE:CZ	1:C:787:VAL:HG23	2.49	0.48
1:D:21:VAL:HA	1:D:62:HIS:NE2	2.28	0.48
1:A:622:LEU:HA	1:A:758:PHE:CE1	2.49	0.48
1:C:528:GLU:OE1	1:C:532:ARG:NH2	2.39	0.48
1:D:42:ASP:OD1	1:D:45:VAL:HG23	2.14	0.48
1:D:665:GLN:HE22	1:D:678:ASN:HA	1.77	0.48
1:A:138:ARG:HG3	1:A:138:ARG:HH11	1.78	0.48
1:A:327:ASP:OD1	1:A:363:LYS:NZ	2.45	0.48
1:B:574:LYS:HB2	1:B:576:GLN:NE2	2.29	0.48
1:C:41:LYS:HG3	1:C:50:ASP:OD2	2.13	0.48
1:C:316:PHE:O	1:C:324:THR:HG22	2.14	0.48
1:A:166:PHE:CD2	1:A:177:GLU:HB3	2.49	0.48
1:A:172:GLY:O	1:A:621:LYS:NZ	2.47	0.48
1:A:196:PHE:HB2	1:A:225:PRO:HG3	1.94	0.48
1:A:592:LYS:NZ	1:A:593:GLU:OE2	2.45	0.48
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.13	0.48
1:B:797:TRP:O	1:B:800:MET:HB2	2.14	0.48
1:C:64:VAL:HG12	1:C:67:TRP:CE3	2.46	0.48
1:C:292:ARG:O	1:C:296:GLU:HG3	2.13	0.48
1:A:80:LYS:HD3	1:A:825:TRP:O	2.13	0.48
1:C:16:ARG:HG3	1:C:16:ARG:O	2.14	0.48
1:C:262:TYR:HD1	1:C:263:ILE:H	1.62	0.48
1:C:759:LYS:HG2	1:C:763:ASN:OD1	2.14	0.48
1:D:49:ARG:HA	1:D:125:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:PHE:O	1:D:316:PHE:HB2	2.13	0.48
1:D:789:ALA:HA	1:D:792:LYS:NZ	2.29	0.48
1:A:326:PHE:HD1	1:A:359:LEU:HD11	1.79	0.48
1:C:23:ASN:CB	1:C:26:GLU:H	2.25	0.48
1:C:85:LEU:HD22	1:C:342:PRO:HB3	1.96	0.48
1:C:703:ALA:HB3	1:C:708:PHE:CE1	2.49	0.48
1:A:252:PHE:CZ	1:A:269:ARG:HB3	2.49	0.47
1:A:499:LEU:HD23	1:A:499:LEU:O	2.13	0.47
1:A:675:GLY:O	1:A:679:MET:HE3	2.14	0.47
1:A:742:ILE:CD1	1:A:765:LEU:HD23	2.44	0.47
1:B:158:GLY:O	1:B:243:LEU:HA	2.14	0.47
1:B:225:PRO:HB2	1:B:242:ARG:HD2	1.96	0.47
1:B:389:VAL:HG12	1:B:439:ILE:CD1	2.44	0.47
1:C:232:GLY:HA3	1:C:235:ASN:HD21	1.79	0.47
1:D:509:GLU:HA	1:D:511:TYR:CD1	2.49	0.47
1:A:356:LEU:H	1:A:356:LEU:HD22	1.78	0.47
1:B:571:HIS:ND1	1:B:572:GLU:N	2.61	0.47
1:B:640:LEU:HD23	1:B:641:ARG:N	2.29	0.47
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.96	0.47
1:D:515:LEU:O	1:D:518:LEU:HB2	2.14	0.47
1:A:756:ASP:OD1	1:D:426:ARG:NH2	2.48	0.47
1:A:759:LYS:HE3	1:A:759:LYS:HB3	1.73	0.47
1:D:53:PHE:CE1	1:D:188:PRO:HD3	2.49	0.47
1:D:374:TYR:HD2	1:D:452:VAL:HG22	1.77	0.47
1:D:521:LEU:HD11	1:D:530:PHE:CE1	2.48	0.47
1:D:802:ILE:HA	1:D:805:ILE:HD12	1.96	0.47
1:A:13:ILE:HG22	1:B:43:ARG:HB2	1.95	0.47
1:A:411:LEU:HD21	1:A:429:SER:CA	2.45	0.47
1:B:163:PHE:HB2	1:B:277:ARG:O	2.15	0.47
1:B:251:ASP:HB3	1:B:255:LYS:CG	2.44	0.47
1:D:754:GLN:HA	1:D:755:PRO:HD3	1.64	0.47
1:A:32:ASN:ND2	1:B:13:ILE:HG23	2.29	0.47
1:B:713:MET:SD	1:B:718:VAL:HA	2.55	0.47
1:C:703:ALA:HB2	1:C:807:THR:HG21	1.96	0.47
1:B:568:LYS:O	1:B:607:GLY:HA3	2.14	0.47
1:B:709:PHE:CD2	1:B:787:VAL:HG23	2.49	0.47
1:A:167:ASN:O	1:A:177:GLU:HA	2.15	0.47
1:A:316:PHE:HE2	1:A:332:LYS:HZ1	1.57	0.47
1:B:569:ARG:O	1:B:574:LYS:HG3	2.15	0.47
1:B:575:ARG:O	1:B:578:LEU:N	2.47	0.47
1:B:590:ILE:CG2	1:B:636:VAL:HG22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:HD23	1:C:187:ASN:HB2	1.96	0.47
1:C:201:HIS:HB3	1:C:218:THR:HG21	1.97	0.47
1:C:446:ILE:HD12	1:C:452:VAL:HG21	1.96	0.47
1:D:315:LYS:O	1:D:319:ARG:HB2	2.15	0.47
1:D:538:LYS:O	1:D:542:LYS:HG3	2.15	0.47
1:D:645:LEU:HD22	1:D:652:LEU:HD13	1.95	0.47
1:A:155:TYR:CD1	1:A:240:THR:HB	2.50	0.47
1:B:713:MET:HE2	1:B:775:ALA:HB1	1.96	0.47
1:C:348:GLU:OE1	1:C:399:HIS:HE1	1.98	0.47
1:B:22:GLU:OE2	1:B:104:LEU:CD1	2.62	0.47
1:B:798:THR:O	1:B:802:ILE:HG13	2.15	0.47
1:C:271:LEU:HA	1:C:274:ASN:HD22	1.79	0.47
1:C:519:ARG:O	1:C:522:LEU:HB2	2.15	0.47
1:C:591:LYS:HZ2	1:C:633:ASP:CG	2.19	0.47
1:D:297:TYR:HB2	1:D:396:LEU:HD21	1.97	0.47
1:A:759:LYS:NZ	1:A:763:ASN:OD1	2.43	0.47
1:B:88:GLU:HG3	1:B:132:GLY:CA	2.42	0.47
1:C:571:HIS:HB3	1:C:574:LYS:HG2	1.96	0.47
1:D:741:ILE:HG22	1:D:744:GLN:HE21	1.80	0.47
1:A:89:PHE:CD2	1:A:241:MET:SD	3.08	0.46
1:A:235:ASN:O	1:A:236:ASN:HB2	2.16	0.46
1:A:493:VAL:HG21	1:A:512:ILE:HD13	1.96	0.46
1:B:603:VAL:HB	1:B:641:ARG:O	2.15	0.46
1:C:585:THR:O	1:C:588:ASN:HB2	2.15	0.46
1:C:792:LYS:C	1:C:794:PRO:HD3	2.40	0.46
1:D:577:LEU:HD13	1:D:765:LEU:CD1	2.39	0.46
1:A:422:VAL:HA	1:A:425:LEU:CD1	2.44	0.46
1:C:14:SEP:HB2	1:C:16:ARG:HG2	1.96	0.46
1:D:64:VAL:O	1:D:68:ILE:HD12	2.15	0.46
1:D:192:ALA:HB2	1:D:226:TYR:CE2	2.50	0.46
1:D:662:LEU:HD23	1:D:687:LEU:O	2.15	0.46
1:A:322:VAL:HG13	1:A:325:ASN:CB	2.45	0.46
1:B:163:PHE:HD2	1:B:277:ARG:HB3	1.81	0.46
1:B:251:ASP:HB3	1:B:255:LYS:CB	2.45	0.46
1:B:369:VAL:HA	1:B:448:GLY:O	2.15	0.46
1:B:554:LYS:HD2	1:B:554:LYS:C	2.40	0.46
1:B:575:ARG:NH1	1:B:666:ILE:O	2.46	0.46
1:B:819:GLN:O	1:B:823:GLU:HB2	2.14	0.46
1:C:157:TYR:CE1	1:C:242:ARG:HG2	2.50	0.46
1:D:147:MET:SD	1:D:154:ALA:CB	3.03	0.46
1:A:203:TYR:CZ	1:A:395:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:HD13	1:A:799:ARG:HG2	1.98	0.46
1:A:629:VAL:HG11	1:A:750:PHE:CE1	2.44	0.46
1:A:744:GLN:HA	1:A:747:SER:OG	2.15	0.46
1:B:182:TRP:H	1:B:182:TRP:CD1	2.33	0.46
1:B:241:MET:SD	1:B:243:LEU:HD11	2.55	0.46
1:B:821:ALA:HB1	1:B:827:VAL:O	2.14	0.46
1:C:28:LYS:HG2	1:C:115:LEU:HD11	1.98	0.46
1:C:254:LEU:HD22	1:C:257:PHE:CZ	2.51	0.46
1:D:790:LEU:C	1:D:797:TRP:HD1	2.24	0.46
1:A:326:PHE:O	1:A:330:PRO:HD3	2.16	0.46
1:A:557:ILE:HD11	1:A:643:ILE:CD1	2.42	0.46
1:A:601:ARG:NH2	1:A:784:GLN:HE22	2.12	0.46
1:B:103:ALA:HB2	1:B:234:ARG:NE	2.31	0.46
1:B:252:PHE:O	1:B:259:VAL:HG11	2.16	0.46
1:D:496:ASN:ND2	1:D:658:PRO:HB3	2.31	0.46
1:D:786:ARG:O	1:D:789:ALA:HB3	2.15	0.46
1:A:486:ILE:HG23	1:A:491:TRP:CD1	2.50	0.46
1:A:670:GLY:H	1:A:693:ASP:CG	2.24	0.46
1:C:456:ALA:HB3	1:C:459:HIS:HB3	1.96	0.46
1:C:574:LYS:HB2	1:C:576:GLN:HE21	1.80	0.46
1:D:169:LYS:HA	1:D:169:LYS:HD2	1.82	0.46
1:D:257:PHE:CD1	1:D:257:PHE:N	2.84	0.46
1:D:486:ILE:HD12	1:D:486:ILE:HA	1.51	0.46
1:D:643:ILE:HD13	1:D:643:ILE:HA	1.72	0.46
1:A:143:PHE:HB3	1:A:147:MET:HE3	1.97	0.46
1:A:191:LYS:HD2	1:A:191:LYS:HA	1.79	0.46
1:A:331:ASP:CB	1:A:332:LYS:HG2	2.45	0.46
1:A:528:GLU:OE2	1:A:795:ARG:HD2	2.15	0.46
1:B:81:ARG:HH11	1:B:81:ARG:HG3	1.79	0.46
1:B:297:TYR:HE1	1:B:348:GLU:OE1	1.99	0.46
1:B:815:ARG:NH1	1:B:819:GLN:OE1	2.48	0.46
1:C:99:MET:SD	1:C:119:MET:HE1	2.55	0.46
1:C:642:VAL:O	1:C:643:ILE:HD13	2.16	0.46
1:C:678:ASN:HB3	1:C:699:MET:HE1	1.98	0.46
1:D:222:LEU:HD23	1:D:222:LEU:HA	1.75	0.46
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.98	0.46
1:A:426:ARG:NH1	1:D:755:PRO:HG2	2.30	0.46
1:A:698:GLU:HB3	1:A:810:LYS:NZ	2.30	0.46
1:B:87:LEU:HD13	1:B:299:VAL:HG11	1.98	0.46
1:B:563:PHE:HD2	1:B:659:ALA:O	1.98	0.46
1:C:386:ARG:HD3	1:C:438:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ILE:HG13	1:D:371:THR:HG22	1.96	0.46
1:D:818:ALA:O	1:D:821:ALA:HB3	2.15	0.46
1:A:49:ARG:O	1:A:53:PHE:HD2	1.99	0.46
1:A:90:TYR:HE2	1:A:134:GLY:HA2	1.81	0.46
1:C:235:ASN:H	1:C:235:ASN:ND2	2.06	0.46
1:C:372:CYS:O	1:C:450:HIS:HD2	1.99	0.46
1:C:792:LYS:O	1:C:794:PRO:HD3	2.16	0.46
1:A:116:GLY:O	1:B:10:ARG:HD3	2.16	0.46
1:A:742:ILE:HD11	1:A:774:PHE:CZ	2.50	0.46
1:C:590:ILE:O	1:C:594:PRO:HA	2.15	0.46
1:D:83:TYR:CE2	1:D:307:ILE:HG12	2.51	0.46
1:D:378:THR:O	1:D:459:HIS:HE1	1.99	0.46
1:A:102:LEU:HB3	1:A:104:LEU:HD22	1.98	0.45
1:A:170:ILE:HD13	1:A:175:GLN:HA	1.97	0.45
1:D:206:VAL:HA	1:D:214:LYS:O	2.16	0.45
1:D:790:LEU:HD21	1:D:800:MET:HG3	1.98	0.45
1:A:582:HIS:HA	1:A:585:THR:HB	1.98	0.45
1:B:304:LEU:HD21	1:B:349:LEU:CA	2.46	0.45
1:D:754:GLN:HB3	1:D:757:LEU:HD13	1.97	0.45
1:D:836:ALA:HA	1:D:837:PRO:HD2	1.78	0.45
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.71	0.45
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.72	0.45
1:A:455:VAL:H	1:A:459:HIS:CD2	2.33	0.45
1:A:599:VAL:HG11	1:A:791:TYR:HD2	1.81	0.45
1:A:730:GLU:O	1:A:734:ARG:HD2	2.16	0.45
1:A:730:GLU:O	1:A:734:ARG:HD3	2.17	0.45
1:B:17:GLY:CA	1:B:18:LEU:HD22	2.46	0.45
1:B:455:VAL:HG13	1:B:484:ASN:ND2	2.31	0.45
1:C:337:LEU:HD11	1:C:345:ALA:HB3	1.99	0.45
1:C:753:LYS:HD2	1:C:753:LYS:N	2.30	0.45
1:D:582:HIS:O	1:D:586:LEU:HD13	2.16	0.45
1:A:18:LEU:HB2	1:B:37:PHE:CZ	2.51	0.45
1:A:304:LEU:HD11	1:A:345:ALA:HB1	1.99	0.45
1:A:490:ARG:HG3	1:A:494:LEU:HD11	1.98	0.45
1:A:544:LYS:O	1:A:547:ALA:HB3	2.16	0.45
1:B:49:ARG:HH11	1:B:125:ILE:HG22	1.82	0.45
1:C:19:ALA:HB1	1:C:21:VAL:H	1.81	0.45
1:C:78:ASP:O	1:C:332:LYS:NZ	2.50	0.45
1:C:543:LEU:HD12	1:C:559:PRO:CB	2.46	0.45
1:D:118:ASP:HB3	1:D:121:GLU:HB3	1.97	0.45
1:D:542:LYS:NZ	1:D:661:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:GLU:HA	1:D:701:GLU:HG2	1.99	0.45
1:D:706:GLU:H	1:D:706:GLU:CD	2.24	0.45
1:A:18:LEU:O	1:A:19:ALA:CB	2.65	0.45
1:B:733:ASP:O	1:B:739:ARG:NH1	2.50	0.45
1:C:155:TYR:N	1:C:155:TYR:CD1	2.84	0.45
1:C:541:ASN:O	1:C:544:LYS:N	2.49	0.45
1:D:244:TRP:CE2	1:D:302:ALA:HB1	2.51	0.45
1:D:279:LEU:HD21	1:D:281:PRO:CD	2.38	0.45
1:D:549:LEU:O	1:D:555:VAL:N	2.50	0.45
1:D:687:LEU:HD12	1:D:797:TRP:CE2	2.51	0.45
1:A:524:TYR:CD1	1:A:524:TYR:N	2.85	0.45
1:A:571:HIS:ND1	1:A:572:GLU:N	2.64	0.45
1:A:834:LEU:HD23	1:A:835:PRO:CD	2.47	0.45
1:B:355:ASP:OD2	1:B:398:ARG:NH1	2.49	0.45
1:C:160:ARG:NH2	1:C:190:GLU:OE2	2.49	0.45
1:D:545:PHE:HD1	1:D:549:LEU:CD2	2.29	0.45
1:D:615:MET:HE3	1:D:615:MET:HB3	1.77	0.45
1:D:758:PHE:CD1	1:D:761:ILE:HD11	2.44	0.45
1:A:455:VAL:H	1:A:459:HIS:HD2	1.65	0.45
1:A:571:HIS:CE1	1:A:613:TYR:OH	2.70	0.45
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.98	0.45
1:C:317:GLY:CA	1:C:320:ASP:HB2	2.46	0.45
1:C:682:MET:CE	1:C:807:THR:HG22	2.46	0.45
1:D:424:ARG:NH2	1:D:473:GLU:OE1	2.46	0.45
1:D:486:ILE:HD11	1:D:680:LYS:CE	2.47	0.45
1:A:24:VAL:CG1	1:A:111:ALA:HA	2.39	0.45
1:A:93:ARG:O	1:A:490:ARG:NH2	2.49	0.45
1:A:157:TYR:CE2	1:A:242:ARG:HG2	2.52	0.45
1:A:460:SER:CB	1:A:481:ASN:HB2	2.46	0.45
1:B:49:ARG:HE	1:B:185:TYR:HD2	1.65	0.45
1:B:575:ARG:HB3	1:B:666:ILE:CD1	2.46	0.45
1:C:19:ALA:HB1	1:C:21:VAL:HA	1.99	0.45
1:C:52:TYR:HH	1:C:189:TRP:HZ2	1.58	0.45
1:C:569:ARG:O	1:C:574:LYS:HG3	2.17	0.45
1:D:60:ARG:O	1:D:64:VAL:HG22	2.16	0.45
1:D:94:THR:H	1:D:126:GLU:CD	2.25	0.45
1:D:159:ILE:HG21	1:D:159:ILE:HD13	1.78	0.45
1:D:297:TYR:CG	1:D:396:LEU:HD21	2.52	0.45
1:D:410:PHE:O	1:D:413:ARG:HB2	2.17	0.45
1:A:24:VAL:HG13	1:A:111:ALA:CA	2.40	0.45
1:A:461:GLU:HB3	1:A:465:LYS:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LYS:NZ	1:A:561:SER:O	2.50	0.45
1:A:725:GLY:HA3	1:D:727:ASN:HD21	1.81	0.45
1:B:138:ARG:HH21	1:B:141:ALA:CB	2.30	0.45
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.32	0.45
1:C:379:VAL:HB	1:C:673:ALA:HB2	1.98	0.45
1:C:566:GLN:HB2	1:C:664:GLU:HB2	1.98	0.45
1:C:573:TYR:CD2	1:C:671:THR:HB	2.52	0.45
1:D:280:TYR:HE2	1:D:289:LYS:HE3	1.82	0.45
1:D:496:ASN:HB2	1:D:684:ASN:OD1	2.17	0.45
1:D:518:LEU:HD12	1:D:518:LEU:HA	1.72	0.45
1:A:97:ASN:HA	1:A:494:LEU:HD22	1.99	0.45
1:A:369:VAL:HA	1:A:448:GLY:O	2.17	0.45
1:B:24:VAL:HG12	1:B:28:LYS:HE2	1.97	0.45
1:B:505:GLU:HB3	1:B:506:ARG:HE	1.82	0.45
1:C:280:TYR:CE2	1:C:289:LYS:CE	2.99	0.45
1:C:379:VAL:HG13	1:C:380:ILE:CD1	2.47	0.45
1:C:571:HIS:ND1	1:C:572:GLU:N	2.65	0.45
1:C:604:MET:HA	1:C:643:ILE:O	2.17	0.45
1:C:727:ASN:HD22	1:C:729:GLN:N	2.15	0.45
1:C:766:MET:HE2	1:C:766:MET:HA	1.99	0.45
1:D:55:LEU:HD23	1:D:95:LEU:HD11	1.98	0.45
1:D:104:LEU:HB3	1:D:108:CYS:SG	2.57	0.45
1:D:191:LYS:HD2	1:D:191:LYS:HA	1.77	0.45
1:D:350:MET:SD	1:D:365:TRP:HE3	2.40	0.45
1:D:361:TRP:CZ3	1:D:409:ARG:HD2	2.51	0.45
1:D:389:VAL:HG22	1:D:437:LYS:O	2.17	0.45
1:D:455:VAL:CG1	1:D:674:SER:HB2	2.47	0.45
1:A:318:CYS:C	1:A:320:ASP:H	2.24	0.44
1:A:455:VAL:C	1:A:483:THR:HA	2.42	0.44
1:A:703:ALA:CB	1:A:807:THR:HG21	2.43	0.44
1:A:746:SER:CB	1:A:762:VAL:HG21	2.47	0.44
1:B:396:LEU:O	1:B:399:HIS:HB2	2.16	0.44
1:B:400:LEU:HD23	1:B:400:LEU:HA	1.78	0.44
1:B:538:LYS:HG3	1:B:542:LYS:HD3	1.99	0.44
1:B:739:ARG:HH11	1:B:739:ARG:CG	2.29	0.44
1:C:13:ILE:O	1:D:43:ARG:NH1	2.50	0.44
1:C:268:ASP:O	1:C:270:ASN:N	2.50	0.44
1:C:543:LEU:HD12	1:C:559:PRO:HB3	1.98	0.44
1:C:682:MET:O	1:C:684:ASN:N	2.51	0.44
1:D:192:ALA:HA	1:D:226:TYR:HA	1.98	0.44
1:D:575:ARG:HD3	1:D:666:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:SER:HB3	1:D:762:VAL:HG21	1.98	0.44
1:A:36:HIS:O	1:A:40:VAL:HA	2.16	0.44
1:A:147:MET:HE2	1:A:825:TRP:HH2	1.83	0.44
1:A:244:TRP:HE1	1:A:303:THR:HG23	1.82	0.44
1:A:413:ARG:HH21	1:A:474:LEU:HD13	1.83	0.44
1:B:40:VAL:O	1:B:40:VAL:HG12	2.17	0.44
1:B:687:LEU:CD1	1:B:709:PHE:HE1	2.30	0.44
1:C:182:TRP:H	1:C:182:TRP:CD1	2.36	0.44
1:C:193:ARG:HB2	1:C:225:PRO:HG2	1.99	0.44
1:C:290:GLU:HG2	1:C:294:LYS:HE2	1.98	0.44
1:C:588:ASN:ND2	1:C:744:GLN:HE22	2.10	0.44
1:D:326:PHE:HD2	1:D:329:PHE:CD2	2.35	0.44
1:D:457:ARG:HB2	1:D:698:GLU:OE1	2.17	0.44
1:A:230:VAL:HG23	1:A:230:VAL:O	2.17	0.44
1:A:320:ASP:HB3	1:A:321:PRO:HA	1.98	0.44
1:A:485:GLY:O	1:A:486:ILE:HD12	2.17	0.44
1:B:211:GLN:HA	1:B:211:GLN:NE2	2.32	0.44
1:B:564:ASP:CG	1:B:601:ARG:HH21	2.26	0.44
1:C:19:ALA:CB	1:C:21:VAL:H	2.30	0.44
1:C:822:ARG:HD3	1:C:828:GLU:OE2	2.16	0.44
1:D:28:LYS:HD2	1:D:115:LEU:HG	2.00	0.44
1:D:63:LEU:HD23	1:D:238:VAL:HG21	1.99	0.44
1:D:122:LEU:O	1:D:125:ILE:HB	2.17	0.44
1:A:316:PHE:HZ	1:A:332:LYS:CE	2.18	0.44
1:A:566:GLN:HB2	1:A:664:GLU:HB2	2.00	0.44
1:A:626:ILE:O	1:A:630:VAL:HG13	2.17	0.44
1:A:678:ASN:HD22	1:A:699:MET:HE1	1.81	0.44
1:A:735:ILE:H	1:A:735:ILE:HG13	1.41	0.44
1:A:796:GLU:HA	1:A:799:ARG:HB2	2.00	0.44
1:B:292:ARG:NH2	1:B:341:HIS:CD2	2.86	0.44
1:B:565:VAL:HG11	1:B:656:VAL:HG21	1.99	0.44
1:C:80:LYS:HG3	1:C:331:ASP:O	2.18	0.44
1:C:163:PHE:HE2	1:C:277:ARG:HH11	1.65	0.44
1:C:418:PHE:CE2	1:C:424:ARG:NE	2.86	0.44
1:D:14:SEP:P	1:D:15:VAL:H	2.40	0.44
1:D:231:PRO:HA	1:D:238:VAL:HA	1.99	0.44
1:D:297:TYR:CD2	1:D:396:LEU:HD11	2.52	0.44
1:D:329:PHE:HB3	1:D:330:PRO:HD3	1.98	0.44
1:D:584:ILE:HG12	1:D:750:PHE:CZ	2.52	0.44
1:A:99:MET:SD	1:A:108:CYS:SG	3.15	0.44
1:A:573:TYR:HB3	1:A:771:PHE:CE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:THR:OG1	1:A:741:ILE:HD13	2.17	0.44
1:A:685:GLY:CA	1:A:805:ILE:HD11	2.43	0.44
1:A:721:LEU:HG	1:A:726:TYR:HB2	1.98	0.44
1:B:596:LYS:NZ	1:B:597:PHE:O	2.51	0.44
1:C:836:ALA:HA	1:C:837:PRO:HD2	1.76	0.44
1:D:647:ASN:O	1:D:649:ARG:HG2	2.18	0.44
1:D:766:MET:HE3	1:D:774:PHE:CE2	2.37	0.44
1:A:69:ARG:HA	1:A:72:GLN:HG2	2.00	0.44
1:A:575:ARG:HG2	1:A:578:LEU:HD22	1.99	0.44
1:A:810:LYS:HG3	1:A:811:PHE:CE1	2.53	0.44
1:B:280:TYR:O	1:B:281:PRO:O	2.36	0.44
1:C:71:GLN:HA	1:C:74:TYR:CD2	2.52	0.44
1:C:282:ASN:C	1:C:284:ASN:H	2.24	0.44
1:C:558:ASN:HA	1:C:559:PRO:HD3	1.85	0.44
1:D:337:LEU:HB2	1:D:373:ALA:O	2.17	0.44
1:D:589:ARG:NH2	1:D:785:GLU:OE2	2.51	0.44
1:A:403:ILE:HG22	1:A:439:ILE:HD13	2.00	0.44
1:A:450:HIS:O	1:A:478:LYS:HA	2.18	0.44
1:C:336:GLN:HG2	1:C:825:TRP:HZ2	1.82	0.44
1:D:36:HIS:CD2	1:D:42:ASP:HA	2.52	0.44
1:D:263:ILE:HG22	1:D:265:ALA:HB3	1.99	0.44
1:D:530:PHE:CE2	1:D:802:ILE:HG12	2.52	0.44
1:D:834:LEU:HA	1:D:835:PRO:HD2	1.69	0.44
1:A:67:TRP:CE3	1:A:229:PRO:HG3	2.53	0.44
1:A:90:TYR:CE1	1:A:650:VAL:HG23	2.52	0.44
1:A:403:ILE:HG21	1:A:439:ILE:HG21	2.00	0.44
1:A:442:ALA:O	1:A:446:ILE:HG13	2.18	0.44
1:A:450:HIS:O	1:A:478:LYS:HG3	2.18	0.44
1:B:320:ASP:HB3	1:B:321:PRO:HA	2.00	0.44
1:B:614:HIS:O	1:B:618:MET:HB2	2.17	0.44
1:B:636:VAL:O	1:B:639:ARG:HD3	2.17	0.44
1:C:19:ALA:HB3	1:C:21:VAL:HG22	1.99	0.44
1:C:461:GLU:HG3	1:C:465:LYS:NZ	2.33	0.44
1:C:571:HIS:CG	1:C:613:TYR:HH	2.35	0.44
1:C:766:MET:HE3	1:C:774:PHE:CE2	2.40	0.44
1:D:502:ILE:CG2	1:D:506:ARG:NH2	2.69	0.44
1:D:626:ILE:CG2	1:D:642:VAL:HG11	2.47	0.44
1:A:102:LEU:HB3	1:A:104:LEU:CD2	2.48	0.44
1:A:555:VAL:CG2	1:A:643:ILE:HD11	2.29	0.44
1:C:18:LEU:O	1:D:33:ARG:NH1	2.50	0.44
1:C:230:VAL:HA	1:C:231:PRO:HD2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:GLU:OE1	1:C:399:HIS:CE1	2.71	0.44
1:C:591:LYS:HD2	1:C:591:LYS:HA	1.82	0.44
1:D:211:GLN:HE21	1:D:211:GLN:HA	1.83	0.44
1:A:82:ILE:HG13	1:A:825:TRP:CD2	2.53	0.43
1:A:555:VAL:CG2	1:A:557:ILE:HD11	2.48	0.43
1:A:756:ASP:N	1:A:756:ASP:CB	2.70	0.43
1:B:197:THR:HG23	1:B:224:MET:CB	2.48	0.43
1:B:337:LEU:HD11	1:B:345:ALA:HB3	1.99	0.43
1:C:246:ALA:HB3	1:C:276:SER:OG	2.18	0.43
1:C:290:GLU:O	1:C:294:LYS:HB2	2.17	0.43
1:C:577:LEU:HD11	1:C:619:ILE:HD11	1.99	0.43
1:C:699:MET:HB3	1:C:708:PHE:CE2	2.49	0.43
1:D:280:TYR:N	1:D:281:PRO:CD	2.78	0.43
1:D:390:HIS:ND1	1:D:391:LEU:HD12	2.32	0.43
1:D:590:ILE:HG22	1:D:590:ILE:O	2.18	0.43
1:D:619:ILE:O	1:D:623:ILE:HG13	2.18	0.43
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.67	0.43
1:A:570:ILE:HG21	1:A:620:ILE:HG13	2.01	0.43
1:B:53:PHE:CE1	1:B:188:PRO:HD3	2.53	0.43
1:B:338:ASN:OD1	1:B:377:HIS:HE1	2.01	0.43
1:B:339:ASP:HB2	1:B:377:HIS:CE1	2.53	0.43
1:B:407:ASN:HB2	1:B:430:LEU:HG	2.00	0.43
1:C:375:THR:HG23	1:C:453:ASN:HD21	1.83	0.43
1:D:387:TRP:O	1:D:438:ARG:HB3	2.18	0.43
1:A:689:ILE:HD12	1:A:784:GLN:HE21	1.83	0.43
1:B:296:GLU:HA	1:B:299:VAL:HG12	1.99	0.43
1:B:455:VAL:HG12	1:B:674:SER:CB	2.45	0.43
1:B:655:LYS:O	1:B:658:PRO:HD2	2.18	0.43
1:D:490:ARG:HA	1:D:494:LEU:HG	2.00	0.43
1:D:498:GLY:O	1:D:500:ALA:N	2.52	0.43
1:D:521:LEU:HA	1:D:524:TYR:CD1	2.53	0.43
1:D:758:PHE:HD1	1:D:761:ILE:CD1	2.26	0.43
1:D:810:LYS:O	1:D:815:ARG:NE	2.47	0.43
1:A:164:GLY:O	1:A:279:LEU:HB2	2.19	0.43
1:A:480:GLN:HE22	1:A:823:GLU:HB3	1.84	0.43
1:A:699:MET:HE3	1:A:699:MET:HB2	1.86	0.43
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.59	0.43
1:A:733:ASP:HA	1:A:739:ARG:HH12	1.83	0.43
1:B:263:ILE:CG2	1:B:266:VAL:HG23	2.48	0.43
1:B:421:ASP:OD2	1:B:424:ARG:HB2	2.19	0.43
1:B:590:ILE:HG22	1:B:590:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:TYR:O	1:C:215:TRP:NE1	2.51	0.43
1:C:746:SER:HB3	1:C:762:VAL:HG11	2.01	0.43
1:D:80:LYS:O	1:D:153:ALA:HB3	2.18	0.43
1:A:24:VAL:HG11	1:A:114:GLN:HE22	1.84	0.43
1:A:445:CYS:O	1:A:449:SER:HB2	2.18	0.43
1:A:509:GLU:HG2	1:A:512:ILE:HD12	1.98	0.43
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.79	0.43
1:B:161:TYR:CE1	1:B:279:LEU:HA	2.53	0.43
1:B:283:ASP:OD1	1:B:383:ALA:HB1	2.17	0.43
1:C:71:GLN:HA	1:C:74:TYR:HD2	1.83	0.43
1:C:138:ARG:NH2	1:C:141:ALA:HB3	2.34	0.43
1:C:159:ILE:HD13	1:C:159:ILE:HG21	1.80	0.43
1:C:252:PHE:HZ	1:C:269:ARG:HB3	1.79	0.43
1:C:386:ARG:HG2	1:C:440:ASN:HA	2.00	0.43
1:D:272:ALA:O	1:D:274:ASN:N	2.52	0.43
1:D:589:ARG:O	1:D:592:LYS:N	2.51	0.43
1:D:665:GLN:HB3	1:D:696:ASN:HD21	1.83	0.43
1:A:93:ARG:HG2	1:A:126:GLU:HG2	2.00	0.43
1:A:338:ASN:OD1	1:A:377:HIS:CE1	2.71	0.43
1:B:434:GLY:HA2	1:C:754:GLN:HE22	1.84	0.43
1:B:703:ALA:CB	1:B:807:THR:HG21	2.48	0.43
1:C:13:ILE:HD11	1:D:115:LEU:HB3	1.99	0.43
1:C:198:LEU:HD13	1:C:305:GLN:HB3	2.01	0.43
1:D:70:THR:HG21	1:D:238:VAL:O	2.19	0.43
1:D:464:LYS:HD2	1:D:472:TYR:CZ	2.54	0.43
1:D:587:TYR:CD1	1:D:630:VAL:HG12	2.53	0.43
1:D:588:ASN:HD21	1:D:744:GLN:HE22	1.67	0.43
1:D:689:ILE:HD12	1:D:784:GLN:HE21	1.83	0.43
1:A:131:LEU:HD21	1:A:243:LEU:HD21	2.00	0.43
1:A:322:VAL:HG13	1:A:325:ASN:HB3	2.01	0.43
1:A:355:ASP:OD1	1:A:398:ARG:NH1	2.51	0.43
1:A:449:SER:O	1:A:478:LYS:HE2	2.18	0.43
1:A:526:ASP:CG	1:A:799:ARG:HH11	2.26	0.43
1:A:575:ARG:HG2	1:A:578:LEU:HB2	2.01	0.43
1:A:591:LYS:HA	1:A:591:LYS:HD2	1.78	0.43
1:B:26:GLU:O	1:B:29:LYS:HB3	2.19	0.43
1:B:692:MET:SD	1:B:697:VAL:HG22	2.57	0.43
1:B:734:ARG:O	1:B:736:PRO:HD3	2.18	0.43
1:B:792:LYS:O	1:B:794:PRO:HD3	2.18	0.43
1:C:133:ASN:HB2	1:C:165:ILE:HG21	1.99	0.43
1:C:270:ASN:HD21	1:D:269:ARG:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:VAL:HG13	1:C:325:ASN:CB	2.48	0.43
1:D:21:VAL:CG1	1:D:22:GLU:N	2.59	0.43
1:A:662:LEU:HD21	1:A:689:ILE:HB	2.01	0.43
1:A:733:ASP:HA	1:A:739:ARG:NH1	2.33	0.43
1:B:735:ILE:HA	1:B:736:PRO:HD2	1.90	0.43
1:C:60:ARG:O	1:C:64:VAL:HG22	2.19	0.43
1:C:88:GLU:CG	1:C:132:GLY:HA2	2.49	0.43
1:C:317:GLY:C	1:C:320:ASP:HB2	2.44	0.43
1:D:203:TYR:CE1	1:D:395:LEU:HD12	2.54	0.43
1:D:509:GLU:OE1	1:D:510:GLU:C	2.61	0.43
1:A:63:LEU:HD12	1:A:98:THR:HG21	1.99	0.43
1:A:354:VAL:HG21	1:A:361:TRP:CD1	2.53	0.43
1:B:485:GLY:HA3	1:B:813:SER:HA	2.01	0.43
1:B:518:LEU:HD12	1:B:518:LEU:HA	1.82	0.43
1:B:587:TYR:CD1	1:B:636:VAL:HG21	2.54	0.43
1:B:698:GLU:HA	1:B:701:GLU:HG2	2.00	0.43
1:C:263:ILE:HG22	1:C:265:ALA:HB3	2.01	0.43
1:C:480:GLN:NE2	1:C:823:GLU:HB3	2.30	0.43
1:D:583:VAL:CG2	1:D:603:VAL:HG21	2.48	0.43
1:A:78:ASP:CG	1:A:332:LYS:HZ1	2.23	0.43
1:B:375:THR:HG22	1:B:377:HIS:CE1	2.53	0.43
1:C:203:TYR:O	1:C:215:TRP:HZ2	2.02	0.43
1:C:325:ASN:C	1:C:327:ASP:N	2.76	0.43
1:C:497:PRO:HA	1:C:500:ALA:HB3	2.01	0.43
1:C:766:MET:HA	1:C:766:MET:CE	2.49	0.43
1:D:352:VAL:O	1:D:356:LEU:HB2	2.18	0.43
1:D:407:ASN:HB2	1:D:430:LEU:HD12	2.00	0.43
1:A:21:VAL:O	1:A:22:GLU:CG	2.67	0.42
1:A:417:ALA:O	1:A:419:PRO:HD3	2.19	0.42
1:B:80:LYS:O	1:B:153:ALA:HB3	2.19	0.42
1:C:133:ASN:OD1	1:C:165:ILE:HD12	2.19	0.42
1:C:533:ASP:O	1:C:534:VAL:C	2.62	0.42
1:D:22:GLU:OE1	1:D:107:ALA:HB2	2.19	0.42
1:D:168:GLN:O	1:D:647:ASN:HB2	2.19	0.42
1:D:570:ILE:HD13	1:D:620:ILE:HG12	2.00	0.42
1:A:118:ASP:O	1:A:121:GLU:HB3	2.20	0.42
1:A:756:ASP:N	1:A:756:ASP:CG	2.76	0.42
1:B:138:ARG:NH2	1:B:142:CYS:SG	2.92	0.42
1:B:304:LEU:O	1:B:308:ILE:HG13	2.19	0.42
1:B:315:LYS:O	1:B:318:CYS:HB2	2.19	0.42
1:B:338:ASN:OD1	1:B:377:HIS:CE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:TRP:CZ3	1:B:409:ARG:HD3	2.54	0.42
1:B:663:SER:HB2	1:B:681:PHE:CD2	2.54	0.42
1:C:396:LEU:HG	1:C:399:HIS:CD2	2.53	0.42
1:C:627:GLY:O	1:C:629:VAL:N	2.52	0.42
1:C:810:LYS:HB3	1:C:811:PHE:CE1	2.54	0.42
1:D:297:TYR:CE1	1:D:399:HIS:CE1	3.07	0.42
1:D:735:ILE:H	1:D:735:ILE:CD1	2.31	0.42
1:A:18:LEU:CB	1:B:37:PHE:CZ	3.03	0.42
1:A:165:ILE:HD12	1:A:166:PHE:HD1	1.82	0.42
1:A:225:PRO:HD3	1:A:244:TRP:HZ3	1.84	0.42
1:B:458:ILE:HD11	1:B:694:GLY:H	1.83	0.42
1:C:407:ASN:OD1	1:C:430:LEU:HG	2.20	0.42
1:D:563:PHE:CD2	1:D:659:ALA:O	2.70	0.42
1:A:90:TYR:HB3	1:A:138:ARG:HA	2.02	0.42
1:A:582:HIS:NE2	1:A:784:GLN:OE1	2.52	0.42
1:B:66:ARG:HB3	1:B:236:ASN:O	2.20	0.42
1:B:157:TYR:HA	1:B:242:ARG:O	2.19	0.42
1:B:515:LEU:HG	1:B:518:LEU:HD22	2.02	0.42
1:B:557:ILE:HD12	1:B:557:ILE:HA	1.79	0.42
1:C:515:LEU:HD22	1:C:812:SER:HB2	2.02	0.42
1:C:692:MET:HE3	1:C:697:VAL:HA	2.02	0.42
1:D:146:SER:OG	1:D:813:SER:HB2	2.19	0.42
1:A:193:ARG:HB2	1:A:225:PRO:HG2	2.02	0.42
1:A:208:HIS:CE1	1:A:213:ALA:HB2	2.54	0.42
1:B:225:PRO:HB3	1:B:244:TRP:CE3	2.54	0.42
1:B:509:GLU:CD	1:B:510:GLU:N	2.78	0.42
1:B:782:LYS:O	1:B:785:GLU:N	2.53	0.42
1:C:206:VAL:HG12	1:C:208:HIS:CE1	2.54	0.42
1:C:225:PRO:HD3	1:C:244:TRP:CZ3	2.54	0.42
1:C:310:ARG:HH11	1:C:310:ARG:HD2	1.69	0.42
1:C:457:ARG:O	1:C:461:GLU:HB2	2.19	0.42
1:C:790:LEU:C	1:C:797:TRP:HD1	2.27	0.42
1:D:492:LEU:HG	1:D:683:LEU:HD22	2.01	0.42
1:D:792:LYS:HE2	1:D:792:LYS:HB2	1.76	0.42
1:A:88:GLU:CD	1:A:133:ASN:H	2.26	0.42
1:A:165:ILE:HB	1:A:279:LEU:HD13	2.00	0.42
1:B:202:PHE:CE1	1:B:297:TYR:HD2	2.36	0.42
1:B:578:LEU:O	1:B:579:ASN:C	2.62	0.42
1:B:592:LYS:C	1:B:594:PRO:HD3	2.44	0.42
1:B:635:VAL:O	1:B:639:ARG:NH1	2.52	0.42
1:C:66:ARG:NH1	1:C:236:ASN:OD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HD23	1:C:344:LEU:HA	1.86	0.42
1:C:492:LEU:CG	1:C:683:LEU:HD22	2.48	0.42
1:C:582:HIS:CD2	1:C:781:VAL:HG22	2.54	0.42
1:D:349:LEU:HD23	1:D:368:THR:HG23	2.01	0.42
1:B:10:ARG:N	1:B:13:ILE:HB	2.34	0.42
1:B:17:GLY:H	1:B:18:LEU:CD2	2.29	0.42
1:B:206:VAL:CG2	1:B:398:ARG:HD2	2.50	0.42
1:B:395:LEU:HA	1:B:395:LEU:HD12	1.84	0.42
1:B:589:ARG:O	1:B:591:LYS:N	2.52	0.42
1:B:790:LEU:HG	1:B:797:TRP:CD1	2.55	0.42
1:C:295:GLN:O	1:C:298:PHE:HB3	2.20	0.42
1:D:100:VAL:HG23	1:D:101:ASN:N	2.34	0.42
1:B:138:ARG:HH21	1:B:141:ALA:HB3	1.85	0.42
1:B:139:LEU:HA	1:B:139:LEU:HD12	1.74	0.42
1:B:423:ASP:CG	1:B:426:ARG:HH11	2.28	0.42
1:C:304:LEU:CD2	1:C:349:LEU:HB2	2.50	0.42
1:C:316:PHE:HA	1:C:319:ARG:CB	2.46	0.42
1:C:322:VAL:HG13	1:C:325:ASN:HB3	2.01	0.42
1:C:464:LYS:HB2	1:C:464:LYS:HE3	1.64	0.42
1:C:737:GLU:C	1:C:740:GLN:HB3	2.44	0.42
1:D:99:MET:O	1:D:103:ALA:N	2.52	0.42
1:D:536:LYS:HE2	1:D:536:LYS:HB2	1.85	0.42
1:D:567:VAL:HB	1:D:648:TYR:CZ	2.55	0.42
1:A:365:TRP:O	1:A:369:VAL:HG12	2.20	0.42
1:A:385:GLU:HB3	1:A:441:MET:HB2	2.02	0.42
1:A:528:GLU:OE1	1:A:532:ARG:NH2	2.53	0.42
1:B:565:VAL:HG13	1:B:604:MET:HE3	2.00	0.42
1:B:571:HIS:ND1	1:B:571:HIS:C	2.78	0.42
1:C:242:ARG:NH2	2:C:902:SO4:O1	2.50	0.42
1:A:781:VAL:O	1:A:785:GLU:HG3	2.20	0.42
1:B:138:ARG:HH11	1:B:491:TRP:HE1	1.64	0.42
1:B:433:GLU:OE2	1:B:437:LYS:NZ	2.53	0.42
1:C:117:LEU:HA	1:C:117:LEU:HD23	1.75	0.42
1:C:149:THR:HG21	1:C:489:ARG:NH2	2.35	0.42
1:C:707:ASN:HA	1:C:800:MET:SD	2.59	0.42
1:C:781:VAL:O	1:C:785:GLU:HG3	2.19	0.42
1:D:206:VAL:HG11	1:D:401:GLN:HE22	1.85	0.42
1:D:515:LEU:CD2	1:D:683:LEU:HD11	2.50	0.42
1:D:566:GLN:O	1:D:605:ILE:HA	2.20	0.42
1:D:682:MET:HE3	1:D:807:THR:HG22	2.02	0.42
1:D:682:MET:SD	1:D:699:MET:HG2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:778:GLU:HB3	1:D:782:LYS:HZ2	1.84	0.42
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.83	0.41
1:A:157:TYR:CE2	1:A:303:THR:CG2	2.89	0.41
1:A:521:LEU:HD12	1:A:521:LEU:HA	1.61	0.41
1:A:594:PRO:O	1:A:639:ARG:NH2	2.51	0.41
1:C:104:LEU:O	1:C:105:GLU:C	2.63	0.41
1:C:133:ASN:OD1	1:C:165:ILE:HG23	2.19	0.41
1:D:374:TYR:CG	1:D:445:CYS:HB3	2.54	0.41
1:D:530:PHE:HB3	1:D:531:ILE:HG13	2.02	0.41
1:D:614:HIS:HE1	1:D:760:ASP:OD2	2.02	0.41
1:D:703:ALA:HA	1:D:807:THR:HG21	2.02	0.41
1:D:707:ASN:CA	1:D:800:MET:SD	3.02	0.41
1:A:32:ASN:HD21	1:B:13:ILE:HG12	1.85	0.41
1:A:413:ARG:NH2	1:A:474:LEU:O	2.53	0.41
1:B:182:TRP:CE2	1:B:183:LEU:HG	2.55	0.41
1:B:338:ASN:O	1:B:339:ASP:HB3	2.20	0.41
1:B:388:PRO:HA	1:B:438:ARG:HG2	2.02	0.41
1:B:564:ASP:HB2	1:B:603:VAL:HA	2.01	0.41
1:B:565:VAL:HG11	1:B:656:VAL:CG2	2.50	0.41
1:B:715:VAL:O	1:B:718:VAL:HG12	2.20	0.41
1:B:778:GLU:HB3	1:B:782:LYS:NZ	2.35	0.41
1:C:81:ARG:HD3	1:C:155:TYR:CE1	2.55	0.41
1:C:304:LEU:N	1:C:304:LEU:HD12	2.35	0.41
1:C:549:LEU:HD23	1:C:557:ILE:HG12	2.02	0.41
1:C:690:GLY:O	1:C:710:ILE:HA	2.20	0.41
1:D:689:ILE:HG23	1:D:689:ILE:O	2.19	0.41
1:A:47:THR:OG1	1:A:50:ASP:OD2	2.38	0.41
1:A:84:TYR:N	1:A:155:TYR:O	2.52	0.41
1:A:575:ARG:O	1:A:577:LEU:N	2.53	0.41
1:B:402:ILE:CG2	1:B:406:ILE:HD11	2.42	0.41
1:B:580:CYS:O	1:B:584:ILE:HG13	2.20	0.41
1:D:570:ILE:HG21	1:D:620:ILE:HG13	2.01	0.41
1:D:757:LEU:C	1:D:759:LYS:H	2.28	0.41
1:A:457:ARG:HH22	1:A:701:GLU:CD	2.29	0.41
1:A:481:ASN:CG	1:A:482:LYS:N	2.78	0.41
1:A:532:ARG:HE	1:A:532:ARG:HB3	1.58	0.41
1:A:824:ILE:C	1:A:826:GLY:H	2.27	0.41
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.79	0.41
1:D:565:VAL:HG22	1:D:660:ALA:HB1	2.02	0.41
1:D:761:ILE:O	1:D:765:LEU:HD22	2.20	0.41
1:A:294:LYS:HE3	1:A:294:LYS:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:VAL:CG2	1:A:557:ILE:CD1	2.99	0.41
1:A:674:SER:OG	1:A:675:GLY:N	2.54	0.41
1:B:233:TYR:OH	1:B:234:ARG:NH1	2.54	0.41
1:B:385:GLU:O	1:B:441:MET:HB2	2.20	0.41
1:C:519:ARG:HA	1:C:806:ALA:O	2.21	0.41
1:C:522:LEU:HD13	1:C:522:LEU:HA	1.80	0.41
1:D:564:ASP:HB3	1:D:603:VAL:HA	2.01	0.41
1:A:356:LEU:HD22	1:A:356:LEU:N	2.35	0.41
1:A:582:HIS:ND1	1:A:582:HIS:C	2.79	0.41
1:A:588:ASN:HD21	1:A:744:GLN:NE2	2.19	0.41
1:B:190:GLU:HA	1:B:227:ASP:O	2.19	0.41
1:B:695:ALA:C	1:B:699:MET:HE3	2.45	0.41
1:B:795:ARG:O	1:B:799:ARG:HG3	2.21	0.41
1:C:31:PHE:O	1:C:31:PHE:CD1	2.74	0.41
1:C:502:ILE:HG13	1:C:503:ILE:N	2.35	0.41
1:D:661:ASP:CB	1:D:797:TRP:HH2	2.26	0.41
1:A:262:TYR:OH	1:D:263:ILE:HD11	2.20	0.41
1:A:293:LEU:HD21	1:A:392:LEU:HD12	2.02	0.41
1:B:13:ILE:HD13	1:B:13:ILE:HG21	1.89	0.41
1:B:242:ARG:C	1:B:243:LEU:HD12	2.46	0.41
1:B:329:PHE:HB3	1:B:330:PRO:HD3	2.03	0.41
1:B:520:LYS:O	1:B:522:LEU:N	2.54	0.41
1:C:530:PHE:O	1:C:533:ASP:N	2.54	0.41
1:C:678:ASN:HD22	1:C:695:ALA:HB3	1.85	0.41
1:D:388:PRO:HD2	1:D:391:LEU:HB2	2.02	0.41
1:D:549:LEU:CB	1:D:557:ILE:HG12	2.50	0.41
1:A:115:LEU:HD22	1:B:13:ILE:HG12	2.02	0.41
1:B:379:VAL:HG22	1:B:462:ILE:HD11	2.03	0.41
1:C:324:THR:O	1:C:325:ASN:C	2.64	0.41
1:D:491:TRP:C	1:D:495:CYS:SG	3.04	0.41
1:A:74:TYR:HE1	1:A:153:ALA:HB2	1.86	0.41
1:A:268:ASP:O	1:A:270:ASN:N	2.53	0.41
1:A:822:ARG:HH11	1:A:822:ARG:HG2	1.86	0.41
1:B:322:VAL:O	1:B:323:ARG:HG2	2.21	0.41
1:B:381:PRO:HG3	1:B:467:ILE:HD12	2.03	0.41
1:B:391:LEU:O	1:B:395:LEU:N	2.54	0.41
1:B:633:ASP:HA	1:B:634:PRO:HD3	1.88	0.41
1:C:110:GLU:O	1:C:113:TYR:HB3	2.20	0.41
1:C:160:ARG:HH21	1:C:190:GLU:CD	2.28	0.41
1:C:381:PRO:O	1:C:384:LEU:HB2	2.20	0.41
1:C:557:ILE:HD11	1:C:643:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:LEU:HB3	1:D:666:ILE:HD12	2.02	0.41
1:D:633:ASP:HA	1:D:634:PRO:HD3	1.82	0.41
1:A:32:ASN:HD22	1:B:13:ILE:HG23	1.86	0.41
1:A:63:LEU:HD21	1:A:229:PRO:HB2	2.03	0.41
1:A:74:TYR:CE1	1:A:153:ALA:HB2	2.55	0.41
1:B:182:TRP:CD1	1:B:182:TRP:N	2.88	0.41
1:B:536:LYS:HZ2	1:B:540:GLU:CD	2.28	0.41
1:C:166:PHE:CD2	1:C:177:GLU:HB3	2.55	0.41
1:C:587:TYR:CZ	1:C:591:LYS:HG3	2.56	0.41
1:C:834:LEU:HD23	1:C:835:PRO:HD2	2.03	0.41
1:D:82:ILE:HD11	1:D:147:MET:SD	2.61	0.41
1:D:279:LEU:CD2	1:D:280:TYR:N	2.84	0.41
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.85	0.40
1:A:49:ARG:HH11	1:A:125:ILE:HG22	1.85	0.40
1:A:492:LEU:HD12	1:A:683:LEU:HD21	2.03	0.40
1:A:698:GLU:HA	1:A:701:GLU:CG	2.47	0.40
1:B:674:SER:OG	1:B:675:GLY:N	2.54	0.40
1:B:810:LYS:O	1:B:815:ARG:NH2	2.50	0.40
1:C:402:ILE:HG21	1:C:402:ILE:HD13	1.90	0.40
1:D:505:GLU:HB2	1:D:506:ARG:HE	1.86	0.40
1:D:542:LYS:HE3	1:D:563:PHE:CD2	2.56	0.40
1:D:699:MET:HB3	1:D:708:PHE:CZ	2.56	0.40
1:D:789:ALA:HA	1:D:792:LYS:HZ1	1.85	0.40
1:B:155:TYR:N	1:B:155:TYR:CD1	2.89	0.40
1:B:417:ALA:C	1:B:419:PRO:HD3	2.46	0.40
1:B:656:VAL:O	1:B:657:ILE:C	2.63	0.40
1:B:716:GLU:CD	1:B:720:ARG:HH11	2.30	0.40
1:B:751:SER:HB3	1:B:758:PHE:HE2	1.86	0.40
1:C:150:LEU:H	1:C:150:LEU:HG	1.58	0.40
1:C:565:VAL:HG12	1:C:604:MET:HE3	2.04	0.40
1:D:159:ILE:HG22	1:D:160:ARG:N	2.36	0.40
1:D:165:ILE:HG12	1:D:279:LEU:HB3	2.02	0.40
1:D:455:VAL:HG13	1:D:674:SER:HB2	2.03	0.40
1:D:531:ILE:HG21	1:D:795:ARG:HG3	2.04	0.40
1:D:835:PRO:HB2	1:D:836:ALA:H	1.70	0.40
1:A:818:ALA:O	1:A:822:ARG:HG3	2.21	0.40
1:B:26:GLU:OE1	1:B:29:LYS:NZ	2.54	0.40
1:B:162:GLU:HB2	1:B:277:ARG:HA	2.03	0.40
1:B:248:ALA:HB2	1:B:269:ARG:HA	2.03	0.40
1:B:469:LYS:O	1:B:472:TYR:HB3	2.21	0.40
1:B:521:LEU:HD11	1:B:530:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:PHE:CE2	1:B:534:VAL:CG2	3.04	0.40
1:B:539:GLN:O	1:B:543:LEU:HD13	2.22	0.40
1:B:581:LEU:HD13	1:B:738:LEU:CD1	2.50	0.40
1:B:590:ILE:HG12	1:B:598:VAL:HG21	2.02	0.40
1:B:665:GLN:NE2	1:B:678:ASN:OD1	2.54	0.40
1:B:713:MET:HG2	1:B:717:ASP:OD2	2.22	0.40
1:B:714:ARG:HH11	1:B:714:ARG:CG	2.34	0.40
1:B:792:LYS:HE2	1:B:792:LYS:HB2	1.74	0.40
1:C:822:ARG:HD3	1:C:822:ARG:HH11	1.75	0.40
1:D:236:ASN:HB2	1:D:834:LEU:O	2.20	0.40
1:D:631:ASN:HD21	1:D:642:VAL:N	2.17	0.40
1:D:692:MET:SD	1:D:710:ILE:HG21	2.60	0.40
1:D:697:VAL:H	1:D:697:VAL:HG23	1.37	0.40
1:D:778:GLU:HB3	1:D:782:LYS:HZ3	1.84	0.40
1:A:143:PHE:HB3	1:A:147:MET:CE	2.52	0.40
1:A:187:ASN:HA	1:A:188:PRO:HD2	1.99	0.40
1:A:365:TRP:CE3	1:A:365:TRP:HA	2.56	0.40
1:A:413:ARG:HH21	1:A:475:GLU:HG3	1.83	0.40
1:A:729:GLN:HA	1:A:732:TYR:HB3	2.03	0.40
1:B:272:ALA:HA	1:B:275:ILE:HG13	2.04	0.40
1:B:497:PRO:O	1:B:498:GLY:C	2.64	0.40
1:B:515:LEU:HD21	1:B:683:LEU:HD11	2.03	0.40
1:C:88:GLU:HG3	1:C:132:GLY:HA2	2.03	0.40
1:C:598:VAL:O	1:C:600:PRO:HD3	2.22	0.40
1:D:231:PRO:HA	1:D:238:VAL:HG22	2.03	0.40
1:D:359:LEU:HD12	1:D:364:ALA:HB2	2.04	0.40
1:D:662:LEU:HA	1:D:687:LEU:O	2.21	0.40
1:A:733:ASP:OD1	1:A:733:ASP:N	2.54	0.40
1:B:198:LEU:HA	1:B:199:PRO:HD2	1.96	0.40
1:B:290:GLU:O	1:B:294:LYS:HD3	2.22	0.40
1:B:426:ARG:NH2	1:C:756:ASP:OD2	2.54	0.40
1:B:536:LYS:O	1:B:540:GLU:HB2	2.20	0.40
1:B:575:ARG:NH2	1:B:776:ASP:OD2	2.53	0.40
1:D:112:THR:CA	1:D:115:LEU:HD12	2.40	0.40
1:D:136:LEU:HD11	1:D:338:ASN:ND2	2.37	0.40
1:D:214:LYS:HB3	1:D:216:VAL:HG13	2.04	0.40
1:D:233:TYR:OH	1:D:234:ARG:NH1	2.54	0.40
1:D:413:ARG:HH21	1:D:475:GLU:CD	2.29	0.40
1:D:620:ILE:O	1:D:624:THR:HG23	2.21	0.40

All (1) 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:21:VAL:O	1:D:370:LYS:NZ[2_646]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	825/842 (98%)	656 (80%)	130 (16%)	39 (5%)	2	7
1	B	822/842 (98%)	674 (82%)	105 (13%)	43 (5%)	1	5
1	C	825/842 (98%)	673 (82%)	100 (12%)	52 (6%)	1	3
1	D	825/842 (98%)	635 (77%)	133 (16%)	57 (7%)	1	2
All	All	3297/3368 (98%)	2638 (80%)	468 (14%)	191 (6%)	1	4

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	166	PHE
1	A	252	PHE
1	A	256	ASP
1	A	265	ALA
1	A	281	PRO
1	A	282	ASN
1	A	283	ASP
1	A	284	ASN
1	A	358	ARG
1	A	553	TYR
1	A	555	VAL
1	A	610	ALA
1	A	730	GLU
1	B	13	ILE
1	B	16	ARG
1	B	166	PHE

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Mol	Chain	Res	Type
1	B	234	ARG
1	B	252	PHE
1	B	265	ALA
1	B	281	PRO
1	B	282	ASN
1	B	283	ASP
1	B	284	ASN
1	B	315	LYS
1	B	436	VAL
1	B	553	TYR
1	B	555	VAL
1	B	590	ILE
1	B	599	VAL
1	B	610	ALA
1	B	637	GLY
1	B	808	SER
1	B	835	PRO
1	B	837	PRO
1	C	16	ARG
1	C	166	PHE
1	C	234	ARG
1	C	281	PRO
1	C	282	ASN
1	C	283	ASP
1	C	284	ASN
1	C	285	PHE
1	C	315	LYS
1	C	555	VAL
1	C	575	ARG
1	C	599	VAL
1	C	610	ALA
1	C	683	LEU
1	C	752	PRO
1	C	836	ALA
1	D	22	GLU
1	D	78	ASP
1	D	281	PRO
1	D	284	ASN
1	D	337	LEU
1	D	358	ARG
1	D	467	ILE
1	D	555	VAL

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Mol	Chain	Res	Type
1	D	610	ALA
1	D	674	SER
1	D	697	VAL
1	D	730	GLU
1	D	751	SER
1	D	835	PRO
1	A	130	GLY
1	A	149	THR
1	A	285	PHE
1	A	288	GLY
1	A	508	GLY
1	A	576	GLN
1	A	769	ASP
1	A	836	ALA
1	B	129	ALA
1	B	272	ALA
1	B	285	PHE
1	B	288	GLY
1	B	510	GLU
1	B	572	GLU
1	B	655	LYS
1	B	730	GLU
1	B	836	ALA
1	C	27	LEU
1	C	324	THR
1	C	506	ARG
1	C	508	GLY
1	C	511	TYR
1	C	531	ILE
1	C	576	GLN
1	C	674	SER
1	C	682	MET
1	C	730	GLU
1	C	809	GLY
1	D	130	GLY
1	D	234	ARG
1	D	273	GLU
1	D	285	PHE
1	D	288	GLY
1	D	313	SER
1	D	314	SER
1	D	315	LYS

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Mol	Chain	Res	Type
1	D	429	SER
1	D	477	HIS
1	D	508	GLY
1	D	509	GLU
1	D	510	GLU
1	D	525	VAL
1	D	599	VAL
1	D	683	LEU
1	D	694	GLY
1	D	725	GLY
1	D	808	SER
1	A	21	VAL
1	A	147	MET
1	A	203	TYR
1	A	755	PRO
1	A	835	PRO
1	B	515	LEU
1	B	656	VAL
1	B	756	ASP
1	C	151	GLY
1	C	269	ARG
1	C	357	GLU
1	C	530	PHE
1	D	17	GLY
1	D	319	ARG
1	D	323	ARG
1	D	499	LEU
1	D	515	LEU
1	D	836	ALA
1	A	78	ASP
1	A	184	ARG
1	A	464	LYS
1	A	492	LEU
1	A	734	ARG
1	C	384	LEU
1	C	510	GLU
1	C	637	GLY
1	C	755	PRO
1	C	758	PHE
1	D	21	VAL
1	D	85	LEU
1	D	166	PHE

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Mol	Chain	Res	Type
1	D	254	LEU
1	D	260	GLY
1	D	466	THR
1	D	629	VAL
1	D	789	ALA
1	A	287	GLU
1	A	320	ASP
1	B	280	TYR
1	B	678	ASN
1	B	729	GLN
1	C	21	VAL
1	C	339	ASP
1	C	694	GLY
1	D	253	ASN
1	D	269	ARG
1	D	282	ASN
1	D	287	GLU
1	D	457	ARG
1	D	723	GLN
1	D	734	ARG
1	A	467	ILE
1	B	358	ARG
1	B	755	PRO
1	C	165	ILE
1	C	280	TYR
1	C	287	GLU
1	C	629	VAL
1	C	735	ILE
1	C	829	PRO
1	D	339	ASP
1	D	755	PRO
1	A	280	TYR
1	B	629	VAL
1	B	773	VAL
1	C	40	VAL
1	A	151	GLY
1	B	130	GLY
1	B	805	ILE
1	C	507	ILE
1	C	537	VAL
1	C	835	PRO
1	D	186	GLY

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Mol	Chain	Res	Type
1	A	193	ARG
1	C	288	GLY
1	C	666	ILE
1	A	40	VAL
1	B	525	VAL
1	C	229	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	714/730 (98%)	565 (79%)	149 (21%)	1	4
1	B	715/730 (98%)	586 (82%)	129 (18%)	2	6
1	C	714/730 (98%)	563 (79%)	151 (21%)	1	4
1	D	714/730 (98%)	546 (76%)	168 (24%)	1	3
All	All	2857/2920 (98%)	2260 (79%)	597 (21%)	1	4

All (597) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	13	ILE
1	A	15	VAL
1	A	18	LEU
1	A	23	ASN
1	A	29	LYS
1	A	30	ASN
1	A	31	PHE
1	A	42	ASP
1	A	43	ARG
1	A	45	VAL
1	A	47	THR
1	A	73	HIS
1	A	75	TYR
1	A	77	LYS

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Mol	Chain	Res	Type
1	A	80	LYS
1	A	82	ILE
1	A	85	LEU
1	A	87	LEU
1	A	95	LEU
1	A	100	VAL
1	A	102	LEU
1	A	112	THR
1	A	125	ILE
1	A	142	CYS
1	A	162	GLU
1	A	165	ILE
1	A	169	LYS
1	A	176	MET
1	A	177	GLU
1	A	187	ASN
1	A	195	GLU
1	A	209	THR
1	A	211	GLN
1	A	219	GLN
1	A	220	VAL
1	A	224	MET
1	A	234	ARG
1	A	240	THR
1	A	242	ARG
1	A	243	LEU
1	A	250	ASN
1	A	251	ASP
1	A	253	ASN
1	A	254	LEU
1	A	263	ILE
1	A	273	GLU
1	A	274	ASN
1	A	279	LEU
1	A	280	TYR
1	A	281	PRO
1	A	286	PHE
1	A	290	GLU
1	A	299	VAL
1	A	300	VAL
1	A	303	THR
1	A	314	SER

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Mol	Chain	Res	Type
1	A	316	PHE
1	A	318	CYS
1	A	319	ARG
1	A	323	ARG
1	A	335	ILE
1	A	339	ASP
1	A	360	ASP
1	A	365	TRP
1	A	366	GLU
1	A	377	HIS
1	A	378	THR
1	A	385	GLU
1	A	391	LEU
1	A	392	LEU
1	A	395	LEU
1	A	396	LEU
1	A	398	ARG
1	A	400	LEU
1	A	412	ASN
1	A	430	LEU
1	A	439	ILE
1	A	449	SER
1	A	450	HIS
1	A	455	VAL
1	A	458	ILE
1	A	462	ILE
1	A	474	LEU
1	A	484	ASN
1	A	492	LEU
1	A	494	LEU
1	A	509	GLU
1	A	510	GLU
1	A	515	LEU
1	A	518	LEU
1	A	523	SER
1	A	536	LYS
1	A	540	GLU
1	A	550	GLU
1	A	554	LYS
1	A	555	VAL
1	A	557	ILE
1	A	558	ASN

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Mol	Chain	Res	Type
1	A	559	PRO
1	A	567	VAL
1	A	575	ARG
1	A	576	GLN
1	A	582	HIS
1	A	586	LEU
1	A	589	ARG
1	A	598	VAL
1	A	622	LEU
1	A	629	VAL
1	A	630	VAL
1	A	636	VAL
1	A	638	ASP
1	A	643	ILE
1	A	652	LEU
1	A	655	LYS
1	A	658	PRO
1	A	662	LEU
1	A	674	SER
1	A	683	LEU
1	A	701	GLU
1	A	706	GLU
1	A	708	PHE
1	A	713	MET
1	A	715	VAL
1	A	716	GLU
1	A	717	ASP
1	A	718	VAL
1	A	720	ARG
1	A	727	ASN
1	A	738	LEU
1	A	742	ILE
1	A	743	GLU
1	A	755	PRO
1	A	756	ASP
1	A	764	MET
1	A	765	LEU
1	A	766	MET
1	A	782	LYS
1	A	787	VAL
1	A	790	LEU
1	A	795	ARG

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Mol	Chain	Res	Type
1	A	800	MET
1	A	807	THR
1	A	808	SER
1	A	810	LYS
1	A	813	SER
1	A	827	VAL
1	A	828	GLU
1	A	833	ARG
1	B	10	ARG
1	B	12	GLN
1	B	15	VAL
1	B	18	LEU
1	B	22	GLU
1	B	23	ASN
1	B	45	VAL
1	B	47	THR
1	B	66	ARG
1	B	76	GLU
1	B	82	ILE
1	B	95	LEU
1	B	102	LEU
1	B	108	CYS
1	B	112	THR
1	B	113	TYR
1	B	120	GLU
1	B	128	ASP
1	B	150	LEU
1	B	159	ILE
1	B	162	GLU
1	B	165	ILE
1	B	169	LYS
1	B	176	MET
1	B	187	ASN
1	B	211	GLN
1	B	214	LYS
1	B	219	GLN
1	B	220	VAL
1	B	224	MET
1	B	241	MET
1	B	242	ARG
1	B	250	ASN
1	B	253	ASN

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Mol	Chain	Res	Type
1	B	255	LYS
1	B	263	ILE
1	B	274	ASN
1	B	278	VAL
1	B	279	LEU
1	B	280	TYR
1	B	281	PRO
1	B	286	PHE
1	B	300	VAL
1	B	304	LEU
1	B	323	ARG
1	B	337	LEU
1	B	344	LEU
1	B	353	LEU
1	B	369	VAL
1	B	375	THR
1	B	379	VAL
1	B	384	LEU
1	B	391	LEU
1	B	392	LEU
1	B	396	LEU
1	B	400	LEU
1	B	412	ASN
1	B	422	VAL
1	B	430	LEU
1	B	444	LEU
1	B	458	ILE
1	B	464	LYS
1	B	467	ILE
1	B	474	LEU
1	B	480	GLN
1	B	486	ILE
1	B	492	LEU
1	B	499	LEU
1	B	502	ILE
1	B	506	ARG
1	B	507	ILE
1	B	515	LEU
1	B	518	LEU
1	B	525	VAL
1	B	536	LYS
1	B	550	GLU

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Mol	Chain	Res	Type
1	B	554	LYS
1	B	555	VAL
1	B	557	ILE
1	B	565	VAL
1	B	571	HIS
1	B	575	ARG
1	B	576	GLN
1	B	577	LEU
1	B	586	LEU
1	B	591	LYS
1	B	592	LYS
1	B	596	LYS
1	B	598	VAL
1	B	602	THR
1	B	603	VAL
1	B	605	ILE
1	B	630	VAL
1	B	633	ASP
1	B	640	LEU
1	B	649	ARG
1	B	650	VAL
1	B	652	LEU
1	B	655	LYS
1	B	662	LEU
1	B	663	SER
1	B	665	GLN
1	B	674	SER
1	B	676	THR
1	B	688	THR
1	B	710	ILE
1	B	714	ARG
1	B	715	VAL
1	B	717	ASP
1	B	721	LEU
1	B	724	ARG
1	B	739	ARG
1	B	740	GLN
1	B	753	LYS
1	B	756	ASP
1	B	757	LEU
1	B	765	LEU
1	B	766	MET

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Mol	Chain	Res	Type
1	B	778	GLU
1	B	779	GLU
1	B	782	LYS
1	B	783	CYS
1	B	787	VAL
1	B	807	THR
1	B	810	LYS
1	B	828	GLU
1	B	831	ARG
1	B	834	LEU
1	B	838	ASP
1	C	10	ARG
1	C	22	GLU
1	C	25	THR
1	C	43	ARG
1	C	45	VAL
1	C	63	LEU
1	C	66	ARG
1	C	68	ILE
1	C	76	GLU
1	C	82	ILE
1	C	87	LEU
1	C	91	MET
1	C	95	LEU
1	C	100	VAL
1	C	102	LEU
1	C	112	THR
1	C	119	MET
1	C	121	GLU
1	C	136	LEU
1	C	150	LEU
1	C	159	ILE
1	C	165	ILE
1	C	170	ILE
1	C	176	MET
1	C	183	LEU
1	C	207	GLU
1	C	211	GLN
1	C	224	MET
1	C	227	ASP
1	C	229	PRO
1	C	235	ASN

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Mol	Chain	Res	Type
1	C	242	ARG
1	C	243	LEU
1	C	250	ASN
1	C	251	ASP
1	C	253	ASN
1	C	259	VAL
1	C	262	TYR
1	C	270	ASN
1	C	273	GLU
1	C	274	ASN
1	C	276	SER
1	C	279	LEU
1	C	280	TYR
1	C	281	PRO
1	C	286	PHE
1	C	292	ARG
1	C	299	VAL
1	C	309	ARG
1	C	319	ARG
1	C	332	LYS
1	C	336	GLN
1	C	353	LEU
1	C	354	VAL
1	C	356	LEU
1	C	358	ARG
1	C	360	ASP
1	C	361	TRP
1	C	368	THR
1	C	372	CYS
1	C	378	THR
1	C	380	ILE
1	C	389	VAL
1	C	391	LEU
1	C	392	LEU
1	C	395	LEU
1	C	396	LEU
1	C	400	LEU
1	C	408	GLN
1	C	413	ARG
1	C	430	LEU
1	C	439	ILE
1	C	444	LEU

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Mol	Chain	Res	Type
1	C	455	VAL
1	C	457	ARG
1	C	460	SER
1	C	461	GLU
1	C	462	ILE
1	C	469	LYS
1	C	474	LEU
1	C	486	ILE
1	C	487	THR
1	C	490	ARG
1	C	492	LEU
1	C	494	LEU
1	C	495	CYS
1	C	502	ILE
1	C	506	ARG
1	C	510	GLU
1	C	519	ARG
1	C	522	LEU
1	C	523	SER
1	C	528	GLU
1	C	531	ILE
1	C	536	LYS
1	C	540	GLU
1	C	549	LEU
1	C	551	ARG
1	C	554	LYS
1	C	555	VAL
1	C	556	HIS
1	C	557	ILE
1	C	558	ASN
1	C	564	ASP
1	C	568	LYS
1	C	575	ARG
1	C	576	GLN
1	C	582	HIS
1	C	586	LEU
1	C	589	ARG
1	C	595	ASN
1	C	619	ILE
1	C	622	LEU
1	C	629	VAL
1	C	635	VAL

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Mol	Chain	Res	Type
1	C	638	ASP
1	C	641	ARG
1	C	646	GLU
1	C	649	ARG
1	C	652	LEU
1	C	655	LYS
1	C	656	VAL
1	C	662	LEU
1	C	665	GLN
1	C	676	THR
1	C	682	MET
1	C	693	ASP
1	C	705	GLU
1	C	713	MET
1	C	724	ARG
1	C	727	ASN
1	C	737	GLU
1	C	738	LEU
1	C	739	ARG
1	C	741	ILE
1	C	742	ILE
1	C	743	GLU
1	C	753	LYS
1	C	755	PRO
1	C	764	MET
1	C	766	MET
1	C	778	GLU
1	C	782	LYS
1	C	787	VAL
1	C	800	MET
1	C	803	ARG
1	C	807	THR
1	C	808	SER
1	C	810	LYS
1	C	813	SER
1	C	831	ARG
1	D	10	ARG
1	D	12	GLN
1	D	16	ARG
1	D	18	LEU
1	D	22	GLU
1	D	39	LEU

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Mol	Chain	Res	Type
1	D	40	VAL
1	D	43	ARG
1	D	45	VAL
1	D	52	TYR
1	D	60	ARG
1	D	61	ASP
1	D	63	LEU
1	D	72	GLN
1	D	77	LYS
1	D	79	PRO
1	D	80	LYS
1	D	82	ILE
1	D	85	LEU
1	D	87	LEU
1	D	88	GLU
1	D	91	MET
1	D	95	LEU
1	D	102	LEU
1	D	104	LEU
1	D	105	GLU
1	D	113	TYR
1	D	127	GLU
1	D	131	LEU
1	D	138	ARG
1	D	147	MET
1	D	165	ILE
1	D	167	ASN
1	D	169	LYS
1	D	181	ASP
1	D	183	LEU
1	D	187	ASN
1	D	195	GLU
1	D	209	THR
1	D	211	GLN
1	D	214	LYS
1	D	229	PRO
1	D	240	THR
1	D	241	MET
1	D	243	LEU
1	D	245	SER
1	D	250	ASN
1	D	251	ASP

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Mol	Chain	Res	Type
1	D	253	ASN
1	D	255	LYS
1	D	263	ILE
1	D	269	ARG
1	D	277	ARG
1	D	279	LEU
1	D	280	TYR
1	D	281	PRO
1	D	283	ASP
1	D	286	PHE
1	D	289	LYS
1	D	291	LEU
1	D	294	LYS
1	D	299	VAL
1	D	304	LEU
1	D	306	ASP
1	D	309	ARG
1	D	314	SER
1	D	319	ARG
1	D	323	ARG
1	D	324	THR
1	D	337	LEU
1	D	339	ASP
1	D	340	THR
1	D	344	LEU
1	D	352	VAL
1	D	356	LEU
1	D	369	VAL
1	D	379	VAL
1	D	380	ILE
1	D	384	LEU
1	D	392	LEU
1	D	396	LEU
1	D	398	ARG
1	D	400	LEU
1	D	403	ILE
1	D	405	GLU
1	D	406	ILE
1	D	408	GLN
1	D	426	ARG
1	D	431	VAL
1	D	436	VAL

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Mol	Chain	Res	Type
1	D	444	LEU
1	D	446	ILE
1	D	455	VAL
1	D	457	ARG
1	D	458	ILE
1	D	461	GLU
1	D	467	ILE
1	D	469	LYS
1	D	474	LEU
1	D	486	ILE
1	D	487	THR
1	D	492	LEU
1	D	493	VAL
1	D	494	LEU
1	D	499	LEU
1	D	506	ARG
1	D	507	ILE
1	D	509	GLU
1	D	533	ASP
1	D	534	VAL
1	D	536	LYS
1	D	543	LEU
1	D	549	LEU
1	D	550	GLU
1	D	554	LYS
1	D	555	VAL
1	D	557	ILE
1	D	561	SER
1	D	562	LEU
1	D	565	VAL
1	D	579	ASN
1	D	582	HIS
1	D	583	VAL
1	D	589	ARG
1	D	592	LYS
1	D	594	PRO
1	D	598	VAL
1	D	600	PRO
1	D	601	ARG
1	D	603	VAL
1	D	605	ILE
1	D	608	LYS

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Mol	Chain	Res	Type
1	D	622	LEU
1	D	624	THR
1	D	626	ILE
1	D	628	ASP
1	D	636	VAL
1	D	650	VAL
1	D	652	LEU
1	D	655	LYS
1	D	656	VAL
1	D	658	PRO
1	D	662	LEU
1	D	672	GLU
1	D	676	THR
1	D	691	THR
1	D	697	VAL
1	D	714	ARG
1	D	718	VAL
1	D	720	ARG
1	D	724	ARG
1	D	735	ILE
1	D	739	ARG
1	D	740	GLN
1	D	743	GLU
1	D	756	ASP
1	D	757	LEU
1	D	761	ILE
1	D	763	ASN
1	D	764	MET
1	D	765	LEU
1	D	766	MET
1	D	770	ARG
1	D	779	GLU
1	D	797	TRP
1	D	824	ILE
1	D	831	ARG
1	D	832	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	44	ASN
1	A	96	GLN
1	A	167	ASN
1	A	208	HIS
1	A	219	GLN
1	A	239	ASN
1	A	250	ASN
1	A	253	ASN
1	A	336	GLN
1	A	408	GLN
1	A	412	ASN
1	A	453	ASN
1	A	459	HIS
1	A	480	GLN
1	A	484	ASN
1	A	566	GLN
1	A	579	ASN
1	A	588	ASN
1	A	614	HIS
1	A	678	ASN
1	A	744	GLN
1	A	754	GLN
1	A	784	GLN
1	B	34	HIS
1	B	73	HIS
1	B	97	ASN
1	B	201	HIS
1	B	211	GLN
1	B	250	ASN
1	B	284	ASN
1	B	295	GLN
1	B	336	GLN
1	B	341	HIS
1	B	377	HIS
1	B	453	ASN
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	560	ASN
1	B	576	GLN
1	B	588	ASN
1	B	614	HIS

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Mol	Chain	Res	Type
1	B	804	ASN
1	C	32	ASN
1	C	34	HIS
1	C	44	ASN
1	C	97	ASN
1	C	167	ASN
1	C	208	HIS
1	C	235	ASN
1	C	270	ASN
1	C	274	ASN
1	C	284	ASN
1	C	336	GLN
1	C	341	HIS
1	C	390	HIS
1	C	399	HIS
1	C	412	ASN
1	C	450	HIS
1	C	453	ASN
1	C	459	HIS
1	C	480	GLN
1	C	481	ASN
1	C	496	ASN
1	C	541	ASN
1	C	556	HIS
1	C	566	GLN
1	C	576	GLN
1	C	588	ASN
1	C	727	ASN
1	C	744	GLN
1	C	754	GLN
1	D	23	ASN
1	D	34	HIS
1	D	71	GLN
1	D	219	GLN
1	D	274	ASN
1	D	284	ASN
1	D	336	GLN
1	D	377	HIS
1	D	390	HIS
1	D	399	HIS
1	D	401	GLN
1	D	412	ASN

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Mol	Chain	Res	Type
1	D	450	HIS
1	D	453	ASN
1	D	459	HIS
1	D	477	HIS
1	D	481	ASN
1	D	496	ASN
1	D	614	HIS
1	D	631	ASN
1	D	665	GLN
1	D	727	ASN
1	D	744	GLN
1	D	754	GLN
1	D	793	ASN
1	D	804	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	C	14	1	8,9,10	1.35	1 (12%)	7,12,14	4.36	2 (28%)
1	SEP	D	14	1	8,9,10	1.26	0	7,12,14	14.68	1 (14%)
1	SEP	A	14	1	8,9,10	1.20	0	7,12,14	3.04	2 (28%)
1	SEP	B	14	1	8,9,10	1.12	0	7,12,14	2.68	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	C	14	1	-	3/6/8/10	-
1	SEP	D	14	1	-	5/6/8/10	-
1	SEP	A	14	1	-	5/6/8/10	-
1	SEP	B	14	1	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	SEP	CA-N	-2.24	1.41	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	SEP	OG-CB-CA	-38.78	70.41	108.14
1	C	14	SEP	OG-CB-CA	11.01	118.86	108.14
1	A	14	SEP	OG-CB-CA	7.29	115.24	108.14
1	B	14	SEP	OG-CB-CA	6.21	114.19	108.14
1	A	14	SEP	O2P-P-OG	2.96	114.38	106.67
1	B	14	SEP	OG-P-O1P	2.61	113.48	106.44
1	C	14	SEP	O2P-P-OG	2.50	113.19	106.67

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	N-CA-CB-OG
1	A	14	SEP	CA-CB-OG-P
1	A	14	SEP	CB-OG-P-O2P
1	A	14	SEP	CB-OG-P-O3P
1	B	14	SEP	C-CA-CB-OG
1	B	14	SEP	CA-CB-OG-P
1	B	14	SEP	CB-OG-P-O2P
1	B	14	SEP	CB-OG-P-O3P
1	C	14	SEP	N-CA-CB-OG
1	C	14	SEP	C-CA-CB-OG
1	C	14	SEP	CA-CB-OG-P
1	D	14	SEP	N-CA-CB-OG
1	D	14	SEP	C-CA-CB-OG
1	D	14	SEP	CB-OG-P-O2P
1	A	14	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
1	B	14	SEP	CB-OG-P-O1P
1	D	14	SEP	CB-OG-P-O1P
1	D	14	SEP	CB-OG-P-O3P
1	B	14	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	14	SEP	1	0
1	D	14	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	901	-	4,4,4	0.36	0	6,6,6	0.70	0
3	PLP	D	999	1	15,15,16	1.49	3 (20%)	21,22,23	1.21	2 (9%)
2	SO4	B	901	-	4,4,4	0.40	0	6,6,6	0.41	0
2	SO4	C	902	-	4,4,4	0.50	0	6,6,6	0.43	0
3	PLP	B	999	1	15,15,16	1.33	2 (13%)	21,22,23	1.73	2 (9%)
2	SO4	C	901	-	4,4,4	0.35	0	6,6,6	0.44	0
3	PLP	A	999	1	15,15,16	2.23	4 (26%)	21,22,23	1.54	5 (23%)
3	PLP	C	999	1	15,15,16	1.37	1 (6%)	21,22,23	1.22	2 (9%)
2	SO4	D	902	-	4,4,4	0.61	0	6,6,6	0.31	0
2	SO4	A	901	-	4,4,4	0.46	0	6,6,6	0.48	0
2	SO4	A	902	-	4,4,4	0.47	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	902	-	4,4,4	0.54	0	6,6,6	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	A	999	1	-	3/6/6/8	0/1/1/1
3	PLP	D	999	1	-	2/6/6/8	0/1/1/1
3	PLP	B	999	1	-	2/6/6/8	0/1/1/1
3	PLP	C	999	1	-	1/6/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C5-C4	-5.43	1.34	1.40
3	C	999	PLP	C3-C2	-3.85	1.37	1.41
3	A	999	PLP	C3-C2	-3.52	1.37	1.41
3	D	999	PLP	C3-C2	-3.39	1.37	1.41
3	A	999	PLP	C2A-C2	-3.34	1.45	1.50
3	A	999	PLP	C4A-C4	-2.55	1.46	1.51
3	B	999	PLP	C3-C2	-2.55	1.38	1.41
3	D	999	PLP	C4A-C4	-2.15	1.47	1.51
3	B	999	PLP	C2-N1	2.13	1.37	1.33
3	D	999	PLP	P-O3P	-2.05	1.47	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	PLP	O4P-C5A-C5	5.48	119.62	109.36
3	A	999	PLP	C4A-C4-C5	-4.17	116.64	120.94
3	C	999	PLP	O4P-C5A-C5	3.58	116.08	109.36
3	D	999	PLP	O4P-C5A-C5	2.73	114.47	109.36
3	C	999	PLP	O3P-P-O4P	2.71	113.75	106.67
3	B	999	PLP	O2P-P-O4P	2.64	113.56	106.67
3	A	999	PLP	O4P-C5A-C5	2.51	114.06	109.36
3	D	999	PLP	O2P-P-O4P	2.40	112.94	106.67
3	A	999	PLP	C5A-C5-C4	-2.17	118.36	122.64
3	A	999	PLP	O3P-P-O4P	2.14	112.25	106.67
3	A	999	PLP	C4A-C4-C3	2.07	123.97	120.52

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C5A-O4P-P-O2P
3	A	999	PLP	C5A-O4P-P-O3P
3	B	999	PLP	C5A-O4P-P-O2P
3	B	999	PLP	C5A-O4P-P-O3P
3	D	999	PLP	C5A-O4P-P-O2P
3	D	999	PLP	C5A-O4P-P-O3P
3	A	999	PLP	C5A-O4P-P-O1P
3	C	999	PLP	C5A-O4P-P-O3P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	902	SO4	1	0
3	C	999	PLP	1	0

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	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	24:VAL	C	25:THR	N	1.95

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.